Supporting Information

Synthesis of Triarylmethanes by Palladium-Catalyzed C-H/C-O Coupling of Oxazoles and Diarylmethanol Derivatives

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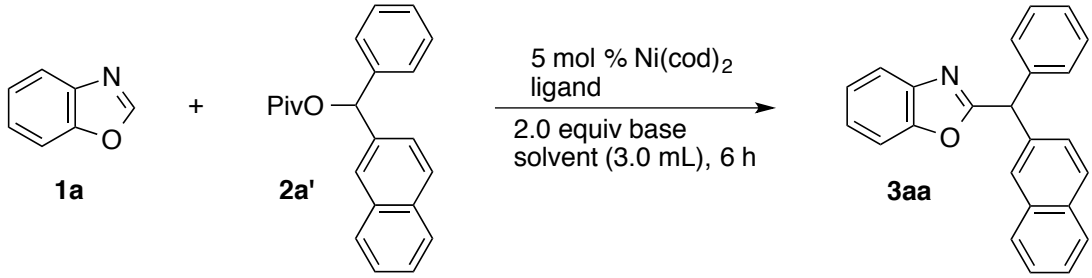
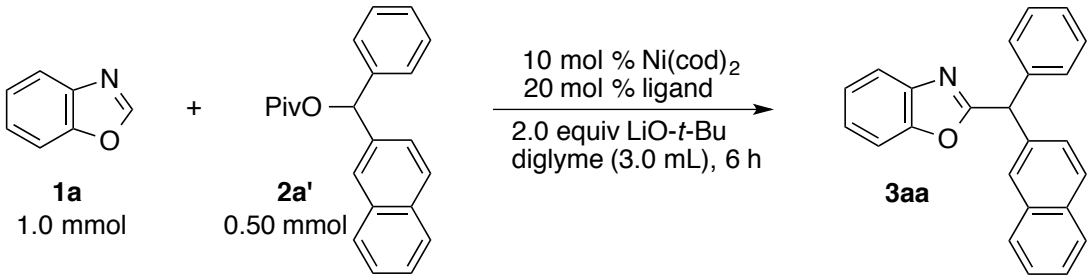
Detailed Optimization Studies for Nickel-Catalyzed C-H/C-O Coupling of 1a with Diarylmethanol Derivatives

Table S1. Optimization Studies for Nickel-Catalyzed C-H/C-O Coupling of **1a** and **2** (1)



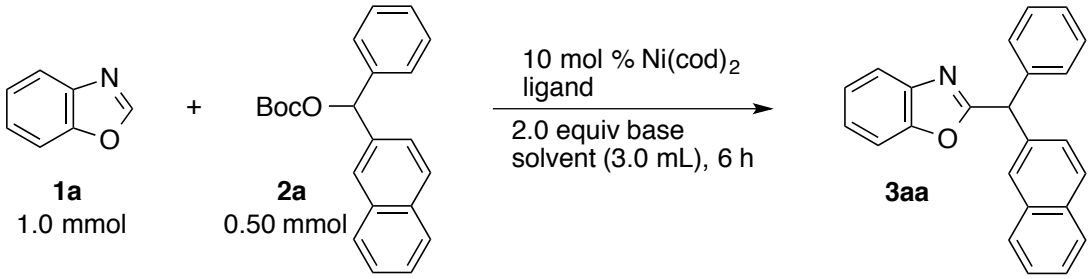
entry	**1a** (mmol)	**2a'** (mmol)	base	solvent	ligand (mol %)	temp (˚C)	yield (%)
1	0.50	0.60	Na_2CO_3	toluene	-	100	0
2	0.50	0.60	K_3PO_4	1,4-dioxane	-	100	0
3	0.50	0.60	Cs_2CO_3	1,4-dioxane	-	100	0
4	0.50	0.60	LiO-*t*-Bu	1,4-dioxane	PCy_3 (10)	100	0
5	0.50	0.60	LiO-*t*-Bu	diglyme	PCy_3 (10)	140	0
6	0.50	0.60	LiO-*t*-Bu	*o*-xylene	PCy_3 (10)	140	0
7	0.50	0.60	LiO-*t*-Bu	DMF	PCy_3 (10)	140	0
8	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	-	100	0
9	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	PCy_3 (10)	100	0
10	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	dppf (5)	100	0
11	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	binap (5)	100	0
12	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	Xantphos (5)	100	0
13	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	IPr•HCl (10)	100	0
14	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	IMes•HCl (10)	100	0
15	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	DPEphos (5)	100	0
16	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	dppe (5)	100	0
17	1.0	0.50	LiO-*t*-Bu	1,4-dioxane	$PCy_2(CH_2)_2PCy_2$(5)	100	0
18	1.0	0.50	NaO-*t*-Bu	*o*-xylene	PCy_3 (10)	100	0
19	1.0	0.50	K_3PO_4	diglyme	PCy_3 (10)	140	0

Table S2. Optimization Studies for Nickel-Catalyzed C-H/C-O Coupling of **1a** and **2** (2)



entry	ligand (mol %)	yield (%)
1	PCy_3 (20)	0
2	Cy-JohnPhos (20)	1
3	DavePhos (20)	0
4	RuPhos (20)	0
5	SPhos (20)	0
6	XPhos (20)	trace
7	JohnPhos (20)	2
8	SIMes•HBF_4 (20)	0
9	PPh_2Cy (20)	0
10	$PPhCy_2$ (20)	0

Table S3. Optimization Studies for Nickel-Catalyzed C-H/C-O Coupling of **1a** and **2** (3)



entry	base	solvent	ligand (mol %)	temp (˚C)	yield (%)
1	LiO-*t*-Bu	diglyme	PCy_3 (20)	140	2
2	LiO-*t*-Bu	diglyme	JohnPhos (20)	140	4
3	LiO-*t*-Bu	diglyme	Cy-JohnPhos (20)	140	5
4	LiO-*t*-Bu	diglyme	DavePhos (20)	140	10
5	LiO-*t*-Bu	diglyme	RuPhos (20)	140	12

6	LiO-*t*-Bu	diglyme	XPhos (20)	140	8
7	LiO-*t*-Bu	diglyme	SPhos (20)	140	7
8	LiO-*t*-Bu	diglyme	IPr•HCl (20)	140	0
9	LiO-*t*-Bu	diglyme	IMes•HCl (20)	140	trace
10	LiO-*t*-Bu	diglyme	DPEphos (10)	140	0
11	LiO-*t*-Bu	diglyme	phen (10)	140	2
12	LiO-*t*-Bu	diglyme	bpy (10)	140	3
13	K_2CO_3	diglyme	RuPhos (20)	140	0
14	K_3PO_4	diglyme	RuPhos (20)	140	0
15	NaO-*t*-Bu	diglyme	RuPhos (20)	140	0
16	KO-*t*-Bu	diglyme	RuPhos (20)	140	0
17	Mg(O-*t*-Bu)$_2$	diglyme	RuPhos (20)	140	0
18	Mg(O-*t*-Bu)$_2$	DMF	RuPhos (20)	140	5
19[a]	LiO-*t*-Bu	diglyme	RuPhos (20)	140	5
20[b]	LiO-*t*-Bu	diglyme	RuPhos (20)	140	3
21	LiO-*t*-Bu	*o*-xylene	RuPhos (20)	140	3
22	LiO-*t*-Bu	DMSO	RuPhos (20)	140	trace
23	LiO-*t*-Bu	toluene	RuPhos (20)	100	3
24	LiO-*t*-Bu	DMF	RuPhos (20)	140	4
25	LiO-*t*-Bu	1,4-dioxane	RuPhos (20)	100	2
26	LiO-*t*-Bu	CH_3CN	RuPhos (20)	80	trace
27	LiO-*t*-Bu	Et_2O	RuPhos (20)	40	0
28	LiO-*t*-Bu	$ClCH_2CH_2Cl$	RuPhos (20)	80	0
29	LiO-*t*-Bu	DME	RuPhos (20)	80	0
30	LiO-*t*-Bu	CPME	RuPhos (20)	100	2
31	LiO-*t*-Bu	DMAc	RuPhos (20)	160	trace
32	LiO-*t*-Bu	NMP	RuPhos (20)	160	2
33	LiO-*t*-Bu	DMI	RuPhos (20)	160	trace
34	LiO-*t*-Bu	triglyme	RuPhos (20)	160	trace

[a] With 1.5 mmol of LiO-*t*-Bu. [b] With 2.0 mmol of LiO-*t*-Bu.

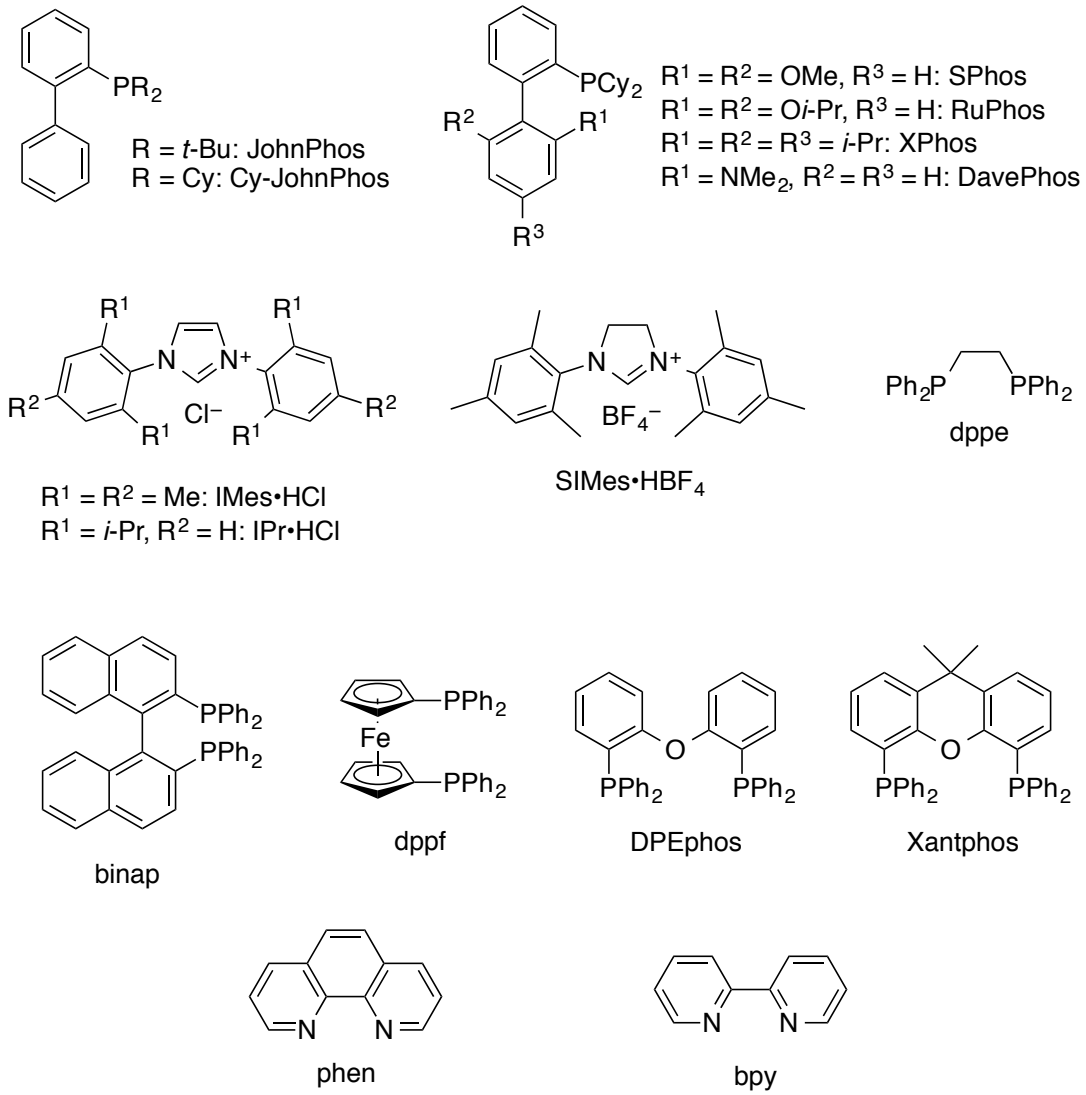
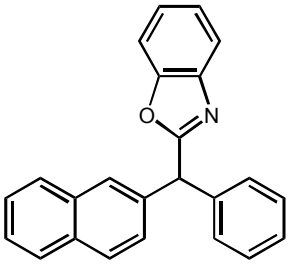
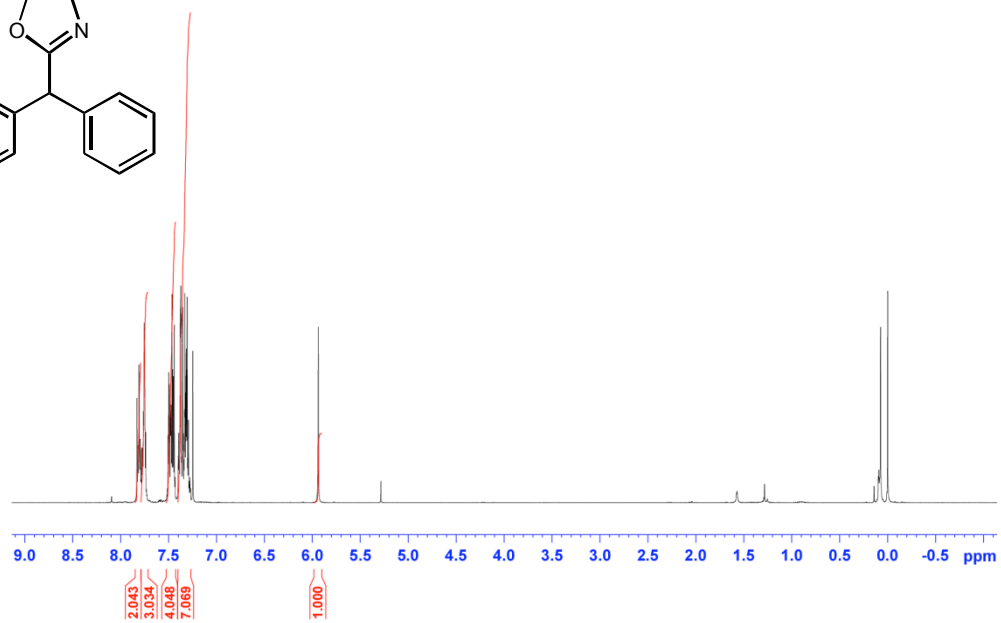
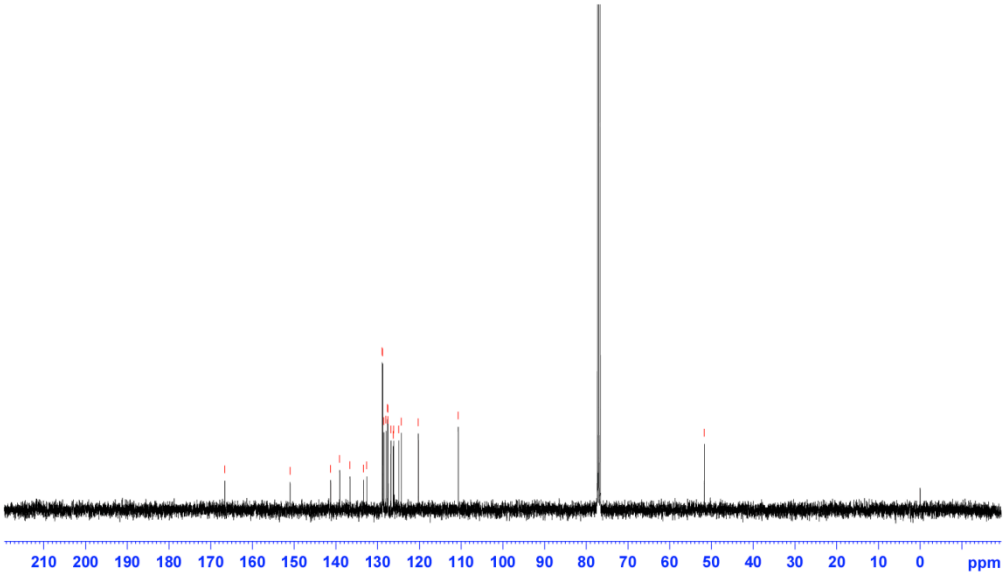


Figure S1. Structures of Ligands Employed in Optimization Studies for Nickel-Catalyzed C-H/C-O Coupling of **1a** and **2**

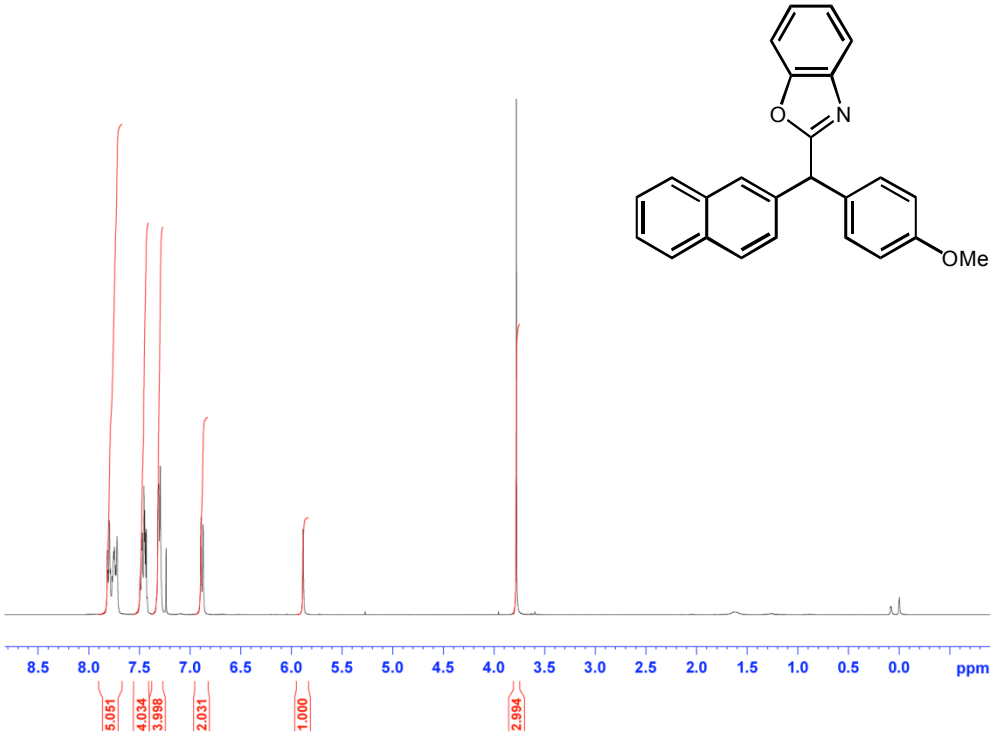
2-(Naphthalen-2-yl(phenyl)methyl)benzo[*d*]oxazole (3aa)

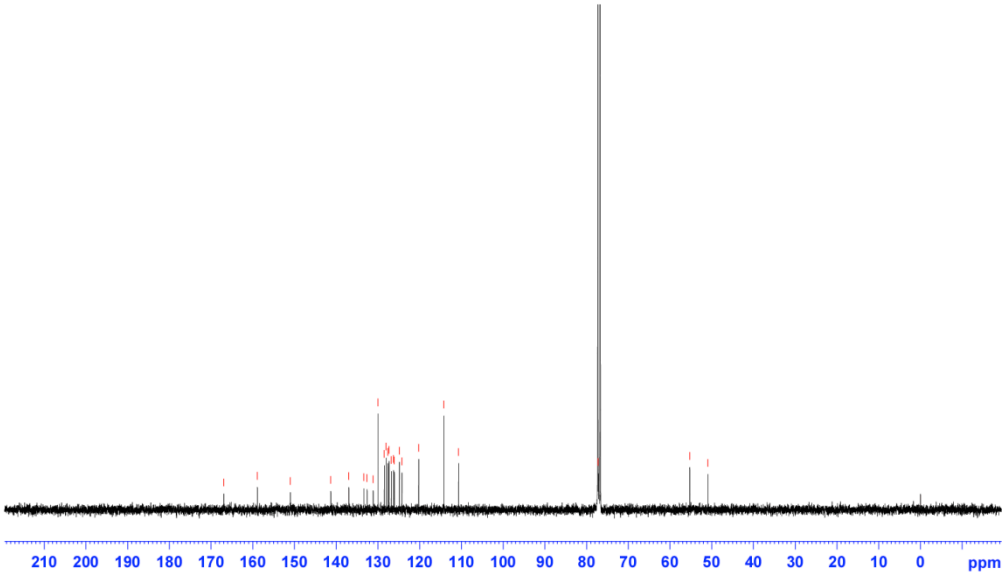




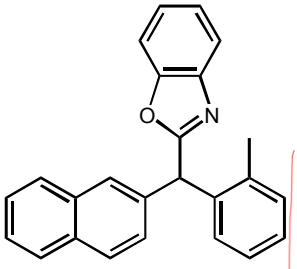


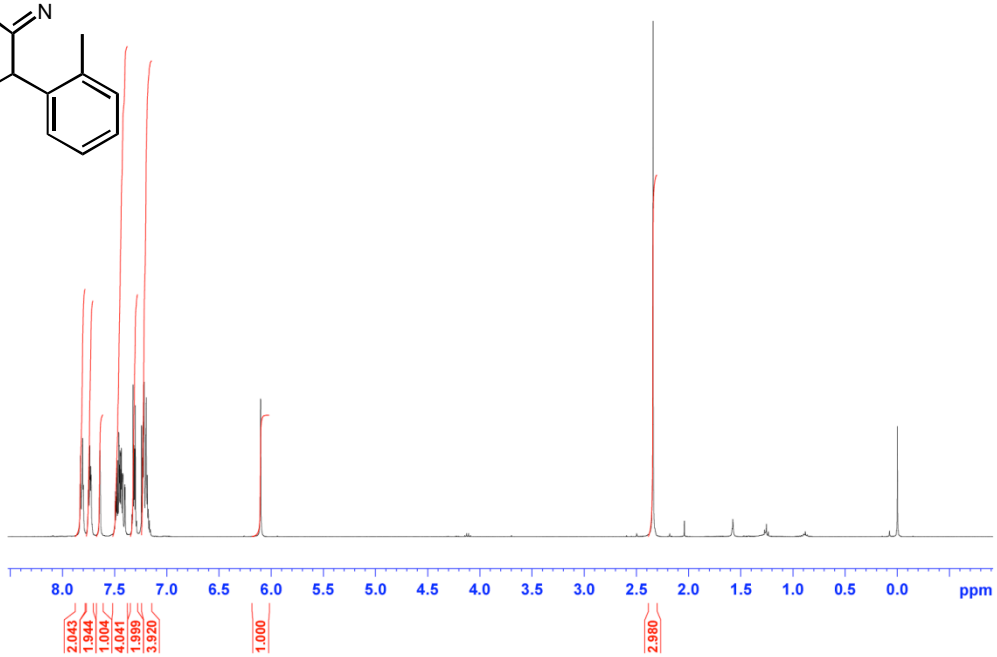
2-[(4-Methoxyphenyl)(naphthalen-2-yl)methyl]benzo[*d*]oxazole (3ab)

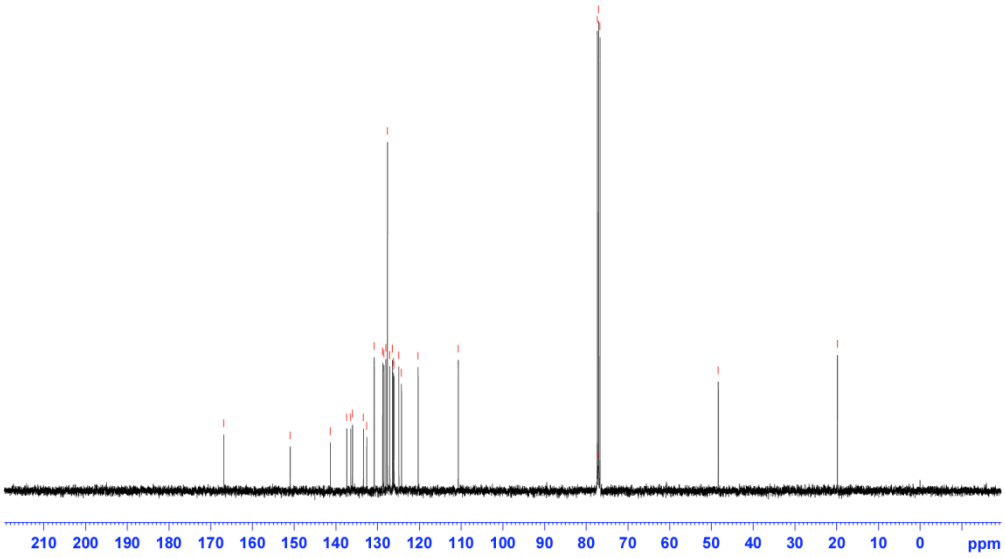




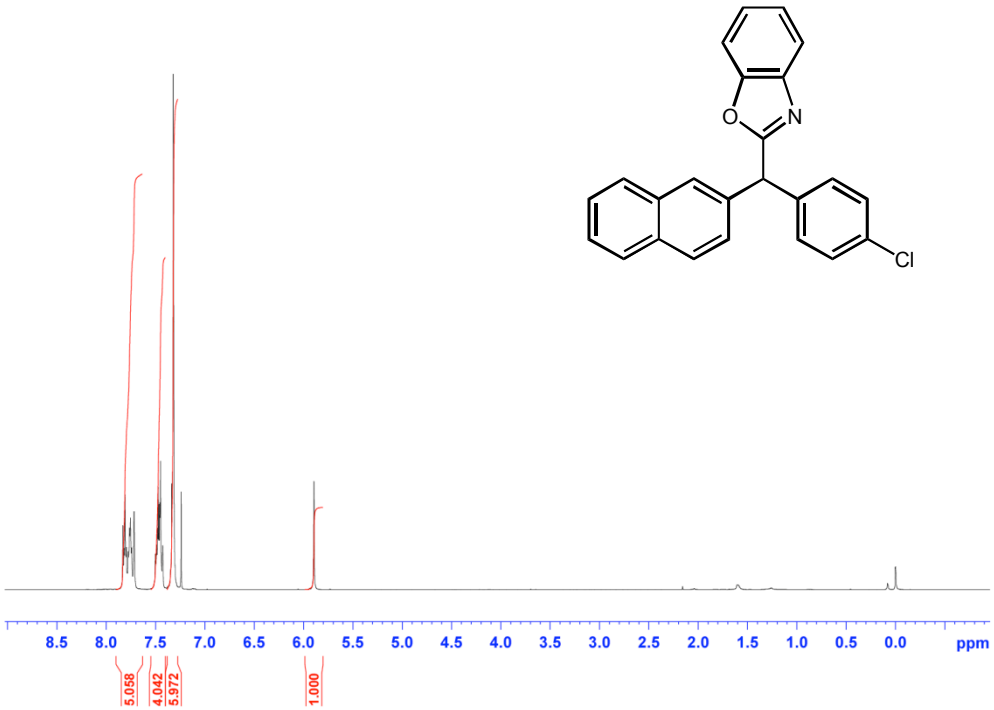
2-[Naphthalen-2-yl(2-methylphenyl)methyl]benzo[*d*]oxazole (3ac)

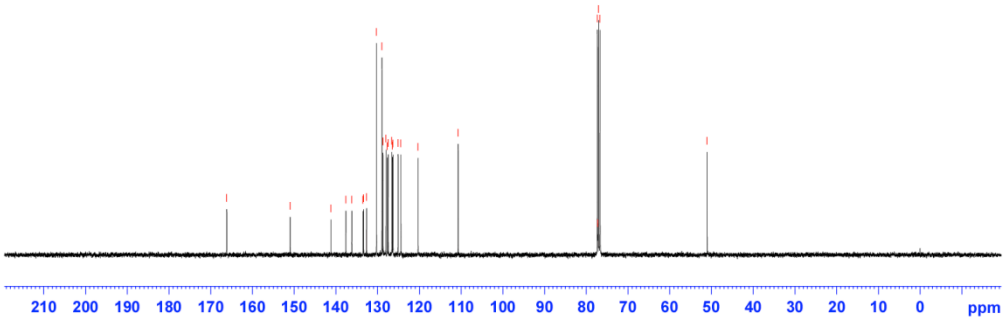






2-[(4-Chlorophenyl)(naphthalen-2-yl)methyl]benzo[*d*]oxazole (3ad)





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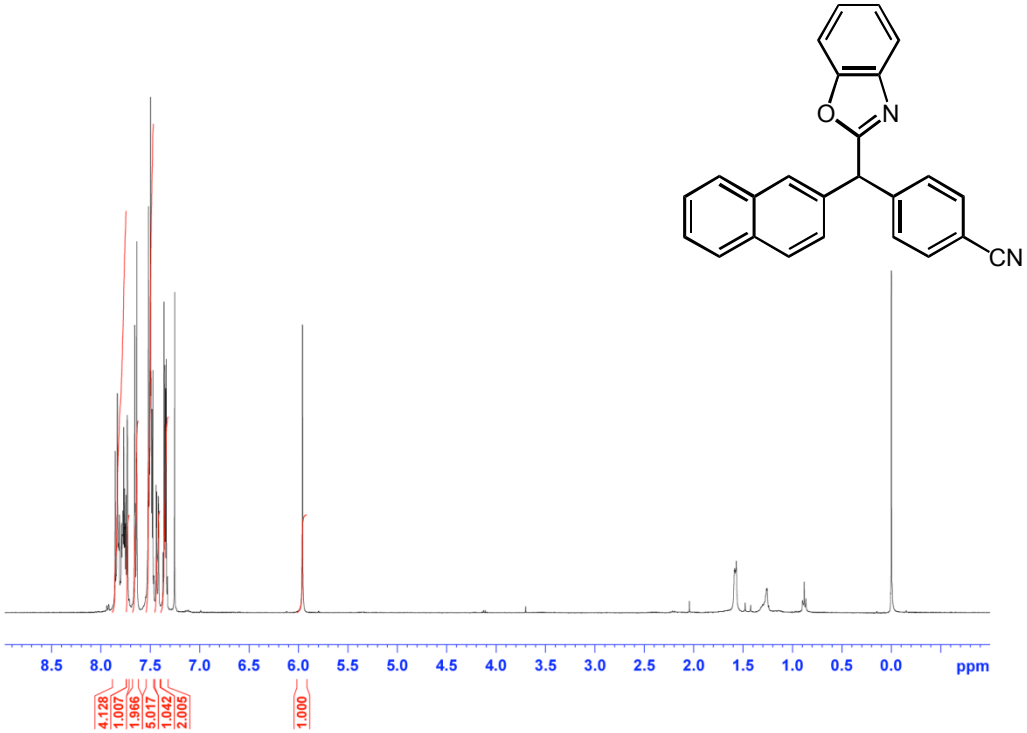

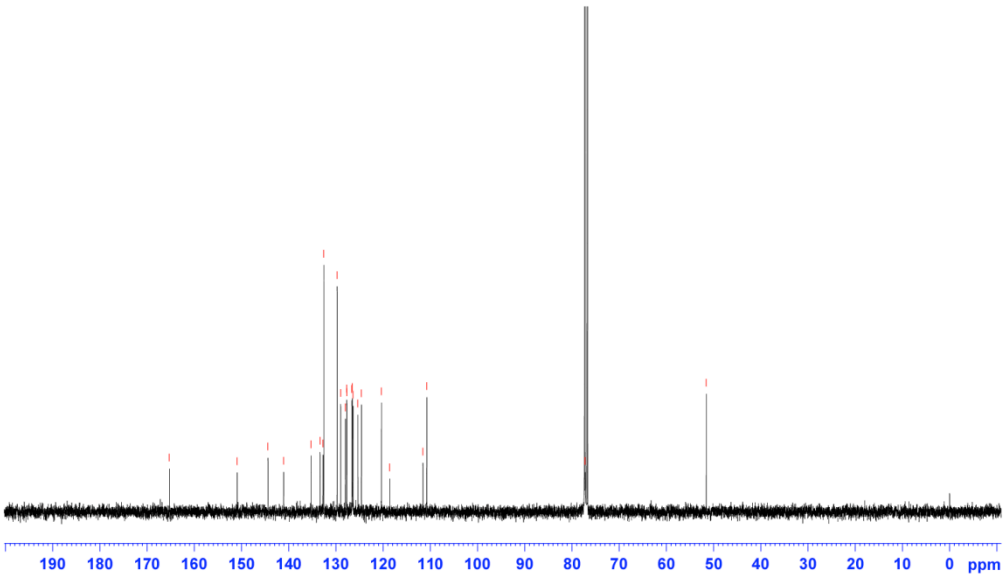

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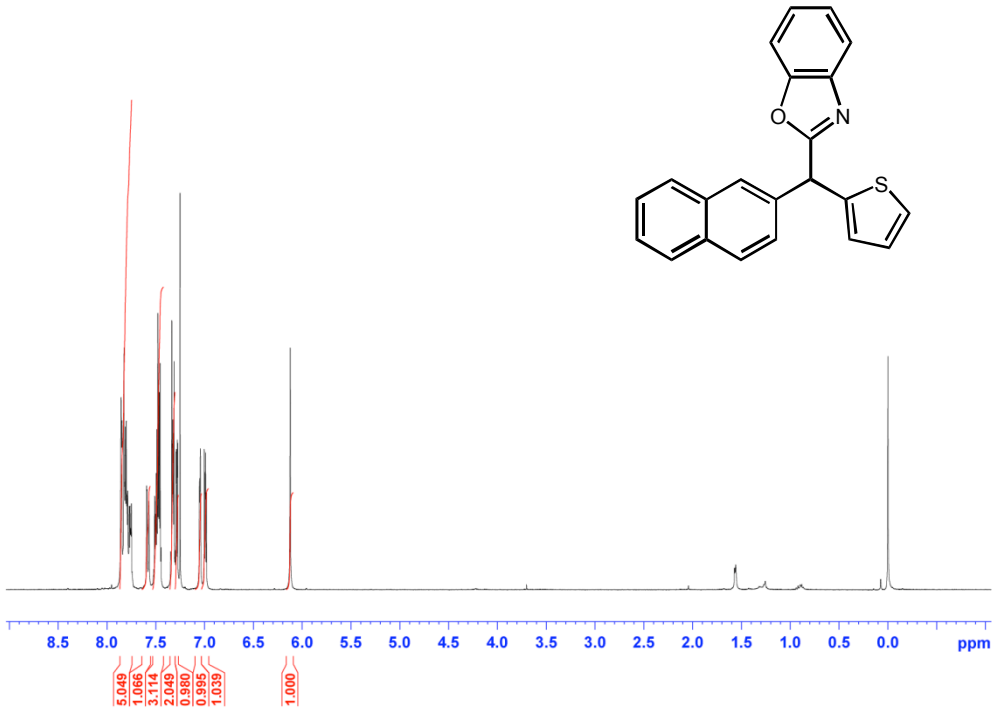

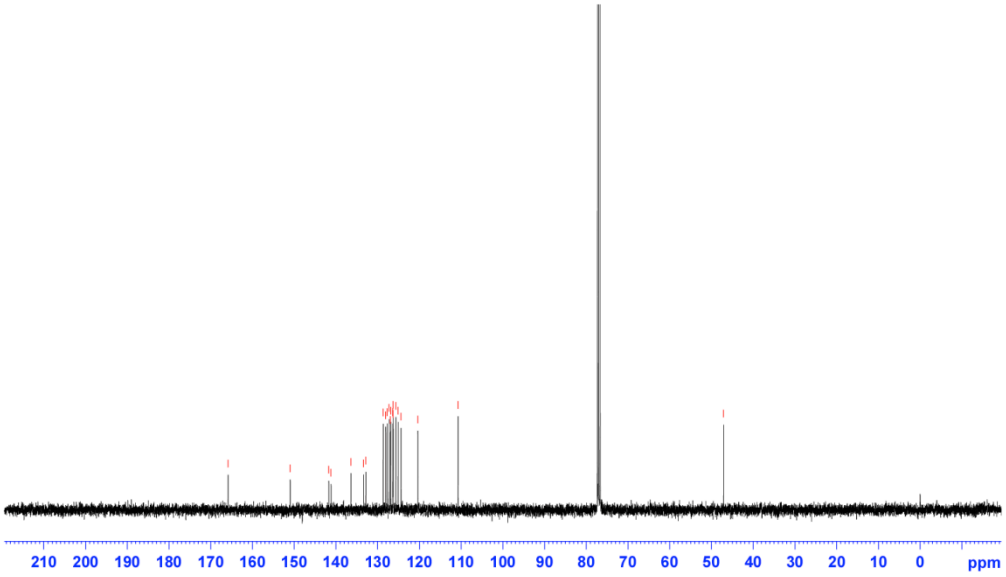

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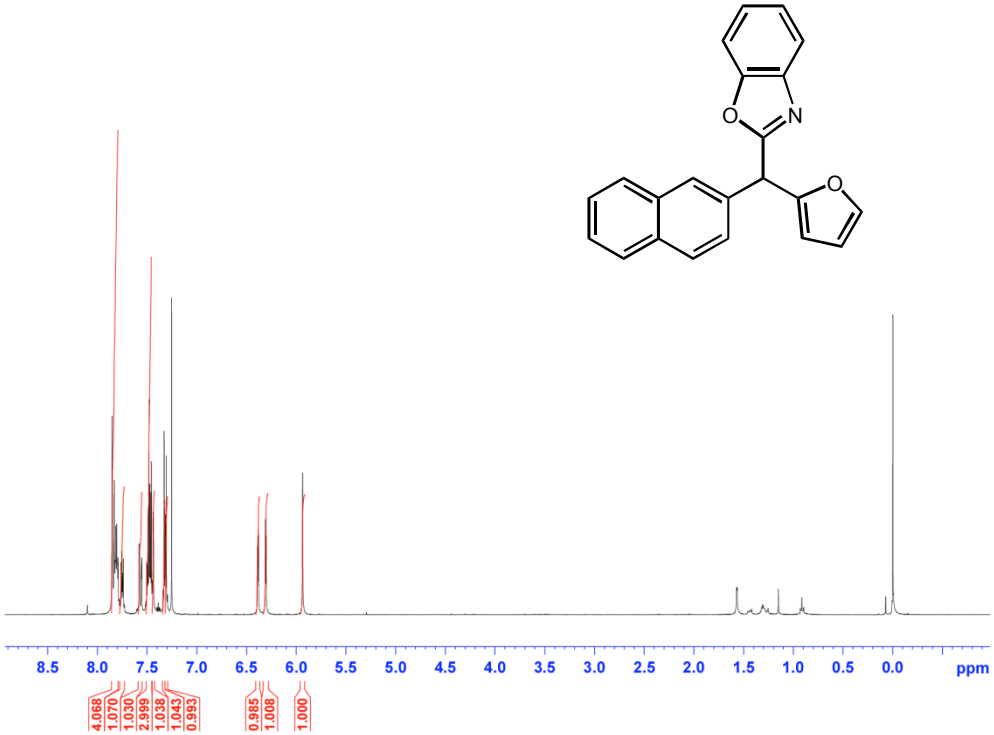
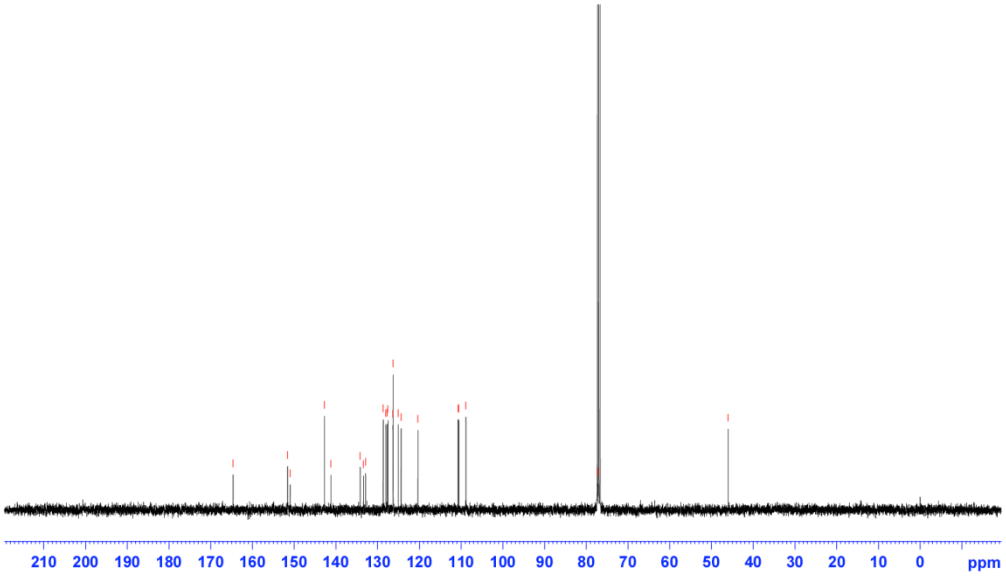
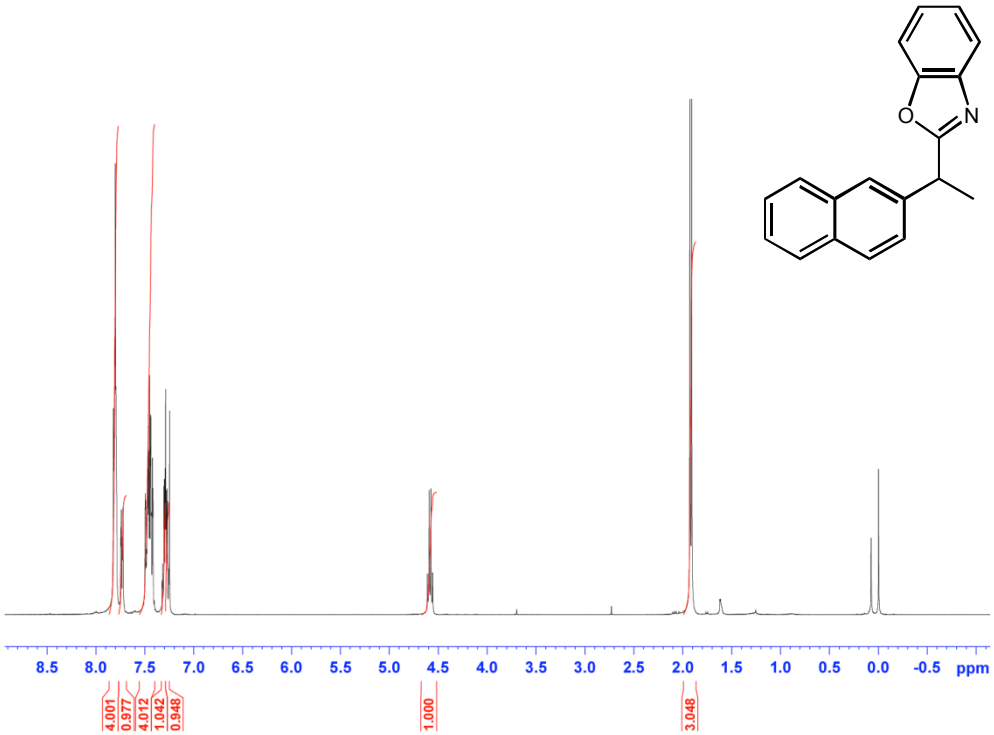
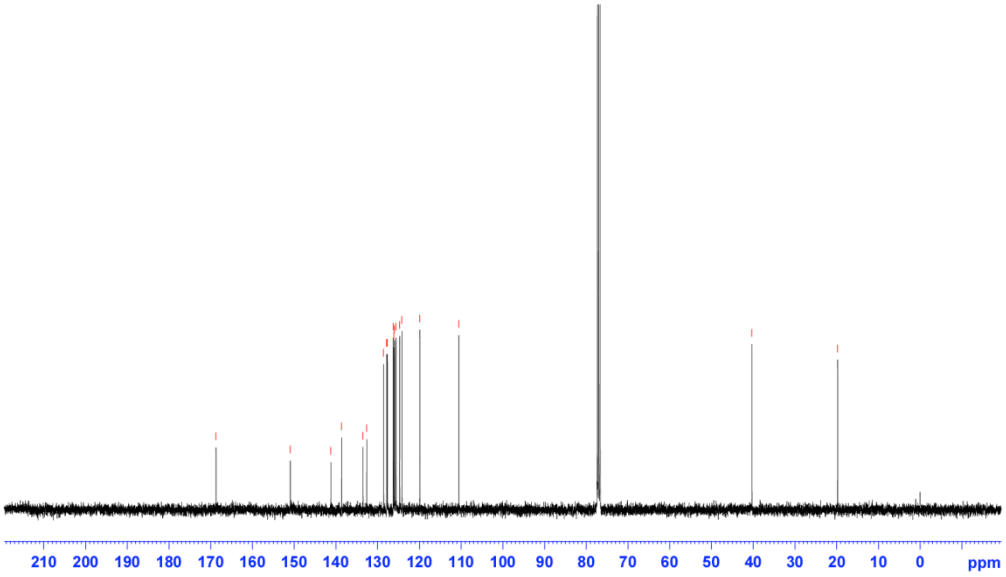




2-[1-(Naphthalen-2-yl)ethyl]benzo[*d*]oxazole (3ah)





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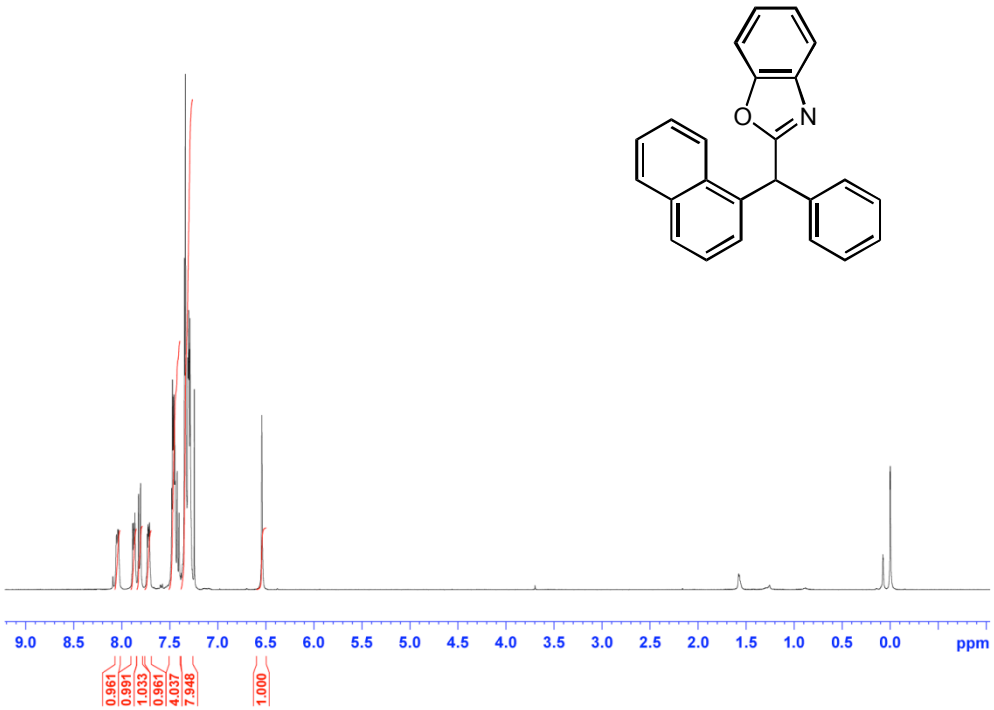

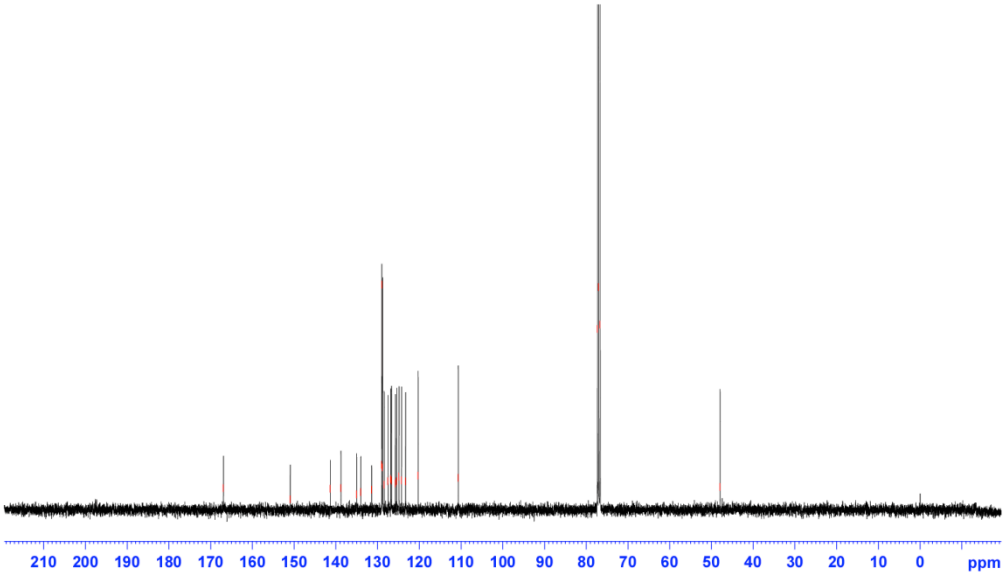

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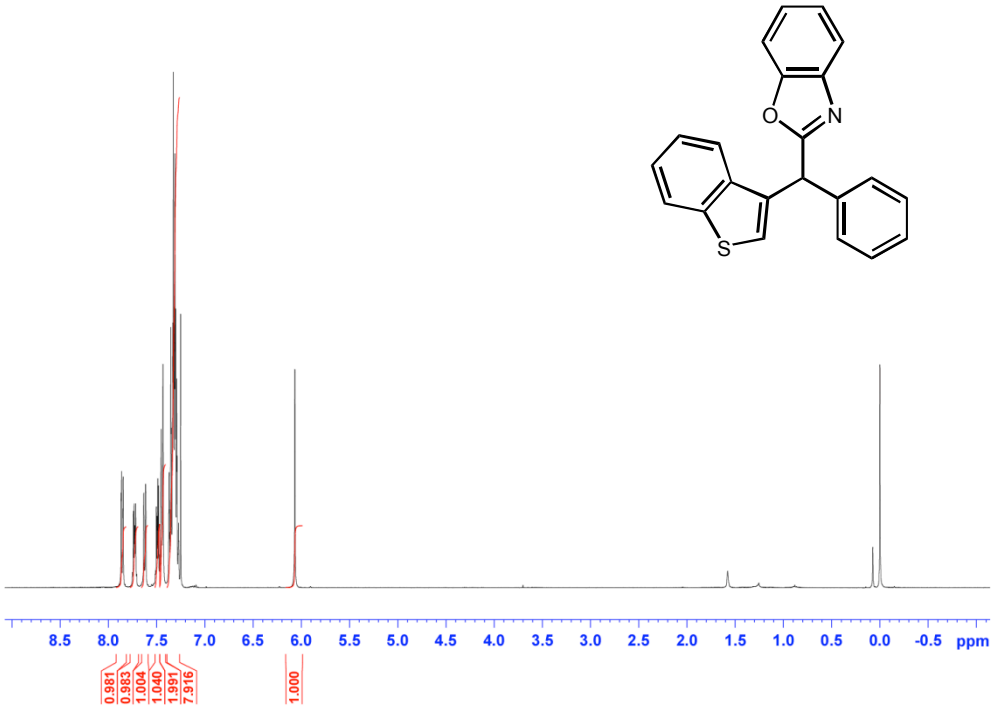

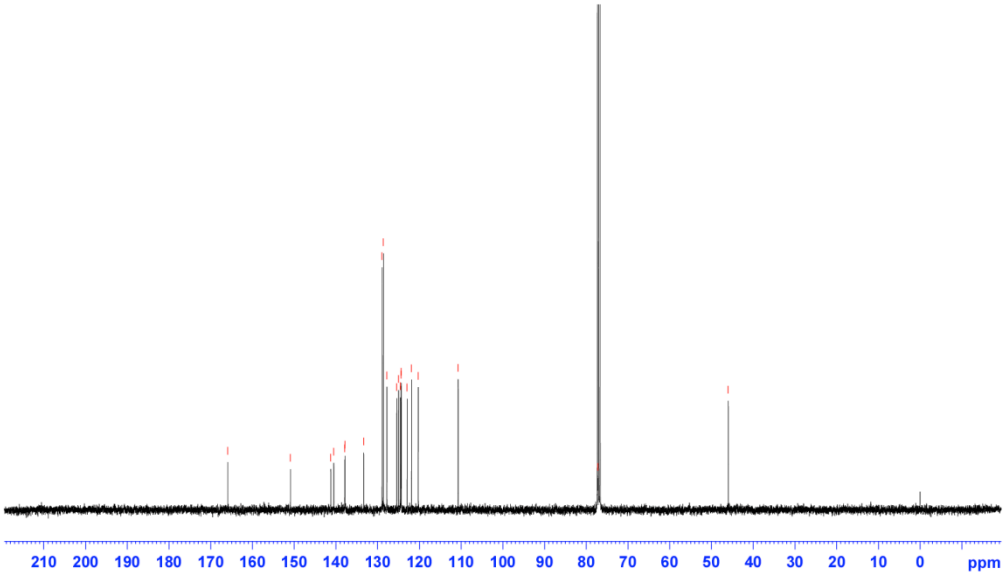

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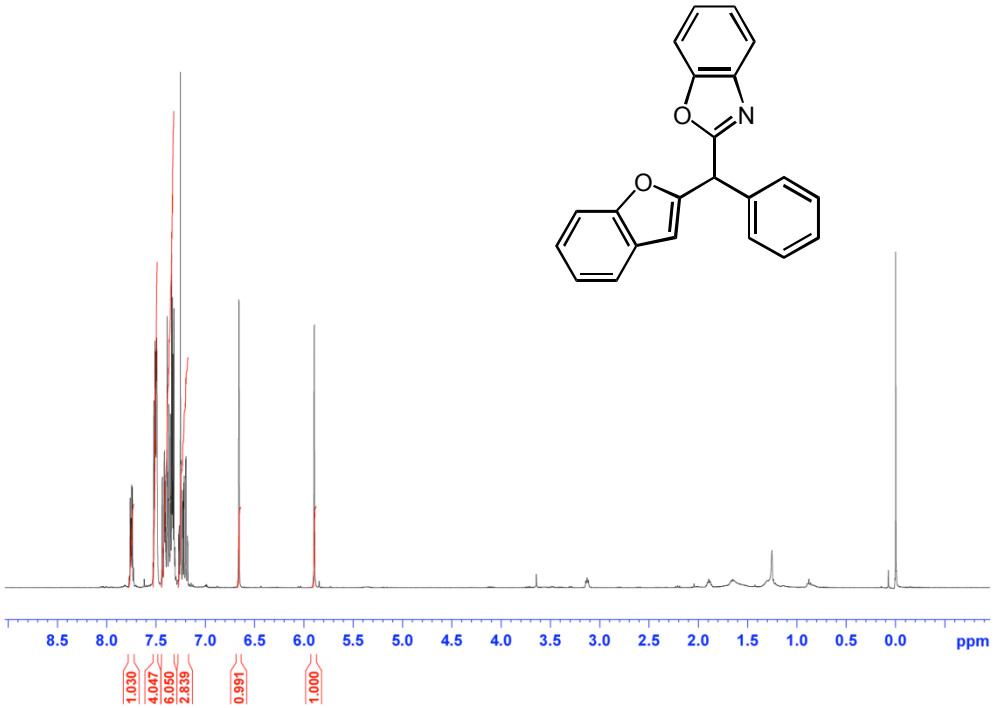
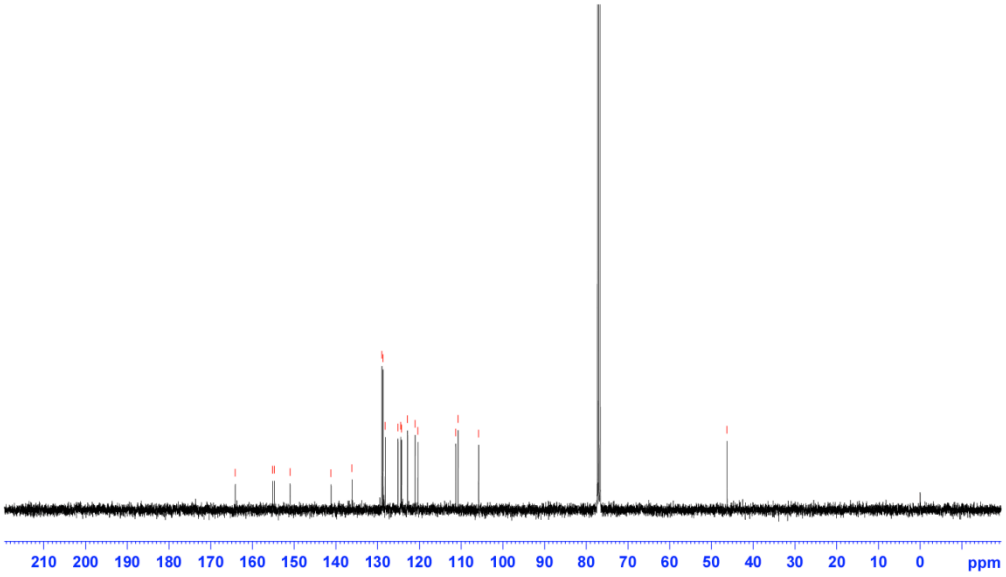
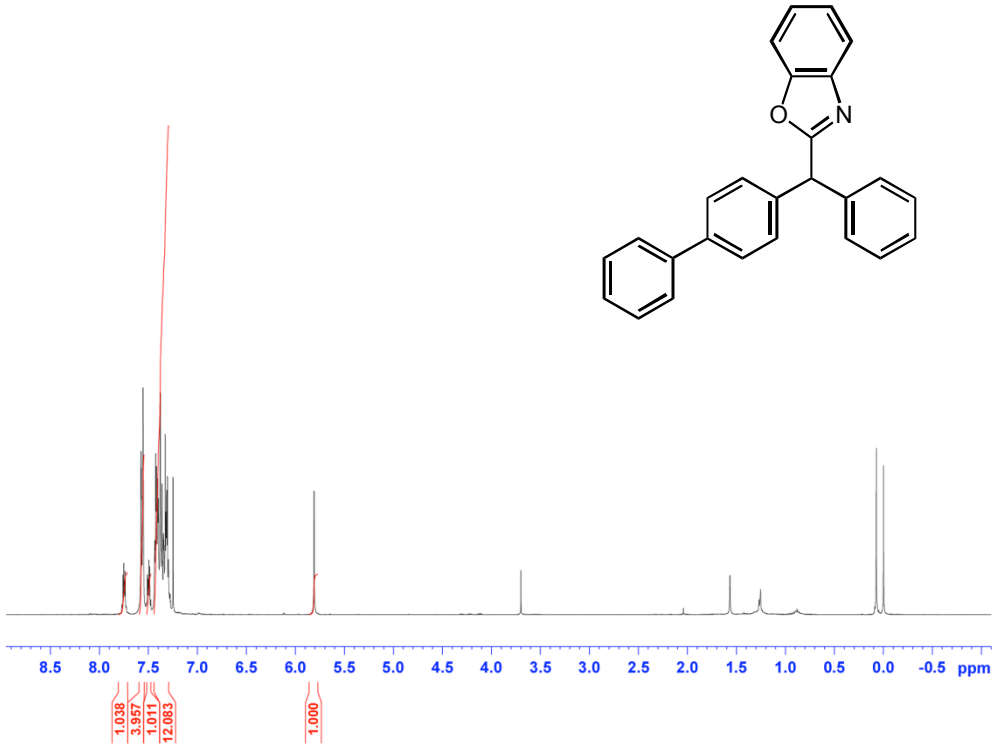
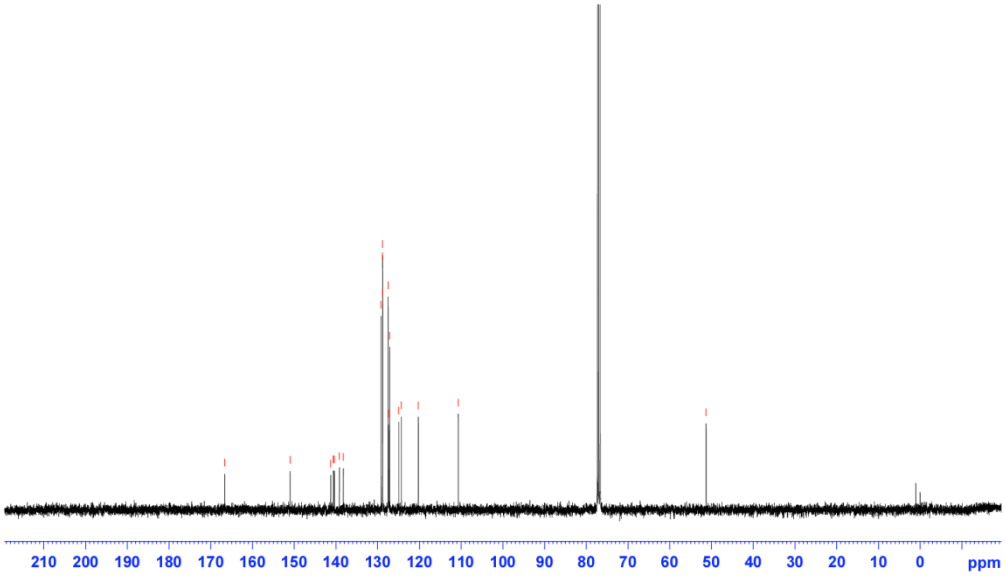




2-[(1,1'-Biphenyl)-4-yl(phenyl)methyl]benzo[*d*]oxazole (3al)





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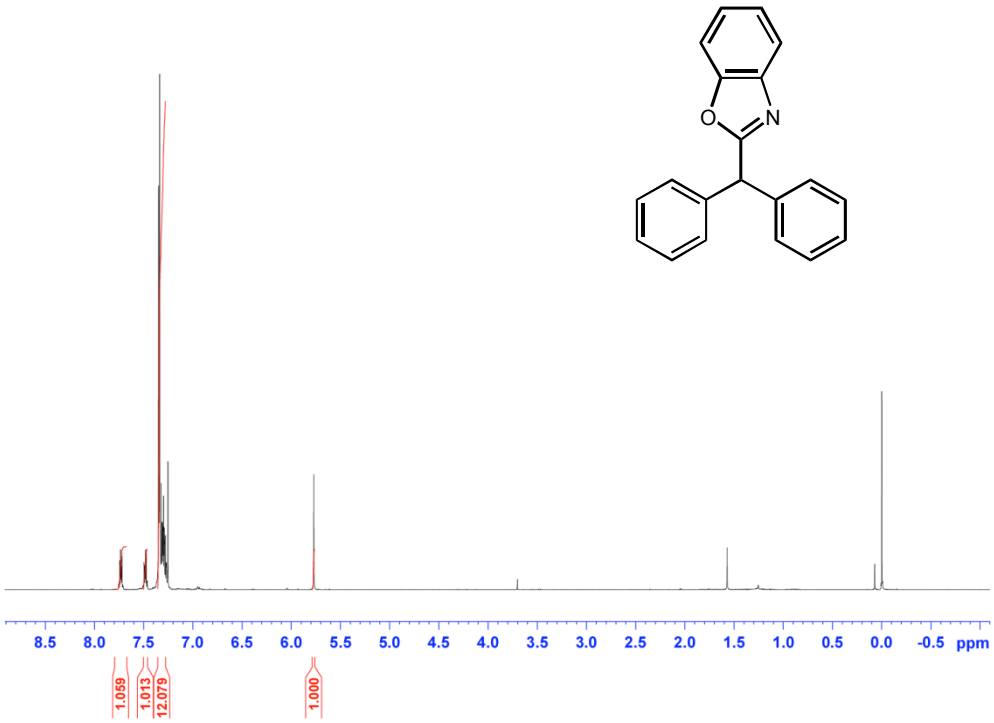
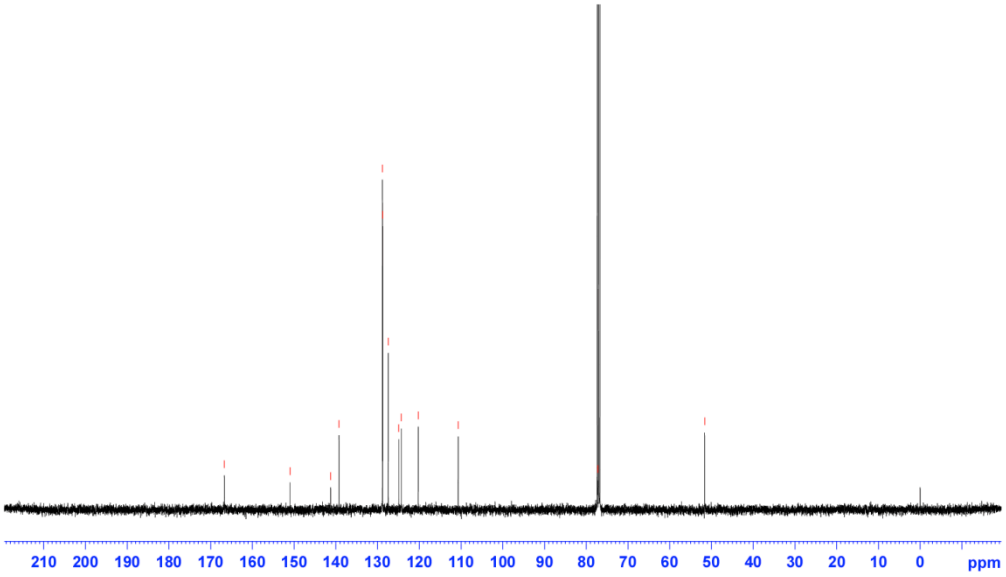
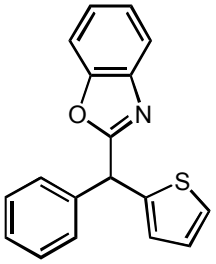
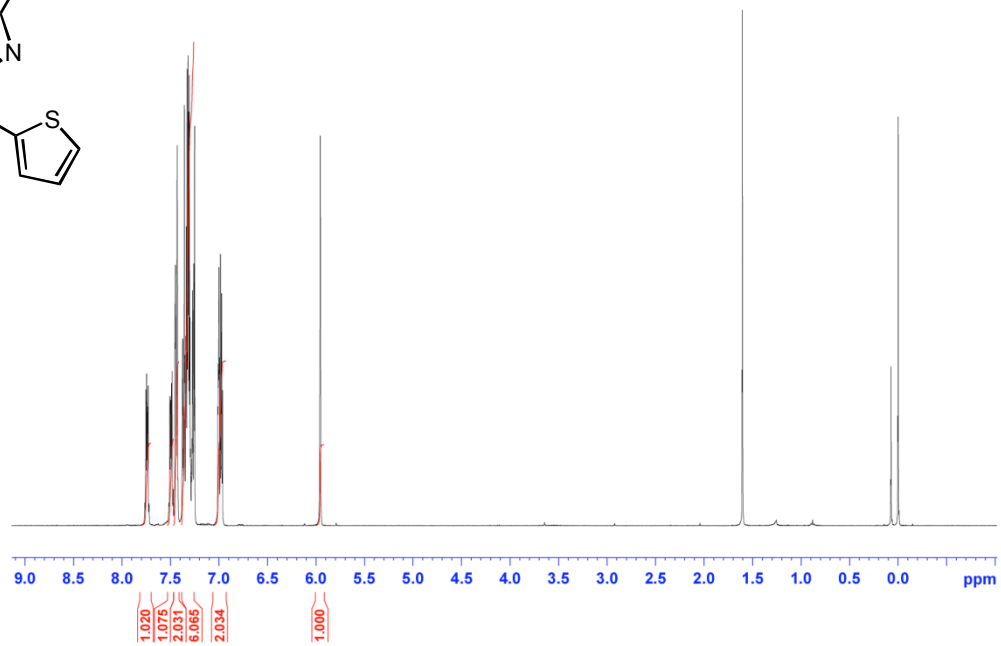
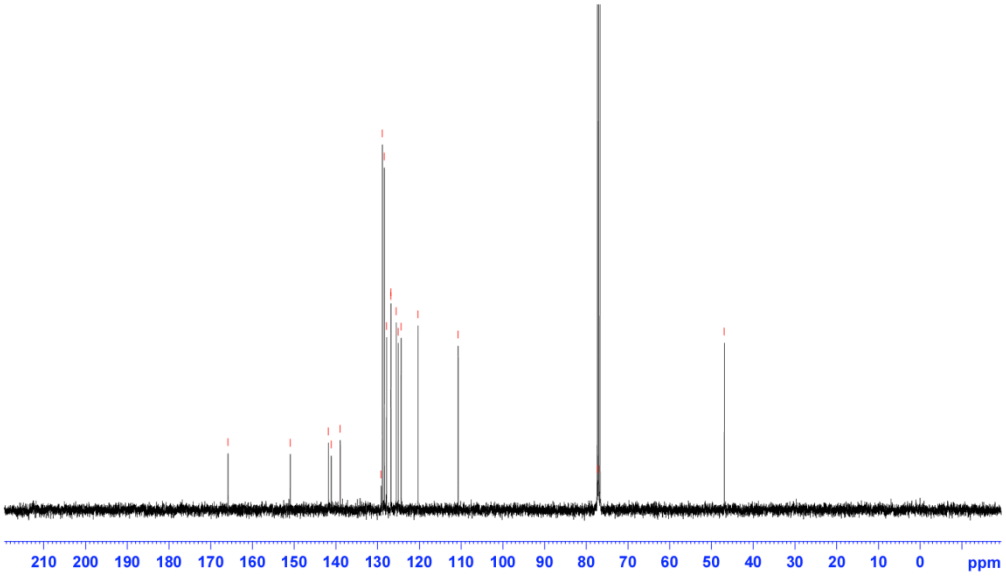




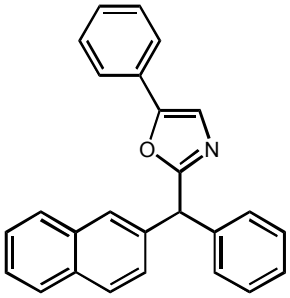
2-[Phenyl(thiophen-2-yl)methyl]benzo[*d*]oxazole (3an)

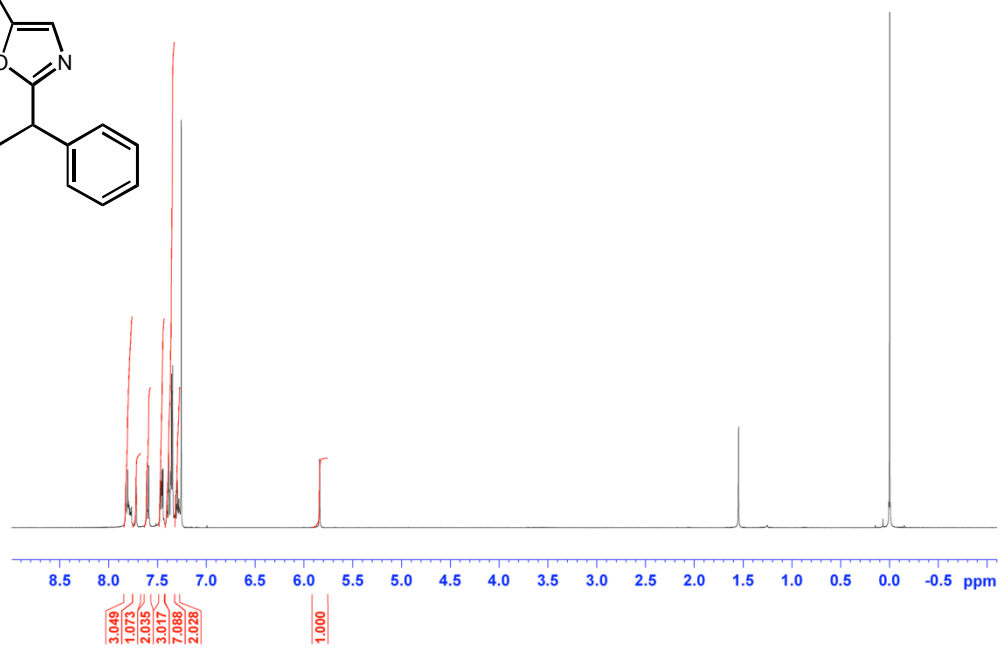


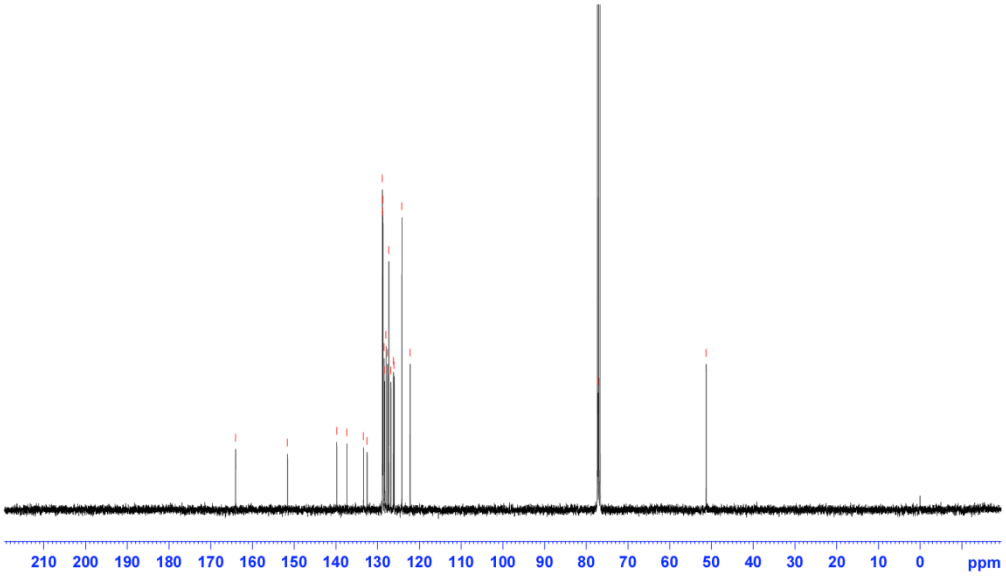




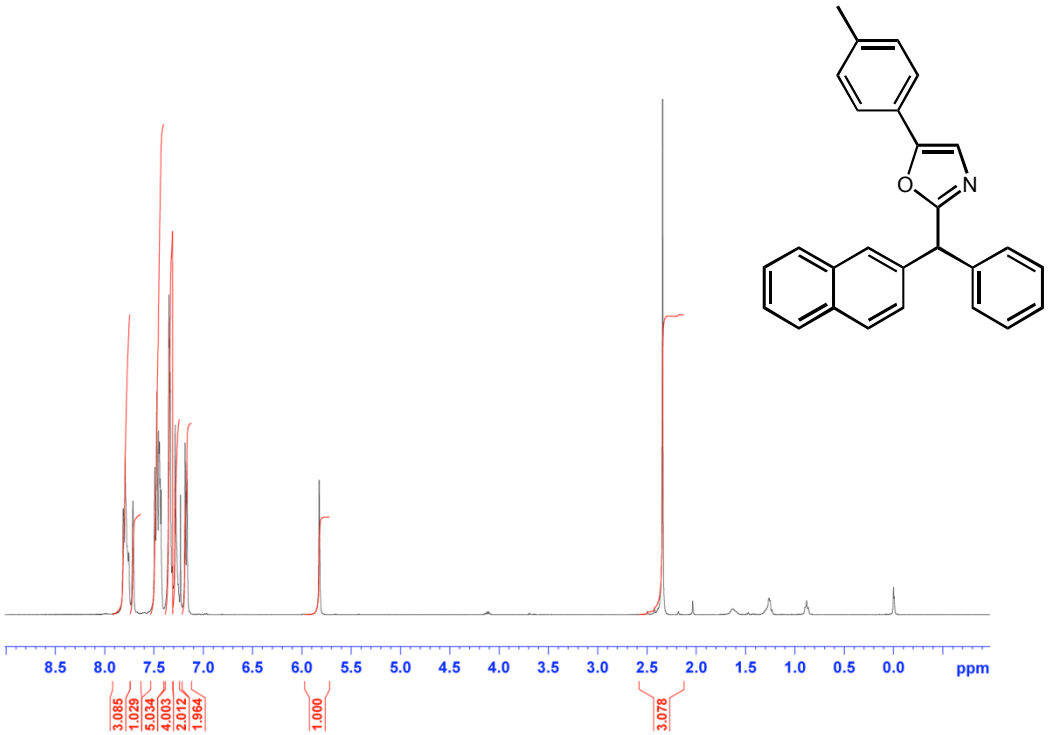
2-[Naphthalen-2-yl(phenyl)methyl]-5-phenyloxazole (3ba)

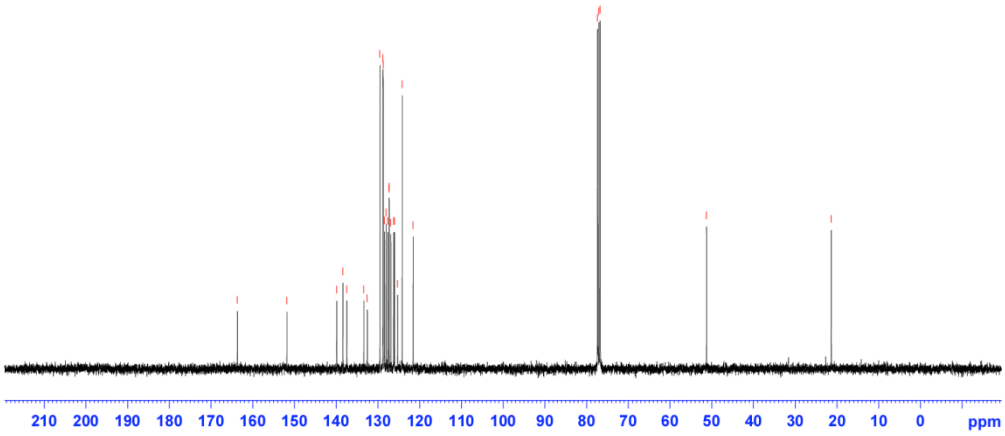




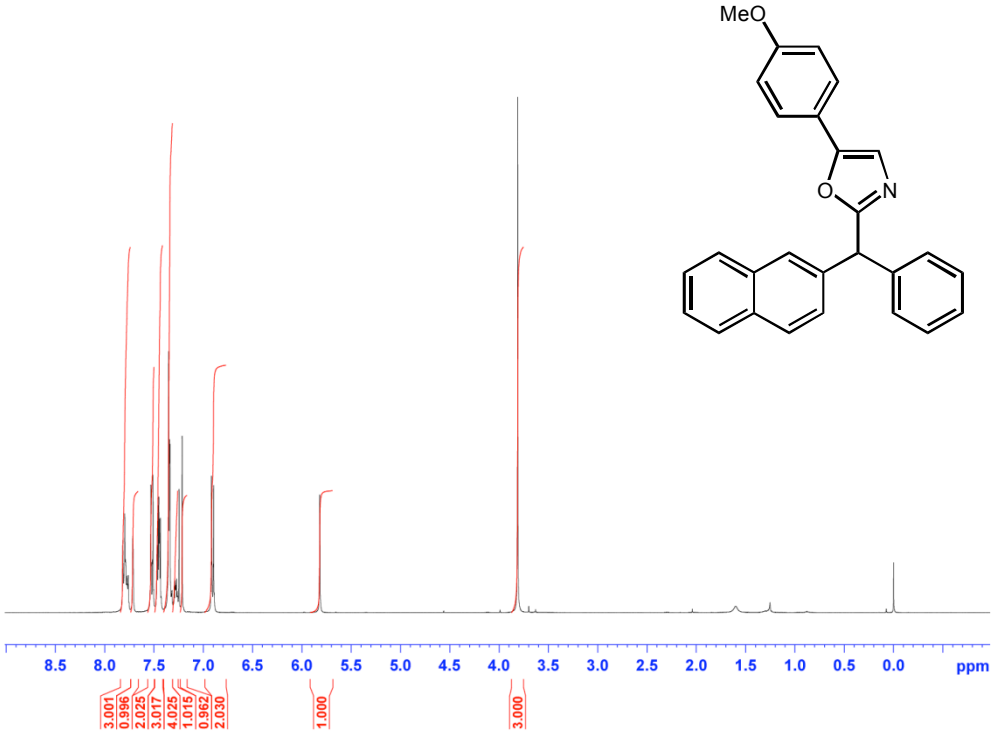


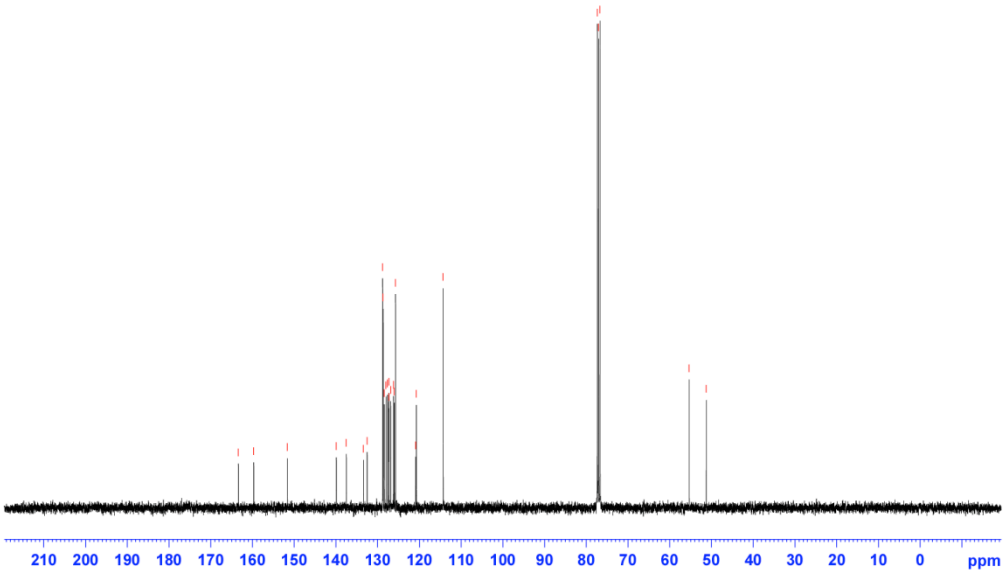
5-(4-Methylphenyl)-2-[naphthalen-2-yl(phenyl)methyl]oxazole (3ca)



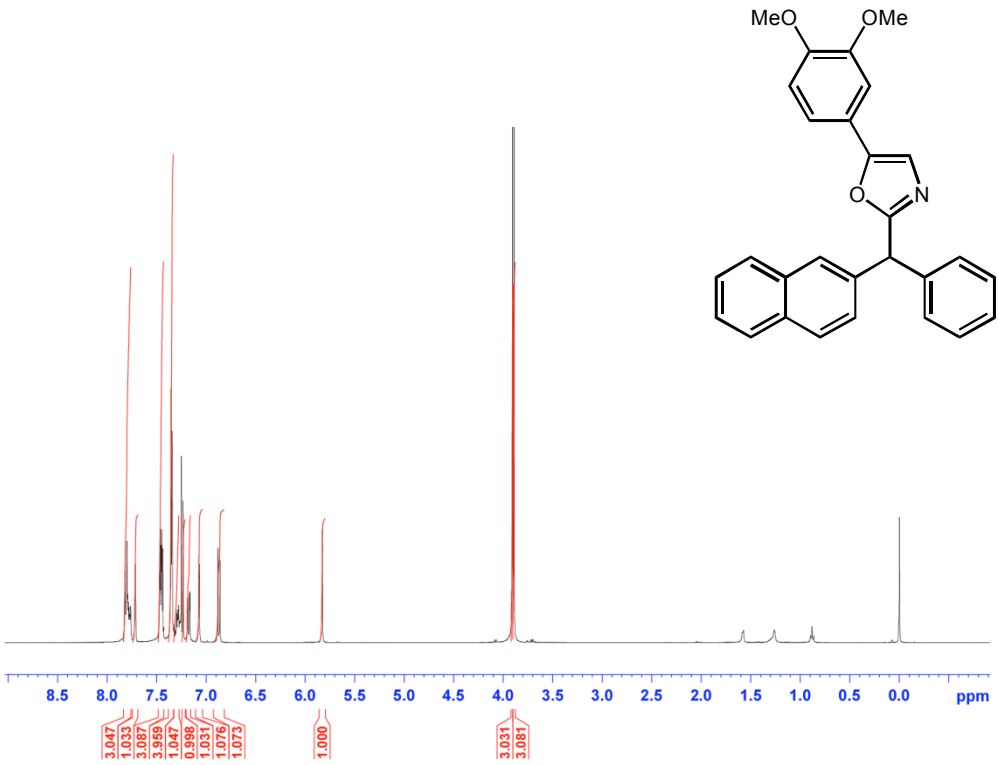


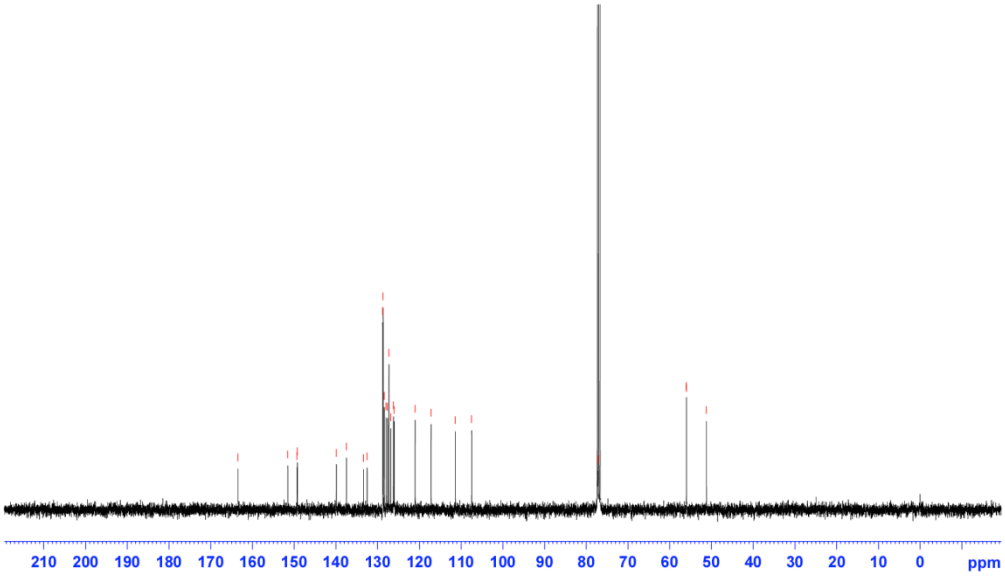
5-(4-Methoxyphenyl)-2-[naphthalen-2-yl(phenyl)methyl]oxazole (3da)



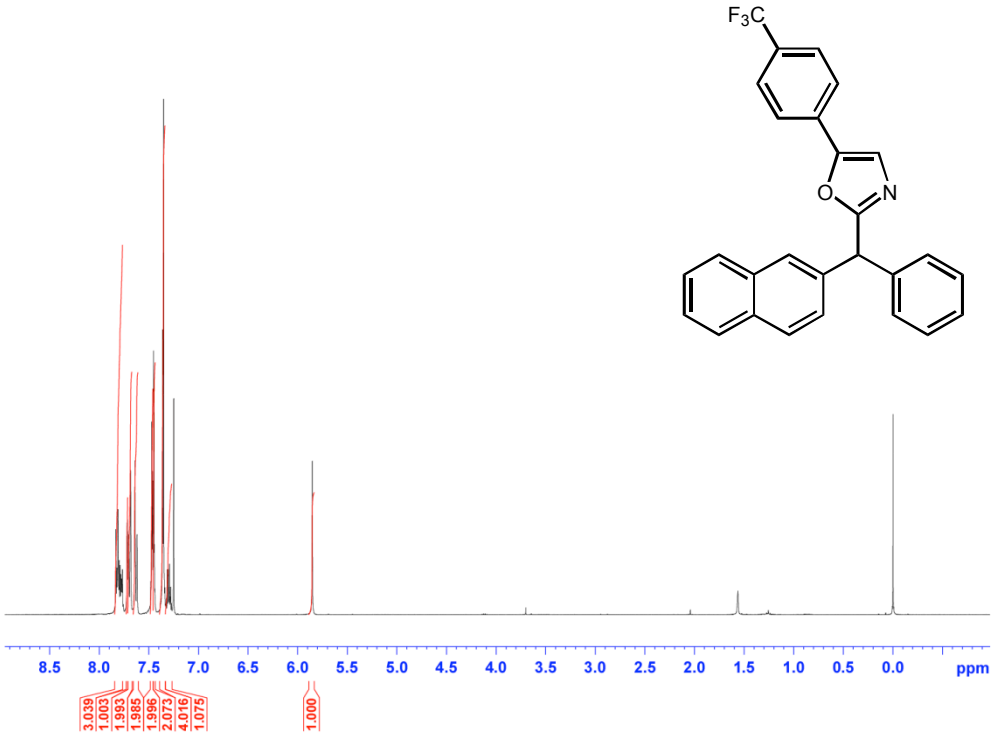


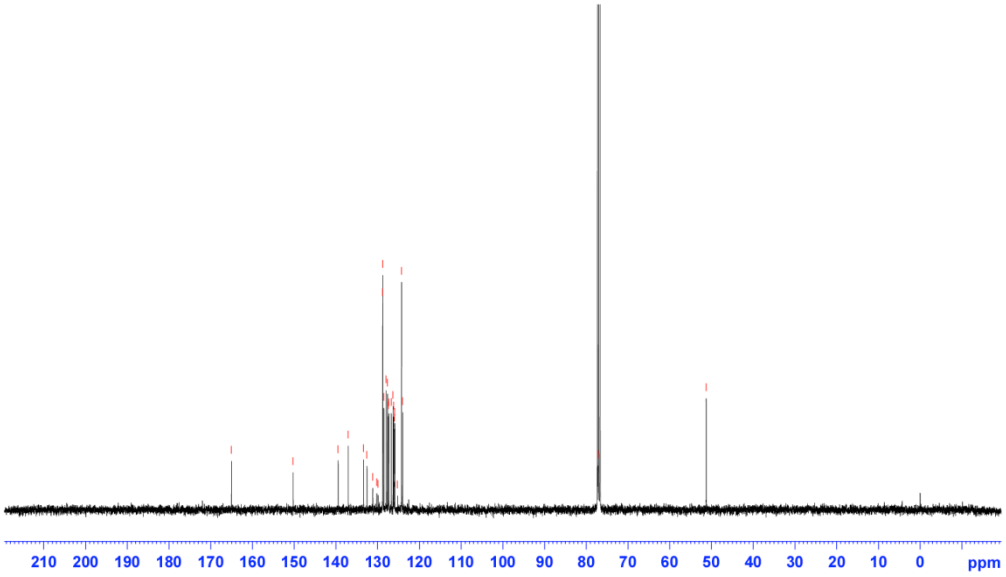
5-(3,4-Dimethoxyphenyl)-2-[naphthalen-2-yl(phenyl)methyl]-4,5-dihydrooxazole (3ea)



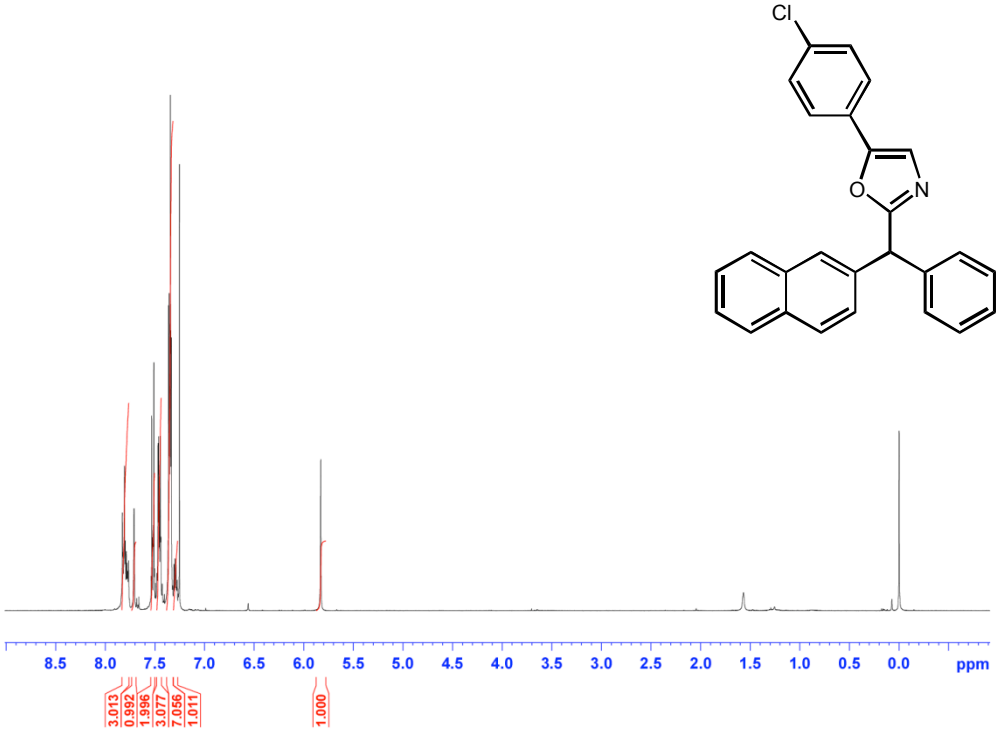


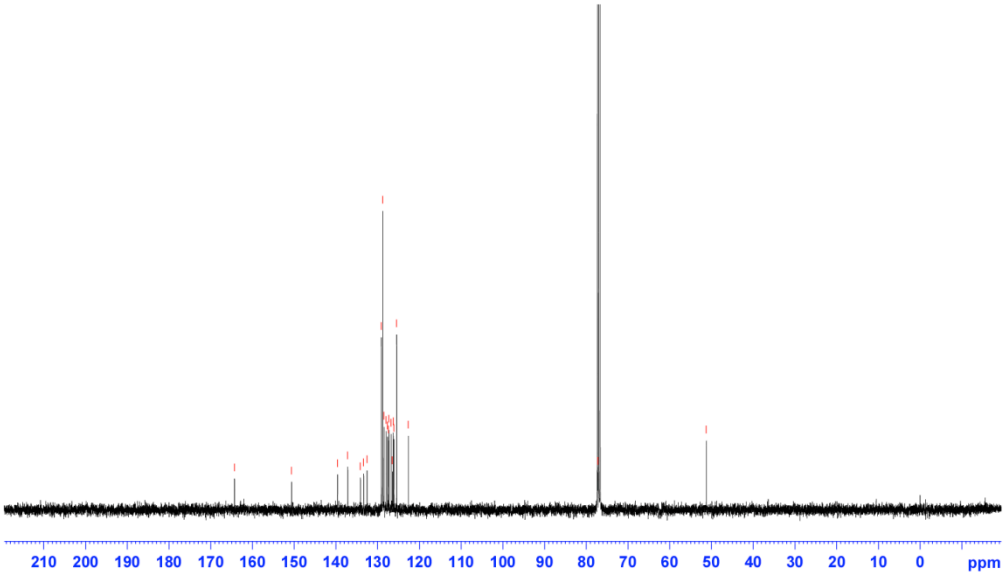
2-(Naphthalen-2-yl(phenyl)methyl)-5-[4-(trifluoromethyl)phenyl]oxazole (3fa)



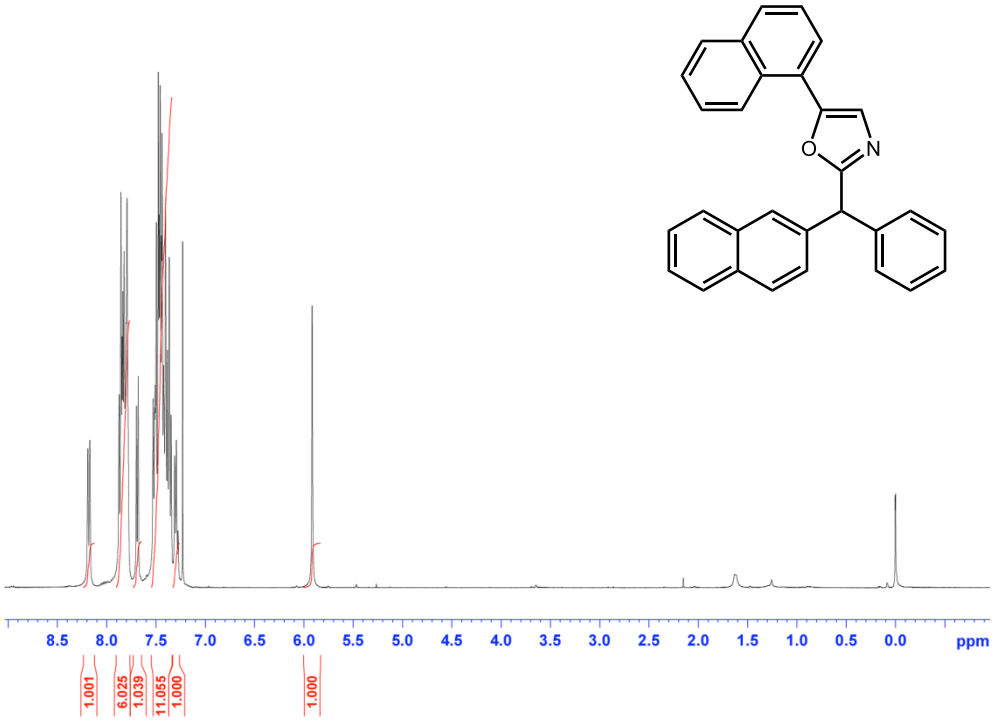


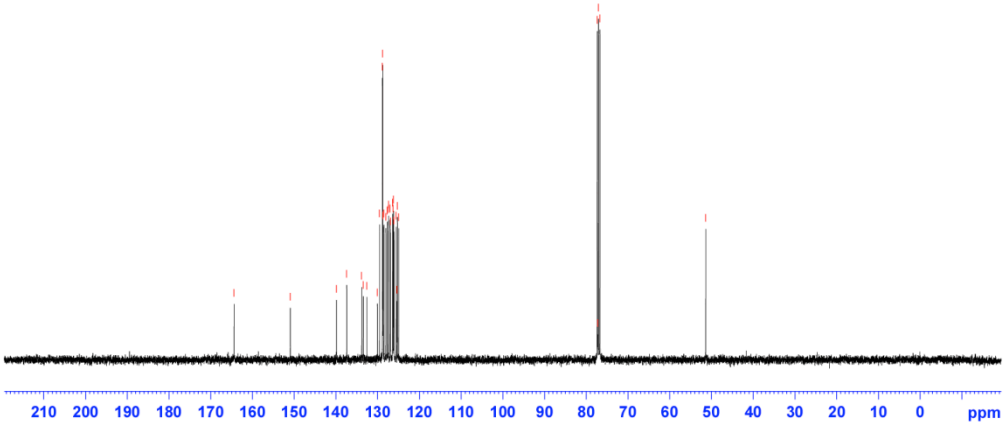
5-(4-Chlorophenyl)-2-[naphthalen-2-yl(phenyl)methyl]oxazole (3ga)



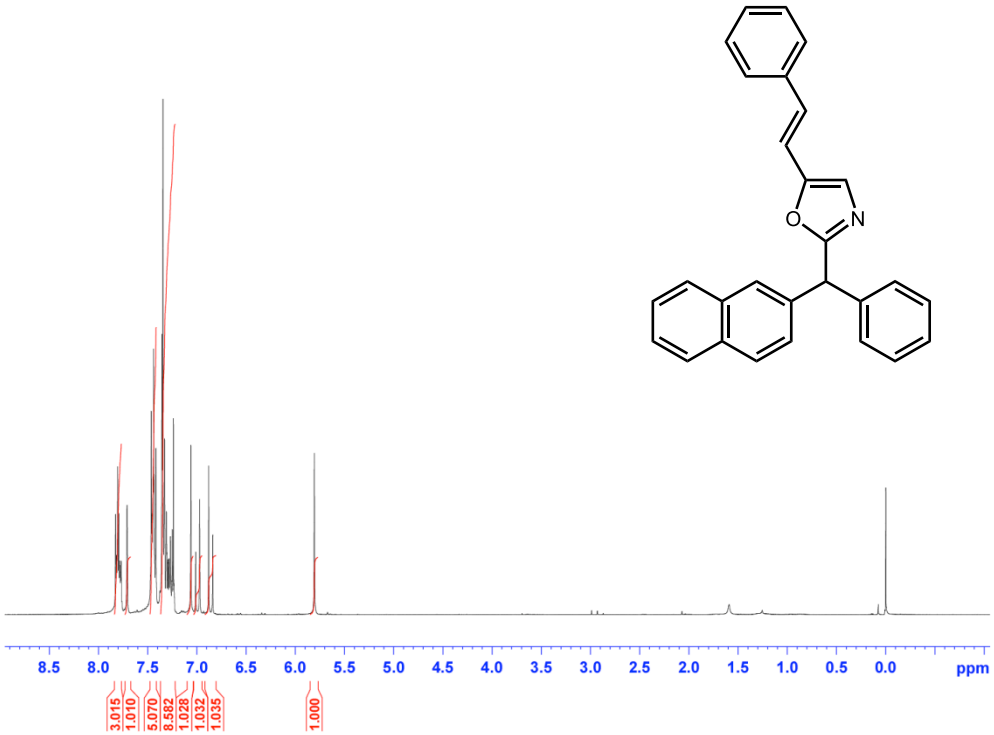


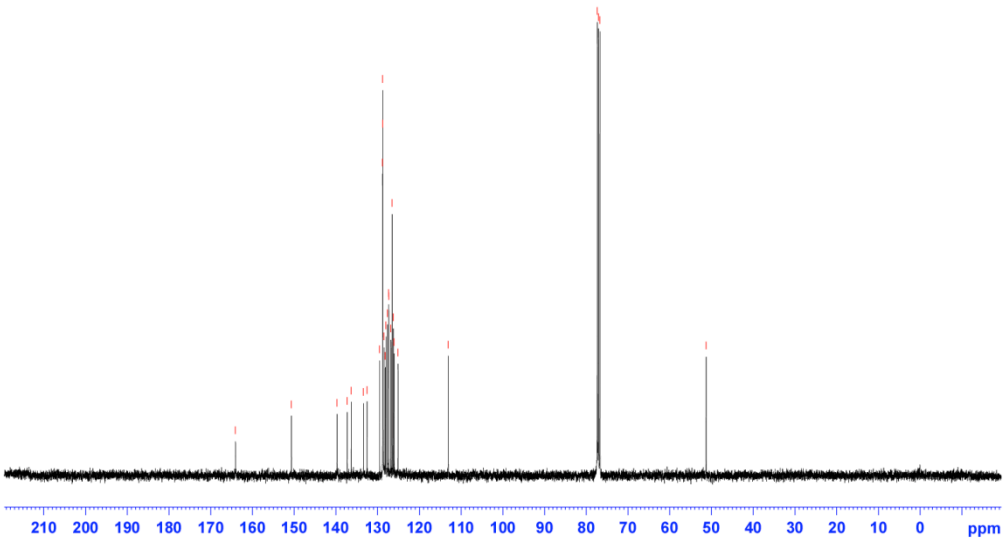
5-(Naphthalen-1-yl)-2-[naphthalen-2-yl(phenyl)methyl]oxazole (3ha)



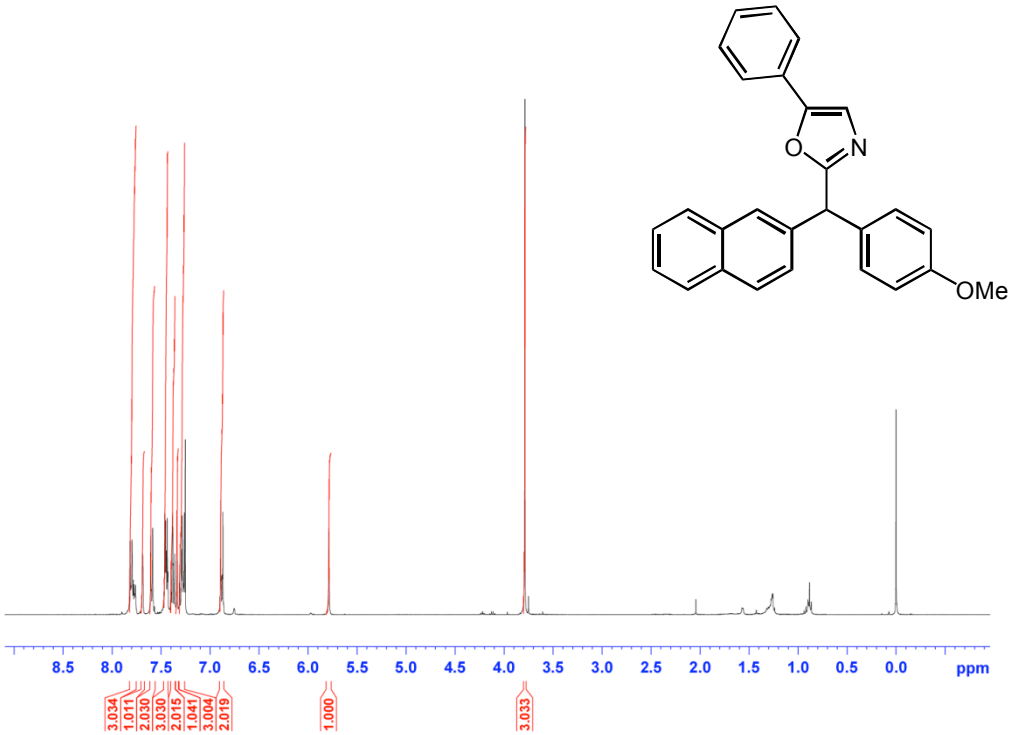


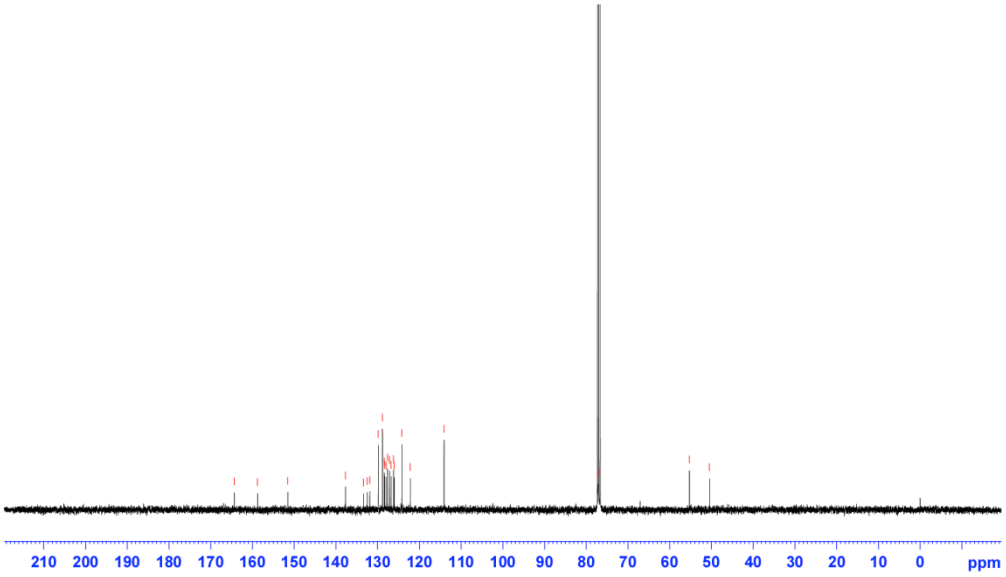
2-[Naphthalen-2-yl(phenyl)methyl]-5-styryloxazole (3ia)



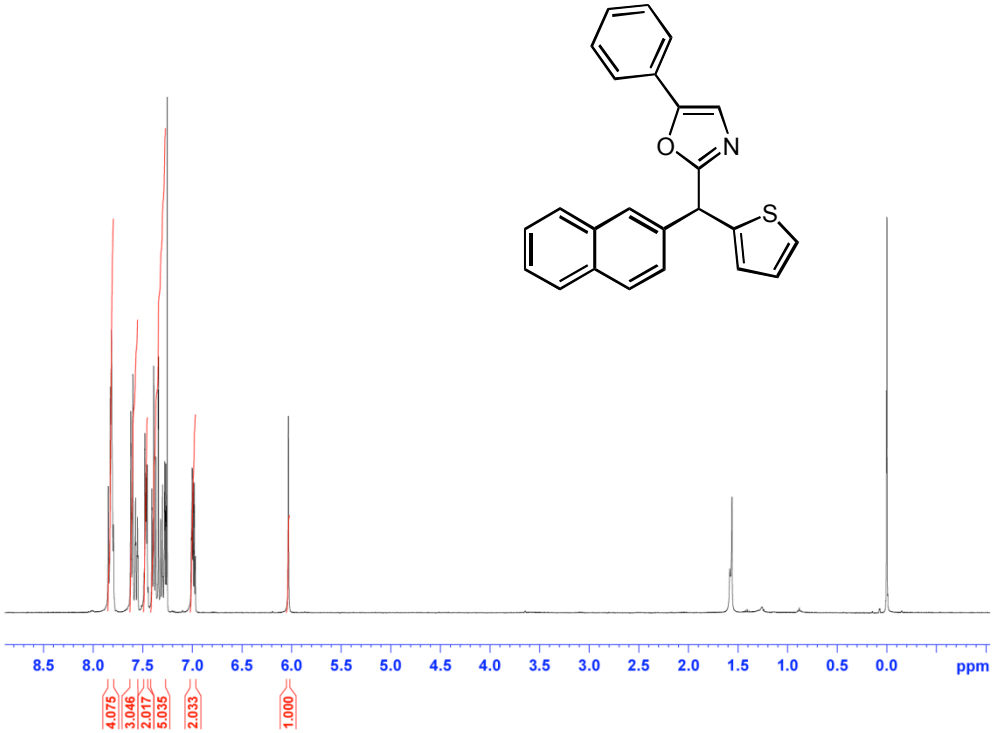


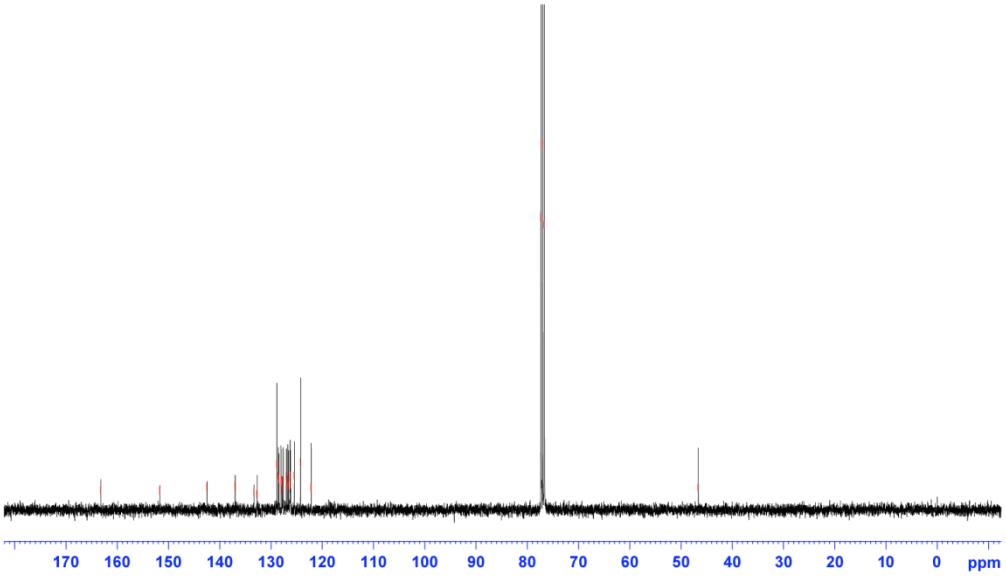
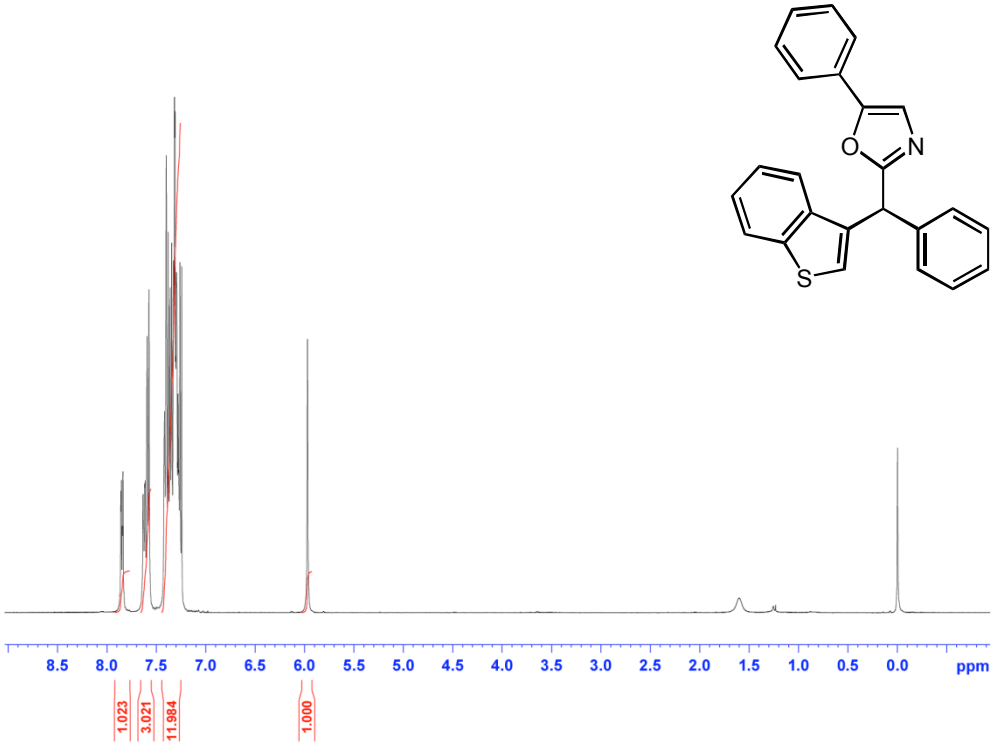
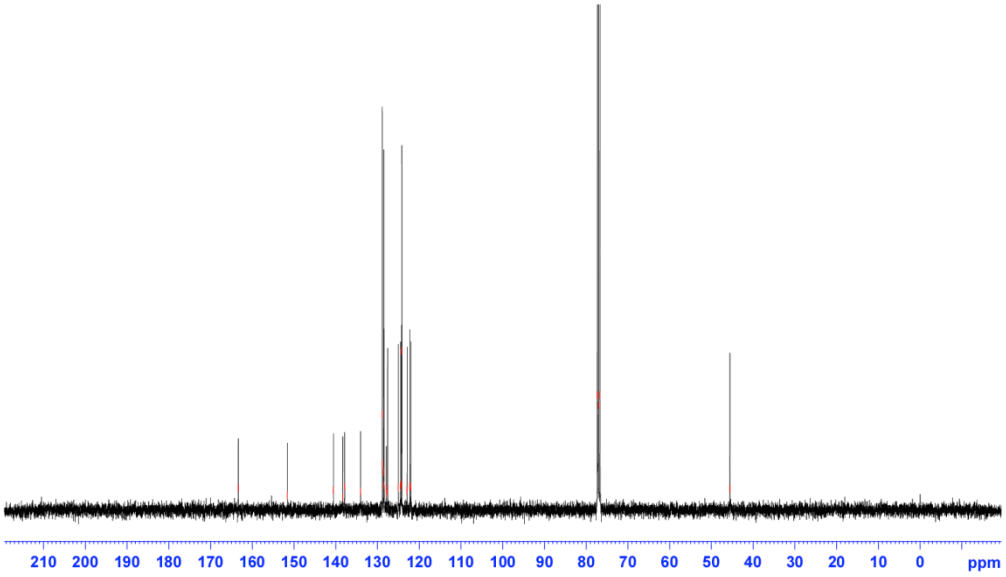
2-[(4-Methoxyphenyl)(naphthalen-2-yl)methyl]-5-phenyloxazole (3bb)





2-[Naphthalen-2-yl(thiophen-2-yl)methyl]-5-phenyloxazole (3bf)





2-[Benzo[*b*]thiophen-3-yl(phenyl)methyl]-5-phenyloxazole (3bj)