Supporting Information for

C-H arylation of azaheterocycles: A direct ligand-free and Cu-catalyzed approach using diaryliodonium salts

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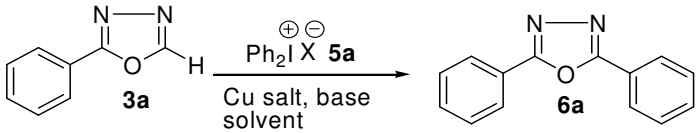
1. General Materials and Methods:

All the laboratory reagents were obtained commercially. The progress of the reaction was monitored by thin layer chromatography, which was performed on Merck precoated plates (silica gel 60, F_{254}, 0.25mm) and it was visualized by fluorescence quenching under hand-UV lamp (254 nm). The column chromatography was performed using 100-200 mesh silica gel. The solvents were evaporated using Buchi rotary evaporator. Microwave reactions were carried out in CEM DISCOVER instrument. Melting points were determined using E-Z melting point apparatus and were uncorrected. ^{1}H and ^{13}C spectra were recorded using Bruker-Avance II (400, 100 MHz) spectrometer. The coupling constants (*J*) were given in Hz, chemical shift (δ) in ppm. TMS was used as an internal standard. The proton multiplicities were described as: s= singlet, d= doublet, t= triplet, q= quartet, dd = doublet of doublet and m= multiplet. Mass spectra were obtained using Hewlett Packard HP 5973 quadrupole Mass Selective Detector with interface for 6890 series GC. All the oxadiazoles **3**[1a], thiadiazole **4**[1b], diaryliodonium salts **5a-o**[1c-f], benzoxazoles **8**[1g] and benzothiazole **9**[1g] were synthesized by the known literature procedures.

2. 2,5-Diaryl-1,3,4-oxadiazoles

(i) Optimization of reaction conditions for 2,5-diaryl-1,3,4-oxadiazoles

Table 1 Optimization of the arylation of 2-phenyl-1,3,4-oxadiazole (**3a**) using **5a**[a]:



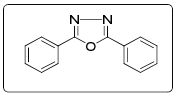
entry	catalyst	base	solvent	X	yield (%)
1[b]	-	Na_2CO_3	PEG-400	OTf	NR
2[b]	-	Cs_2CO_3	PEG-400	OTf	NR
3[b]	-	Na_2CO_3	DMSO	OTf	NR
4[b]	-	Cs_2CO_3	DMSO	OTf	NR
5[b]	-	*t*-BuOK	DMSO	OTf	NR
6[b]	CuBr	*t*-BuOK	PEG-400	OTf	68
7[c]	CuBr	*t*-BuOK	PEG-400	OTf	80
8[c]	CuBr	Cs_2CO_3	PEG-400	OTf	Trace
9[c]	CuBr	K_3PO_4	PEG-400	OTf	NR
10[d]	CuI	*t*-BuOK	PEG-400	OTf	Trace
11[d]	CuBr	*t*-BuOK	DMSO	OTf	80
12[d]	CuBr	*t*-BuOLi	DMSO	OTf	89
13[d]	CuBr	Cs_2CO_3	DMSO	OTf	NR
14[d]	CuBr	*t*-BuOLi	DMSO	BF_4	65

[a] A mixture of **3a** (1 equiv.), **5a** (1 equiv.), Cu catalyst (20 mol %), base (3 equiv.) was stirred in DMSO for 15 min. at rt. [b] Conventional heating at 100 °C for 18-24 h. [c] reaction under microwave irradiation at 100 °C for 30 min. [d] stirring at rt for 10-15 min, NR = no reaction

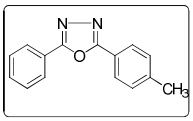
(ii) Typical experimental procedure for 2,5-diaryl-1,3,4-oxadiazoles (**6a**)

To a stirred solution of oxadiazole **3a** (100 mg, 0.684 mmol) and CuBr (20 mg, 0.136 mmol) in DMSO (2 mL), *t*-BuOLi (164 mg, 2.05 mmol) was charged and continued stirring at room temperature for 5 min. Then the required amount of diphenyliodonium triflate **5a** (294 mg, 0.684 mmol) was added portionwise and stirred at room temperature for 15 min. Completion of the reaction was confirmed by the TLC (4:1 hexane:ethylacetate). Then the resulting reaction mixture was added to ice-cold water and extracted with EtOAc (3 × 5 mL). The combined organic layer was washed with ammonia solution, brine and dried over anhydrous Na_2SO_4 and the solvent was removed in vacuo. The obtained crude product was purified by column chromatography using EtOAc/hexane (10%) as an eluent to afford **6a** in 89% yield.

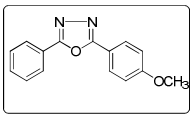
(iii) Analytical data for 2,5-diaryl-1,3,4-oxadiazoles (**6a-q**)



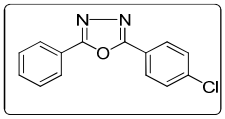
2,5-Diphenyl-1,3,4-oxadiazole (**6a**)[2a]: White solid (135 mg, 89%), mp 138 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.15-8.13 (m, 4H), 7.69-7.63 (m, 6H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.46, 132.55, 129.78, 127.19, 123.78; GC-MS m/z calcd. for $C_{14}H_{10}N_2O$: 222.1, found: 222.0



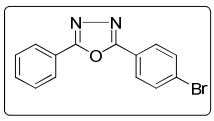
2-(4'-Methylphenyl)-5-phenyl-1,3,4-oxadiazole (**6b**)[2b]: White solid (63 mg, 79%), mp 125-126 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.13 (m, 2H), 8.03 (d, *J* = 8.0 Hz, 2H), 7.54-7.52 (m, 3H), 7.34 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.83, 164.20, 142.36, 131.62, 129.64, 128.81, 126.90, 123.82, 121.20, 21.49; GC-MS m/z calcd. for $C_{15}H_{12}N_2O$: 236.1, found: 236.0



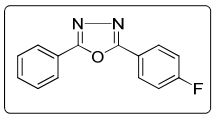
2-(4'-Methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (**6c**)[2a]: White solid (75 mg, 75%), mp 147 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-8.11 (m, 2H), 8.09 (d, *J* = 8.8 Hz 2H), 7.54-7.52 (m, 3H), 7.05 (d, *J* = 8.8 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.55, 164.14, 162.37, 131.50, 129.06, 128.72, 126.84, 124.02, 116.46, 114.53, 55.24; GC-MS m/z calcd. for $C_{15}H_{12}N_2O_2$: 252.1, found: 252.0



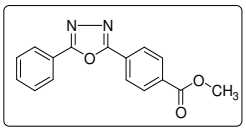
2-(4'-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (**6d**)[2b]: Off white solid (79 mg, 89%), mp 161 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.08 (m, 4H), 7.58-7.50 (m, 5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.15, 160.21, 134.43, 128.30, 125.84, 125.54, 124.60, 123.38, 120.09, 118.81; GC-MS m/z calcd. for $C_{14}H_9ClN_2O$: 256.0, found: 256.0



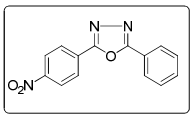
2-(4'-Bromophenyl)-5-phenyl-1,3,4-oxadiazole (**6e**)[2b]: White solid (90 mg, 88%), mp 171 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 7.6, 1.5 Hz, 2H), 8.03 (d, *J* = 8.5 Hz, 2H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.58-7.54 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.77, 163.89, 132.46, 131.84, 129.14, 128.33, 126.99, 126.54, 123.73, 122.80; GC-MS m/z calcd. for $C_{14}H_9BrN_2O$: 300.0, found: 300.0



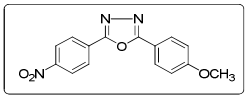
2-(4'-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (**6f**)[2b]: Light pink solid (72 mg, 88%), mp 154 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17-8.11 (m, 4H), 7.56-7.54 (m, 3H), 7.27-7.21 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 207.30, 166.05, 164.64, 163.81, 163.57, 131.84, 129.19, 129.13, 126.94, 123.80, 120.29, 116.58, 116.35; GC-MS m/z calcd. for $C_{14}H_9FN_2O$: 240.1, found: 240.0



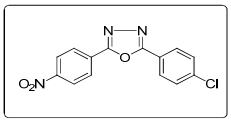
Methyl-4'-(5-phenyl-1,3,4-oxadiazol-2-yl)benzoate (6g): White solid (67 mg, 70%), mp 171 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29-8.21 (m, 4H), 8.21-8.16 (m, 2H), 7.63-7.54 (m, 3H), 3.99 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.13, 165.10, 163.86, 132.84, 132.04, 130.22, 129.18, 127.71, 127.08, 126.87, 123.67, 52.32. GC-MS m/z calcd. for $C_{16}H_{12}N_2O_3$: 280.1, found: 280.0



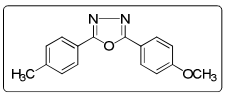
2-(4'-Nitrophenyl)-5-phenyl-1,3,4-oxadiazole (**6h**)[2c]: Yellow solid (70 mg, 77%), mp 207 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.40 (m, 2H), 8.39-8.33 (m, 2H), 8.18 (dd, *J* = 8.1, 1.5 Hz, 2H), 7.65-7.53 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.48, 162.96, 149.50, 132.26, 129.43, 129.28, 127.82, 127.24, 124.45, 123.24.



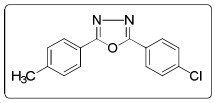
2-(4'-Methoxyphenyl)-5-(4''-nitrophenyl)-1,3,4-oxadiazole (**6i**)[2d]: Yellow solid (60 mg, 75%), mp 250 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42-8.38 (m, 2H), 8.33-8.29 (m, 2H), 8.12-8.08 (m, 2H), 7.08-7.04 (m, 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.53, 162.83, 162.37, 149.43, 129.61, 128.95, 127.67, 124.34, 115.68, 114.72, 55.59.GC-MS m/z calcd. for $C_{15}H_{11}N_3O_4$: 297.1, found: 297.0



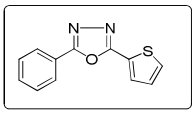
2-(4'-Chlorophenyl)-5-(4''-nitrophenyl)-1,3,4-oxadiazole (**6j**)[2d] : Yellow solid (65 mg, 81%), mp 238 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45-8.27 (m, 4H), 8.16-8.01 (m, 2H), 7.62-7.47 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.79, 162.94, 149.66, 138.80, 129.71, 129.24, 128.43, 127.87, 124.49, 121.80; GC-MS m/z calcd. for $C_{14}H_8ClN_3O_3$: 301.0, found: 301.0



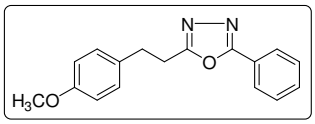
2-(4'-Methoxyphenyl)-5-(4''-methylphenyl)-1,3,4-oxadiazole (**6k**)[2b] : Off white solid, yield 78%, mp 138 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.06 (d, J = 8.9 Hz, 2H), 8.00 (d, J = 8.1 Hz, 2H), 7.43 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 8.9 Hz, 2H), 3.87 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.18, 162.43, 142.20, 130.40, 128.95, 126.98, 121.20, 116.21, 115.32, 55.93, 21.61; GC-MS m/z calcd. for $C_{16}H_{14}N_2O_2$: 266.1, found: 266.0



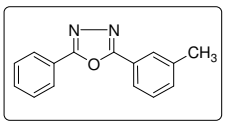
2-(4'-Chlorophenyl)-5-(4''-methylphenyl)-1,3,4-oxadiazole (**6l**): White solid (74 mg, 88%), mp 209 °C. ^{1}H NMR (400 MHz, DMSO-d_6) ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11-7.99 (m, 4H), 7.64-7.39 (m, 4H), 2.42 (s, 3H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.78, 163.34, 142.62, 137.23, 130.26, 129.87, 128.58, 126.95, 122.65, 120.67, 21.69; GC-MS m/z calcd. for $C_{15}H_{11}ClN_2O$: 270.1, found: 270.0



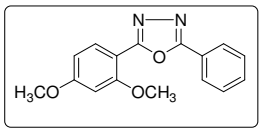
2-Phenyl-5-(thiophen-2'-yl)-1,3,4-oxadiazole (**6m**)[2b]: Yellow solid (66 mg, 85%), mp 114-115 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.09 (m, 2H), 7.85-7.79 (m, 1H), 7.61-7.50 (m, 4H), 7.19 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.01, 160.83, 131.79, 130.11, 129.80, 129.10, 126.97, 125.26, 123.72; GC-MS m/z calcd. for $C_{12}H_8N_2OS$: 228.0, found: 228.0



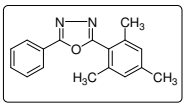
2-(4'-Methoxyphenethyl)-5-phenyl-1,3,4-oxadiazole (**6n**) : Yellow liquid (50 mg, 74%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, J = 7.7, 1.4Hz, 1H), 7.51-7.46 (m, 2H), 7.16-7.11 (m, 3H), 6.85-6.81 (m, 3H), 3.76 (s, 3H), 3.22 (t, J = 7.7 Hz, 1H), 3.12 (t, J = 7.5 Hz, 1H), 2.90 (t, J = 7.7 Hz, 1H), 2.64 (t, J = 7.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.62, 158.28, 132.43, 129.46, 129.29, 129.17, 126.96, 114.28, 114.14, 55.48, 35.50, 29.52; GC-MS m/z calcd. for $C_{17}H_{16}N_2O_2$: 280.1, found: 280.0



2-(3'-Methylphenyl)-5-phenyl-1,3,4-oxadiazole (6o) : Light pink solid, (56 mg, 70%), mp 92 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20-8.15 (m, 2H), 8.01-7.94 (m, 2H), 7.59-7.54 (m, 3H), 7.47-7.37 (m, 2H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.77, 164.53, 138.99, 132.56, 131.69, 129.08, 129.00, 127.47, 126.94, 124.10, 124.01, 123.81, 21.41. GC-MS m/z calcd. for $C_{15}H_{12}N_2O$: 236.1, found: 236.0



2-(2',4'-Dimethoxyphenyl)-5-phenyl-1,3,4-oxadiazole (6p): White solid (41 mg, 60%), mp 85°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.0 Hz, 2H), 7.94 (d, *J* = 8.6 Hz, 1H), 7.51-7.49 (m, 3H), 6.61 (d, *J* = 8.6 Hz, 1H), 6.57 (s, 1H), 3.96 (s, 3H), 3.87 (s, 3H) ; ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.76, 163.42, 159.45, 131.88, 131.40, 129.05, 126.95, 124.42, 106.11, 105.62, 99.20, 56.22, 55.73. GC-MS m/z calcd. for $C_{16}H_{14}N_2O_3$: 282.1, found: 282.0

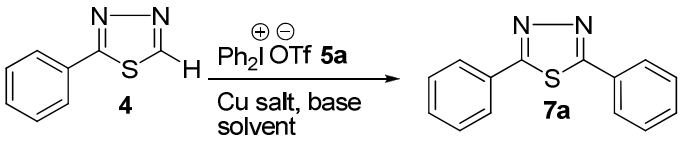


2-(Mesityl)-5-phenyl-1,3,4-oxadiazole (6q)[2e]**:** White solid (7 mg, 8%), mp 93 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.08 (m, 2H), 7.58-7.48 (m, 3H), 7.00 (s, 2H), 2.36 (s, 3H), 2.33 (s, 6H). GC-MS m/z calcd. for $C_{17}H_{16}N_2O$: 264.1, found: 264.0

3. 2,5-Diaryl-1,3,4-thiadiazoles

(i) Optimization of reaction conditions for 2,5-diaryl-1,3,4-thiadiazoles

Table 2 Optimization for the arylation of 2-phenyl-1,3,4-thiadiazole **4** using **5a**[a]



entry	catalyst	base	solvent	yield (%)
1[b]	CuBr	*t*-BuOK	PEG-400	trace
2[b]	CuBr	Cs_2CO_3	PEG-400	trace
3[b]	CuBr	K_3PO_4	PEG-400	NR
4[b]	CuI	*t*-BuOK	DMSO	30
5[b]	CuBr	*t*-BuOK	DMSO	35
6[b]	CuBr	*t*-BuOLi	DMF	83

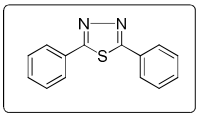
[a]A mixture of **4** (1 equiv.), **5a** (1 equiv.), Cu catalyst (30 mol%), base (3.5 equiv) was stirred in DMF for 15 min. at rt. [b]stirring at rt for 10-15 min, NR = no reaction

(ii) Typical experimental procedure for 2,5-diaryl-1,3,4-thiadiazoles (**7a**)

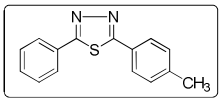
To a stirred solution of thiadiazole **4** (100 mg, 0.617 mmol) and CuBr (26.4 mg, 0.136 mmol) in DMF (2 mL), *t*-BuOLi (172 mg, 2.16 mmol,) was charged and stirred at room temperature for 5 min. Then appropriate amount of diaryliodonium triflate **5a** (265 mg, 0.617 mmol) was added in portions. The reaction mixture was stirred at room temperature for 15 min. Completion of the reaction was confirmed by TLC (4:1 hexane:ethylacetate). Then the resulting reaction mixture was added to ice-cold water and extracted with EtOAc (3 × 5 mL). The combined organic layer was washed with ammonia, brine solution

and dried over Na_2SO_4. The solvent was removed and the obtained crude product was purified by column chromatography eluting with 10% EtOAc/hexane to afford **7a** in 83% yield.

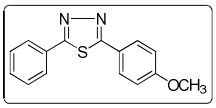
(iii) Analytical data for 2,5-diaryl-1,3,4-thiadiazoles (**7a-f**)



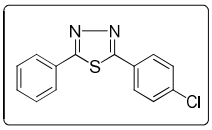
2,5-Diphenyl-1,3,4-thiadiazole (**7a**)[3]: White solid (121 mg, 83%), mp 132 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.18-8.13 (m, 4H), 7.70-7.62 (m, 6H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 164.48, 132.55, 129.92, 127.19, 123.77.



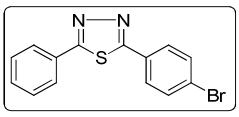
2-(4'-Methylphenyl)-5-phenyl-1,3,4-thiadiazole (**7b**)[3]: White solid (56 mg, 72%), mp 122 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.13 (m, 2H), 8.03 (d, *J* = 8.1 Hz, 2H), 7.55-7.52 (m, 3H), 7.34 (d, *J* = 8.1Hz, 2H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.71, 164.32, 142.29, 131.62, 129.73, 128.99, 126.81, 124.06, 121.18, 21.57.



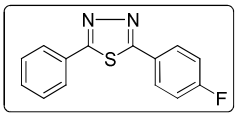
2-(4'-Methoxylphenyl)-5-phenyl-1,3,4-thiadiazole (**7c**)[3]: White solid, (64 mg, 78%), mp 136 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.13 (m, 2H), 8.11-8.06 (dd, *J* = 8.96, 2.1 Hz, 2H), 7.56-7.55 (m, 3H), 7.07(dd, *J* = 8.96, 2.1 Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.55, 164.16, 162.39, 131.54, 128.98, 128.73, 126.80, 124.08, 116.42, 114.48, 55.24.



2-(4'-Chlorophenyl)-5-phenyl-1,3,4-thiadiazole (**7d**)[3]: White solid (70 mg, 84%), mp 180 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.00 (m, 2H), 7.99-7.95 (m, 2H), 7.54-7.47 (m, 5H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.33, 166.88, 137.24, 131.27, 130.03, 129.49, 129.24, 129.09, 128.70, 127.98.



2-(4'-Bromophenyl)-5-phenyl-1,3,4-thiadiazole (**7e**)[3]: White solid (80 mg, 82%), mp 152 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 7.5, 1.9 Hz, 2H), 8.12-8.06 (m, 2H), 7.59-7.53 (m, 4H), 7.52 (d, *J* = 1.6 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.99, 160.09, 134.43, 128.30, 125.90, 125.54, 124.60, 123.38, 120.09, 118.69.



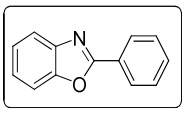
2-(4-Fluorophenyl)-5-phenyl-1,3,4-thiadiazole (**7f**): White solid (65 mg, 83%), mp 173 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.00 (m, 4H), 7.54-7.52 (m, 3H), 7.22 (t, *J* = 8.6 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.72, 163.18, 131.20, 130.12, 129.98, 129.90, 129.23, 127.95, 116.53, 116.31. GC-MS m/z calcd. for $C_{14}H_9FN_2S$: 256.0, found: 256.0

4. 2-Arylbenzoxazoles

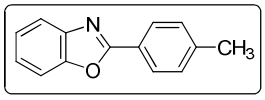
(i) Typical experimental procedure for 2-arylbenzoxazoles (**10a)**

To the oven dried 10 mL round bottomed flask, benzoxazole **8a** (100 mg, 0.840 mmol), CuBr (24 mg, 0.136 mmol) and DMSO (2 mL) were added. Then *t*-BuOLi (201 mg, 2.52 mmol) was charged and stirred at room temperature for 5 min. Then diphenyliodonium triflate **5a** (361mg, 0.840 mmol) was added portionwise. The reaction mixture was allowed to stir for 15 min. After completion, the reaction mixture was added to ice-cold water and extracted with EtOAc (3 × 5 mL). The combined organic layer was washed with ammonia and brine solutions, and dried over Na_2SO_4. The combined organic layer was evaporated and crude product was obtained. The pure **10a** was isolated in 89%yield by column chromatography using 10% EtOAc/Hexane as an eluent.

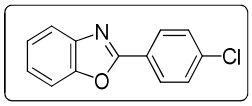
(ii) Analytical data for 2-arylbenzoxazoles (**10a-n)**



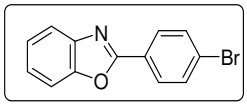
2-Phenylbenzoxazole (**10a**)[4a]**:** White solid (145 mg, 89%), mp 102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28-8.25 (m, 2H), 7.79-7.77 (m,1H), 7.60-7.58 (m, 1H), 7.55-7.52 (m, 3H), 7.37-7.35 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.08, 150.81, 142.16, 131.62, 129.01, 127.74, 127.29, 125.21, 124.68, 120.13, 110.59; GC-MS m/z calcd. for $C_{13}H_9NO$: 195.1, found: 195.0



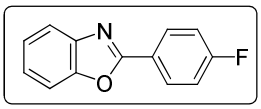
2-(4'-Methylphenyl)benzoxazole (**10b**)[4a]: White solid (69 mg, 79%), mp 113 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.2 Hz, 2H), 7.79-7.73 (m, 1H), 7.59-7.53 (m, 1H), 7.35-7.32 (m, 4H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.33, 150.72, 142.20, 142.08, 129.63, 127.62, 124.88, 124.50, 124.43, 119.99, 110.73, 21.74; GC-MS m/z calcd. for $C_{14}H_{11}NO$: 209.1, found: 209.0



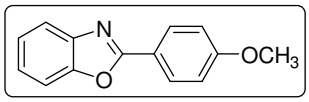
2-(4'-Chlorophenyl)benzoxazole (**10c**)[4a]**:** White solid, (79 mg, 83%), mp 148 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.4 Hz, 2H), 7.79-7.76 (m,1H), 7.60-7.56 (m, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.37-7.36 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.09, 150.85, 142.06, 137.74, 129.22, 128.88, 125.69, 125.37, 124.77, 119.94, 110.65; GC-MS m/z calcd. for $C_{13}H_8ClNO$: 229.0, found: 229.0



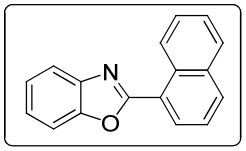
2-(4'-Bromophenyl)benzoxazole (10d)[4b]**:** Off white solid (102 mg, 89%), mp 158 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.0 Hz, 2H), 7.79-7.76 (m, 1H), 7.68 (d, *J* = 8.0 Hz, 2H), 7.60-7.57 (m, 1H), 7.38-7.36 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.02, 150.70, 142.02, 132.23, 129.00, 126.17, 126.11, 125.39, 124.77, 120.13, 110.65; GC-MS m/z calcd. for $C_{13}H_8BrNO$: 273.0, found: 273.0



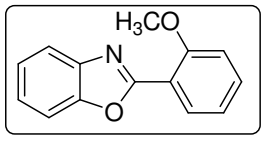
2-(4'-Fluorophenyl)benzoxazole (10e)[4b]**:** Off white solid (78 mg, 88%), mp 97 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28-8.25 (m, 2H), 7.78-7.76 (m, 1H), 7.59-7.56 (m, 1H), 7.37-7.35 (m, 2H), 7.26-7.20 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.08, 163.57, 150.75, 142.06, 129.89, 129.80, 125.13, 124.68, 123.53, 123.50, 120.00, 116.32, 116.10, 110.32. GC-MS m/z calcd. for $C_{13}H_8FNO$: 213.1, found: 213.0



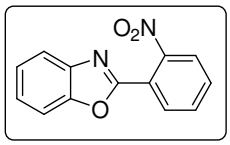
2-(4'-Methoxyphenyl)benzoxazole(10f)[4c]: White solid (68 mg, 72%), mp 98 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.9, 2.1Hz, 3H), 7.91-7.84 (m, 1H), 7.50-7.43 (m, 1H), 7.38-7.34 (m, 1H), 7.03 (dd, *J* = 8.8, 2.0Hz, 2H), 3.88 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.27, 162.02, 134.53, 129.03, 126.70, 124.37, 122.88, 121.67, 114.31, 55.68, 7.71. GC-MS m/z calcd. for $C_{14}H_{11}NO_2$: 225.0, found: 225.0



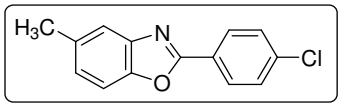
2-(Naphthalen-1'-yl)benzoxazole (10g)[4c]: Pale yellow solid (68 mg, 67%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.50 (dd, *J* = 8.6, 1.1Hz, 1H), 8.47 (dd, *J* = 7.3, 1.2 Hz, 1H), 8.07 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.94-7.89 (m, 1H), 7.74-7.71 (m, 1H), 7.69-7.59 (m, 3H), 7.46-7.41 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.84, 150.20, 142.33, 133.98, 132.33, 130.71, 129.35, 128.69, 127.94, 126.48, 126.29, 125.30, 124.97, 123.65, 120.30, 110.54. GC-MS m/z calcd. for $C_{17}H_{11}NO$: 245.1, found: 245.0



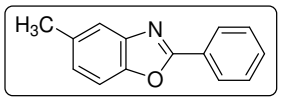
2-(2'-Methoxyphenyl)benzoxazole (10h)[4d]: White solid (68 mg, 72%), mp 54 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 9.3 Hz, 1H), 7.87-7.80 (m, 1H), 7.63-7.57 (m, 1H), 7.53 (t, *J* = 7.1 Hz, 1H), 7.39-7.32 (m, 2H), 7.14-7.10 (m, 2H), 4.04 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.45, 150.26, 142.15, 132.66, 131.29, 124.96, 124.29, 120.73, 120.13, 111.91, 110.38, 56.21. GC-MS m/z calcd. for $C_{14}H_{11}NO_2$: 225.1, found: 225.0



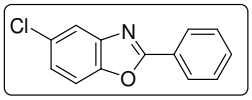
2-(2'-Nitrophenyl)benzoxazole (10i): Yellow solid (80 mg, 80%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.87 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.83-7.78 (m, 1H), 7.75-7.63 (m, 2H), 7.59-7.52 (m, 1H), 7.43-7.35 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.64, 154.10, 137.06, 135.04, 132.19, 129.30, 128.70, 126.57, 125.39, 123.33, 121.68. GC- MS m/z calcd. for $C_{13}H_8N_2O_3$: 240.1, found: 240.0



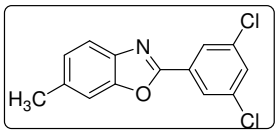
2-(4'-Chlorophenyl)-5-methylbenzoxazole (10j)[4f]**:** White solid (77 mg, 85%), mp 151 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.5 Hz, 2H), 7.56-7.42 (m, 4H), 7.17 (d, *J* = 8.2 Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.10, 162.69, 149.62, 142.94, 138.20, 135.14, 129.86, 129.42, 127.20, 126.57, 120.93, 110.57, 22.15; GC-MS m/z calcd. for $C_{14}H_{10}ClNO$: 243.0, found: 243.0



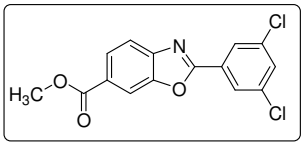
5-(Methyl-2-phenyl)benzoxaozle (10k)[4a]**:** White solid (66 mg, 85%), mp 102 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25-8.23 (m, 2H), 7.55-7.44 (m, 5H), 7.17-7.15 (m, 1H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.07, 148.99, 142.25, 134.30, 131.38, 128.88, 127.57, 127.26, 126.24, 119.94, 109.95, 21.35; GC-MS m/z calcd. for $C_{14}H_{11}NO$: 209.1, found: 209.0



5-(Chloro-2-phenyl)benzoxaozle (10l)[4a]**:** White solid (60 mg, 80%), mp 105 °C. ^{1}H NMR (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (dd, *J* = 7.6, 1.5 Hz, 2H), 7.75 (d, *J* = 2.0 Hz, 1H), 7.58-7.49 (m, 4H), 7.33 (dd, *J* = 8.6, 2.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.64, 154.10, 137.06, 135.04, 132.19, 129.30, 128.70, 126.57, 125.39, 123.33, 121.68; GC-MS m/z calcd. for $C_{13}H_8ClNO$: 229.0, found: 229.0



2-(3',5'-Dichlorophenyl)-6-methylbenzoxazole (10m)[4e]**:** White solid (72 mg, 69%), mp 146 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 1.9 Hz, 2H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.51 (d, *J* = 1.9 Hz, 1H), 7.28 (s, 1H), 7.22 (dd, *J* = 8.1, 0.9 Hz, 1H), 2.54 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.81, 151.03, 139.48, 136.56, 135.68, 130.92, 129.97, 126.30, 125.59, 119.68, 110.86, 21.87. GC-MS m/z calcd. for $C_{14}H_9Cl_2NO$: 277.0, found: 277.0

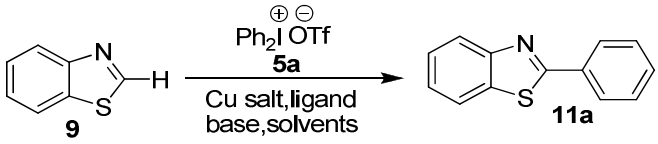


Methyl-2-(3',5'-dichlorophenyl)benzoxazole-6-carboxylate (10n)[4e]: White solid (60 mg, 67%), mp 151 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 1.4 Hz, 1H), 8.20-8.14 (m, 2H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 2.0 Hz, 1H), 7.46 (dd, *J* = 8.5, 2.1 Hz, 1H), 4.00 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.52, 162.63, 150.20, 145.33, 138.30, 134.59, 132.61, 131.61, 127.56, 126.55, 120.17, 112.49, 52.60. GC-MS m/z calcd. for $C_{15}H_9Cl_2NO_3$: 321.0, found: 321.0

5. 2-Arylbenzothiazoles

(i) Optimization of reaction conditions for 2-arylbenzothiazoles

Table 3 Optimization for the arylation of benzothiazole (**9**) using diphenyliodonium triflate (**5a**)

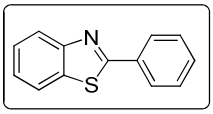


entry	catalyst/ligand	Base	solvent	yield (%)
1[a]	CuI/PPh_3	K_3PO_4	DMSO	NR
2[a]	CuBr	*t*-BuOK	DMSO	NR
3[b]	CuI/PPh_3	K_3PO4	DMSO	NR
4[b]	CuI/Phen	K_3PO4	DMF	NR
5[b]	CuI	Cs_2CO_3	DMF	NR
6[b]	CuI	*t*-BuOLi	DMF	Trace
7[b]	CuBr	*t*-BuOK	DMSO	NR
8[b]	CuBr	AgOAc	DMSO	NR
9[b]	CuBr	*t*-BuOLi	DMSO	Trace
10[b]	$Cu(OAc)_2$	*t*-BuOK	DMSO	NR
11[b]	$Cu(OAc)_2$	AgOAc	DMF	NR
12[b]	$CuCl_2$	*t*-BuOK	DMSO	NR
13[b]	$Cu(OAc)_2$	NaOAc	DMF	NR
14[b]	$Cu(OTf)_2$	AgOAc	DMF	NR
15[b]	$Pd(OAc)_2$	K_2CO_3	DMF	Trace
16[b]	$Pd(OAc)_2$/ $Cu(OAc)_2$	K_2CO_3	DMF	NR
17[c]	$Pd(OAc)_2$	*t*-BuOLi	DMF	Trace
18[c]	$Pd(OAc)_2$	AgOAc	DMF	60
19[c]	$CuBr_2$	AgOAc	DMF	NR
20[c]	CuI	Cs_2CO_3	DMSO	Trace
21[c]	CuI	AgOAc	DMSO	NR
22[c]	CuI	*t*-BuOLi	DMF	40
23[c]	CuI	*t*-BuOLi	DMSO	40
24[c]	CuI	*t*-BuOLi	PEG-400	NR
25[c]	CuI	*t*-BuOLi	NMP	NR
26[c]	CuI	*t*-BuOLi	DMA	Trace
27[c]	CuI	*t*-BuOLi	1,4-dioxane	85

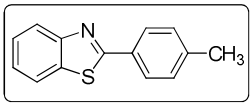
[a]A mixture of **9** (1 equiv.), **5a** (1 equiv.), Cu catalyst (30 mol%), ligand (10 mol%), and base (3.5 equiv) was stirred in DMSO for 24 h at rt. [b] Conventional heating at 130 °C for 18-24 h. [c] reaction under microwave irradiation at 130 °C for 25-30 min., NR = no reaction

(ii) Typical experimental procedure for 2-arylbenzothiazoles (**11a**):
Benzothiazole **9** (100 mg, 0.740 mmol), CuI (42 mg, 0.222 mmol) diphenyliodonium triflate **5a** (318 mg, 0.740 mmol), *t*-BuOLi (207 mg, 2.59 mmol) and 1,4-dioxane (2 mL) were charged in a sealed vial and irradiated under microwave (CEM Discover) with P = 200 w/ 100 psi at 130 °C for 30 min. Completion of the reaction was confirmed by the TLC (4:1 hexane:ethylacetate). The solvent was evaporated and extracted with EtOAc (3 × 5 mL). The organic layer was washed with ammonia and brine solutions, and dried over anhydrous Na_2SO_4 and the solvent was removed *in vacuo*. The obtained crude product was purified by column chromatography using 10% EtOAc/hexane as an eluent to obtain **11a** in 85% yield.

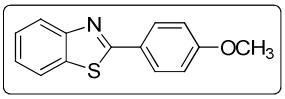
(iii) Analytical data for 2-arylbenzoxazoles **(11a-h)**



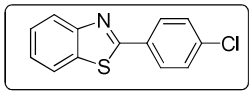
2-Phenylbenzothiazole (**11a**)[5a]**:** Yellow solid (132 mg, 85%), mp 113 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 – 8.07 (m, 3H), 7.93-7.90 (m, 1H), 7.52-7.48 (m, 4H), 7.41-7.37 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.06, 154.13, 135.09, 133.66, 130.92, 129.05, 127.59, 126.34, 125.21, 123.27, 121.61, 119.59.



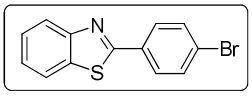
2-(4'-Methylphenyl)benzothiazole (**11b**)[5a]**:** Light yellow solid (62 mg, 75%), mp 85 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 1H), 8.01 (dd, *J* = 8.2, 1.7 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.52-7.48 (m, 1H), 7.40-7.36 (m, 1H), 7.31 (d, *J* = 7.9 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.25, 154.08, 141.44, 134.96, 130.97, 129.73, 127.51, 126.26, 125.02, 123.06, 121.58, 21.34.



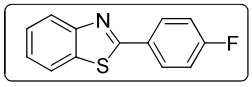
2-(4'-Methoxylphenyl)benzothiazole (**11c**)[5a]**:** Yellow solid (69 mg, 78%), mp 120 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 8.9, 2.0 Hz, 3H), 7.90 (d, *J* = 7.5 Hz, 1H), 7.52-7.47 (m, 1H), 7.47-7.35 (m, 1H), 7.03 (dd, *J* = 8.9, 2.0 Hz 2H), 3.90 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.82, 161.81, 154.09, 134.75, 129.05, 126.40, 126.24, 124.83, 122.82, 121.33, 114.45, 55.23.



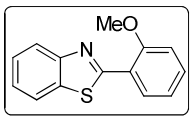
2-(4'-Chlorophenyl)benzothiazole (**11d**)[5a]**:** Yellow solid (72 mg, 80%), mp 118°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08-8.00 (m, 3H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.53-7.44 (m, 3H), 7.40 (t, *J* = 8.1 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.56, 154.15, 136.96, 135.04, 132.19, 129.30, 128.70, 126.51, 125.44, 123.33, 121.68.



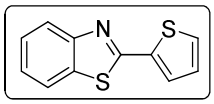
2-(4'-Bromophenyl)benzothiazole (**11e**)[5b]**:** Off white solid (89 mg, 83%), mp 133 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 7.6 Hz, 1H), 7.98 (dd, *J* =8.6, 1.9 Hz, 2H), 7.92-7.90 (m, 1H), 7.65 (dd, *J* =8.6, 1.9 Hz, 2H), 7.54-7.50 (m, 1H), 7.44-7.40 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.70, 154.04, 134.97, 132.52, 132.24, 128.91, 126.53, 125.45, 123.19, 121.68.



2-(4'-Fluorophenyl)benzothiazole (**11f**)[5a]: Yellow solid (72 mg, 85%), mp 99 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-8.04 (m, 3H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 8.2 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 8.6 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.69, 165.73, 163.28, 154.05, 135.08, 129.51, 126.44, 125.27, 123.22, 121.54, 116.08.



2-(2'-Methoxyphenyl)benzothiazole (11g)[5c]: Yellow solid (65 mg, 73%), mp 121 °C ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (dd, *J* = 7.9, 1.7 Hz, 1H), 8.10 (d, *J* = 8.2 Hz, 1H), 7.92 (d, *J* = 7.9 Hz, 1H), 7.51-7.42 (m, 2H), 7.39-7.34 (m, 1H), 7.16-7.10 (m, 1H), 7.05 (d, *J* = 8.3 Hz, 1H), 4.03 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.17, 157.21, 151.89, 135.97, 131.84, 129.53, 125.93, 124.61, 122.68, 122.09, 121.18, 111.64, 55.68. GC-MS m/z calcd. for $C_{14}H_{11}NOS$: 241.1, found: 241.0



2-(Thiophen-2'-yl)benzothiazole (**11h**)[5d]: Brown solid (62 mg, 78%), mp 99 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.2 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.65-7.64 (m, 1H), 7.50-7.45 (m, 2H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.13 (t, *J* = 8.1 Hz 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.37, 153.64, 137.35, 134.64, 129.35, 128.68, 128.10, 126.47, 125.27, 122.99, 121.51.

6. References:

1. (a) C. Ainsworth, *J. Am. Chem. Soc.*, 1955, **77**, 1148; (b) V. Polshettiwar and R. S. Varma, *Tetrahedron Lett.*, 2008, **49**, 879; (c) M. Bielawski, M. Zhu and B. Olofsson, *Adv. Synth. Catal.*, 2007, **349**, 2610; (d) M. Bielawski and B. Olofsson, *Chem. Commun.*, 2007, 2521; (e) J.-H. Chun, S. Lu and V. W. Pike, *Eur. J. Org. Chem.*, 2011, **2011**, 4439; (f) L. Kraszkiewicz and L. Skulski, *Synthesis*, 2008, **15**, 2373; (g) G. Jenkins, A. Knevel and C. Davis, *J. Org. Chem.*, 1961, **26**, 274.
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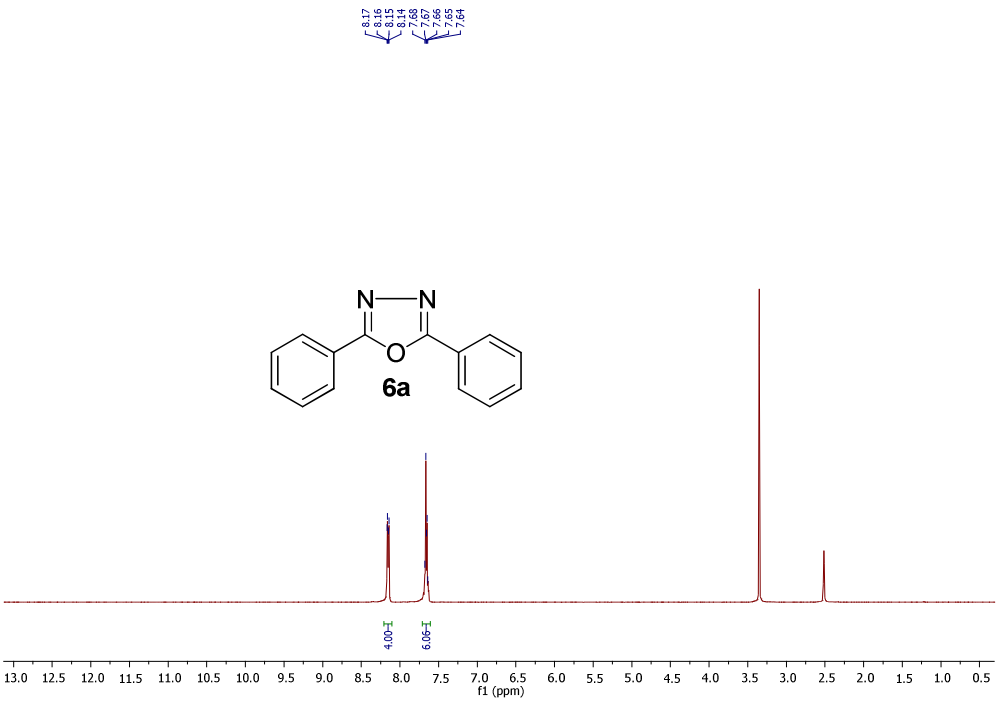
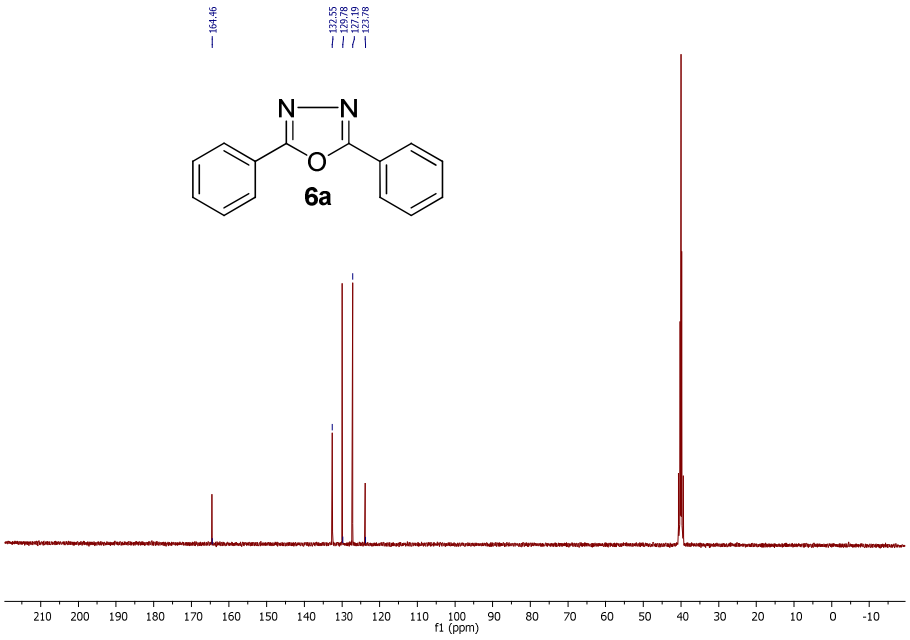
5. (a) J. R. M. Canivet, J. Yamaguchi, I. Ban and K. Itami, *Org. Lett.*, 2009, **11**, 1733; (b) U. R. Pratap, J. R. Mali, D. V. Jawale and R. A. Mane, *Tetrahedron Lett.*, 2009, **50**, 1352; (c) Z. Yang, X. Chen, S. Wang, J. Liu, K. Xie, A. Wang and Z. Tan, *J. Org. Chem.*, 2012, **77**, 7086; (d) Y.-H. Cho, C.-Y. Lee and C.-H. Cheon, *Tetrahedron*, 2013, **69**, 6565.

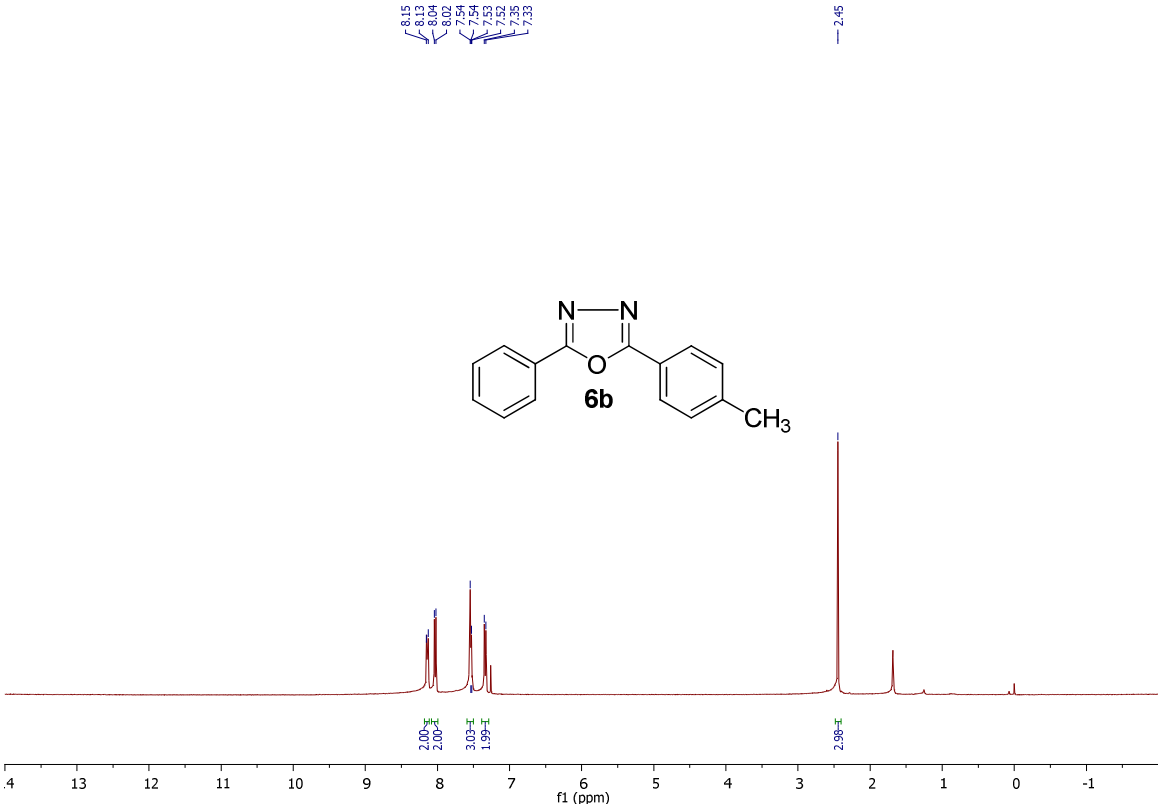
7. NMR spectra of isolated 2,5-diaryl-1,3,4-oxadiazoles **6** and 2,5-diaryl-1,3,4-thiadiazoles **7**

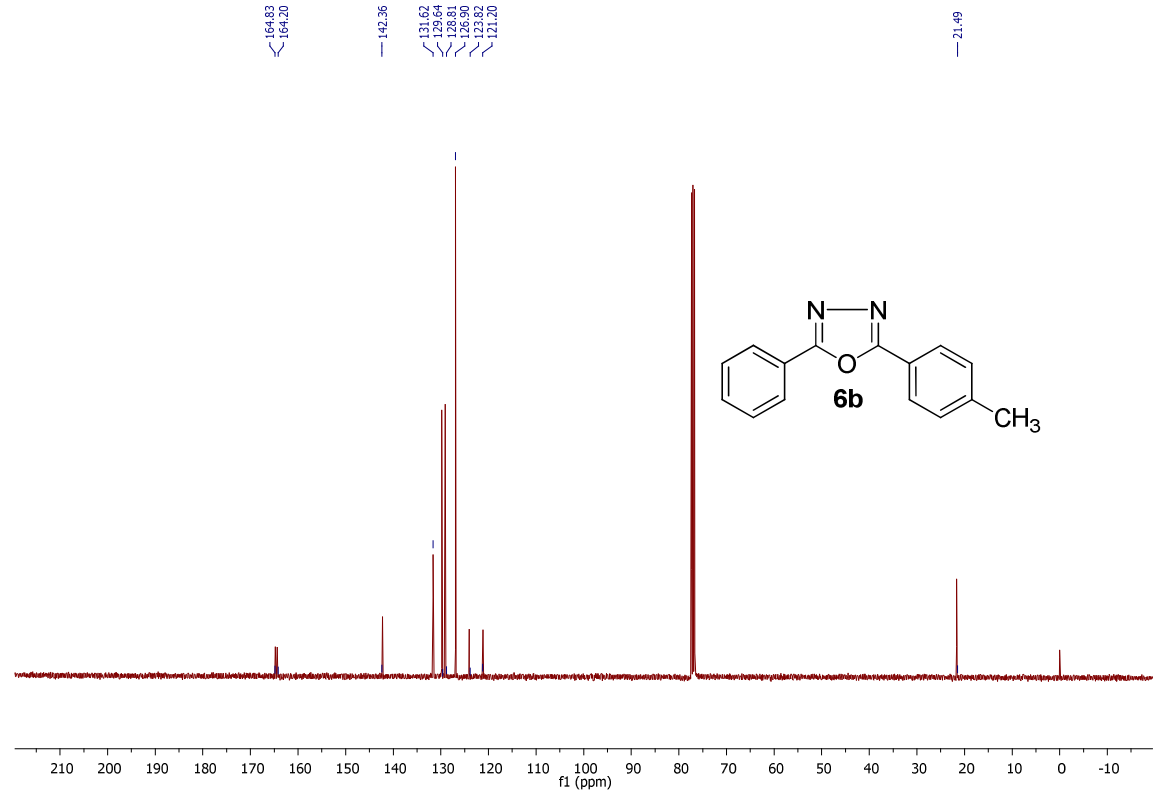
2,5-Diphenyl-1,3,4-oxadiazole (**6a**)



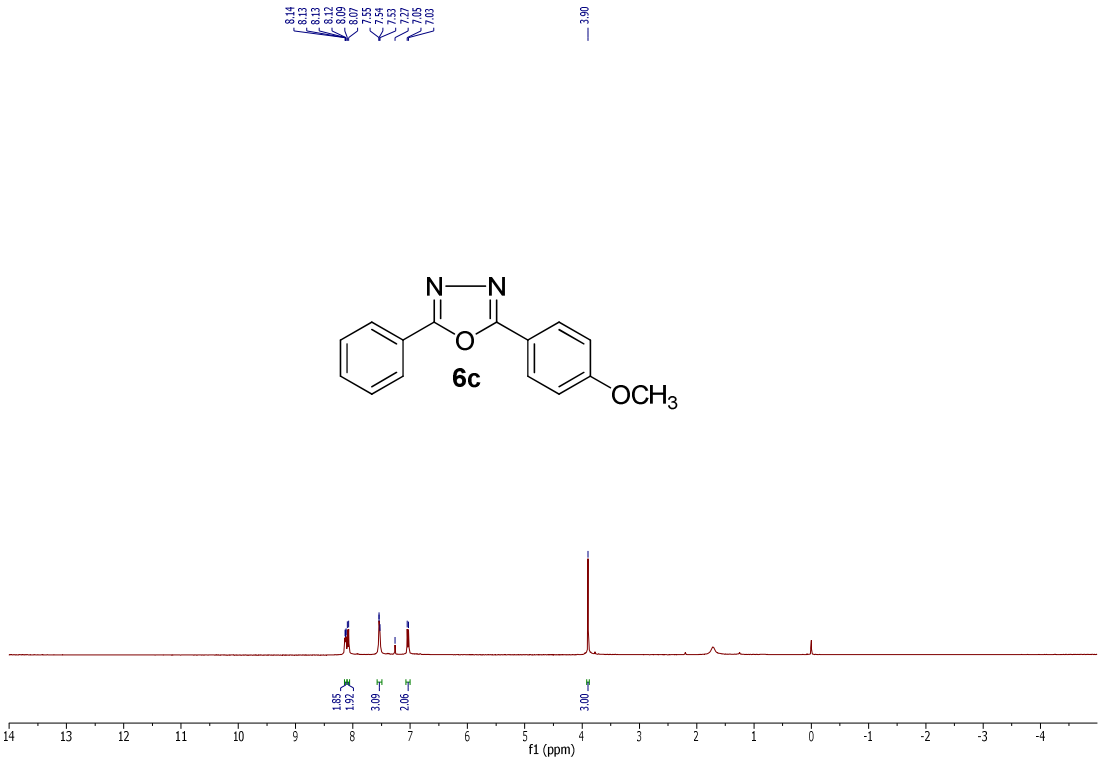


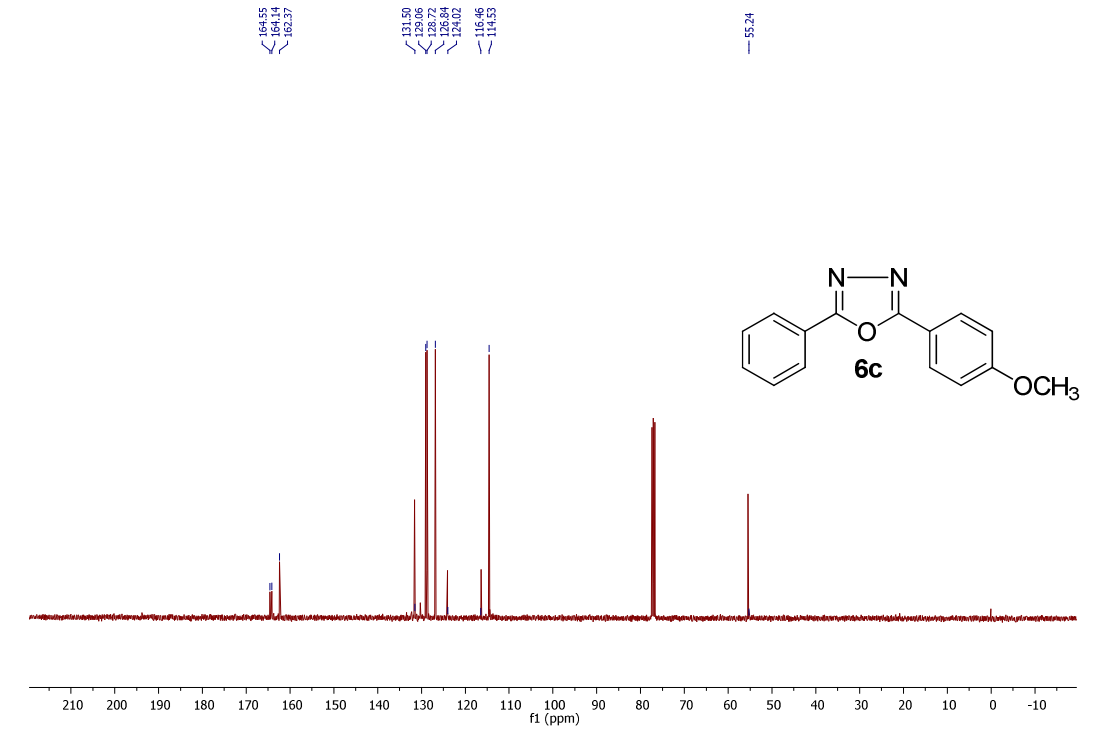
2-(4'-Methylphenyl)-5-phenyl-1,3,4-oxadiazole (6b)



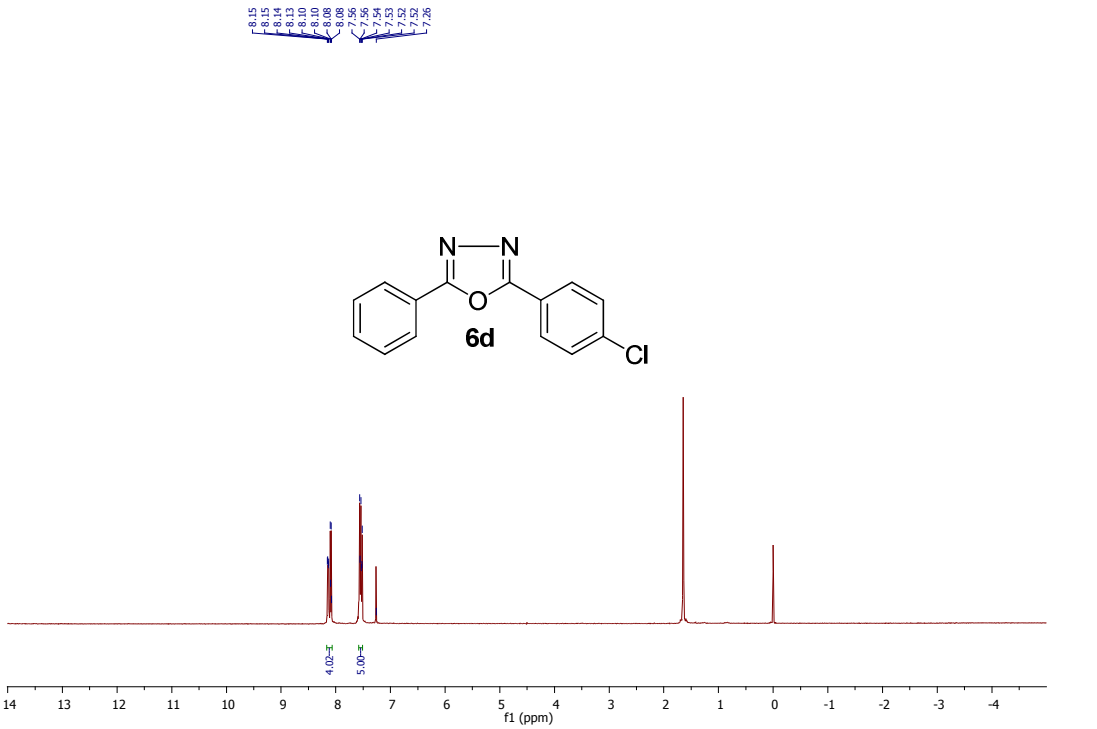


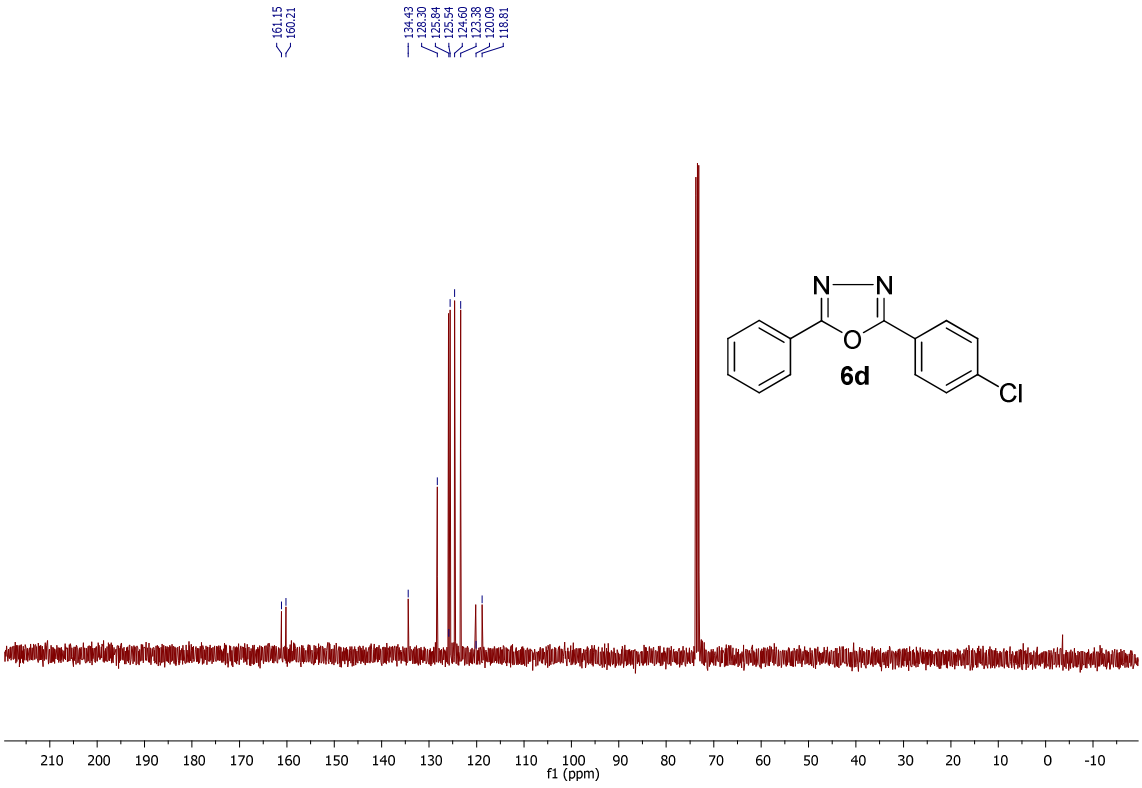
2-(4'-Methoxyphenyl)-5-phenyl-1,3,4-oxadiazole (6c)



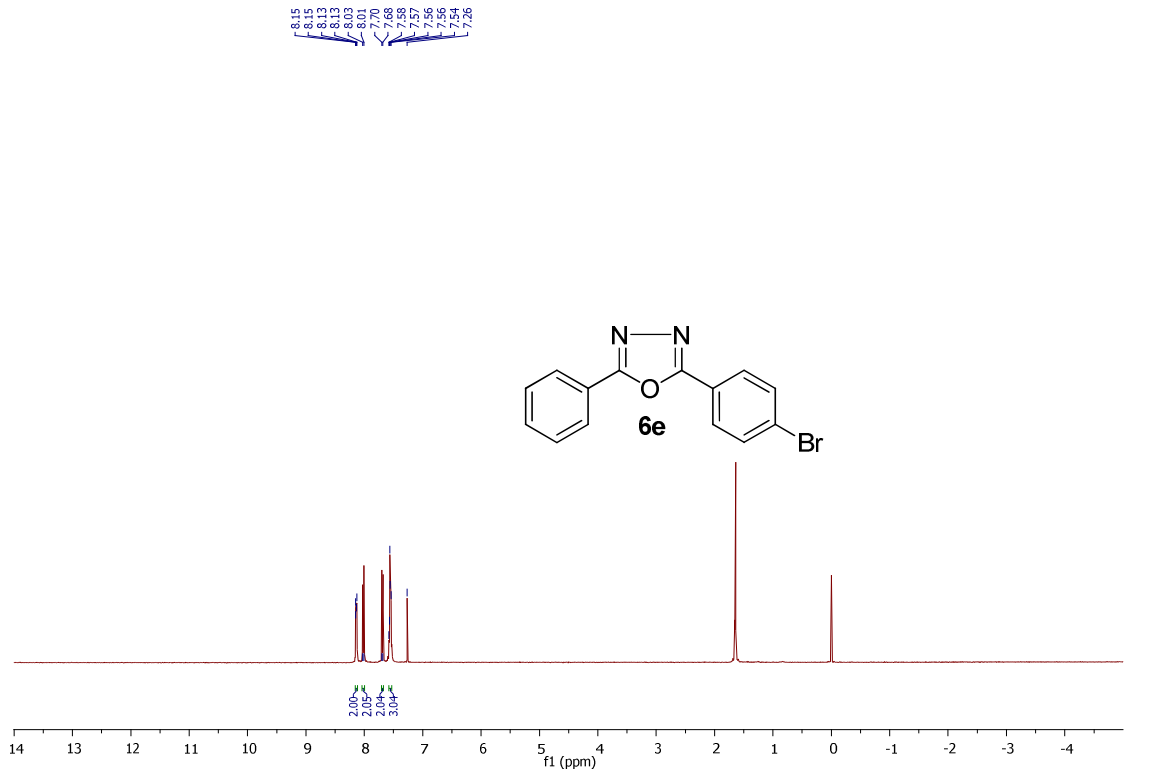


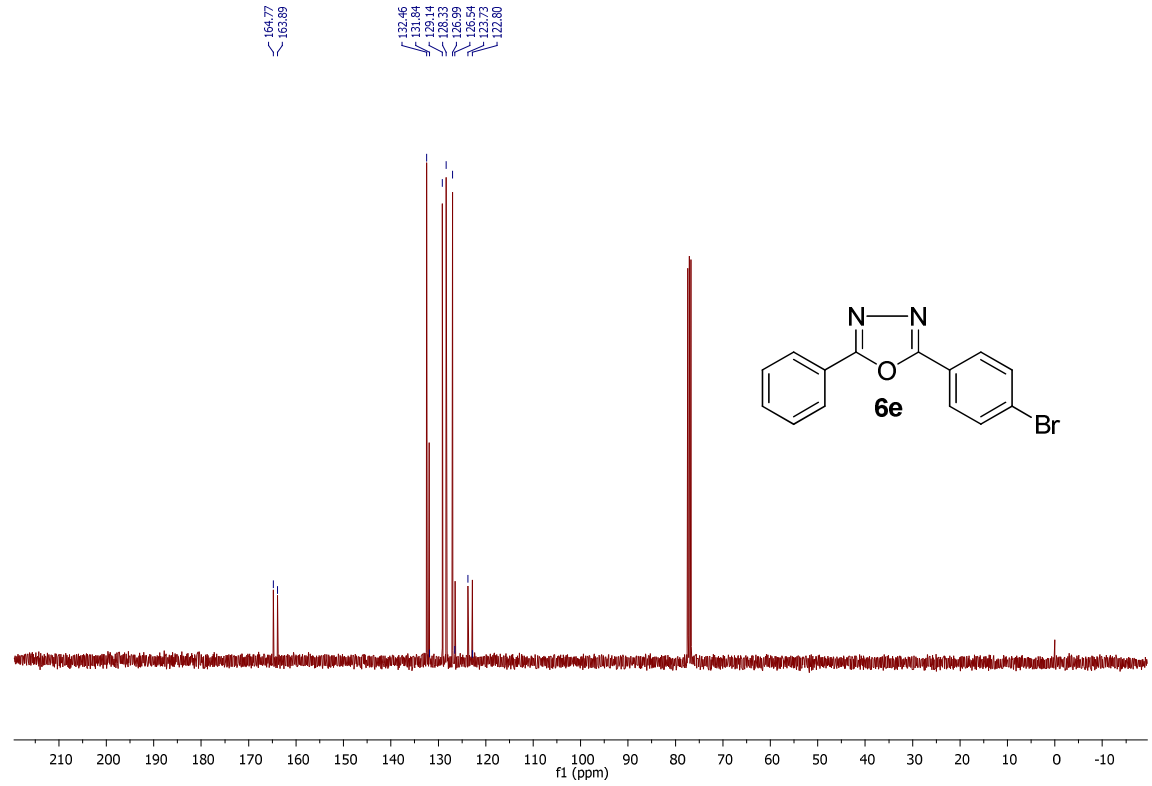
2-(4'-Chlorophenyl)-5-phenyl-1,3,4-oxadiazole (6d)



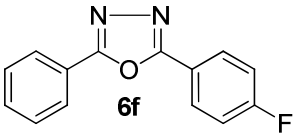


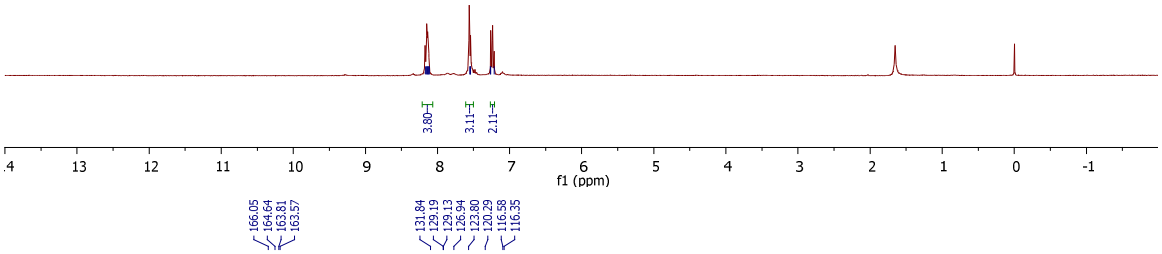
2-(4'-Bromophenyl)-5-phenyl-1,3,4-oxadiazole (6e)

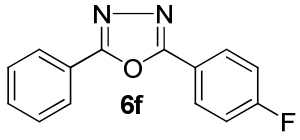


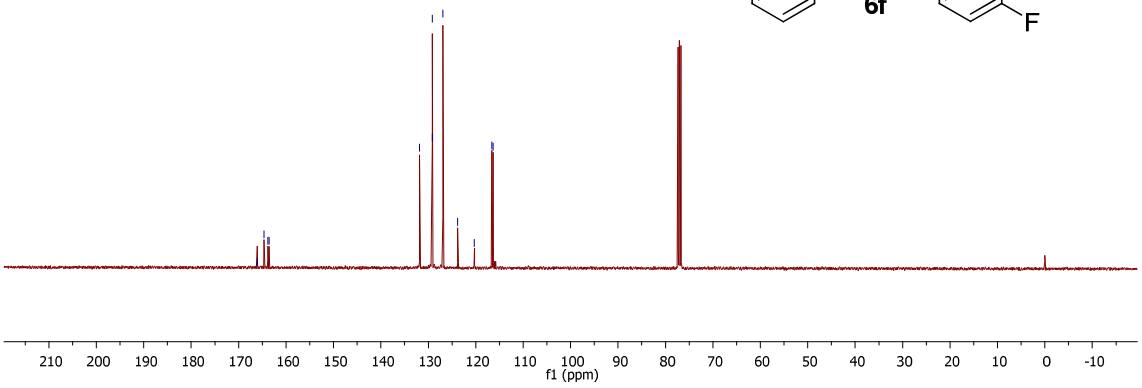


2-(4'-Fluorophenyl)-5-phenyl-1,3,4-oxadiazole (6f)

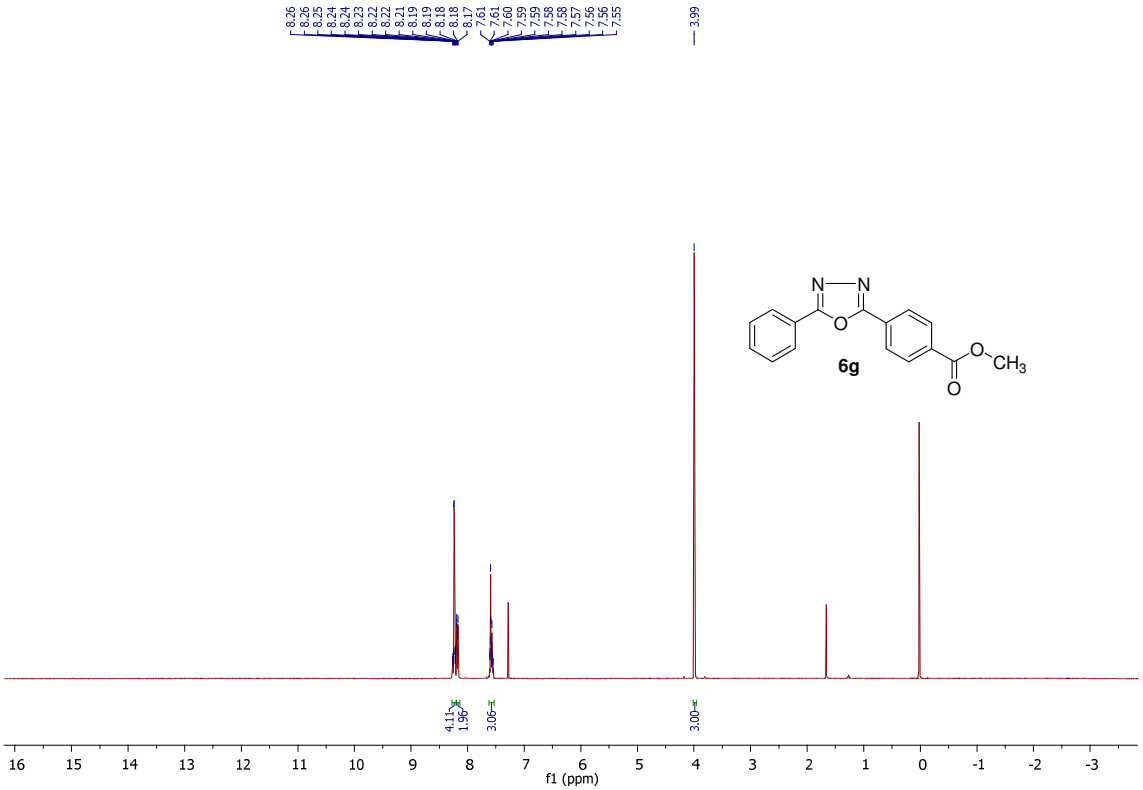


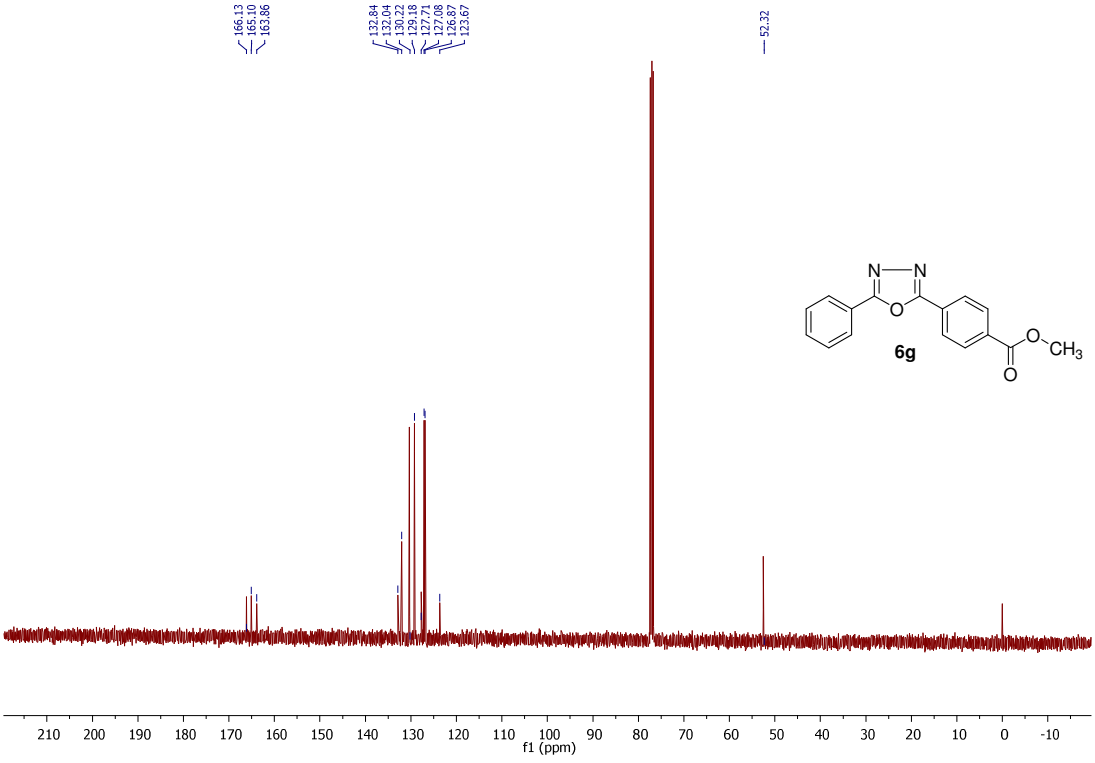




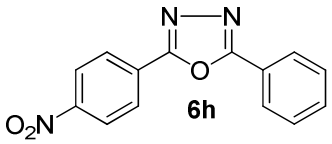


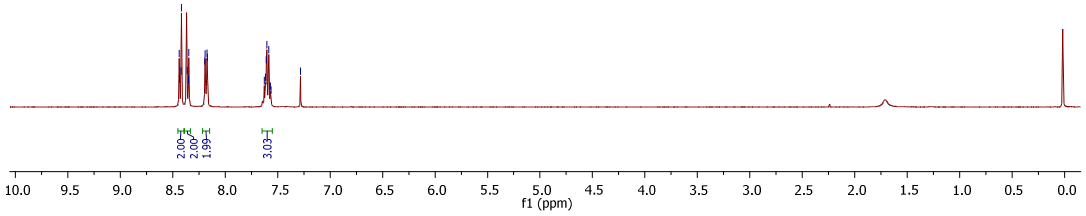
Methyl-4'-(5-phenyl-1,3,4-oxadiazol-2-yl)benzoate (6g)

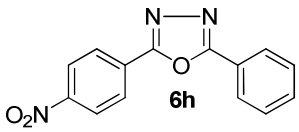




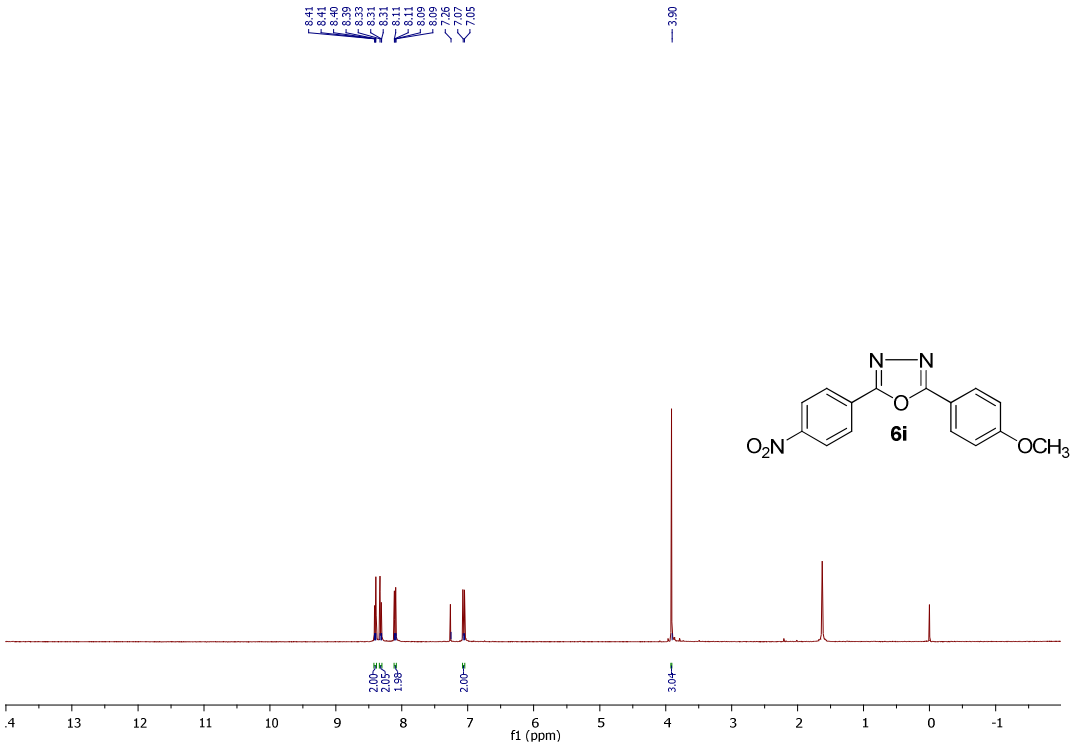
2-(4'-Nitrophenyl)-5-phenyl-1,3,4-oxadiazole (6h)

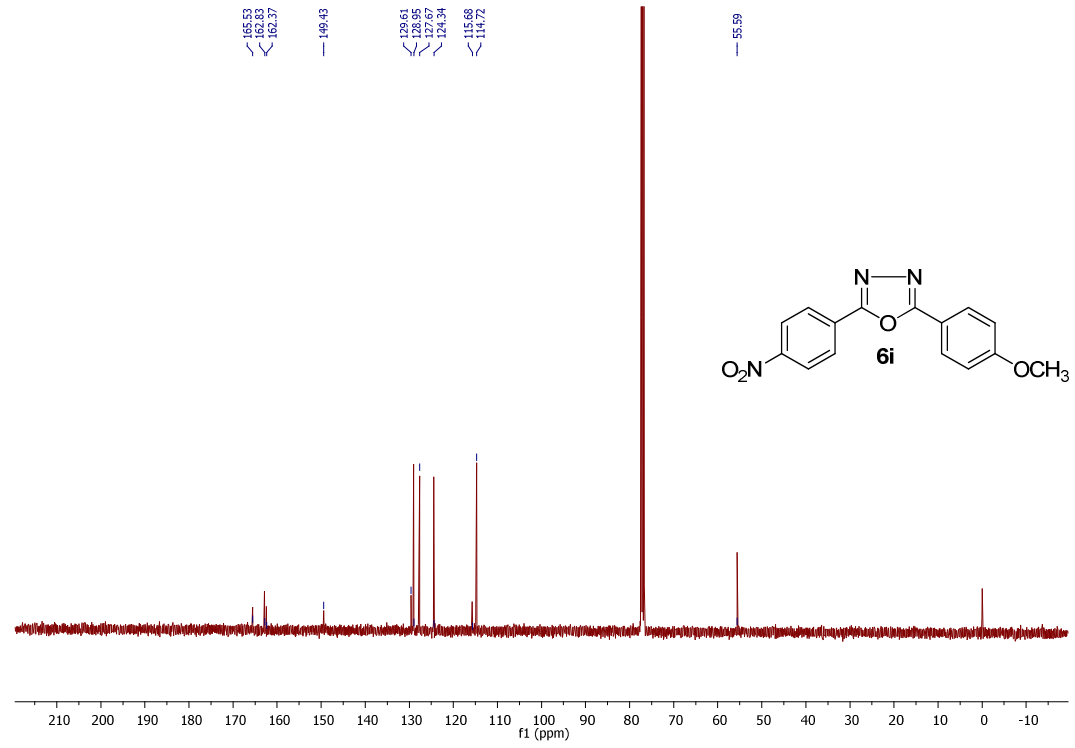




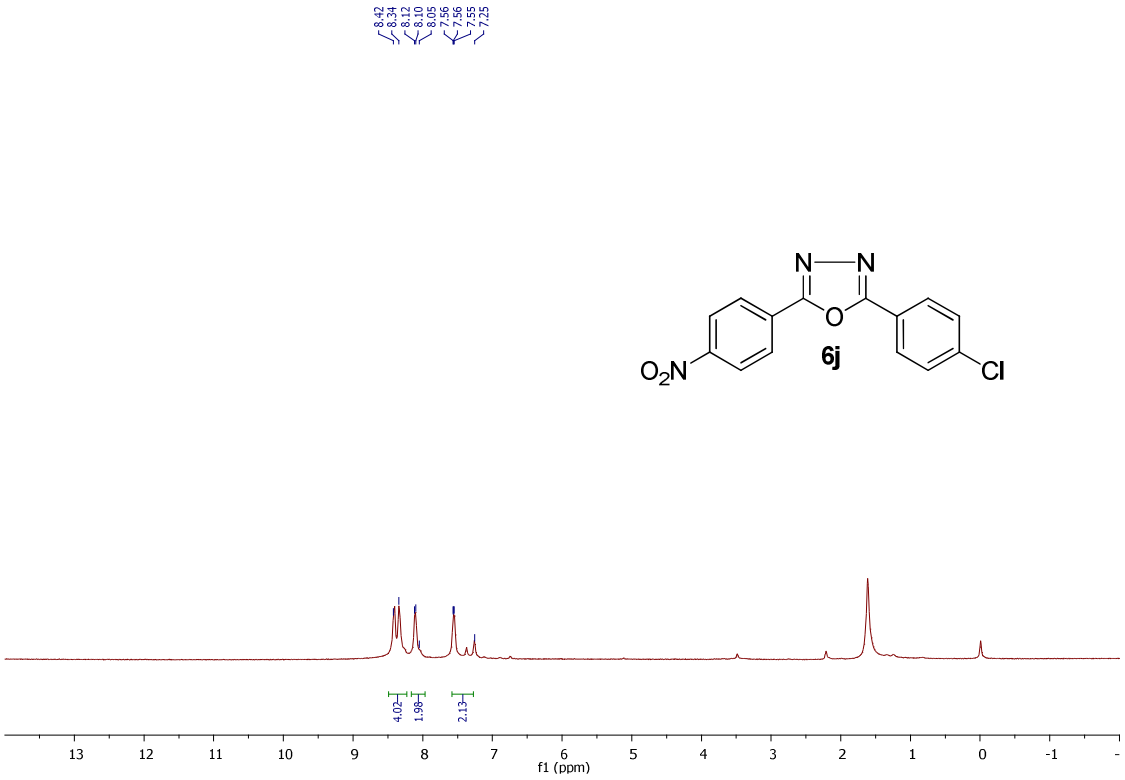


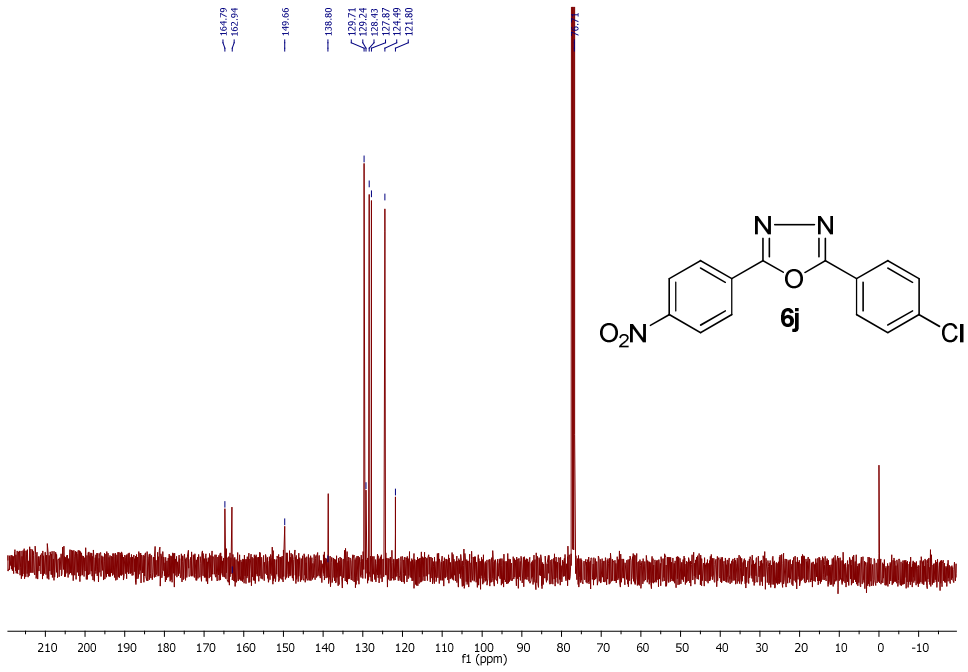
2-(4'-Methoxyphenyl)-5-(4''-nitrophenyl)-1,3,4-oxadiazole (6i)



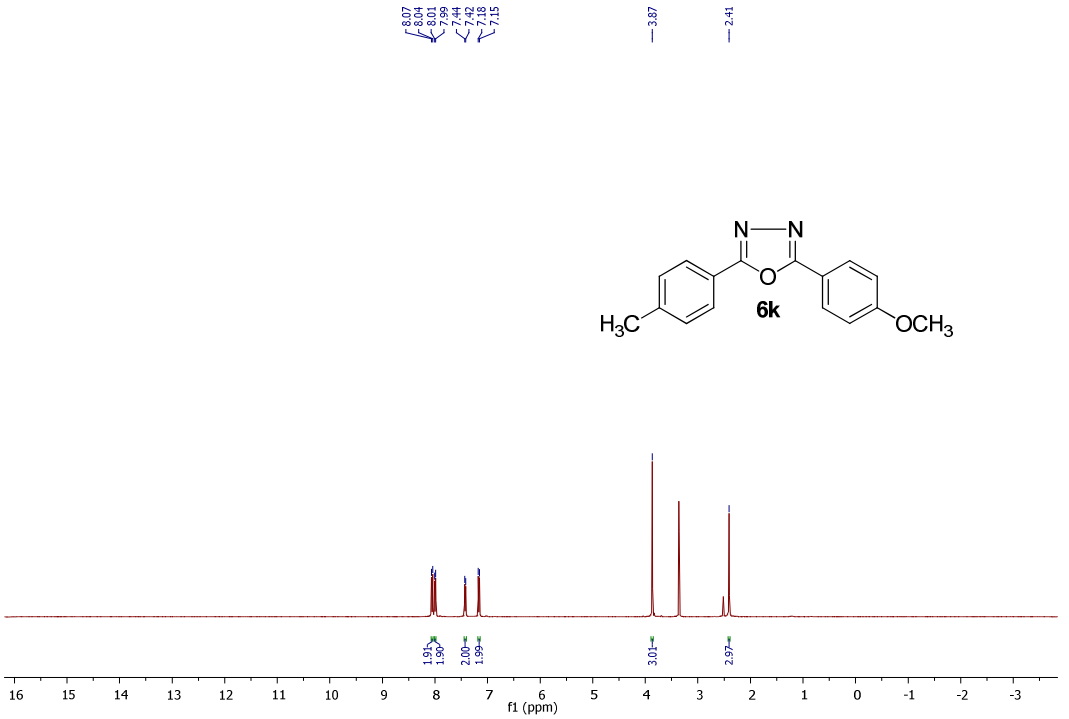


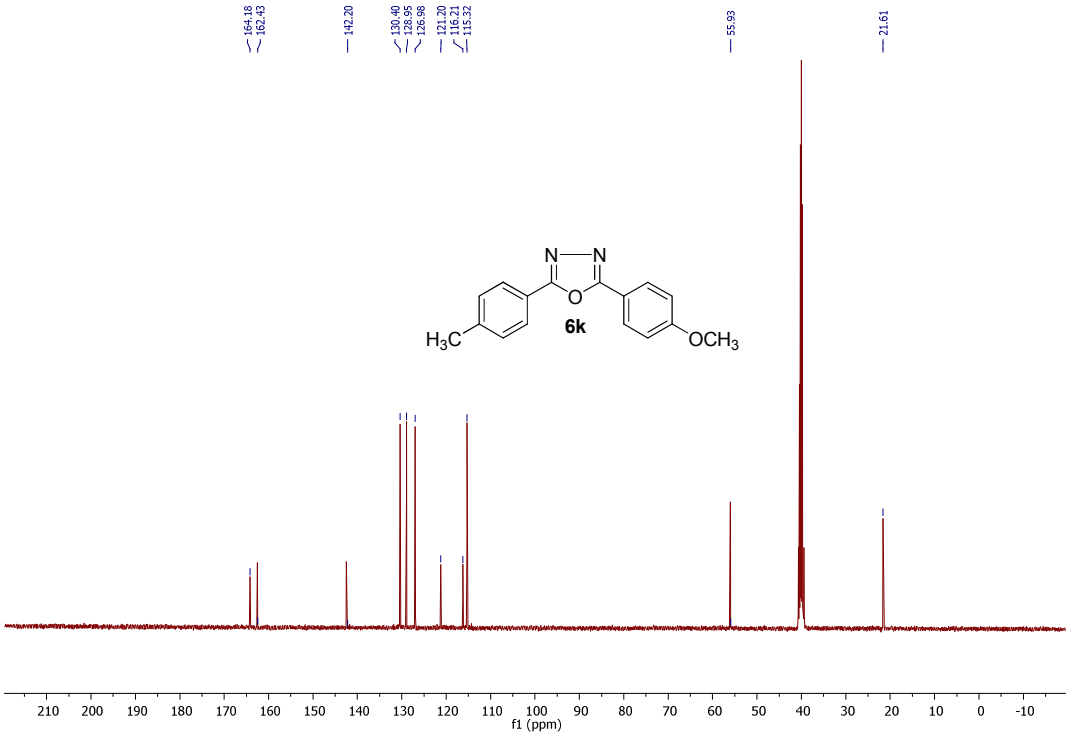
2-(4'-Chlorophenyl)-5-(4''-nitrophenyl)-1,3,4-oxadiazole (6j)



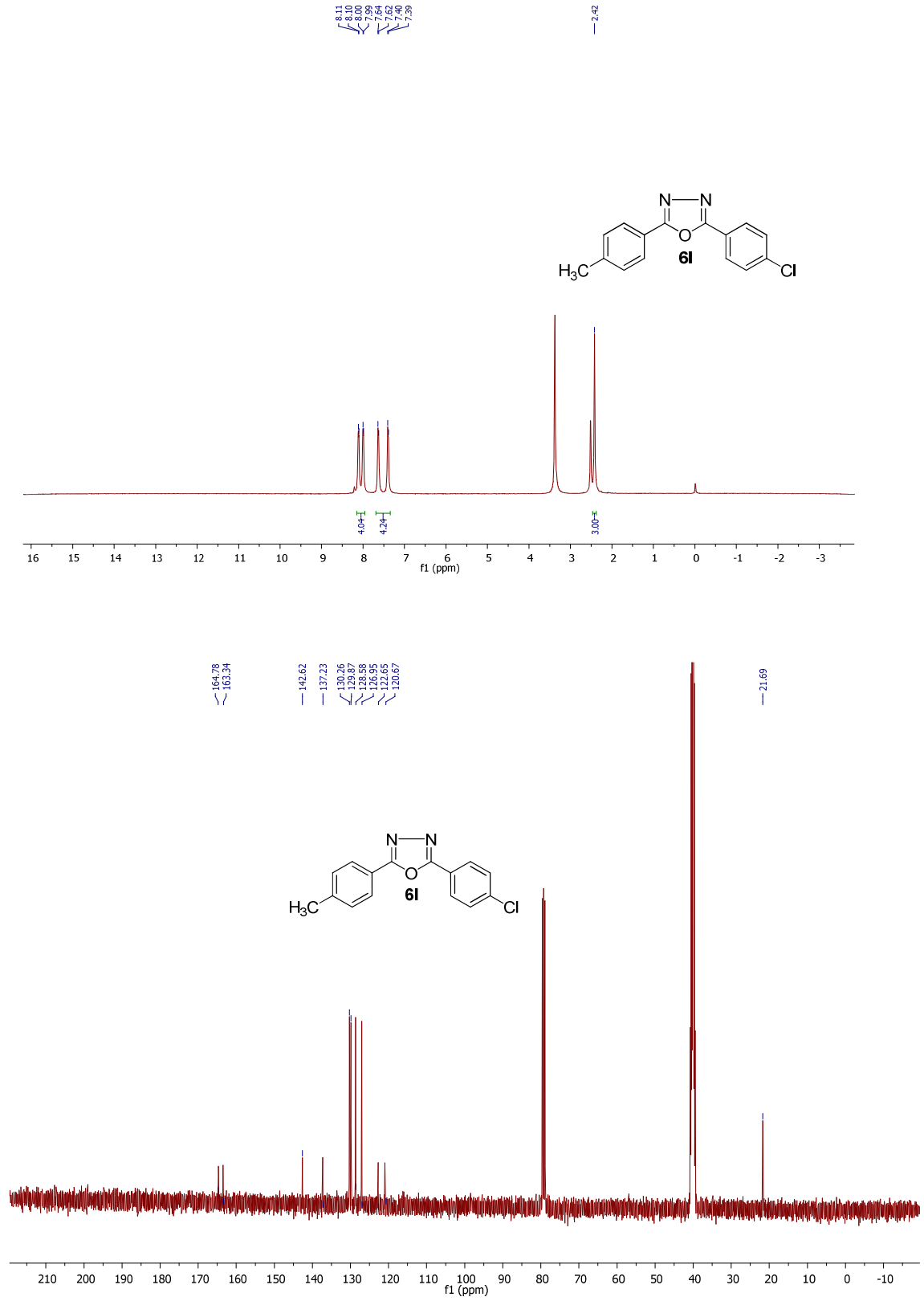


2-(4'-Methoxyphenyl)-5-(4''-methylphenyl)-1,3,4-oxadiazole (6k)

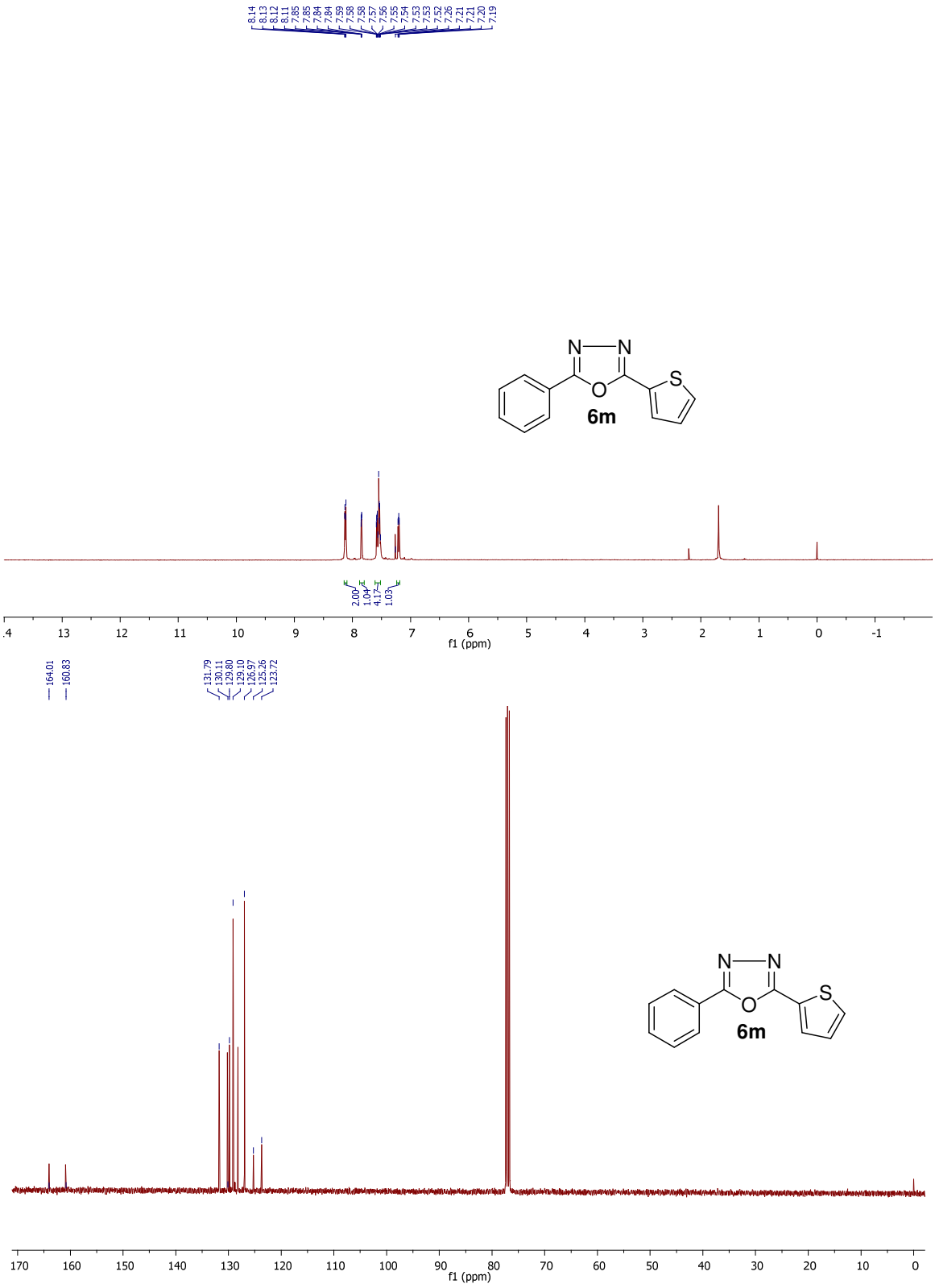




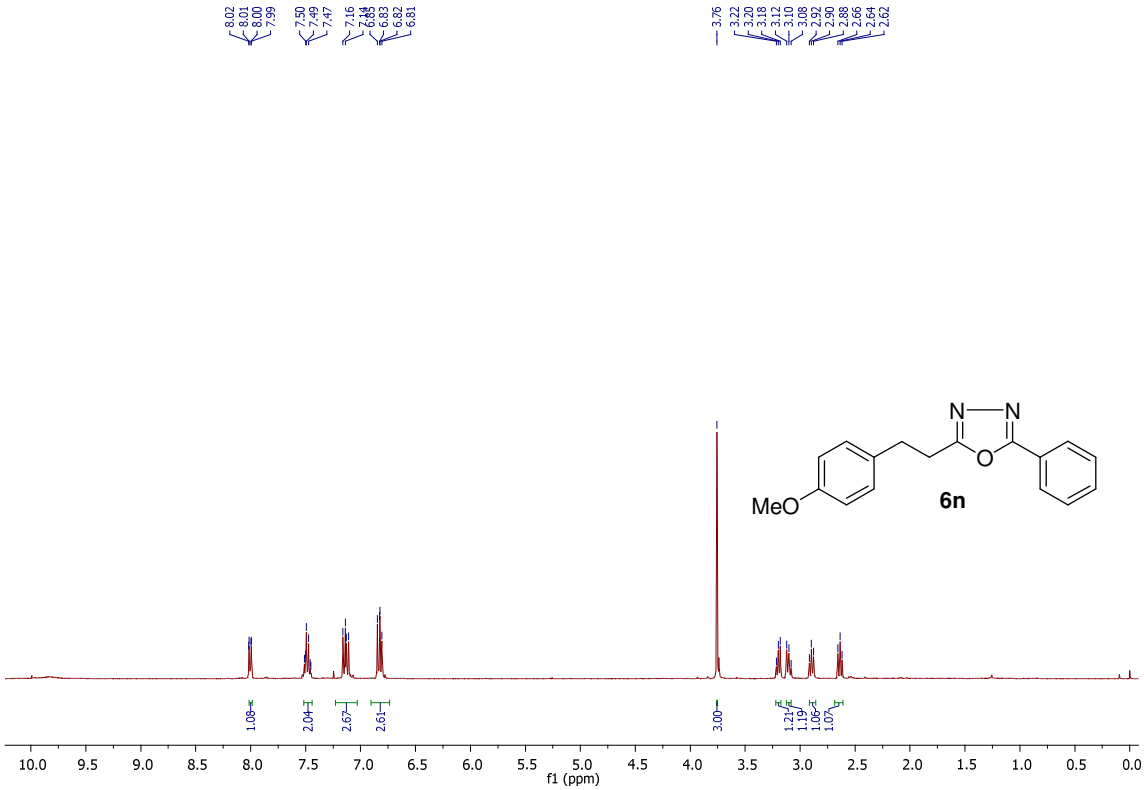
2-(4'-Chlorophenyl)-5-(4''-methylphenyl)-1,3,4-oxadiazole (6l)

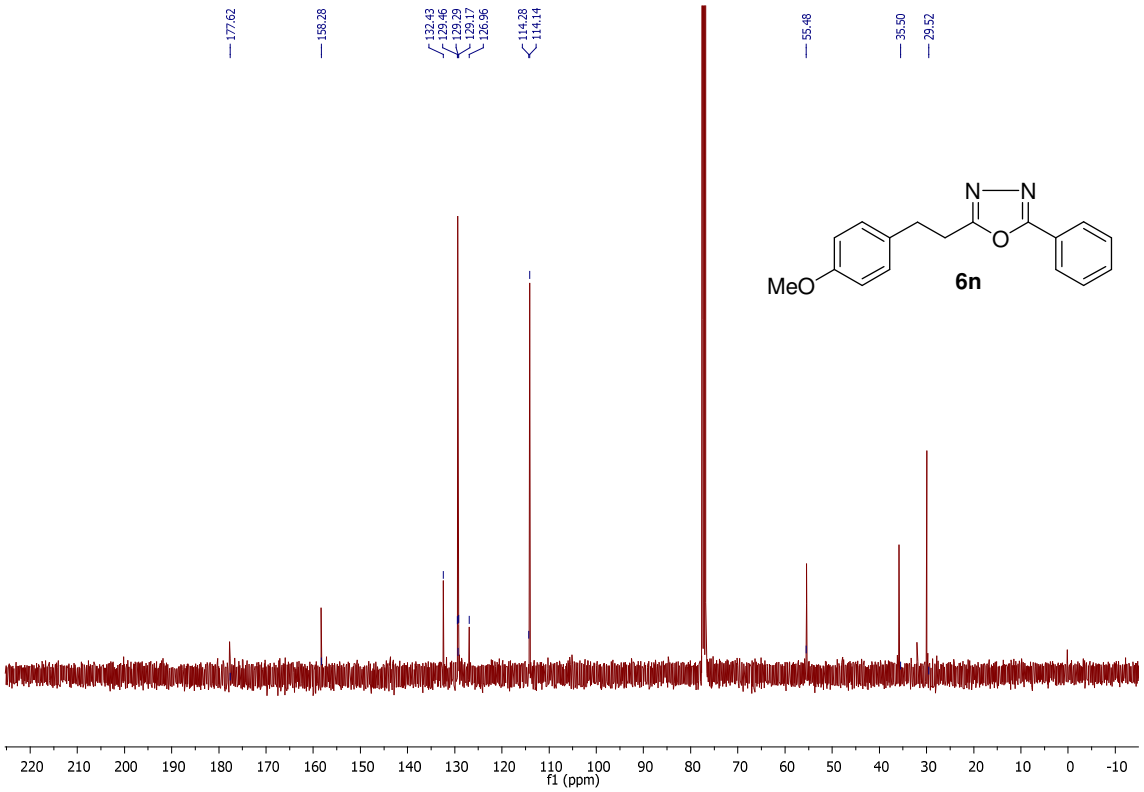


2-Phenyl-5-(thiophen-2'-yl)-1,3,4-oxadiazole (6m)

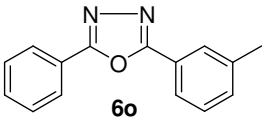


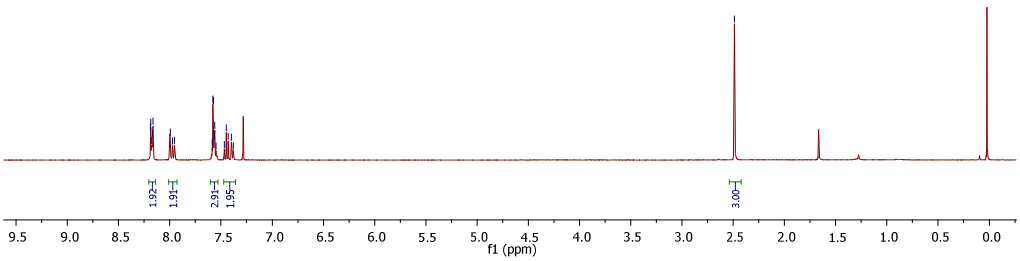
2-(4'-Methoxyphenethyl)-5-phenyl-1,3,4-oxadiazole (6n)

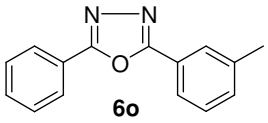




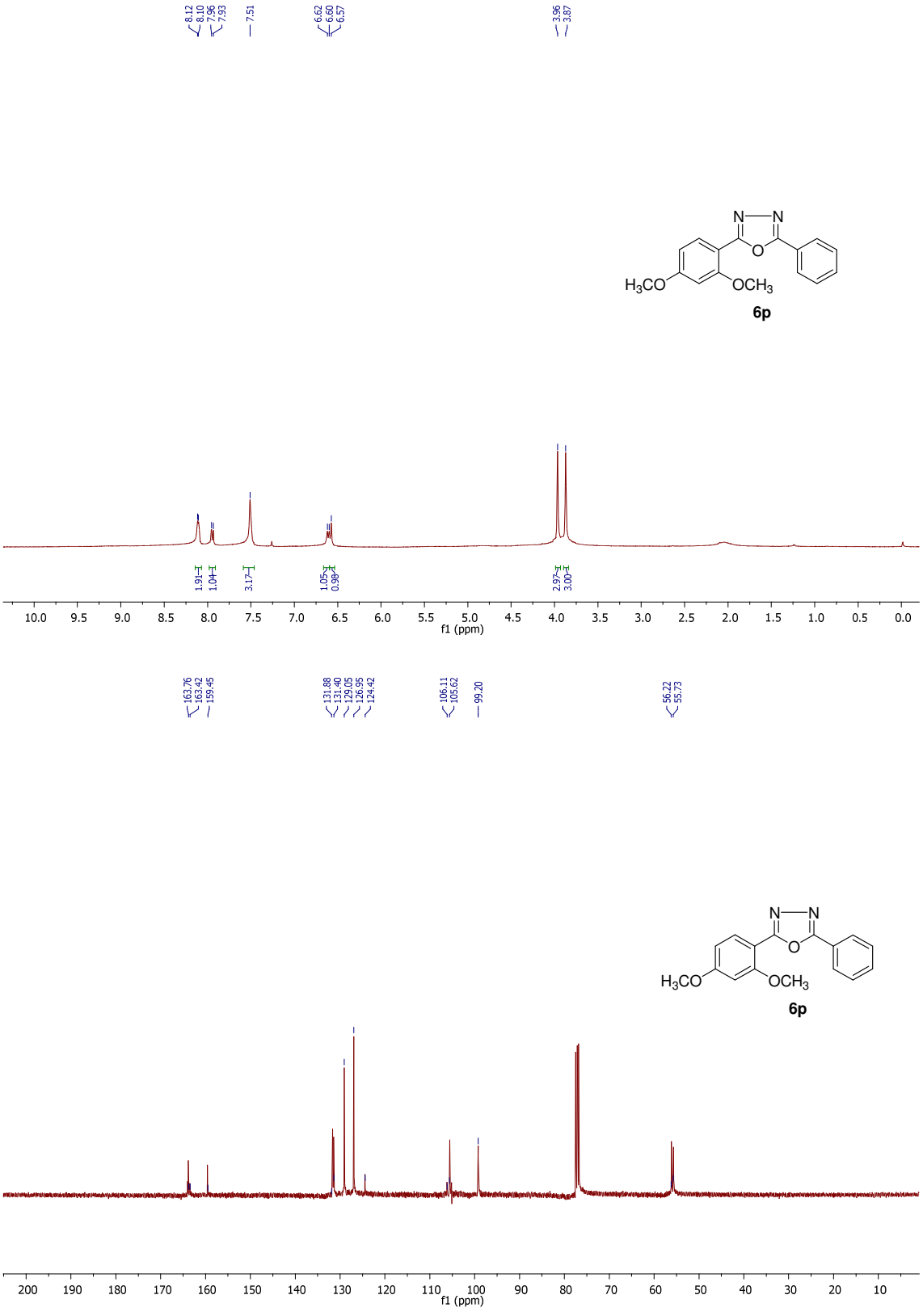
2-(3'-Methylphenyl)-5-phenyl-1,3,4-oxadiazole (6o)



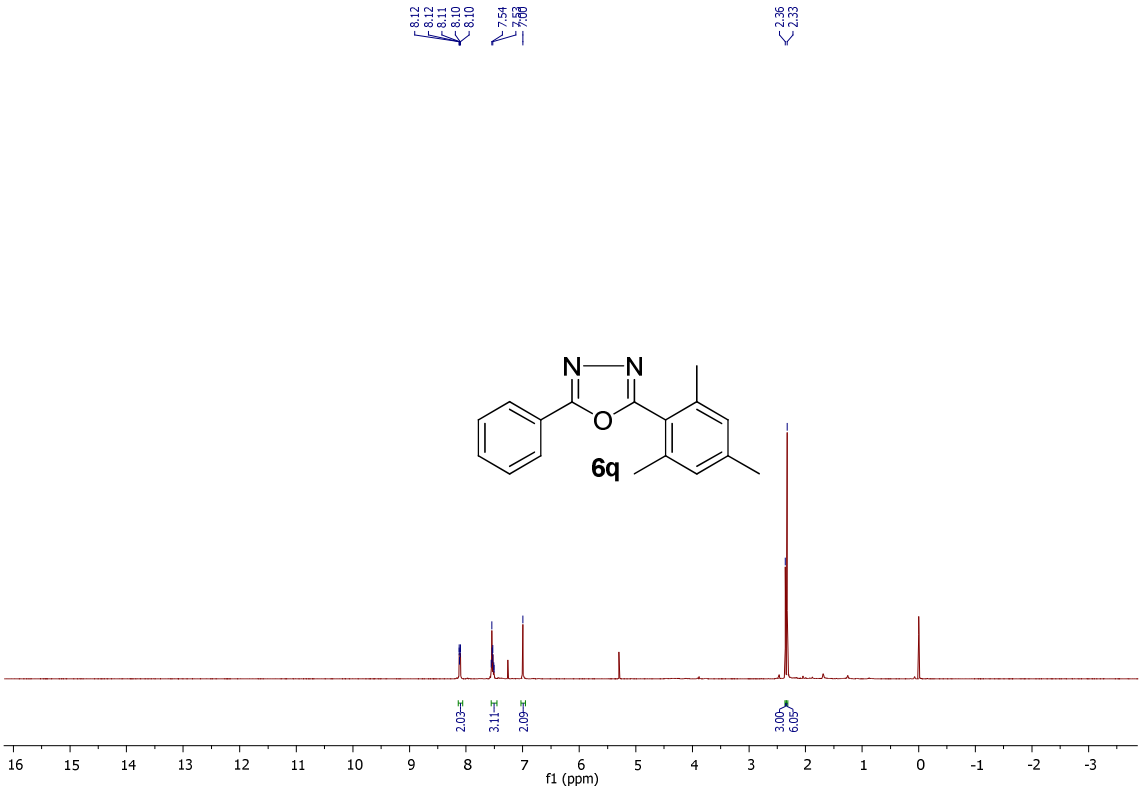




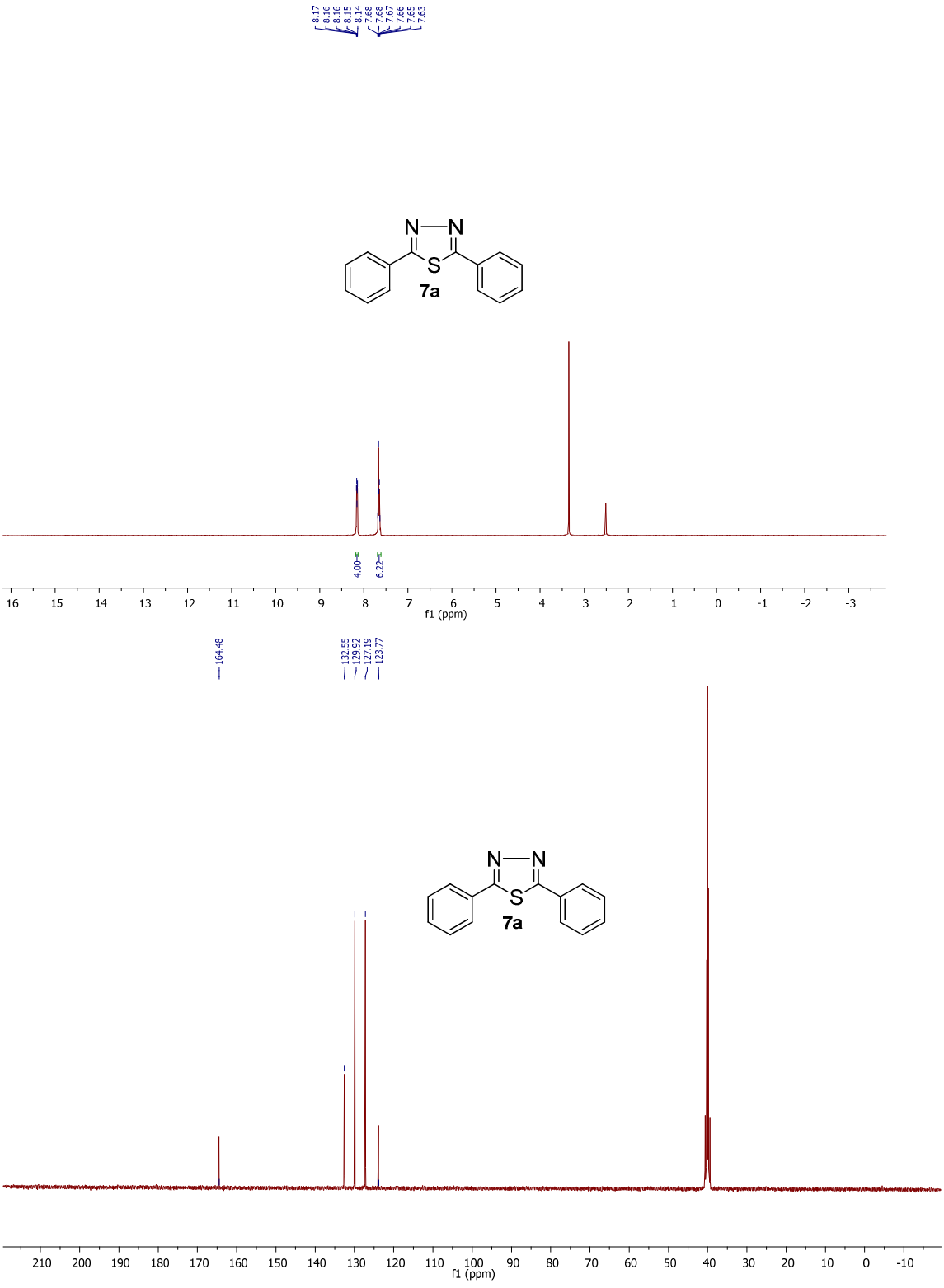
2-(2',4'-Dimethoxyphenyl)-5-phenyl-1,3,4-oxadiazole (6p)



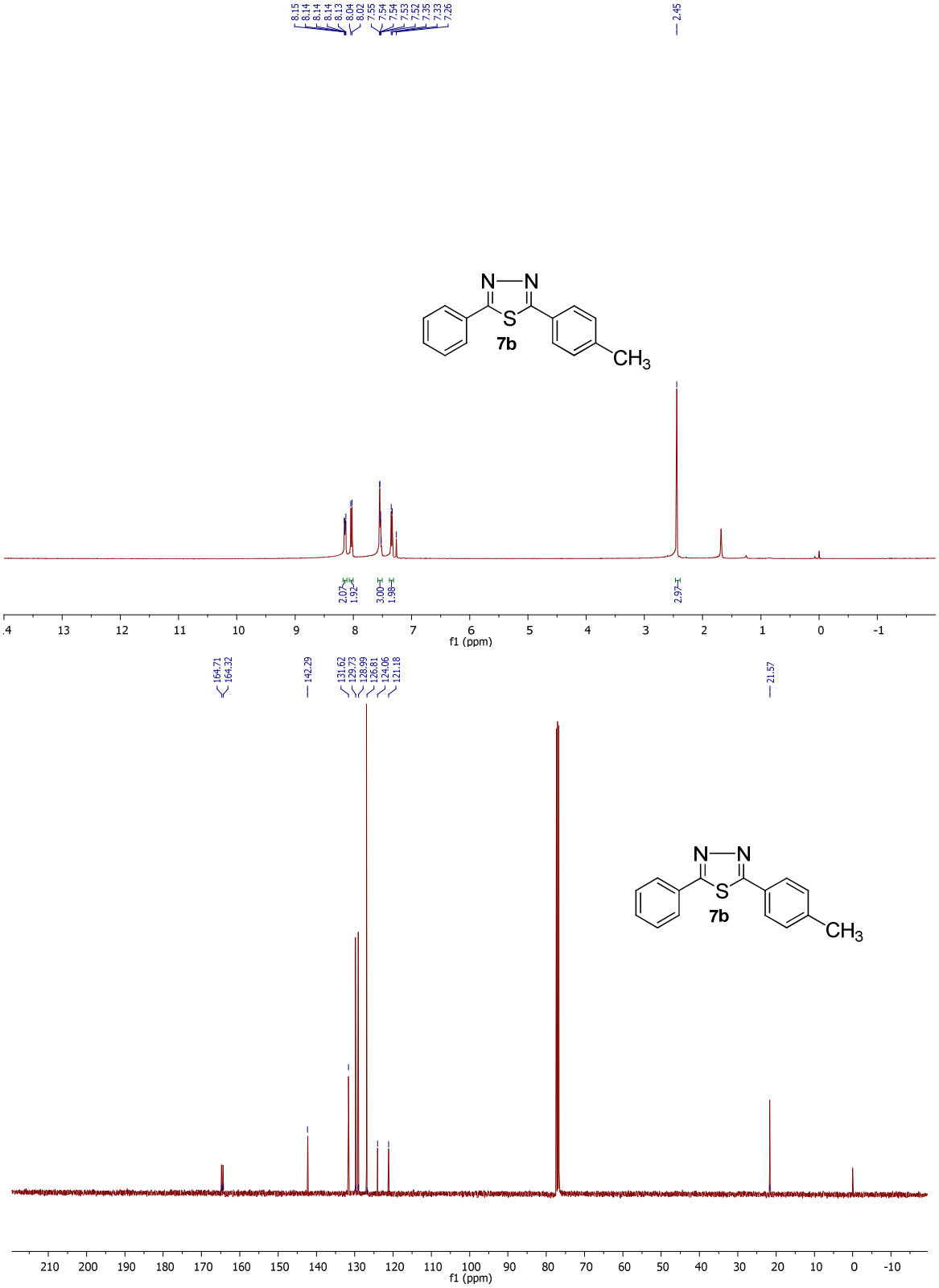
2-(Mesityl)-5-phenyl-1,3,4-oxadiazole (6q)



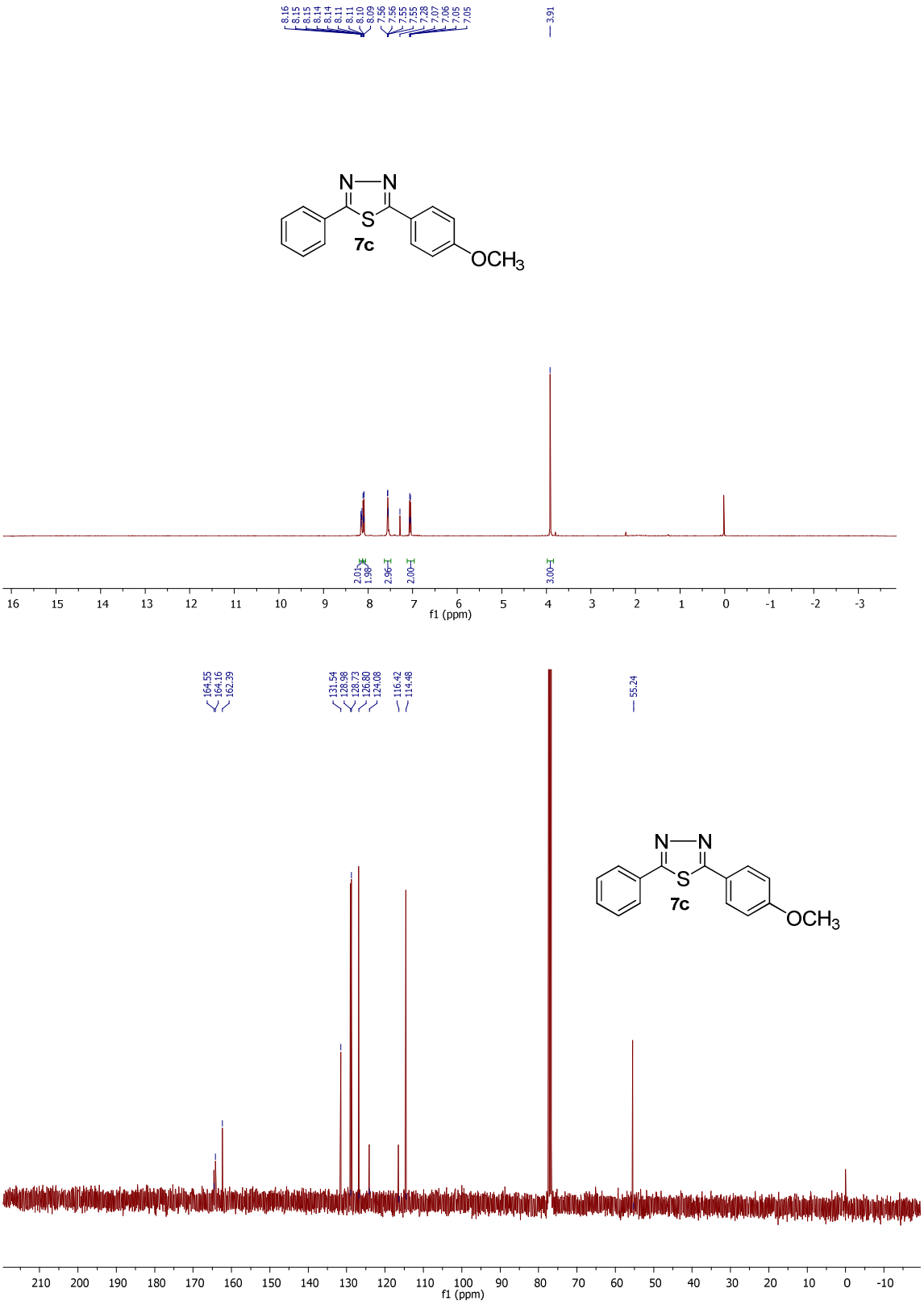
2,5-Diphenyl-1,3,4-thiadiazole (7a)



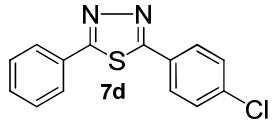
2-(4'-Methylphenyl)-5-phenyl-1,3,4-thiadiazole (7b)

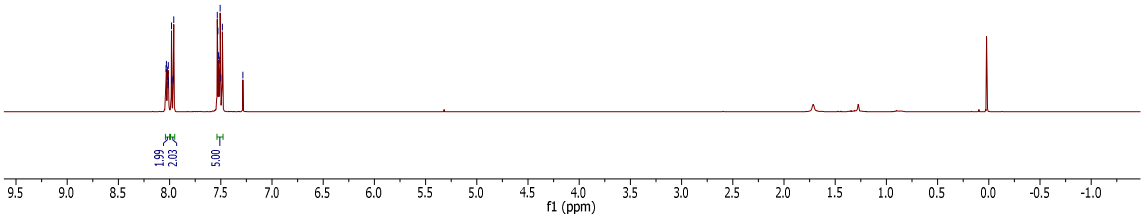


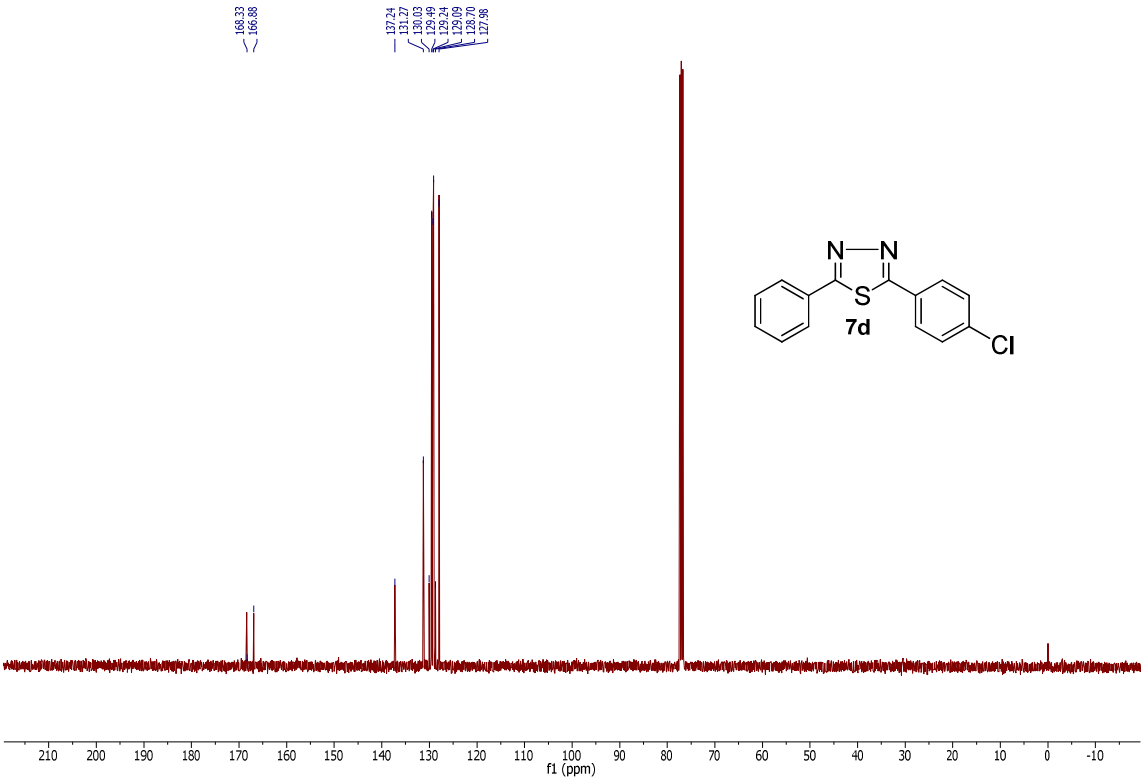
2-(4'-Methoxylphenyl)-5-phenyl-1,3,4-thiadiazole (7c)



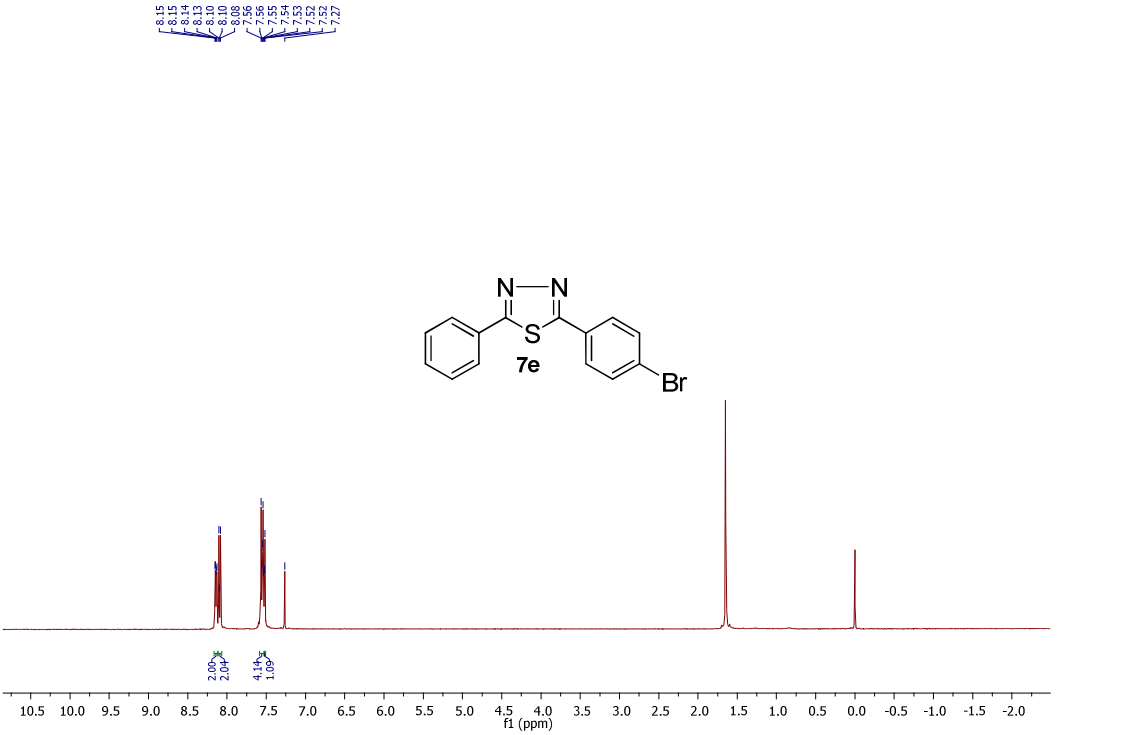
2-(4'-Chlorophenyl)-5-phenyl-1,3,4-thiadiazole (7d)

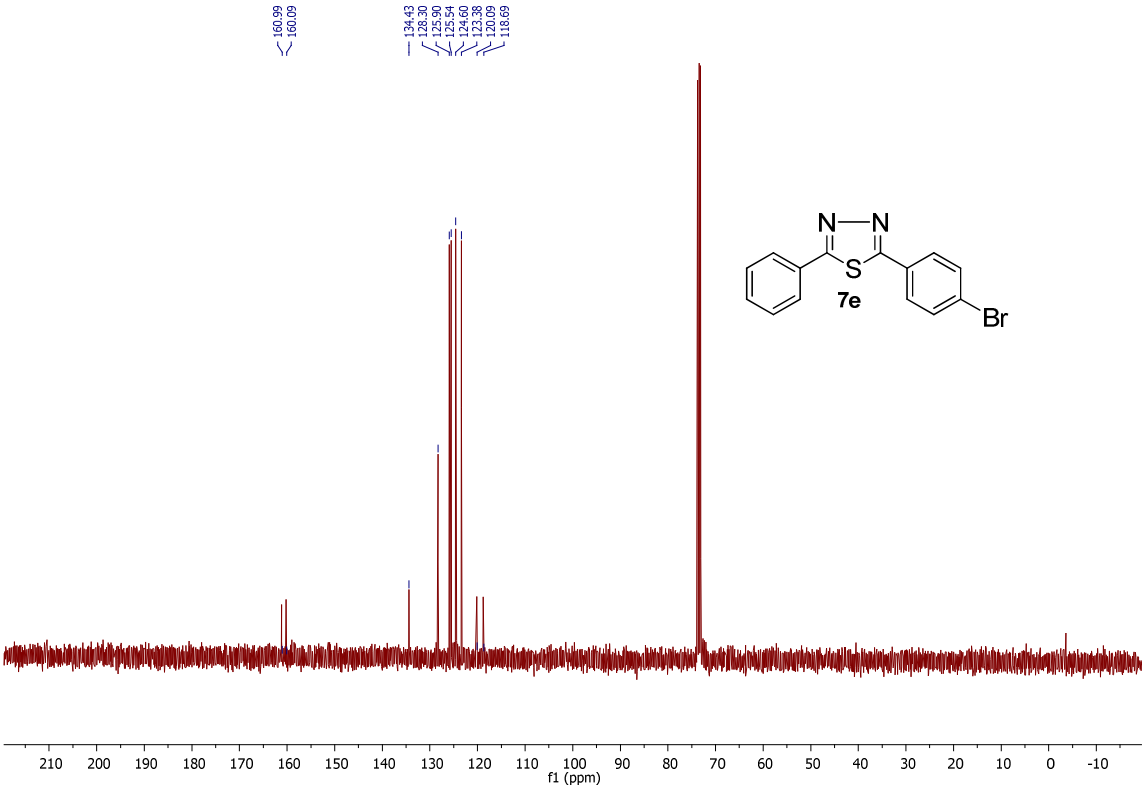




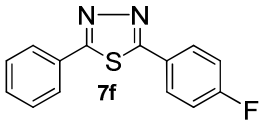


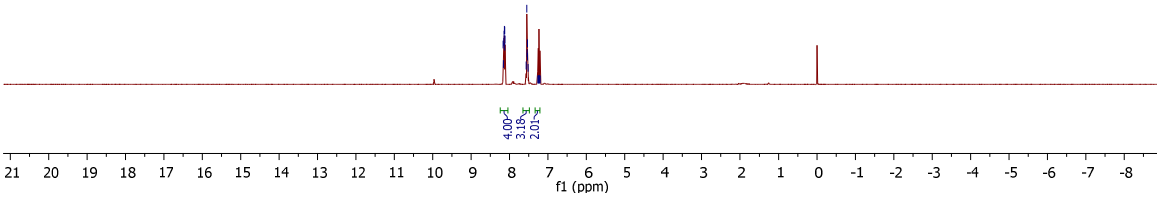
2-(4'-Bromophenyl)-5-phenyl-1,3,4-thiadiazole (7e)

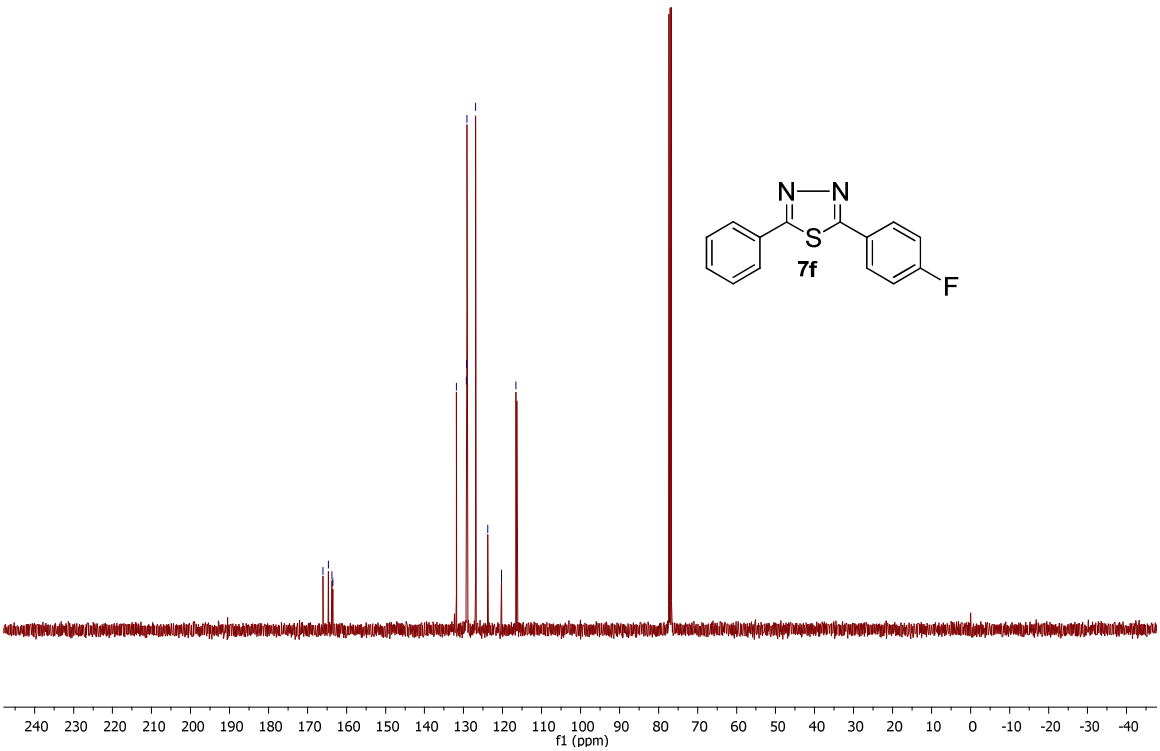




2-(4'-Fluorophenyl)-5-phenyl-1,3,4-thiadiazole (7f)

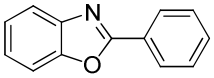




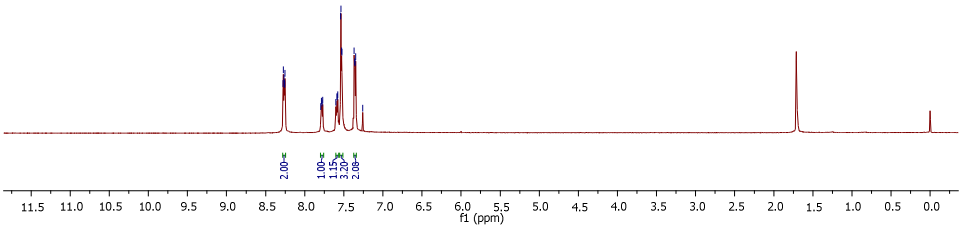


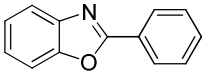
8. NMR spectra of isolated 2-arylbenzoxazoles **10** and 2-arylbenzothiazoles**11**

2-Phenylbenzoxazole (**10a**)



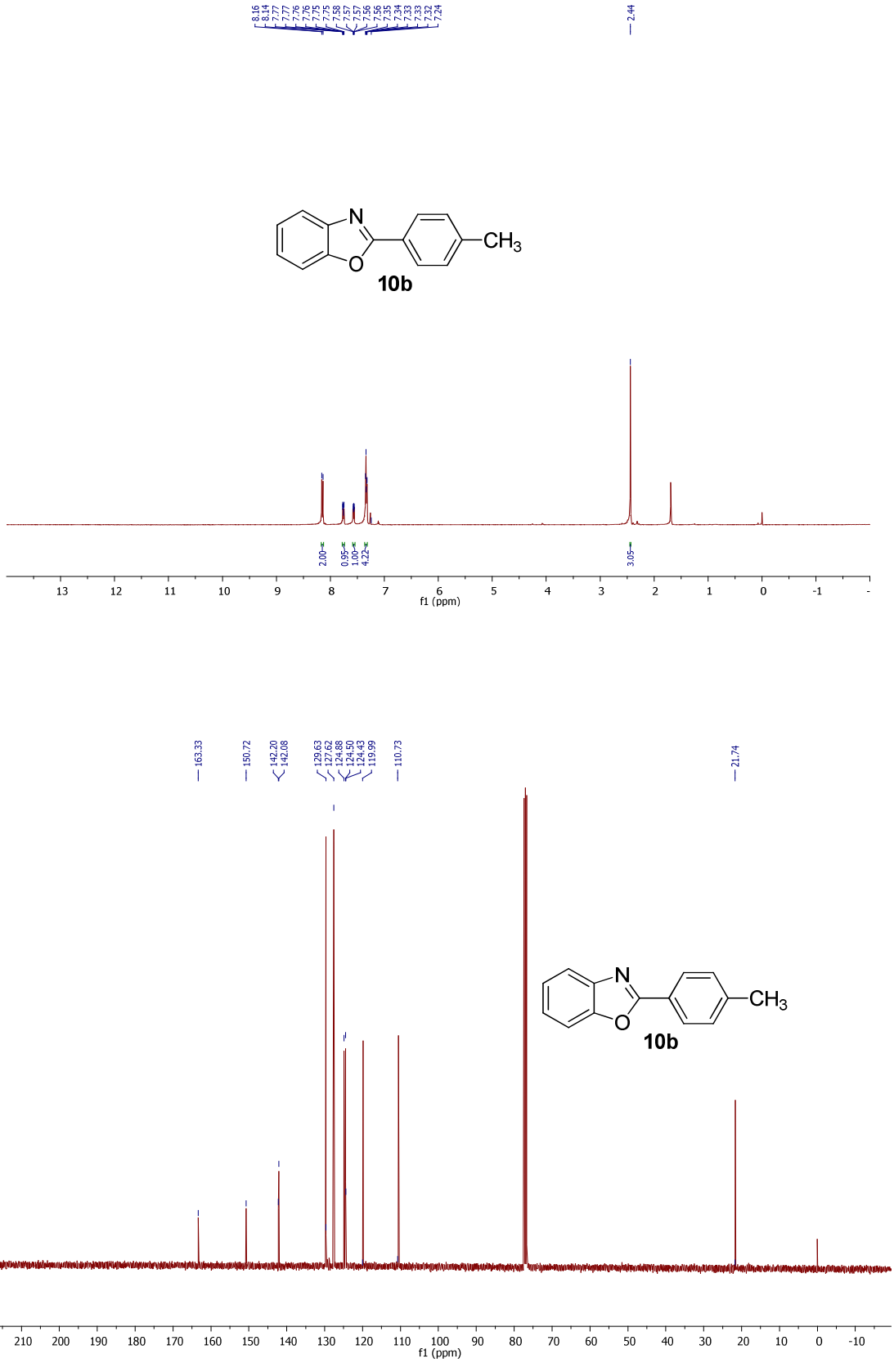
10a



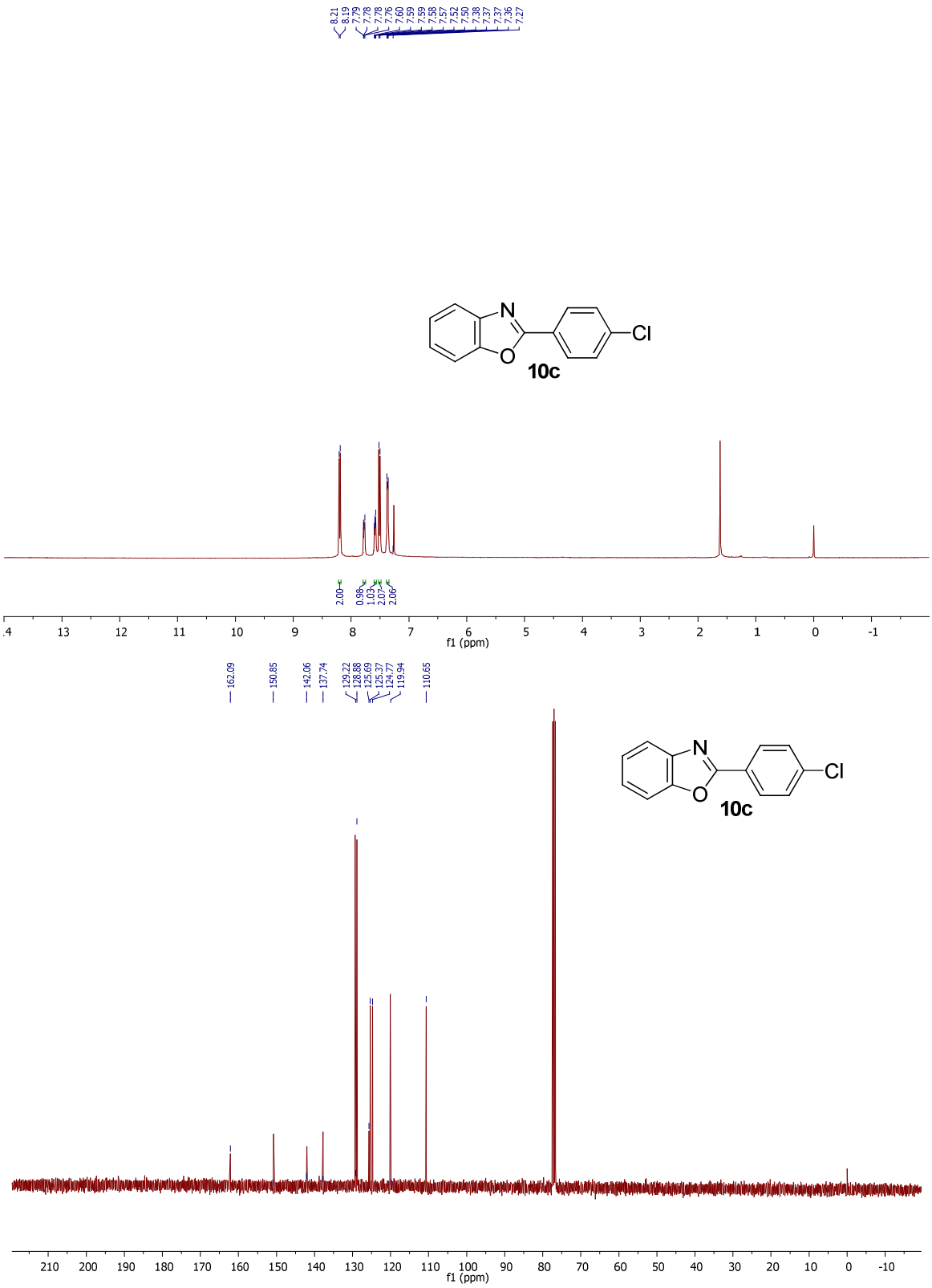


10a

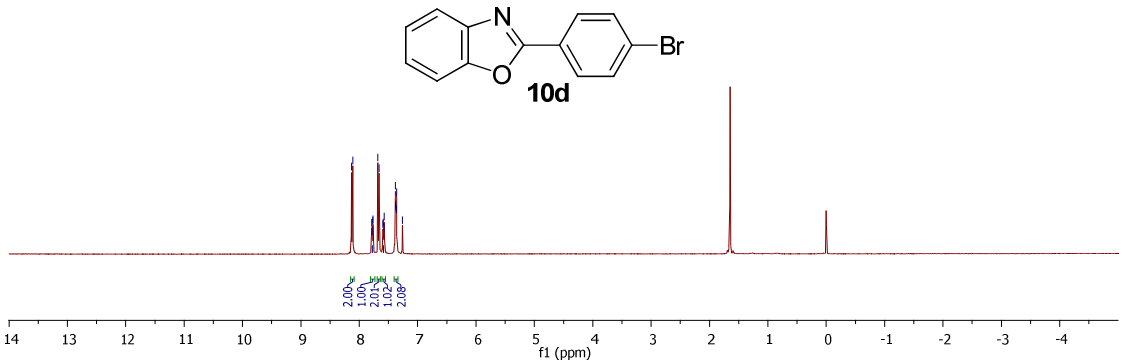
2-(4'-Methylphenyl)benzoxazole (10b)

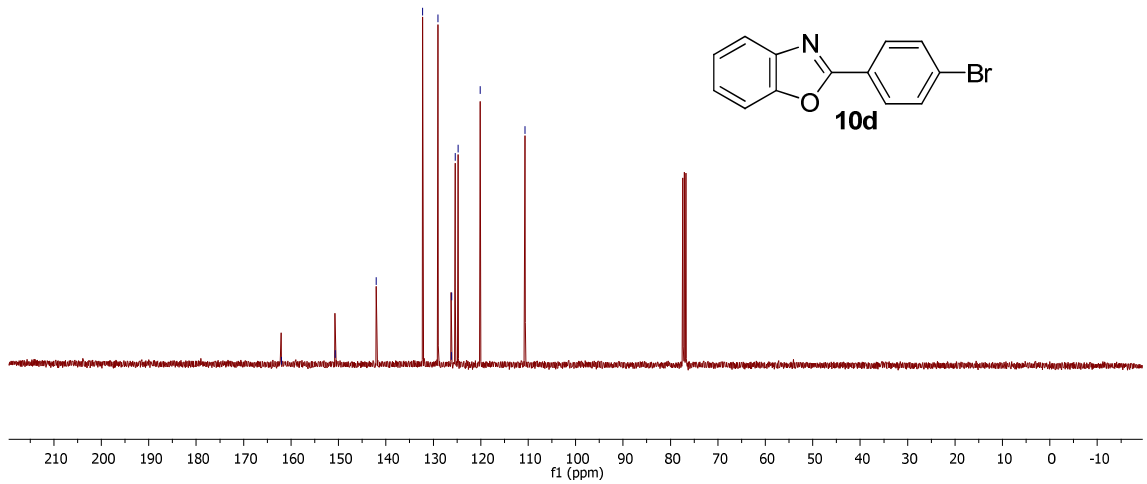


2-(4'-Chlorophenyl)benzoxazole (10c)

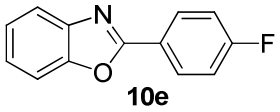


2-(4'-Bromophenyl)benzoxazole (10d)

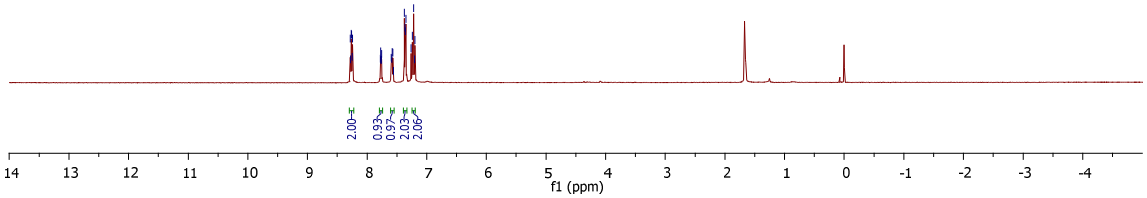


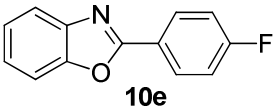


2-(4'-Fluorophenyl)benzoxazole (10e)



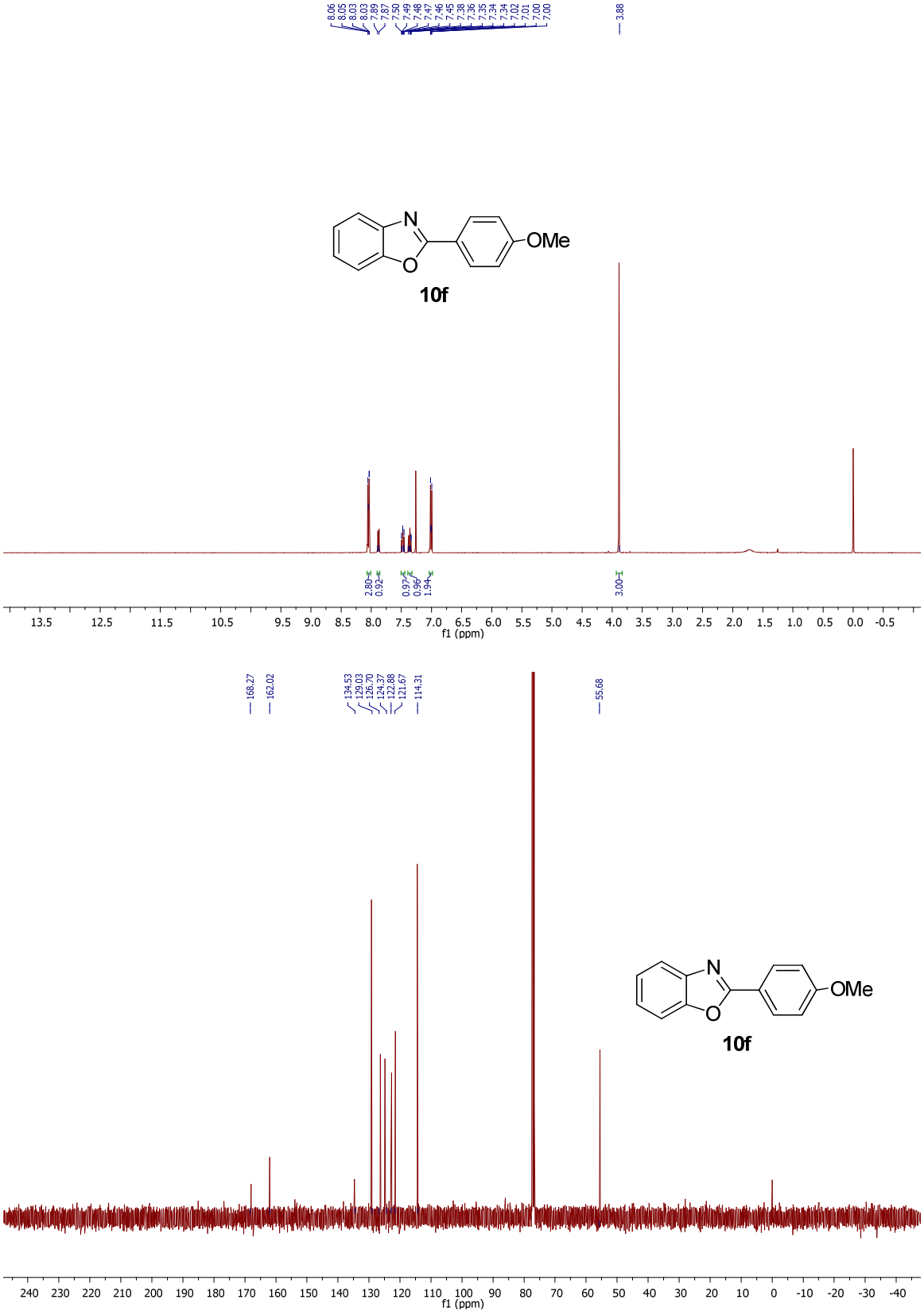
10e



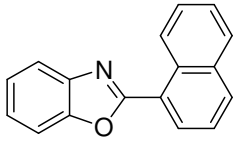


10e

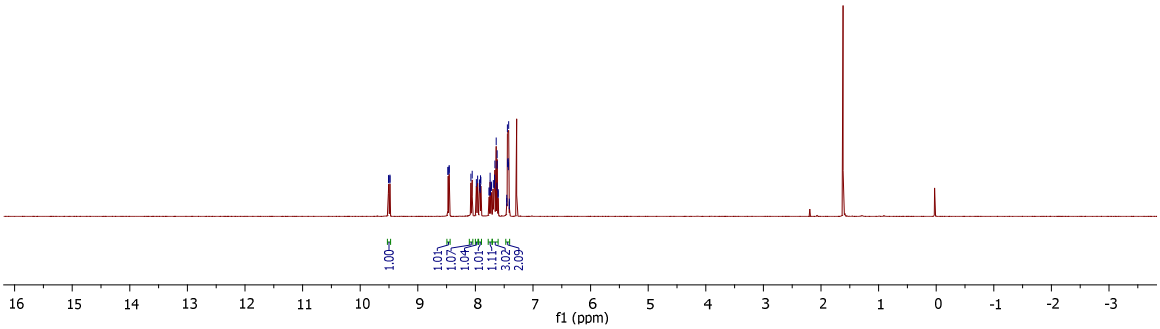
2-(4'-Methoxyphenyl)benzoxazole (10f)

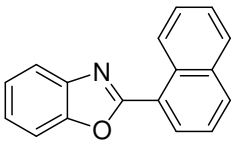


2-(Napthalen-1'-yl)benzoxazole (10g)



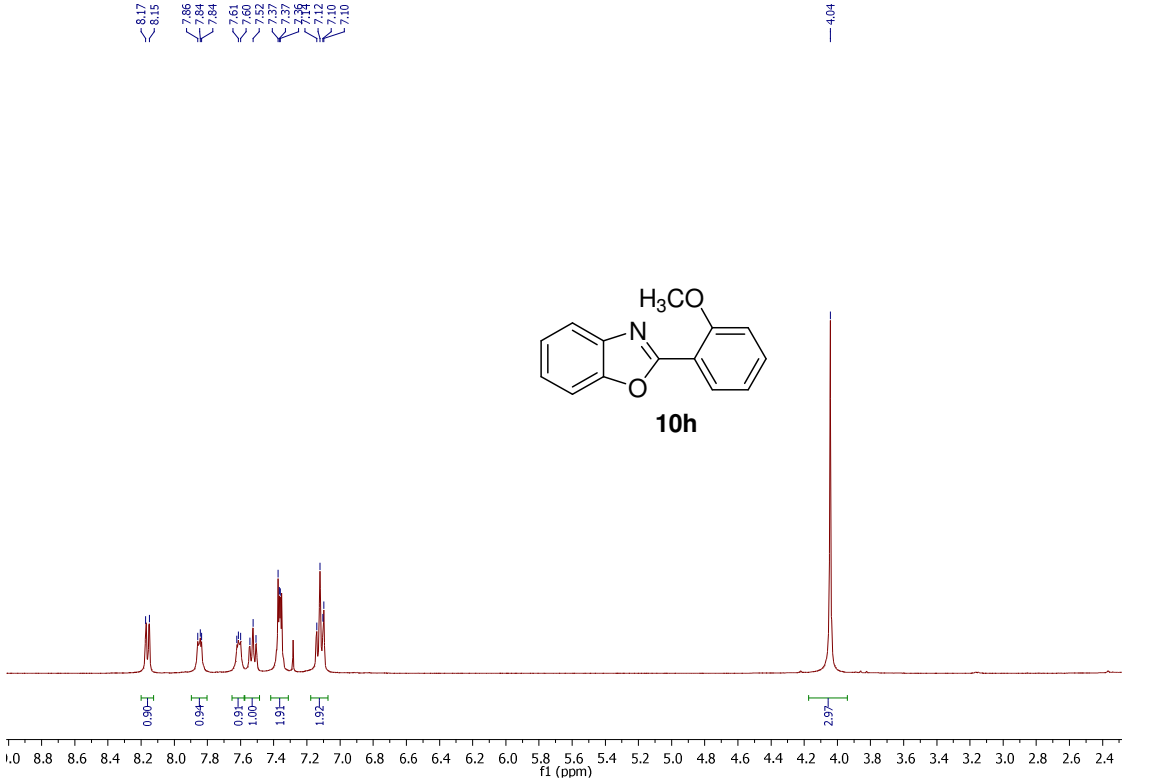
10g

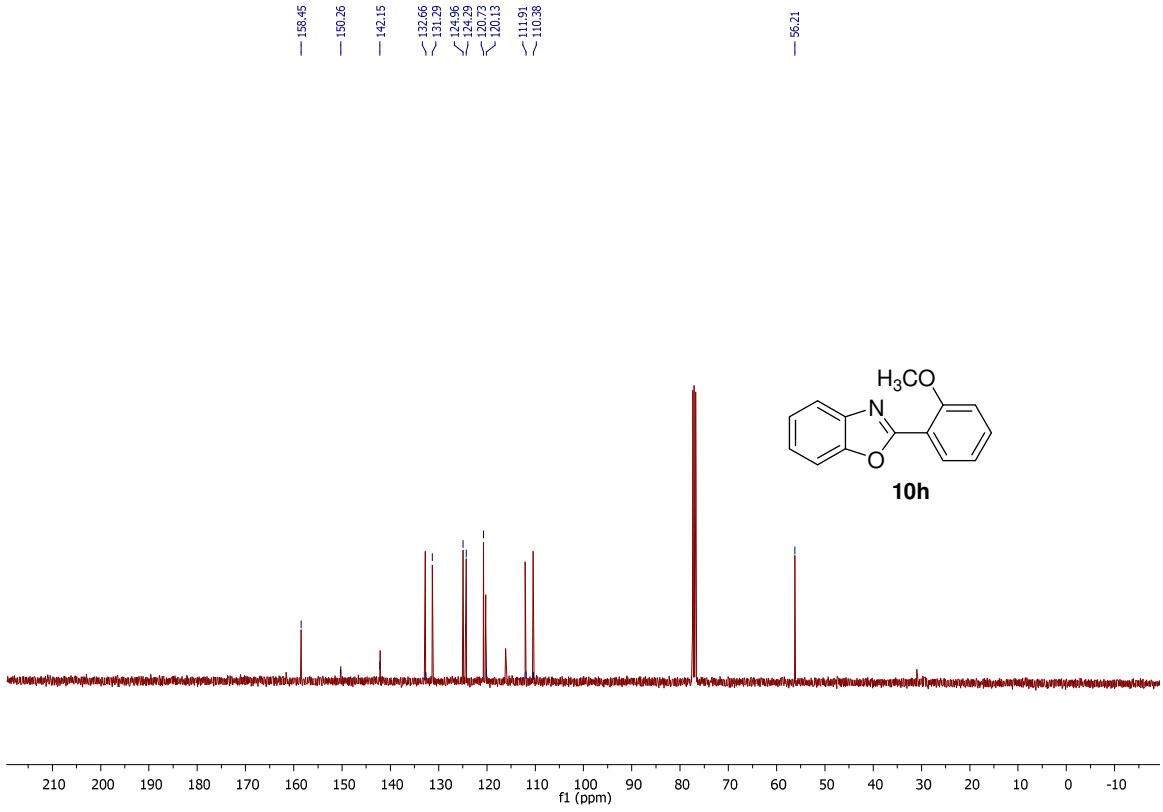




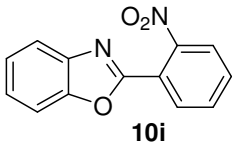
10g

2-(2'-Methoxyphenyl)benzoxazole (10h)

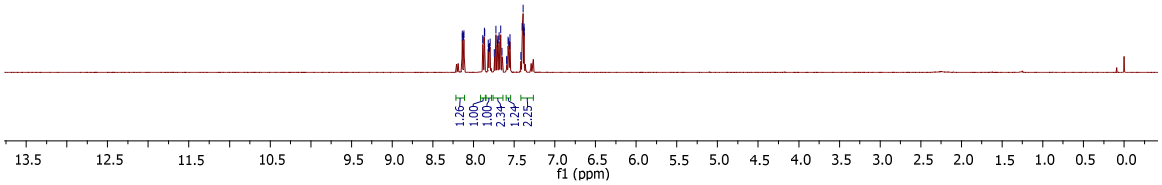


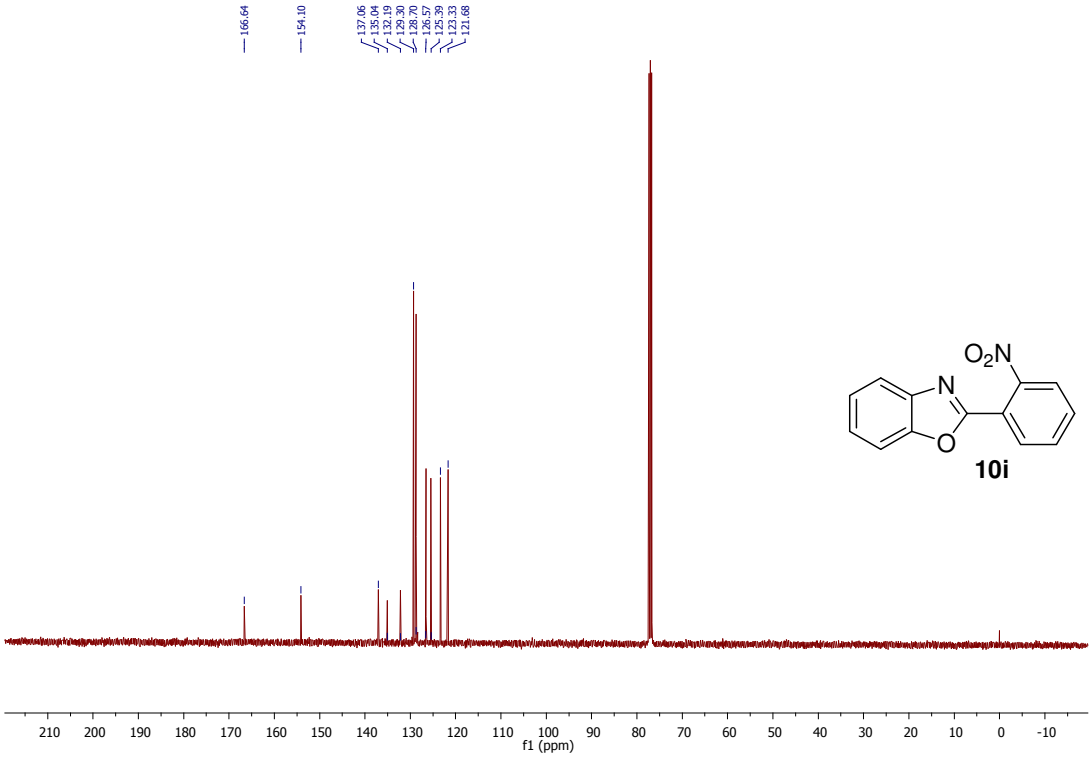


2-(2'-Nitrophenyl)benzoxazole (10i)



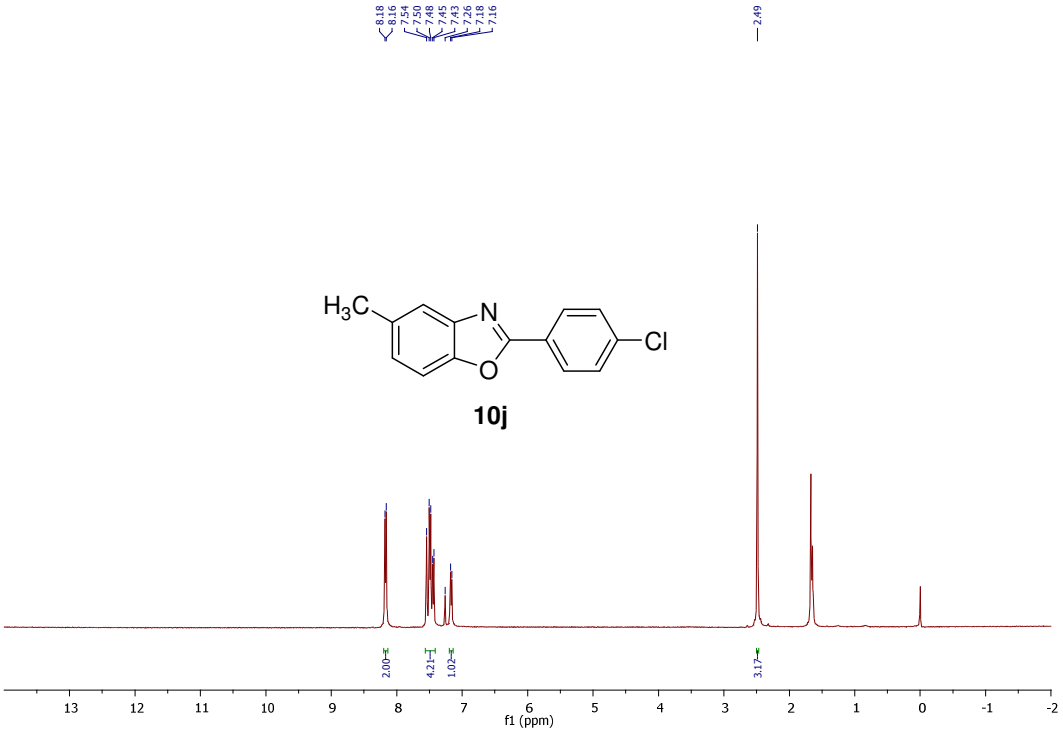
10i

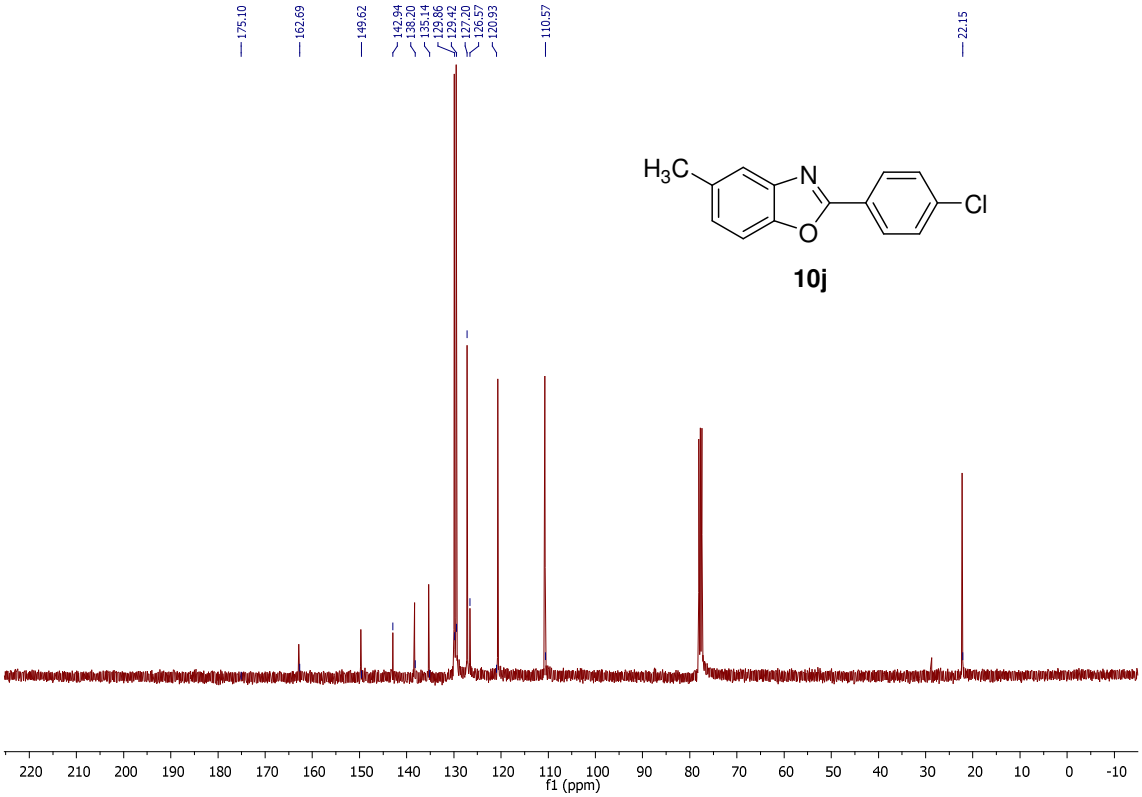




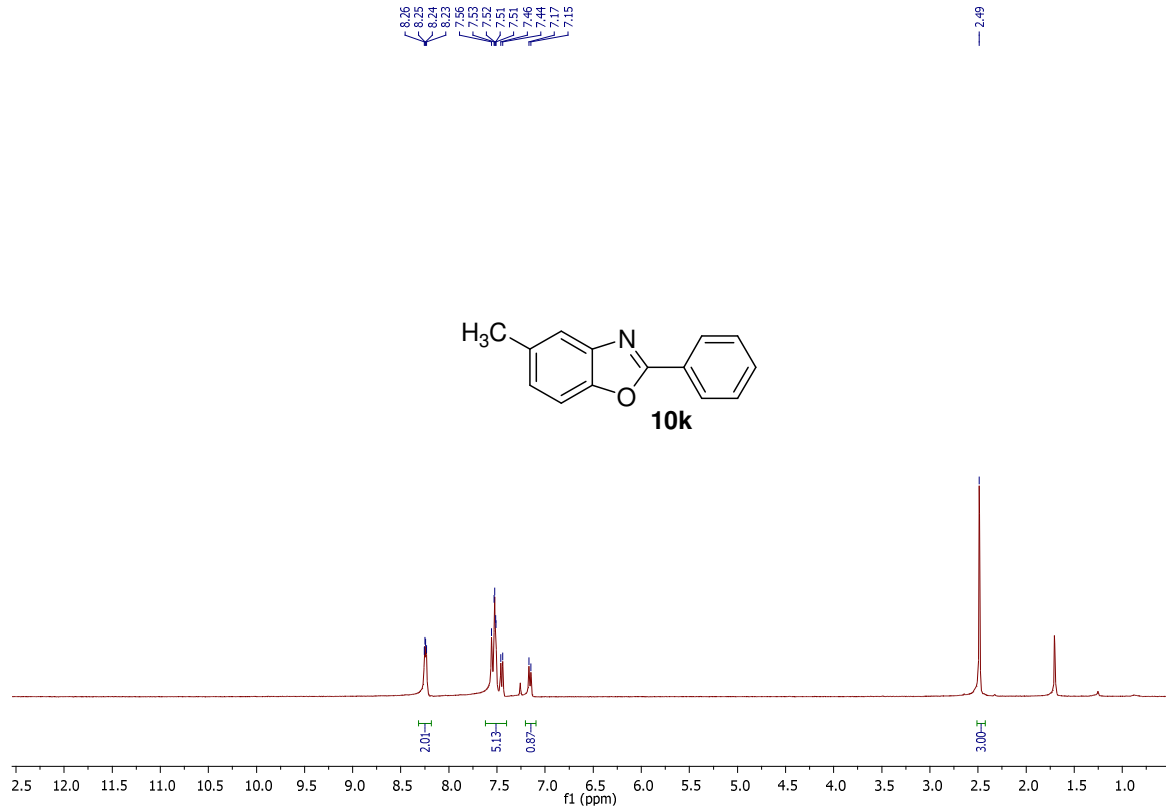
10i

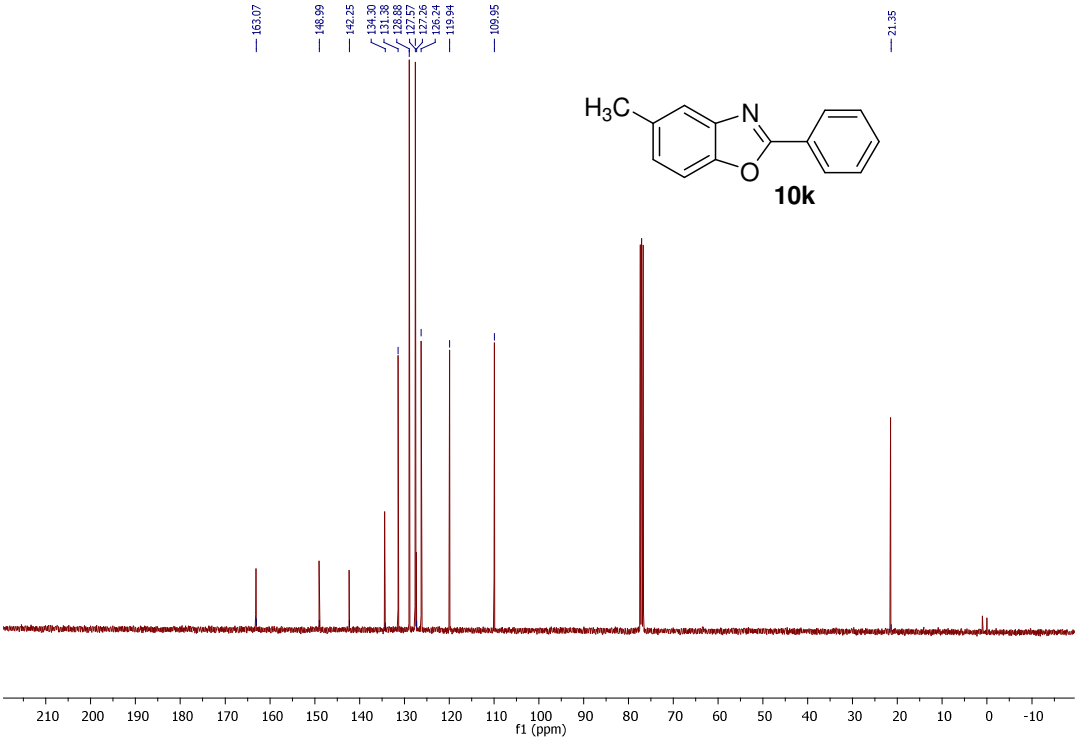
2-(4'-Chlorophenyl)-5-methylbenzoxazole (10j)



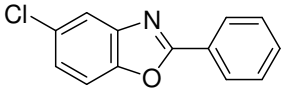


5-Methyl-2-phenylbenzoxazole (10k)

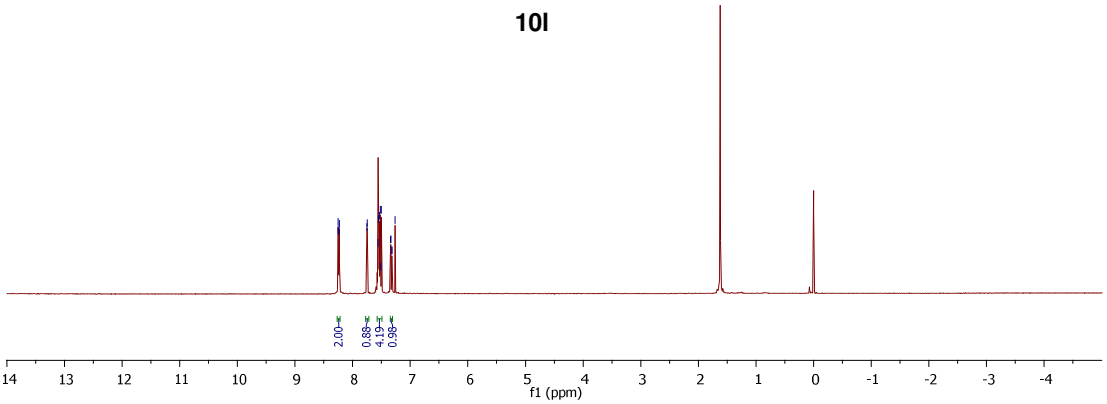


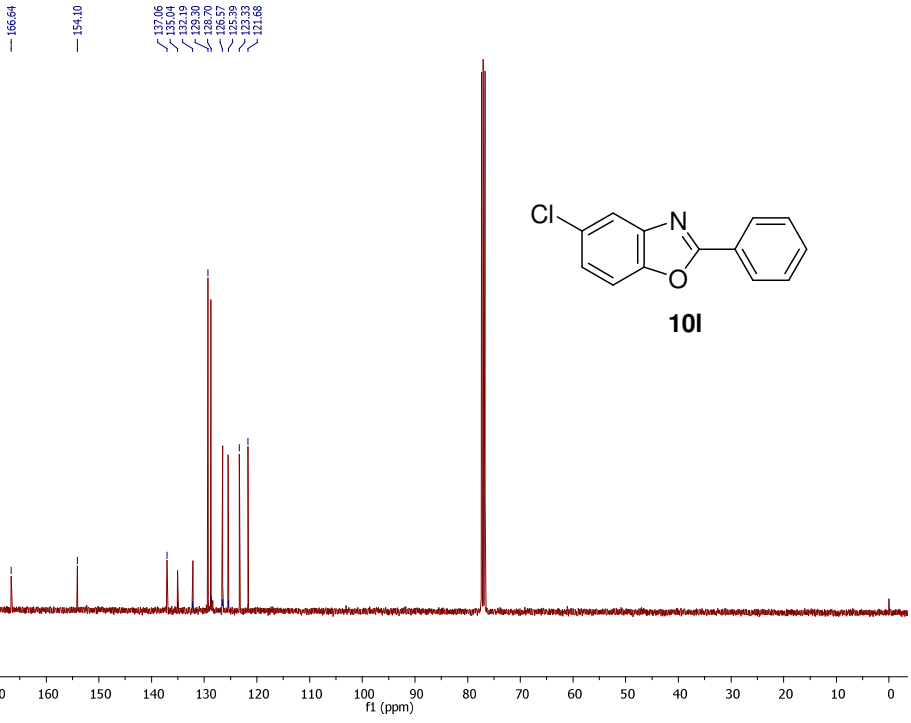


5-Chloro-2-phenylbenzoxaozle (10l)

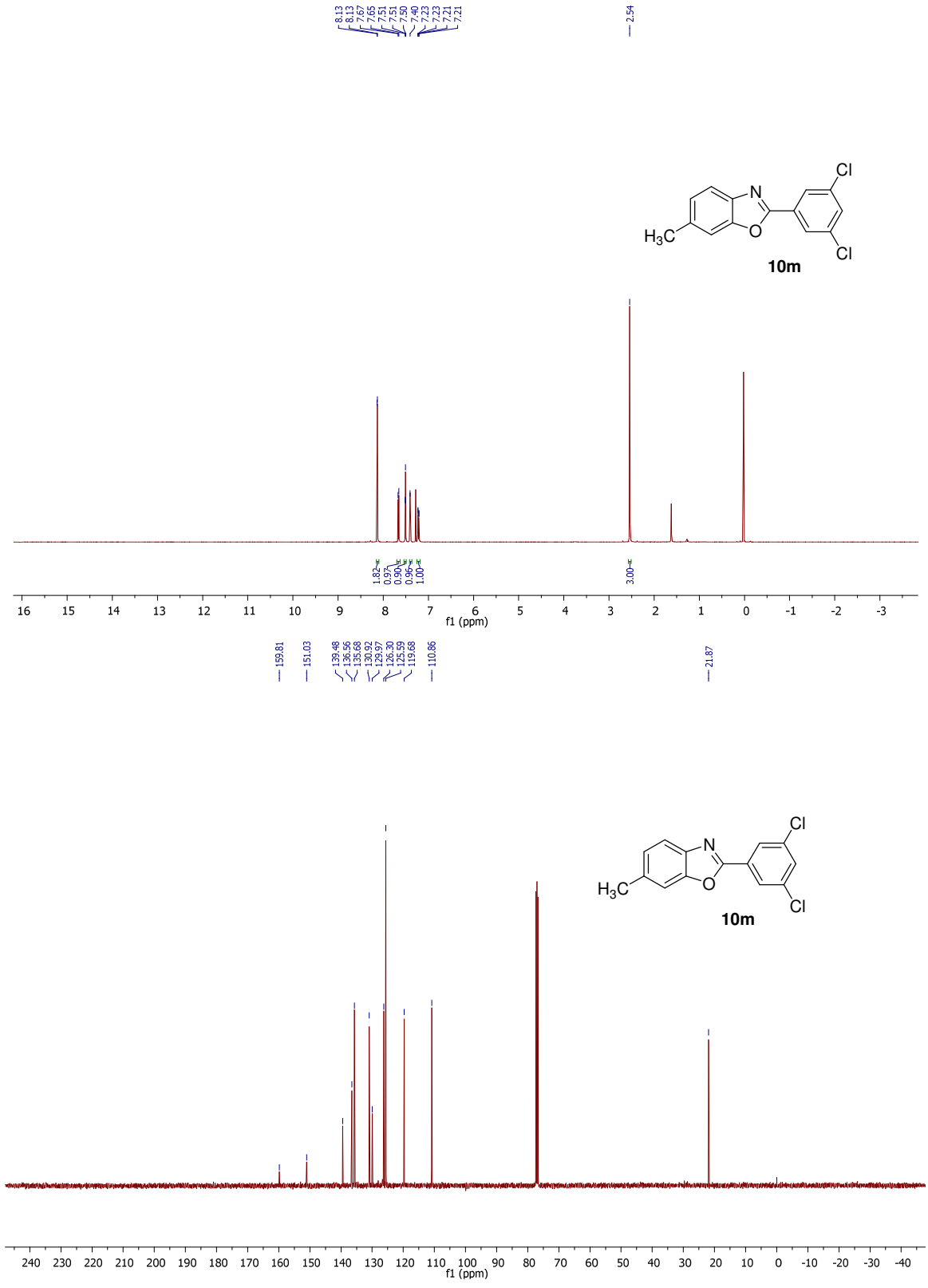


10l

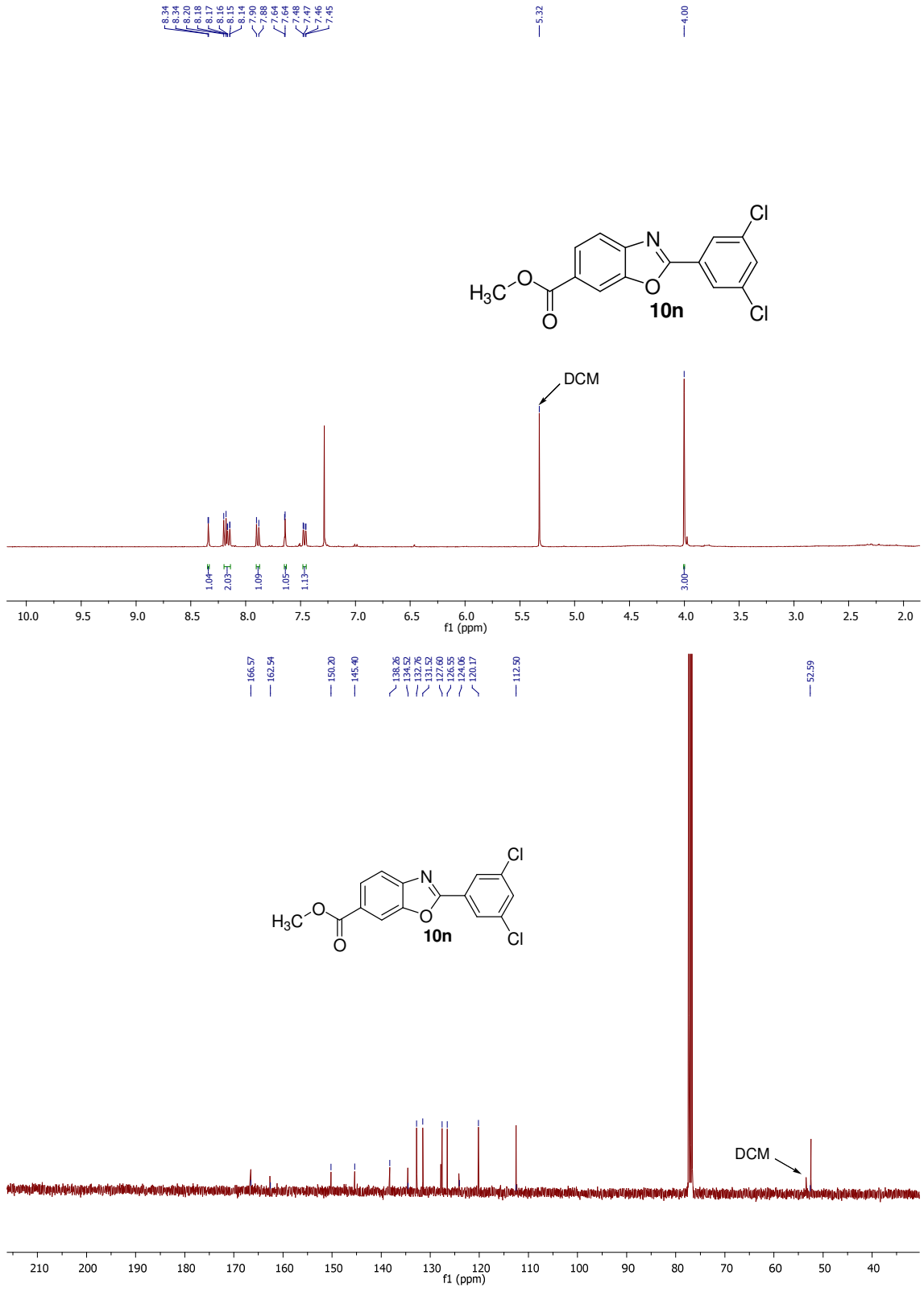




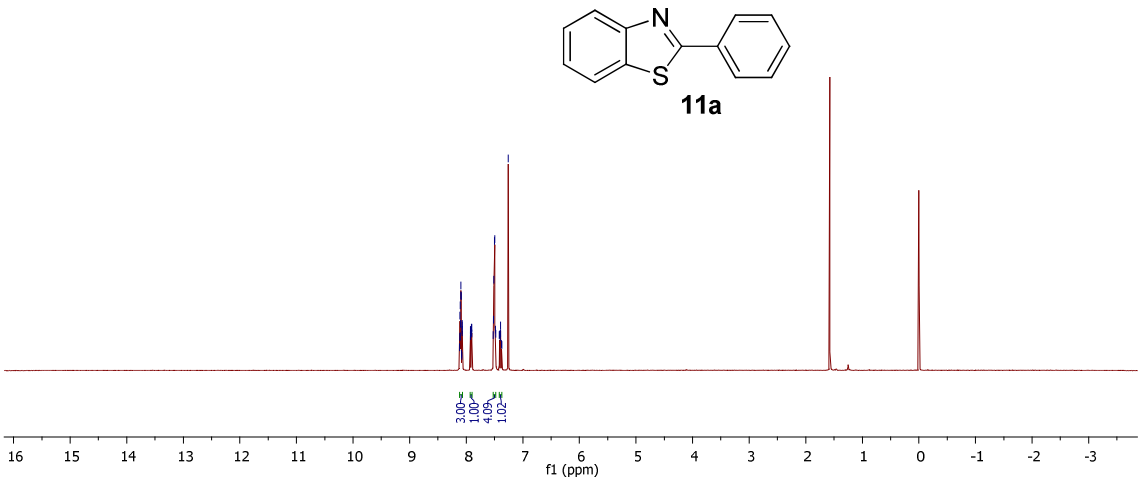
2-(3',5'-Dichlorophenyl)-6-methylbenzoxazole (10m)

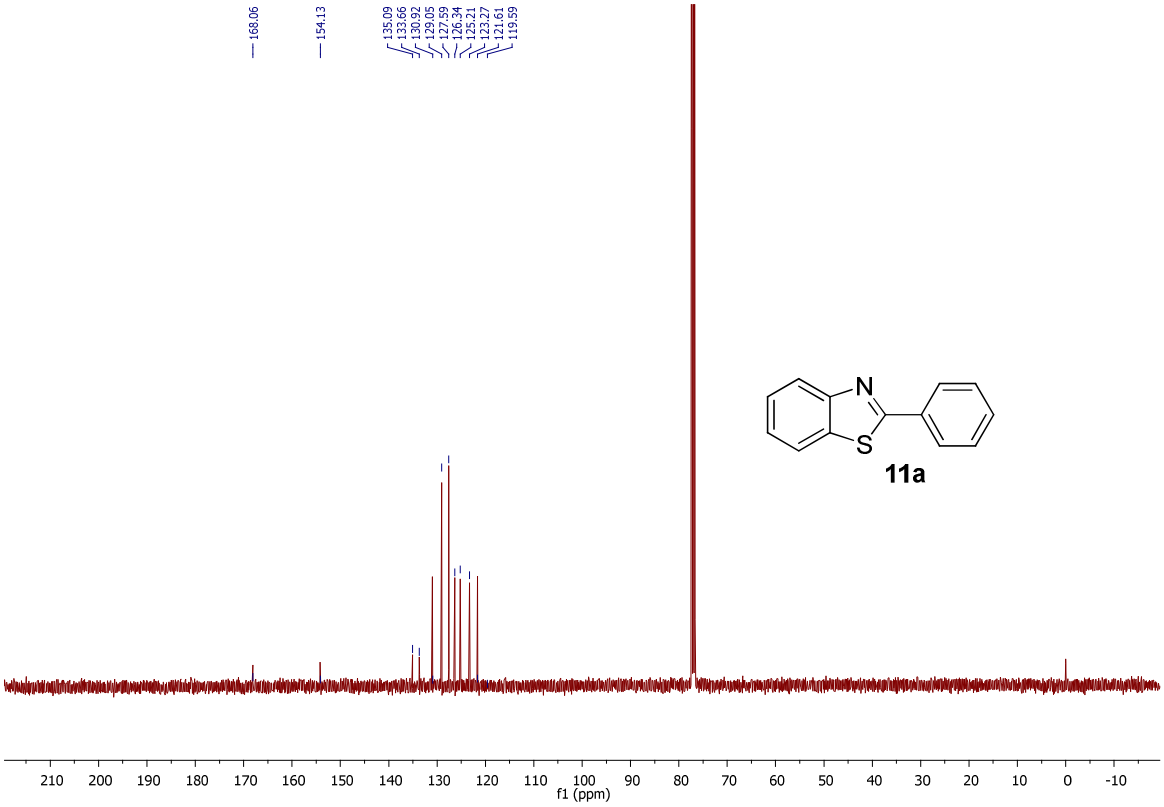


Methyl-2-(3',5'-dichlorophenyl) benzoxazole-6-carboxylate (10n)

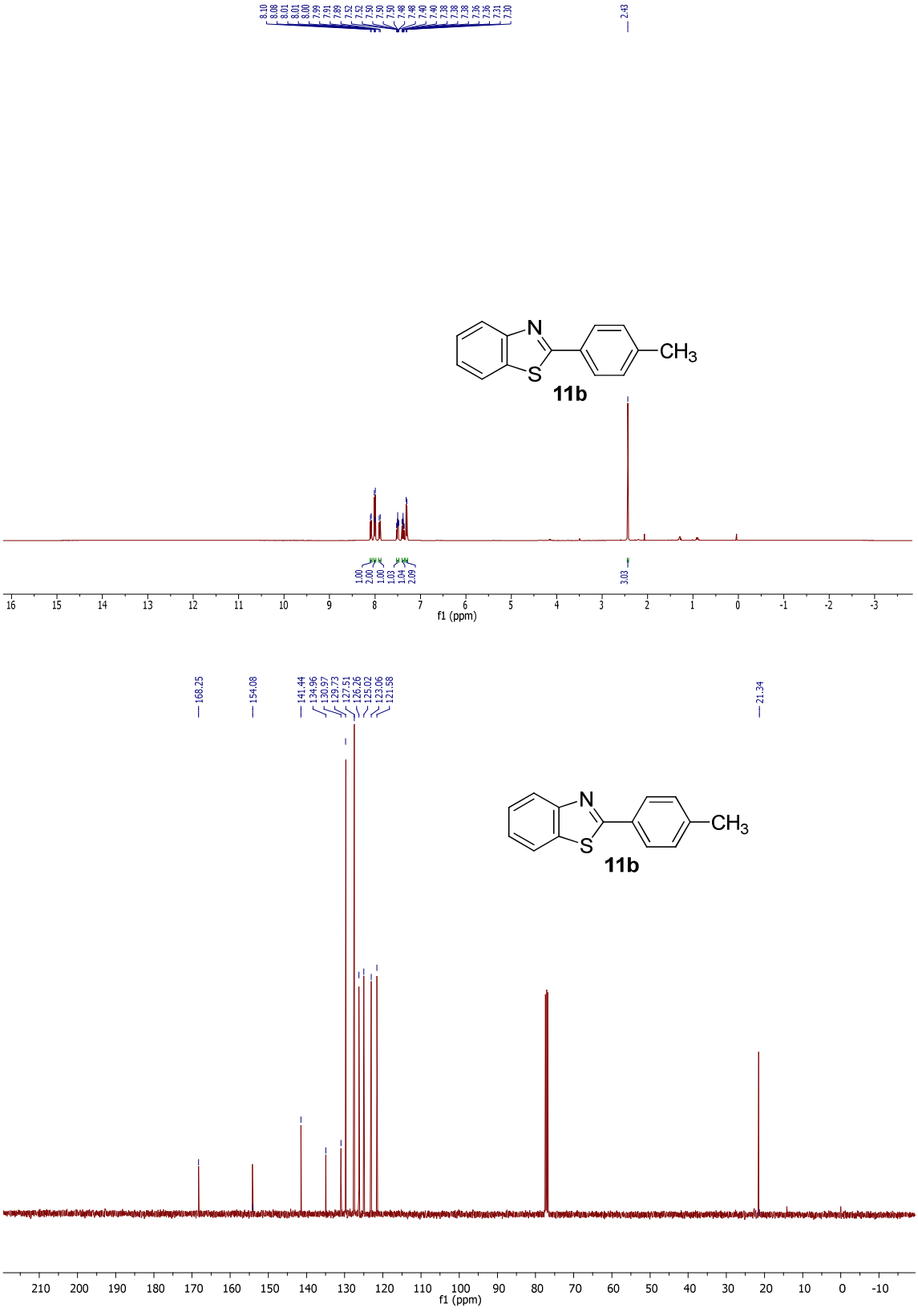


2-Phenylbenzothiazole (11a)

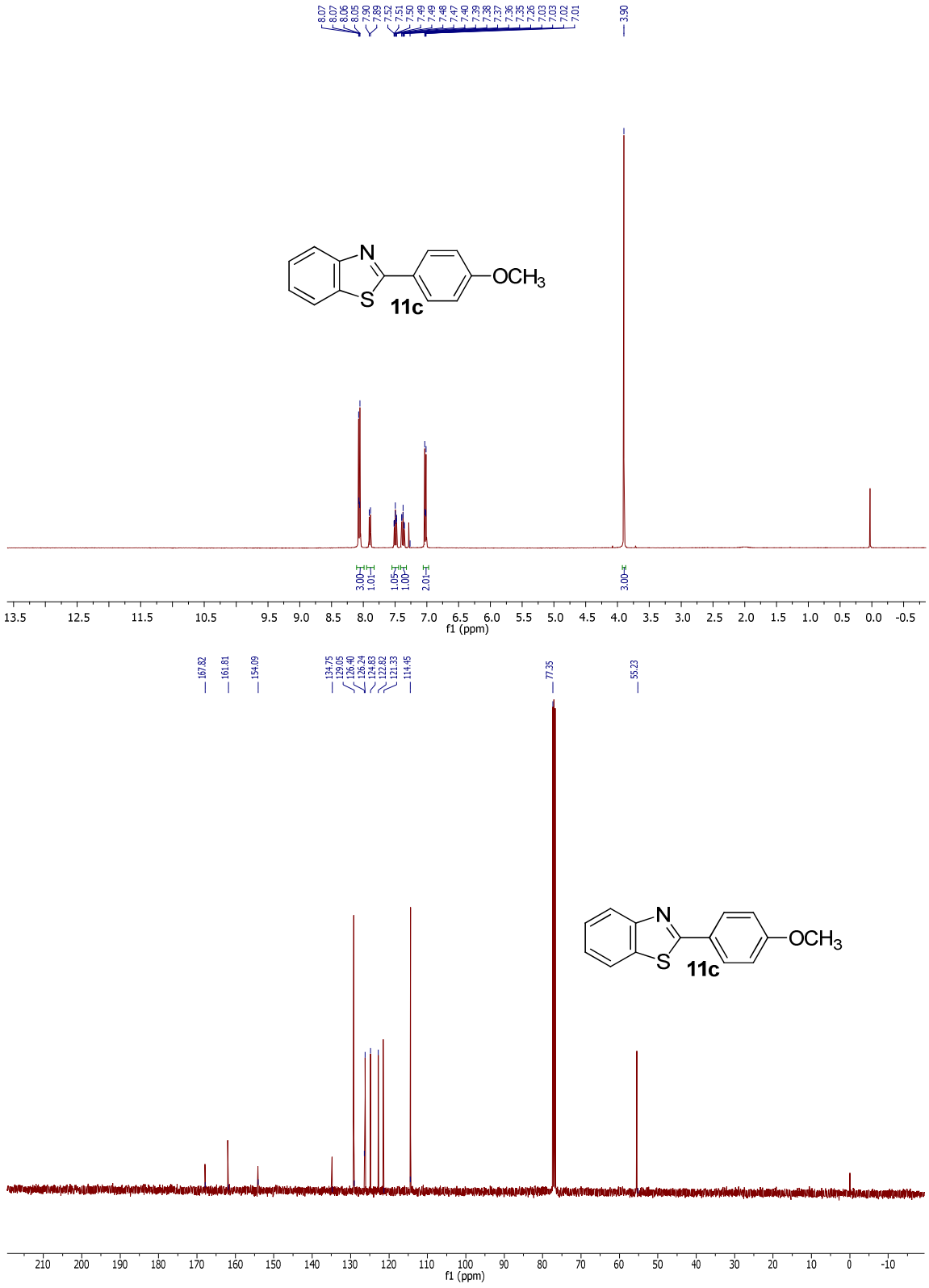




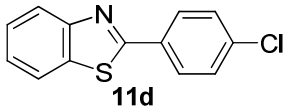
2-(4'-Methylphenyl)benzothiazole (11b)

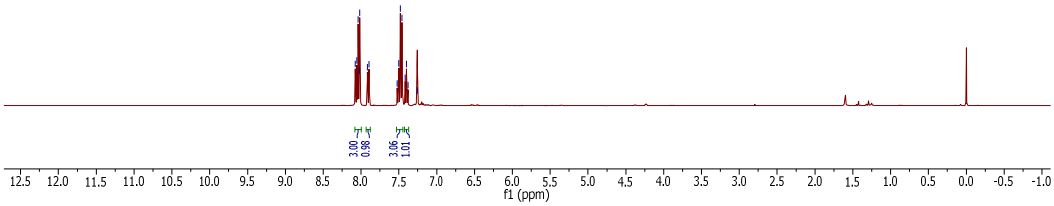


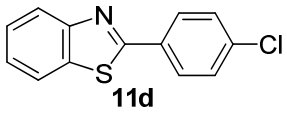
2-(4'-Methoxyphenyl) benzothiazole (11c)



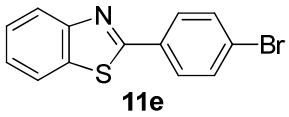
2-(4'-Chlorophenyl)benzothiazole (11d)



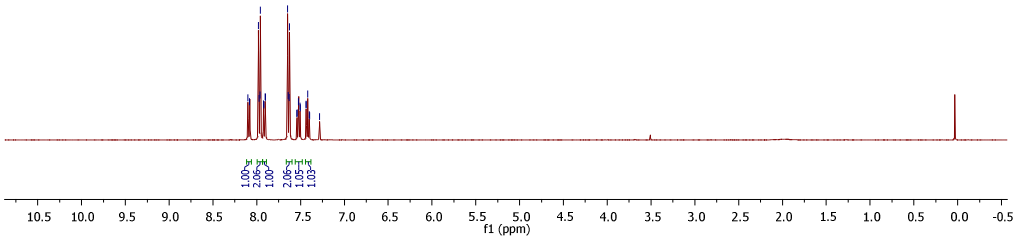


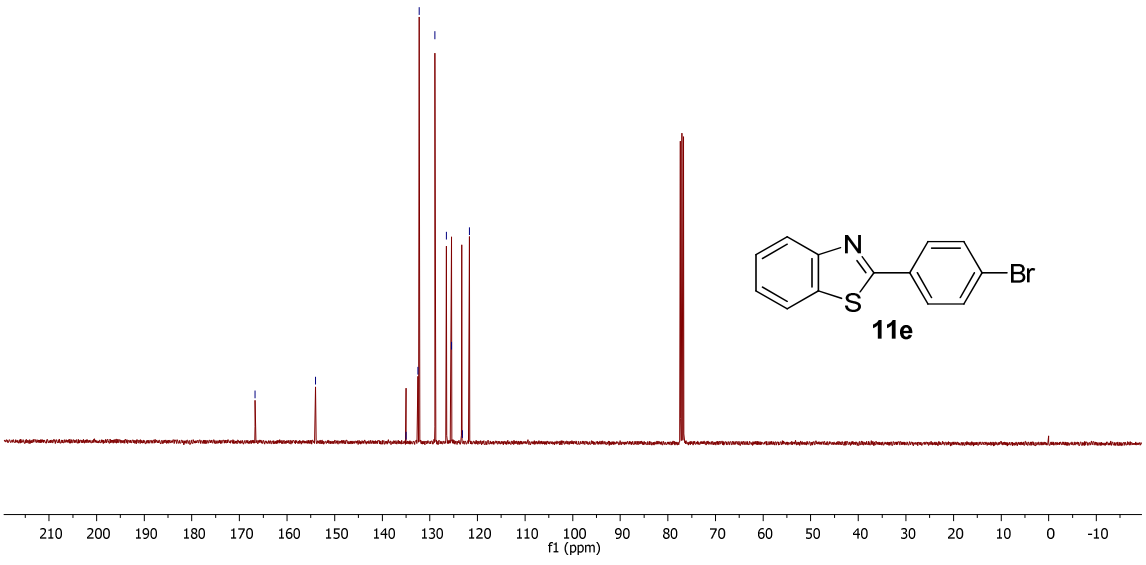


2-(4'-Bromophenyl)benzothiazole (11e)



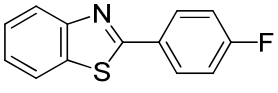
11e



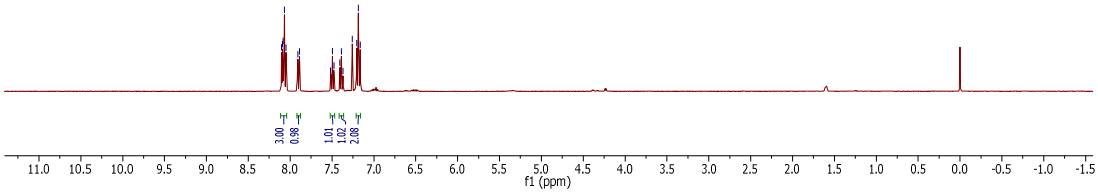


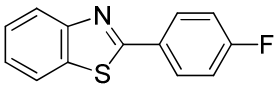
11e

2-(4'-Fluorophenyl)benzothiazole (11f)



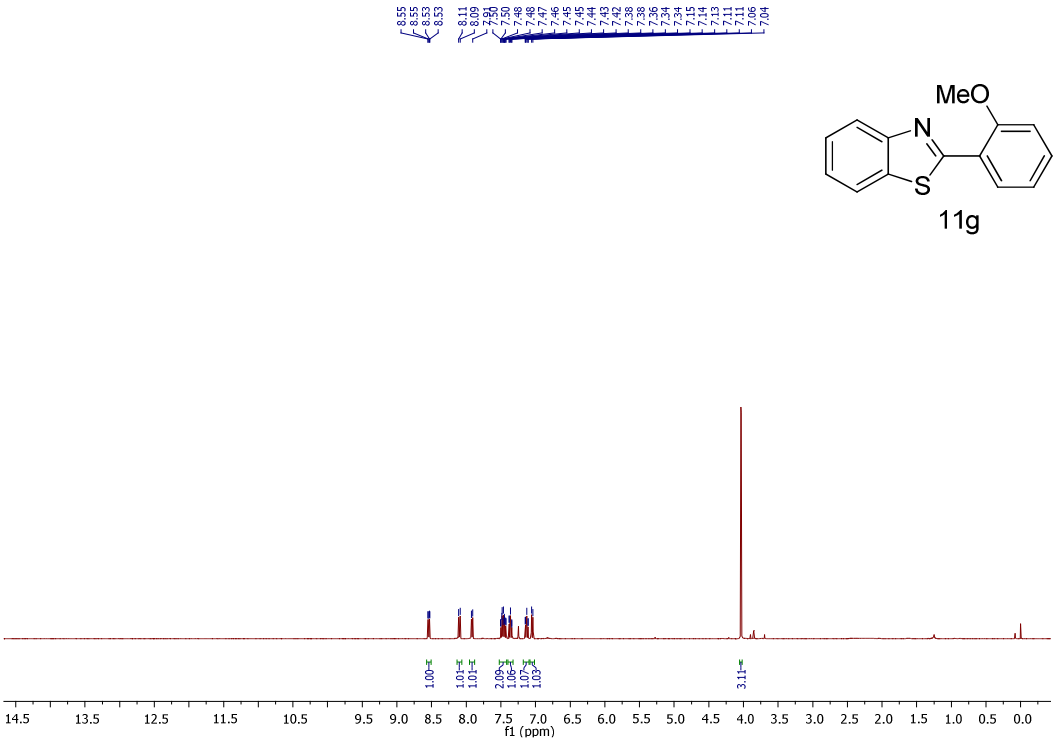
11f

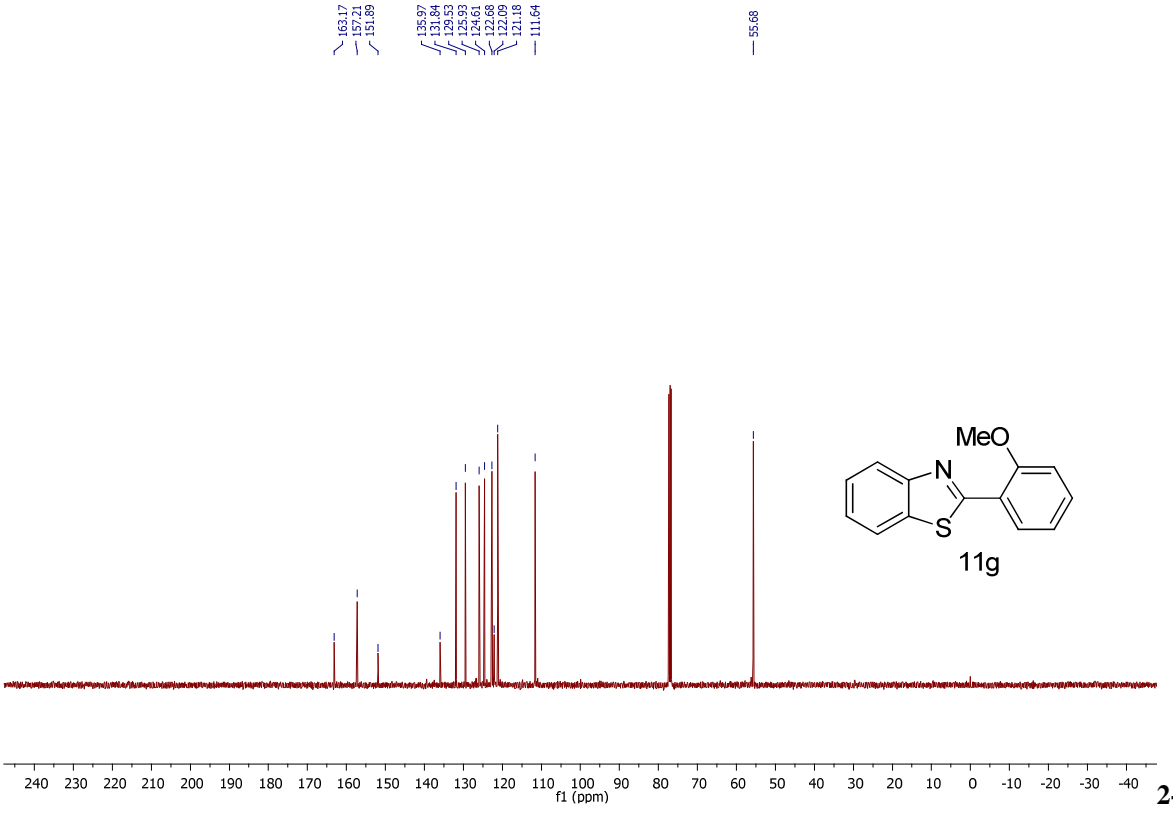




11f

2-(2'-Methoxyphenyl)benzothiazole (11g)





2-

2-(Thiophen-2'-yl)benzothiazole (11h)