Supporting Information

Facile synthesis of benzoxazole derivatives by a multi-component reaction catalysed by copper complexes capable of generating phenoxyl radical complex

Virendra Kumar Chaudhary[a], Sain Singh[a], Kapil Kumar[a], Angshuman R. Choudhury[c], and Kaushik Ghosh [a,b] *

[a]Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India

[b]Department of Biosciences and Bioengineering, Indian Institute of Technology Roorkee, Roorkee 247667, Uttarakhand, India

[c]Department of Chemical Sciences, Indian Institute of Science Education and Research, Mohali, India

E-mail: kaushik.ghosh@cy.iitr.ac.in

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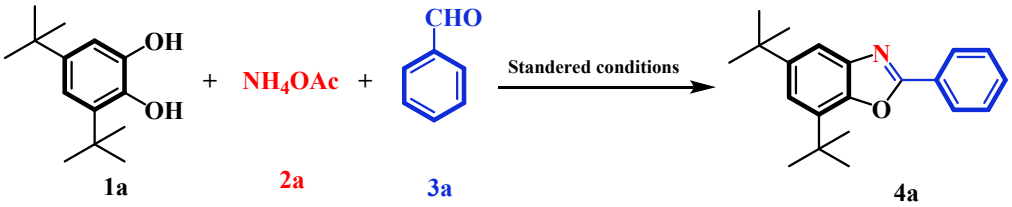
Table S1. Optimization of Benzoxazole with different catalysts.

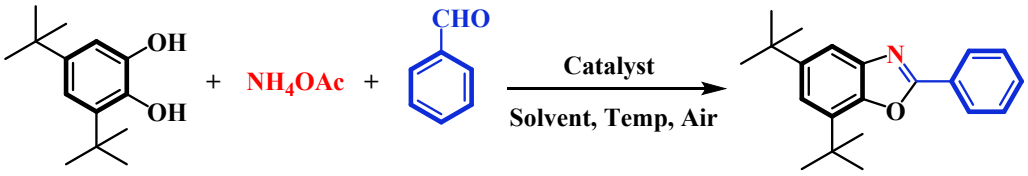


1a 2a 3a 4a

S.N.	Complexes	Yields (%)
[1]1	$[Cr(phimp)_2]ClO_4$ (**1**)	24
	$[Cr(N\text{-}phimp)_2]ClO_4$ (**2**)	20
	$[Cr(Me\text{-}phimp)_2]ClO_4$ (**3**)	25
[2-3]2	$[Fe(^{H}phimp)_2]ClO_4$ (**1**)	45
	$[Fe(^{OCH3}phimp)_2]ClO_4$ (**2**)	52
	$[Fe(^{Me}phimp)_2]ClO_4$ (**3**)	50
	$[Fe(^{tBu}phimp)_2]ClO_4$ (**4**)	68
	$[Fe(^{NO2}phimp)_2]ClO_4$ (**5**)	28
[4]3	$[Fe(^{Me}phimp)Cl_2]$(**1**)	70
	$[Fe(^{NO2}phimp)Cl_2]$(**2**)	65
	$[Fe(^{OMe}phimp)Cl_2]$(**3**)	78
	$[Fe(^{ditertbutyl}phimp)Cl_2]$(**4**)	86
[5]4	$[Co^{II}(L)(L^{+})]NO_3$	30

[6]5	$[Ni_2(L1)H_2O(CH_3COO)]$(**1**) $[Ni_2(L2)H_2O(CH_3COO)]$(**2**)	40 46
[7]- [9]6	[Cu(^{tBu}Phimp)(Cl)] (**1**) Cu(Phimp)(L)](**2**); L= -$OOCCH_3$ [Cu(L^1)]ClO_4(**3**)	90 70 65
[10]7	$Zn_2(Phimp)_2(Cl)_2$](**1**) Zn_2(Me-Phimp)$_2(Cl)_2$](**2**) Zn_2(OMe-Phimp)$_2(Cl)_2$](**3**)	18 18 22

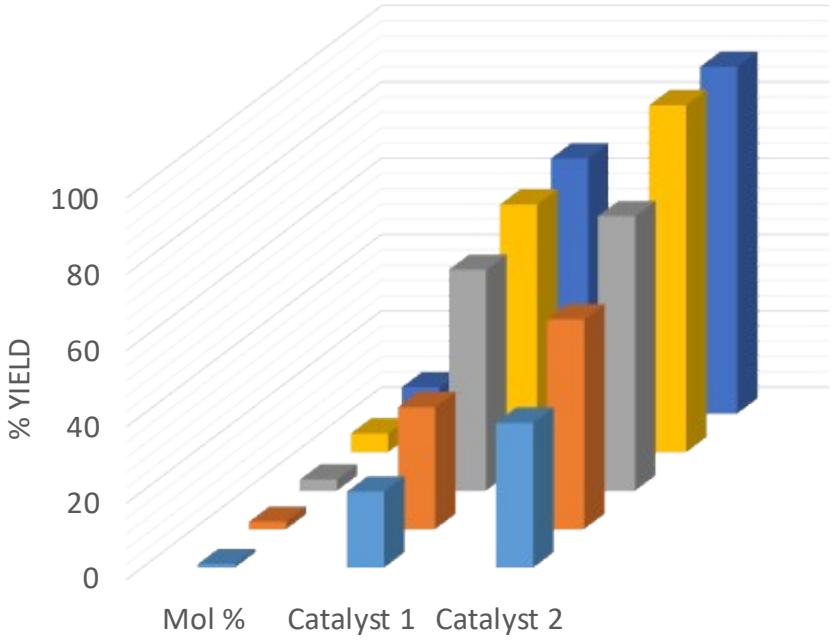
Table S2. Optimization of the Reaction Conditions for Synthesis of 5,7-di-tert-butyl-2-phenylbenzo[d]oxazole.

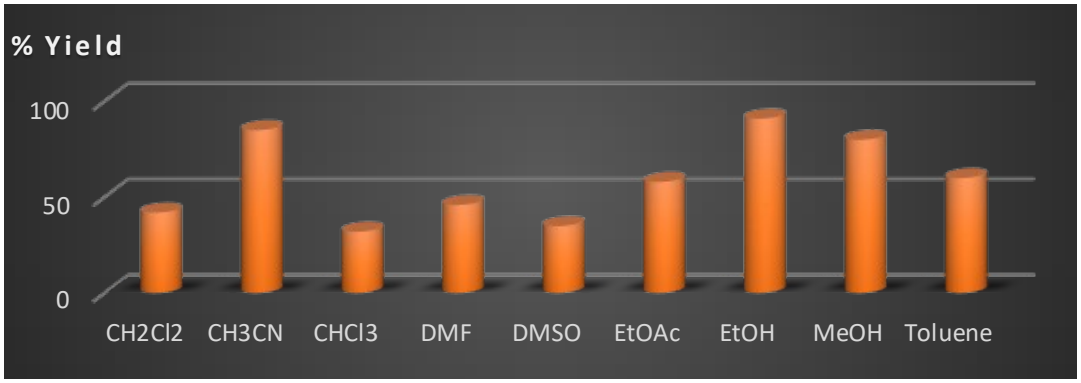


1a **2a** **3a** **4a**

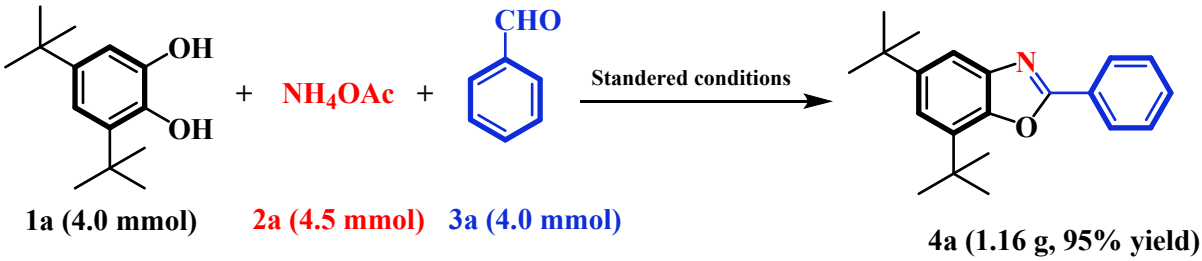
Entry	Catalyst/mol %	Solvent	Temp.	Time (h)	Yield (%)
1.	Complex (**1**)/**3**	C_2H_5OH	25 °C	12	58
2.	Complex (**1**)/**5**	C_2H_5OH	25 °C	12	60
3.	Complex (**1**)/**5**	C_2H_5OH	50 °C	24	65
4.	Complex (**2**)/**3**	C_2H_5OH	25 °C	24	72
5.	Complex (**2**)/**3**	C_2H_5OH	25 °C	48	75
6.	Complex (**2**)/**5**	C_2H_5OH	25 °C	24	75
7.	**Complex (2)/3**	**C_2H_5OH**	**50 °C**	**6**	**91**
8.	Complex (**2**)/**3**	C_2H_5OH	reflux	6	85
9.	Complex (**2**)/**3**	C_2H_5OH	50 °C	24	91
[b]10.	Complex (**2**)/**3**	C_2H_5OH	50 °C	6	91
[c]11.	Complex (**2**)/**3**	C_2H_5OH	50 °C	6	83
12.	Complex (**2**)/**3**	CH_3OH	50 °C	24	80
13.	Complex (**2**)/**3**	$CHCl_3$	50 °C	24	32
14.	Complex (**2**)/**3**	EtOAc	50 °C	24	58
15.	Complex (**2**)/**3**	CH_2Cl_2	25 °C	24	42

16.	Complex (**2**)/**3**	CH_3CN	50 °C	24	85
17.	Complex (**2**)/**3**	DMSO	50 °C	24	35
18.	Complex (**2**)/**3**	DMF	50 °C	24	46
19.	Complex (**2**)/**3**	Toluene	50 °C	24	60
[d]20.	-	C_2H_5OH	50 °C	24	0
[e]21.	Complex (**2**)/**3**	-	50 °C	24	0
22.	$CuCl_2$/**3**	C_2H_5OH	50 °C	24	43
[a]General conditions: 3,5-Di-tert-butylcatechol (1.0 mmol), ammonium acetate (1.2mmol), benzaldehyde (1.0 mmol), solvent (3.0mL), and air. [b]Ammonium acetate (2.0 mmol). [c]Ammonium acetate (4.0 mmol). [d] without catalyst. [e] without solvent					



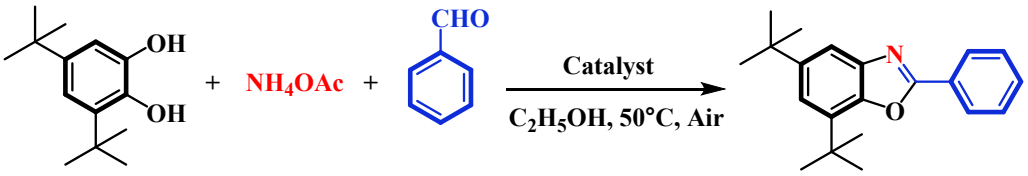


Scheme S1. Gram-Scale Synthesis of 5,7-di-tert-butyl-2-phenylbenzo[d]oxazole (**4a**).



1a (4.0 mmol) **2a (4.5 mmol)** **3a (4.0 mmol)** **4a (1.16 g, 95% yield)**

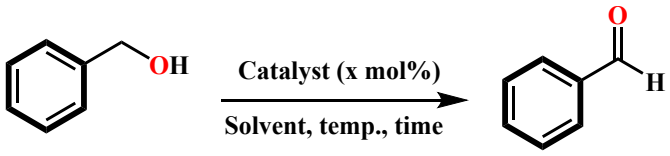
Table S3. Optimization of the Reaction Conditions with radical scavenger for Synthesis of 5,7-di-tert-butyl-2-phenylbenzo[d]oxazole.



1a **2a** **3a** **4a**

S.N.	Catalysts/mol%	Time(h)	Yields(%)
1.	Complex (**2**)/3	6	80
2	Complex (**2**)/3	12	95
3	Complex (**2**)/3 + TEMPO/0.5 equivalent	12	60
4	Complex (**2**)/3 + TEMPO/1.0 equivalent	12	trace
5	Complex (**2**)/3 + TEMPO/2.0 equivalent	12	trace
6.	TEMPO/3	6	38
7.	TEMPO/5	6	55
8.	TEMPO/10	6	71
9.	TEMPO/20	6	80
10.	TEMPO/100	6	30
11.	TEMPO/100	24	trace

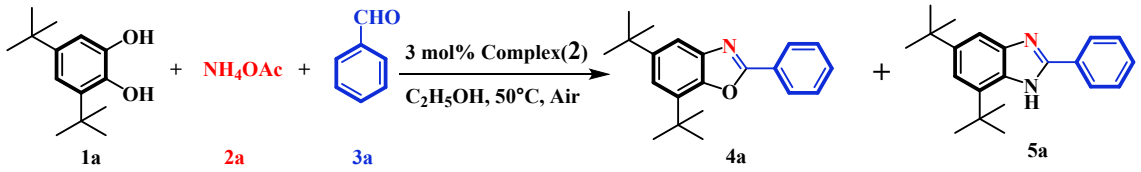
Table S4 Conversion of alcohol to aldehyde



S.N.	Catalysts/mol%	Solvent	Temp.	Time(h)	Yields(%)
1.	Complex (**2**)/3	C_2H_5OH	50	12	8
2	Complex (**2**)/5	C_2H_5OH	50	12	8
3	Complex (**2**)/3	C_2H_5OH	80	12	17
4	Complex (**2**)/3	C_2H_5OH	100	12	22
5	Complex (**2**)/3	Toluene	50	12	20
6.	Complex (**2**)/3	Toluene	80	12	40
7.	Complex (**2**)/3	Toluene	100	12	71
8.	Complex (**2**)/3	Toluene	100	24	71
9.	Complex (**2**)/3	THF	100	12	19
10.	Complex (**2**)/3	Xylene	100	12	58
11.	Complex (**2**)/3	Benzene	100	12	60
12.	Complex (**2**)/3	DMSO	100	12	20

Scheme S2. Control Experiments (A-G)

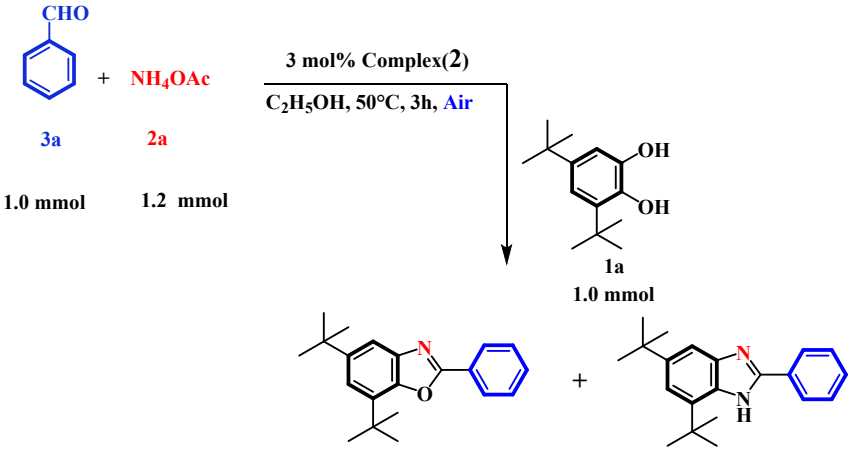
A



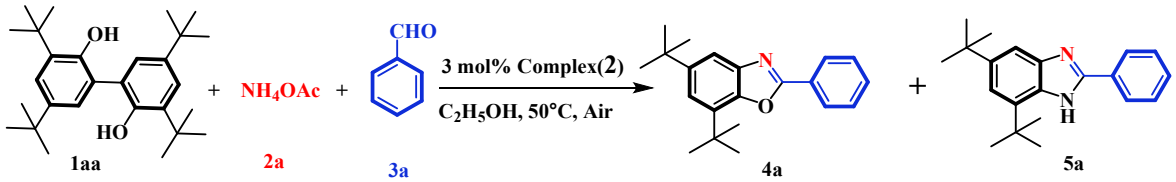
1a 2a 3a 4a 5a

1.0 mmol	1.2 mmol	1.0 mmol	91%	0%
1.0 mmol	2.0 mmol	1.0 mmol	91%	0%
1.0 mmol	4.0 mmol	1.0 mmol	83%	0%

B

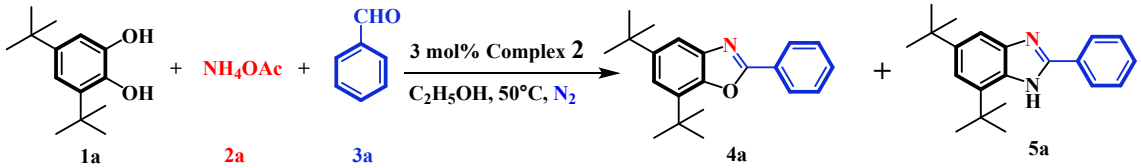


C

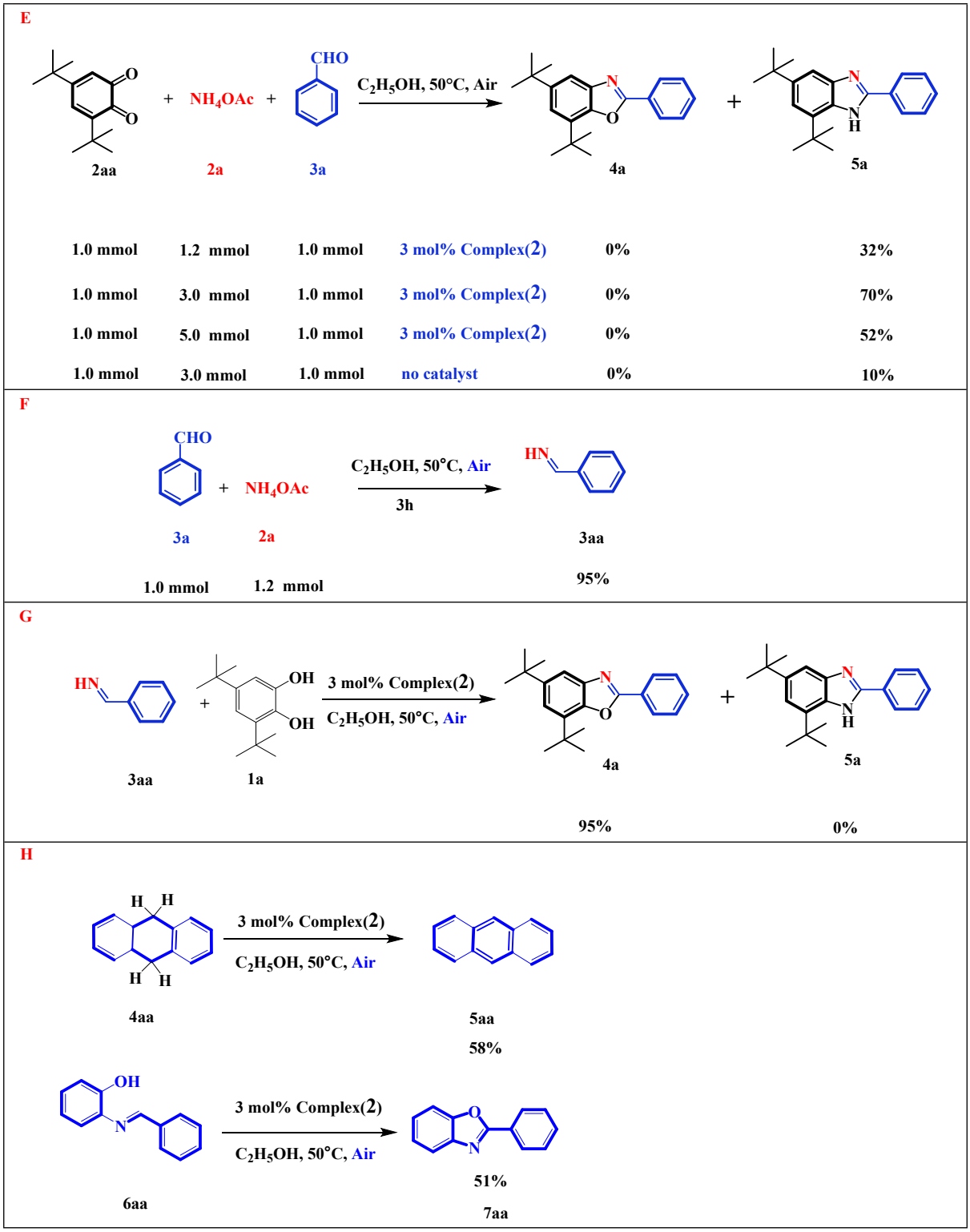


1.0 mmol	1.2 mmol	1.0 mmol	0%	0%

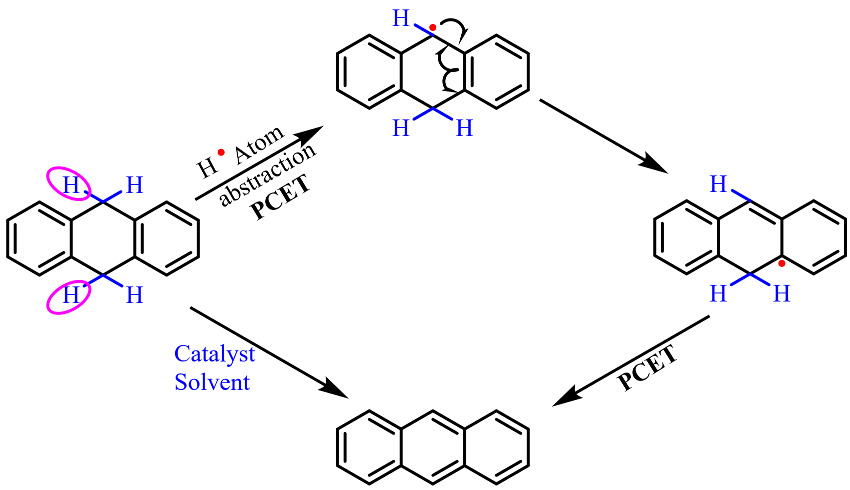
D



1.0 mmol	1.2 mmol	1.0 mmol	15 %	0%



Scheme S3. Proposed mechanism for the hydrogen atom abstraction reaction from 9,10-dihydroanthracene leading to the synthesis of anthracene.



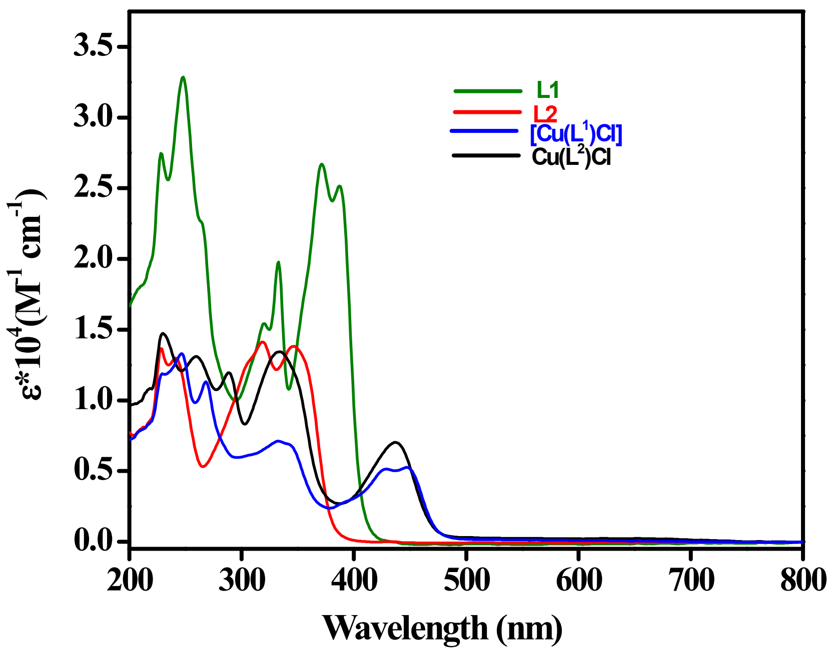
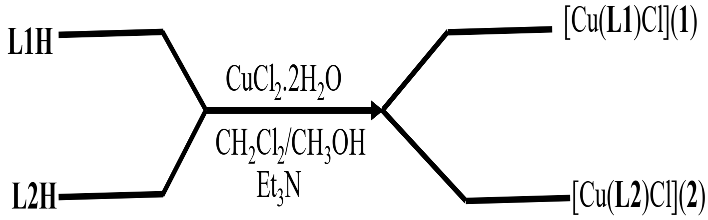


Figure S1. Electronic absorption spectra of ligands and metal complexes in dichloromethane.



Scheme S4. Schematic drawing for the synthesis of complexes **1**–**2**.

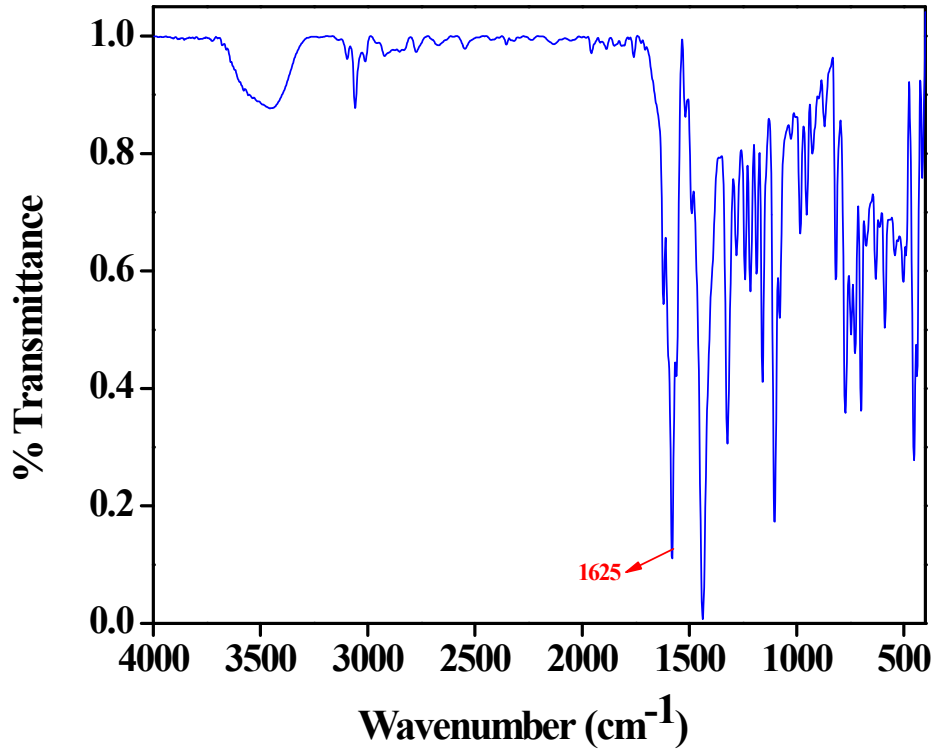


Figure S2. IR spectra of the ligand L^1H

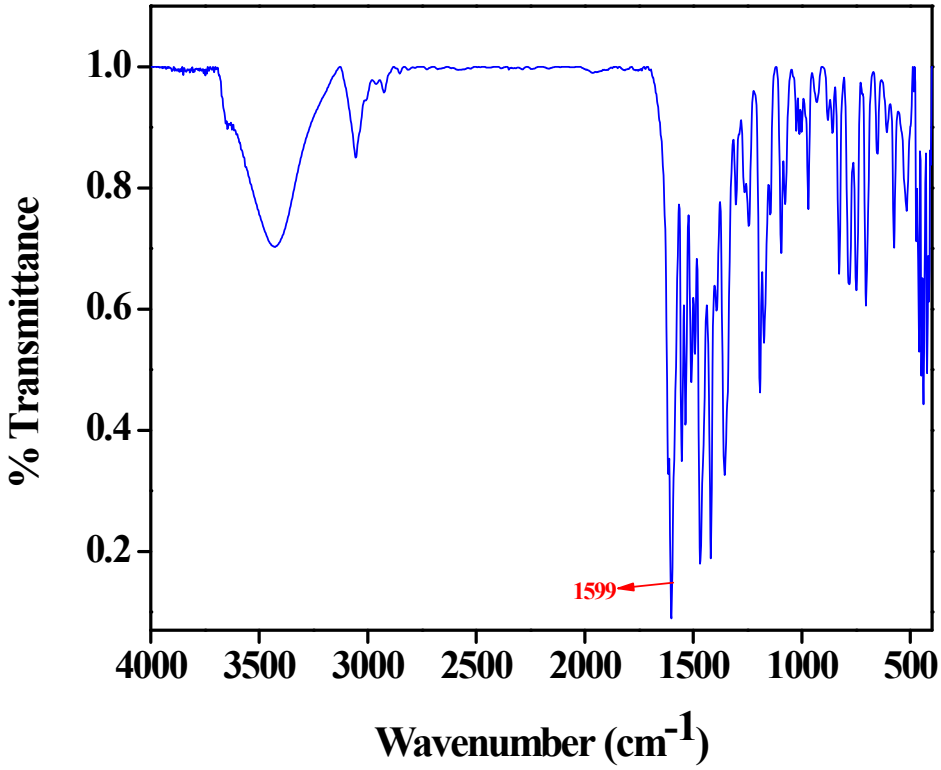


Figure S3. IR spectra of the complex [Cu(L1)Cl] (1)

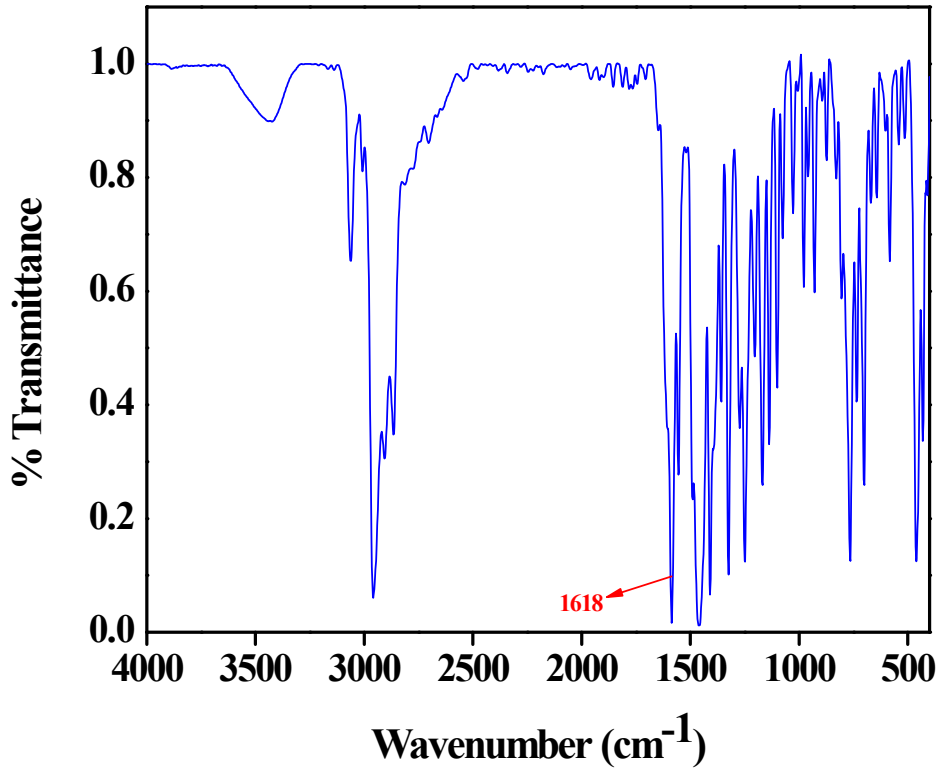


Figure S4. IR spectra of the ligand L^2H

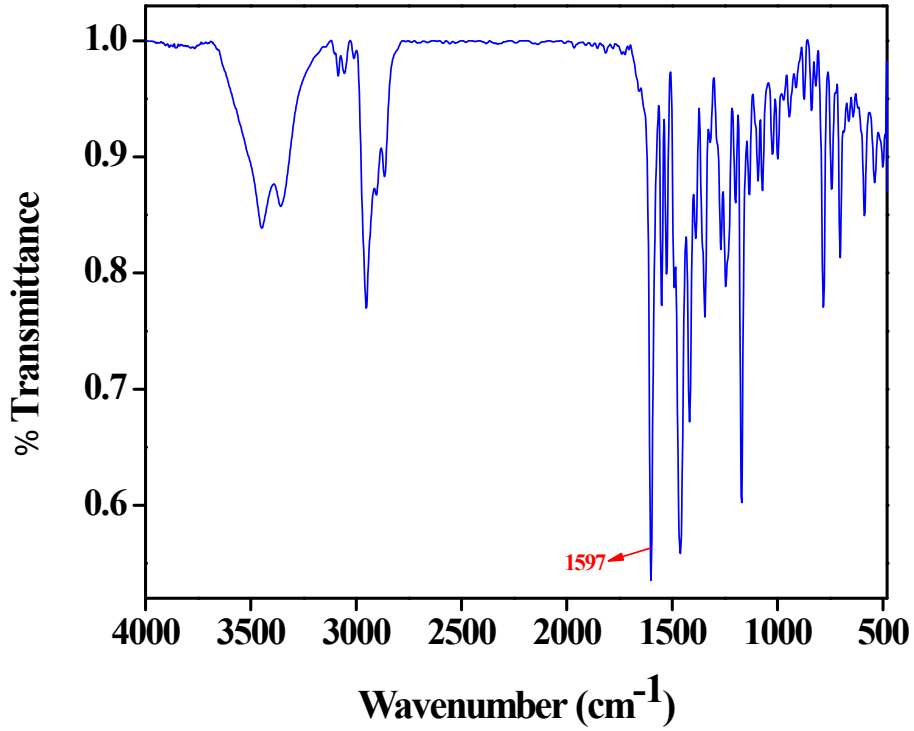


Figure S5. IR spectra of the complex [Cu(L2)Cl] (2)

Table S5. Crystal data and structural refinement parameters for complexes **1** and **2**.

	2	**1**
Chemical formula	$C_{26}H_{29}Cl_2CuN_3O$	$C_{23}H_{19}Cl_2CuN_3O_2$
T(K)	296.0 K	293.0 K
λ(A)(Mo-Kα)	0.71073	0.71073
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$
V(Å^3)	2574.46(16)	2180.8(3)
Z	4	4
ρ_{calc} (g/cm^3)	1.378	1.535
F(000)	1108.0	1028.0
Data/Restraints/parameters	8962/0/304	5358/0/282
GOF[a] on F^2	1.035	1.087
R_1[b][I>2σ(I)]	0.0568	0.0767
R_1[all data]	0.0999	0.0896
R_{int}	0.0350	0.0392
Formula weight	533.96	503.86
a(Å)	13.9524(5)	9.0804(7)
b(Å)	12.3044(4)	20.1924(16)
c(Å)	15.0863(6)	11.8970(9)
α(°)	90°	90°
β(°)	96.271(3)°	91.264(4)°
γ(°)	90°	90°
Crystal size/mm^3	0.5 × 0.38 × 0.26	0.27 × 0.27 × 0.27
Theta range(°)	2.6470−27.8870	1.14−28.402
Index ranges	–21<*h* < 19, –18 <*k* < 18, –20 <*l* < 18	–12<*h* < 11, –26 <*k* < 26, –15 <*l* < 15
wR_2 [all data]	0.1933	0.2539
Largest diff. peak/hole / e Å^{-3}	1.15/-0.64	1.64/-0.83
wR_2[c] [I>2σ(I)]	0.1561	0.2455

R_{sigma}	0.0398	0.0310

[a]*GOF* = $[\Sigma[w(F_o^2-F_c^2)^2]/M-N]^{1/2}$ (*M* = number of reflections, *N* = number of parameters refined). [b]$R1 = \Sigma \| F_o | - | F_c | / \Sigma | F_o |$. [c]$wR2 = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[(F_o^2)^2]]^{1/2}$.

Table S6. Selected bond lengths (Å) and bond angles (º) of complex **2**.

Bond lengths(Length/Å)			
Cu(1)—Cl(1)	2.2018(8)	N(1)—N(2)	1.399(3)
Cu(1)—O(1)	1.8768(16)	C(1)—Cl(2)	1.728(3)
Cu(1)—N(3)	2.008(2)	O(1)—C(14)	1.316(3)
Cu(1)—N(1)	1.951(2)	C13—C14	1.416(3)
C16—C17	1.404(4)	C14—C15	1.437(3)
C17—C18	1.372(3)	C15—C16	1.386(3)
Bond angles(Angle/Å)			
O(1)—Cu(1)—Cl(1)	97.59(6)	C14—O1—Cu1	127.41(15)
O(1)—Cu(1)—N(3)	155.09(9)	N2—N1—Cu1	113.20(15)
O(1)—Cu(1)—N(1)	91.01(8)	C12—N1—Cu1	126.95(17)
N(1)—Cu(1)—Cl(1)	147.80(7)	C5—N3—Cu1	111.89(15)
N(1)—Cu(1)—N(3)	80.55(8)	C1—N3—Cu1	129.20(19)
N(3)—Cu(1)—Cl(1)	102.01(6)	N3—C1—Cl2	116.4(2)
C5—N2—C6	123.5(2)	C2—C1—Cl2	119.9(2)

Table S7. Selected bond lengths (Å) and bond angles (º) of complex **1**.

Bond lengths(Length/Å)			
Cu(1)—Cl(1)	2.2141(16)	N(1)—N(2)	1.387(6)
Cu(1)—O(1)	1.890(4)	C(3)—N(1)	1.306(7)
Cu(1)—N(3)	2.028(5)	O(1)—C(1)	1.315(7)
Cu(1)—N(1)	1.942(5)	N(2)—C(16)	1.378(7)
C12—Cl2	1.718(6)	N(2)—C(17)	1.435(6)
Bond angles(Angle/Å)			
O(1)—Cu(1)—Cl(1)	93.89(15)	C1—O1—Cu1	126.7(4)
O(1)—Cu(1)—N(3)	156.1(2)	N2—N1—Cu1	114.0(3)
O(1)—Cu(1)—N(1)	90.64(19)	C12—N3—Cu1	130.7(4)
N(1)—Cu(1)—Cl(1)	147.45(16)	C16—N3—Cu1	112.2(4)
N(1)—Cu(1)—N(3)	80.79(19)	C3—N1—Cu1	126.5(4)
N(3)—Cu(1)—Cl(1)	105.38(13)	N3—C12—Cl2	116.0(5)
C16—N2—C17	123.2(5)	C13—C12—Cl2	119.7(5)

Figure S6. Electronic absorption spectra change during the formation of I_3^- ion in presence of H_2O_2 (detection of H_2O_2).

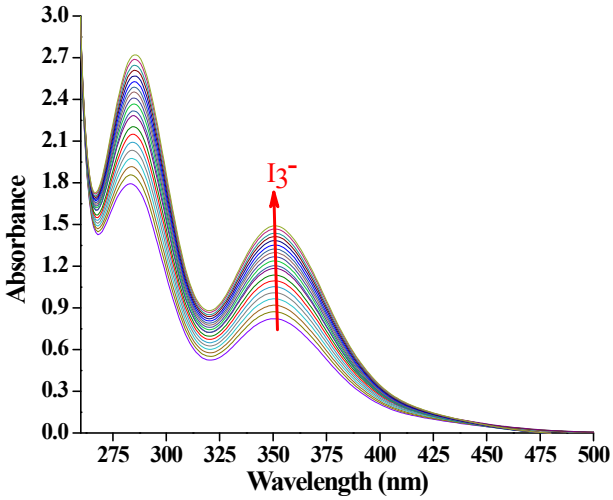


Figure S7. X-band EPR spectra of complex **2** in DMF at 100K

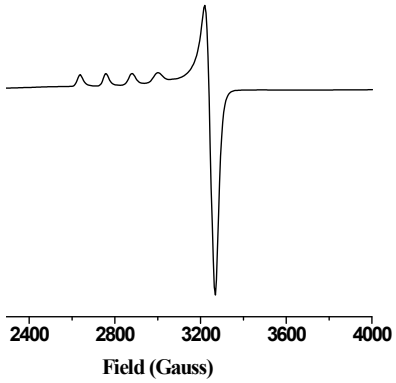


Figure S8. X-band EPR spectra of complex **2** + 3,5-DTBC (1:100) in ACN at 100K

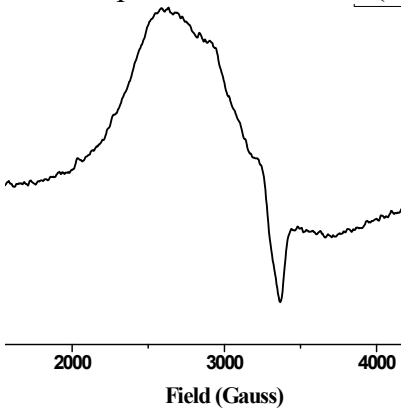


Figure S9: X-band EPR spectra at 100K in DMF (**A**) of complex **2** with CAN, (**B**) reaction mixture of complex **2** and 3,5-DTBC (1:1).

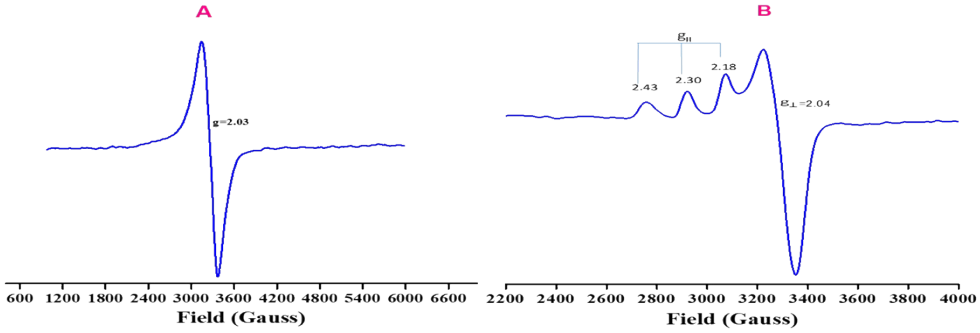
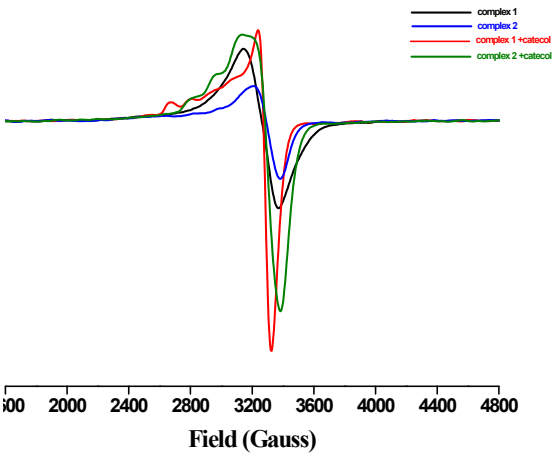
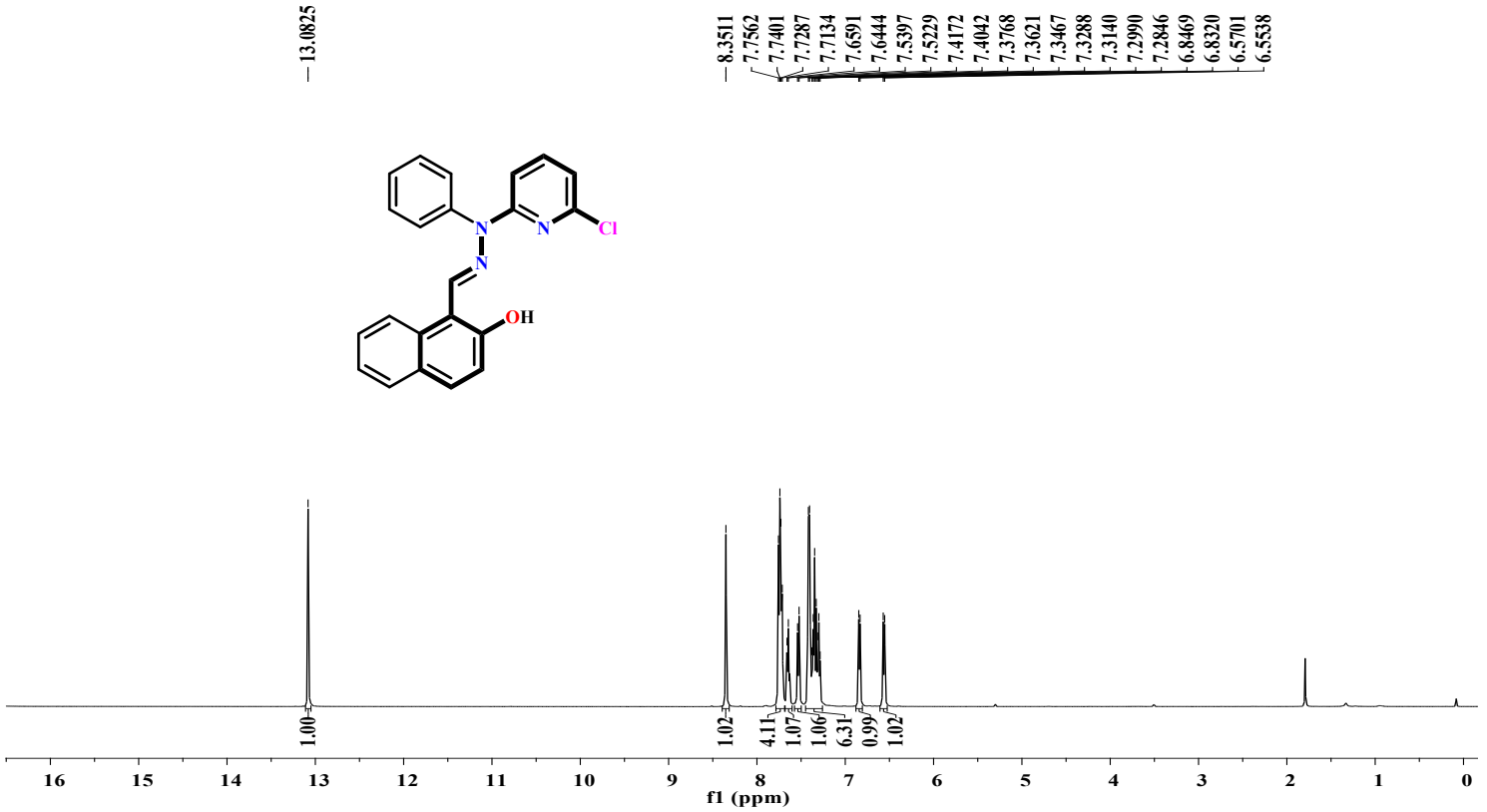


Figure S10. EPR spectra of crude product recorded in CH_3CN at 100K





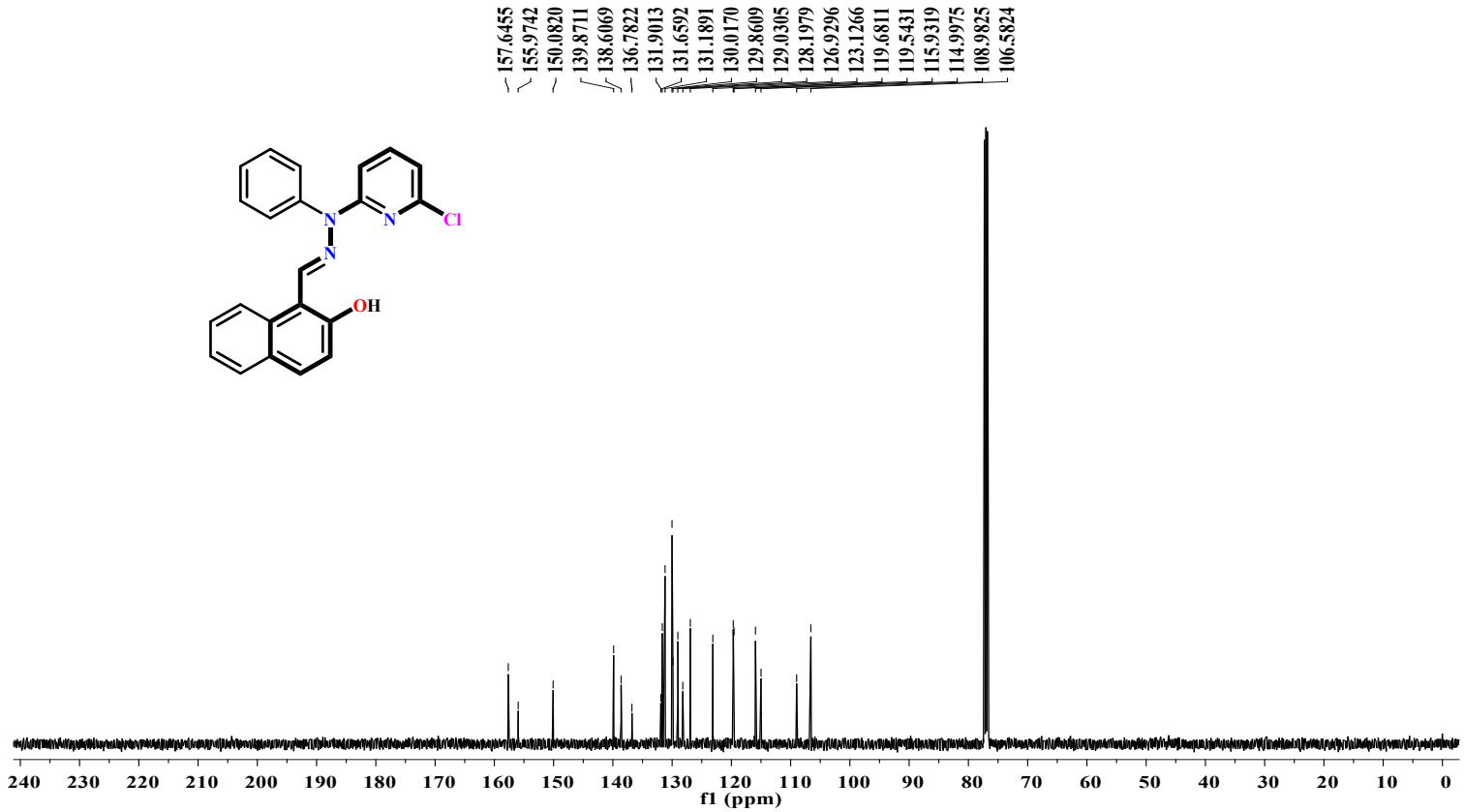


Figure S11. ^{1}H NMR spectrum of ligand **L^{1}H** in $CDCl_3$ (500 MHz).

Figure S12. ^{13}C NMR spectrum of ligand **L^{1}H** in $CDCl_3$ (500 MHz).

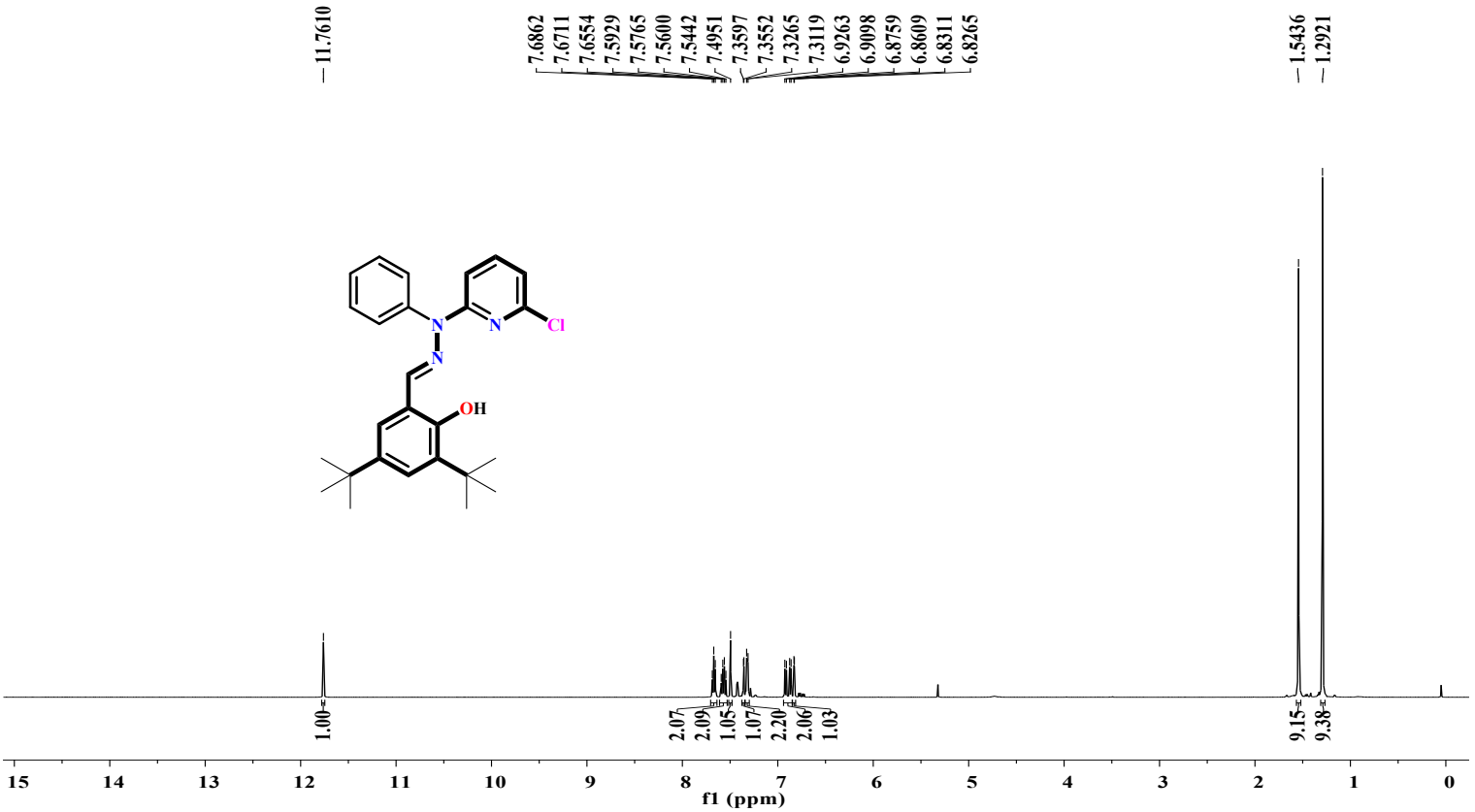


Figure S13. ^{1}H NMR spectrum of ligand **L^{2}H** in $CDCl_3$ (500 MHz).

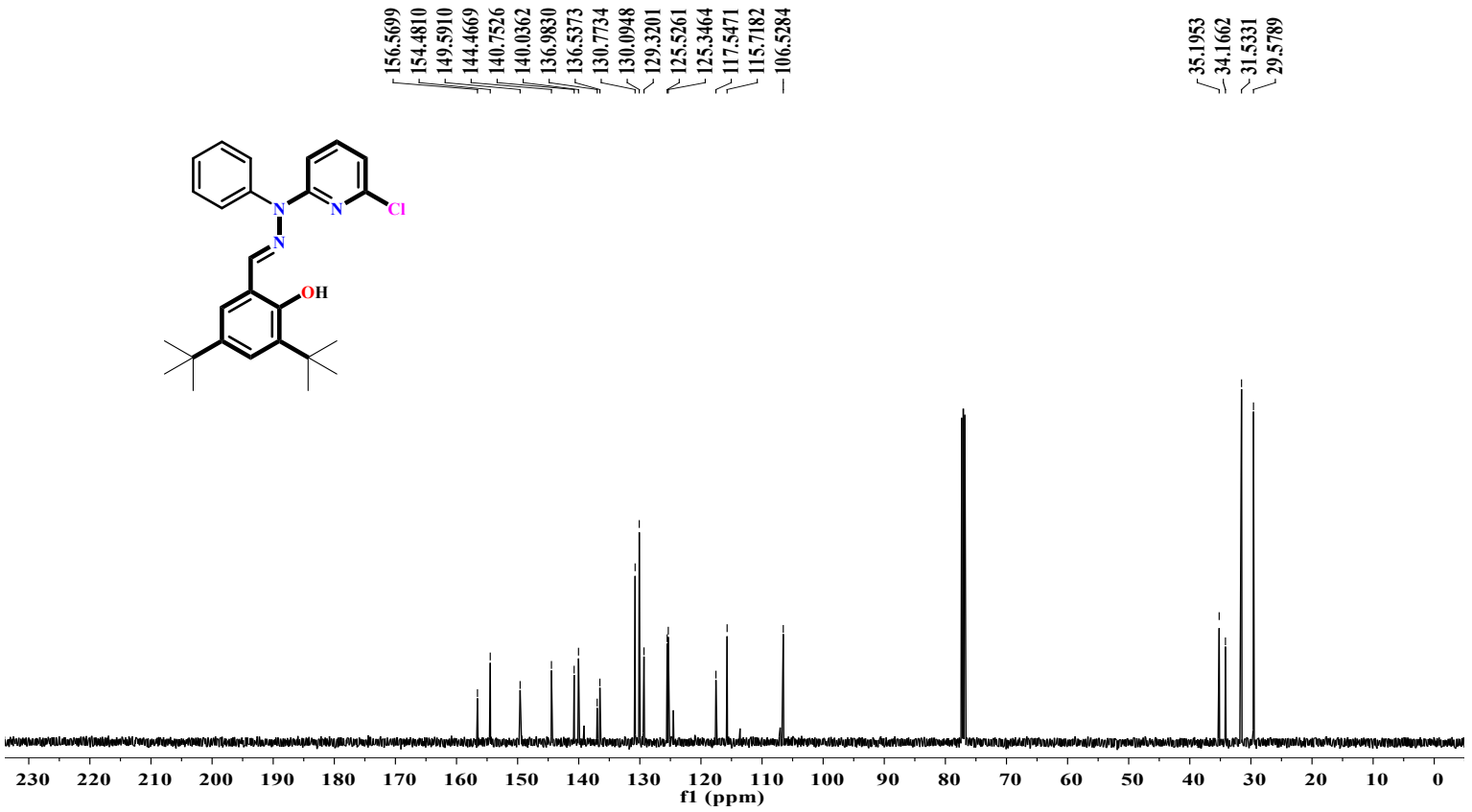


Figure S14. ^{13}C NMR spectrum of ligand **L^{2}H** in $CDCl_3$ (500 MHz).

5,7-di-tert-butyl-2-(4-chlorophenyl)benzo[d]oxazole (4aa).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 320 mg, 94%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, J = 8.6 Hz, 2H), 7.69 (s, 1H), 7.52 (d, J = 8.6 Hz, 2H), 7.36 (s, 1H), 1.59 (s, 9H), 1.44 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.52 (s), 147.99 (s), 147.00 (s), 142.31 (s), 137.39 (s), 133.81 (s), 129.24 (s), 128.64 (s), 126.11 (s), 119.86 (s), 115.00 (s), 114.32 (s), 35.12 (s), 34.52 (s), 31.83 (s), 30.08 (s).

4-(5,7-di-tert-butylbenzo[d]oxazol-2-yl)-N,N-dimethylaniline (4ab).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 318 mg, 91%. White solid, mp: 138−140 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (d, J = 9.0 Hz, 2H), 7.58 (s, 1H), 7.22 (s, 1H), 6.77 (d, J = 9.0 Hz, 2H), 3.05 (s, 6H), 1.53 (s, 9H), 1.38 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.62 (s), 152.25 (s), 147.25 (s), 146.66 (s), 142.76 (s), 133.20 (s), 128.85 (s), 118.39 (s), 115.00 (s), 113.56 (s), 111.65 (s), 40.14 (s), 35.05 (s), 34.45 (s), 31.89 (s), 30.08 (s).

5,7-di-tert-butyl-2-(4-ethoxyphenyl)benzo[d]oxazole (4ac).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 351 mg, 95%. Crystaline solid, mp: 90−92 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, J = 8.6 Hz, 2H), 7.68 (s, 1H), 7.32 (s, 1H), 7.04 (d, J = 8.6 Hz, 2H), 4.12 (q, J = 7.0 Hz, 2H), 1.59 (s, 9H), 1.47 (t, J = 7.0 Hz, 3H), 1.44 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.53 (s), 147.54 (s), 142.55 (s), 133.50 (s), 129.13 (s), 119.96 (s), 119.03 (s), 114.81 (s), 113.95 (s), 63.67 (s), 35.08 (s), 34.50 (s), 31.88 (s), 30.10 (s), 14.73 (s).

5,7-di-tert-butyl-2-(p-tolyl)benzo[d]oxazole (4ad).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 305 mg, 95%. Cream solid, mp: 93−95 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (d, J = 8.1 Hz, 2H), 7.74 (s, 1H), 7.38 (s, 1H), 7.35 (d, J = 8.0 Hz, 2H), 2.44 (s, 3H), 1.63 (s, 9H), 1.47 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.78 (s), 147.66 (s), 146.93 (s), 142.51 (s), 141.63 (s), 133.65 (s), 129.63 (s), 127.43 (s), 124.87 (s), 119.35 (s), 115.00 (s), 114.20 (s), 35.12 (s), 34.53 (s), 31.92 (s), 30.13 (s), 21.63 (s).

5,7-di-tert-butyl-2-phenylbenzo[d]oxazole (4ae).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 280 mg, 91%. Brown liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (dd, J = 6.7, 3.0 Hz, 2H), 7.69 (d, J = 1.8 Hz, 1H), 7.58 – 7.52 (m, 3H), 7.34 (d, J = 1.8 Hz, 1H), 1.59 (s, 9H), 1.43

(s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.50 (s), 147.77 (s), 146.97 (s), 142.34 (s), 133.75 (s), 131.20 (s), 128.90 (s), 127.42 (s), 119.59 (s), 115.00 (s), 114.25 (s), 35.11 (s), 34.51 (s), 31.85 (s), 30.06 (s).

5,7-di-tert-butyl-2-(2-nitrophenyl)benzo[d]oxazole (4af).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:90). Isolated yield: 300 mg, 85%. Crystaline solid, mp: 124−126 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, J = 7.7 Hz, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.75 – 7.69 (m, 2H), 7.64 (m, 1H), 7.42 (s, 1H), 1.52 (s, 9H), 1.43 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.27 (s), 149.40 (s), 148.27 (s), 147.42 (s), 141.84 (s), 134.34 (s), 132.16 (s), 131.65 (s), 131.18 (s), 123.94 (s), 121.33 (s), 120.59 (s), 114.74 (s), 35.16 (s), 34.39 (s), 31.83 (s), 29.94 (s).

5,7-di-tert-butyl-2-(naphthalen-1-yl)benzo[d]oxazole (4ag).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 318 mg, 89%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.52 (d, J = 8.5 Hz, 1H), 8.45 (d, J = 7.3 Hz, 1H), 8.06 (d, J = 8.2 Hz, 1H), 7.98 (d, J = 8.1 Hz, 1H), 7.84 (d, J = 1.8 Hz, 1H), 7.75 (ddd, J = 8.4, 6.8, 1.3 Hz, 1H), 7.69 – 7.60 (m, 2H), 7.42 (d, J = 1.8 Hz, 1H), 1.65 (s, 9H), 1.49 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.36 (s), 147.74 (s), 146.43 (s), 142.63 (s), 134.02 (s), 133.72 (s), 131.97 (s), 130.76 (s), 129.02 (s), 128.65 (s), 127.83 (s), 126.44 (s), 125.01 (s), 124.17 (s), 119.77 (s), 114.53 (s), 35.19 (s), 34.55 (s), 31.93 (s), 30.14 (s).

5,7-di-tert-butyl-2-(4-methoxyphenyl)benzo[d]oxazole (4ah).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 320 mg, 95%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (d, J = 8.8 Hz, 2H), 7.70 (s, 1H), 7.34 (s, 1H), 7.04 (d, J = 8.8 Hz, 2H), 3.84 (s, 3H), 1.60 (s, 9H), 1.45 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.64 (s), 162.11 (s), 147.55 (s), 146.87 (s), 142.58 (s), 133.50 (s), 129.14 (s), 120.15 (s), 119.05 (s), 115.00 (s), 114.33 (s), 114.00 (s), 55.32 (s), 35.09 (s), 34.49 (s), 31.90 (s), 30.11 (s).

5,7-di-tert-butyl-2-(4-fluorophenyl)benzo[d]oxazole (4ai).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 303 mg, 93%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (dd, J = 8.8, 5.3 Hz, 2H), 7.70 (s, 1H), 7.36 (s, 1H), 7.24 (t, J = 8.6 Hz, 2H), 1.59 (s, 9H), 1.44 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.65 (s), 163.64 (s), 161.63 (s), 147.92 (s), 147.00 (s), 142.34 (s), 133.73 (s), 129.61 (s), 123.93 (s), 119.63 (s), 116.23 (s), 116.05 (s), 114.25 (s), 35.11 (s), 34.51 (s), 31.85 (s), 30.08 (s).

5,7-di-tert-butyl-2-(thiophen-2-yl)benzo[d]oxazole (4aj).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 291 mg, 93%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (d, J = 4.7 Hz, 1H), 7.68 (s, 1H), 7.52 (d, J = 6.0 Hz, 1H), 7.35 (s, 1H), 7.18 (dd, J = 4.9, 3.8 Hz, 1H), 1.58 (s, 9H), 1.43 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.53 (s), 147.91 (s), 146.65 (s), 142.30 (s), 133.62 (s), 130.18 (s), 129.73 (s), 129.35 (s), 128.14 (s), 119.58 (s), 115.00 (s), 114.15 (s), 35.11 (s), 34.50 (s), 31.87 (s), 30.07 (s).

2-(5-bromothiophen-2-yl)-5,7-di-tert-butylbenzo[d]oxazole (4ak).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 380 mg, 97%. White solid, mp: 115−117 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, J = 3.9 Hz, 1H), 7.63 (s, 1H), 7.33 (s, 1H), 7.16 (d, J = 3.9 Hz, 1H), 1.54 (s, 9H), 1.41 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.24 (s), 148.14 (s), 146.55 (s), 142.09 (s), 133.68 (s), 131.53 (s), 131.14 (s), 129.34 (s), 119.88 (s), 117.32 (s), 114.17 (s), 35.11 (s), 34.48 (s), 31.81 (s), 30.02 (s).

5,7-di-tert-butyl-2-(3,4-dimethoxyphenyl)benzo[d]oxazole (4al).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:50). Isolated yield: 338 mg, 92%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, J = 8.4 Hz, 1H), 7.80 (s, 1H), 7.66 (s, 1H), 7.30 (s, 1H), 7.01 (d, J = 8.4 Hz, 1H), 4.04 (s, 3H), 3.98 (s, 3H), 1.57 (s, 9H), 1.42 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.59 (s), 151.80 (s), 149.30 (s), 147.63 (s), 146.88 (s), 142.42 (s), 133.52 (s), 120.82 (s), 120.27 (s), 119.19 (s), 113.94 (s), 111.01 (s), 110.00 (s), 56.14(s), 56.03(s), 35.09 (s), 34.48 (s), 31.86 (s), 30.08 (s).

2-(anthracen-9-yl)-5,7-di-tert-butylbenzo[d]oxazole (4am).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 366 mg, 90%. Yellowish-green crystals, mp: 175−177 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.27 – 8.19 (m, 2H), 8.15 – 8.07 (m, 2H), 7.95 (s, 1H), 7.61 – 7.49 (m, 5H), 1.61 (s, 9H), 1.55 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.46 (s), 147.92 (s), 147.45 (s), 142.29 (s), 134.30 (s), 131.43 (s), 131.20 (s), 130.62 (s), 128.70 (s), 127.23 (s), 125.75 (s), 125.56 (s), 121.89 (s), 119.89 (s), 114.70 (s), 35.28 (s), 34.63 (s), 32.00 (s), 30.12 (s).

5,7-di-tert-butyl-2-(pyridin-3-yl)benzo[d]oxazole (4an).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 247 mg, 80%. White solid, mp: 98−100 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.46 (s, 1H), 8.69 (s, 1H), 8.46 (d, J = 7.8 Hz, 1H), 7.64 (s, 1H), 7.38 (s, 1H), 7.31 (s, 1H), 1.51 (s, 9H),

1.36 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.02 (s), 151.67 (s), 148.54 (s), 148.08 (s), 146.97 (s), 142.07 (s), 134.36 (s), 133.87 (s), 123.62 (s), 120.14 (s), 115.00 (s), 114.43 (s), 35.06 (s), 34.46 (s), 31.77 (s), 30.00 (s).

5,7-di-tert-butyl-2-(furan-2-yl)benzo[d]oxazole (4ao).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 279 mg, 94%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, J = 1.8 Hz, 1H), 7.64 (s, 1H), 7.33 (d, J = 1.8 Hz, 1H), 7.26 (d, J = 3.2 Hz, 1H), 6.58 (dd, J = 3.3, 1.5 Hz, 1H), 1.55 (s, 9H), 1.41 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.90 (s), 148.00 (s), 146.40 (s), 145.34 (s), 143.04 (s), 141.95 (s), 133.77 (s), 119.72 (s), 114.35 (s), 113.53 (s), 112.07 (s), 35.07 (s), 34.46 (s), 31.82 (s), 30.00 (s).

2-(4-bromophenyl)-5,7-di-tert-butylbenzo[d]oxazole (4ap).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 365 mg, 95%. Viscous liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, J = 8.5 Hz, 2H), 7.68 (m, 3H), 7.35 (s, 1H), 1.57 (s, 9H), 1.42 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.59 (s), 148.01 (s), 146.99 (s), 142.26 (s), 133.82 (s), 132.22 (s), 128.80 (s), 126.51 (s), 125.82 (s), 119.91 (s), 114.30 (s), 35.12 (s), 34.52 (s), 31.83 (s), 30.07 (s).

5,7-di-tert-butyl-2-(4-nitrophenyl)benzo[d]oxazole (4aq).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:30). Isolated yield: 314 mg, 89%. light yellow solid, mp: 199−200 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (q, J = 9.1 Hz, 4H), 7.71 (s, 1H), 7.41 (s, 1H), 1.59 (s, 9H), 1.43 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.11 (s), 149.19 (s), 148.58 (s), 147.34 (s), 142.24 (s), 134.16 (s), 133.19 (s), 128.11 (s), 124.24 (s), 120.92 (s), 114.72 (s), 35.18 (s), 34.57 (s), 31.78 (s), 30.06 (s).

5,7-di-tert-butylbenzo[d]oxazole (4ar).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:80). Isolated yield: 92 mg, 40%. Viscous liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.69 (d, J = 1.8 Hz, 1H), 7.37 (d, J = 1.8 Hz, 1H), 1.52 (s, 9H), 1.42 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.00 (s), 147.75 (s), 146.35 (s), 140.35 (s), 134.14 (s), 119.90 (s), 115.00 (s), 114.65 (s), 35.07 (s), 34.42 (s), 31.85 (s), 29.91 (s).

2-(5,7-di-tert-butylbenzo[d]oxazol-2-yl)phenol (4as).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 258 mg, 80%. White solid, mp: 120−122 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.63 (s, 1H), 8.09 (d, J = 7.8 Hz, 1H), 7.66 (s, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.39 (s, 1H), 7.18 (d, J = 8.3

Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H), 1.61 (s, 9H), 1.46 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.33 (s), 158.64 (s), 148.32 (s), 145.38 (s), 140.30 (s), 133.88 (s), 133.21 (s), 126.93 (s), 119.93 (s), 119.47 (s), 117.40 (s), 115.00 (s), 113.57 (s), 110.95 (s), 35.18 (s), 34.57 (s), 31.86 (s), 30.07 (s).

2-(5,7-di-tert-butylbenzo[d]oxazol-2-yl)-4-methylphenol (4at).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 286 mg, 85%. White solid, mp: 107−109 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.44 (s, 1H), 7.82 (s, 1H), 7.63 (d, J = 1.8 Hz, 1H), 7.37 (d, J = 1.8 Hz, 1H), 7.27 (d, J = 8.4 Hz, 1H), 7.06 (d, J = 8.4 Hz, 1H), 2.43 (s, 3H), 1.61 (s, 9H), 1.44 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.45 (s), 156.57 (s), 148.24 (s), 145.36 (s), 140.35 (s), 134.17 (s), 133.83 (s), 128.62 (s), 126.63 (s), 119.80 (s), 117.19 (s), 113.51 (s), 110.48 (s), 35.16 (s), 34.56 (s), 31.85 (s), 30.09 (s), 20.60 (s).

1,3-bis(5,7-di-tert-butylbenzo[d]oxazol-2-yl)benzene (4au).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:90). Isolated yield: 440 mg, 82%. White solid, mp: 189−191 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.15 (s, 1H), 8.47 (dd, J = 7.8, 1.6 Hz, 2H), 7.75 (d, J = 1.8 Hz, 2H), 7.73 (d, J = 7.8 Hz, 1H), 7.41 (d, J = 1.8 Hz, 2H), 1.65 (s, 18H), 1.46 (s, 18H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.58 (s), 148.01 (s), 147.08 (s), 142.40 (s), 133.89 (s), 129.79 (s), 128.51 (s), 126.22 (s), 120.02 (s), 115.00 (s), 114.48 (s), 35.16 (s), 34.59 (s), 31.88 (s), 30.13 (s).

1,4-bis(5,7-di-tert-butylbenzo[d]oxazol-2-yl)benzene (4av).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 482 mg, 90%. White solid, mp: 248−250 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (s, 4H), 7.72 (d, J = 1.8 Hz, 2H), 7.38 (d, J = 1.8 Hz, 2H), 1.60 (s, 18H), 1.44 (s, 18H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.62 (s), 148.10 (s), 147.12 (s), 142.39 (s), 133.91 (s), 129.77 (s), 127.82 (s), 120.12 (s), 114.43 (s), 35.15 (s), 34.55 (s), 31.83 (s), 30.08 (s).

2,4-di-tert-butyl-6-(5,7-di-tert-butylbenzo[d]oxazol-2-yl)phenol (4aw).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 370 mg, 85%. Crystaline solid, mp: 155−157 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.05 (s, 1H), 8.00 (s, 1H), 7.66 (s, 1H), 7.59 (s, 1H), 7.40 (s, 1H), 1.64 (s, 9H), 1.59 (s, 9H), 1.48 (d, J = 5.8 Hz, 18H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.46 (s), 155.78 (s), 148.08 (s), 145.31 (s), 140.97 (s), 140.38 (s), 137.27 (s), 133.70 (s), 128.09 (s), 120.94 (s), 119.61 (s), 115.00 (s),

113.37 (s), 110.10 (s), 35.35 (s), 35.17 (s), 34.56 (s), 34.35 (s), 31.90 (s), 31.51 (s), 30.09 (s), 29.54 (s).

4-(5,7-di-tert-butylbenzo[d]oxazol-2-yl)-2-methoxyphenol (4ax).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:10). Isolated yield: 318 mg, 90%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, J = 7.2 Hz, 2H), 7.66 (s, 1H), 7.32 (s, 1H), 7.09 (d, J = 8.7 Hz, 1H), 6.64 (br s, 1H), 4.01 (s, 3H), 1.58 (s, 9H), 1.42 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.77 (s), 148.95 (s), 147.68 (s), 147.03 (s), 146.82 (s), 142.25 (s), 133.56 (s), 121.50 (s), 119.63 (s), 119.19 (s), 114.84 (s), 113.83 (s), 109.75 (s), 56.15 (s), 35.10 (s), 34.49 (s), 31.86 (s), 30.08 (s).

2-(5,7-di-tert-butylbenzo[d]oxazol-2-yl)benzoic acid (4ay).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:30). Isolated yield: 309 mg, 88%. Crystaline solid, mp: 205−207 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, J = 7.7 Hz, 1H), 8.28 (d, J = 8.9 Hz, 1H), 7.76 – 7.66 (m, 3H), 7.42 (s, 1H), 1.55 (s, 9H), 1.42 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.30 (s), 161.71 (s), 148.94 (s), 146.51 (s), 139.53 (s), 134.35 (s), 133.89 (s), 132.23 (s), 131.68 (s), 130.20 (s), 125.14 (s), 121.04 (s), 115.00 (s), 113.96 (s), 35.24 (s), 34.49 (s), 31.77 (s), 30.01 (s).

2-(2-bromophenyl)-5,7-di-tert-butylbenzo[d]oxazole (4az).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 332 mg, 82%. Crystaline solid, mp: 140−142 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (dd, J = 7.8, 1.6 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.76 (d, J = 1.8 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.42 – 7.36 (m, 2H), 1.59 (s, 9H), 1.44 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.18 (s), 147.90 (s), 147.07 (s), 141.84 (s), 134.67 (s), 134.15 (s), 132.26 (s), 131.78 (s), 128.84 (s), 127.49 (s), 121.67 (s), 119.98 (s), 114.56 (s), 35.16 (s), 34.45 (s), 31.86 (s), 30.03 (s).

5,7-di-tert-butyl-2-(1H-indol-3-yl)benzo[d]oxazole (4ba).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:55). Isolated yield: 284 mg, 82%. White crystaline solid, mp: 208−210 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.81 (s, 1H), 8.52 (d, J = 7.9 Hz, 1H), 8.11 (s, 1H), 7.70 (d, J = 1.7 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.40 (t, J = 7.5 Hz, 1H), 7.37 – 7.30 (m, 2H), 1.65 (s, 9H), 1.45 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.13 (s), 147.54 (s), 146.16 (s), 142.23 (s), 136.50 (s), 133.37 (s), 127.56 (s), 125.04 (s), 123.38 (s), 121.91 (s), 121.20 (s), 118.53 (s), 115.00 (s), 113.29 (s), 111.96 (s), 105.41 (s), 35.13 (s), 34.49 (s), 31.94 (s), 30.15 (s).

4-(5,7-di-tert-butylbenzo[d]oxazol-2-yl)-N,N-diethylaniline (4bb)

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 341 mg, 90%. White solid, mp: 135−140 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 8.7 Hz, 2H), 7.63 (s, 1H), 7.26 (s, 1H), 6.78 (d, J = 8.4 Hz, 2H), 3.47 (q, J = 7.0 Hz, 4H), 1.58 (s, 9H), 1.42 (s, 9H), 1.25 (t, J = 7.0 Hz, 6H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.77 (s), 149.84 (s), 147.16 (s), 146.68 (s), 142.94 (s), 133.15 (s), 129.18 (s), 118.25 (s), 113.57 (s), 111.10 (s), 44.48 (s), 35.07 (s), 34.48 (s), 31.96 (s), 30.13 (s), 12.57 (s).

5-(tert-butyl)-2-(4-chlorophenyl)benzo[d]oxazole (4a'a).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 213 mg, 75%. Colorless liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (d, J = 8.6 Hz, 2H), 7.68 (d, J = 8.4 Hz, 1H), 7.60 (s, 1H), 7.49 (d, J = 8.6 Hz, 2H), 7.43 (d, J = 8.4 Hz, 1H), 1.40 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.91 (s), 151.05 (s), 149.60 (s), 139.64 (s), 137.50 (s), 129.26 (s), 128.69 (s), 125.91 (s), 122.48 (s), 119.17 (s), 107.36 (s), 35.23 (s), 31.69 (s).

5-(tert-butyl)-2-(3-fluorophenyl)benzo[d]oxazole (4a'b).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 188 mg, 70%. Viscous liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.56 (d, J = 7.8 Hz, 1H), 8.37 (dd, J = 8.2, 2.1 Hz, 1H), 7.84 (d, J = 1.6 Hz, 1H), 7.72 (t, J = 8.0 Hz, 1H), 7.55 (d, J = 8.6 Hz, 1H), 7.50 (dd, J = 8.6, 1.8 Hz, 1H), 1.43 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.64 (s), 148.90 (s), 148.78 (s), 141.71 (s), 132.88 (s), 130.09 (s), 129.09 (s), 125.59 (s), 123.93 (s), 122.33 (s), 116.90 (s), 115.00 (s), 110.02 (s), 35.02 (s), 31.74 (s).

5-(tert-butyl)-2-(3-nitrophenyl)benzo[d]oxazole (4a'c).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:80). Isolated yield: 213 mg, 72%. Crystaline solid, mp: 156−158 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.04 (s, 1H), 8.53 (d, J = 7.8 Hz, 1H), 8.34 (dd, J = 7.8, 1.7 Hz, 1H), 7.70 (t, J = 8.5 Hz, 2H), 7.64 (d, J = 1.5 Hz, 1H), 7.47 (dd, J = 8.4, 1.7 Hz, 1H), 1.43 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.32 (s), 151.12 (s), 150.39 (s), 148.64 (s), 139.40 (s), 132.77 (s), 130.05 (s), 125.48 (s), 122.90 (s), 122.22 (s), 119.55 (s), 115.00 (s), 107.53 (s), 35.31 (s), 31.65 (s).

5-(tert-butyl)-2-(naphthalen-1-yl)benzo[d]oxazole (4a'd).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 183 mg, 61%. Pale yellow liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.48 (dd, J = 12.3, 8.7 Hz, 1H), 8.34 (d, J = 7.3 Hz, 1H), 7.93 – 7.74 (m, 3H), 7.72 – 7.56 (m, 2H), 7.55 – 7.43 (m, 2H), 7.40 (td, J = 10.2, 1.8 Hz, 1H), 1.38 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.74 (s), 149.48 (s), 140.12 (s), 134.05 (s), 132.12 (s), 129.15 (s), 128.72 (s), 127.91 (s), 126.50 (s), 126.47 (s),

125.01 (s), 124.99 (s), 122.30 (s), 119.50 (s), 116.86 (s), 109.75 (s), 107.31 (s), 35.30 (s), 31.83 (s).

5-(tert-butyl)-2-(4-methoxyphenyl)benzo[d]oxazole (4a'e).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 191 mg, 68%. Light brown solid, mp: 105−107 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, J = 8.8 Hz, 2H), 7.68 (d, J = 8.4 Hz, 1H), 7.61 (d, J = 1.5 Hz, 1H), 7.42 (dd, J = 8.4, 1.7 Hz, 1H), 7.04 (d, J = 8.8 Hz, 2H), 3.90 (s, 3H), 1.42 (s, 9H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.02 (s), 162.15 (s), 150.94 (s), 148.73 (s), 139.90 (s), 129.20 (s), 122.06 (s), 119.98 (s), 118.71 (s), 114.34 (s), 107.17 (s), 55.44 (s), 35.15 (s), 31.74 (s).

2-(4-methoxyphenyl)-5-methylbenzo[d]oxazole (4a'f).

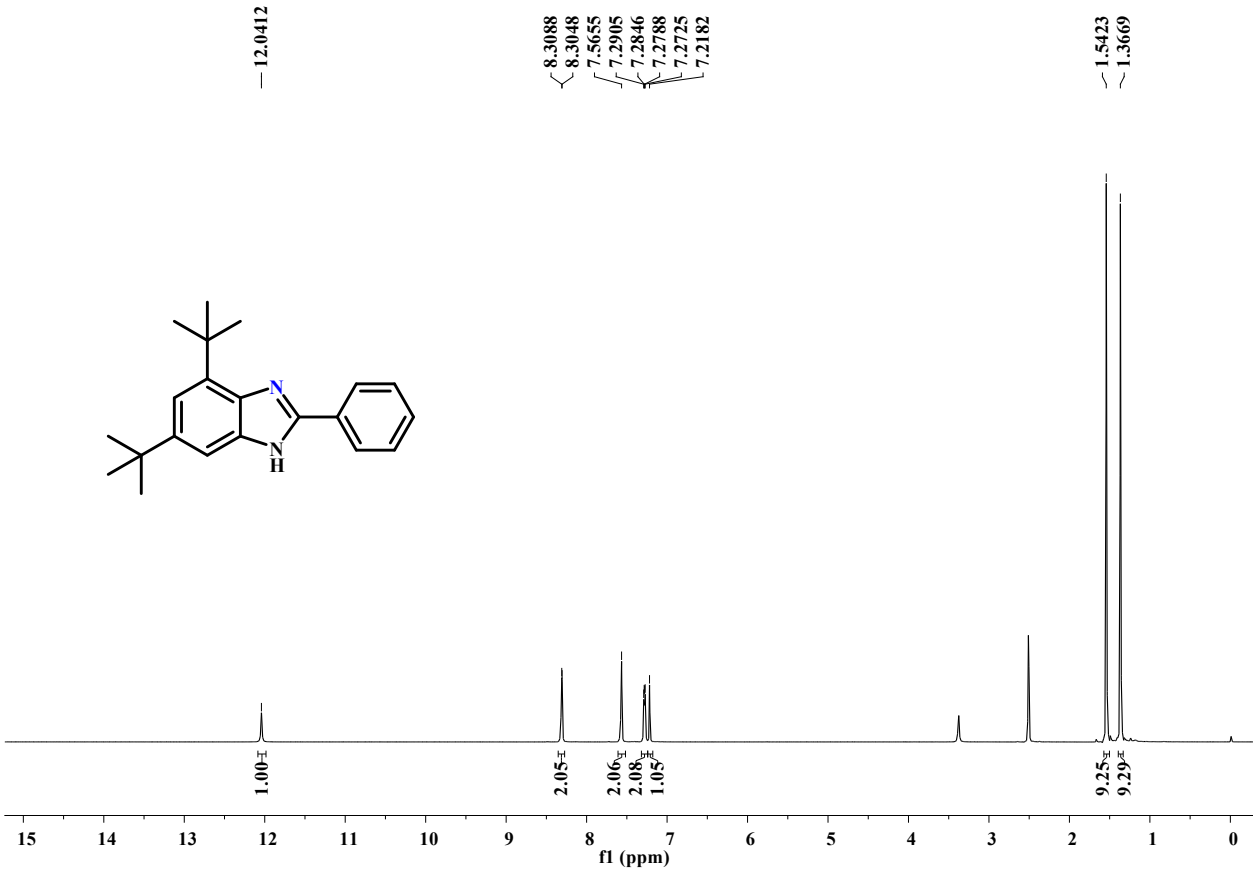
Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:100). Isolated yield: 124 mg, 52%. White solid, mp: 107−109 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, J = 8.9 Hz, 2H), 7.54 (s, 1H), 7.44 (d, J = 8.3 Hz, 1H), 7.14 (d, J = 9.2 Hz, 1H), 7.04 (d, J = 8.9 Hz, 2H), 3.91 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 163.27 (s), 162.23 (s), 148.93 (s), 142.49 (s), 134.20 (s), 129.31 (s), 125.67 (s), 119.59 (s), 115.00 (s), 114.32 (s), 109.72 (s), 55.44 (s), 21.52 (s).

5-methyl-2-(3-nitrophenyl)benzo[d]oxazole (4a'g).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (1:90). Isolated yield: 127 mg, 50%. White solid, mp: 174−176 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.57 (d, J = 7.8 Hz, 1H), 8.38 (dd, J = 8.2, 1.2 Hz, 1H), 7.73 (t, J = 8.0 Hz, 1H), 7.60 (s, 1H), 7.51 (d, J = 8.3 Hz, 1H), 7.24 (d, J = 7.4 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.61 (s), 149.13 (s), 148.68 (s), 141.99 (s), 135.05 (s), 132.92 (s), 130.05 (s), 129.10 (s), 127.25 (s), 125.61 (s), 122.38 (s), 120.32 (s), 110.23 (s), 21.52 (s).

4,6-di-tert-butyl-2-phenyl-1H-benzo[d]imidazole (5a).

Purified by silica gel column chromatography with ethyl acetate/petroleum ether (10:90). Isolated yield: 215 mg, 70%. semisolid; ^{1}H NMR (500 MHz, DMSO) δ 12.04 (s, 1H), 8.31 (d, J = 2.0 Hz, 2H), 7.57 (s, 2H), 7.28 (dd, J = 6.0, 3.0 Hz, 2H), 7.22 (s, 1H), 1.54 (s, 9H), 1.37 (s, 9H); ^{13}C NMR (126 MHz, DMSO) δ 160.96 (s), 147.20 (s), 145.76 (s), 142.92 (s), 137.12 (s), 133.00 (s), 129.44 (s), 125.12 (s), 123.13 (s), 121.62 (s), 120.73 (s), 118.10 (s), 113.60 (s), 112.98 (s), 103.61 (s), 35.17 (s), 34.49 (s), 32.14 (s), 30.29 (s) (Figure S12-S13).



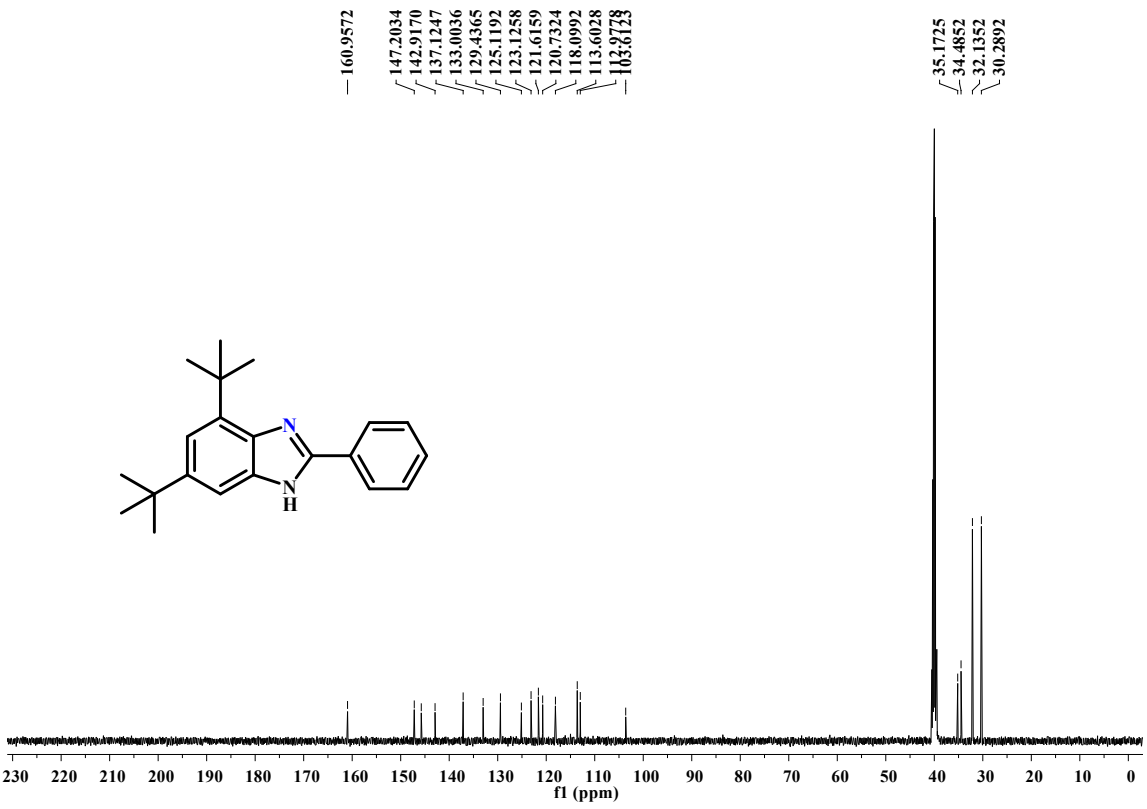


Figure S15. ^{1}H NMR spectrum of compound **5a** in DMSO-d6 (500 MHz).

Figure S16. ^{13}C NMR spectrum of compound **5a** in DMSO-d6 (500 MHz).

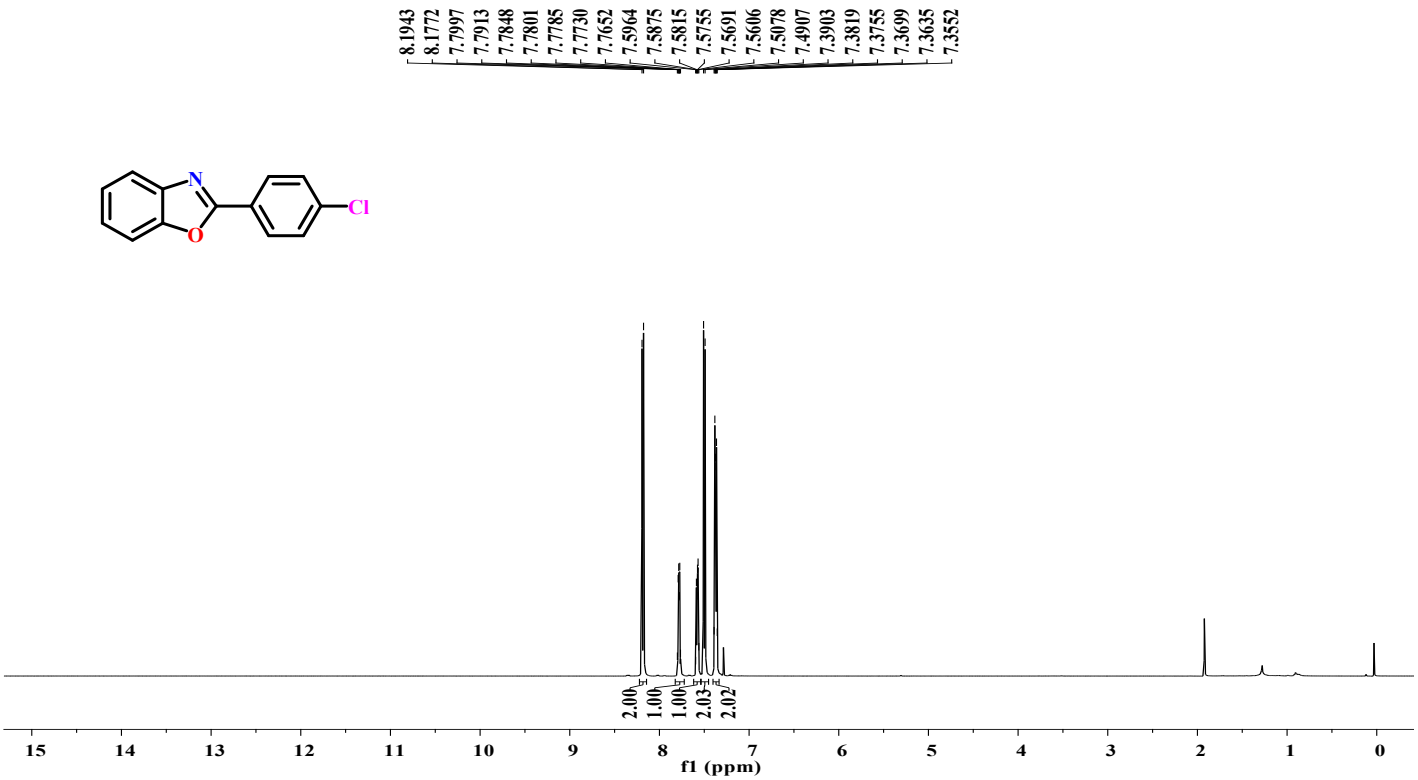


Figure S17. ^{1}H NMR spectrum of compound **7aa** in $CDCl_3$ (500 MHz).

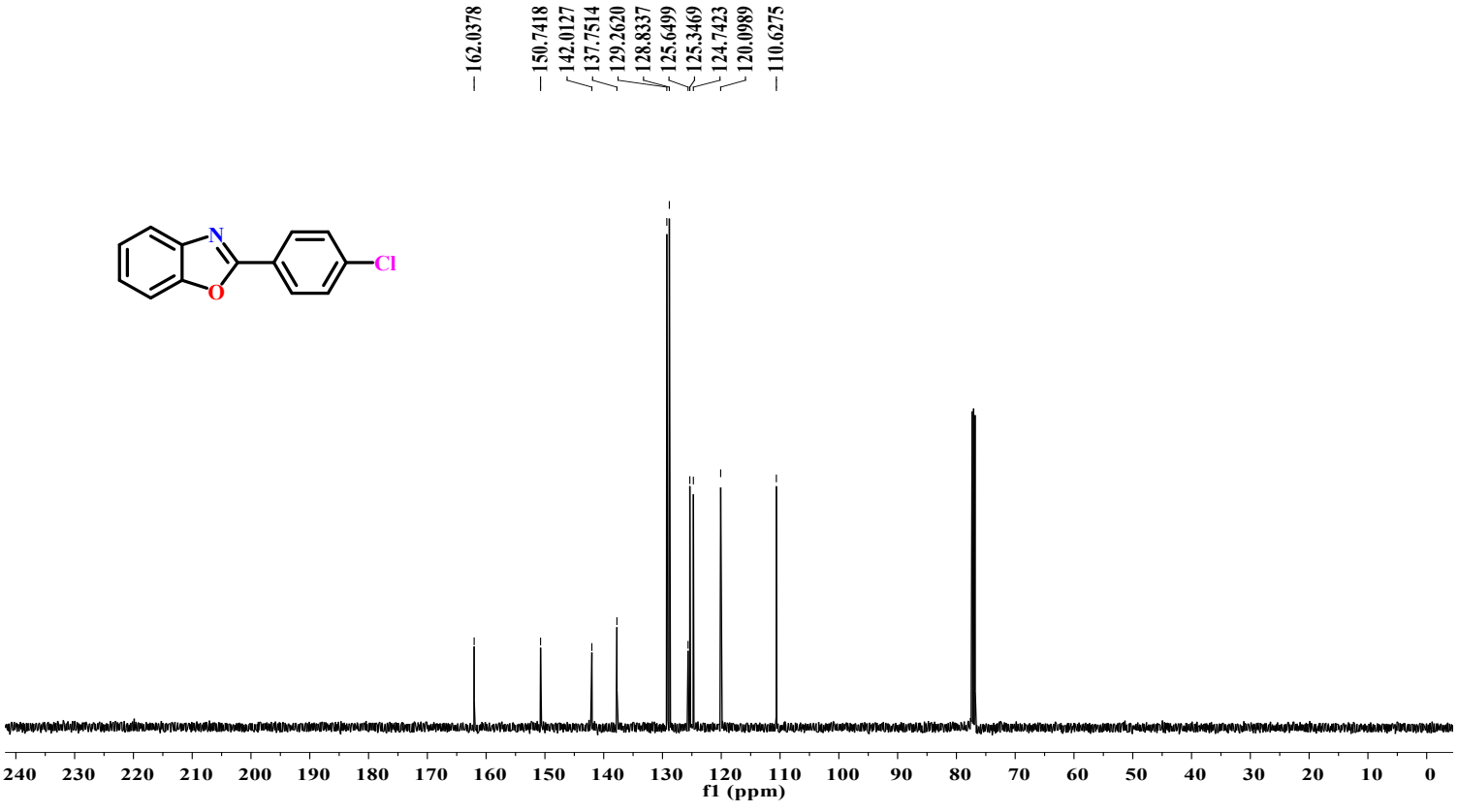


Figure S18. ^{13}C NMR spectrum of compound **7aa** in $CDCl_3$ (500 MHz).

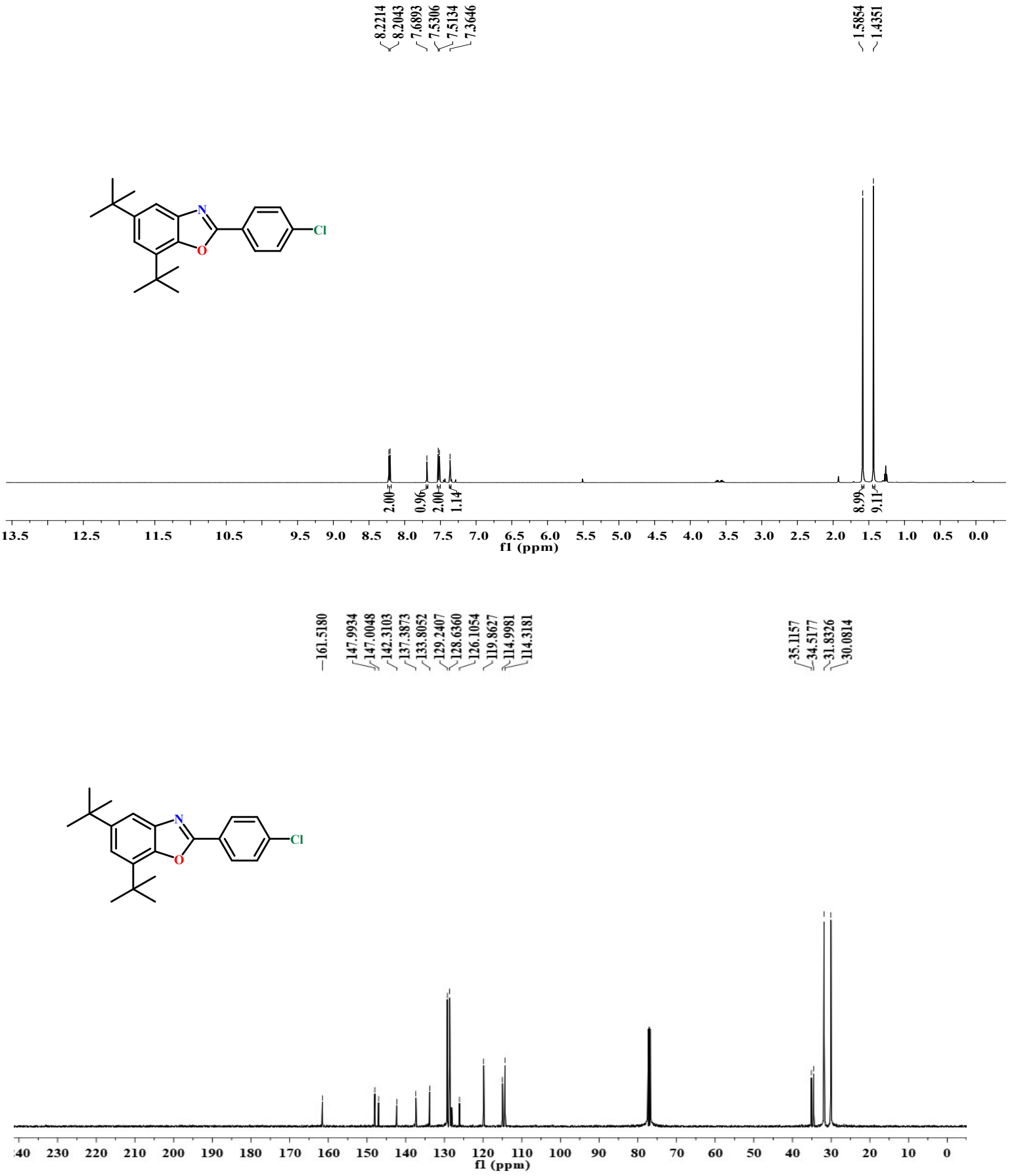


Figure S19. ^{1}H NMR spectrum of compound 4aa in $CDCl_3$ (500 MHz).

Figure S20. ^{13}C NMR spectrum of compound 4aa in $CDCl_3$ (500 MHz).

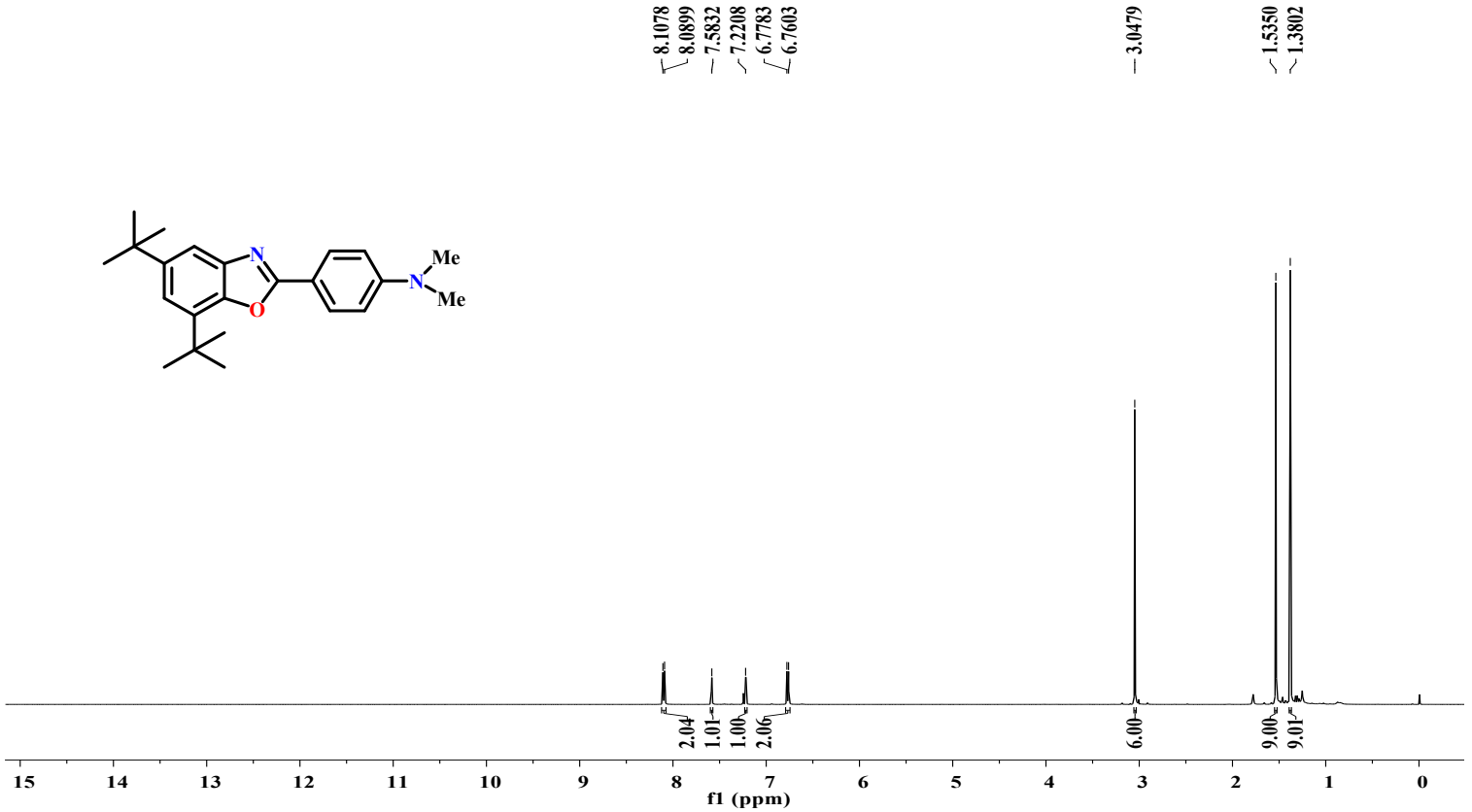


Figure S21. ^{1}H NMR spectrum of compound 4ab in $CDCl_3$ (500 MHz).

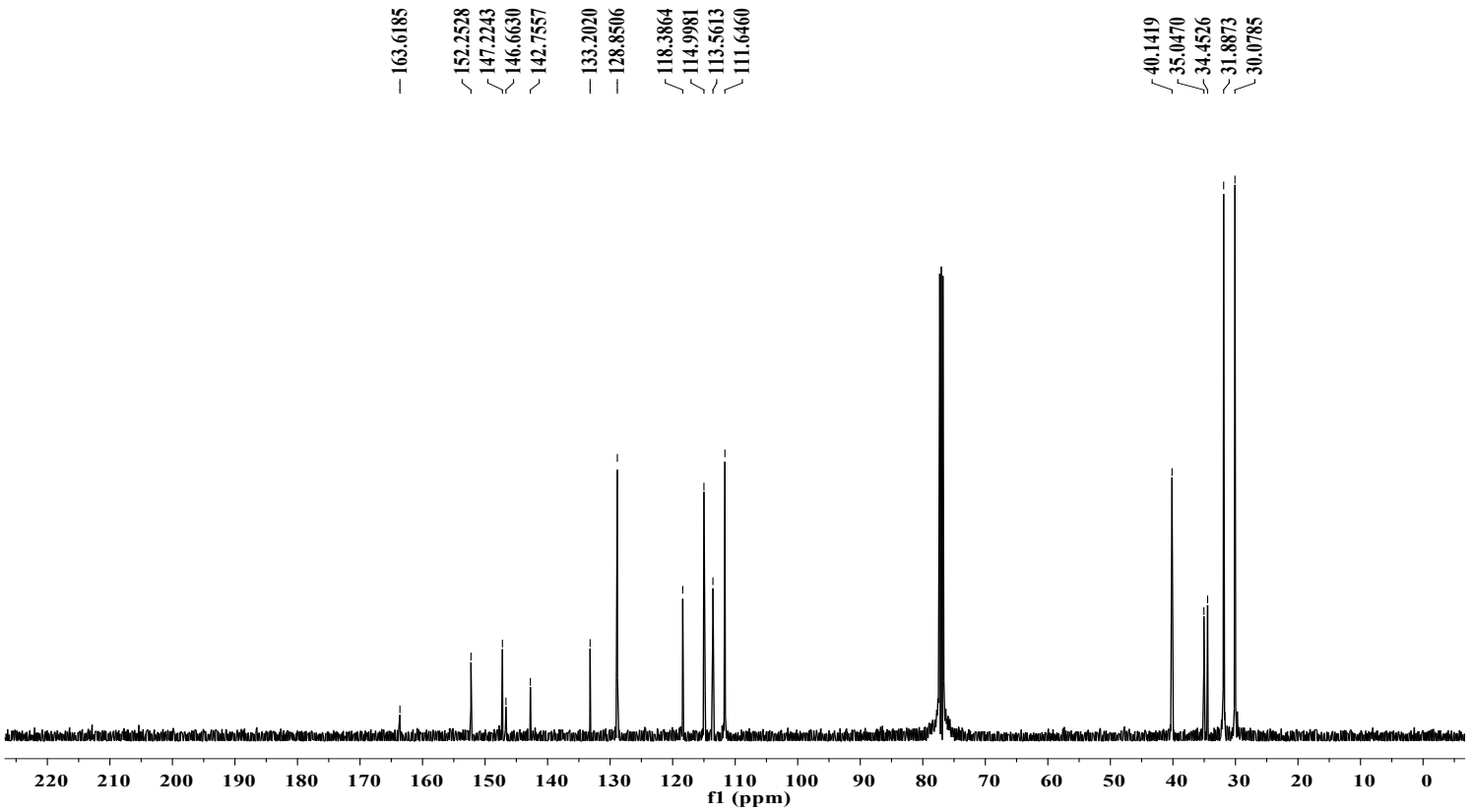


Figure S22. ^{13}C NMR spectrum of compound 4ab in $CDCl_3$ (500 MHz).

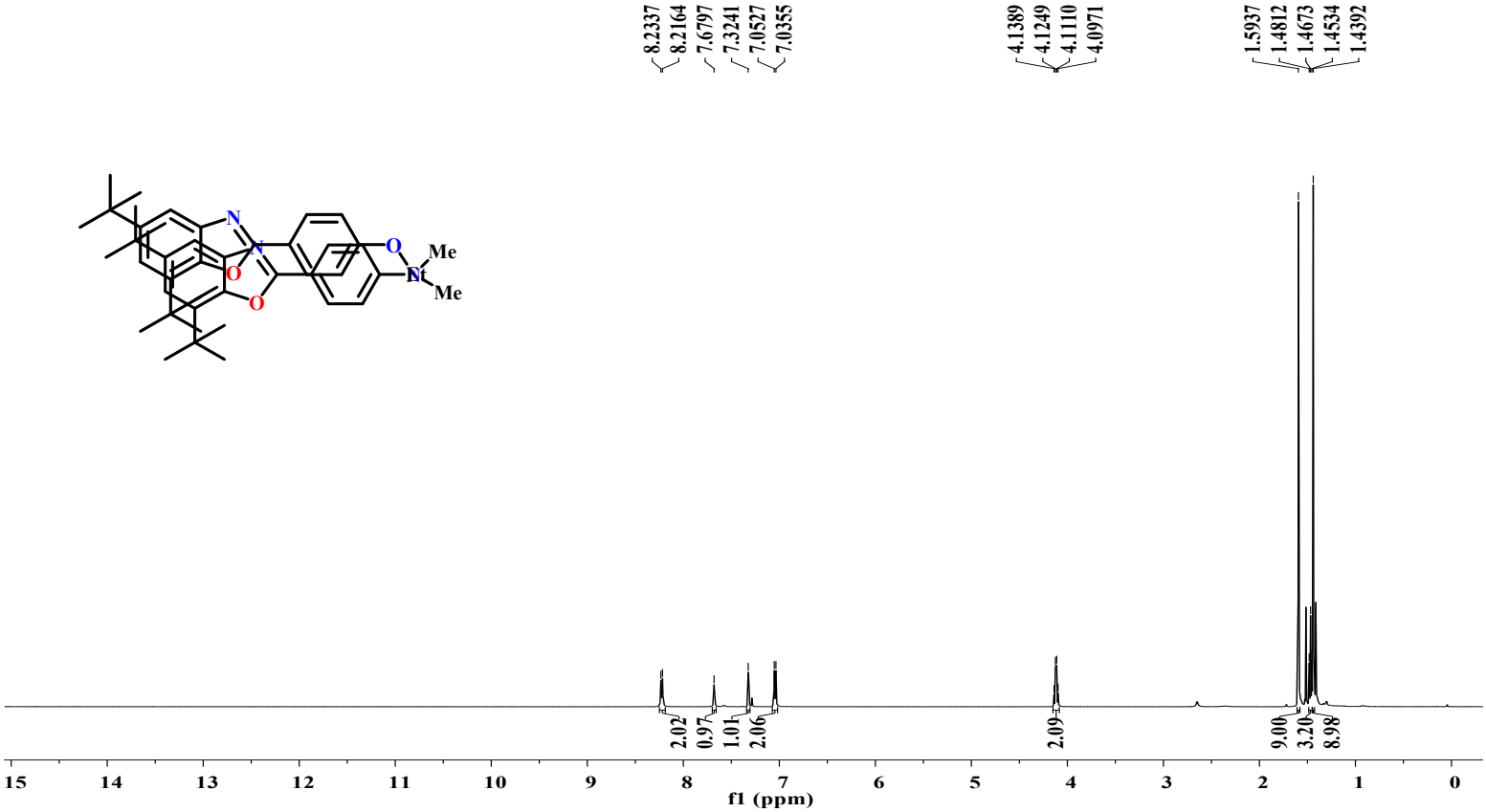


Figure S23. ^{1}H NMR spectrum of compound 4ac in $CDCl_3$ (500 MHz).

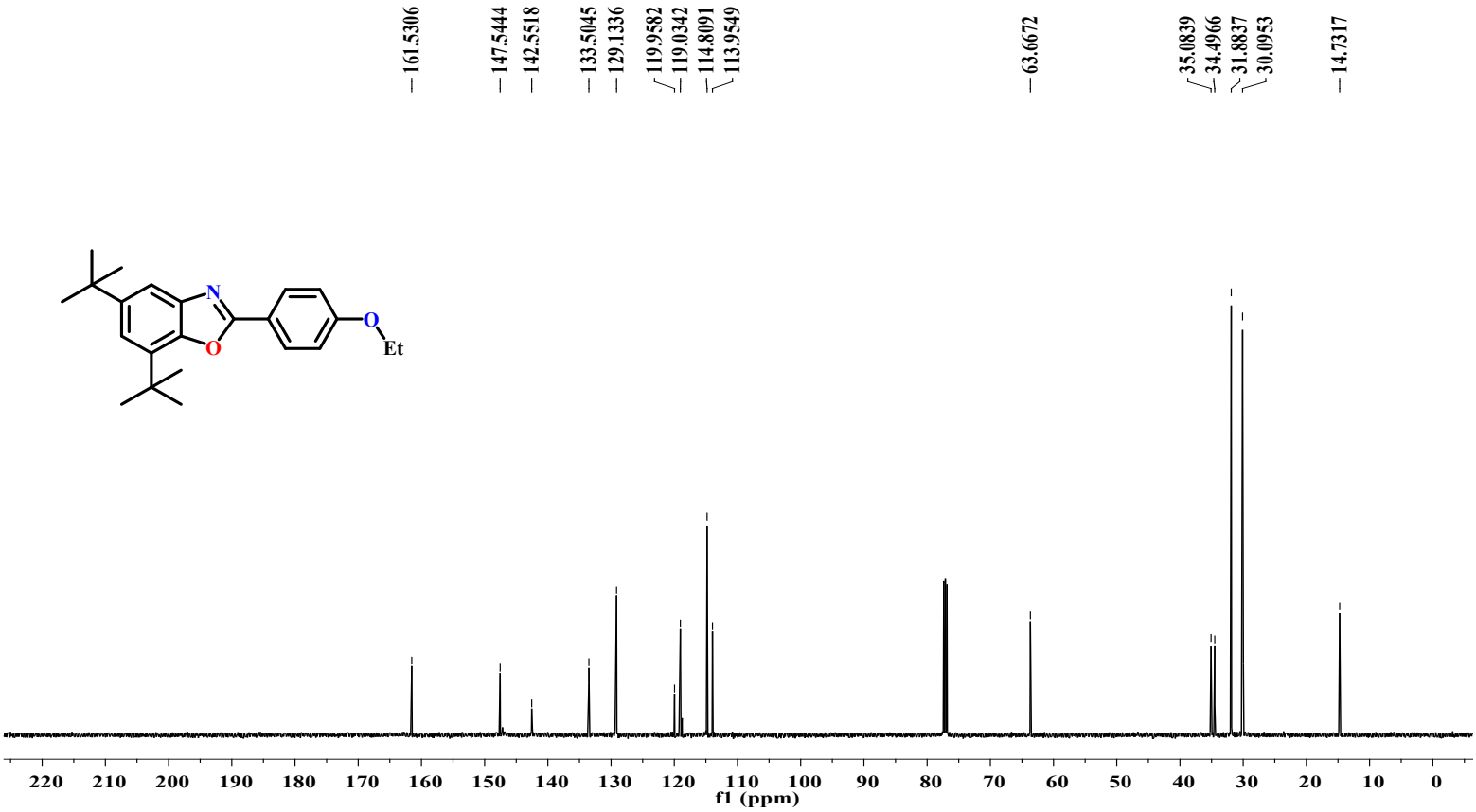


Figure S24. ^{1}H NMR spectrum of compound 4ac in $CDCl_3$ (500 MHz).

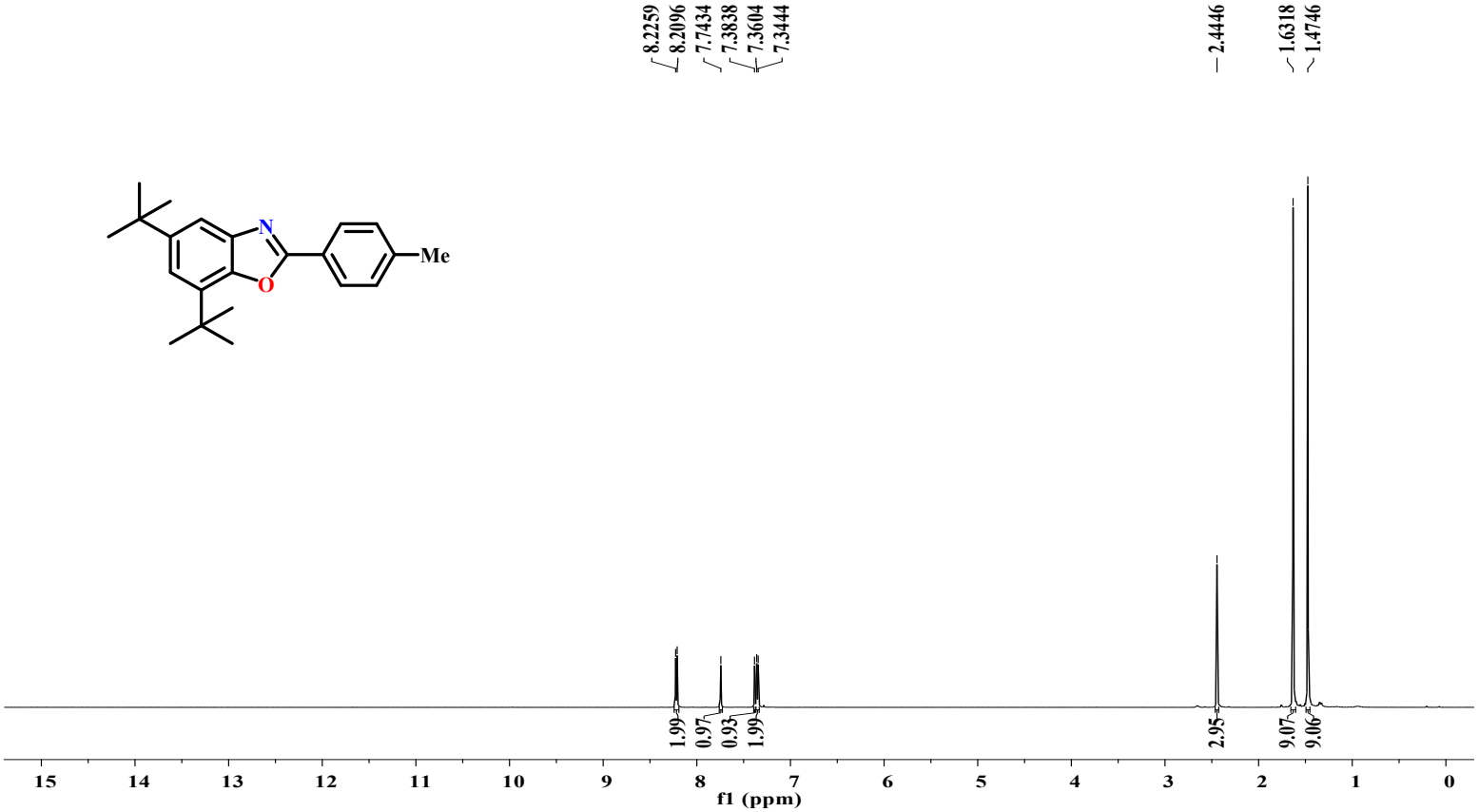


Figure S25. ^{1}H NMR spectrum of compound 4ad in $CDCl_3$ (500 MHz).

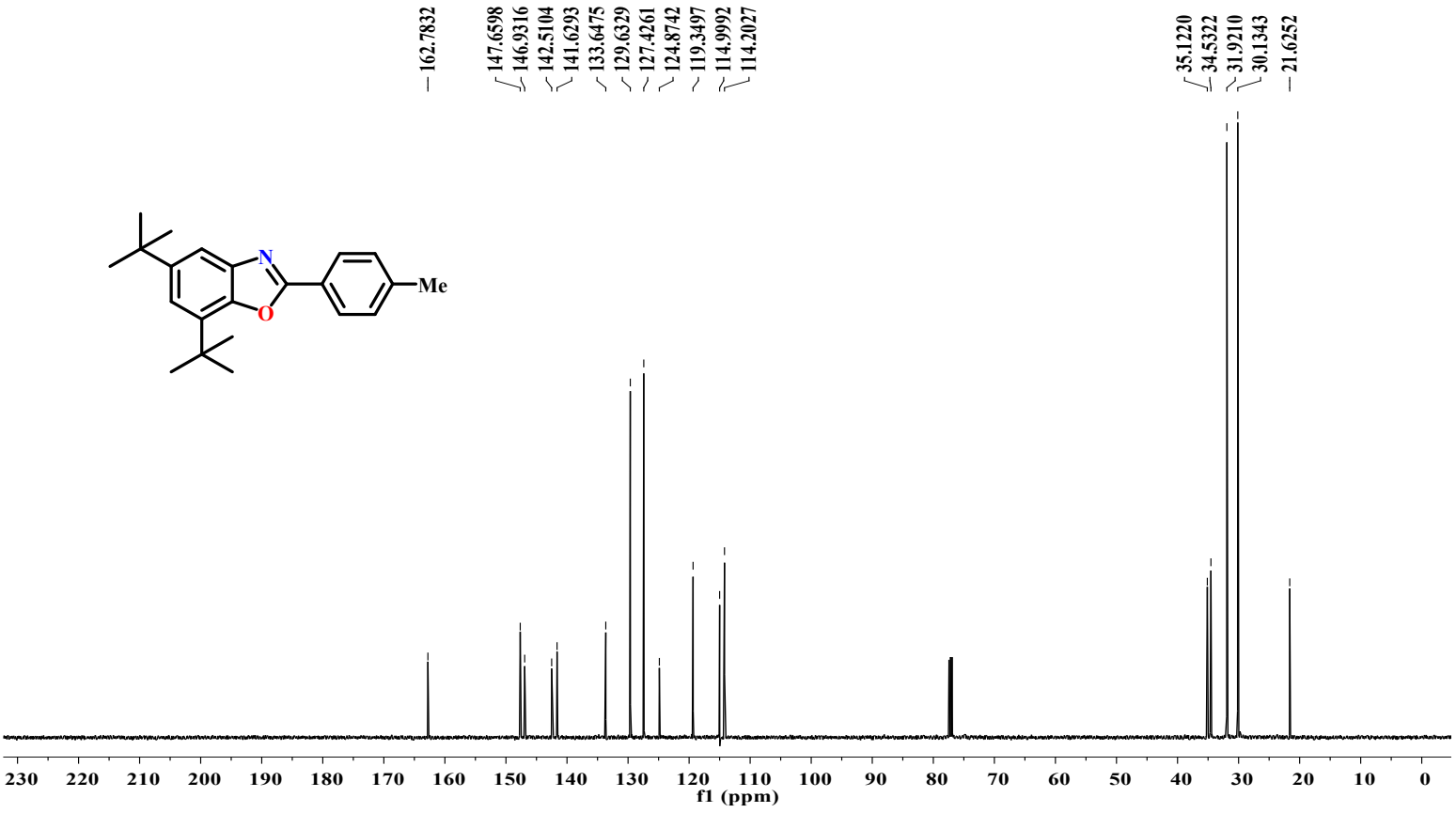


Figure S26. ^{13}C NMR spectrum of compound 4ad in $CDCl_3$ (500 MHz).

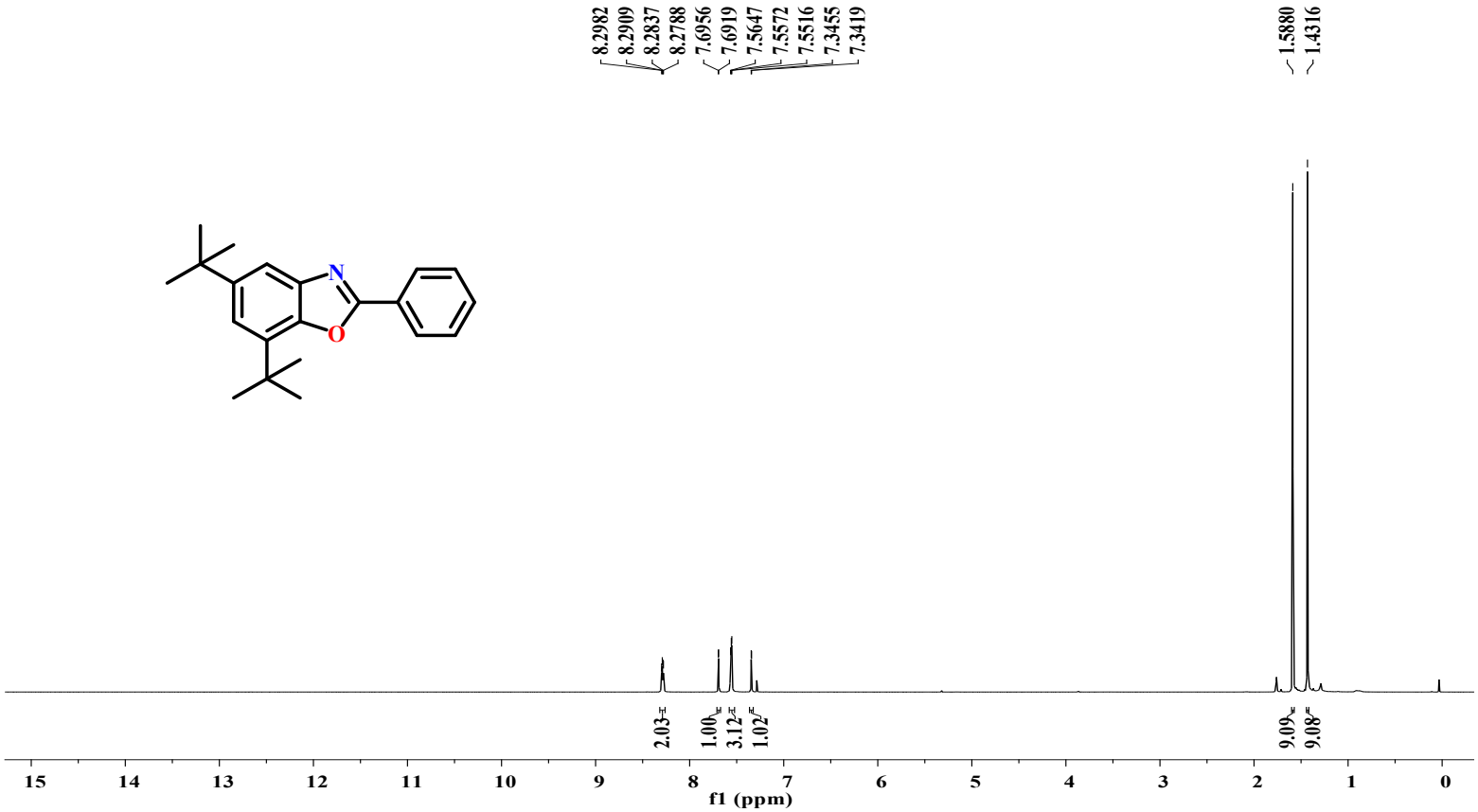


Figure S27. ^{1}H NMR spectrum of compound 4ae in $CDCl_3$ (500 MHz).

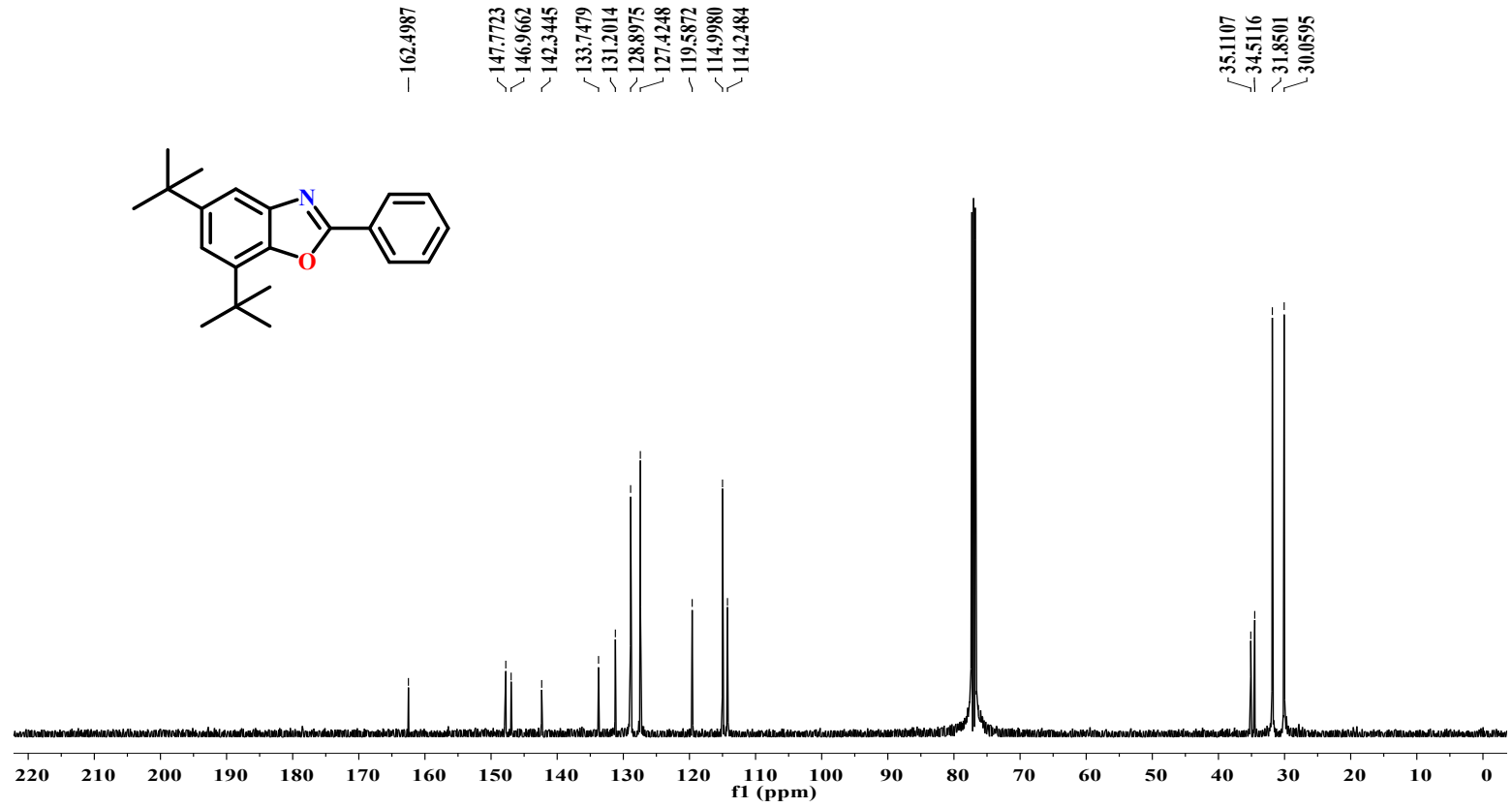
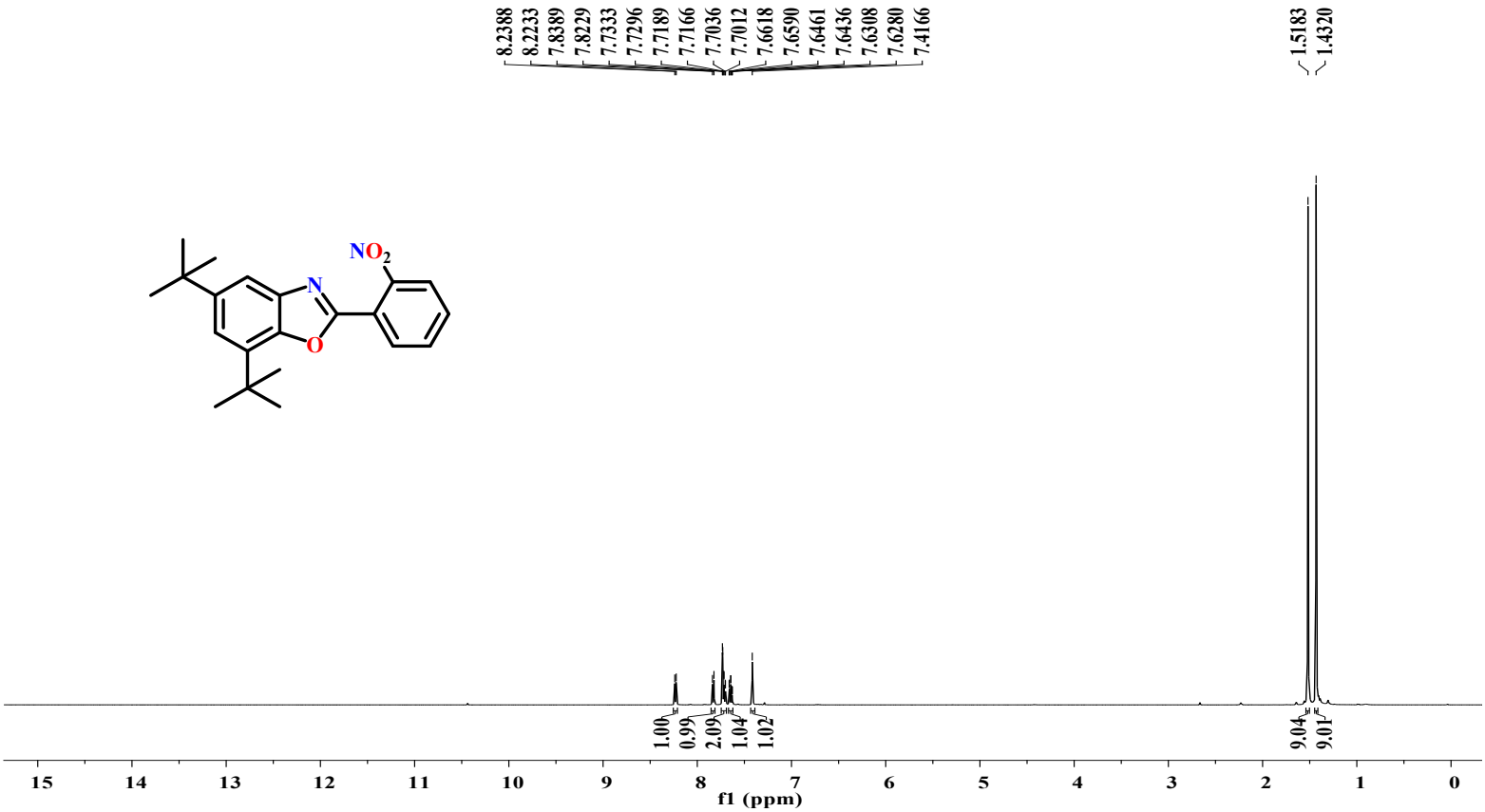


Figure S28. ^{13}C NMR spectrum of compound 4ae in $CDCl_3$ (500 MHz).



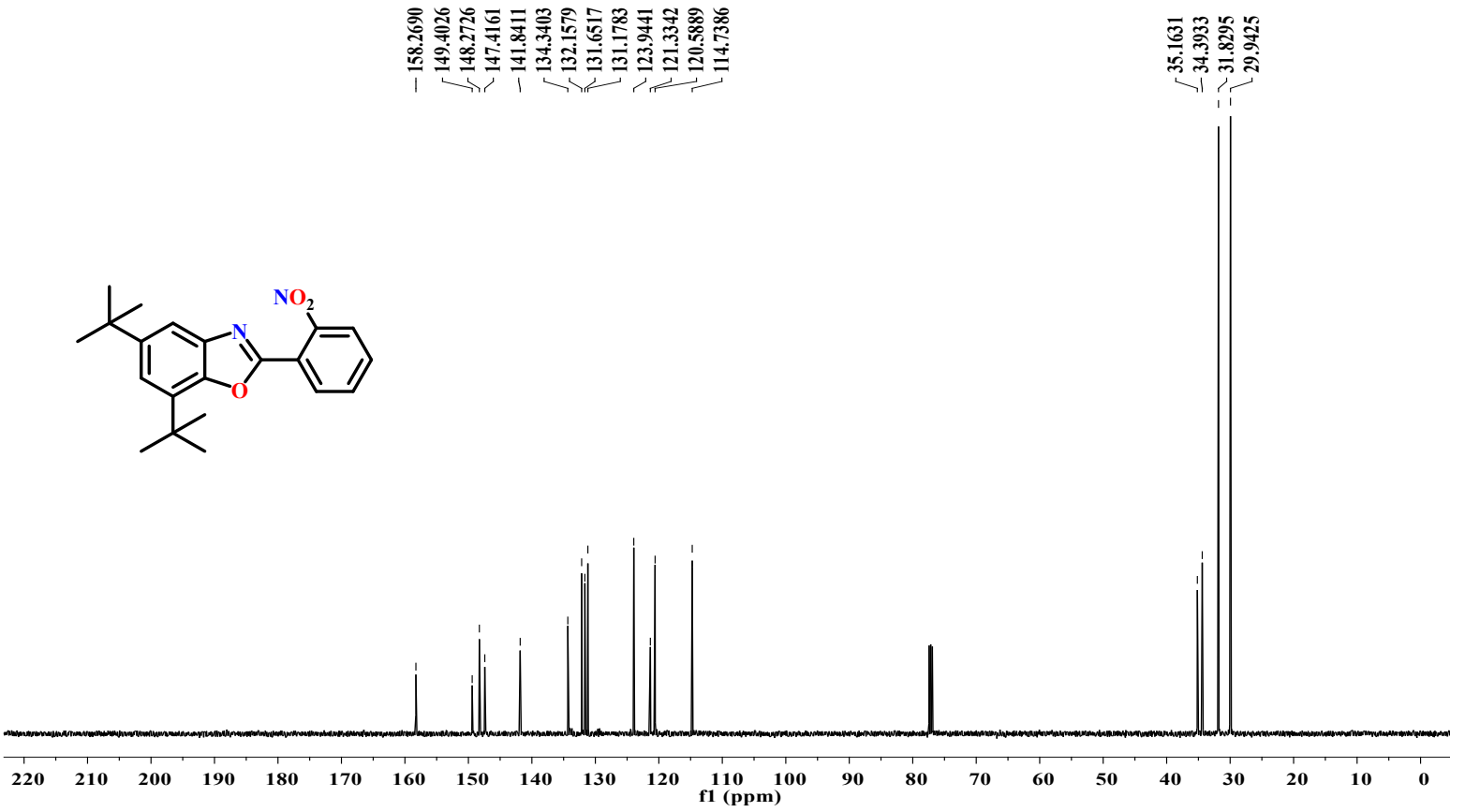


Figure S29. ^{1}H NMR spectrum of compound 4af in $CDCl_3$ (500 MHz).

Figure S30. ^{13}C NMR spectrum of compound 4af in $CDCl_3$ (500 MHz).

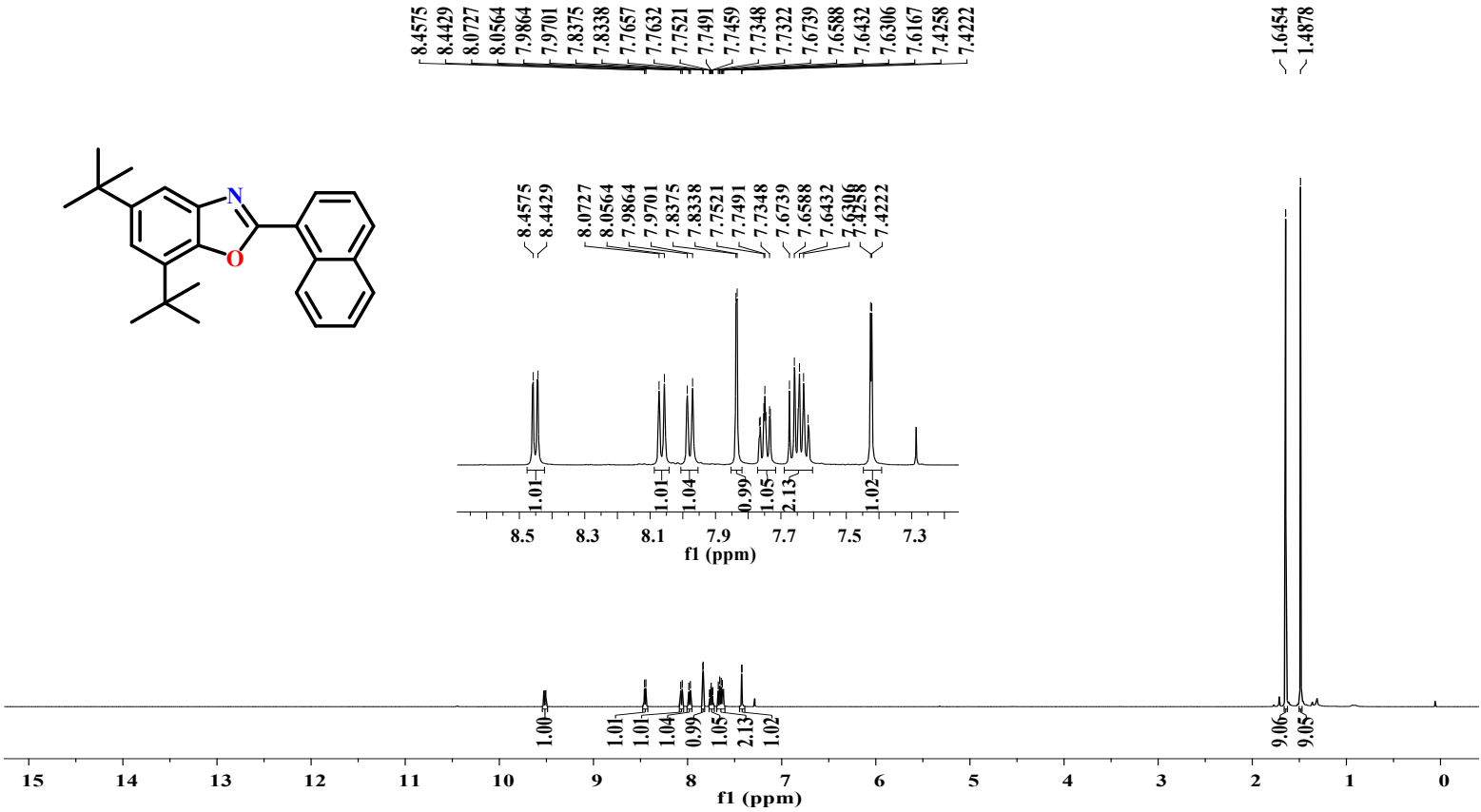


Figure S31. ^{1}H NMR spectrum of compound 4ag in $CDCl_3$ (500 MHz).

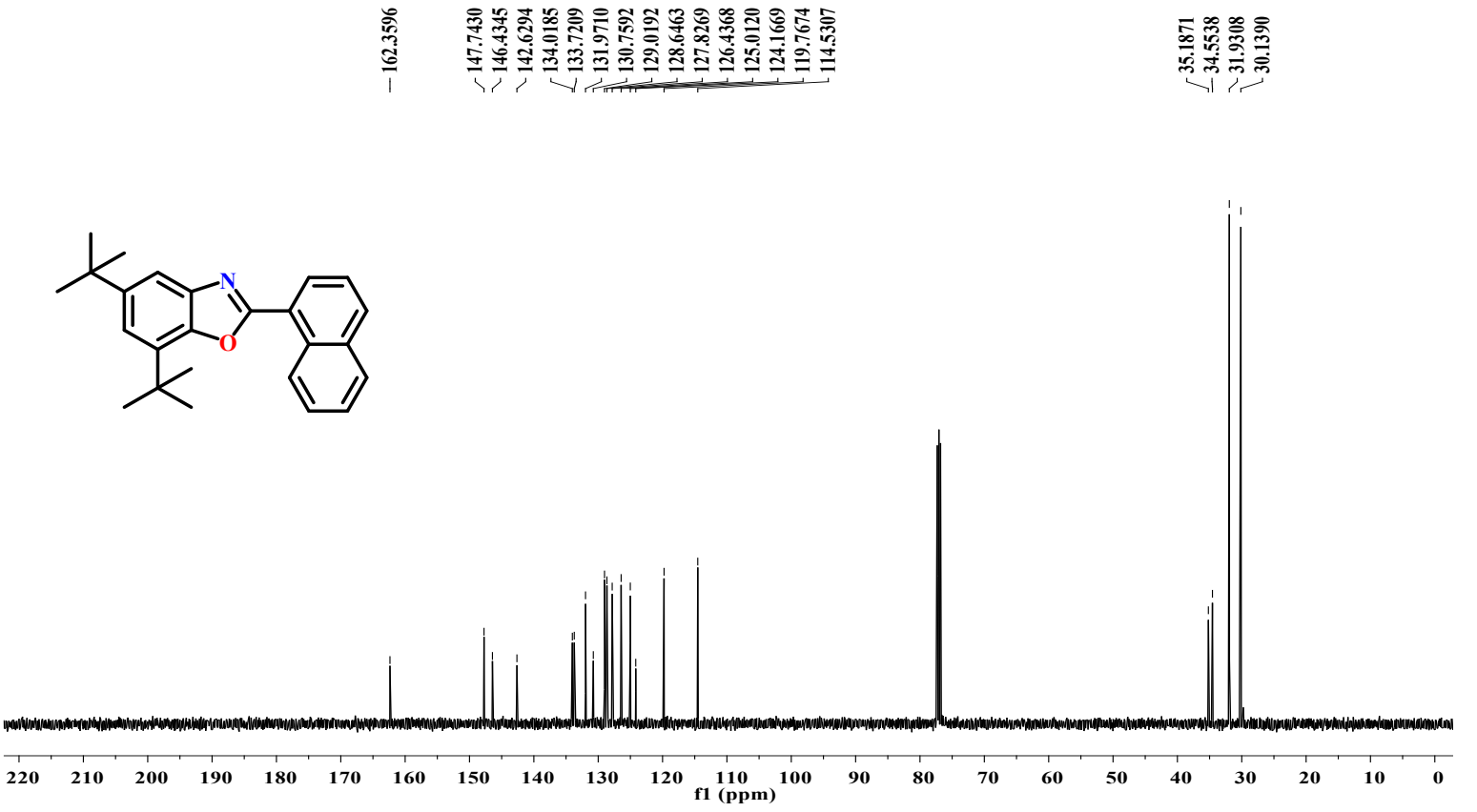


Figure S32. ^{13}C NMR spectrum of compound 4ag in $CDCl_3$ (500 MHz).

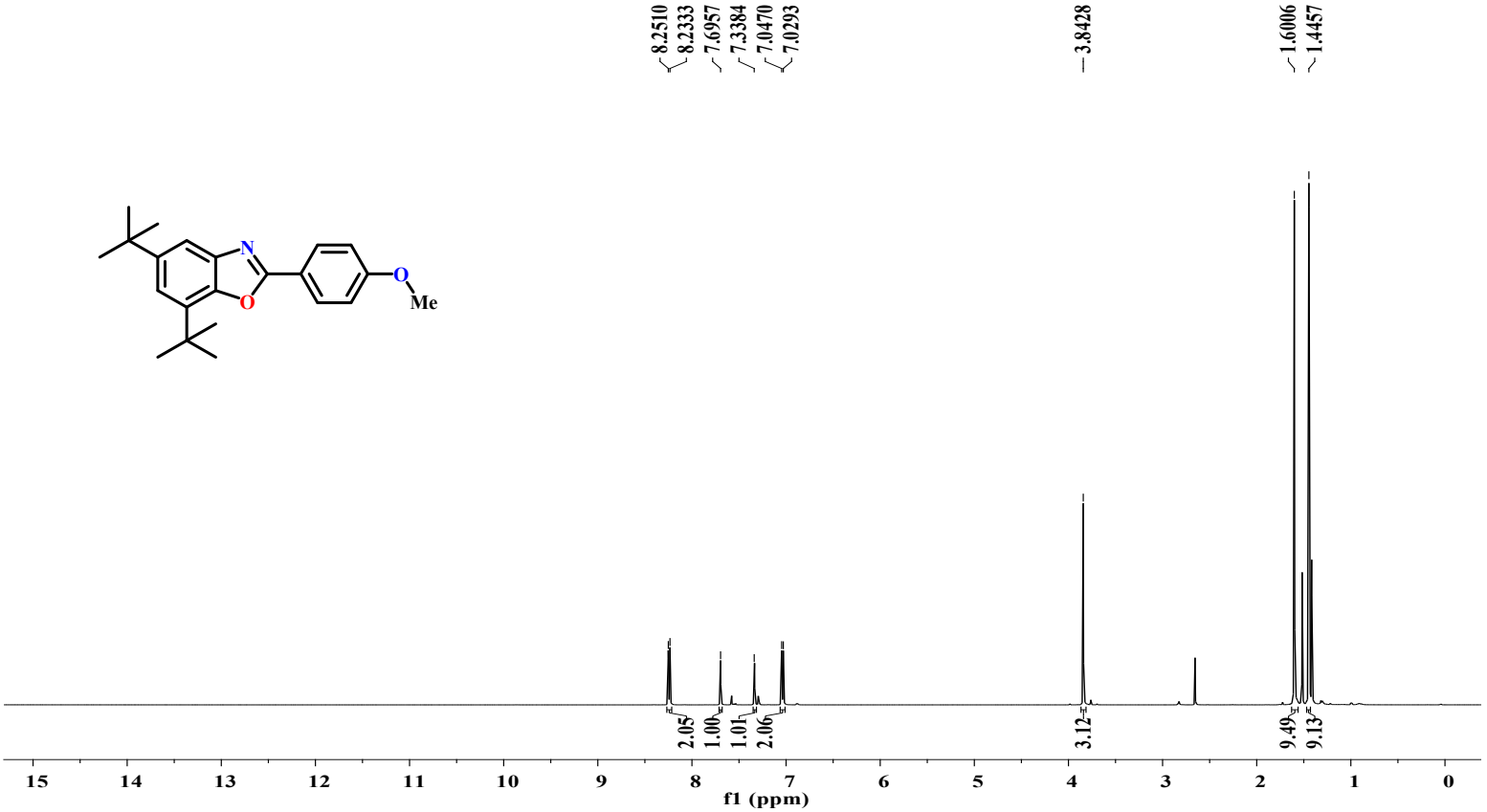


Figure S33. ^{1}H NMR spectrum of compound 4ah in $CDCl_3$ (500 MHz).

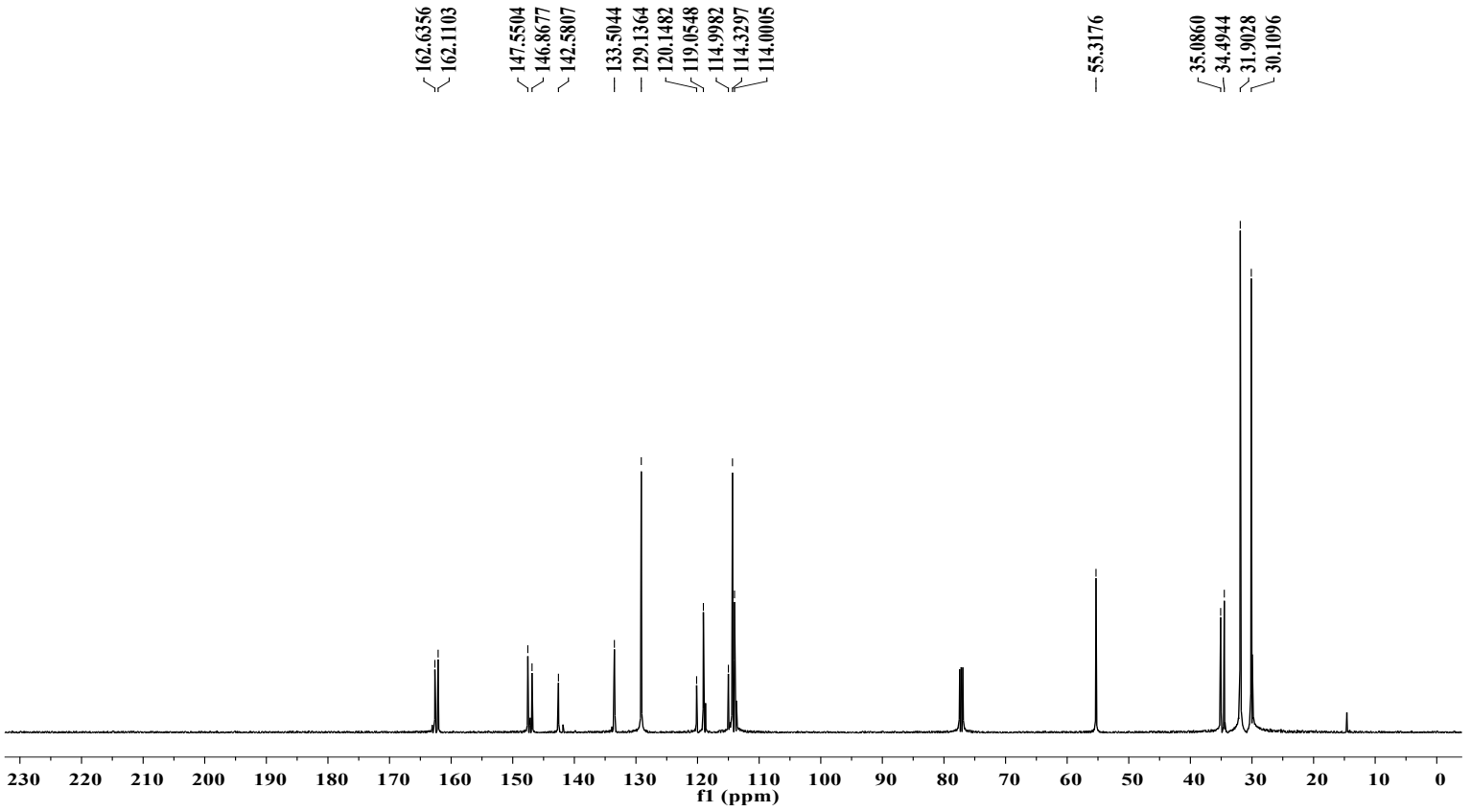


Figure S34. ^{13}C NMR spectrum of compound 4ah in $CDCl_3$ (500 MHz).

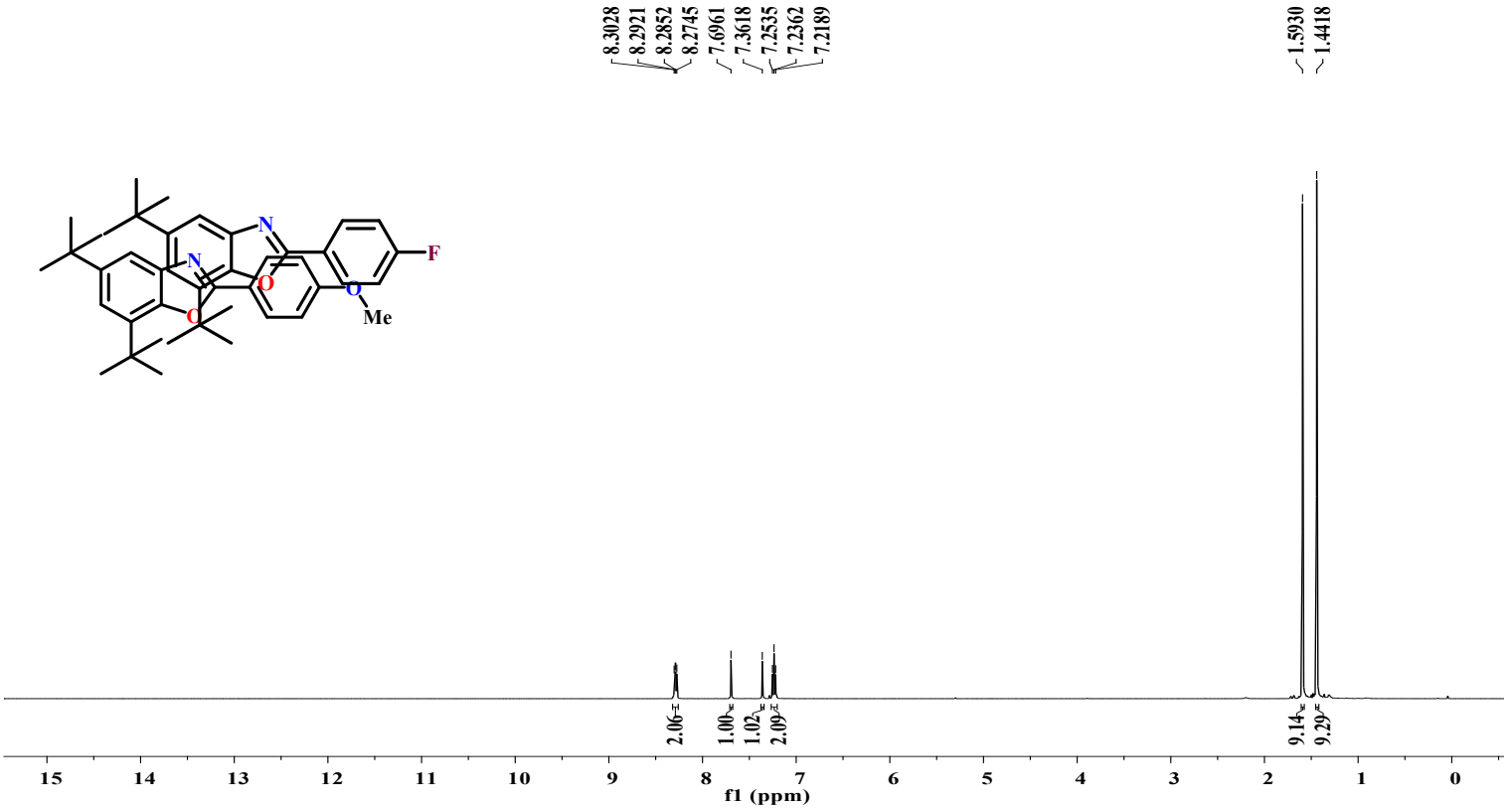


Figure S35. ^{1}H NMR spectrum of compound 4ai in $CDCl_3$ (500 MHz).

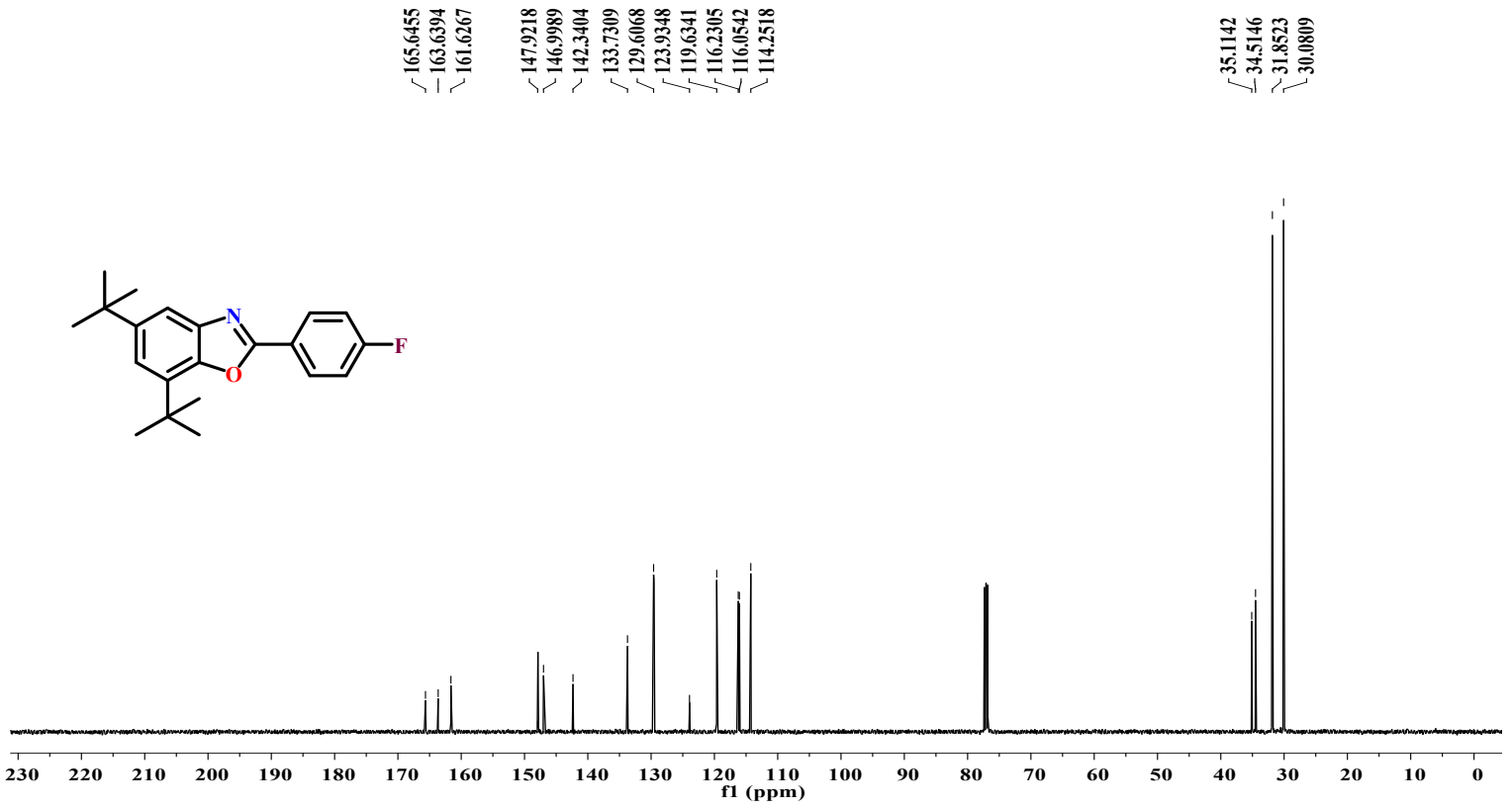


Figure S36. ^{13}C NMR spectrum of compound 4ai in $CDCl_3$ (500 MHz).

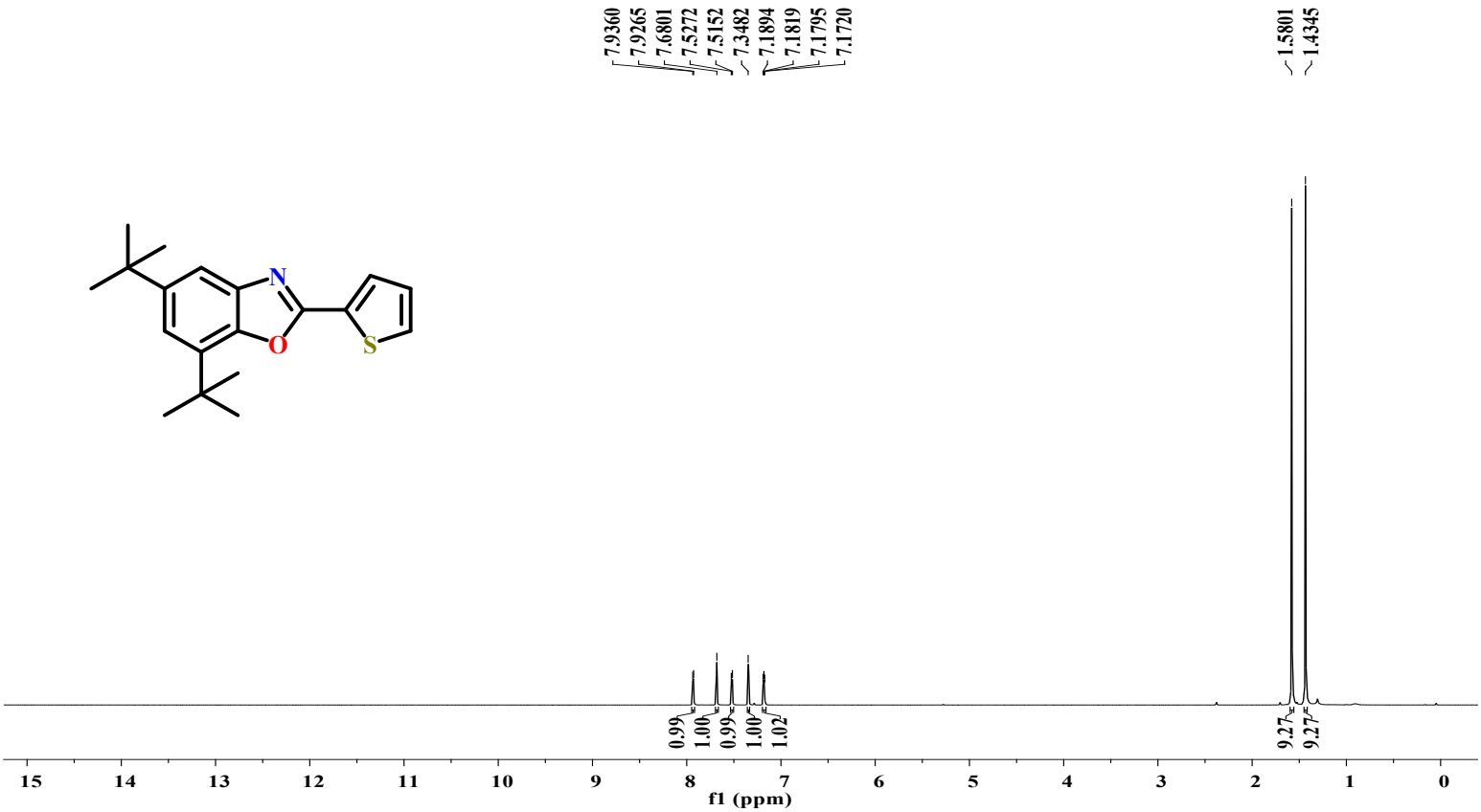


Figure S37. ^{1}H NMR spectrum of compound 4aj in $CDCl_3$ (500 MHz).

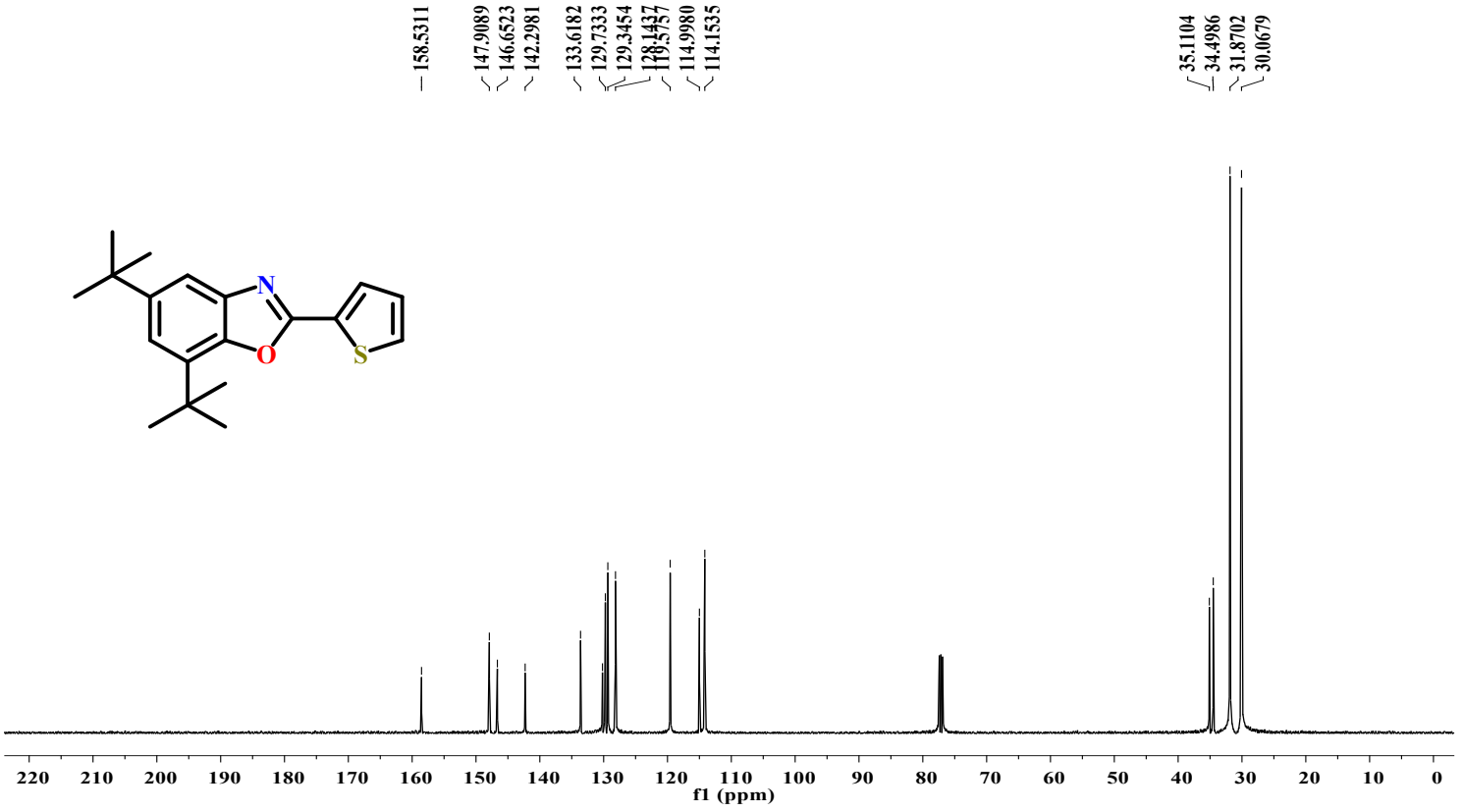


Figure S38. ^{13}C NMR spectrum of compound 4aj in $CDCl_3$ (500 MHz).

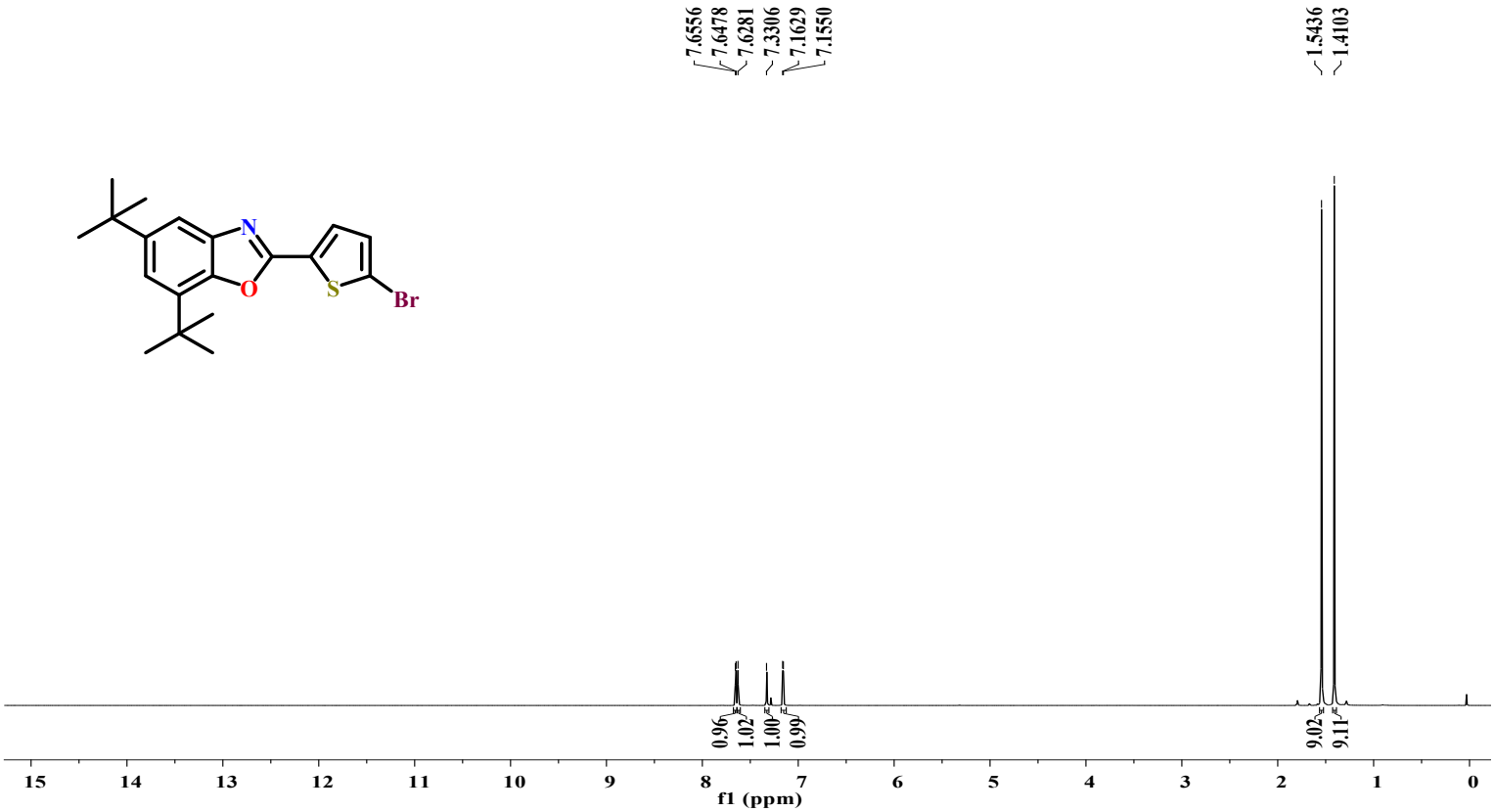


Figure S39. ^{1}H NMR spectrum of compound 4ak in $CDCl_3$ (500 MHz).

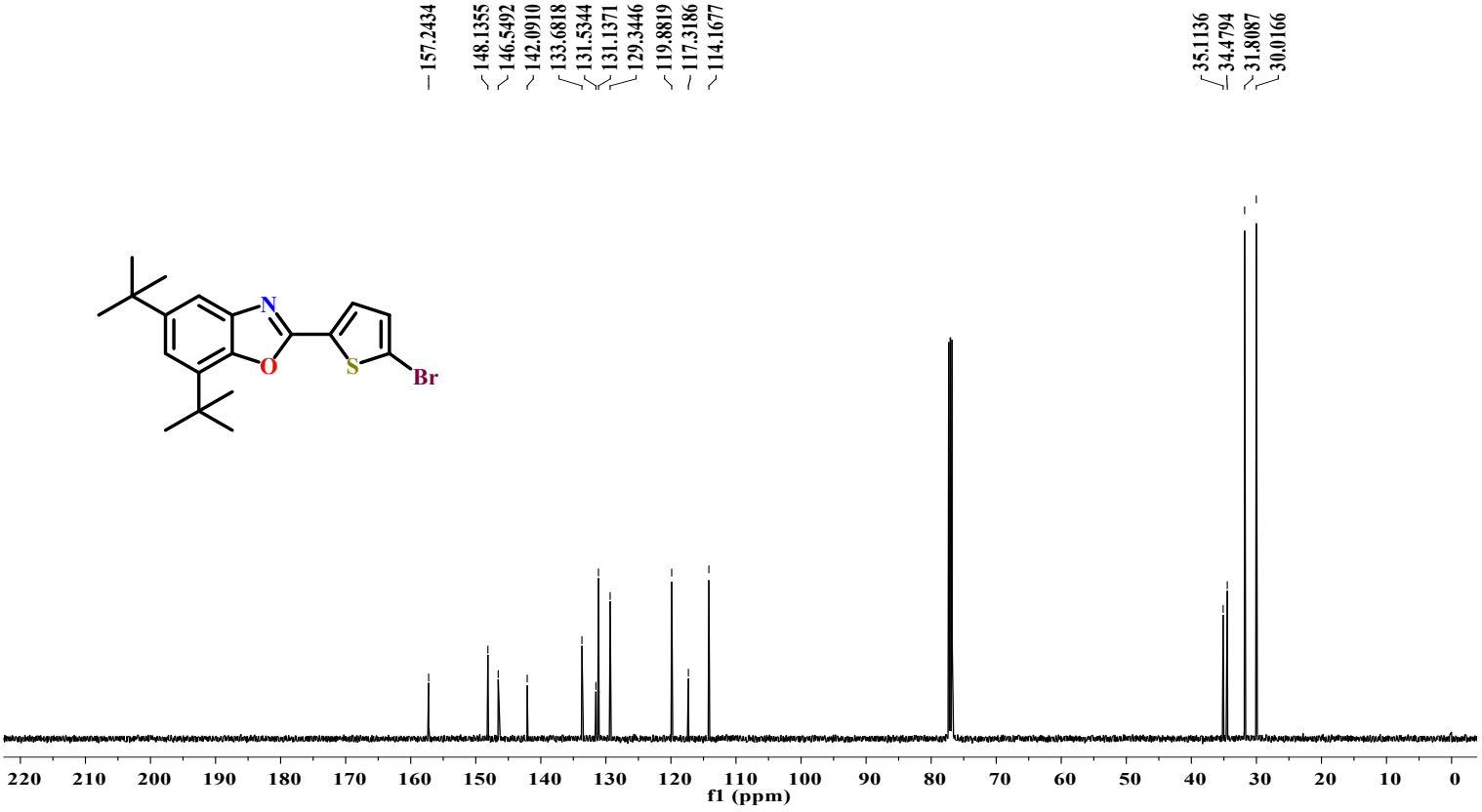


Figure S40. ^{13}C NMR spectrum of compound 4ak in $CDCl_3$ (500 MHz).

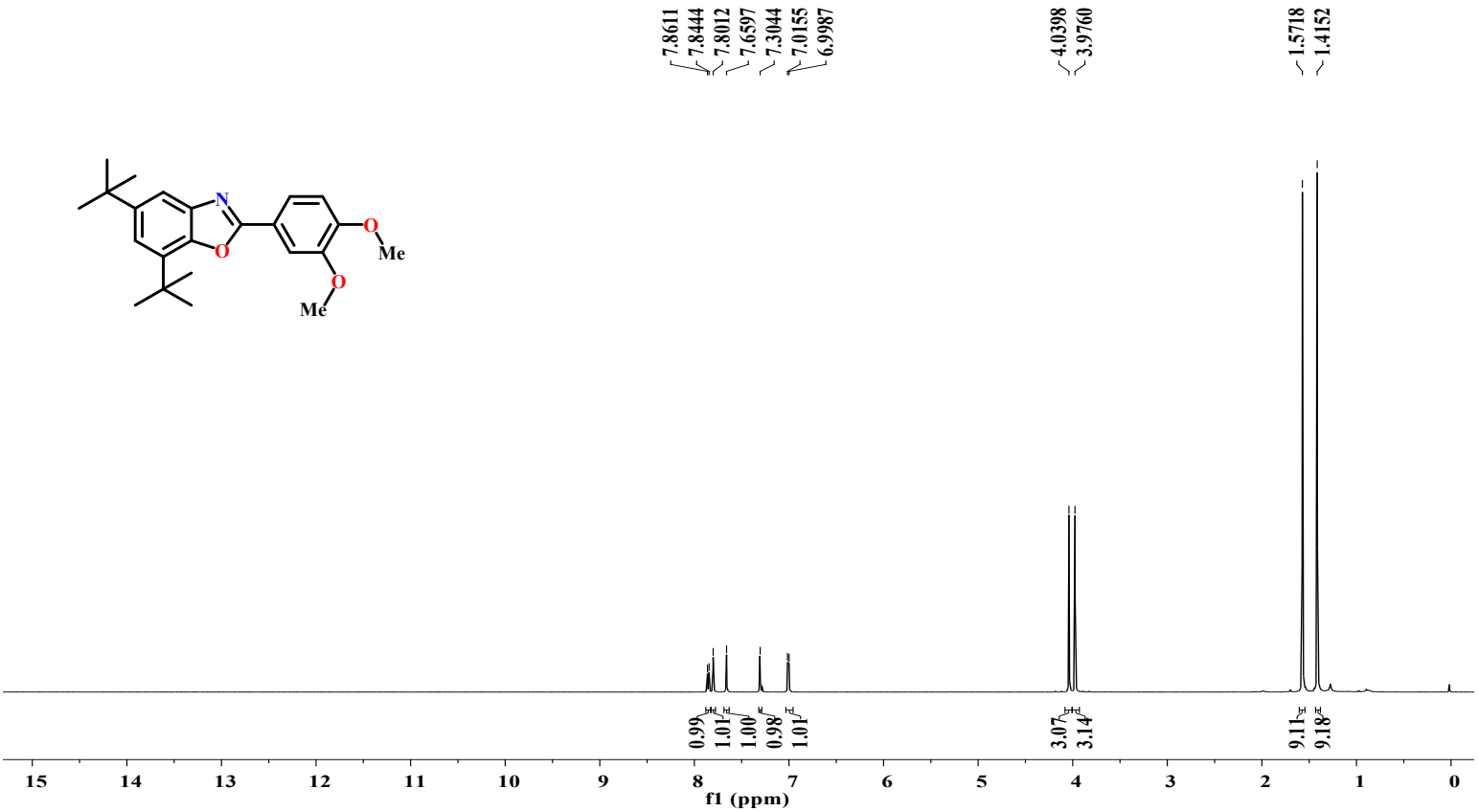


Figure S41. ^{1}H NMR spectrum of compound 4al in $CDCl_3$ (500 MHz).

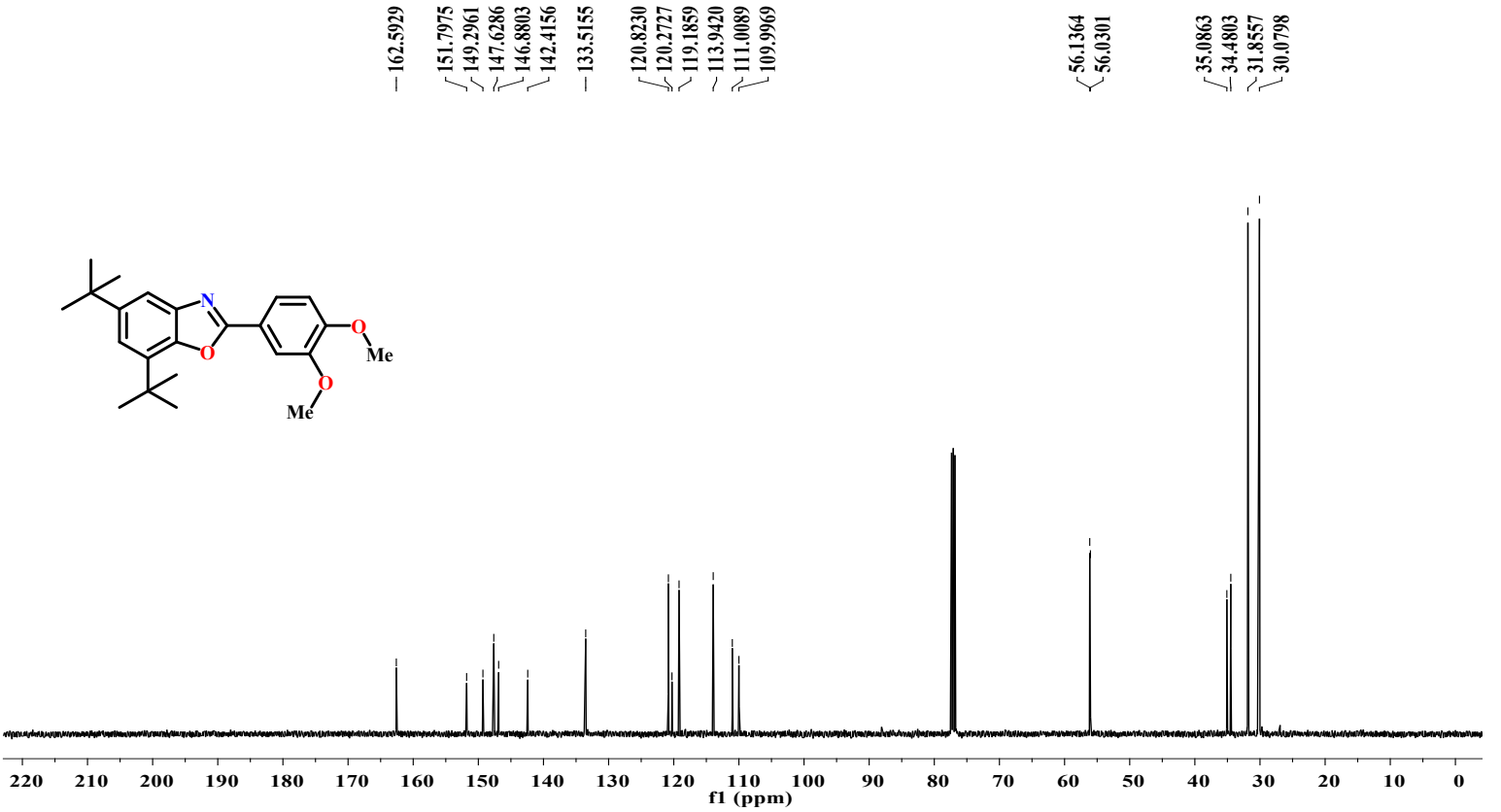


Figure S42. ^{13}C NMR spectrum of compound 4al in $CDCl_3$ (500 MHz).

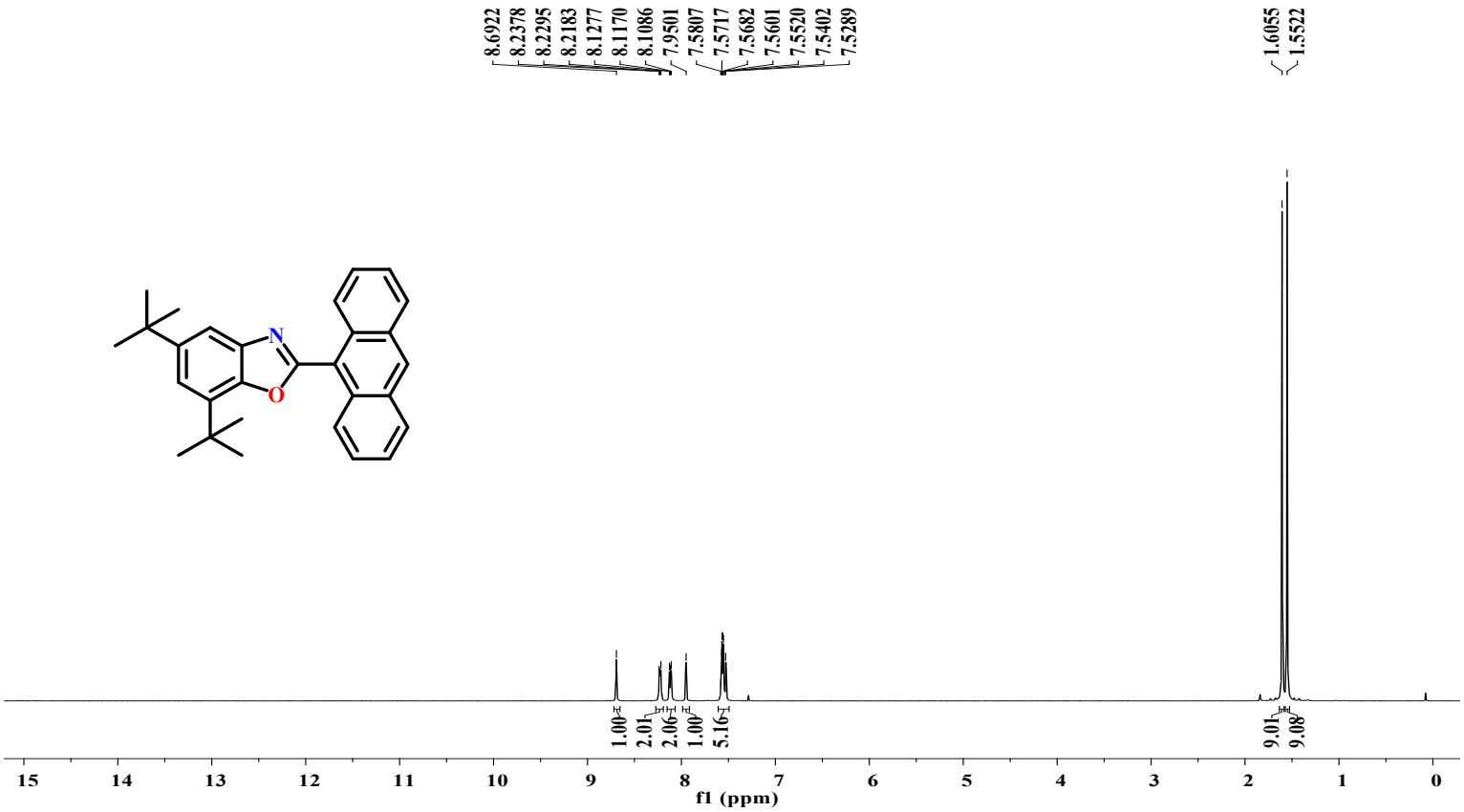


Figure S43. ^{1}H NMR spectrum of compound 4am in $CDCl_3$ (500 MHz).

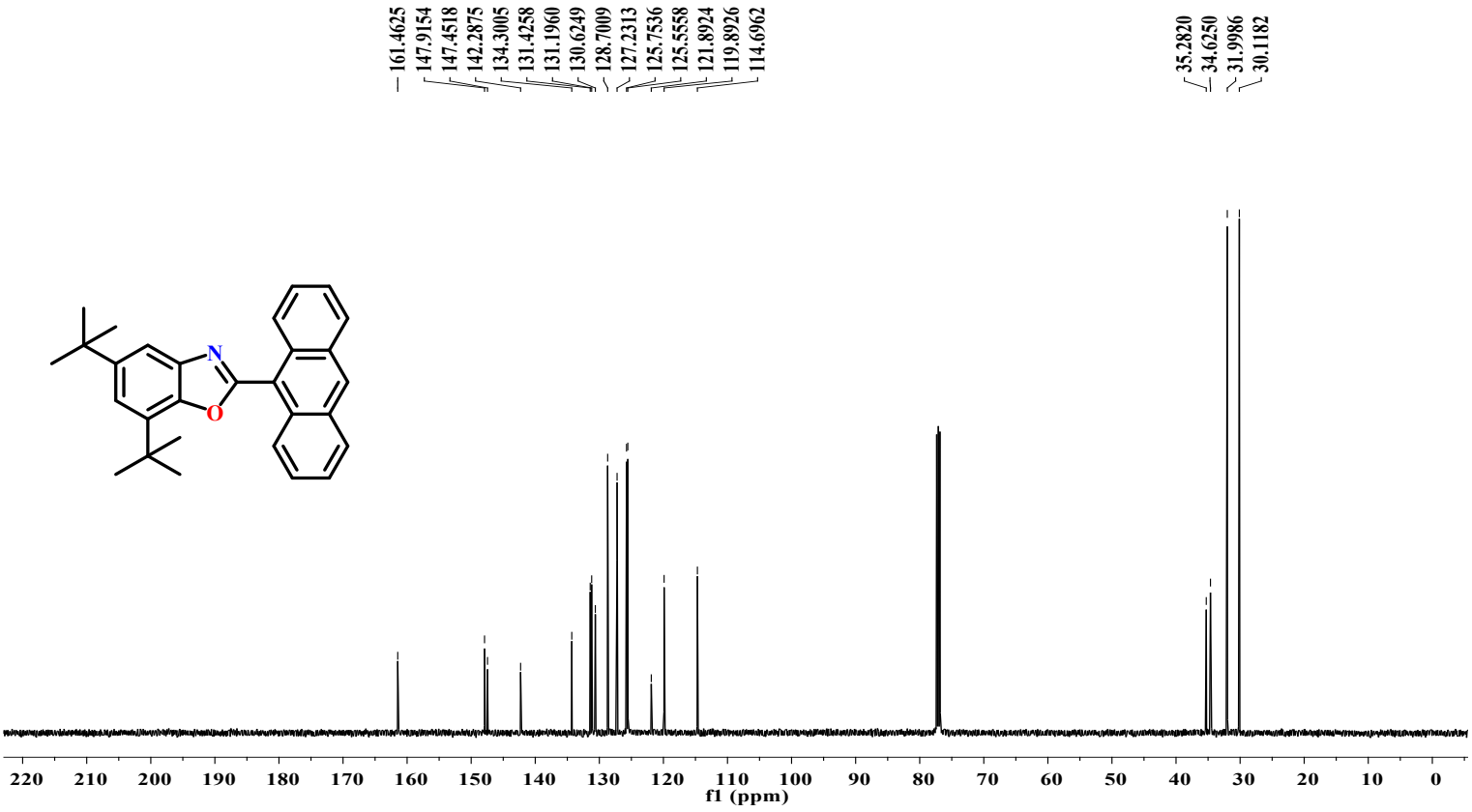


Figure S44. ^{13}C NMR spectrum of compound 4am in $CDCl_3$ (500 MHz).

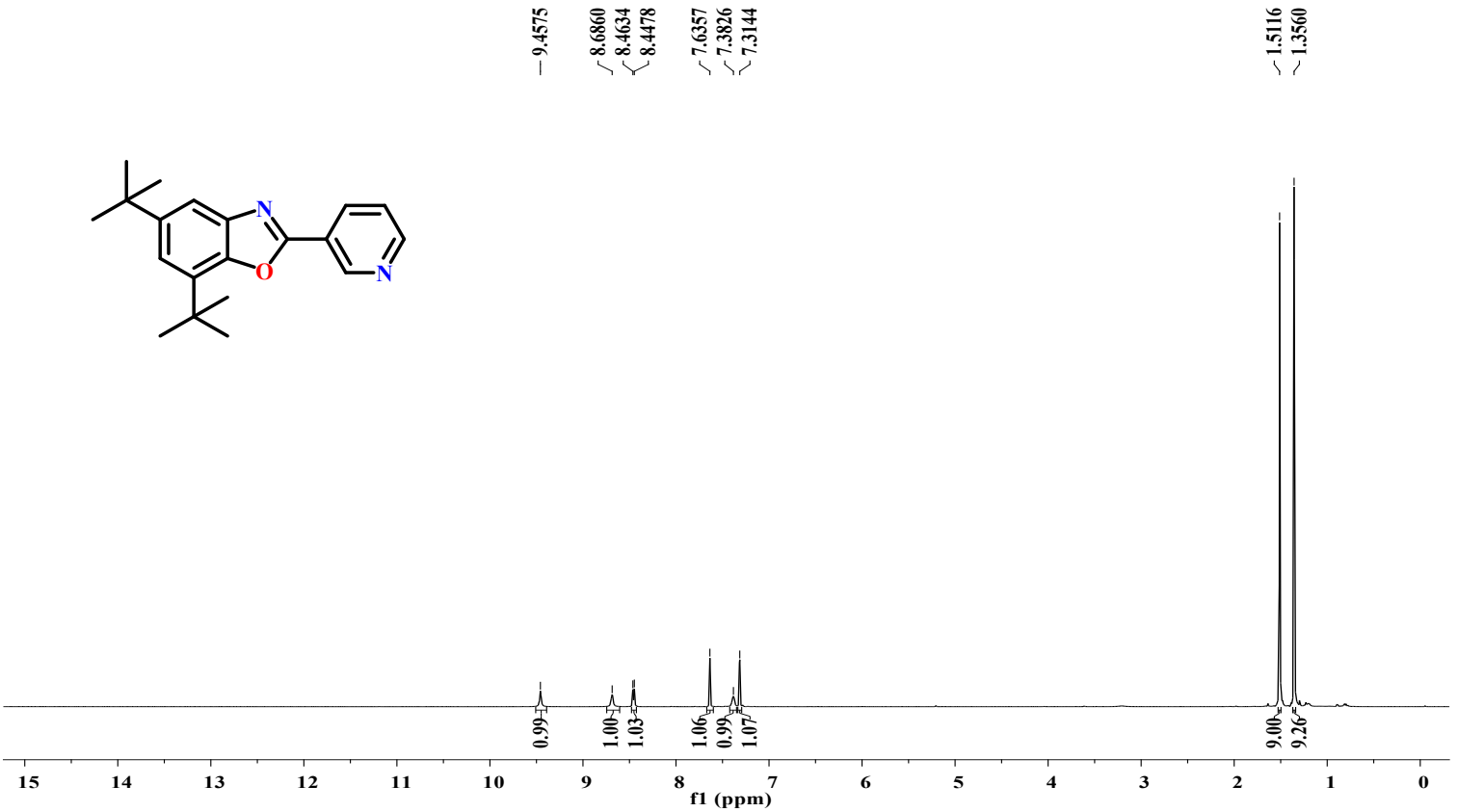


Figure S45. ^{1}H NMR spectrum of compound 4an in $CDCl_3$ (500 MHz).

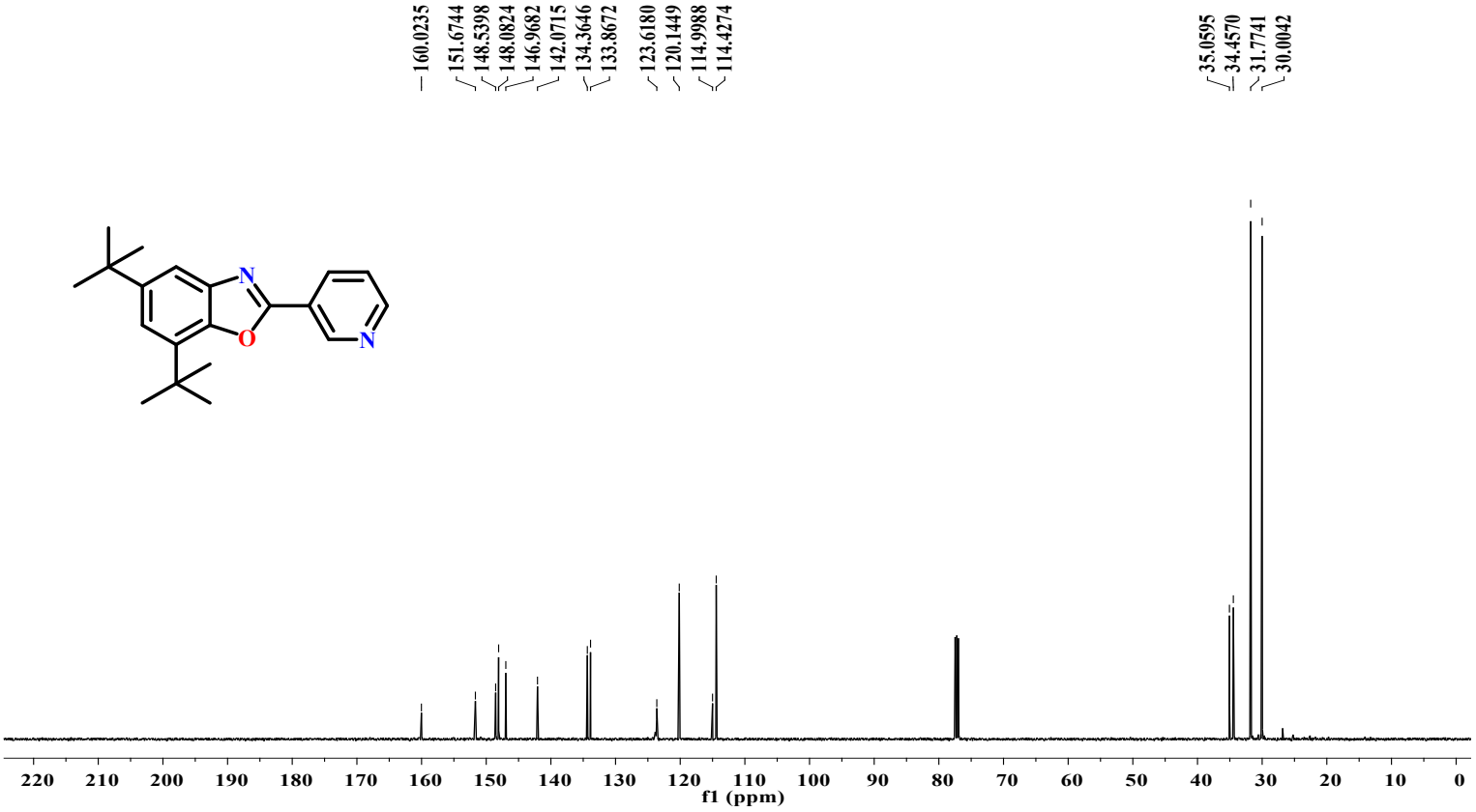


Figure S46. ^{13}C NMR spectrum of compound 4an in $CDCl_3$ (500 MHz).

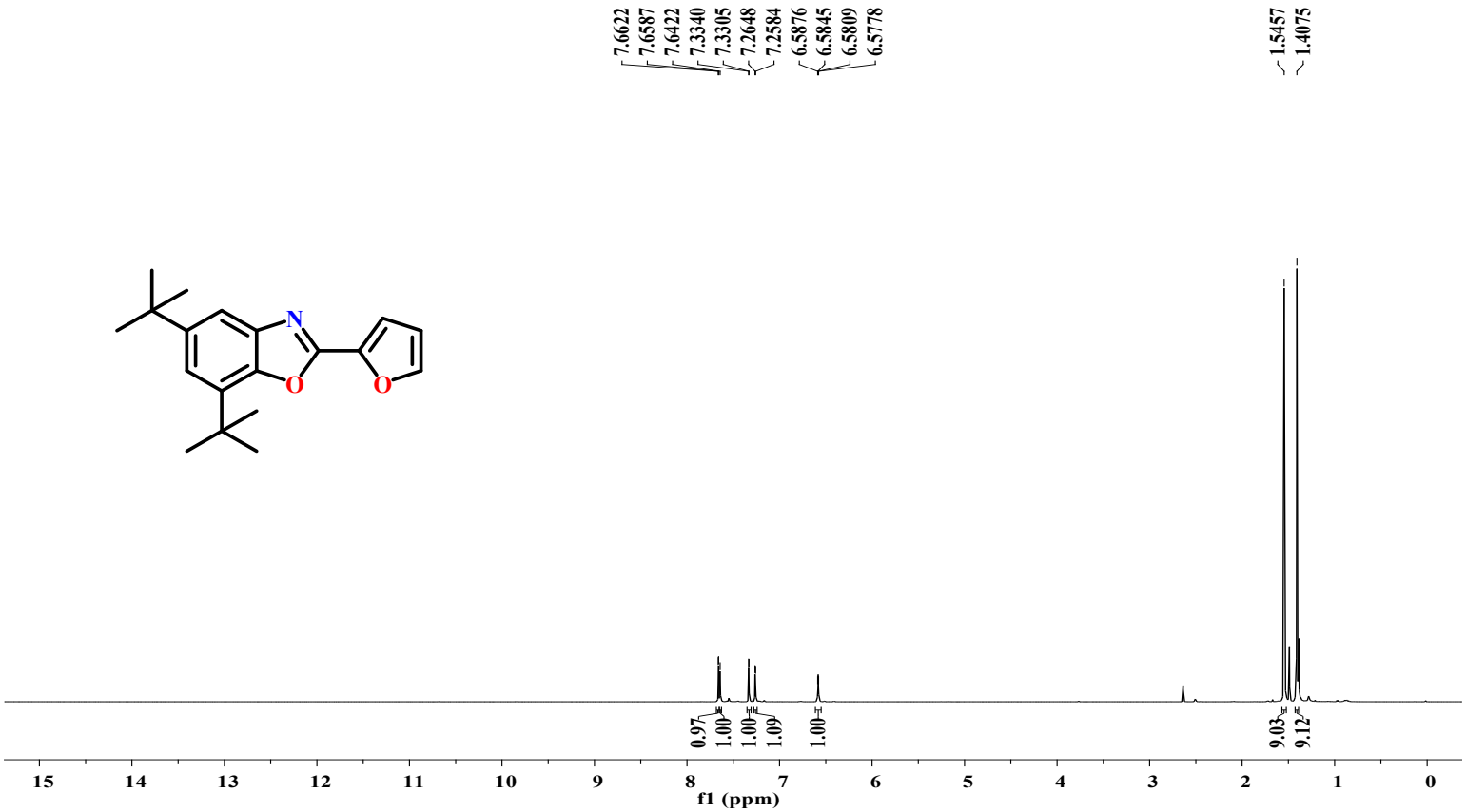


Figure S47. ^{1}H NMR spectrum of compound 4ao in $CDCl_3$ (500 MHz).

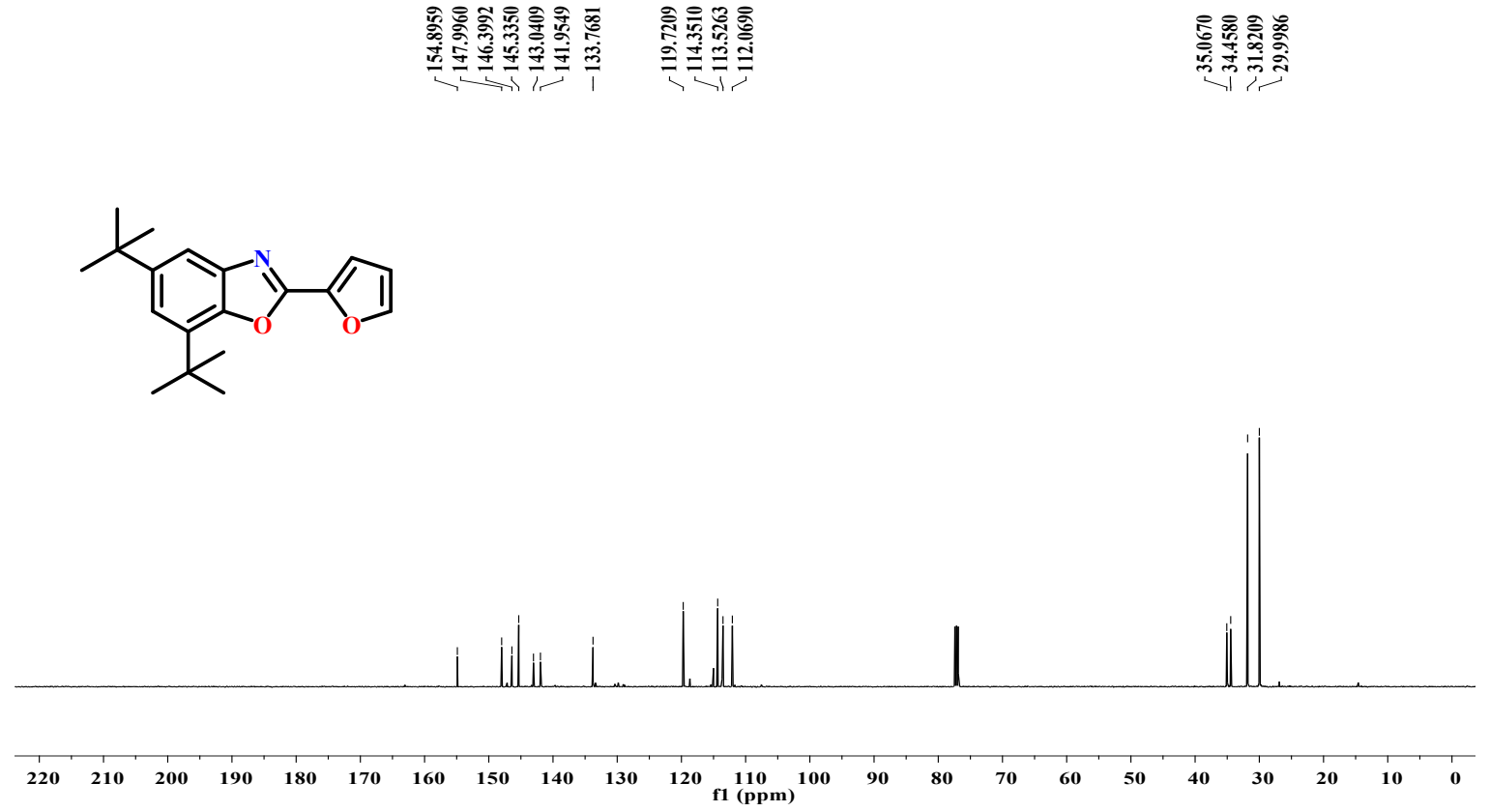


Figure S48. ^{13}C NMR spectrum of compound 4ao in $CDCl_3$ (500 MHz).

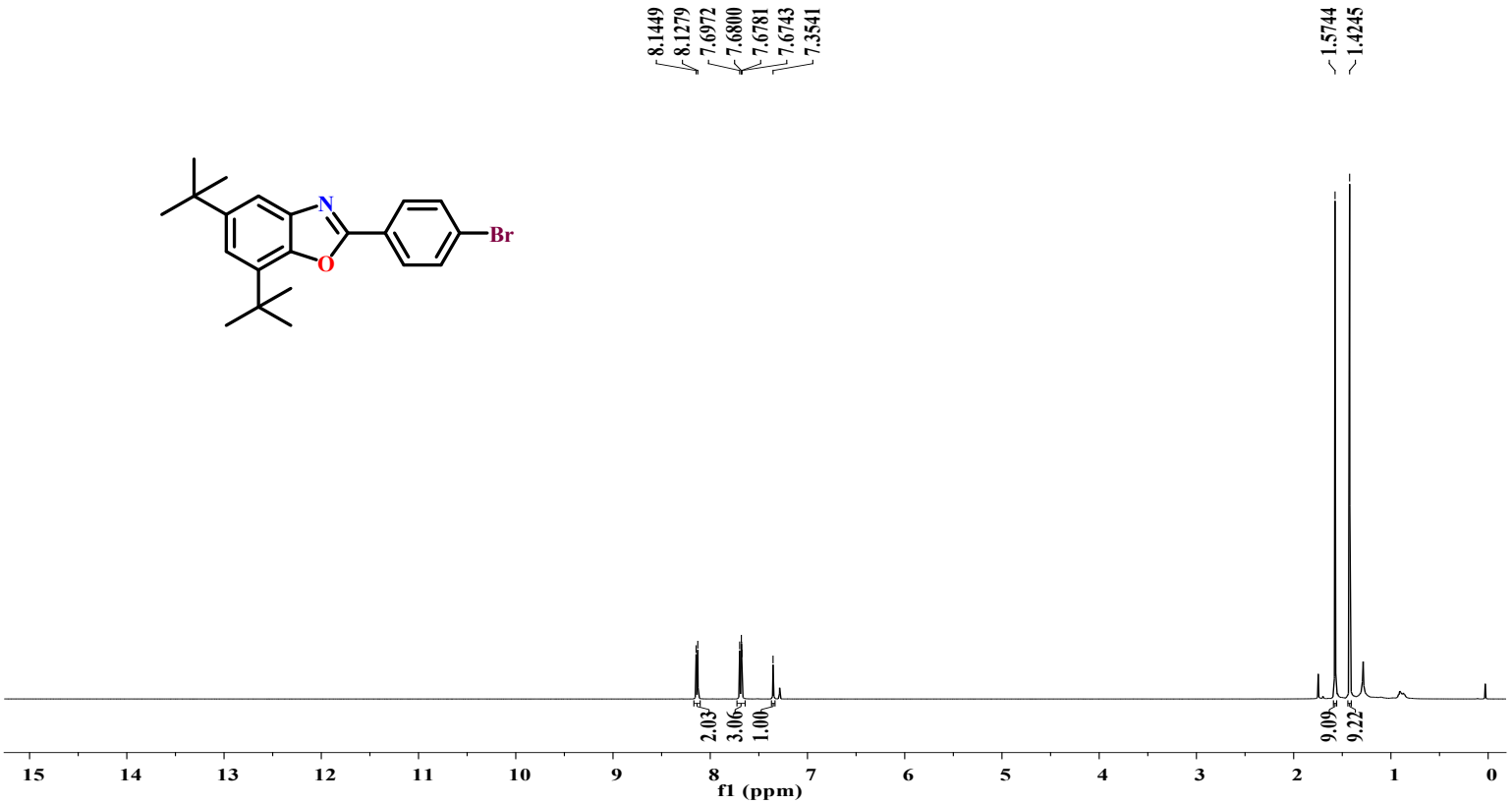


Figure S49. ^{1}H NMR spectrum of compound 4ap in $CDCl_3$ (500 MHz).

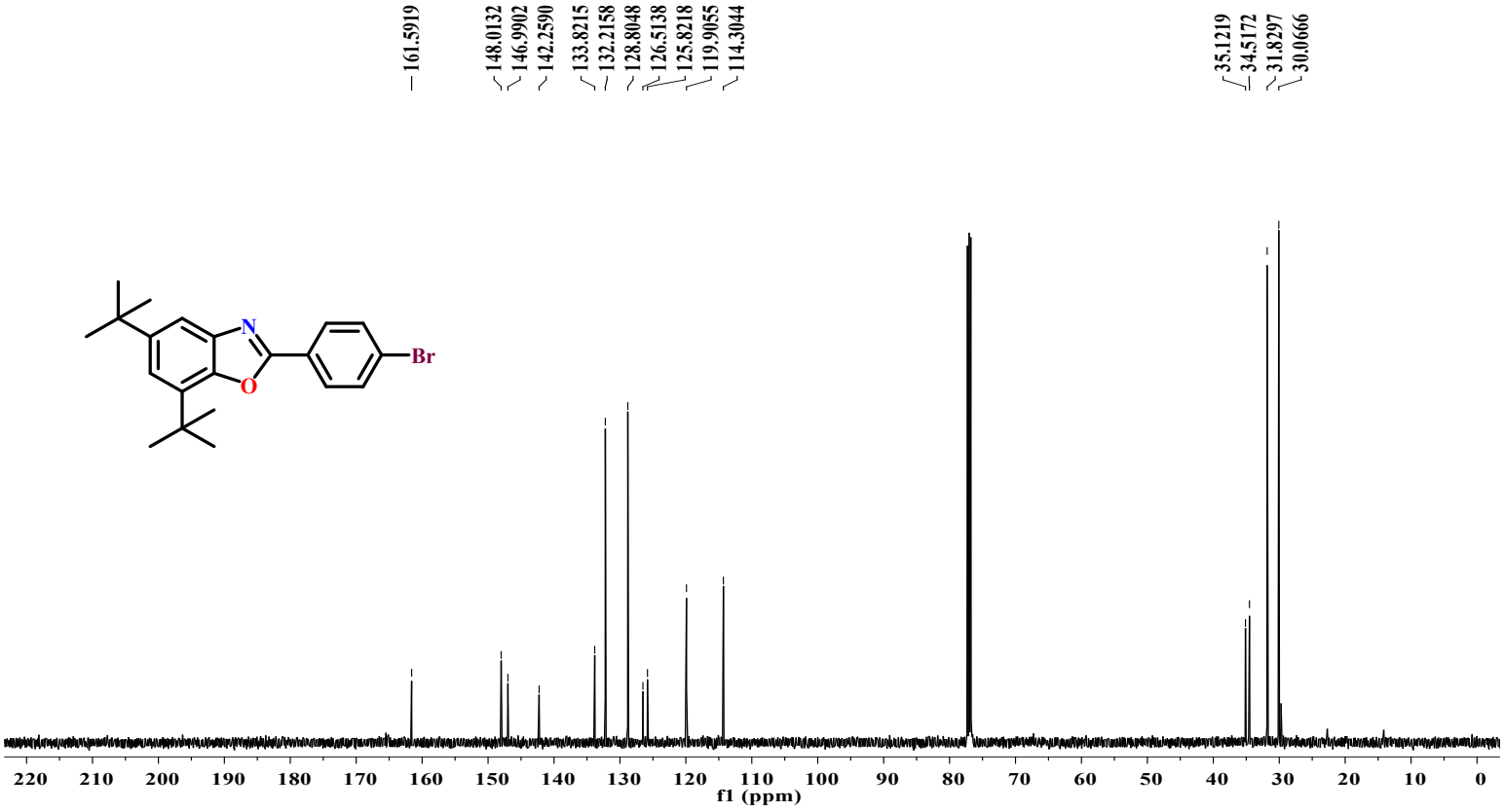


Figure S50. ^{13}C NMR spectrum of compound 4ap in $CDCl_3$ (500 MHz).

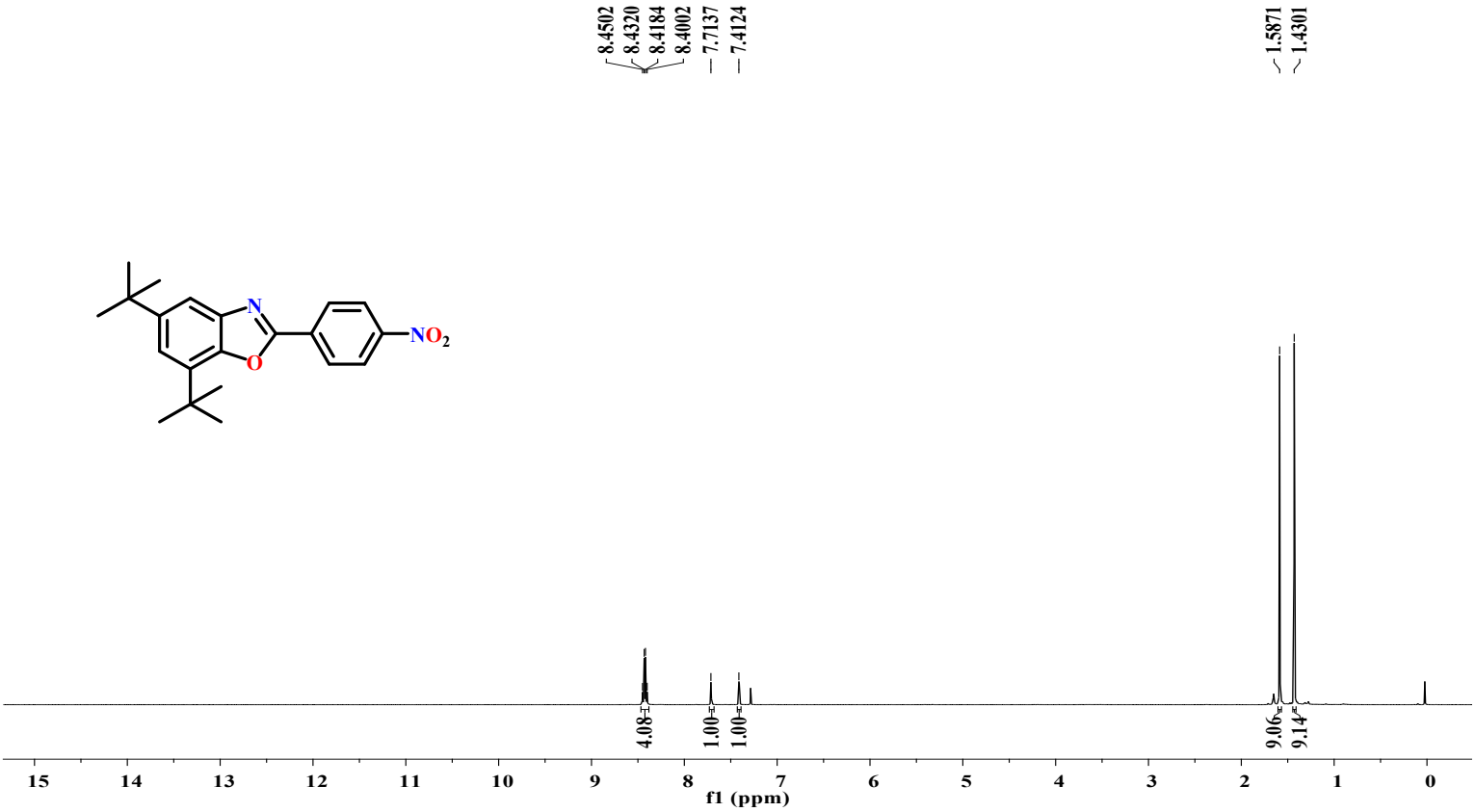


Figure S51. ^{1}H NMR spectrum of compound 4aq in $CDCl_3$ (500 MHz).

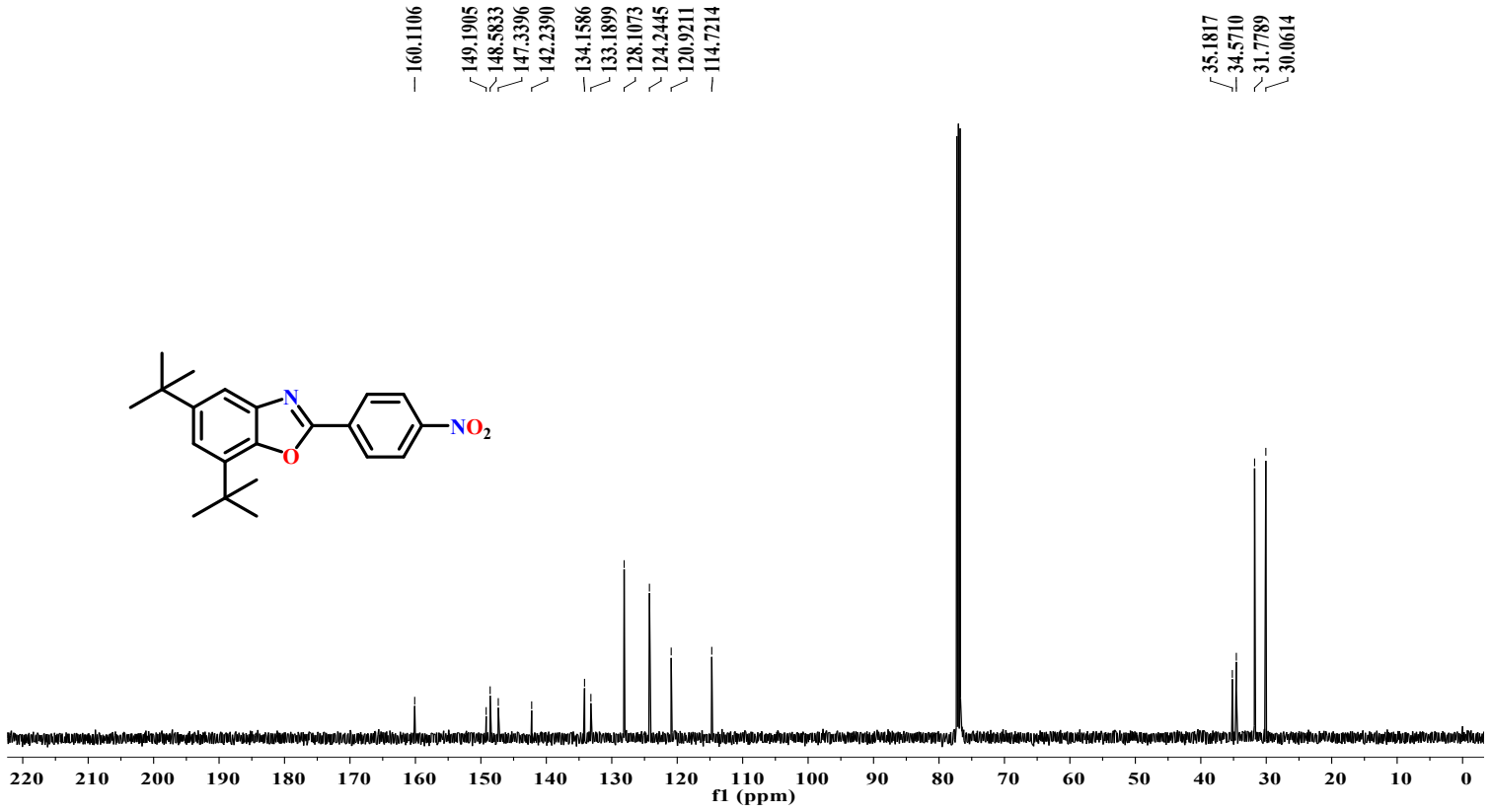


Figure S52. ^{13}C NMR spectrum of compound 4aq in $CDCl_3$ (500 MHz).

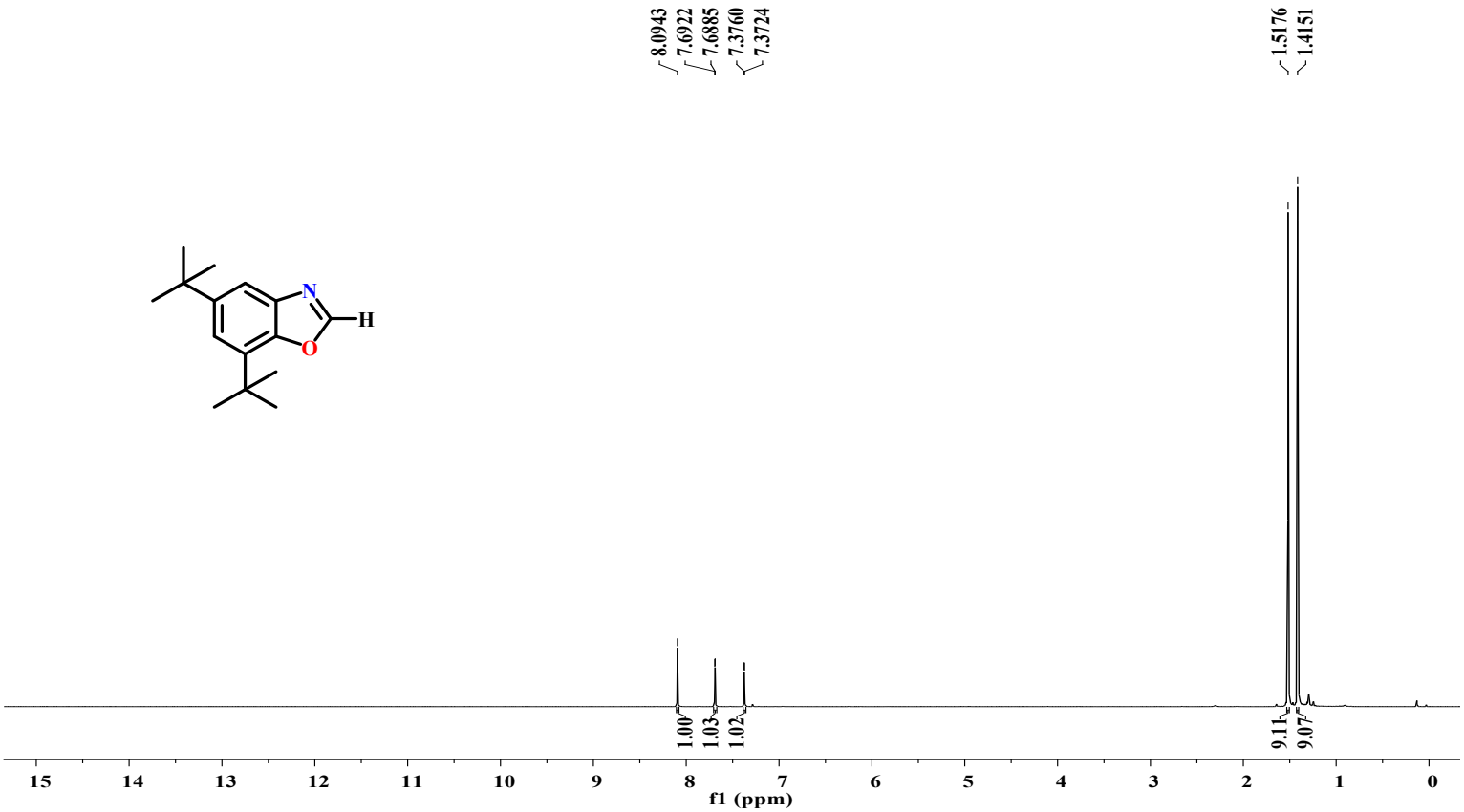


Figure S53. ^{1}H NMR spectrum of compound 4ar in $CDCl_3$ (500 MHz).

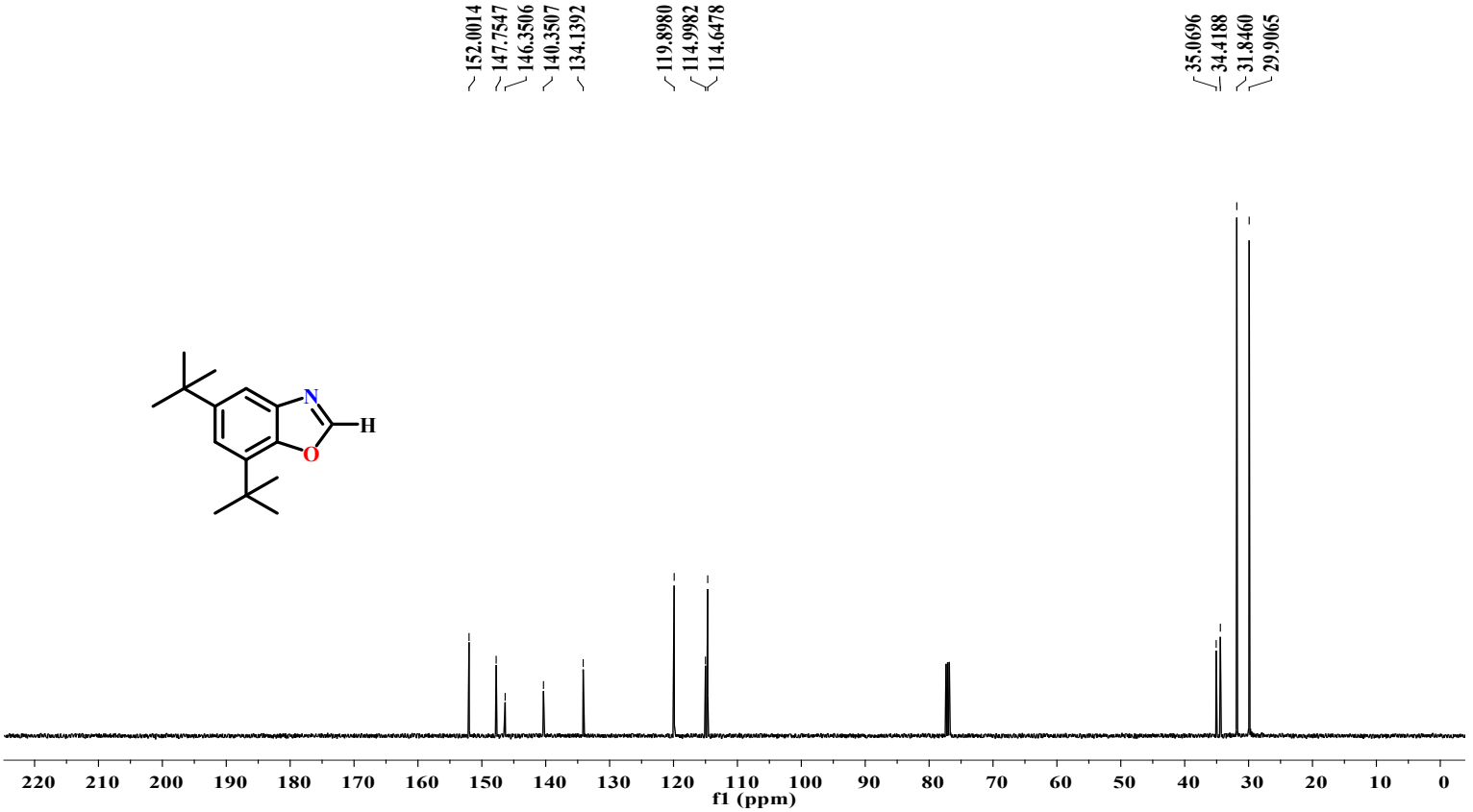


Figure S54. ^{13}C NMR spectrum of compound 4ar in $CDCl_3$ (500 MHz).

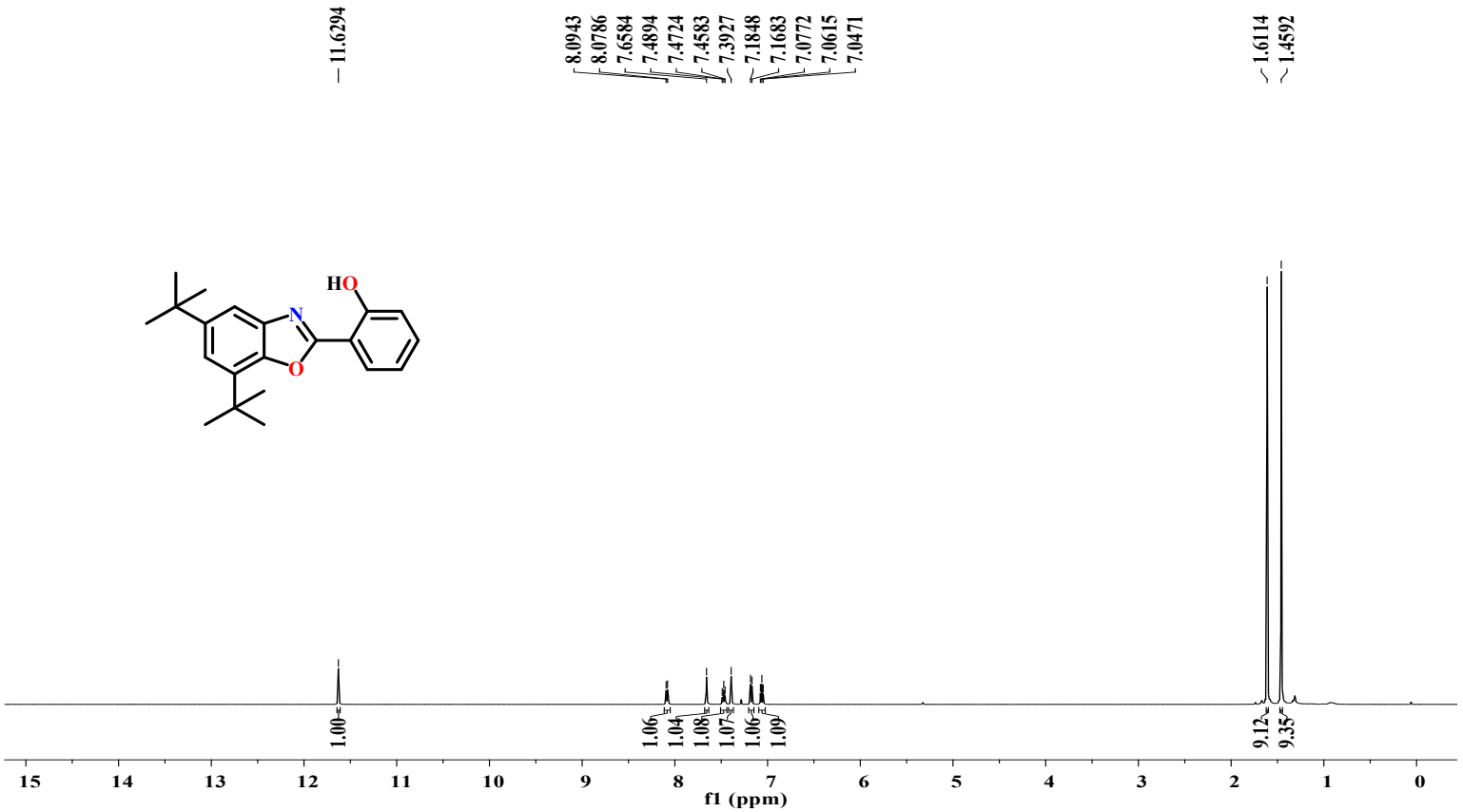


Figure S55. ^{1}H NMR spectrum of compound 4as in $CDCl_3$ (500 MHz).

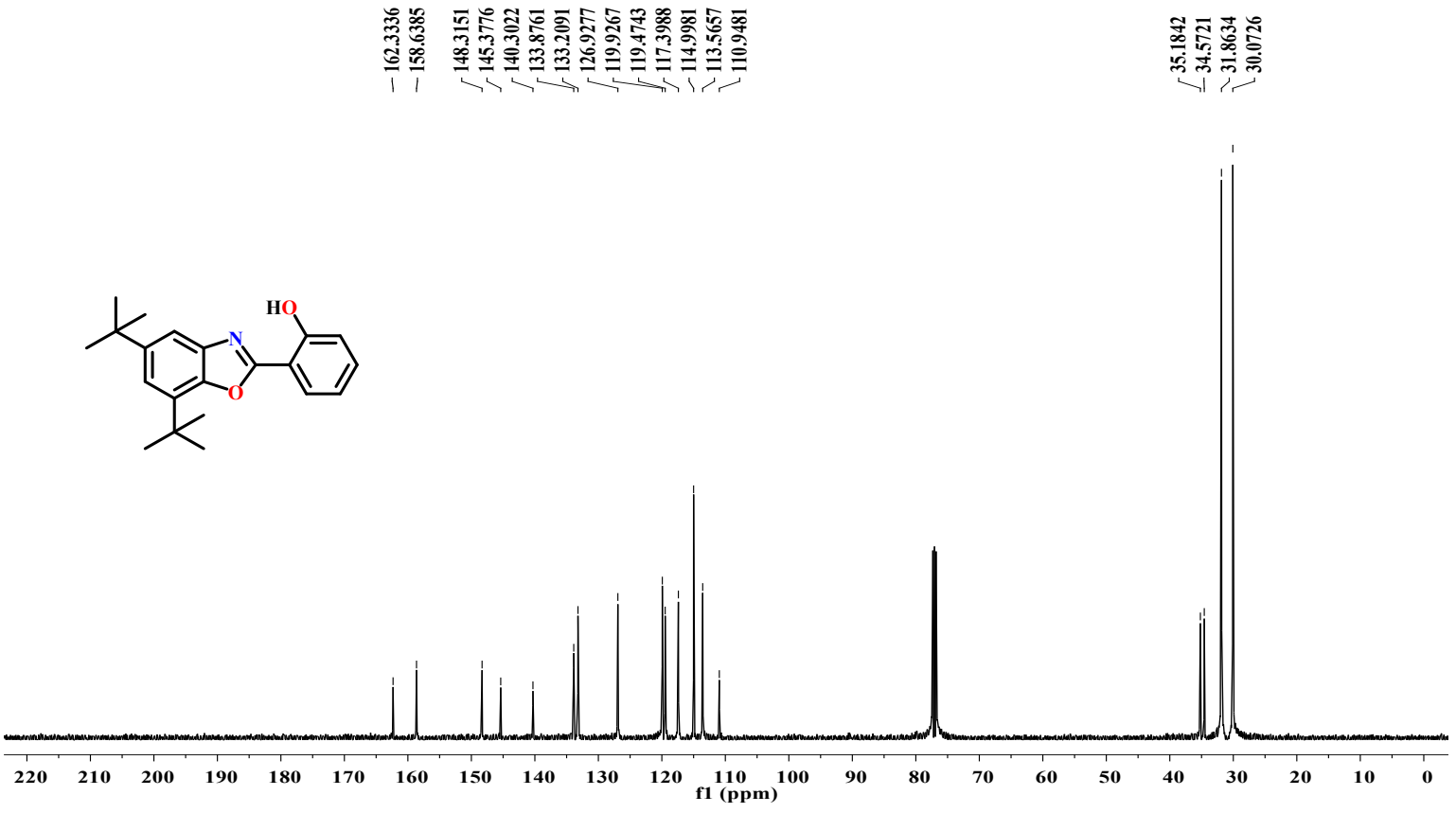


Figure S56. ^{13}C NMR spectrum of compound 4as in $CDCl_3$ (500 MHz).

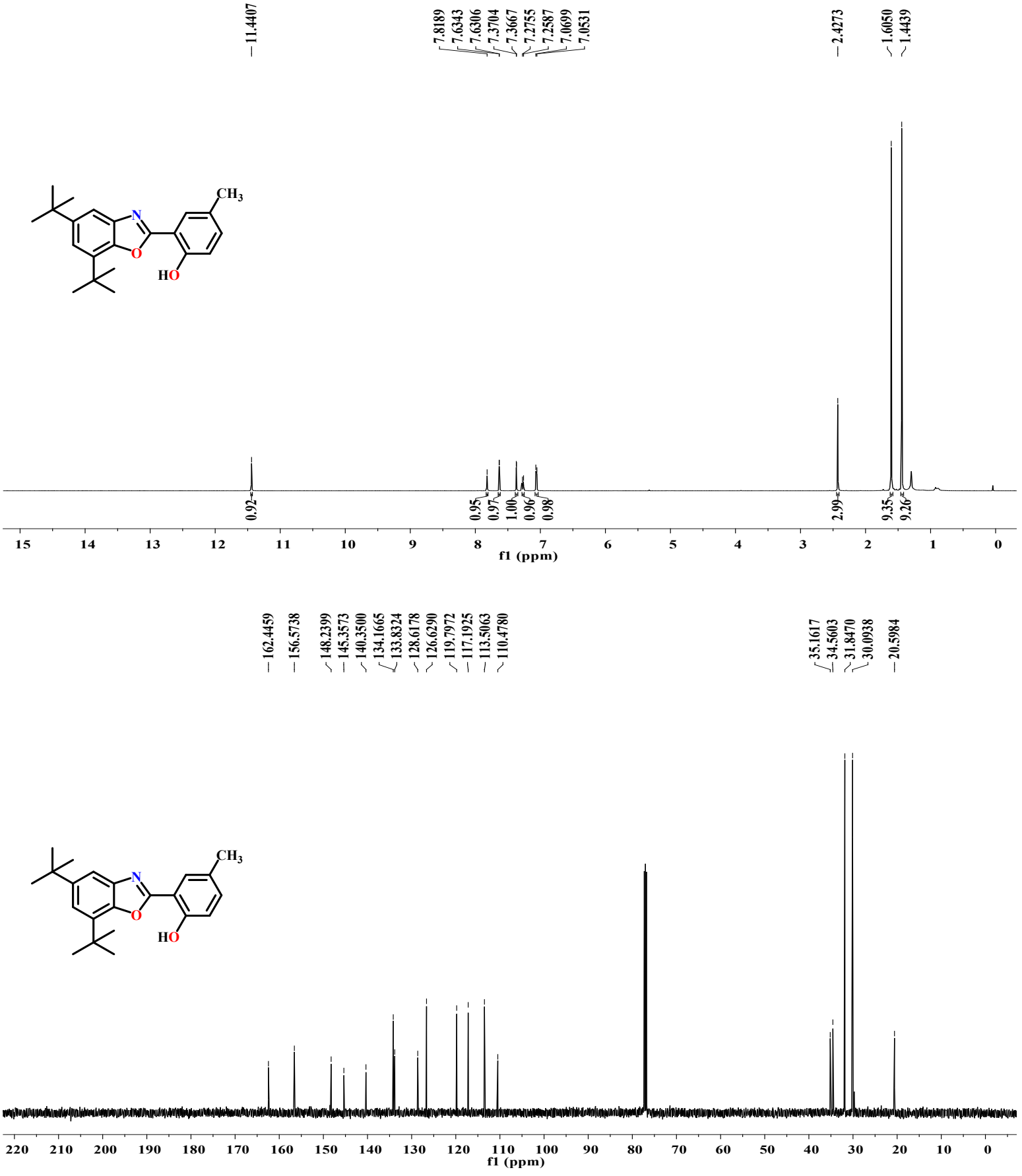


Figure S57. ^{1}H NMR spectrum of compound 4at in $CDCl_3$ (500 MHz).

Figure S58. ^{13}C NMR spectrum of compound 4at in $CDCl_3$ (500 MHz).

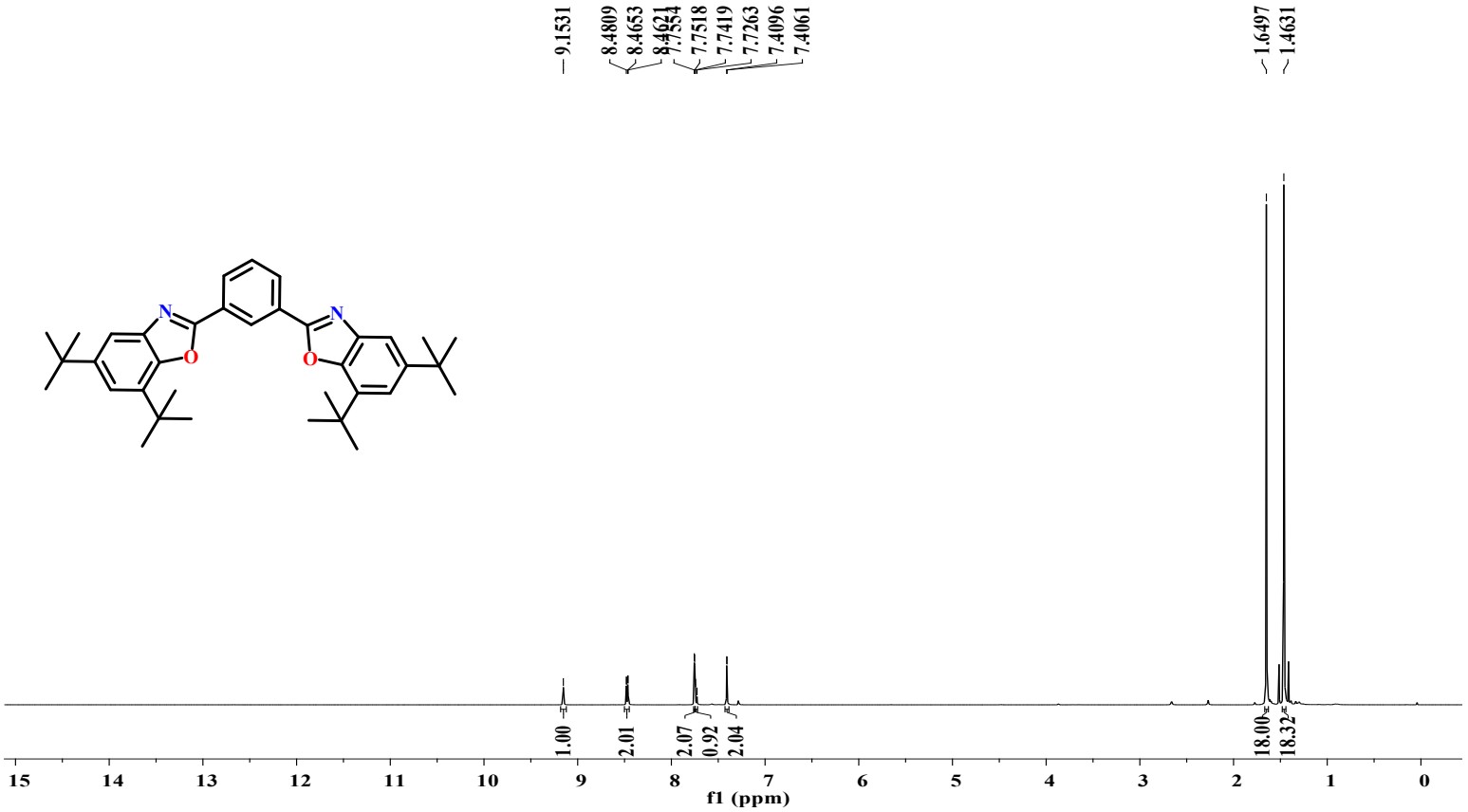


Figure S59. ^{1}H NMR spectrum of compound 4au in $CDCl_3$ (500 MHz).

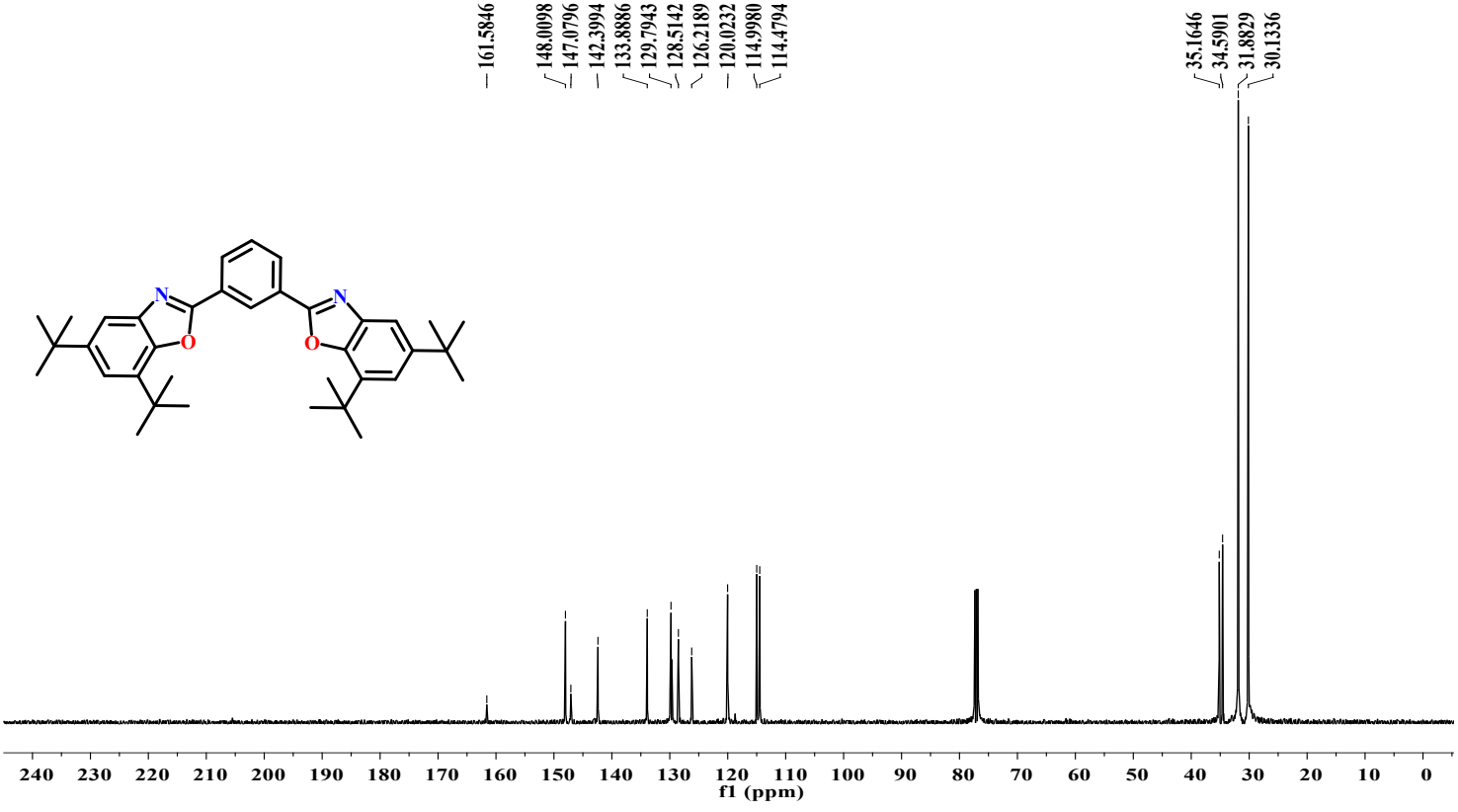
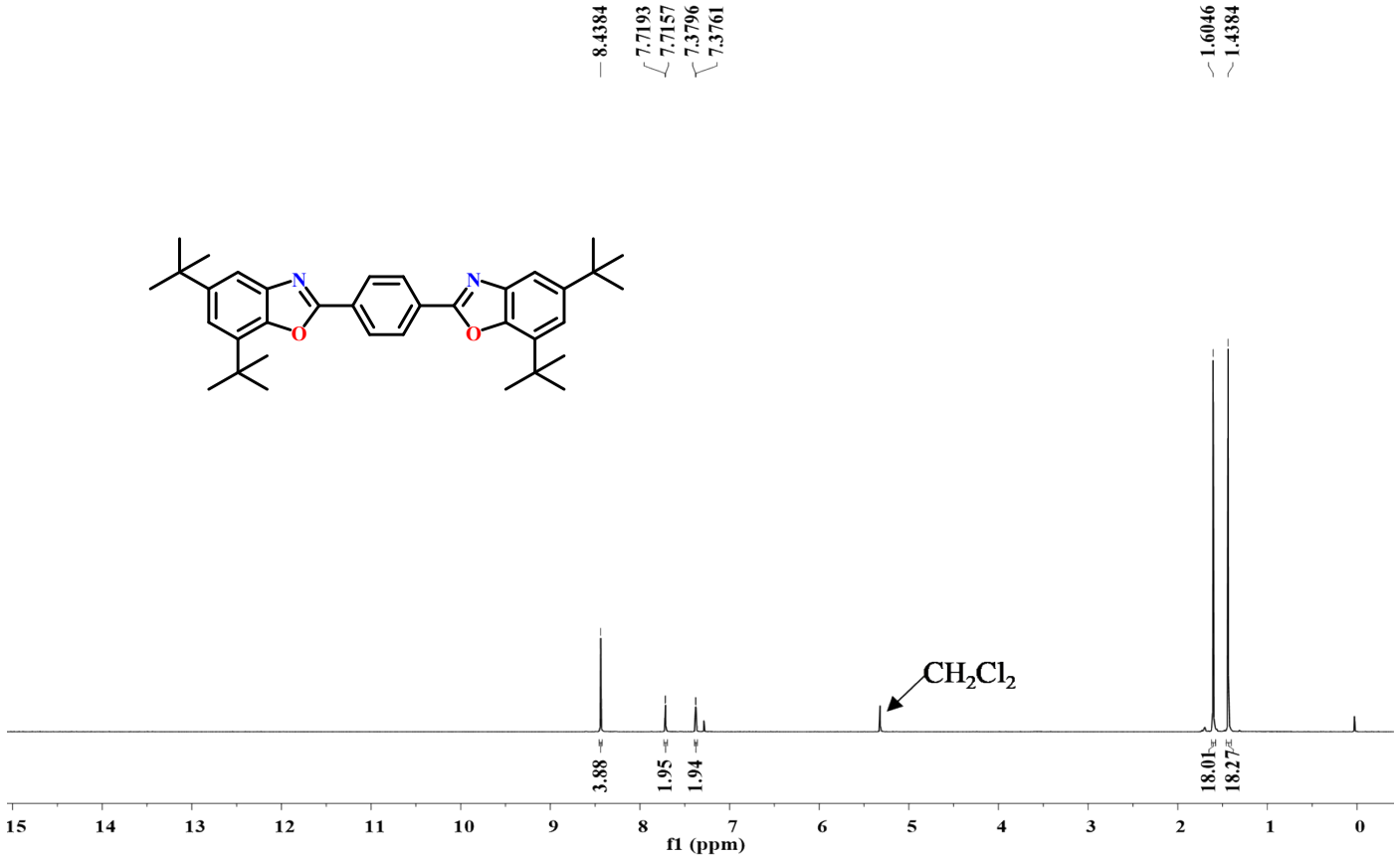


Figure S60. ^{13}C NMR spectrum of compound 4au in $CDCl_3$ (500 MHz).



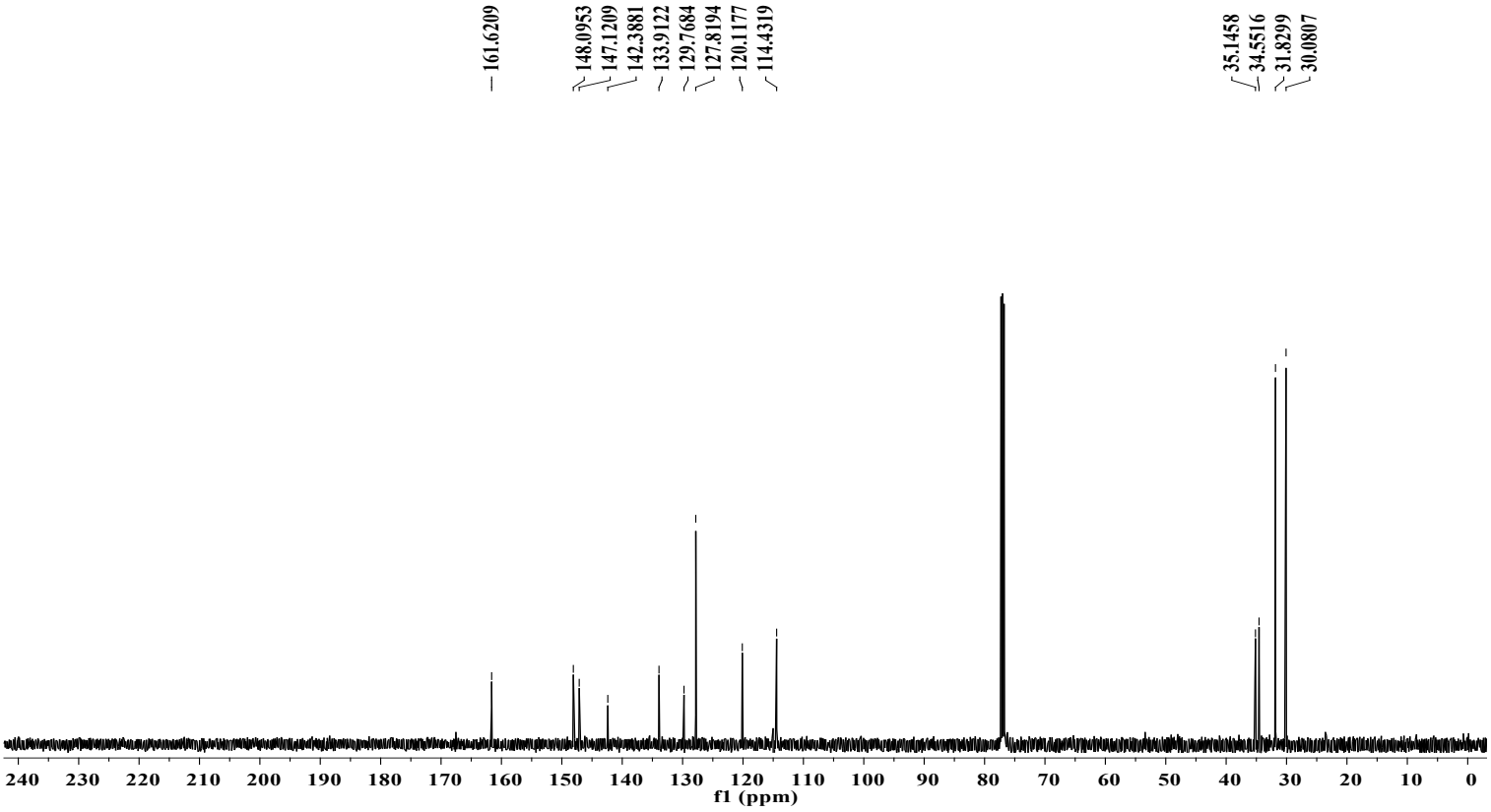


Figure S61. ^{1}H NMR spectrum of compound 4av in $CDCl_3$ (500 MHz).

Figure S62. ^{13}C NMR spectrum of compound 4av in $CDCl_3$ (500 MHz).

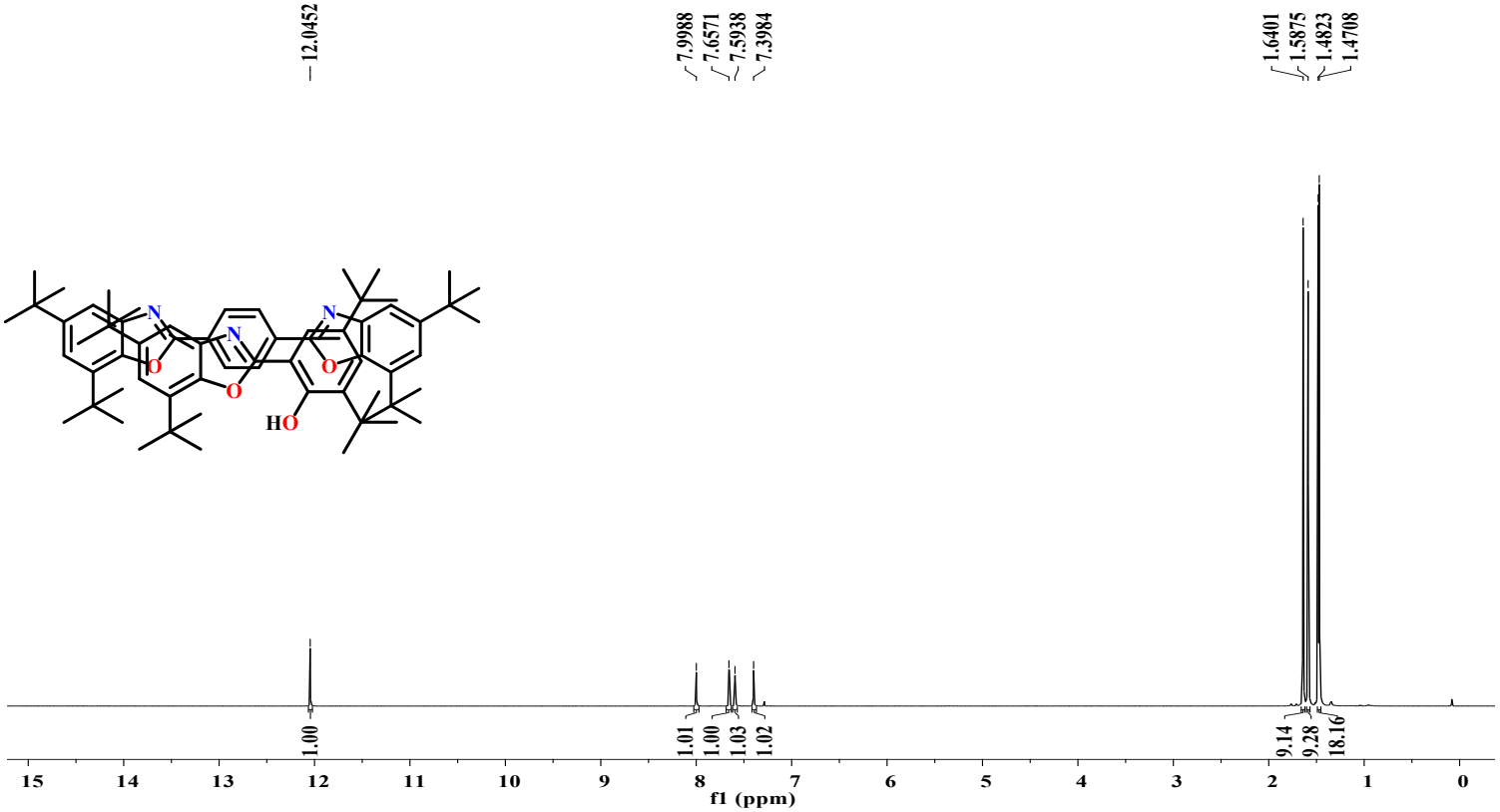


Figure S63. ^{1}H NMR spectrum of compound 4aw in $CDCl_3$ (500 MHz).

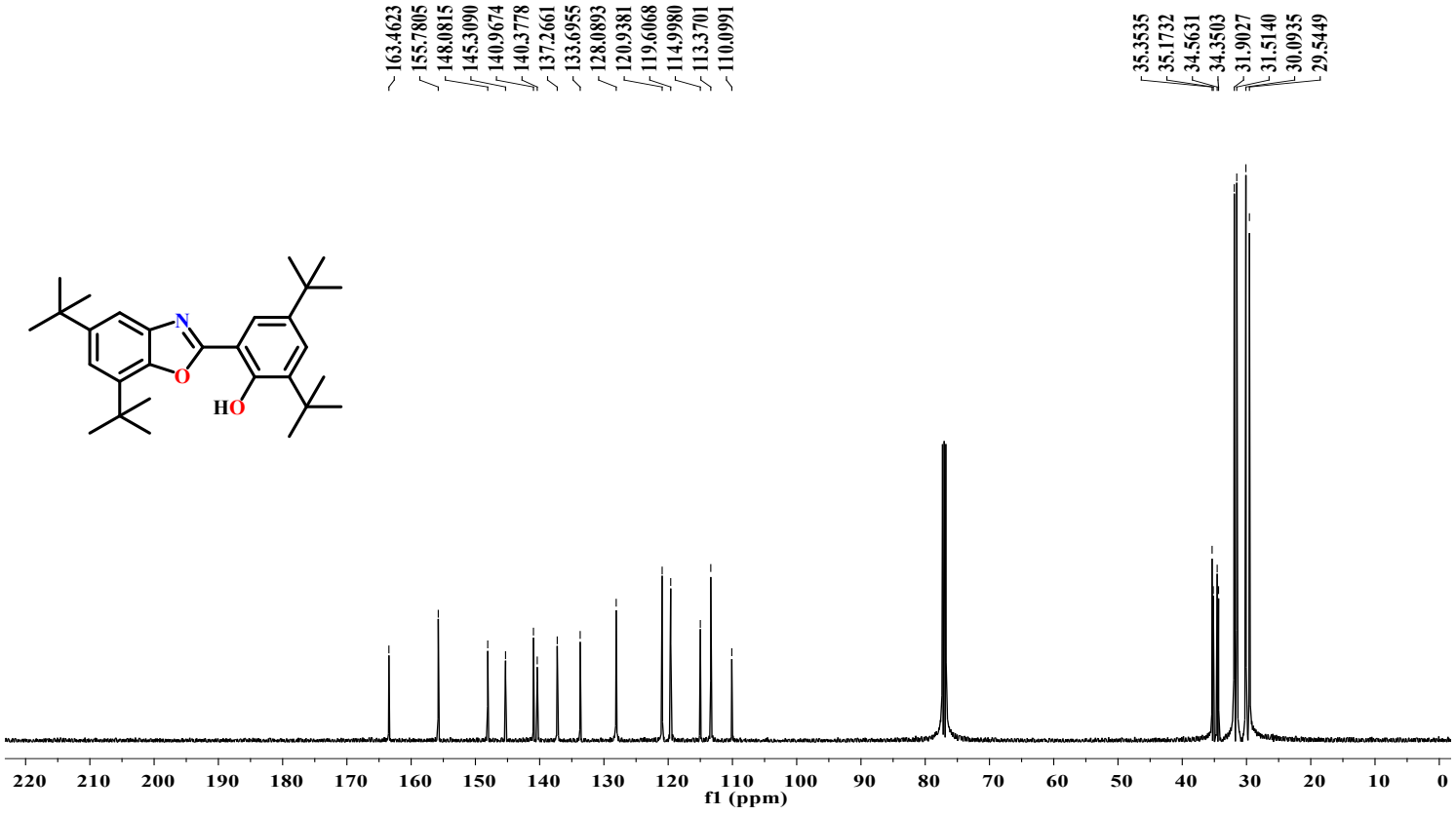


Figure S64. ^{13}C NMR spectrum of compound 4aw in $CDCl_3$ (500 MHz).

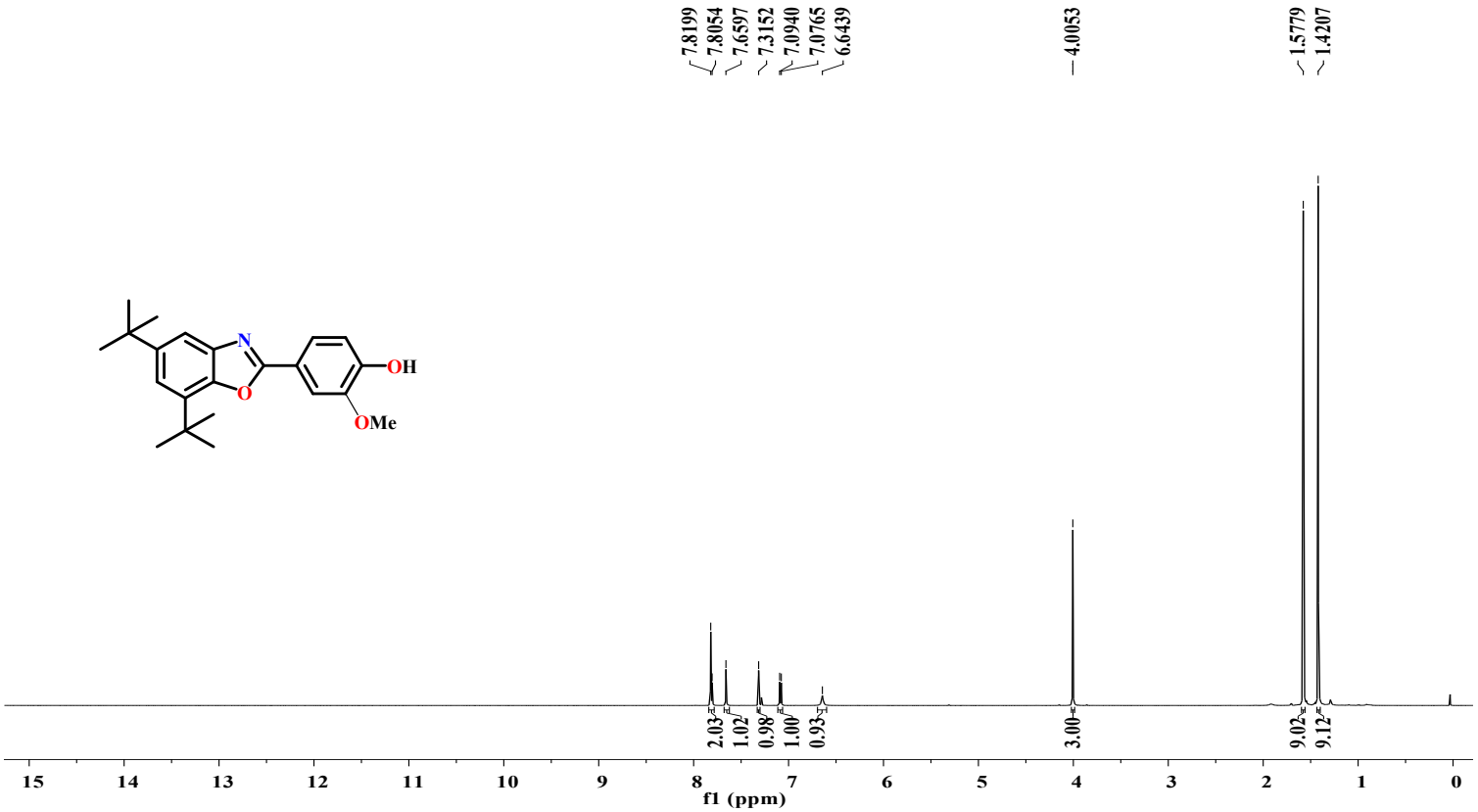


Figure S65. ^{1}H NMR spectrum of compound 4ax in $CDCl_3$ (500 MHz).

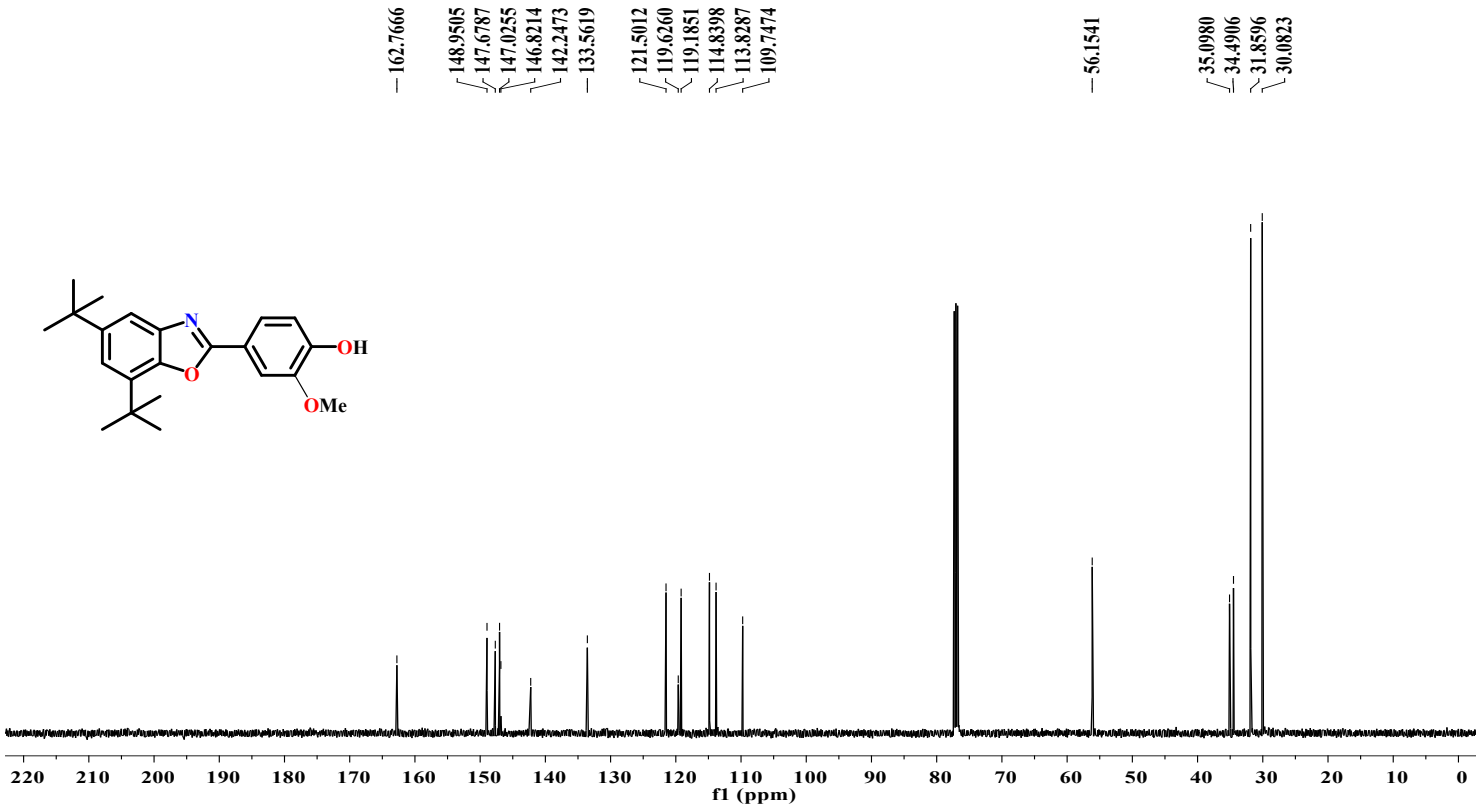


Figure S66. ^{13}C NMR spectrum of compound 4ax in $CDCl_3$ (500 MHz).

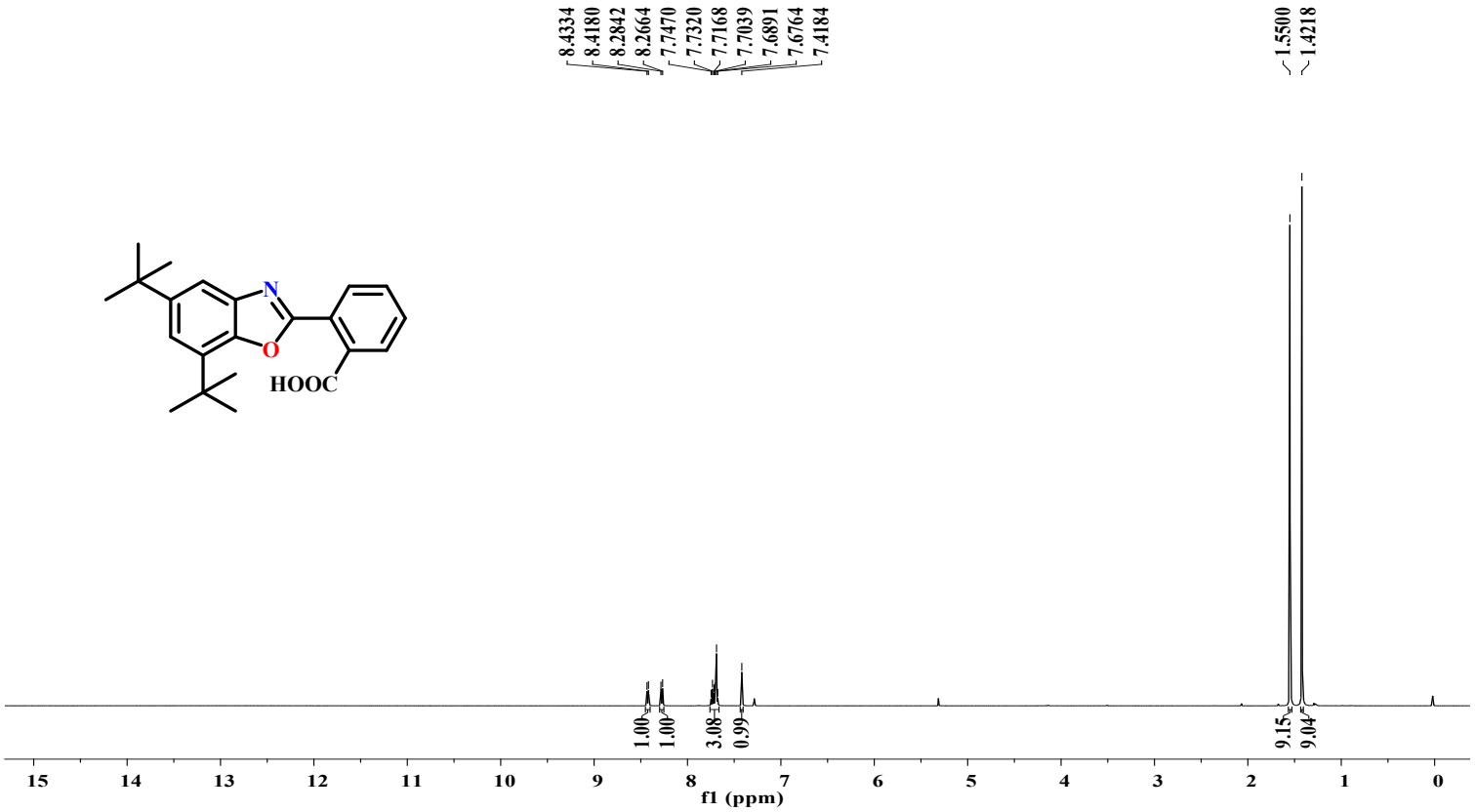


Figure S67. ^{1}H NMR spectrum of compound 4ay in $CDCl_3$ (500 MHz).

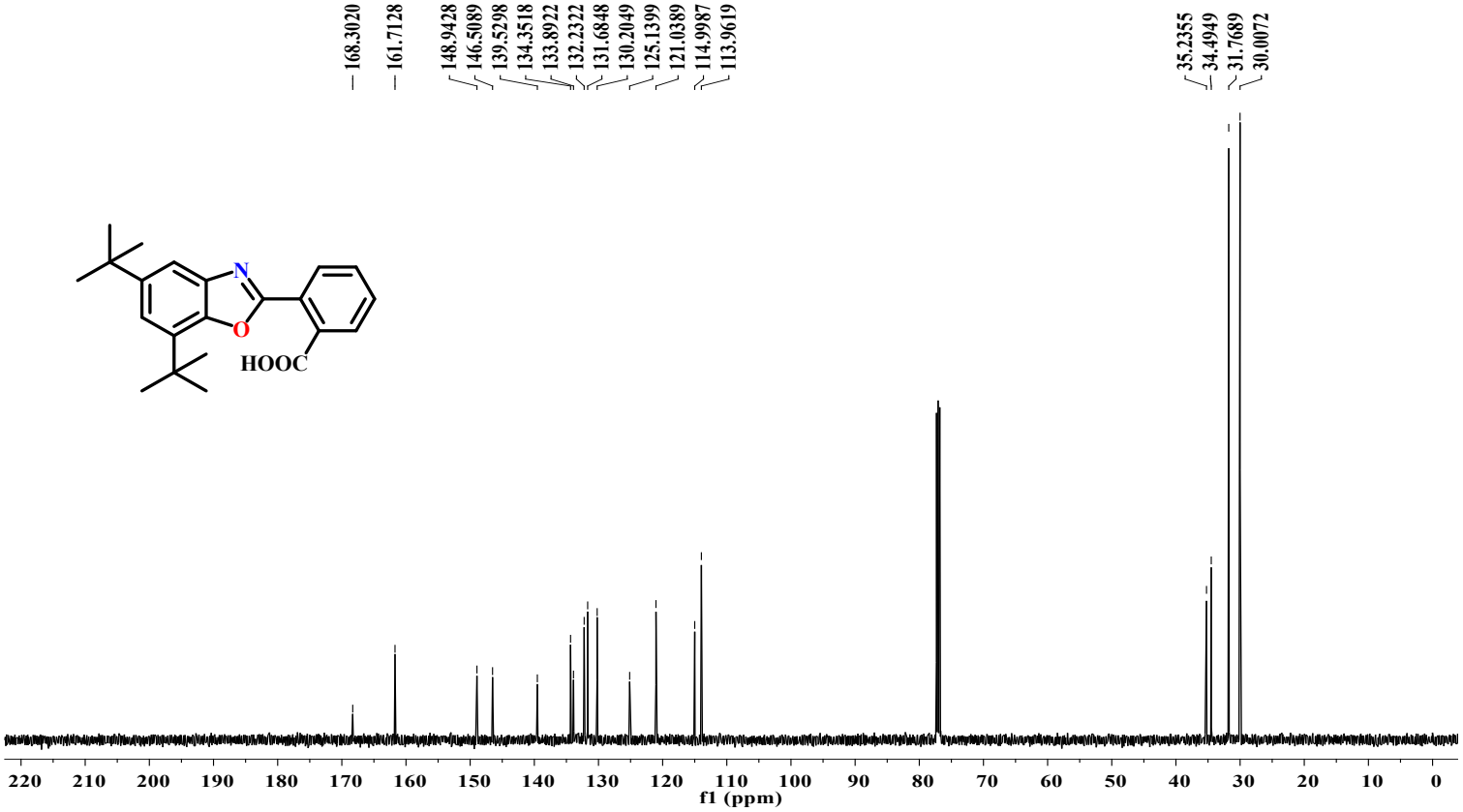
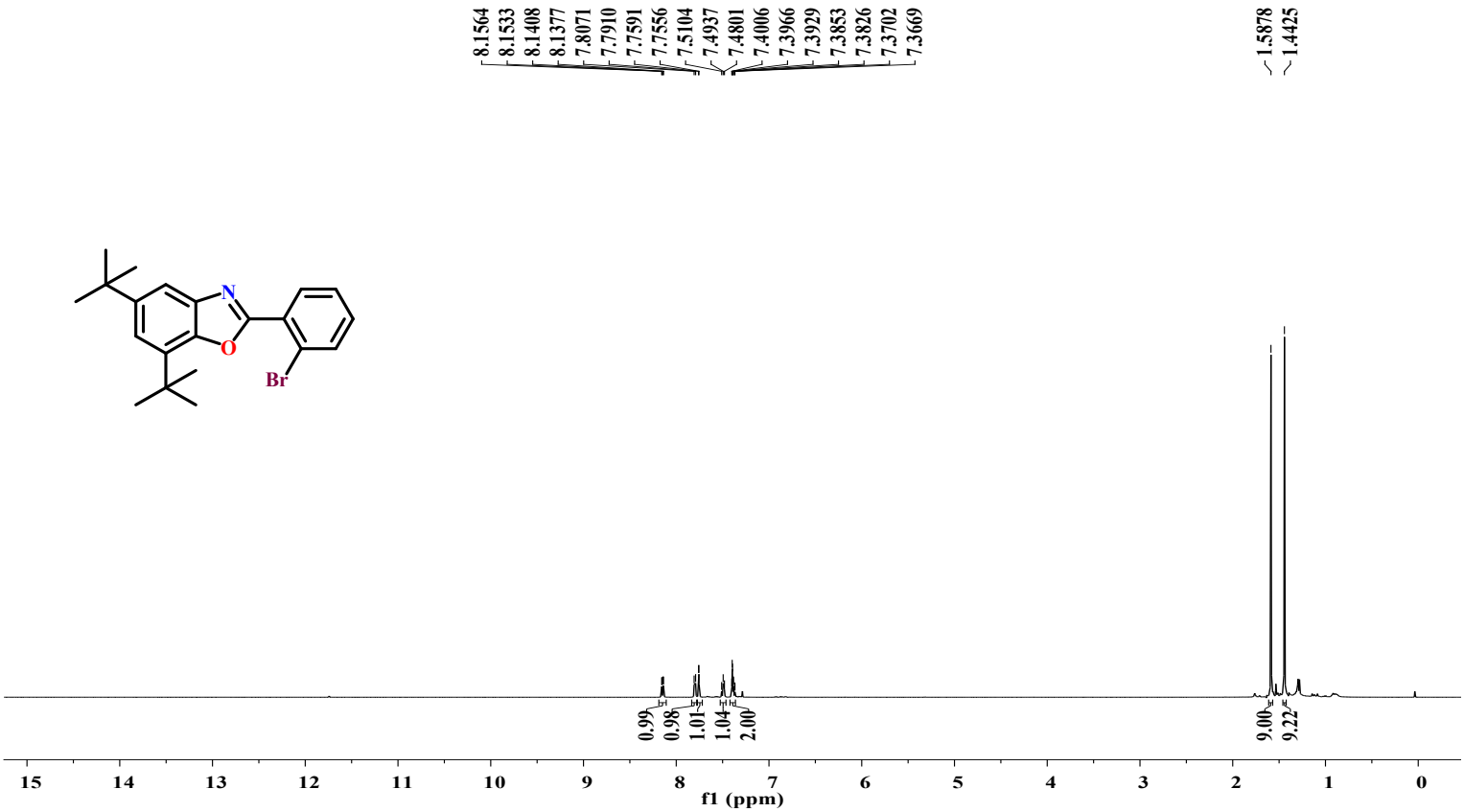


Figure S68. ^{13}C NMR spectrum of compound 4ay in $CDCl_3$ (500 MHz).



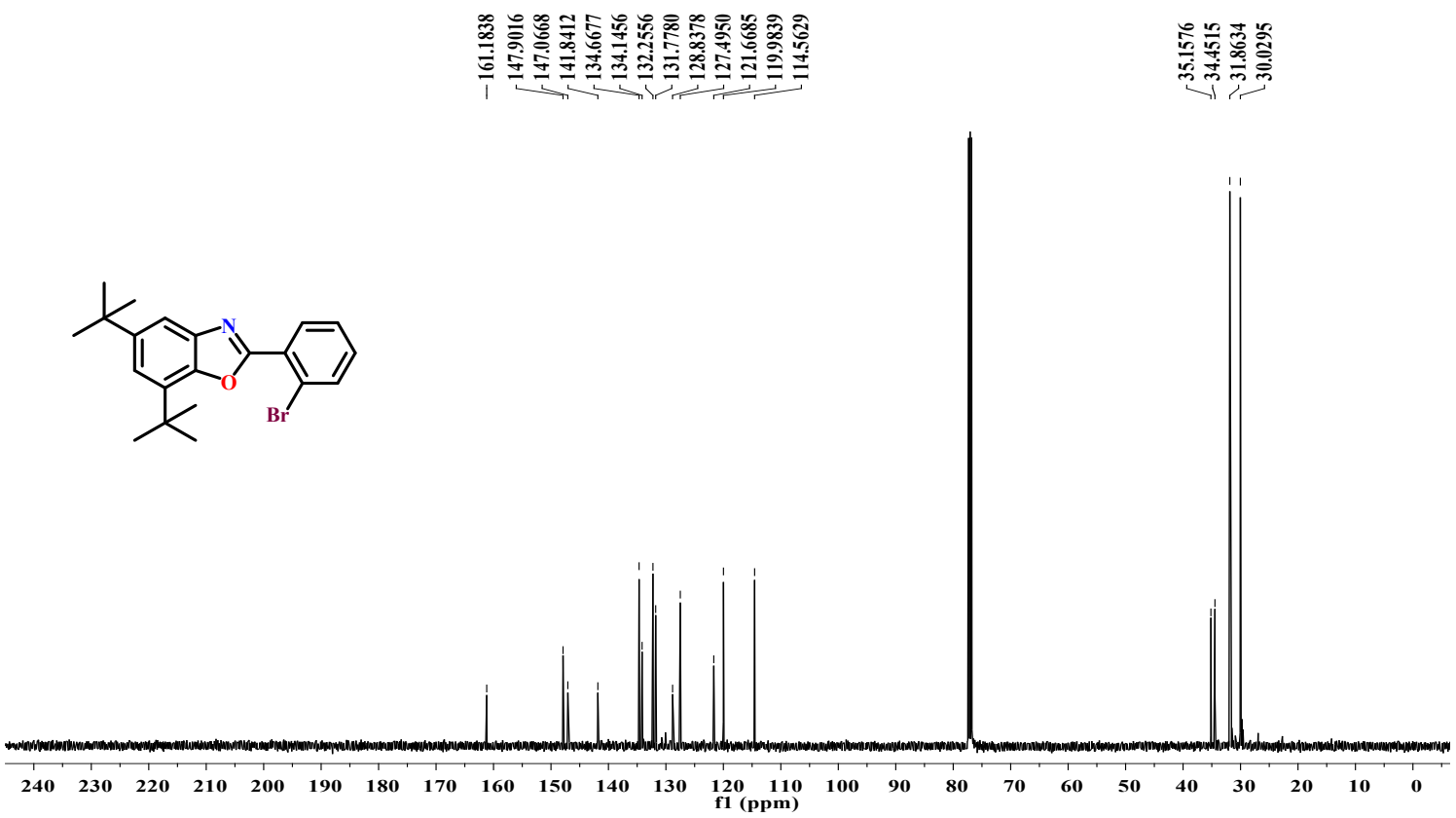


Figure S69. ^{1}H NMR spectrum of compound 4az in $CDCl_3$ (500 MHz).

Figure S70. ^{13}C NMR spectrum of compound 4az in $CDCl_3$ (500 MHz).

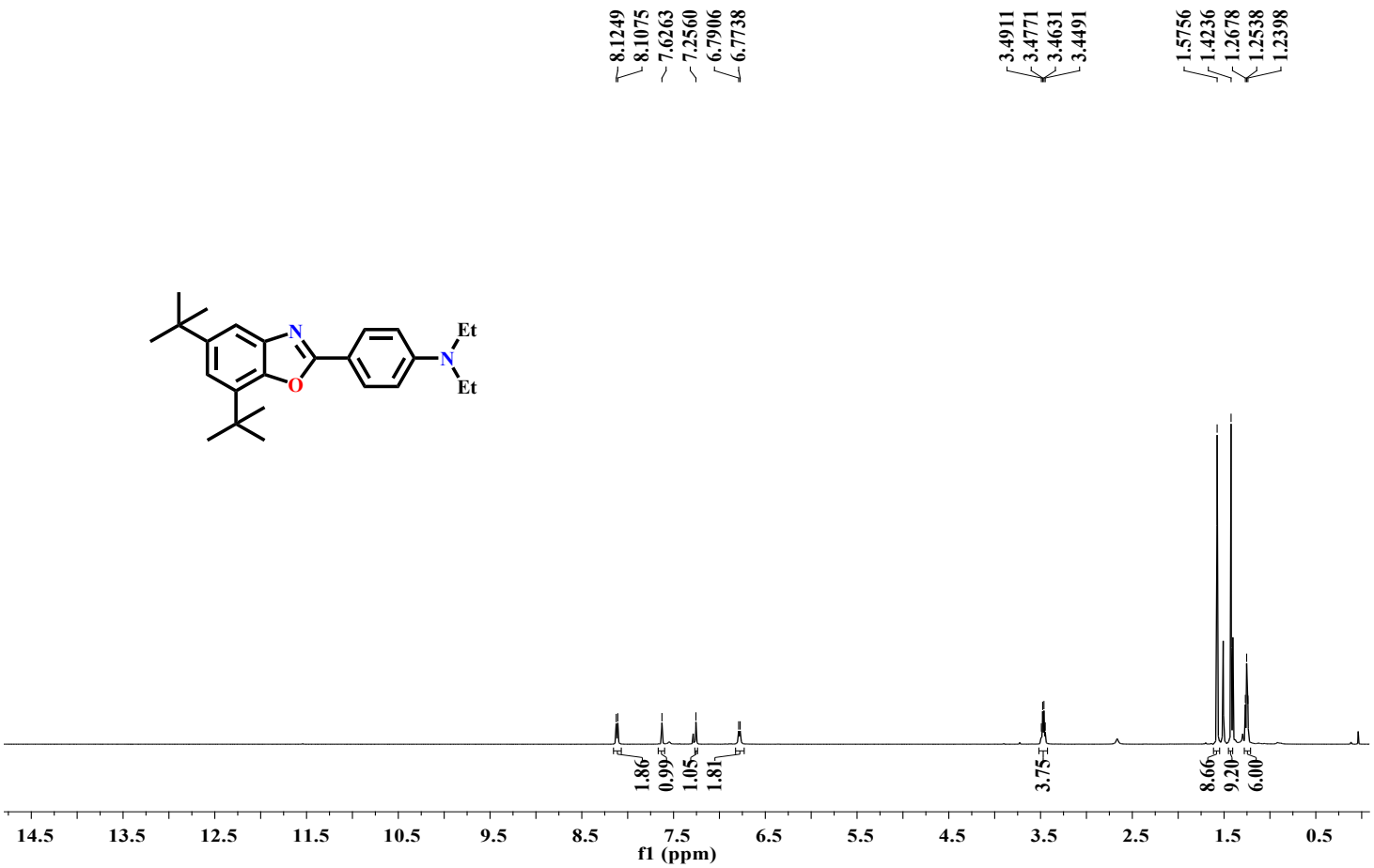


Figure S71. ^{1}H NMR spectrum of compound 4bb in $CDCl_3$ (500 MHz).

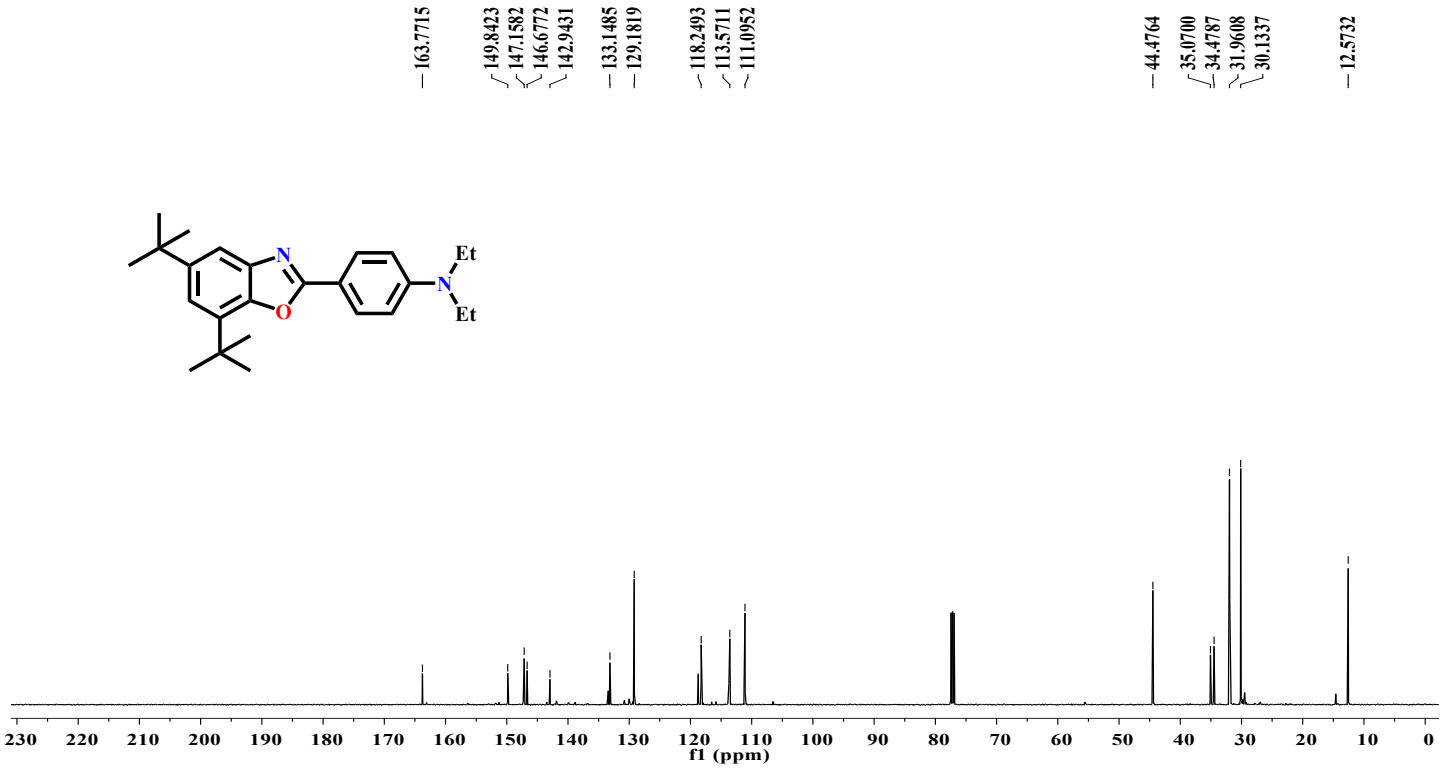


Figure S72. ^{13}C NMR spectrum of compound 4bb in $CDCl_3$ (500 MHz).

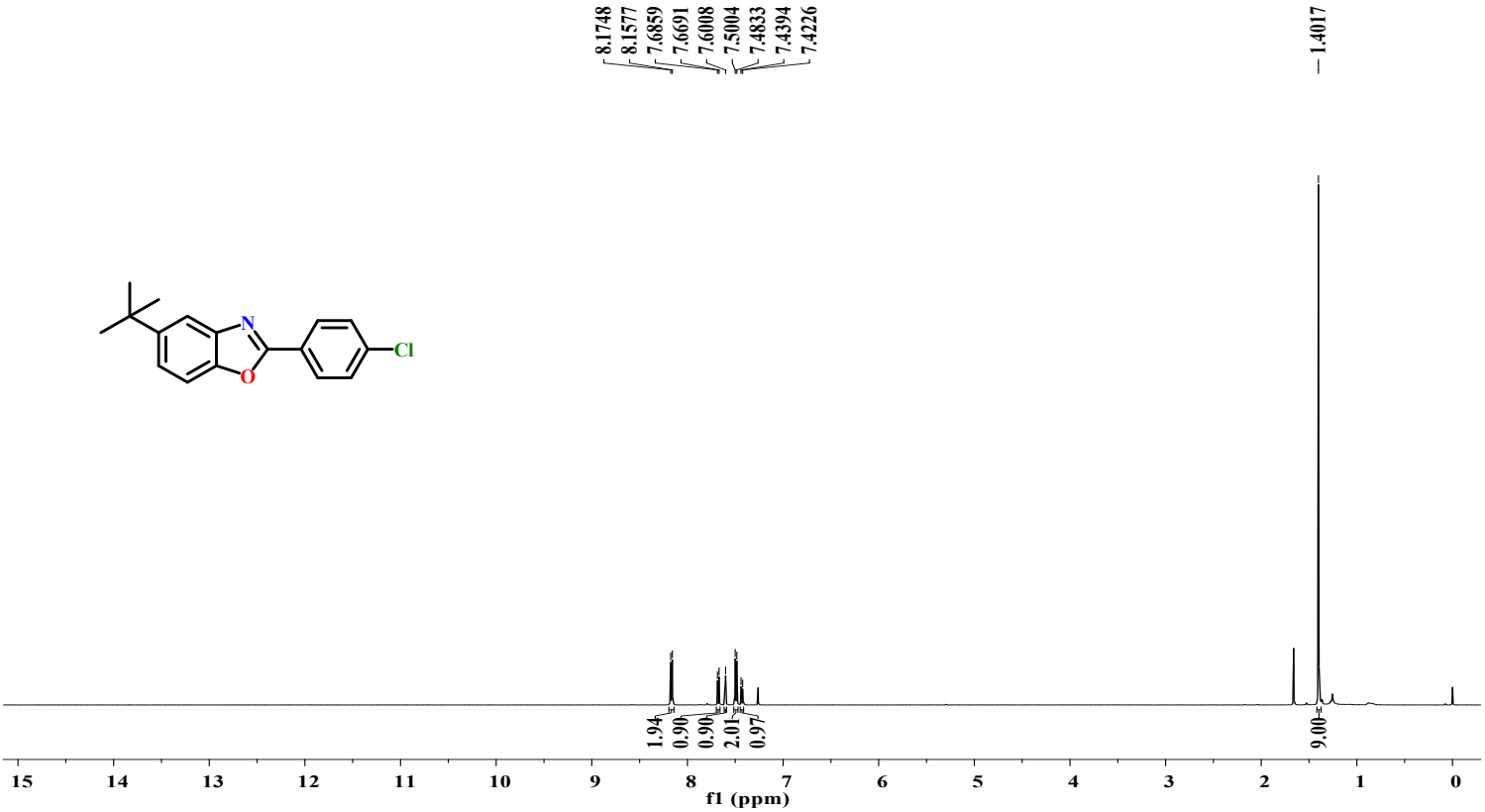


Figure S73. ^{1}H NMR spectrum of compound 4a'a in $CDCl_3$ (500 MHz).

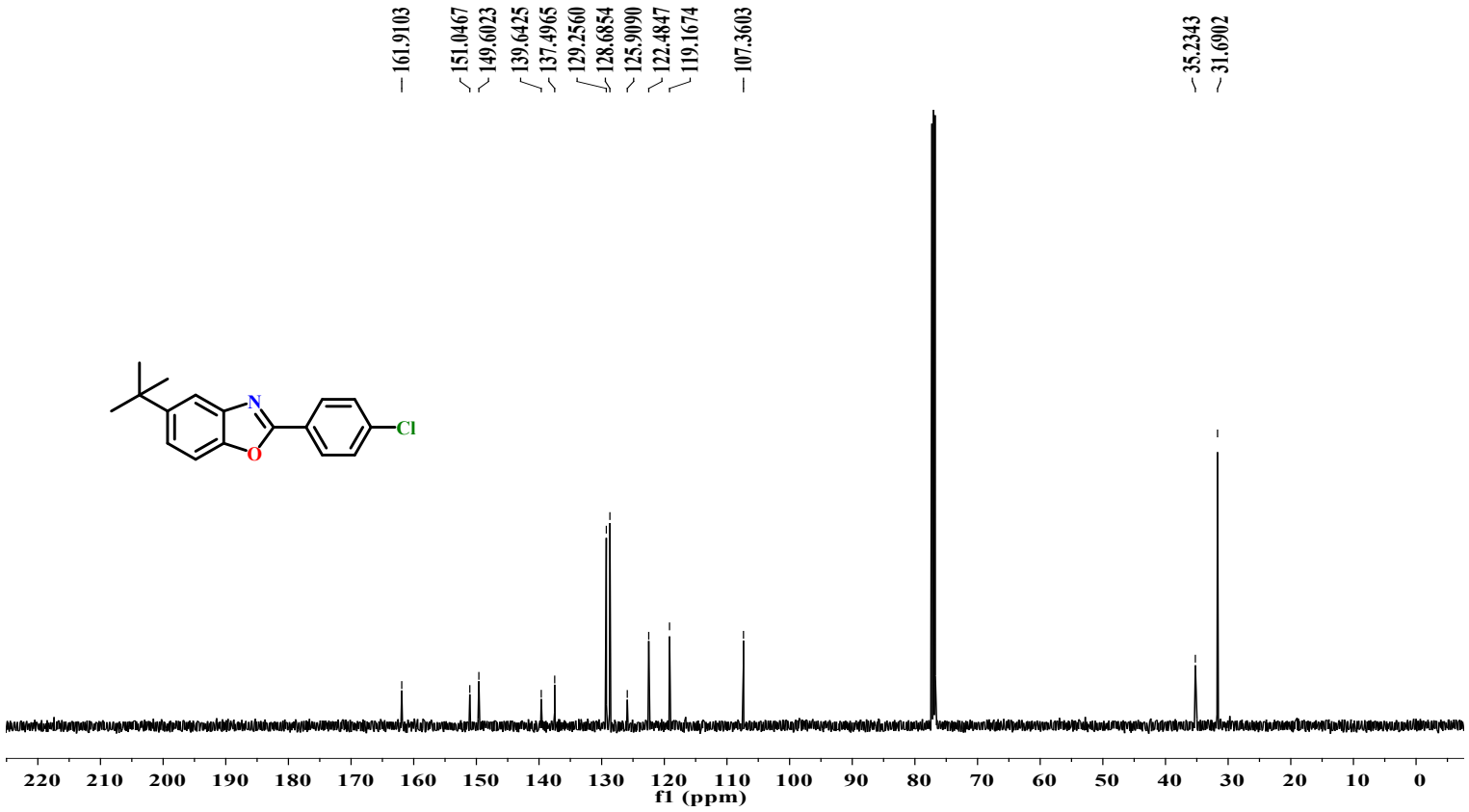
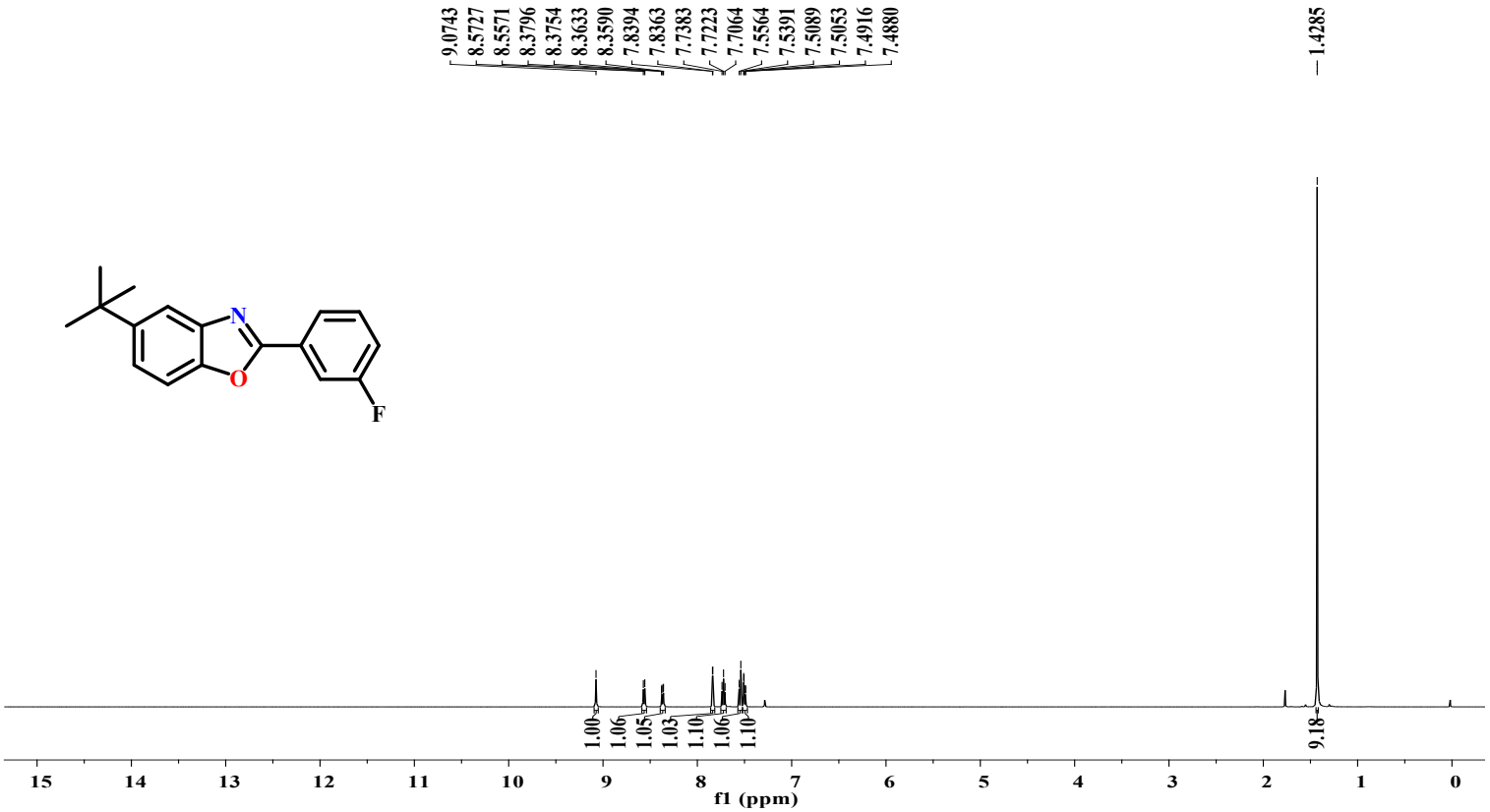


Figure S74. ^{13}C NMR spectrum of compound 4a'a in $CDCl_3$ (500 MHz).



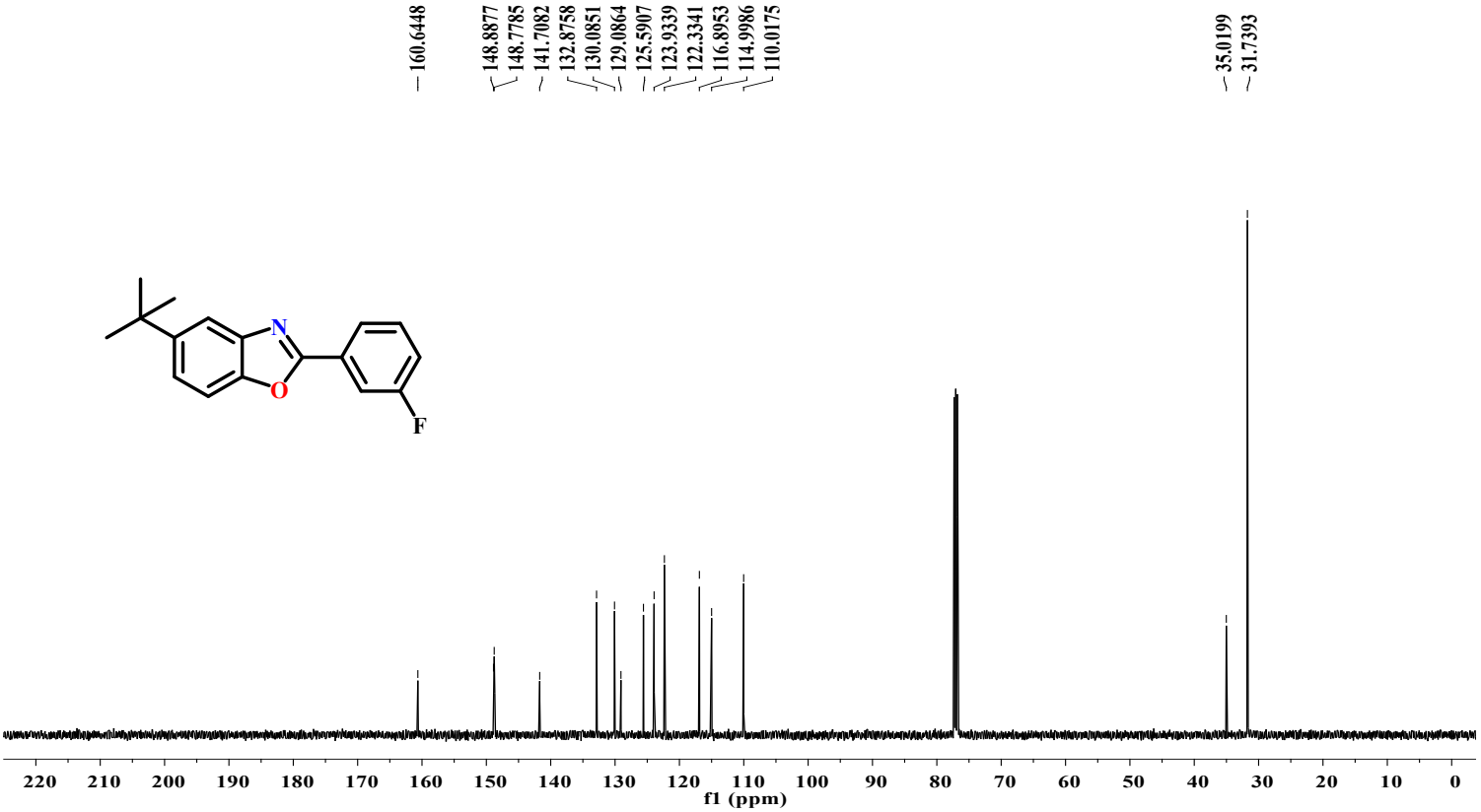


Figure S75. ^{1}H NMR spectrum of compound 4a'b in $CDCl_3$ (500 MHz).

Figure S76. ^{13}C NMR spectrum of compound 4a'b in $CDCl_3$ (500 MHz).

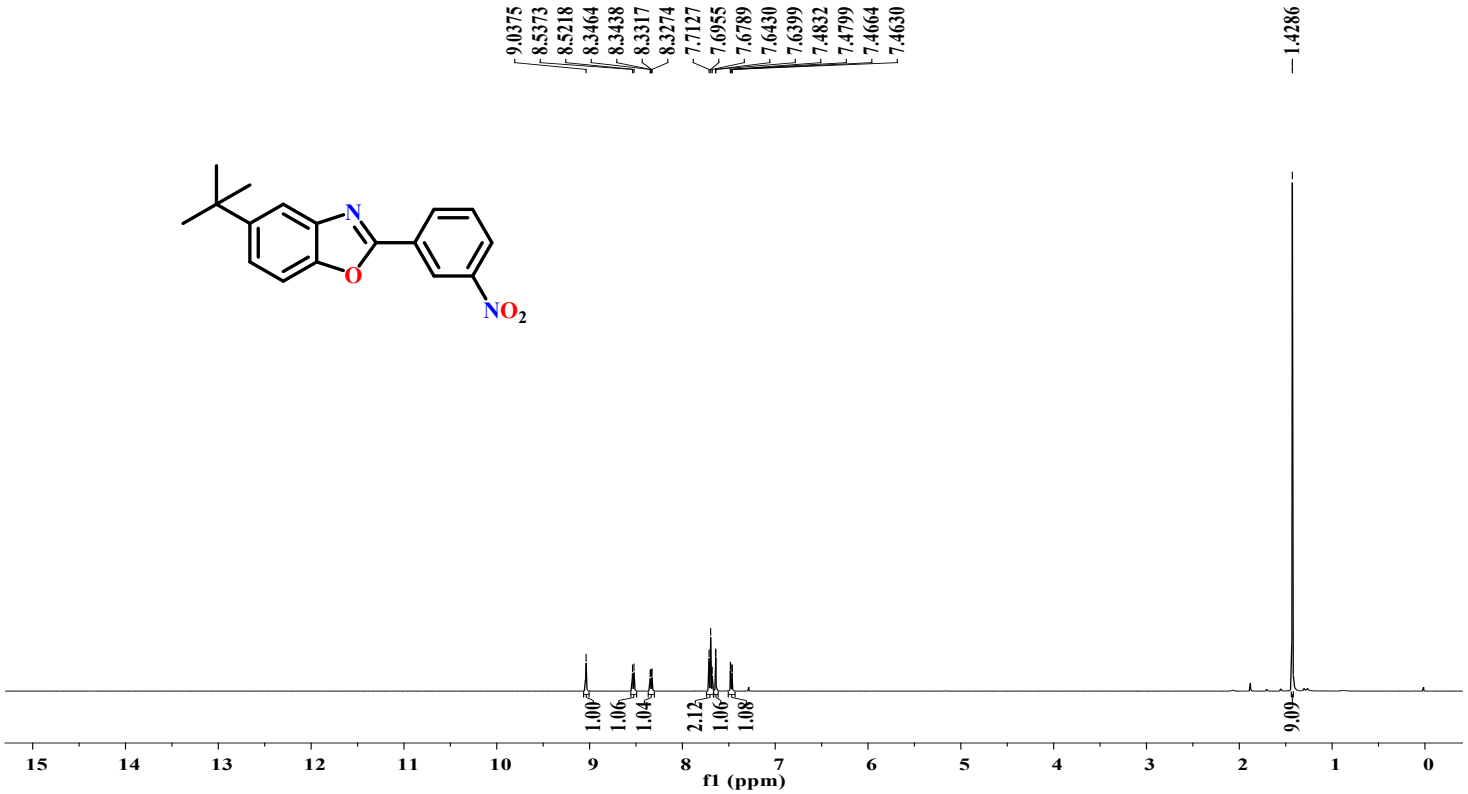


Figure S77. ^{1}H NMR spectrum of compound 4a'c in $CDCl_3$ (500 MHz).

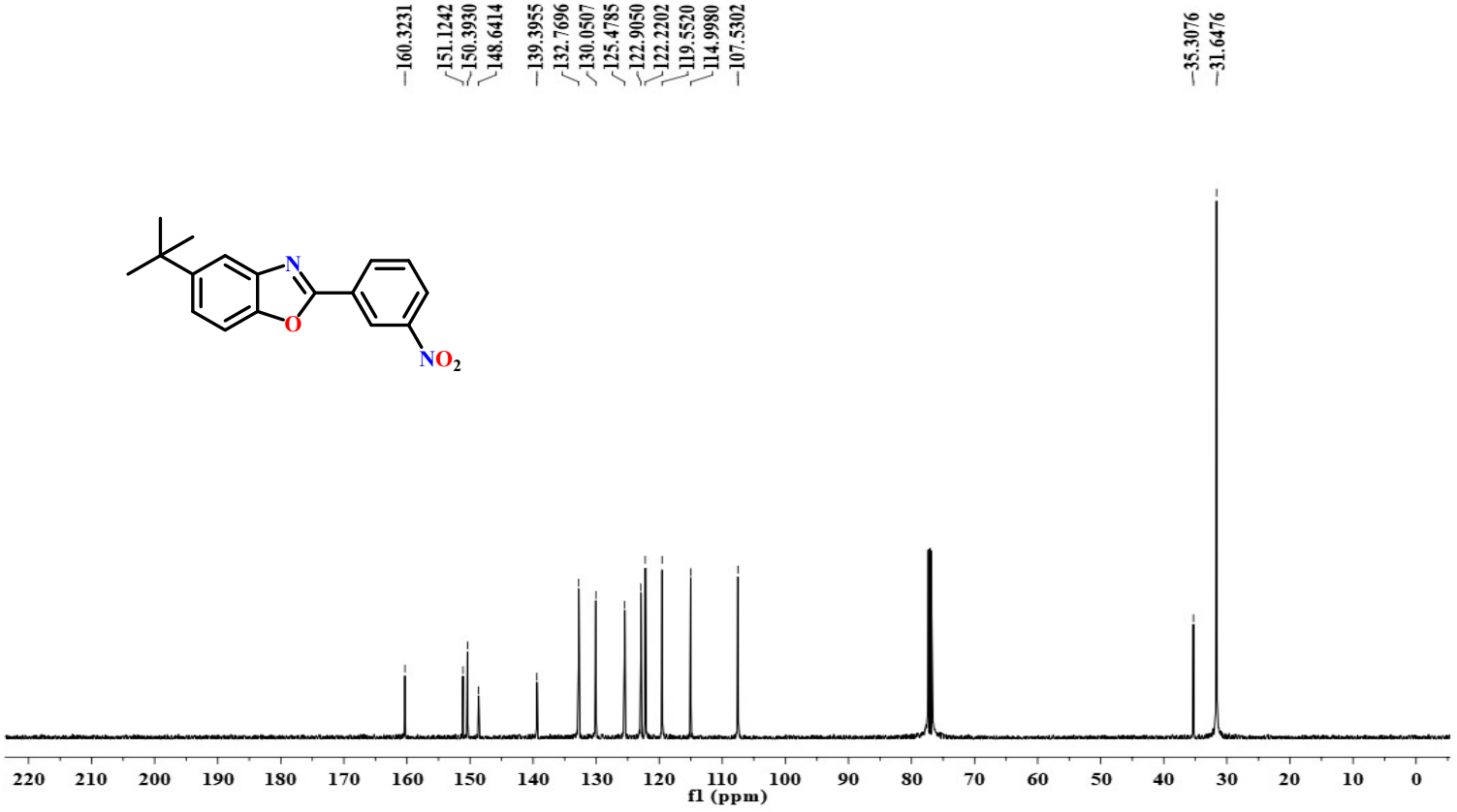


Figure S78. ^{13}C NMR spectrum of compound 4a'c in $CDCl_3$ (500 MHz).

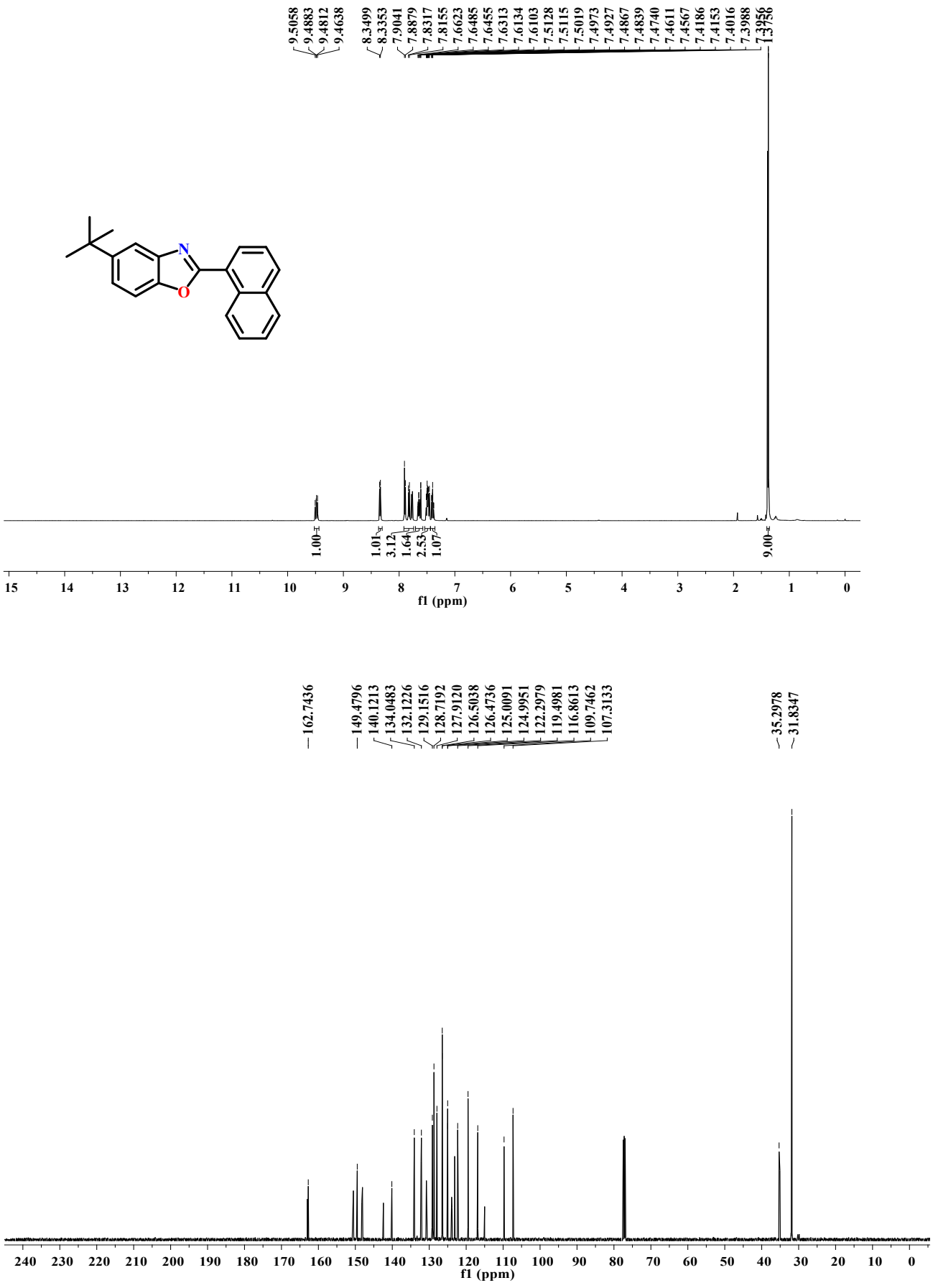


Figure S79. ^{1}H NMR spectrum of compound 4a'd in $CDCl_3$ (500 MHz).

Figure S80. ^{13}C NMR spectrum of compound 4a'd in $CDCl_3$ (500 MHz).

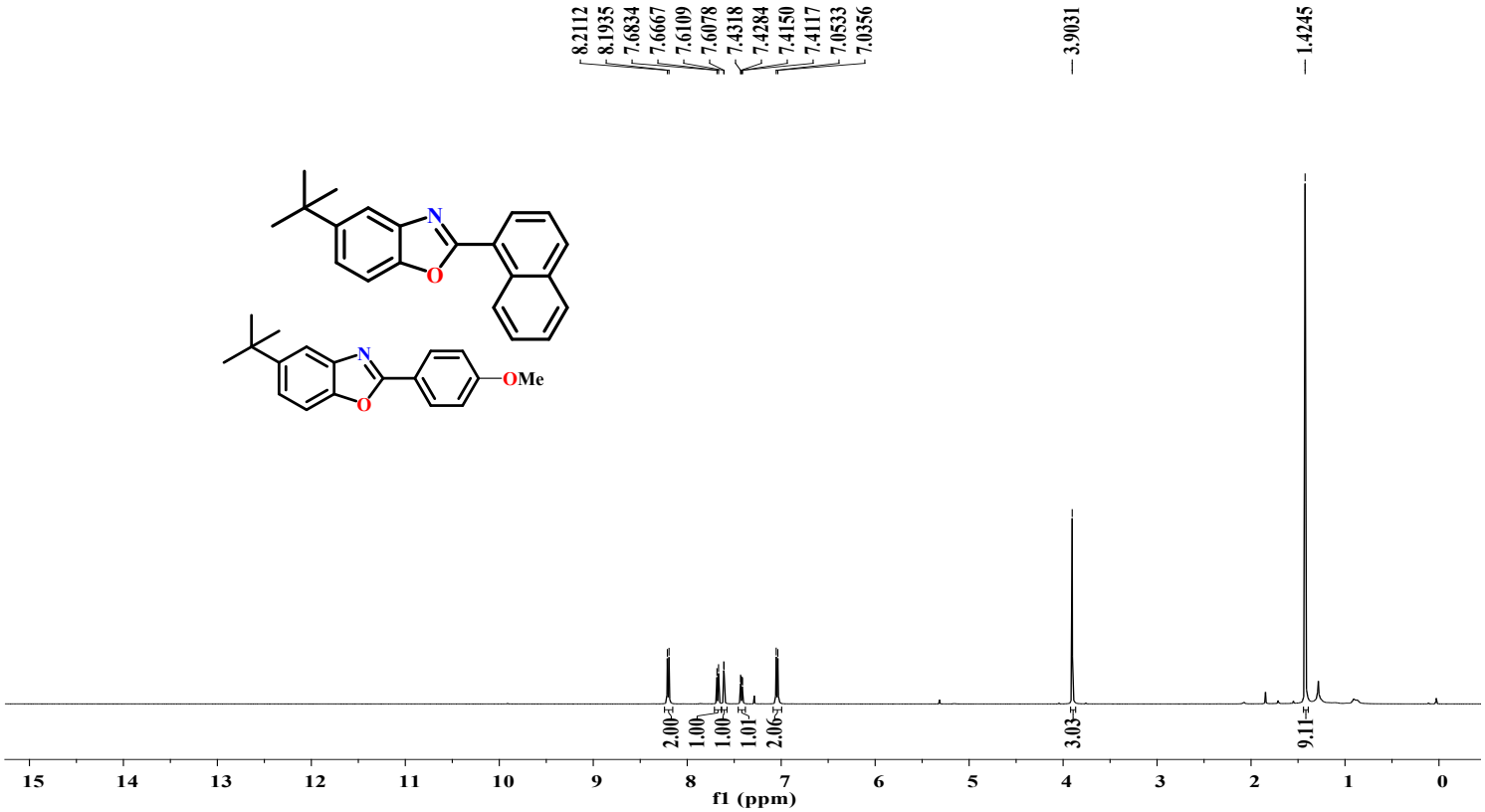


Figure S81. ^{13}C NMR spectrum of compound 4a'e in $CDCl_3$ (500 MHz).

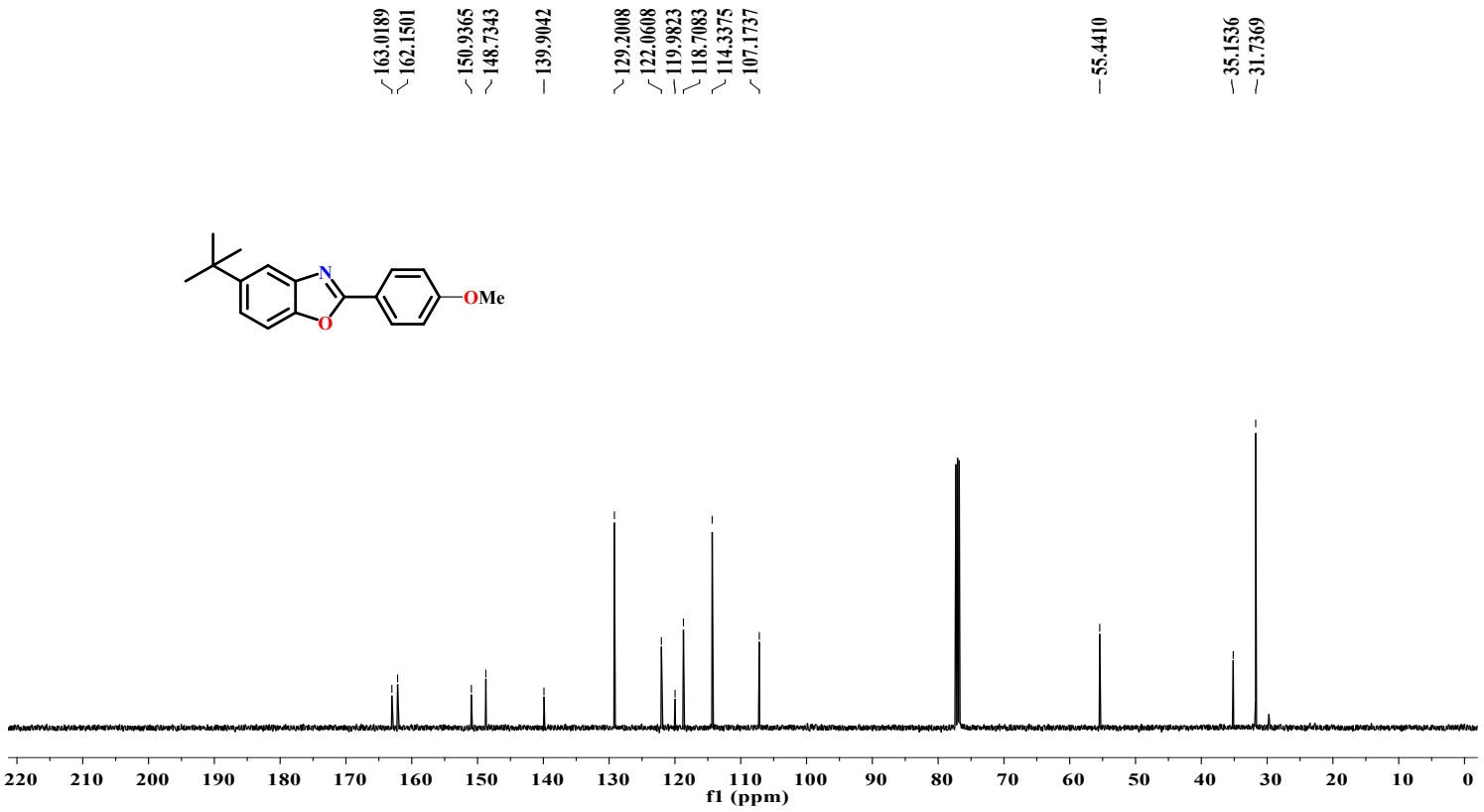


Figure S82. ^{13}C NMR spectrum of compound 4a'e in $CDCl_3$ (500 MHz).

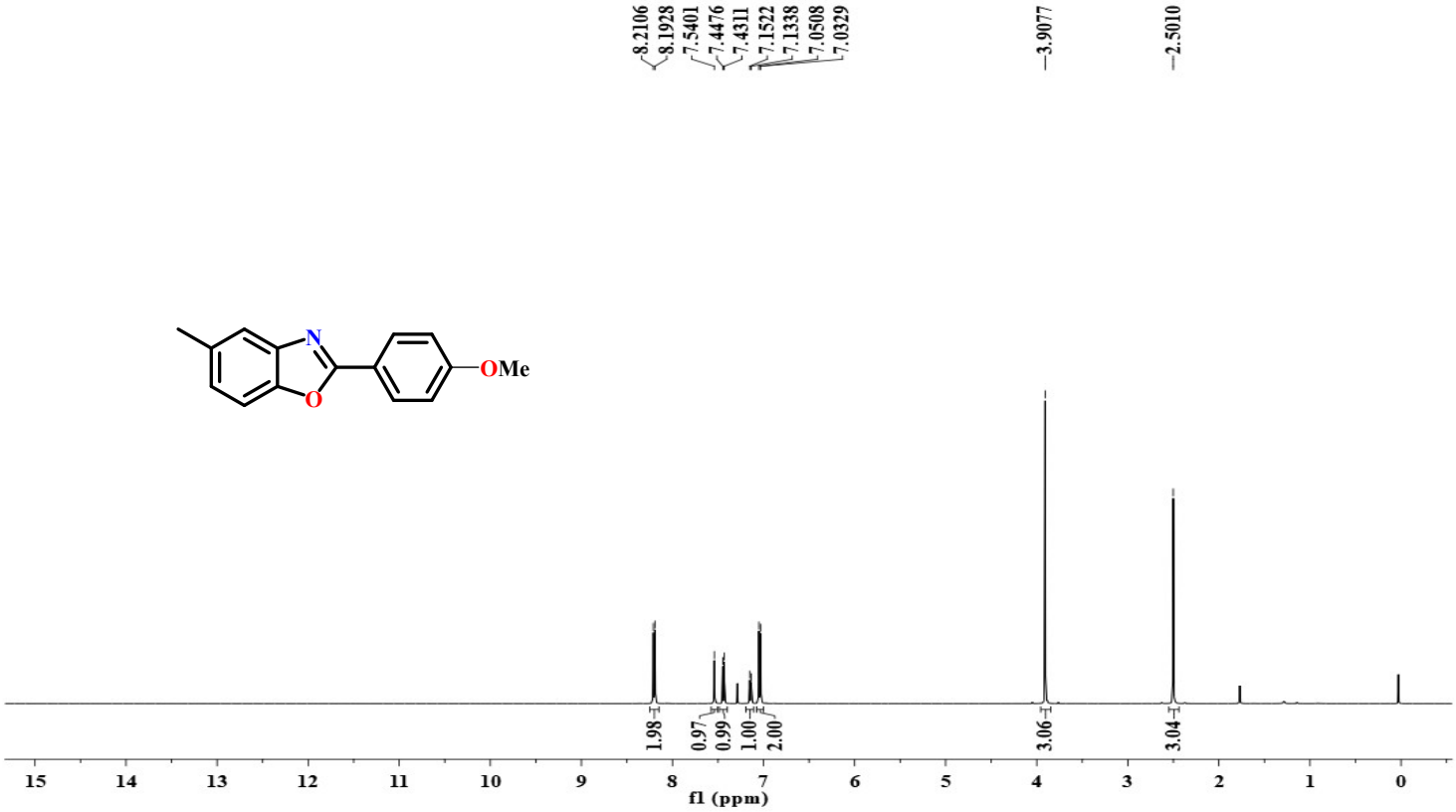


Figure S83. ^{1}H NMR spectrum of compound 4a'f in $CDCl_3$ (500 MHz).

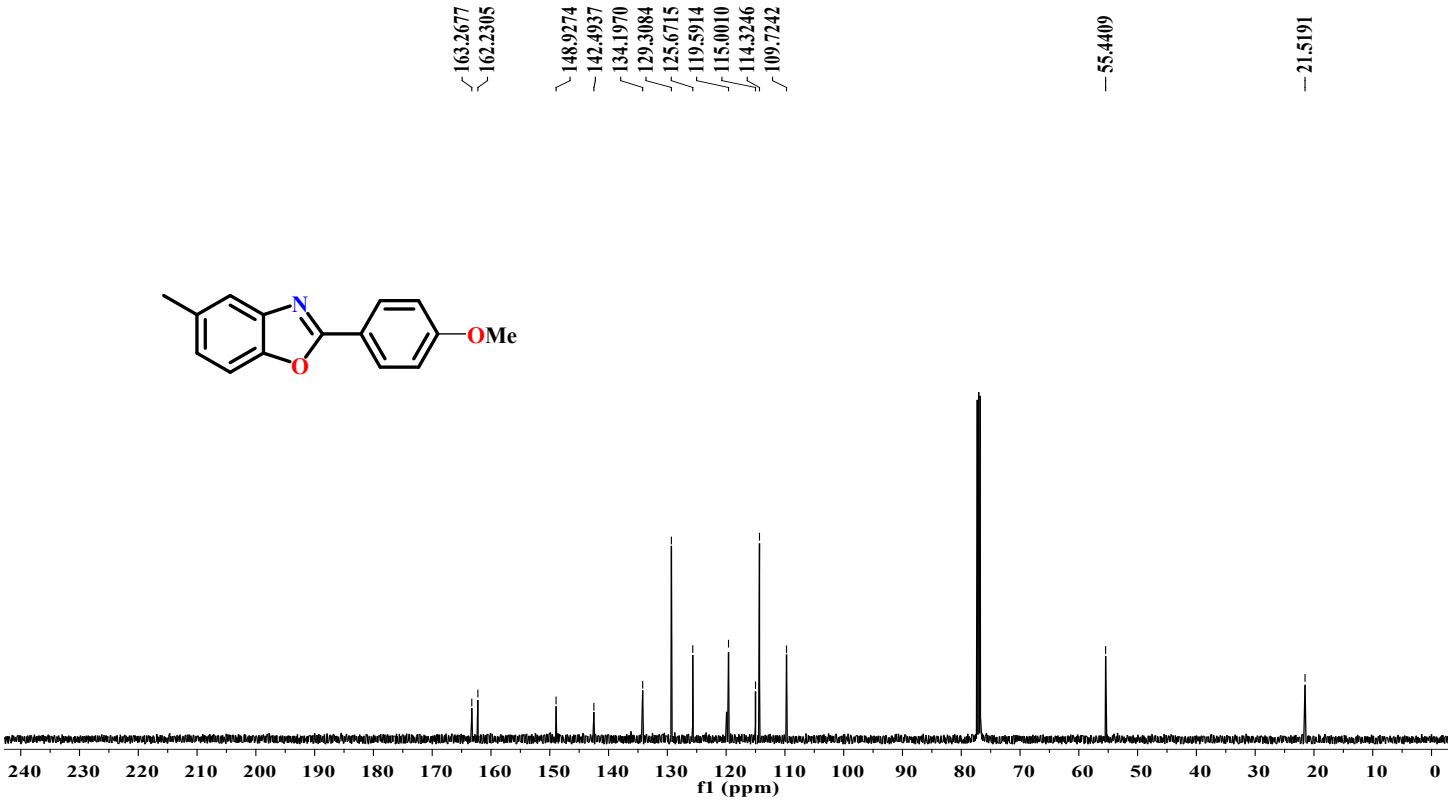


Figure S84. ^{13}C NMR spectrum of compound 4a'f in $CDCl_3$ (500 MHz).

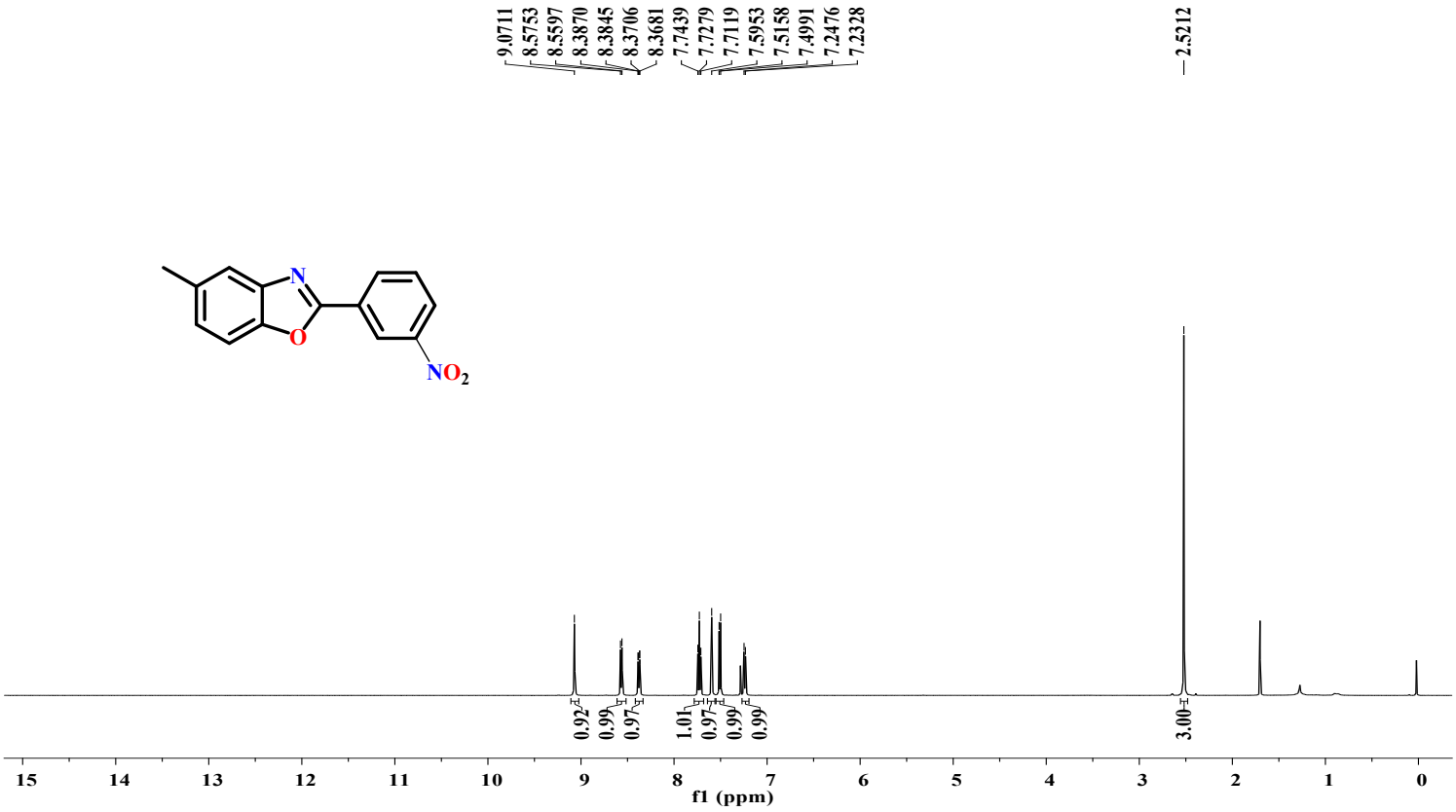


Figure S85. ^{1}H NMR spectrum of compound 4a'g in $CDCl_3$ (500 MHz).

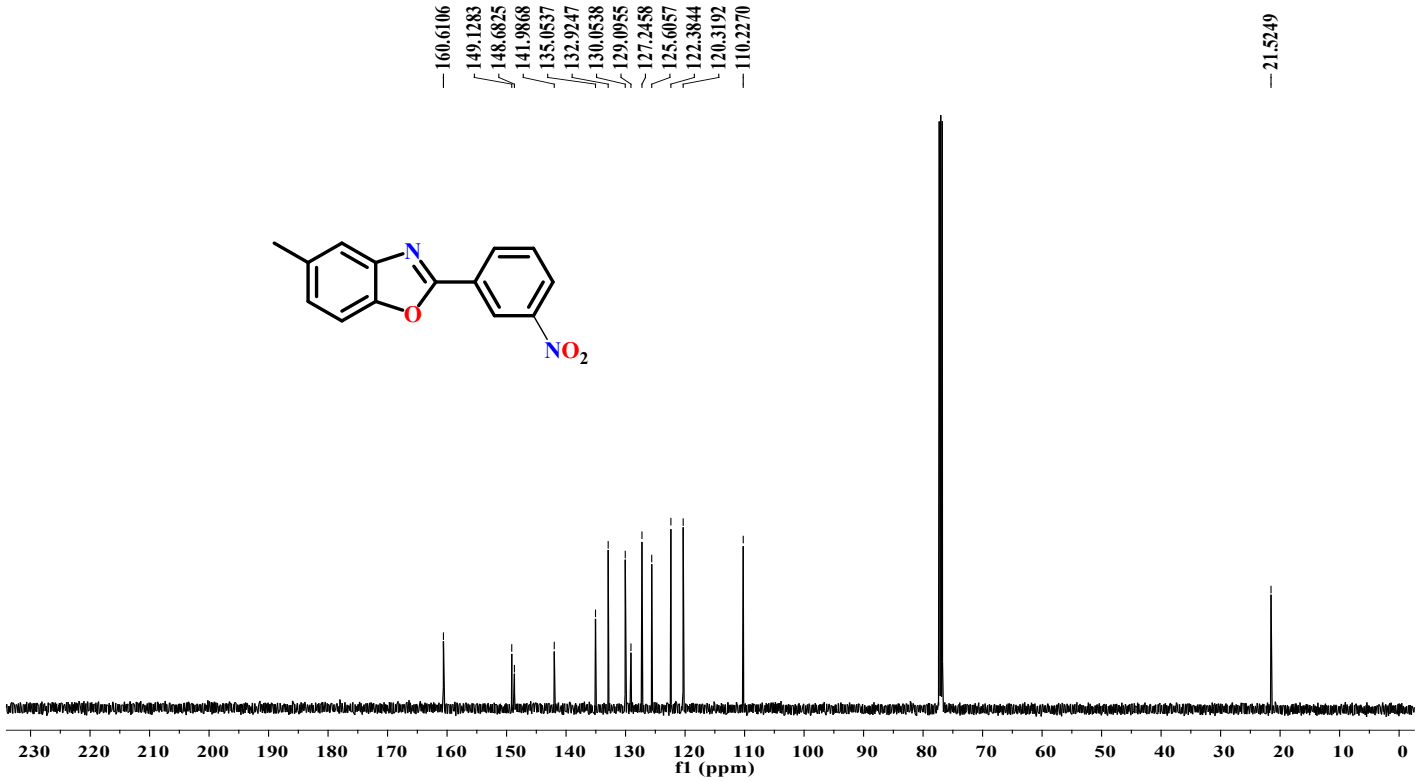


Figure S86. ^{13}C NMR spectrum of compound 4a'g in $CDCl_3$ (500 MHz).

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