Supporting Information

Selective Aerobic C–H Amination of Phenols with Primary Amines over Copper toward Benzoxazoles

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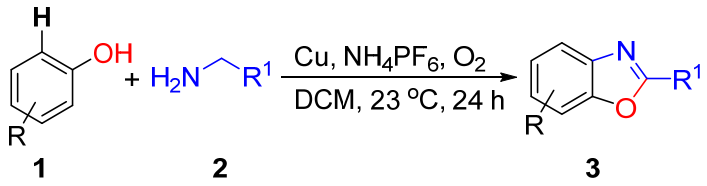
1. General Information

The reactions were carried out in schlenk tubes of 25 mL under O_2 atmosphere. Reagents were used as received unless otherwise noted, and solvents were purified according to standard operation procedure. Column chromatography was performed using Silica Gel 60 (300–400 mesh). The reactions were monitored by GC and GC-MS, GC-MS results were recorded on GC-MS QP2010, and GC analysis was performed on GC 2010 plus. The ^{1}H, and ^{13}C NMR spectra were recorded on a Brucker ADVANCE III spectrometer at 400 MHz, and 100 MHz respectively, and chemical shifts were reported in parts per million (ppm). The electron ionization (EI) method was used as the ionization method for the HRMS measurement, and the mass analyzer type is TOF for EI. All solvents and reagents were purchased from Energy Chemical, Alfa Aesar, and Aladdin.

2. Experimental Procedure

2.1 General Experimental Procedure for the Synthesis of Benzo[*d*]oxazoles



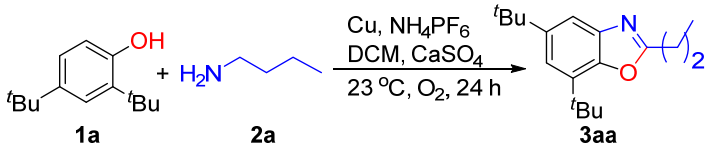
In an oven dried Schlenk tube of 25 mL was charged with phenol **1** (0.2 mmol), copper powder (0.12 mmol, 60 mol %), NH_4PF_6 (0.09 mmol, 45 mol %) and unhydrous $CaSO_4$ (200 mg), after charging oxygen for three times, the amine **2** (0.4 mmol, 2.0 equiv), and DCM (2 mL) were added. The reaction mixture was reacted at 23 °C for 24 h. After completion of the reaction, the reaction mixture was filtered and the filtrate was concentrated under vacuum. The desired product was isolated by column chromatography over silica gel (300-400 mesh) using petroleum ether-ethyl acetate as eluent.

2.2 Experimental Procedure for the Preparation of 5, 7-Di-*tert*-butyl-2-propylbenzo[*d*]oxazole for 1 mmol scale.

In an oven dried Schlenk tube of 100 mL was charged with 2,4-di-*tert*-butylphenol **1a** (1.0 mmol), copper powder (0.60 mmol, 60 mol %), NH_4PF_6 (0.45 mmol, 45 mol %) and unhydrous $CaSO_4$ (1000 mg), after charging oxygen for three times, the butan-1-amine **2a** (2.0 mmol, 2.0 equiv), and DCM (10 mL) were added. The reaction mixture was reacted at 23 °C for 24 h. After completion of the reaction, the reaction mixture was filtered and the filtrate was concentrated under vacuum. The desired product was isolated by column chromatography over silica gel (300-400 mesh) using petroleum ether-ethyl acetate (20/1) as eluent to afford a pale yellow oil in 64% yield (177.5 mg).

2.3 Loadings of Cu powder and NH_4PF_6 screening.

Table S1 Loadings screening of Cu powder and NH_4PF_6.[a,b]



1a **2a** **3aa**

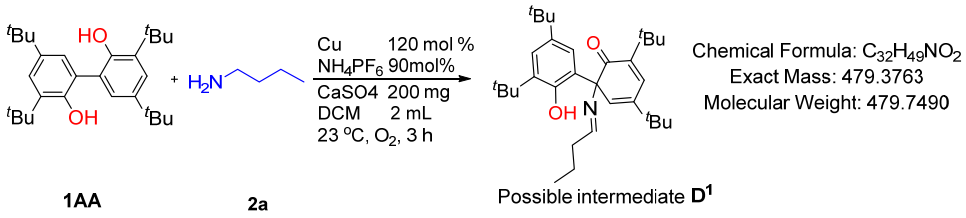
Run	Cu (mol %)	NH_4PF_6 (mol %)	Yield of **3aa** (%)
1	50	40	50
2	60	40	63
3	60	45	69
4	60	50	54
5	65	45	59
6	65	50	55
7	65	55	51
8	70	45	58
9	70	50	65
10	70	55	54
11	70	60	53
12	75	50	61
13	75	55	55
14	90	90	47
15	100	70	48
16	100	80	54
17	100	90	49
18	100	100	38
19	110	110	33

[a]Reaction conditions:**1a** (0.2 mmol), **2a** (0.4 mmol, 2.0 equiv), $CaSO_4$ (200 mg) in the DCM (2 mL) at 23 °C under O_2 for 24 h. [b]GC yield using dodecane as an internal standard.

Loading of copper powder and NH_4PF_6 were screened (Table S1), results showed that when 60 mol % of Cu and 45 mol % of NH_4PF_6 were added, **3aa** could obtain in 69% yield (Run 3). However, when 1 equiv of Cu, with different loadings of NH_4PF_6, was added, the yield of **3aa** was restricted to 54% (Runs 15–18).

2.4 GC-MS Analysis of Intermediate D[1]

In an oven dried Schlenk tube of 25 mL was charged with **1AA** (0.1 mmol), copper powder (0.12 mmol, 120 mol %), NH_4PF_6 (0.09 mmol, 90 mol %) and unhydrous CaSO4 (200 mg), after charging oxygen for three times, the amine **2a** (0.4 mmol, 4.0 equiv), and DCM (2 mL) were added. The reaction mixture was reacted at 23 °C for 3 h. After completion, the reaction mixture was filtered and the filtrate was detected by GC-MS, and the result is show in Figure S1.



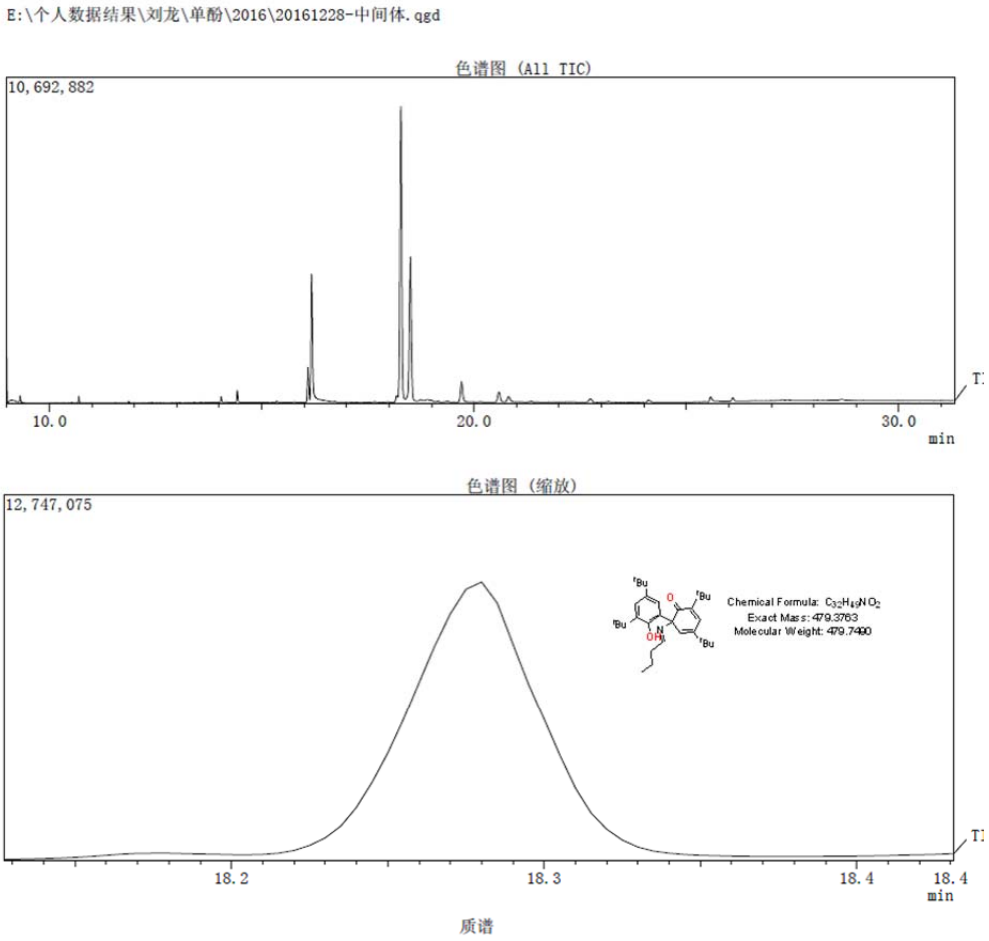
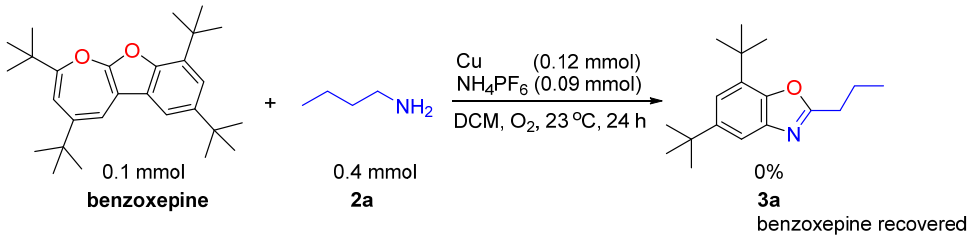


Figure S1 GC-MS Analysis of Intermediate D[1]

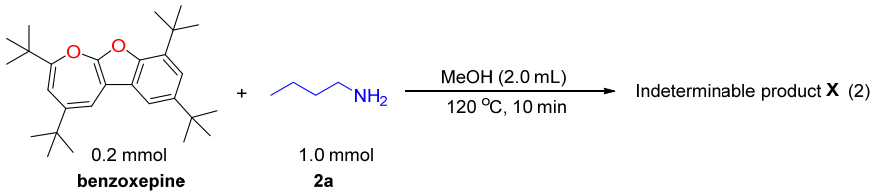
2.5 Control Experiment Related to Benzoxepine

Benzoxepine was prepared according the corresponding literature as a colorless oil.[1] ^{1}H NMR (400 M, $CDCl_3$): δ 7.26 (s, 1H), 7.15 (s, 1H), 6.39 (s, 1H), 5.53 (s, 1H), 1.46 (s, 9H), 1.37 (s, 9H), 1.26 (s, 9H), 1.21 (s,

9H).



In an oven dried Schlenk tube of 25 mL was charged with benzoxepine (0.1 mmol), copper powder (0.12 mmol, 120 mol %), NH_4PF_6 (0.09 mmol, 90 mol %), after charging oxygen for three times, amine **2a** (0.4 mmol, 4.0 equiv), and DCM (2 mL) were added. The reaction mixture was reacted at 23 °C for 24 h (eq 1). After completion of the reaction, the reaction mixture was monitored by TLC. Benzoxepine remained, and **3a** was not observed. This result showed that benzoxepine did not act as an intermediate during the reaction.



In an oven dried Schlenk tube of 25 mL was charged with benzoxepine (0.2 mmol), after charging nitrogen for three times, amine **2a** (1.0 mmol), and MeOH (2 mL) were added. The reaction mixture was reacted at 120 °C for 10 min. After completion of the reaction, the reaction mixture was monitored by GC-MS, and the result of indeterminable product **X** was showed in Figure S2.

The mass spectra of **X** (Figure S2, base peak, 424, MW, 438) further demonstrated that **X** was not intermediate **C** (MW, 481). Obviously, **X** was not intermediate $\mathbf{D}^1$ (Figure S1, base peak, 436, MW, 479) neither.

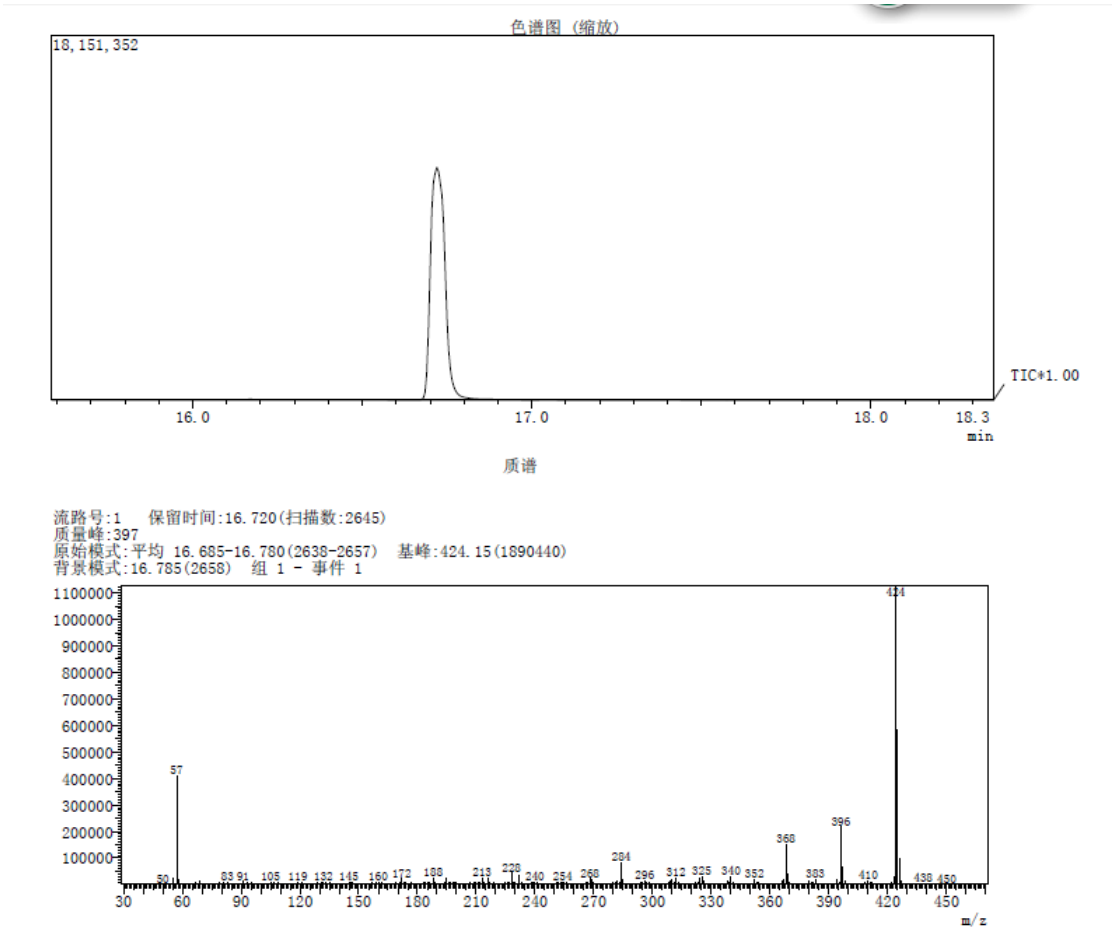
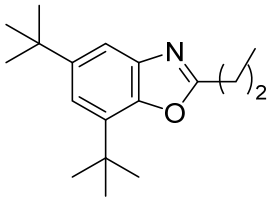


Figure S2 GC-MS Analysis of Indeterminable Product X

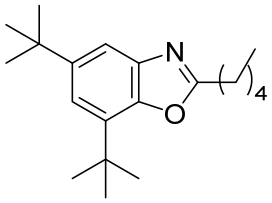
3. Characterization Data for the Products

5, 7-di-*tert*-butyl-2-propylbenzo[*d*]oxazole (3a)[2]



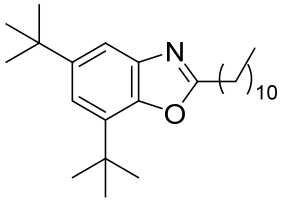
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 65% yield (35.5 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.56 (s, 1H), 7.25 (s, 1H), 2.91 (t, *J* =7.2 Hz, 2H), 1.97–1.88(m, 2H), 1.48 (s, 9H), 1.37 (s, 9H), 1.06 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.5, 147.1, 147.0, 141.6, 133.4, 118.6, 113.8, 35.0, 34.4, 31.9, 30.6, 29.9, 20.4, 13.7.

5, 7-di-*tert*-butyl-2-pentylbenzo[*d*]oxazole (3b)[3]



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a yellow oil in 64% yield (38.6 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.54 (s, 1 H), 7.24 (s, 1H), 2.92 (t, *J* =7.2 Hz, 2H), 1.92–1.85(m, 2H), 1.47 (s, 9H), 1.42–1.39 (m, 3H), 1.37 (s, 9H), 0.91 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ166.7, 147.1, 147.0, 141.6, 133.4, 118.6, 113.7, 35.0, 34.4, 31.9, 31.3, 29.9, 28.6, 26.6, 22.3, 13.9.

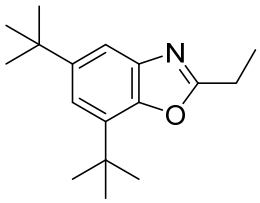
5, 7-di-*tert*-butyl-2-undecylbenzo[*d*]oxazole (3c)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a yellow oil in 58% yield (44.7 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.55 (d, *J* = 1.6 Hz, 1H), 7.24 (d, *J* = 1.6 Hz, 1H), 2.92 (t, *J* = 7.6 Hz, 2H), 1.92–1.84 (m,

2H), 1.48 (s, 9H), 1.40–1.33 (m, 11H), 1.31–1.21 (m, 14H), 0.89–0.86 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 166.7, 147.0, 146.9, 141.5, 133.4, 118.6, 113.7, 35.0, 34.3, 31.9, 31.8, 29.9, 29.6, 29.4, 29.3, 29.2, 29.1, 28.6, 26.9, 22.6, 14.1. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{26}H_{43}NO$: 385.3345; found: 385.3340.

5, 7-di-*tert*-butyl-2-ethylbenzo[*d*]oxazole (3d)[3]



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a colorless oil in 45% yield (23.3 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.55 (s, 1H), 7.24 (s, 1H), 2.96 (q, J_1 =7.6 Hz, J_2 =15.2 Hz, 2H), 1.48 (s, 9H), 1.45 (t, J = 7.6 Hz, 3H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.4, 147.1, 147.0, 141.5, 133.4, 118.6, 113.7, 35.0, 34.4, 31.8, 29.9, 22.2, 11.0.

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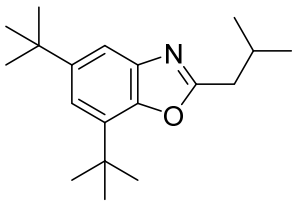
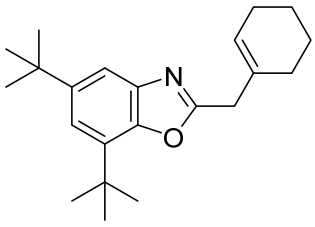
5, 7-di-*tert*-butyl-2-isobutylbenzo[*d*]oxazole (3e)[2]



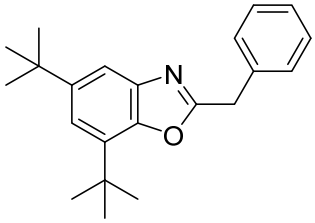
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 40% yield (23.0 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.54 (s, 1H), 7.24 (s, 1H), 2.81 (d, J = 6.8 Hz, 2H), 2.34–2.24 (m, 1H), 1.48 (s, 9H), 1.37 (s, 9H), 1.05 (d, J = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.9, 147.1, 147.0, 141.5, 133.4, 118.6, 113.7, 37.6, 35.0, 34.3, 31.8, 29.9, 27.5, 22.4.

5, 7-di-*tert*-butyl-2-(cyclohex-1-en-1-ylmethyl)benzo[*d*]oxazole (3f)



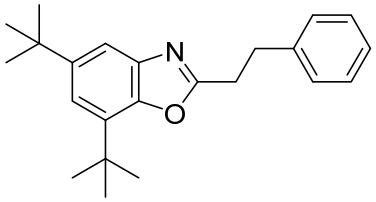
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a yellow oil in 30% yield (19.5 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.55 (s, 1H), 7.24 (s, 1H), 5.67 (s, 1H), 3.56 (s, 2H), 2.06–2.04 (m, 4H), 1.65–1.62 (m, 2H), 1.58–1.55 (m, 2H), 1.47 (s, 9H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.9, 147.1, 147.0, 141.6, 133.4, 132.0, 125.4, 118.7, 113.8, 37.6, 35.0, 34.3, 31.8, 29.9, 28.3, 25.3, 22.7, 22.0. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{22}H_{31}NO$: 325.2406; found: 325.2400.

2-benzyl-5, 7-di-*tert*-butylbenzo[*d*]oxazole (3h)[3]



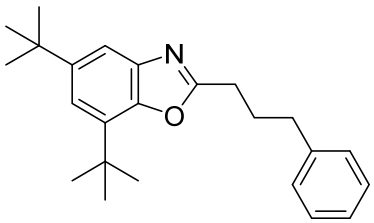
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 25% yield (16.1 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.54 (s, 1H), 7.40–7.38 (m, 2H), 7.34–7.30 (m, 2H), 7.27–7.24 (m, 2H), 4.26 (s, 2H), 1.44 (s, 9H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.6, 147.3, 147.2, 141.5, 135.2, 133.5, 128.9, 128.7, 127.1, 118.9, 114.0, 35.3, 35.0, 34.4, 31.8, 29.9.

5, 7-di-*tert*-butyl-2-phenethylbenzo[*d*]oxazole (3i)[3]



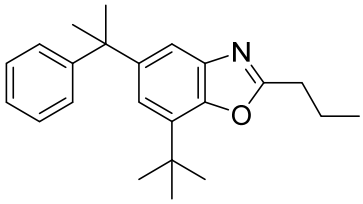
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 51% yield (34.2 mg). Yield 51%; ^{1}H NMR (400 M, $CDCl_3$): δ 7.55 (s, 1H), 7.31–7.24 (m, 5H), 7.22–7.28 (m, 1H), 3.27–3.20 (m, 4H), 1.45 (s, 9H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.7, 147.3, 147.0, 141.5, 140.2, 133.5, 128.6, 128.3, 126.4, 118.9, 113.8, 35.0, 34.4, 33.0, 31.9, 30.5, 30.0.

5, 7-di-*tert*-butyl-2-(3-phenylpropyl)benzo[*d*]oxazole (3j)



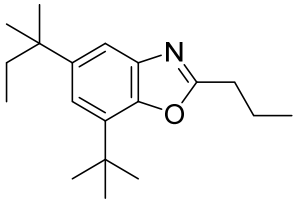
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 61% yield (42.6 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.56 (s, 1H), 7.30–7.25 (m, 3H), 7.22–7.17 (m, 3H), 2.96–2.93 (m, 2H), 2.78–2.74 (m, 2H), 2.26–2.18 (m, 2H), 1.48 (s, 9H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.1, 147.1, 146.9, 141.5, 141.2, 133.4, 128.5, 128.4, 126.0, 118.7, 113.7, 35.0, 34.9, 34.3, 31.8, 29.9, 28.4, 27.9. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{24}H_{31}NO$: 349.2406; found: 349.2395.

7-(*tert*-butyl)-5-(2-phenylpropan-2-yl)-2-propylbenzo[*d*]oxazole (3l)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 68% yield (45.6 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.44 (s, 1H), 7.27–7.24 (m, 4H), 7.18–7.13 (m, 1H), 7.00 (s, 1H), 2.90 (t, J = 7.6 Hz, 2H), 1.96–1.86 (m, 2H), 1.73 (s, 6H), 1.39 (s, 9H), 1.06 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.6, 150.7, 147.0, 146.7, 141.4, 133.4, 127.9, 126.7, 125.5, 120.5, 115.1, 43.1, 34.2, 31.2, 30.5, 29.8, 20.3, 13.7. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{23}H_{29}NO$: 335.2249; found: 335.2239.

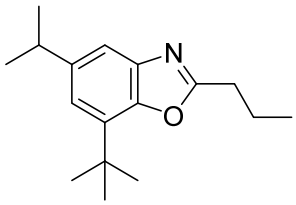
7-(*tert*-butyl)-5-(*tert*-pentyl)-2-propylbenzo[*d*]oxazole (3m)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 67% yield (38.5 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.40 (s, 1H), 7.09 (s, 1H), 2.85–2.81 (m, 2H), 1.89–1.80 (m, 2H), 1.63–1.57 (m, 2H),

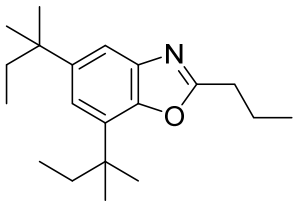
1.39 (s, 9H), 1.25 (s, 6H), 0.99 (t, J = 7.2 Hz, 3H), 0.63–0.59 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.5, 146.9, 145.4, 141.6, 133.3, 119.2, 114.5, 38.2, 37.2, 34.4, 30.6, 30.0, 28.9, 20.4, 13.8, 9.2. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{19}H_{29}NO$: 287.2249; found: 287.2238.

7-(*tert*-butyl)-5-isopropyl-2-propylbenzo[*d*]oxazole (3n)



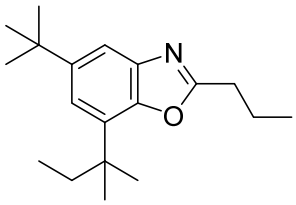
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 43% yield (22.3 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.38 (s, 1H), 7.04 (s, 1H), 3.03–2.96 (m, 1H), 2.93–2.89 (m, 2H), 1.96–1.87 (m, 2H), 1.47 (s, 9H), 1.29 (d, J = 6.8 Hz, 6H), 1.08–1.04 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.5, 147.3, 144.9, 141.8, 133.9, 120.0, 114.2, 34.4, 34.2, 30.6, 29.9, 24.5, 20.4, 13.7. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{17}H_{25}NO$: 259.1936; found: 259.1927.

5, 7-di-*tert*-pentyl-2-propylbenzo[*d*]oxazole (3o)



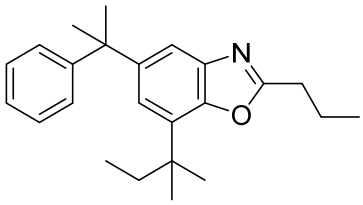
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 61% yield (36.8 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.48 (s, 1H), 7.11 (s, 1H), 2.92–2.88 (m, 2H), 1.96–1.88 (m, 2H), 1.86–1.82 (m, 2H), 1.67 (q, J_1 = 7.2 Hz, J_2 = 14.4 Hz, 2H), 1.43 (s, 6H), 1.32 (s, 6H), 1.08-1.04 (m, 3H), 0.68–0.65 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.3, 146.9, 145.2, 141.5, 131.8, 120.5, 114.4, 38.1, 37.8, 37.2, 34.6, 30.6, 28.9, 27.4, 20.3, 13.7, 9.2, 9.1. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{20}H_{31}NO$: 301.2406; found: 301.2395.

5-(*tert*-butyl)-7-(*tert*-pentyl)-2-propylbenzo[*d*]oxazole (3p)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 60% yield (34.5 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.45 (s, 1 H), 7.19 (s, 1 H), 2.92–2.88 (m, 2 H), 1.96–1.88 (m, 2 H), 1.87–1.83 (m, 2 H), 1.43 (s, 6 H), 1.36 (s, 9 H), 1.07–1.04 (m, 3 H), 0.70–0.67 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.4, 147.1, 147.0, 141.5, 132.0, 120.0, 113.6, 37.9, 34.9, 34.6, 31.8, 30.6, 27.4, 20.4, 13.7, 9.3. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{19}H_{29}NO$: 287.2249; found: 287.2248.

7-(*tert*-pentyl)-5-(2-phenylpropan-2-yl)-2-propylbenzo[*d*]oxazole (3q)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow oil in 61% yield (42.6 mg). ^{1}H NMR (400 M, $CDCl_3$): δ 7.46 (s, 1 H), 7.27–7.21 (m, 4H), 7.16–7.13 (m, 1H), 6.93 (s, 1H), 2.91–2.87 (m, 2H), 1.95–1.86 (m, 2H), 1.81–1.75 (m, 2H), 1.72 (s, 6H), 1.34 (s, 6H), 1.08-1.04 (m, 3H), 0.62–0.58 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.6, 150.9, 147.1, 146.6, 141.4, 132.0, 127.9, 126.7, 125.6, 122.1, 115.0, 43.2, 37.8, 34.6, 31.2, 30.6, 27.3, 20.4, 13.8, 9.2. HRMS (EI) m/z: $[M]^+$ calcd. for $C_{24}H_{31}NO$: 349.2406; found: 349.2404.

4. References

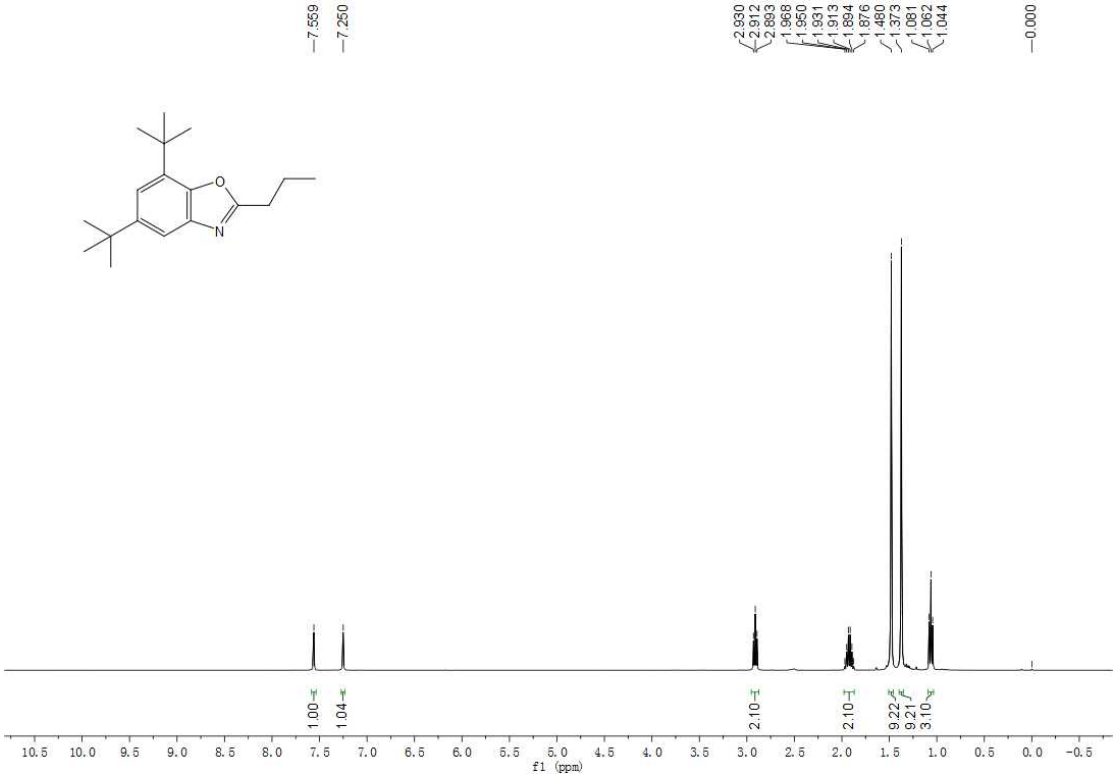
(1) Esguerra, K. V. N.; Fall, Y.; Petitjean, L.; Lumb, J.-P. *J. Am. Chem. Soc*. **2014**, *136*, 7662.

(2) Jarmila, V.; Vaclav, H.; Vladimir, B.; Jarmila, K. *Molecules* **2005**, *10*, 783.

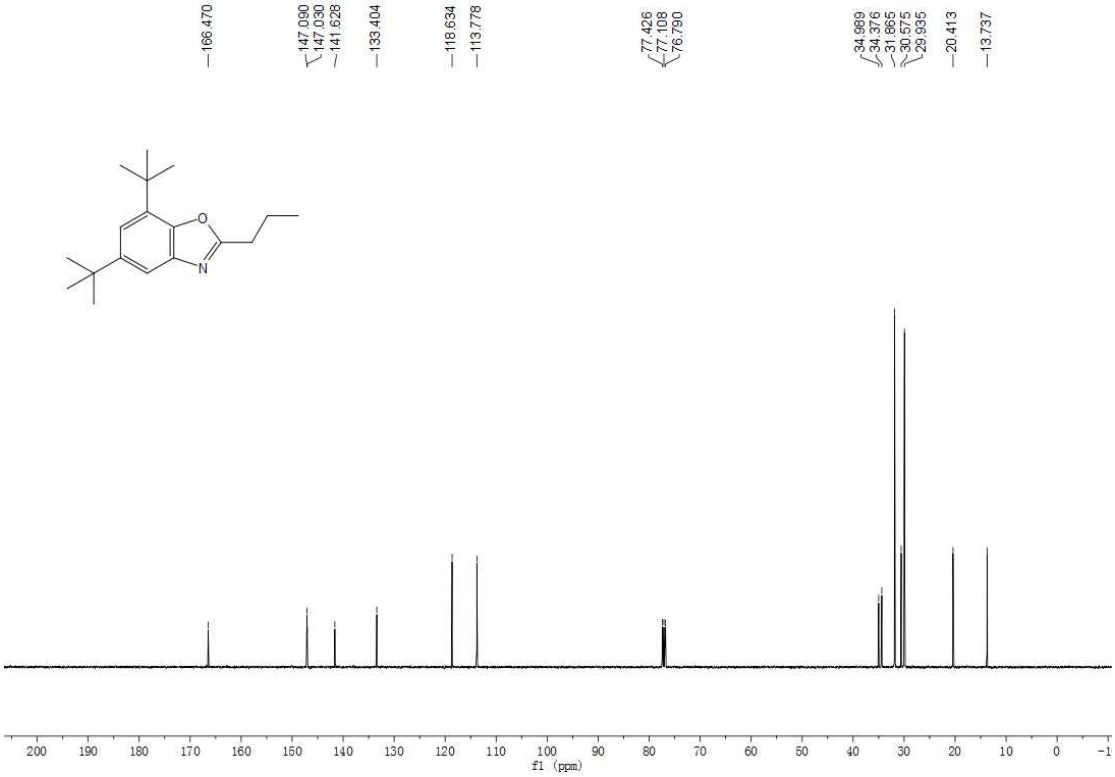
(3) Chen, X.; Ji, F.; Zhao, Y.; Liu, Y.; Zhou, Y.; Chen, T.; Yin, S-F. *Adv. Synth. Catal*. **2015**, *357*, 2924.

5. Copies of ^{1}H, ^{13}C NMR Spectra of the Products

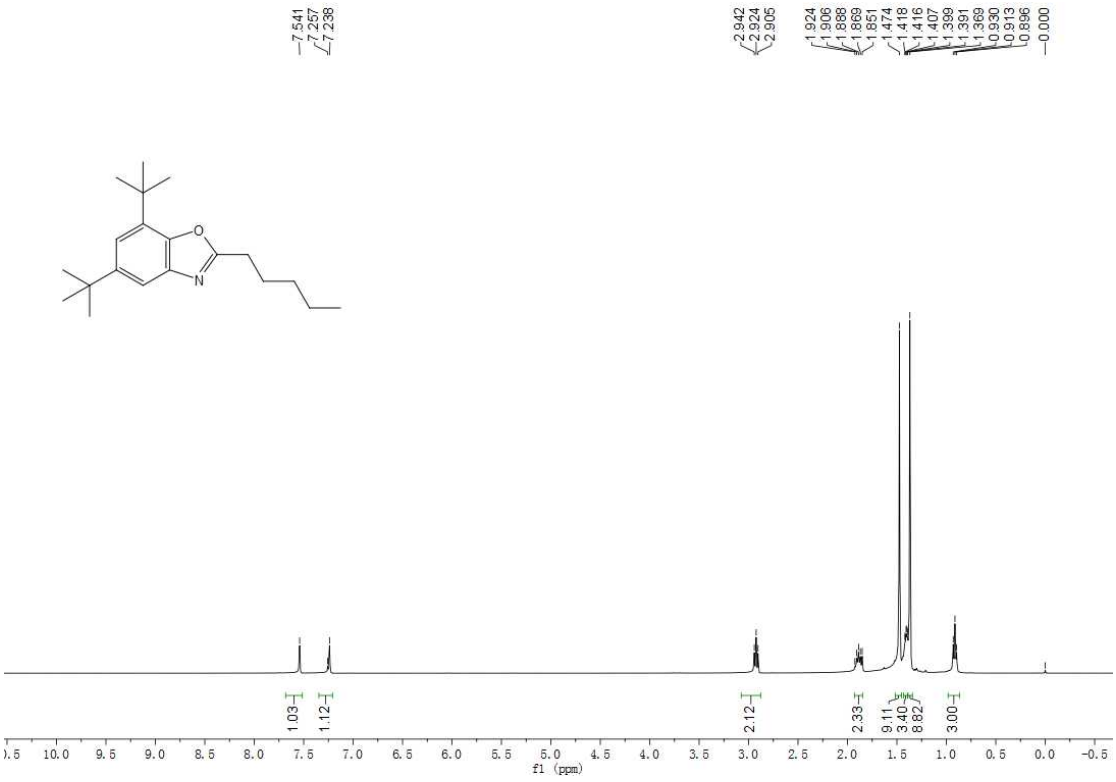
^{1}H NMR Spectrum of 5, 7-di-*tert*-butyl-2-propylbenzo[*d*]oxazole **(3a)**



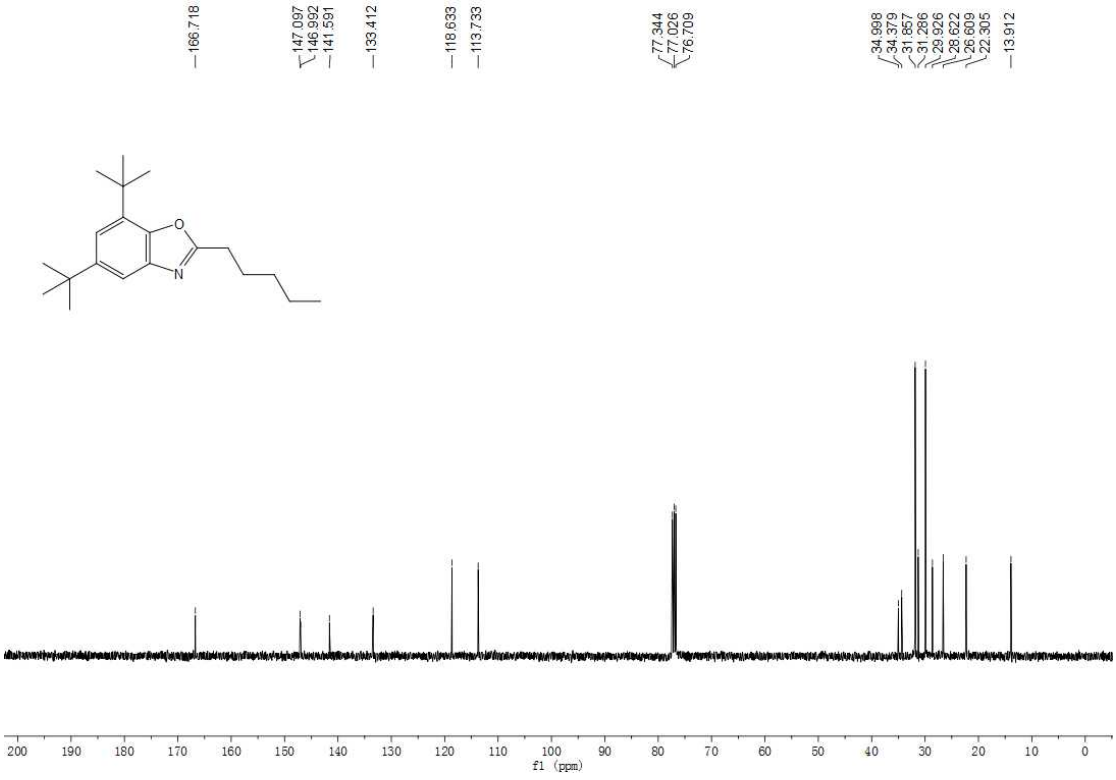
^{13}C NMR Spectrum of 5, 7-di-*tert*-butyl-2-propylbenzo[*d*]oxazole **(3a)**



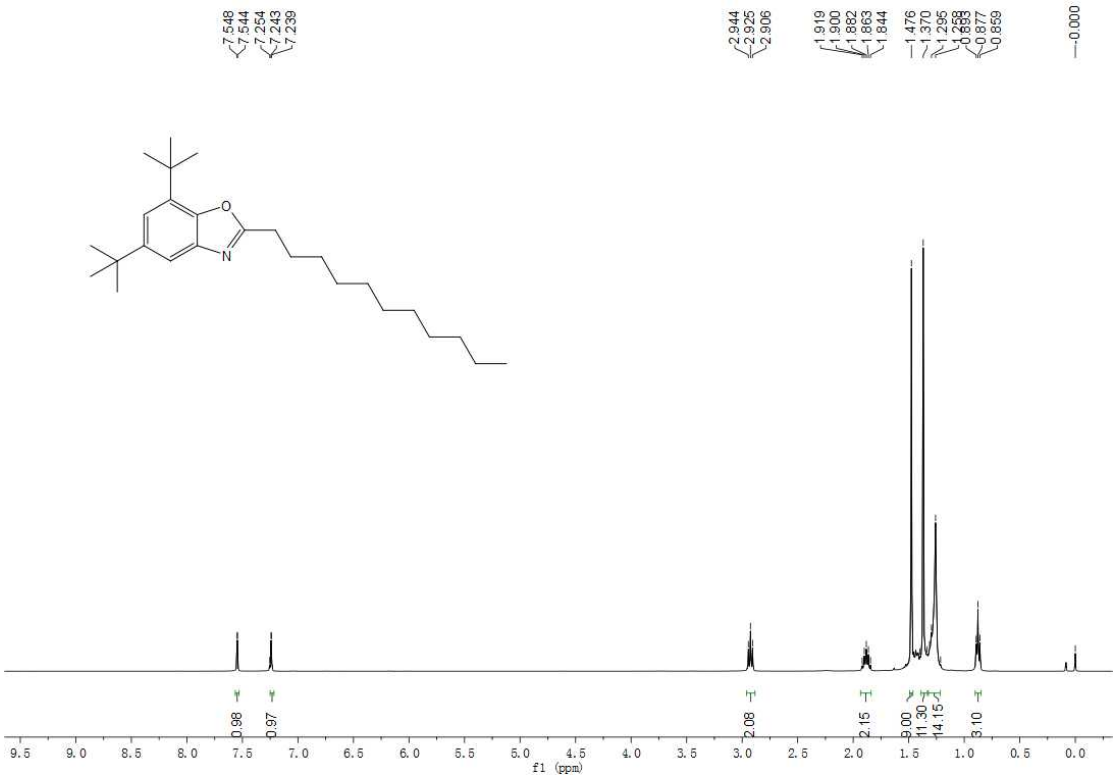
^{1}H NMR Spectrum of 5, 7-di-*tert*-butyl-2-pentylbenzo[*d*]oxazole **(3b)**



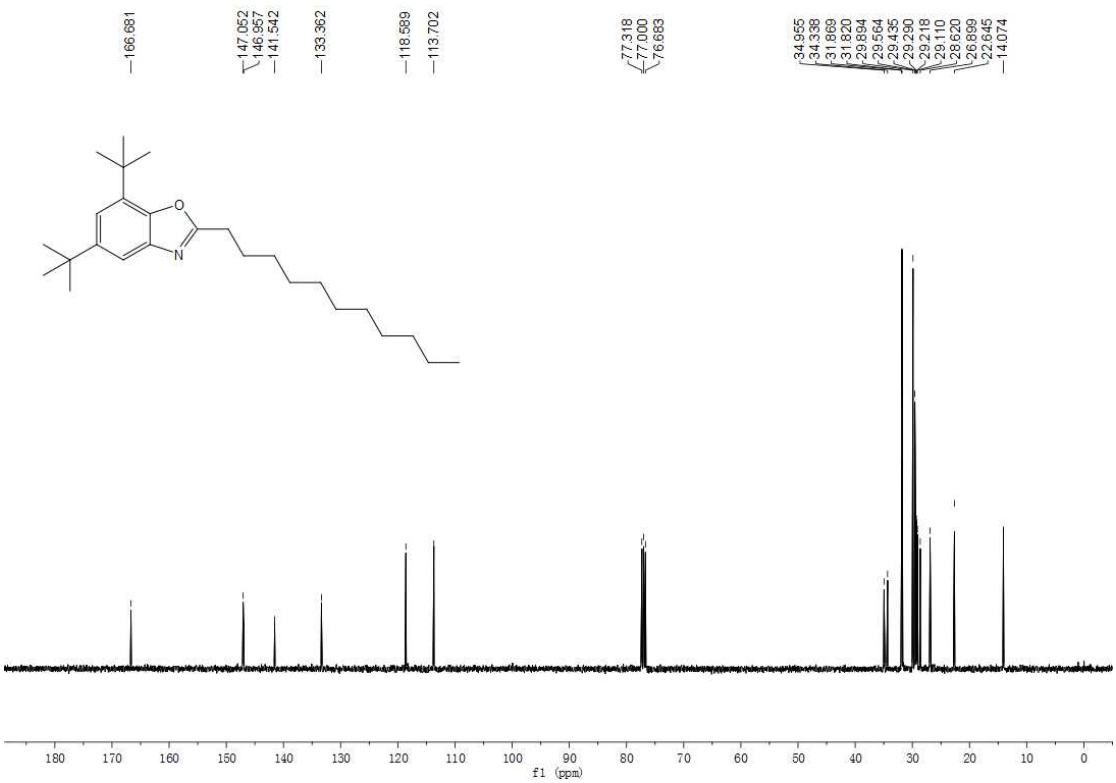
^{13}C NMR Spectrum of 5, 7-di-*tert*-butyl-2-pentylbenzo[*d*]oxazole **(3b)**



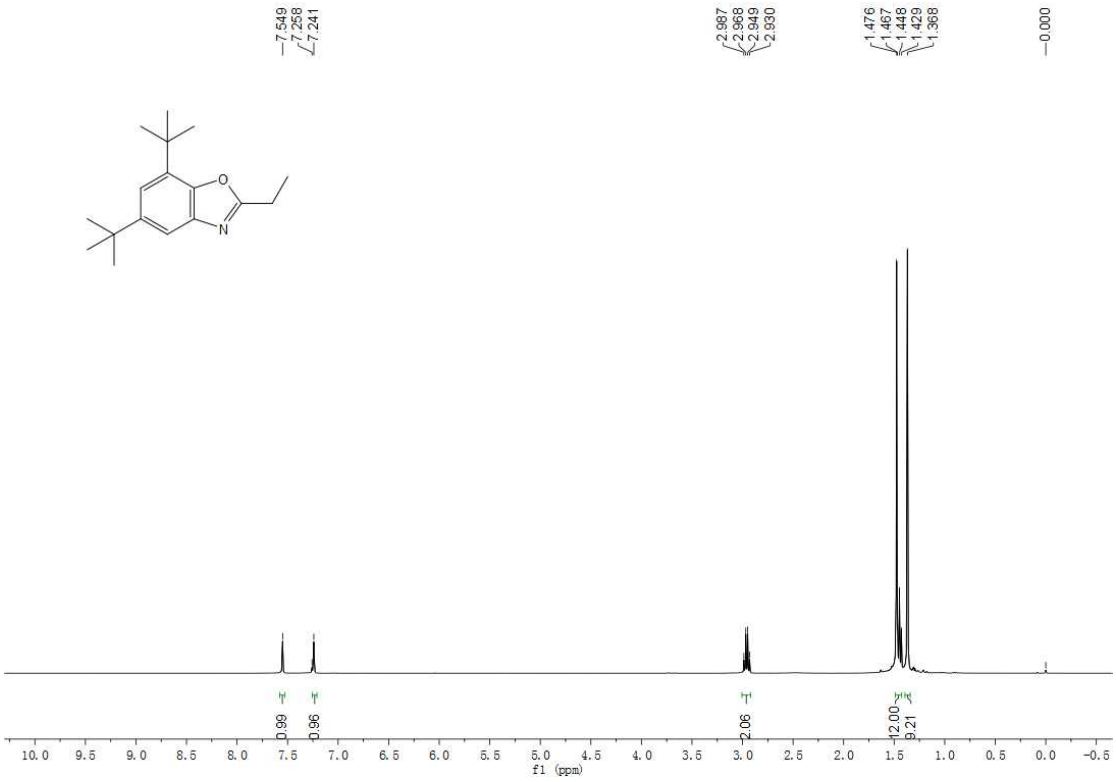
^{1}H NMR Spectrum of 5, 7-di-*tert*-butyl-2-undecylbenzo[*d*]oxazole **(3c)**



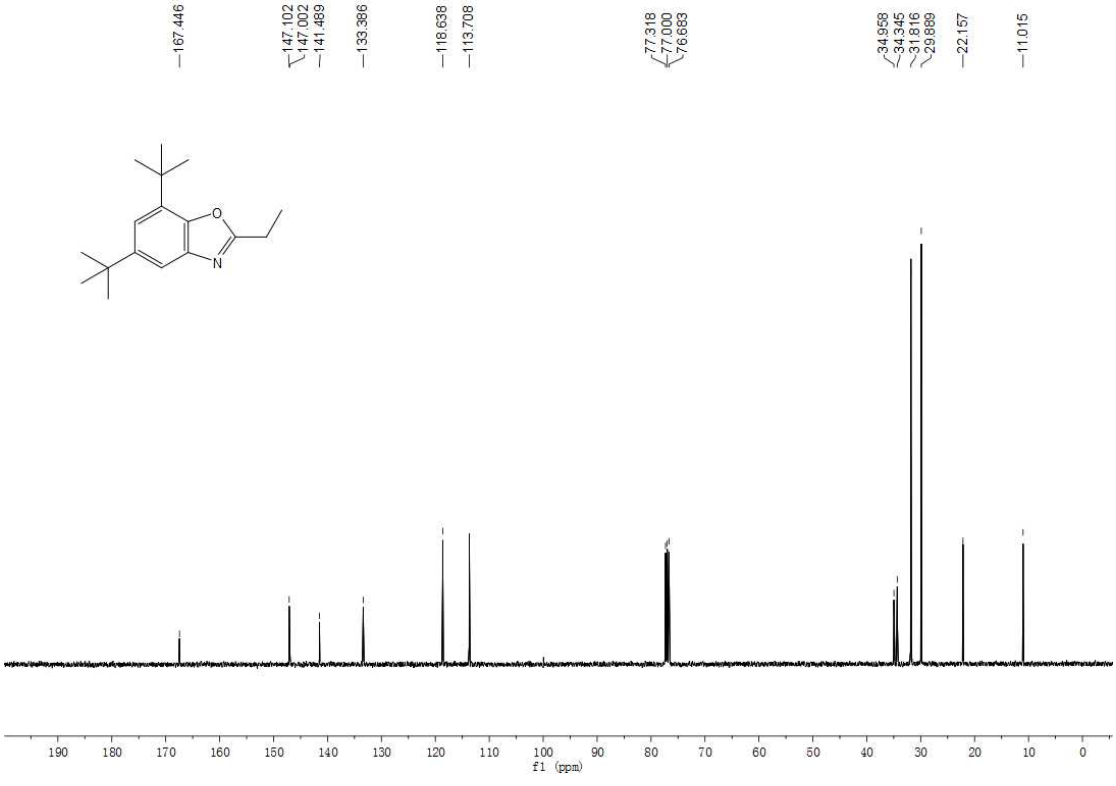
^{13}C NMR Spectrum of 5, 7-di-*tert*-butyl-2-undecylbenzo[*d*]oxazole **(3c)**



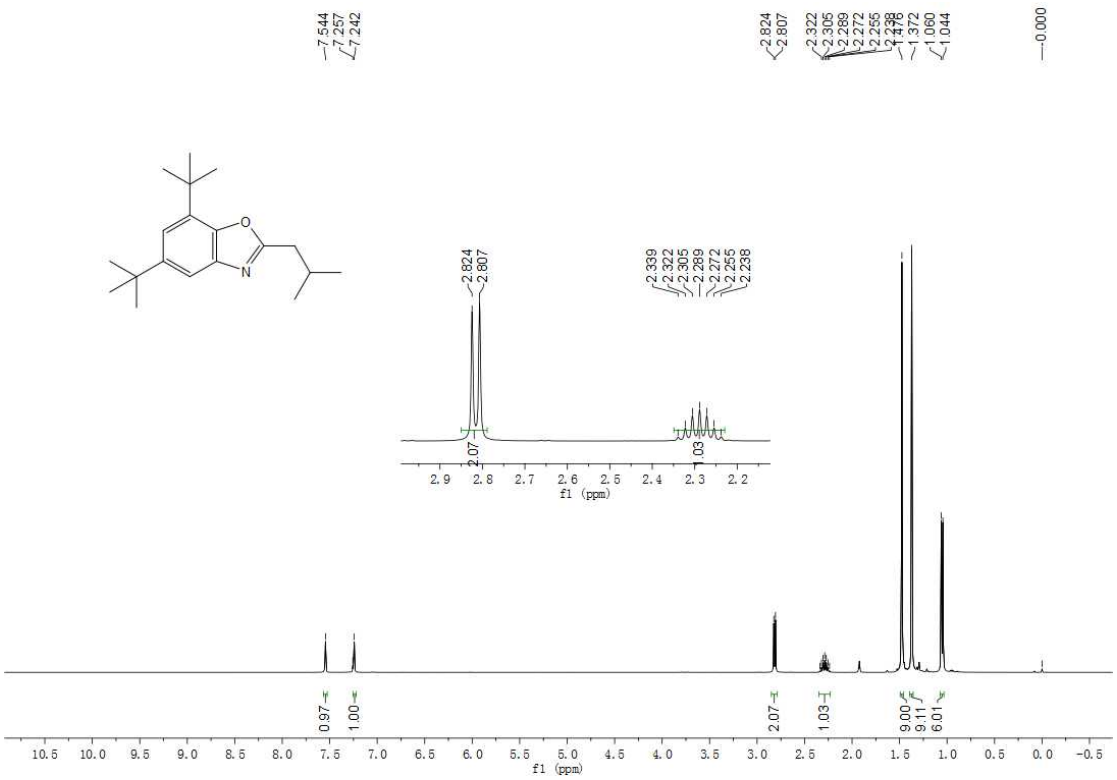
^{1}H NMR Spectrum of 5, 7-di-*tert*-butyl-2-ethylbenzo[*d*]oxazole **(3d)**



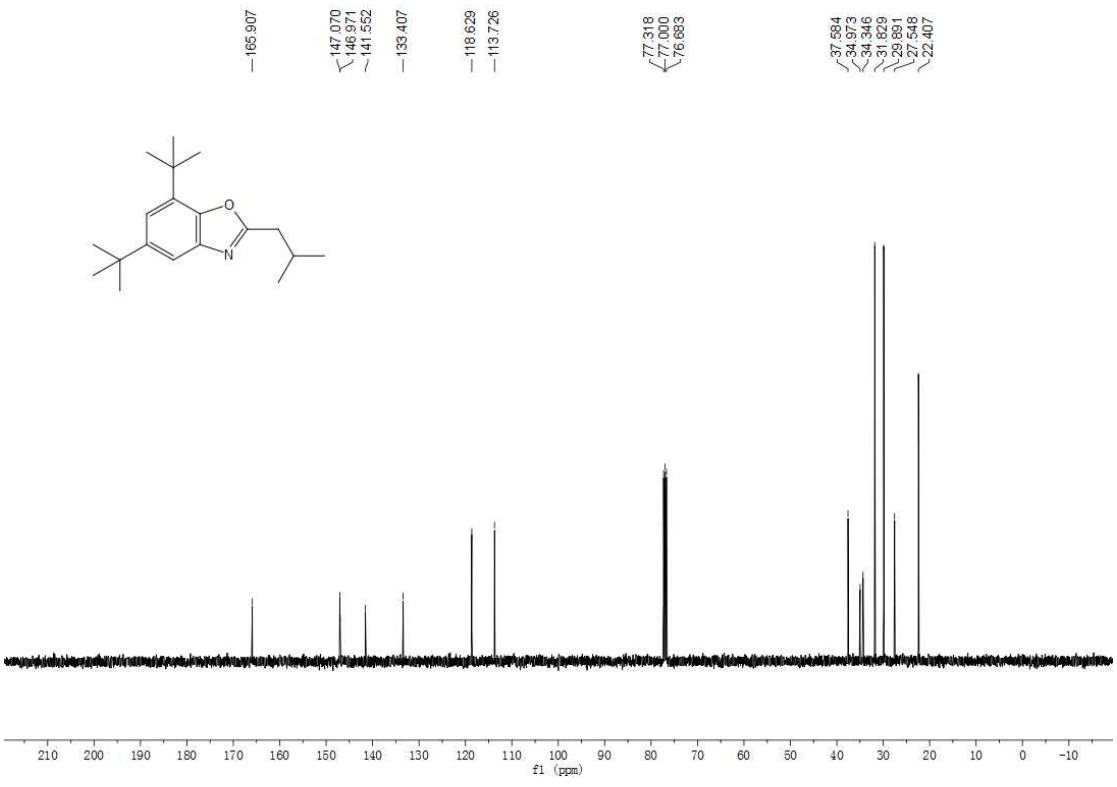
^{13}C NMR Spectrum of 5, 7-di-*tert*-butyl-2-ethylbenzo[*d*]oxazole **(3d)**



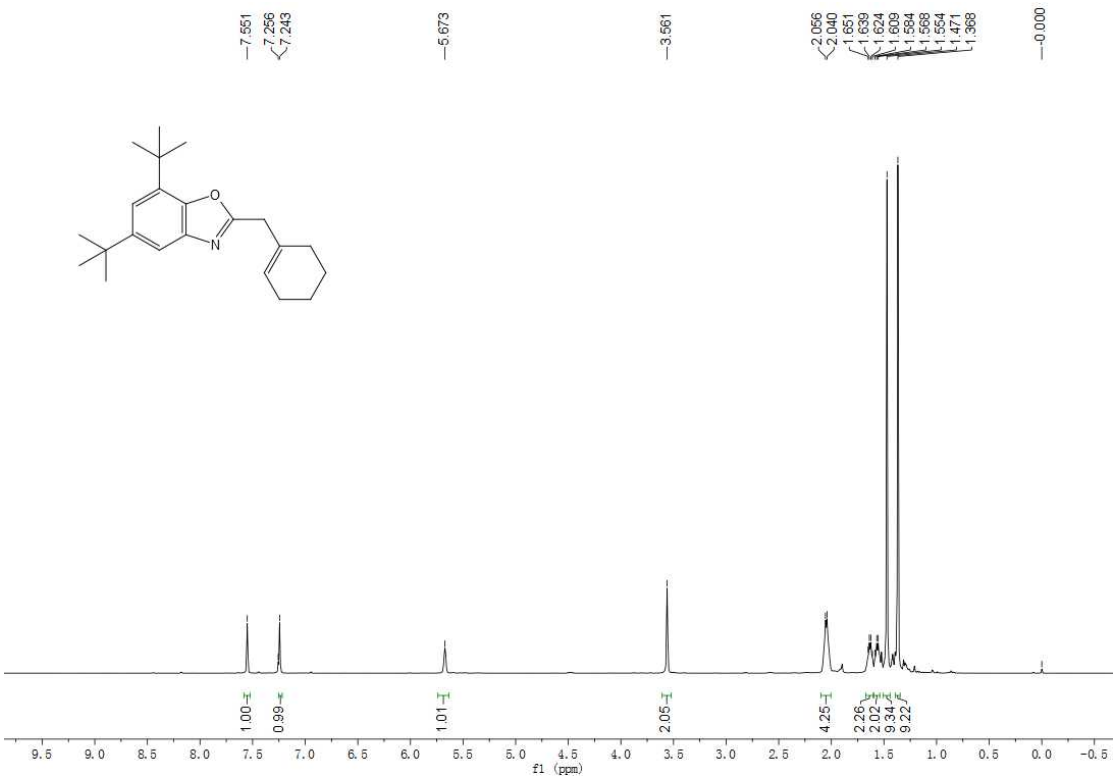
^{1}H NMR Spectrum of 5, 7-di-*tert*-butyl-2-isobutylbenzo[*d*]oxazole **(3e)**



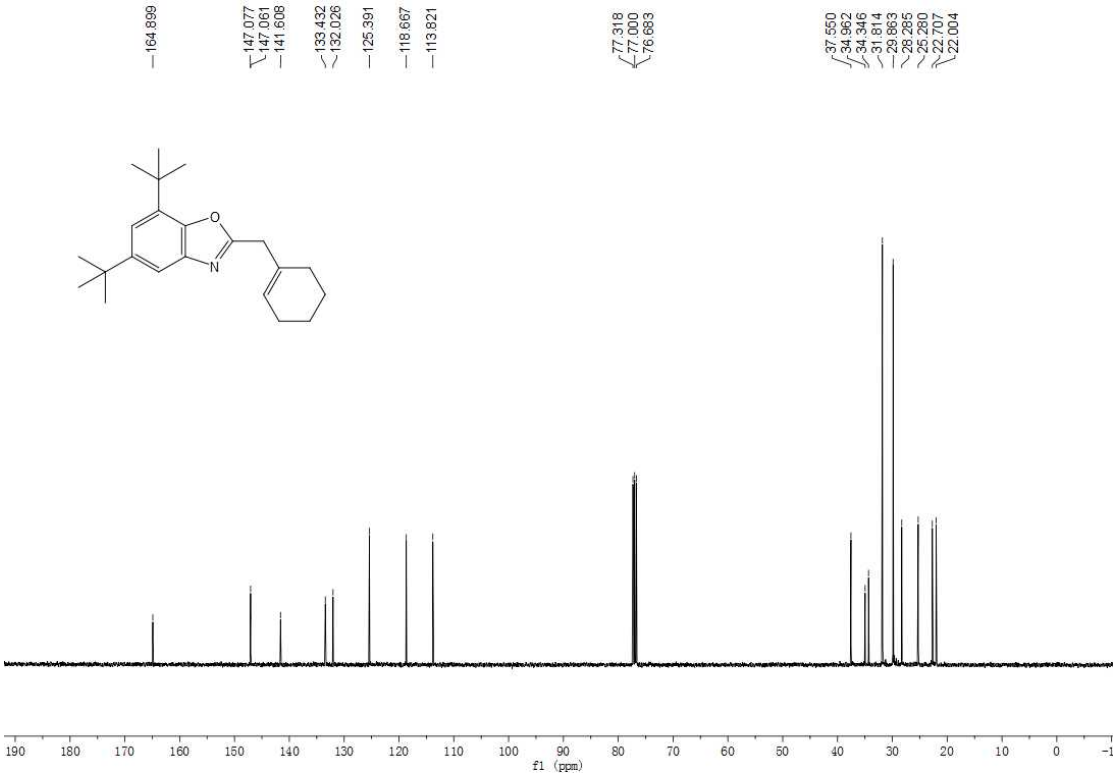
^{13}C NMR Spectrum of 5, 7-di-*tert*-butyl-2-isobutylbenzo[*d*]oxazole **(3e)**



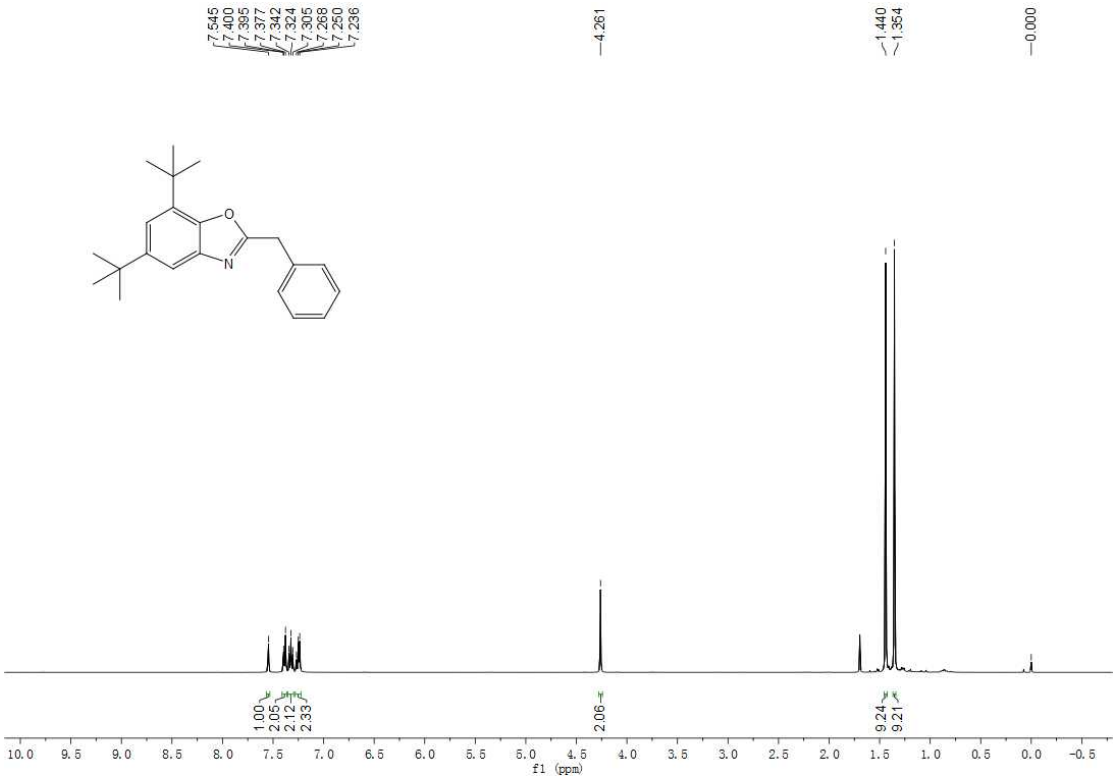
^{1}H NMR Spectrum of 5, 7-di-*tert*-butyl-2-(cyclohex-1-en-1-ylmethyl)benzo[*d*]oxazole **(3f)**



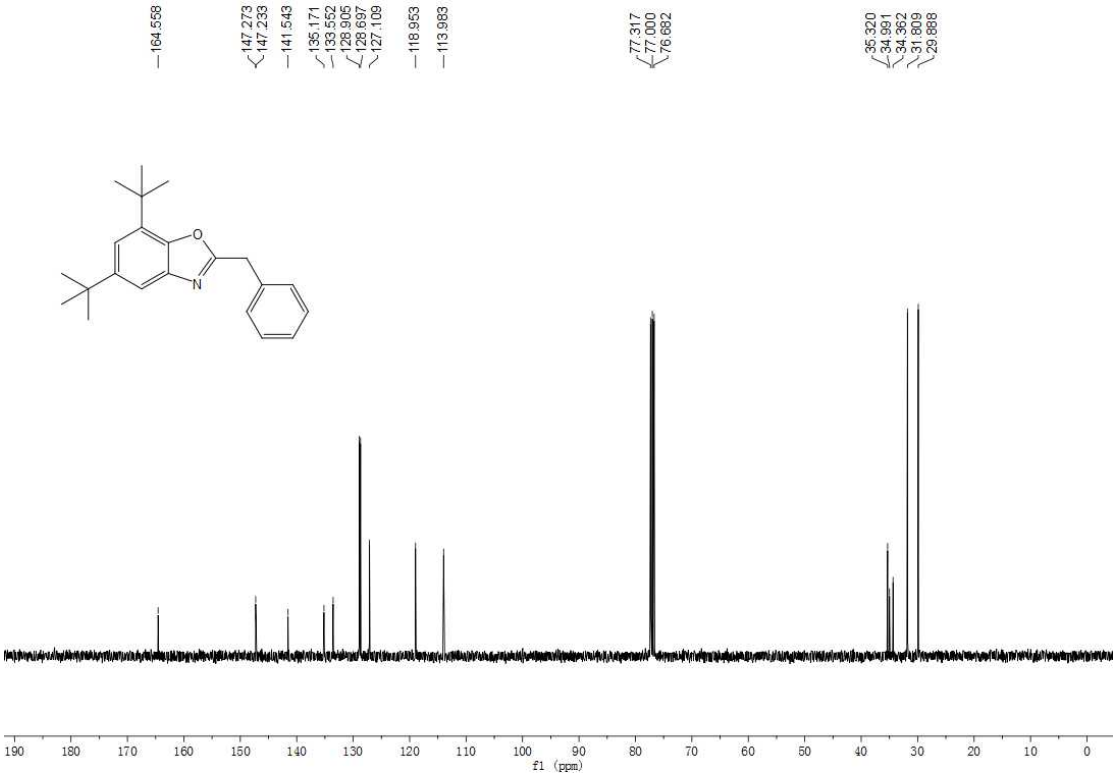
^{13}C NMR Spectrum of 5, 7-di-*tert*-butyl-2-(cyclohex-1-en-1-ylmethyl)benzo[*d*]oxazole **(3f)**



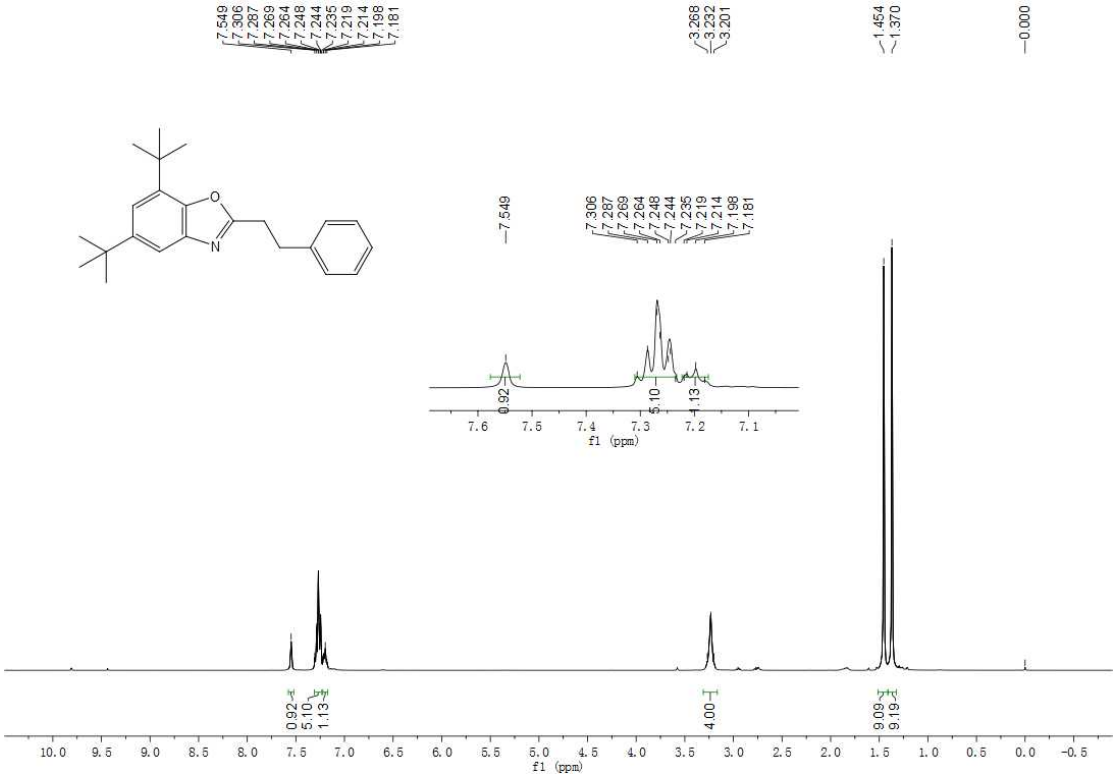
^{1}H NMR Spectrum of 2-benzyl-5, 7-di-*tert*-butylbenzo[*d*]oxazole **(3h)**



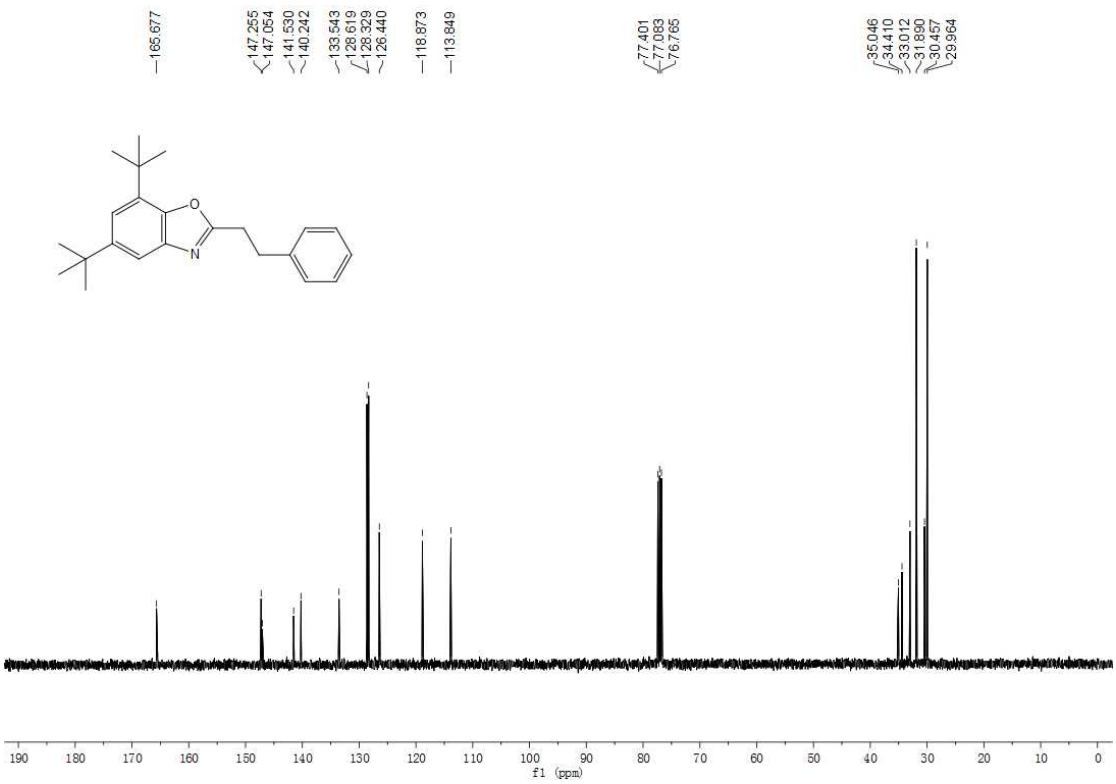
^{13}C NMR Spectrum of 2-benzyl-5, 7-di-*tert*-butylbenzo[*d*]oxazole **(3h)**



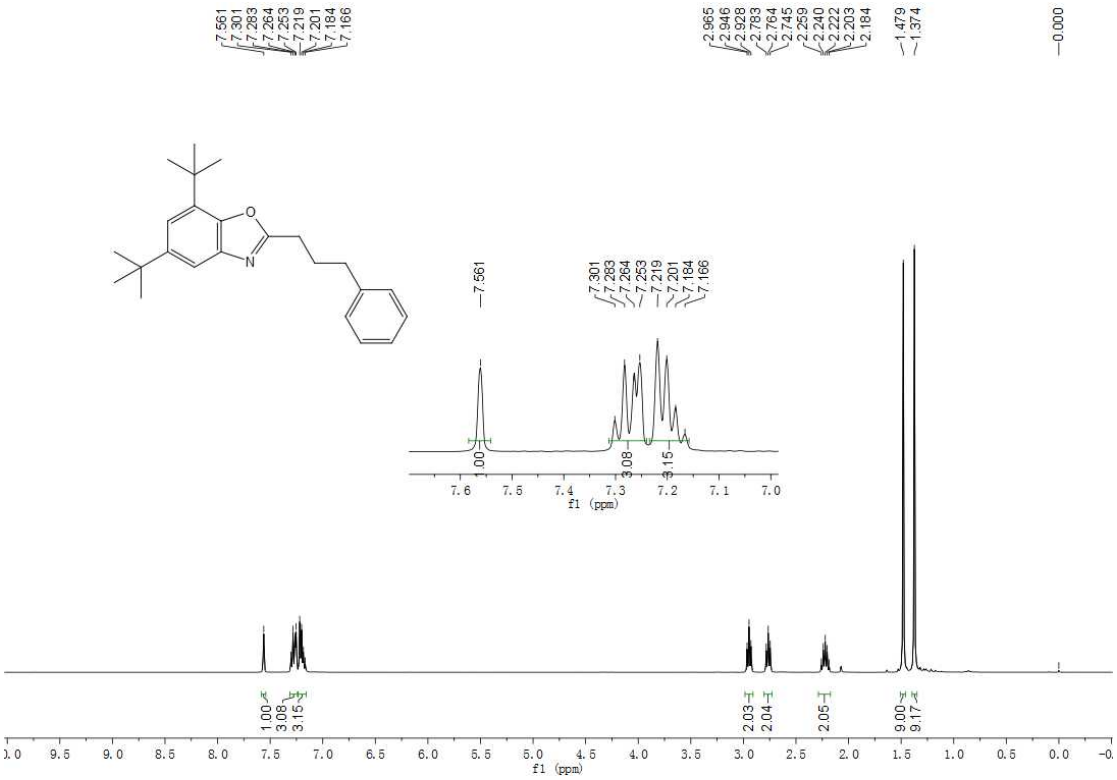
^{1}H NMR Spectrum of 5, 7-di-*tert*-butyl-2-phenethylbenzo[*d*]oxazole **(3i)**



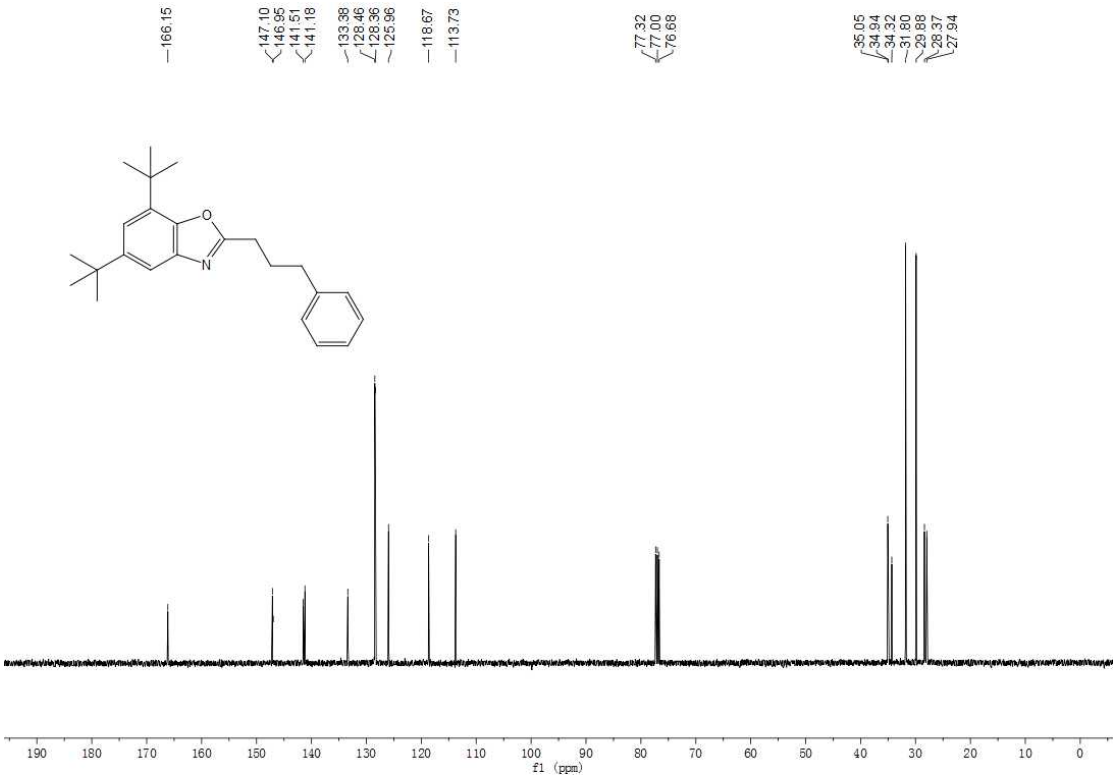
^{13}C NMR Spectrum of 5, 7-di-*tert*-butyl-2-phenethylbenzo[*d*]oxazole **(3i)**



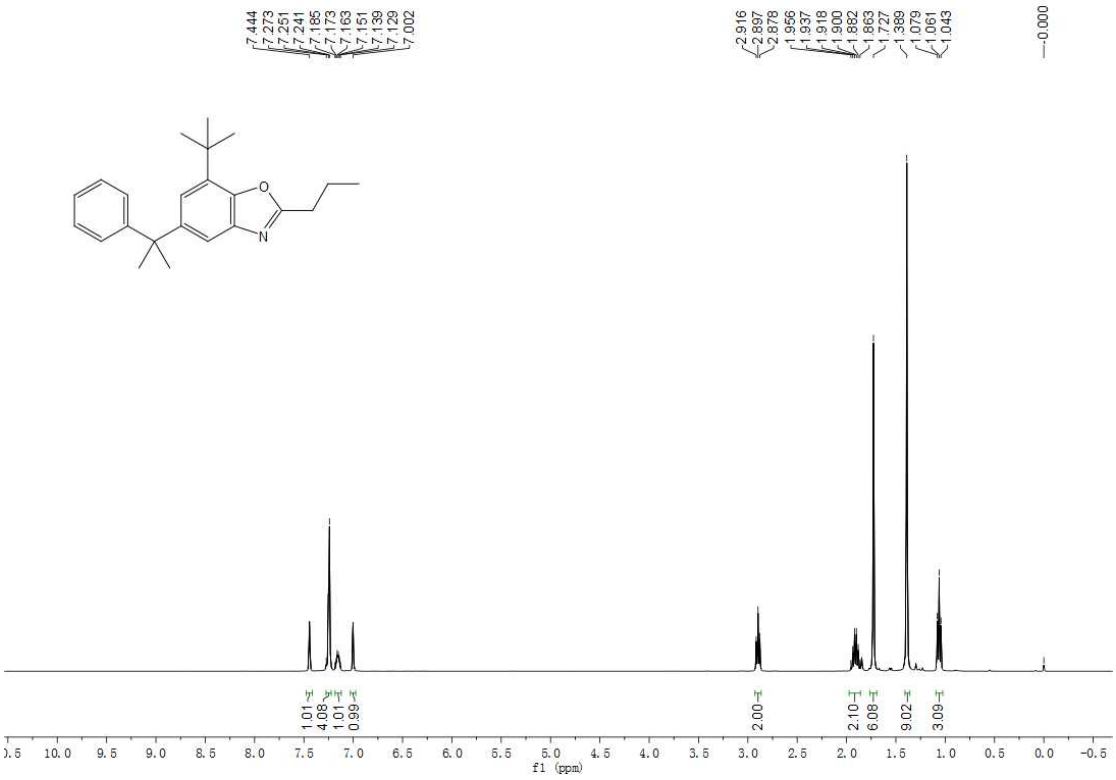
^{1}H NMR Spectrum of 5, 7-di-*tert*-butyl-2-(3-phenylpropyl)benzo[*d*]oxazole **(3j)**



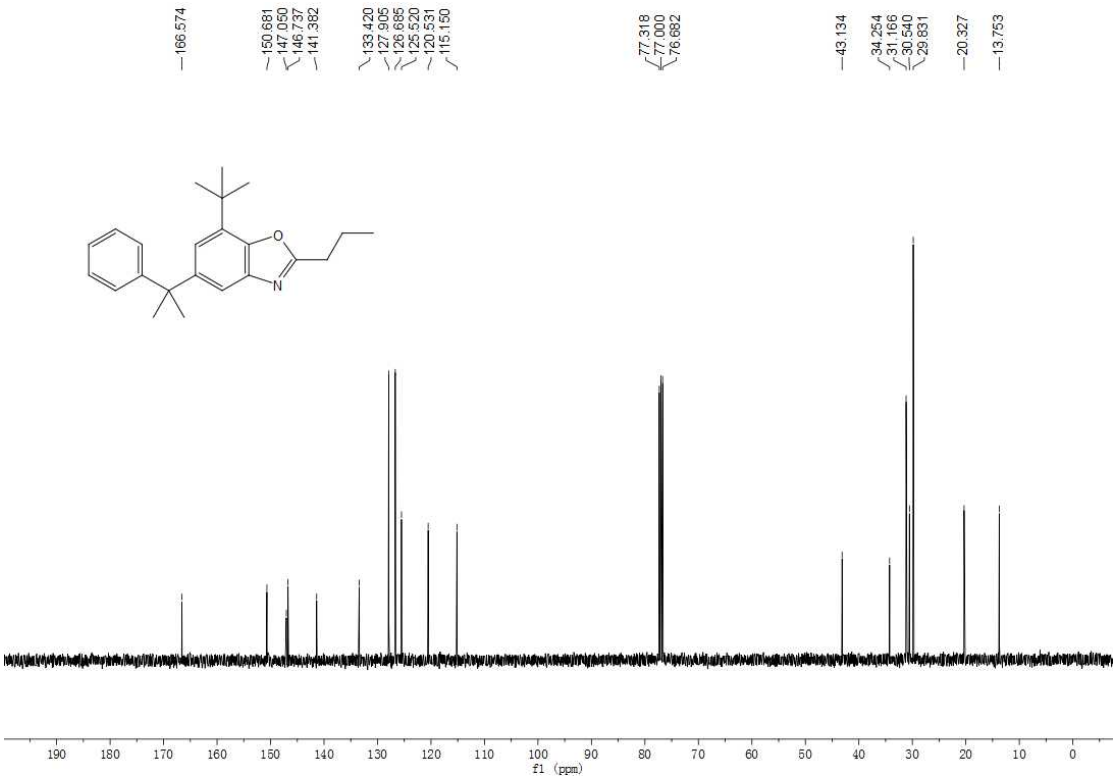
^{13}C NMR Spectrum of 5, 7-di-*tert*-butyl-2-(3-phenylpropyl)benzo[*d*]oxazole **(3j)**



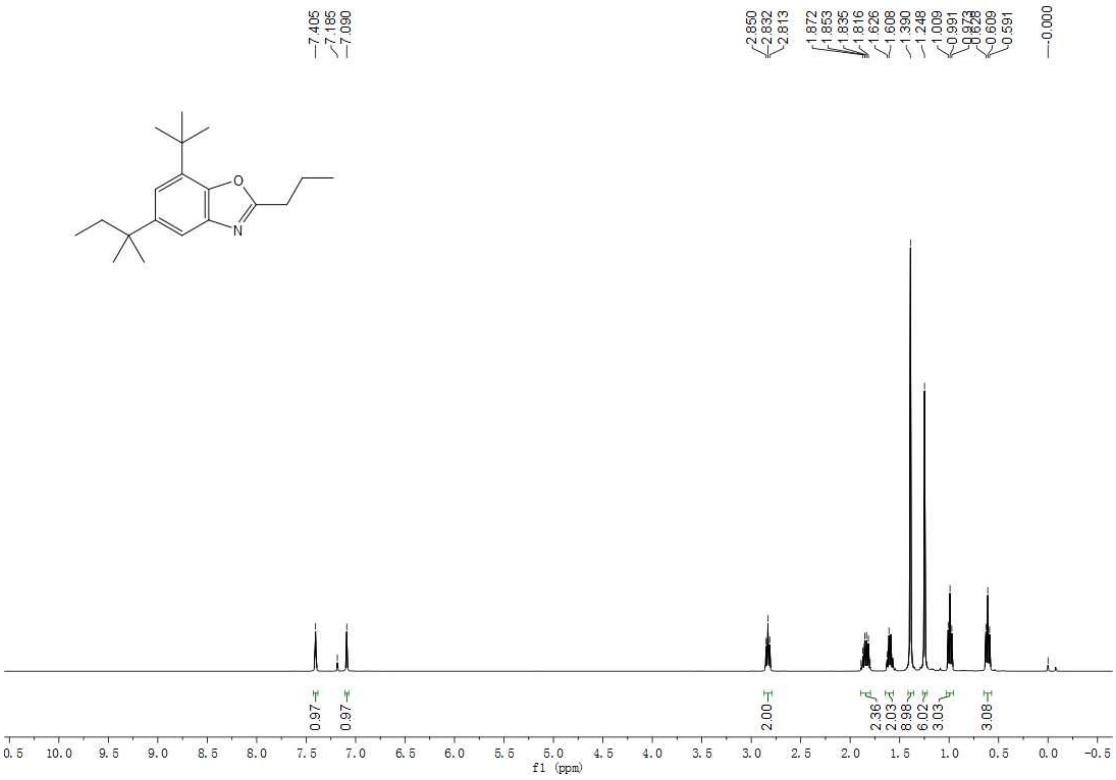
^{1}H NMR Spectrum of 7-(*tert*-butyl)-5-(2-phenylpropan-2-yl)-2-propylbenzo[*d*]oxazole **(3l)**



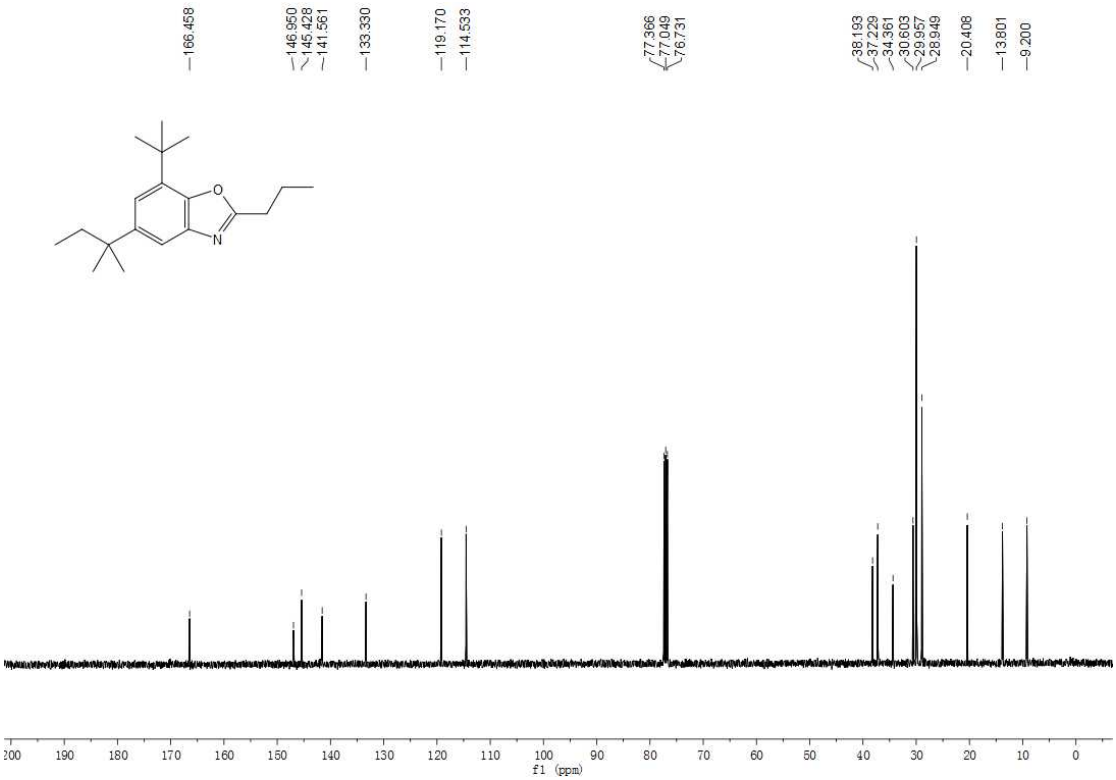
^{13}C NMR Spectrum of 7-(*tert*-butyl)-5-(2-phenylpropan-2-yl)-2-propylbenzo[*d*]oxazole **(3l)**



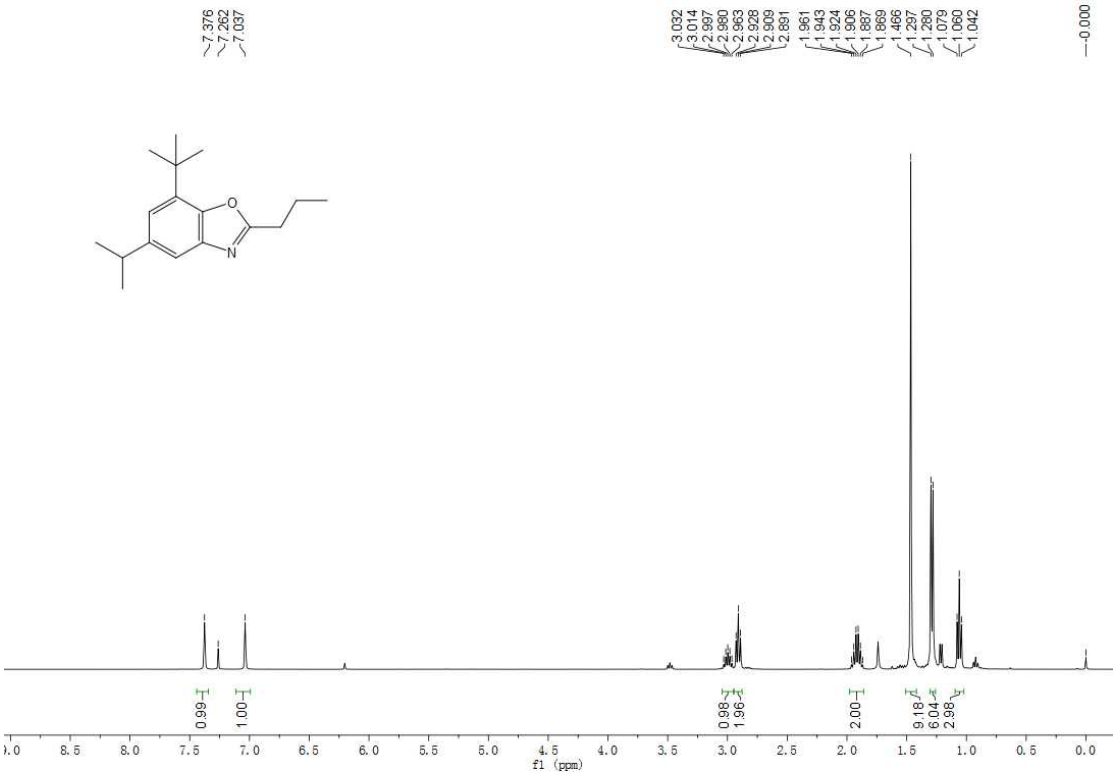
^{1}H NMR Spectrum of 7-(*tert*-butyl)-5-(*tert*-pentyl)-2-propylbenzo[*d*]oxazole **(3m)**



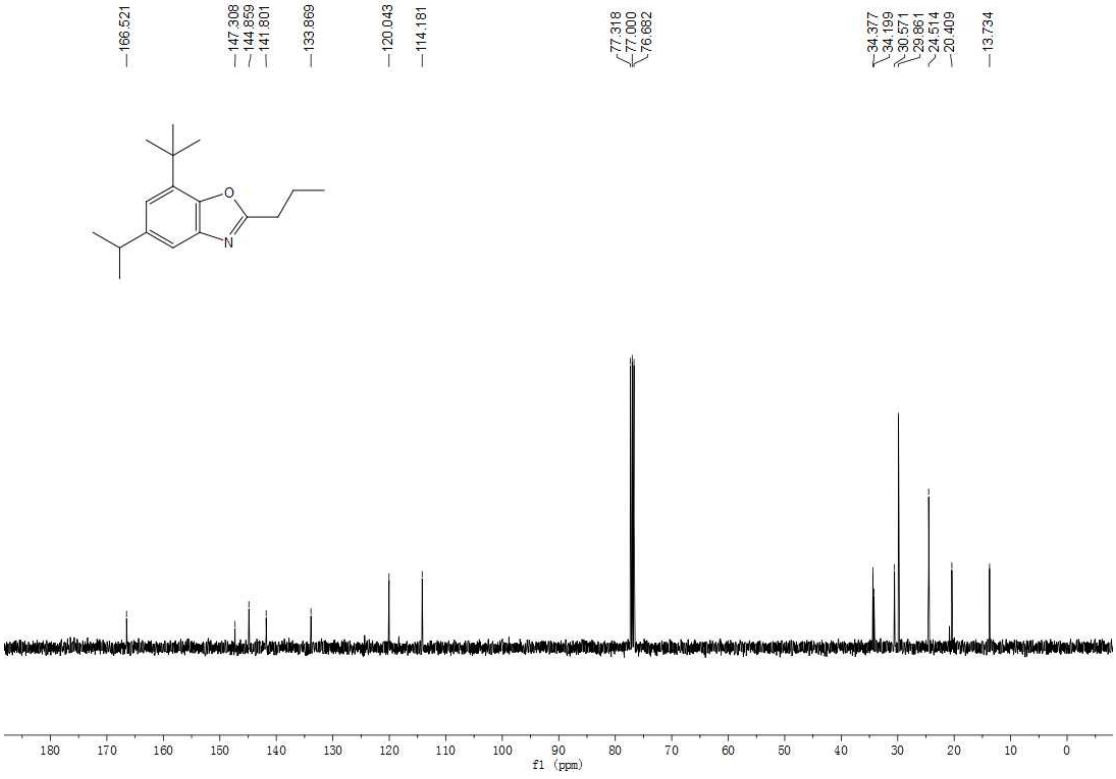
^{13}C NMR Spectrum of 7-(*tert*-butyl)-5-(*tert*-pentyl)-2-propylbenzo[*d*]oxazole **(3m)**



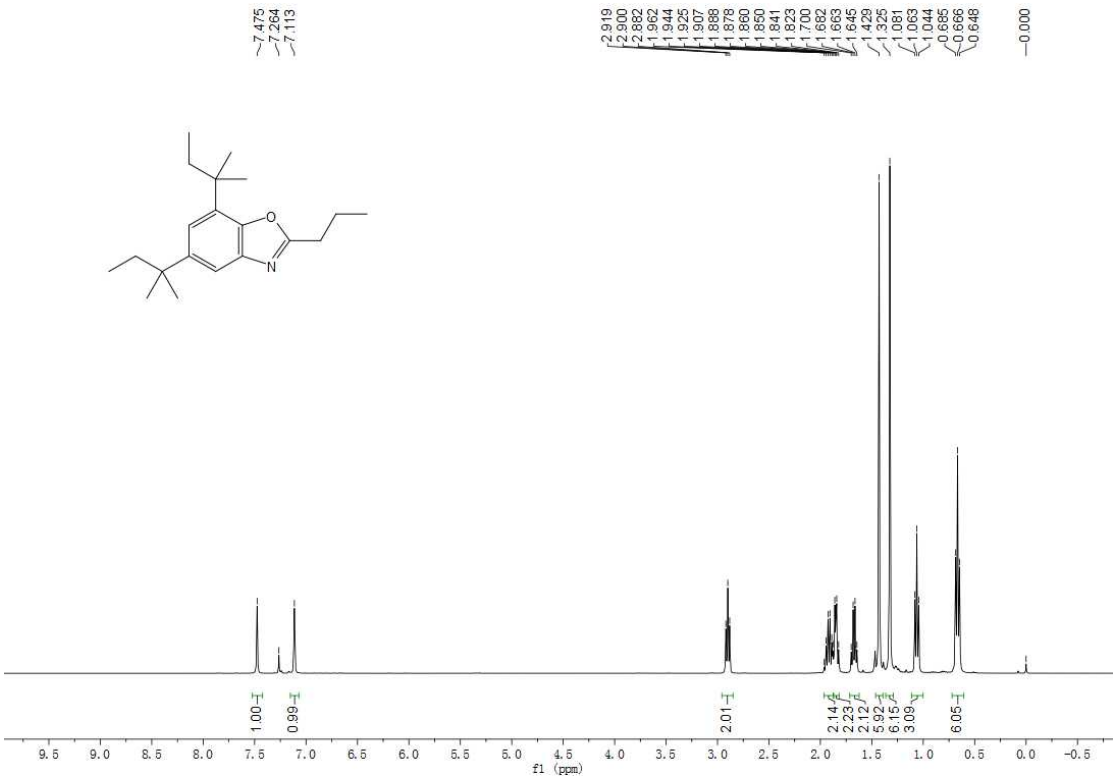
^{1}H NMR Spectrum of 7-(*tert*-butyl)-5-isopropyl-2-propylbenzo[*d*]oxazole **(3n)**



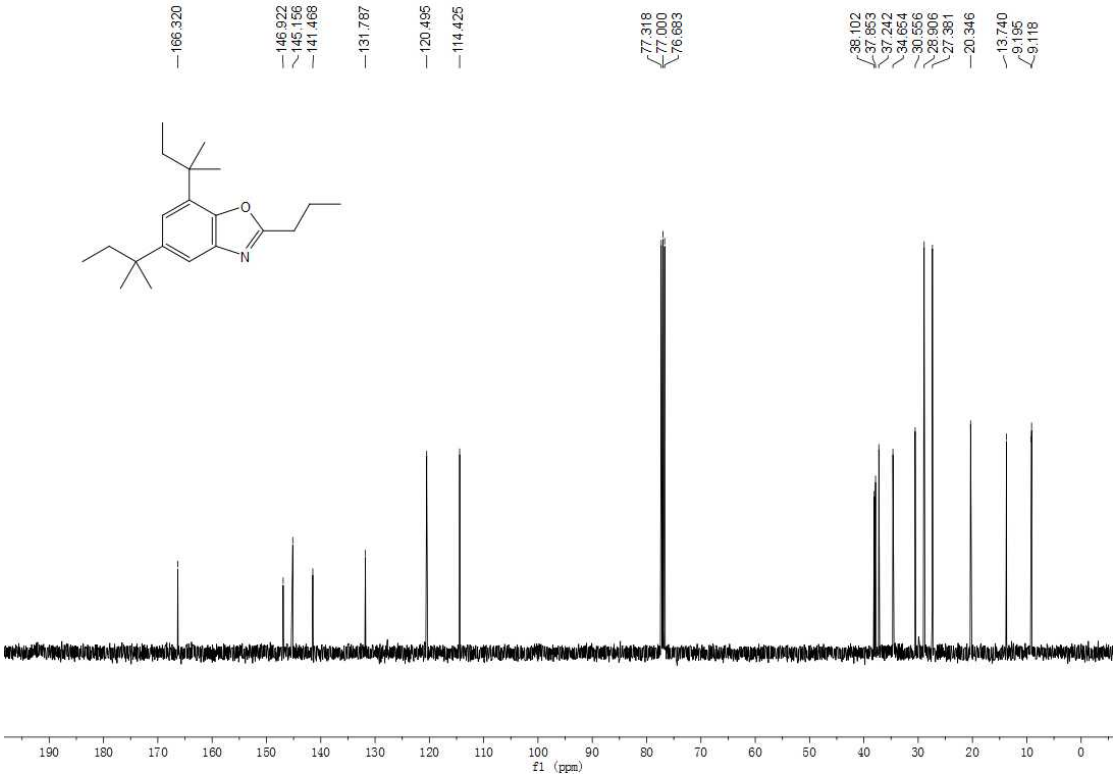
^{13}C NMR Spectrum of 7-(*tert*-butyl)-5-isopropyl-2-propylbenzo[*d*]oxazole **(3n)**



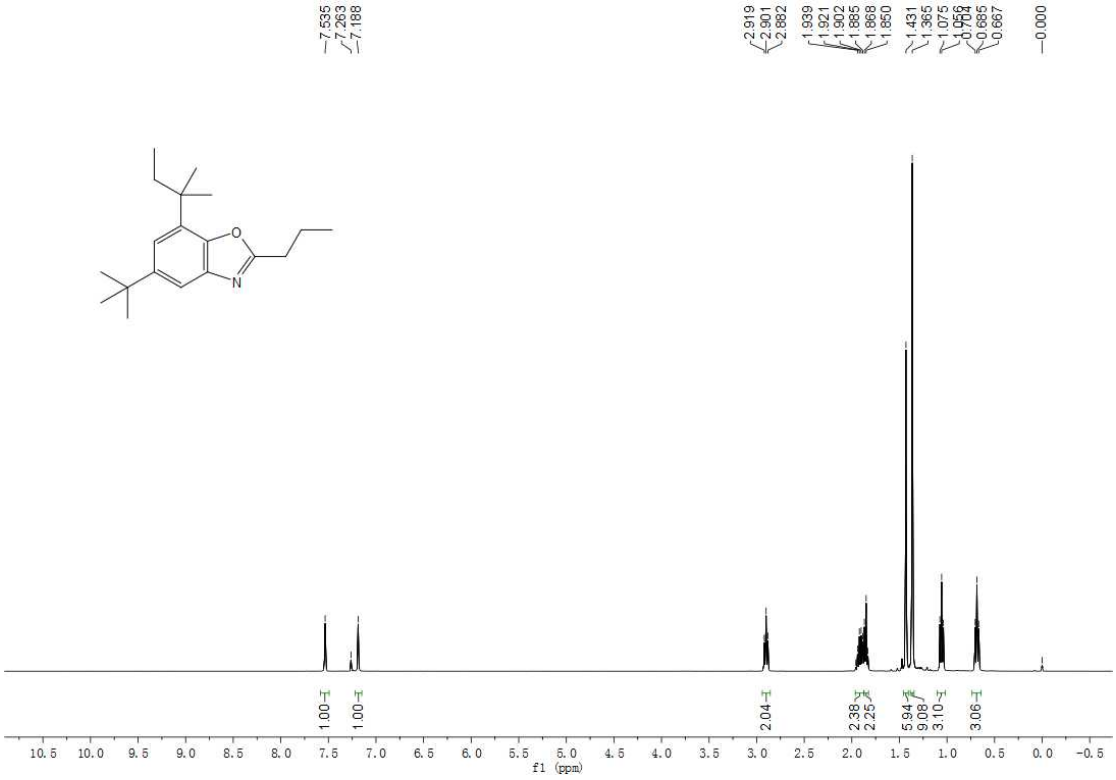
^{1}H NMR Spectrum of 5, 7-di-*tert*-pentyl-2-propylbenzo[*d*]oxazole **(3o)**



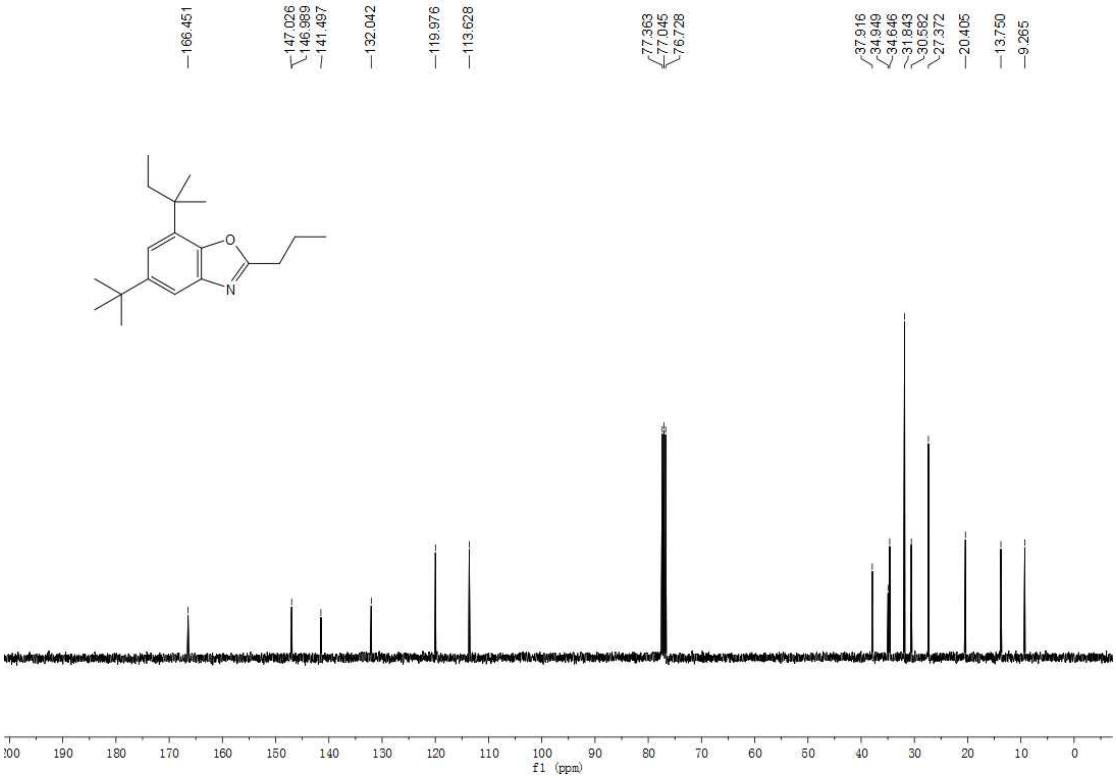
^{13}C NMR Spectrum of 5, 7-di-*tert*-pentyl-2-propylbenzo[*d*]oxazole **(3o)**



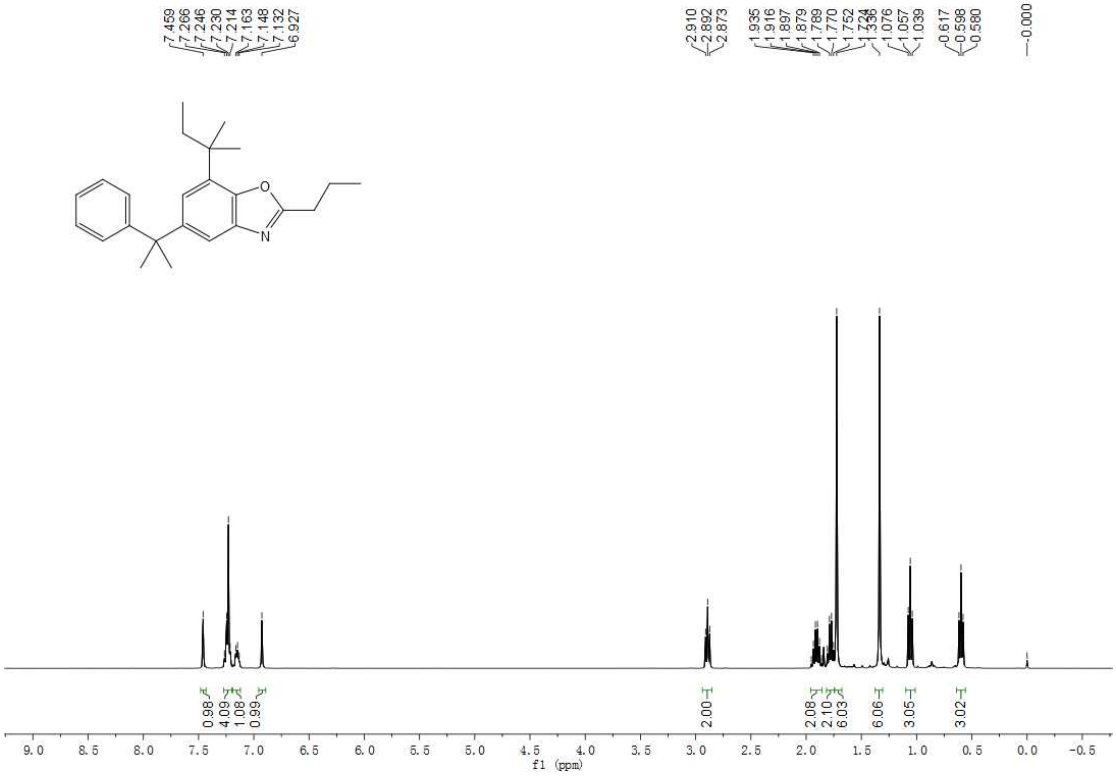
^{1}H NMR Spectrum of 5-(*tert*-butyl)-7-(*tert*-pentyl)-2-propylbenzo[*d*]oxazole **(3p)**



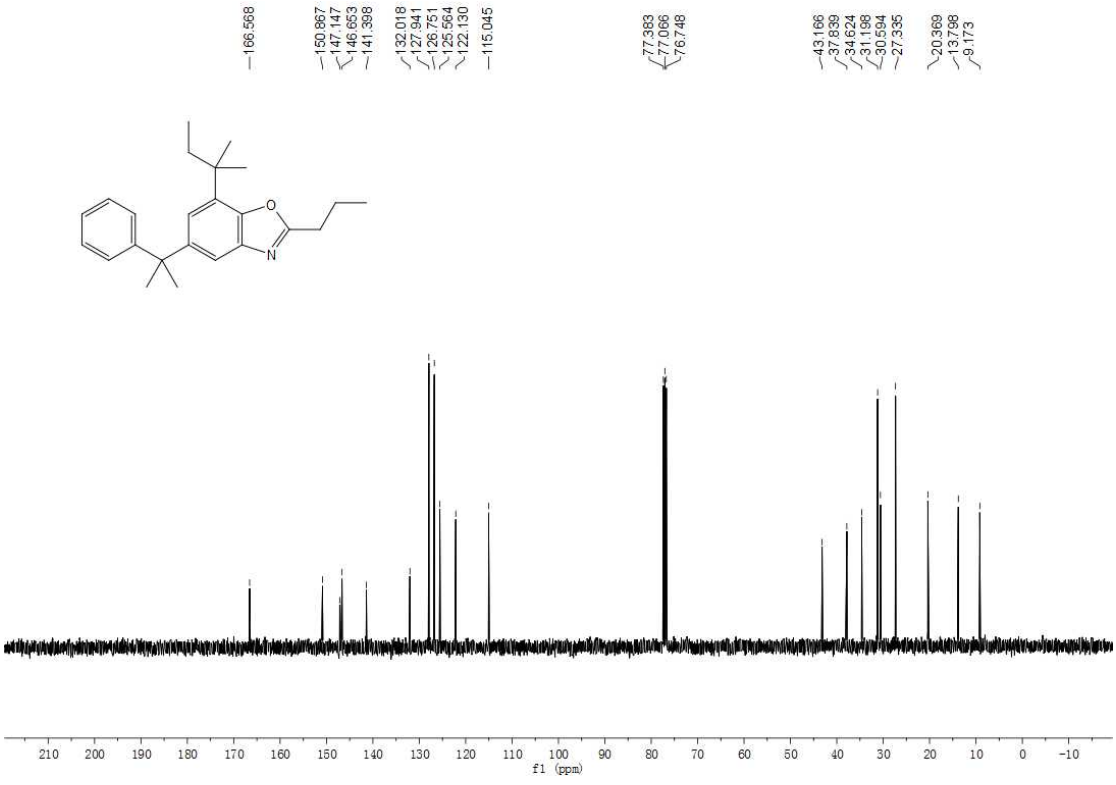
^{13}C NMR Spectrum of 5-(*tert*-butyl)-7-(*tert*-pentyl)-2-propylbenzo[*d*]oxazole **(3p)**



^{1}H NMR Spectrum of 7-(*tert*-pentyl)-5-(2-phenylpropan-2-yl)-2-propylbenzo[*d*]oxazole **(3q)**



^{13}C NMR Spectrum of 7-(*tert*-pentyl)-5-(2-phenylpropan-2-yl)-2-propylbenzo[*d*]oxazole **(3q)**



^{1}H NMR Spectrum of benzoxepine **4a**