

## Supporting Information

### Catalytic Direct C2-Alkenylation of Oxazoles at ppm Levels of Palladium-PhMezole-Phos Complex

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## 1. General considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All arylation reactions were performed in resealable screw-capped Schlenk tube (approx. 20 mL volume) in the presence of Teflon-coated magnetic stirrer bar (4 mm × 10 mm). Tetrahydrofuran (THF) and 1,4-Dioxane were distilled from sodium benzophenone ketyl under nitrogen. Toluene was distilled from sodium under nitrogen. *t*-BuOH and dichloromethane were distilled from calcium hydride under nitrogen. Li<sub>2</sub>CO<sub>3</sub>, NaOt-Bu, KOt-Bu and LiOH were purchased from Aldrich. LiOt-Bu was purchased from J&K scientific. Pd<sub>2</sub>(dba)<sub>3</sub>, Pd(dba)<sub>2</sub> and Pd(OAc)<sub>2</sub> were purchased from Strem. PdCl<sub>2</sub>(ACN)<sub>2</sub> and Pd(TFA)<sub>2</sub> were purchased from Aldrich. **L1**,<sup>1</sup> **L2**,<sup>2</sup> **L3**,<sup>3</sup> **L4**,<sup>4</sup> and **L5**,<sup>5</sup> were prepared according to reported literature procedures. **L6** – **L8**, **L11**, **L13** were purchased from Strem. **L9**, **L10** and **L12** were purchased from Aldrich. Commercially available azoles (liquid form only) were purified by passed through a short plug (0.5 cm width × 4 cm height) of neutral alumina. Thin layer chromatography was performed on Merck precoated silica gel 60 F<sub>254</sub> plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected Büchi Melting Point B-545 instrument. <sup>1</sup>H NMR spectra were recorded on a Bruker (400 MHz) spectrometer. Spectra were referenced internally to the residual proton resonance in CDCl<sub>3</sub> (δ 7.26 ppm), or with tetramethylsilane (TMS, δ 0.00 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. <sup>13</sup>C NMR spectra were referenced to CDCl<sub>3</sub> (δ 77.00 ppm, the middle peak). <sup>31</sup>P NMR spectra were referenced to 85% H<sub>3</sub>PO<sub>4</sub> externally. <sup>19</sup>F NMR spectra were referenced to trifluorotoluene externally. Coupling constants (J) were reported in Hertz (Hz). Mass spectra (EI-MS and ES-MS) were recorded on a HP 5989B Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on a Brüker APEX 47e FTICR mass spectrometer (ESIMS). GC-MS analysis was conducted on a HP 5973 GCD system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from HP 6890 GC-FID system. All yields reported refer to isolated yield of compounds estimated to be greater than 95% purity as determined by capillary gas chromatography (GC) or <sup>1</sup>H NMR. Compounds described in the literature were characterized by comparison of their <sup>1</sup>H, and/or <sup>13</sup>C NMR spectra to the previously reported data. The procedures in this section are representative, and thus the yields may differ from those reported in tables.

## 2. General procedures for ligand and reaction condition screenings

*General procedure for screening (Pd catalysts loading ranging from 5000-100 ppm):*

A Schlenk tube equipped with a Teflon-coated stir bar was carefully evacuated and backfilled with nitrogen for three cycles. Pd source (0.0075 mmol) and ligand with corresponding ratio in 10.0 mL DCM (0.25 mol% Pd per 1.00 mL stock solution) was then prepared under N<sub>2</sub> with stirring until all of the solids are dissolved (usually within 1 min). The corresponding volume of stock solution was then immediately added to the Schlenk tube by syringe (In case of 250 ppm Pd, 100  $\mu$ L of stock solution was added). The solvent was then evaporated under high vacuum. 3,4-Dihydronaphthalen-2-yl tosylate (0.3 mmol) and base (0.6 mmol) were loaded into the tube, and the system was further evacuated and flushed with nitrogen for three cycles. Benzoxazole (0.45 mmol) and subsequently solvent were added with stirring by syringe at room temperature. After that, the tube was further stirred (1000 rpm) at room temperature for 5 minutes. The tube was then placed into a preheated oil bath at indicated temperature and stirred for 18 h. Ethyl acetate (~3 mL), dodecane (114  $\mu$ L, internal standard), water (~2 mL) were added. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

## 3. General procedures for direct C2-alkenylation of azoles

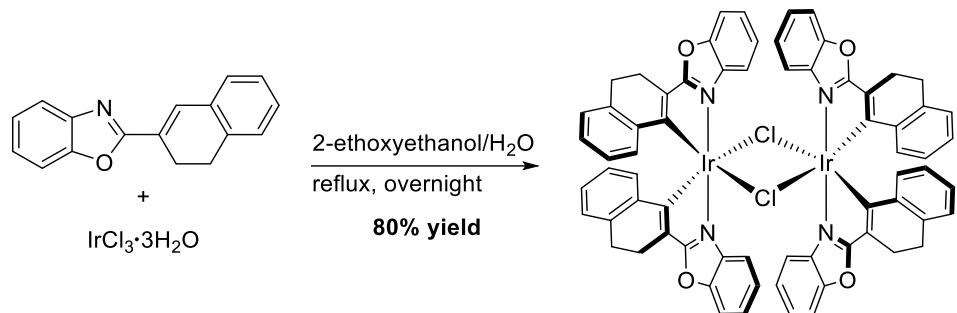
*General procedure for direct C2-alkenylation of azoles with alkenyl tosylates:* A Schlenk tube equipped with a Teflon-coated stir bar was carefully evacuated and backfilled with nitrogen for three cycles. Pd(OAc)<sub>2</sub> (0.0075 mmol) and **PhMezole-Phos** (0.030 mmol) in 10.0 mL DCM (0.25 mol% Pd per 1.00 mL stock solution) was then prepared under N<sub>2</sub> with stirring until all of the solids are dissolved (usually within 1 min). The corresponding volume of stock solution was then immediately added to the Schlenk tube by syringe (In case of 250 ppm Pd, 100  $\mu$ L of stock solution was added). The solvent was then evaporated under high vacuum. Alkenyl tosylate (if solid, 0.3 mmol), oxazole (if solid, 0.45 mmol) and LiOt-Bu (0.6 mmol) were loaded into the tube, and the system was further evacuated and flushed with nitrogen for three cycles. Benzoxazole (if liquid, 0.45 mmol), alkenyl tosylate (if liquid, 0.3 mmol) and subsequently *t*-BuOH (1.0 mL) were added with stirring by syringe at room temperature. After that, the tube was further stirred (1000 rpm) at room temperature for 5 minutes. The tube was then placed into a preheated oil bath at indicated

temperature and stirred for 18 h. Ethyl acetate (~3 mL), and water (~2 mL) were added. The organic layer was separated and the aqueous layer was washed with ethyl acetate. The combined organic layer was concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired product.

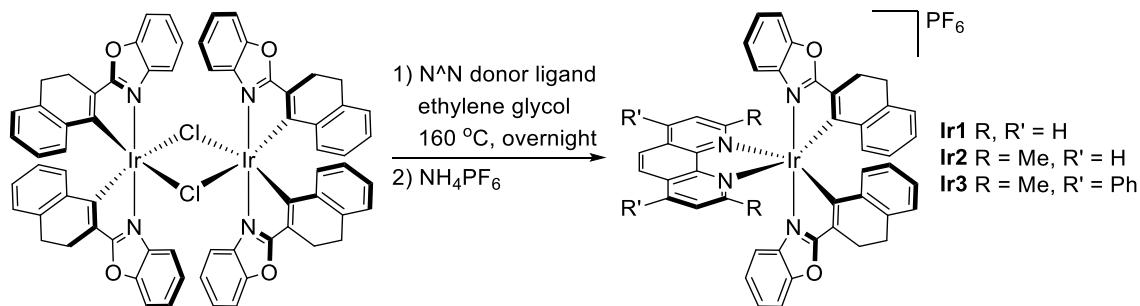
#### 4. Gram-scale synthesis of **1a**

**Pd(OAc)<sub>2</sub>** (2.25 mg, 0.01 mmol) in 4.0 mL DCM was prepared under N<sub>2</sub> with stirring until all of the solids are dissolved (usually within 1 min). 1.0 mL of stock solution was then immediately added to a Schlenk tube (100.0 mL, equipped with a Teflon-coated stir bar) by syringe and the solvent was then evaporated under high vacuum. After that, 3,4-Dihydronaphthalen-2-yl tosylate (3.00 g, 10 mmol), **PhMezole-Phos** (4.04 mg, 0.01 mmol), LiOt-Bu (1.60 g, 20 mmol), benzoxazole (1.79 g, 15 mmol) were added to the Schlenk tube. The Schlenk tube was then carefully evacuated and backfilled with nitrogen for three cycles and *t*-BuOH (33.0 mL) were added with stirring by syringe at room temperature. After that, the tube was further stirred (1000 rpm) at room temperature for 5 minutes. The tube was then placed into a preheated oil bath at indicated temperature and stirred for 18 h. Ethyl acetate (~3 mL), and water (~2 mL) were added. The organic layer was separated and the aqueous layer was washed with ethyl acetate. The combined organic layer was concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel (230-400 mesh) to afford the desired product.

## 5. General procedures for preparation of Ir(III) complexes



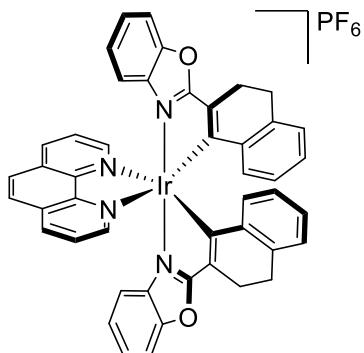
*General procedure for synthesis of the dichlorobridged iridium dimer:* A mixture of  $\text{IrCl}_3 \cdot 3\text{H}_2\text{O}$  (448 mg, 1.5 mmol) and 2-(3,4-dihydronaphthalen-2-yl)benzo[*d*]oxazole (815 mg, 3.3 mmol) in 2-ethoxyethanol/ $\text{H}_2\text{O}$  (40 mL, 3:1, v/v) was refluxed under an inert atmosphere of nitrogen for 16 h. The solution was then cooled to room temperature, and the precipitate was filtered and washed with water and diethyl ether successively. The product was dried under high vacuum to provide an orange solid (865 mg, 80% yield). The product was used in the next step without any further purification.



*General procedure for synthesis of the iridium complexes:* A mixture of the dichlorobridged iridium dimer obtained from the previous step (144.4 mg, 0.10 mmol) and 1,10-phenanthroline or neocuproine or bathocuproine (0.21 mmol) in ethylene glycol (8.0 mL) was heated at 160 °C under an inert atmosphere of nitrogen in the dark for 16 h. The reaction mixture was then cooled to room temperature and poured into water (30 mL). The aqueous layer was washed with diethyl ether ( $3 \times 30$  mL) and  $\text{NH}_4\text{PF}_6$  (0.22 mmol) was added to the aqueous solution. The precipitate was filtered and washed with water and diethyl ether successively. The solid obtained was dried under high vacuum and recrystallized by vapor diffusion of diethyl ether into a dichloromethane solution

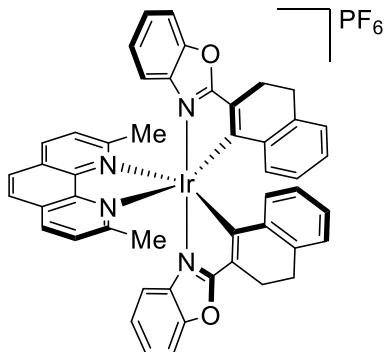
containing the solid. The solution was removed by dropper and the solid was dried under high vacuum to provide the final product.

**Ir 1(Scheme 4, entry Ir1).**



Yield: 81% (163.7 mg); Orange solid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  2.30 – 2.50 (m, 6H), 2.60 – 2.78 (m, 2H), 4.99 (d,  $J$  = 8.0 Hz, 2H), 6.46 (t,  $J$  = 7.9 Hz, 2H), 6.56 (d,  $J$  = 7.7 Hz, 2H), 6.89 (t,  $J$  = 7.8 Hz, 2H), 7.05 (t,  $J$  = 7.4 Hz, 2H), 7.12 – 7.17 (m, 4H), 7.26 (s, 1H), 7.39 (d,  $J$  = 8.2 Hz, 2H), 8.00 (dd,  $J$  = 8.2, 5.1 Hz, 2H), 8.37 (s, 2H), 8.84 – 8.97 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  21.4, 29.7, 111.7, 112.1, 124.5, 124.6, 125.8, 126.6, 127.0, 127.3, 127.5, 129.0, 131.3, 137.4, 137.7, 139.1, 140.0, 148.2, 149.0, 153.8, 168.2, 178.5; HRMS: calcd. for  $\text{C}_{46}\text{H}_{32}\text{N}_4\text{O}_2\text{Ir}$  : 863.2126, found 863.2091.

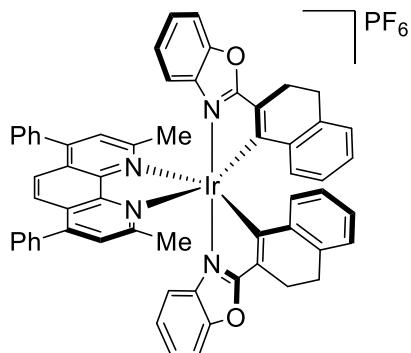
**Ir 2(Scheme 4, entry Ir2).**



Yield: 70% (145.2 mg); Yellow solid;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  1.92 (td,  $J$  = 15.2, 6.8 Hz, 2H), 2.15 – 2.36 (m, 4H), 2.40 – 2.54 (m, 2H), 2.76 (s, 6H), 5.17 (d,  $J$  = 8.1 Hz, 2H), 6.28 (d,  $J$  = 7.8 Hz, 2H), 6.53 (t,  $J$  = 6.1 Hz, 2H), 6.91 (t,  $J$  = 7.8 Hz, 2H), 7.04 – 7.13 (m, 4H), 7.21 (t,  $J$  = 7.9 Hz, 2H), 7.47 (d,  $J$  = 8.2 Hz, 2H), 7.85 (d,  $J$  = 8.3 Hz, 2H), 8.18 (s, 2H), 8.71 (d,  $J$  = 8.3 Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  21.2, 28.7, 29.0, 111.7, 112.6, 122.1, 124.7, 125.5, 126.5, 127.6, 127.7, 127.8, 128.0, 129.1, 129.7, 137.5, 138.2,

138.4, 140.4, 148.9, 149.3, 165.8, 178.6; HRMS: calcd. for  $C_{48}H_{36}N_4O_2Ir$ : 891.2438, found 891.2439.

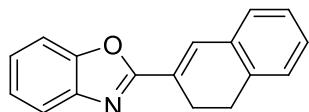
**Ir 3 (Scheme 4, entry Ir3).**



Yield: 74% (176.2 mg); Dark yellow solid;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  1.93 (td,  $J$  = 15.2, 6.7 Hz, 2H), 2.15 – 2.37 (m, 4H), 2.40 – 2.57 (m, 2H), 2.82 (s, 6H), 5.40 (d,  $J$  = 8.0 Hz, 2H), 6.33 (d,  $J$  = 7.8 Hz, 2H), 6.55 (td,  $J$  = 8.1, 7.2, 2.5 Hz, 2H), 7.01 (t,  $J$  = 7.8 Hz, 2H), 7.11 (q,  $J$  = 4.6, 4.0 Hz, 4H), 7.29 (dd,  $J$  = 14.5, 6.9 Hz, 2H), 7.46 – 7.70 (m, 14H), 7.77 (s, 2H), 8.15 (s, 2H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  21.3, 28.8, 29.2, 111.9, 112.7, 122.3, 124.9, 125.4, 125.6, 126.4, 127.6, 127.8, 127.9, 128.1, 129.2, 129.2, 129.7, 130.0, 135.1, 137.5, 138.3, 138.4, 149.0, 150.2, 152.2, 165.3, 166.1, 178.8; HRMS: calcd. for  $C_{60}H_{44}N_4O_2Ir$ : 1043.3105, found 1043.3065.

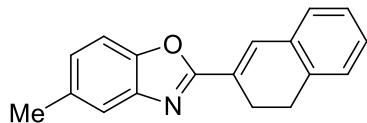
## 6. Characterization data for coupling products

### 2-(3,4-Dihydronaphthalen-2-yl)benzo[d]oxazole (Scheme 2, entry 1a).<sup>6</sup>



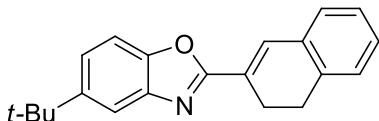
Flash chromatography: Hexane:EA = 50:1; Yield: 89% (66.0 mg);  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  2.99 (s, 4H), 7.18 – 7.22 (m, 1H), 7.22 – 7.29 (m, 3H), 7.30 – 7.41 (m, 2H), 7.46 – 7.59 (m, 1H), 7.66 (s, 1H), 7.70 – 7.80 (m, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  22.9, 27.3, 110.2, 119.7, 124.3, 125.1, 125.4, 126.7, 127.6, 127.9, 128.9, 132.1, 132.8, 136.2, 142.0, 150.4, 163.5

**2-(3,4-Dihydronaphthalen-2-yl)-5-methylbenzo[d]oxazole (Scheme 2, entry 1b).**



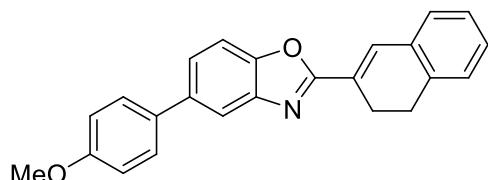
Flash chromatography: Hexane:EA = 50:1; Yield: 89% (69.8 mg); Light yellow solid; Melting point 106.5 – 108.6 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.47 (s, 3H), 2.98 (s, 4H), 7.13 (d, *J* = 8.3 Hz, 1H), 7.17 – 7.30 (m, 4H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.52 (s, 1H), 7.63 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 21.4, 23.0, 27.4, 109.5, 119.7, 125.6, 126.2, 126.7, 127.6, 127.9, 128.8, 131.8, 132.9, 134.1, 136.2, 142.3, 148.7, 163.6; HRMS: calcd. for C<sub>18</sub>H<sub>15</sub>ONH<sup>+</sup> : 262.1226, found 262.1235.

**5-*tert*-Butyl-2-(3,4-dihydronaphthalen-2-yl)benzo[d]oxazole (Scheme 2, entry 1c).**



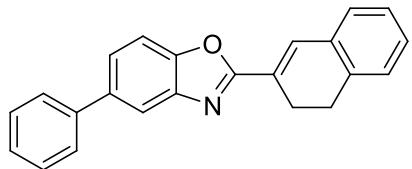
Flash chromatography: Hexane:EA = 70:1; Yield: 70% (63.7 mg); Light yellow solid; Melting point 114.4 – 116.8 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.40 (s, 9H), 3.00 (s, 4H), 7.15 – 7.30 (m, 4H), 7.36 – 7.48 (m, 2H), 7.64 (s, 1H), 7.78 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 23.0, 27.4, 31.7, 34.8, 109.3, 116.3, 122.8, 125.6, 126.7, 127.6, 127.9, 128.8, 131.7, 132.9, 136.2, 142.0, 147.8, 148.5, 163.6; HRMS: calcd. for C<sub>21</sub>H<sub>21</sub>ONH<sup>+</sup> : 304.1696, found 304.1705.

**2-(3,4-Dihydronaphthalen-2-yl)-5-(4-methoxyphenyl)benzo[d]oxazole (Scheme 2, entry 1d).**



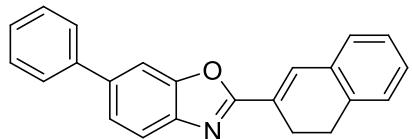
Flash chromatography: Hexane:EA = 40:1; Yield: 76% (80.5 mg); Light orange solid; Melting point 141.0 – 142.6 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 3.01 (s, 4H), 3.86 (s, 3H), 7.01 (d, *J* = 8.7 Hz, 2H), 7.18 – 7.32 (m, 4H), 7.47 – 7.61 (m, 4H), 7.67 (s, 1H), 7.88 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 23.0, 27.4, 55.3, 110.1, 114.3, 117.7, 124.4, 125.5, 126.8, 127.7, 128.0, 128.3, 129.0, 132.3, 132.9, 133.6, 136.3, 137.9, 142.7, 149.7, 159.1, 164.1; HRMS: calcd. for C<sub>24</sub>H<sub>19</sub>O<sub>2</sub>NH<sup>+</sup> : 354.1505, found 354.1489.

**2-(3,4-Dihydronaphthalen-2-yl)-5-phenylbenzo[d]oxazole (Scheme 2, entry 1e).**



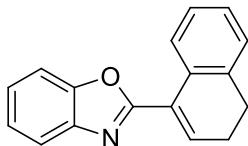
Flash chromatography: Hexane:EA = 50:1; Yield: 73% (70.8 mg); White solid; Melting point 155.3 – 157.0 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 3.02 (s, 4H), 7.19 – 7.32 (m, 4H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 2H), 7.57 (s, 2H), 7.64 (d, *J* = 7.5 Hz, 2H), 7.69 (s, 1H), 7.94 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 23.0, 27.4, 110.2, 118.2, 124.8, 125.5, 126.8, 127.2, 127.4, 127.7, 128.0, 128.8, 129.0, 132.4, 132.9, 136.4, 138.2, 141.0, 142.8, 150.1, 164.2; HRMS: calcd. for C<sub>23</sub>H<sub>17</sub>ONH<sup>+</sup> : 324.1383, found 324.1388.

**2-(3,4-Dihydronaphthalen-2-yl)-6-phenylbenzo[d]oxazole (Scheme 2, entry 1f).**



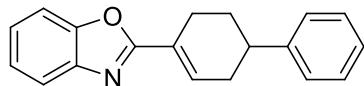
Flash chromatography: Hexane:EA = 50:1; Yield: 70% (67.9 mg); Light orange solid; Melting point 116.0 – 121.7 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 3.02 (s, 4H), 7.22 – 7.28 (m, 4H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.57 – 7.59 (m, 1H), 7.64 – 7.69 (m, 3H), 7.74 – 7.79 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 23.0, 27.4, 108.7, 119.7, 124.0, 125.5, 126.8, 127.3, 127.4, 127.7, 128.0, 128.9, 129.0, 132.3, 132.9, 136.4, 139.0, 140.8, 141.5, 151.2, 164.0; HRMS: calcd. for C<sub>23</sub>H<sub>17</sub>ONH<sup>+</sup> : 324.1383, found 324.1399.

**2-(3,4-Dihydronaphthalen-1-yl)benzo[d]oxazole (Scheme 2, entry 1g).**



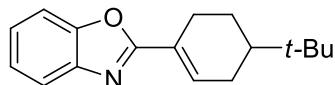
Flash chromatography: Hexane:EA = 50:1; Yield: 70% (51.8 mg); Light yellow oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.39 – 2.44 (m, 2H), 2.75 (t, *J* = 7.9 Hz, 2H), 7.09 – 7.19 (m, 2H), 7.20 – 7.26 (m, 4H), 7.39 – 7.47 (m, 1H), 7.65 – 7.73 (m, 1H), 8.12 (d, *J* = 7.7 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 23.6, 27.5, 110.2, 120.1, 124.2, 125.0, 126.2, 126.7, 127.0, 127.6, 127.8, 130.7, 136.2, 137.1, 141.9, 149.9, 162.1; HRMS: calcd. for C<sub>17</sub>H<sub>13</sub>ONH<sup>+</sup> : 248.1122, found 248.1119.

**2-(4-Phenylcyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1h).**



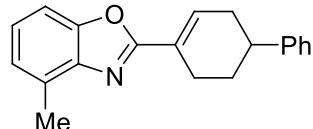
Flash chromatography: Hexane:EA = 50:1; Yield: 90% (74.3 mg); White solid; Melting point 77.5 – 80.9 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.87 – 1.98 (m, 1H), 2.14 – 2.21 (m, 1H), 2.40 – 2.51 (m, 1H), 2.61 – 2.74 (m, 2H), 2.86 – 3.00 (m, 2H), 7.15 – 7.20 (m, 1H), 7.23 – 7.36 (m, 7H), 7.46 – 7.53 (m, 1H), 7.69 – 7.76 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 25.4, 29.3, 33.8, 39.3, 110.2, 119.8, 124.2, 124.8, 126.2, 126.3, 126.8, 128.5, 134.7, 141.9, 145.9, 150.3, 163.8; HRMS: calcd. for C<sub>19</sub>H<sub>17</sub>ONH<sup>+</sup> : 276.1383, found 276.1387.

**2-(4-*tert*-Butylcyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1i).**



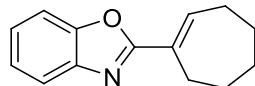
Flash chromatography: Hexane:EA = 70:1; Yield: 86% (65.9 mg); White solid; Melting point 124.6 – 129.3 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 0.92 (s, 9H), 1.22 – 1.46 (m, 2H), 1.97 – 2.13 (m, 2H), 2.31 – 2.51 (m, 2H), 2.80 – 2.95 (m, 1H), 7.02 – 7.12 (m, 1H), 7.24 – 7.32 (m, 2H), 7.46 (dd, *J* = 6.0, 3.3 Hz, 1H), 7.69 (dd, *J* = 5.9, 3.2 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 23.5, 26.2, 27.1, 27.6, 32.2, 43.5, 110.1, 119.7, 124.1, 124.6, 126.1, 135.8, 142.0, 150.3, 164.0; HRMS: calcd. for C<sub>17</sub>H<sub>21</sub>ONH<sup>+</sup> : 256.1696, found 256.1701.

**4-Methyl-2-(4-phenylcyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1j).**



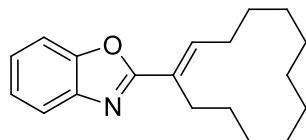
Flash chromatography: Hexane:EA = 50:1; Yield: 97% (84.2 mg); Light yellow solid; Melting point 106.1 – 108.0 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.87 – 2.00 (m, 1H), 2.14 – 2.23 (m, 1H), 2.39 – 2.51 (m, 1H), 2.60 – 2.77 (m, 5H), 2.90 – 3.00 (m, 2H), 7.08 – 7.43 (m, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 16.5, 25.5, 29.3, 33.8, 39.3, 107.4, 124.3, 124.6, 126.3, 126.3, 126.8, 128.4, 130.2, 133.9, 141.2, 146.0, 150.0, 163.0; HRMS: calcd. for C<sub>20</sub>H<sub>19</sub>ONH<sup>+</sup> : 290.1539, found 290.1547.

**2-Cycloheptenylbenzo[*d*]oxazole (Scheme 2, entry 1k).**



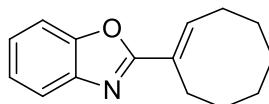
Flash chromatography: Hexane:EA = 50:1; Yield: 91% (58.2 mg); Orange solid; Melting point 55.0 – 57.2 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.56 – 1.64 (m, 2H), 1.64 – 1.71 (m, 2H), 1.80 – 1.91 (m, 2H), 2.42 (q, *J* = 6.4 Hz, 2H), 2.85 – 2.94 (m, 2H), 7.23 – 7.33 (m, 3H), 7.41 – 7.49 (m, 1H), 7.64 – 7.72 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 26.1, 26.4, 28.7, 29.1, 32.2, 110.1, 119.6, 124.0, 124.6, 132.7, 140.2, 142.1, 150.7, 165.0; HRMS: calcd. for C<sub>14</sub>H<sub>15</sub>ONH<sup>+</sup> : 214.1226, found 214.1225.

**(*E*)-2-Cyclododecenylbenzo[*d*]oxazole (Scheme 2, entry 1l).**



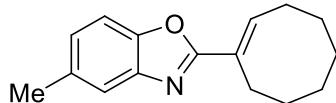
Flash chromatography: Hexane:EA = 50:1; Yield: 76% (64.6 mg); Light yellow solid; Melting point 77.6 – 79.5 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.22 – 1.33 (m, 3H), 1.33 – 1.42 (m, 6H), 1.43 – 1.51 (m, 3H), 1.57 – 1.70 (m, 2H), 1.70 – 1.83 (m, 2H), 2.34 (q, *J* = 7.6 Hz, 2H), 2.70 (t, *J* = 6.8 Hz, 2H), 6.89 (t, *J* = 8.2 Hz, 1H), 7.25 – 7.32 (m, 2H), 7.41 – 7.57 (m, 1H), 7.63 – 7.80 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 22.1, 23.0, 23.4, 24.2, 24.8, 25.0, 25.2, 25.8, 26.3, 26.5, 110.1, 119.7, 124.0, 124.5, 128.2, 139.3, 142.1, 150.2, 164.7; HRMS: calcd. for C<sub>19</sub>H<sub>25</sub>ONH<sup>+</sup> : 284.2009, found 284.2018.

**(*E*)-2-Cyclooctenylbenzo[*d*]oxazole (Scheme 2, entry 1m).**



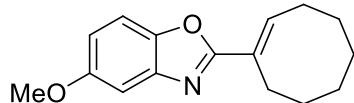
Flash chromatography: Hexane:EA = 50:1; Yield: 95% (64.8 mg); Light yellow solid; Melting point 66.9 – 69.7 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.47 – 1.58 (m, 4H), 1.62 – 1.71 (m, 2H), 1.71 – 1.81 (m, 2H), 2.36 – 2.46 (m, 2H), 2.83 (t, *J* = 6.2 Hz, 2H), 7.09 (t, *J* = 8.5 Hz, 1H), 7.24 – 7.32 (m, 2H), 7.43 – 7.50 (m, 1H), 7.66 – 7.74 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 25.6, 26.0, 26.5, 27.2, 29.0, 29.5, 110.1, 119.7, 124.0, 124.6, 129.4, 138.1, 142.1, 150.5, 164.3; HRMS: calcd. for C<sub>15</sub>H<sub>17</sub>ONH<sup>+</sup> : 228.1383, found 228.1394.

**(E)-2-Cyclooctenyl-5-methylbenzo[d]oxazole (Scheme 2, entry 1n).**



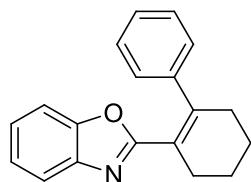
Flash chromatography: Hexane:EA = 50:1; Yield: 97% (70.2 mg); Light beige solid; Melting point 89.1 – 92.3 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.52 (p, *J* = 2.7 Hz, 4H), 1.59 – 1.68 (m, 2H), 1.69 – 1.80 (m, 2H), 2.36 – 2.43 (m, 2H), 2.44 (s, 3H), 2.80 (t, *J* = 6.2 Hz, 2H), 7.02 – 7.10 (m, 2H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.47 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 21.4, 25.6, 26.0, 26.5, 27.1, 29.0, 29.4, 109.4, 119.6, 125.6, 129.5, 133.7, 137.6, 142.3, 148.6, 164.3; HRMS: calcd. for C<sub>16</sub>H<sub>19</sub>ONH<sup>+</sup> : 242.1539, found 242.1550.

**(E)-2-Cyclooctenyl-5-methoxybenzo[d]oxazole (Scheme 2, entry 1o).**



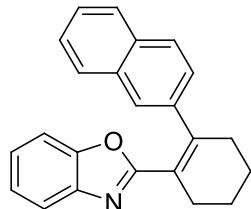
Flash chromatography: Hexane:EA = 40:1; Yield: 95% (73.2 mg); White solid; Melting point 61.1 – 62.2 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.45 – 1.57 (m, 4H), 1.61 – 1.69 (m, 2H), 1.69 – 1.80 (m, 2H), 2.40 (td, *J* = 8.5, 6.2 Hz, 2H), 2.76 – 2.83 (m, 2H), 3.83 (s, 3H), 6.88 (dd, *J* = 8.8, 2.6 Hz, 1H), 7.05 (t, *J* = 8.5 Hz, 1H), 7.20 (d, *J* = 2.6 Hz, 1H), 7.34 (d, *J* = 8.8 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 25.6, 26.0, 26.5, 27.2, 29.0, 29.5, 55.9, 102.8, 110.2, 113.0, 129.5, 137.8, 142.9, 145.1, 157.0, 165.1; HRMS: calcd. for C<sub>16</sub>H<sub>19</sub>O<sub>2</sub>NH<sup>+</sup> : 258.1501, found 258.1516.

**2-(2-Phenylcyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1p).**



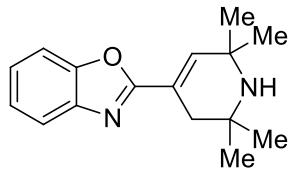
Flash chromatography: Hexane:EA = 50:1; Yield: 73% (60.3 mg); Colorless oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.82 – 1.91 (m, 4H), 2.51 – 2.60 (m, 2H), 2.73 – 2.85 (m, 2H), 7.08 – 7.30 (m, 8H), 7.63 (d, *J* = 7.2 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 22.2, 22.6, 28.1, 33.6, 110.1, 119.6, 122.3, 123.9, 124.5, 127.0, 127.5, 128.0, 141.3, 143.3, 147.0, 150.0, 164.7; HRMS: calcd. for C<sub>19</sub>H<sub>17</sub>ONH<sup>+</sup> : 276.1383, found 276.1388.

**2-(2-(Naphthalen-2-yl)cyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1q).**



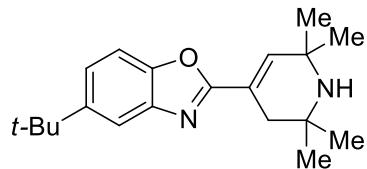
Flash chromatography: Hexane:EA = 50:1; Yield: 74% (72.2 mg); White oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  1.85 – 2.00 (m, 4H), 2.58 – 2.70 (m, 2H), 2.77 – 2.96 (m, 2H), 6.99 (d,  $J$  = 8.1 Hz, 1H), 7.11 (t,  $J$  = 7.7 Hz, 1H), 7.18 – 7.28 (m, 2H), 7.43 – 7.49 (m, 2H), 7.64 (d,  $J$  = 7.9 Hz, 1H), 7.69 – 7.83 (m, 4H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  22.2, 22.7, 28.2, 33.8, 110.1, 119.5, 122.6, 123.9, 124.4, 125.7, 125.8, 126.0, 126.4, 127.4, 127.5, 128.0, 132.5, 133.2, 140.8, 141.3, 146.7, 149.9, 164.6; HRMS: calcd. for  $\text{C}_{23}\text{H}_{19}\text{ONH}^+$  : 326.1539, found 326.1535.

**2-(2,2,6,6-Tetramethyl-1,2,3,6-tetrahydropyridin-4-yl)benzo[d]oxazole (Scheme 2, entry 1r).**



Flash chromatography: Hexane:EA = 5:1; Yield: 91% (69.9 mg); Light orange oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  1.21 (s, 6H), 1.30 (s, 6H), 2.46 (s, 2H), 6.95 (s, 1H), 7.23 – 7.30 (m, 2H), 7.41 – 7.49 (m, 1H), 7.63 – 7.71 (m, 1H);  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  30.0, 31.0, 36.9, 49.3, 51.6, 110.2, 119.8, 121.9, 124.2, 124.9, 141.3, 141.7, 150.3, 163.6; HRMS: calcd. for  $\text{C}_{16}\text{H}_{20}\text{ON}_2\text{H}^+$  : 257.1648, found 257.1650.

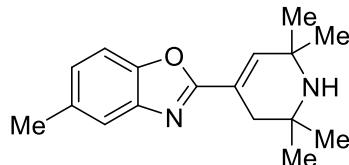
**5-*tert*-Butyl-2-(2,2,6,6-tetramethyl-1,2,3,6-tetrahydropyridin-4-yl)benzo[d]oxazole (Scheme 2, entry 1s).**



Flash chromatography: Hexane:EA = 5:1; Yield: 70% (65.6 mg); Light yellow solid; Melting point 82.3 – 84.0 °C;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  1.21 (s, 6H), 1.31 (s, 6H), 1.34 (s, 9H), 2.46 (s, 2H), 6.92 (s, 1H), 7.27 – 7.46 (m, 2H), 7.71 (s, 1H);  $^{13}\text{C}$  NMR (100

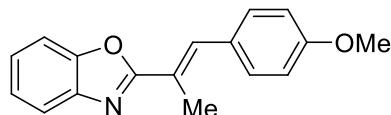
MHz, CDCl<sub>3</sub>) δ 30.0, 31.0, 31.7, 34.8, 36.9, 49.3, 51.6, 109.2, 116.3, 122.0, 122.6, 140.8, 141.6, 147.7, 148.2, 163.7; HRMS: calcd. for C<sub>20</sub>H<sub>28</sub>ON<sub>2</sub>H<sup>+</sup> : 313.2274, found 313.2285.

**5-Methyl-2-(2,2,6,6-tetramethyl-1,2,3,6-tetrahydropyridin-4-yl)benzo[d]oxazole (Scheme 2, entry 1t).**



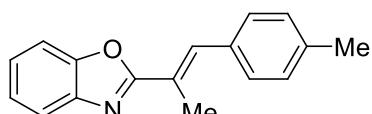
Flash chromatography: Hexane:EA = 5:1; Yield: 98% (79.5 mg); Light yellow solid; Melting point 80.8 – 84.2 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 1.20 (s, 6H), 1.29 (s, 6H), 2.41 (s, 3H), 2.43 (s, 2H), 6.91 (s, 1H), 7.06 (d, *J* = 8.3 Hz, 1H), 7.31 (d, *J* = 8.3 Hz, 1H), 7.43 (s, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 21.4, 29.9, 31.0, 36.8, 49.2, 51.6, 109.4, 119.6, 122.0, 125.9, 133.9, 140.8, 141.9, 148.4, 163.6; HRMS: calcd. for C<sub>17</sub>H<sub>22</sub>ON<sub>2</sub>H<sup>+</sup> : 271.1805, found 271.1811.

**(E)-2-(1-(4-Methoxyphenyl)prop-1-en-2-yl)benzo[d]oxazole (Scheme 2, entry 1u).**



Flash chromatography: Hexane:EA = 40:1; Yield: 89% (70.8 mg); Orange oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.40 (d, *J* = 1.6 Hz, 3H), 3.81 (s, 3H), 6.82 (d, *J* = 8.8 Hz, 2H), 6.95 (s, 1H), 7.23 (d, *J* = 8.7 Hz, 3H), 7.28 – 7.40 (m, 2H), 7.74 (dd, *J* = 7.5, 1.7 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 23.0, 55.2, 110.5, 113.4, 119.9, 121.8, 124.3, 125.1, 128.8, 130.4, 136.2, 141.5, 149.9, 159.3, 163.7; HRMS: calcd. for C<sub>17</sub>H<sub>15</sub>O<sub>2</sub>NH<sup>+</sup> : 266.1176, found 266.1182.

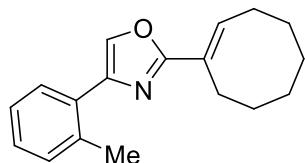
**(E)-2-(1-*p*-tolylprop-1-en-2-yl)benzo[d]oxazole (Scheme 2, entry 1v).**



Flash chromatography: Hexane:EA = 50:1; Yield: 80% (59.8 mg); Yellow oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 2.36 (s, 3H), 2.42 (d, *J* = 1.6 Hz, 3H), 6.99 (s, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.26 – 7.40 (m, 3H), 7.75 (d, *J* = 6.3 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 21.3, 23.0, 110.5, 119.9, 122.8, 124.2, 125.1, 128.7, 128.8, 133.4,

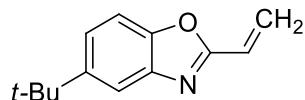
136.5, 137.7, 141.4, 149.9, 163.6; HRMS: calcd. for  $C_{17}H_{15}ONH^+$  : 250.1226, found 250.1234.

**(E)-2-Cyclooctenyl-4-*o*-tolyloxazole (Scheme 2, entry 1w).**



Flash chromatography: Hexane:EA = 50:1; Yield: 71% (56.9 mg); Colorless oil;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  1.54 (p,  $J$  = 2.6 Hz, 4H), 1.61 – 1.68 (m, 2H), 1.70 – 1.77 (m, 2H), 2.31 – 2.42 (m, 2H), 2.49 (s, 3H), 2.71 – 2.81 (t,  $J$  = 6.2 Hz, 2H), 6.86 (t,  $J$  = 8.5 Hz, 1H), 7.13 – 7.32 (m, 4H), 7.70 (d,  $J$  = 7.0 Hz, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  21.8, 25.5, 26.0, 26.5, 26.9, 29.0, 29.6, 125.6, 126.1, 126.6, 127.5, 128.0, 129.1, 131.1, 134.1, 134.6, 149.8, 162.2; HRMS: calcd. for  $C_{18}H_{21}ONH^+$  : 268.1695, found 268.1696.

**5-*tert*-Butyl-2-vinylbenzo[*d*]oxazole (Scheme 2, entry 1x).**



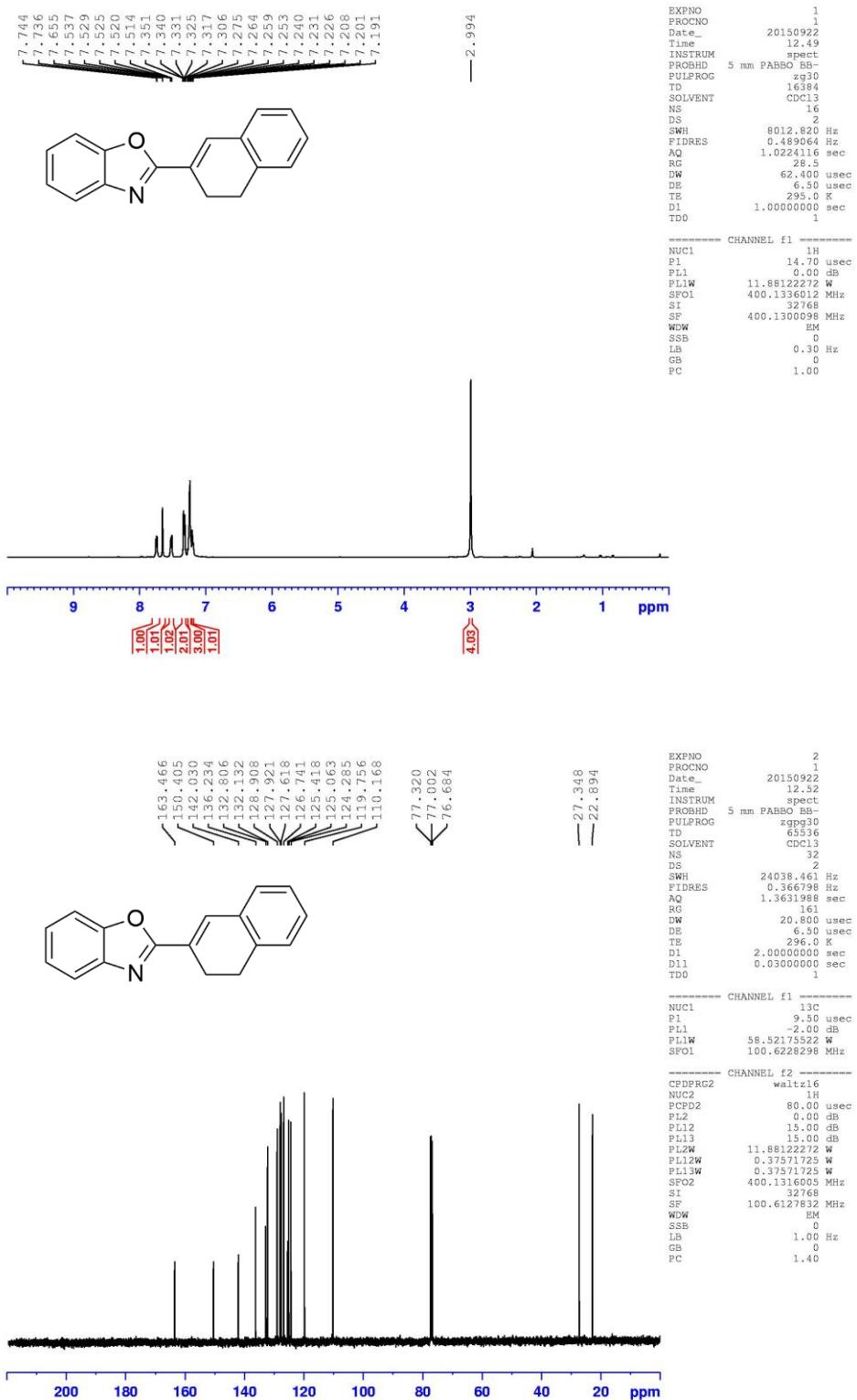
Flash chromatography: Hexane:EA = 50:1; Yield: 70% (42.2 mg); Light yellow oil;  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  1.37 (s, 9H), 5.81 (d,  $J$  = 11.1 Hz, 1H), 6.44 (d,  $J$  = 17.6 Hz, 1H), 6.74 (dd,  $J$  = 17.6, 11.1 Hz, 1H), 7.30 – 7.50 (m, 1H), 7.73 (s, 1H);  $^{13}C$  NMR (100 MHz,  $CDCl_3$ )  $\delta$  31.7, 34.9, 109.5, 116.6, 123.2, 124.0, 124.8, 141.7, 148.0, 148.3, 162.2; HRMS: calcd. for  $C_{13}H_{15}ONH^+$  : 202.1226, found 202.1233.

## 7. References

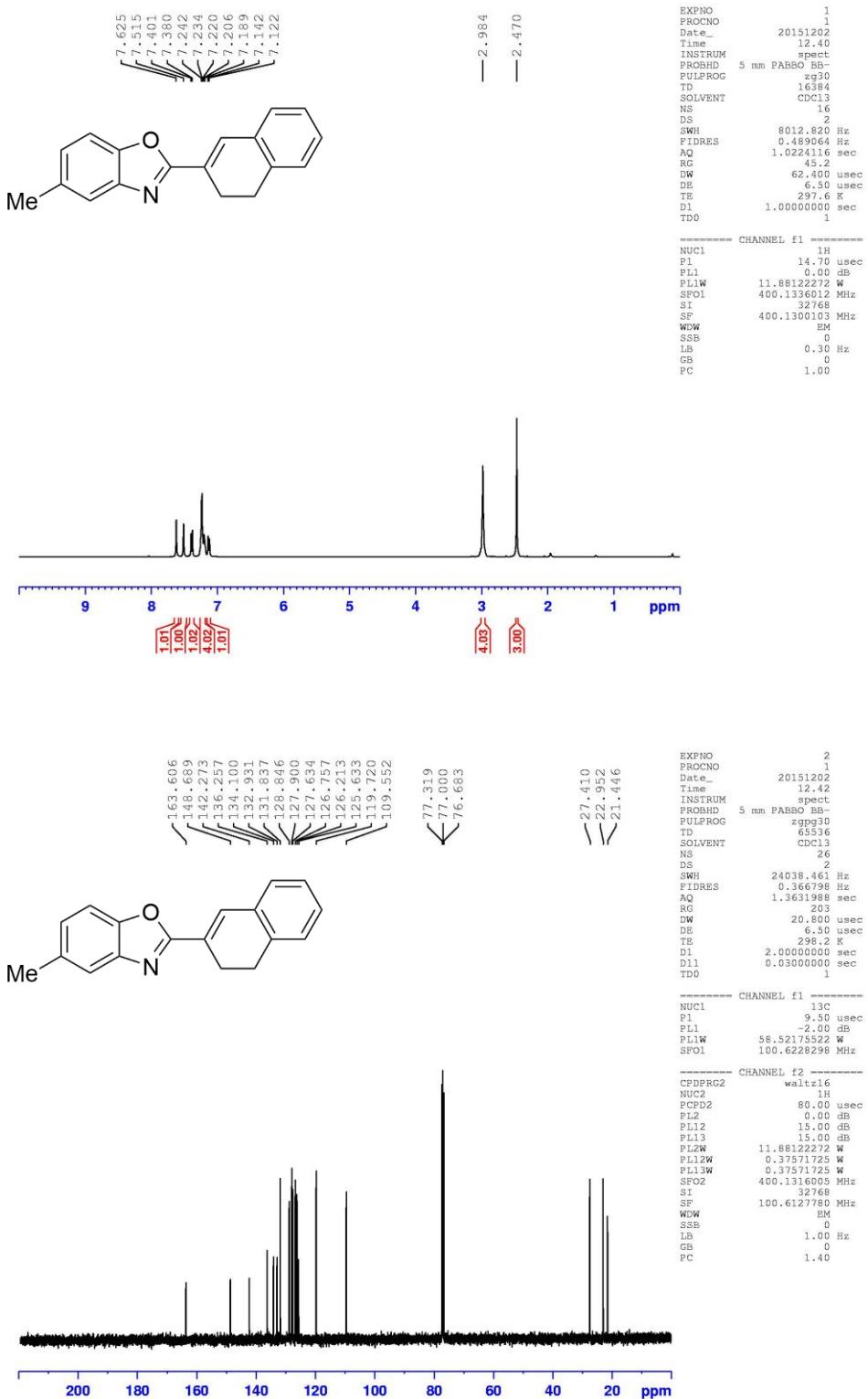
- (1) So, C. M.; Lau, C. P.; Kwong, F. Y. *Angew. Chem. Int. Ed.* **2008**, *47*, 8059.
- (2) Chung, K. H.; So, C. M.; Wong, S. M.; Luk, C. H.; Zhou, Z.; Lau, C. P.; Kwong, F. Y. *Chem. Commun.* **2012**, *48*, 1967.
- (3) Chow, W. K.; Yuen, O. Y.; So, C. M.; Wong, W. T.; Kwong, F. Y. *J. Org. Chem.* **2012**, *77*, 3543.
- (4) Fu, W. C.; So, C. M.; Chow, W. K.; Yuen, O. Y.; Kwong, F. Y. *Org. Lett.* **2015**, *17*, 4612.
- (5) To, S. C.; Kwong, F. Y. *Chem. Commun.* **2011**, *47*, 5079.
- (6) Meng, L.; Kamada, Y.; Muto, K.; Yamaguchi, J.; Itami, K. *Angew. Chem. Int. Ed.* **2013**, *52*, 10048.

## 8. $^1\text{H}$ and $^{13}\text{C}$ NMR spectra

**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(3,4-Dihydronaphthalen-2-yl)benzo[d]oxazole (Scheme 2, entry 1a)**



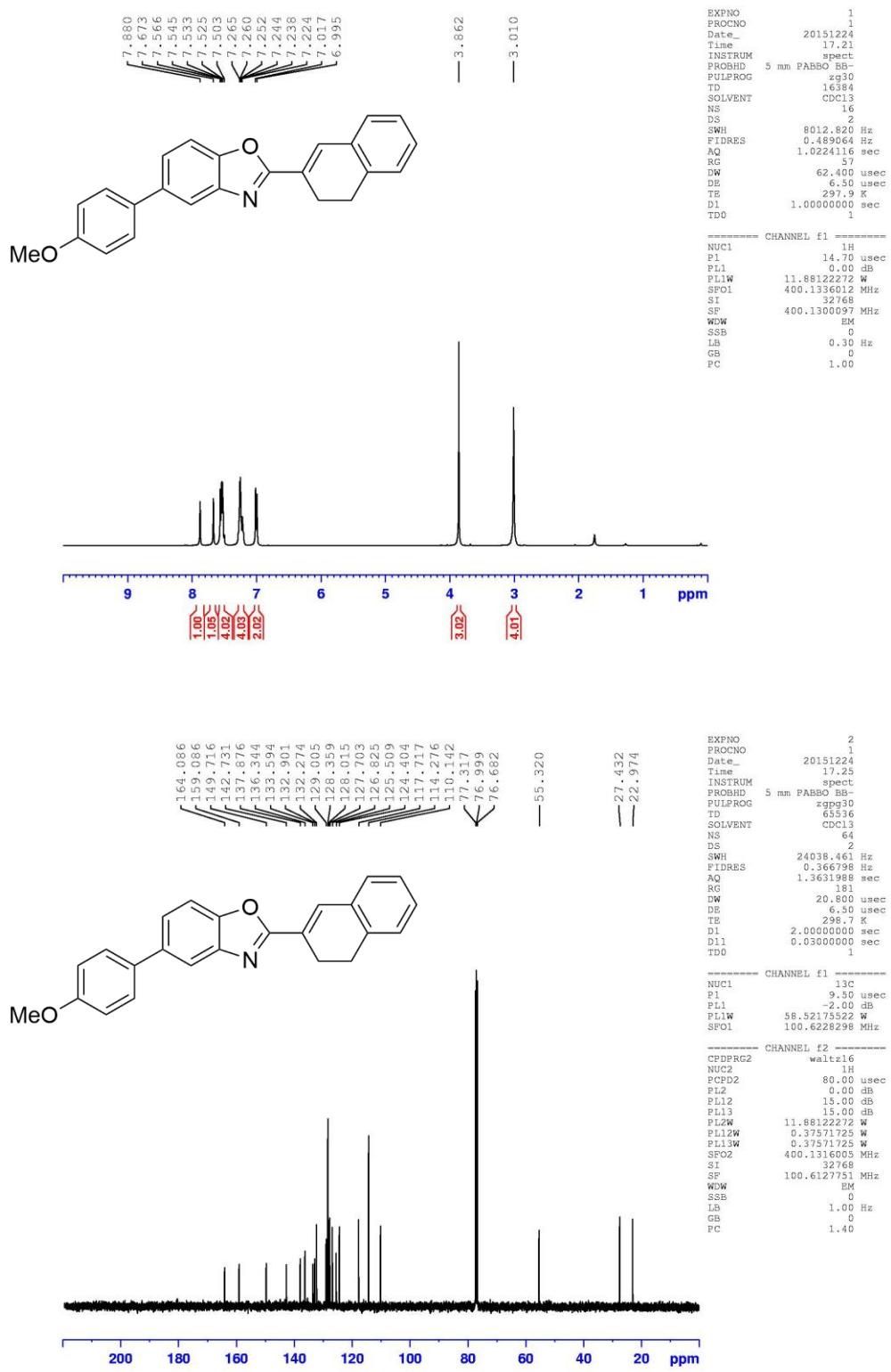
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(3,4-Dihydronaphthalen-2-yl)-5-methylbenzo[d]oxazole (Scheme 2, entry 1b)**



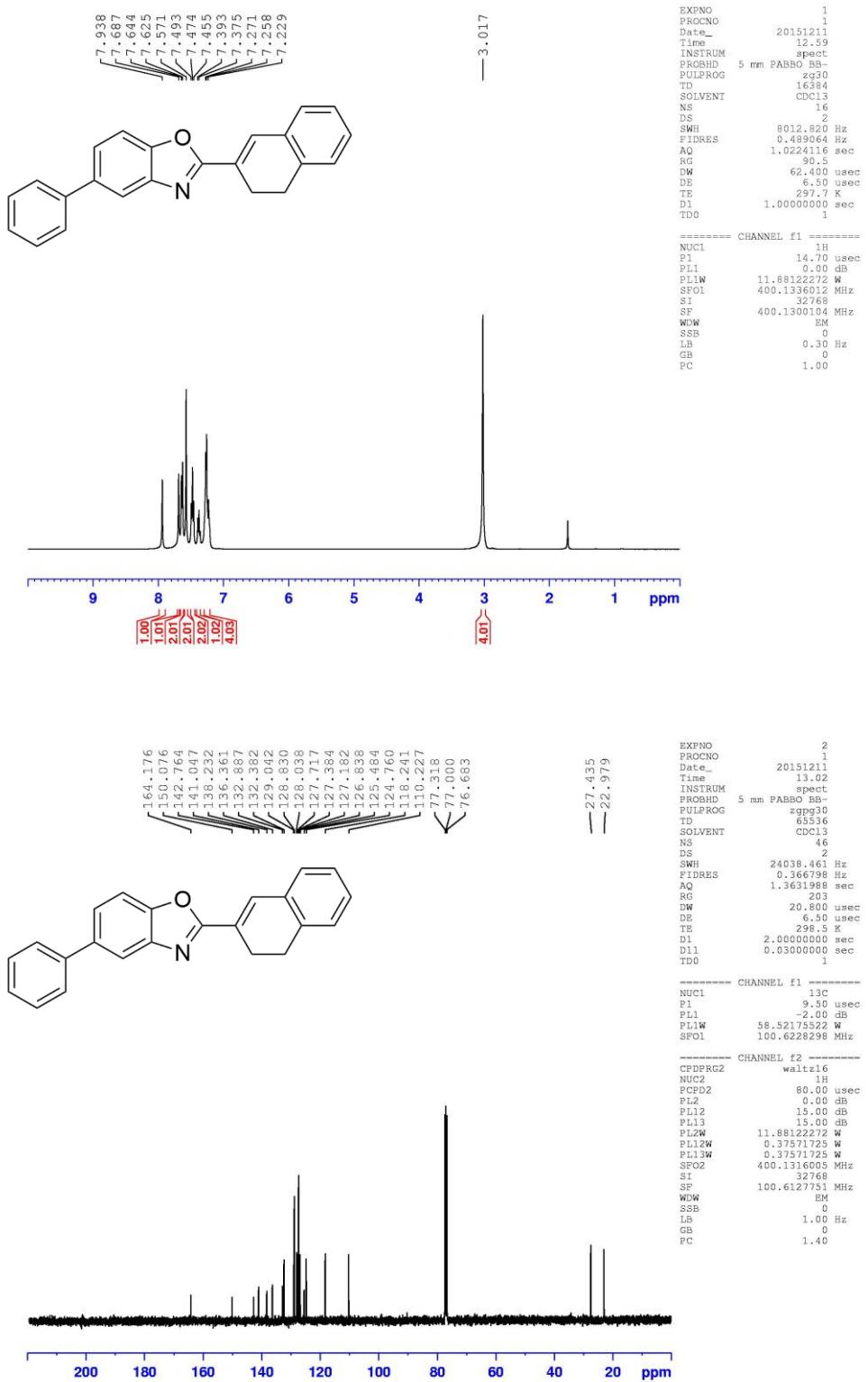
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 5-*tert*-Butyl-2-(3,4-dihydronaphthalen-2-yl)benzo[d]oxazole (Scheme 2, entry 1c)**



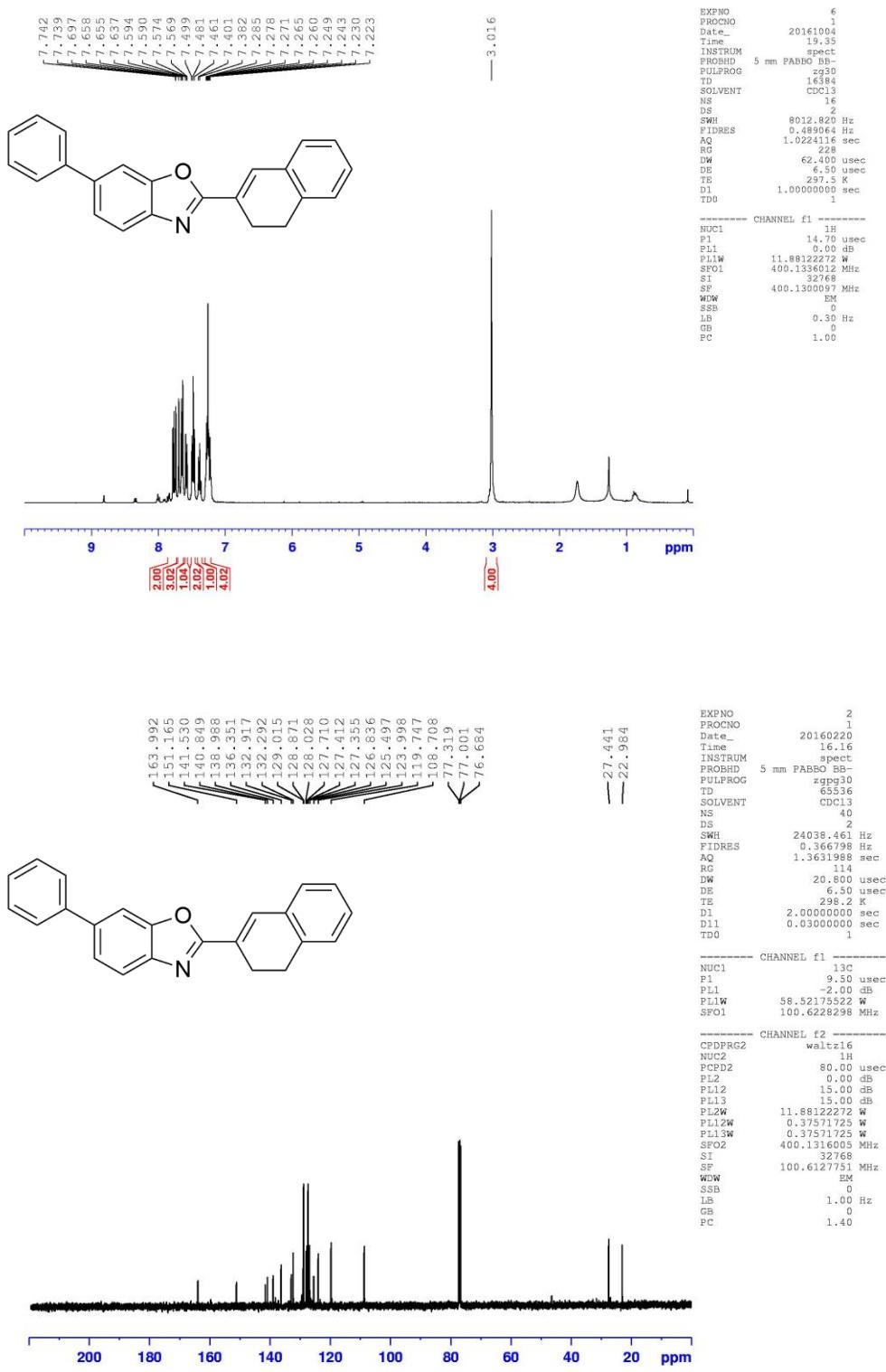
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(3,4-Dihydronaphthalen-2-yl)-5-(4-methoxyphenyl)benzo[d]oxazole (Scheme 2, entry 1d)**



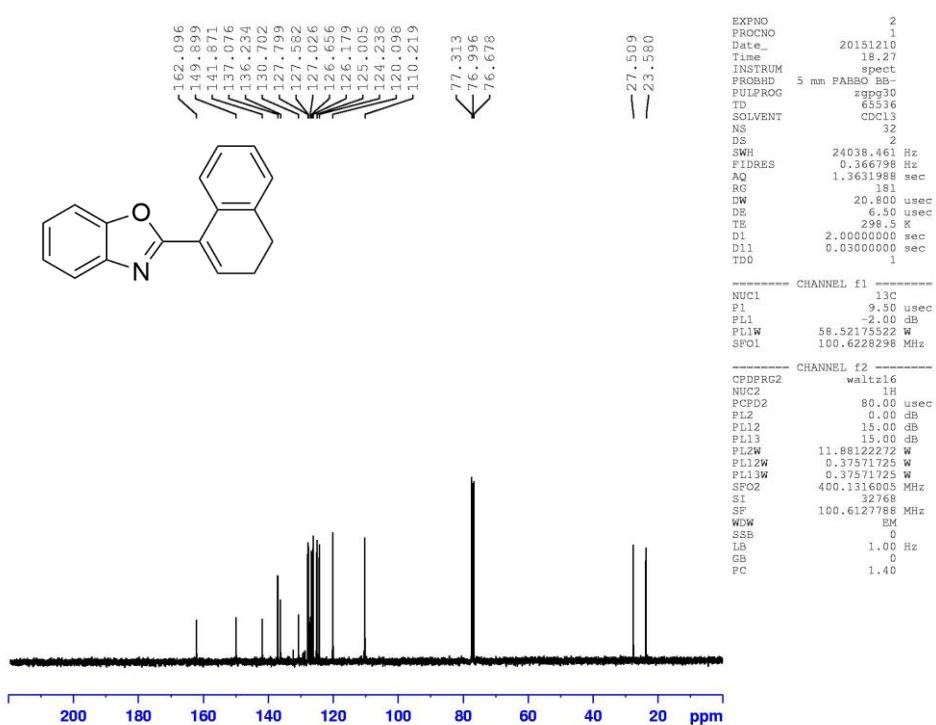
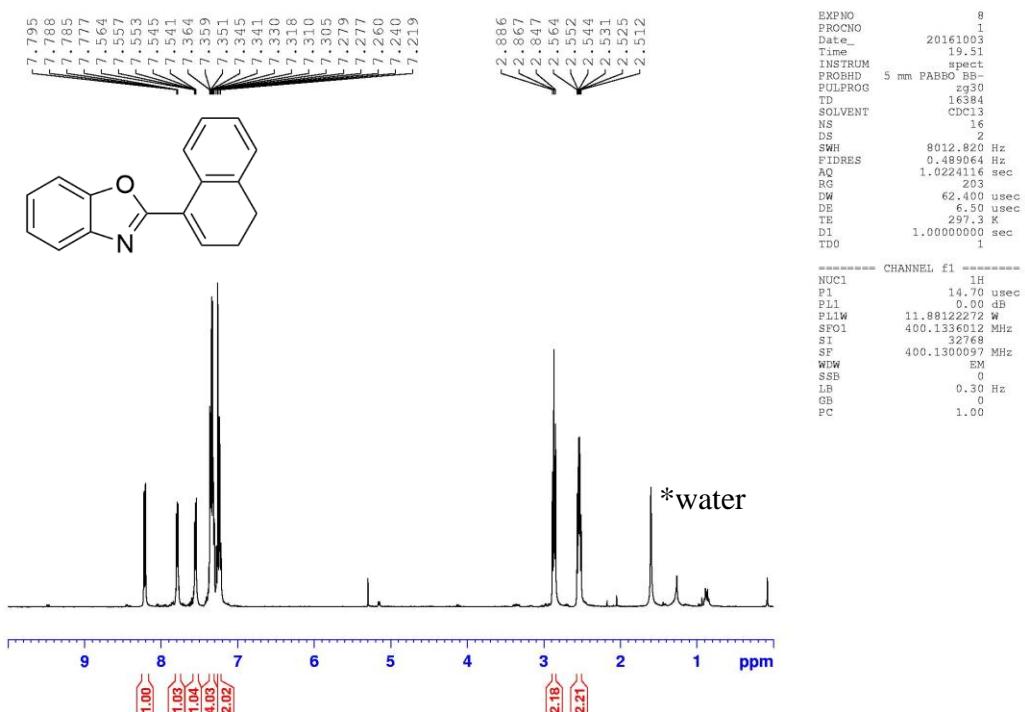
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(3,4-Dihydronaphthalen-2-yl)-5-phenylbenzo[d]oxazole (Scheme 2, entry 1e)**



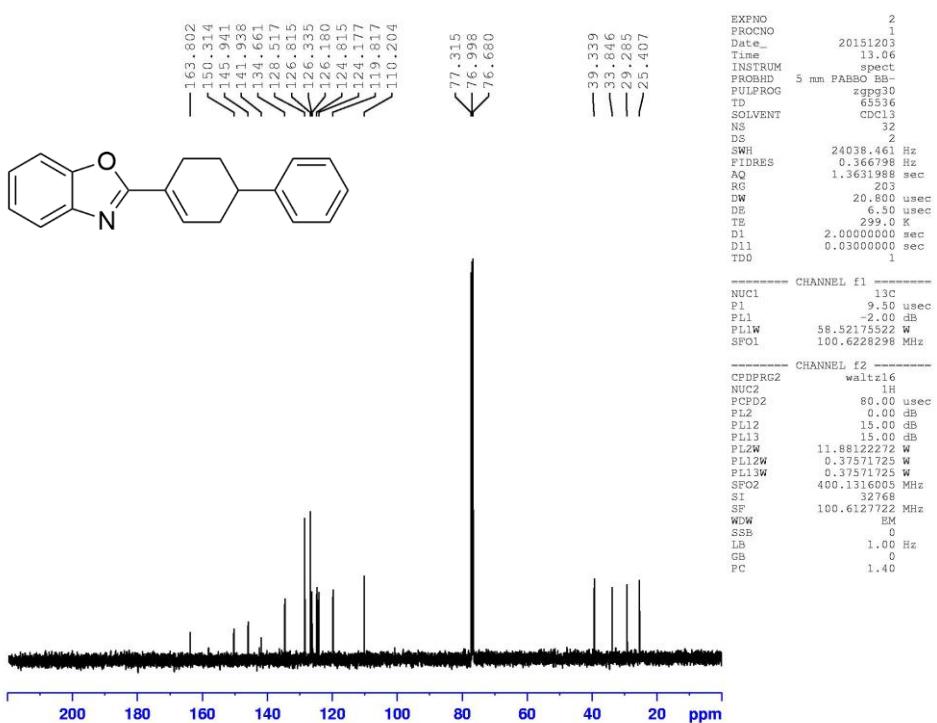
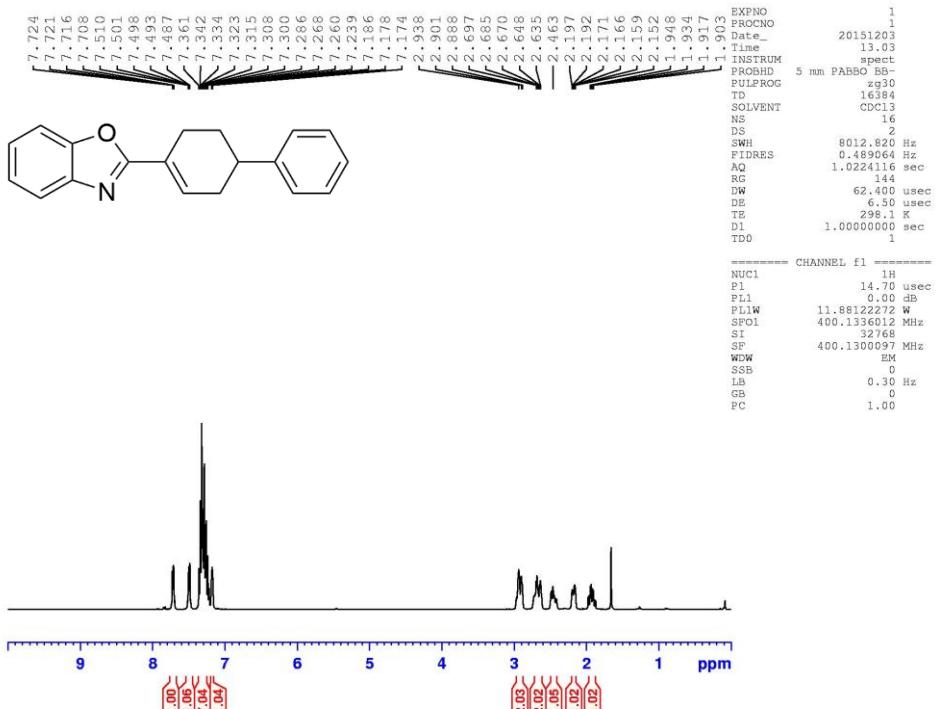
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(3,4-Dihydronaphthalen-2-yl)-6-phenylbenzo[d]oxazole (Scheme 2, entry 1f)**



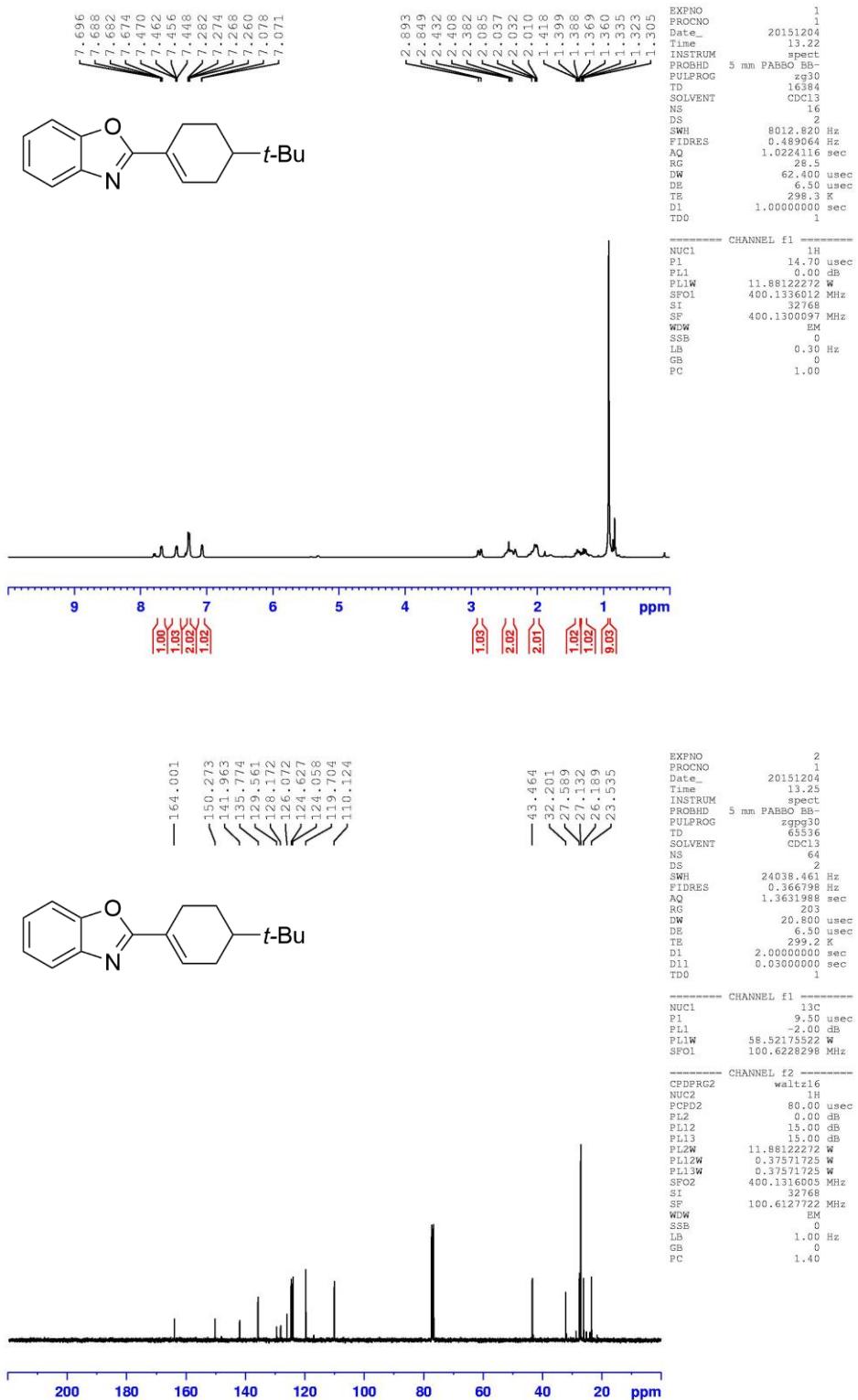
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(3,4-Dihydronaphthalen-1-yl)benzo[d]oxazole (Scheme 2, entry 1g)**



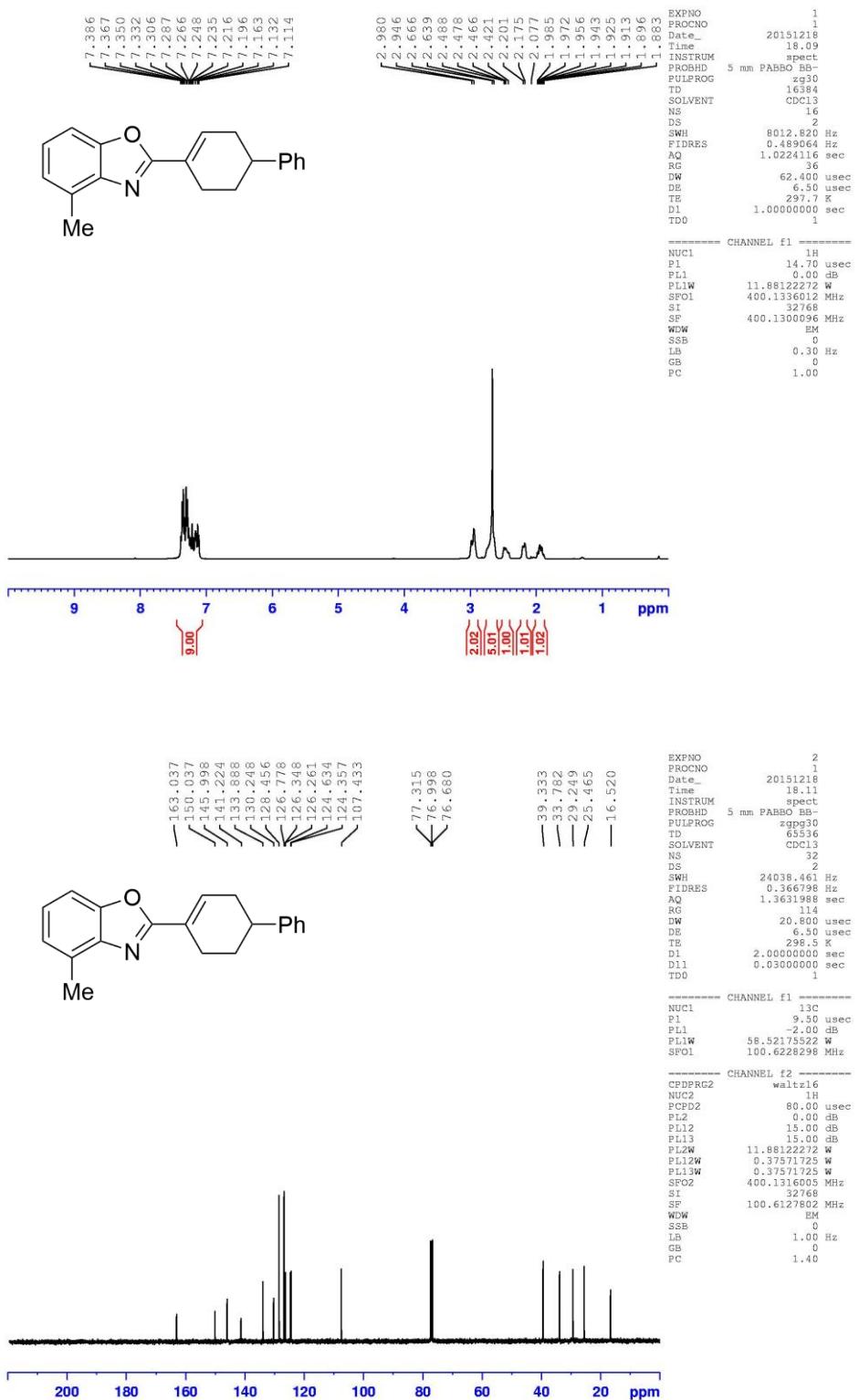
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(4-Phenylcyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1h)**



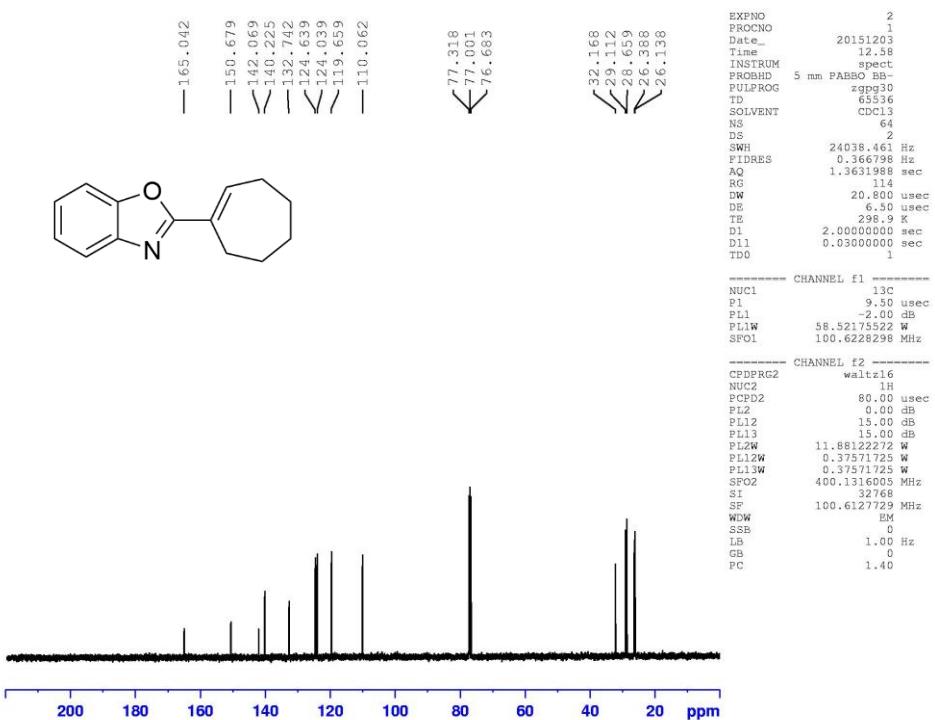
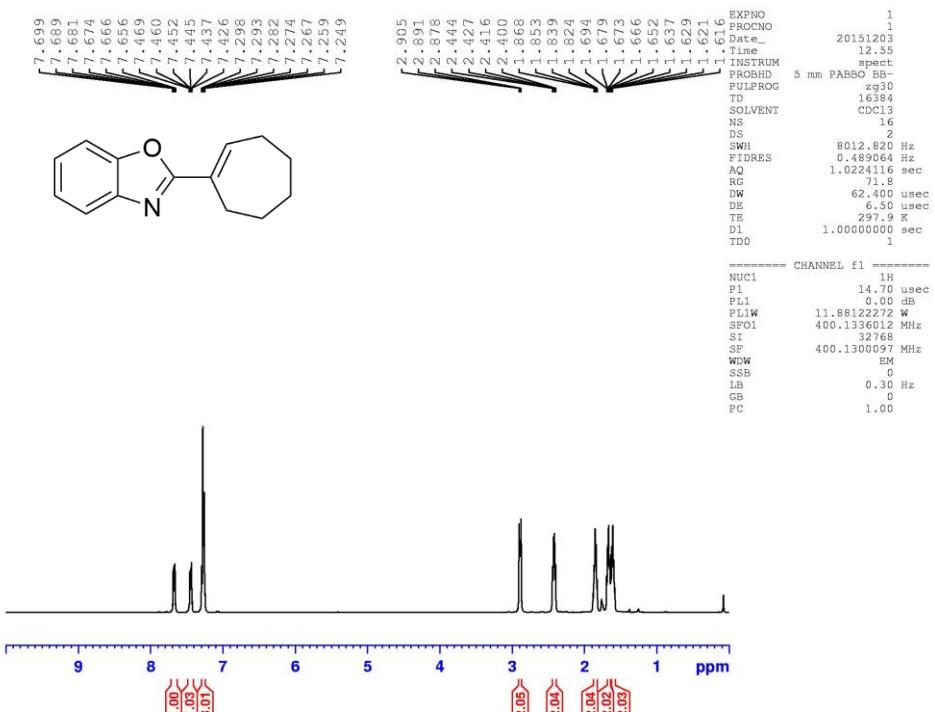
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(4-*tert*-Butylcyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1i)**



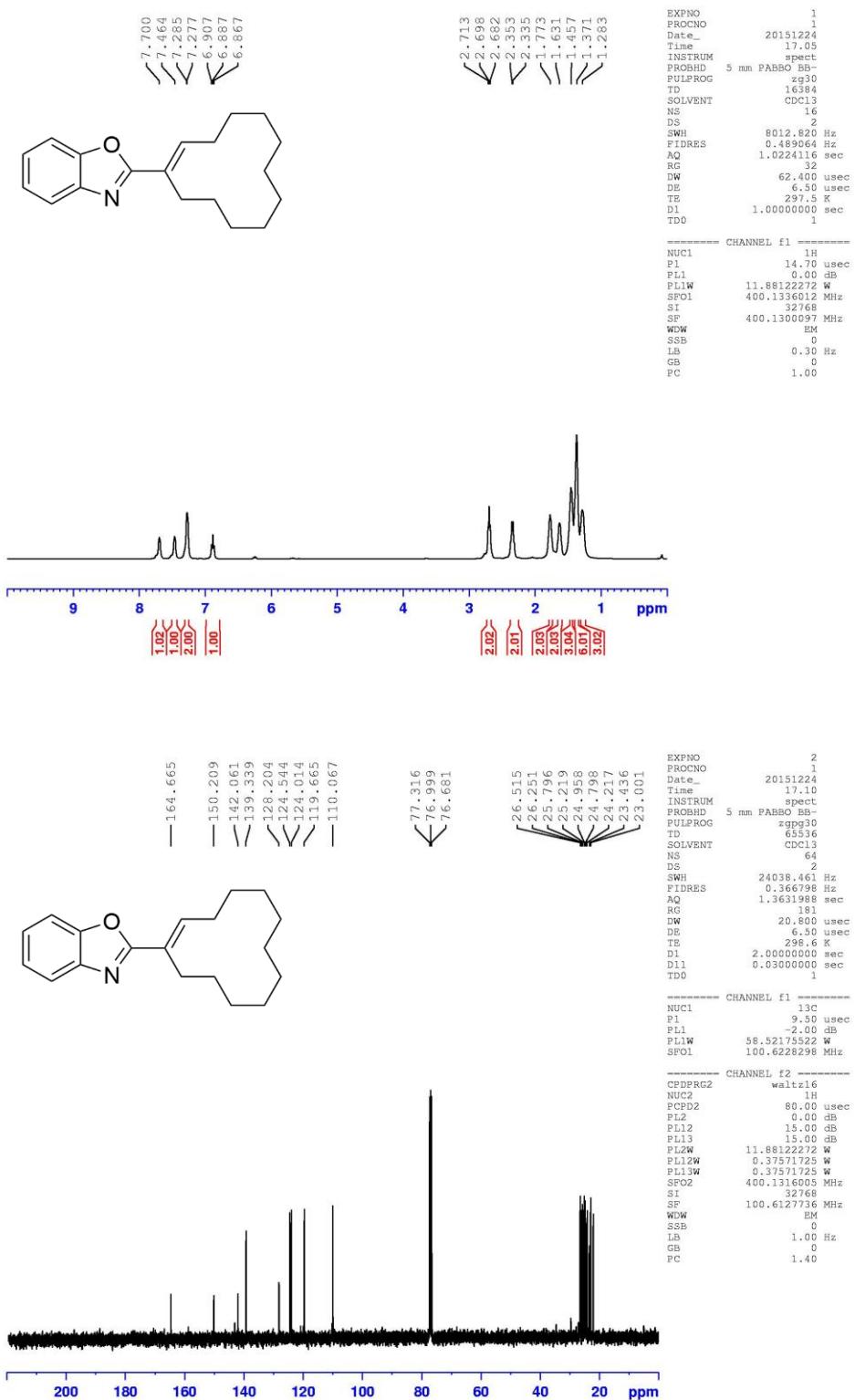
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 4-Methyl-2-(4-phenylcyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1j)**



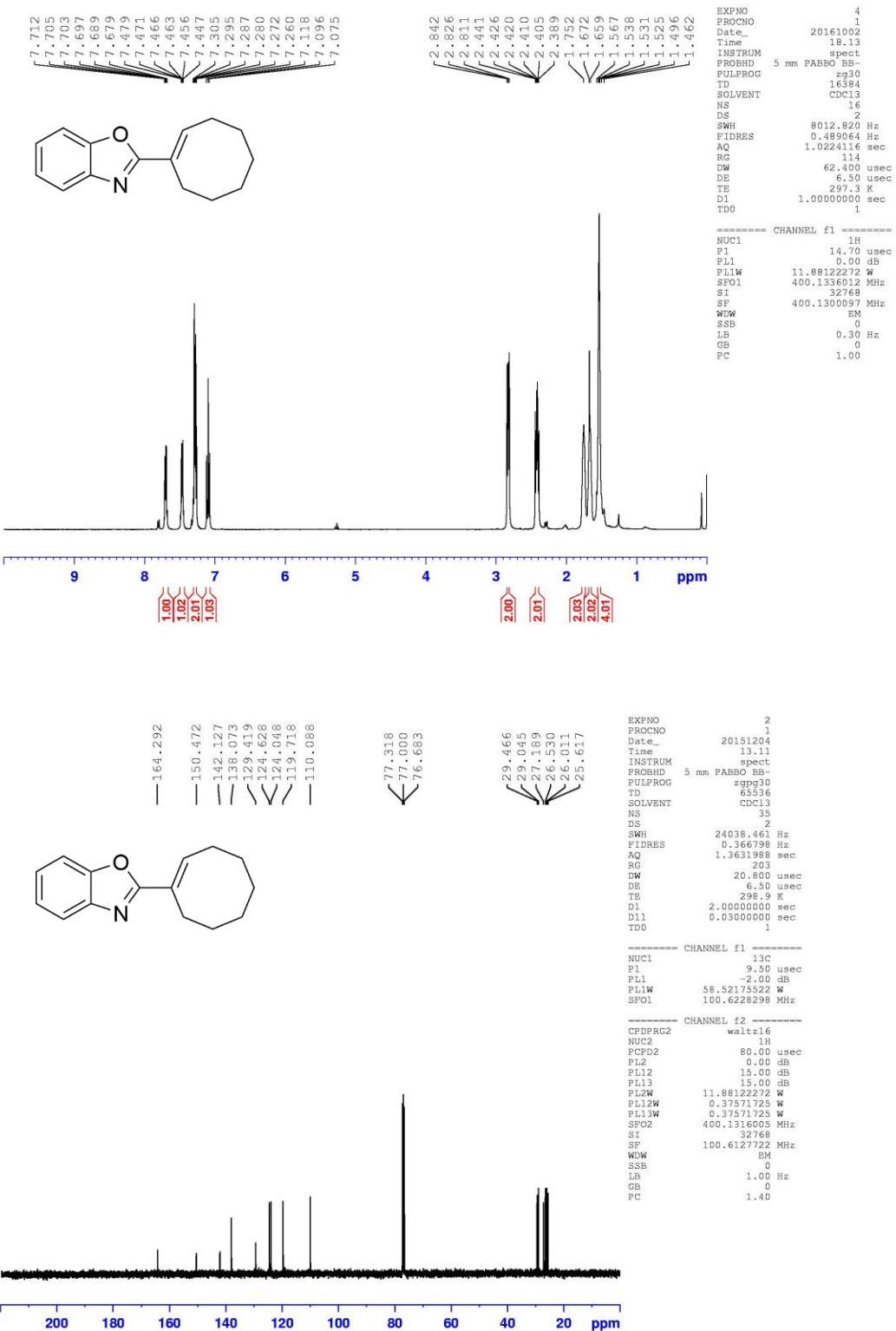
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-Cycloheptenylbenzo[d]oxazole (Scheme 2, entry 1k)**



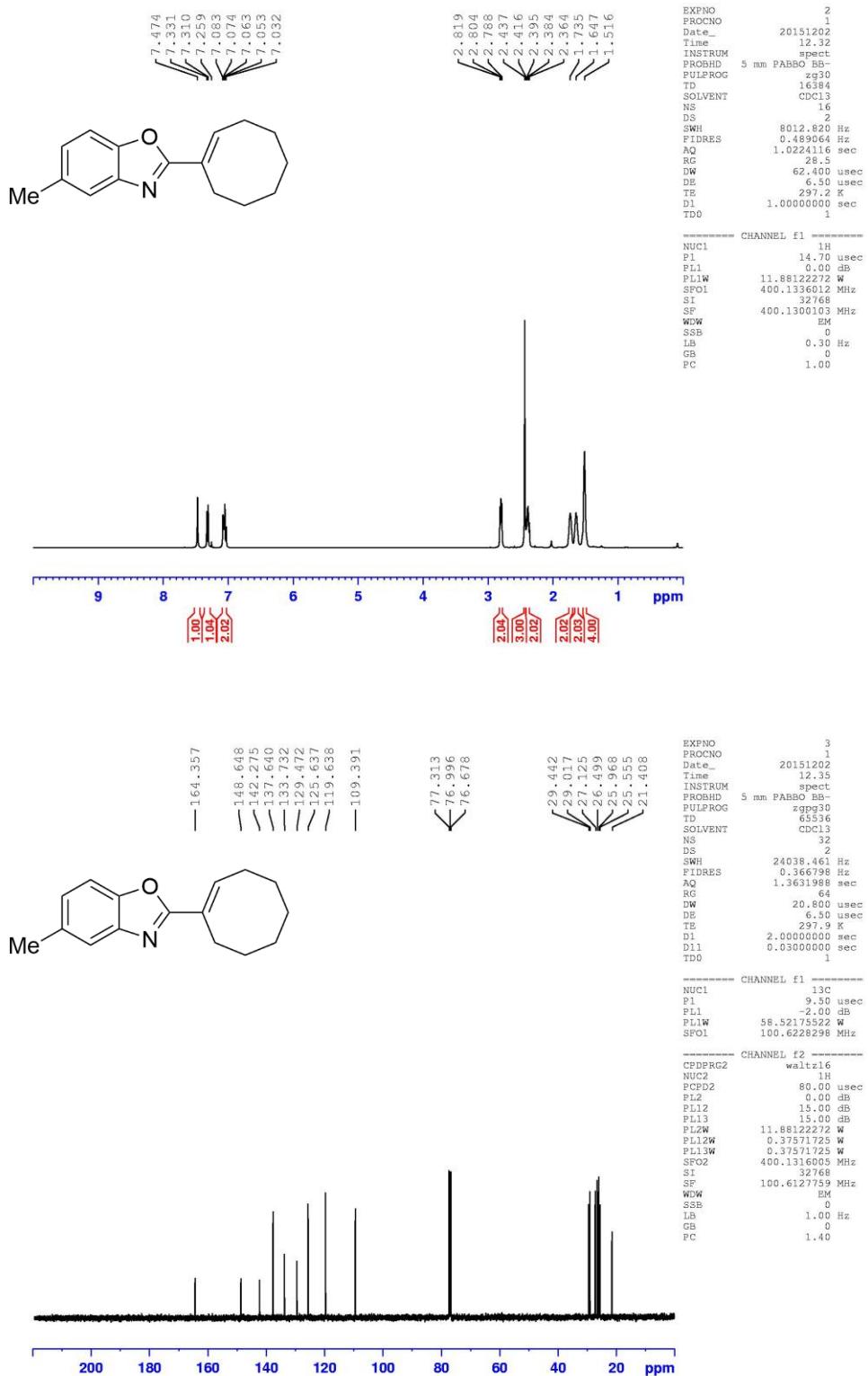
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for (E)-2-Cyclododecenylbenzo[d]oxazole (Scheme 2, entry 1l)**



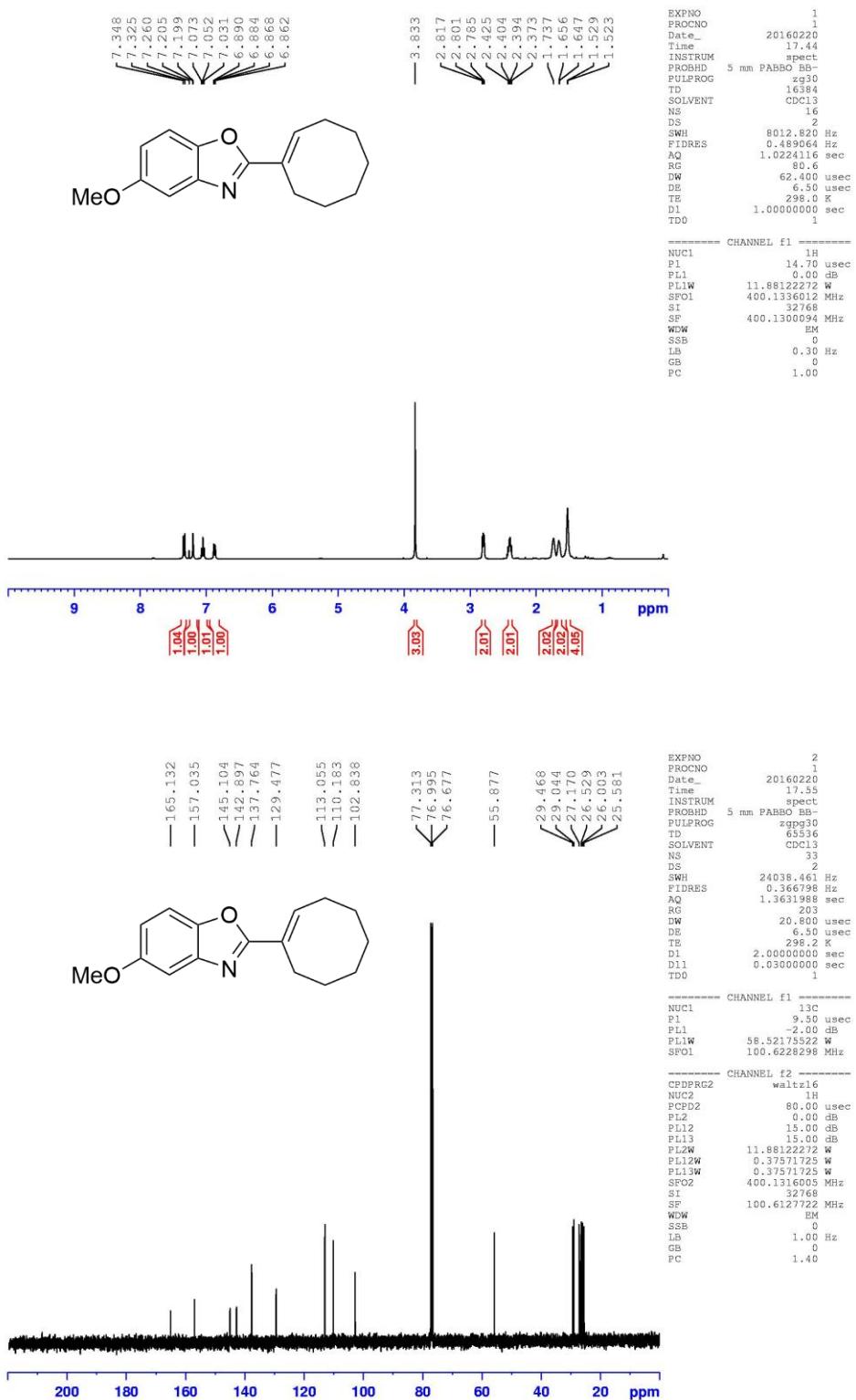
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for (E)-2-Cyclooctenylbenzo[d]oxazole (Scheme 2, entry 1m)**



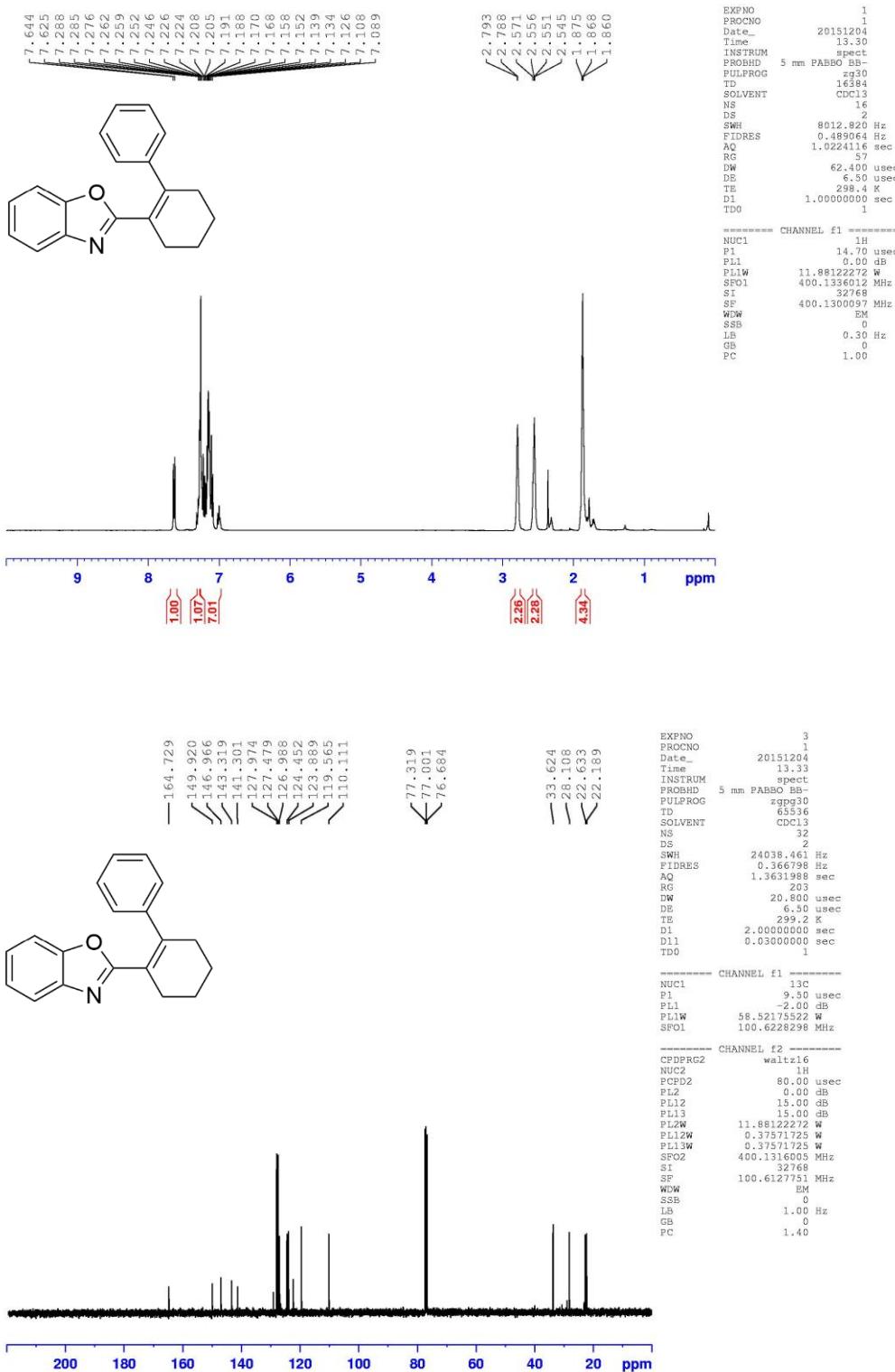
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for (E)-2-Cyclooctenyl-5-methylbenzo[d]oxazole (Scheme 2, entry 1n)**



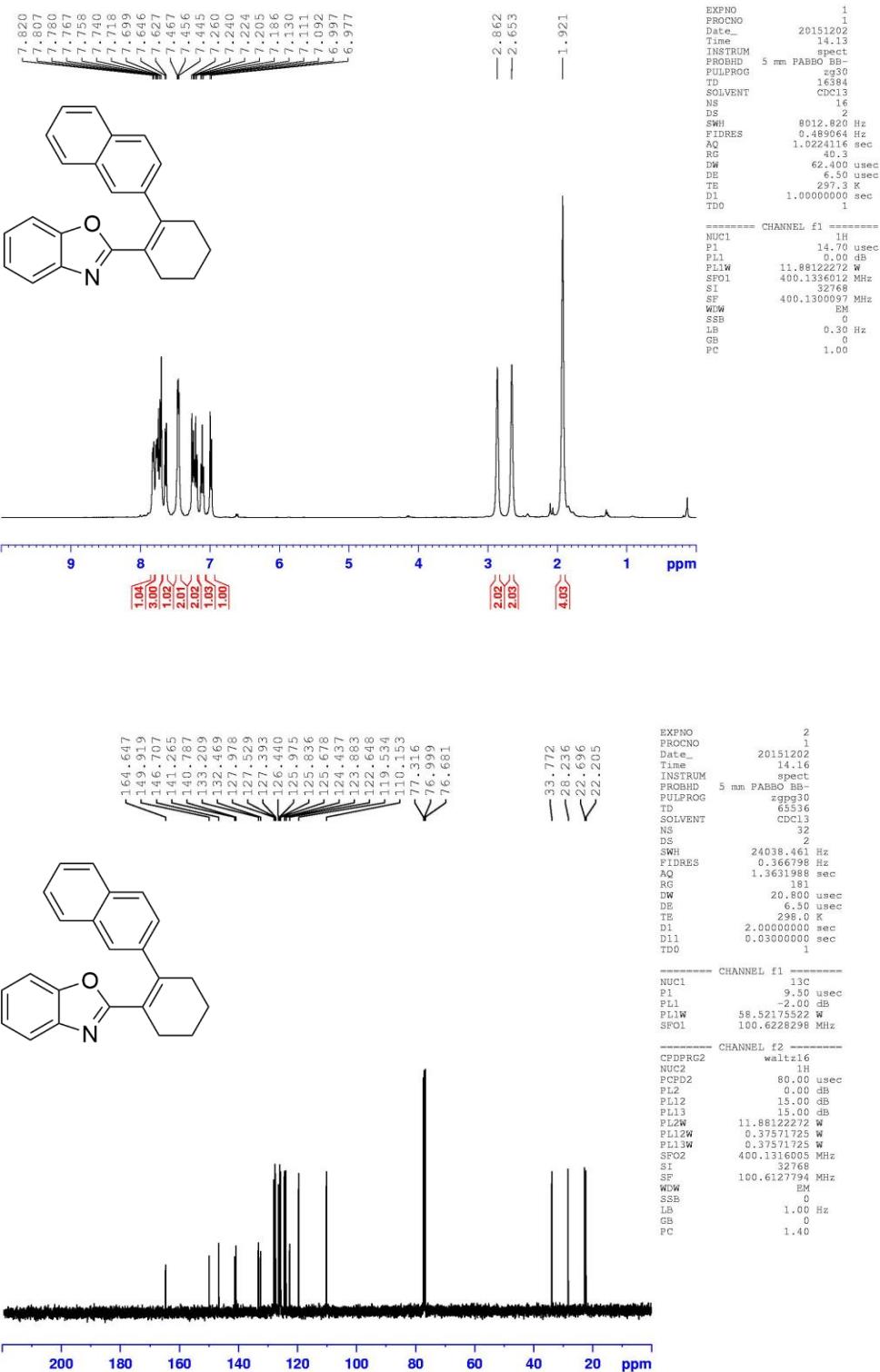
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for (E)-2-Cyclooctenyl-5-methoxybenzo[d]oxazole (Scheme 2, entry 1o)**



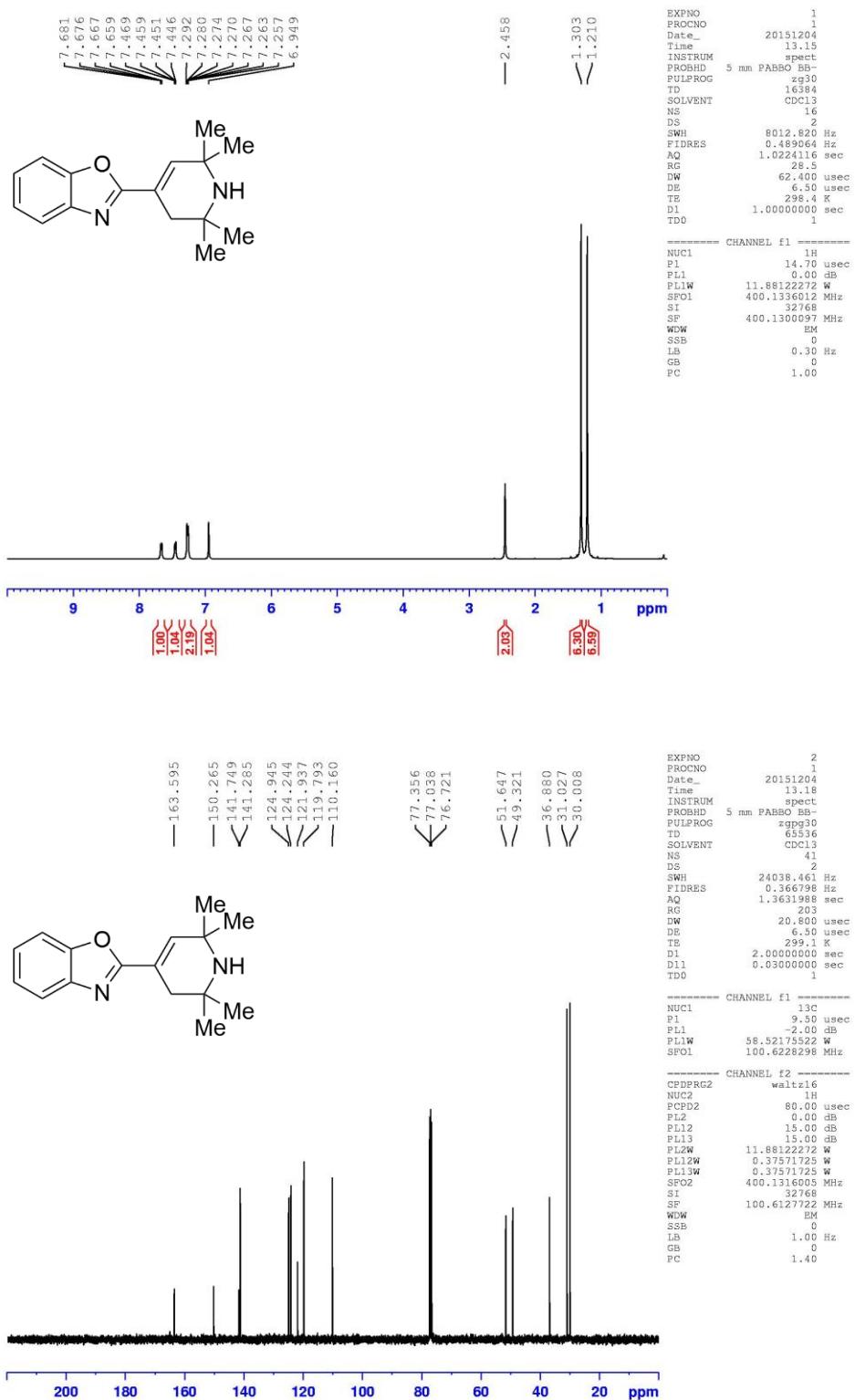
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(2-Phenylcyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1p)**



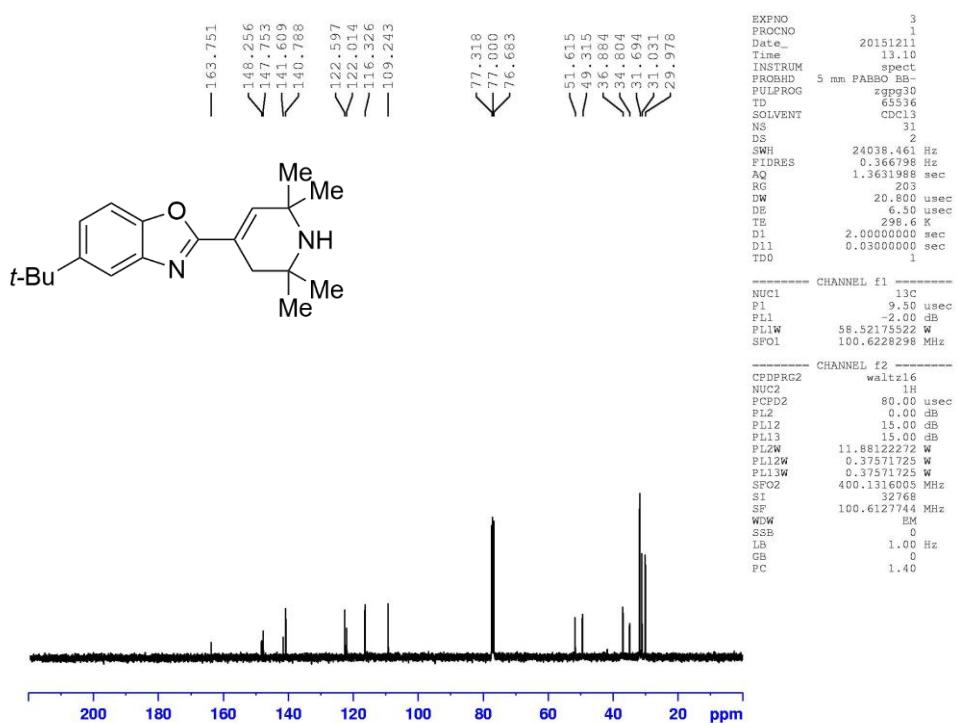
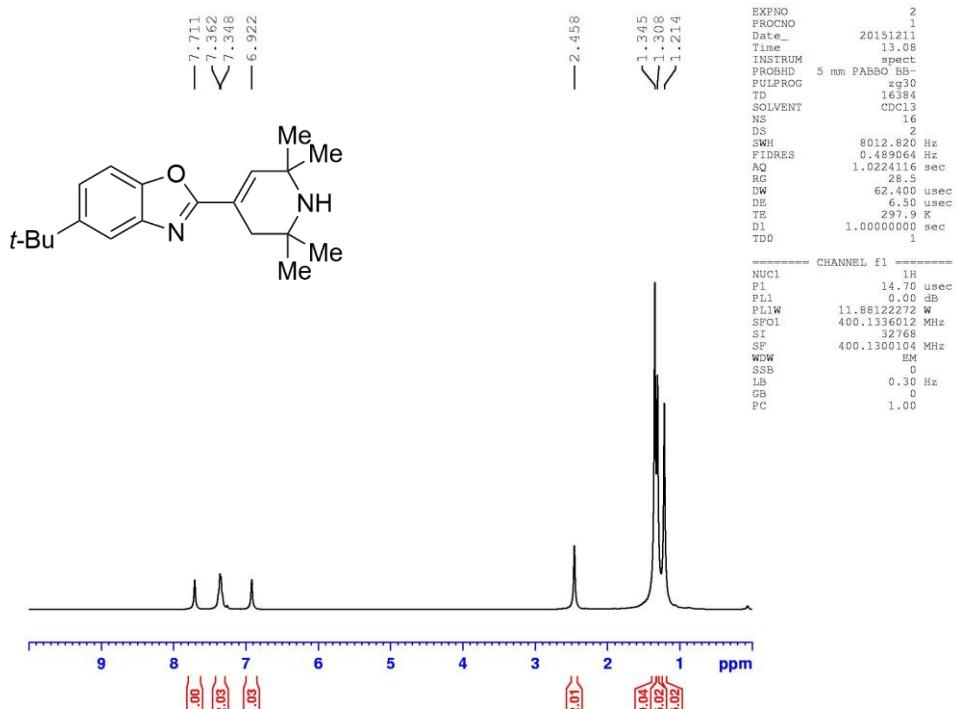
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(2-(Naphthalen-2-yl)cyclohex-1-enyl)benzo[d]oxazole (Scheme 2, entry 1q)**



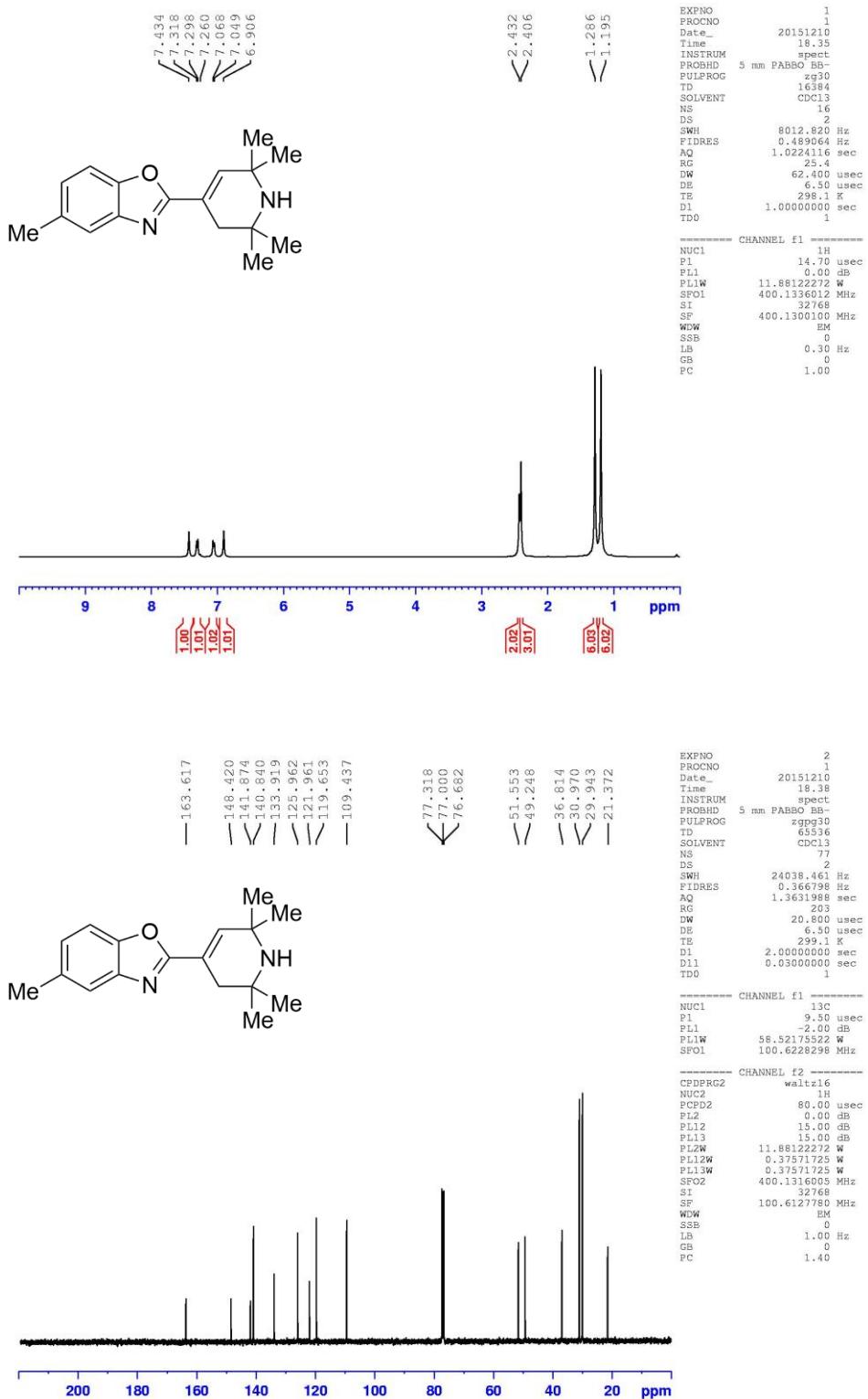
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 2-(2,2,6,6-Tetramethyl-1,2,3,6-tetrahydropyridin-4-yl)benzo[d]oxazole (Scheme 2, entry 1r)**



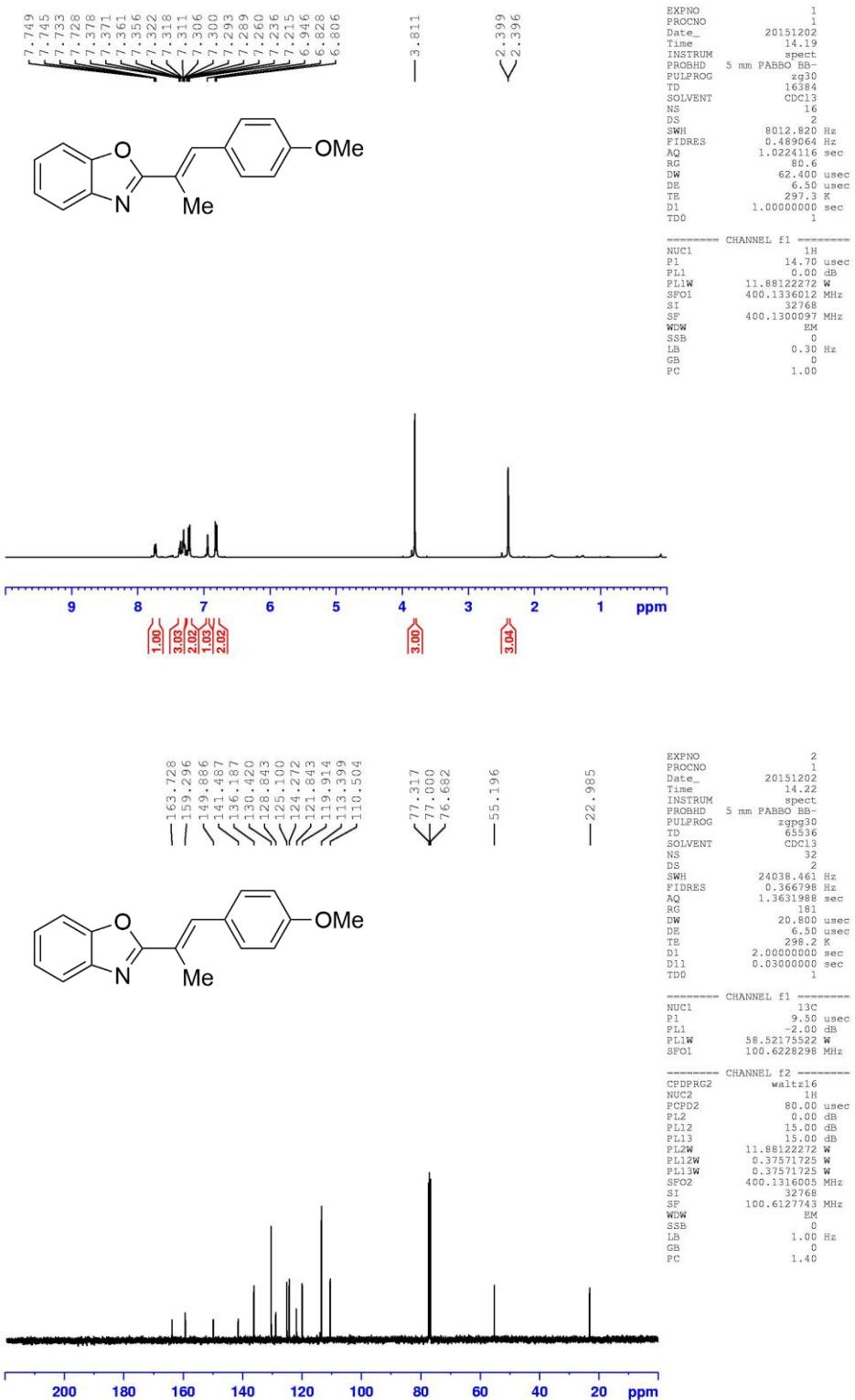
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 5-*tert*-Butyl-2-(2,2,6,6-tetramethyl- 1,2,3,6-tetrahydropyridin-4-yl)benzo[d]oxazole (Scheme 2, entry 1s)**



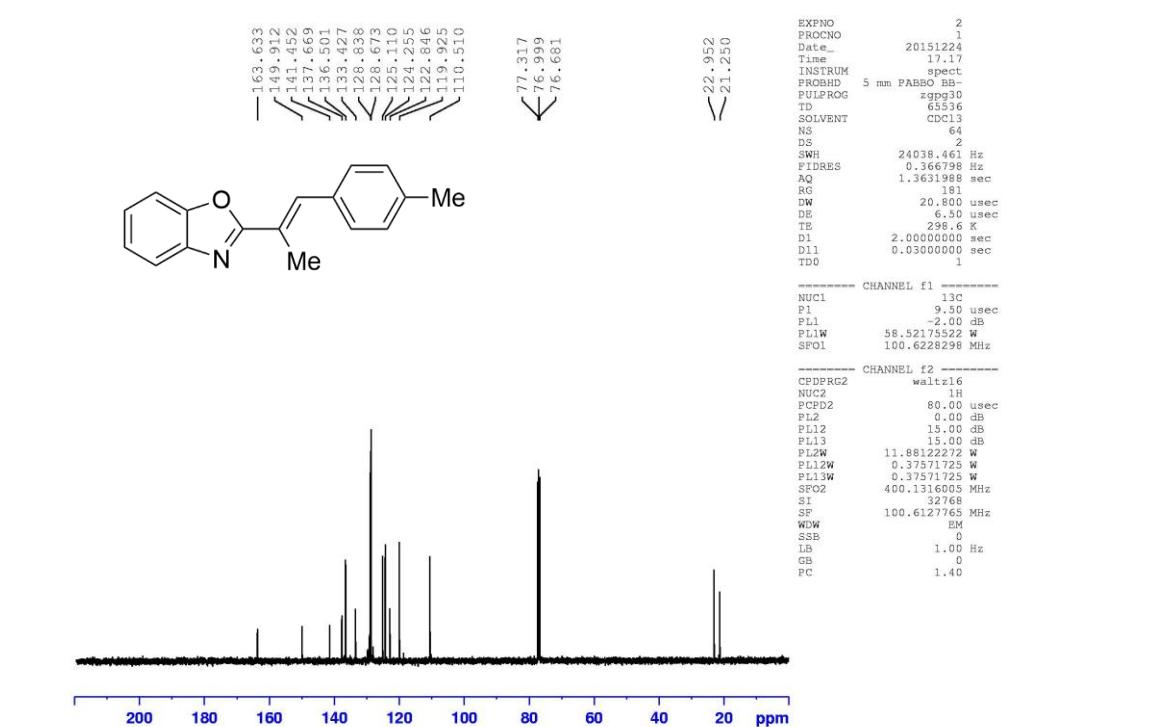
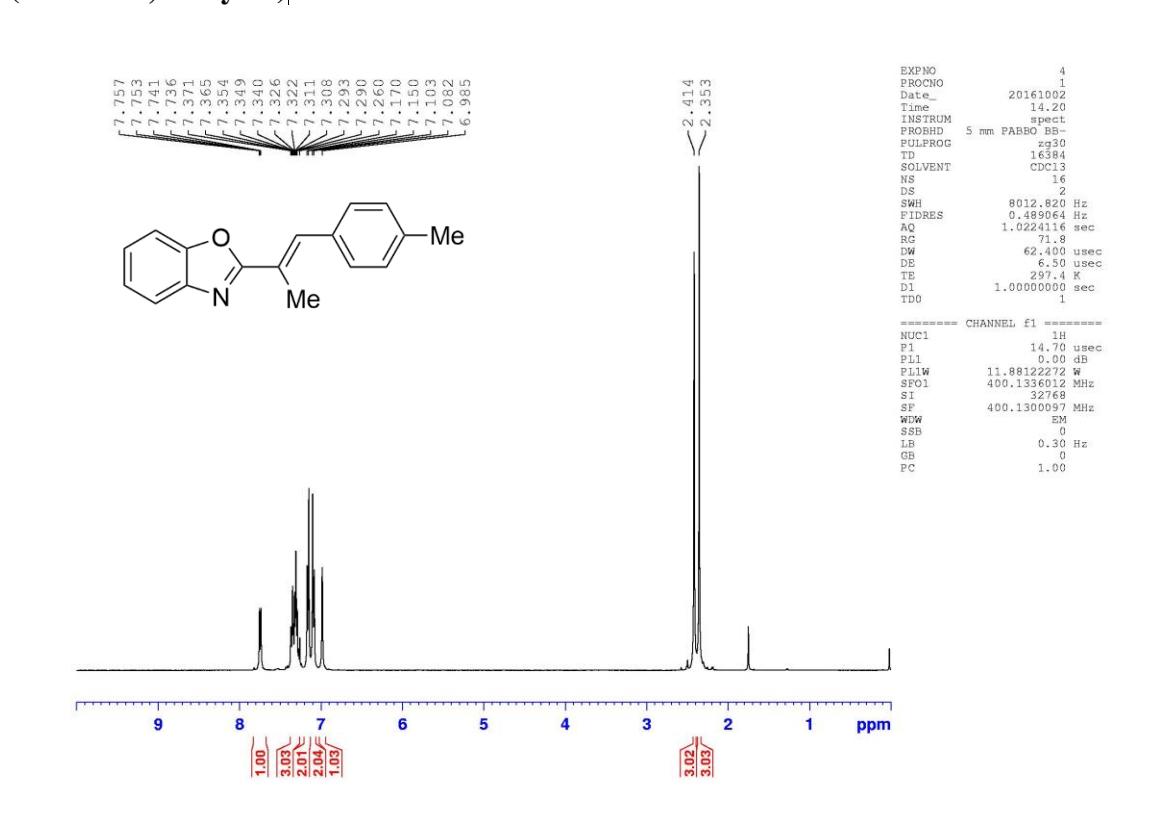
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 5-Methyl-2-(2,2,6,6-tetramethyl- 1,2,3,6-tetrahydropyridin-4-yl)benzo[d]oxazole (Scheme 2, entry 1t)**



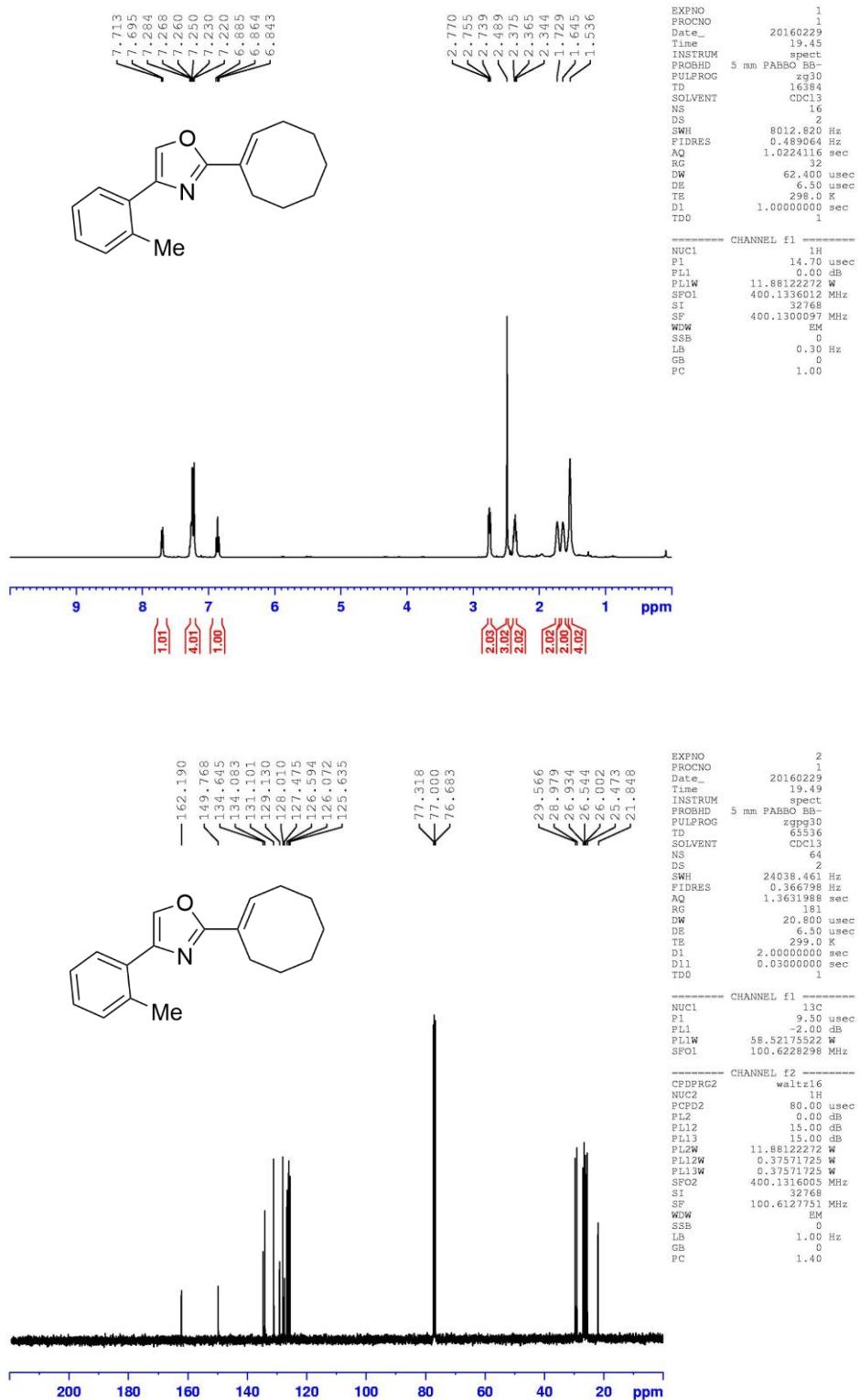
<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for (E)-2-(1-(4-Methoxyphenyl)prop-1-en-2-yl)benzo[d]oxazole (Scheme 2, entry 1u)



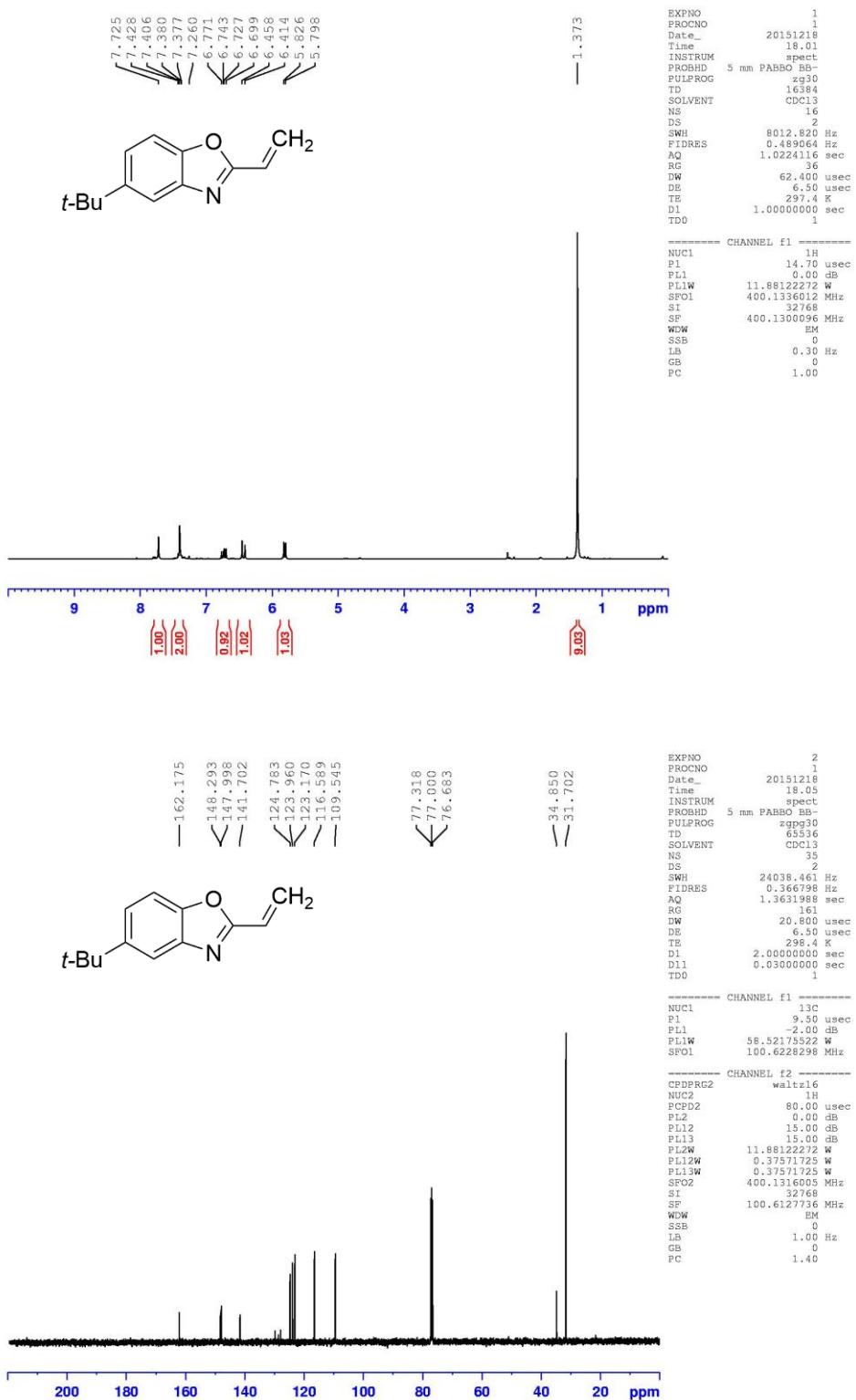
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for (E)-2-(1-p-tolylprop-1-en-2-yl)benzo[d]oxazole (Scheme 2, entry 1v)**



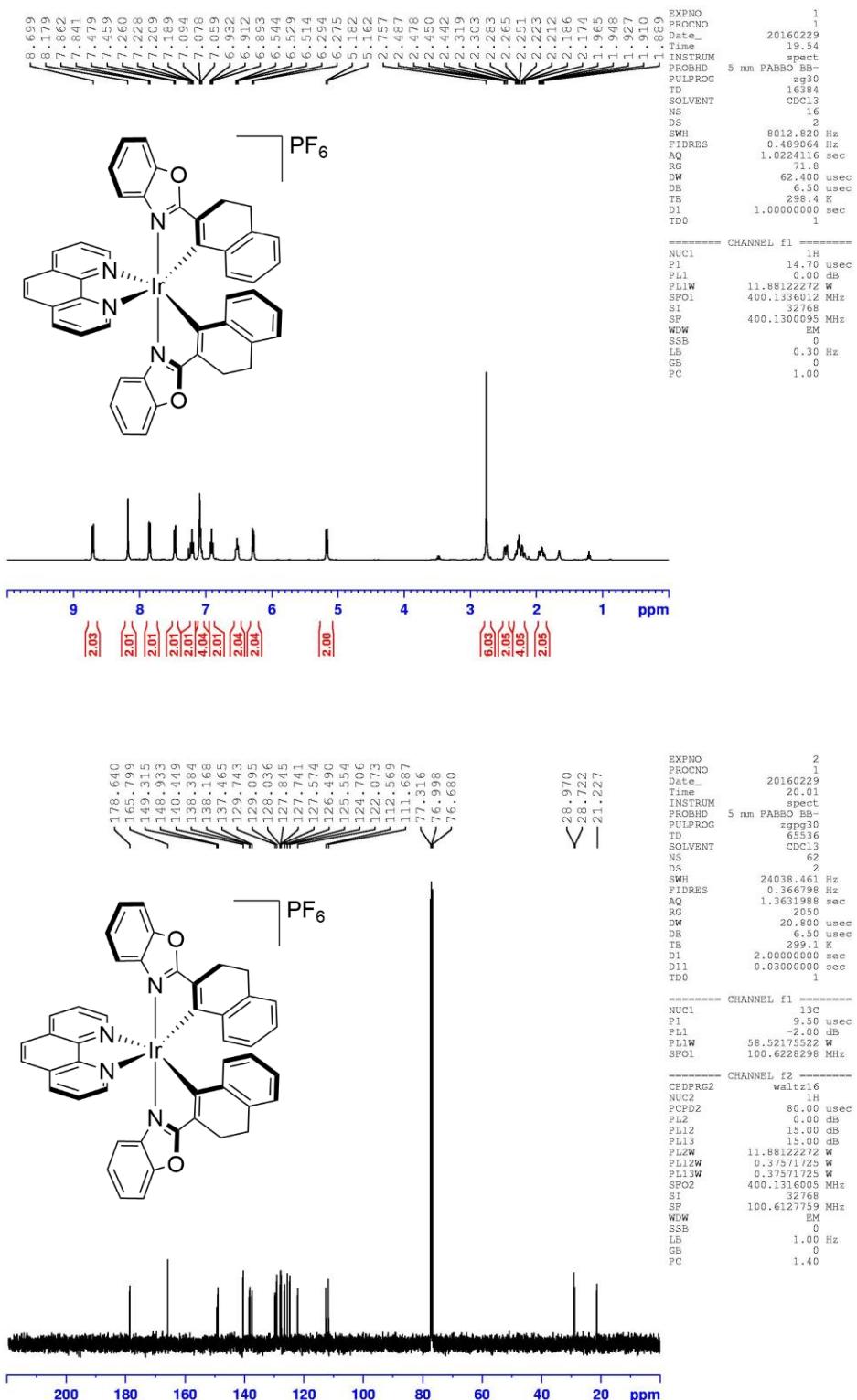
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for (E)-2-Cyclooctenyl-4-*o*-tolyloxazole (Scheme 2, entry 1w)**



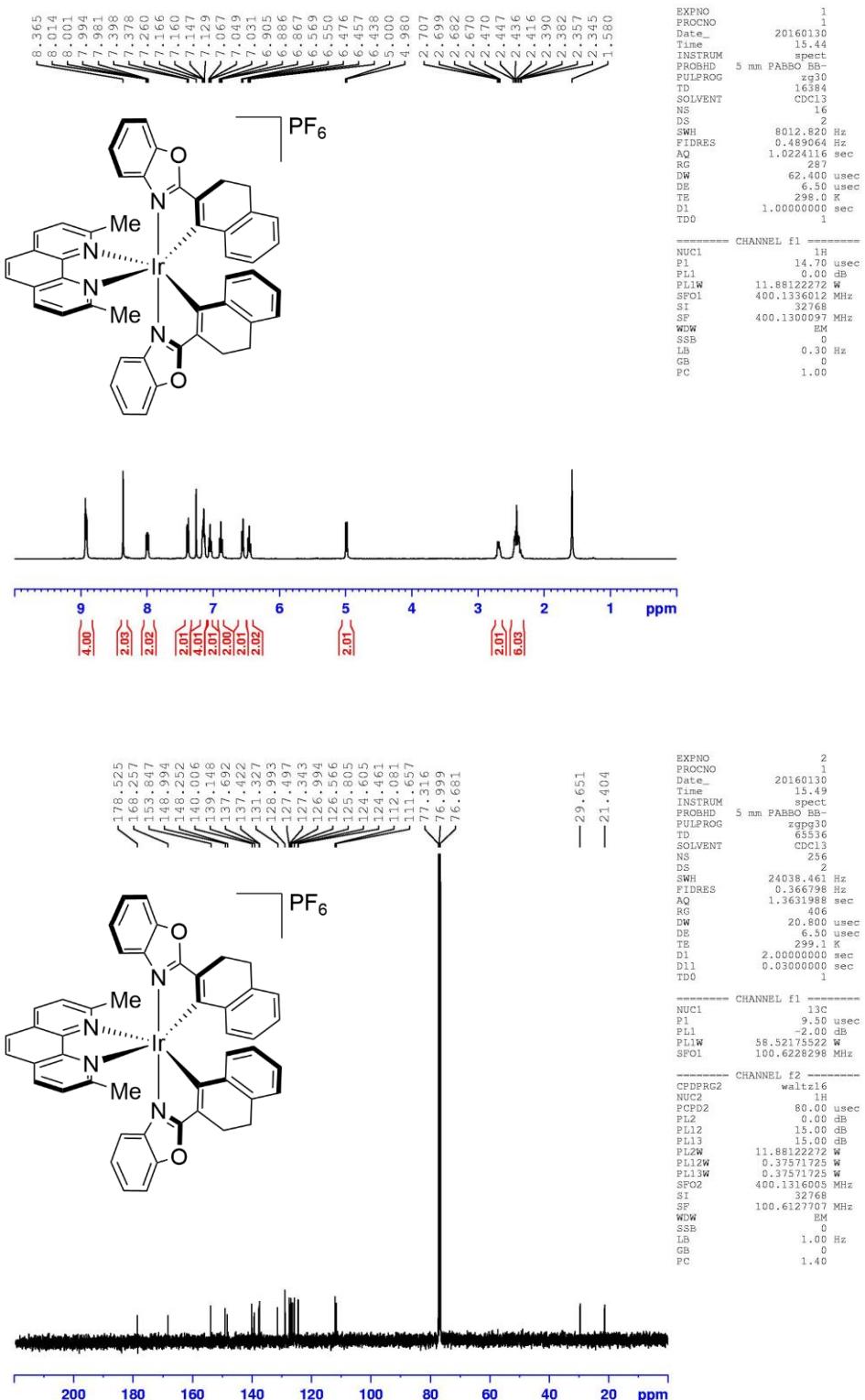
**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for 5-*tert*-Butyl-2-vinylbenzo[d]oxazole (Scheme 2, entry 1x)**



**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for Ir1 (Scheme 4, entry Ir1).**



**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for Ir2 (Scheme 4, entry Ir2)**



**<sup>1</sup>H NMR and <sup>13</sup>C NMR spectra for Ir3 (Scheme 4, entry Ir3)**

