Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Experimental section

General Information. All reagents and solvents were obtained from commercial sources. All known products were identified by comparing of their physical characteristics and spectral data with those in the valid samples. ^{1}H NMR (250, 300, 400 MHz) and ^{13}C NMR (62.5, 75, 100 MHz), spectra were recorded on Brucker Avance DRX. Melting points were checked by a Büchi B-545 apparatus in open capillary tubes. All reactions were monitored by thin-layer chromatography (TLC) using silica gel plates (silica gel 60 F254 Merck chemical company).

General experimental procedure for the synthesis of 2-aryl benzoxazoles *via* alkene/alkyne/ketone

Sequentially, to a round-bottomed flask (equipped air condensation), the reaction was carried out with catechol (1.0 mmol), ammonium acetate (1.2 mmol), alkene/alkyne/ketone (1.0 mmol), and I_2 (10 mol %) in DMSO (5.0 mL) heated at 150 °C (oil bath) for the appropriate time. Then, the resulting mixture was cooled to room temperature and extracted with ethyl acetate. Afterward, the combined organic layer was washed with saturated $Na_2S_2O_3$ and brine. Next, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. Finally, the crude mixtures were purified by column chromatography using eluent to afford the corresponding the pure 2-aryl benzoxazoles 4.

Table S1. Investigation of different type of solvent.[a]

Entry	Catalyst (mol %)	Solvent	Temp.	Yield %[b]
1	I_2 (10)	DMSO	140 °C	75
2	I_2 (10)	DMF	140 °C	30
3	I_2 (10)	Toluene	140 °C	-
4	I_2 (10)	Xylene	140 °C	-
5	I_2 (10)	PEG	140 °C	-
6	**I_2 (10)**	**DMSO**	**150 °C**	**92**

[a]General conditions: 3,5-di-*tert*-butylbenzene-1,2-diol (1.0 mmol), ammonium acetate (1.2 mmol), acetophenone (1.0 mmol), solvent (5.0 mL), open air, 12h. [b]Isolated yield.

Table S2. Iodine sources were employed in the reaction.[a]

Entry	Catalyst (mol %)	Solvent	Temp.	Yield %[b]
1	I_2 (10)	DMSO	140 °C	75
2	TBAI (10)	DMSO	140 °C	0
3	AgI (10)	DMSO	140 °C	10
4	CuI (10)	DMSO	140 °C	20
5	KIO_4 (10)	DMSO	140 °C	35
6	KI (10)	DMSO	140 °C	5
7	**I_2 (10)**	**DMSO**	**150 °C**	**92**

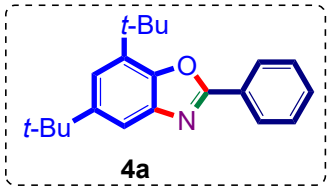
[a]General conditions: 3,5-di-*tert*-butylbenzene-1,2-diol (1.0 mmol), ammonium acetate (1.2 mmol), acetophenone (1.0 mmol), DMSO (5.0 mL), open air, 12h. [b]Isolated yield.

Table S3. Various sources of ammonia in the reaction.[a]

Entry	Catalyst (mol %)	Ammonia source	Solvent	Temp.	Yield %[b]
1	I_2 (10)	NH_4OAc	DMSO	150 °C	92
2	I_2 (10)	$(NH_4)_2CO_3$	DMSO	150 °C	30
3	I_2 (10)	$(NH_4)_2SO_4$	DMSO	150 °C	35
4	I_2 (10)	Bu_4NOH	DMSO	150 °C	0
5	I_2 (10)	NH_4OH	DMSO	150 °C	50
6	I_2 (10)	NH_4Cl	DMSO	150 °C	60
7	I_2 (10)	NH_4CN	DMSO	150 °C	20
8	I_2 (10)	NH_4SCN	DMSO	150 °C	45

[a]General conditions: 3,5-di-*tert*-butylbenzene-1,2-diol (1.0 mmol), ammonia sources (1.2 mmol), acetophenone (1.0 mmol), DMSO (5.0 mL), open air, 12h. [b]Isolated yield.

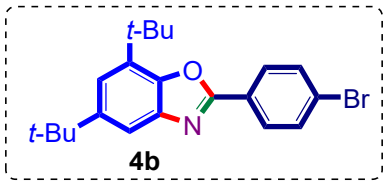
5,7-Di-*tert*-butyl-2-phenylbenzo[*d*]oxazole (4a).[1]



4a

Yield: 92% (282 mg); Brown liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (300 MHz, $CDCl_3$):** δ (ppm) 8.29 (s, 2H), 7.70 (s, 1H), 7.56 (s, 3H), 7.33 (s, 1H), 1.58 (s, 9H), 1.42 (s, 9H); **^{13}C{H} NMR (75 MHz, $CDCl_3$):** δ (ppm) 162.5, 147.7, 146.9, 142.3, 133.7, 131.2, 128.9, 127.5, 127.4, 119.6, 114.2, 35.1, 34.5, 31.8, 30.0; **Anal. Calcd for $C_{21}H_{25}NO$:** C, 82.04; H, 8.20; N, 4.56; Found: C, 81.90; H, 8.08; N, 4.43.

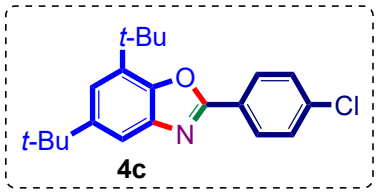
5,7-Di-*tert*-butyl-2-(4-bromophenyl)benzo[*d*]oxazole (4b).[2]



4b

Yield: 92% (355 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (250 MHz, $CDCl_3$):** δ (ppm) 8.03 (d, *J*= 7.5 Hz, 2H), 7.59-7.55 (m, 3H), 7.24 (d, *J*= 2.5 Hz, 1H), 1.46 (s, 9H), 1.31 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 161.6, 148.0, 147.0, 142.2, 133.8, 132.2, 128.8, 126.5, 125.8, 119.9, 114.3, 35.1, 34.5, 31.8, 30.0; **Anal. Calcd for $C_{21}H_{24}BrNO$:** C, 65.29; H, 6.26; N, 3.63; Found: C, 65.05; H, 6.10; N, 3.76.

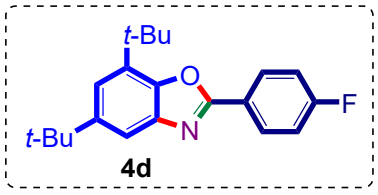
5,7-Di-*tert*-butyl-2-(4-chlorophenyl)benzo[*d*]oxazole (4c).[3]



4c

Yield: 94% (321 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.10 (d, *J*= 8.0 Hz, 2H), 7.56 (d, *J*= 4.0 Hz, 1H), 7.41 (d, *J*= 12.0 Hz, 2H), 7.24 (d, *J*= 4.0 Hz, 1H), 1.46 (s, 9H), 1.31 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 161.5, 147.9, 146.9, 142.2, 137.3, 133.8, 129.2, 128.6, 126.0, 119.8, 114.3, 35.1, 34.5, 31.8, 30.0; **Anal. Calcd for $C_{21}H_{24}ClNO$:** C, 73.78; H, 7.08; N, 4.10; Found: C, 73.64; H, 6.91; N, 4.21.

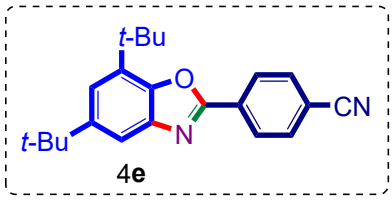
5,7-Di-*tert*-butyl-2-(4-fluorophenyl)benzo[*d*]oxazole (4d).[1]



4d

Yield: 89% (289 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.27 (dd, *J*= 8.0, 4.0 Hz, 2H), 7.67 (d, *J*= 4.0 Hz, 1H), 7.33 (d, *J*= 4.0 Hz, 1H), 7.24 (t, *J*= 8.0 Hz, 2H), 1.57 (s, 9H), 1.42 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 164.6 (d, $J_{C\text{-}F}$= 250.0 Hz), 161.6, 147.8, 146.9, 142.2, 133.7, 129.5 (d, $J_{C\text{-}F}$= 8.0 Hz), 123.8 (d, $J_{C\text{-}F}$= 3.0 Hz), 119.6, 116.1 (d, $J_{C\text{-}F}$= 22.0 Hz), 114.2, 35.1, 34.5, 31.8, 30.0; **Anal. Calcd for $C_{21}H_{24}FNO$:** C, 77.51; H, 7.43; N, 4.30; Found: C, 77.39; H, 7.31; N, 4.40.

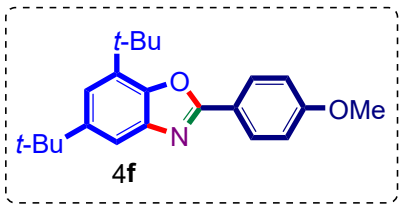
4-(5,7-Di-*tert*-butylbenzo[*d*]oxazol-2-yl)benzonitrile (4e).[1]



4e

Yield: 85% (282 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (300 MHz, $CDCl_3$):** δ (ppm) 8.28 (d, *J*= 9.0 Hz, 2H), 7.75 (d, *J*= 9.0 Hz, 2H), 7.60 (d, *J*= 3.0 Hz, 1H), 7.30 (d, *J*= 3.0 Hz, 1H), 1.48 (s, 9H), 1.33 (s, 9H); **^{13}C{H} NMR (75 MHz, $CDCl_3$):** δ (ppm) 160.3, 148.4, 147.1, 142.1, 134.0, 132.7, 131.5, 127.7, 120.7, 118.3, 114.6, 114.3, 35.1, 34.5, 31.7, 30.0; **Anal. Calcd for $C_{22}H_{24}N_2O$:** C, 79.48; H, 7.28; N, 8.43; Found: C, 79.11; H, 7.06; N, 8.30.

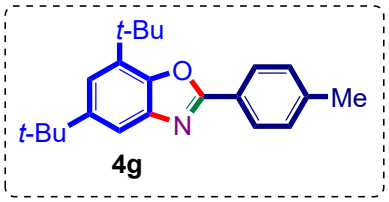
5,7-Di-*tert*-butyl-2-(4-methoxyphenyl)benzo[*d*]oxazole (4f).[4]



4f

Yield: 91% (307 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (300 MHz, $CDCl_3$):** δ (ppm) 8.10 (d, *J*= 9.0 Hz, 2H), 7.53 (d, *J*= 3.0 Hz, 1H), 7.18 (d, *J*= 3.0 Hz, 1H), 7.93 (d, *J*= 9.0 Hz, 2H), 3.76 (s, 3H), 1.45 (s, 9H), 1.30 (s, 9H); **^{13}C{H} NMR (75 MHz, $CDCl_3$):** δ (ppm) 162.6, 162.1, 147.5, 146.8, 142.4, 133.5, 129.1, 120.1, 119.0, 114.3, 113.9, 55.4, 35.0, 34.4, 31.8, 30.0; **Anal. Calcd for $C_{22}H_{27}NO_2$:** C, 78.30; H, 8.06; N, 4.15; Found: C, 78.16; H, 8.12; N, 4.23.

5,7-Di-*tert*-butyl-2-(*p*-tolyl)benzo[*d*]oxazole (4g).[5]

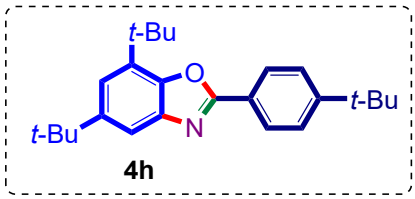


4g

Yield: 93% (298 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.06 (d, *J*= 8.0 Hz, 2H), 7.57 (d, *J*= 4.0 Hz, 1H), 7.25 (d, *J*= 8.0 Hz, 2H), 7.21 (d, *J*= 4.0 Hz, 1H), 2.36 (s, 3H), 1.47 (s, 9H), 1.32 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 162.7, 147.6, 146.8, 142.3,

141.6, 133.6, 129.6, 127.3, 124.8, 119.3, 114.1, 35.1, 34.5, 31.8, 30.0, 21.6; **Anal. Calcd for $C_{22}H_{27}NO$:** C, 82.20; H, 8.47; N, 4.36; Found: C, 82.09; H, 8.40; N, 4.42.

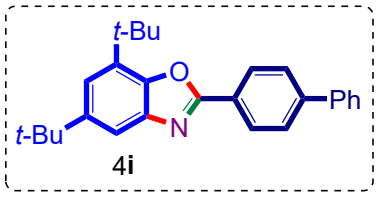
5,7-Di-*tert*-butyl-2-(4-(*tert*-butyl)phenyl)benzo[*d*]oxazole (4h).[2]



4h

Yield: 94% (341 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (250 MHz, $CDCl_3$):** δ (ppm) 8.11 (d, *J*= 10.0 Hz, 2H), 7.58 (d, *J*= 2.5 Hz, 1H), 7.47 (d, *J*= 7.5 Hz, 2H), 7.21 (d, *J*= 2.5 Hz, 1H), 1.47 (s, 9H), 1.32 (s, 9H), 1.30 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 162.6, 154.7, 147.6, 146.8, 142.3, 133.6, 127.2, 125.9, 124.7, 119.3, 114.1, 35.1, 35.0, 34.5, 31.8, 31.2, 30.0; **Anal. Calcd for $C_{25}H_{33}NO$:** C, 82.60; H, 9.15; N, 3.85; Found: C, 82.49; H, 9.04; N, 3.94.

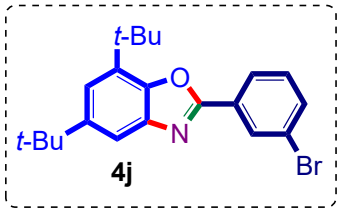
2-([1,1'-Biphenyl]-4-yl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4i).



4i

Yield: 85% (326 mg); Pale brown liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.35 (d, *J*= 8.0 Hz, 2H), 7.79 (d, *J*= 8.0 Hz, 2H), 7.71-7.68 (m, 3H), 7.52 (t, *J*= 8.0 Hz, 2H), 7.45-7.41 (m, 1H), 7.35 (d, *J*= 4.0 Hz, 1H), 1.60 (s, 9H), 1.43 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 162.3, 147.8, 146.9, 144.0, 140.1, 133.7, 128.9, 128.0, 127.9, 127.6, 127.1, 126.2, 119.6, 114.1, 35.1, 34.5, 31.8, 30.0; **Anal. Calcd for $C_{27}H_{29}NO$:** C, 84.55; H, 7.62; N, 3.65; Found: C, 84.42; H, 7.50; N, 3.57.

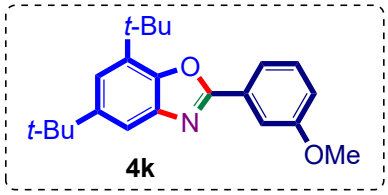
2-(3-Bromophenyl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4j).[5]



4j

Yield: 87% (336 mg); Pale green solid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.40 (d, *J*= 4.0 Hz, 1H), 8.20 (d, *J*= 8.0 Hz, 1H), 7.67 (d, *J*= 4.0 Hz, 1H), 7.66 (s, 1H), 7.42 (t, *J*= 8.0 Hz, 1H), 7.35 (d, *J*= 4.0 Hz, 1H), 1.58 (s, 9H), 1.42 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 160.9, 148.0, 147.0, 142.1, 134.1, 133.9, 130.4, 130.2, 129.4, 125.9, 123.0, 120.0, 114.3, 35.1, 34.5, 31.8, 30.0; **Anal. Calcd for $C_{21}H_{24}BrNO$:** C, 65.29; H, 6.26; N, 3.63; Found: C, 65.15; H, 6.07; N, 3.42.

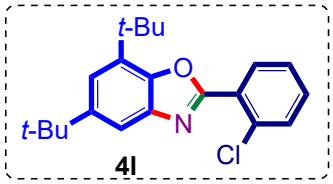
5,7-Di-*tert*-butyl-2-(3-methoxyphenyl)benzo[*d*]oxazole (4k).[3]



4k

Yield: 89% (300 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 7.89-7.86 (m, 1H), 7.83 (d, *J*= 4.0 Hz, 1H), 7.70 (d, *J*= 4.0 Hz, 1H), 7.47 (t, *J*= 8.0 Hz, 1H), 7.34 (d, *J*= 4.0 Hz, 1H), 7.12-7.09 (m, 1H), 3.95 (s, 3H), 1.58 (s, 9H), 1.43 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 162.4, 159.9, 147.7, 146.9, 142.2, 133.7, 130.0, 128.7, 119.8, 119.6, 117.6, 114.2, 112.0, 55.5, 35.1, 34.5, 31.8, 30.0; **Anal. Calcd for $C_{22}H_{27}NO_2$:** C, 78.30; H, 8.06; N, 4.15; Found: C, 78.20; H, 8.02; N, 4.07.

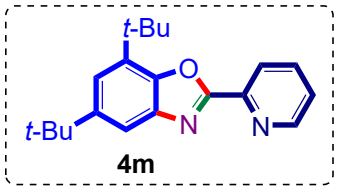
5,7-Di-*tert*-butyl-2-(2-chlorophenyl)benzo[*d*]oxazole (4l).[4]



4l

Yield: 84% (287 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.14-8.10 (m, 1H), 7.65 (d, *J*= 4.0 Hz, 1H), 7.51-7.48 (m, 1H), 7.39-7.33 (m, 2H), 7.28 (d, *J*= 4.0 Hz, 1H), 1.47 (s, 9H), 1.33 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 160.6, 148.0, 146.9, 141.4, 134.1, 133.3, 131.9, 131.8, 131.4, 127.0, 126.4, 120.0, 114.4, 35.1, 34.4, 31.8, 29.9; **Anal. Calcd for $C_{21}H_{24}ClNO$:** C, 73.78; H, 7.08; N, 4.10; Found: C, 73.69; H, 7,03; N, 4.05.

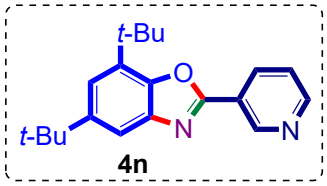
5,7-Di-*tert*-butyl-2-(pyridin-2-yl)benzo[*d*]oxazole (4m).[1]



4m

Yield: 91% (280 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (300 MHz, $CDCl_3$):** δ (ppm) 8.84 (d, *J*= 6.0 Hz, 1H), 8.30 (d, *J*= 6.0 Hz, 1H), 7.91-7.85 (m, 1H), 7.70 (d, *J*= 3.0 Hz, 1H), 7.45-7.40 (m, 1H), 7.37 (d, *J*= 3.0 Hz, 1H), 1.58 (s, 9H), 1.41 (s, 9H); **^{13}C{H} NMR (75 MHz, $CDCl_3$):** δ (ppm) 161.1, 150.4, 148.0, 147.3, 146.4, 142.1, 136.9, 134.1, 125.2, 123.1, 120.4, 114.8, 35.1, 34.5, 31.8, 30.1; **Anal. Calcd for $C_{20}H_{24}N_2O$:** C, 77.89; H, 7.84; N, 9.08; Found: C, 77.80; H, 7.77; N, 9.02.

5,7-Di-*tert*-butyl-2-(pyridin-3-yl)benzo[*d*]oxazole (4n).[3]

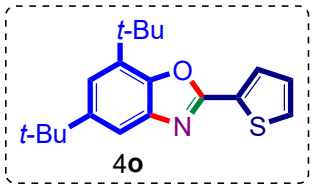


4n

Yield: 96% (296 mg); White solid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.48 (s, 1H), 8.76 (s, 1H), 8.50 (d, *J*= 8.0 Hz, 1H), 7.67 (d, *J*= 4.0 Hz, 1H), 7.49-7.46 (m, 1H), 7.35 (d, *J*= 4.0 Hz, 1H), 1.55 (s, 9H), 1.40 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 160.0, 151.7, 148.5, 148.2, 147.0, 142.0, 134.4, 133.9, 123.8, 123.7, 120.2, 114.4, 35.1, 34.5, 31.8, 30.0; **Anal. Calcd for $C_{20}H_{24}N_2O$:** C, 77.89; H, 7.84; N, 9.08; Found: C, 77.80; H, 7.71; N, 9.15.

5,7-Di-*tert*-butyl-2-(thiophen-2-yl)benzo[*d*]oxazole (4o).[3]

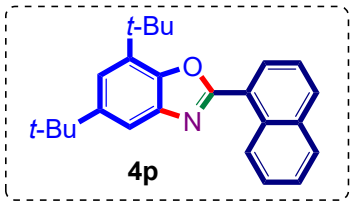


4o

Yield: 92% (288 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1).

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.79 (d, *J*= 6.0 Hz, 1H), 7.52 (d, *J*= 3.0 Hz, 1H), 7.42-7.39 (m, 1H), 7.19 (d, *J*= 3.0 Hz, 1H), 7.08-7.04 (m, 1H), 1.43 (s, 9H), 1.29 (s, 9H); **^{13}C{H} NMR (75 MHz, $CDCl_3$):** δ (ppm) 158.5, 147.9, 146.6, 142.2, 133.6, 130.1, 129.7, 129.3, 128.1, 119.5, 114.1, 35.1, 34.4, 31.8, 30.0; **Anal. Calcd for $C_{19}H_{23}NOS$:** C, 72.80; H, 7.40; N, 4.47; Found: C, 72.71; H, 7.30; N, 4.43.

5,7-Di-*tert*-butyl-2-(naphthalen-1-yl)benzo[*d*]oxazole (4p).[3]

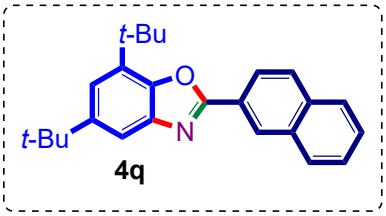


4p

Yield: 82% (293 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.38 (d, *J*= 12.0 Hz, 1H), 8.32 (d, *J*= 8.0 Hz, 1H), 7.95 (d, *J*= 8.0 Hz, 1H), 7.86 (d, *J*= 8.0 Hz, 1H), 7.69 (d, *J*= 4.0 Hz, 1H), 7.62 (t, *J*= 8.0 Hz, 1H), 7.56-7.49 (m, 2H), 7.28 (d, *J*= 4.0 Hz, 1H), 1.51 (s, 9H), 1.35 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 162.3, 147.7, 146.4, 142.5, 133.9, 133.7, 131.9, 130.7, 129.0, 128.6, 127.8, 126.4, 126.3, 125.0, 124.1, 119.7, 114.4, 35.1, 34.5, 31.9, 30.1; **Anal. Calcd for $C_{25}H_{27}NO$:** C, 83.99; H, 7.61; N, 3.92; Found: C, 83.83; H, 7.52; N, 4.01.

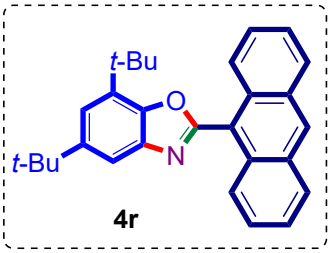
5,7-Di-*tert*-butyl-2-(naphthalen-2-yl)benzo[*d*]oxazole (4q).[6]



4q

Yield: 88% (314 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.78 (s, 1H), 8.36-8.33 (m, 1H), 8.05-8.00 (m, 2H), 7.94-7.91 (m, 1H), 7.72 (d, *J*= 4.0 Hz, 1H), 7.62-7.59 (m, 2H), 7.36 (d, *J*= 4.0 Hz, 1H), 1.63 (s, 9H), 1.44 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 162.6, 147.8, 147.0, 142.3, 134.6, 133.7, 133.0, 128.9, 128.7, 127.9, 127.7, 127.6, 126.8, 124.7, 123.9, 119.7, 114.2, 35.1, 34.5, 31.8, 30.1; **Anal. Calcd for $C_{25}H_{27}NO$:** C, 83.99; H, 7.61; N, 3.92; Found: C, 83.88; H, 7.55; N, 3.98.

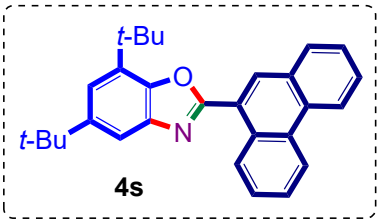
2-(Anthracen-9-yl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4r).



4r

Yield: 72% (293 mg); Pale brown liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.56 (s, 1H), 8.08-8.04 (m, 2H), 8.00-7.96 (m, 2H), 7.77 (d, *J*= 4.0 Hz, 1H), 7.43-7.39 (m, 4H), 7.36 (d, *J*= 4.0 Hz, 1H), 1.44 (s, 9H), 1.39 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 161.4, 147.8, 147.4, 142.2, 134.2, 131.3, 131.1, 130.6, 128.6, 127.2, 125.7, 125.5, 121.8, 119.8, 114.6, 35.2, 34.6, 31.9, 30.0; **Anal. Calcd for $C_{29}H_{29}NO$:** C, 85.47; H, 7.17; N, 3.44; Found: C, 85.10; H, 6.92; N, 3.25.

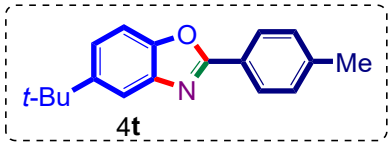
5,7-Di-*tert*-butyl-2-(phenanthren-9-yl)benzo[*d*]oxazole (4s).



4s

Yield: 80% (326 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 9.53-9.50 (m, 1H), 8.83 (d, *J*= 8.0 Hz, 1H), 8.77 (d, *J*= 8.0 Hz, 1H), 8.69 (s, 1H), 8.09 (d, *J*= 8.0 Hz, 1H), 7.83 (d, *J*= 4.0 Hz, 1H), 7.82-7.77 (m, 3H), 7.70 (d, *J*= 8.0 Hz, 1H), 7.42 (d, *J*= 4.0 Hz, 1H), 1.56 (s, 9H), 1.48 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 162.3, 147.7, 146.4, 142.5, 133.7, 131.6, 131.1, 130.8, 130.6, 129.8, 128.8, 128.5, 127.5, 127.1 (2C), 123.1, 122.9, 122.7, 119.8, 114.5, 35.1, 34.5, 31.9, 30.1; **Anal. Calcd for $C_{29}H_{29}NO$:** C, 85.47; H, 7.17; N, 3.44; Found: C, 85.20; H, 6.97; N, 3.32.

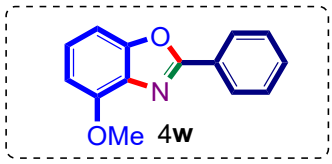
5-(*Tert*-butyl)-2-(*p*-tolyl)benzo[*d*]oxazole (4t).[4]



4t

Yield: 85% (225 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.06 (d, *J*= 12.0 Hz, 2H), 7.60 (d, *J*= 12.0 Hz, 1H), 7.53 (d, *J*= 4.0 Hz, 1H), 7.36-7.31 (m, 1H), 7.25 (d, *J*= 12.0 Hz, 2H), 2.37 (s, 3H), 1.33 (s, 9H); **^{13}C{H} NMR (75 MHz, $CDCl_3$):** δ (ppm) 163.1, 150.9, 149.0, 141.8, 139.6, 129.6, 127.4, 124.5, 122.2, 118.8, 107.2, 35.2, 31.7, 21.6; **Anal. Calcd for $C_{18}H_{19}NO$:** C, 81.47; H, 7.22; N, 5.28; Found: C, 81.07; H, 6.95; N, 5.10.

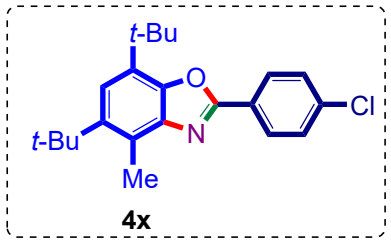
4-methoxy-2-phenylbenzo[*d*]oxazole (4w).[7]



4**w**

Yield: 50% (112 mg); Yellow liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.25-8.22 (m, 2H), 7.46-7.42 (m, 3H), 7.22 (t, *J*= 8.0 Hz, 1H), 7.14 (d, *J*= 8.0 Hz, 1H), 6.75 (d, *J*= 8.0 Hz, 1H), 4.00 (s, 3H); **^{13}C{H} NMR (75 MHz, $CDCl_3$):** δ (ppm) 162.8, 152.2, 151.8, 131.7, 131.3, 128.8, 127.6, 127.1, 125.7, 105.8, 103.4, 56.1; **Anal. Calcd for $C_{14}H_{11}NO_2$:** C, 74.65; H, 4.92; N, 6.22; Found: C, 74.48; H, 4.76; N, 6.12.

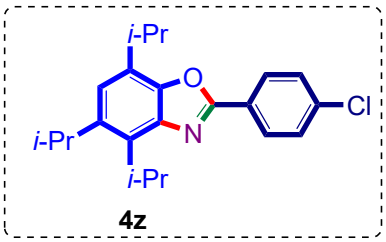
5,7-Di-*tert*-butyl-2-(4-chlorophenyl)-4-methylbenzo[*d*]oxazole (4x).



4x

Yield: 80% (284 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 8.22 (d, *J*= 8.0 Hz, 1H), 7.51 (d, *J*= 12.0 Hz, 2H), 7.35 (s, 1H), 2.87 (s, 3H), 1.55 (s, 9H), 1.52 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 160.5, 146.4, 143.7, 143.5, 137.1, 130.3, 129.1, 128.7, 126.3, 126.1, 120.3, 36.2, 34.3, 31.3, 30.0, 16.3; **Anal. Calcd for $C_{22}H_{26}ClNO$:** C, 74.24; H, 7.36; N, 3.94; Found: C, 74.09; H, 7.22; N, 4.04.

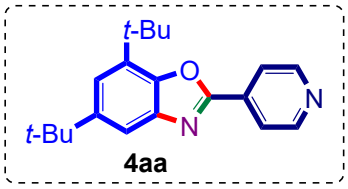
2-(4-chlorophenyl)-4,5,7-triisopropylbenzo[*d*]oxazole (4z).



4z

Yield: 75% (266 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** *δ* (ppm) 8.10 (d, *J*= 8.0 Hz, 1H), 7.39 (d, *J*= 8.0 Hz, 2H), 7.02 (s, 1H), 3.38-3.53 (m, 2H), 3.23-3.33 (m, 1H), 1.42 (d, *J*= 8.0 Hz, 6H), 1.34 (d, *J*= 8.0 Hz, 6H), 1.22 (d, *J*= 8.0 Hz, 6H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** *δ* (ppm) 160.2, 149.5, 142.5, 138.6, 138.1, 136.9, 129.1, 128.6, 126.5, 126.2, 118.2, 29.8, 29.3, 27.1, 24.4, 23.2, 22.1; **Anal. Calcd for $C_{22}H_{26}ClNO$:** C, 74.24; H, 7.36; N, 3.94; Found: C, 73.95; H, 7.13; N, 3.81.

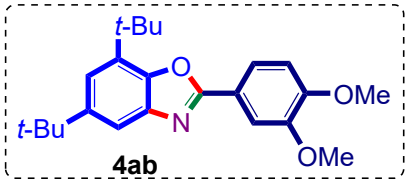
5,7-Di-*tert*-butyl-2-(pyridin-4-yl)benzo[*d*]oxazole (4aa).[5]



4aa

Yield: 72% (222 mg); White solid; Purified by column chromatography (petroleum ether/ethyl acetate 100/1). **^{1}H NMR (400 MHz, $CDCl_3$):** *δ* (ppm) 8.82 (d, *J*= 4.0 Hz, 2H), 8.09 (d, *J*= 8.0 Hz, 2H), 7.69 (d, *J*= 4.0 Hz, 1H), 7.38 (d, *J*= 4.0 Hz, 1H), 1.56 (s, 9H), 1.41 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** *δ* (ppm) 160.0, 150.7, 148.4, 147.1, 142.0, 134.6, 134.1, 120.8, 114.7, 35.1, 34.5, 31.7, 30.0; **Anal. Calcd for $C_{20}H_{24}N_2O$:** C, 77.89; H, 7.84; N, 9.08; Found: C, 77.75; H, 7.78; N, 9.13.

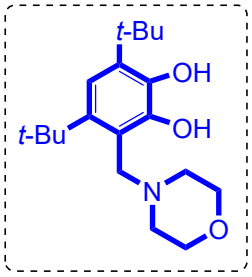
5,7-Di-*tert*-butyl-2-(3,4-dimethoxyphenyl)benzo[*d*]oxazole (4ab).[5]



4ab

Yield: 81% (297 mg); Colorless liquid; Purified by column chromatography (petroleum ether/ethyl acetate 50/1). **^{1}H NMR (400 MHz, $CDCl_3$):** δ (ppm) 7.75 (dd, *J*= 4.0, 8.0 Hz, 1H), 7.68 (d, *J*= 4.0 Hz, 1H), 7.56 (d, *J*= 4.0 Hz, 1H), 7.19 (d, *J*= 4.0 Hz, 1H), 6.89 (d, *J*= 8.0 Hz, 1H), 3.93 (s, 3H), 3.86 (s, 3H), 1.46 (s, 9H), 1.30 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 162.6, 151.7, 149.2, 147.6, 146.8, 142.32, 133.5, 120.8, 120.2, 119.1, 113.9, 110.9, 109.8, 56.1, 56.0, 35.0, 34.4, 31.8, 30.0. Anal. Calcd for $C_{23}H_{29}NO_3$: C, 75.17; H, 7.95; N, 3.81. Found: C, 75.08; H, 7.88; N, 3.70.

4,6-Di-*tert*-butyl-3-morpholinobenzene-1,2-diol (1g).[8]



Yield: 94% (302 mg); Colorless crystal; Purified by wash with glacial acetic acid and water.

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 12.36 (S, 1H), 6.81 (s, 1H), 6.06 (S, 1H), 4.05 (s, 2H), 3.87-3.59 (m, 4H), 2.86-2.39 (m, 4H), 1.43 (s, 9H), 1.39 (s, 9H); **^{13}C{H} NMR (100 MHz, $CDCl_3$):** δ (ppm) 146.0, 141.6, 138.0, 132.8, 115.8, 114.5, 66.8, 58.8, 52.4, 35.4, 34.7, 32.0, 29.4; **Anal. Calcd for $C_{19}H_{31}NO_3$:** C, 70.99; H, 9.72; N, 4.36; Found: C, 70.72; H, 9.56; N, 4.24.

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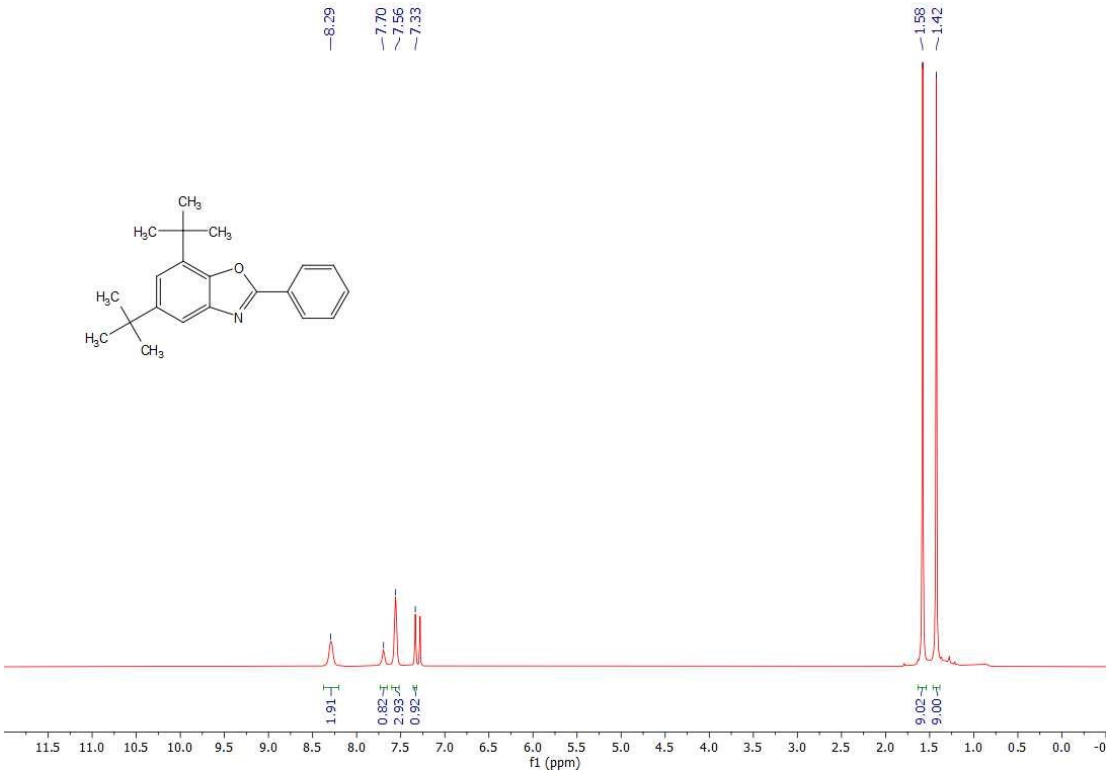

Figure S1. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-phenylbenzo[*d*]oxazole (4a) in $CDCl_3$ at 300 MHz.

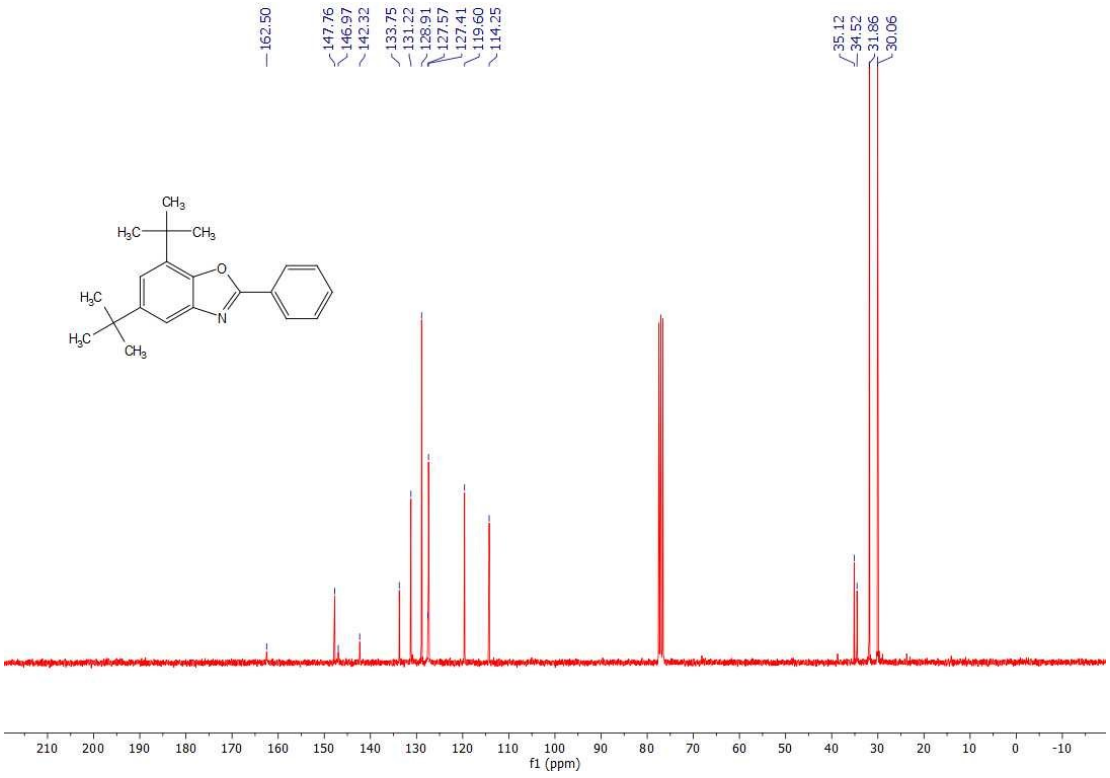

Figure S2. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-phenylbenzo[*d*]oxazole (4a) in $CDCl_3$ at 75 MHz.

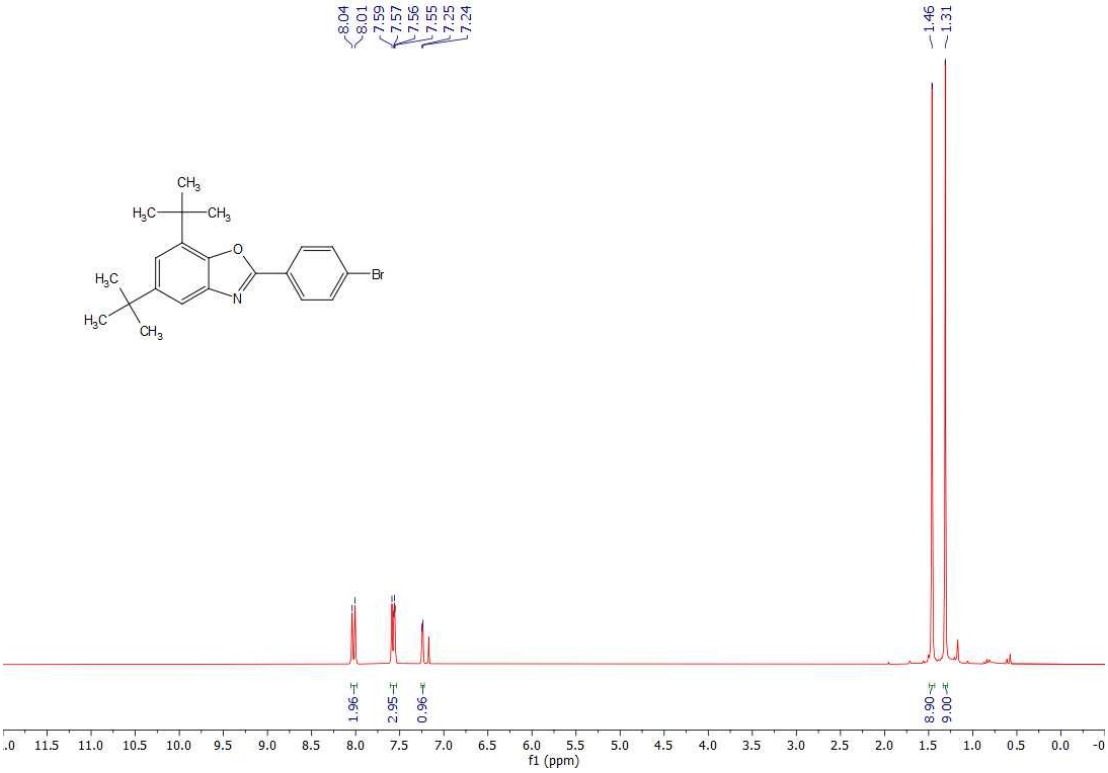

Figure S3. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(4-bromophenyl)benzo[*d*]oxazole (4b) in $CDCl_3$ at 250 MHz.

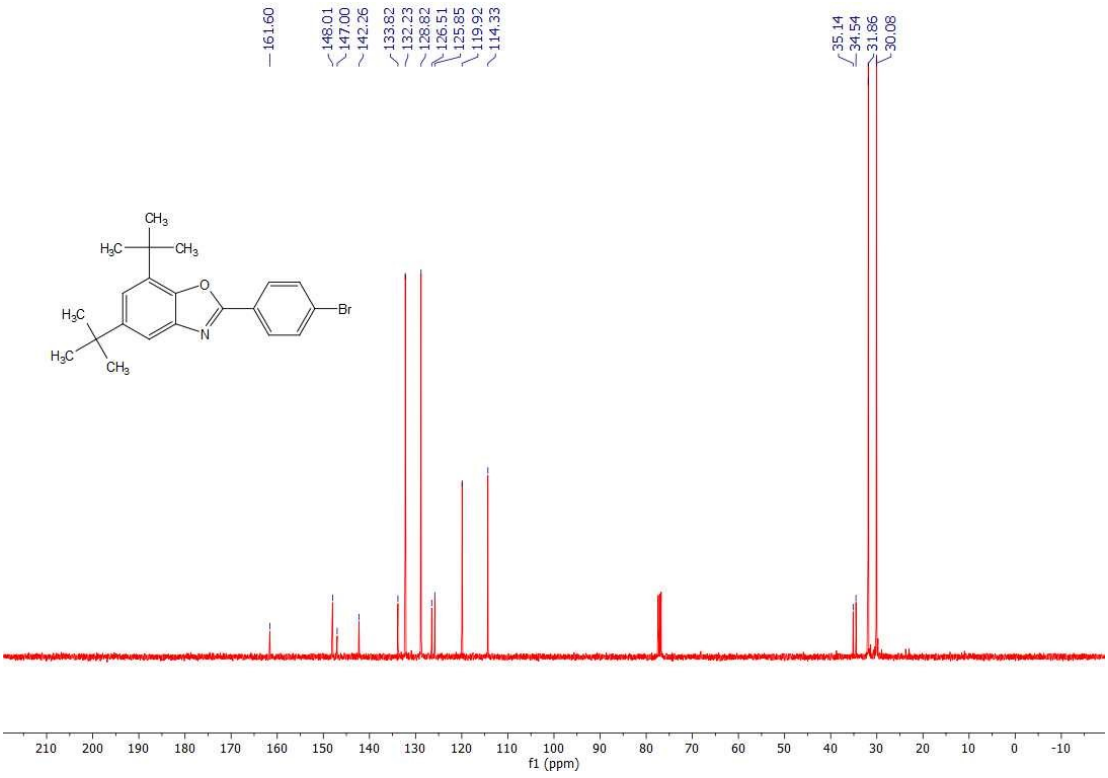

Figure S4. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(4-bromophenyl)benzo[*d*]oxazole (4b) in $CDCl_3$ at 100 MHz.

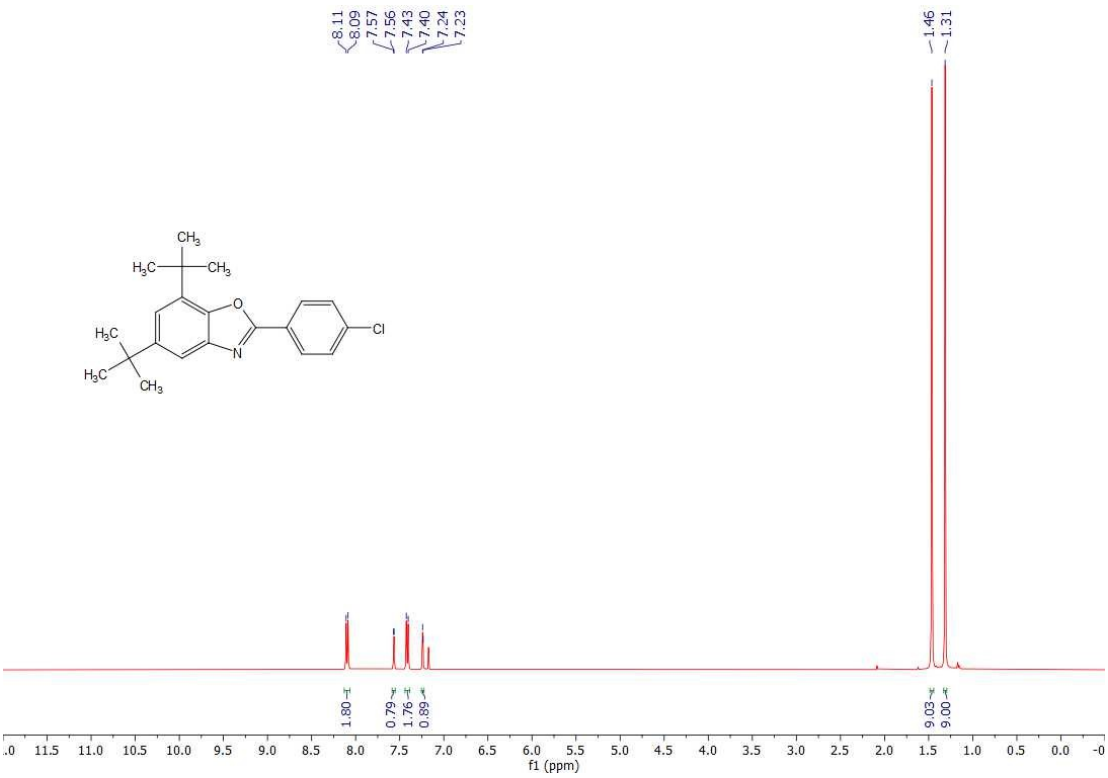

Figure S5. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(4-chlorophenyl)benzo[*d*]oxazole (4c) in $CDCl_3$ at 400 MHz.

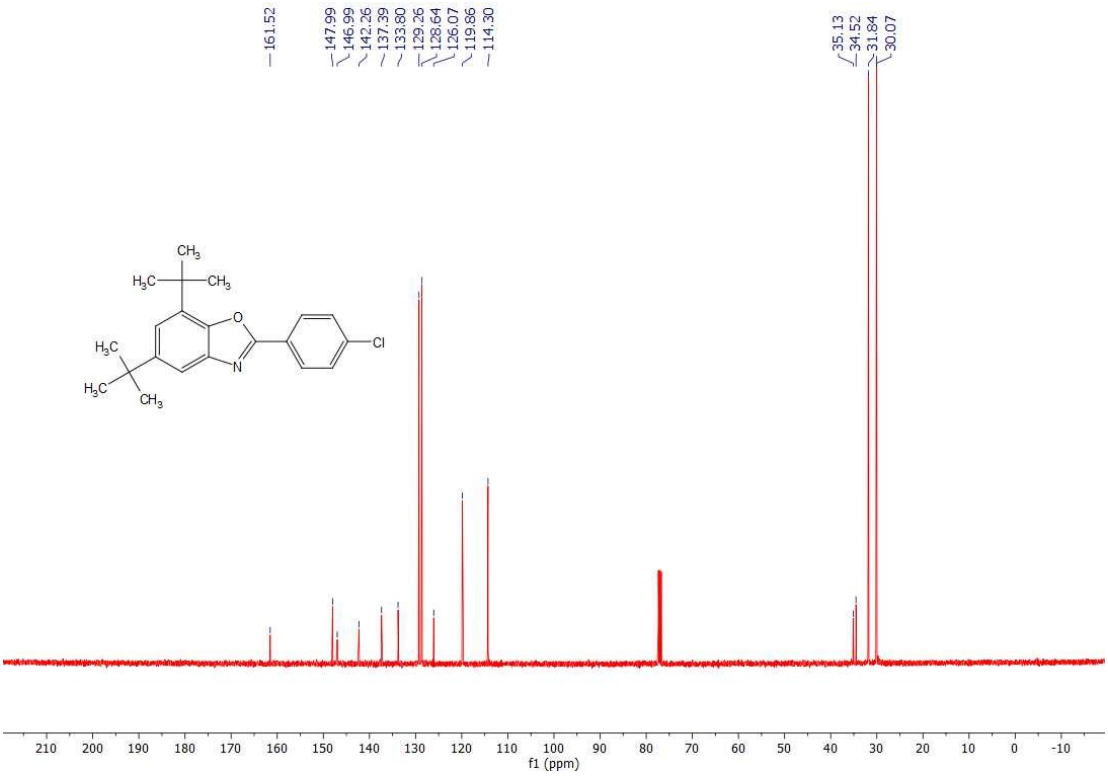

Figure S6. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(4-chlorophenyl)benzo[*d*]oxazole (4c) in $CDCl_3$ at 100 MHz.

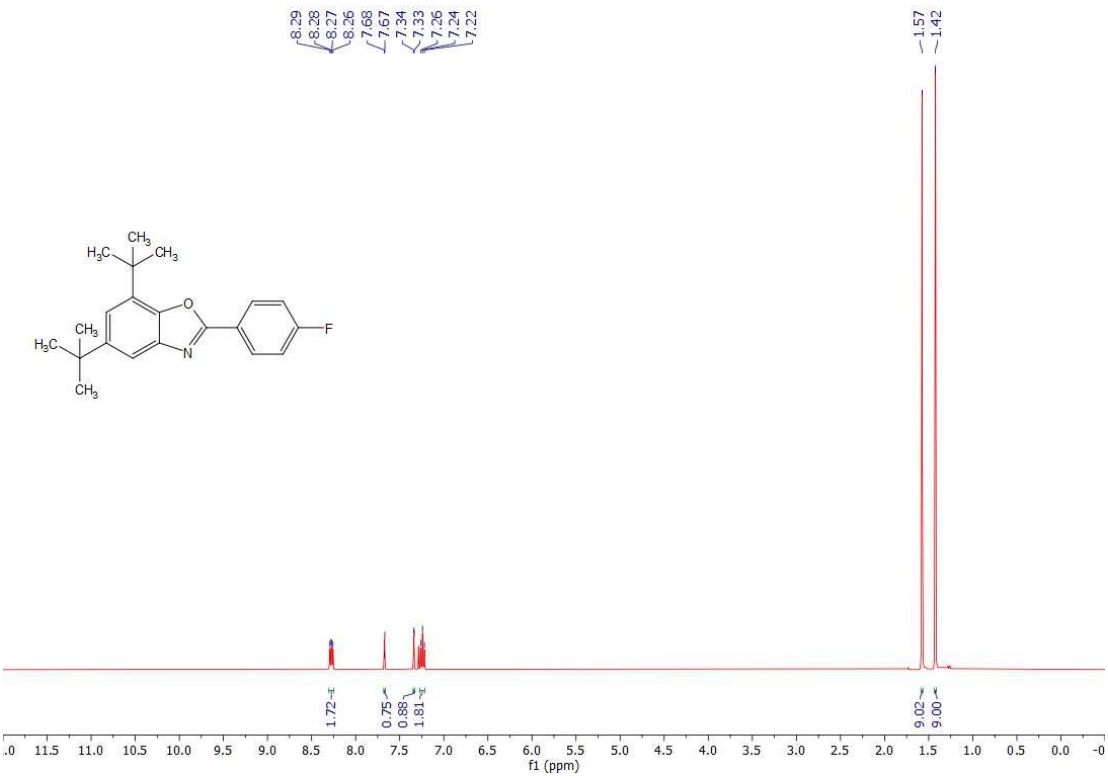

Figure S7. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(4-fluorophenyl)benzo[*d*]oxazole (4d) in $CDCl_3$ at 400 MHz.

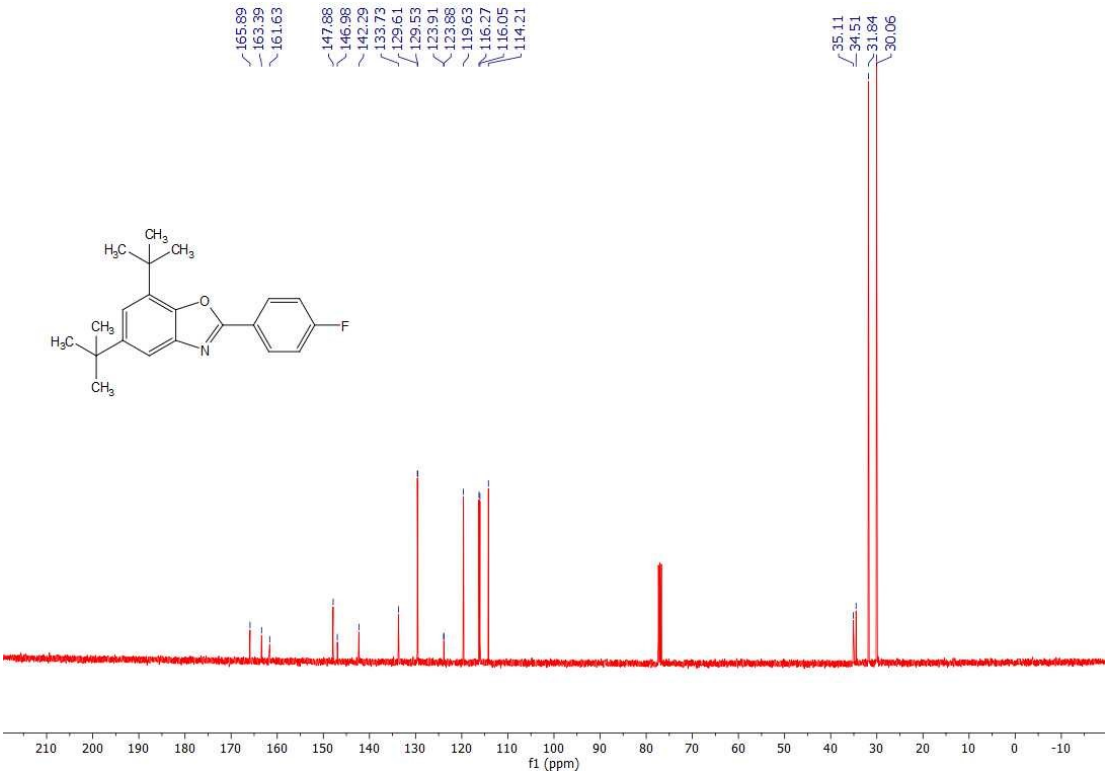

Figure S8. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(4-fluorophenyl)benzo[*d*]oxazole (4d) in $CDCl_3$ at 100 MHz.

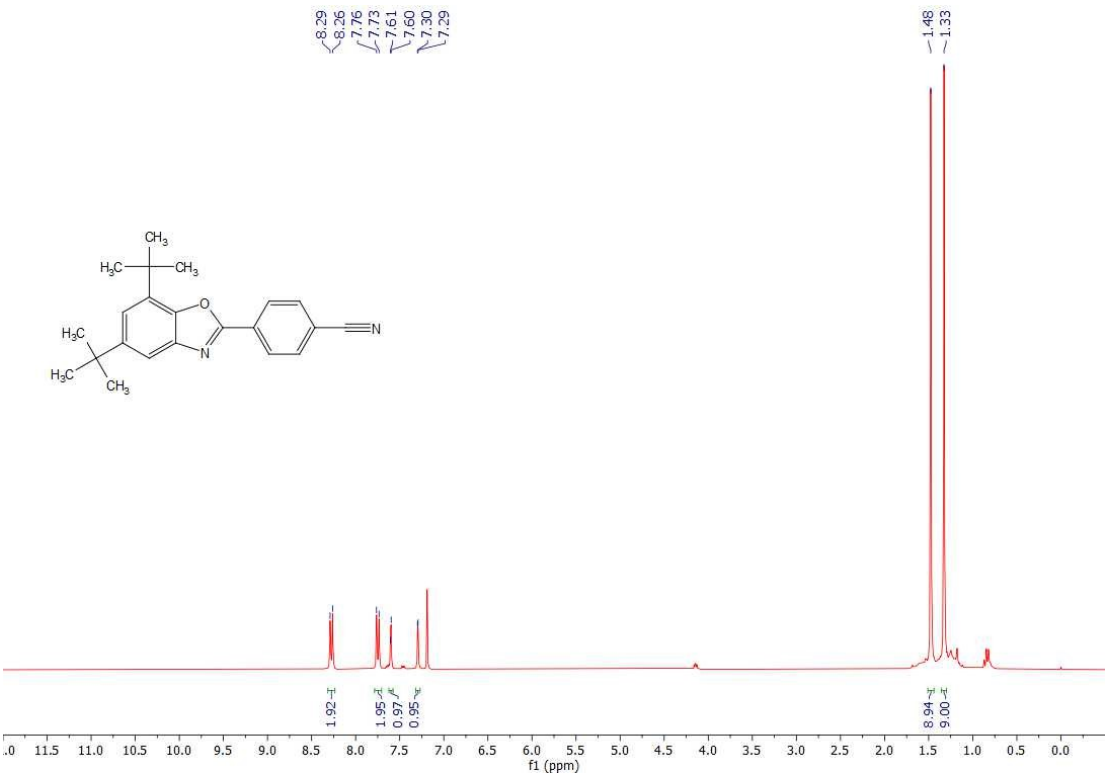

Figure S9. ^{1}H NMR spectrum of 4-(5,7-di-*tert*-butylbenzo[*d*]oxazol-2-yl)benzonitrile (4e) in $CDCl_3$ at 300 MHz.

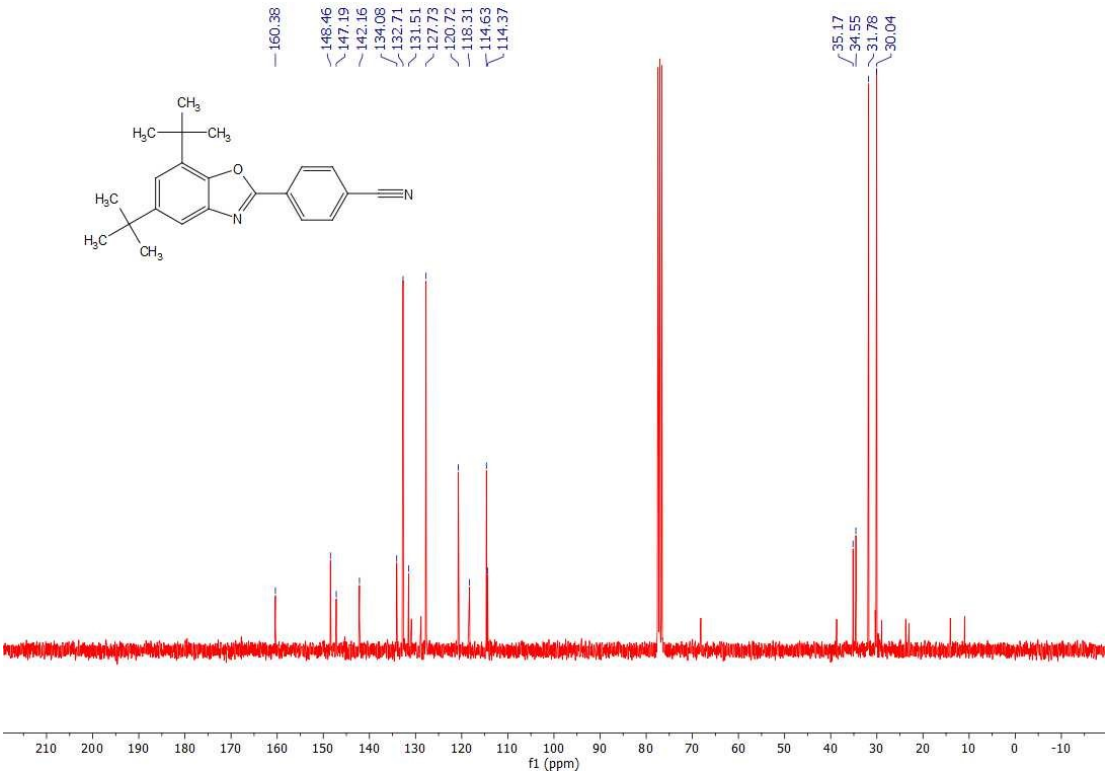

Figure S10. ^{13}C NMR spectrum of 4-(5,7-di-*tert*-butylbenzo[*d*]oxazol-2-yl)benzonitrile (4e) in $CDCl_3$ at 75 MHz.

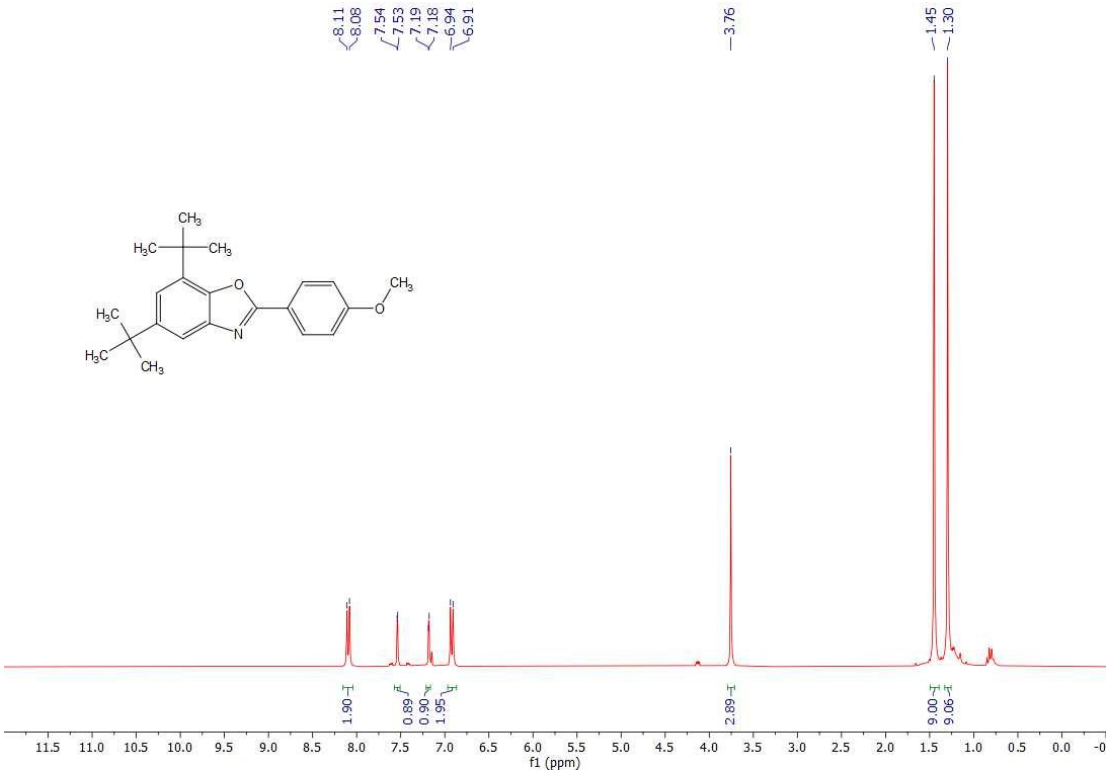

Figure S11. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(4-methoxyphenyl)benzo[*d*]oxazole (4f) in $CDCl_3$ at 300 MHz.

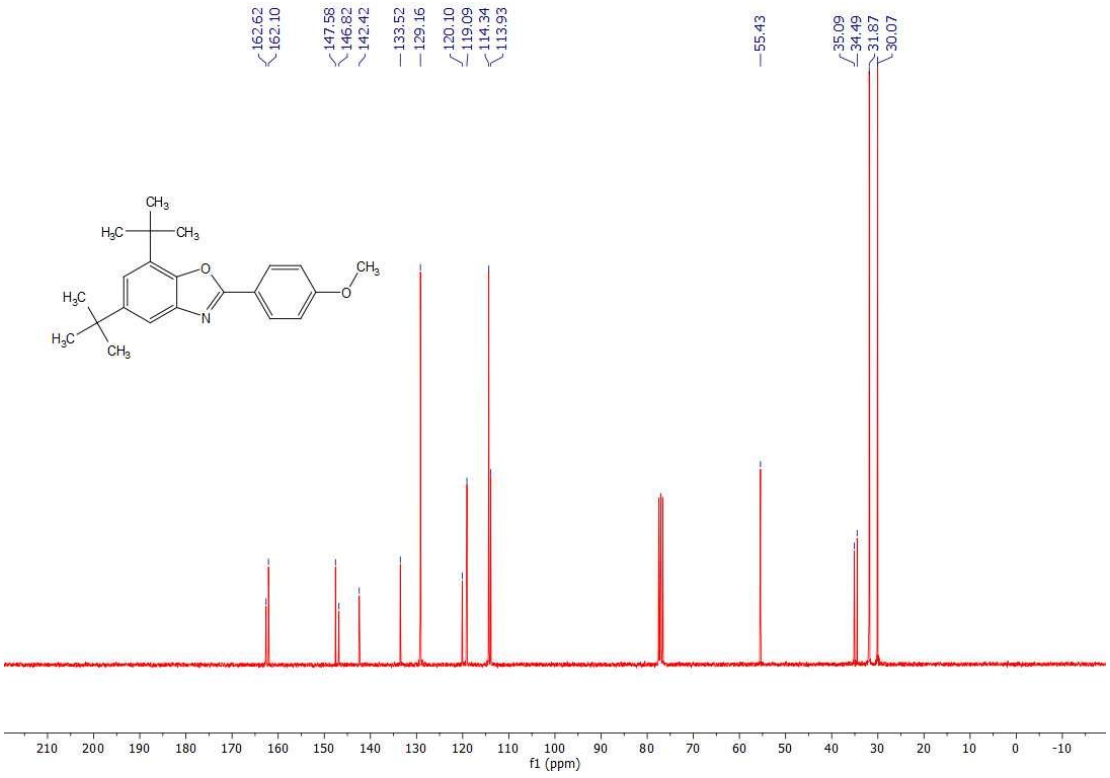

Figure S12. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(4-methoxyphenyl)benzo[*d*]oxazole (4f) in $CDCl_3$ at 75 MHz.

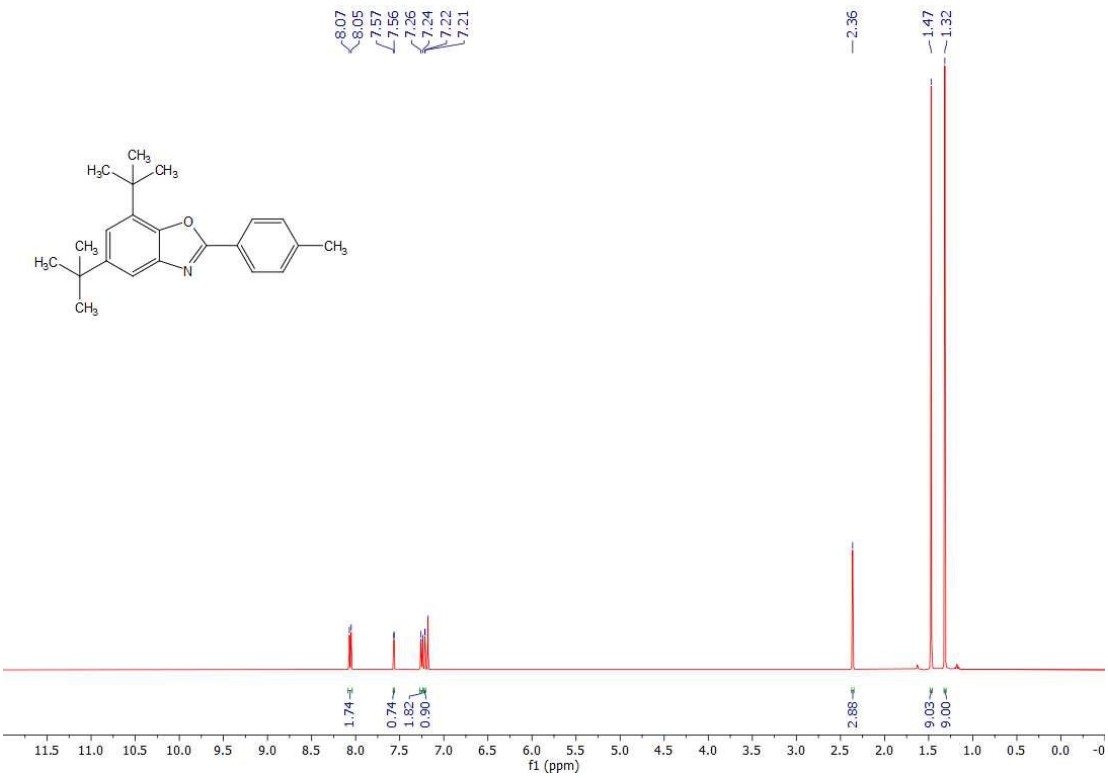

Figure S13. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(*p*-tolyl)benzo[*d*]oxazole (4g) in $CDCl_3$ at 400 MHz.

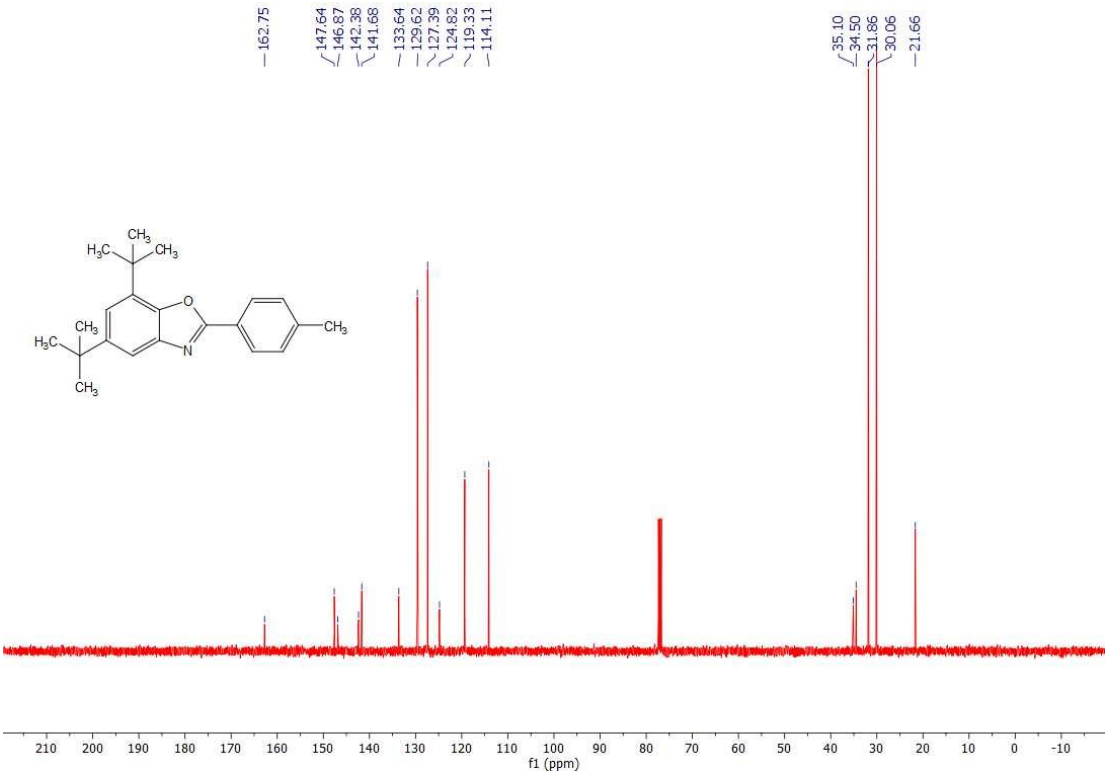

Figure S14. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(*p*-tolyl)benzo[*d*]oxazole (4g) in $CDCl_3$ at 100 MHz.

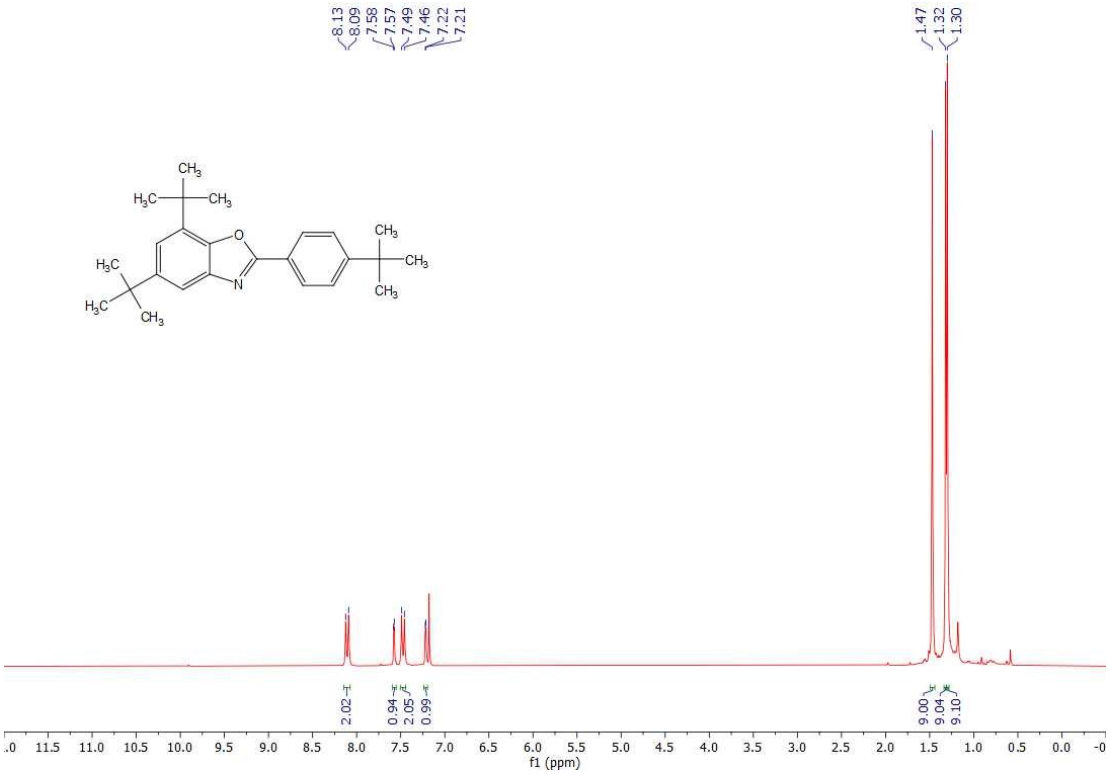

Figure S15. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(4-(*tert*-butyl)phenyl)benzo[*d*]oxazole (4h) in $CDCl_3$ at 250 MHz.

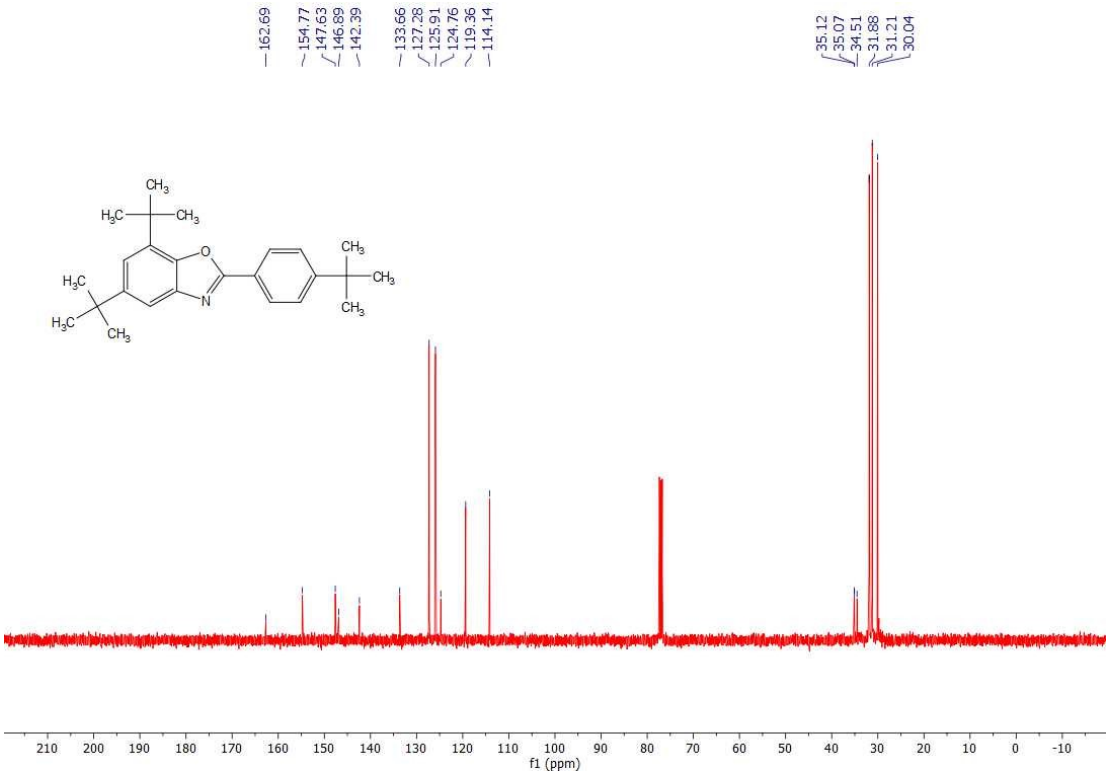

Figure S16. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(4-(*tert*-butyl)phenyl)benzo[*d*]oxazole (4h) in $CDCl_3$ at 100 MHz.

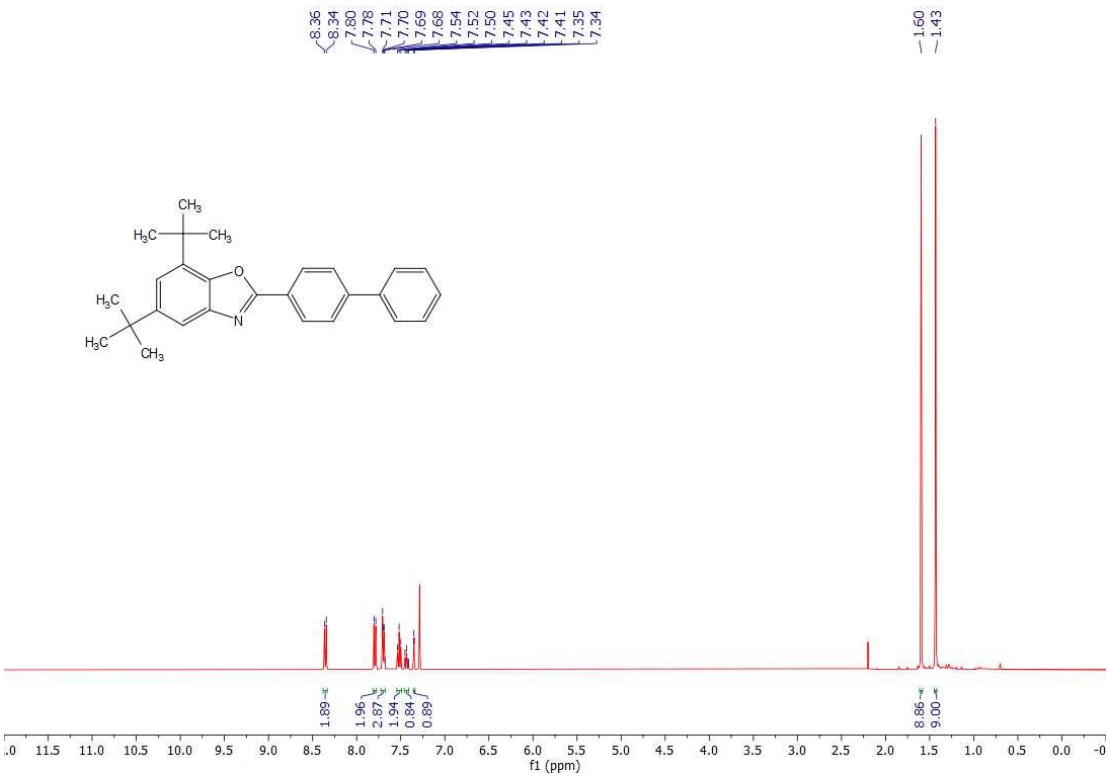

Figure S17. ^{1}H NMR spectrum of 2-([1,1'-biphenyl]-4-yl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4i) in $CDCl_3$ at 400 MHz.

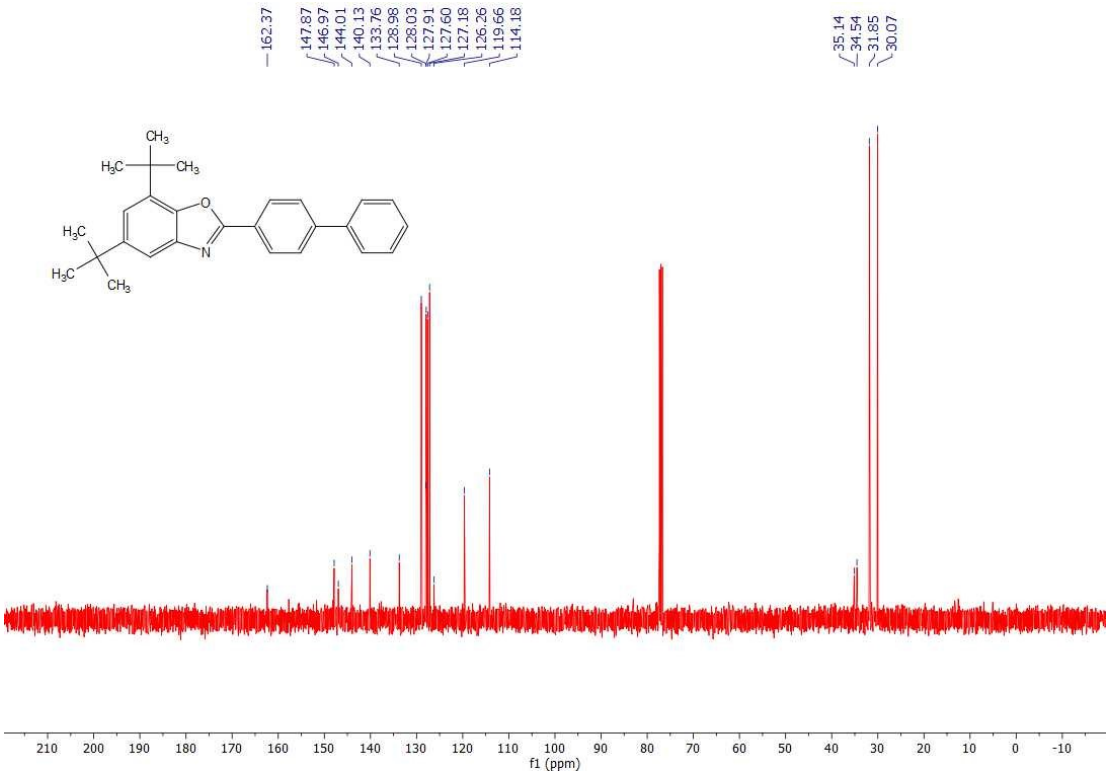

Figure S18. ^{13}C NMR spectrum of 2-([1,1'-biphenyl]-4-yl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4i) in $CDCl_3$ at 100 MHz.

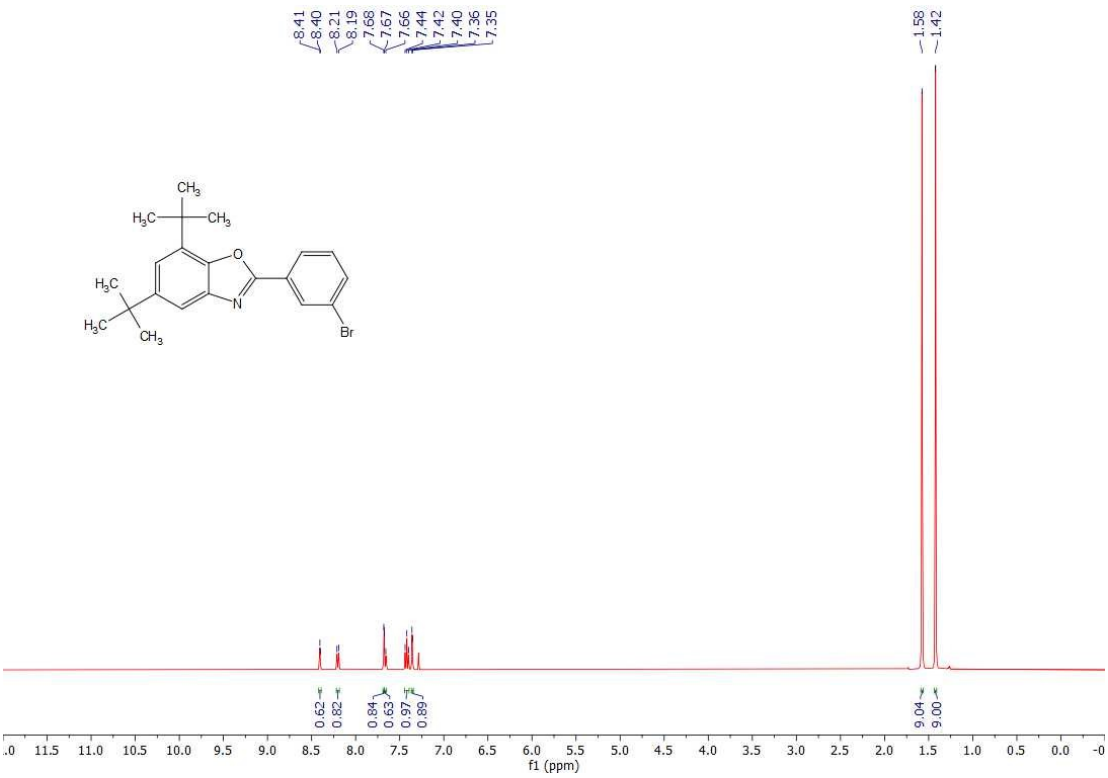

Figure S19. ^{1}H NMR spectrum of 2-(3-bromophenyl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4j) in $CDCl_3$ at 400 MHz.

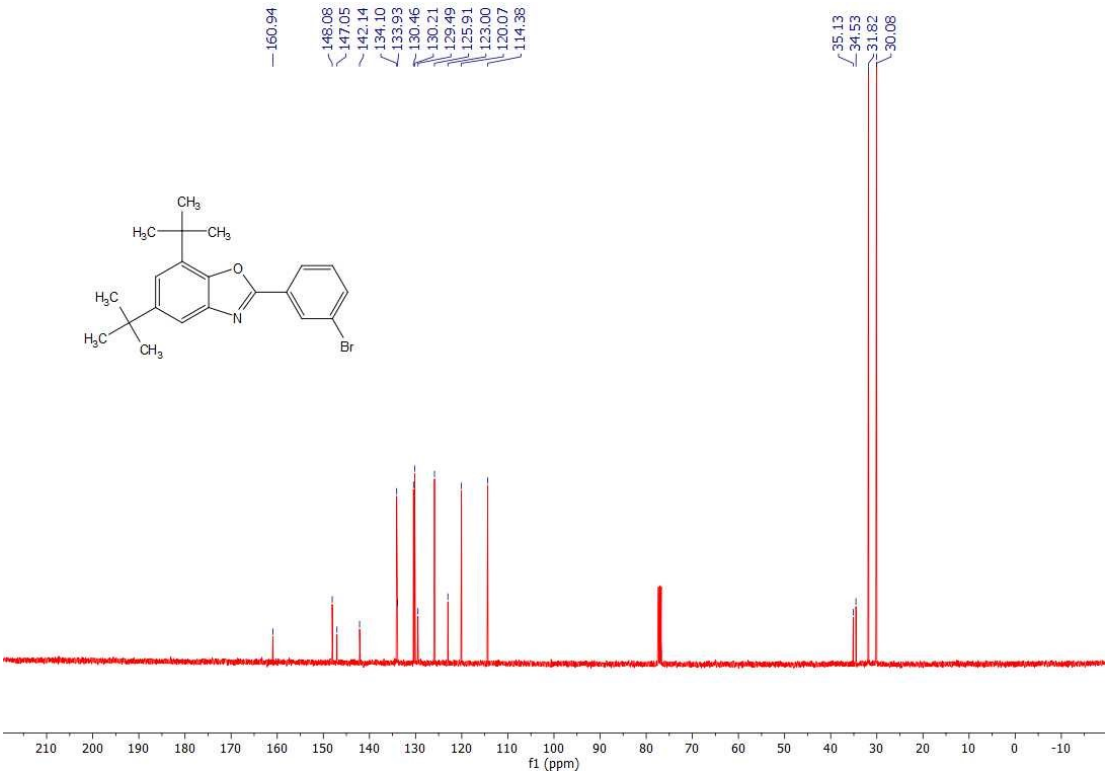

Figure S20. ^{13}C NMR spectrum of 2-(3-bromophenyl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4j) in $CDCl_3$ at 100 MHz.

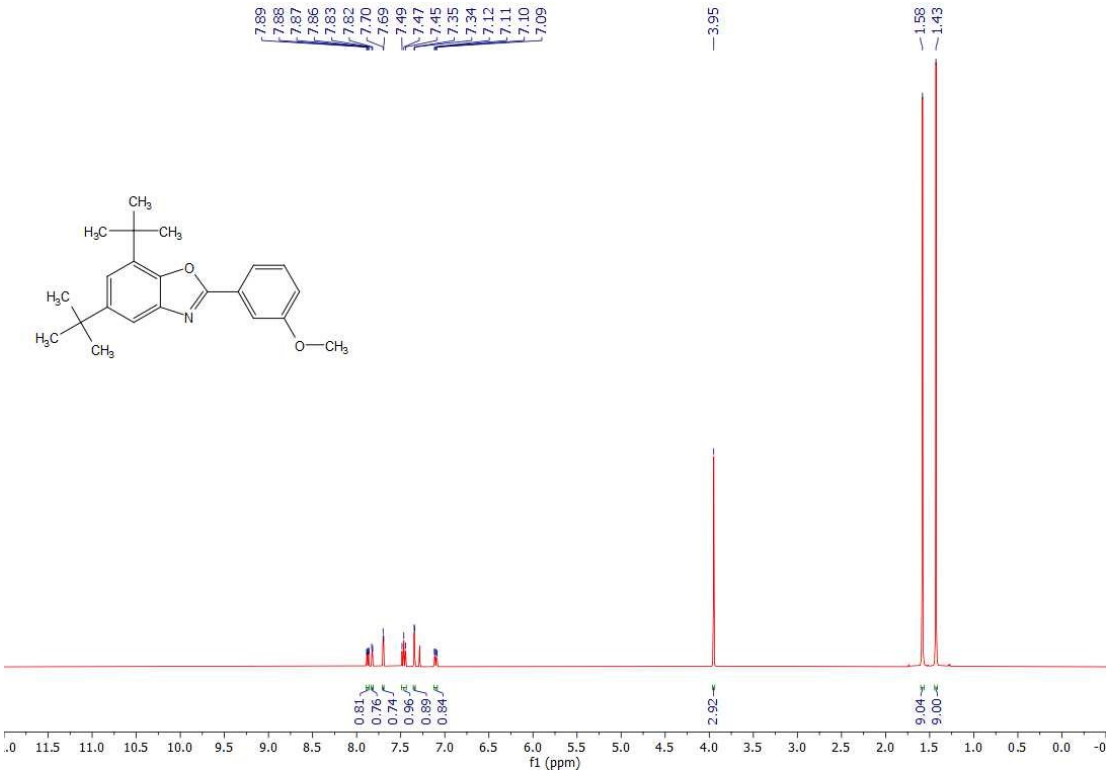

Figure S21. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(3-methoxyphenyl)benzo[*d*]oxazole (4k) in $CDCl_3$ at 400 MHz.

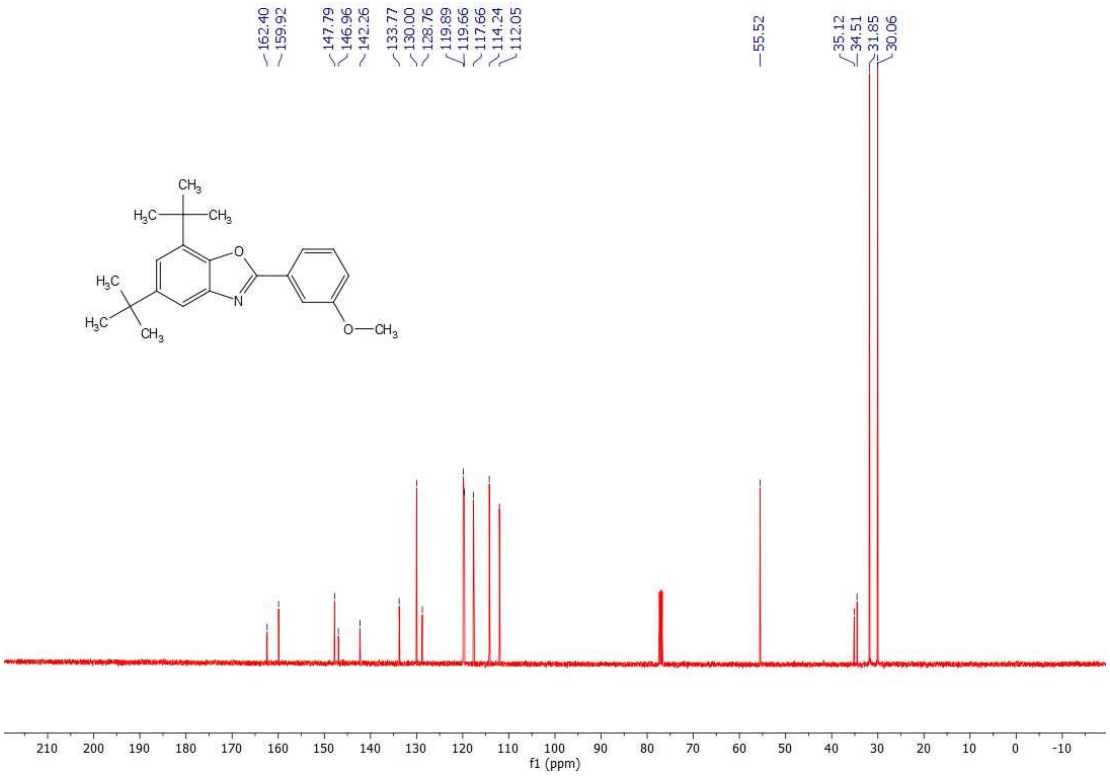

Figure S22. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(3-methoxyphenyl)benzo[*d*]oxazole (4k) in $CDCl_3$ at 100 MHz.

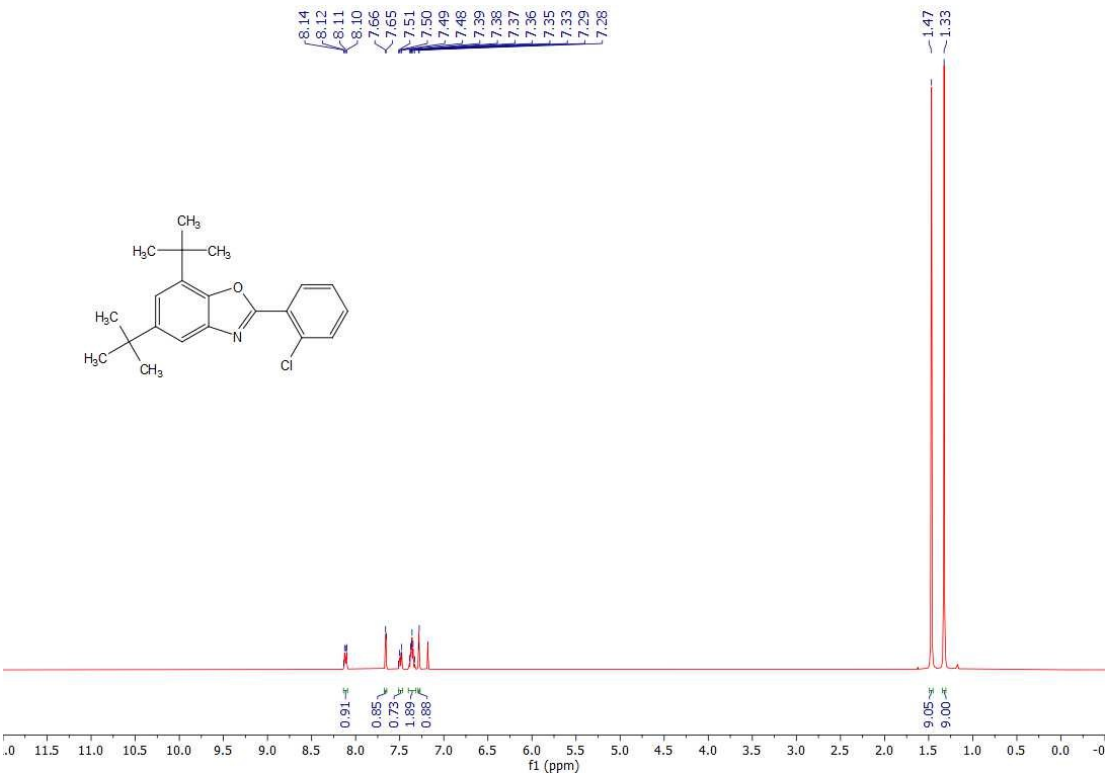

Figure S23. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(2-chlorophenyl)benzo[*d*]oxazole (4l) in $CDCl_3$ at 400 MHz.

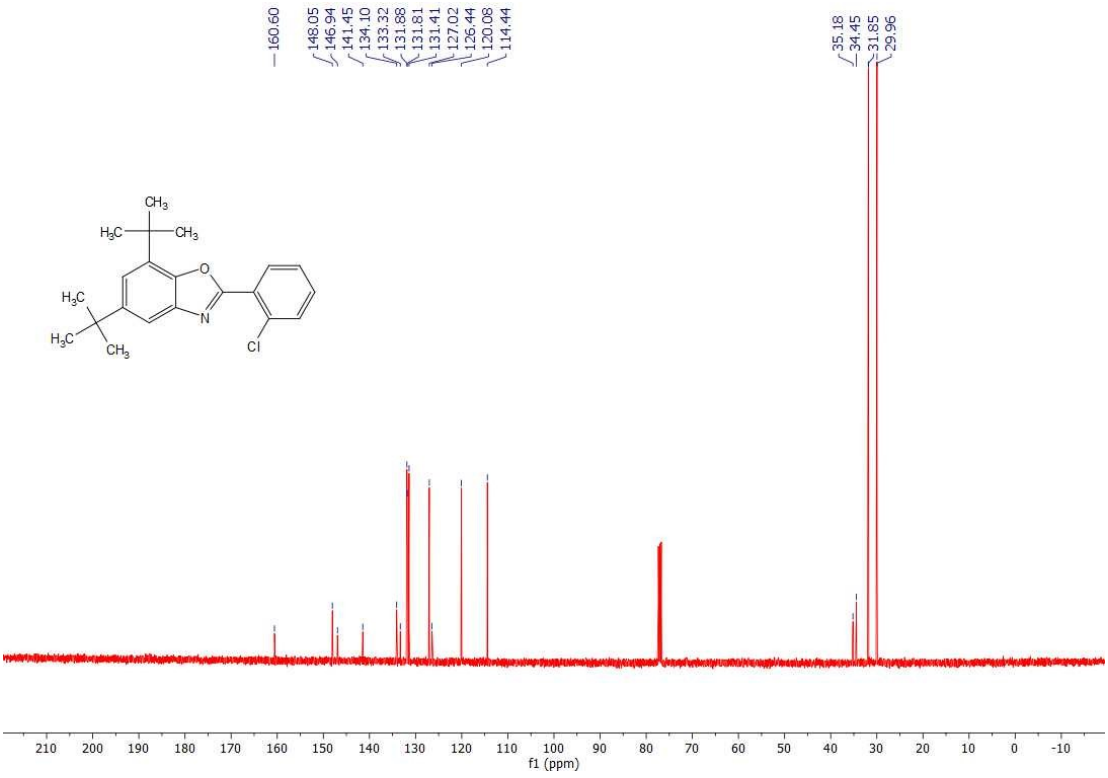

Figure S24. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(2-chlorophenyl)benzo[*d*]oxazole (4l) in $CDCl_3$ at 100 MHz.

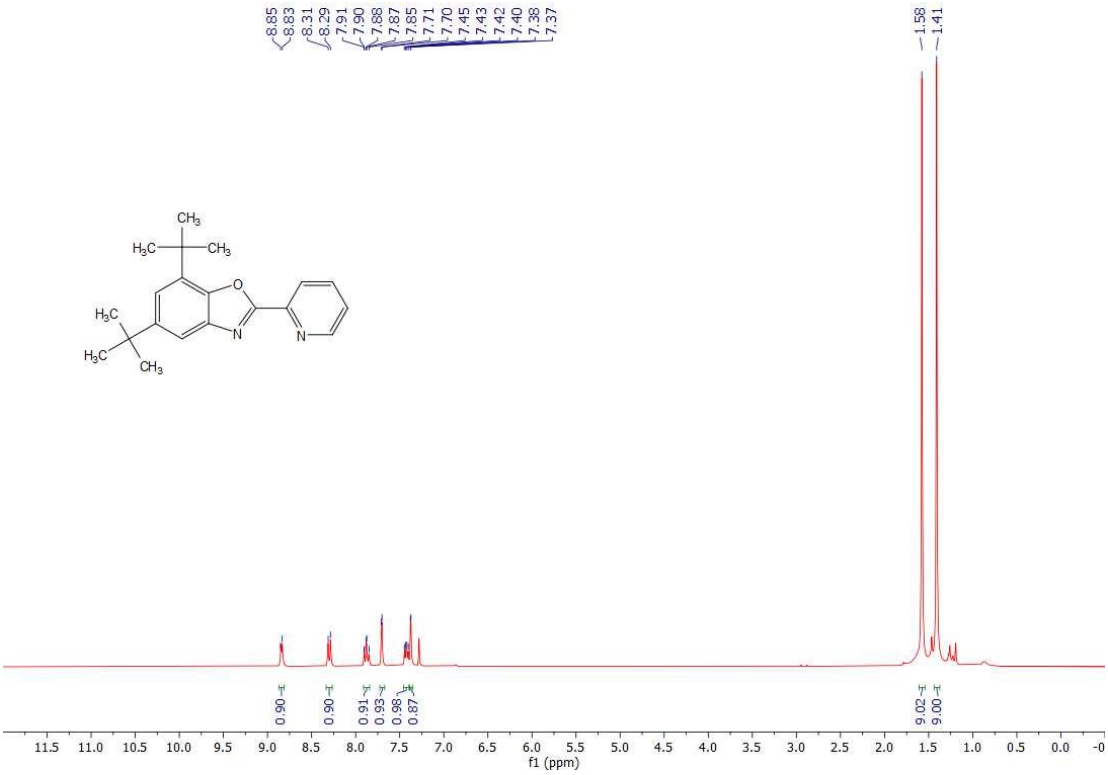

Figure S25. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(pyridin-2-yl)benzo[*d*]oxazole (4m) $CDCl_3$ at 300 MHz.

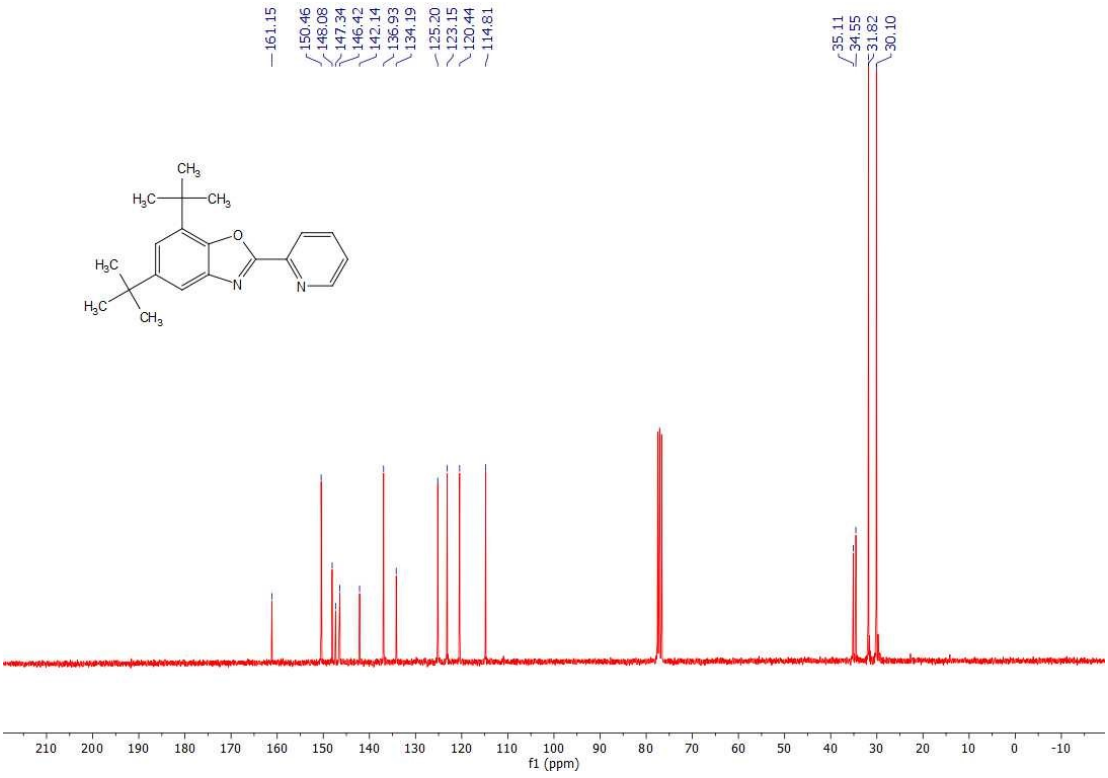

Figure S26. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(pyridin-2-yl)benzo[*d*]oxazole (4m) in $CDCl_3$ at 75 MHz.

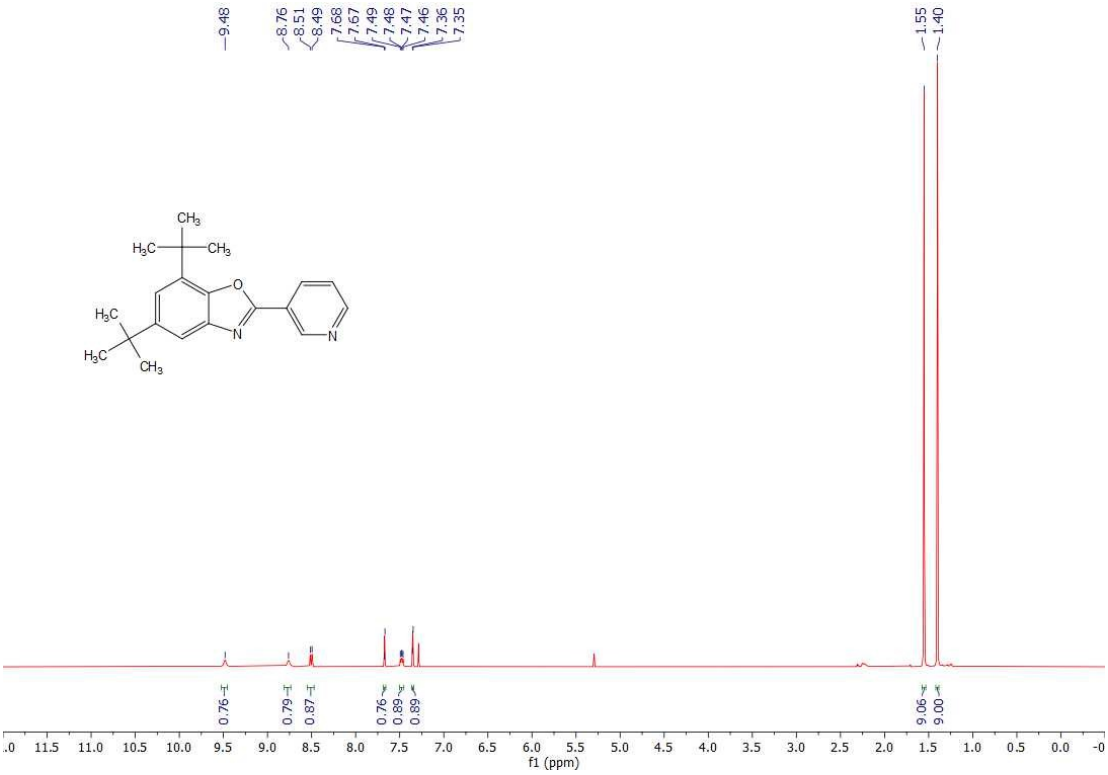

Figure S27. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(pyridin-3-yl)benzo[*d*]oxazole (4n) $CDCl_3$ at 400 MHz.

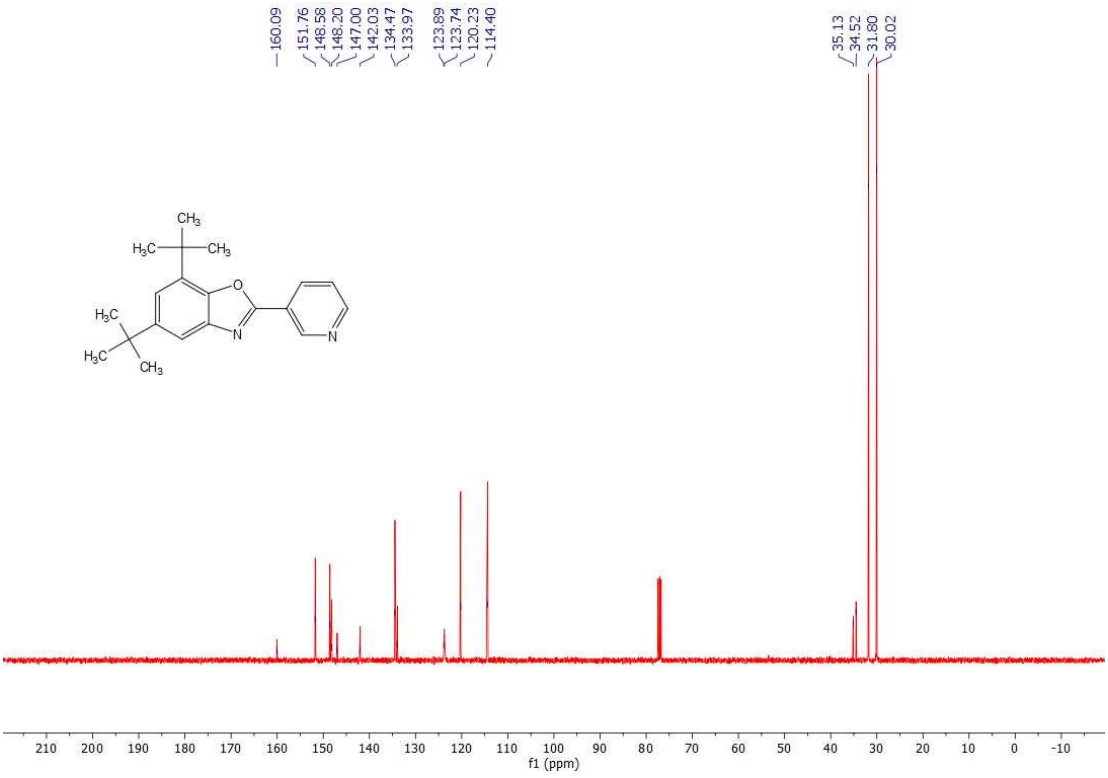

Figure S28. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(pyridin-3-yl)benzo[*d*]oxazole (4n) in $CDCl_3$ at 100 MHz.

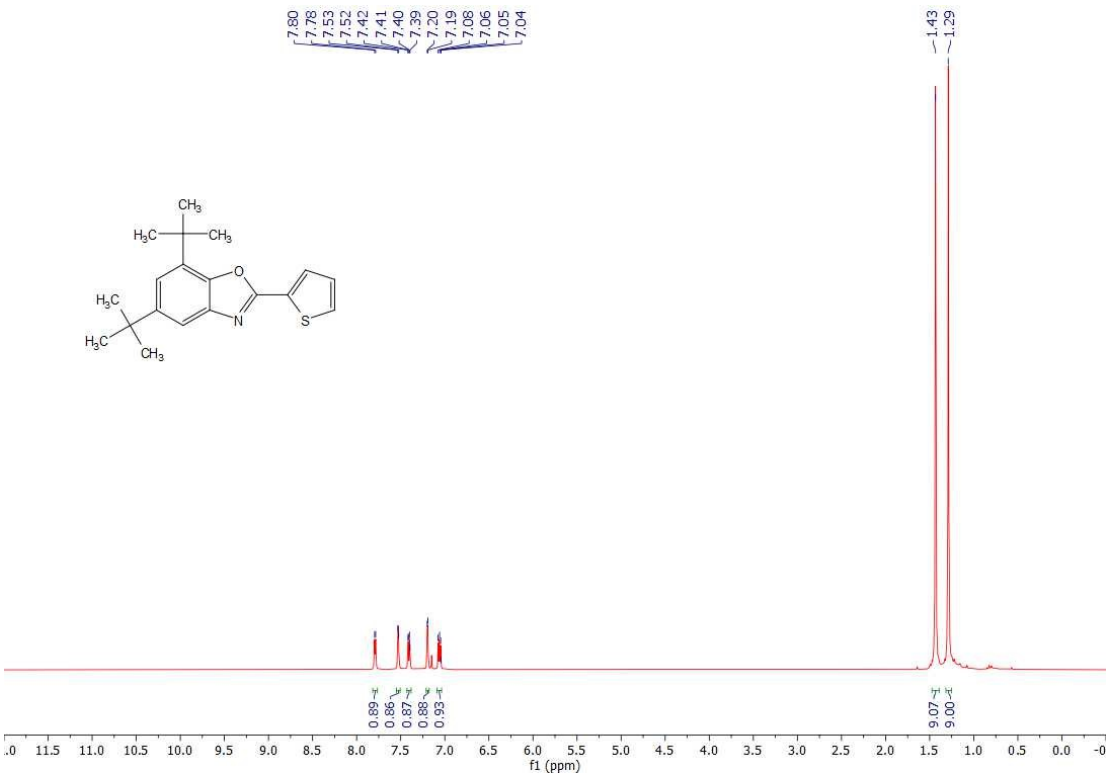

Figure S29. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(thiophen-2-yl)benzo[*d*]oxazole (4o) in $CDCl_3$ at 300 MHz.

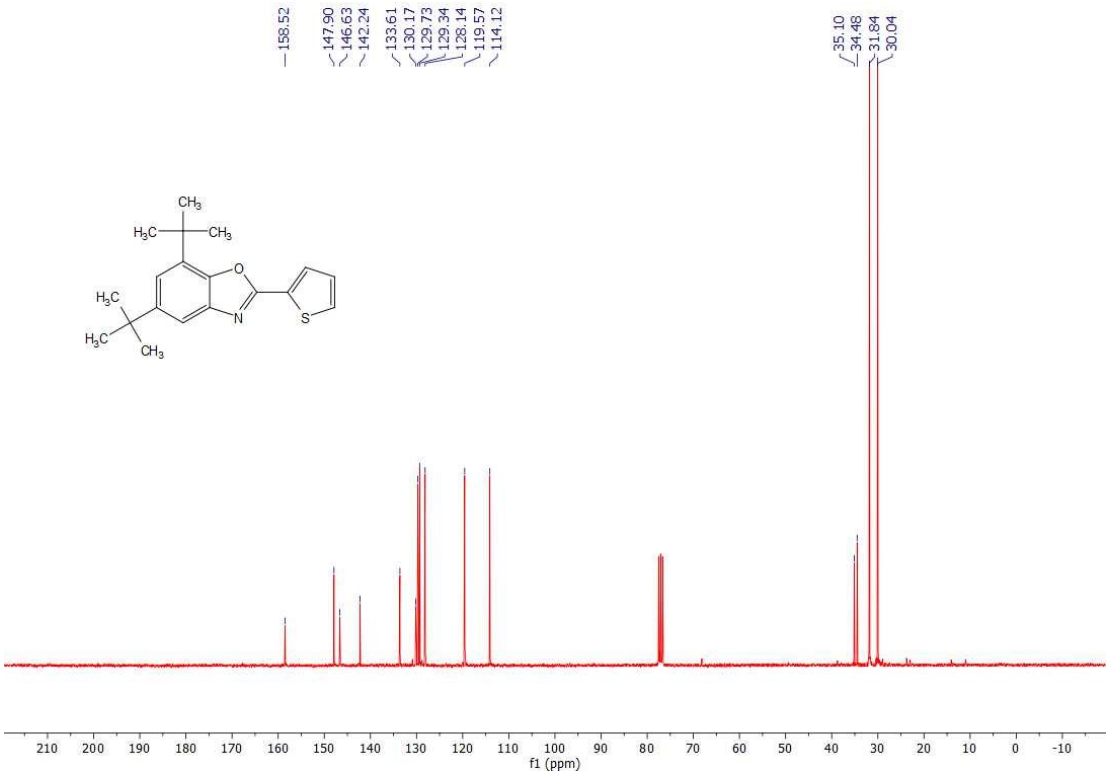

Figure S30. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(thiophen-2-yl)benzo[*d*]oxazole (4o) in $CDCl_3$ at 75 MHz.

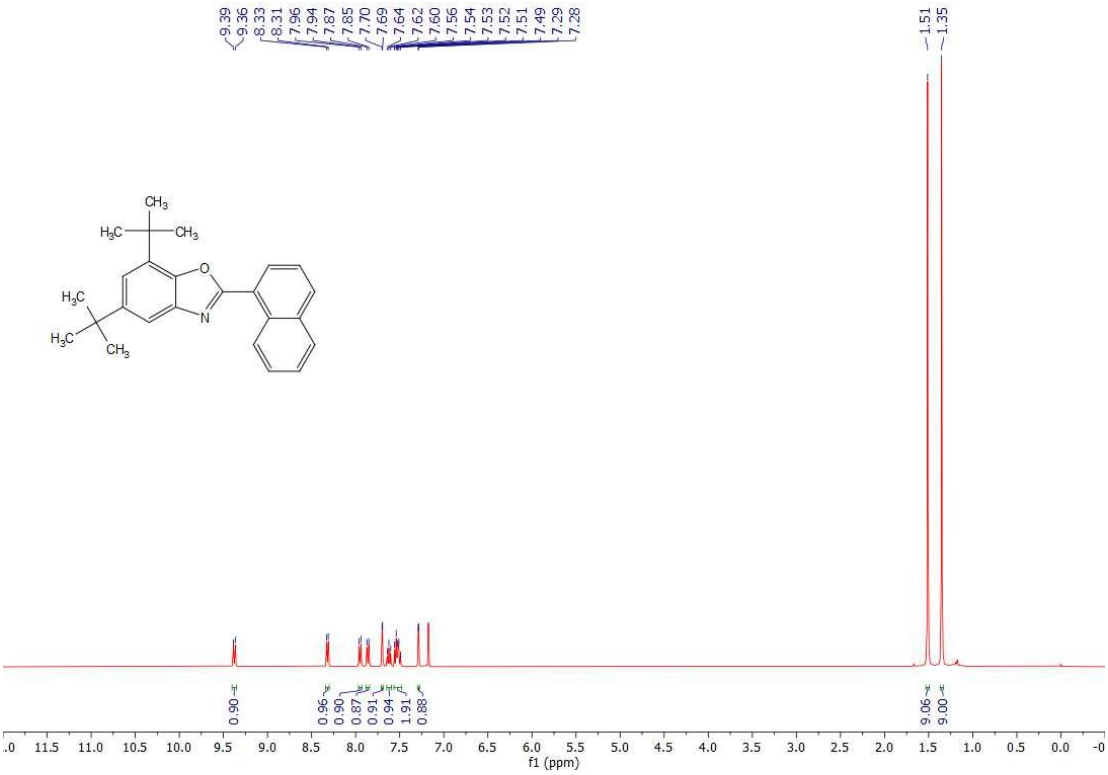

Figure S31. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(naphthalen-1-yl)benzo[*d*]oxazole (4p) $CDCl_3$ at 400 MHz.

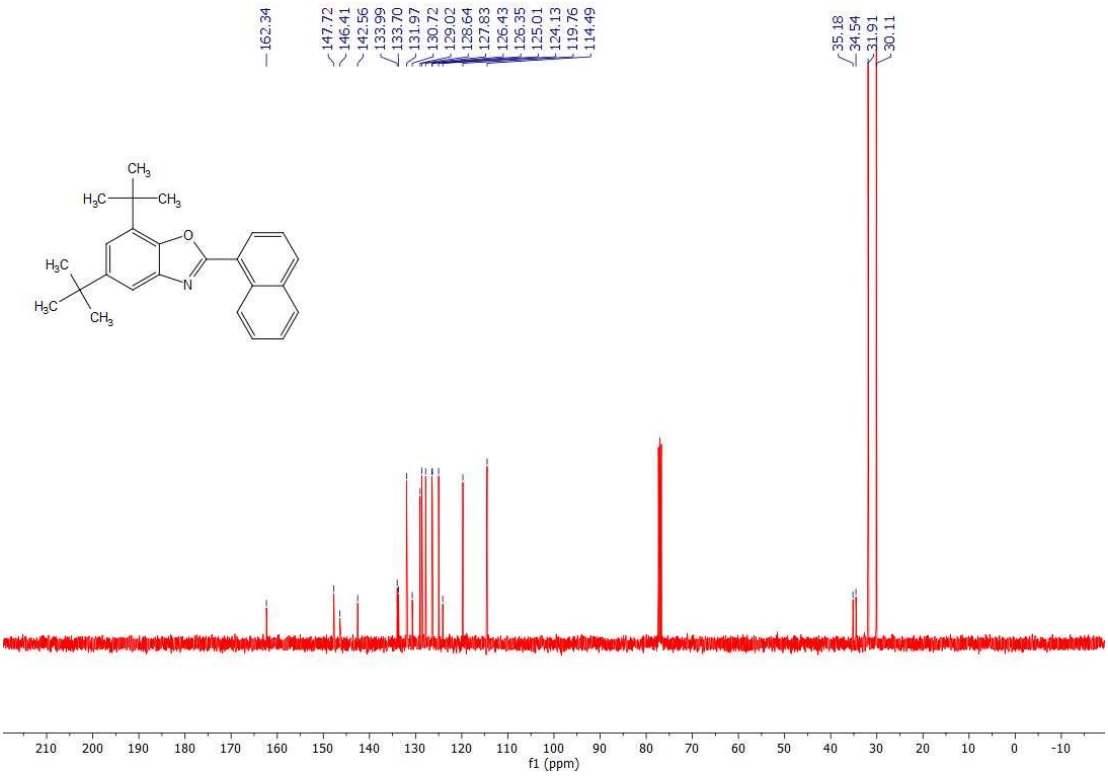

Figure S32. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(naphthalen-1-yl)benzo[*d*]oxazole (4p) in $CDCl_3$ at 100 MHz.

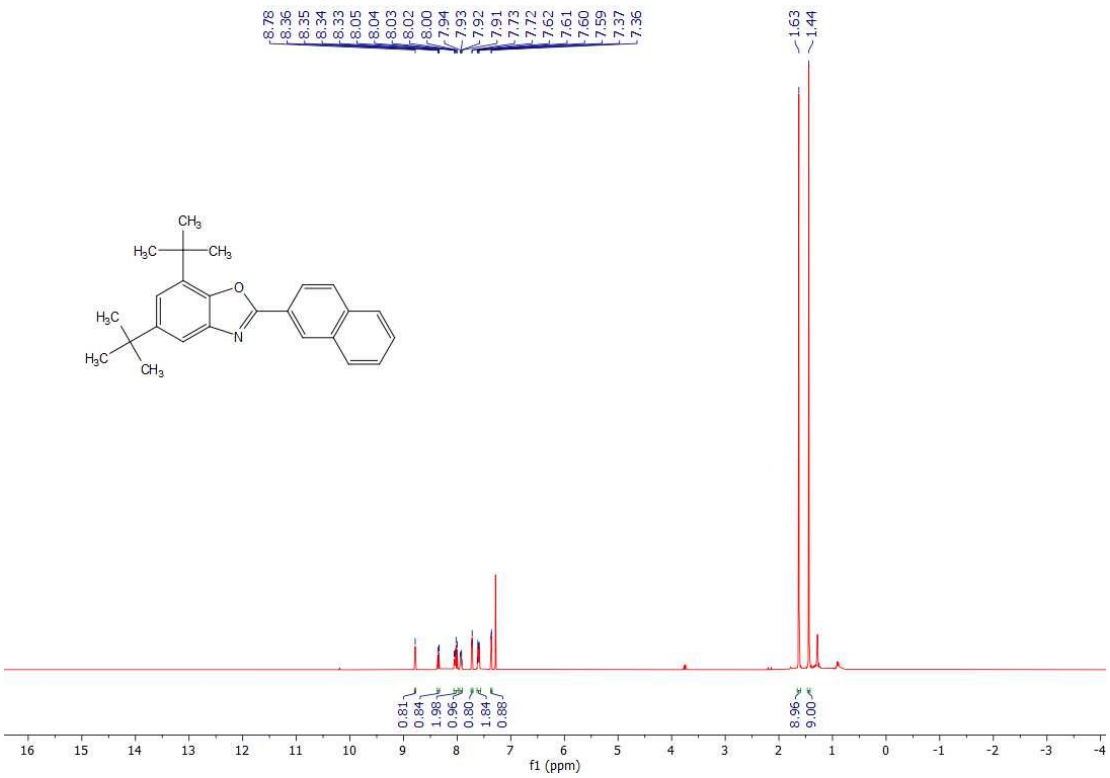

Figure S33. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(naphthalen-2-yl)benzo[*d*]oxazole (4q) in $CDCl_3$ at 400 MHz.

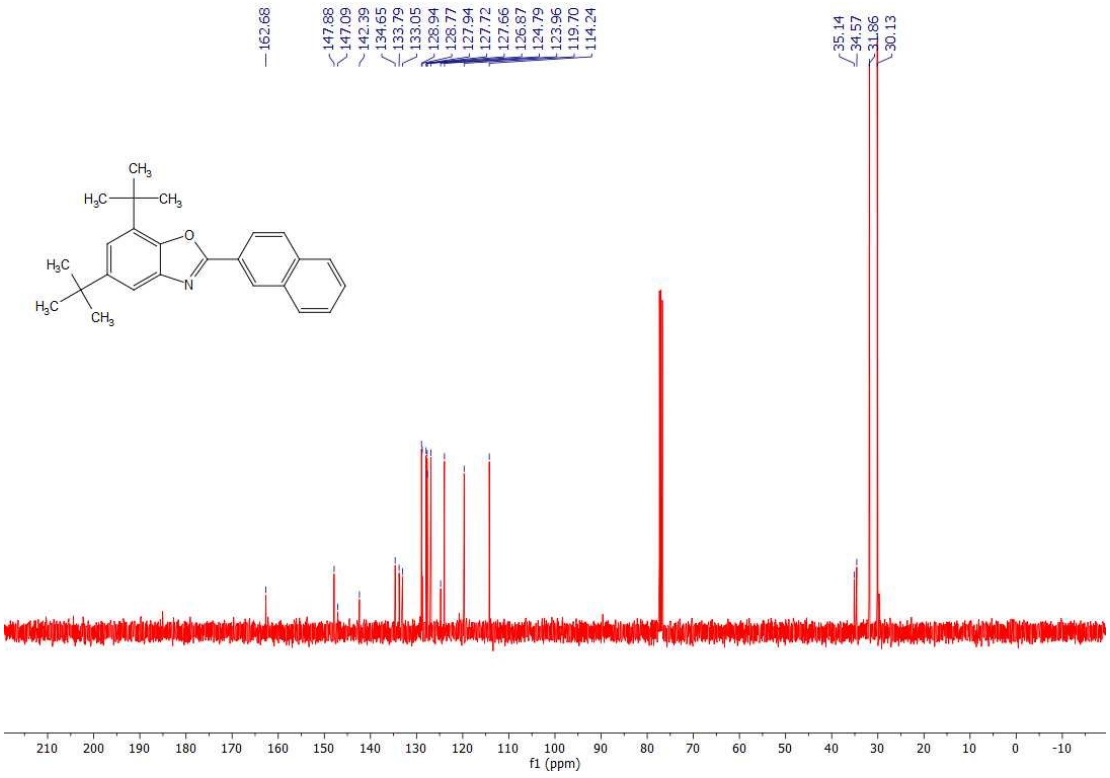

Figure S34. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(naphthalen-2-yl)benzo[*d*]oxazole (4q) in $CDCl_3$ at 100 MHz.

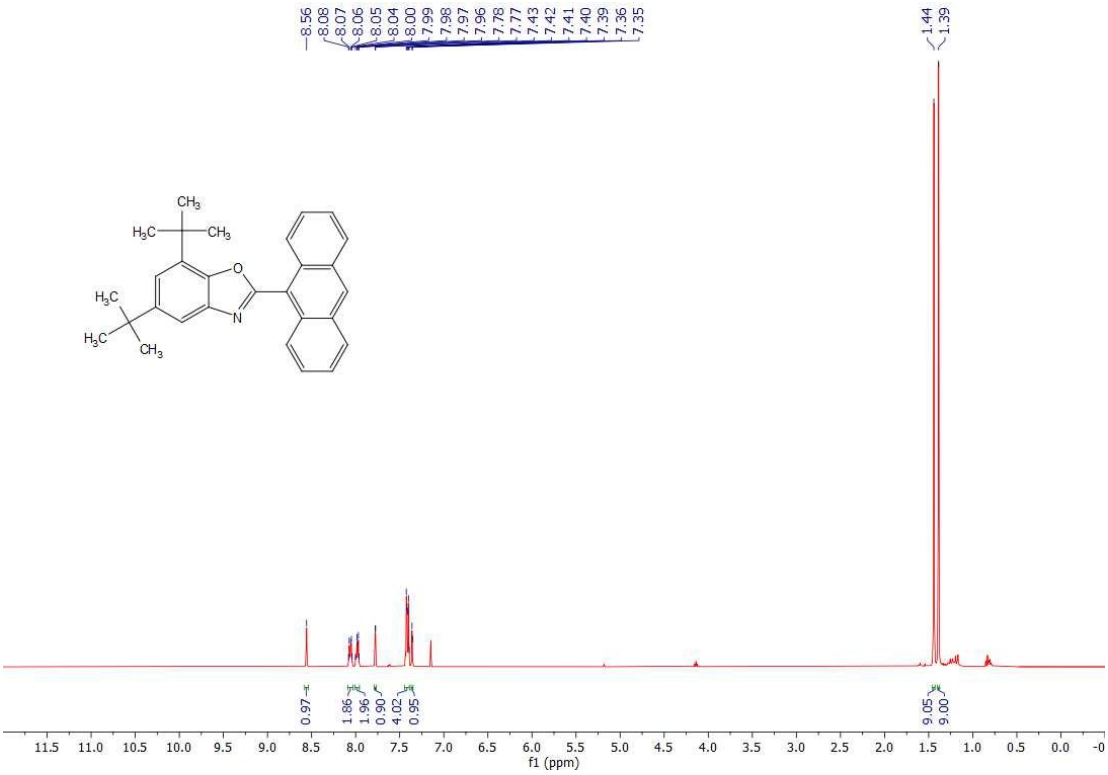

Figure S35. ^{1}H NMR spectrum of 2-(anthracen-9-yl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4r) in $CDCl_3$ at 400 MHz.

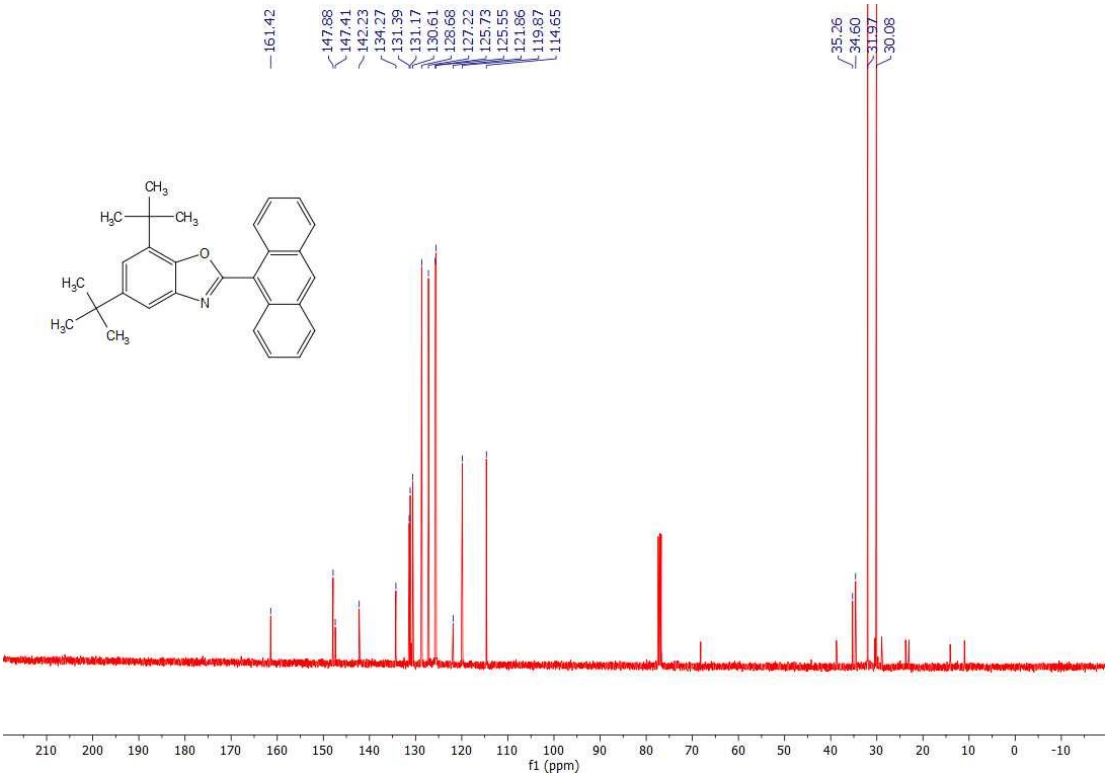

Figure S36. ^{13}C NMR spectrum of 2-(anthracen-9-yl)-5,7-di-*tert*-butylbenzo[*d*]oxazole (4r) in $CDCl_3$ at 100 MHz.

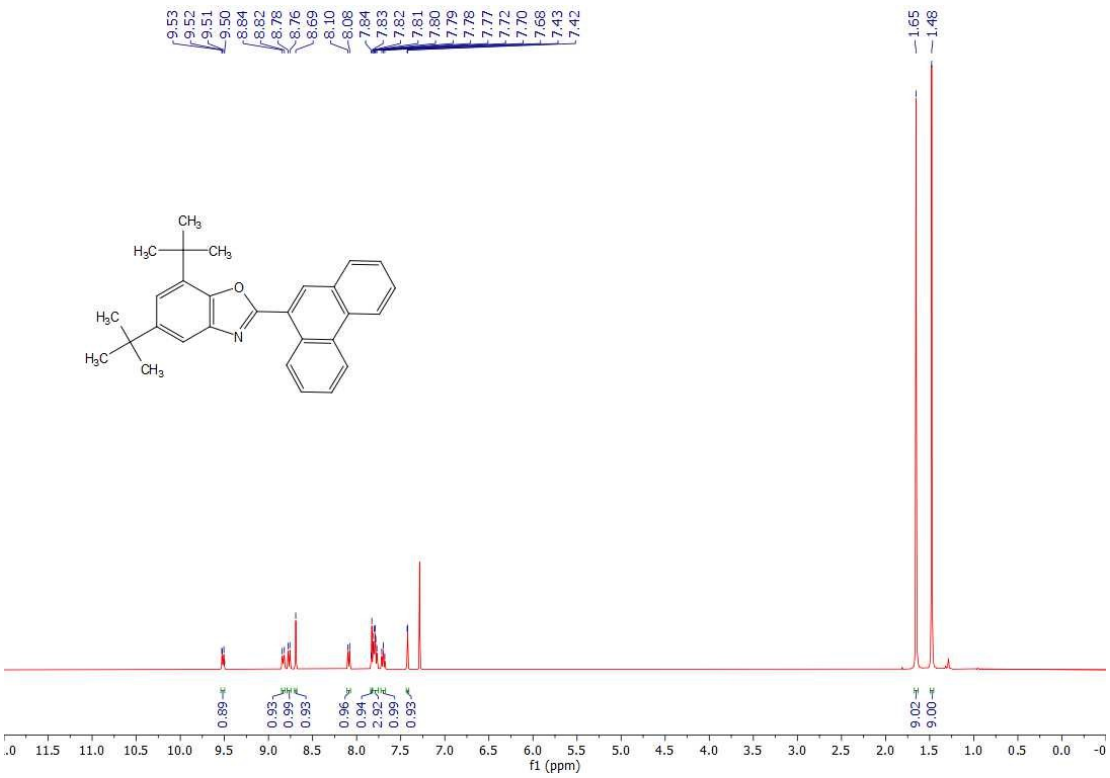

Figure S37. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(phenanthren-9-yl)benzo[*d*]oxazole (4s) in $CDCl_3$ at 400 MHz.

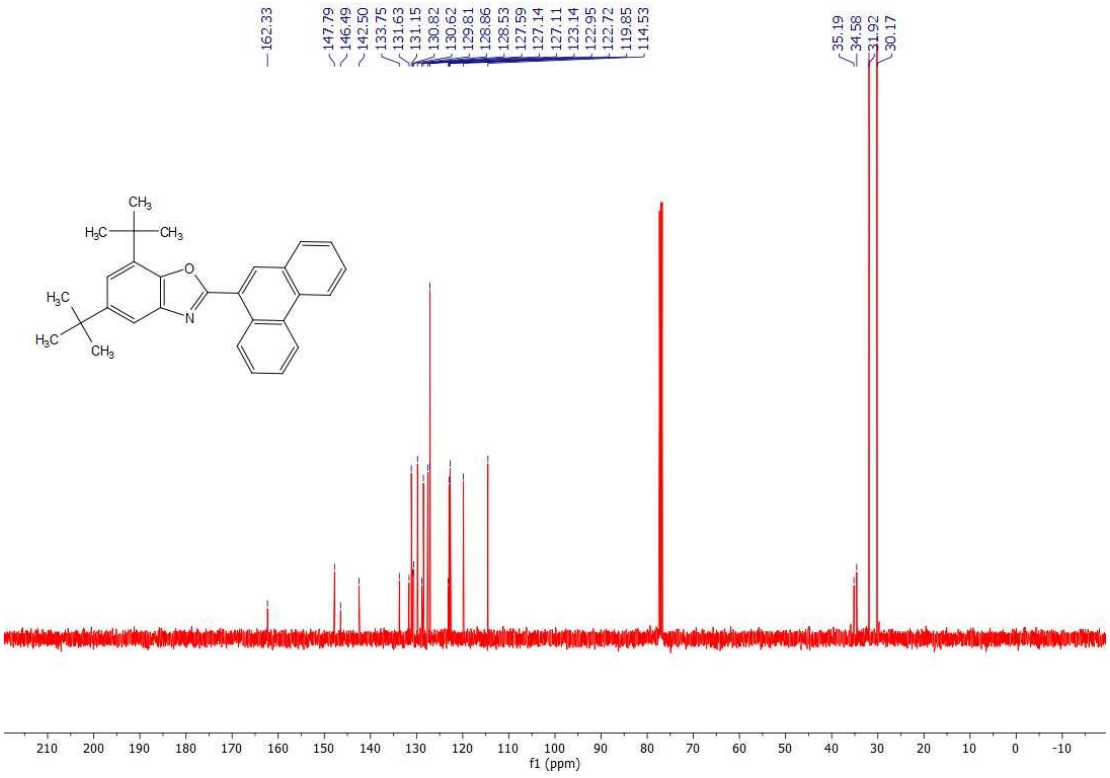

Figure S38. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(phenanthren-9-yl)benzo[*d*]oxazole (4s) in $CDCl_3$ at 100 MHz.

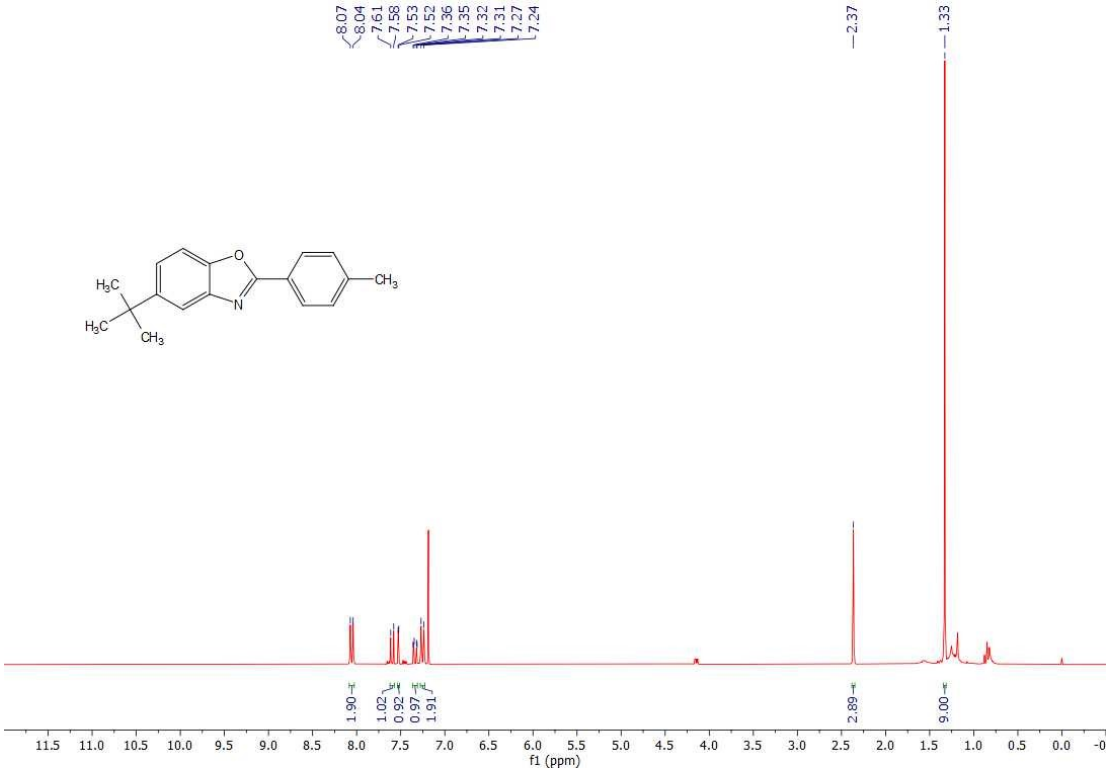

Figure S39. ^{1}H NMR spectrum of 5-(*tert*-butyl)-2-(*p*-tolyl)benzo[*d*]oxazole (4t) in $CDCl_3$ at 400 MHz.

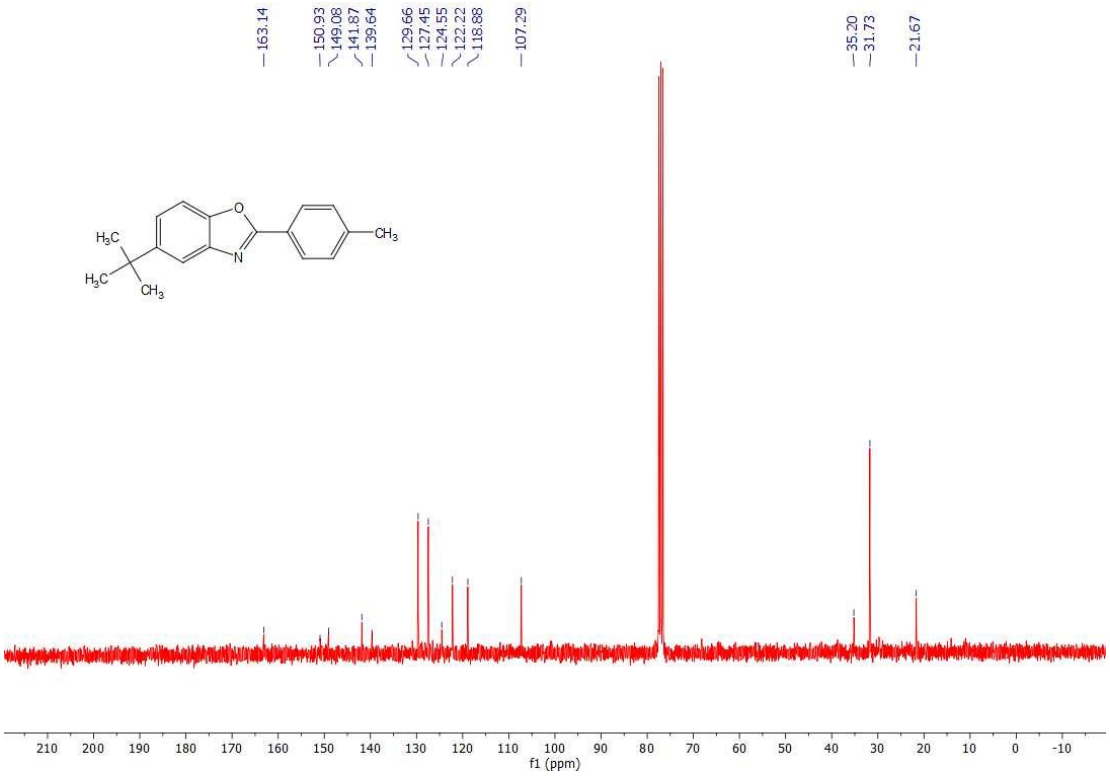

Figure S40. ^{13}C NMR spectrum of 5-(*tert*-butyl)-2-(*p*-tolyl)benzo[*d*]oxazole (4t) in $CDCl_3$ at 75 MHz.

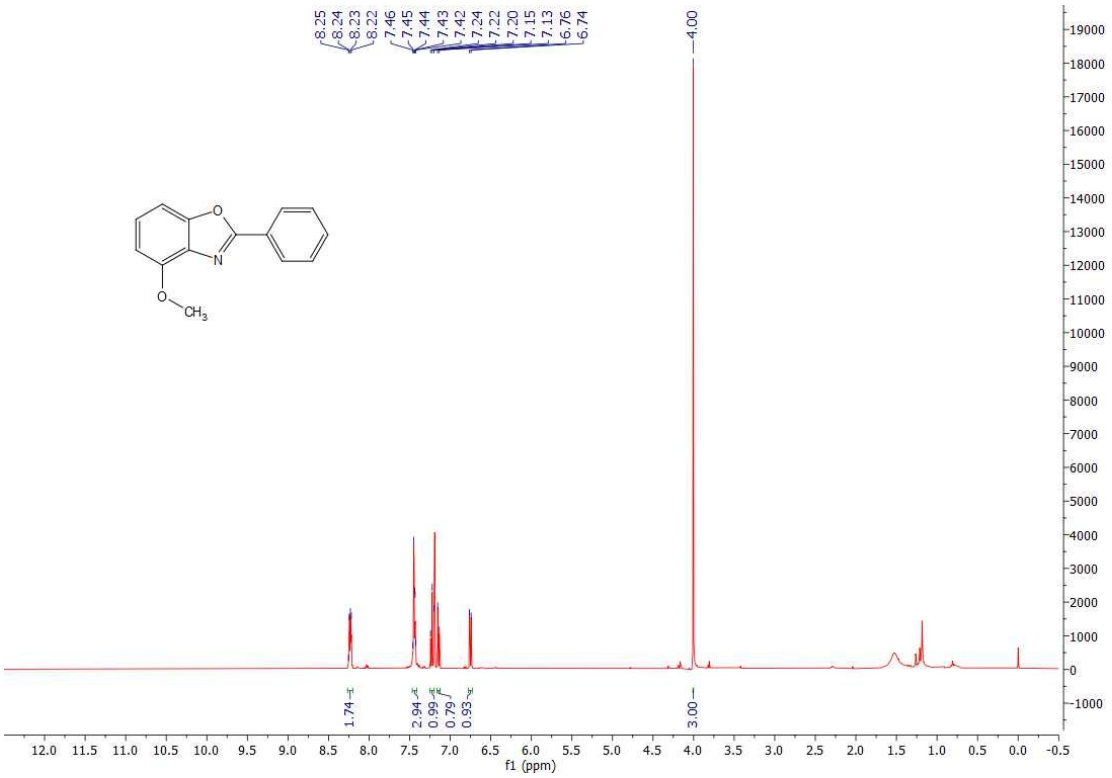

Figure S41. ^{1}H NMR spectrum of 4-methoxy-2-phenylbenzo[*d*]oxazole (4w) in $CDCl_3$ at 400 MHz.

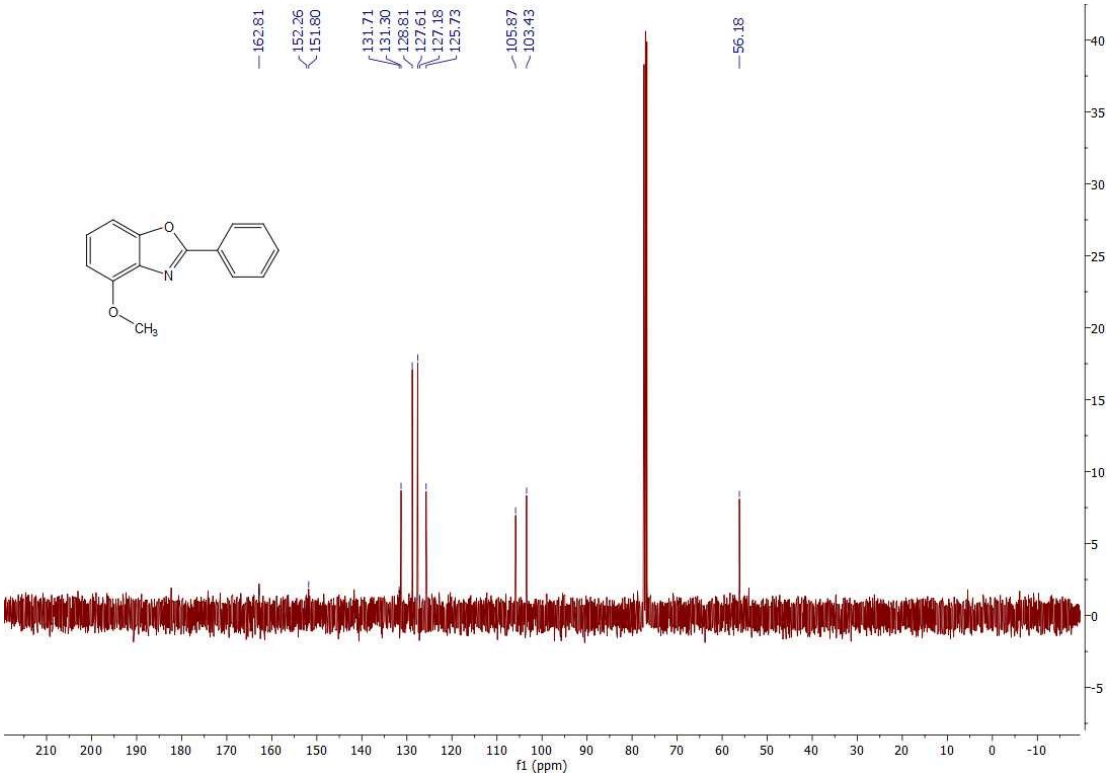

Figure S42. ^{13}C NMR spectrum of 4-methoxy-2-phenylbenzo[*d*]oxazole (4w) in $CDCl_3$ at 100 MHz.

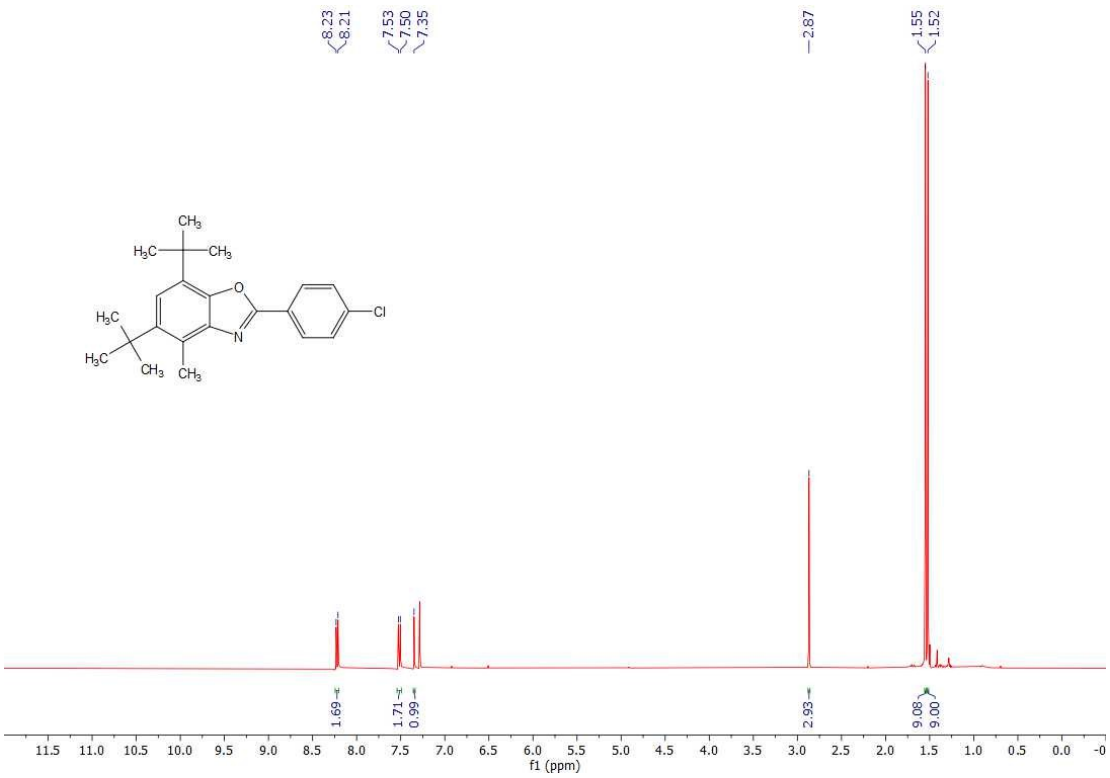

Figure S43. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(4-chlorophenyl)-4-methylbenzo[*d*]oxazole (4x) in $CDCl_3$ at 400 MHz.

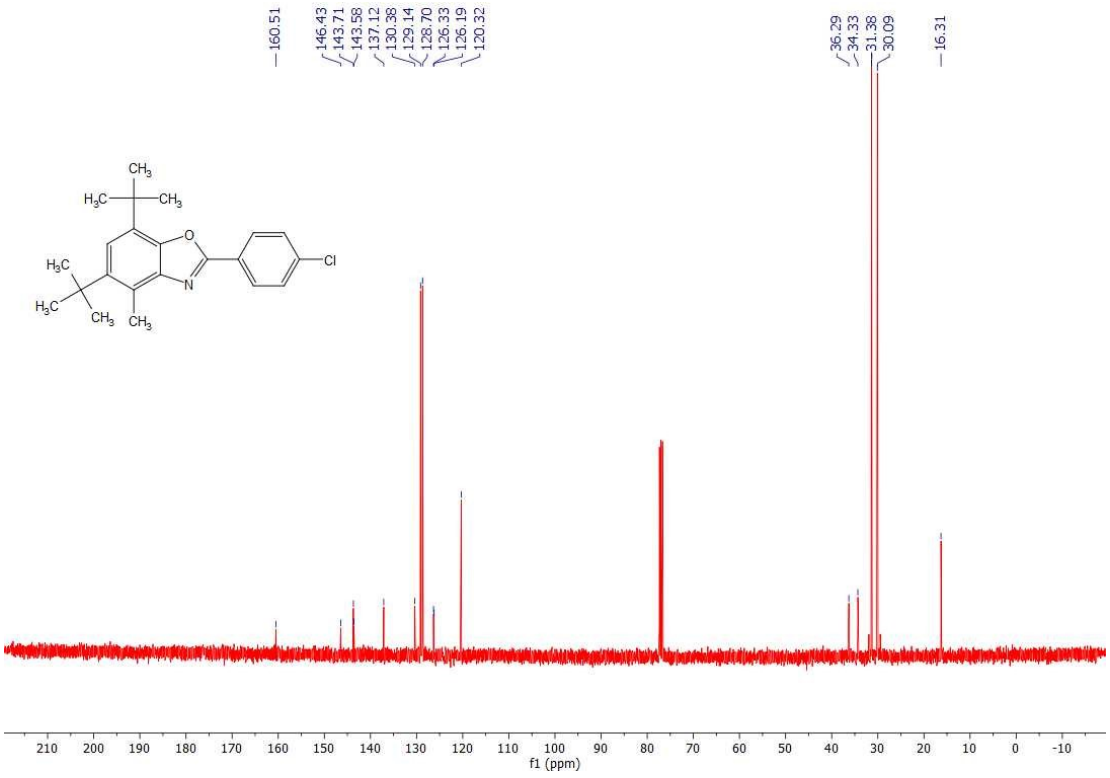

Figure S44. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(4-chlorophenyl)-4-methylbenzo[*d*]oxazole (4x) in $CDCl_3$ at 100 MHz.

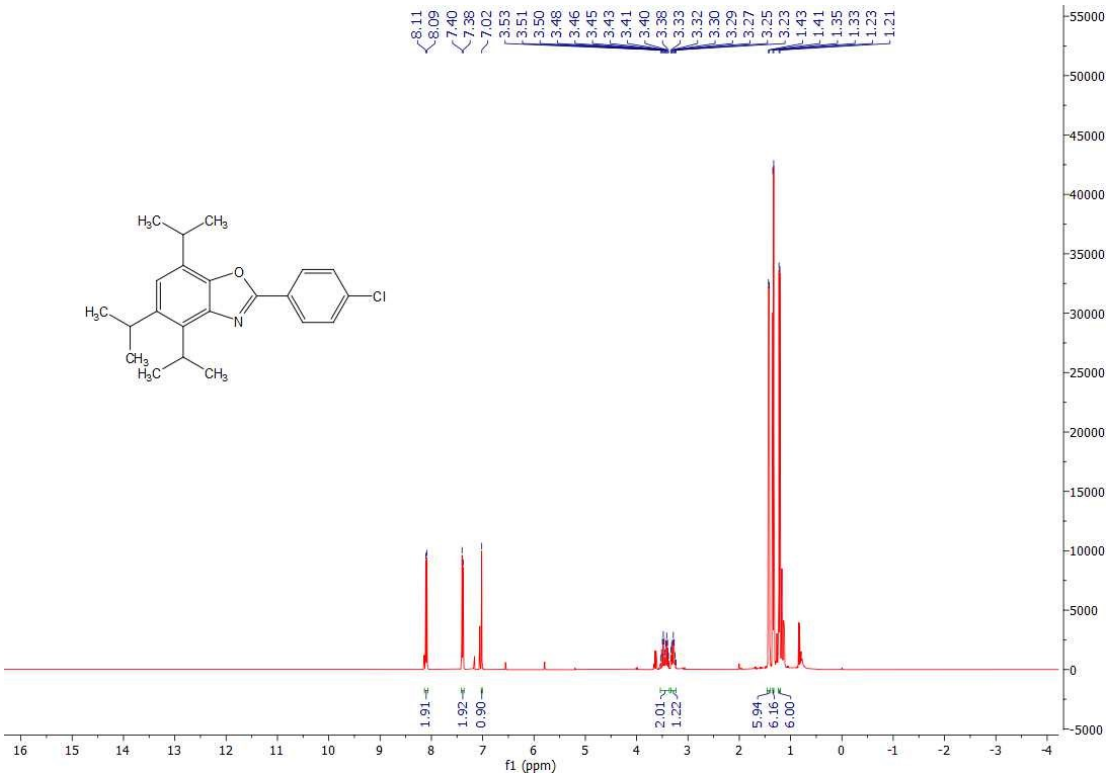

Figure S45. ^{1}H NMR spectrum of 2-(4-chlorophenyl)-4,5,7-triisopropylbenzo[*d*]oxazole (4z) in $CDCl_3$ at 400 MHz.

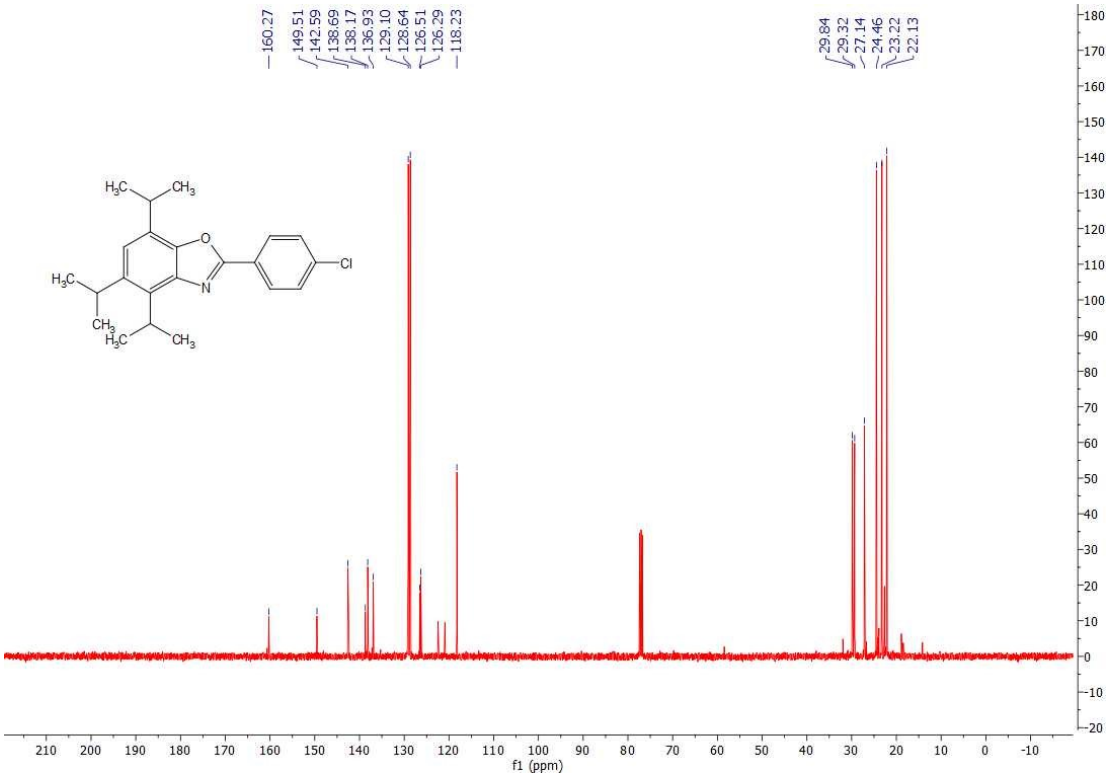

Figure S46. ^{13}C NMR spectrum of 2-(4-chlorophenyl)-4,5,7-triisopropylbenzo[*d*]oxazole (4z) in $CDCl_3$ at 100 MHz.

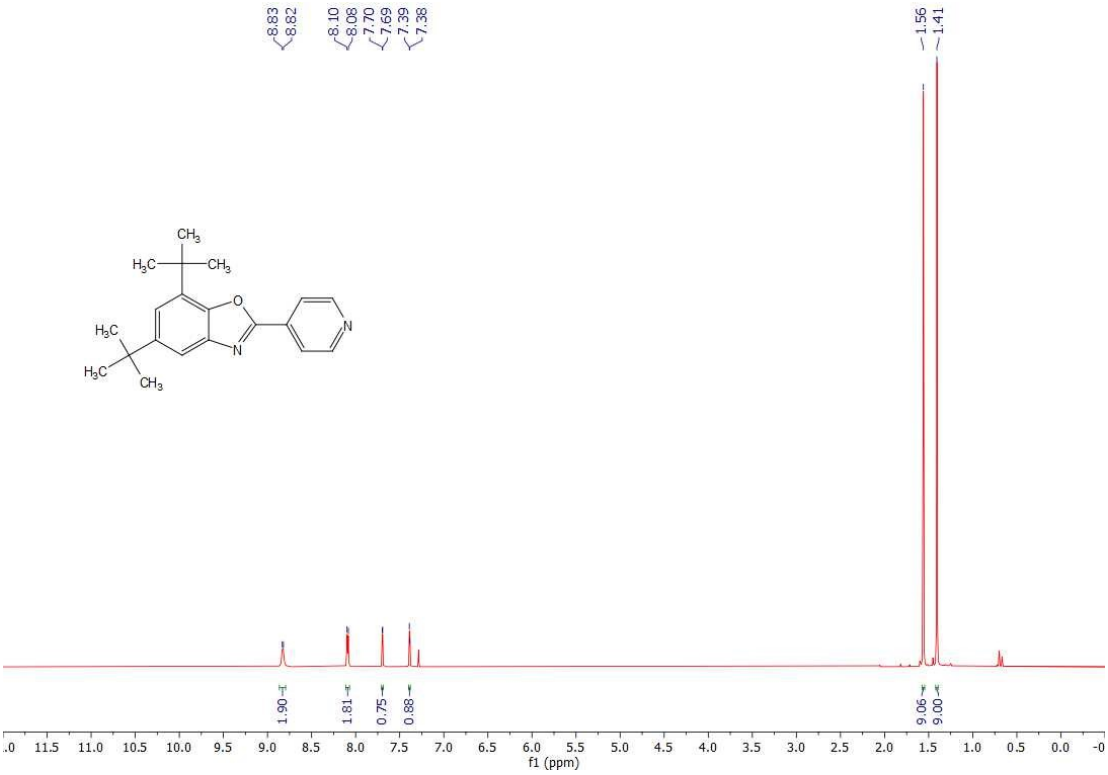

Figure S47. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(pyridin-4-yl)benzo[*d*]oxazole (4aa) in $CDCl_3$ at 400 MHz.

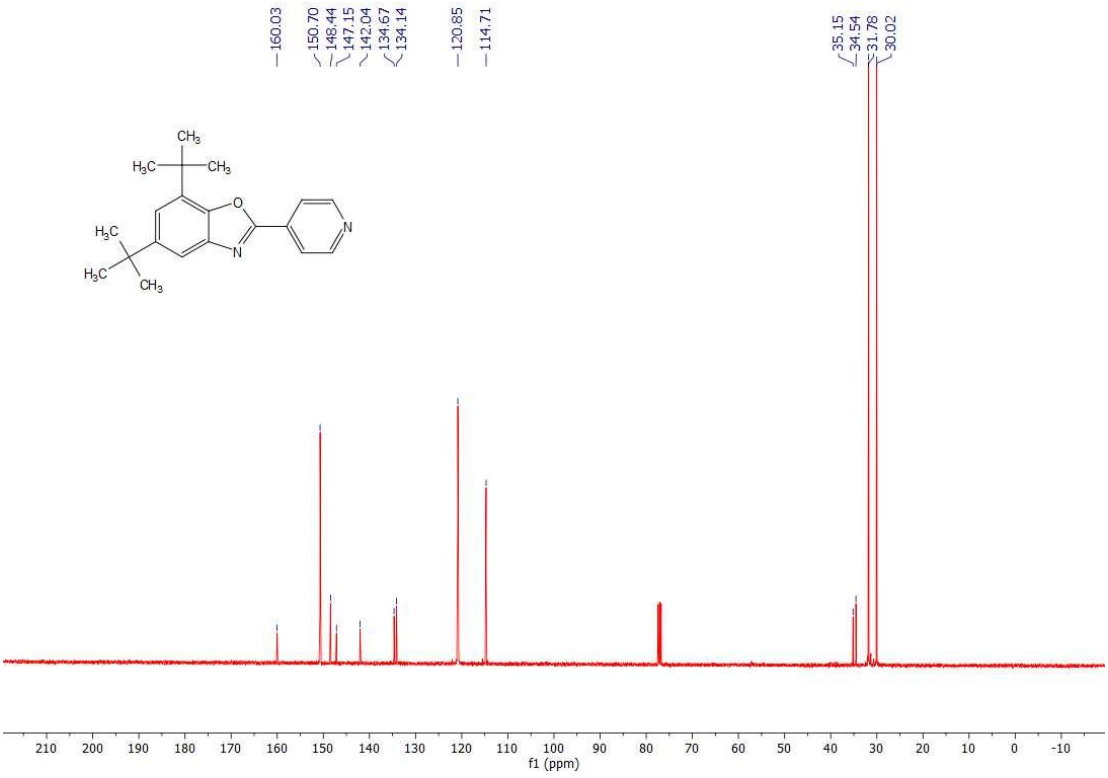

Figure S48. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(pyridin-4-yl)benzo[*d*]oxazole (4aa) in $CDCl_3$ at 100 MHz.

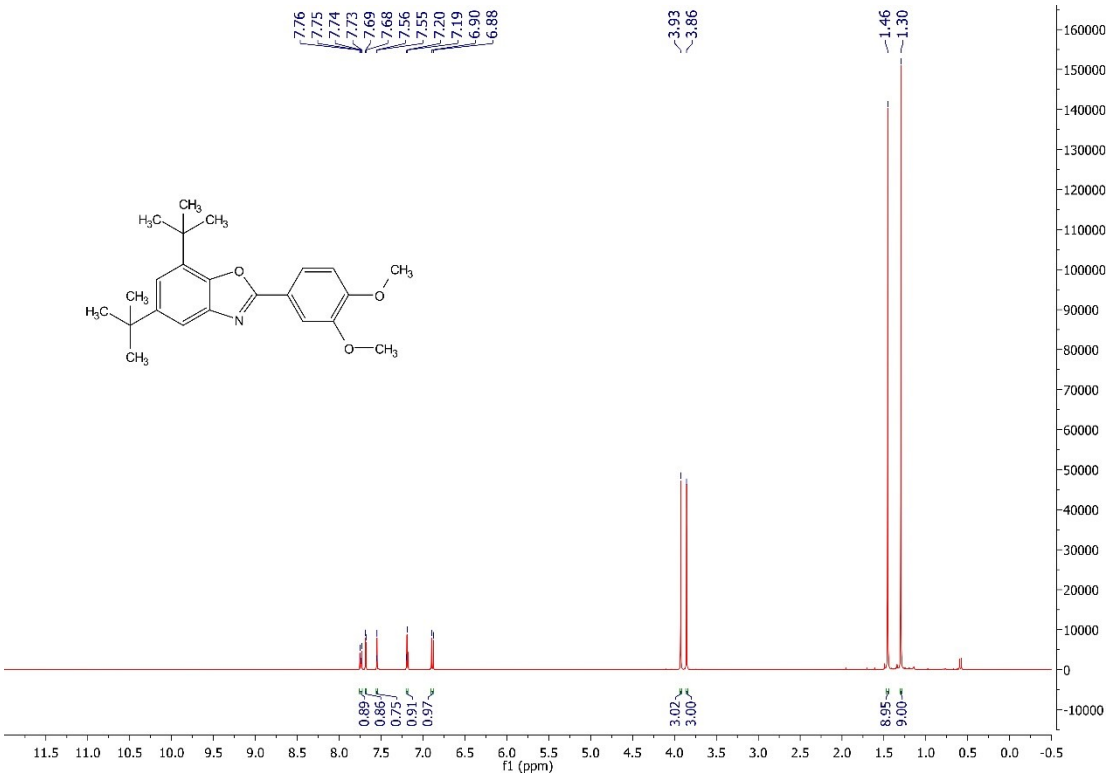

Figure S49. ^{1}H NMR spectrum of 5,7-di-*tert*-butyl-2-(3,4-dimethoxyphenyl)benzo[*d*]oxazole (4ab) in $CDCl_3$ at 400 MHz.

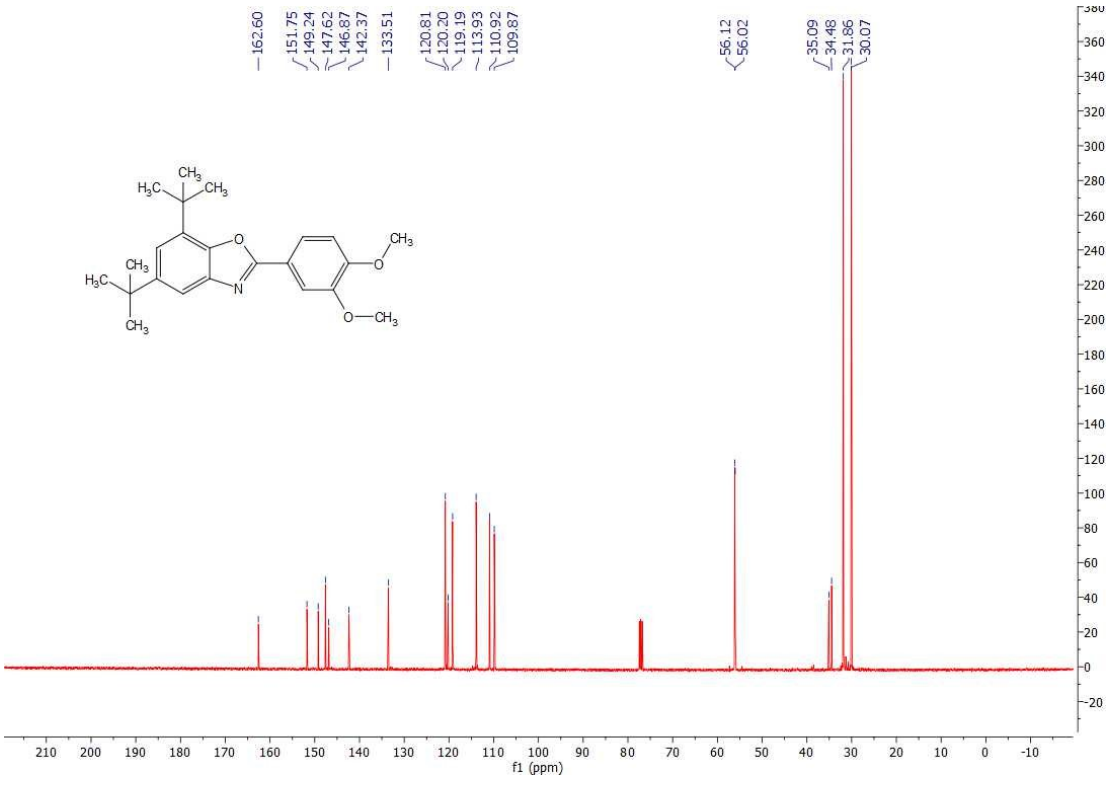

Figure S50. ^{13}C NMR spectrum of 5,7-di-*tert*-butyl-2-(3,4-dimethoxyphenyl)benzo[*d*]oxazole (4ab) in $CDCl_3$ at 100 MHz.

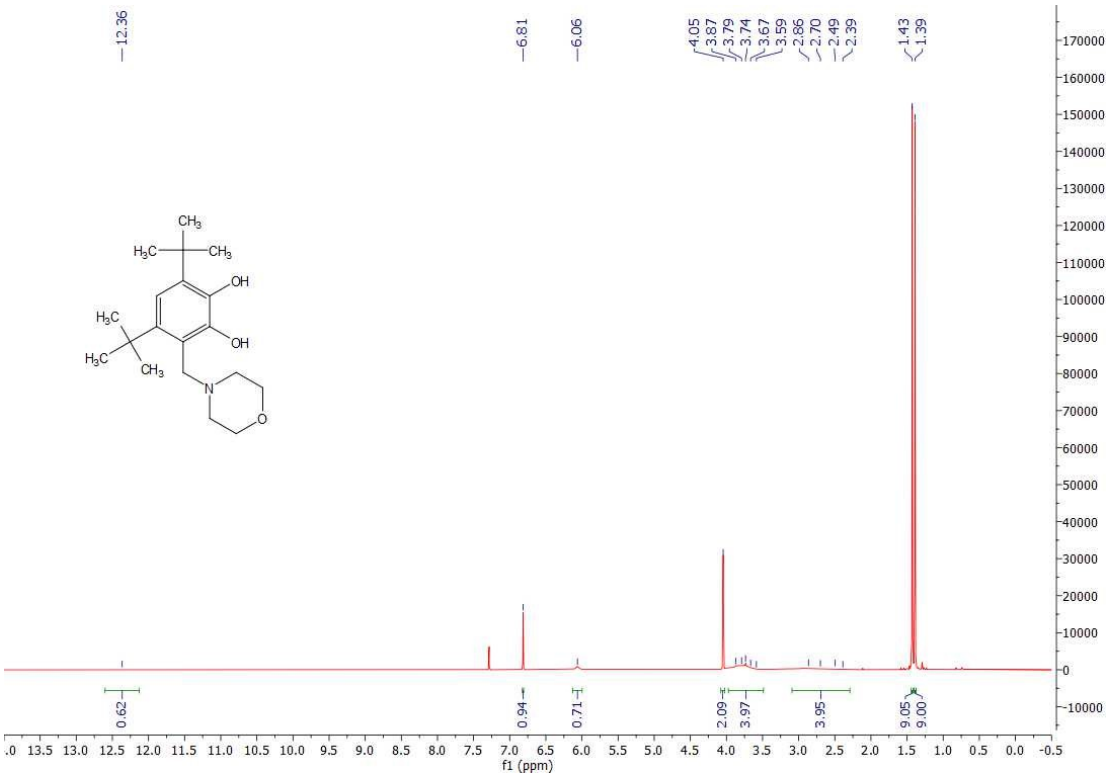

Figure S51. ^{1}H NMR spectrum of 4,6-di-*tert*-butyl-3-morpholinobenzene-1,2-diol (1g) in $CDCl_3$ at 400 MHz.

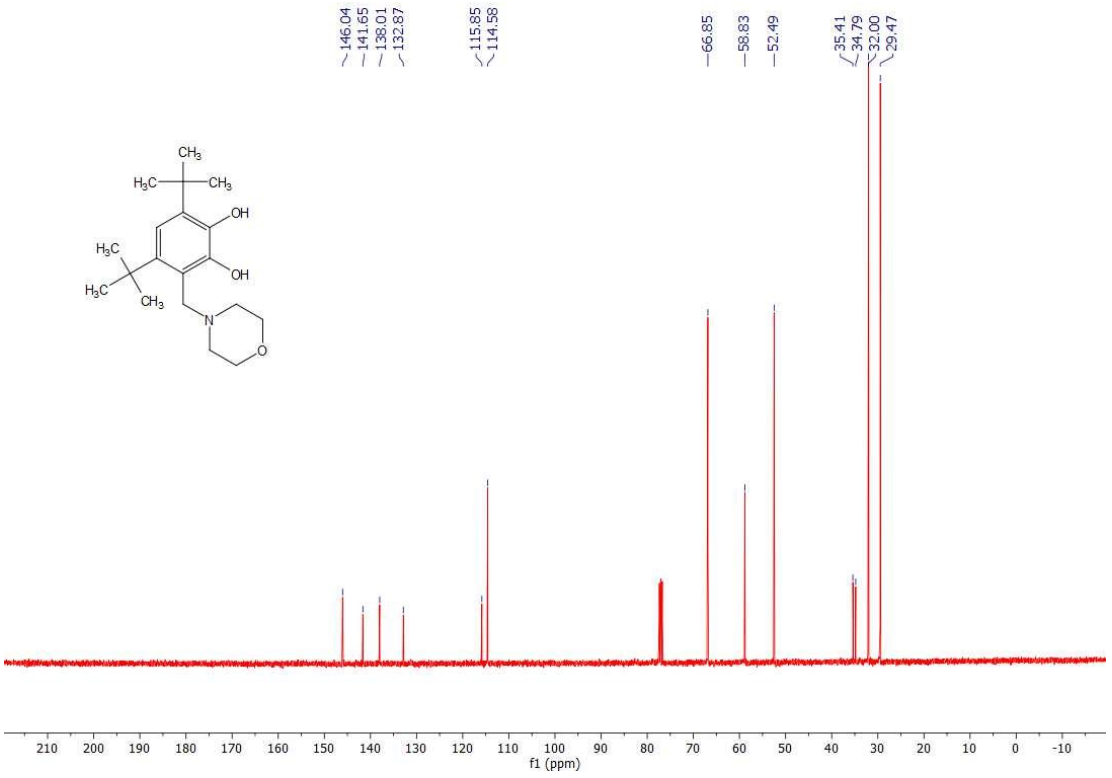

Figure S52. ^{13}C NMR spectrum of 4,6-di-*tert*-butyl-3-morpholinobenzene-1,2-diol (1g) in $CDCl_3$ at 100 MHz.