Copper-Catalyzed Oxidative Cyclization of Glycine Derivatives for Synthesis of 2-Substituted Benzoxazoles

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Supporting Information

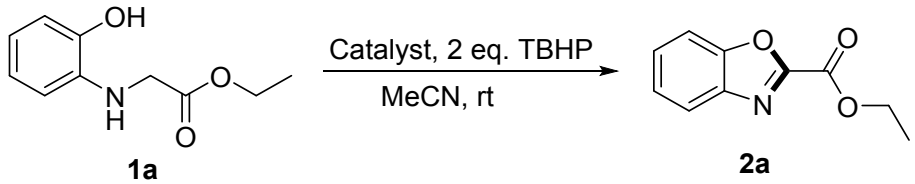
Contents:

1. General Information

Unless otherwise indicated, all reagents were purchased from commercial distributors and used without further purification. ^{1}H NMR and ^{13}C NMR were recorded at 400 MHz and 100 MHz, respectively, using tetramethylsilane as an internal reference. High-resolution mass spectra (HRMS) were measured on a quadrupole time-of-flight (Q-TOF) mass spectrometer instrument with an electrospray ionization (ESI) source. Melting points were uncorrected. Flash column chromatography was performed over silica gel 200-300 mesh. Thin-layer chromatography (TLC) was carried out with silica gel GF254 plates. Glycine derivatives **1** were prepared according to the previous reported protocols.[1]

2. Optimization of the Reaction Conditions

Table S1. Screening of Catalysts[a,b]

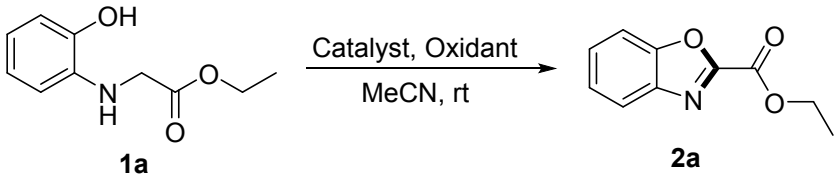


1a **2a**

Entry	Catalyst	Oxidant	Solvent	Yield (%)[b]
1	CuI	TBHP	MeCN	27
2	CuBr	TBHP	MeCN	20
3	**CuCl**	**TBHP**	**MeCN**	**53**
4	$CuBr_2$	TBHP	MeCN	7
5	$CuCl_2$	TBHP	MeCN	10
6	$Cu(OAc)_2$	TBHP	MeCN	26
7	$Cu(OTf)_2$	TBHP	MeCN	10
8	$FeCl_3$	TBHP	MeCN	30
9	$FeCl_2$	TBHP	MeCN	trace
10	$CoCl_2$	TBHP	MeCN	trace

(a) Reaction conditions: **1a** (0.2 mmol), catalyst (5 mol %), TBHP (70 % solution in water, 2 eq.), MeCN (2 mL) at room temperature for 2-4 hrs. (b) Isolated yield.

Table S2. Screening of Oxidants[a,b]

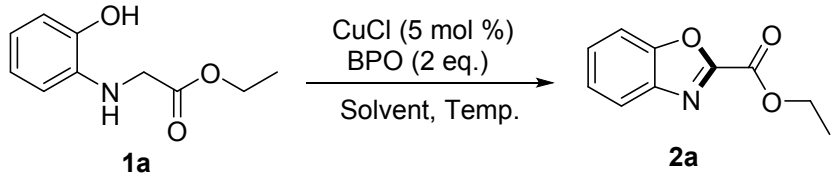


1a **2a**

Entry	Catalyst	Oxidant	Solvent	Yield (%)[b]
1	CuCl	TBHP	MeCN	53
2	CuCl	DTBP	MeCN	15
4	CuCl	TBPB	MeCN	46
5	CuCl	DCP	MeCN	trace
6	**CuCl**	**BPO**	**MeCN**	**66**
7	CuCl	$PhI(OAc)_2$	MeCN	31
8	CuCl	$K_2S_2O_8$	MeCN	trace
9	CuCl	O_2	MeCN	trace
10	CuCl	--	MeCN	trace
11	CuCl	N_2	MeCN	0
12[c]	CuCl	BPO	MeCN	22
13[d]	CuCl	BPO	MeCN	27

(a) Reaction conditions: **1a** (0.2 mmol), CuCl (5 mol %), oxidant (2 eq.), MeCN (2 mL) at room temperature for 2-4 hrs. BPO (75%(wetted with ca. 25% Water).). (b) Isolated yield. (c) BPO (1 eq.). (d) BPO (3.0 eq.).

Table S3. Screening of Solvents and Temperature[a,b]



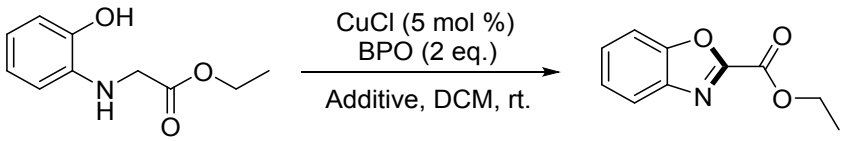
1a **2a**

Entry	Catalyst	Temperature (°C)	Solvent	Yield (%)[b]
1	CuCl	rt	MeCN	66
2	CuCl	rt	Tolnene	35
3	CuCl	rt	EtOAc	51
4	CuCl	rt	DCE	40

5	**CuCl**	**rt**	**DCM**	**72**
6	CuCl	rt	DMF	23
7	CuCl	rt	EtOH	14
8	CuCl	rt	PhCl	25
9	CuCl	rt	DMSO	33
10	CuCl	40	DCM	67
11	CuCl	60	DCM	60

(a) Reaction conditions: **1a** (0.2 mmol), CuCl (5 mol %), BPO (2 equiv), solvent (2 mL) at room temperature for 2-4 hrs. (b) Isolated yield.

Table S4. Screening of Additives.[a]



Entry	Catalyst	Additive	Solvent	Yield (%)[b]
1	CuCl	$CsCO_3$	DCM	64
2	CuCl	*t*BuOK	DCM	49
3	CuCl	*t*BuONa	DCM	65
4	CuCl	$LiCO_3$	DCM	70
5	CuCl	DBU	DCM	61
6	CuCl	DABCU	DCM	52
7	CuCl	$NaHCO_3$	DCM	69
8	CuCl	Na_2CO_3	DCM	73
9	**CuCl**	**K_2CO_3**	**DCM**	**84**
10	CuCl	NaOH	DCM	66
11[c]	CuCl	K_2CO_3	DCM	69
12[d]	CuCl	K_2CO_3	DCM	58

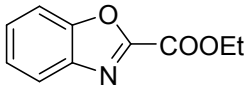
(a) Reaction conditions: **1a** (0.2 mmol), CuCl (5 mol %), BPO (2 equiv), Base (1 equiv), Solvent (2 mL) at room temperature for 2-4 hours. (b) Isolated yield based on **2a**. (c) K_2CO_3 (0.5 eq.). (d) K_2CO_3 (2.0 eq.).

3. General Procedure

General procedure for the synthesis of 2-substituted benzoxazoles. To a mixture of glycine derivatives **1** (0.2 mmol) in MeCN (2 mL) was added CuCl (0.01 mmol, 1.0 mg) and BPO (0.4 mmol, 96.9 mg). Then, the reaction mixture was stirred at room temperature for 2-4 hours. After the reaction was completed, the resulting mixture was concentrated under vacuum and the residue was subjected to column chromatography (silica gel, petroleum ether/ethyl acetate as an eluent) to afford the desired cyclization products **2**.

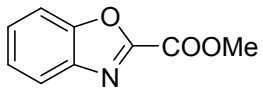
4. Characterization Data

Ethyl benzo[*d*]oxazole-2-carboxylate (2a)[2]



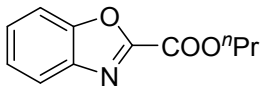
Yellowish-brown solid; mp 88-92.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.54 (t, *J* = 8.0 Hz, 1H), 7.47 (t, *J* = 8.4 Hz, 1H), 4.57 (q, *J* = 7.2 Hz, 2H), 1.51 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.5, 152.8, 150.9, 140.6, 128.1, 125.7, 122.1, 111.7, 63.2, 14.2; HRMS (ESI) calcd for $C_{10}H_{10}NO_3$ $(M+H)^+$ 192.0655, found 192.0653.

Methyl benzo[*d*]oxazole-2-carboxylate (2b)[3]



Yellowish-brown solid; mp 95.2-97.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 4.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 152.5, 150.9, 140.5, 128.2, 125.8, 122.2, 111.8, 53.7; HRMS (ESI) calcd for $C_9H_8NO_3$ $(M+H)^+$ 178.0499, found 178.0498.

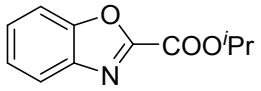
Propyl benzo[*d*]oxazole-2-carboxylate (2c)



Yellowish-brown solid; mp 60.1-63.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.52 (t, *J* = 8.4 Hz, 1H), 7.45 (t, *J* = 8.4 Hz, 1H), 4.46 (t, *J* = 6.8 Hz, 2H), 1.97-1.81 (m, 2H), 1.07 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.6, 152.8, 150.9, 140.6, 128.0, 125.7, 122.1, 111.7, 68.6, 21.9, 10.2; HRMS (ESI) calcd for $C_{11}H_{12}NO_3$

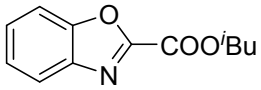
$(M+H)^+$ 206.0812, found 206.0813.

Isopropyl benzo[*d*]oxazole-2-carboxylate (2d)



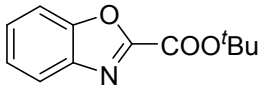
Yellow soild; mp 54.6-58.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.52 (t, *J* = 8.8 Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 1H), 5.42 (dt, *J* = 6.4, 6.0 Hz, 1H), 1.48 (d, *J* = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.1, 153.1, 150.9, 140.6, 128.0, 125.6 122.1, 111.7, 71.5, 21.7. HRMS (ESI) calcd for $C_{11}H_{12}NO_3$ $(M+H)^+$ 206.0812, found 206.0812.

Isobutyl benzo[*d*]oxazole-2-carboxylate (2e)



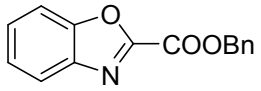
Yellowi solid; mp 97.4-97.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.0 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 4.28 (d, *J* = 6.8 Hz, 2H), 2.20 (dt, *J* = 13.2, 6.8 Hz, 1H), 1.06 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.6, 152.8, 150.9, 140.6, 128.1, 125.7, 122.2, 111.7, 73.0, 27.8, 19.0. HRMS (ESI) calcd for $C_{12}H_{14}NO_3$ $(M+H)^+$ 220.0968, found 220.0970.

***tert*-Butyl benzo[*d*]oxazole-2-carboxylate (2f)**[4]



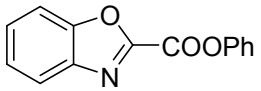
Yellow oil liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 8.5 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 1.69 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 153.7, 150.8, 140.6, 127.9, 125.6, 122.1, 111.7, 85.2, 28.1; HRMS (ESI) calcd for $C_{12}H_{14}NO_3$ $(M+H)^+$ 220.0968, found 220.0967.

Benzyl benzo[*d*]oxazole-2-carboxylate (2g)[5]



Yellowish solid; mp 91.1 -93.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.61-7.28 (m, 7H), 5.51 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.4, 152.6, 150.9, 140.6, 134.5, 128.9, 128.9, 128.8, 128.2, 125.8, 122.2, 111.7, 68.6; HRMS (ESI) calcd for $C_{11}H_{12}NO_3$ $(M+H)^+$ 206.0812, found 206.0813.

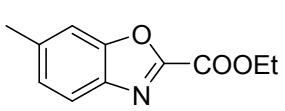
Phenyl benzo[*d*]oxazole-2-carboxylate (2h)



Orange solid; m.p. 152.1-155.8°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 2H), 7.81 (d, *J* = 7.8 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 2H),

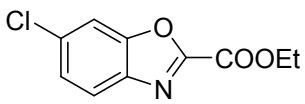
7.44-7.30 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 146.4, 146.3, 132.1, 131.2, 129.6, 125.7, 116.8. HRMS (ESI) calcd for $C_{14}H_{10}NO_3$ $(M+H)^+$ 240.0655, found 240.0645.

Ethyl 6-methylbenzo[*d*]oxazole-2-carboxylate (2i)



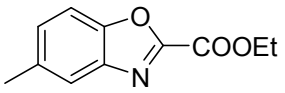
Yellowish solid; m.p. 85.3-86.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 8.4 Hz, 1H), 7.44 (s, 1H), 7.26 (d, J = 8.0 Hz, 1H), 4.55 (q, J = 7.2 Hz, 2H), 2.53 (s, 3H), 1.49 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.6, 152.4, 151.2, 139.1, 138.4, 127.3, 121.4, 111.5, 63.0, 22.0, 14.1; HRMS (ESI) calcd for $C_{11}H_{12}NO_3$ $(M+H)^+$ 206.0811, found 206.0812.

Ethyl 6-chlorobenzo[*d*]oxazole-2-carboxylate (2j)[6]

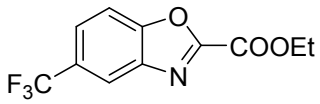


Yellow solid; mp 98.2-103.2 °C; 1H NMR (400 MHz, CDCl3) δ 7.88 (d, J = 2.0 Hz, 1H), 7.68-7.40 (m, 2H), 4.57 (q, J = 7.2 Hz, 2H), 1.50 (t, J = 7.2 Hz, 3H); 13C NMR (100 MHz, CDCl3) δ 156.1, 153.9, 149.4, 141.5, 131.5, 128.7, 121.9, 112.6, 63.5, 14.1; HRMS (ESI) calcd for $C_{10}H_9ClNO_3$ $(M+H)^+$ 226.0262, found 226.0266.

Ethyl 5-methylbenzo[*d*]oxazole-2-carboxylate (2k)

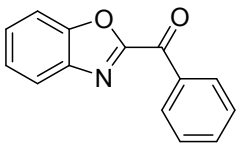


Yellow solid; mp 97.4-98.6 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (s, 1H), 7.53 (d, J = 8.5 Hz, 1H), 7.33 (d, J = 8.4 Hz, 1H), 4.56 (q, J = 7.1 Hz, 2H), 2.50 (s, 3H), 1.50 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.56, 152.83, 149.18, 140.74, 135.83, 129.54, 121.66, 111.06, 63.15, 21.49, 14.18. HRMS (ESI) calcd for $C_{11}H_{12}NO_3$ $(M+H)^+$ 206.0811, found 206.0812. **Ethyl 5-(trifluoromethyl)benzo[*d*]oxazole-2-carboxylate (2l)**



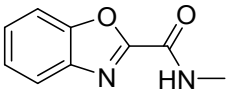
Yellow oil liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (s, 1H), 7.92 – 7.67 (m, 2H), 4.60 (q, J = 7.2 Hz, 2H), 1.52 (t, J = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.0, 154.3, 152.4, 140.5, 128.7 (q, J = 32.5 Hz), 125.3 (q, J = 3.75 Hz), 123.7 (q, J = 271.3 Hz), 120.0 (q, J = 3.75 Hz), 112.6, 63.7, 14.2. HRMS (ESI) calcd for $C_{11}H_8F_3NO_3$ $(M+H)^+$ 260.0529, found 260.0526.

Benzo[*d*]oxazol-2-yl(phenyl)methanone (2m)



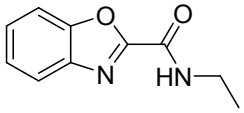
Yellow solid; mp 66.3-68.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (d, *J* = 8.5 Hz, 2H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.69 (dd, *J* = 14.5, 7.7 Hz, 2H), 7.56 (dd, *J* = 15.1, 7.7 Hz, 3H), 7.47 (t, *J* = 8.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.5, 157.2, 150.5, 140.8, 135.1, 134.3, 131.0, 128.6, 128.4, 125.7, 122.4, 111.8. HRMS (ESI) calcd for $C_{14}H_9NO_2$ $(M+H)^+$ 224.0706, found 224.0700.

***N*-Methylbenzo[*d*]oxazole-2-carboxamide (2n)**[6]



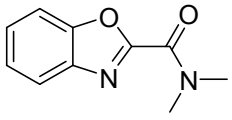
Yellow solid; mp 97.4-98.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.46 (dt, *J* = 11.6, 7.6 Hz, 2H), 7.34 (s, 1H), 3.09 (d, *J* = 5.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.3, 155.5, 151.1, 140.3, 127.3, 125.5, 121.2, 111.9, 26.5; HRMS (ESI) calcd for $C_9H_9N_2O_3$ $(M+H)^+$ 177.0659, found 177.0657.

***N*-ethylbenzo[*d*]oxazole-2-carboxamide (2o)**[6]



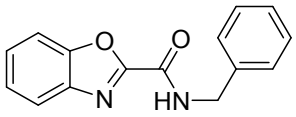
Yellow solid; mp 94.2-95.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.55-7.38 (m, 2H), 7.32 (s, 1H), 3.67-3.47 (m, 2H), 1.31 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 155.6, 151.1, 140.3, 127.3, 125.5, 121.3, 111.9, 34.8, 14.6; HRMS (ESI) calcd for $C_{10}H_{11}N_2O_2$ $(M+H)^+$ 191.0815, found 191.0814.

***N*,*N*-dimethylbenzo[*d*]oxazole-2-carboxamide (2p)**



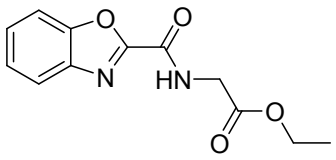
Yellow solid; mp 79.2-81.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.6 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.44 (dt, *J* = 15.2, 7.2 Hz, 2H), 3.52 (s, 3H), 3.21 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.6, 155.2, 159.0, 140.3, 127.1, 125.2, 121.3, 111.6, 38.9, 36.5. HRMS (ESI) calcd for $C_{10}H_{10}N_2O_2$ $(M+H)^+$ 191.0815, found 191.0813.

***N*-Benzylbenzo[*d*]oxazole-2-carboxamide (2q)**[6]



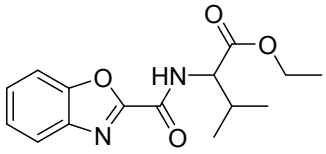
Yellow solid; mp 93.4-95.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.50-7.33 (m, 6H), 4.70 (d, *J* = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 155.5, 151.3, 140.3, 137.0, 128.9, 128.0, 127.9, 127.4, 125.6, 121.2, 111.9, 43.9; HRMS (ESI) calcd for $C_{15}H_{13}N_2O_2$ $(M+H)^+$ 253.0972, found 253.0971.

Ethyl (benzo[*d*]oxazole-2-carbonyl)glycinate (2r)



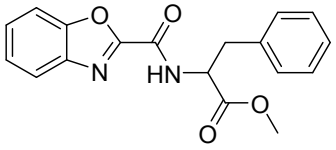
Yellow solid; mp 109.9-110.4 °C ; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.0 Hz, 1H), δ 7.81 (s, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.5-7.36 (m, 2H), 4.58-3.95 (m, 4H), 1.32 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 155.8, 154.9, 151.2, 140.2, 127.6, 125.6, 121.5, 111.9, 61.9, 41.6, 14.2. HRMS (ESI) calcd for $C_{12}H_{13}N_2O_3$ $(M+H)^+$ 249.0870, found 249.0868.

Ethyl (benzo[*d*]oxazole-2-carbonyl)valinate (2s)



Yellow oil liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.54-7.38 (m, 2H), 4.77 (dd, *J* = 9.2, 4.8 Hz, 1H), 4.27 (q, *J* = 6.8 Hz, 2H), 2.67-2.14 (m, 1H), 1.32 (t, *J* = 7.2 Hz, 3H), 1.11-0.96 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 155.5, 155.1, 151.2, 140.3, 127.5, 125.6, 121.4, 111.8, 61.6, 57.6, 31.6, 19.0, 17.8, 14.2; HRMS (ESI) calcd for $C_{18}H_{17}N_2O_4$ $(M+H)^+$ 325.1183, found 325.1184.

Methyl (benzo[*d*]oxazole-2-carbonyl)phenylalaninate (2t)



Yellow oil liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.53-7.39 (m, 2H), 7.33-7.16 (m, 5H), 5.11 (dt, *J* = 8.0, 6.0 Hz, 1H), 3.77 (s, 3H), 3.28 (qd, *J* = 12.8, 6.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 155.2, 154.8, 151.2, 140.2, 135.4, 129.3, 128.8, 127.5, 127.4, 125.6, 121.5, 111.8, 53.6, 52.6, 38.0; HRMS (ESI) calcd for $C_{15}H_{19}N_2O_4$ $(M+H)^+$ 291.1339, found 291.1338.

5. References

(1) Z. Nace and K. Danijel, *Tetrahedron* 2008, **24**, 5756-5761.

(2) W.-M. Shi, X. H. Li, C. Liang and D.-L. Mo, *Adv. Synth. Catal.* 2017, **359**, 4129-4135.

(3) J.-H. Chen, C.-H. Deng, S. Fang, J.-G. Ma and P. Cheng, *Green Chem.* 2018, **20**, 989-996.

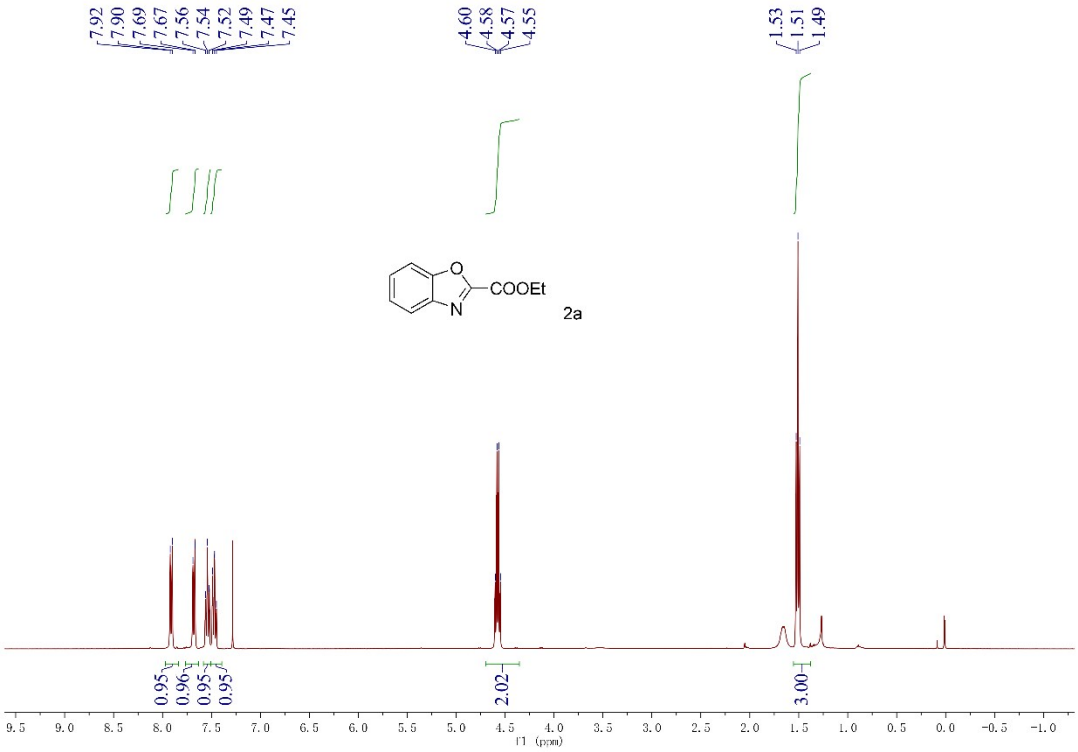
(4) M. Baltas, K. Raouf-Benchekroun, A.-D. L. Blica, Cazaux, P. Tisnes, L. Gorrichon, K. Hussein and J.-C Barthelat, *Tetrahedron* 1996, **52**, 14865-14876.

(5) A. Thorarensen, C.-J Ruble and D.-L. Romero, *Antibacterial benzoic acid derivatives*: US 2004.

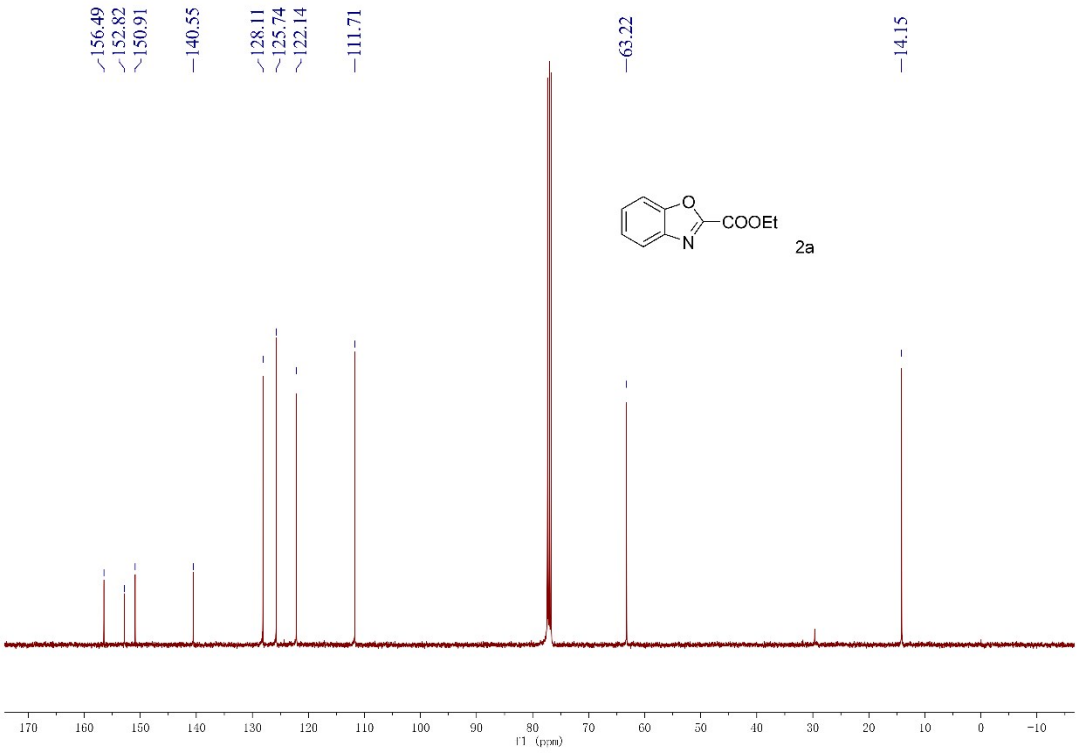
(6) K. DickoreK.; K. Sasse and K.-D. Bode, *Liebigs Ann. Chem*. 1970, **733**, 70-87.

6. ^{1}H NMR and ^{13}C NMR Spectra of Products

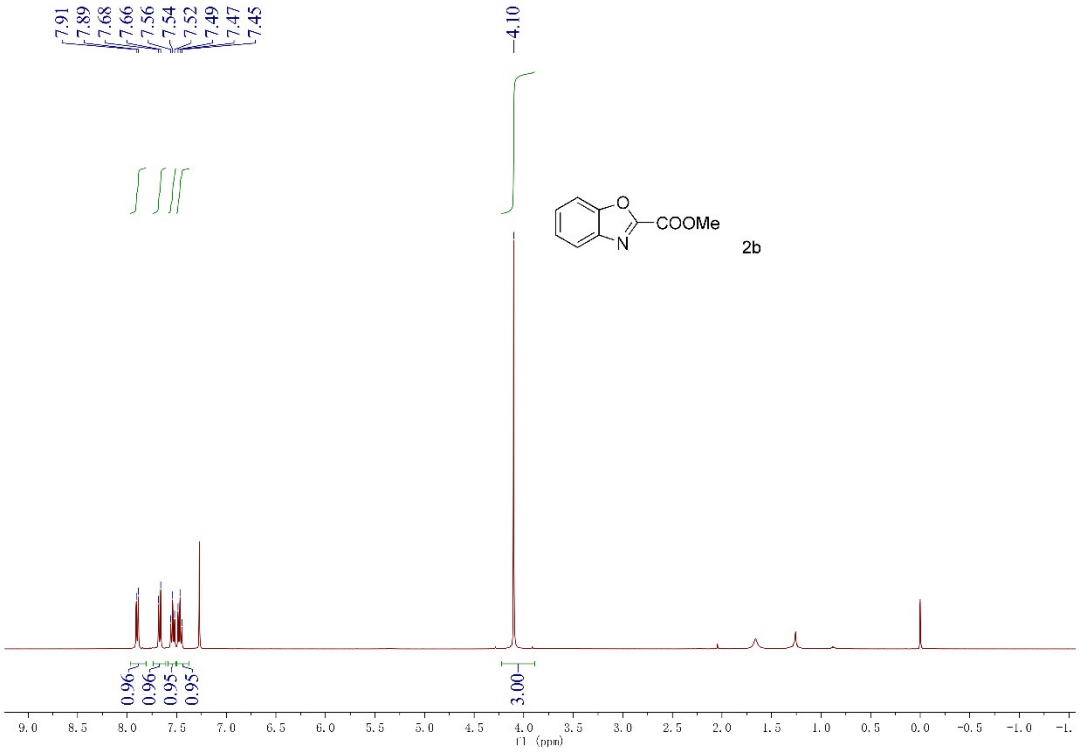
^{1}H NMR Spectra of ethyl benzo[*d*]oxazole-2-carboxylate (**2a**)



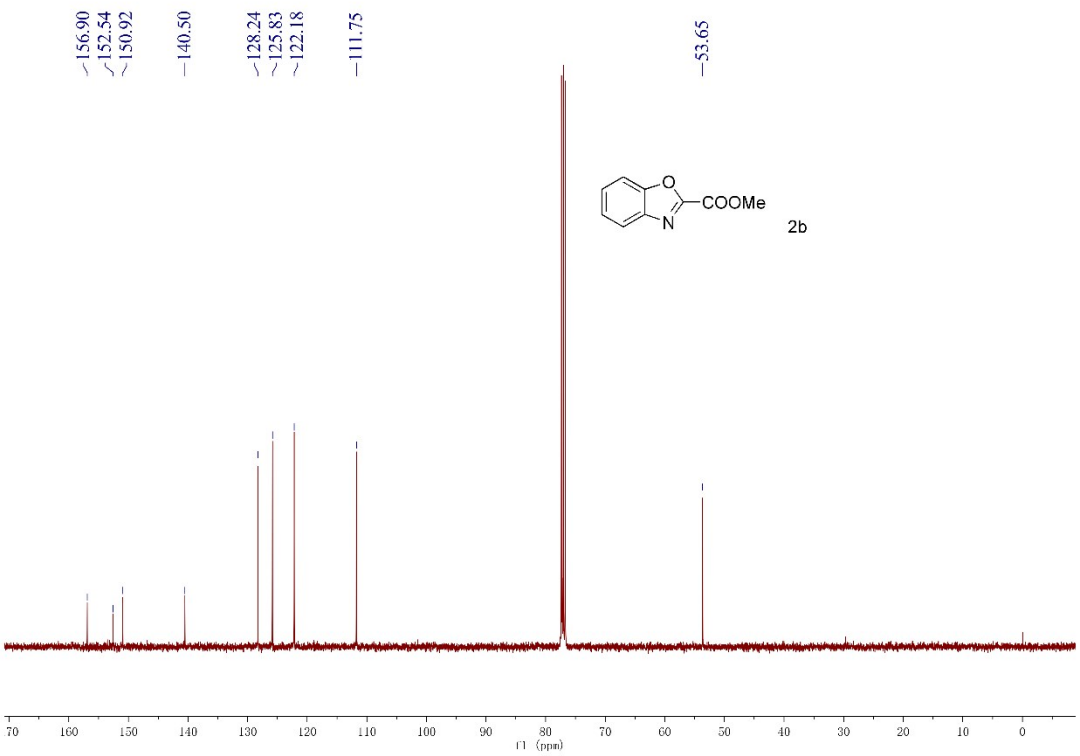
^{13}C NMR Spectra of ethyl benzo[*d*]oxazole-2-carboxylate (**2a**)



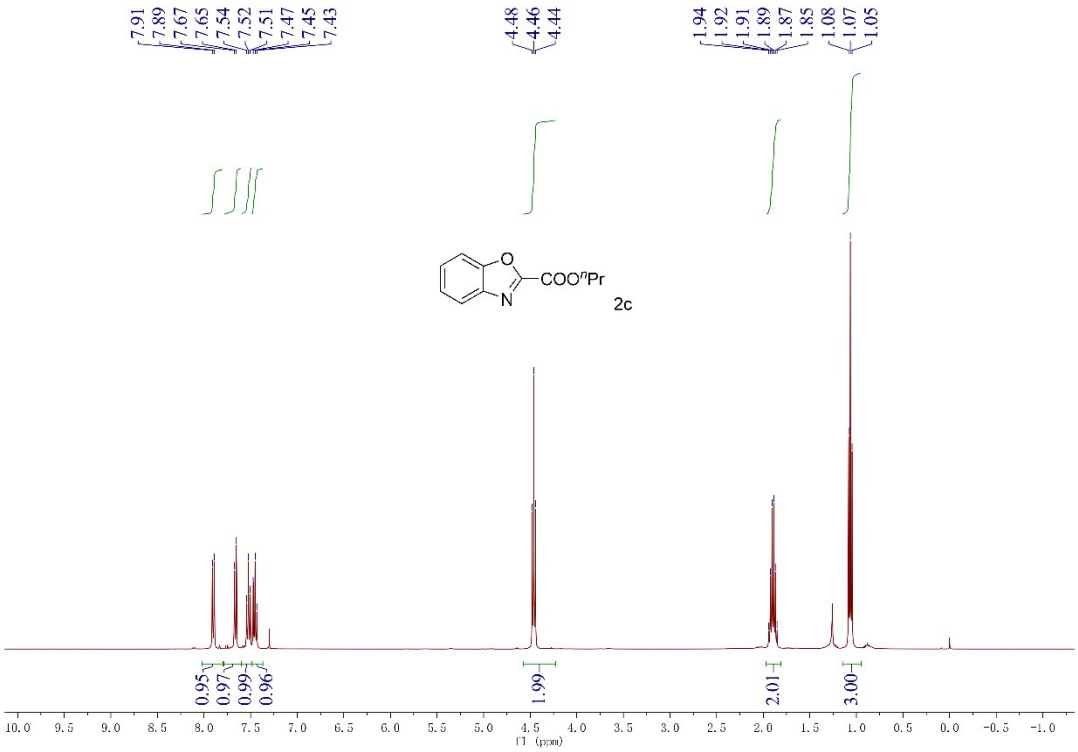
^{1}H NMR Spectra of methyl benzo[*d*]oxazole-2-carboxylate (**2b**)



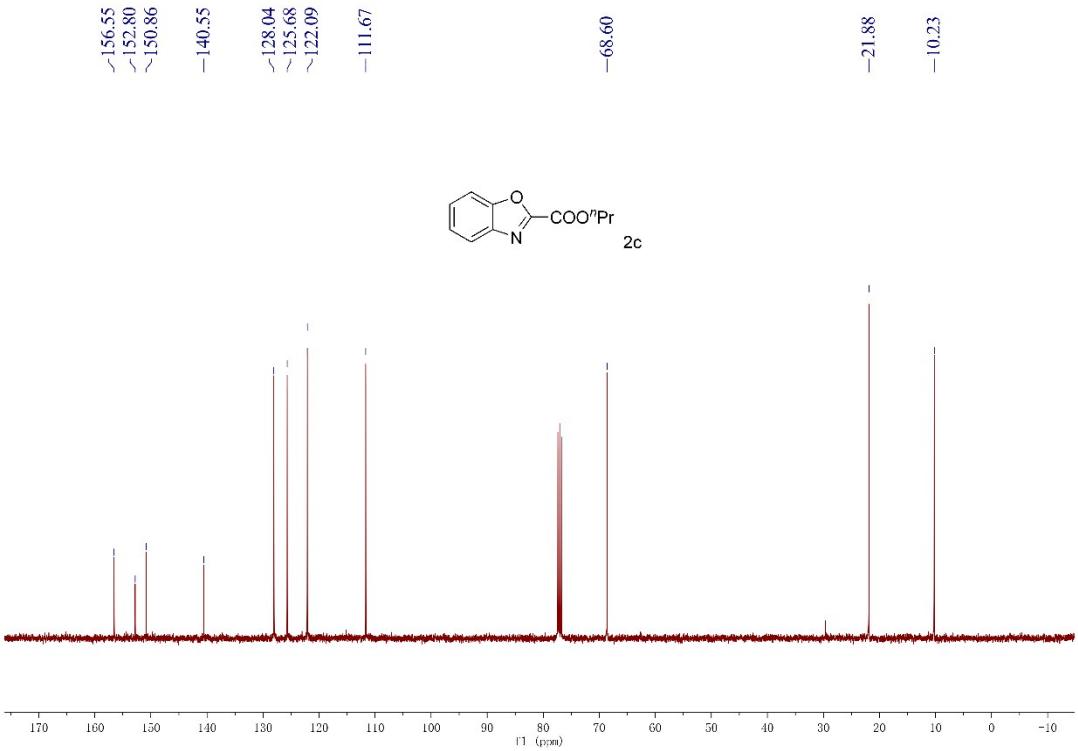
^{13}C NMR Spectra of methyl benzo[*d*]oxazole-2-carboxylate (**2b**)



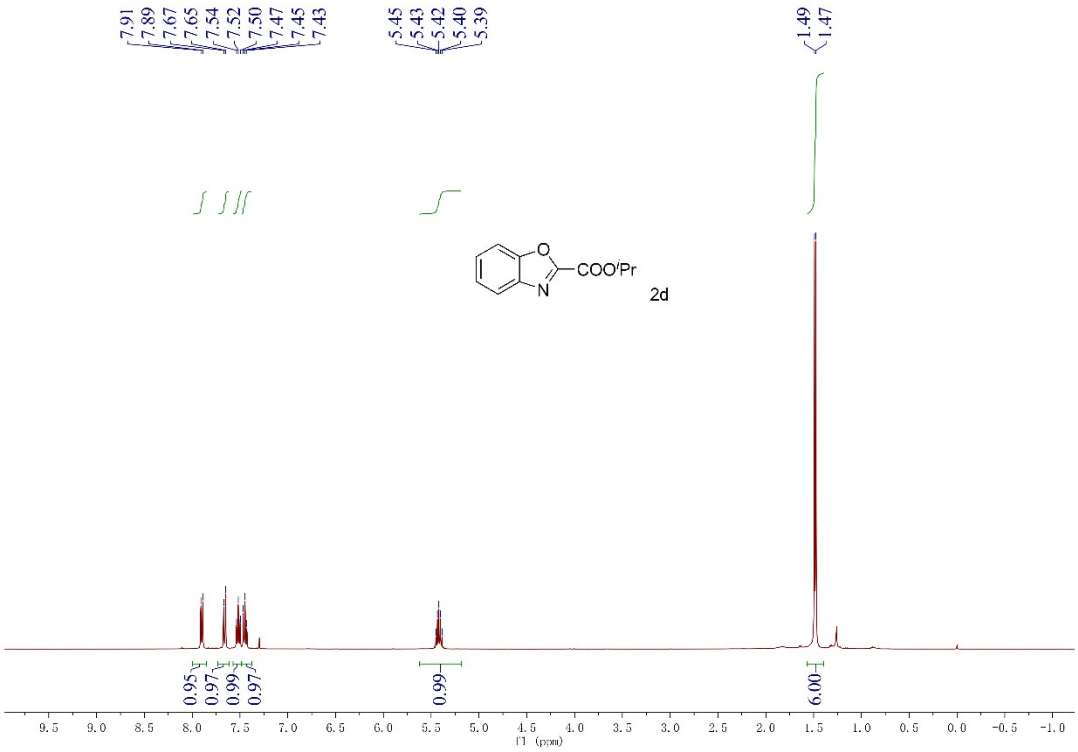
^{1}H NMR Spectra of propyl benzo[*d*]oxazole-2-carboxylate (**2c**)



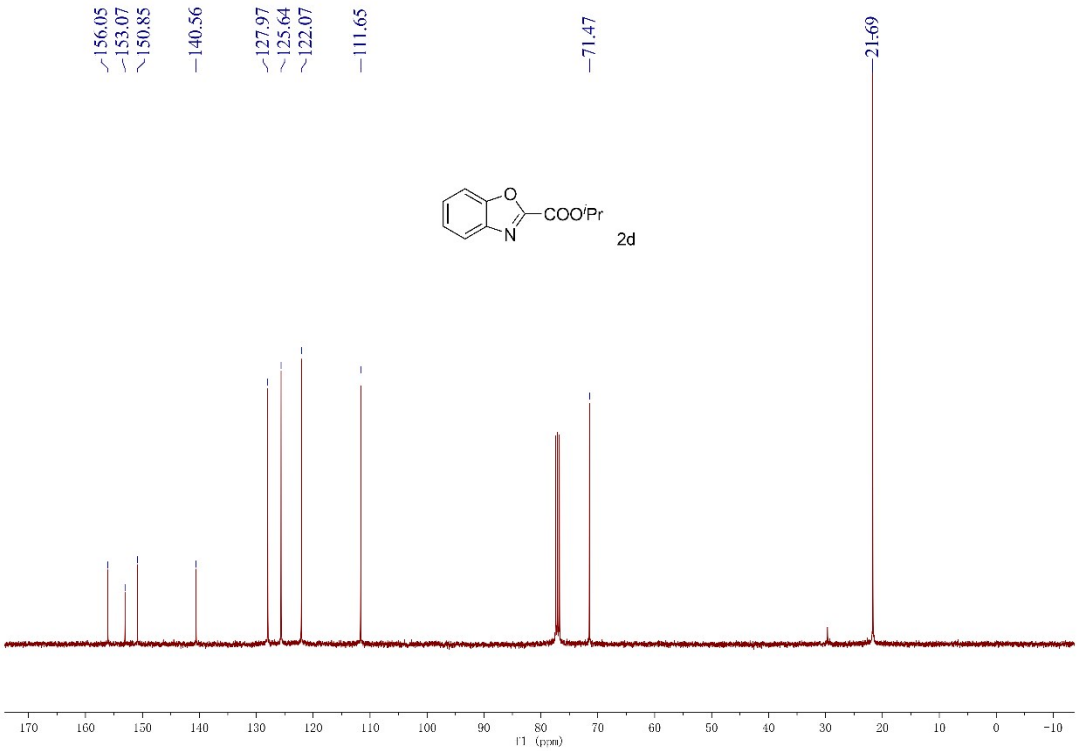
^{13}C NMR Spectra of propyl benzo[*d*]oxazole-2-carboxylate (**2c**)



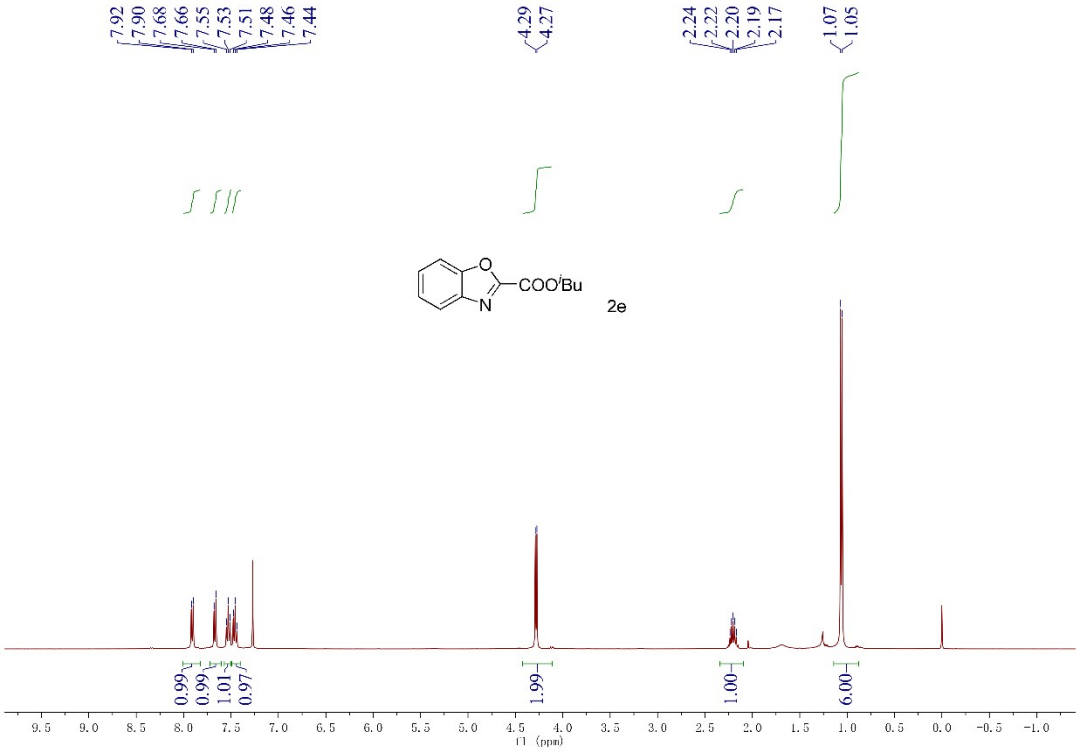
^{1}H NMR Spectra of isopropyl benzo[*d*]oxazole-2-carboxylate (**2d**)



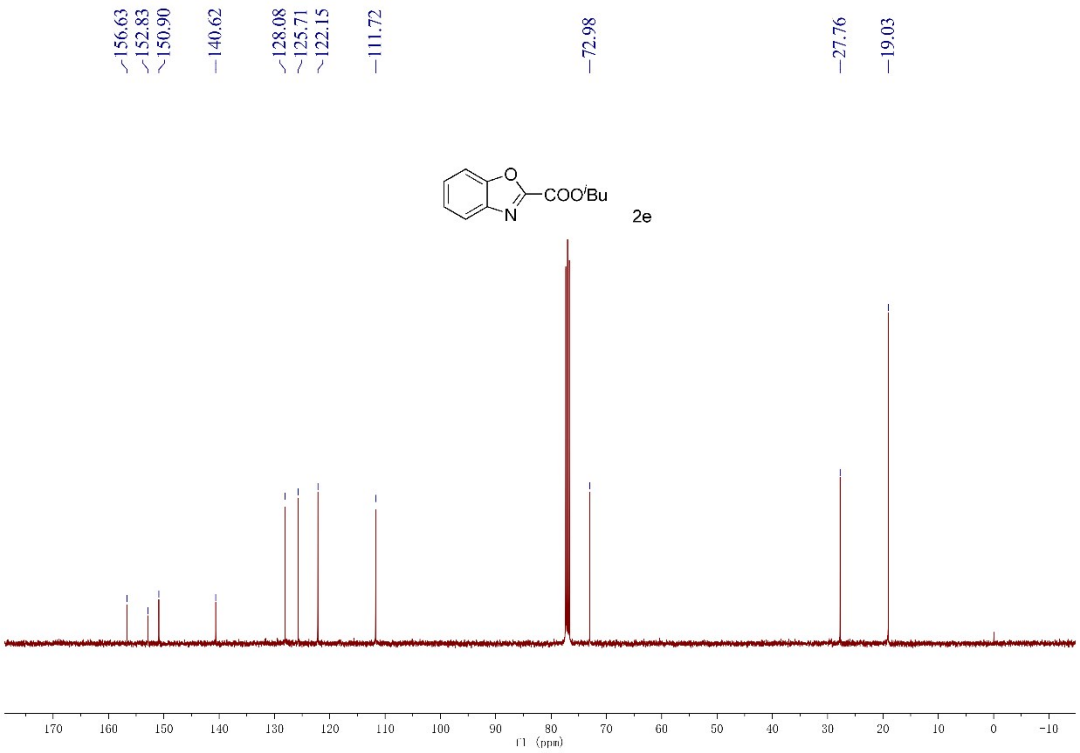
^{13}C NMR Spectra of isopropyl benzo[*d*]oxazole-2-carboxylate (**2d**)



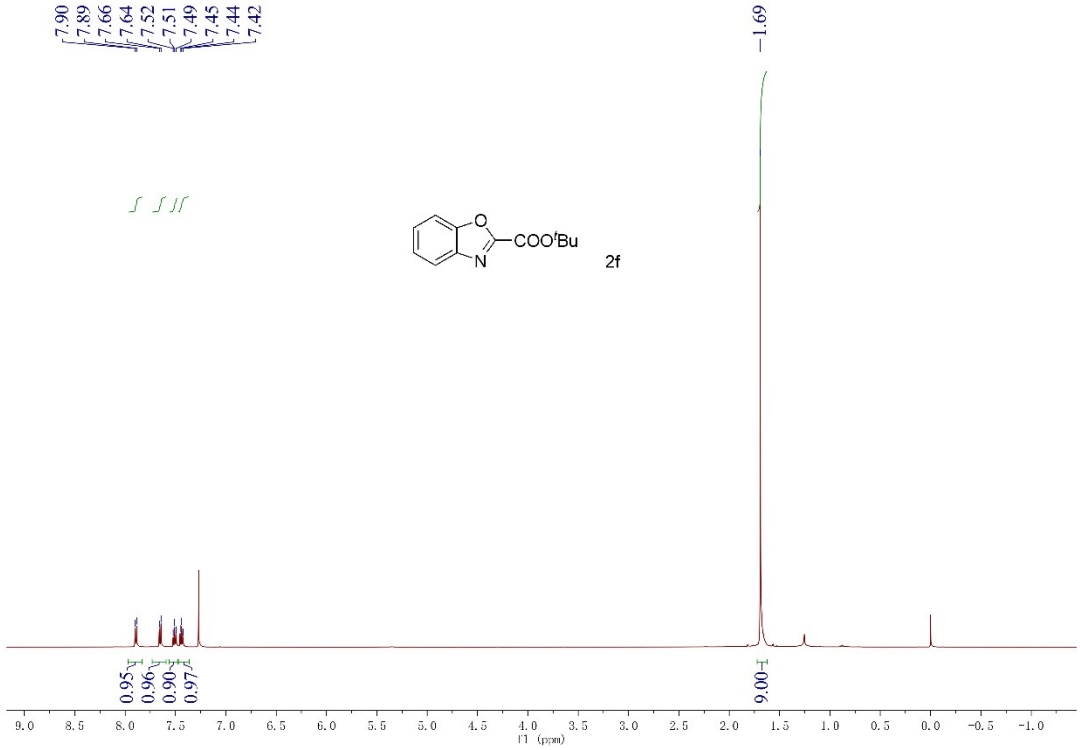
^{1}H NMR Spectra of isobutyl benzo[*d*]oxazole-2-carboxylate (**2e**)



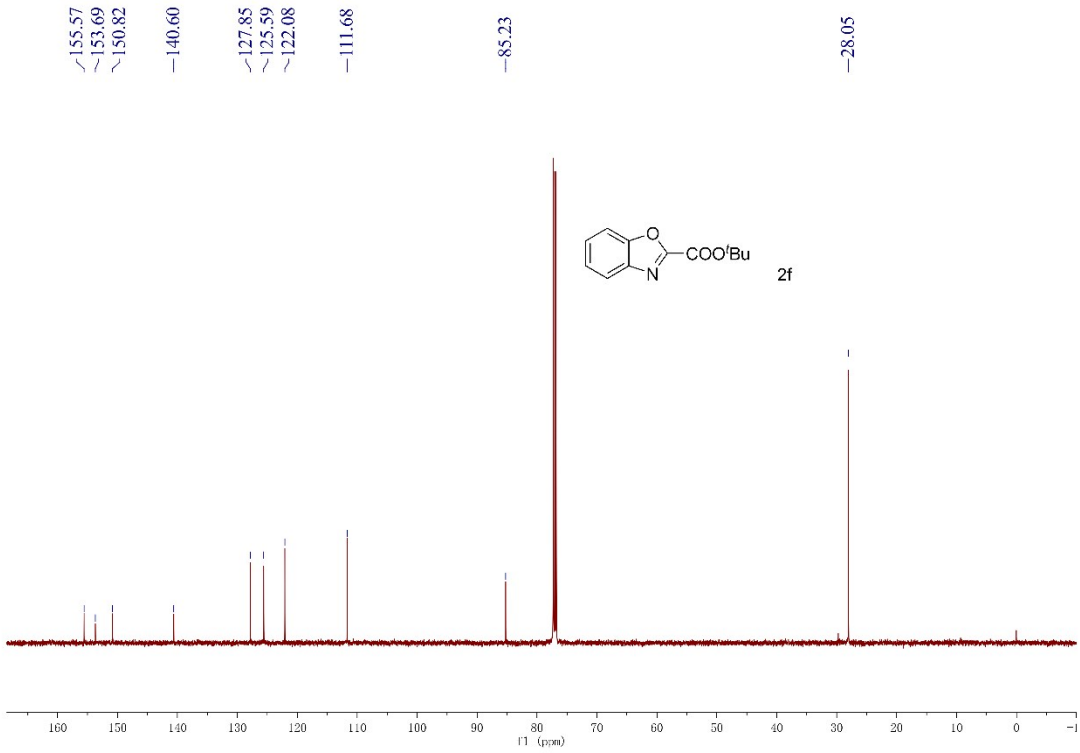
^{13}C NMR Spectra of isobutyl benzo[*d*]oxazole-2-carboxylate (**2e**)



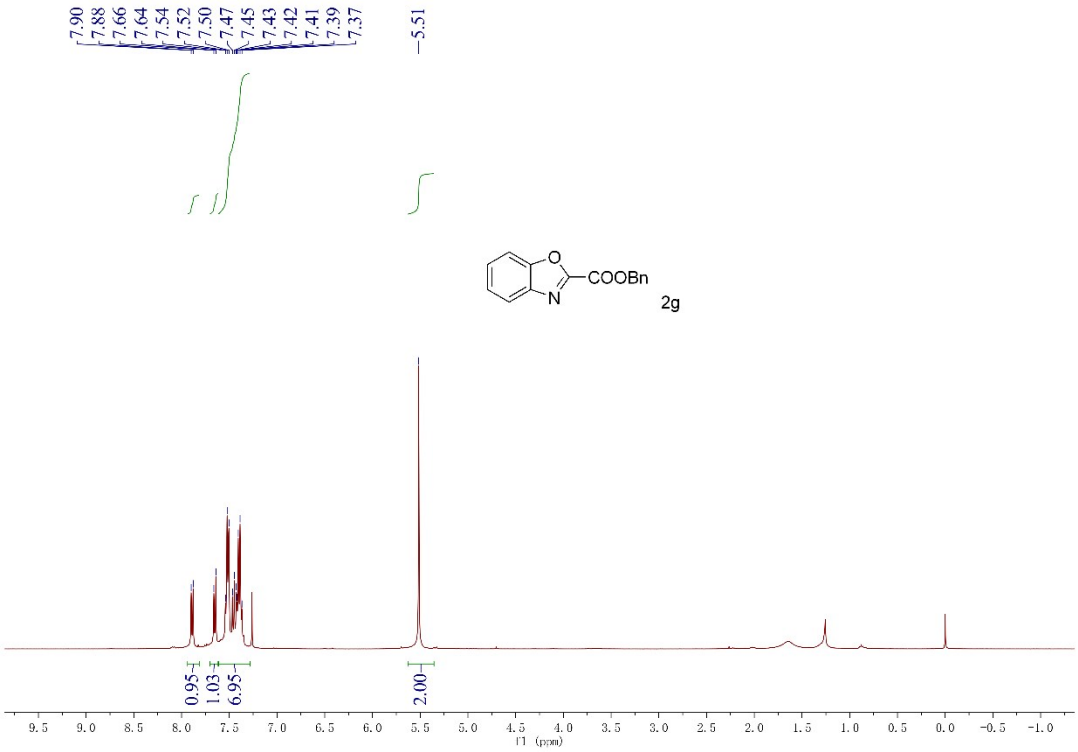
^{1}H NMR Spectra of *tert*-butyl benzo[*d*]oxazole-2-carboxylate (**2f**)



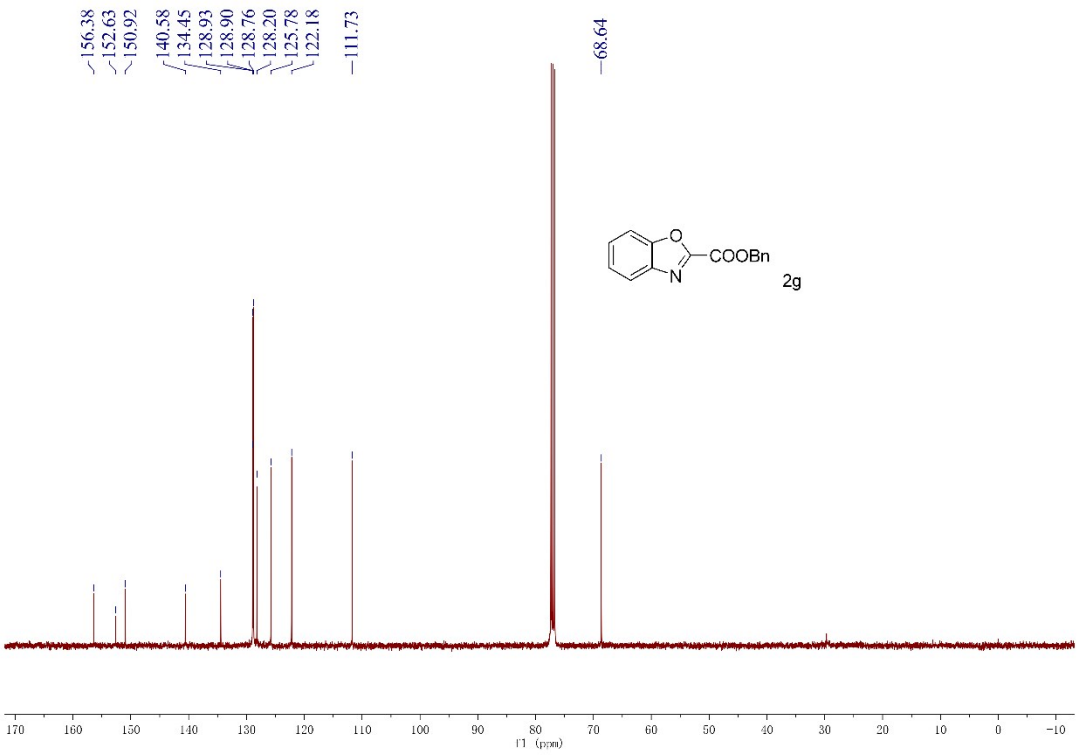
^{13}C NMR Spectra of *tert*-butyl benzo[*d*]oxazole-2-carboxylate (**2f**)



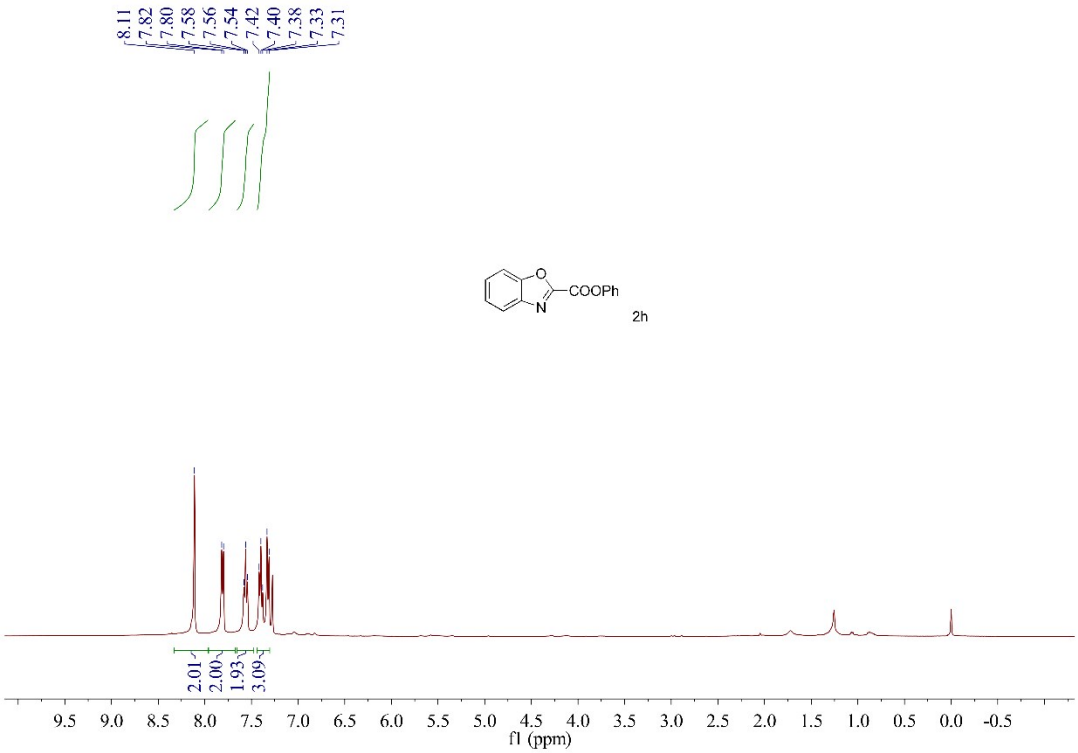
^{1}H NMR Spectra of benzyl benzo[*d*]oxazole-2-carboxylate (**2g**)



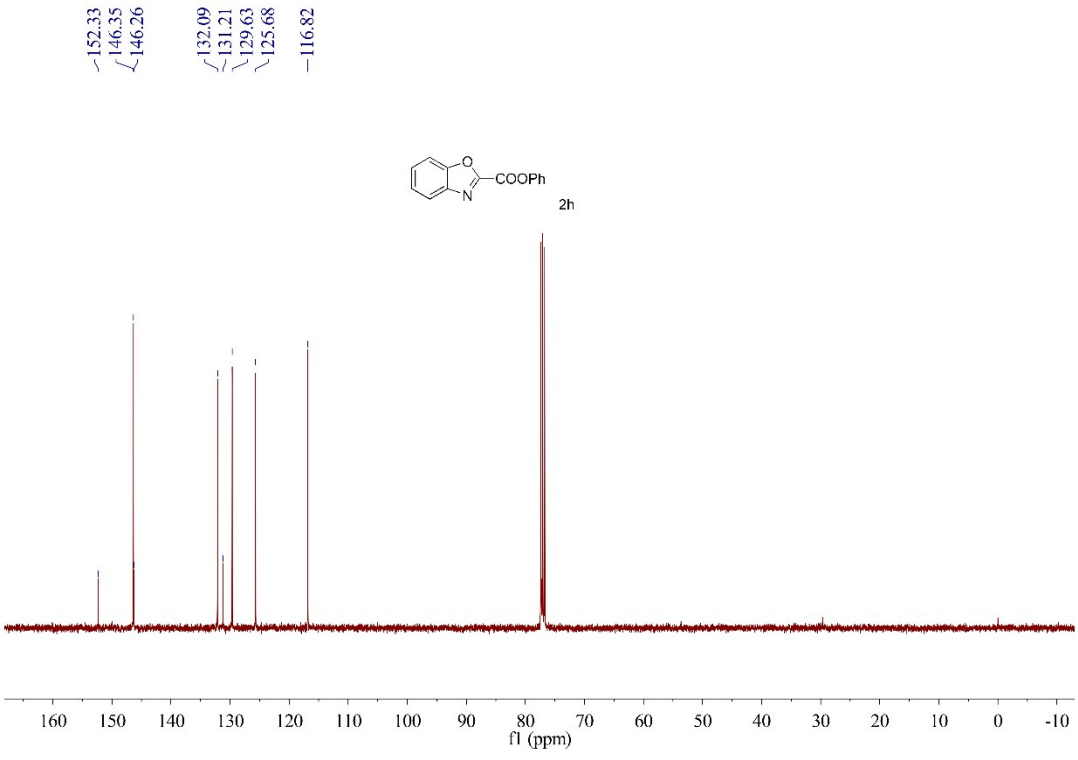
^{13}C NMR Spectra of benzyl benzo[*d*]oxazole-2-carboxylate (**2g**)



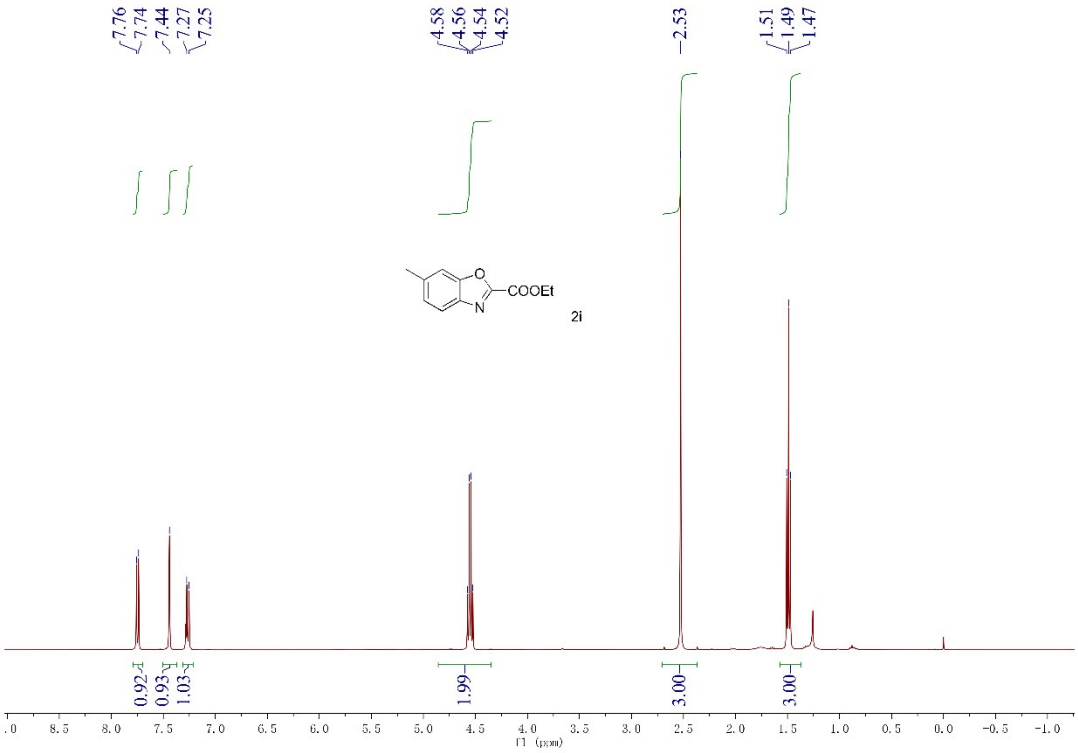
^{1}H NMR Spectra of phenyl benzo[*d*]oxazole-2-carboxylate (**2h)**



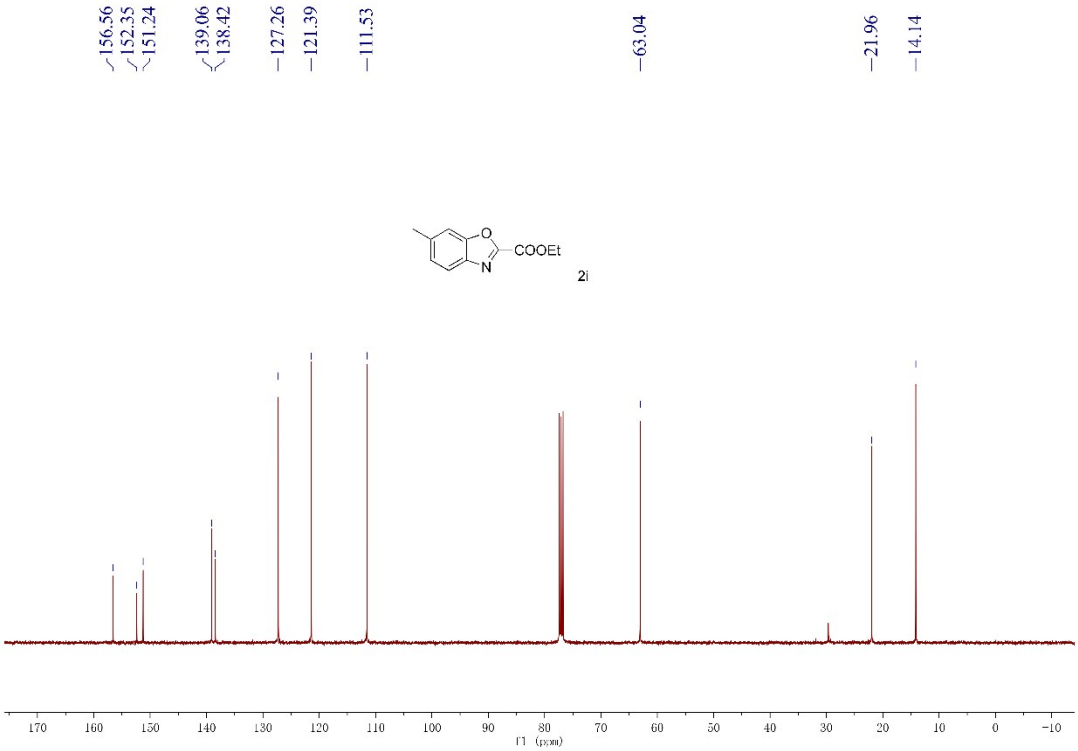
^{13}C NMR Spectra of phenyl benzo[*d*]oxazole-2-carboxylate (**2h)**



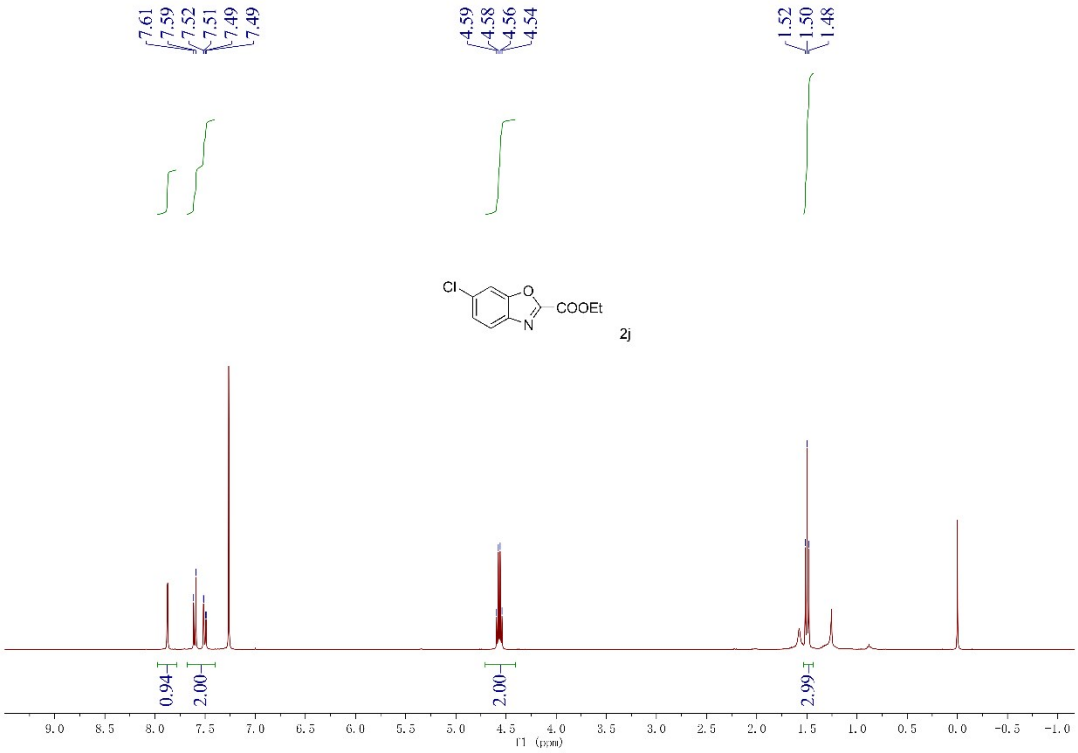
^{1}H NMR Spectra of ethyl 6-methylbenzo[*d*]oxazole-2-carboxylate (**2i**)



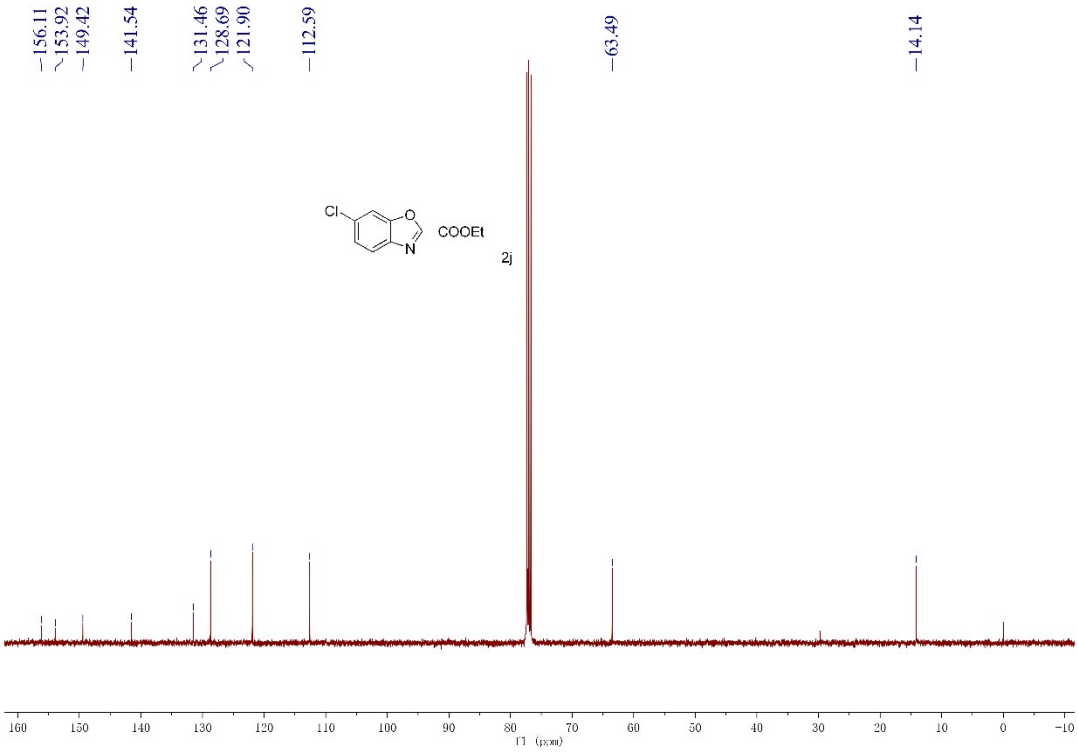
^{13}C NMR Spectra of ethyl 6-methylbenzo[*d*]oxazole-2-carboxylate (**2i**)



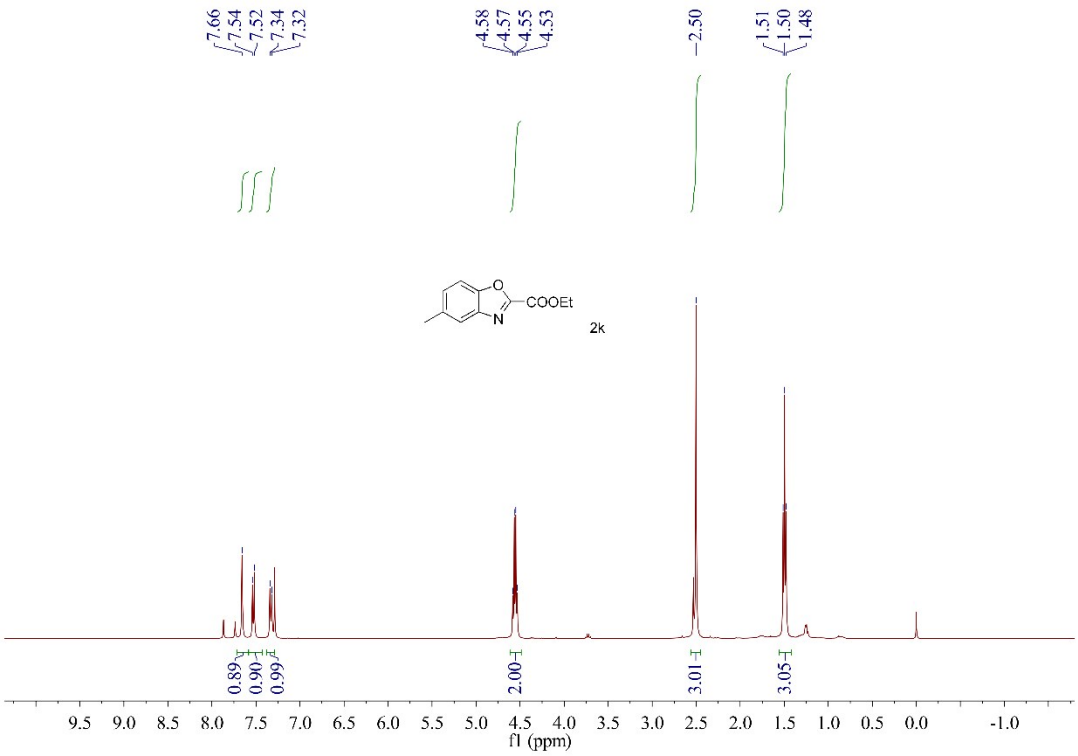
^{1}H NMR Spectra of ethyl 6-chlorobenzo[*d*]oxazole-2-carboxylate (**2j**)



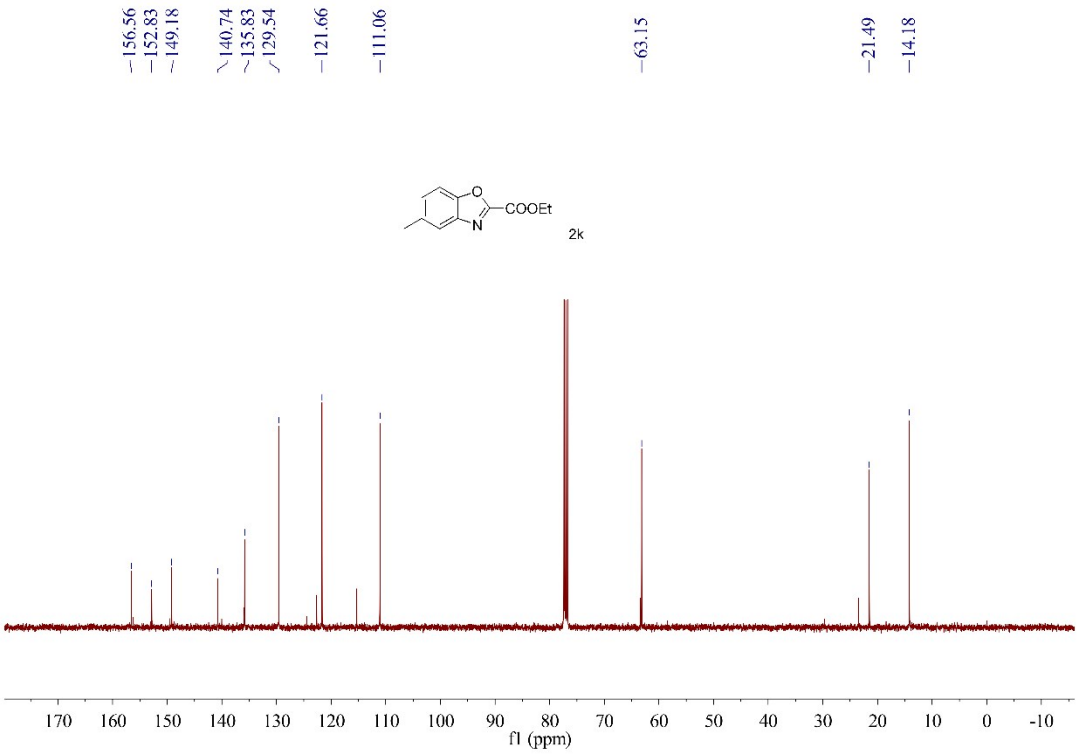
^{13}C NMR Spectra of ethyl 6-chlorobenzo[*d*]oxazole-2-carboxylate (**2j**)



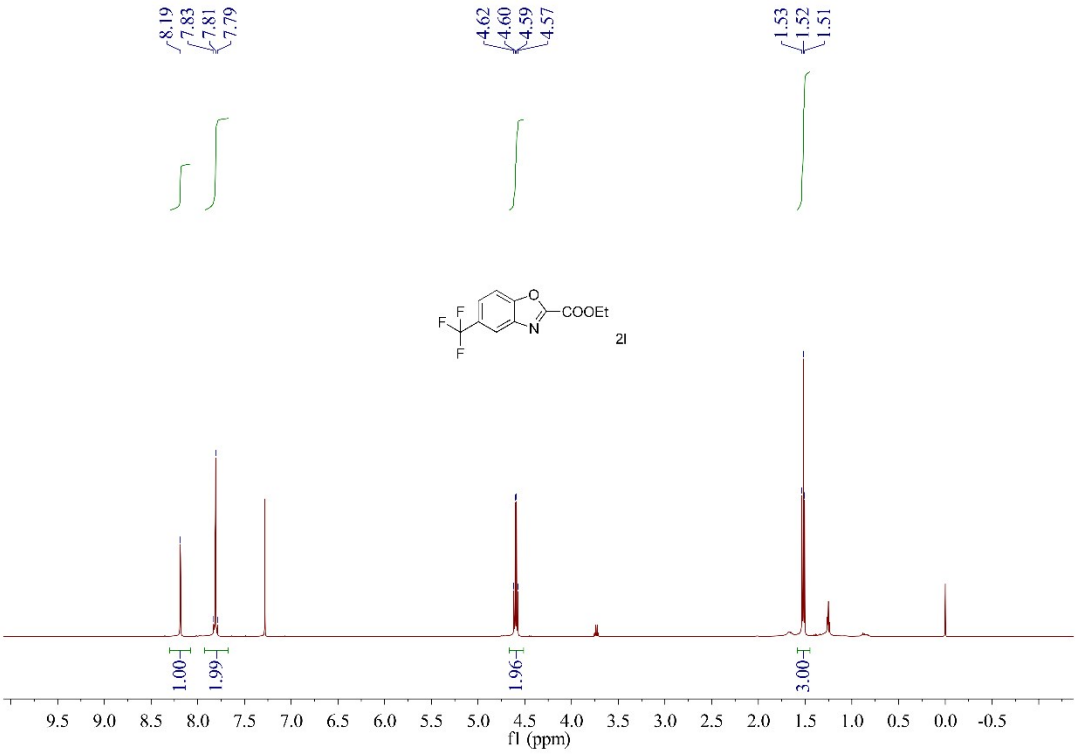
^{1}H NMR Spectra of ethyl 5-methylbenzo[*d*]oxazole-2-carboxylate (**2k**)



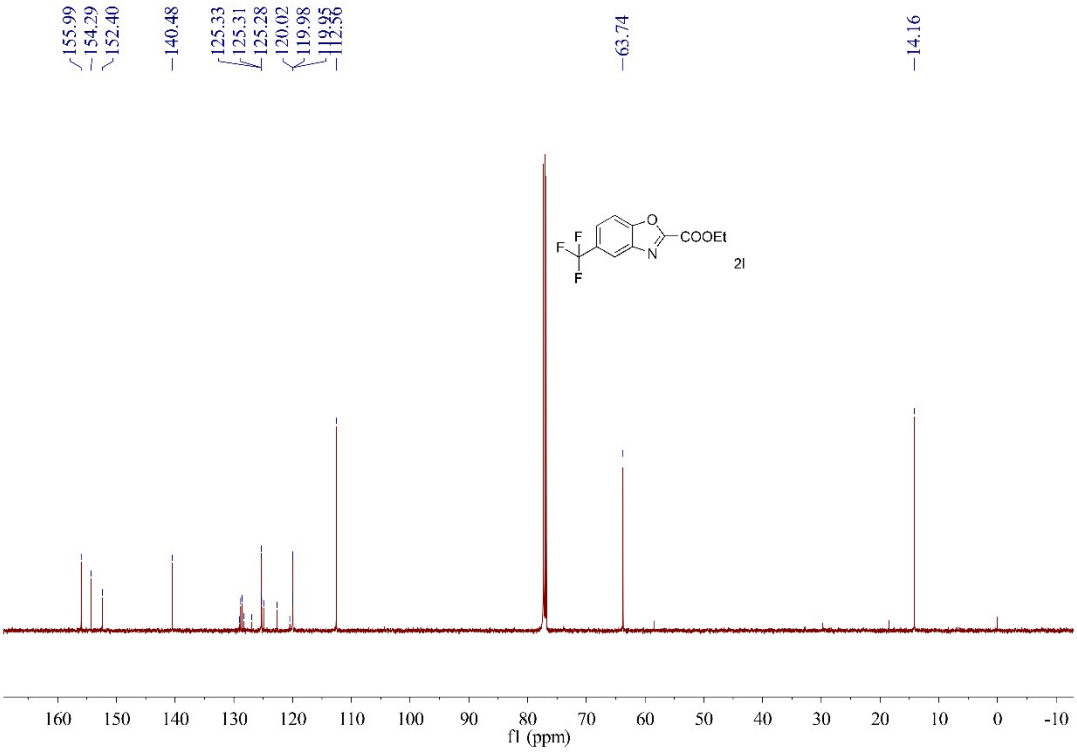
^{13}C NMR Spectra of ethyl 5-methylbenzo[*d*]oxazole-2-carboxylate (**2k**)



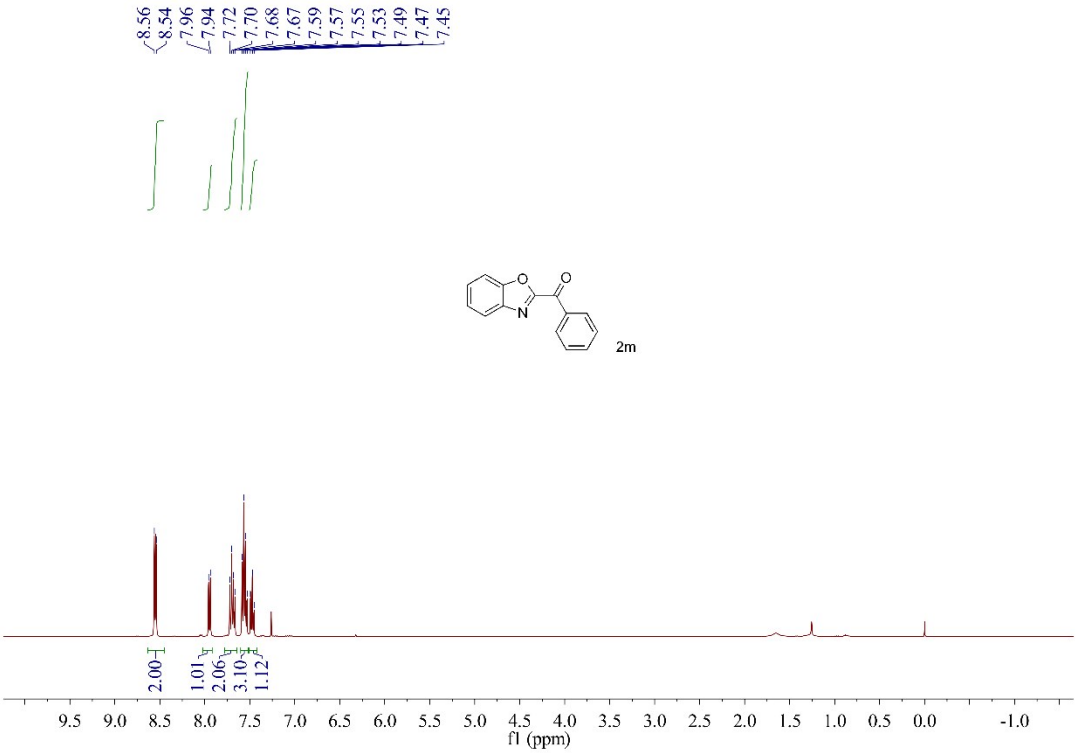
^{1}H NMR Spectra of ethyl 5-(trifluoromethyl)benzo[*d*]oxazole-2-carboxylate (**2l**)



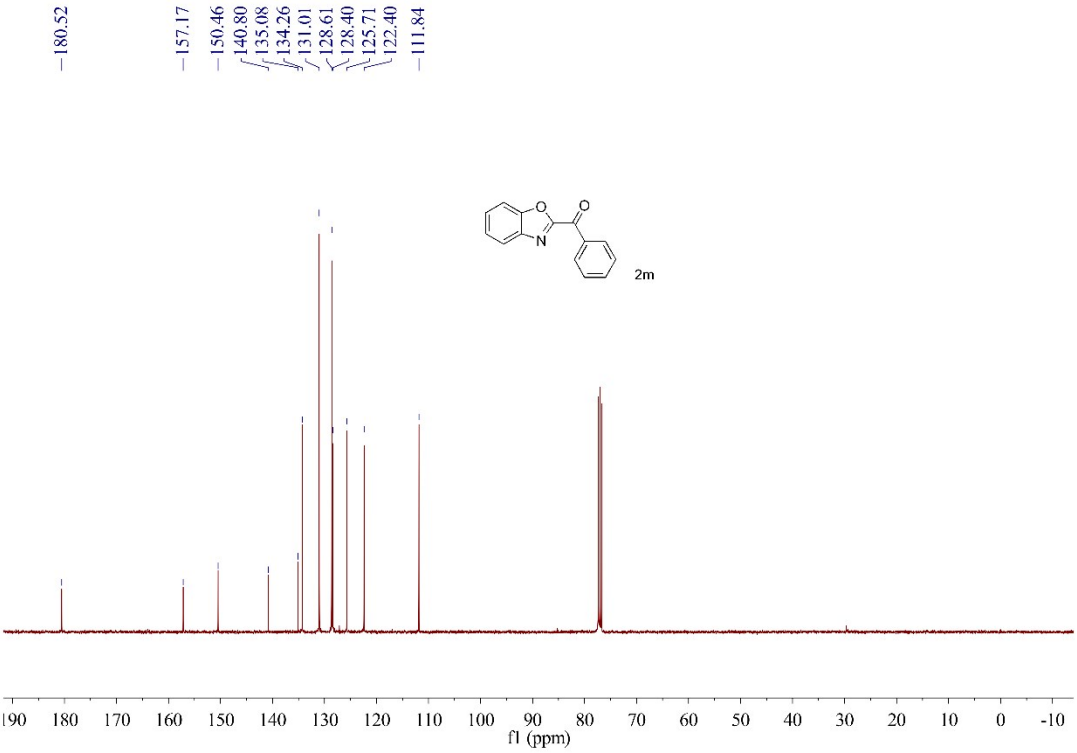
^{13}C NMR Spectra of ethyl 5-(trifluoromethyl)benzo[*d*]oxazole-2-carboxylate (**2l**)



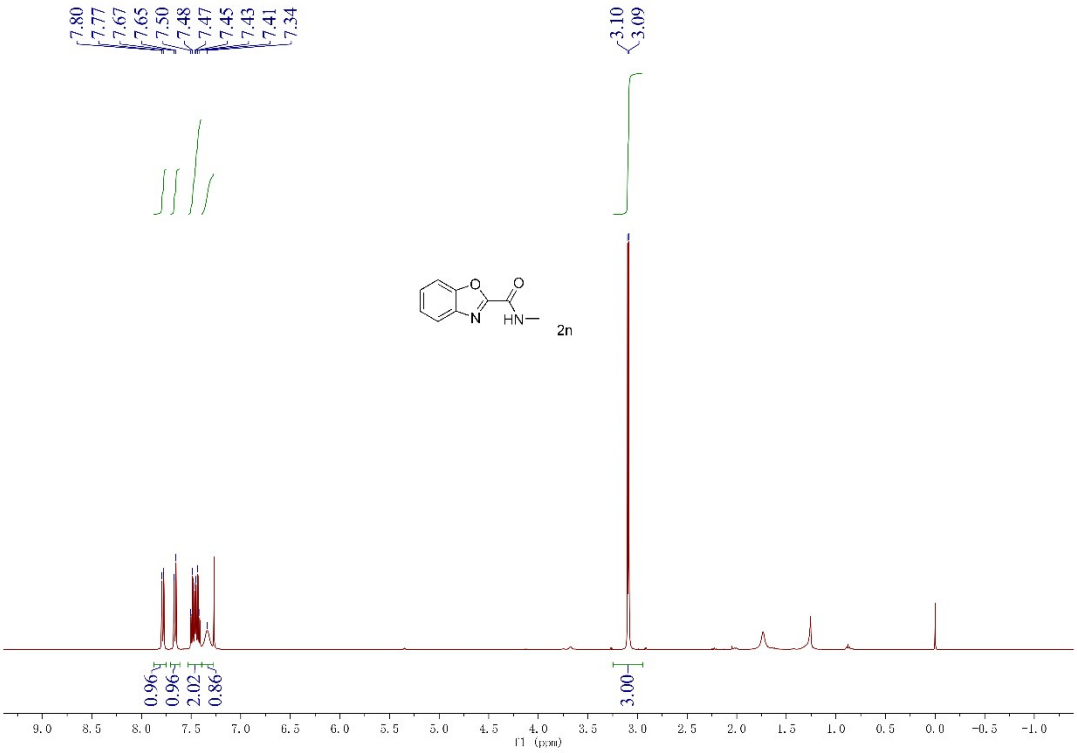
^{1}H NMR Spectra of Benzo[*d*]oxazol-2-yl(phenyl)methanone (**2m**)



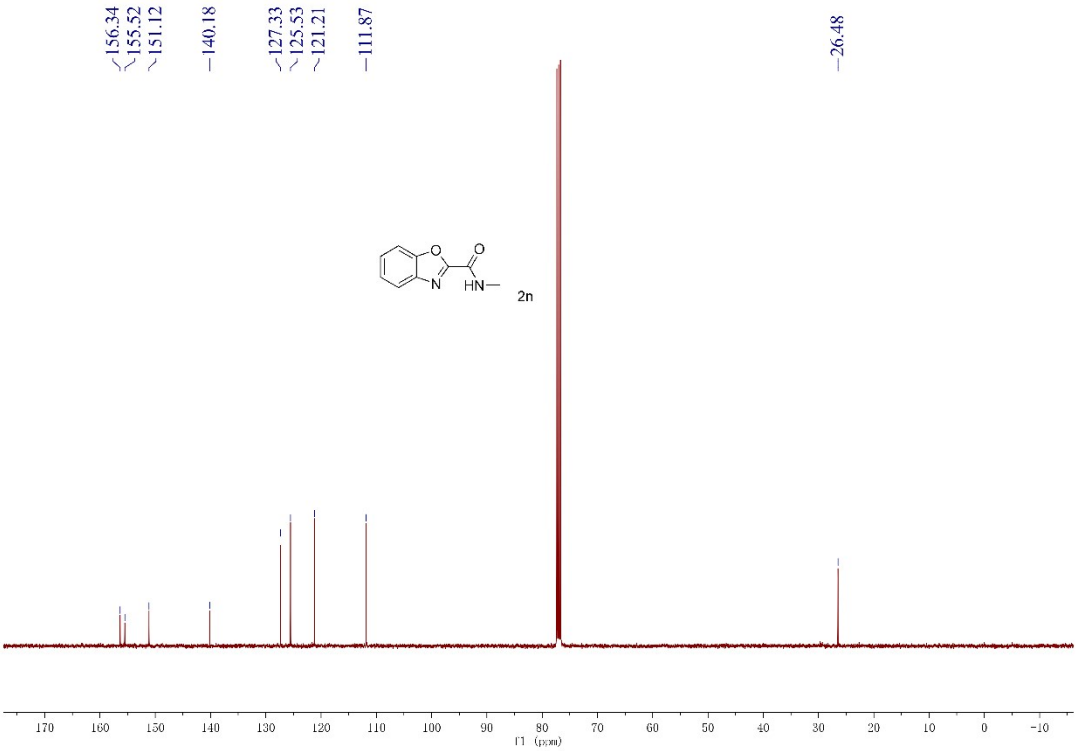
^{13}C NMR Spectra of Benzo[*d*]oxazol-2-yl(phenyl)methanone (**2m**)



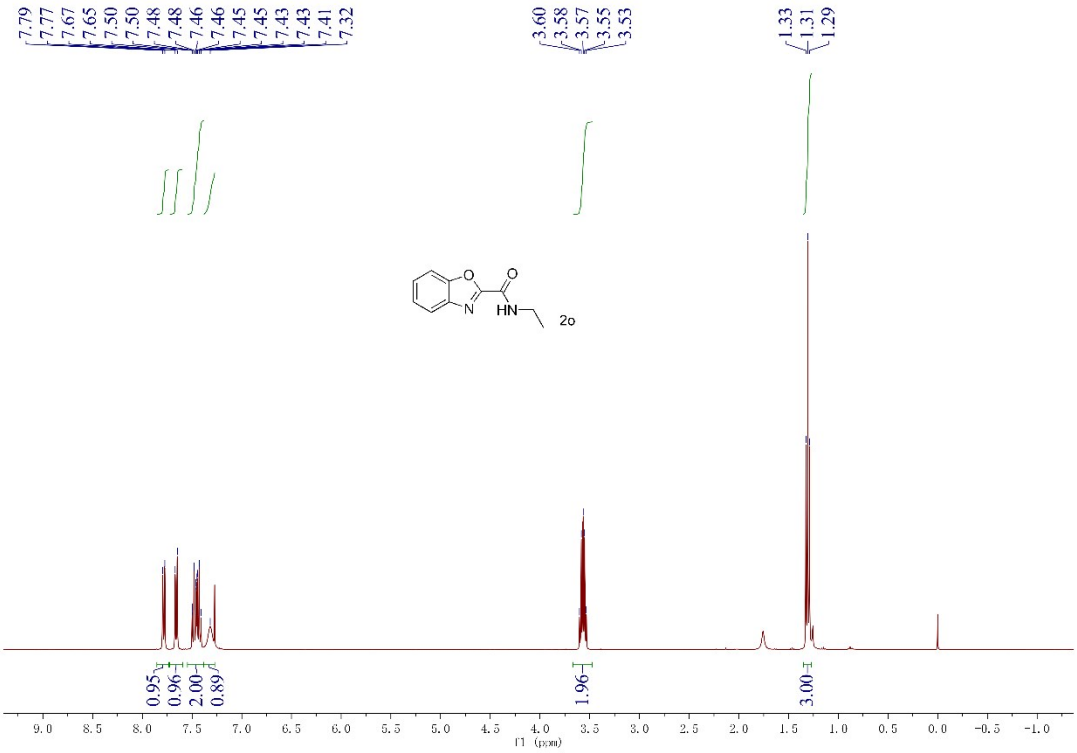
^{1}H NMR Spectra of *N*-methylbenzo[*d*]oxazole-2-carboxamide (**2n**)



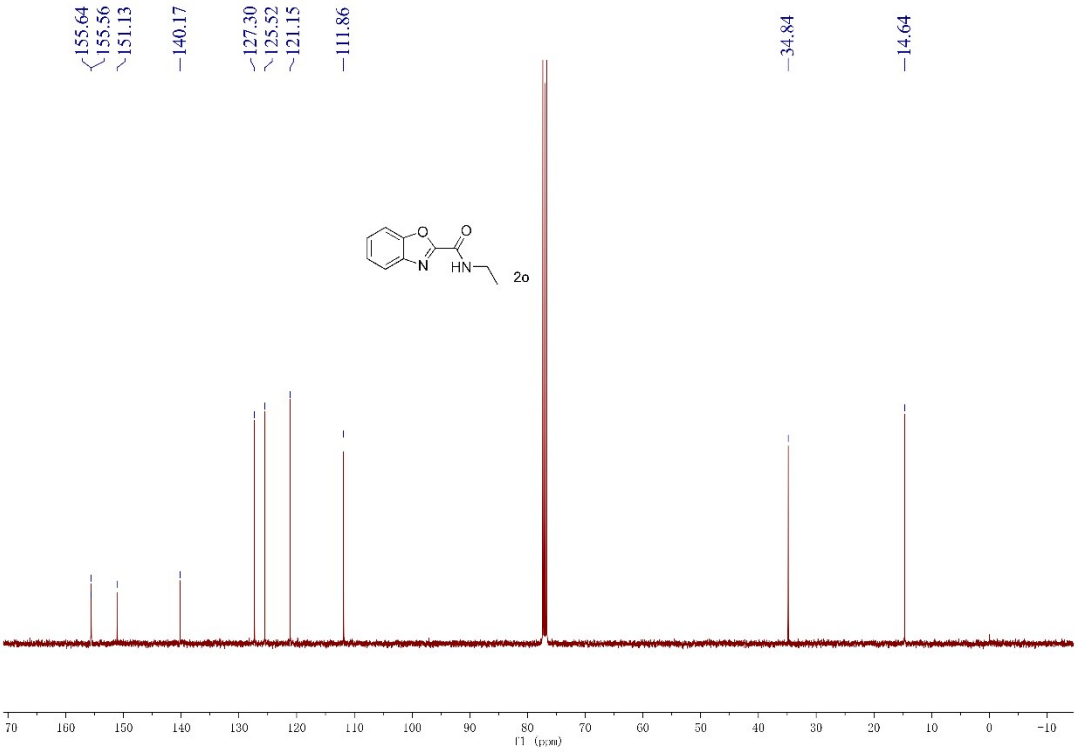
^{13}C NMR Spectra of *N*-methylbenzo[*d*]oxazole-2-carboxamide (**2n**)



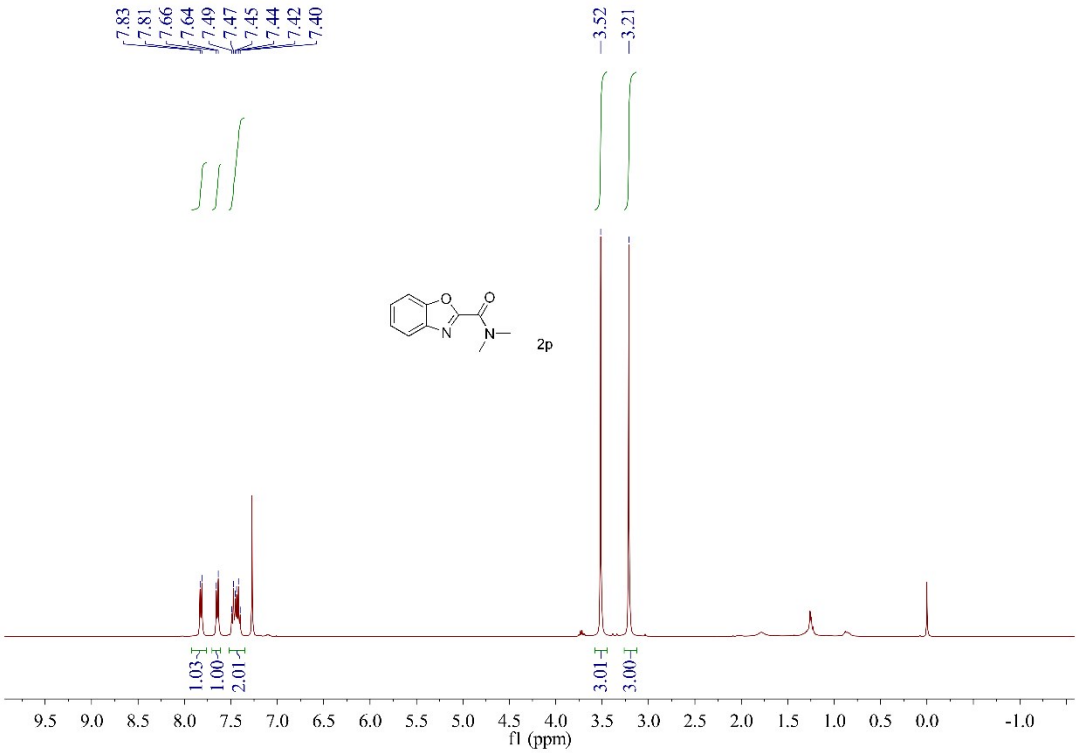
^{1}H NMR Spectra of *N*-ethylbenzo[*d*]oxazole-2-carboxamide (**2o**)



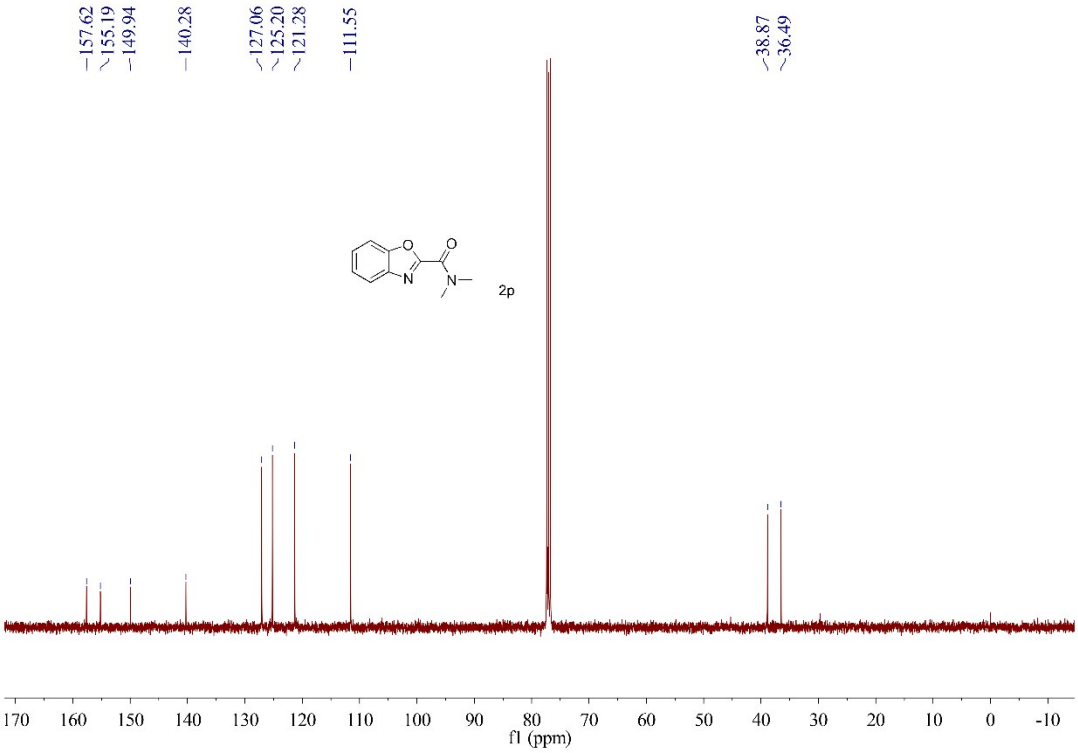
^{13}C NMR Spectra of *N*-ethylbenzo[*d*]oxazole-2-carboxamide (**2o**)



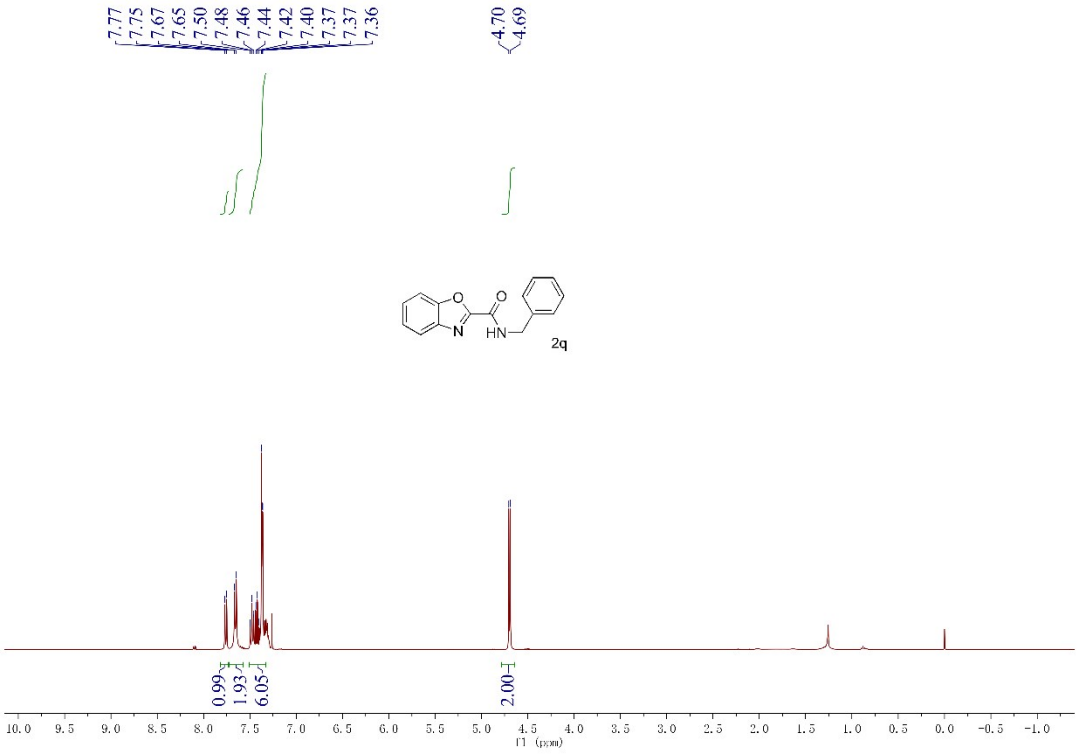
^{1}H NMR Spectra of *N,N*-dimethylbenzo[*d*]oxazole-2-carboxamide (**2p**)



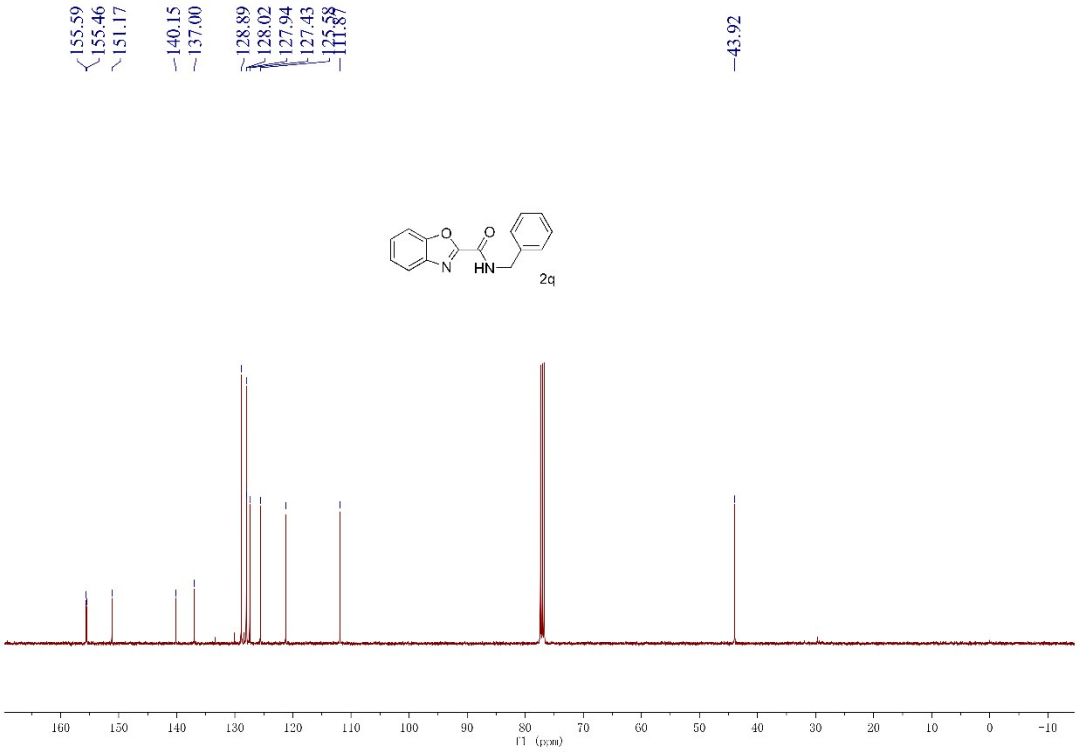
^{13}C NMR Spectra of *N,N*-dimethylbenzo[*d*]oxazole-2-carboxamide (**2p**)



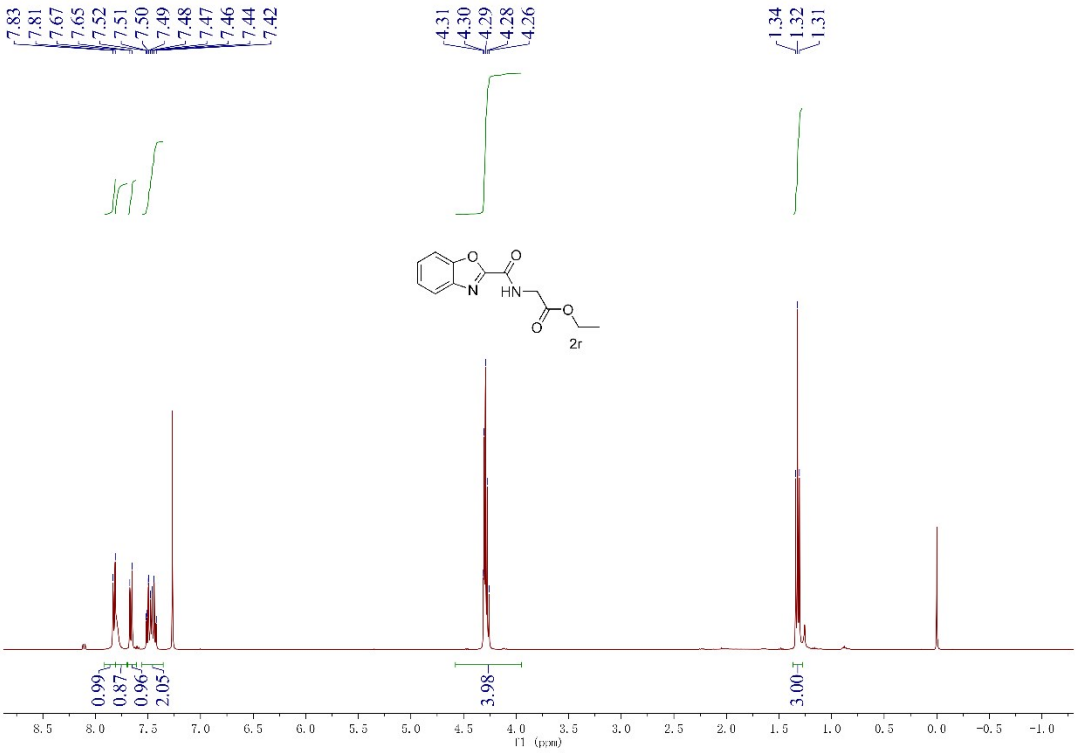
^{1}H NMR Spectra of *N*-benzylbenzo[*d*]oxazole-2-carboxamide (**2q**)



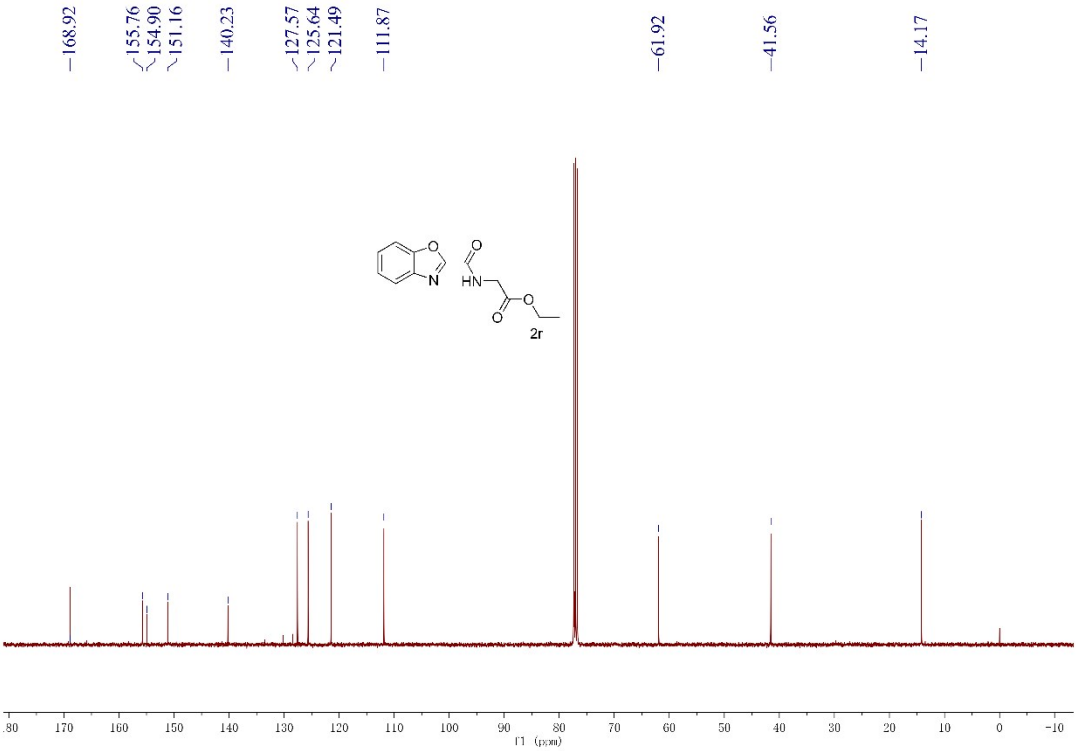
^{13}C NMR Spectra of *N*-benzylbenzo[*d*]oxazole-2-carboxamide (**2q**)



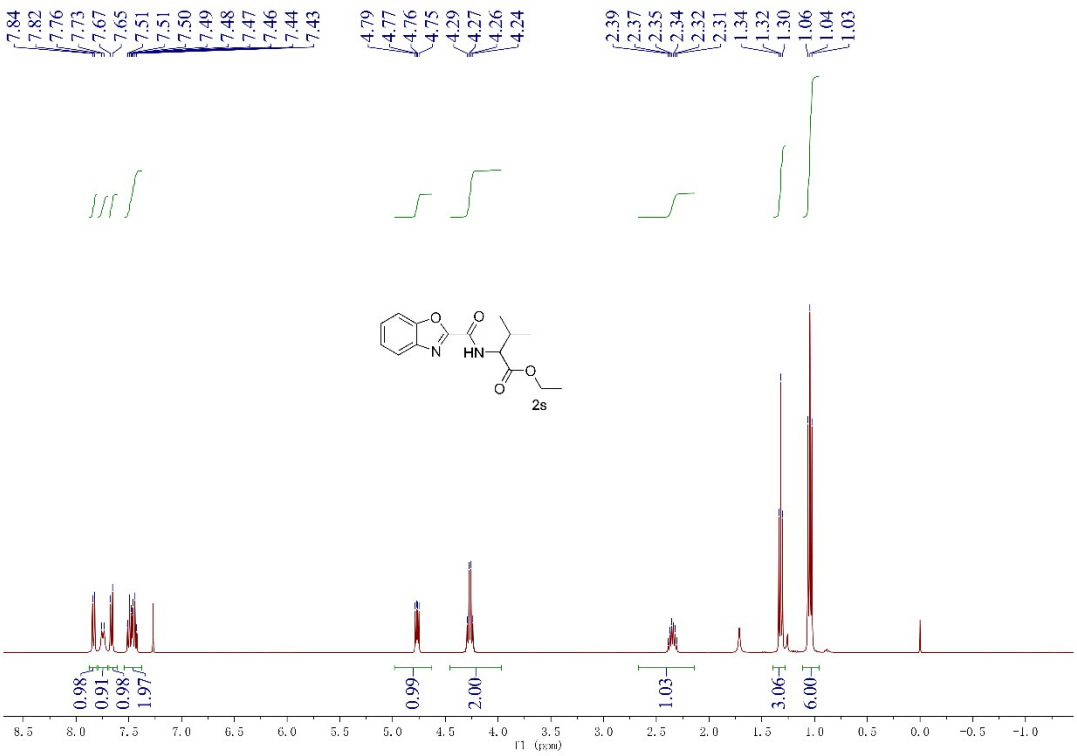
^{1}H NMR Spectra of ethyl (benzo[*d*]oxazole-2-carbonyl)glycinate (**2r**)



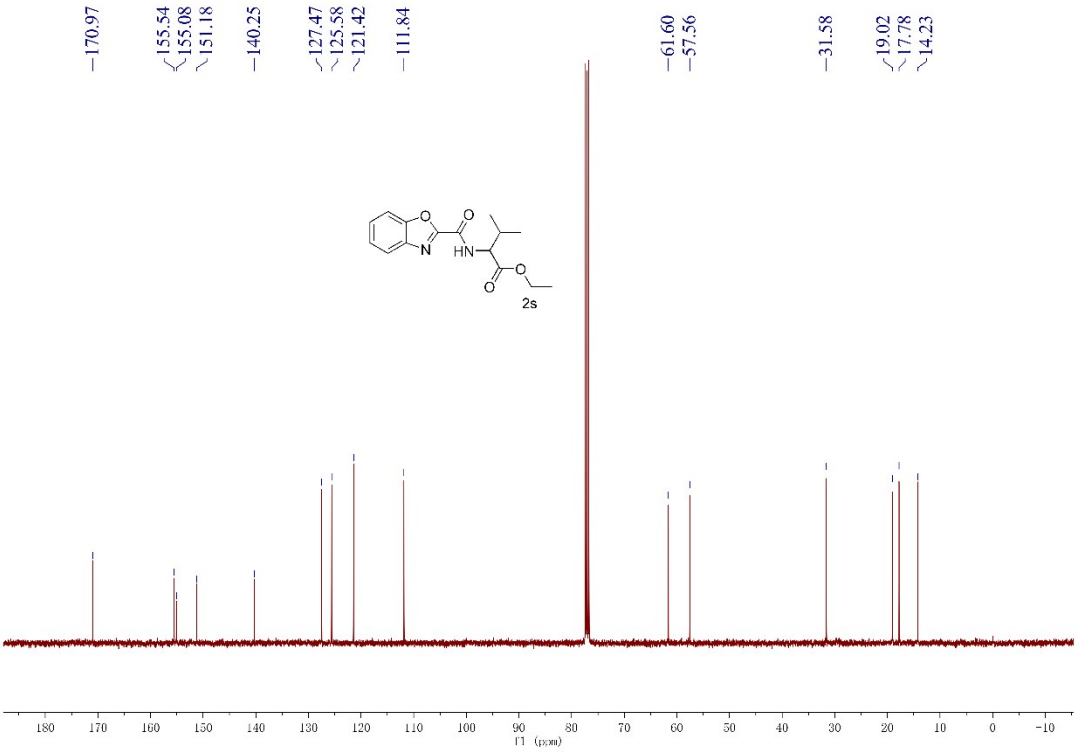
^{13}C NMR Spectra of ethyl (benzo[*d*]oxazole-2-carbonyl)glycinate (**2r**)



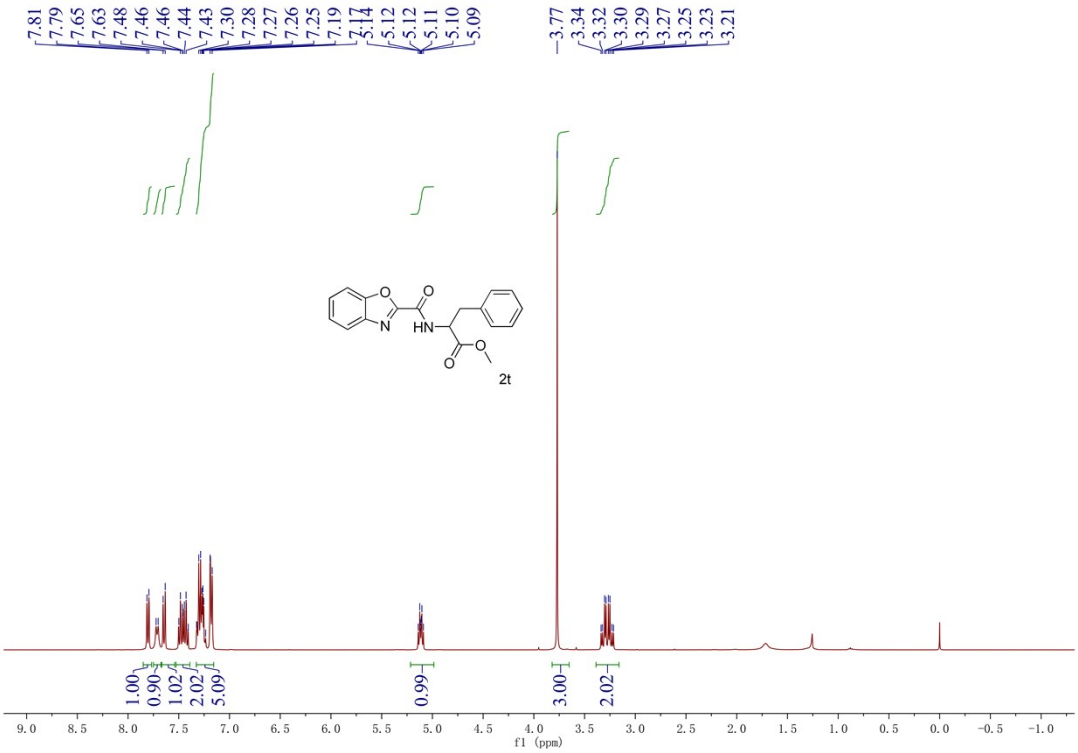
^{1}H NMR Spectra of ethyl (benzo[*d*]oxazole-2-carbonyl)valinate (**2s**)



^{13}C NMR Spectra of ethyl (benzo[*d*]oxazole-2-carbonyl)valinate (**2s**)



^{1}H NMR Spectra of methyl (benzo[*d*]oxazole-2-carbonyl)phenylalaninate (**2t**)



^{13}C NMR Spectra of methyl (benzo[*d*]oxazole-2-carbonyl)phenylalaninate (**2t**)