Supporting Information

Cu^{II}/H-USY as a regenerable bifunctional catalyst for the additive-free C–H amination of azoles

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Contents

General Information. Except for azoles **1m-p**, all reagents, solvents and zeolite materials (Zeolyst International) were commercial and used as received. Catalytic reactions were monitored by GC/MS using a GC Shimadzu 2014 GC instrument equipped with a FID detector and a CP-Sil 5 CB column. Mass spectra were recorded with a GC/MS Agilent 6890 gas chromatograph equipped with a HP-5MS column coupled to a 5973 MSD mass spectrometer with electron impact ionization. Liquid ^{1}H and ^{13}C NMR spectra were recorded with a Bruker AVANCE 400 MHz spectrometer in $CDCl_3$ with TMS as an internal standard at room temperature. Powder X-ray diffraction (PXRD) patterns were recorded with a Malvern PANalytical Empyrean diffractometer in transmission mode over a 1.3–45° 2θ range, using a PIXcel3D solid state detector and Cu anode (Cu $K_{\alpha1}$: 1.5406; Cu $K_{\alpha2}$: 1.5444). Cu K-edge X-ray absorption spectroscopy (XAS) spectra were collected at the DUBBLE XAFS beam line (BM26A) of the European Synchrotron Radiation Facility and analyzed with the Athena software package.[S1] Nitrogen sorption measurements were performed on a Micromeritics 3Flex surface analyzer at -196 °C. Prior to measurements, samples were evacuated under vacuum at 150 °C for 4 hours. Surface areas were calculated using the multi-point BET method applied to the isotherm adsorption branch, taking into account the Rouquerol consistency criteria.[S2] TGA analyses were performed under air at 4 °C/min on a NETZSCH STA 449 F3 Jupiter® thermal analyser.

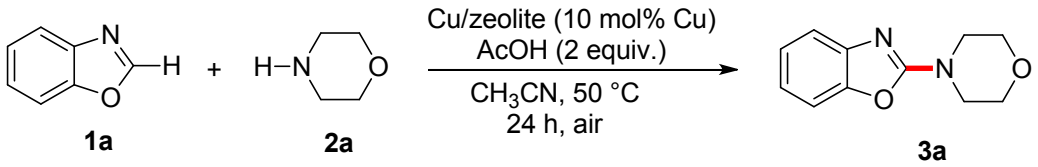
General procedure for the preparation of Cu-exchanged zeolites

Cu-zeolites were prepared using standard ion exchange method, by stirring 1.00 g of the commercial zeolite (Zeolyst International) with 100 mL of a 0.05 M aqueous solution of $Cu(OAc)_2.H_2O$ at room temperature for 24 h. The resulting light blue Cu-zeolite was filtrated and thoroughly washed with deionized water before drying overnight at 110 °C. The final copper loading was determined by ICP-MS.

Catalyst screening for the reaction between benzoxazole (1a) and morpholine (2a)

For initial optimization of the reaction conditions, we started to study the reaction between benzoxazole **1a** and morpholine **2a** as a model reaction. Similar to the procedure described by Cao *et al.*,[S3] a Cu catalyst (10 mol% metal content) was employed with acetic acid as an additive in acetonitrile for 24 h at 50 °C under air. Table S1 displays the results obtained depending on the initial zeolite support used.

Table S1 Influence of the zeolite support in the Cu/zeolite-catalyzed model reaction



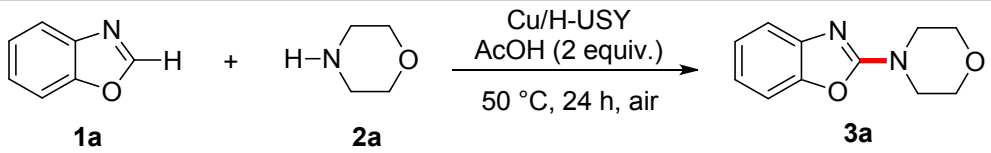
1a + **2a** → **3a**

Entry	Zeolite	Ref. Zeolyst	Form	SiO_2/Al_2O_3 ratio	Cu content (wt %)	Conversion (%)[b]
1	ZSM-5	CBV 2314	NH_4^+	23	2.0	n.d.
2	ZSM-5	CBV 28014	NH_4^+	280	0.2	n.d.
3	MOR	CBV21A	NH_4^+	20	2.2	4
4	*BEA	CP814E-22	NH_4^+	25	2.0	6
5	*BEA	CP811C-300	H^+	300	0.2	3
6	Y	CBV400	H^+	5.1	7.7	11
7	Y	CBV600	H^+	5.2	7.5	2
8	Y	CBV712	NH_4^+	12	3.8	5
9	USY	CBV720	H^+	30	1.3	20
10	**USY**	**CBV780**	**H^+**	**80**	**0.5**	**45**
11	USY	CBV780	Na^+	80	0.3	18
12	USY	CBV780	NH_4^+	80	0.7	23
13	USY	CBV780	H^+	80	0.5	21[c]
14	USY	CBV780	H^+	80	0.5	12[d]
15	USY	CBV780	H^+	80	0.5	16[e]
16	USY	CBV780	H^+	80	0.5	8[f]

[a]*Conditions*: benzoxazole (0.5 mmol), morpholine (1.2 equiv.), Cu/zeolite (10 mol% Cu) and AcOH (2 equiv.) in CH_3CN (2 mL) at 50 °C for 24 h under air. [b]Conversions determined by GC after correction using the effective carbon numbers. [c]Cu/zeolite synthesized from $CuBr_2$. [d]Cu/zeolite synthesized from $CuCl_2.H_2O$. [e]Cu/zeolite synthesized from $Cu(NO_3)_2.3H_2O$. [f]Cu/zeolite synthesized from $CuSO_4.5H_2O$.

Optimization of the conditions for reaction between (1a) and (2a)

Table S2 Optimization of the model reaction with Cu/H-USY

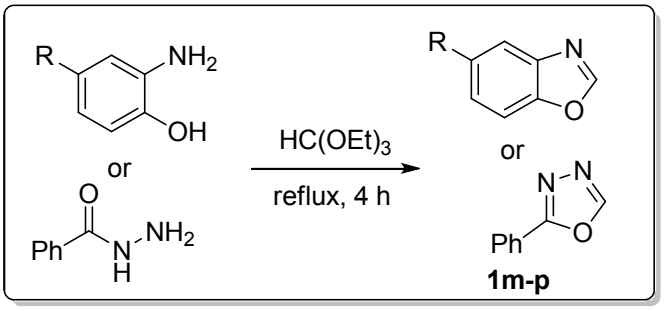


1a **2a** **3a**

Entry	Catalyst (mol%)	Solvent	Additive	Conversion (%)[b]
1	Cu/H-USY (10)	MeCN	AcOH	45
2	Cu/H-USY (10)	EtOH	AcOH	12
3	Cu/H-USY (10)	hexanes	AcOH	5
4	Cu/H-USY (10)	DMF	AcOH	n.d.
5	Cu/H-USY (10)	DMSO	AcOH	n.d.
6	Cu/H-USY (10)	toluene	AcOH	n.d.
7	Cu/H-USY (10)	dioxane	AcOH	n.d.
8	Cu/H-USY (10)	EtOAc	AcOH	n.d.
9	Cu/H-USY (10)	HFIP	AcOH	>97
10	Cu/H-USY (5)	HFIP	AcOH	>97
11	Cu/H-USY (3)	HFIP	AcOH	62
12	Cu/H-USY (3)	HFIP	None	60
13	**Cu/H-USY (3)**	**HFIP**	**None**	**>97[c] (91)[c,d]**
10	H-USY	HFIP	None	0[c]
11	$Cu(OAc)_2.H_2O$ (3)	HFIP	None	0[c]
12	$Cu(OAc)_2.H_2O$ (3) + H-USY	HFIP	None	24[c]
13	Cu/H-USY (3)	HFIP	None	0[c,e]

[a]*Conditions*: benzoxazole (0.5 mmol), morpholine (1.2 equiv.), Cu/H-USY and additive (2 equiv.) in solvent (2 mL) at 50 °C for 24 h under air. [b]Conversions determined by GC after correction using the effective carbon numbers. [c]2 equiv. of morpholine were used. [d]Isolated yield [e]reaction performed under Ar

General procedure for the synthesis of azoles 1m-p[S4]



A solution containing the corresponding 2-aminophenol or benzhydrazide (5 mmol) in triethyl orthoformate (15 mL) was heated at reflux for 4 h. The excess of triethyl orthoformate was then removed under reduced pressure, and the resulting residue was

purified by column chromatography using the appropriate eluent to afford the pure azoles **1m-p**.

Typical procedure for the Cu/zeolite-catalyzed amination of benzoxazole

A 10 mL vial equipped with a magnetic stirbar was loaded with benzoxazole (60 mg, 0.500 mmol), CH_3CN (2 mL), morpholine (52.5 μL, 0.600 mmol) and finally the Cu-zeolite catalyst (3 mol% Cu), in this order. The suspension was stirred under air at the desired temperature and time. The reaction mixture was eventually centrifuged before purification of the liquid phase by column chromatography, using the appropriate eluent. The solid was recovered, and washed with ethanol (5 x 5 mL) before drying overnight at 110 °C, followed by calcination at 550 °C for 5 h (1 °C/min ramp). The resulting solid was regenerated by another ion exchange in the presence of aqueous copper acetate, following the same procedure as described above.

Recycling and Stability experiments

- *Hot filtration tests*

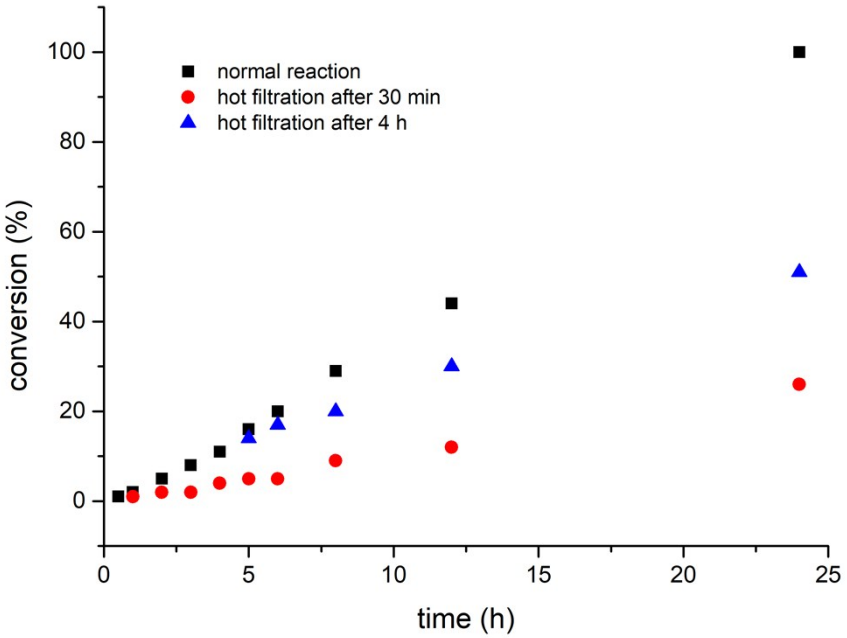


Fig S1 Hot filtration tests with catalyst removal during the reaction course. Conversion percentage as a function of reaction time in the presence of the Cu/H-USY catalyst (black) and once Cu/H-USY was removed 30 min (red) or 4 h (blue) after the reaction started.

- *Recyclability tests*

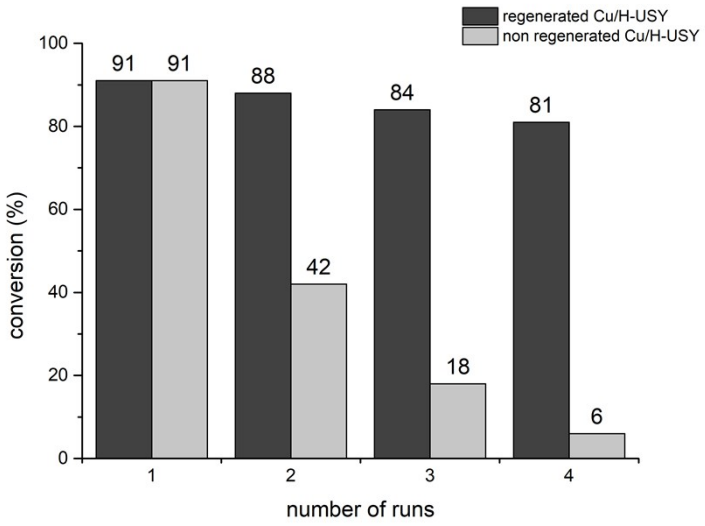


Fig S2 Comparative catalyst recycling study between regenerated (dark grey) and non-regenerated (light grey) Cu/H-USY.

- *PXRD patterns of Cu/H-USY*

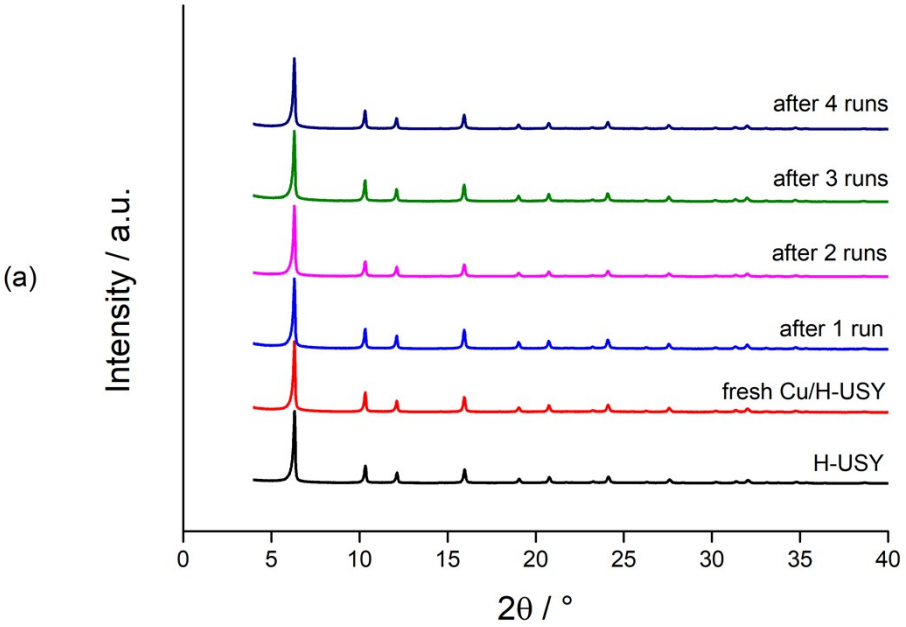


Fig S3 Powder X-ray diffraction (PXRD) patterns of the initial H-USY, the ion-exchanged Cu/H-USY as well as Cu/H-USY after regeneration and subsequent re-use. For comparability, all PXRD pattern intensities have been normalized.

- *XAS spectra*

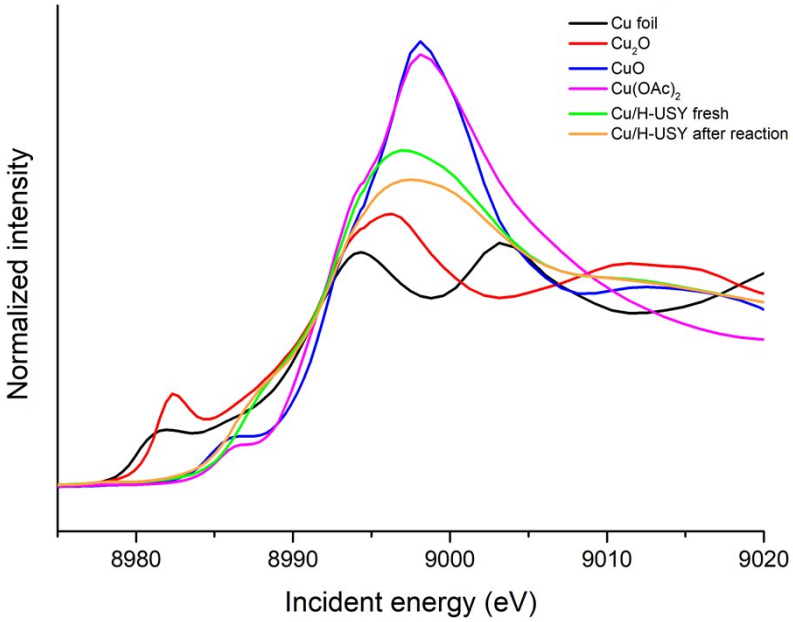


Fig S4 Overall normalized Cu-XANES spectra of Cu(0), Cu(I) and Cu(II) reference materials, and of Cu/H-USY before and after catalysis.

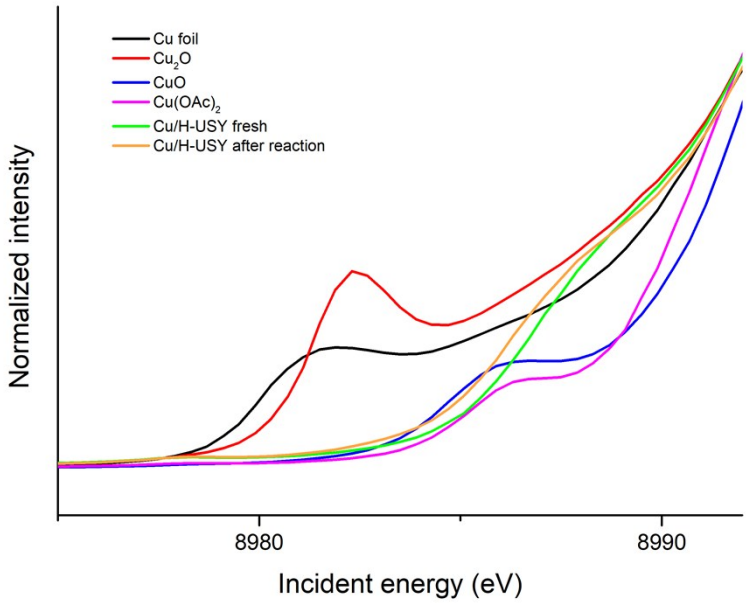


Fig S5 Normalized Cu-XANES spectra of Cu(0), Cu(I) and Cu(II) materials, and of Cu/H-USY before and after catalysis (zoomed-in).

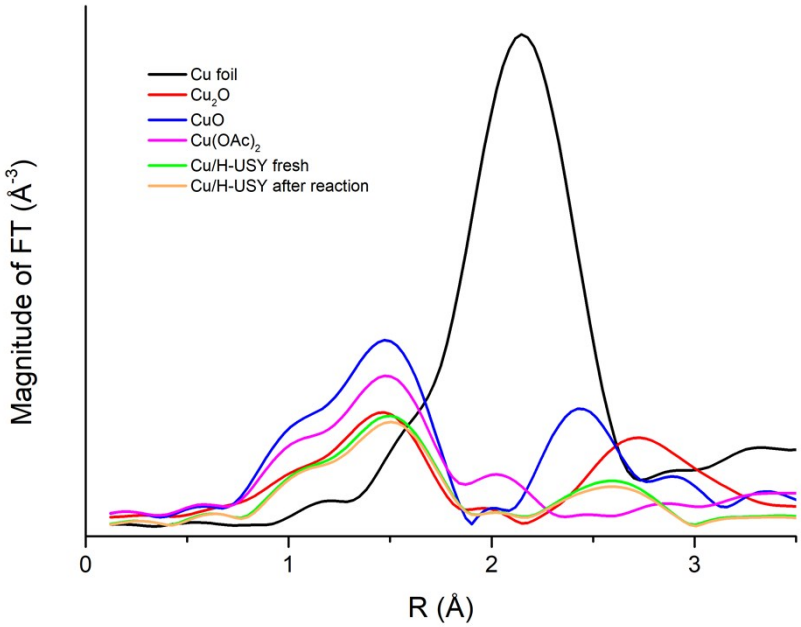
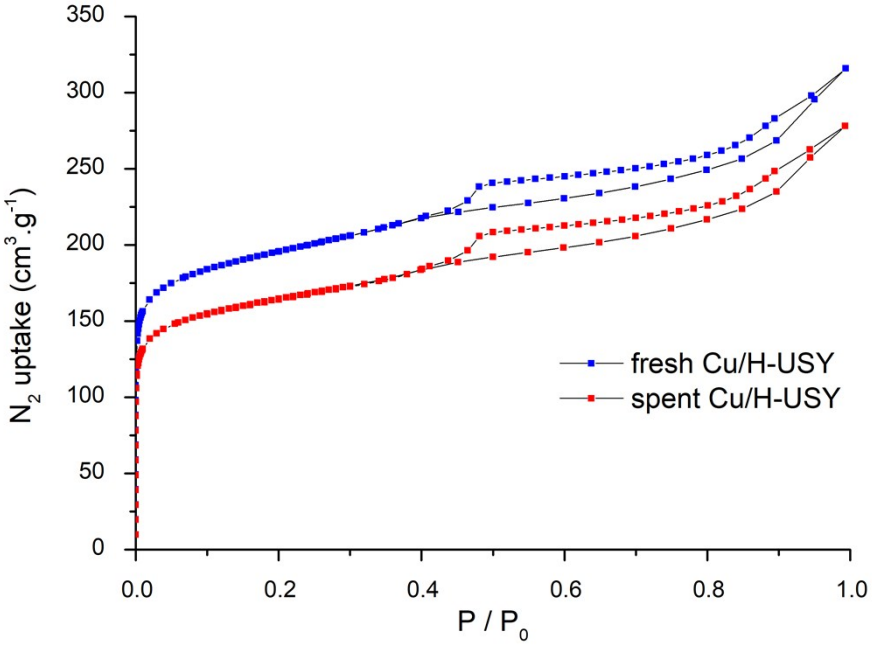


Fig S6 EXAFS spectra of Cu(0), Cu(I) and Cu(II) references with Cu/H-USY before and after catalysis.

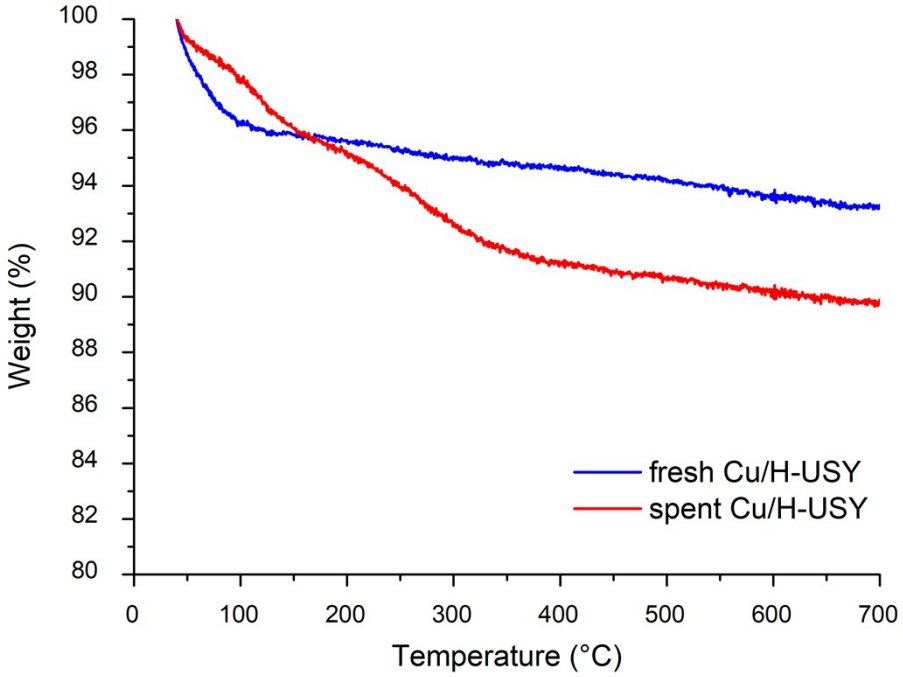
- *Nitrogen sorption*



S_{BET}(fresh) = 734 $m^2.g^{-1}$

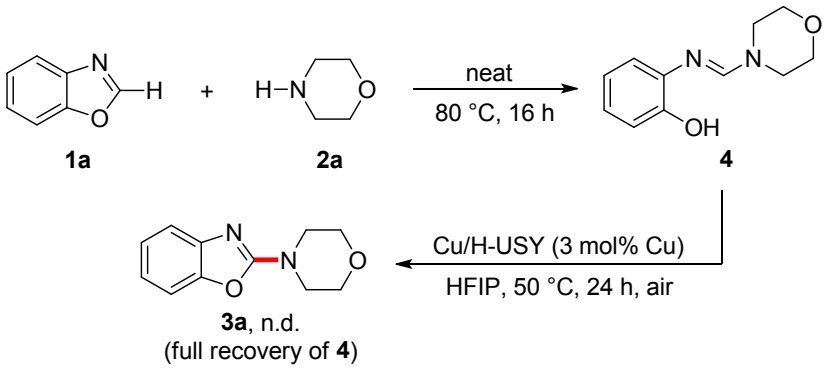
S_{BET}(spent) = 618 $m^2.g^{-1}$

- *TGA analysis*



Synthesis and evaluation of amidine 4 as a potential reaction intermediate

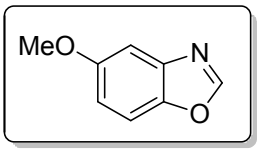
Amidine **4** was synthesized according to the literature by reacting **1a** with 2 equiv. **2a** under neat conditions. After isolation, **4** was reacted alone in the optimized conditions. No product formed at all, and **4** was fully recovered. This precludes its participation in the present Cu/H-USY catalyzed azole amination (Scheme S1).



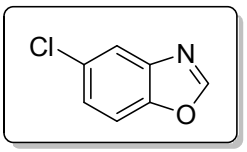
Scheme S1 (a) procedure for the preparation of **4**, (b) reaction of **4** with Cu/H-USY under the optimized conditions.

Spectroscopic data

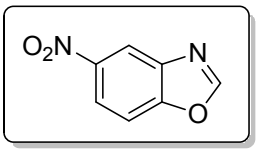
Azoles **1m-p** and aminoazoles **3a-p** are all known compounds.



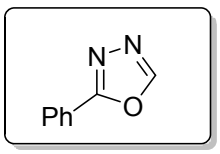
5-Methoxybenzoxazole[S4] **(1m):** Prepared as described in the general experimental procedure. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.46 (d, 1H), 7.26 (d, 1H), 7.00 (dd, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.6, 153.3, 144.8, 141.0, 114.6, 111.2, 103.4, 56.0.



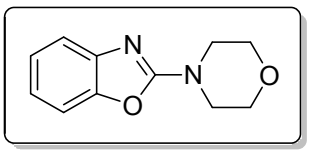
5-Chlorobenzoxazole[S5] **(1n):** Prepared as described in the general experimental procedure. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.79 (s, 1H), 7.53 (d, 1H), 7.38 (d, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.8, 148.7, 141.3, 130.3, 126.2, 120.7, 111.8.



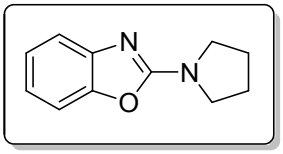
5-Nitrobenzoxazole[S4] **(1o):** Prepared as described in the general experimental procedure. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.71 (s, 1H), 8.38 (d, 1H), 8.28 (s, 1H), 7.72 (d, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.3, 153.6, 145.7, 140.6, 121.8, 117.3, 111.5.



2-Phenyl-1,3,4-oxadiazole[S4] **(1p):** Prepared as described in the general experimental procedure. White solid (mg, mmol, %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.07 (d, 2H), 7.52 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.7, 152.7, 131.9, 129.1, 127.1, 123.5.

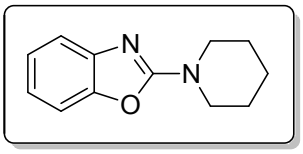


2-(4-Morpholinyl)benzoxazole[S5] **(3a):** Prepared as described in the general experimental procedure. Light yellow solid (93 mg, 0.455 mmol, 91 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (d, 1H), 7.27 (d, 1H), 7.18 (dd, 1H), 7.05 (dd, 1H), 3.83 (t, 4H), 3.70 (t, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.0, 148.6, 142.8, 124.0, 120.8, 116.5, 116.3, 108.8, 108.6, 66.0, 45.6.

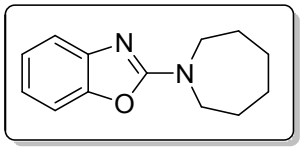


2-(Pyrrolidin-1-yl)benzoxazole[S5] **(3b):** Prepared as described in the general experimental procedure. White solid (87 mg, 0.461 mmol,

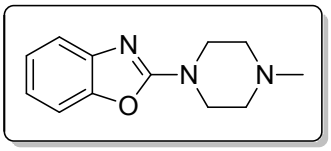
92 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (d, 1H), 7.23 (d, 1H), 7.13 (dd, 1H), 6.96 (dd, 1H), 3.63 (m, 4H), 2.01 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.1, 149.1, 143.8, 123.9, 120.1, 116.0, 108.6, 47.5, 22.7.



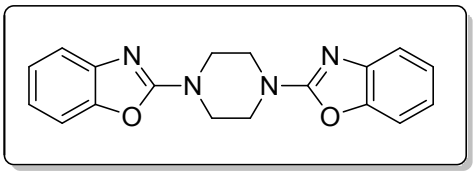
2-(Piperidin-1-yl)benzoxazole[S5] **(3c):** Prepared as described in the general experimental procedure. White solid (97 mg, 0.482 mmol, 96 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (d, 1H), 7.23 (d, 1H), 7.14 (dd, 1H), 6.99 (dd, 1H), 3.66 (t, 4H), 1.68 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.5, 148.7, 143.4, 123.9, 120.3, 116.1, 108.6, 46.6, 25.3, 24.1.



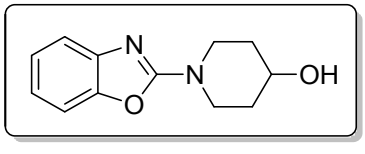
2-(Hexahydro-1*H*-azepin-1-yl)benzoxazole[S5] **(3d):** Prepared as described in the general experimental procedure. White solid (96 mg, 0.445 mmol, 89 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (d, 1H), 7.19 (d, 1H), 7.09 (dd, 1H), 6.92 (dd, 1H), 3.63 (t, 4H), 1.77 (m, 4H), 1.55 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.5, 148.8, 143.6, 123.7, 119.8, 115.7, 108.4, 47.9, 28.2, 27.3.



2-(4-methylpiperazin-1-yl)benzoxazole[S7] **(3e):** Prepared as described in the general experimental procedure. Light yellow solid (85 mg, 0.391 mmol, 78 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (d, 1H), 7.25 (d, 1H), 7.16 (dd, 1H), 7.01 (dd, 1H), 3.74 (t, 4H), 2.55 (t, 4H), 2.36 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.3, 148.9, 143.2, 124.1, 120.85, 116.4, 108.9, 54.3, 46.3, 45.5.

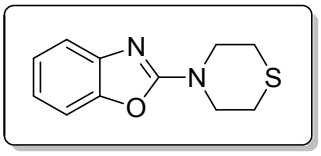


2,2'-(1,4-Piperazinediyl)-bis(benzoxazole)[S5] **(3f):** Prepared as described in the general experimental procedure, except that 0.250 mmol (0.5 equiv.) piperazine was used instead. Light yellow solid (65 mg, 0.204 mmol, 82 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.39 (d, 2H), 7.28 (d, 2H), 7.20 (dd, 2H), 7.07 (dd, 2H), 3.87 (s, 8H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.9, 149.0, 142.9, 124.4, 121.3, 116.8, 109.1, 45.2.

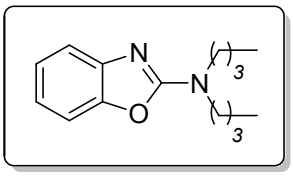


1-(Benzo[d]oxazol-2-yl)piperidin-4-ol[S8] **(3g):** Prepared as described in the general experimental procedure. White solid

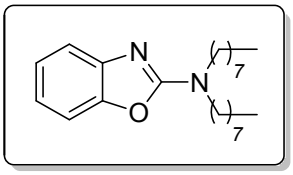
(74 mg, 0.340 mmol, 68 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (d, 1H), 7.24 (d, 1H), 7.15 (dd, 1H), 7.00 (dd, 1H), 4.06 (m, 4H), 3.97 (m, 1H), 3.43 (m, 2H), 2.16 (bs, 1H), 1.97 (m, 2H), 1.67 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.3, 148.8, 143.2, 124.1, 120.7, 116.2, 108.8, 66,7, 43.3, 33.6.



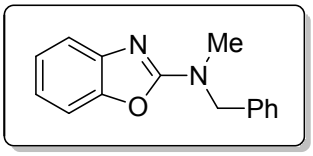
2-(4-Thiomorhophonyl)benzoxazole[S7] **(3h):** Prepared as described in the general experimental procedure. Light yellow solid (37 mg, 0.170 mmol, 34 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (d, 1H), 7.25 (d, 1H), 7.17 (dd, 1H), 7.02 (dd, 1H), 3.99 (t, 4H), 2.72 (t, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.8, 148.8, 124.2, 120.9, 116.4, 108.8, 48.2, 26.8.



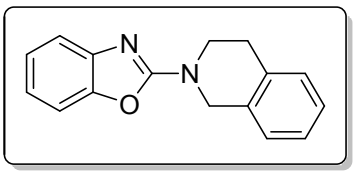
2-(*N*,*N*-Dibutyl)benzoxazole[S6] **(3i):** Prepared as described in the general experimental procedure. (117 mg, 0.474 mmol, 95 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (d, 1H), 7.23 (d, 1H), 7.13 (dd, 1H), 6.97 (dd, 1H), 3.50 (t, 4H), 1.66 (m, 4H), 1.38 (m, 4H), 0.96 (t, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.5, 148.6, 143.6, 123.6, 119.7, 115.7, 115.5, 108.3, 48.2, 30.0, 19.8, 13.7.



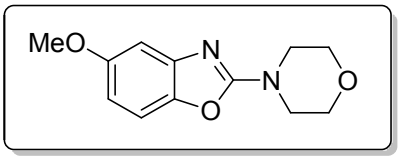
2-(*N*,*N*-Dioctyl)benzoxazole[S9] **(3j):** Prepared as described in the general experimental procedure. (162 mg, 0.453 mmol, 91 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.34 (d, 1H), 7.23 (d, 1H), 7.12 (dd, 1H), 6.96 (dd, 1H), 3.49 (t, 4H), 1.78 (m, 6H), 1.52 (m, 22H), 0.88 (t, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.7, 148.8, 143.8, 123.8, 119.9, 115.8, 108.5, 48.7, 31.9, 29.3, 28.1, 26.8, 22.7, 14.1.



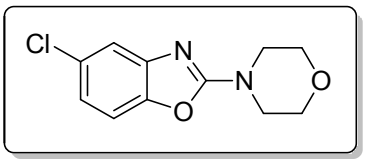
2-(*N*-Benzyl-*N*-methyl)benzoxazole[S5] **(3k):** Prepared as described in the general experimental procedure. (106 mg, 0.446 mmol, 89 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (m, 7H), 7.17 (dd, 1H), 7.01 (dd, 1H), 4.75 (s, 2H), 3.12 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.1, 149.1, 143.7, 136.5, 128.9, 127.9, 127.8, 124.1, 120.5, 116.3, 108.8, 53.9, 35.3.



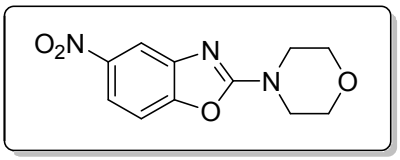
2-(3,4-Dihydroisoquinolin-2(1*H*)-yl)benzoxazole[S5] **(3l):** Prepared as described in the general experimental procedure. White solid (105 mg, 0.419 mmol, 84 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.38 (d, 1H), 7.25 (d, 1H), 7.14 (m, 5H), 6.99 (dd, 1H), 4.80 (s, 2H), 3.89 (t, 2H), 2.94 (t, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.0, 148.8, 143.2, 133.9, 132.3, 128.7, 126.7, 126.5, 126.3, 124.0, 120.5, 116.2, 108.7, 47.1, 43.0, 28.4.



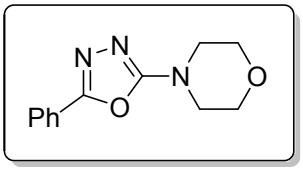
5-Methoxy-2-(morpholinyl)benzoxazole[S10] **(3m):** Prepared as described in the general experimental procedure. White solid (98 mg, 0.417 mmol, 83 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.05 (d, 1H), 6.87 (d, 1H), 6.52 (dd, 1H), 3.72 (s, 3H), 3.72 (t, 4H), 3.58 (t, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.7, 157.0, 143.8, 143.2, 108.6, 107.3, 101.4, 66.1, 55.7, 45.5.



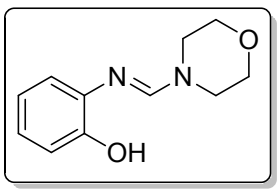
5-Chloro-2-(morpholinyl)benzoxazole[S6] **(3n):** Prepared as described in the general experimental procedure. White solid (112 mg, 0.469 mmol, 94 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (s, 1H), 7.14 (d, 1H), 6.98 (d, 1H), 3.80 (t, 4H), 3.67 (t, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.8, 147.3, 144.3, 129.4, 120.7, 116.5, 109.3, 66.1, 45.6.



5-Nitro-2-(morpholinyl)benzoxazole[S10] **(3o):** Prepared as described in the general experimental procedure. Yellow solid (31 mg, 0.125 mmol, 25 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17 (s, 1H), 8.01 (d, 1H), 7.32 (d, 1H), 3.84 (t, 4H), 3.73 (t, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.7, 152.8, 145.5, 144.1, 117.5, 112.2, 108.6, 66.2, 45.9.



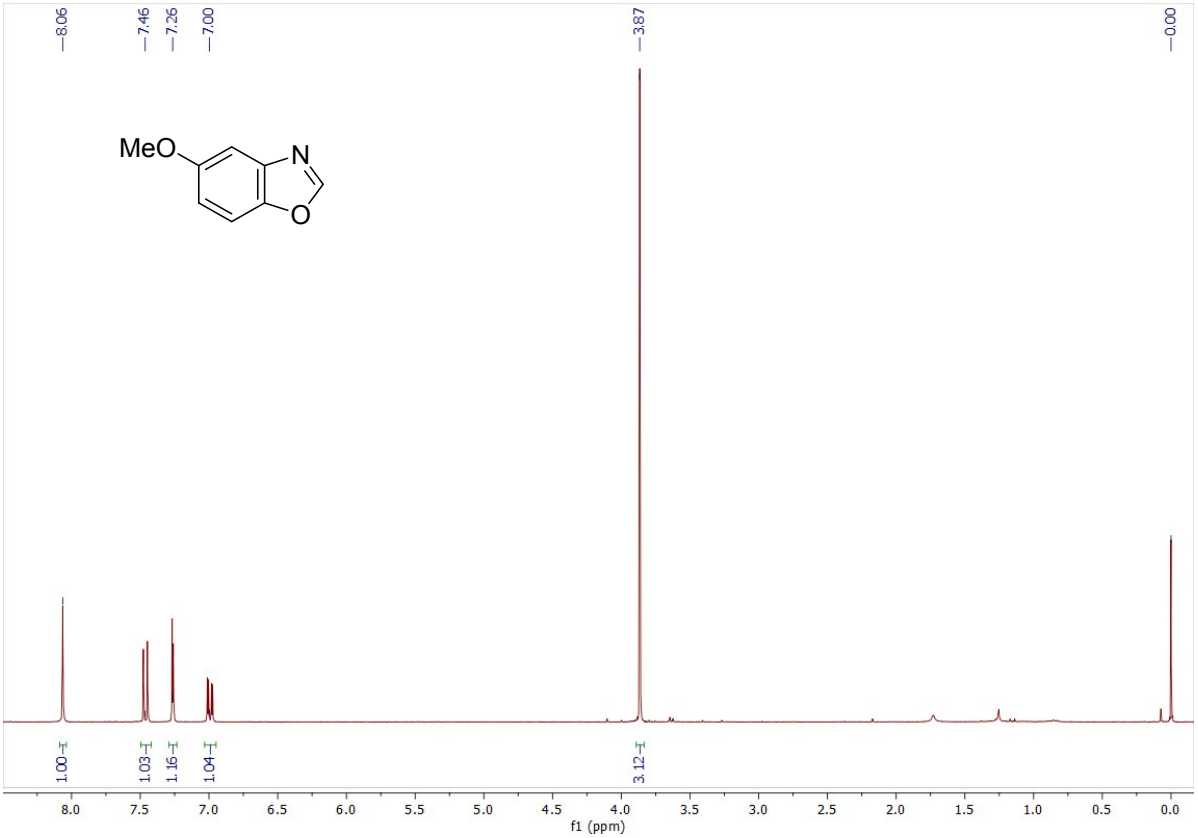
2-Phenyl-5-(morpholinyl)-1,3,4-oxadiazole[S6] **(3p):** Prepared as described in the general experimental procedure. White solid (71 mg, 0.306 mmol, 61 %). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (m, 2H), 7.45 (m, 3H), 3.83 (t, 4H), 3.58 (t, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.2, 159.7, 130.7, 129.0, 126.0, 124.6, 66.1, 46.4.

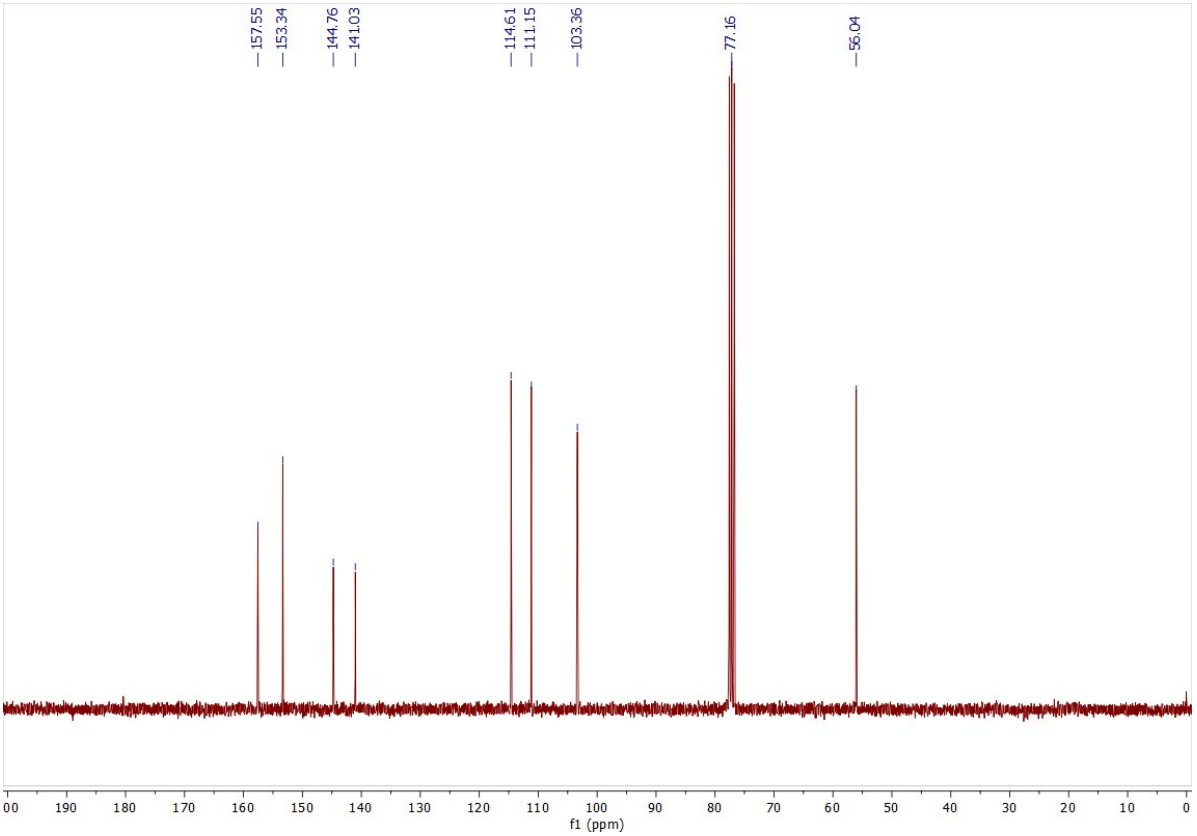


2-(4-morholonylmethyleneamino)phenol[S4] **(4):** Prepared as described above. Viscous liquid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.73 (s, 1H), 7.06-6.70 (m, 4H), 3.85-3.37 (m, 8H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.5, 150.3, 136.7, 124.3, 120.0, 115.7, 113.7, 68.2, 66.7, 46.6.

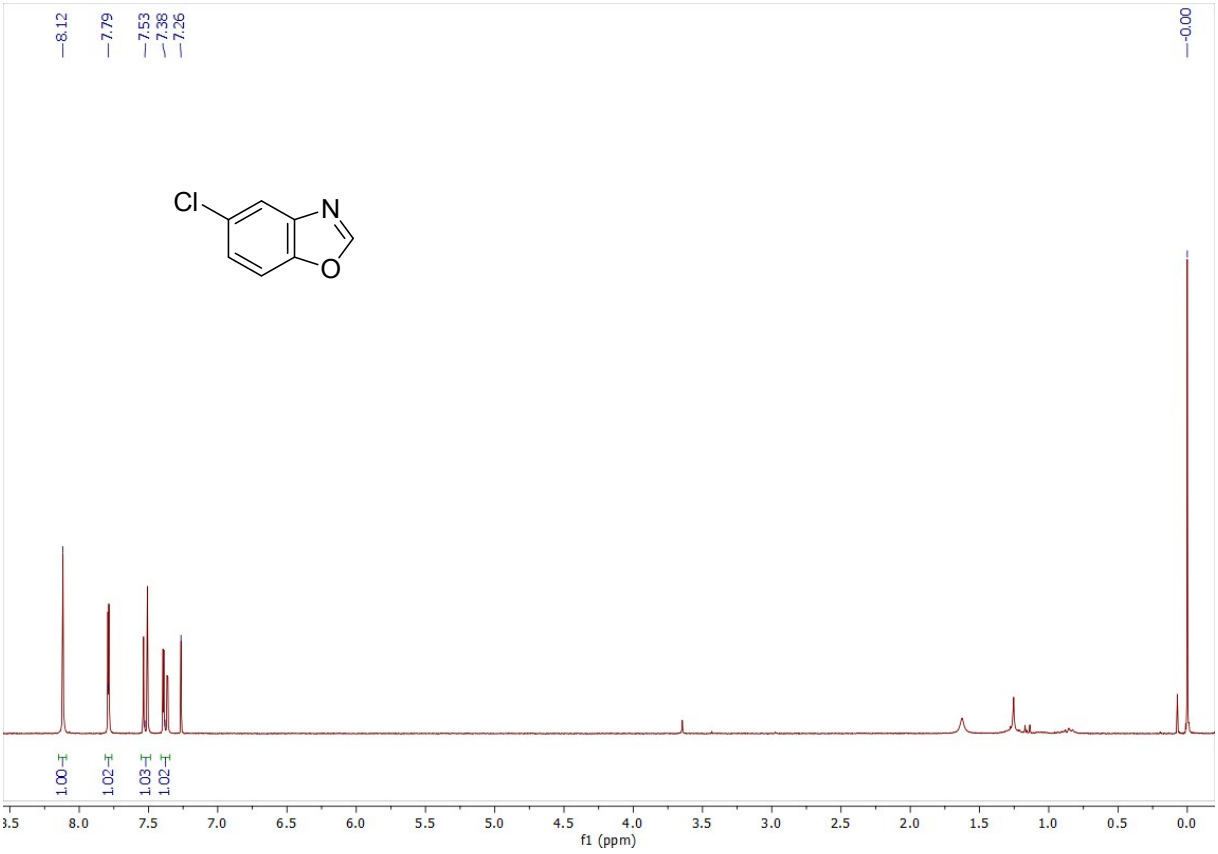
NMR spectra of compounds 1m-p and 3a-p

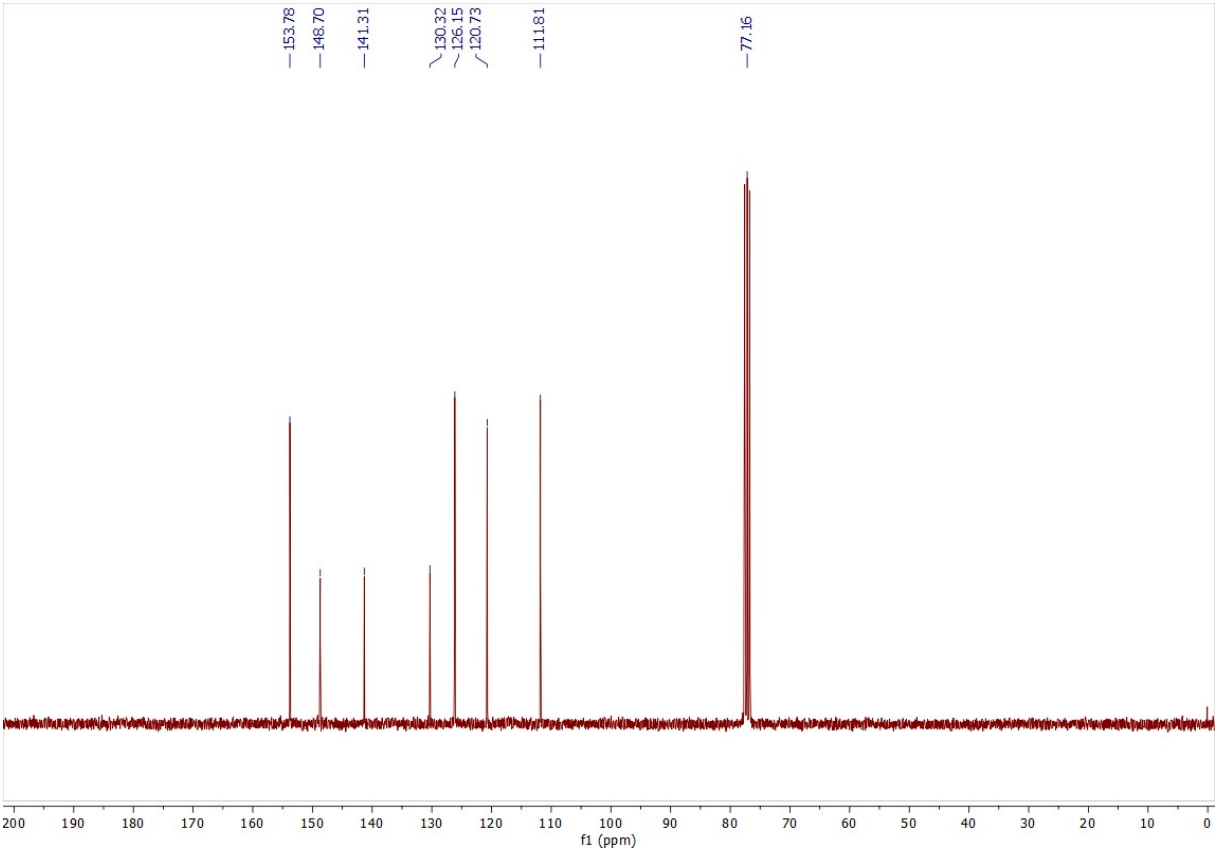
5-Methoxybenzoxazole (1m)



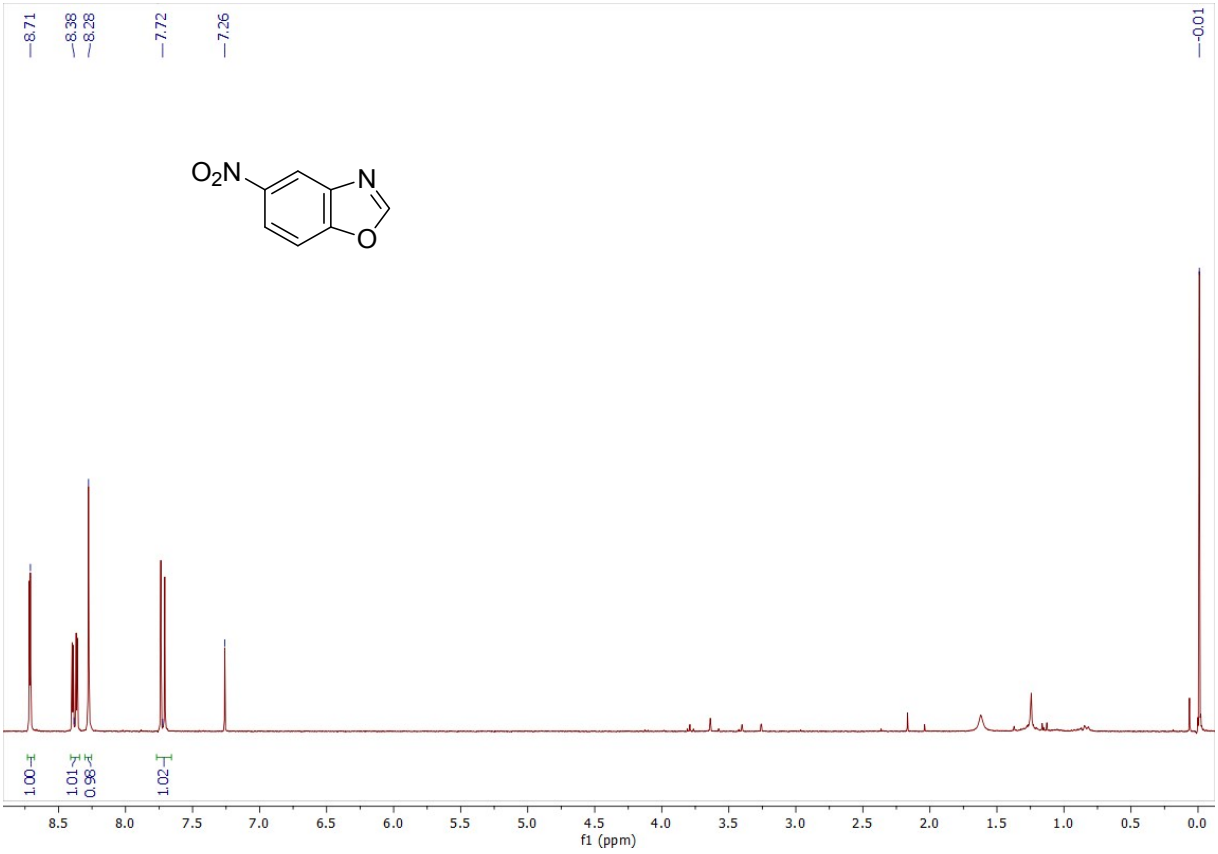


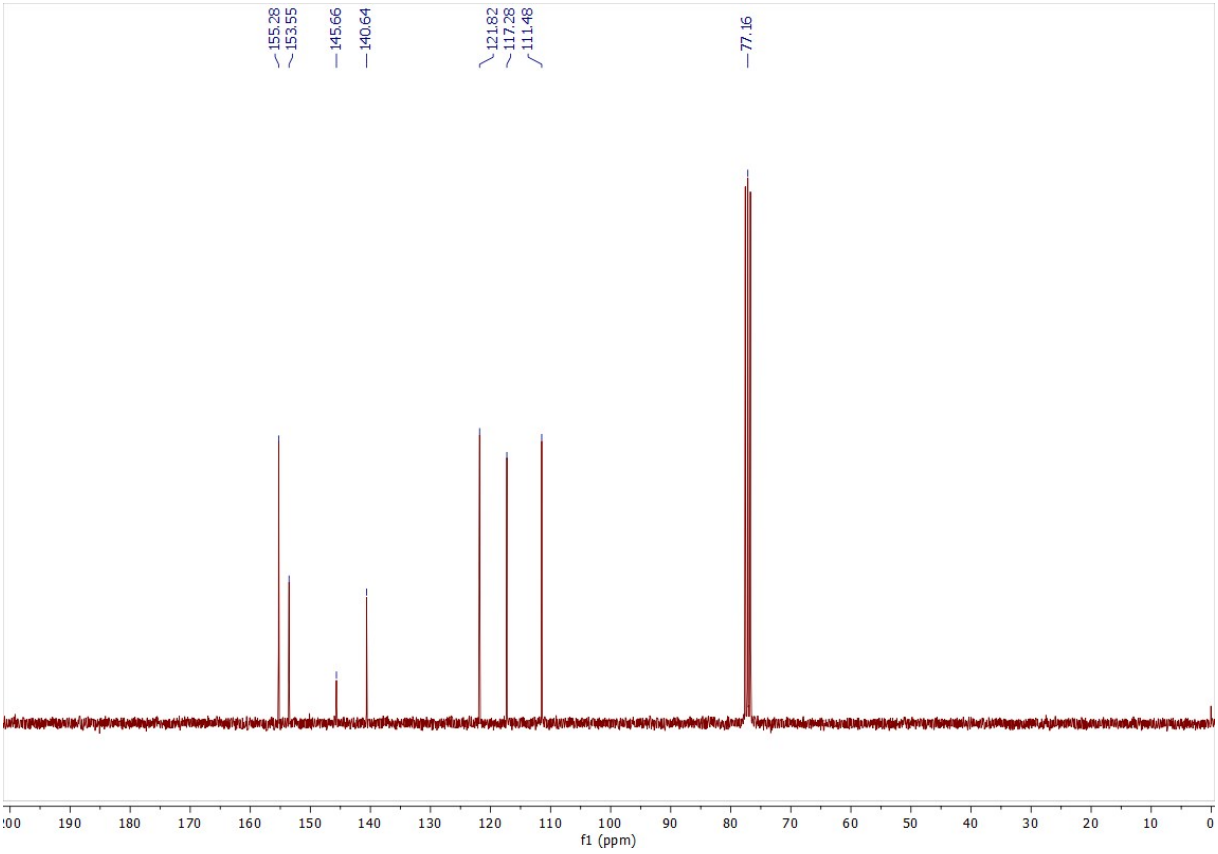
5-Chlorobenzoxazole (1n)



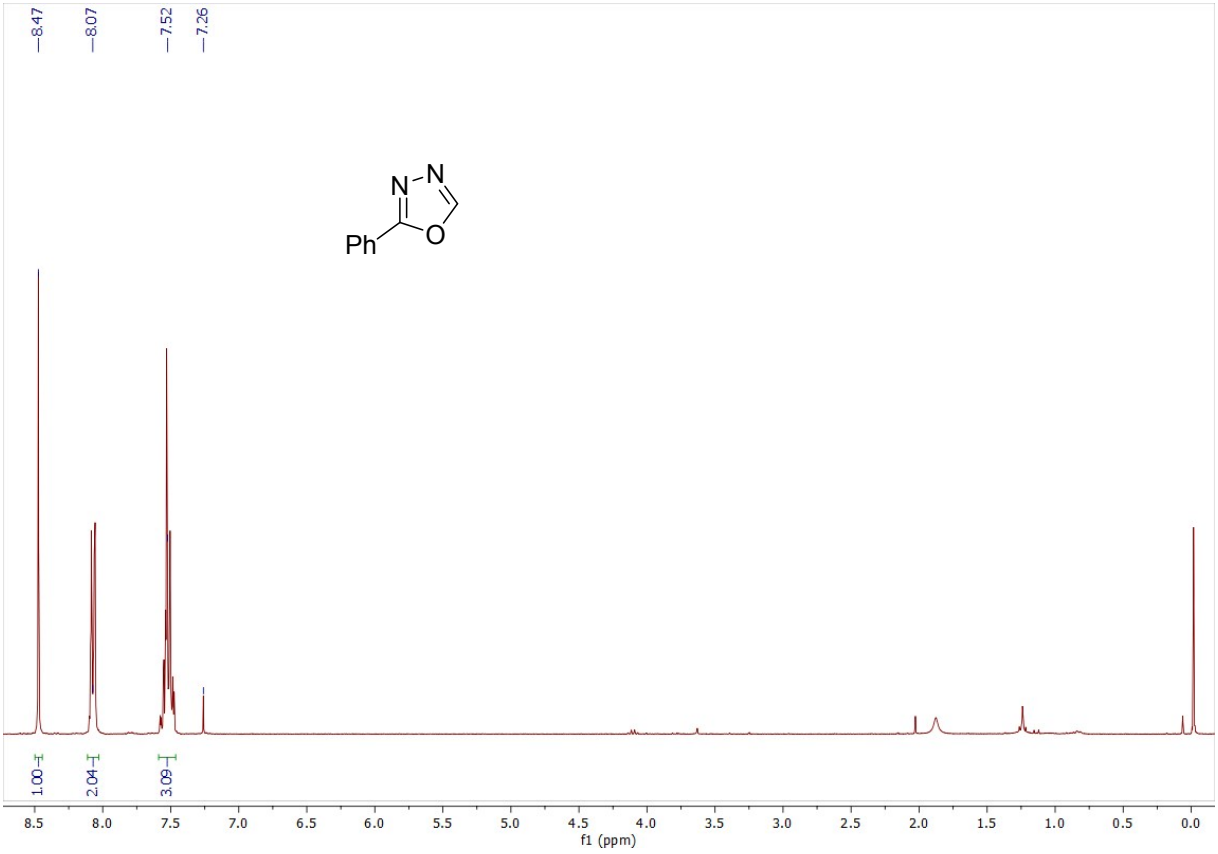


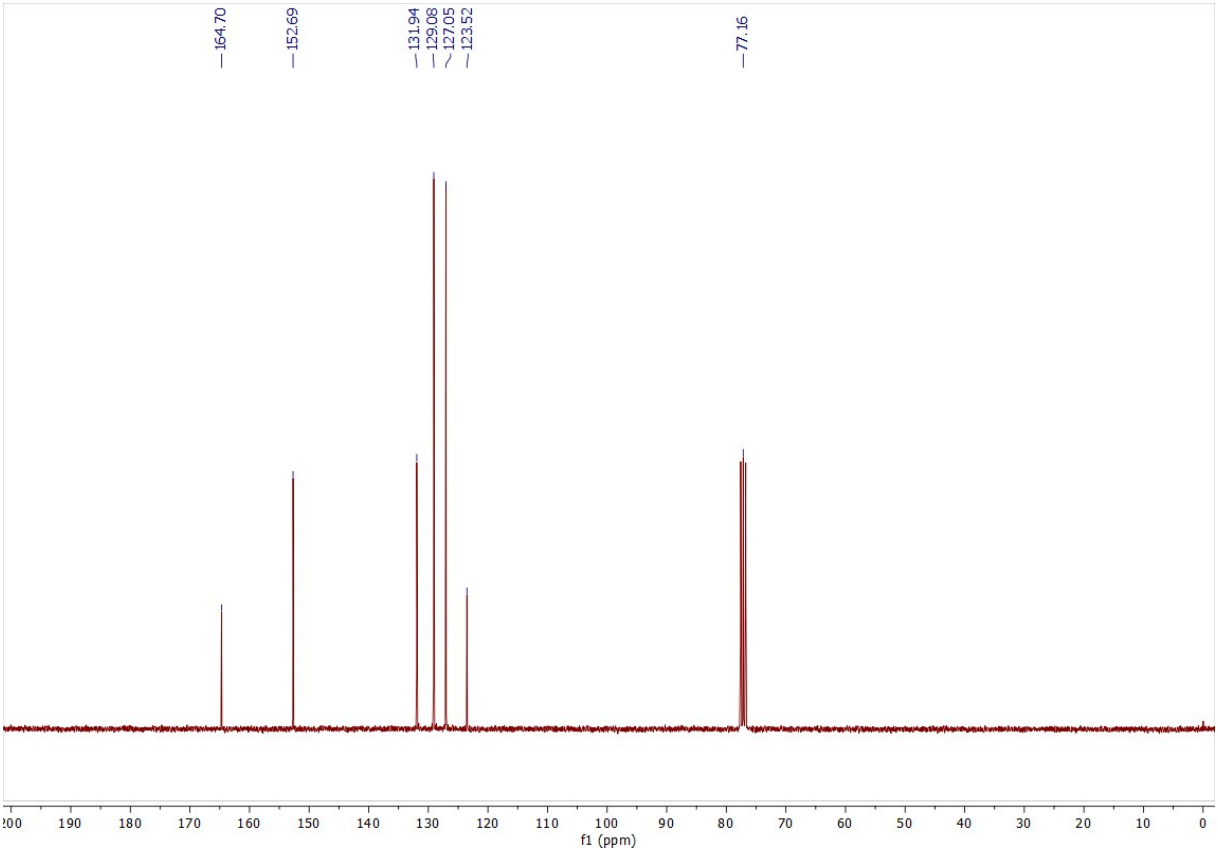
5-Nitrobenzoxazole (1o)



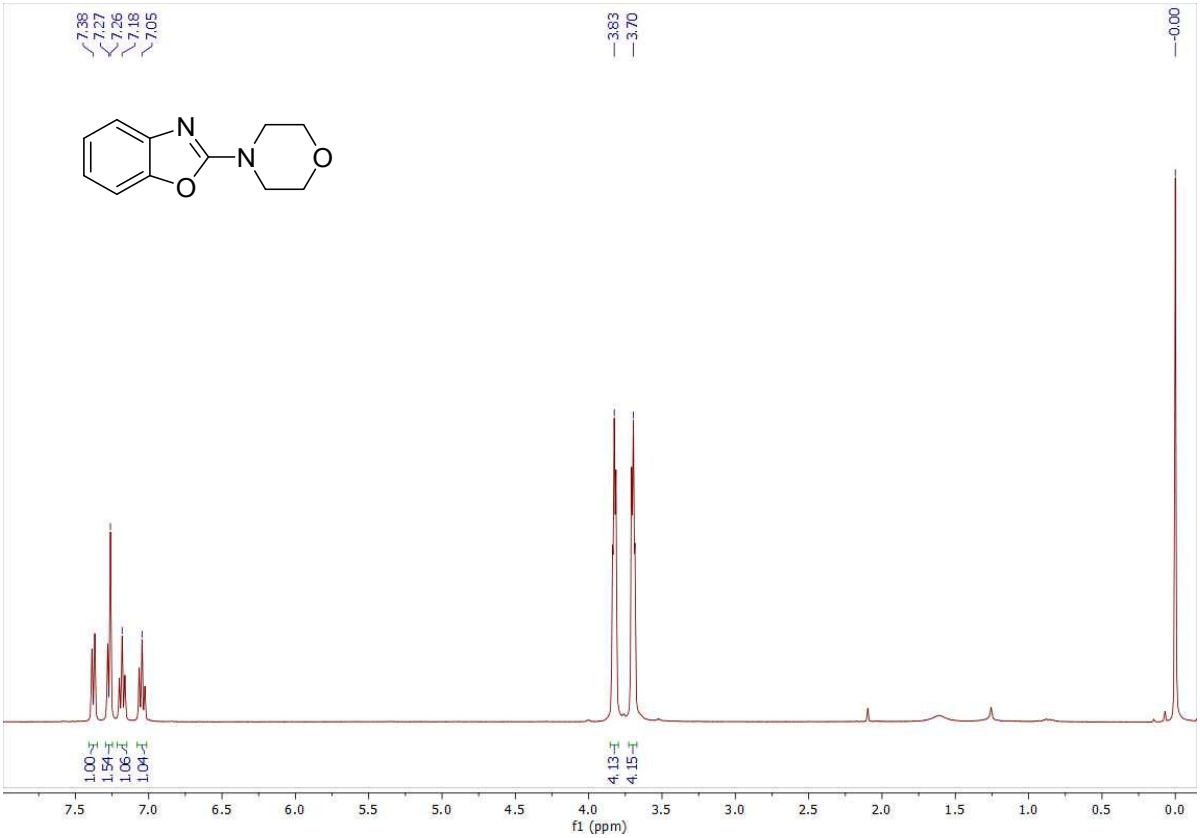


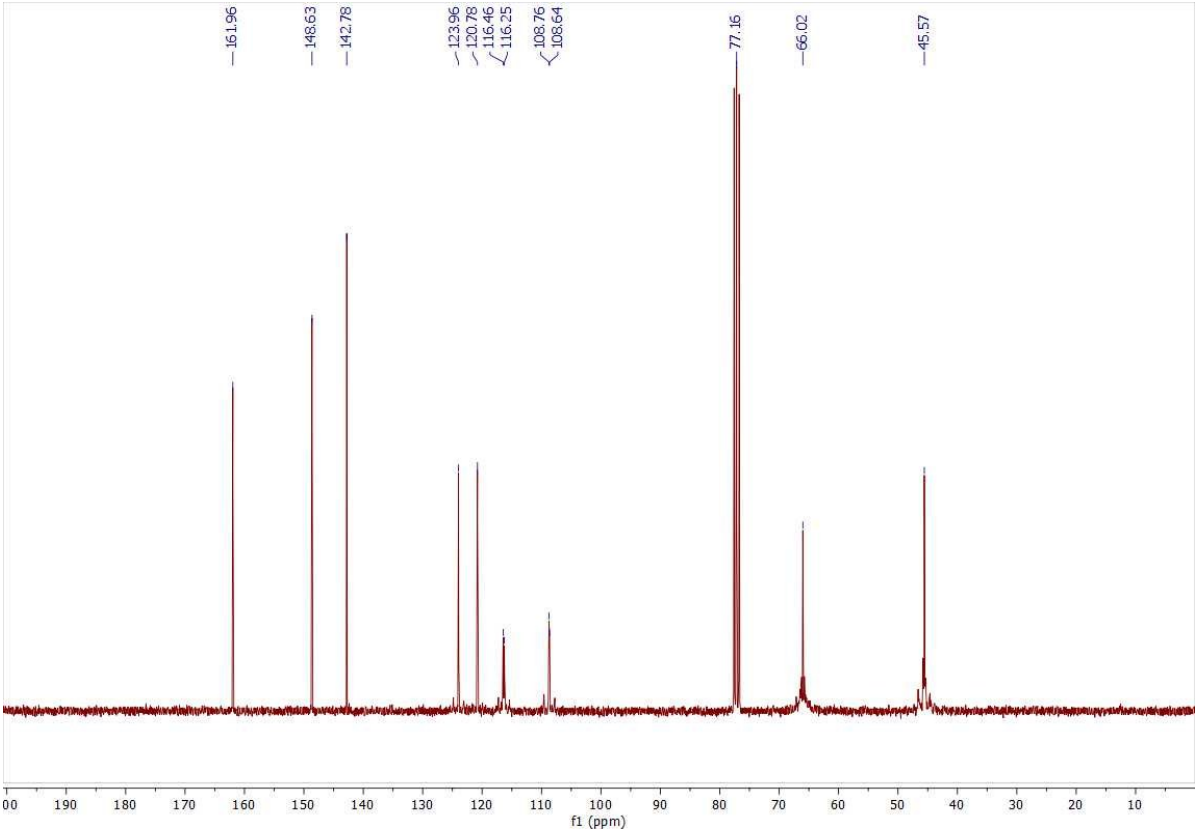
2-Phenyl-1,3,4-oxadiazole (1p)



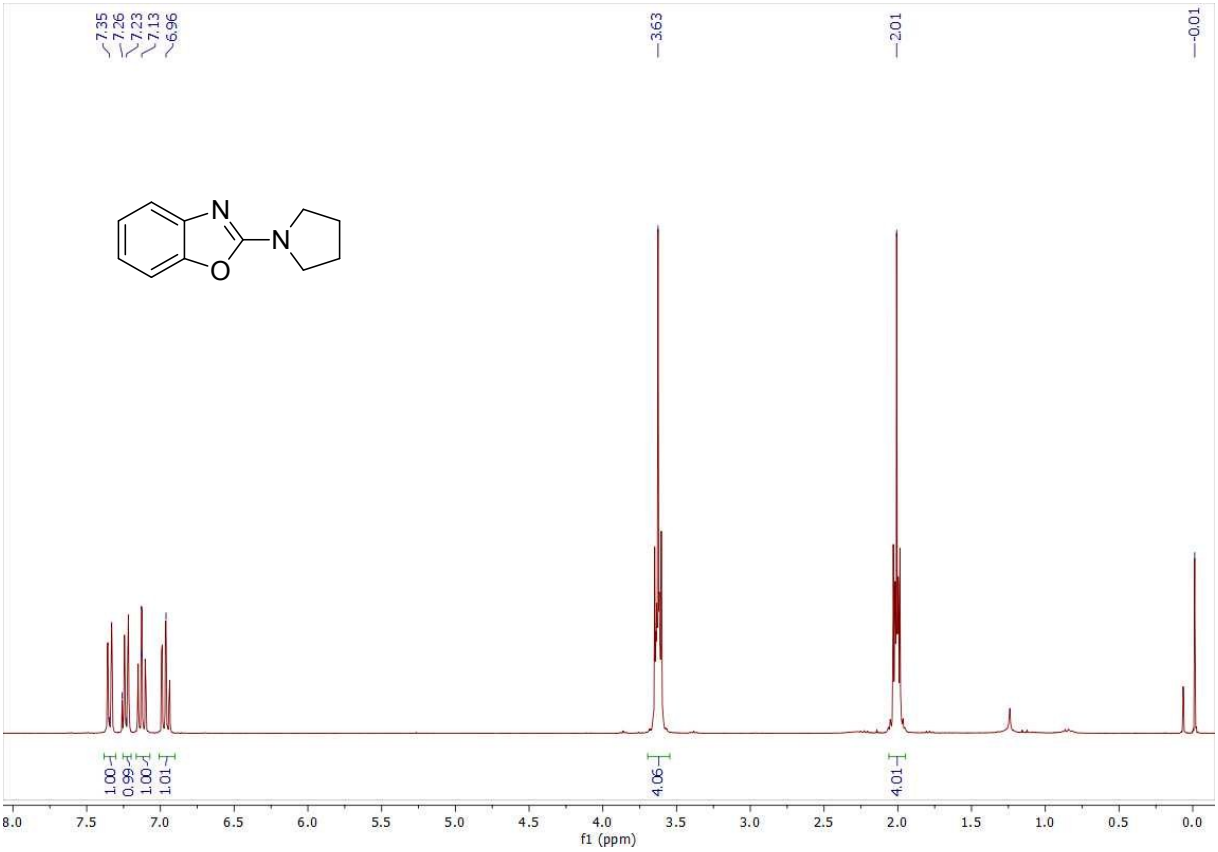


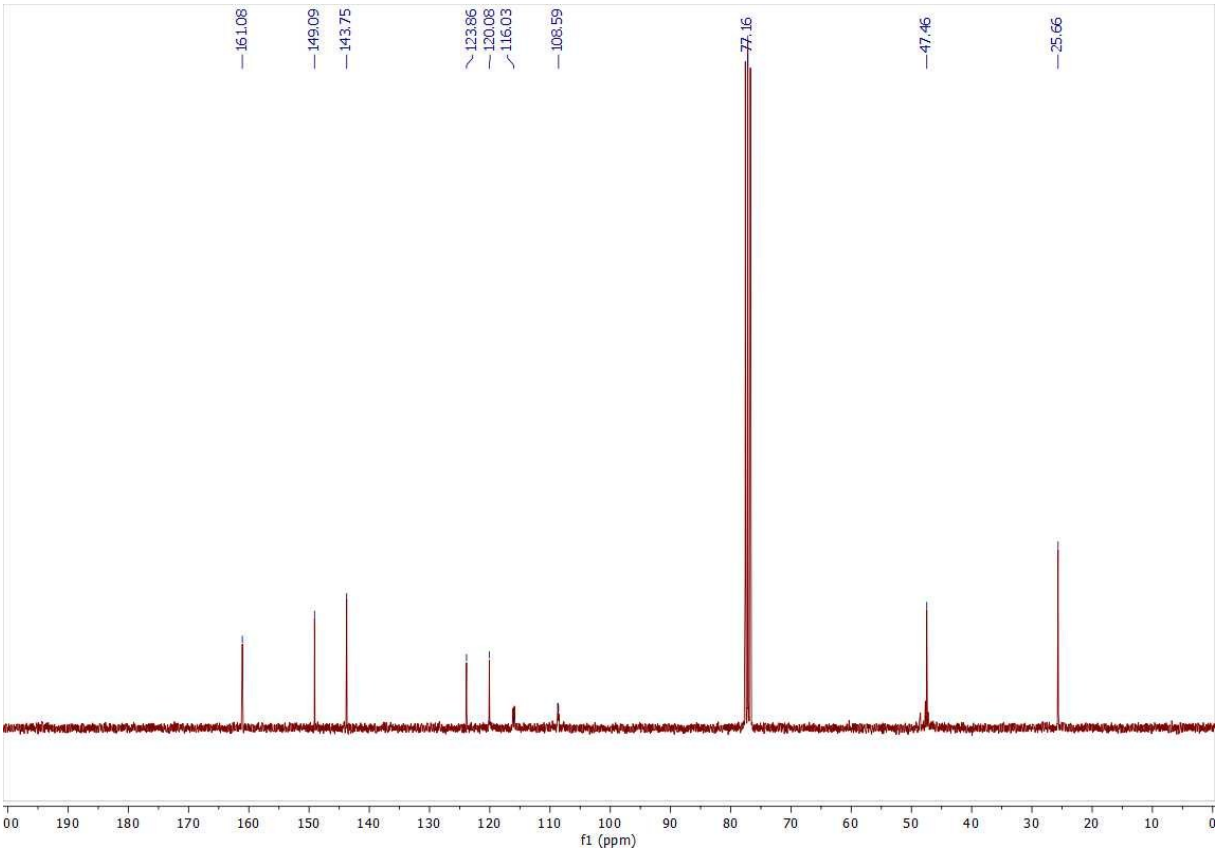
2-(4-Morpholinyl)benzoxazole (3a)



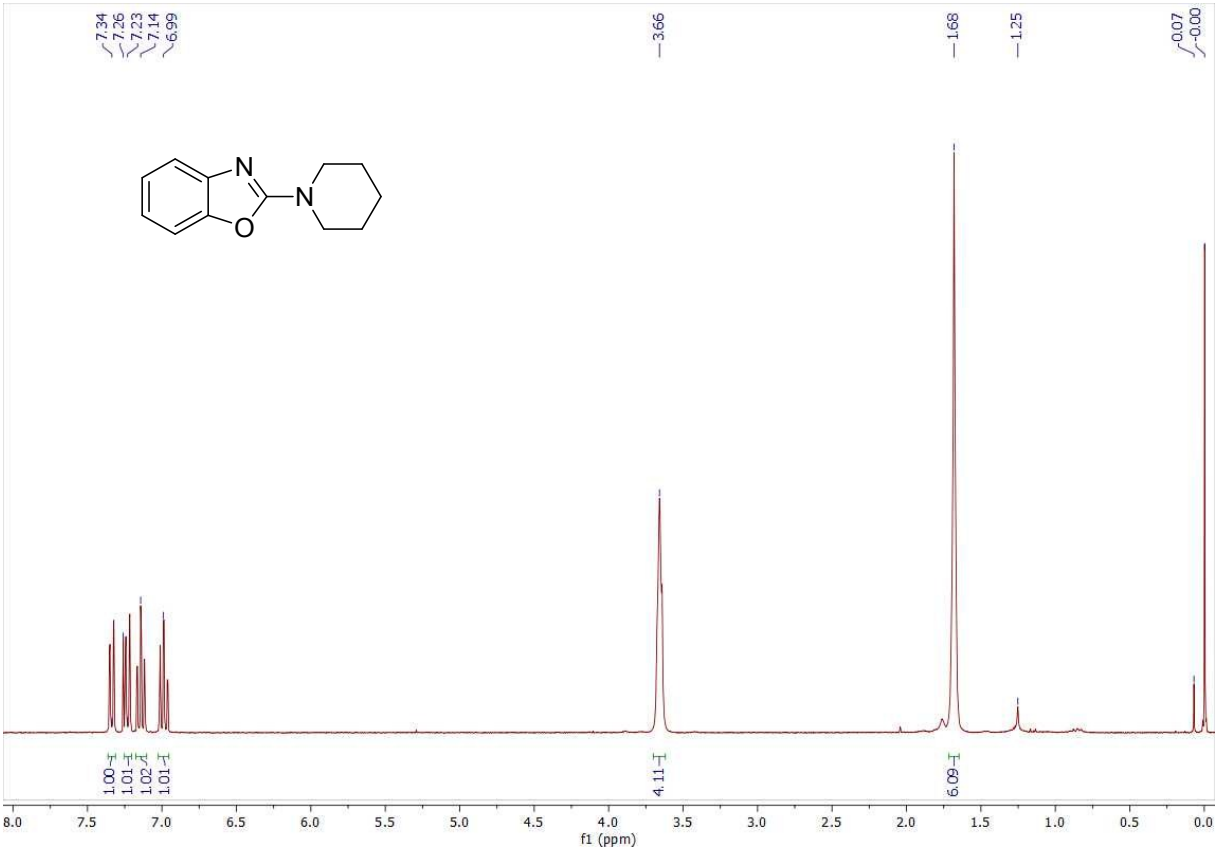


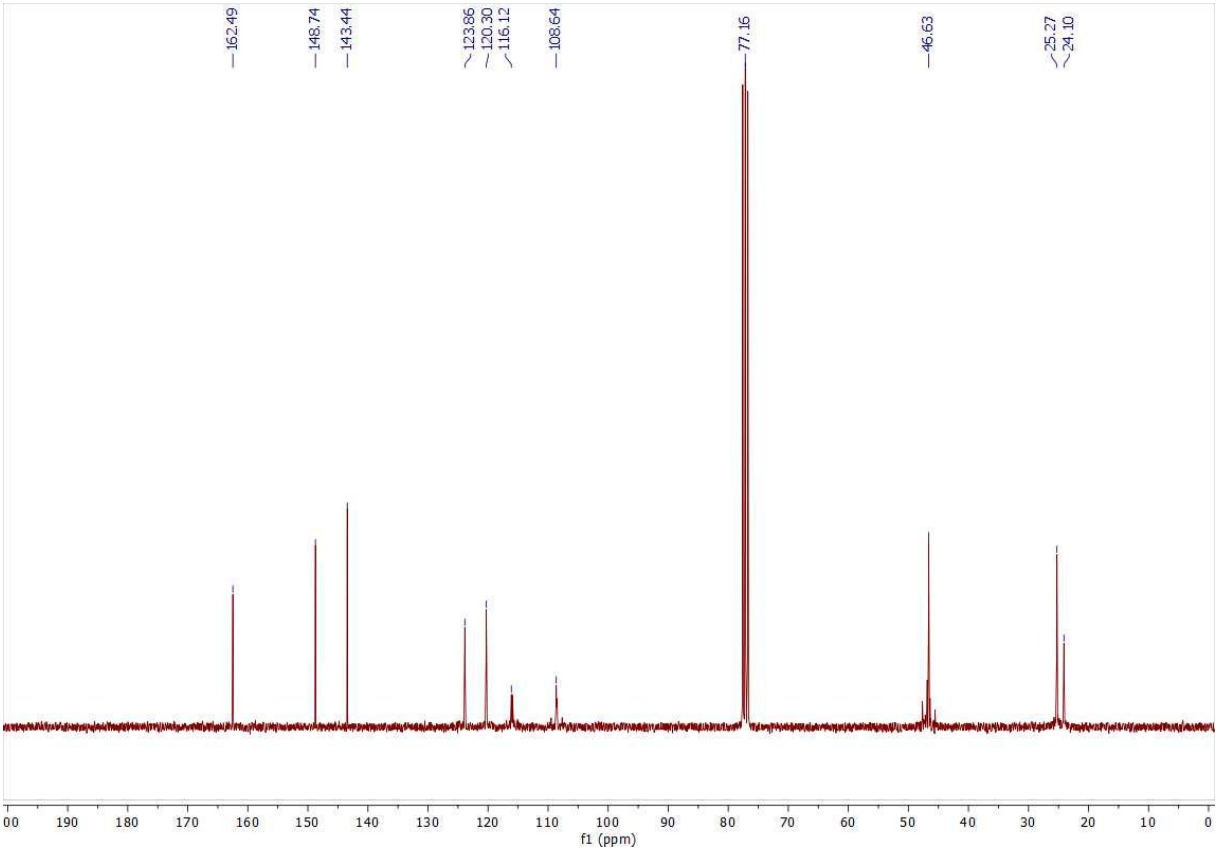
2-(Pyrrolidin-1-yl)benzoxazole (3b)



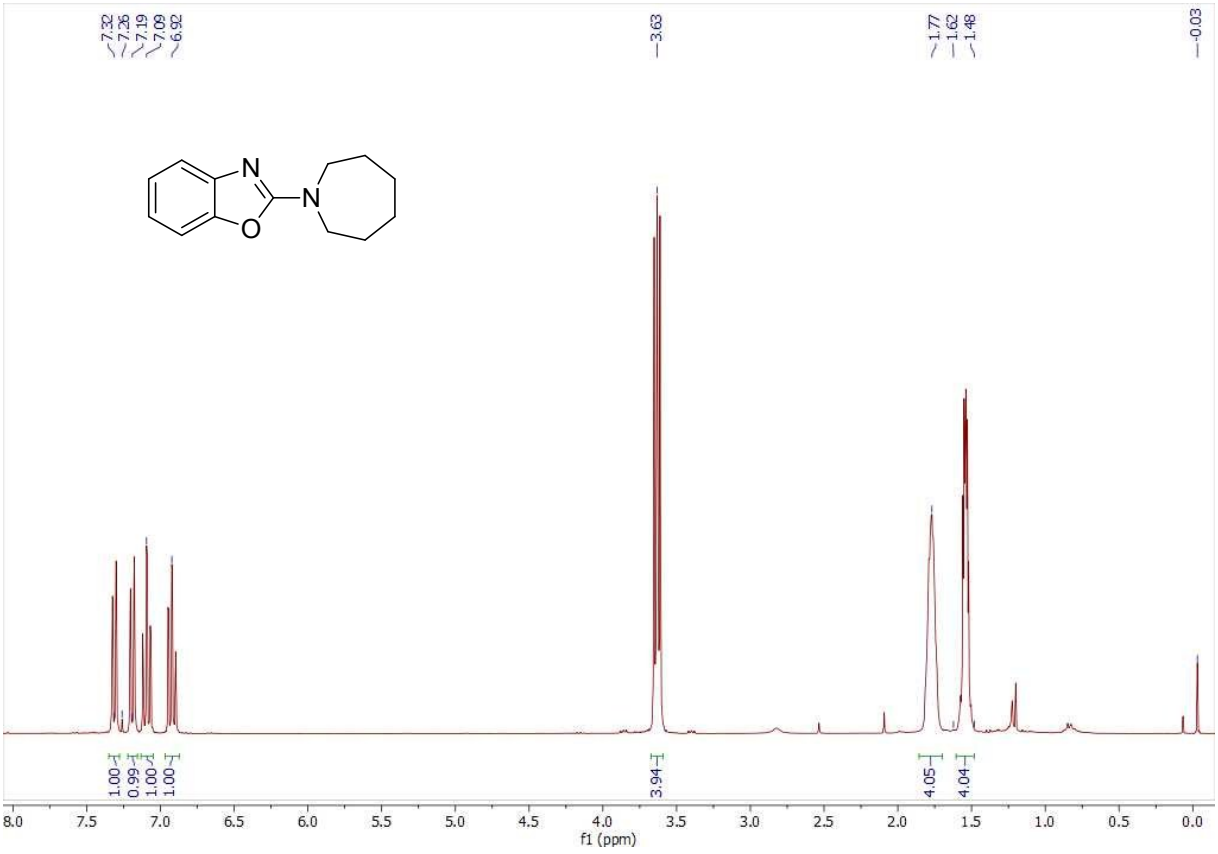


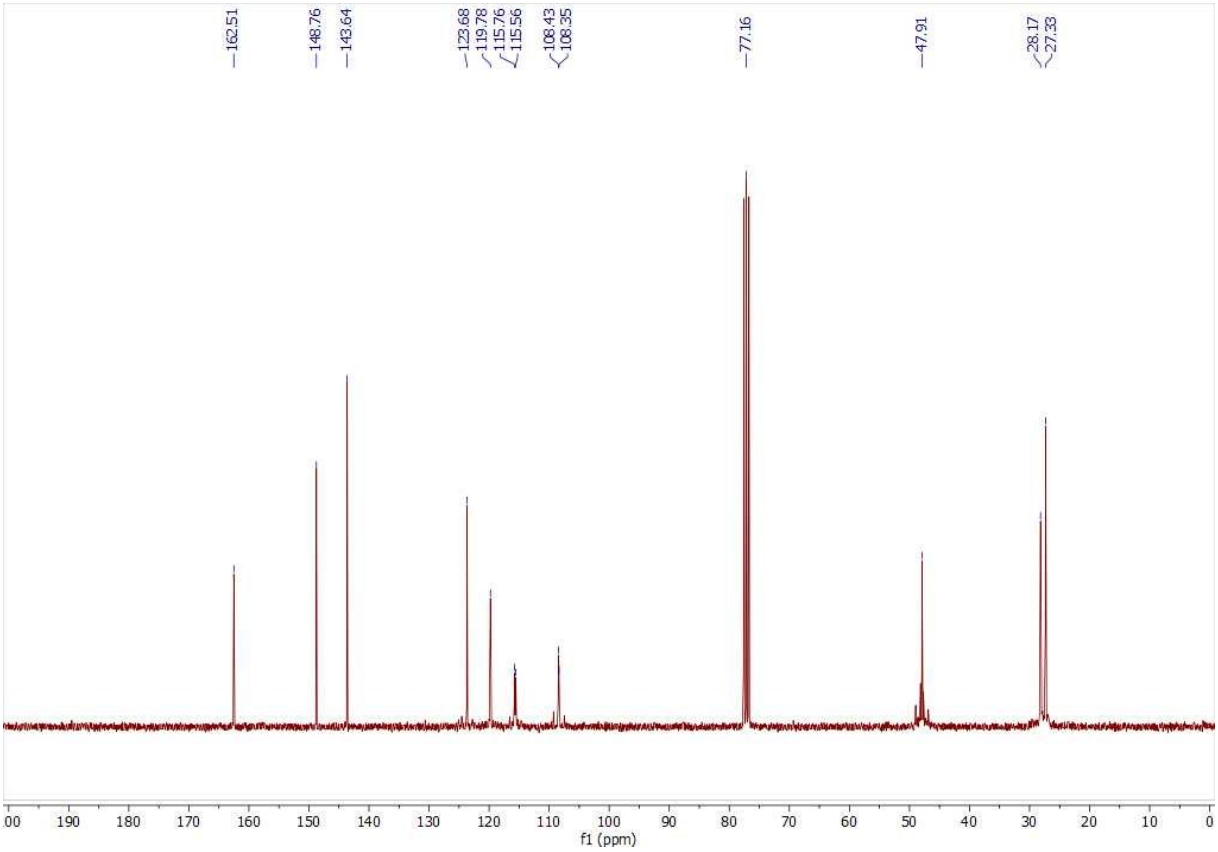
2-(Piperidin-1-yl)benzoxazole (3c)



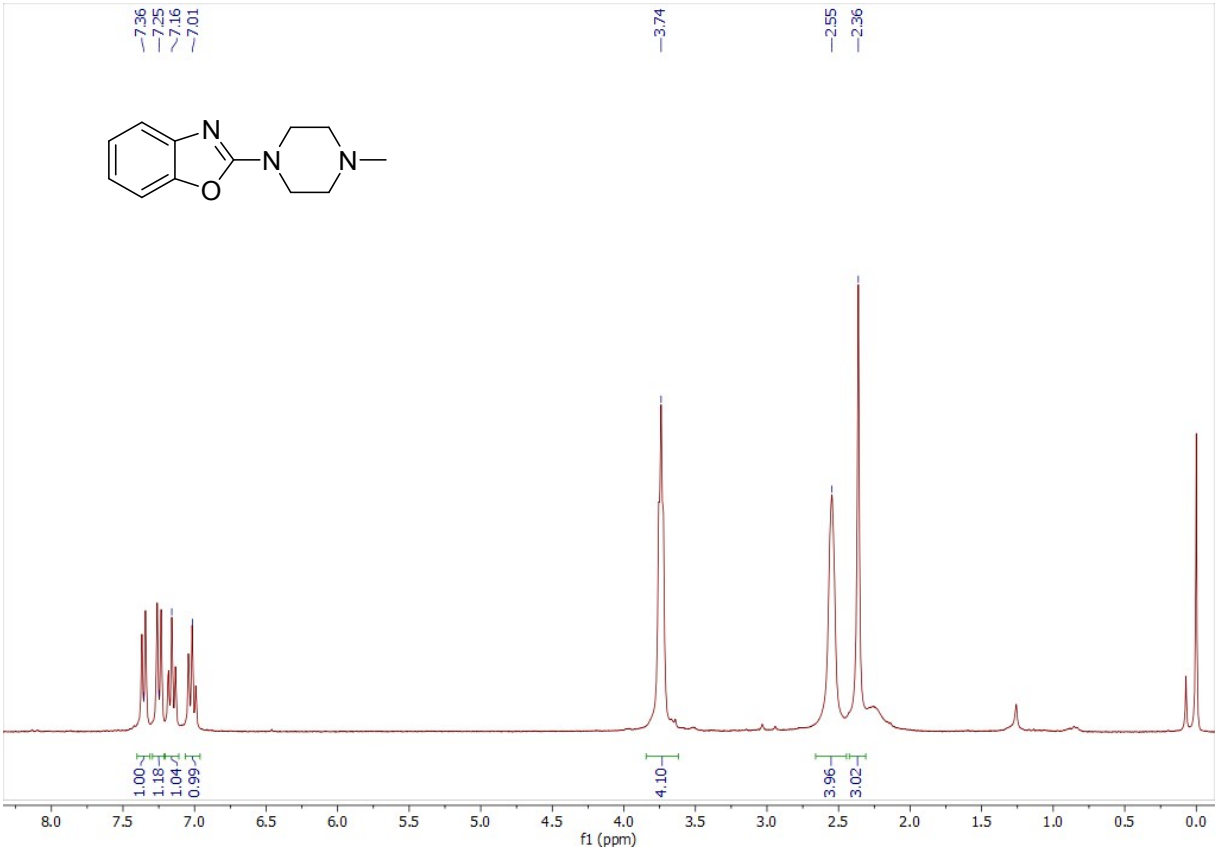


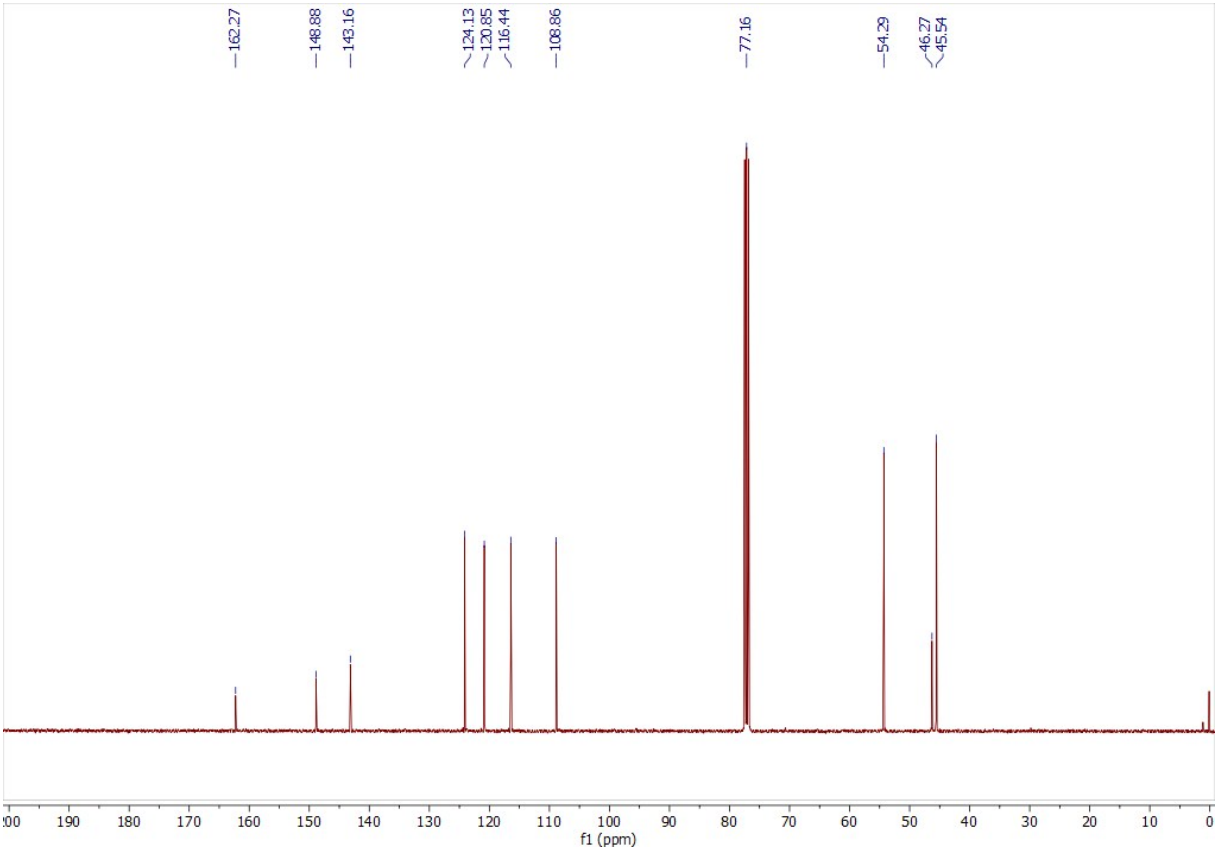
2-(Hexahydro-1*H*-azepin-1-yl)benzoxazole (3d)



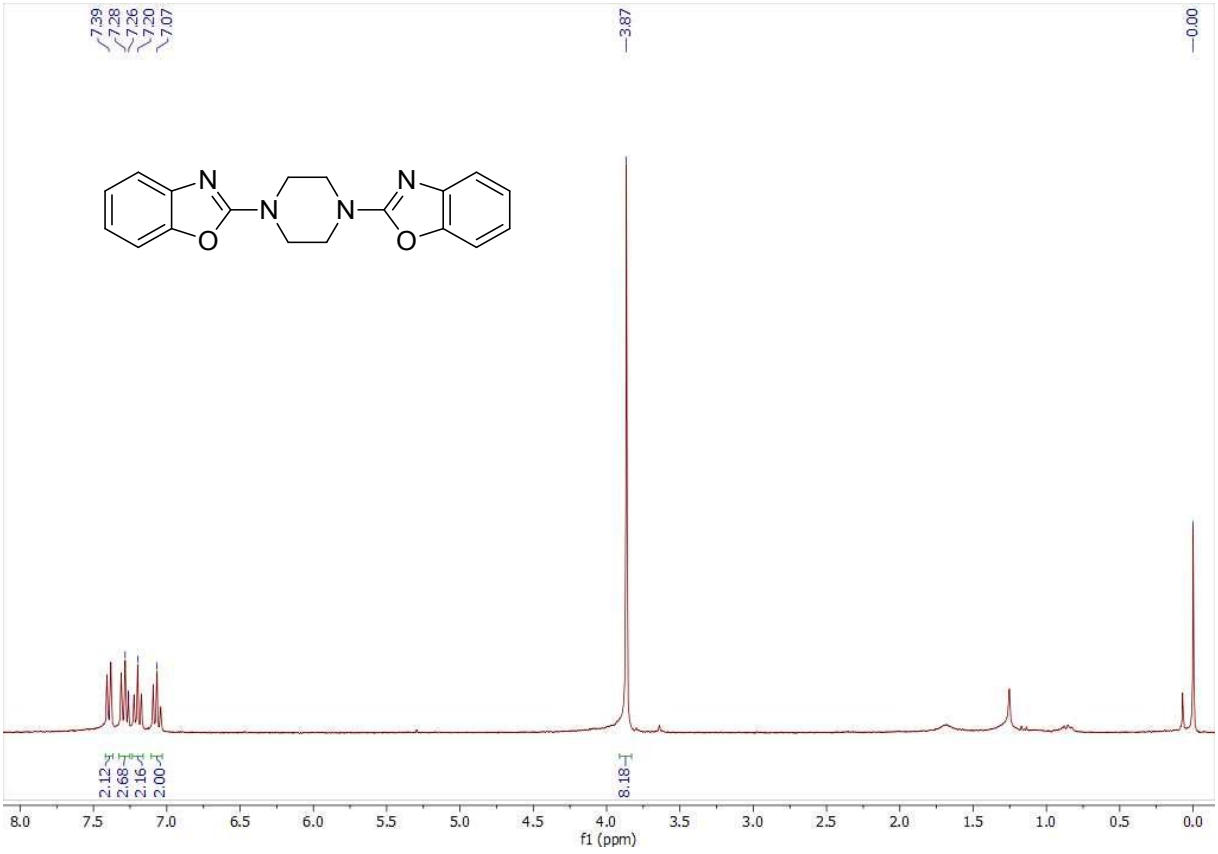


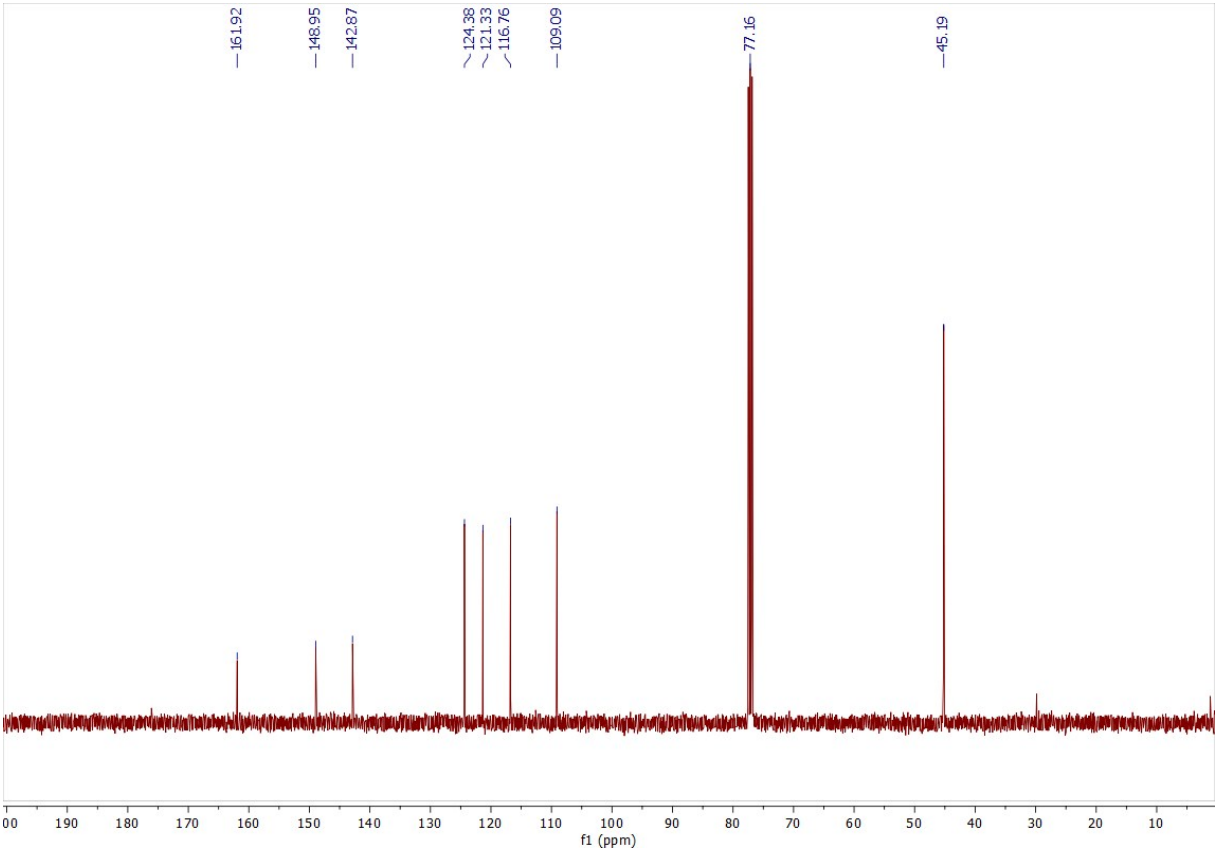
2-(4-methylpiperazin-1-yl)benzoxazole (3e)



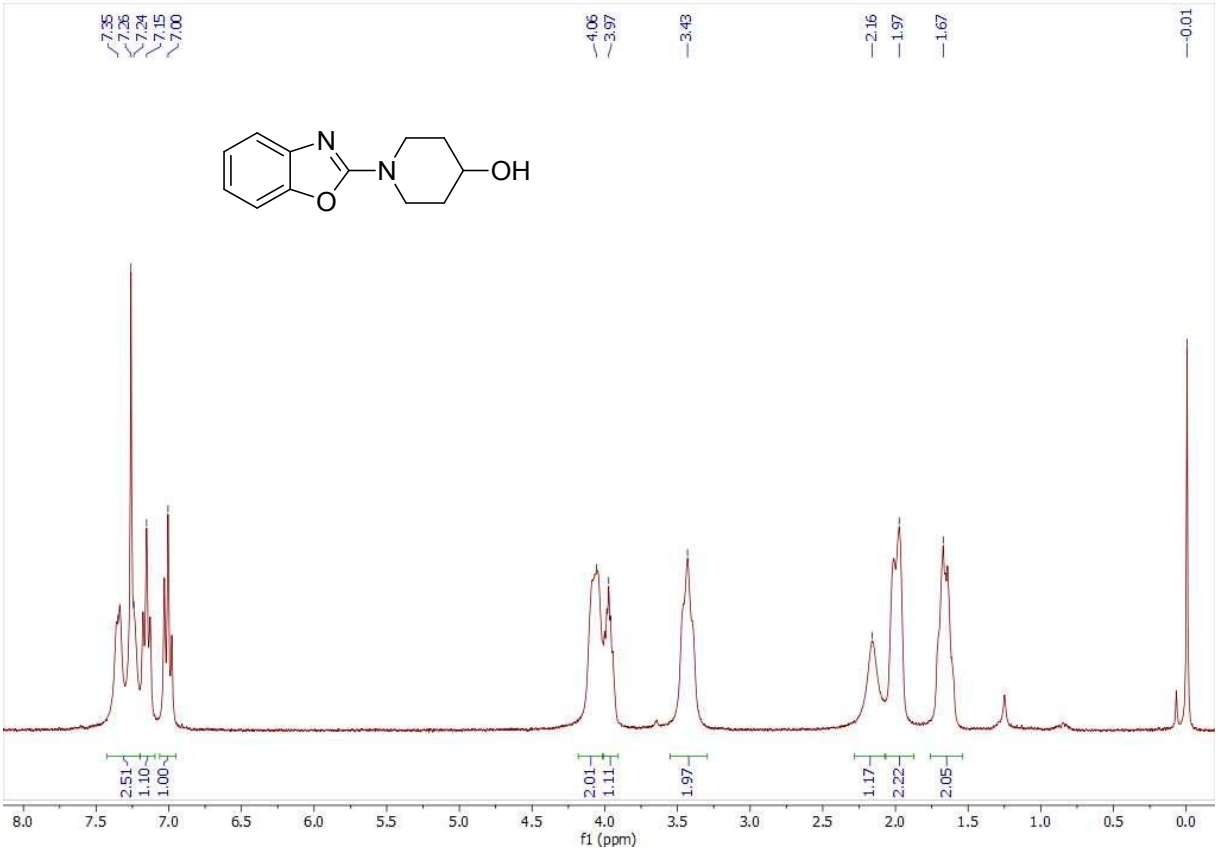


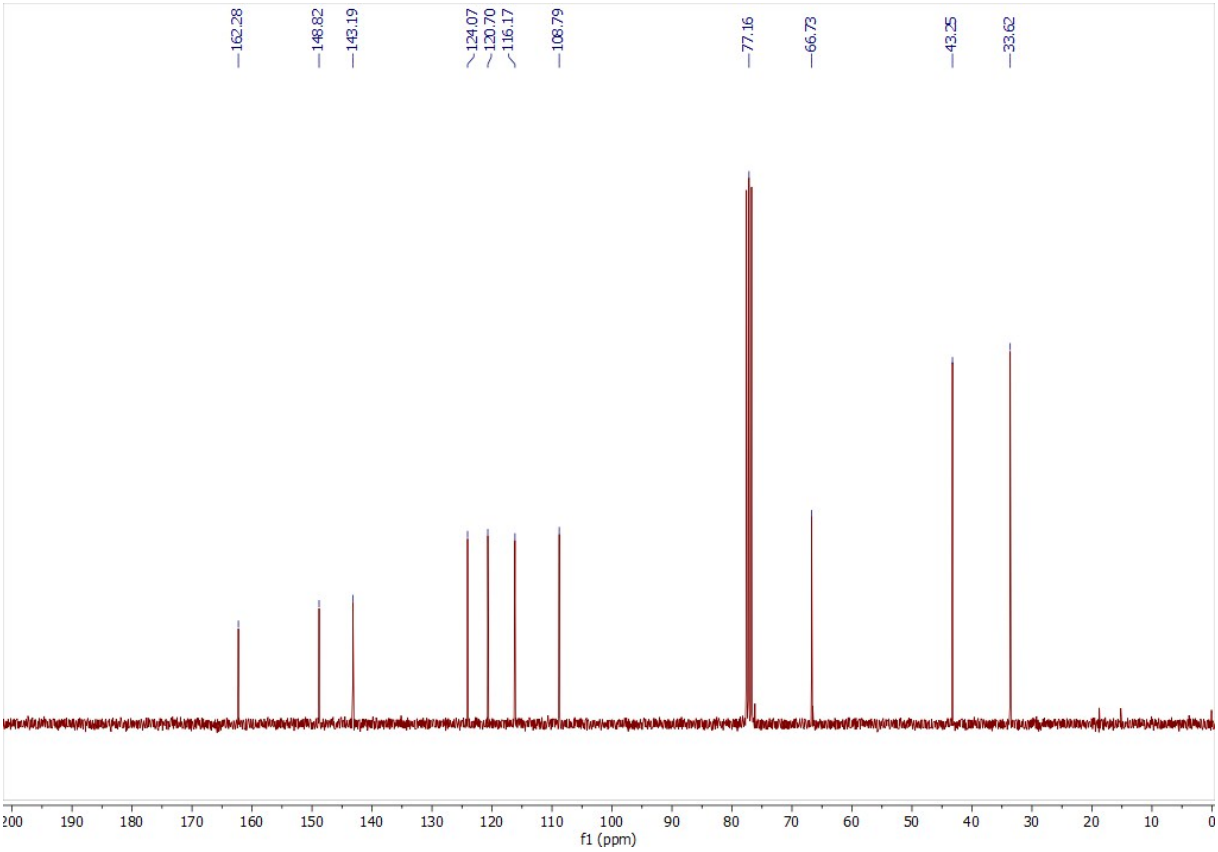
2,2’-(1,4-Piperazinediyl)-bis(benzoxazole) (3f)



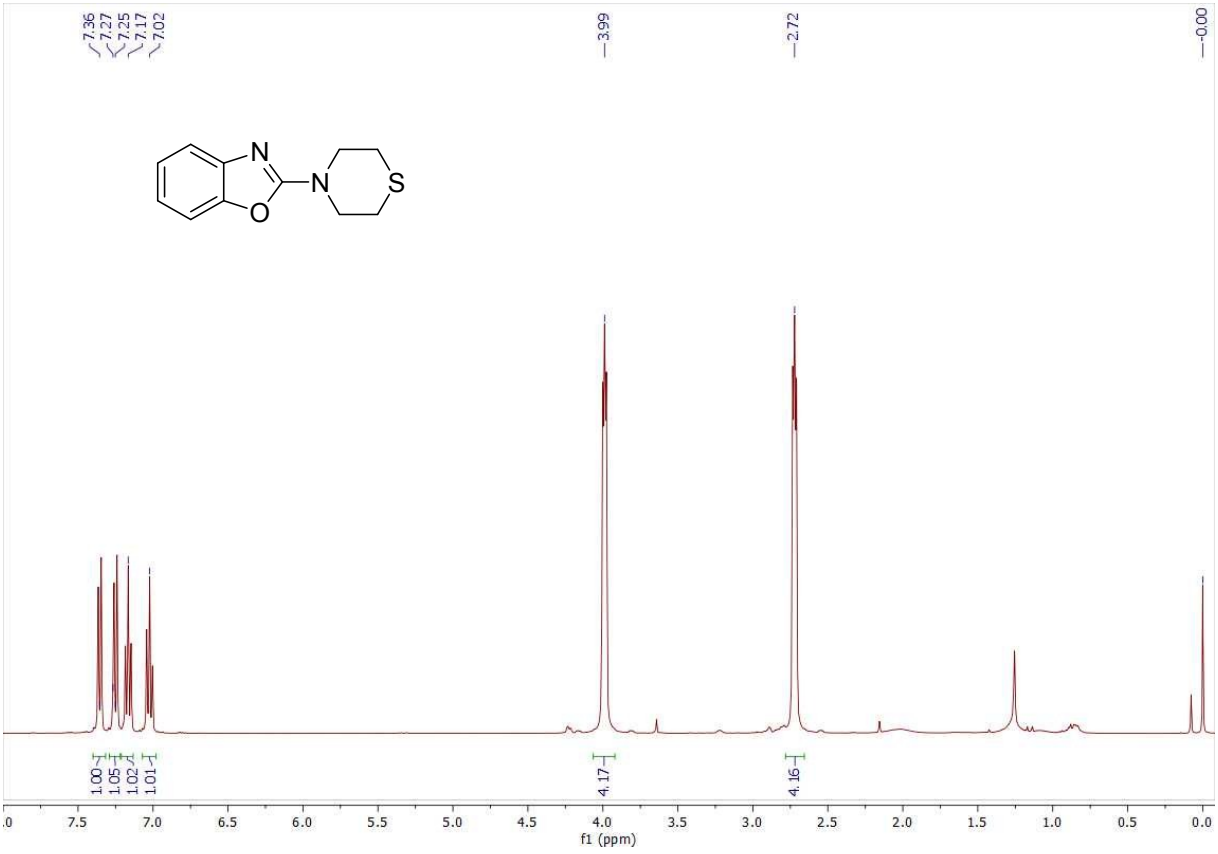


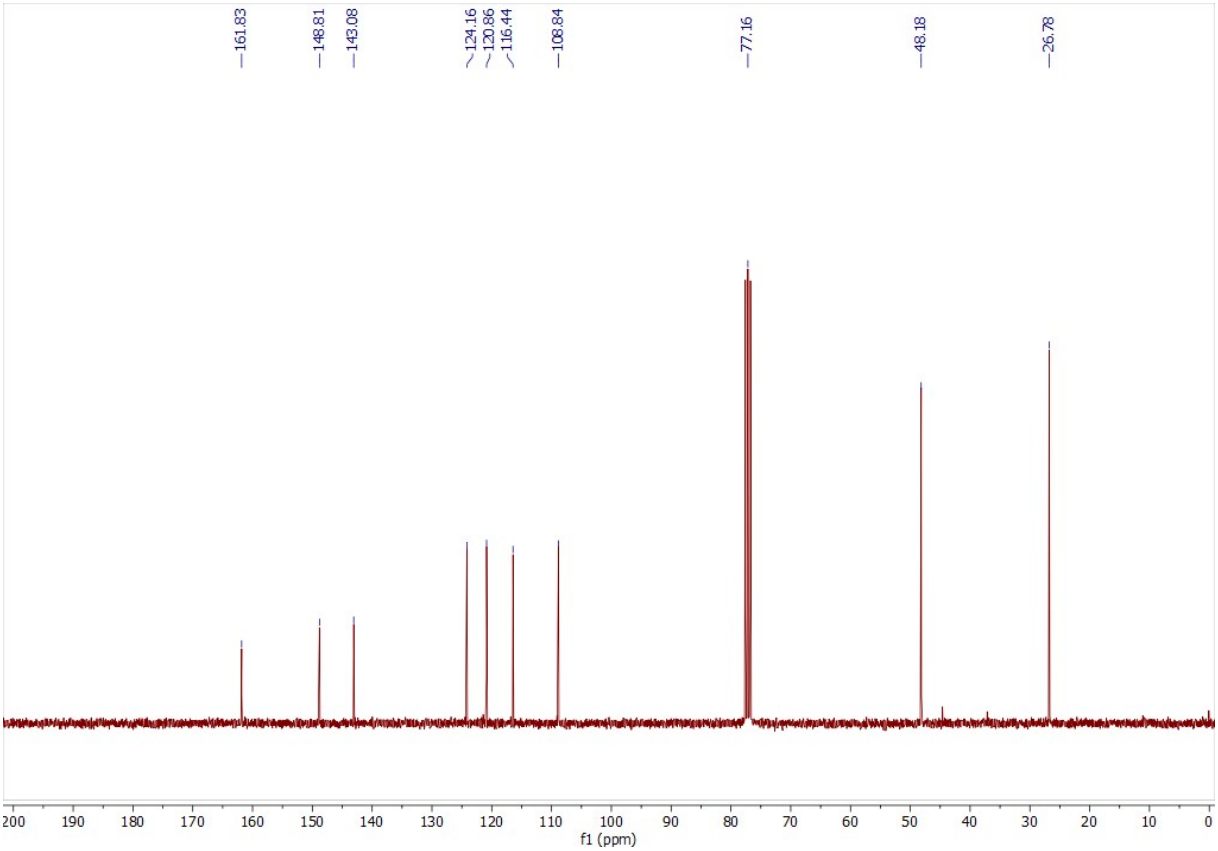
1-(Benzo[d]oxazol-2-yl)piperidin-4-ol (3g)



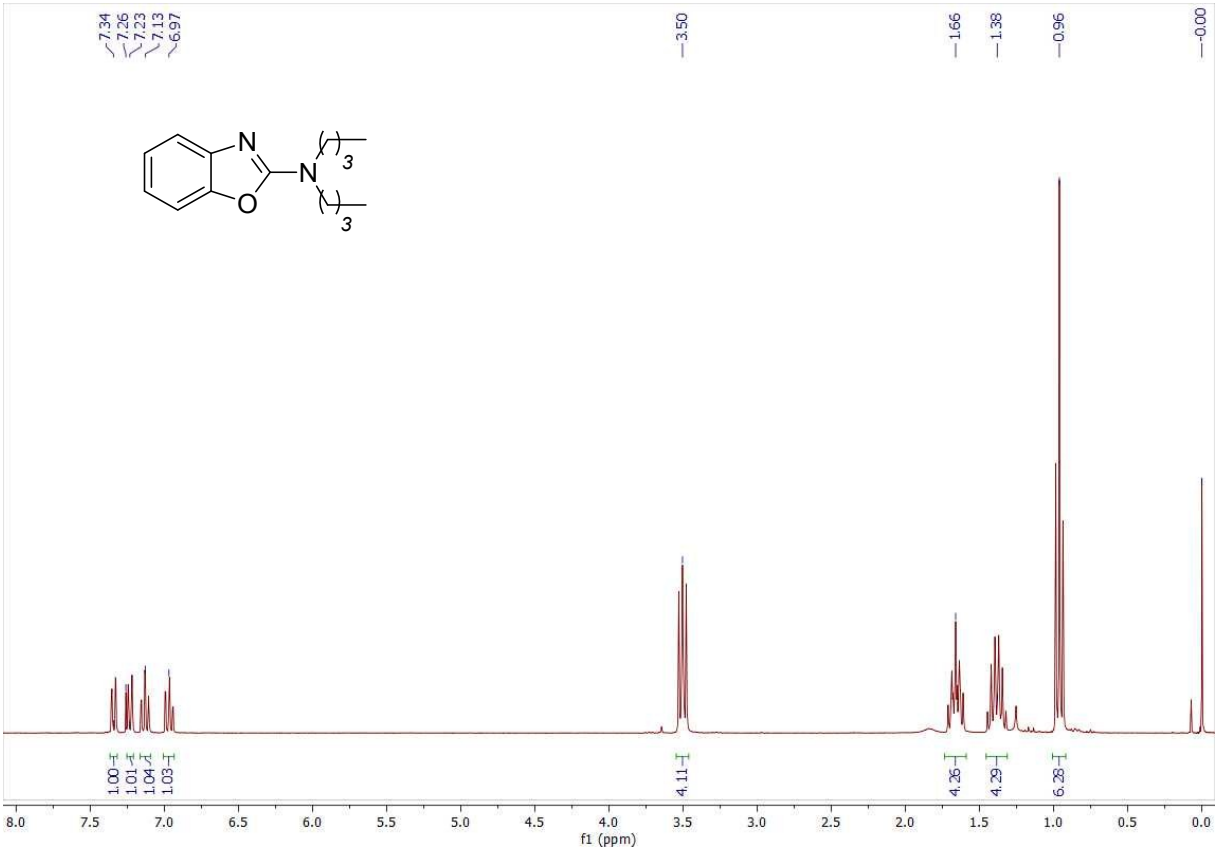


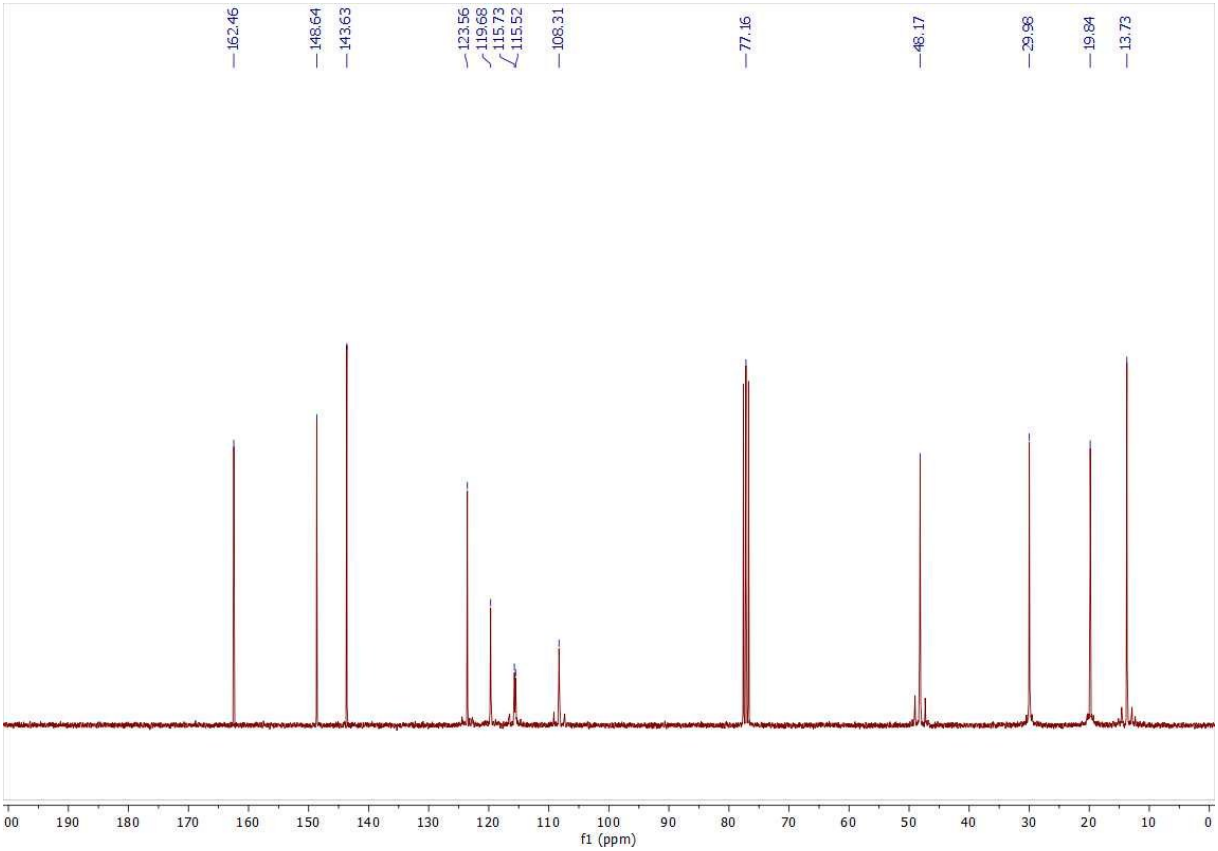
2-(4-Thiomorhophonyl)benzoxazole (3h)



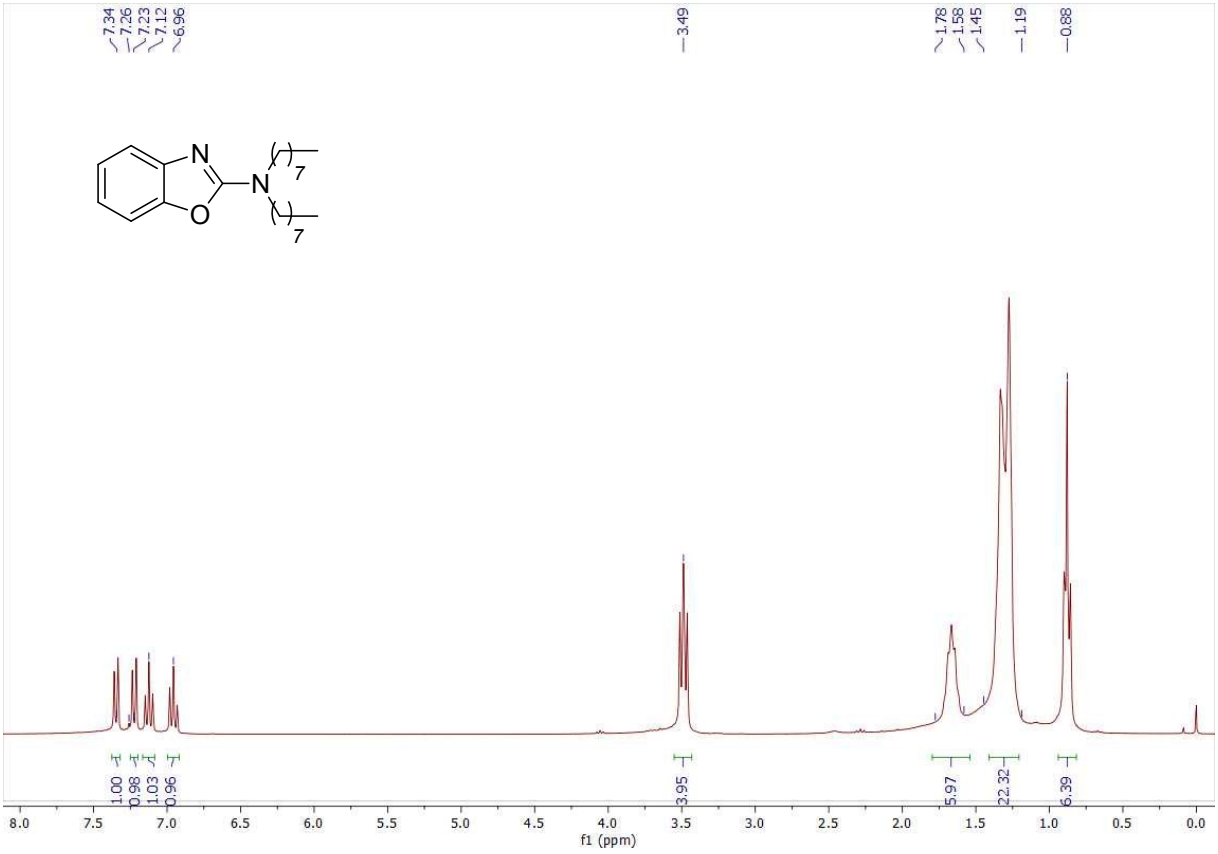


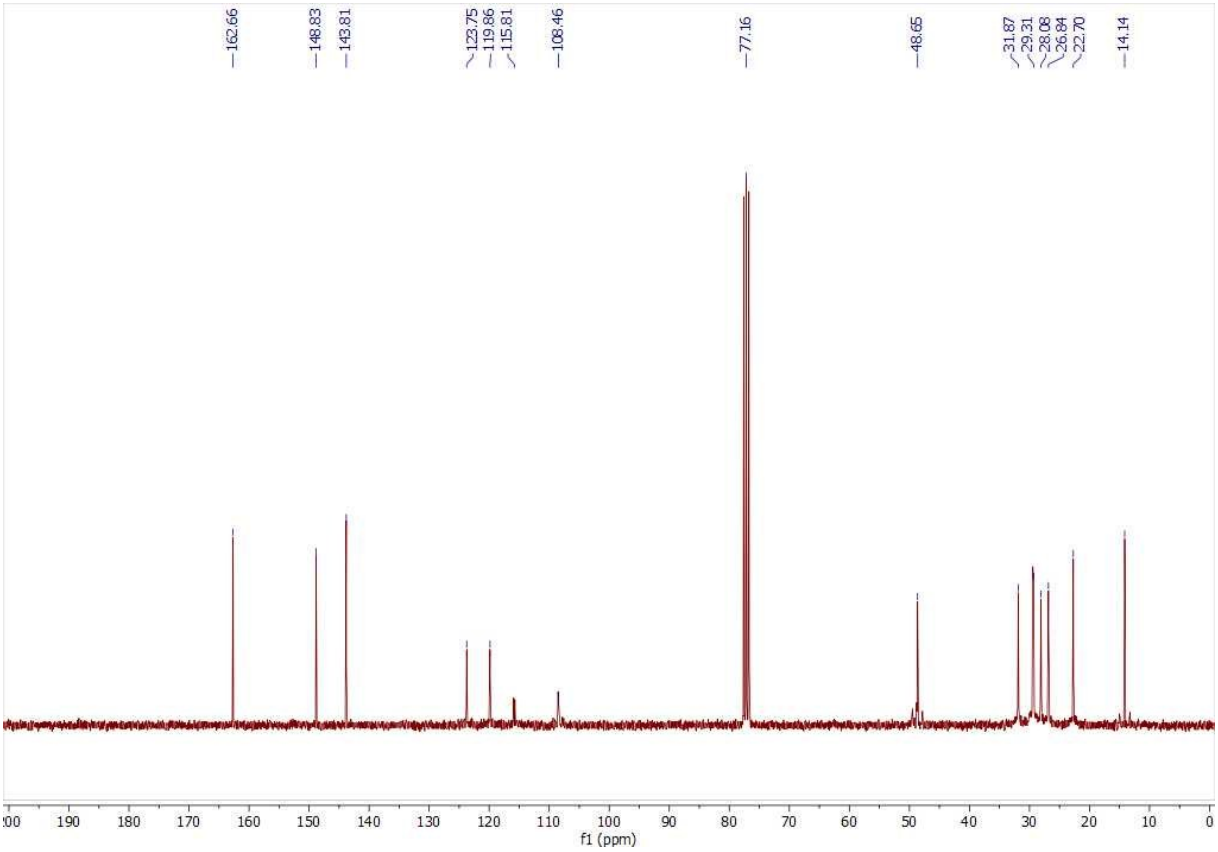
2-(*N*,*N*-Dibutyl)benzoxazole (3i)


7.34
7.26
7.23
7.13
6.97
3.50
1.66
1.38
0.96
0.00
N
N
O
3
3
1.00
1.01
1.04
1.03
4.11
4.26
4.29
6.28
f1 (ppm)

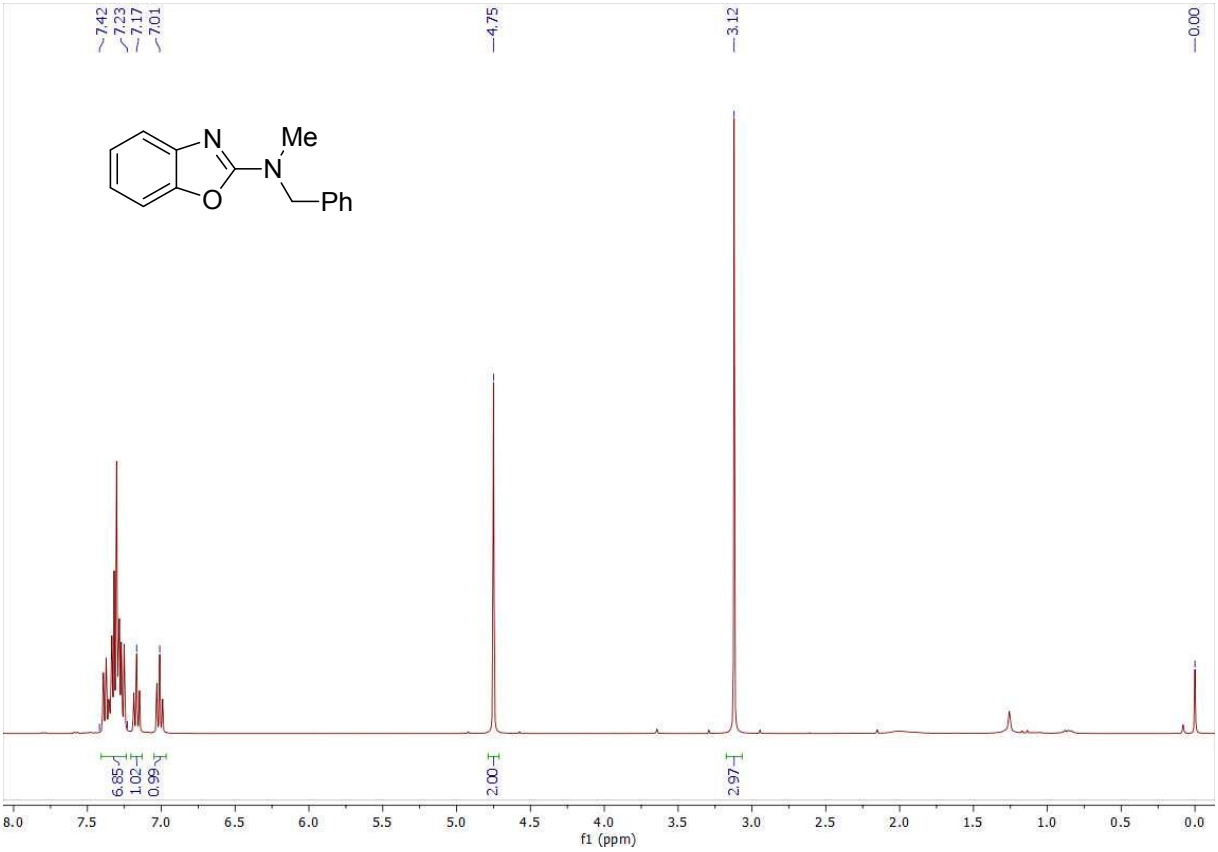

162.46
148.64
143.63
123.56
119.68
115.73
115.52
108.31
77.16
48.17
29.98
19.84
13.73
f1 (ppm)

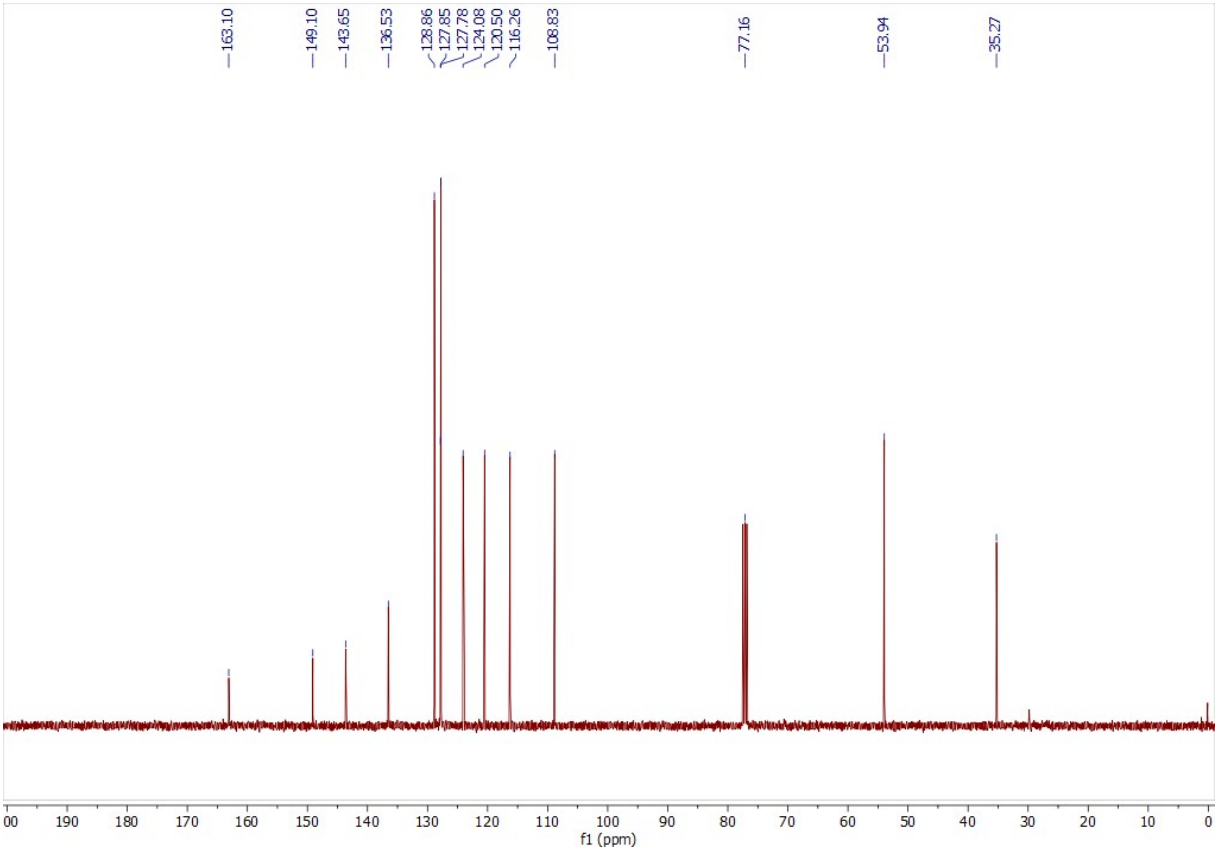
2-(*N*,*N*-Dioctyl)benzoxazole (3j)



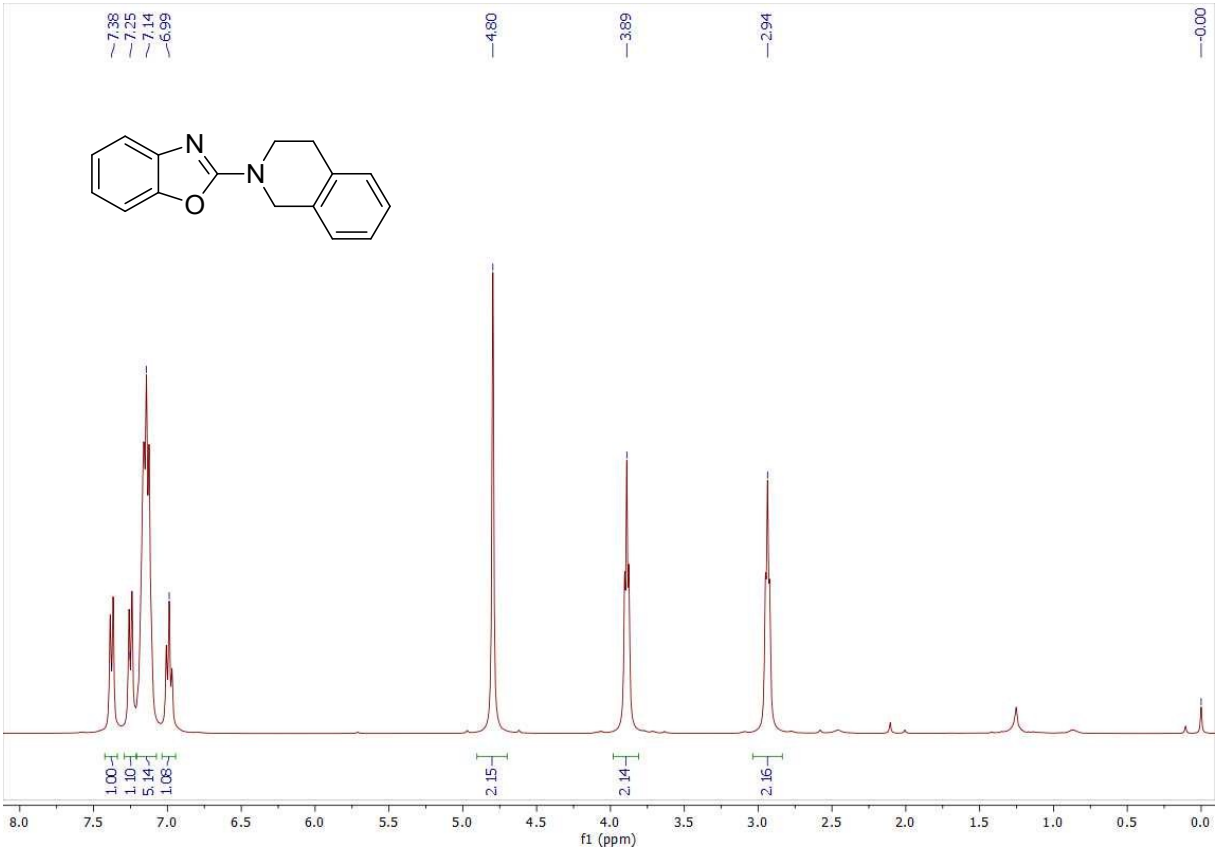


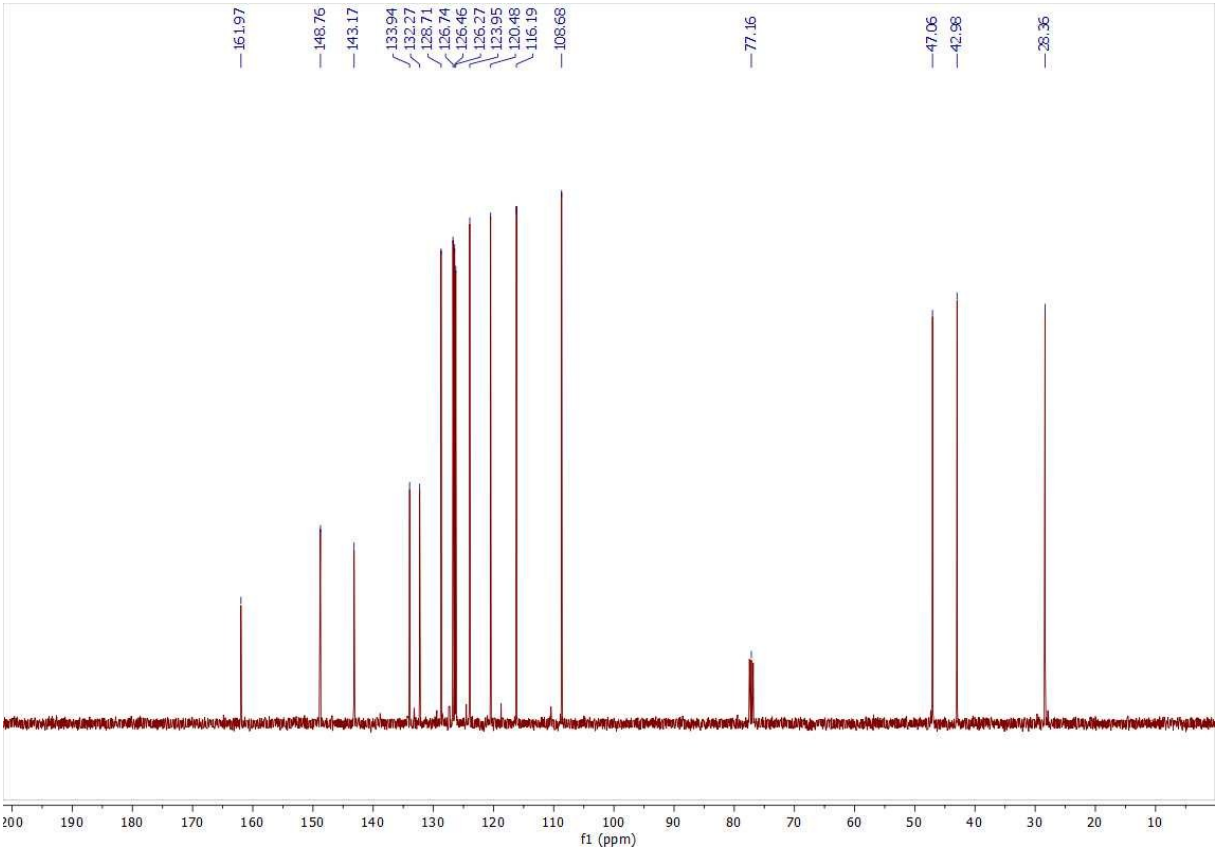
2-(*N*-Benzyl-*N*-methyl)benzoxazole (3k)



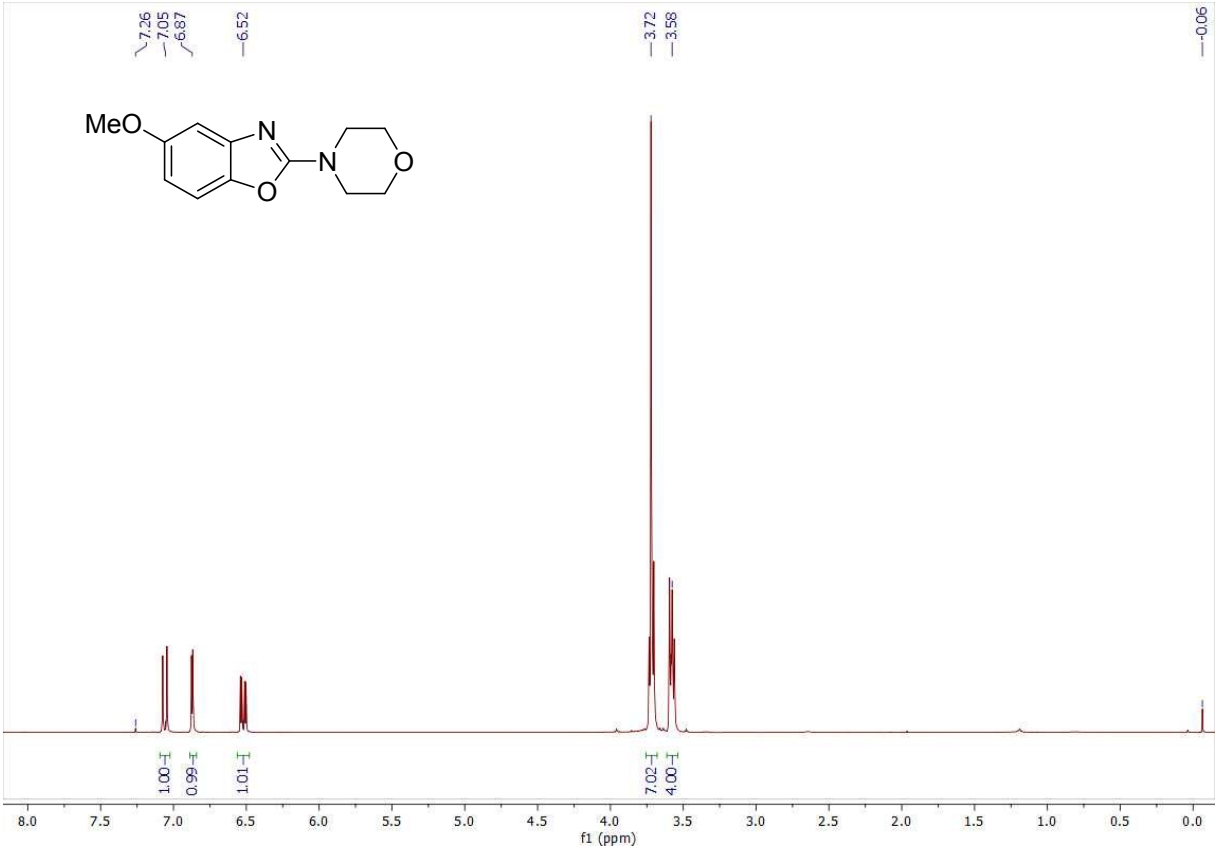


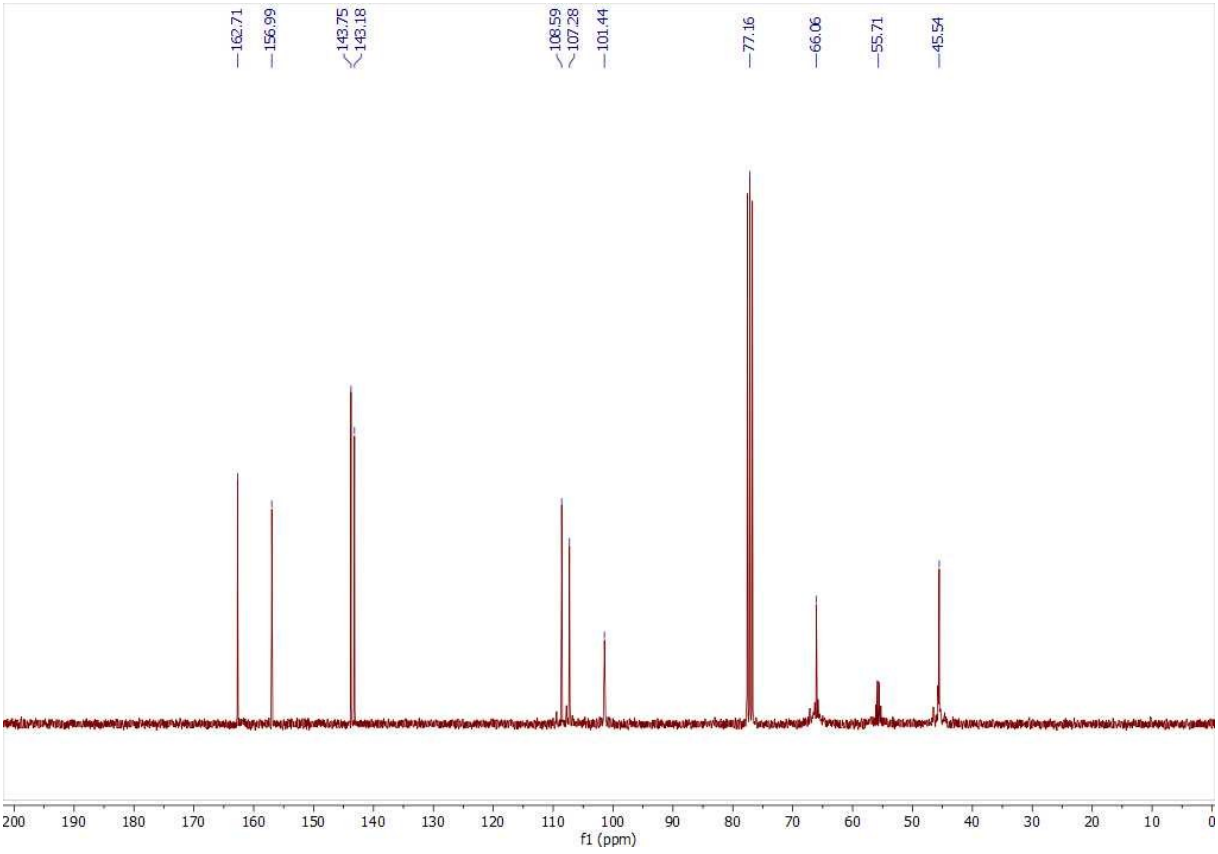
2-(3,4-Dihydroisoquinolin-2(1*H*)-yl)benzoxazole (3l)



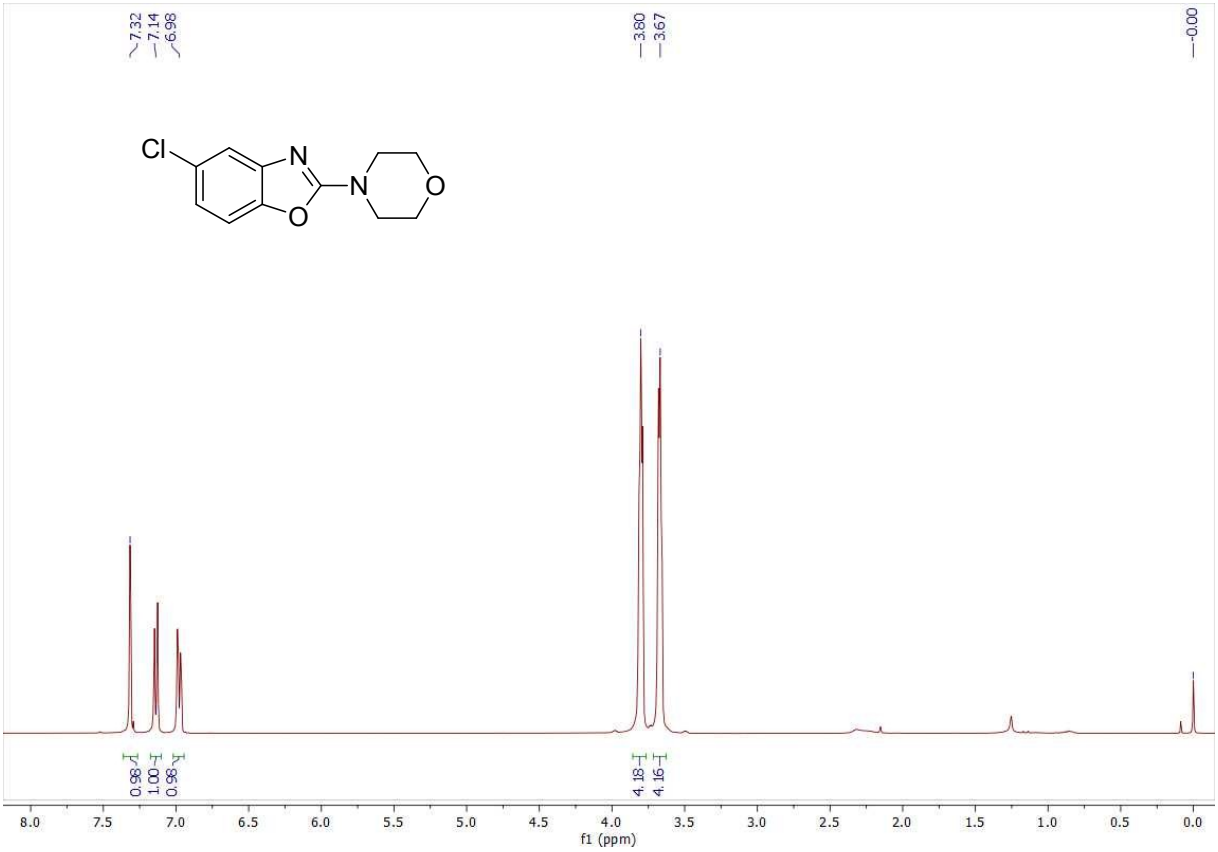


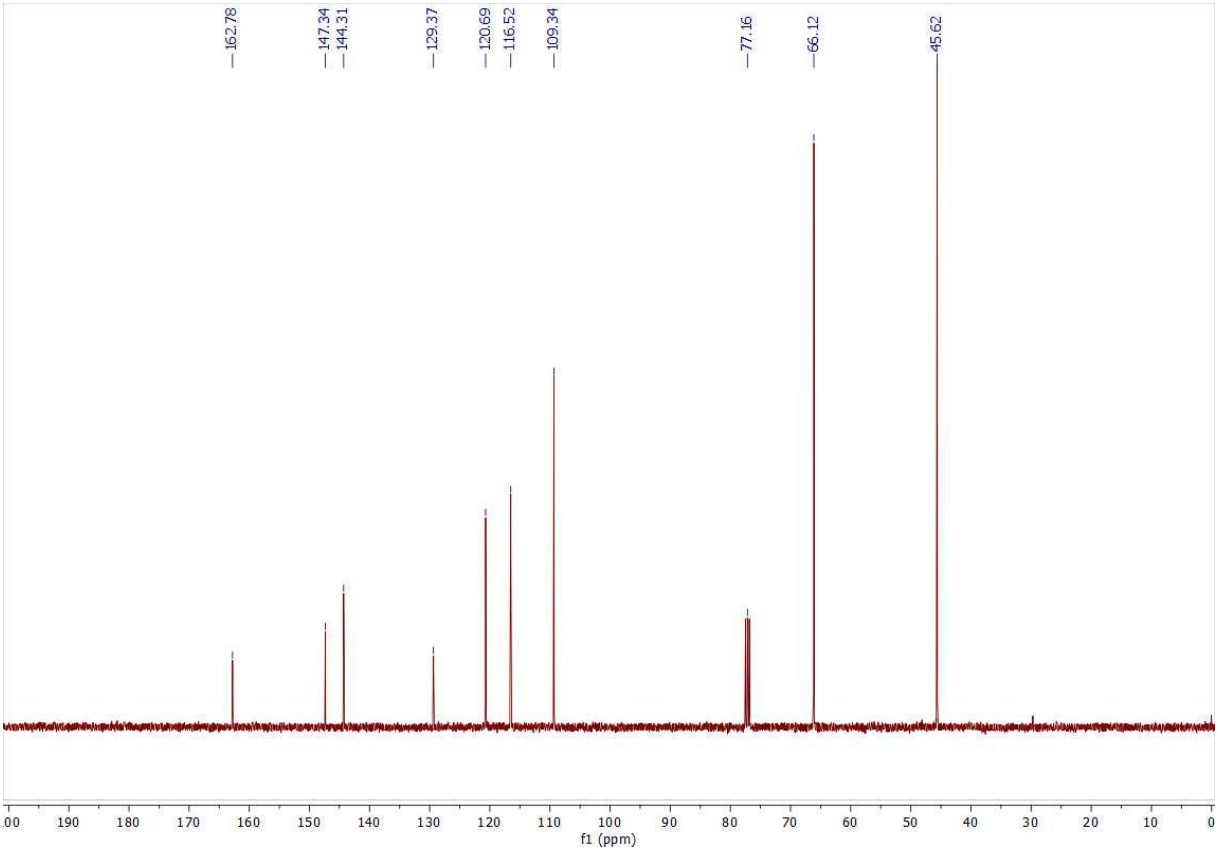
5-Methoxy-2-(morpholinyl)benzoxazole (3m)



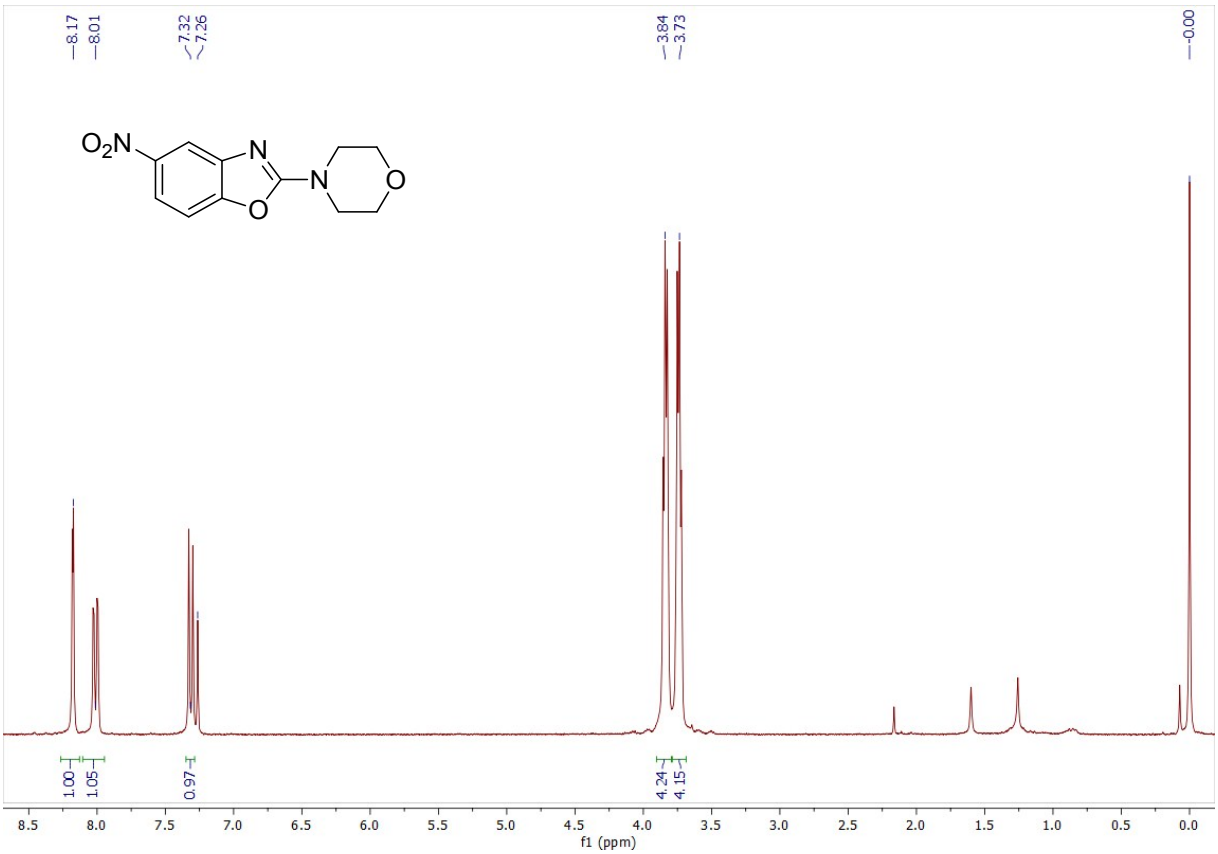


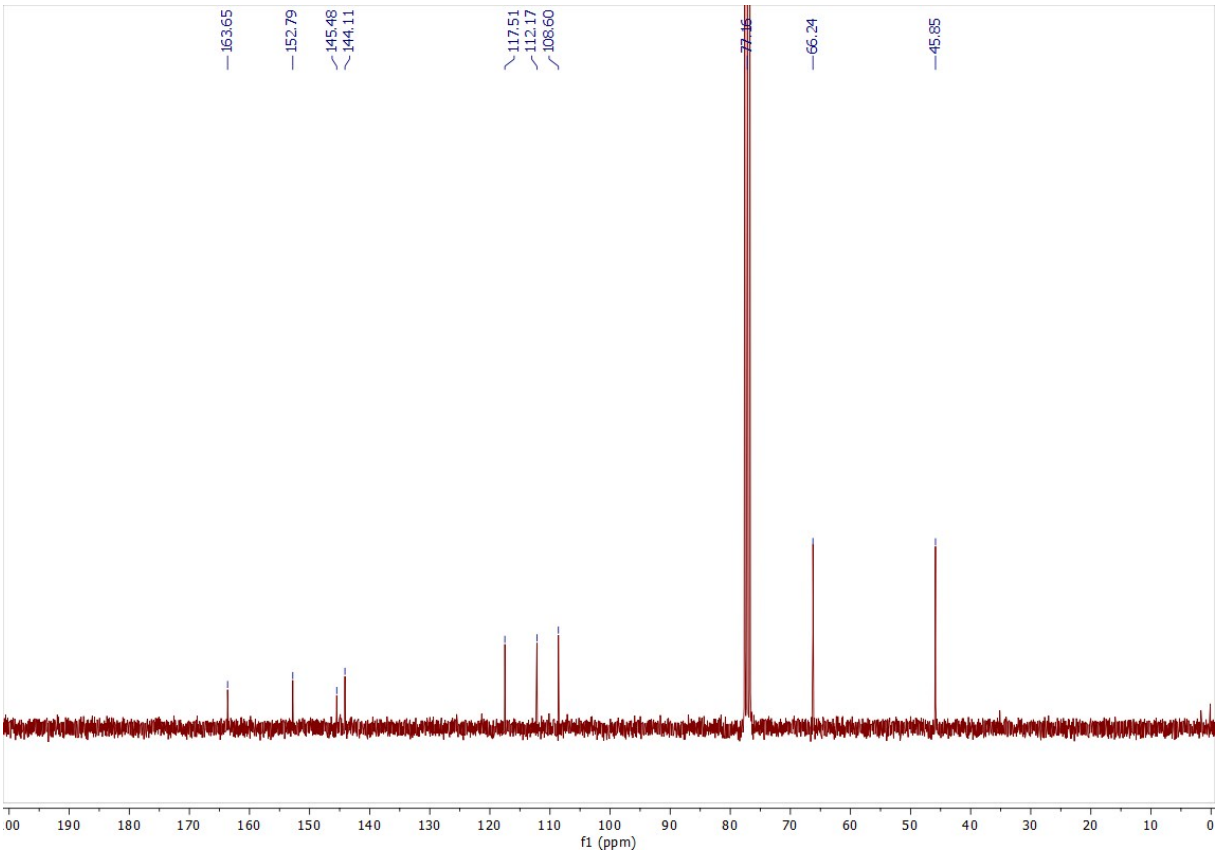
5-Chloro-2-(morpholinyl)benzoxazole (3n)



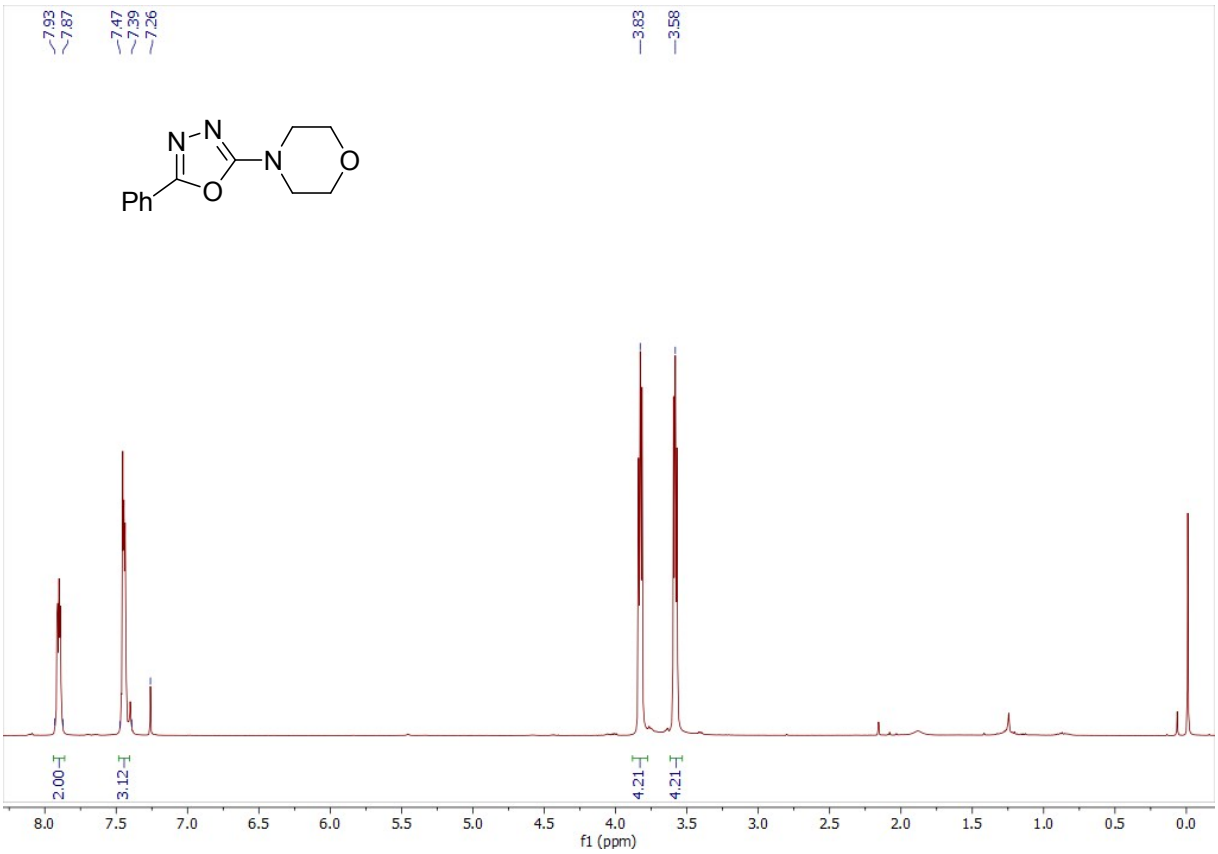


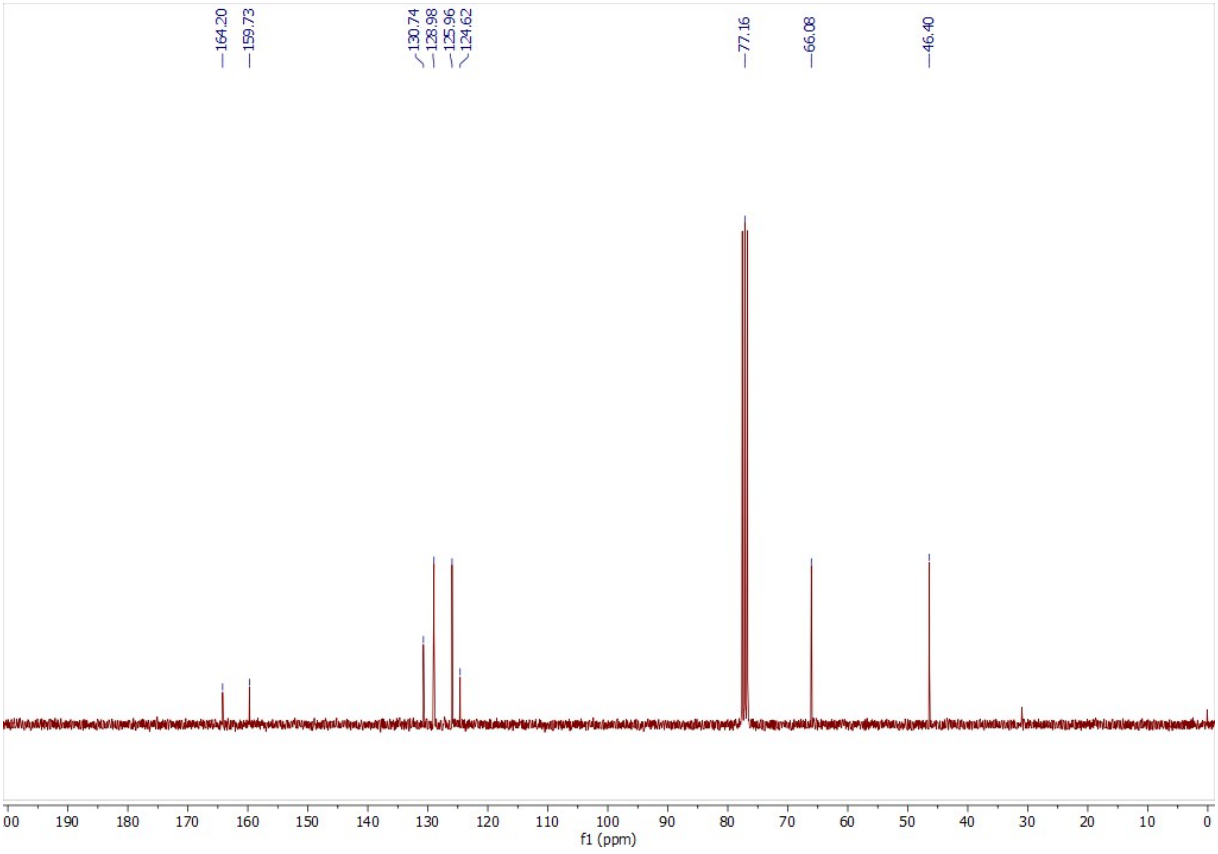
5-Nitro-2-(morpholinyl)benzoxazole (3o)



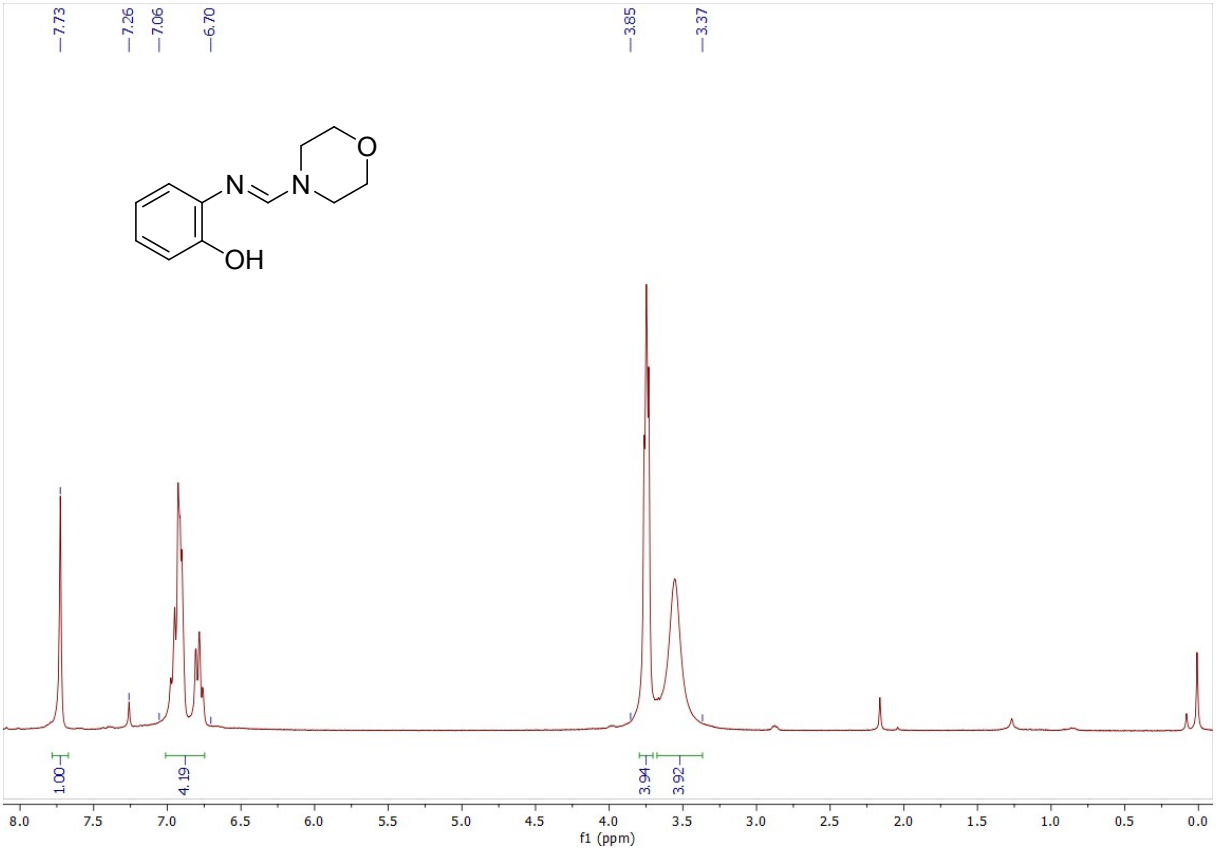


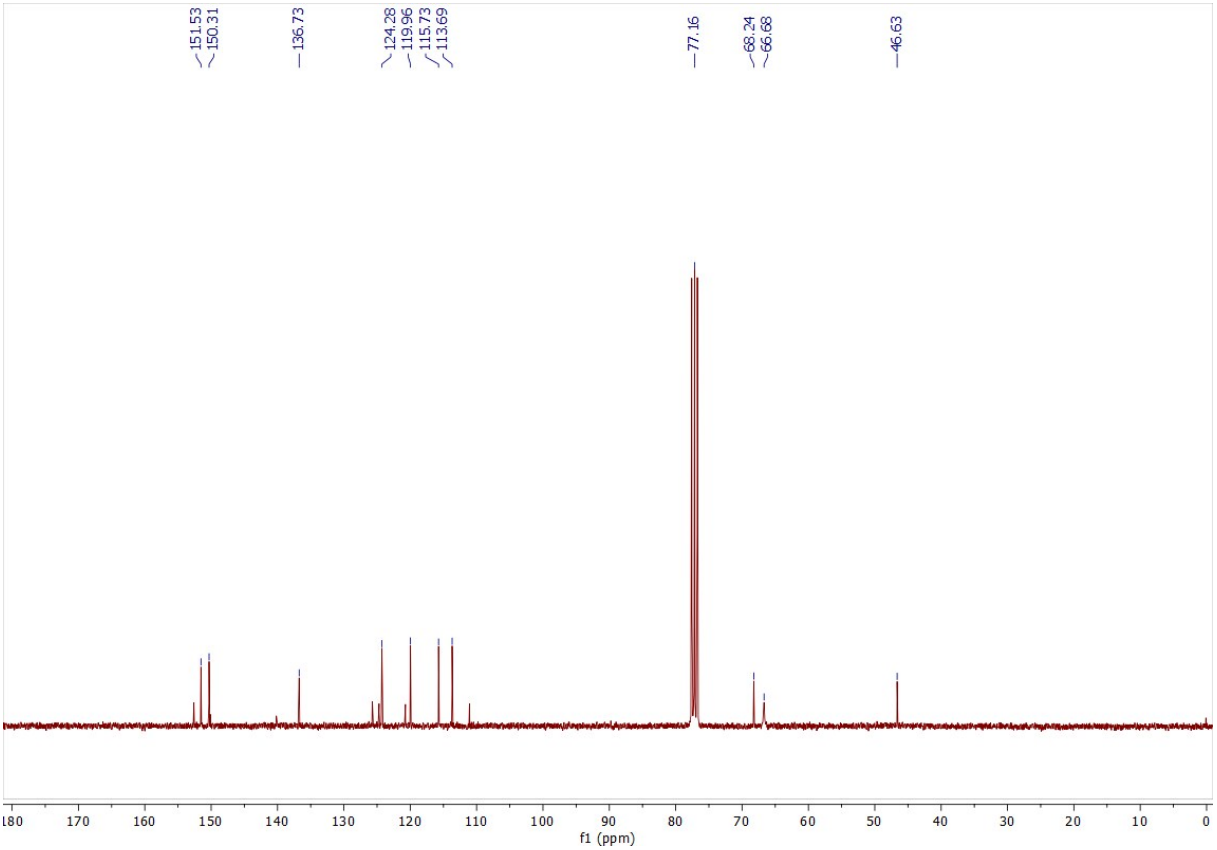
2-Phenyl-5-(morpholinyl)-1,3,4-oxadiazole (3p)





2-(4-morholonylmethyleneamino)phenol (4)





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