A Facile Approach to 3,5-Disubstituted-1,2,4-Oxadiazoles via Copper-Catalyzed Cascade Annulation Amidines and Methylarenes

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Supporting Information

A. General methods

Melting points were measured using a melting point instrument and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer. IR spectra were obtained with an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets. GC−MS data were obtained using electron ionization. HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). TLC was performed using commercially available 100−400 mesh silica gel plates (GF254). Unless otherwise noted, purchased chemicals were used without further purification.

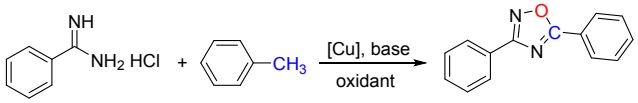
B. General procedure for the synthesis of disubstituted 1,2,4-oxadiazoles

General procedure for **3aa**: A mixture of benzamidine hydrochloride **1a** (0.25 mmol), toluene **2a** (0.50 mmol), $Cu(OAc)_2$ (4.5 mg, 10 mol %), K_3PO_4 (159 mg, 3 equiv), 70% TBHP (63 mg, 3 equiv) and DCE (1 mL) in a test tube (10 mL) equipped with a magnetic stirring bar. The mixture was stirred at room temperature for 12 h. After the reaction was completed, 10 mL ethyl acetate (3 × 10 mL) was added into the tube. The combined organic layers were washed with brine to neutral, dried over $MgSO_4$, and concentrated in vacuum. Purification of the residue on a preparative TLC afforded **3aa** as a white solid.

C. Screening reaction conditions

We initiated our investigations by examining the reaction of benzamidine hydrochloride (**1a**) with toluene (**2a**) in the presence of copper salts, bases and oxidants (Table 1). Fortunately, the desired product **3aa** was obtained in 24% isolated yield with $CuCl_2$ as catalyst, K_3PO_4 as base and 70% TBHP as oxidant at room temperature (entry 1). A screening of copper catalysts revealed that $Cu(OAc)_2$ was most effective, and its use resulted in the formation of **3aa** in 81% isolated yield (entries 2-5). A higher temperature led to a decreased yield due to the transformation of **1a** to benzonitrile (entries 6-7). No products were obtained in the absence of copper salt, base or oxidant (entries 8-10). The examination of different bases were also performed, however, no desired product could be obtained with the use of DBU (entry 11). Evaluation of additional bases such as KOH, Na_2CO_3 and Cs_2CO_3 provided conditions that resulted in a much lower yield of **3aa** relative to K_3PO_4 (entries 12-14). Some commonly used oxidants, such as TBHP, DTBP, H_2O_2, $K_2S_2O_8$ and O_2 were also tested, in which TBHP was found to be the best one, while others showed little effect (entries 4, 15-18). When the amount of copper, base and oxidant were decreased, dramatic lowering of yields were observed (entries 19-21). When the reaction was performed in N_2 atmosphere, 79% yield of **3aa** was isolated (entry 22). A gram scale preparation was performed and the isolated yield was 63% (entry 23).

Table 1. Screening for optimal reaction conditions.[a]

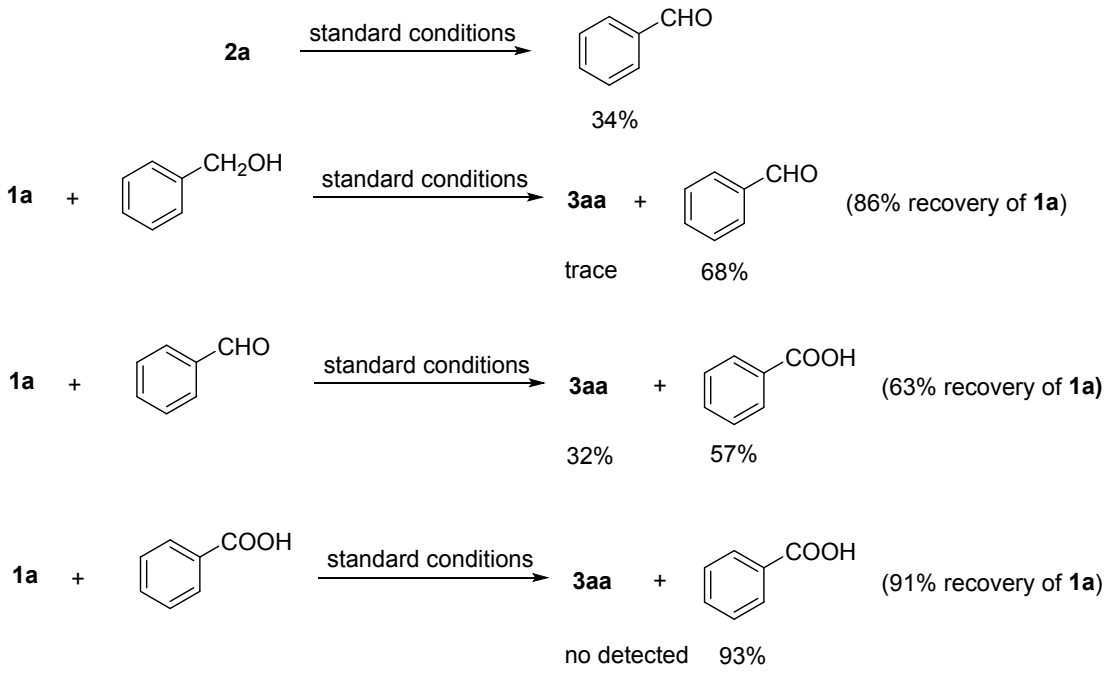


1a **2a** **3aa**

Entry	[Cu]	Base	Oxidant	Yield (%)[b]
1	$CuCl_2$	K_3PO_4	70%TBHP	18
2	$CuBr_2$	K_3PO_4	70%TBHP	33
3	CuI	K_3PO_4	70%TBHP	0
4	$Cu(OAc)_2$	K_3PO_4	70%TBHP	81
5	$Cu(OTf)_2$	K_3PO_4	70%TBHP	15
6[c]	$Cu(OAc)_2$	K_3PO_4	70%TBHP	21
7[d]	$Cu(OAc)_2$	K_3PO_4	70%TBHP	trace
8	none	K_3PO_4	70%TBHP	0
9	$Cu(OAc)_2$	none	70%TBHP	0
10	$Cu(OAc)_2$	K_3PO_4	none	0
11	$Cu(OAc)_2$	DBU	70%TBHP	0
12	$Cu(OAc)_2$	KOH	70%TBHP	11
13	$Cu(OAc)_2$	Na_2CO_3	70%TBHP	14
14	$Cu(OAc)_2$	Cs_2CO_3	70%TBHP	28
15	$Cu(OAc)_2$	K_3PO_4	DTBP	0
16	$Cu(OAc)_2$	K_3PO_4	H_2O_2	0
17	$Cu(OAc)_2$	K_3PO_4	$K_2S_2O_8$	0
18	$Cu(OAc)_2$	K_3PO_4	O_2	0
19[e]	$Cu(OAc)_2$	K_3PO_4	70%TBHP	43
20[f]	$Cu(OAc)_2$	K_3PO_4	70%TBHP	46
21[g]	$Cu(OAc)_2$	K_3PO_4	70%TBHP	28
22[h]	$Cu(OAc)_2$	K_3PO_4	70%TBHP	79
23[i]	$Cu(OAc)_2$	K_3PO_4	70%TBHP	63

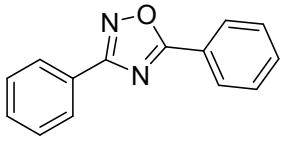
[a] Reaction conditions: unless otherwise noted, all reaction were performed with **1a** (0.25 mmol), **2a** (0.5 mmol), [Cu] catalyst (10 mol %), 70% TBHP (3 equiv) and base (3 equiv) in a 1.0 mL DCE at room temperature for 12 h. [b] Isolated yield based on **1a**. [c] 60 °C for 12 h. [d] 80 °C for 12 h. [e] 5 mol % $Cu(OAc)_2$ was used . [f] 1.5 equiv K_3PO_4 was used. [g] 1.5 equiv 70% TBHP was used. [h] The reaction proceeded with N_2 atmosphere. [i] A gram scale preparation were performed with **1a** (10 mmol), **2a** (20 mmol), $Cu(OAc)_2$ (10 mol %), K_3PO_4 (3 equiv), 70% TBHP (3 equiv) and DCE (20 mL) at room temperature for 12 h.

D. Control experiments



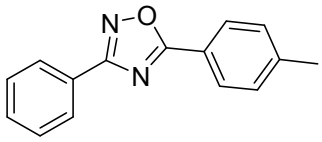
Without benzamidine hydrochloride, the toluene was oxidized to benzaldehyde by TBHP with a low yield under the standard conditions. The reactions failed to give the desired product **3aa** when benzamidine hydrochloride was reacted with benzylic alcohol or benzoic acid under the standard conditions, and we found that benzylic alcohol was converted to benzaldehyde. For benzaldehyde, 32% yield of the desired product was obtained.

E. Characterization data for all products



3,5-Diphenyl-1,2,4-oxadiazole[1] (3aa)

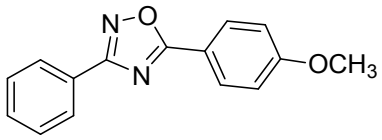
Yield: 0.045 g (81%), white solid, m. p. 108-109 ^{o}C; IR (KBr, cm^{-1}): ν = 3057, 1607, 1556, 1533, 1494, 1440, 1362, 1263, 1171, 1129, 720, 682; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.19-8.18 (m, 4H), 7.55-7.49 (m, 6H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.71, 168.99, 132.70, 131.18, 129.09, 128.86, 128.17, 127.56, 127.05, 124.35; HRMS (ESI) calc. $C_{14}H_{10}N_2ONa$ $[M+Na]^+$: 245.0685, found: 245.0687.



3-Phenyl-5-p-tolyl-1,2,4-oxadiazole[2] (3ab)

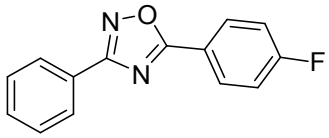
Yield: 0.041 g (68%), white solid, m. p. 112-114 ^{o}C; IR (KBr, cm^{-1}): ν = 3067, 3032,

2922, 2851, 1610, 1526, 1443, 1362, 1267, 1177, 1128, 739, 691; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.18 (d, 2H, *J* = 8.0 Hz), 8.10 (d, 2H, *J* = 8.0 Hz), 7.51-7.50 (m, 3H), 7.34 (d, 2H, *J* = 8.0 Hz), 2.44 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.86, 168.90, 143.48, 131.11, 129.81, 128.83, 128.15, 127.53, 127.12, 121.63, 21.75; HRMS (ESI) calc. $C_{15}H_{12}N_2ONa$ $[M+Na]^+$: 259.0842, found: 259.0837.



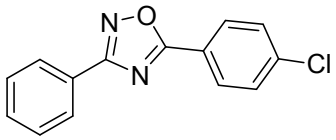
5-(4-Methoxyphenyl)-3-phenyl-1,2,4-oxadiazole[3] (3ac)

Yield: 0.043 g (68%), white solid, m. p. 95-97 °C; IR (KBr, cm^{-1}): ν = 3069, 2977, 2919, 2844, 1609, 1510, 1468, 1368, 1263, 1179, 1022, 836, 749, 692; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.16-8.14 (m, 4H), 7.51-7.49 (m, 3H), 7.04-7.01 (m, 2H), 3.88 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.60, 168.83, 163.18, 131.06, 130.07, 128.81, 127.51, 127.18, 116.91, 114.51, 55.50; HRMS (ESI) calc. $C_{15}H_{12}N_2O_2Na$ $[M+Na]^+$: 275.0791, found: 275.0792.



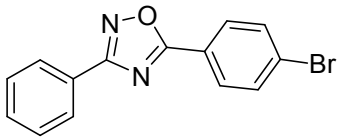
5-(4-Fluorophenyl)-3-phenyl-1,2,4-oxadiazole (3ad)

Yield: 0.042 g (70%), white solid, m. p. 119-120 °C; IR (KBr, cm^{-1}): ν = 3072, 1602, 1524, 1470, 1414, 1362, 1283, 1077, 843, 747, 694; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.22-8.29 (m, 2H), 8.15 (d, 2H, *J* = 8.0 Hz), 7.50-7.49 (m, 3H), 7.24-7.19 (m, 2H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.78, 168.99, 165.47 (d, *J* = 253 Hz), 131.24, 130.60 (d, *J* = 9 Hz), 128.86, 127.52, 126.87, 120.71 (d, J = 3 Hz), 116.46 (d, *J* = 22 Hz); HRMS (ESI) calc. $C_{14}H_9FN_2ONa$ $[M+Na]^+$: 263.0591, found: 263.0589.



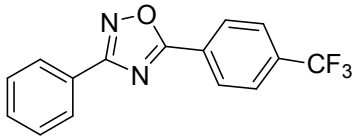
5-(4-Chlorophenyl)-3-phenyl-1,2,4-oxadiazole[4] (3ae)

Yield: 0.047 g (74%), white solid, m. p. 118-121 °C; IR (KBr, cm^{-1}): ν = 3062, 1604, 1554, 1522, 1494, 1399, 1361, 1267, 1082, 836, 738, 698; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.15 (d, 4H, *J* = 8.0 Hz), 7.54-7.42 (m, 5H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.81, 169.07, 139.20, 131.29, 129.52, 129.45, 128.88, 127.53, 126.79, 122.79; HRMS (ESI) calc. $C_{14}H_9ClN_2ONa$ $[M+Na]^+$: 279.0296, found: 279.0301.



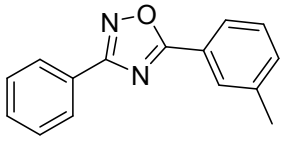
5-(4-Bromophenyl)-3-phenyl-1,2,4-oxadiazole[5] (3af)

Yield: 0.055 g (72%), white solid, m. p. 118-121 ^{o}C; IR (KBr, cm^{-1}): ν = 3061, 1603, 1581, 1551, 1519, 1475, 1401, 1365, 1266, 832, 737, 714, 681; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.16 (d, 2H, *J* = 8.0 Hz), 8.08 (d, 2H, *J* = 8.0 Hz), 7.70 (d, 2H, *J* = 8.0 Hz), 7.52-7.51 (m, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.92, 169.09, 132.51, 131.31, 129.56, 128.89, 127.73, 127.54, 126.77, 123.22; HRMS (ESI) calc. $C_{14}H_9BrN_2ONa$ $[M+Na]^+$: 322.9790, found: 322.9787.



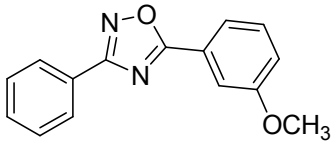
3-Phenyl-5-(4-(trifluoromethyl)phenyl)-1,2,4-oxadiazole (3ag)

Yield: 0.047 g (65%), white solid, m. p. 101-102 ^{o}C; IR (KBr, cm^{-1}): ν = 3076, 3036, 1598, 1564, 1526, 1508, 1470, 1449, 1413, 1326, 1170, 1118, 850, 792, 757, 721, 686; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.35 (d, 2H, *J* = 8.0 Hz), 8.17 (d, 2H, *J* = 4.0 Hz), 7.82 (d, 2H, *J* = 8.0 Hz), 7.53-7.52 (m, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.38, 169.24, 134.27 (d, *J* = 32 Hz), 131.43, 128.93, 128.55, 127.56, 127.47, 126.61, 126.14 (q, *J* = 8 Hz), 124.31 (d, *J* = 271 Hz); HRMS (ESI) calc. $C_{15}H_{10}F_3N_2O$ $[M+H]^+$: 291.0740, found: 291.0736.



3-Phenyl-5-m-tolyl-1,2,4-oxadiazole[6] (3ah)

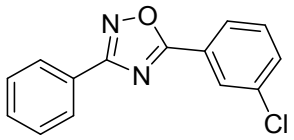
Yield: 0.039 g (65%), white solid, m. p. 72-73 ^{o}C; IR (KBr, cm^{-1}): ν = 3064, 2922, 2851, 1611, 1559, 1529, 1478, 1441, 1361, 1283, 1068, 917, 737, 690; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.18-8.17 (m, 2H), 8.04-8.00 (m, 2H), 7.51-7.50 (m, 3H), 7.45-7.39 (m, 2H), 2.46 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.92, 168.94, 139.03, 129.01, 128.84, 128.67, 127.54, 127.06, 125.33, 124.22, 21.33; HRMS (ESI) calc. $C_{15}H_{12}N_2ONa$ $[M+Na]^+$: 259.0842, found: 259.0845.



5-(3-Methoxyphenyl)-3-phenyl-1,2,4-oxadiazole[5] (3ai)

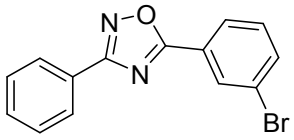
Yield: 0.045 g (71%), white solid, m. p. 81-83 ^{o}C; IR (KBr, cm^{-1}): ν = 3068, 3005, 2931, 2840, 1605, 1559, 1483, 1439, 1363, 1287, 1229, 1181, 1129, 1041, 992, 849,

793, 744, 691; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.17 (d, 2H, *J* = 4.0 Hz), 7.80 (d, 1H, *J* = 8.0 Hz), 7.72 (s, 1H), 7.51-7.43 (m, 4H), 7.13 (d, 1H, *J* = 12.0 Hz), 3.90 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.66, 168.99, 159.99, 131.19, 130.24, 128.85, 127.55, 126.99, 125.41, 120.61, 119.29, 112.64, 55.56; HRMS (ESI) calc. $C_{15}H_{12}N_2O_2Na$ $[M+Na]^+$: 275.0791, found: 275.0792.



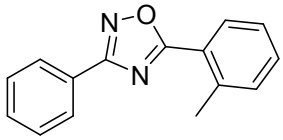
5-(3-Chlorophenyl)-3-phenyl-1,2,4-oxadiazole[5] (3aj)

Yield: 0.047 g (73%), white solid, m. p. 102-103 °C; IR (KBr, cm^{-1}): ν = 3073, 1604, 1554, 1522, 1475, 1439, 1362, 1282, 1074, 733, 682; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.20 (s, 1H), 8.15 (d, 2H, *J* = 8.0 Hz), 8.08 (d, 2H, *J* = 8.0 Hz), 7.57-7.47 (m, 5H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.45, 169.08, 135.29, 132.74, 131.33, 130.45, 128.89, 128.17, 127.54, 126.71, 126.19, 125.90; HRMS (ESI) calc. $C_{14}H_9ClN_2ONa$ $[M+Na]^+$: 279.0296, found: 279.0297.



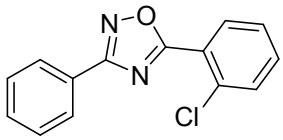
5-(3-Bromophenyl)-3-phenyl-1,2,4-oxadiazole[5] (3ak)

Yield: 0.057 g (76%), white solid, m. p. 107-109 °C; IR (KBr, cm^{-1}): ν = 3061, 3031, 1603, 1551, 1521, 1480, 1439, 1356, 1271, 1075, 793, 737, 680; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.35 (s, 1H), 8.16-8.11 (m, 3H), 7.71 (d, 1H, *J* = 8.0 Hz), 7.51-7.50 (m, 3H), 7.39 (d, 1H, *J* = 8.0 Hz); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.30, 169.06, 135.66, 131.34, 131.05, 130.65, 128.90, 127.54, 126.70, 126.63, 126.10, 123.16; HRMS (ESI) calc. $C_{14}H_9BrN_2ONa$ $[M+Na]^+$: 322.9790, found: 322.9790.



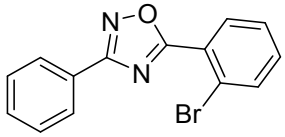
3-Phenyl-5-o-tolyl-1,2,4-oxadiazole[7] (3al)

Yield: 0.036 g (61%), white solid, m. p. 51-52 °C; IR (KBr, cm^{-1}): ν = 3065, 2968, 2927, 2854, 1604, 1555, 1520, 1440, 1361, 1298, 1255, 1174, 1065, 799, 740, 691; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.19-8.14 (m, 3H), 7.51-7.50 (m, 3H), 7.44 (d, 1H, *J* = 8.0 Hz), 7.35 (d, 2H, *J* = 8.0 Hz), 2.77 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 176.35, 168.60, 139.16, 132.18, 131.91, 131.13, 130.21, 128.85, 127.55, 127.17, 126.28, 123.51, 21.97; HRMS (ESI) calc. $C_{15}H_{12}N_2ONa$ $[M+Na]^+$: 259.0842, found: 259.0846.



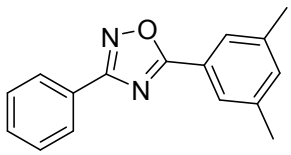
5-(2-Chlorophenyl)-3-phenyl-1,2,4-oxadiazole (3am)

Yield: 0.041 g (63%), white solid, m. p. 56-57 ^{o}C; IR (KBr, cm^{-1}): ν = 3067, 1605, 1571, 1519, 1482, 1445, 1362, 1301, 1134, 1045, 967, 915, 743, 689; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.18 (d, 2H, *J* = 8.0 Hz), 8.12 (d, 1H, *J* = 8.0 Hz), 7.56-7.45 (m, 5H), 7.41-7.38 (m, 1H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.31, 166.70, 133.88, 133.12, 131.94, 131.45, 131.29, 128.90, 127.59, 127.09, 126.81, 123.67; HRMS (ESI) calc. $C_{14}H_9ClN_2ONa$ $[M+Na]^+$: 279.0296, found: 279.0301.



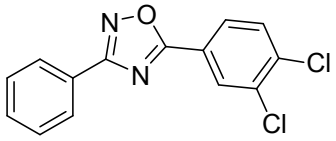
5-(2-Bromophenyl)-3-phenyl-1,2,4-oxadiazole (3an)

Yield: 0.046 g (62%), white solid, m. p. 56-57 ^{o}C; IR (KBr, cm^{-1}): ν = 3069, 1600, 1570, 1543, 1480, 1446, 1359, 1312, 1139, 1028, 974, 740, 691; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.18 (d, 2H, *J* = 8.0 Hz), 8.06 (d, 1H, *J* = 8.0 Hz), 7.77 (d, 1H, *J* = 8.0 Hz), 7.51-7.38 (m, 5H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.85, 168.71, 134.81, 132.16, 131.31, 128.91, 127.60, 126.79, 125.80, 122.16; HRMS (ESI) calc. $C_{14}H_9BrN_2ONa$ $[M+Na]^+$: 322.9790, found: 322.9793.



5-(3,5-Dimethylphenyl)-3-phenyl-1,2,4-oxadiazole (3ao)

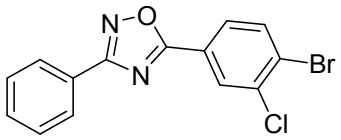
Yield: 0.043 g (69%), white solid, m. p. 87-88 ^{o}C; IR (KBr, cm^{-1}): ν = 3066, 2920, 2850, 1610, 1562, 1445, 1363, 1300, 1224, 1028, 919, 833, 748, 690; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.18-8.17 (m, 2H), 7.84 (s, 2H), 7.51-7.50 (m, 3H), 7.23 (s, 1H), 2.42 (s, 6H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 176.1, 168.89, 138.90, 134.49, 131.11, 128.83, 127.53, 127.10, 125.87, 124.09, 21.20; HRMS (ESI) calc. $C_{16}H_{14}N_2ONa$ $[M+Na]^+$: 273.0998, found: 273.1005.



5-(3,4-Dichlorophenyl)-3-phenyl-1,2,4-oxadiazole (3ap)

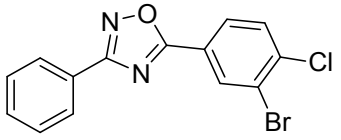
Yield: 0.054 g (74%), white solid, m. p. 133-134 ^{o}C; IR (KBr, cm^{-1}): ν = 3068, 1608, 1574, 1546, 1480, 1448, 1396, 1361, 1289, 1269, 1031, 912, 893, 829, 803, 740, 685; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.29 (s, 1H), 8.14-8.13 (m, 2H), 8.01 (d, 1H, *J* =

8.0 Hz), 7.61 (d, 1H, *J* = 8.0 Hz), 7.51-7.50 (m, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 173.72, 169.14, 137.40, 133.82, 131.42, 131.31, 129.92, 128.91, 127.53, 127.06, 126.54, 124.02; HRMS (ESI) calc.$C_{14}H_9Cl_2N_2O$ $[M+H]^+$: 291.0086, found: 291.0086.



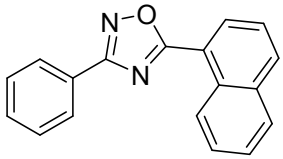
5-(4-Bromo-3-chlorophenyl)-3-phenyl-1,2,4-oxadiazole (3aq)

Yield: 0.061 g (73%), white solid, m. p. 107-108 °C; IR (KBr, cm^{-1}): ν = 3066, 1604, 1545, 1524, 1476, 1447, 1393, 1360, 1118, 1021, 741, 685; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.30 (s, 1H), 8.15 (d, 2H, *J* = 8.0 Hz), 7.94 (d, 1H, *J* = 8.0 Hz), 7.81 (d, 1H, *J* = 8.0 Hz), 7.52-7.51 (m, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 173.85, 169.18, 135.83, 134.65, 131.44, 129.64, 128.93, 127.75, 127.55, 127.04, 126.54, 124.71; HRMS (ESI) calc.$C_{14}H_9BrClN_2O$ $[M+H]^+$: 334.9738, found: 334.9728.



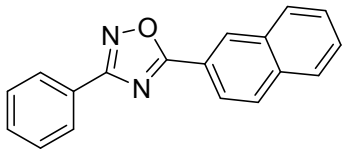
5-(3-Bromo-4-chlorophenyl)-3-phenyl-1,2,4-oxadiazole (3ar)

Yield: 0.062 g (75%), white solid, m. p. 148-149 °C; IR (KBr, cm^{-1}): ν = 3064, 1604, 1544, 1525, 1478, 1447, 1391, 1361, 1289, 1268, 1123, 1025, 981, 913, 895, 830, 741, 685; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.47 (s, 1H), 8.14 (d, 2H, *J* = 8.0 Hz), 8.06 (d, 1H, *J* = 8.0 Hz), 7.62 (d, 1H, *J* = 8.0 Hz), 7.52-7.50 (m, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 173.58, 169.14, 139.36, 133.17, 131.43, 131.10, 128.92, 127.73, 127.54, 126.54, 124.08, 123.51; HRMS (ESI) calc.$C_{14}H_9BrClN_2O$ $[M+H]^+$: 334.9738, found: 334.9731.



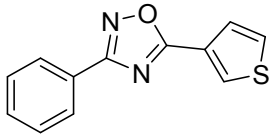
5-(Naphthalen-1-yl)-3-phenyl-1,2,4-oxadiazole[8] (3as)

Yield: 0.038 g (56%), white solid, m. p. 87-89 °C; IR (KBr, cm^{-1}): ν = 3054, 1598, 1579, 1551, 1514, 1474, 1445, 1358, 1306, 1288, 1252, 1143, 1071, 966, 844, 773, 750, 730, 694; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 9.26 (d, 1H, *J* = 8.0 Hz), 8.41 (d, 1H, *J* = 8.0 Hz), 8.26-8.25 (m, 2H), 8.08 (d, 1H, *J* = 8.0 Hz), 7.93 (d, 1H, *J* = 8.0 Hz), 7.71-7.69 (m, 1H), 7.61-7.54 (m, 5H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.89, 168.85, 133.92, 133.62, 131.23, 130.32, 130.00, 128.91, 128.81, 128.31, 127.64, 127.64, 126.74, 125.84, 124.93, 120.84; HRMS (ESI) calc. $C_{18}H_{12}N_2ONa$ $[M+Na]^+$: 295.0842, found: 295.0850.



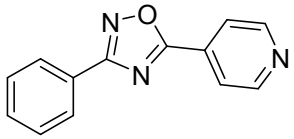
5-(Naphthalen-2-yl)-3-phenyl-1,2,4-oxadiazole (3at)

Yield: 0.030 g (43%), white solid, m. p. 121-122 ^{o}C; IR (KBr, cm^{-1}): ν = 3053, 1608, 1585, 1554, 1526, 1473, 1444, 1367, 1290, 1134, 1071, 905, 824, 759, 737, 694; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.77 (s, 1H), 8.25-8.21 (m, 3H), 8.02-7.99 (m, 2H), 7.91 (d, 1H, *J* = 8.0 Hz), 7.62-7.54 (m, 5H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.90, 169.09, 135.24, 132.80, 131.24, 129.25, 129.19, 129.08, 128.88, 128.65, 128.46, 127.99, 127.58, 127.19, 123.93, 121.55; HRMS (ESI) calc. $C_{18}H_{12}N_2ONa$ $[M+Na]^+$: 295.0842, found: 295.0845.



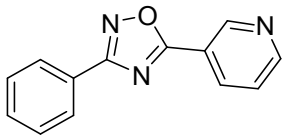
3-Phenyl-5-(thiophen-3-yl)-1,2,4-oxadiazole (3au)

Yield: 0.035 g (54%), white solid, m. p. 77-78 ^{o}C; IR (KBr, cm^{-1}): ν = 3104, 1637, 1600, 1525, 1471, 1443, 1416, 1384, 1353,1299, 1125, 1070, 1023, 914, 855, 804,736, 690; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.18 (s, 1H), 8.07-8.06 (m, 2H), 7.66-7.65 (m, 1H), 7.42-7.38(m, 4H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 171.96, 168.81, 131.18, 130.17, 128.85, 127.55, 127.44, 126.95, 126.71, 126.01; HRMS (ESI) calc.$C_{12}H_9N_2OS$ $[M+H]^+$: 229.0587, found: 229.0585.



4-(3-Phenyl-1,2,4-oxadiazol-5-yl)pyridine (3av)

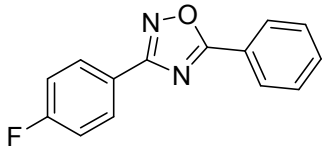
Yield: 0.037 g (67%), white solid, m. p. 155-157 ^{o}C; IR (KBr, cm^{-1}): ν = 3065, 3031, 1644, 1608, 1572, 1545, 1471, 1445, 1410, 1363, 1284, 1222, 1174, 1132, 1065, 1023, 915, 834, 767, 734, 719, 688; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.88 (s, 2H), 8.17 (d, 2H, J = 8.0 Hz), 8.05 (d, 2H, J = 4.0 Hz), 7.53-7.50 (m, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 173.79, 169.37, 151.03, 131.55, 131.18, 128.97, 127.57, 126.38, 121.37; HRMS (ESI) calc. $C_{13}H_{10}N_3O$ $[M+H]^+$: 224.0818, found: 224.0818.



3-(3-Phenyl-1,2,4-oxadiazol-5-yl)pyridine[9] (3aw)

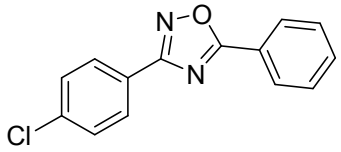
Yield: 0.035 g (63%), white solid, m. p. 120-122 ^{o}C; IR (KBr, cm^{-1}): ν = 3063, 1634,

1603, 1578, 1550, 1519, 1439, 1357, 1283, 1129, 1071, 965, 896, 734, 687; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 9.44 (s, 1H), 8.84 (d, 1H, *J* = 8.0 Hz), 8.46 (d, 1H, *J* = 8.0 Hz), 8.17 (d, 2H, *J* = 8.0 Hz), 7.52-7.48 (m, 4H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 173.65, 169.10, 153.26, 149.16, 135.24, 131.43, 128.92, 127.56, 126.53, 123.80, 120.76; HRMS (ESI) calc. $C_{13}H_{10}N_3O$ $[M+H]^+$: 224.0818, found: 224.0815.



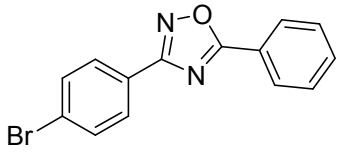
3-(4-Fluorophenyl)-5-phenyl-1,2,4-oxadiazole (3ba)

Yield: 0.045 g (74%), white solid, m. p. 116-117 °C; IR (KBr, cm^{-1}): ν = 3063, 1603, 1558, 1488, 1446, 1359, 1319, 1282, 1223, 1130, 1097, 1064, 843, 742, 683; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.19-8.14 (m, 4H), 7.57-7.51 (m, 3H), 7.19-7.15 (t, 2H, *J* = 8.0 Hz); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.78, 168.13, 164.60 (d, *J* = 250 Hz), 132.78, 129.68 (d, *J* = 9 Hz), 129.10, 128.15, 124.22, 123.24 (d, *J* = 3 Hz), 116.01 (d, *J* = 22 Hz); HRMS (ESI) calc. $C_{14}H_9FN_2ONa$ $[M+Na]^+$: 263.0591, found: 263.0593.



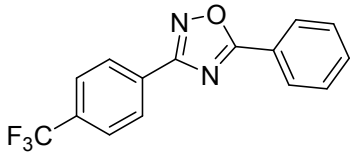
3-(4-Chlorophenyl)-5-phenyl-1,2,4-oxadiazole[2] (3ca)

Yield: 0.046 g (72%), white solid, m. p. 77-79 °C (108-110) ; IR (KBr, cm^{-1}): ν = 3061, 1604, 1554, 1518, 1489, 1445, 1405, 1356, 1271, 1088, 1017, 966, 918, 834, 738, 707, 683; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.13 (d, 2H, *J* = 8.0 Hz), 8.05 (d, 2H, *J* = 8.0 Hz), 7.54-7.40 (m, 5H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.80, 168.07, 137.27, 132.78, 129.12, 129.07, 128.80, 128.13, 125.49, 124.13; HRMS (ESI) calc. $C_{14}H_9ClN_2ONa$ $[M+Na]^+$: 279.0296, found: 279.0294.



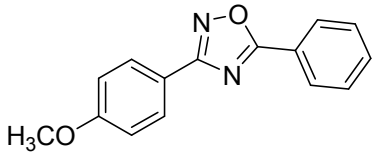
3-(4-Bromophenyl)-5-phenyl-1,2,4-oxadiazole[2] (3da)

Yield: 0.054 g (72%), white solid, m. p. 102-103 °C; IR (KBr, cm^{-1}): ν = 3059, 1595, 1553, 1516, 1489, 1445, 1403, 1356, 1318, 1271, 1176, 1131, 1104, 1072, 919, 834, 737, 684; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.20 (d, 2H, *J* = 8.0 Hz), 8.04 (d, 2H, *J* = 8.0 Hz), 7.65-7.60 (m, 3H), 7.57-7.53 (m, 2H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.93, 168.27, 132.88, 132.15, 129.15, 129.04, 128.19, 125.95, 125.75, 124.15; HRMS (ESI) calc. $C_{14}H_9BrN_2ONa$ $[M+Na]^+$: 322.9790, found: 322.9791.



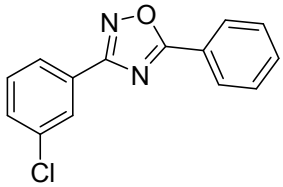
5-Phenyl-3-(4-(trifluoromethyl)phenyl)-1,2,4-oxadiazole (3ea)

Yield: 0.044 g (61%), white solid, m. p. 93-95 ^{o}C; IR (KBr, cm^{-1}): ν = 3065, 1614, 1558, 1494, 1446, 1414, 1360, 1324, 1269, 1172, 1105, 1062, 1017, 848, 750, 726, 686; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.30 (d, 2H, *J* = 8.0 Hz), 8.22 (d, 2H, *J* = 8.0 Hz), 7.81-7.76 (m, 2H), 7.63-7.55 (m, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 176.14, 167.91, 132.94, 132.86 (d, *J* = 32 Hz), 130.40 , 129.13, 128.17, 127.84, 125.79 (dd, *J* = 3 Hz, *J* = 11 Hz), 124.01, 123.83 (d, *J* = 270 Hz); HRMS (ESI) calc.$C_{15}H_{10}F_3N_2O$ $[M+H]^+$: 291.0740, found: 291.0740.



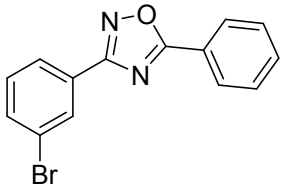
3-(4-Methoxyphenyl)-5-phenyl-1,2,4-oxadiazole[10] (3fa)

Yield: 0.049 g (78%), white solid, m. p. 97-98 ^{o}C; IR (KBr, cm^{-1}): ν = 3059, 3006, 2968, 2916, 2839, 1610, 1558, 1494, 1450, 1419, 1364, 1303, 1256, 1172, 1026, 835, 746, 684; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.20 (d, 2H, *J* = 8.0 Hz), 8.11 (d, 2H, *J* = 8.0 Hz), 7.59-7.52 (m, 3H), 7.01 (d, 2H, *J* = 8.0 Hz), 3.87 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.44, 168.68, 161.96, 132.63, 129.14, 129.07, 128.15, 124.44, 119.47, 114.26, 55.39; HRMS (ESI) calc. $C_{15}H_{12}N_2O_2Na$ $[M+Na]^+$: 275.0791, found: 275.0799.



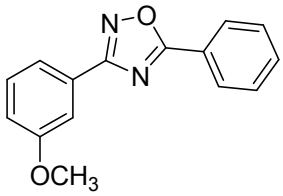
3-(3-Chlorophenyl)-5-phenyl-1,2,4-oxadiazole[2] (3ga)

Yield: 0.049 g (77%), white solid, m. p. 102-103 ^{o}C; IR (KBr, cm^{-1}): ν = 3089, 1608, 1553, 1514, 1471, 1457, 1440, 1361, 1280, 1140, 1072, 885, 764, 677; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.20 (s, 1H), 8.17 (d, 2H, *J* = 8.0 Hz), 8.04 (d, 1H, *J* = 4.0 Hz), 7.62-7.52 (m, 3H), 7.49-7.40 (m, 2H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.97, 167.96, 134.95, 132.89, 131.21, 130.16, 129.14, 128.73, 128.18, 127.65, 125.57, 124.11; HRMS (ESI) calc. $C_{14}H_9ClN_2ONa$ $[M+Na]^+$: 279.0296, found: 279.0303.



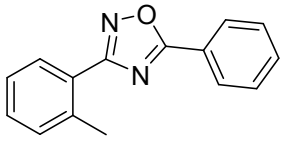
3-(3-Bromophenyl)-5-phenyl-1,2,4-oxadiazole (3ha)

Yield: 0.061 g (81%), white solid, m. p. 106-107 ^{o}C; IR (KBr, cm^{-1}): ν = 3067, 1607, 1550, 1512, 1484, 1426, 1339, 1267, 1062, 970, 926, 887, 804, 742, 676; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.28 (s, 1H), 8.14 (d, 2H, *J* = 8.0 Hz), 8.05 (d, 2H, *J* = 8.0 Hz), 7.60-7.54 (m, 2H), 7.49 (t, 2H, *J* = 8.0 Hz), 7.31 (t, 1H, *J* = 8.0 Hz); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.90, 167.76, 134.10, 132.86, 130.48, 130.37, 129.10, 128.93, 128.15, 126.00, 124.05, 122.94; HRMS (ESI) calc. $C_{14}H_9BrN_2ONa$ $[M+Na]^+$: 322.9790, found: 322.9796.



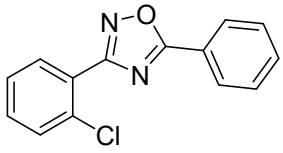
3-(3-Methoxyphenyl)-5-phenyl-1,2,4-oxadiazole (3ia)

Yield: 0.053 g (83%), white solid, m. p. 82-83 ^{o}C; IR (KBr, cm^{-1}): ν = 3066, 3004, 2963, 2836, 1612, 1561, 1523, 1465, 1365, 1318, 1281, 1242, 1182, 1043, 844, 795, 743, 687; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.19 (d, 2H, *J* = 8.0 Hz), 7.76 (d, 1H, *J* = 8.0 Hz), 7.69 (s, 1H), 7.57-7.49 (m, 3H), 7.39 (t, 1H, *J* = 8.0 Hz), 7.04 (d, 1H, *J* = 12.0 Hz), 3.87 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.68, 168.91, 159.92, 129.96, 129.08, 128.19, 128.16, 124.31, 120.01, 117.64, 112.15, 55.43; HRMS (ESI) calc. $C_{15}H_{13}N_2O_2$ $[M+H]^+$: 253.0972, found: 253.0970.



5-Phenyl-3-o-tolyl-1,2,4-oxadiazole (3ja)

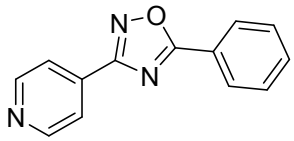
Yield: 0.044 g (75%), white solid, m. p. 79-81 ^{o}C; IR (KBr, cm^{-1}): ν = 3036, 2922, 2850, 1610, 1561, 1516, 1480, 1449, 1348, 1278, 1171, 1115, 1066, 900, 740, 688; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.21 (d, 1H, *J* = 8.0 Hz), 8.09 (d, 1H, *J* = 8.0 Hz), 7.61-7.52 (m, 3H), 7.42-7.34 (m, 3H), 2.68 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 174.73, 169.61, 138.28, 132.67, 131.38, 130.58, 130.15, 129.11, 128.18, 126.27, 126.00, 124.39, 22.11; HRMS (ESI) calc. $C_{15}H_{13}N_2O$ $[M+H]^+$: 237.1022, found: 237.1025.



3-(2-Chlorophenyl)-5-phenyl-1,2,4-oxadiazole[11] **(3ka)**

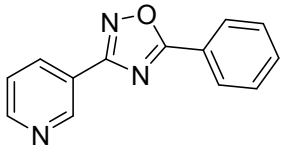
Yield: 0.051 g (79%), white solid, m. p. 86-88 ^{o}C; IR (KBr, cm^{-1}): ν = 3071, 1610, 1561, 1491, 1347, 1278, 1092, 895, 739, 685; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.20 (d, 2H, *J* = 8.0 Hz), 8.01 (d, 1H, *J* = 8.0 Hz), 7.61-7.51 (m, 4H), 7.44-7.37 (m,

2H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.28, 167.78, 133.55, 132.87, 131.79, 131.69, 130.94, 129.14, 128.21, 126.90, 126.30, 124.10; HRMS (ESI) calc. $C_{14}H_9ClN_2ONa$ $[M+Na]^+$: 279.0296, found: 279.0300.



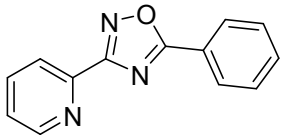
4-(5-Phenyl-1,2,4-oxadiazol-3-yl)pyridine (3la)

Yield: 0.034 g (61%), white solid, m. p. 152-153 °C; IR (KBr, cm^{-1}): ν = 3006, 1605, 1548, 1517, 1486, 1412, 1366, 1308, 1268, 1137, 1060, 743, 680; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.80 (d, 2H, *J* = 4.0 Hz), 8.20 (d, 2H, *J* = 8.0 Hz), 8.02 (d, 2H, *J* = 4.0 Hz), 7.62-7.53 (m, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 176.46, 167.41, 150.62, 134.43, 133.10, 129.19, 128.20, 123.83, 121.32; HRMS (ESI) calc. $C_{13}H_{10}N_3O$ $[M+H]^+$: 224.0818, found: 224.0820.



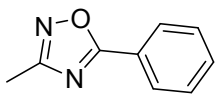
3-(5-Phenyl-1,2,4-oxadiazol-3-yl)pyridine[12] (3ma)

Yield: 0.035 g (63%), white solid, m. p. 140-141 °C; IR (KBr, cm^{-1}): ν = 3065, 1587, 1551, 1445, 140, 1364, 1272, 1187, 1063, 1019, 967, 787, 734, 687; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 9.39 (s, 1H), 8.76 (d, 1H, *J* = 4.0 Hz), 8.42 (d, 1H, *J* = 4.0 Hz), 8.19 (d, 2H, *J* = 8.0 Hz), 7.62-7.52 (m, 3H), 7.43 (t, 1H, *J* = 8.0 Hz); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 176.11, 166.98, 151.98, 148.69, 134.70, 132.98, 129.14, 128.18, 123.92, 123.61, 123.25; HRMS (ESI) calc. $C_{13}H_{10}N_3O$ $[M+H]^+$: 224.0818, found: 224.0821.



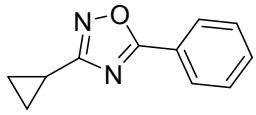
2-(5-Phenyl-1,2,4-oxadiazol-3-yl)pyridine[10] (3na)

Yield: 0.033 g (59%), white solid, m. p. 131-132 °C; IR (KBr, cm^{-1}): ν = 3066, 1610, 1557, 1514, 1489, 1447, 1366, 1278, 1156, 1039, 925, 50, 723; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.84 (d, 1H, *J* = 4.0 Hz), 8.27 (d, 2H, *J* = 8.0 Hz), 8.21 (d, 1H, *J* = 8.0 Hz), 7.86 (t, 1H, *J* = 8.0 Hz), 7.58-7.52 (m, 3H), 7.44 (m, 1H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 176.43, 168.75, 150.40, 146.45, 137.02, 132.91, 129.06, 128.29, 125.48, 123.98, 123.24; HRMS (ESI) calc. $C_{13}H_{10}N_3O$ $[M+H]^+$: 224.0818, found: 224.0818.



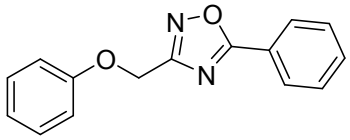
3-Methyl-5-phenyl-1,2,4-oxadiazole[13] (3oa)

Yield: 0.030 g (75%), white solid, m. p. 57-58 ^{o}C; IR (KBr, cm^{-1}): ν = 3064, 2923, 2851, 1613, 1562, 1448, 1395, 1342, 1274, 1101, 1070, 786, 722, 688; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.11 (d, 2H, J = 8.0 Hz), 7.60-7.49 (m, 3H), 2.47 (s, 3H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.42, 167.77, 132.62, 129.07, 127.99, 124.23, 11.69; HRMS (ESI) calc. $C_9H_9N_2O$ $[M+H]^+$: 161.0709, found: 161.0707.



3-Cyclopropyl-5-phenyl-1,2,4-oxadiazole (3pa)

Yield: 0.034 g (73%), pale yellow oil; IR (KBr, cm^{-1}): ν = 3095, 3065, 3013, 2930, 2850, 1614, 1563, 1530, 1485, 1451, 1376, 1279, 1248, 1179, 1116, 1060, 905, 822, 788, 743, 697; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.05 (d, 2H, *J* = 4.0 Hz), 7.53-7.43 (m, 3H), 2.14-2.11 (m, 1H), 1.11-1.05 (m, 4H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 175.02, 172.90, 132.39, 128.90, 127.91, 124.34, 7.70, 6.90; HRMS (ESI) calc. $C_{11}H_{10}N_2ONa$ $[M+Na]^+$: 209.0685, found: 209.0685.



3-(Phenoxymethyl)-5-phenyl-1,2,4-oxadiazole (3qa)

Yield: 0.047 g (68%), white solid, m. p. 67-69 ^{o}C; IR (KBr, cm^{-1}): ν = 3066, 2931, 2861, 1598, 1561, 1491, 1451, 1397, 1352, 1301, 1242, 1076, 754, 722, 689; ^{1}H NMR (400 Hz, $CDCl_3$, ppm): δ = 8.09 (d, 2H, *J* = 8.0 Hz), 7.51 (t, 1H, *J* = 8.0 Hz), 7.44 (t, 2H, *J* = 8.0 Hz), 7.27 (t, 2H, *J* = 8.0 Hz), 7.04 (d, 2H, *J* = 8.0 Hz), 6.97 (t, 1H, *J* = 8.0 Hz), 5.21 (s, 2H); ^{13}C NMR (100 Hz, $CDCl_3$, ppm): δ = 176.40, 167.50, 158.06, 133.02, 129.64, 129.14, 128.23, 123.89, 121.85, 114.98, 61.23; HRMS (ESI) calc. $C_{15}H_{12}N_2O_2Na$ $[M+Na]^+$: 275.0791, found: 275.0796.

E. References

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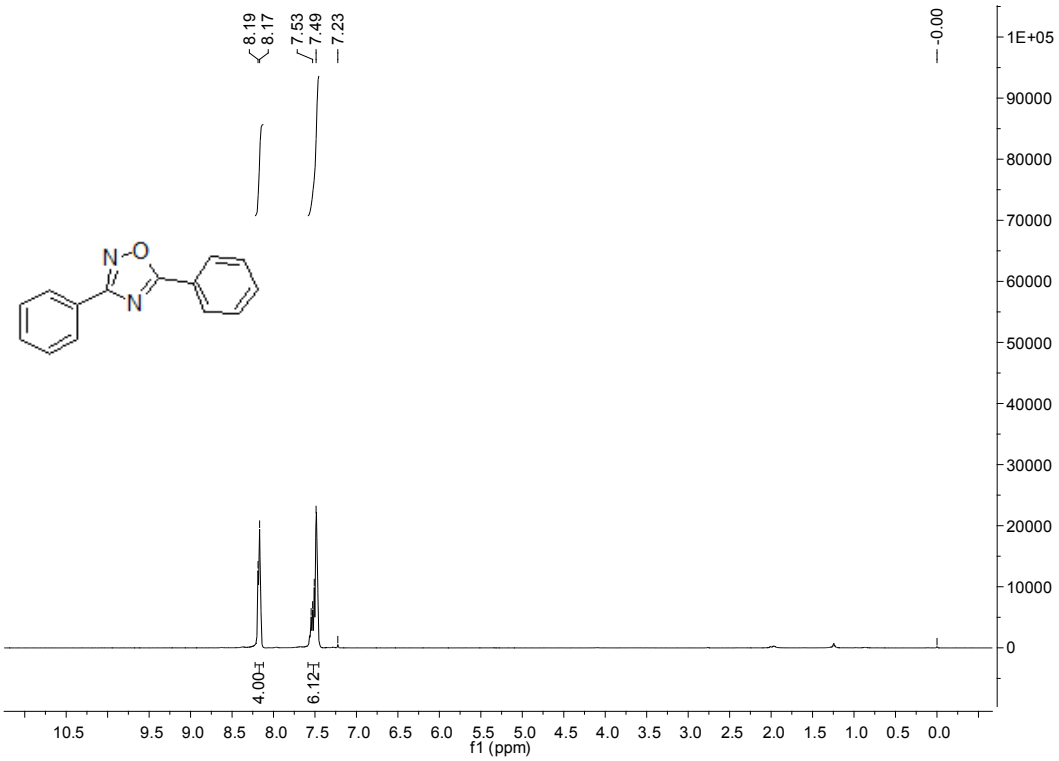
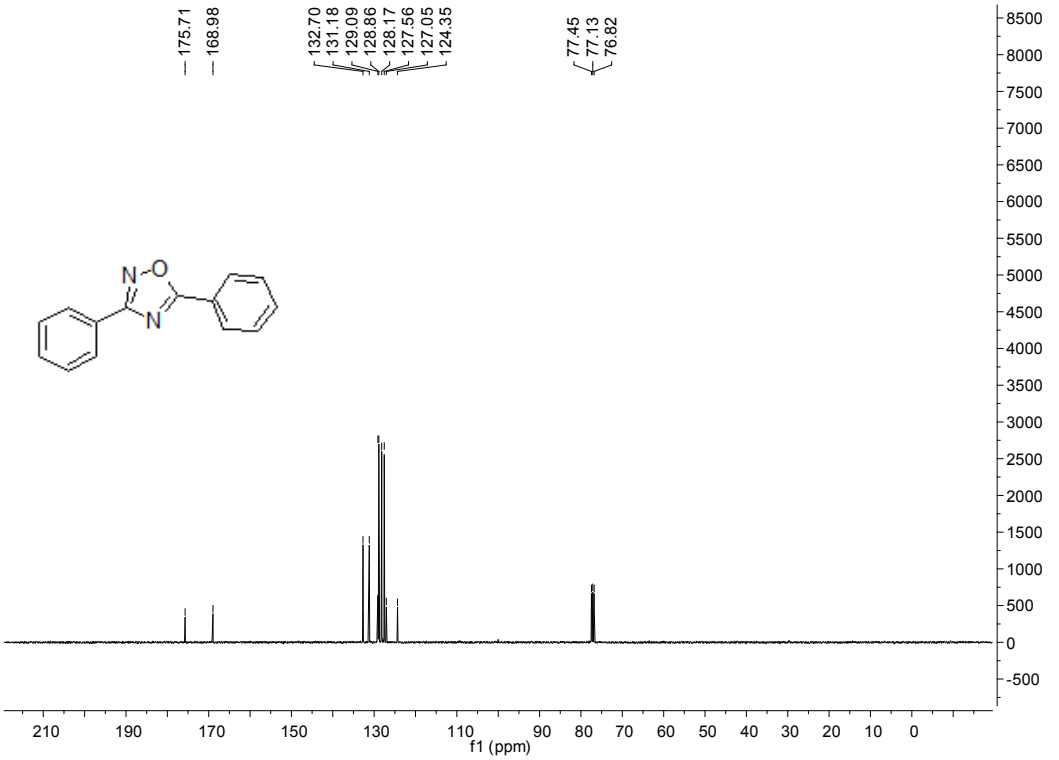
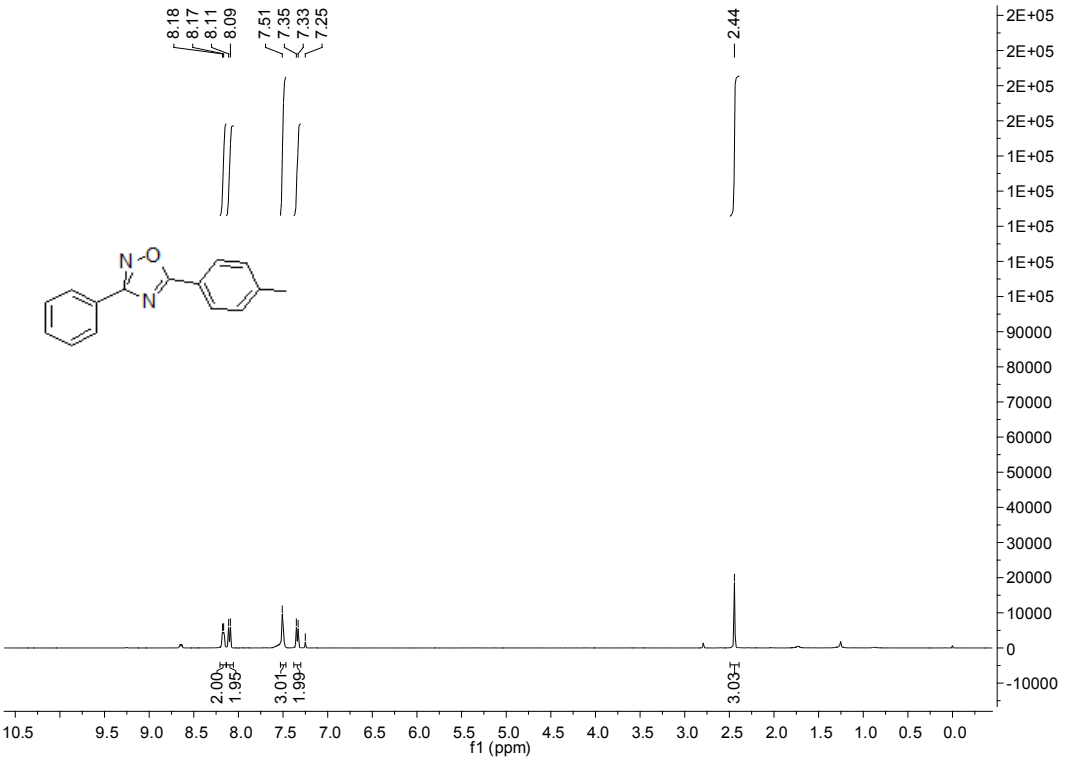
F. NMR spectra for all compounds



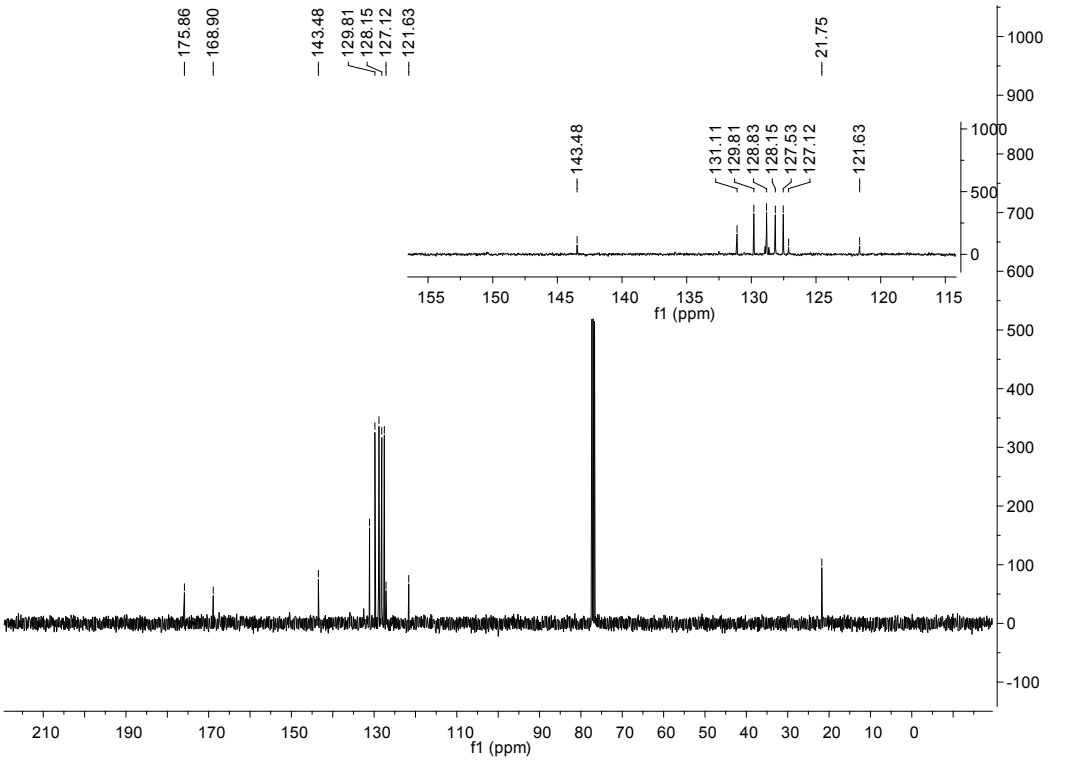
^{1}H NMR of **3aa**



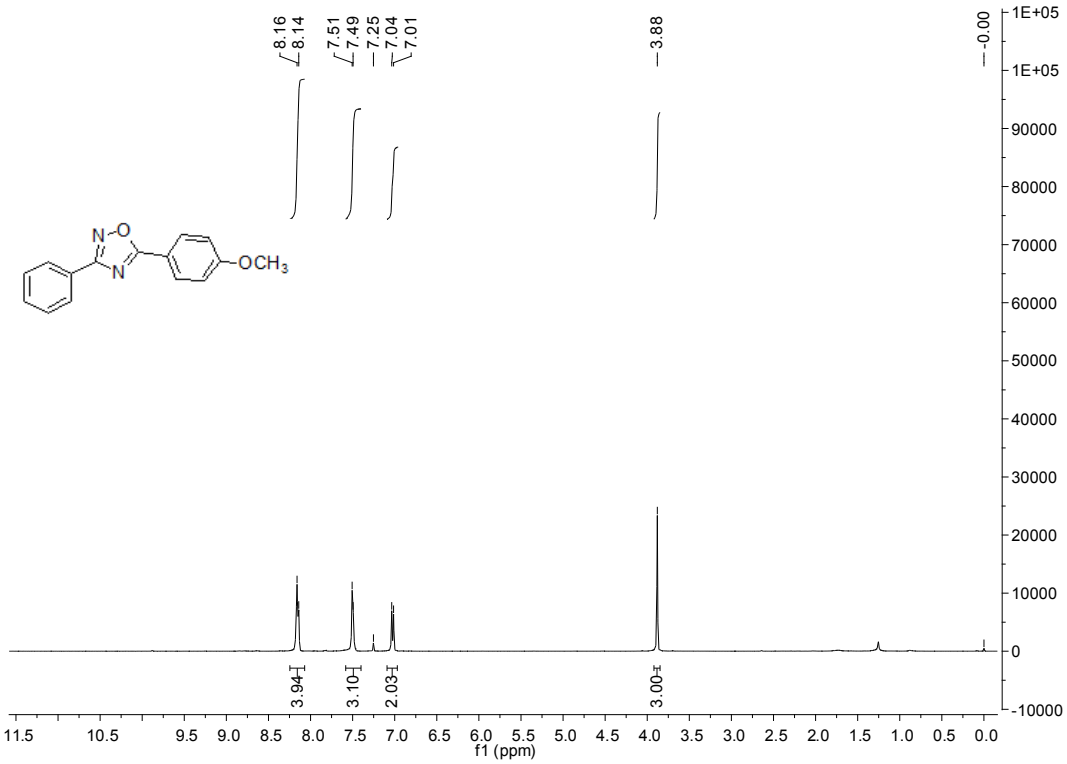
^{13}C NMR of **3aa**



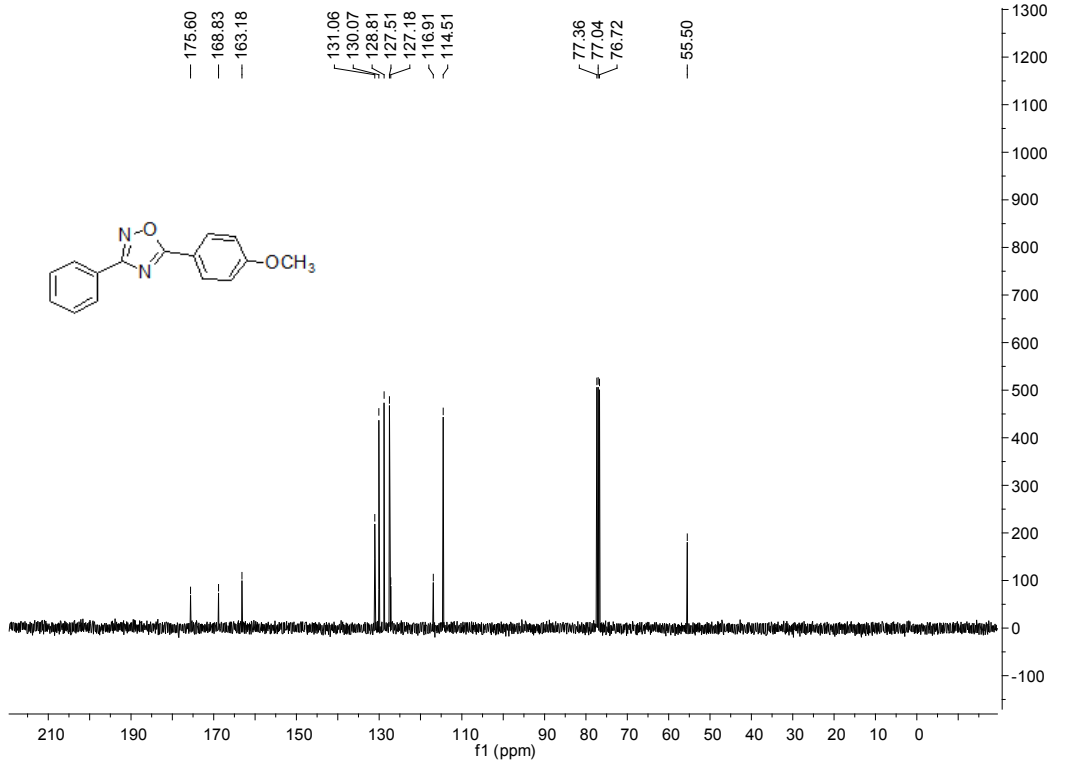
^{1}H NMR of **3ab**



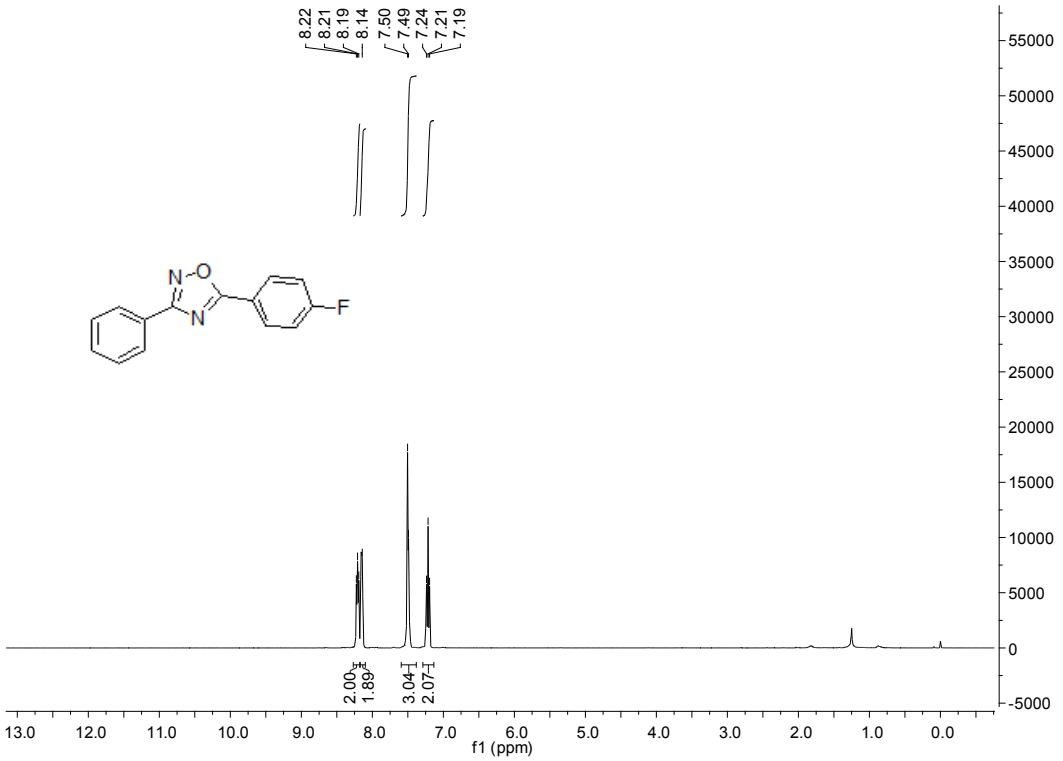
^{13}C NMR of **3ab**



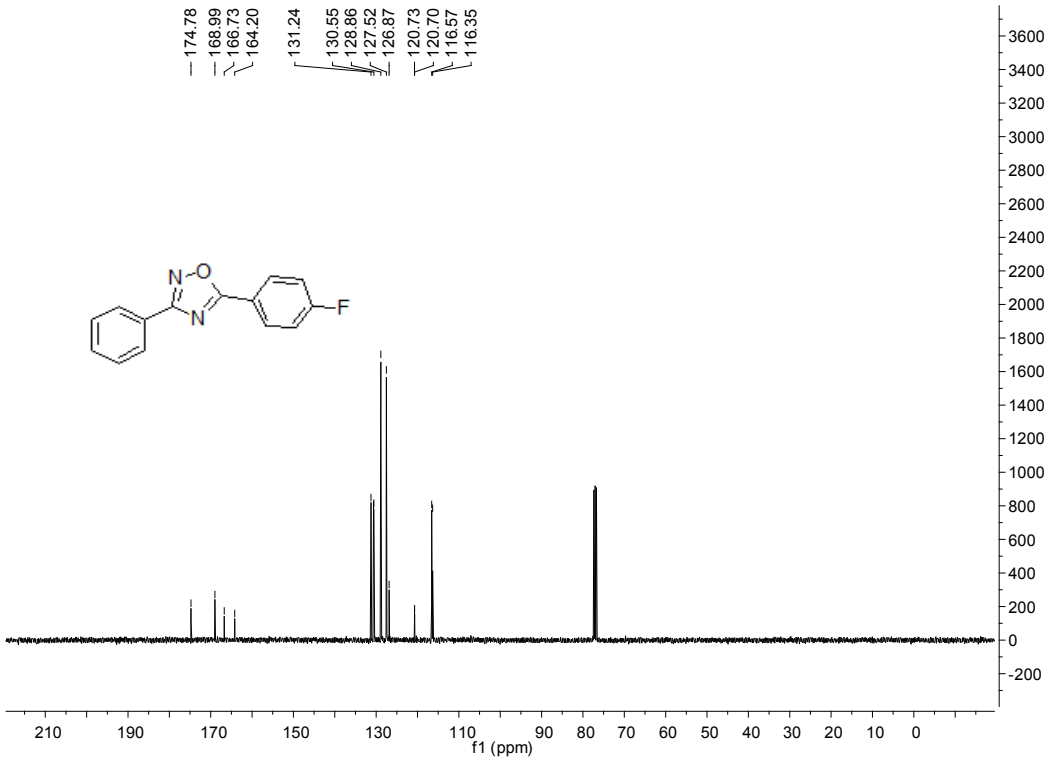
^{1}H NMR of **3ac**



^{13}C NMR of **3ac**



^{1}H NMR of **3ad**



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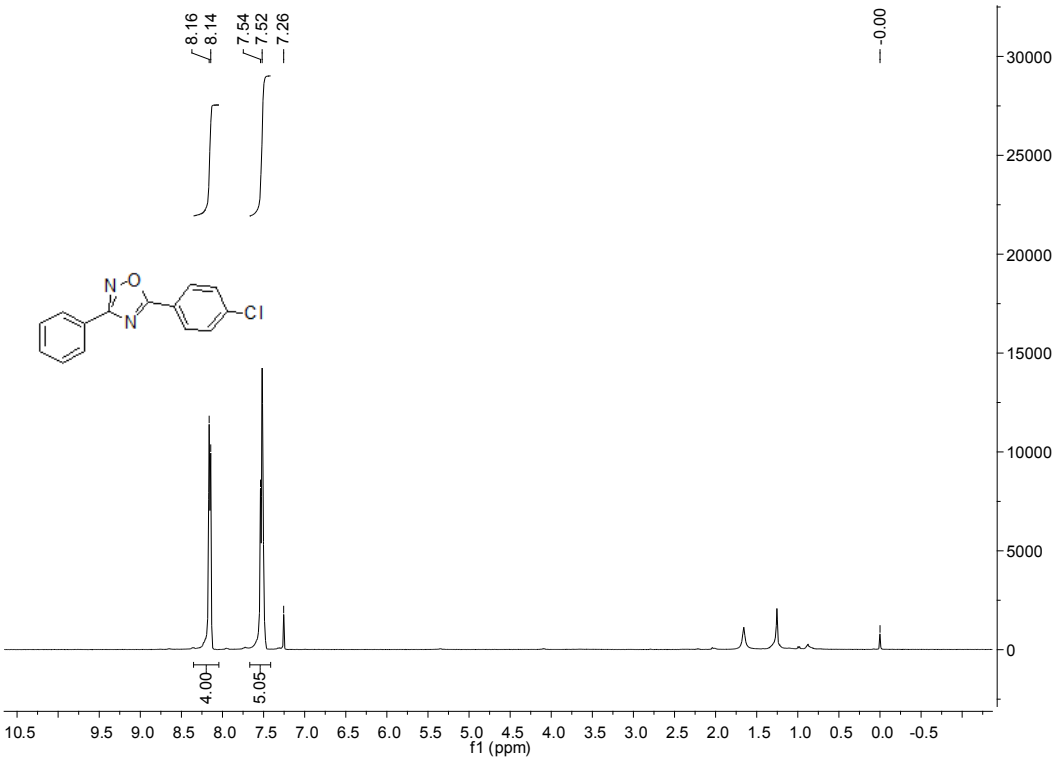
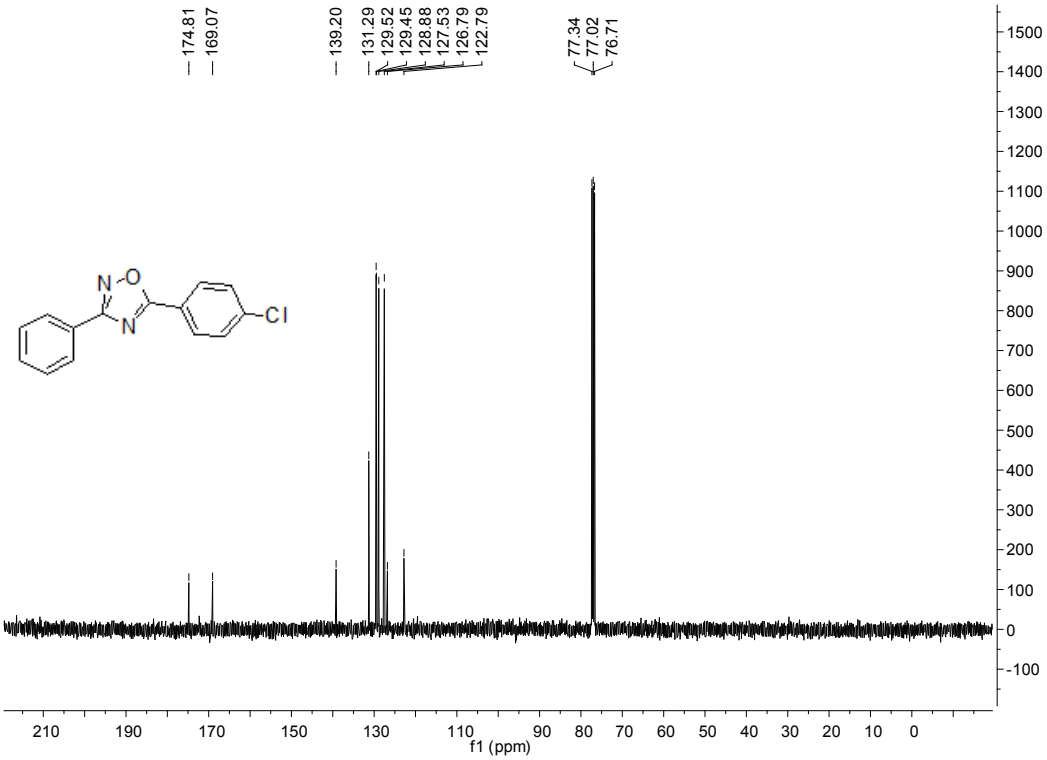


^{1}H NMR of **3ae**



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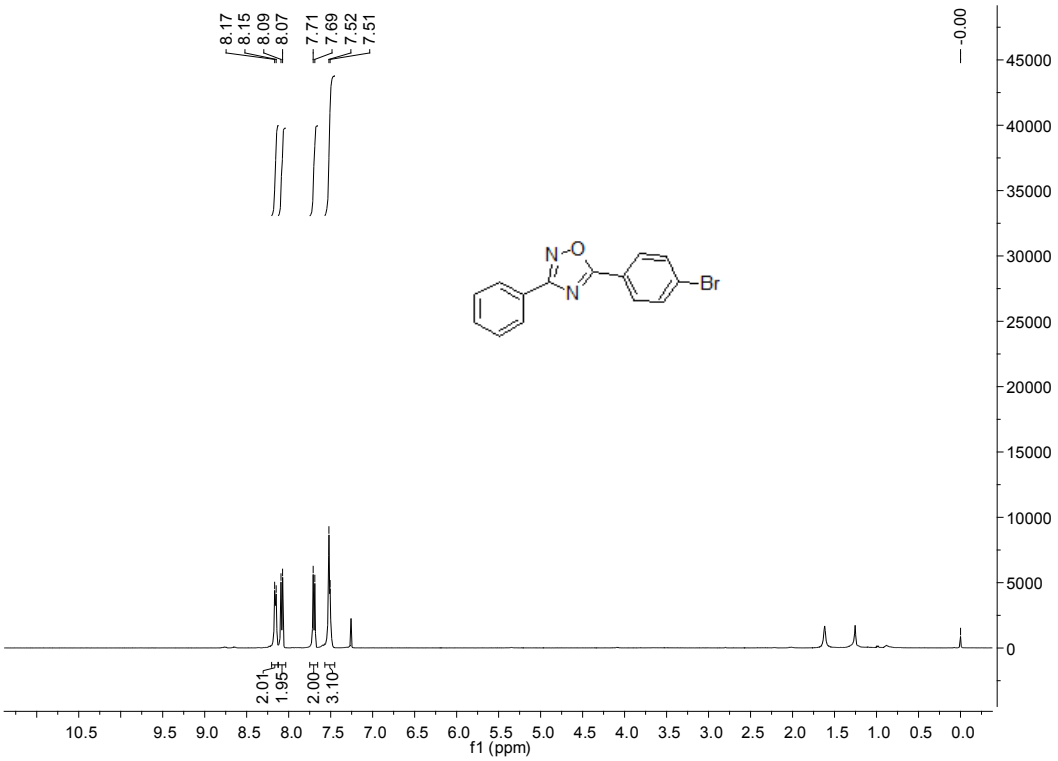
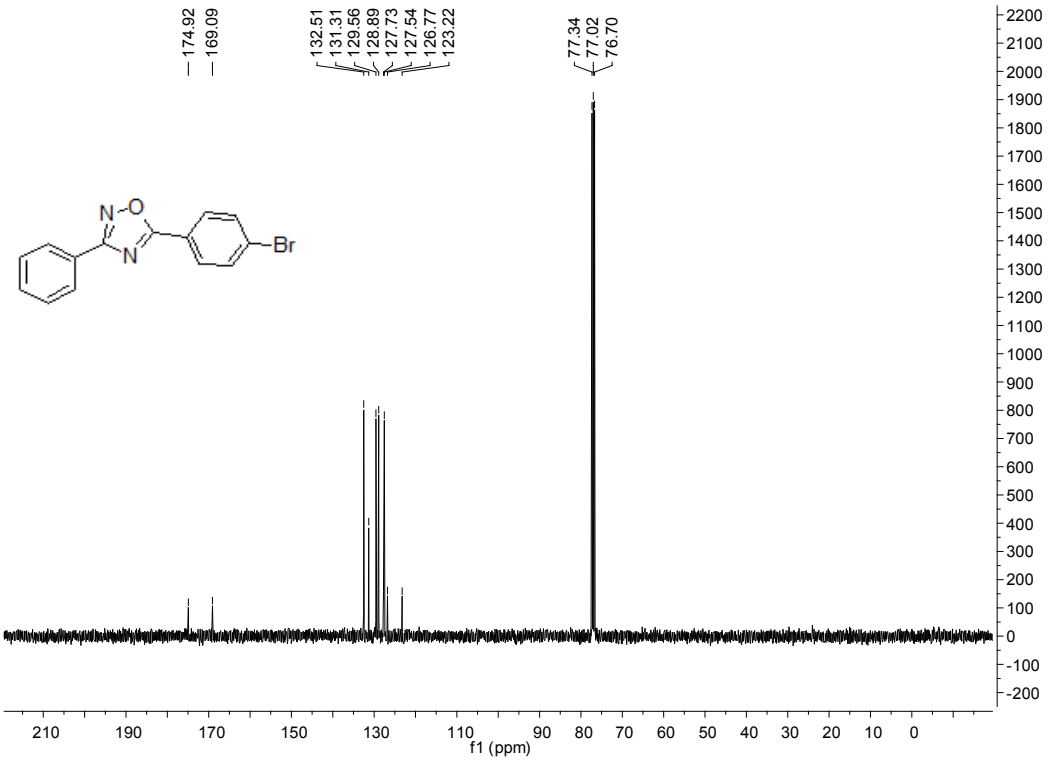
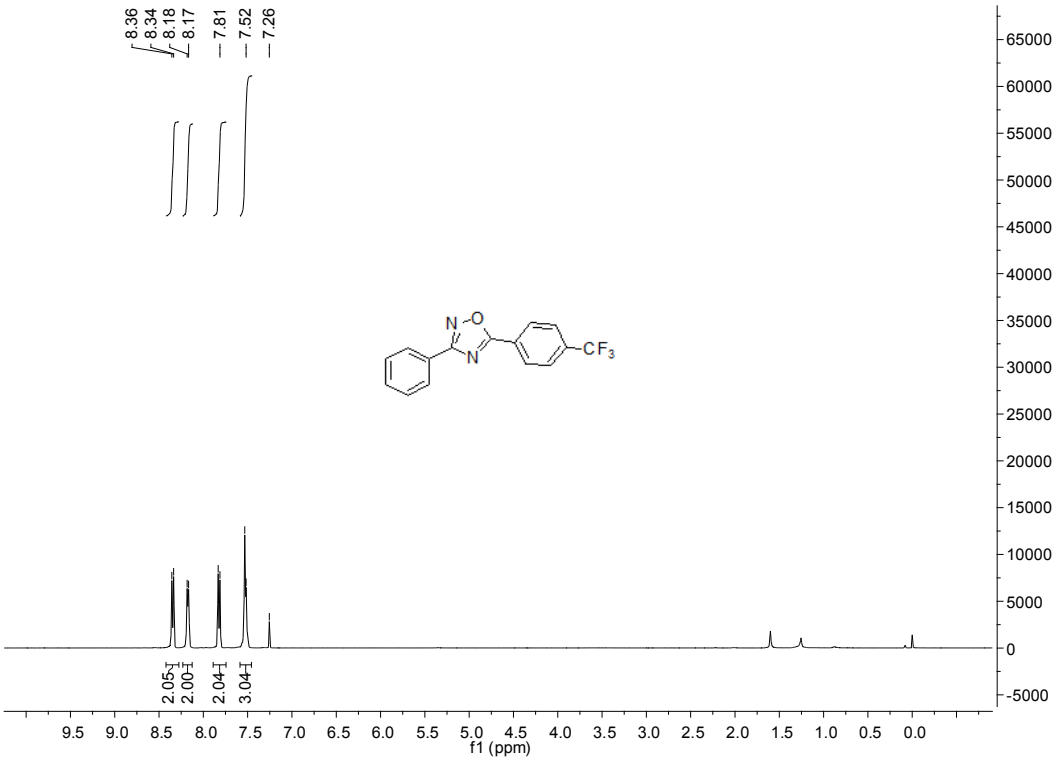


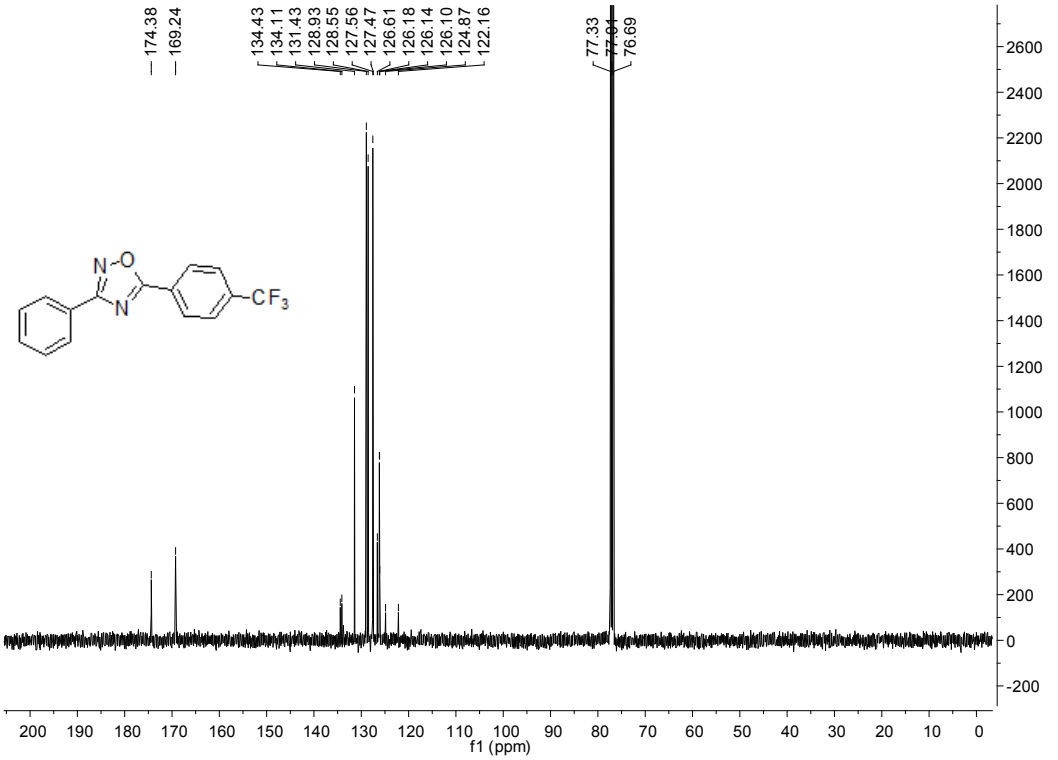
^{1}H NMR of **3af**



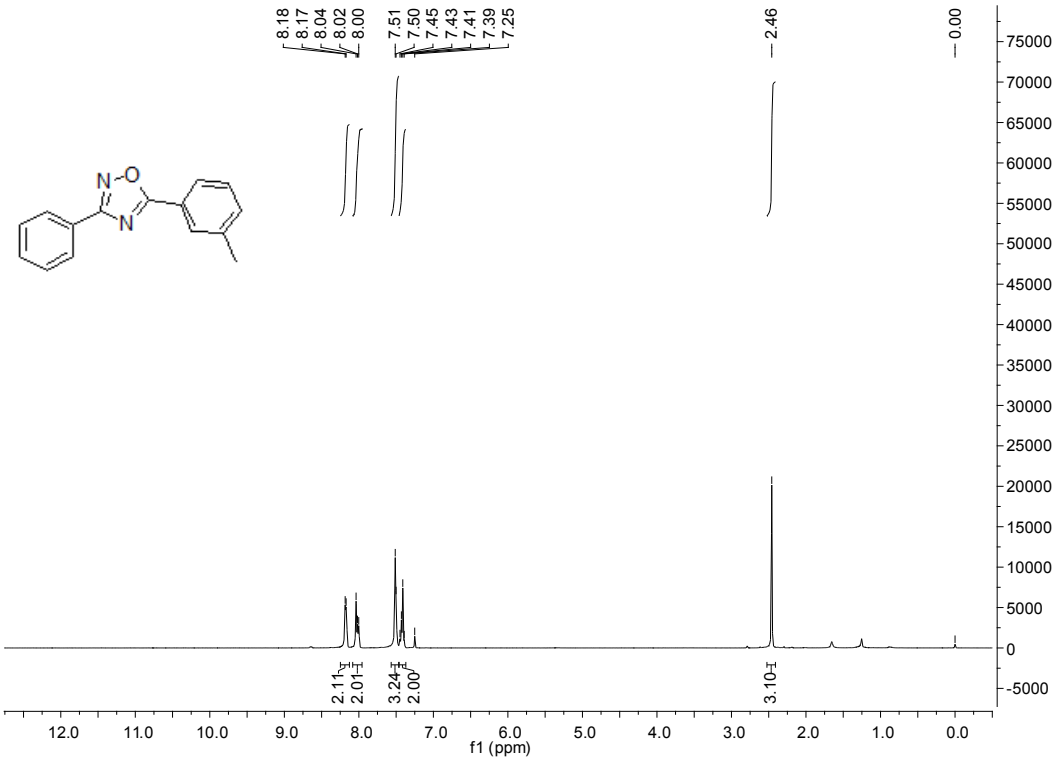
^{13}C NMR of **3af**



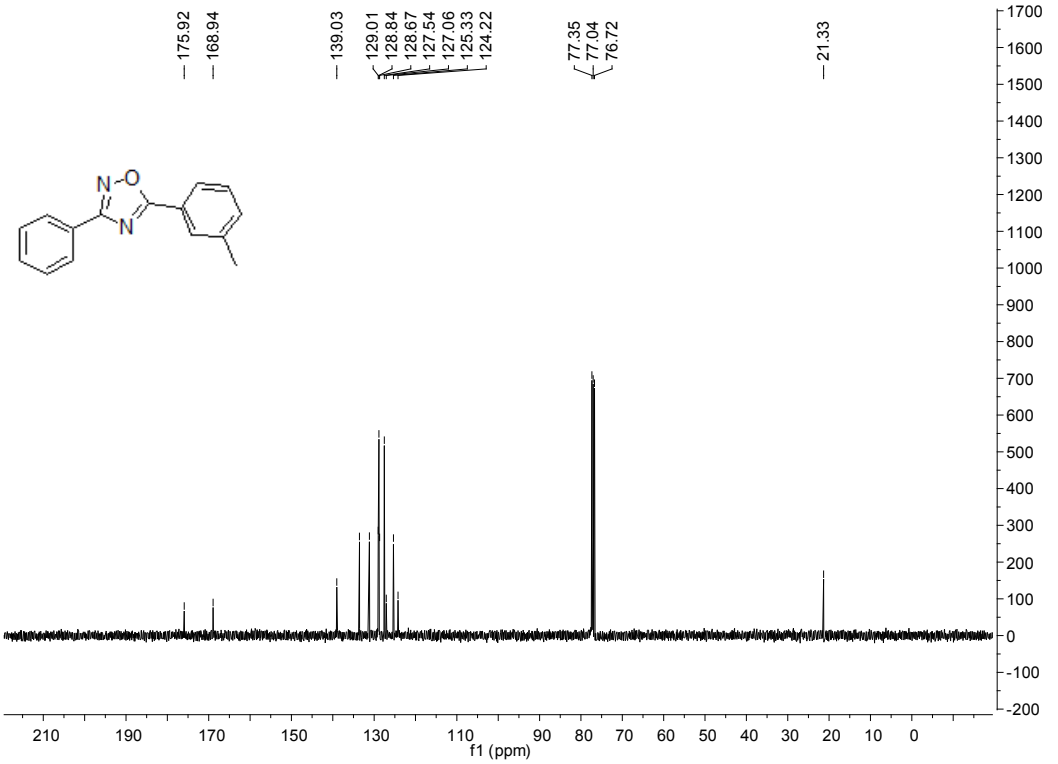
^{1}H NMR of **3ag**



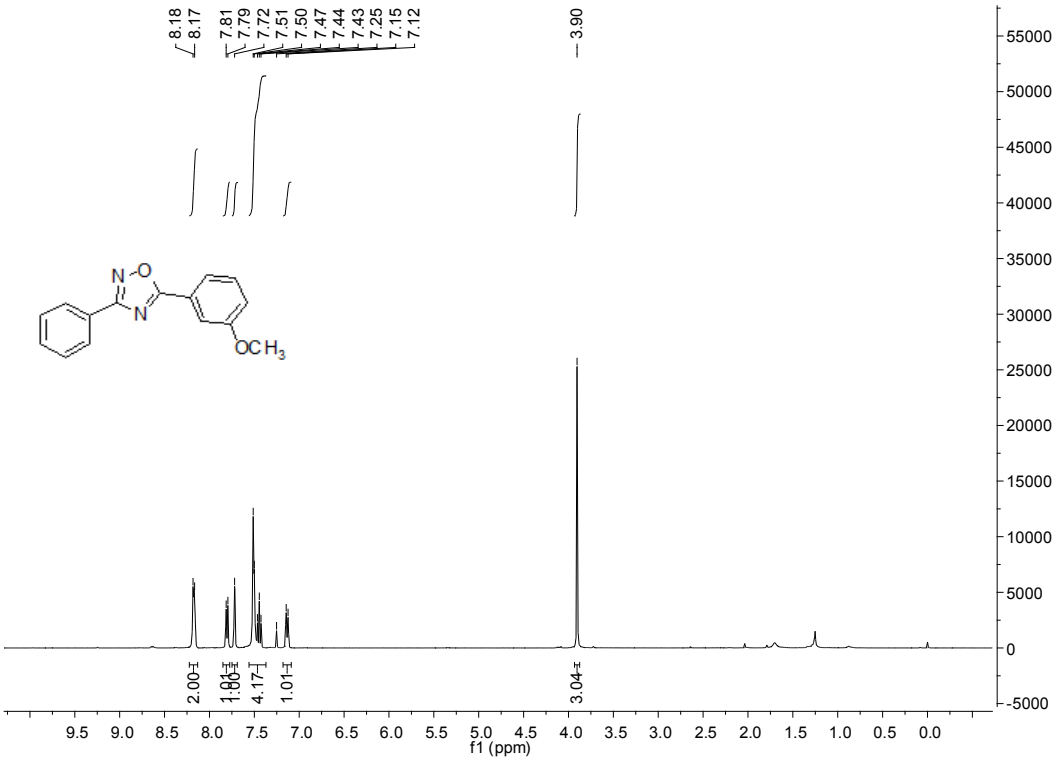
^{13}C NMR of **3ag**



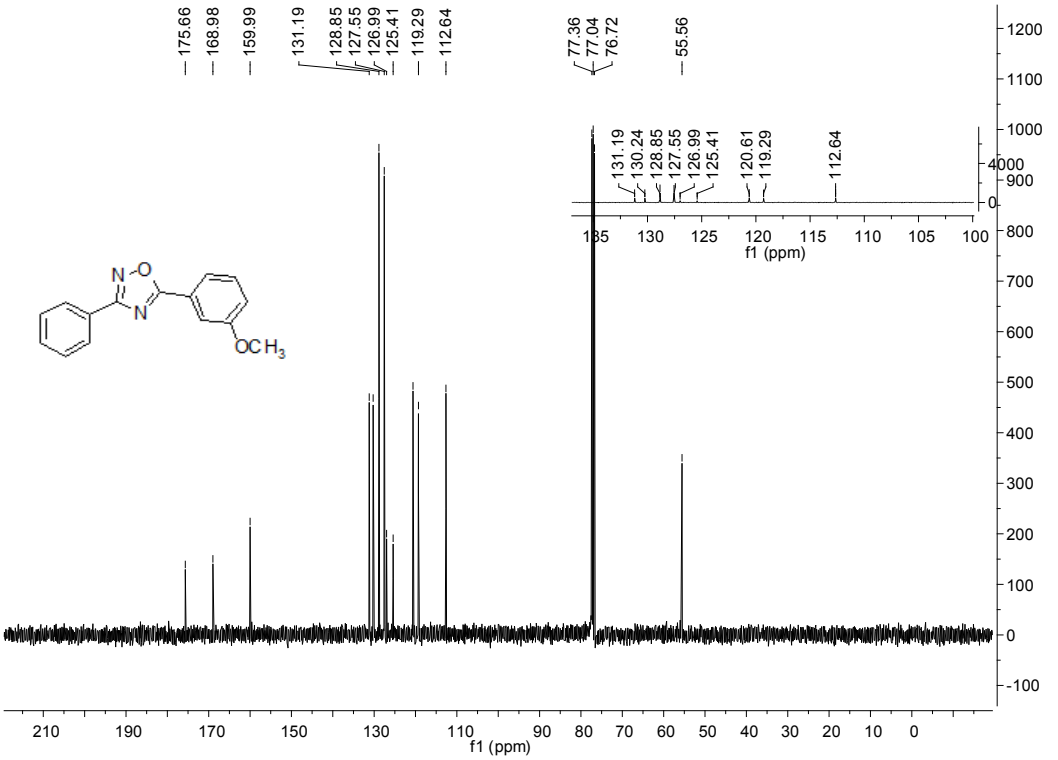
^{1}H NMR of **3ah**



^{13}C NMR of **3ah**



^{1}H NMR of **3ai**



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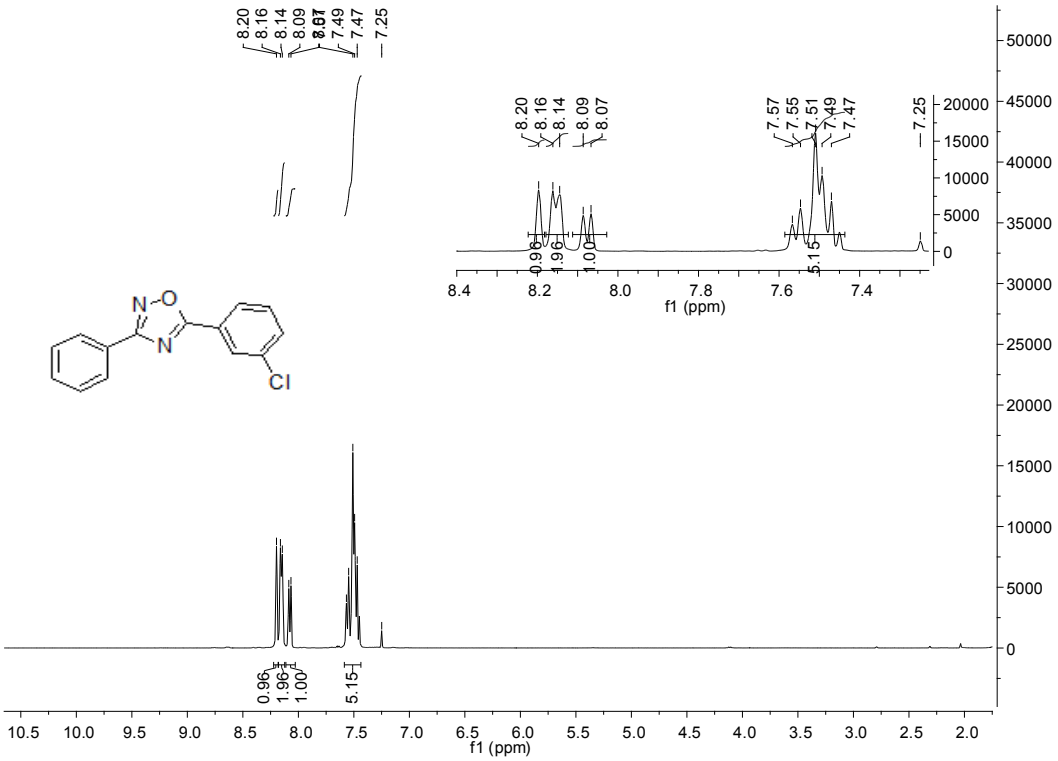
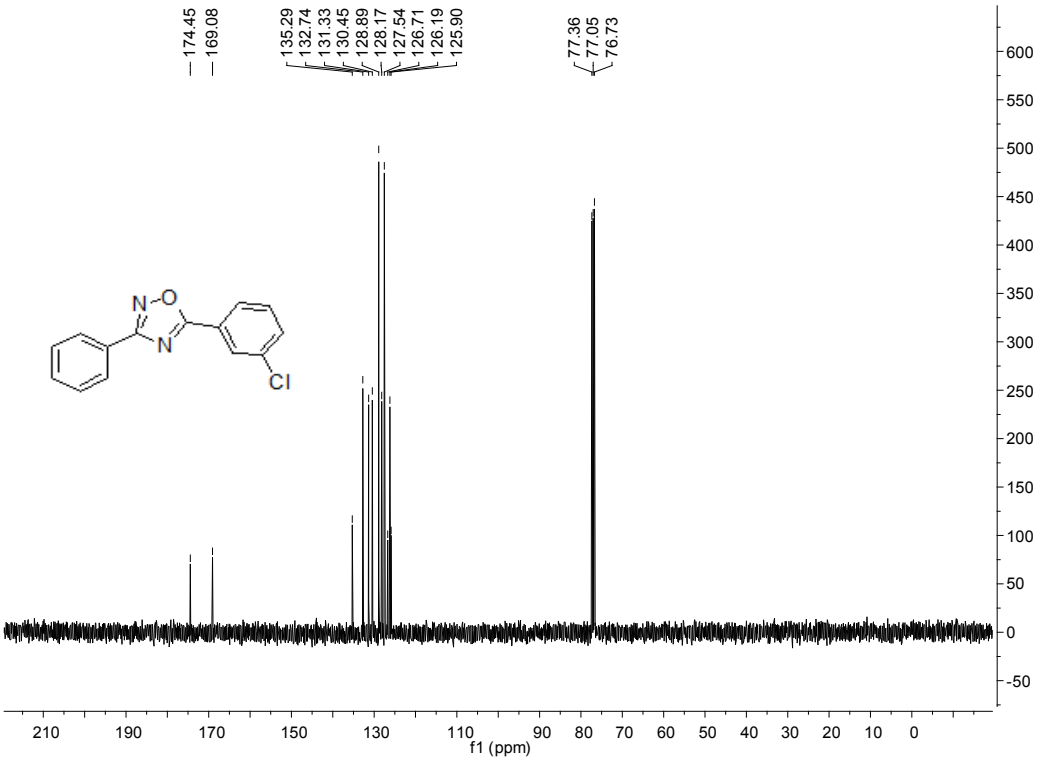


^{1}H NMR of **3aj**



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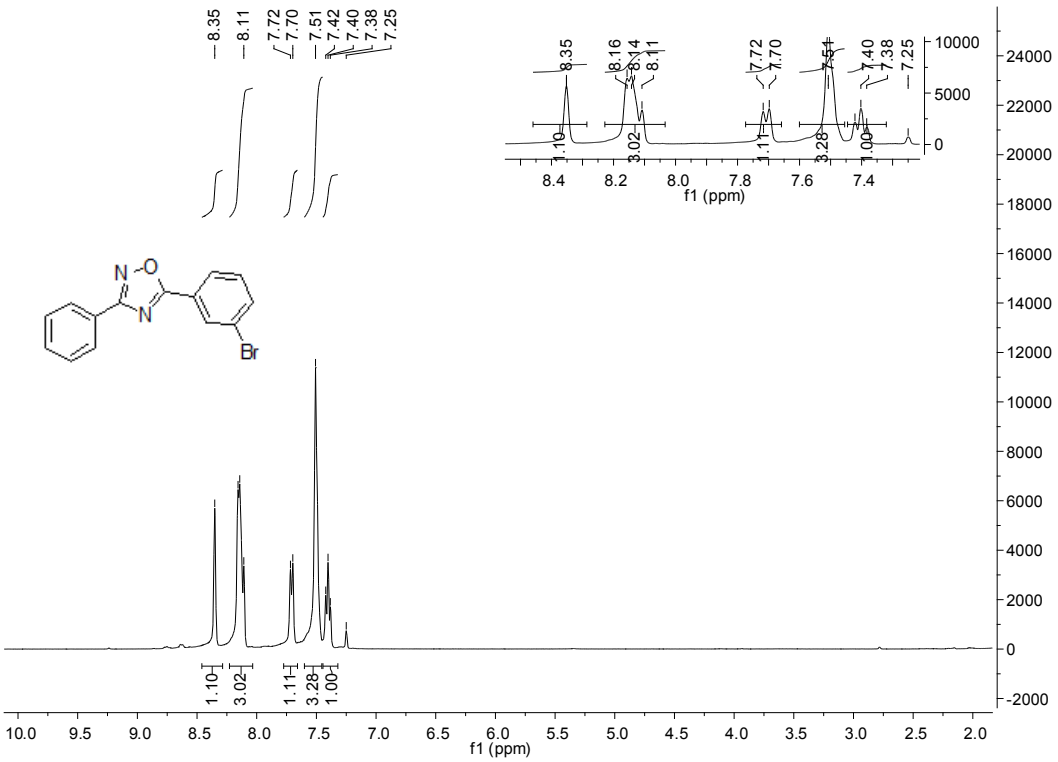

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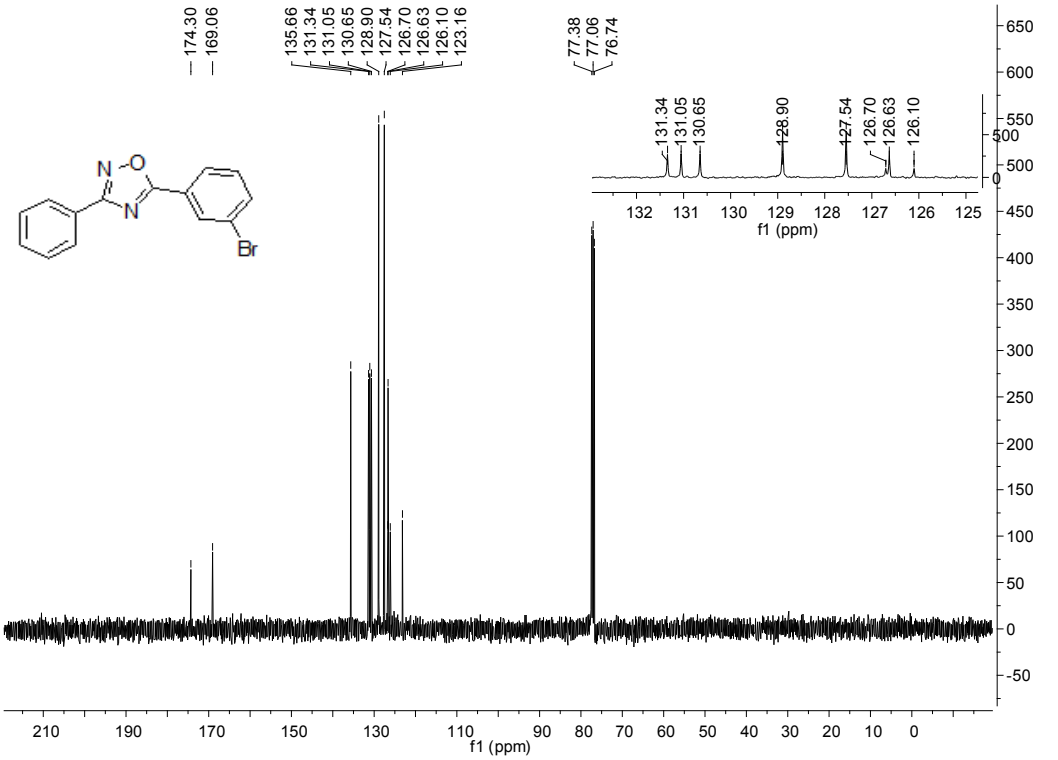

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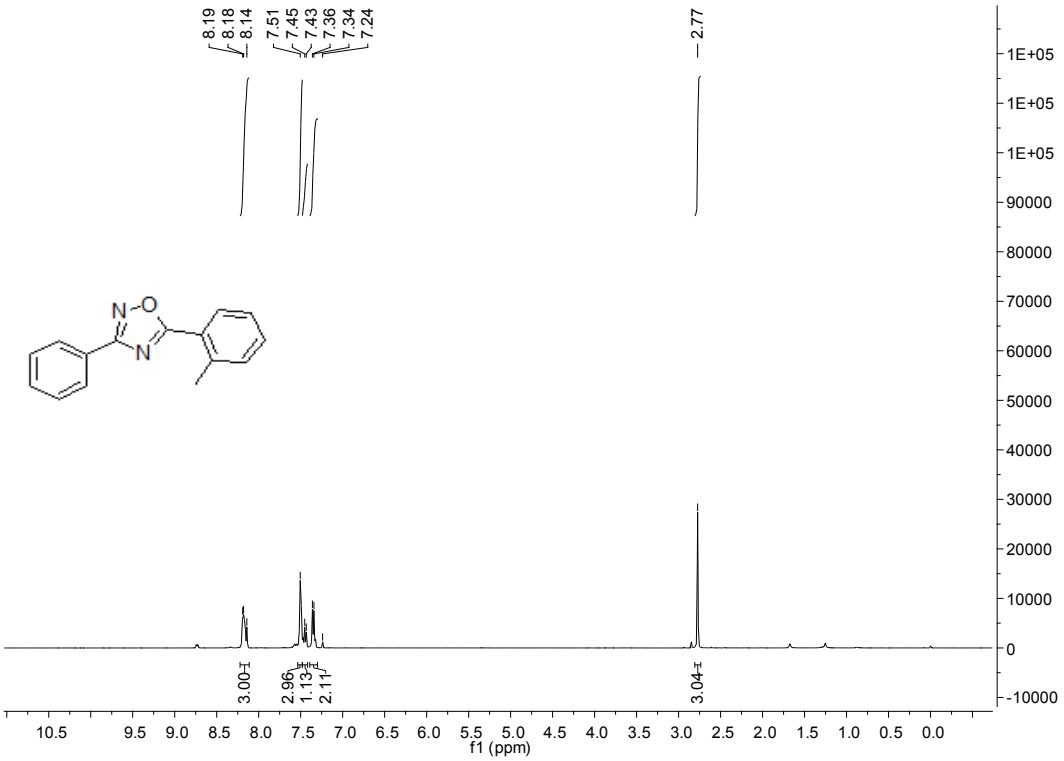
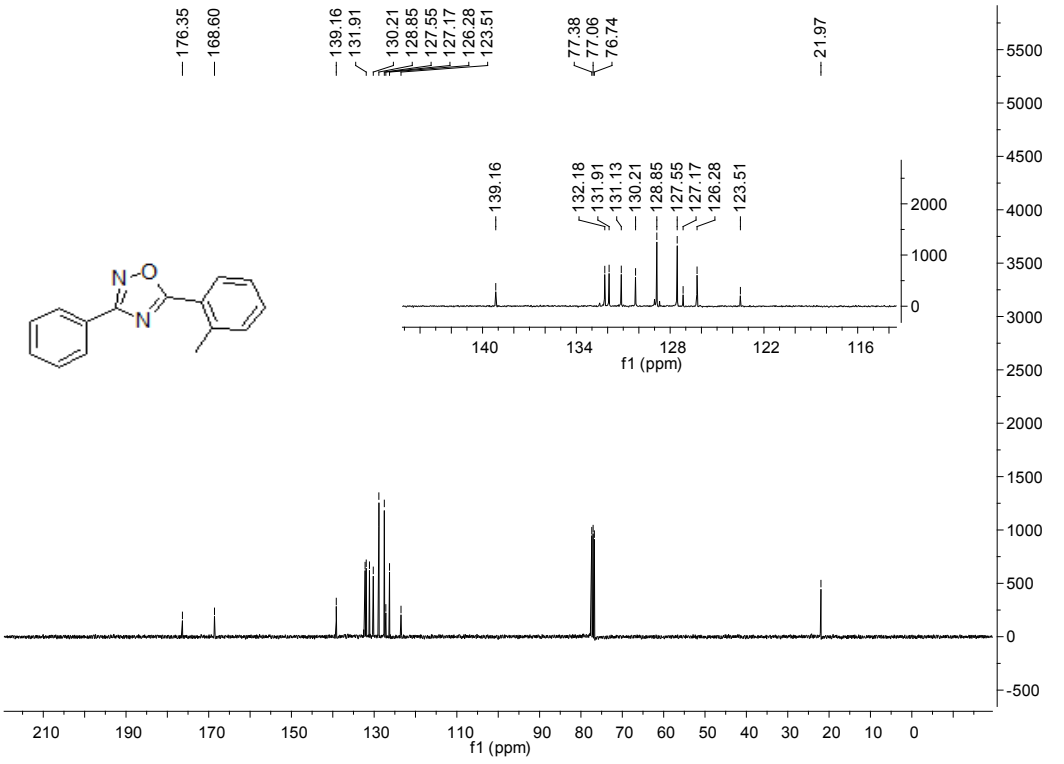
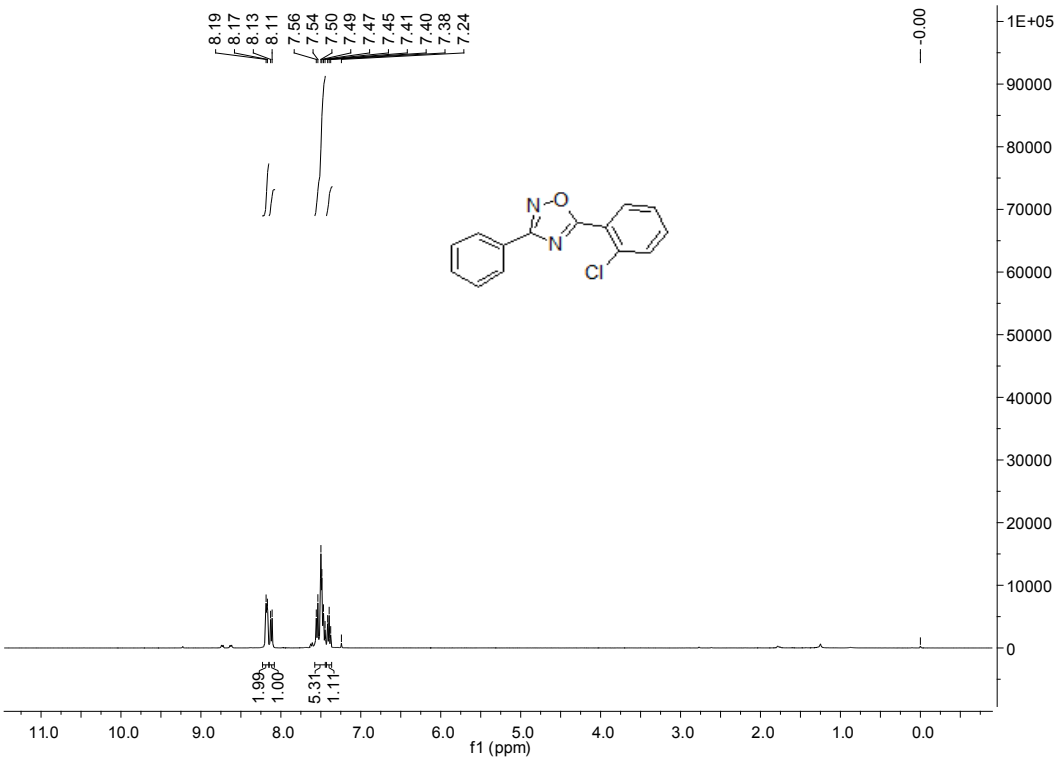


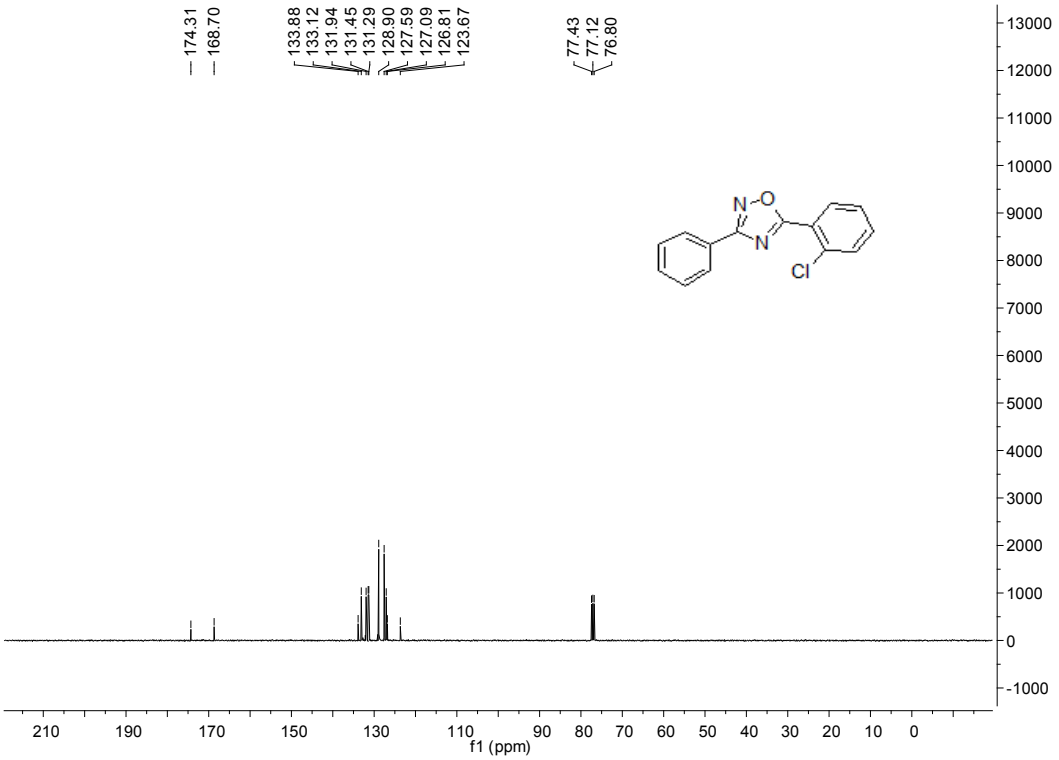
^{1}H NMR of **3al**



^{13}C NMR of **3al**



^{1}H NMR of **3am**



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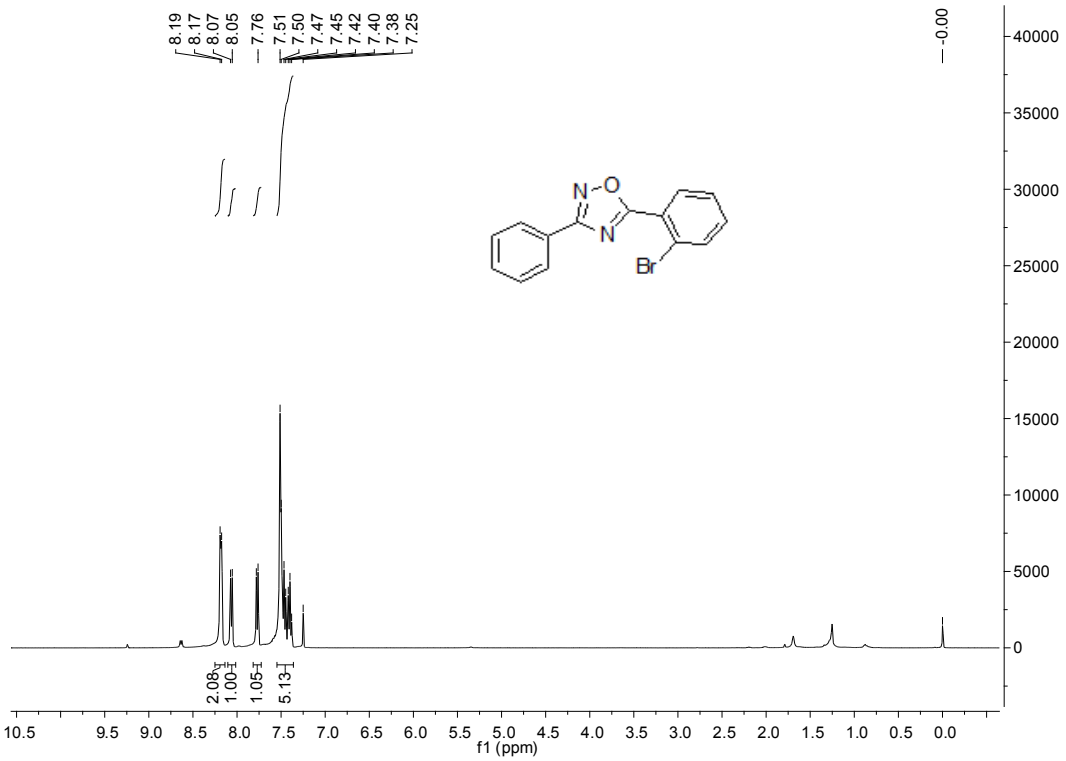

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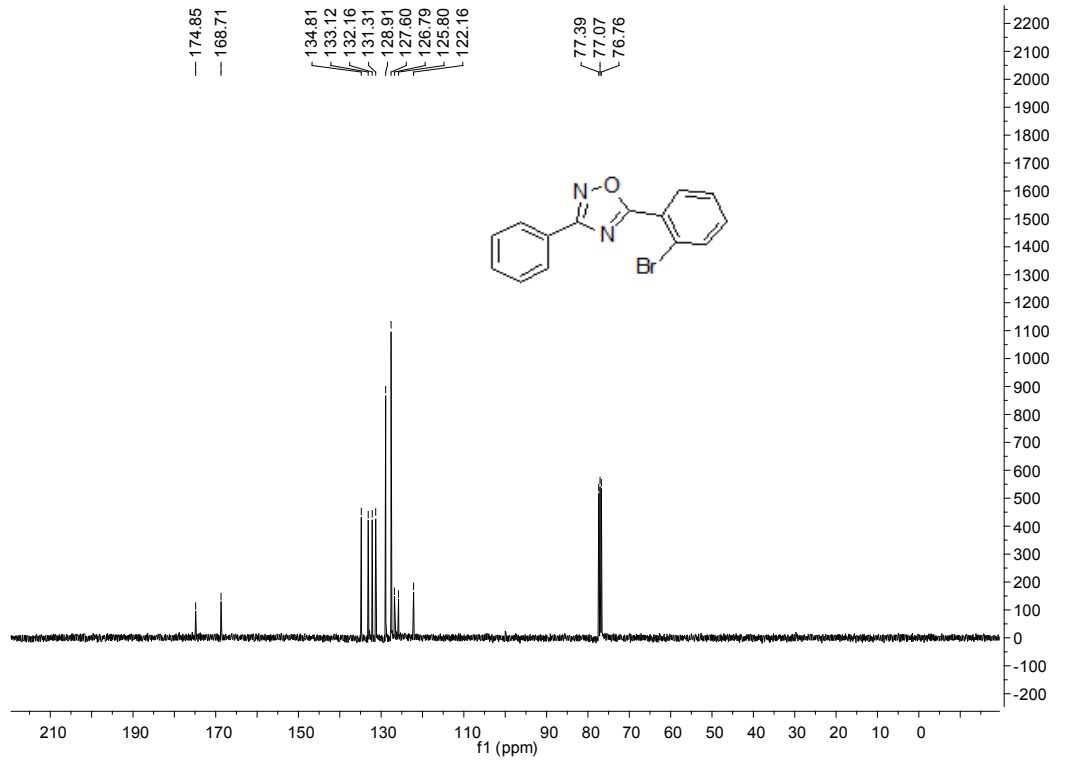

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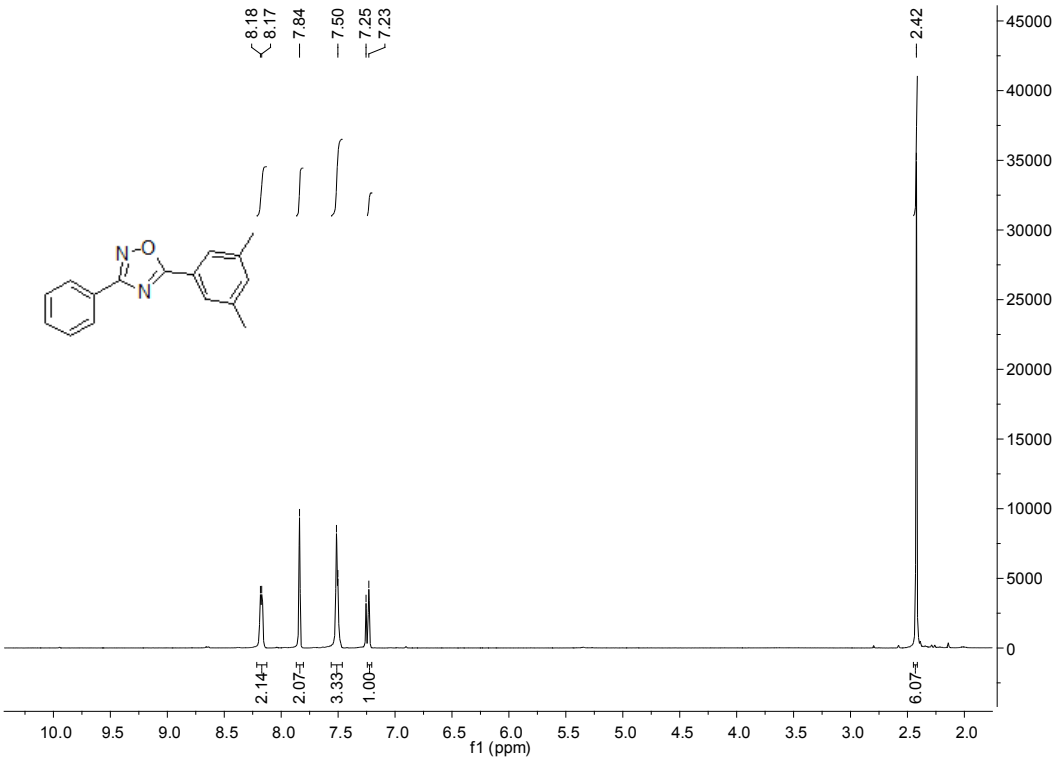
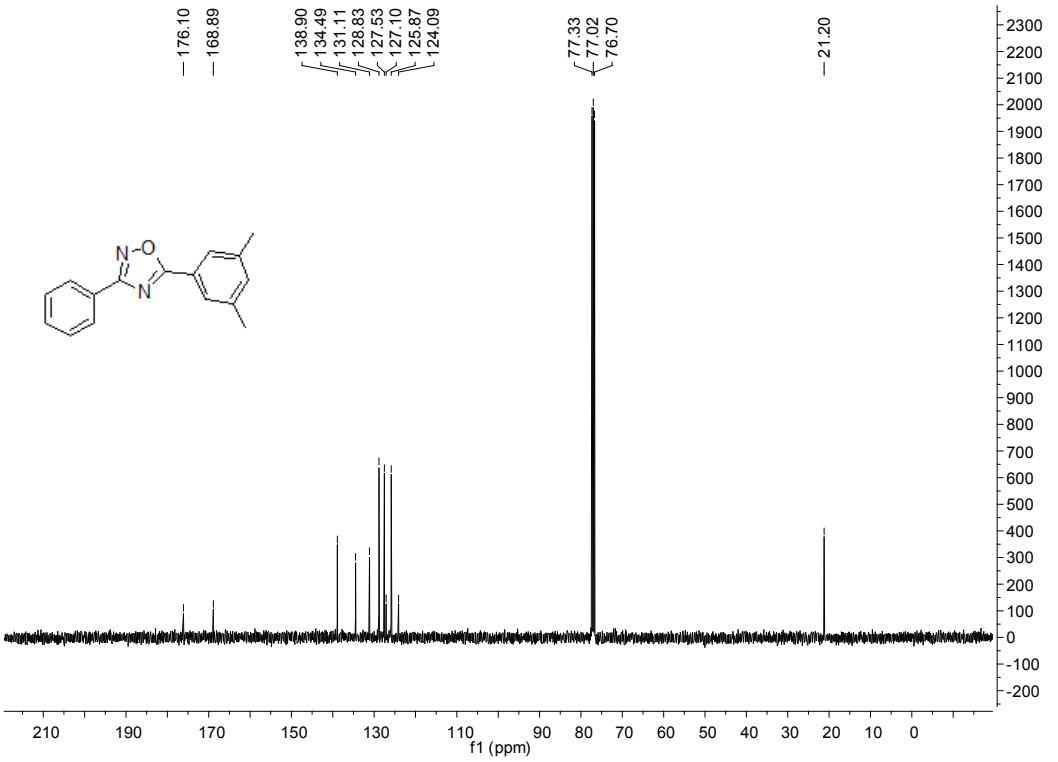
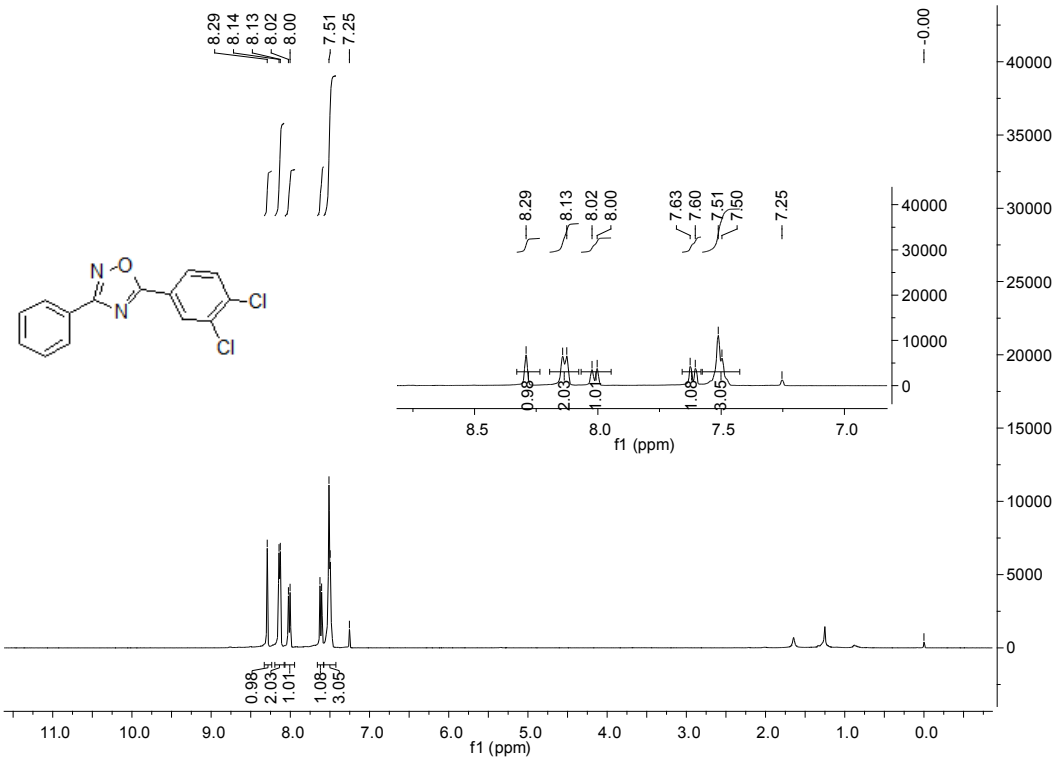


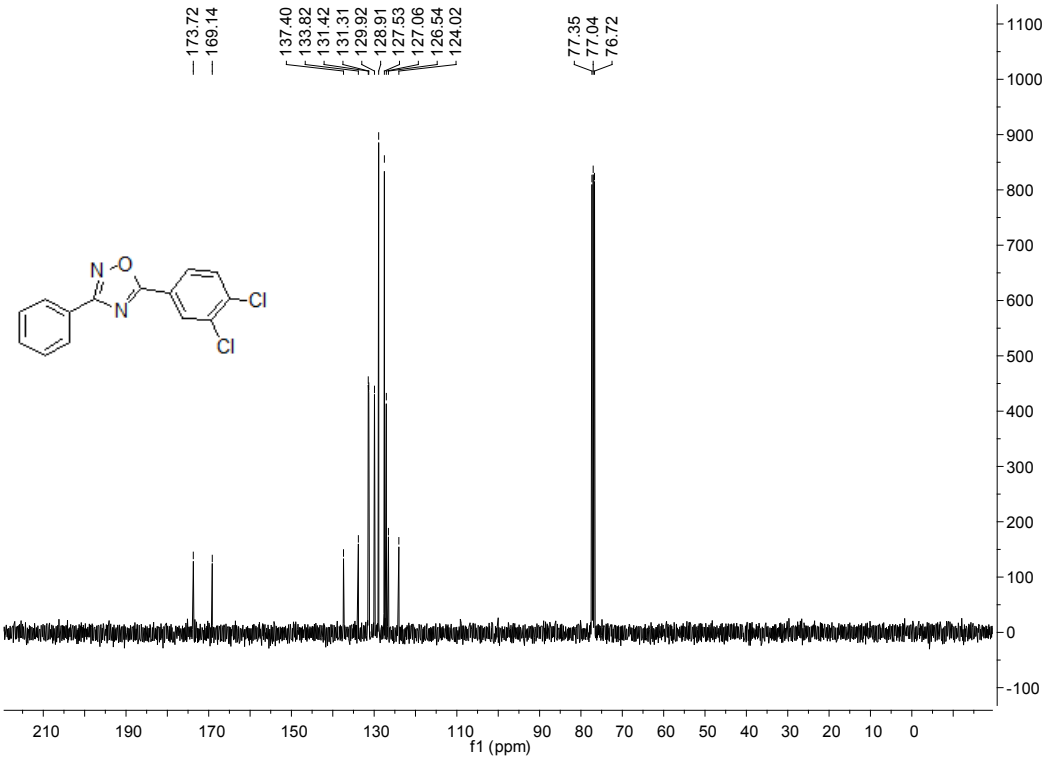
^{1}H NMR of **3ao**



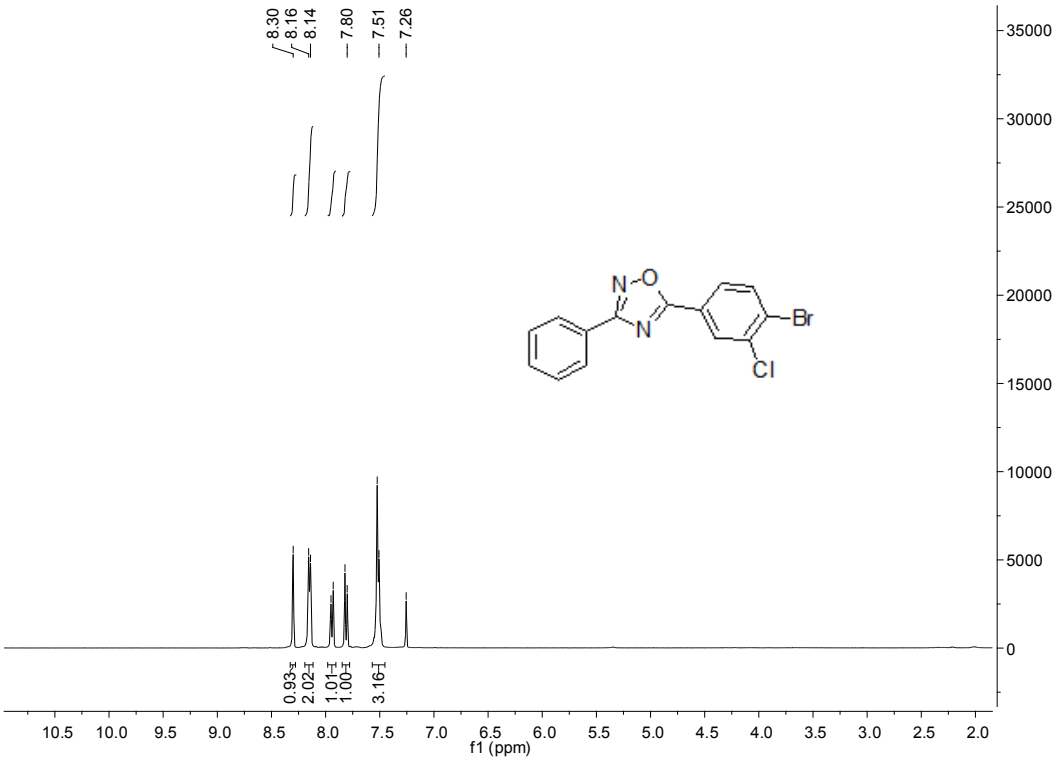
^{13}C NMR of **3ao**



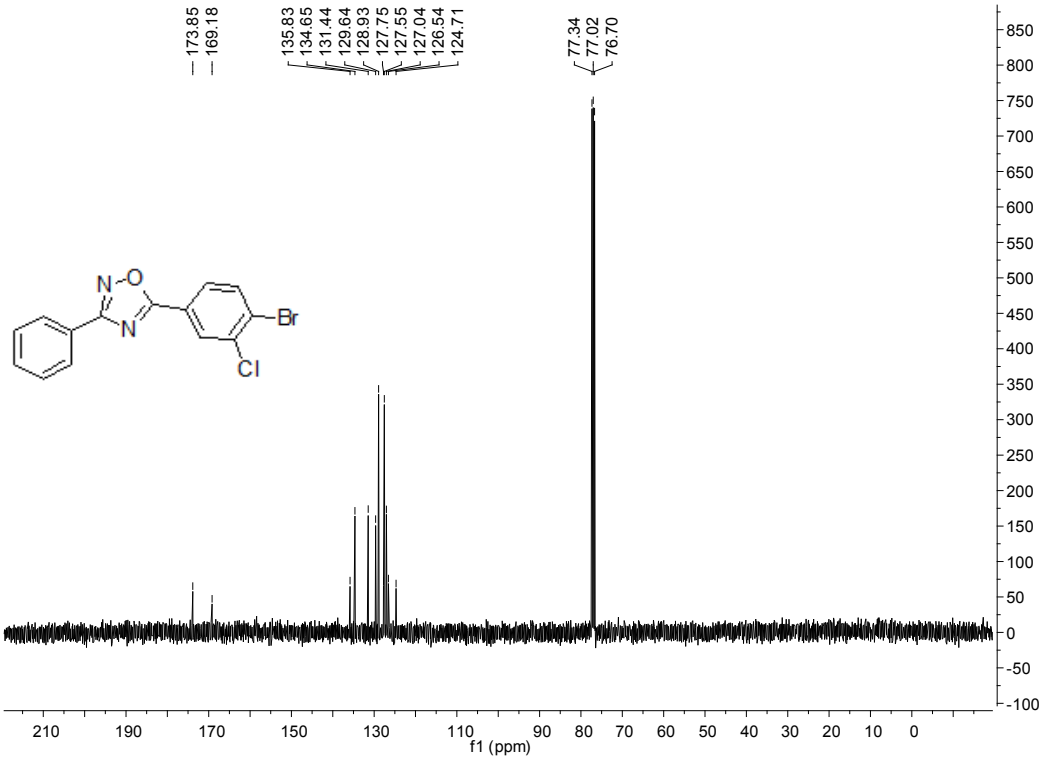
^{1}H NMR of **3ap**



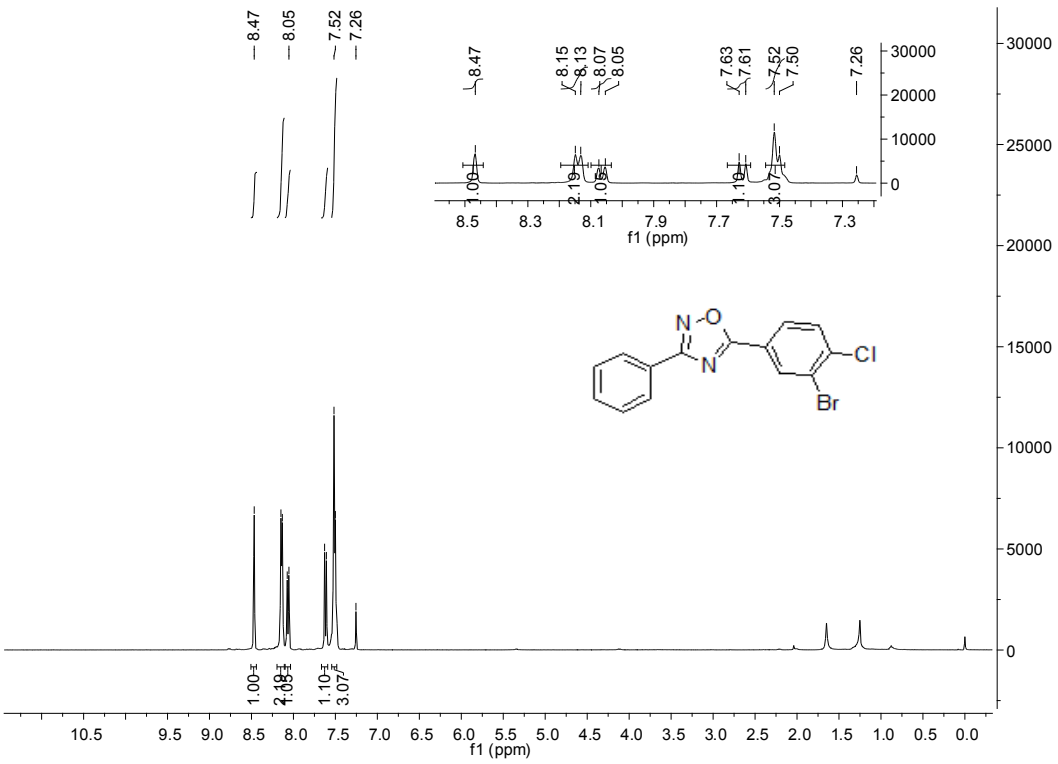
^{13}C NMR of **3ap**



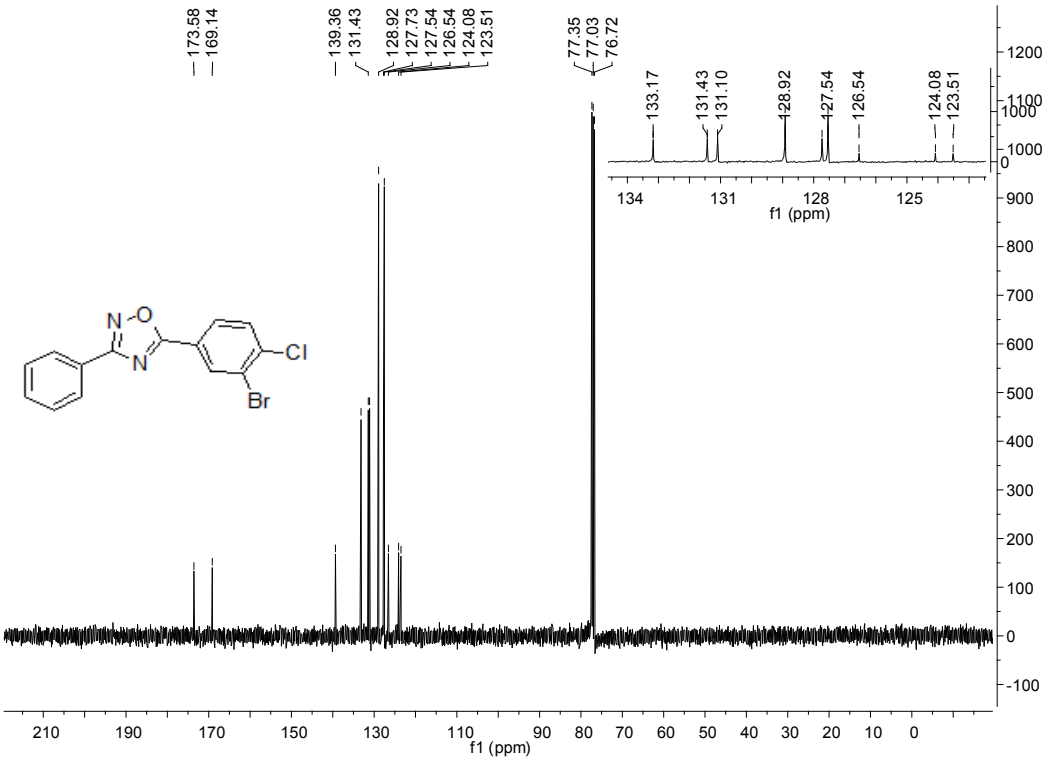
^{1}H NMR of **3aq**



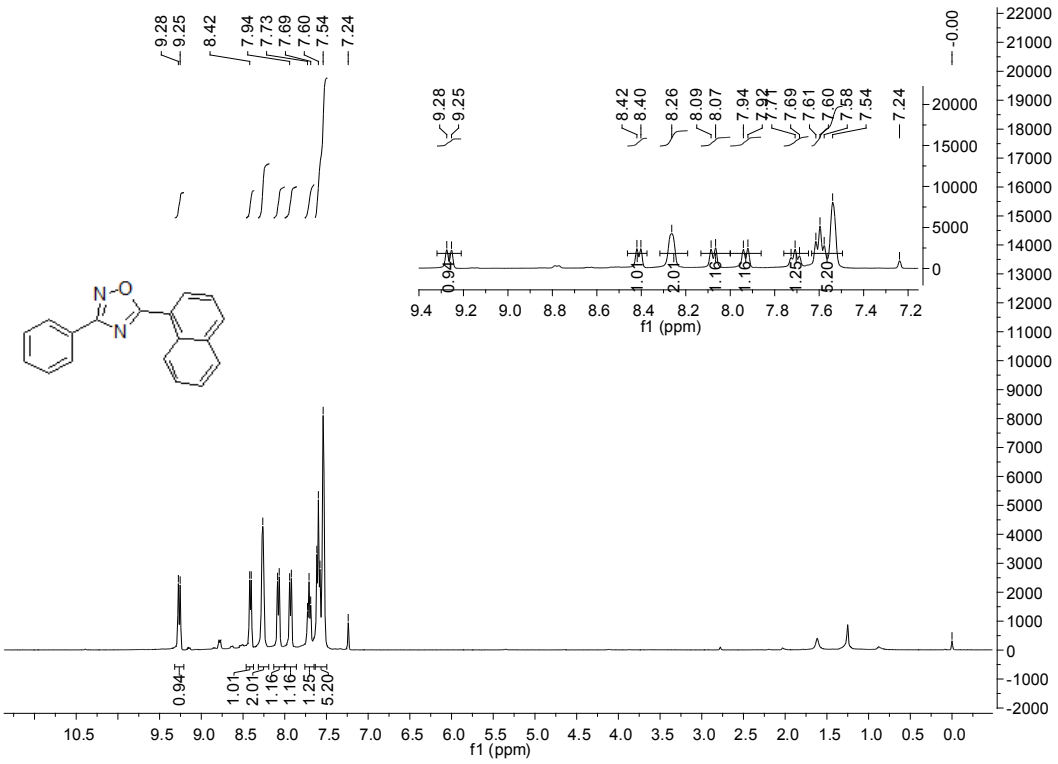
^{13}C NMR of **3aq**



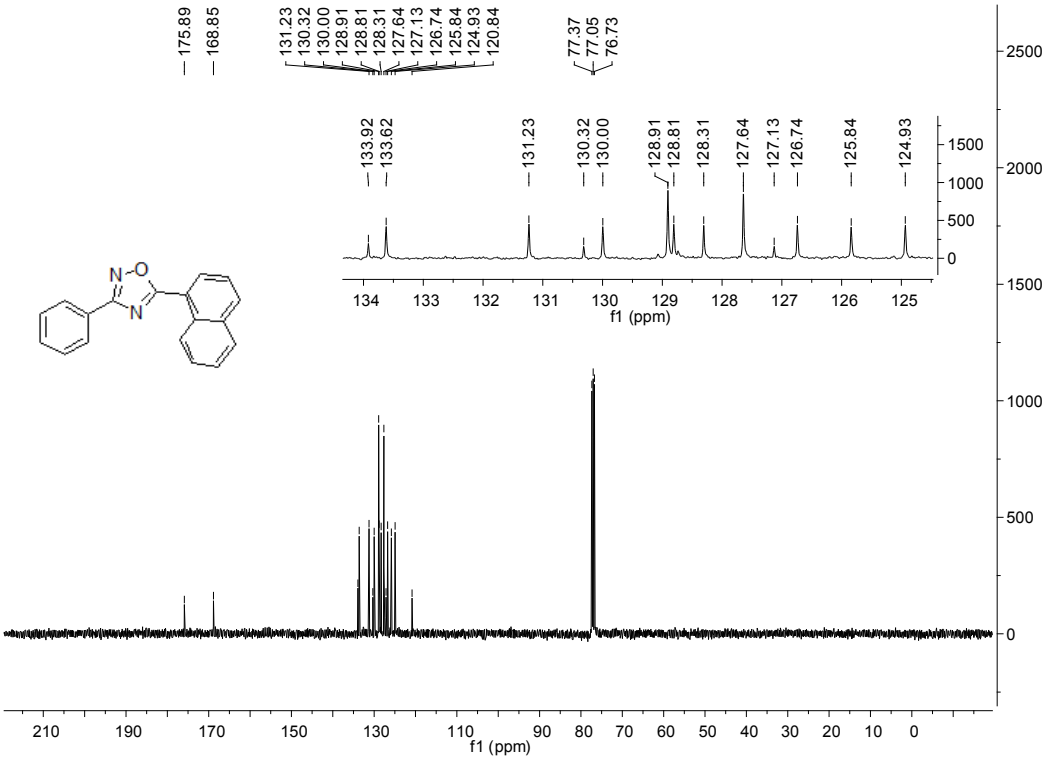
^{1}H NMR of **3ar**



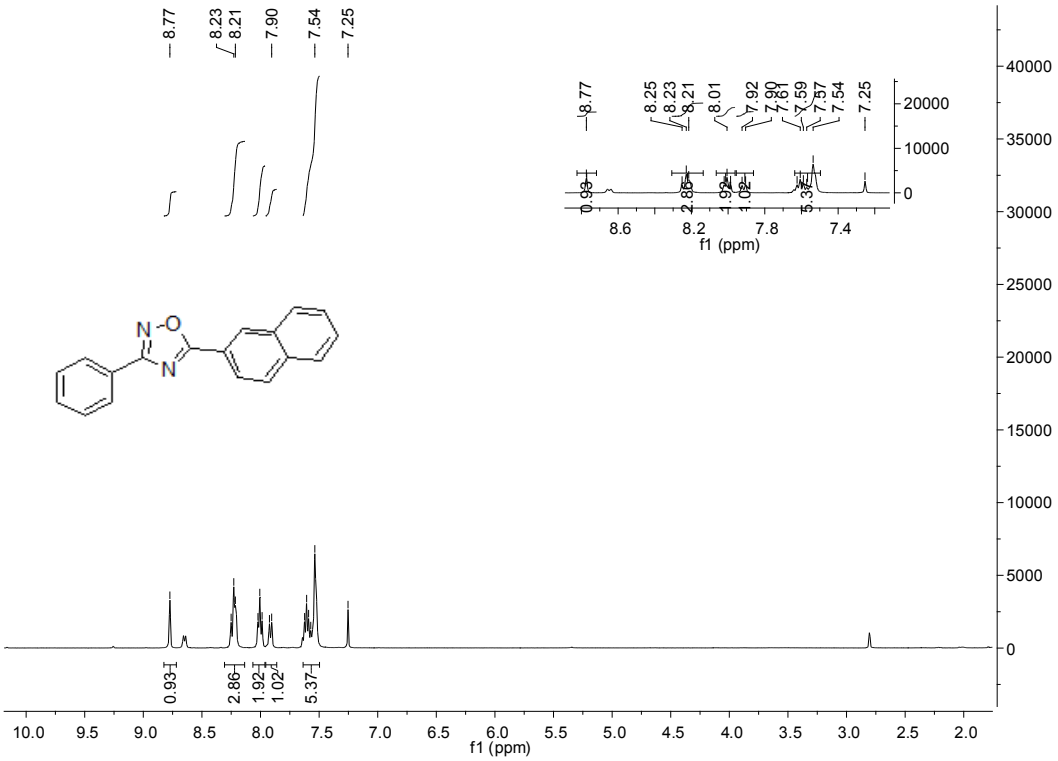
^{13}C NMR of **3ar**



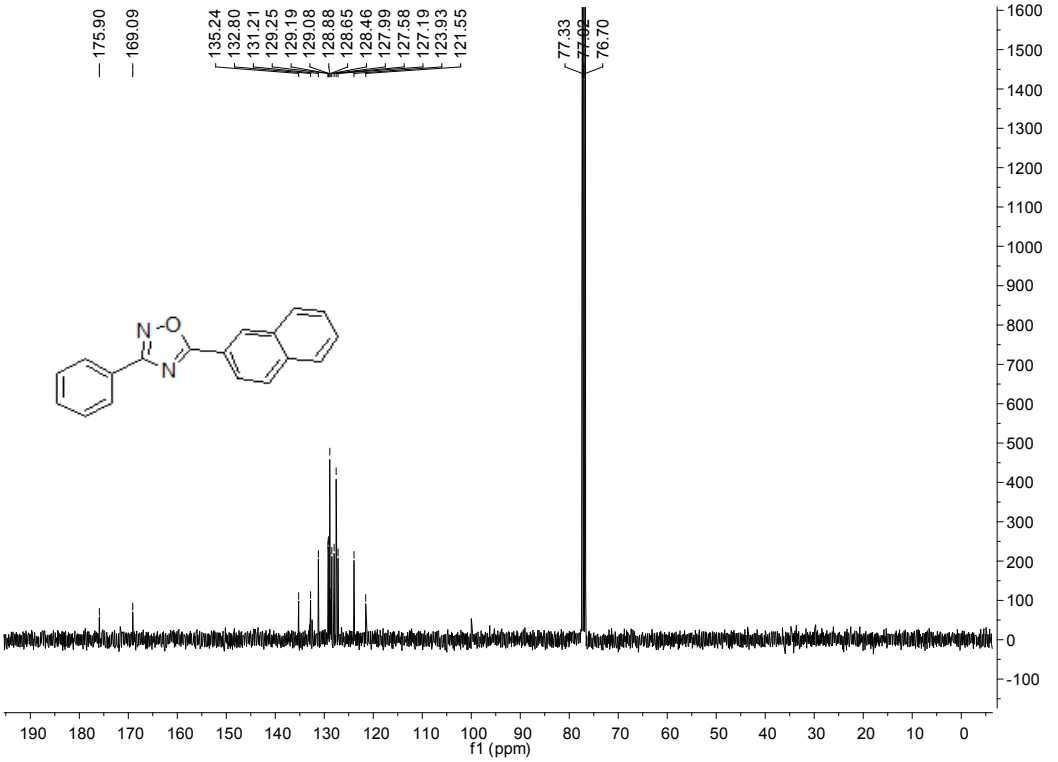
^{1}H NMR of **3as**



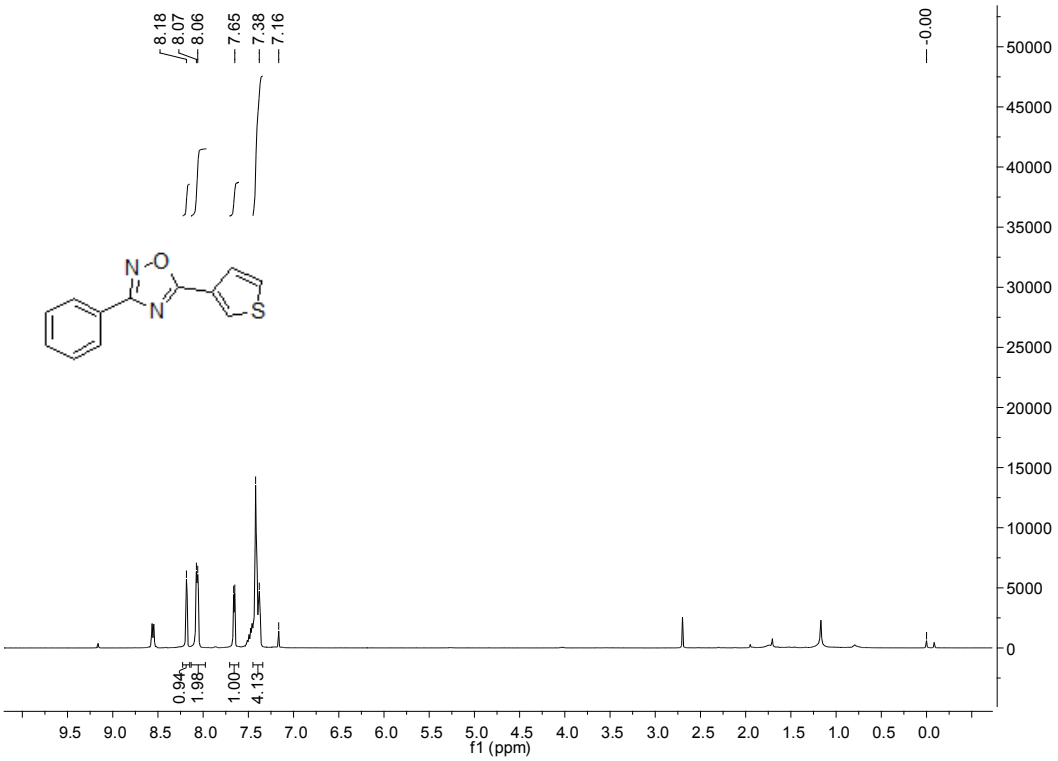
^{13}C NMR of **3as**



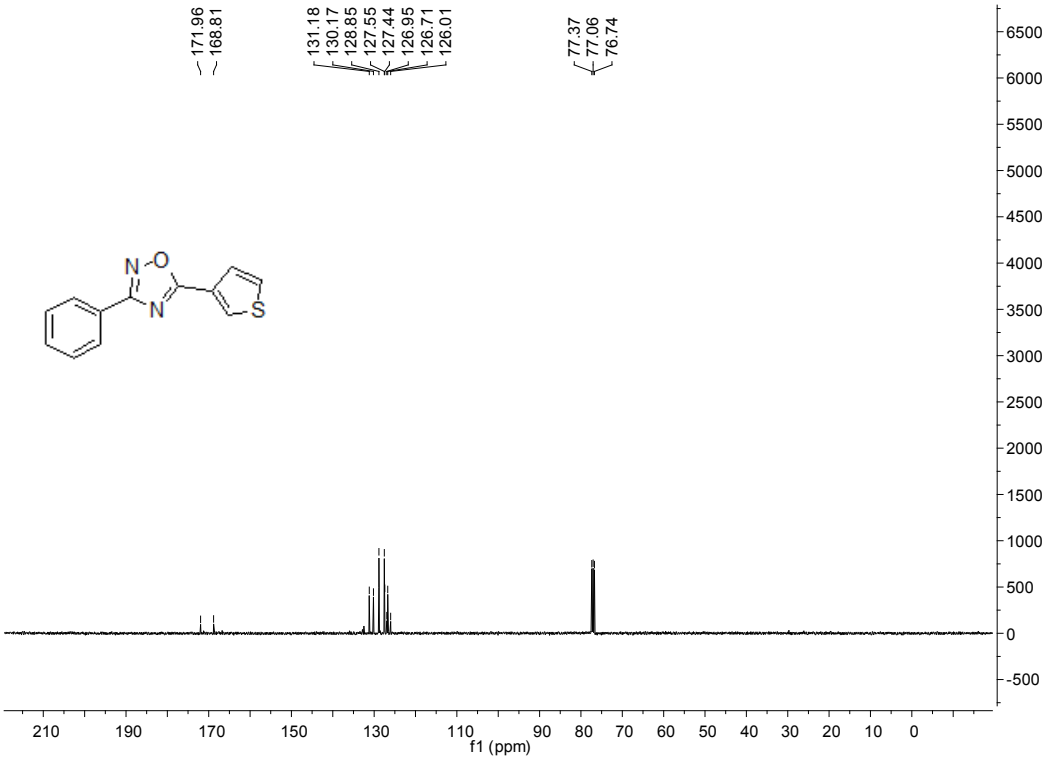
^{1}H NMR of **3at**



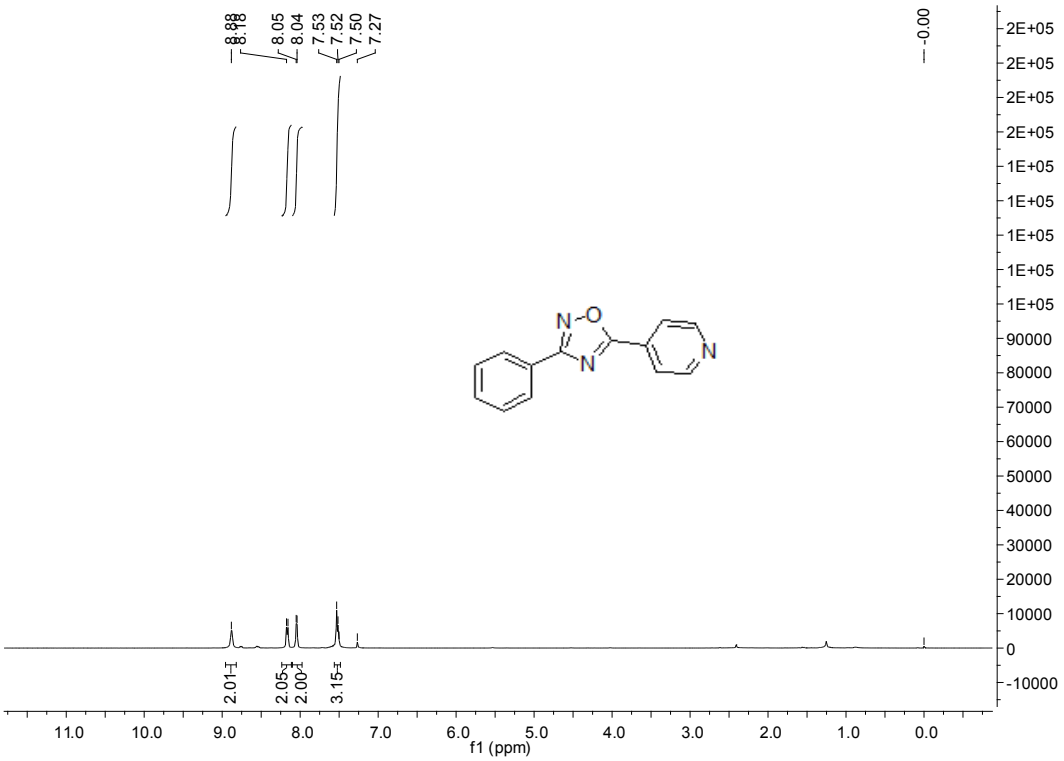
^{13}C NMR of **3at**



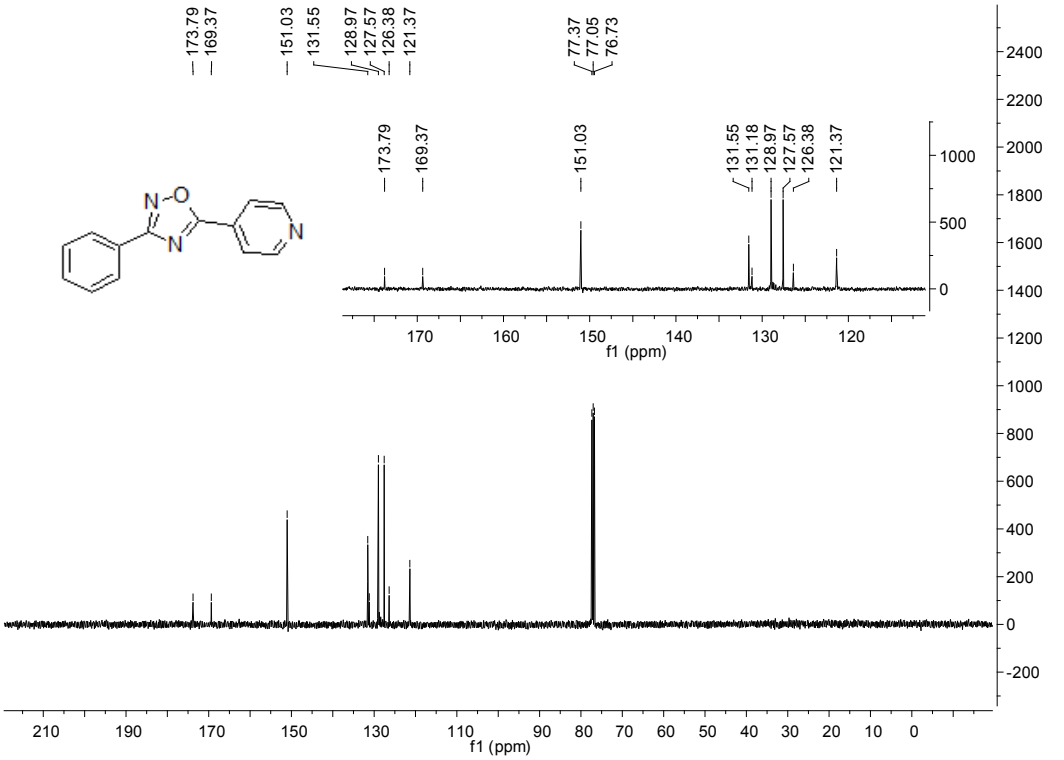
^{1}H NMR of **3au**



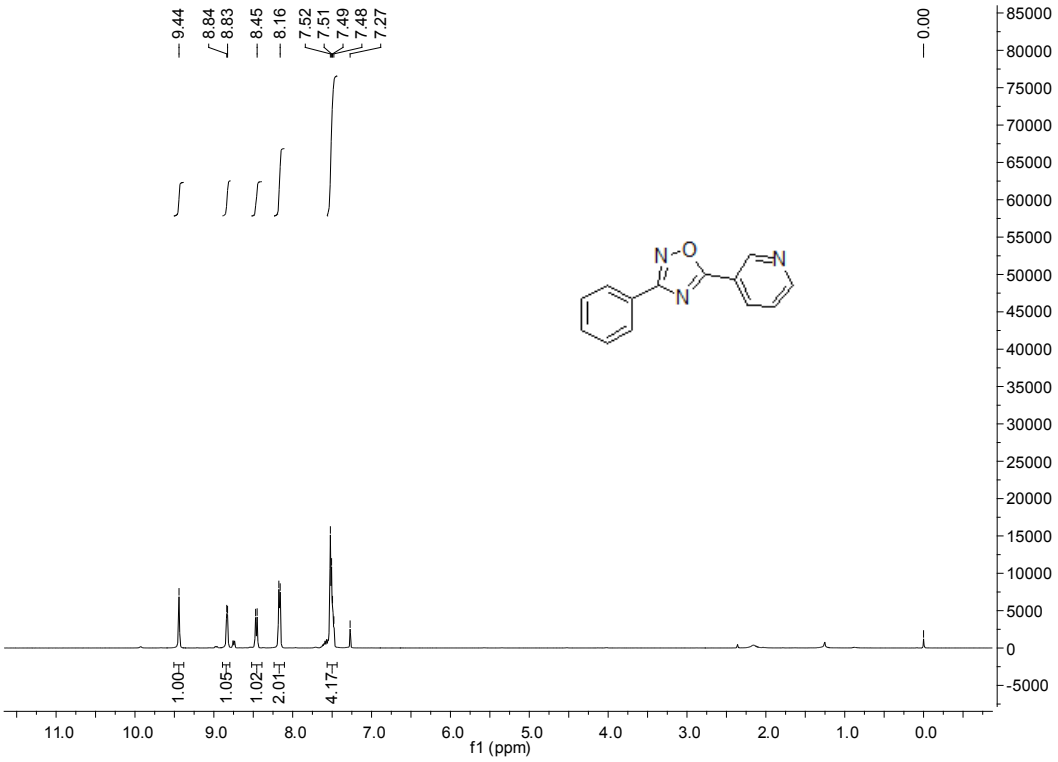
^{13}C NMR of **3au**



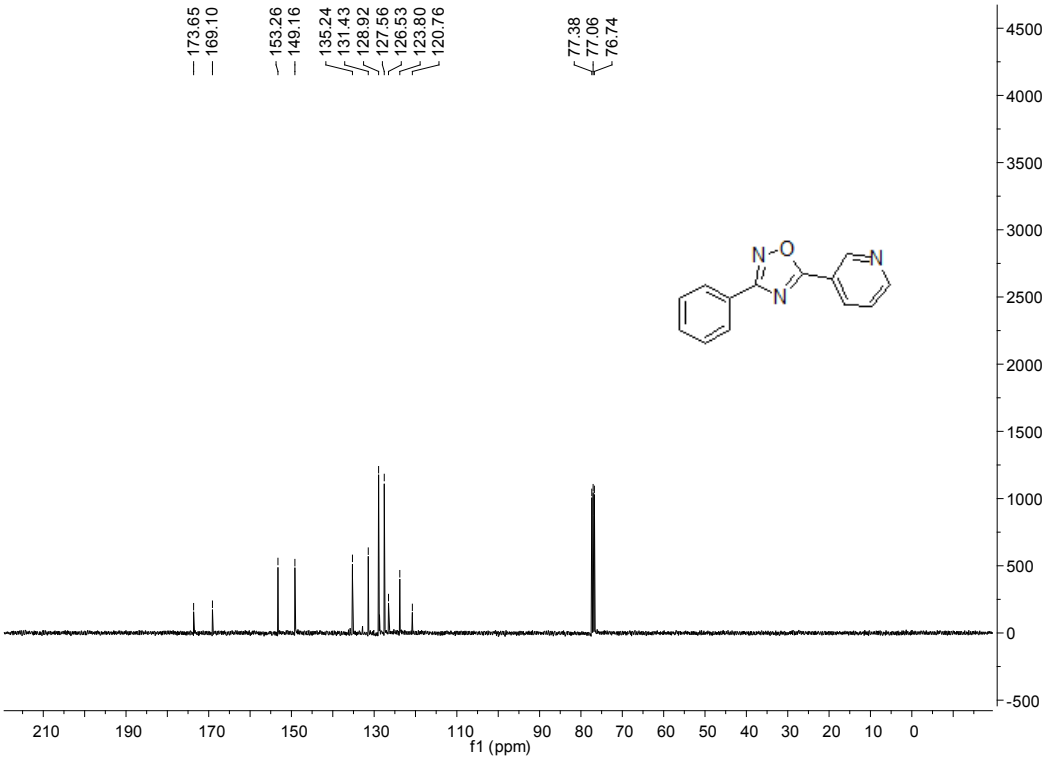
^{1}H NMR of **3av**



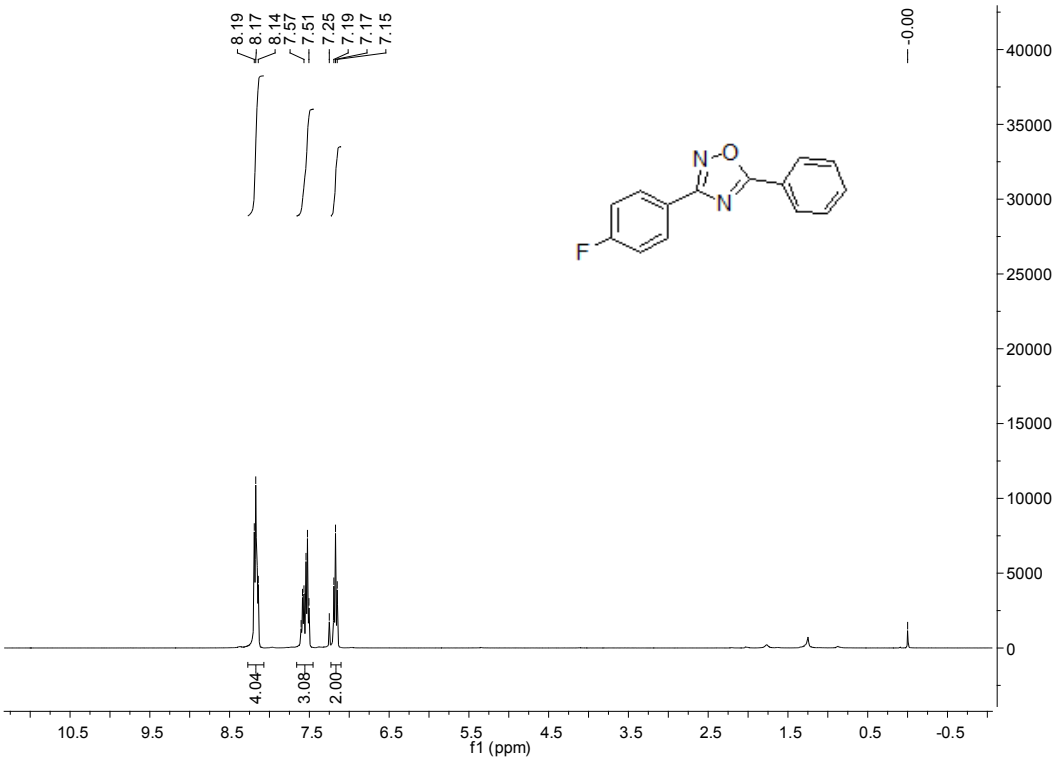
^{13}C NMR of **3av**



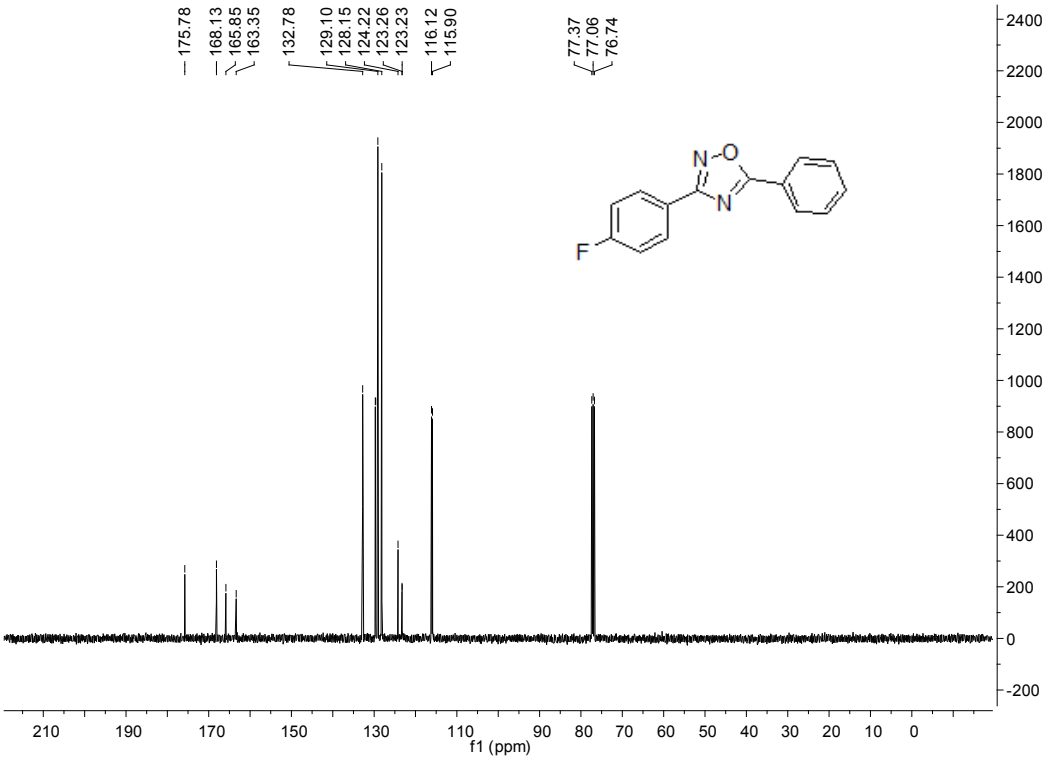
^{1}H NMR of **3aw**



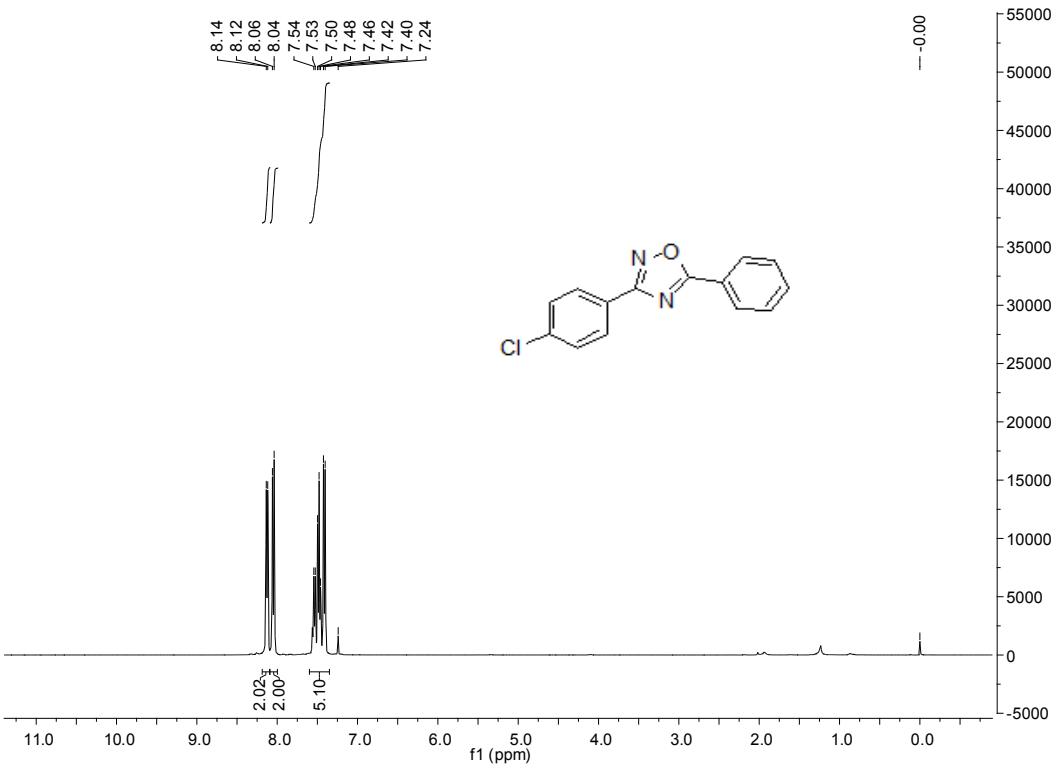
^{13}C NMR of **3aw**



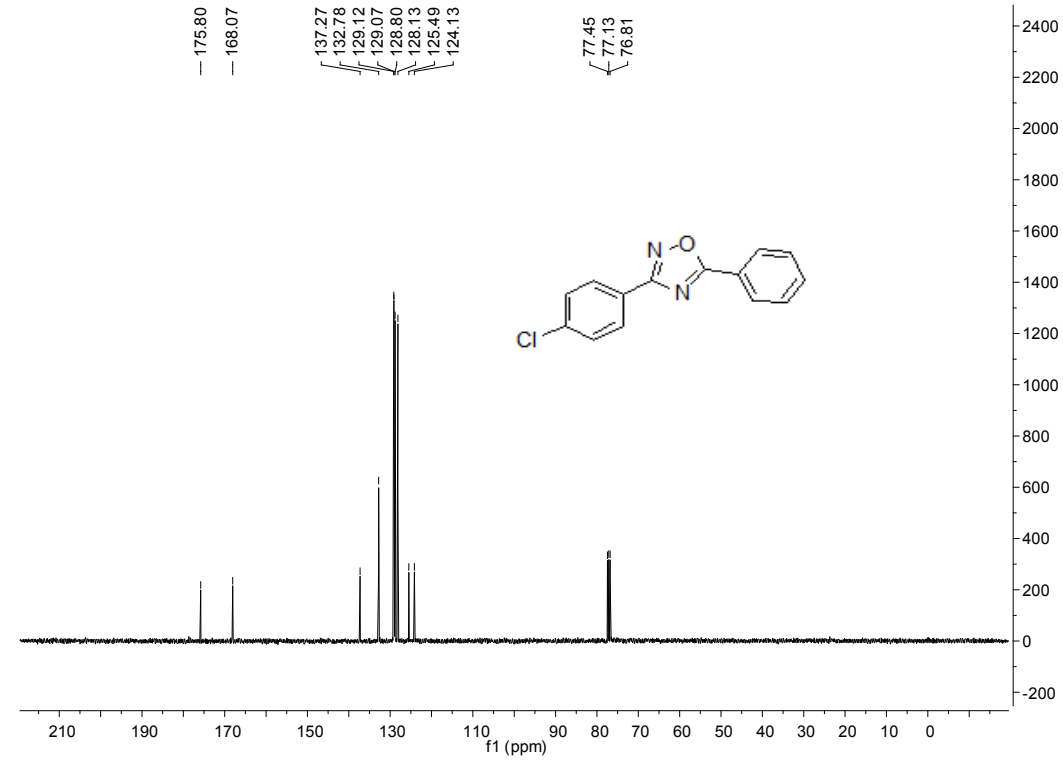
^{1}H NMR of **3ba**



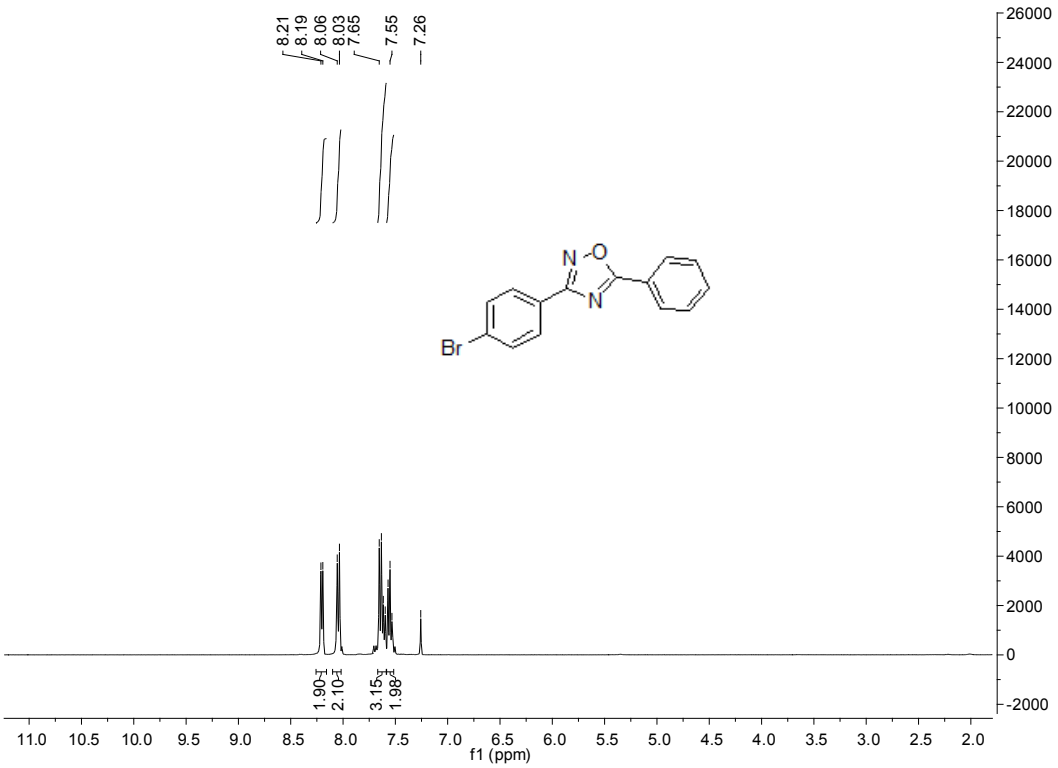
^{13}C NMR of **3ba**



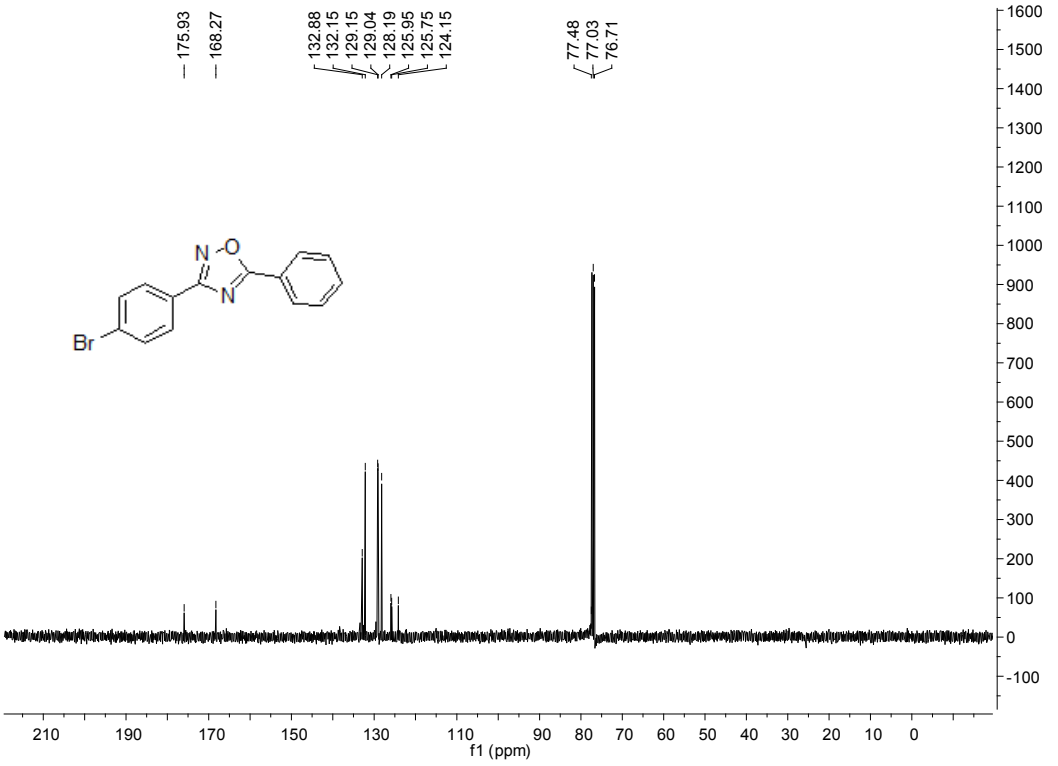
^{1}H NMR of **3ca**



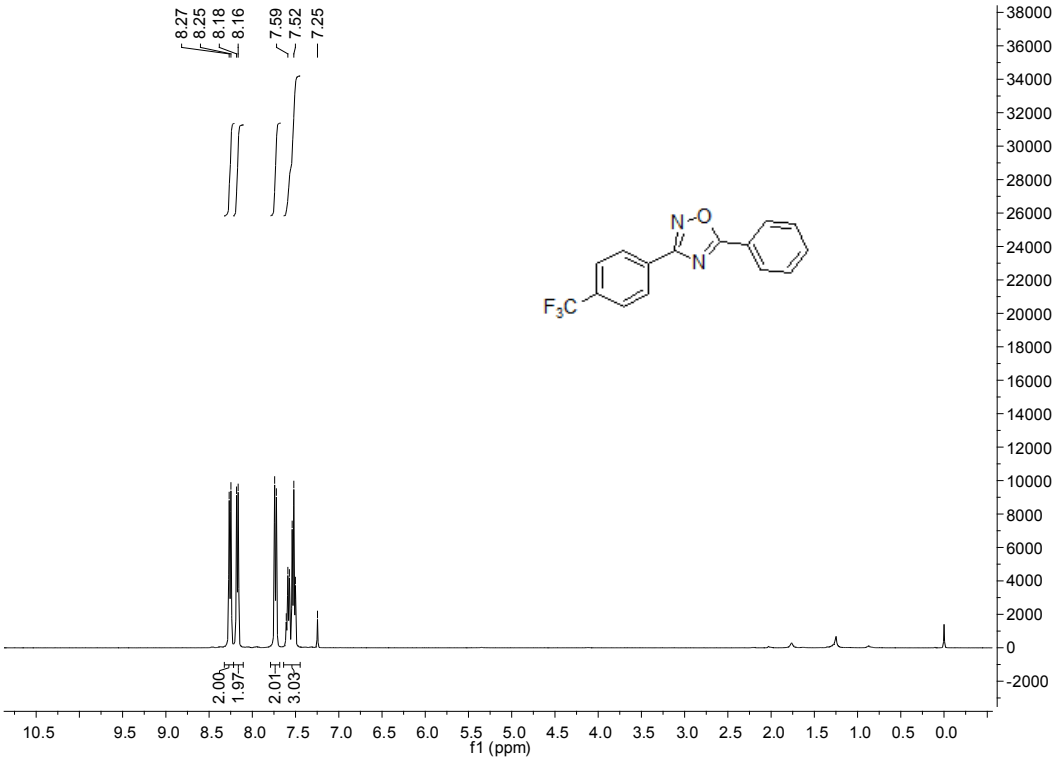
^{13}C NMR of **3ca**



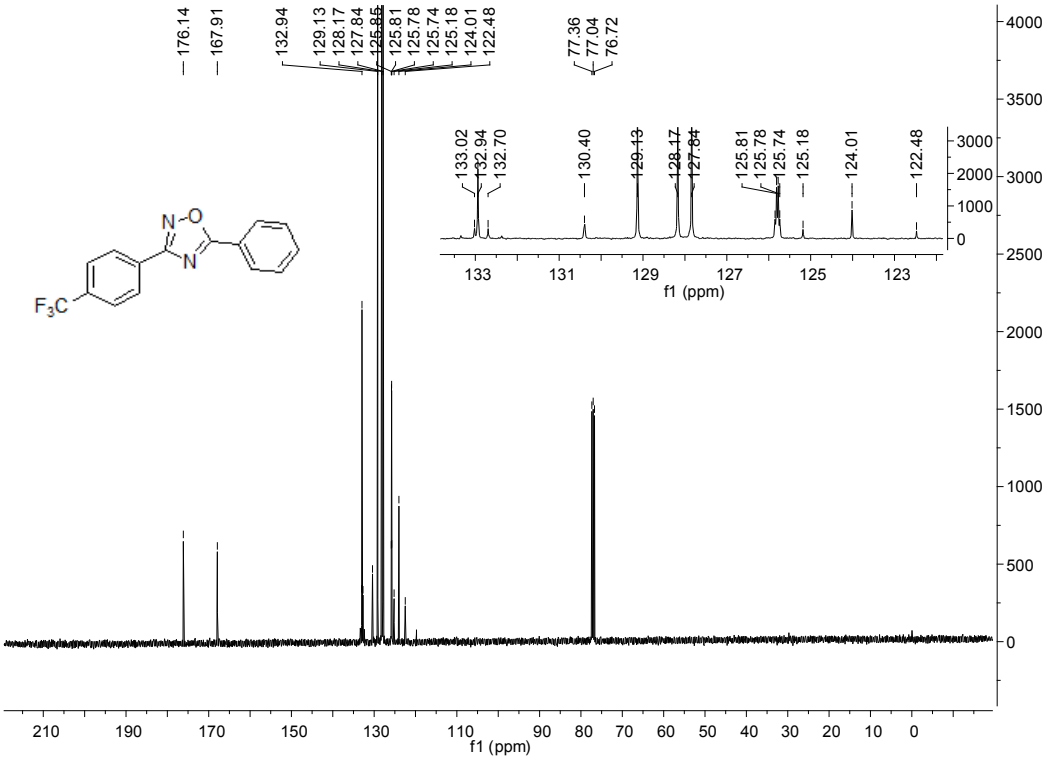
^{1}H NMR of **3da**



^{13}C NMR of **3da**



^{1}H NMR of **3ea**



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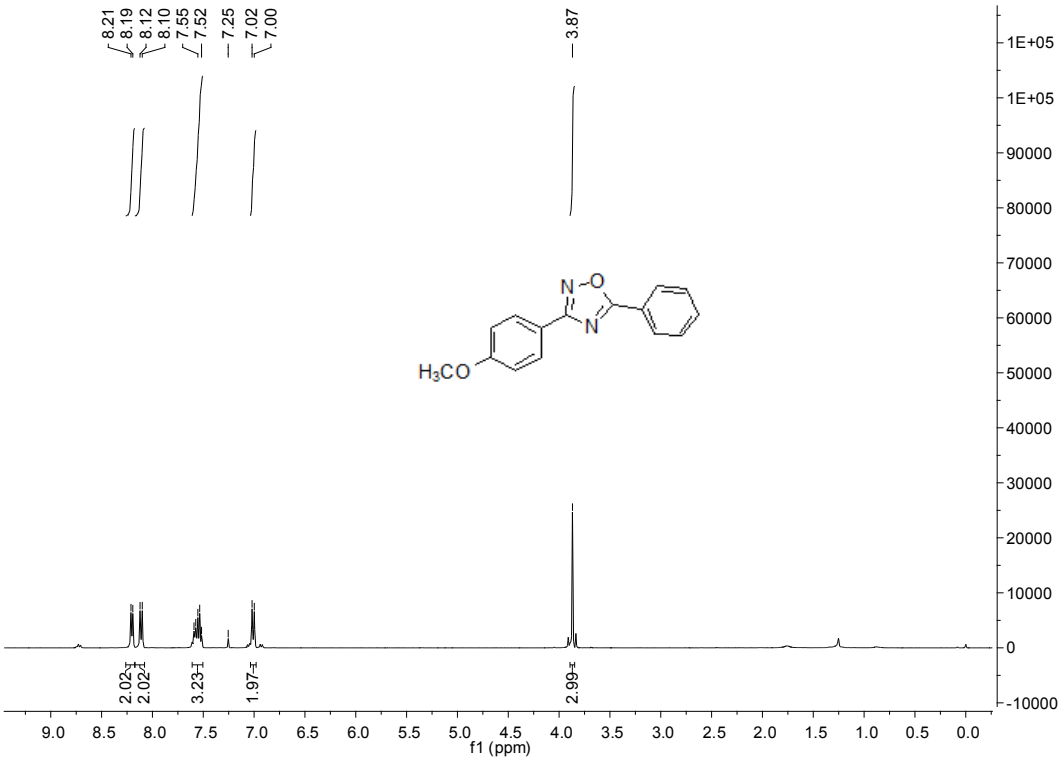
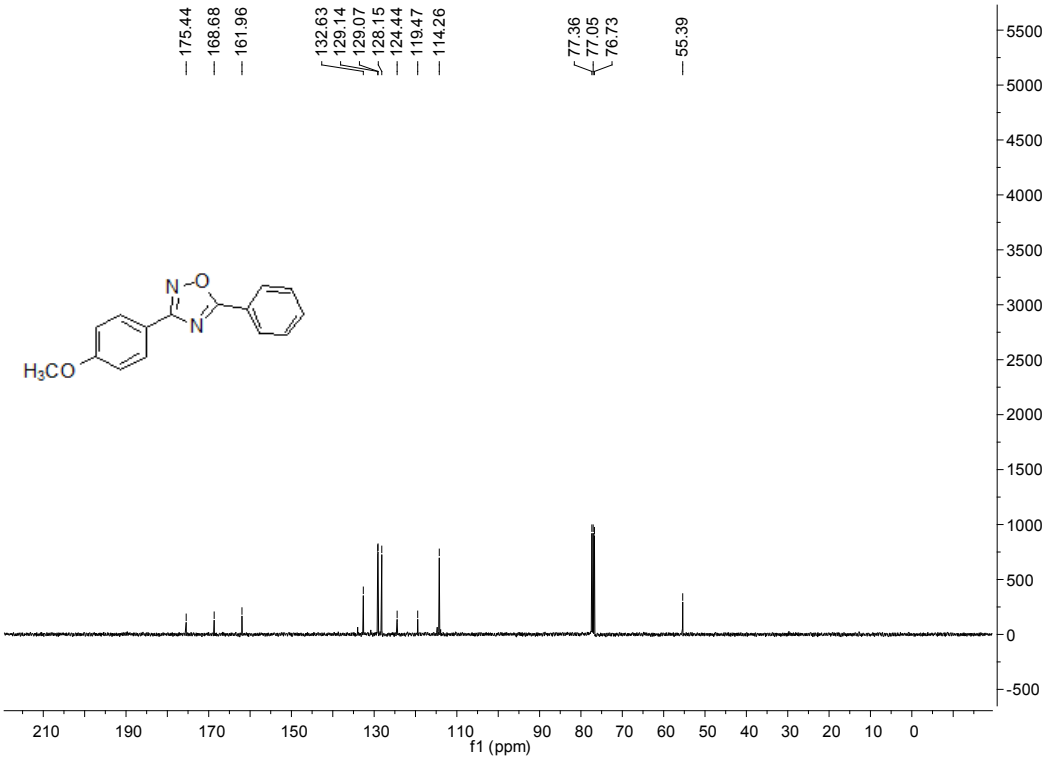
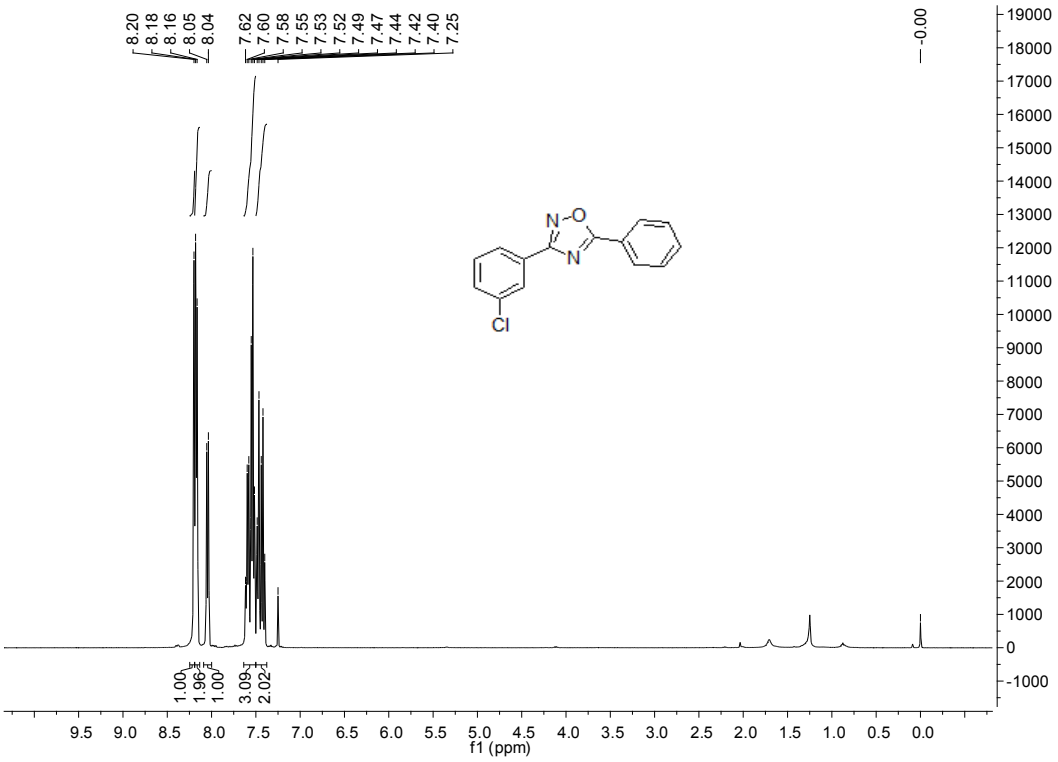


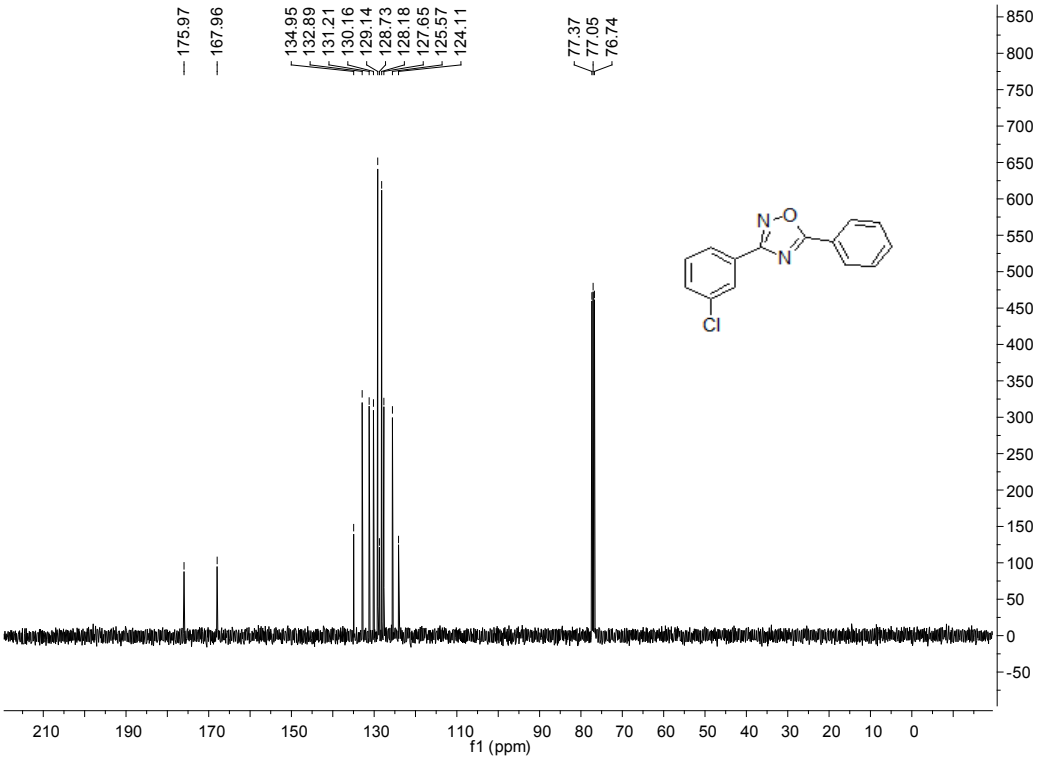
^{1}H NMR of **3fa**



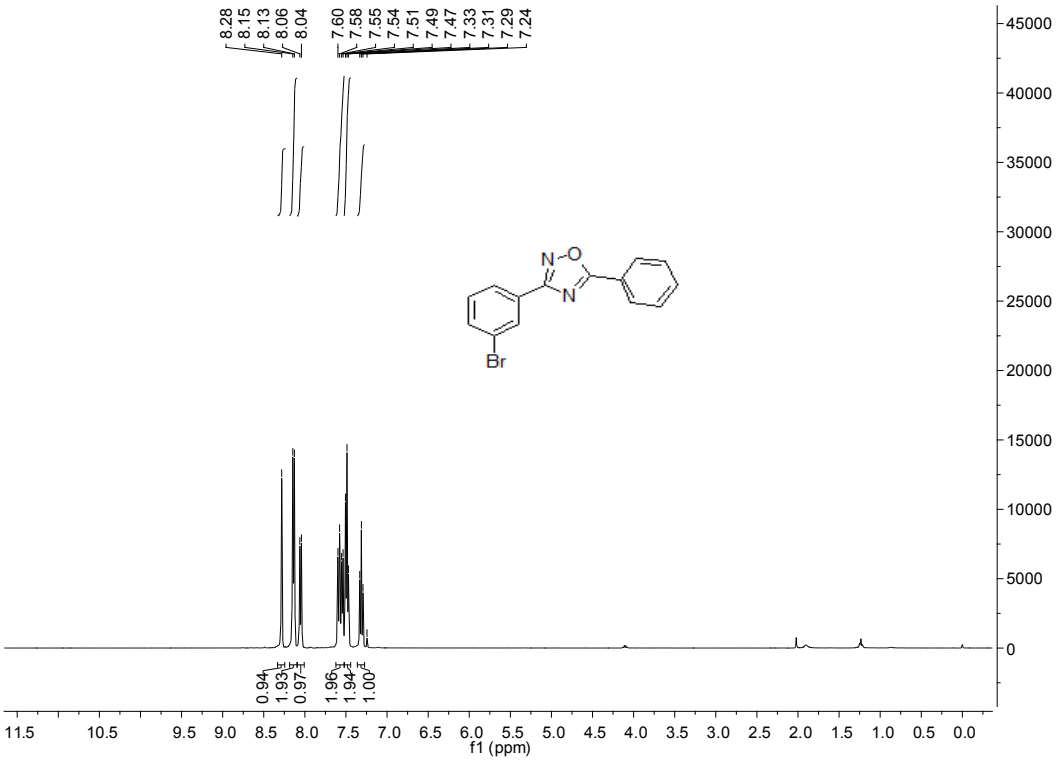
^{13}C NMR of **3fa**



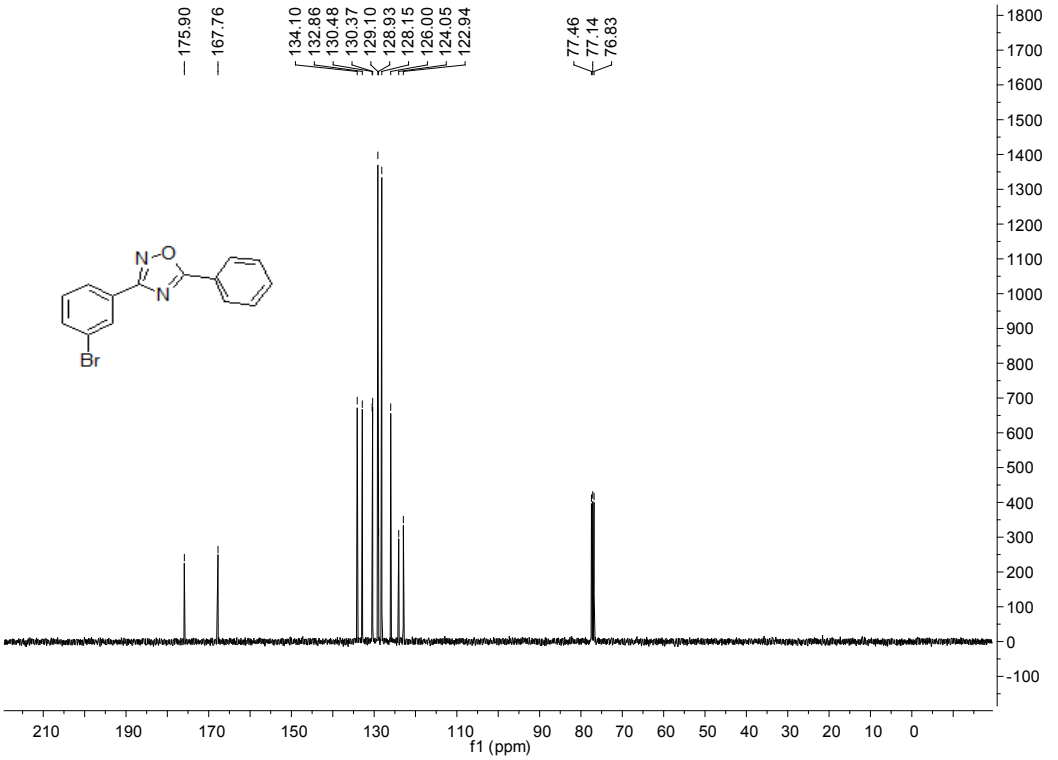
^{1}H NMR of **3ga**



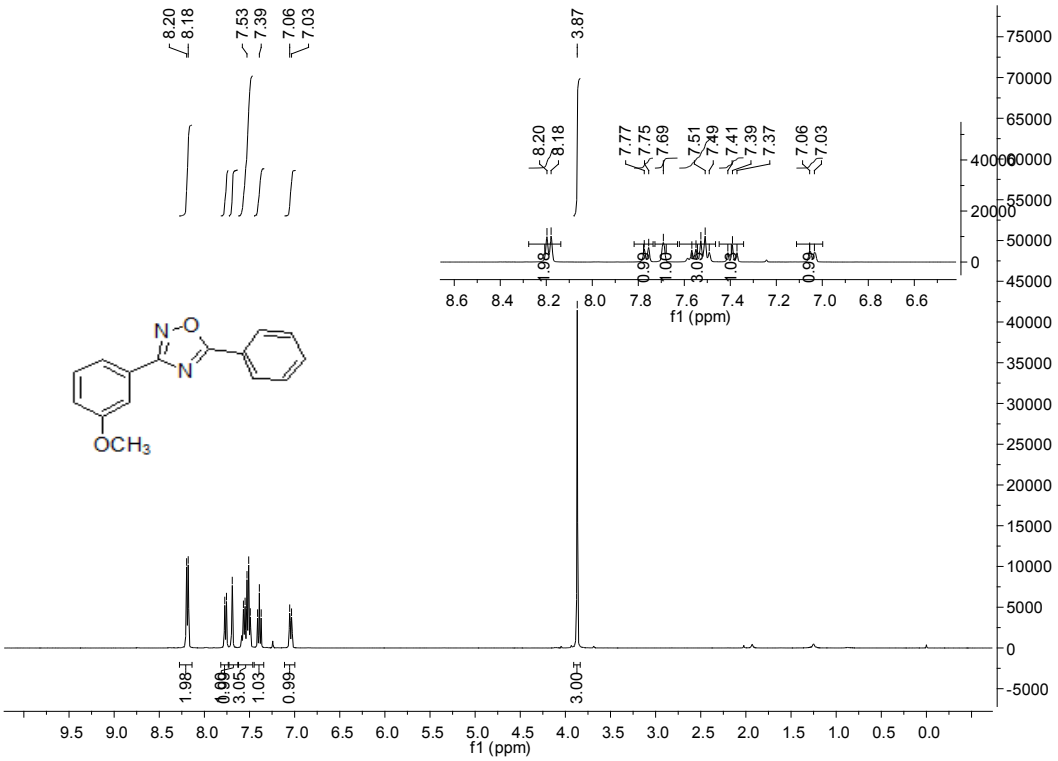
^{13}C NMR of **3ga**



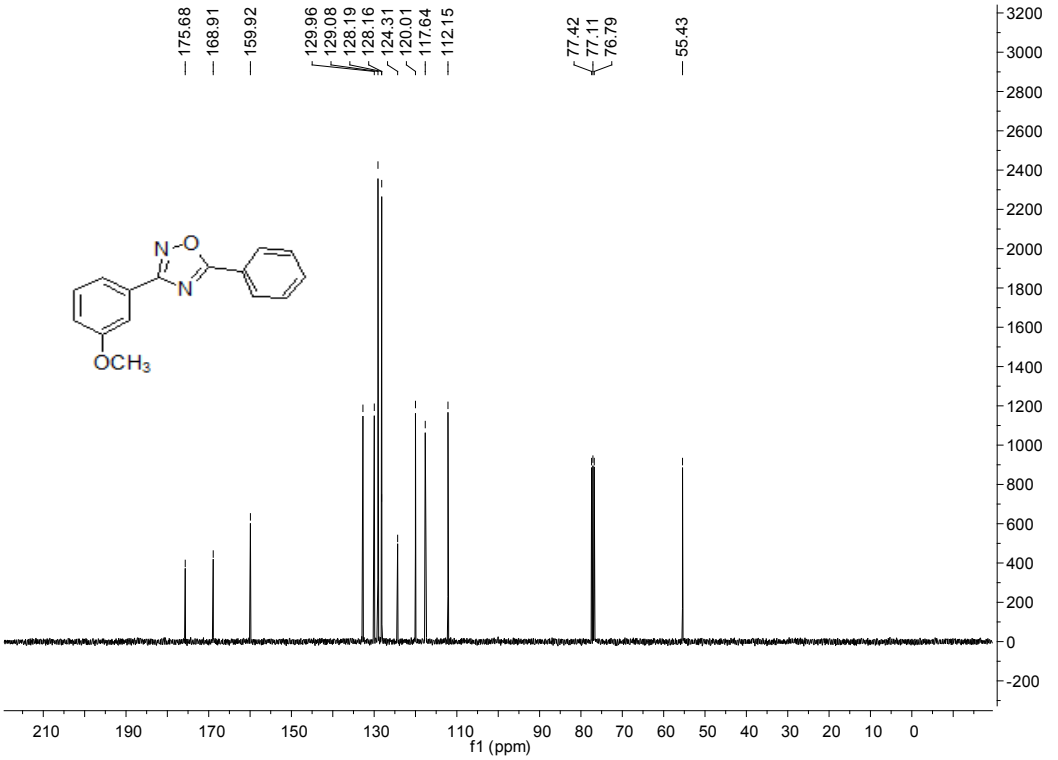
^{1}H NMR of **3ha**



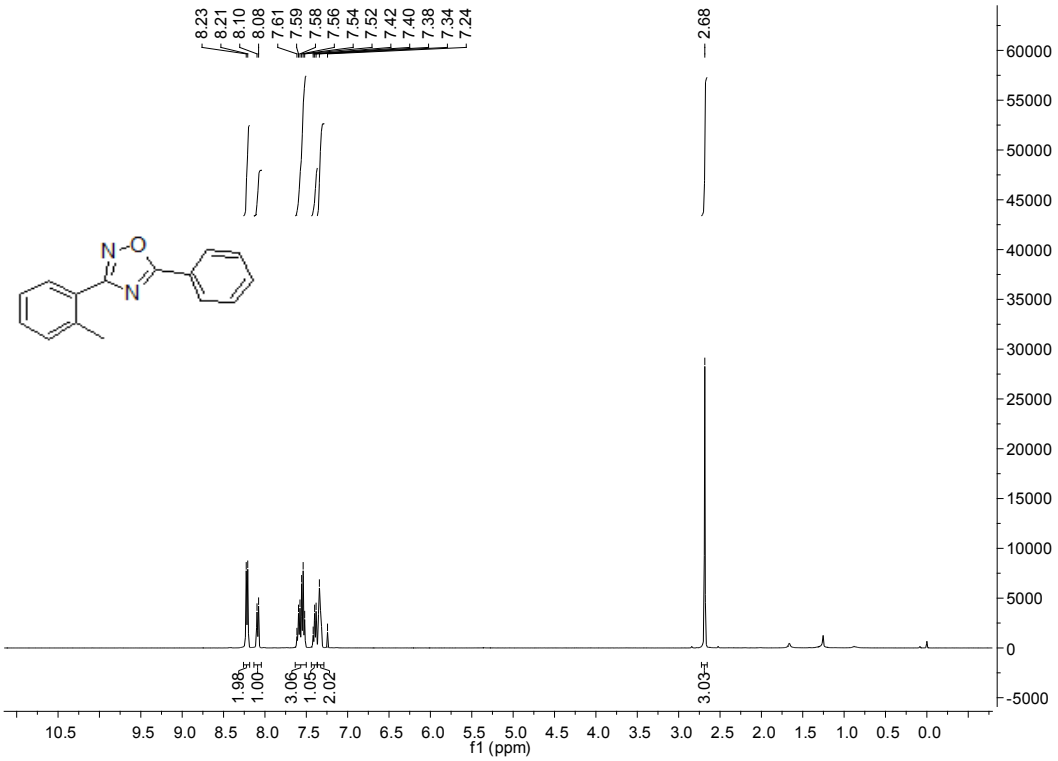
^{13}C NMR of **3ha**



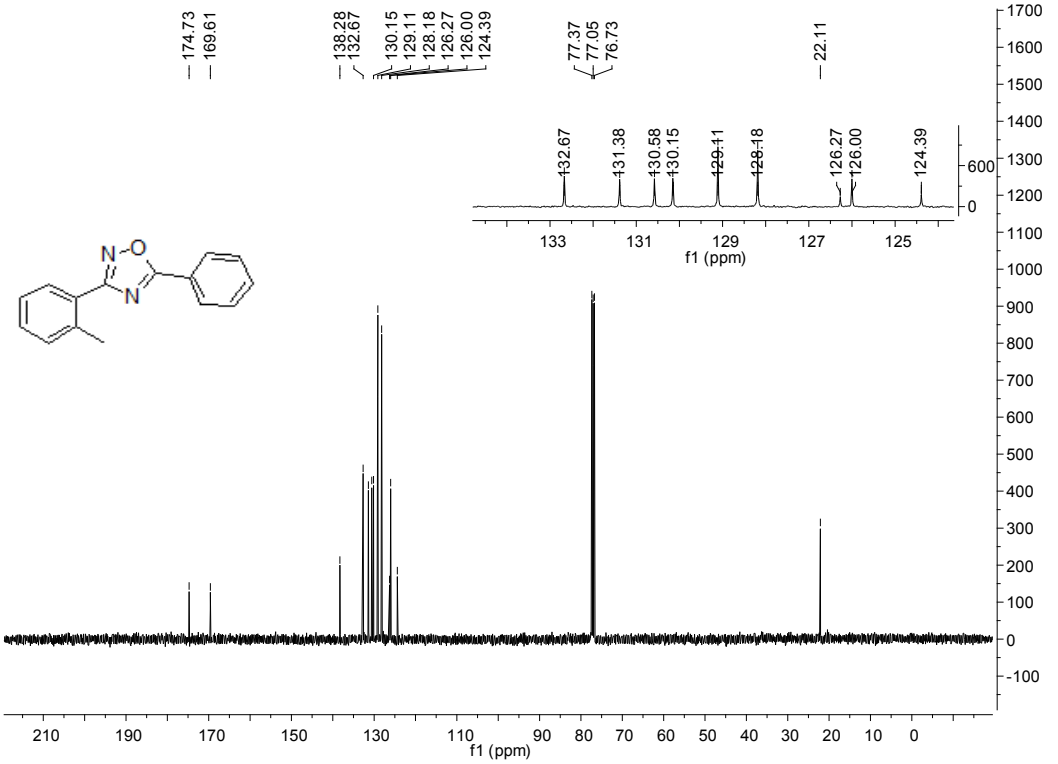
^{1}H NMR of **3ia**



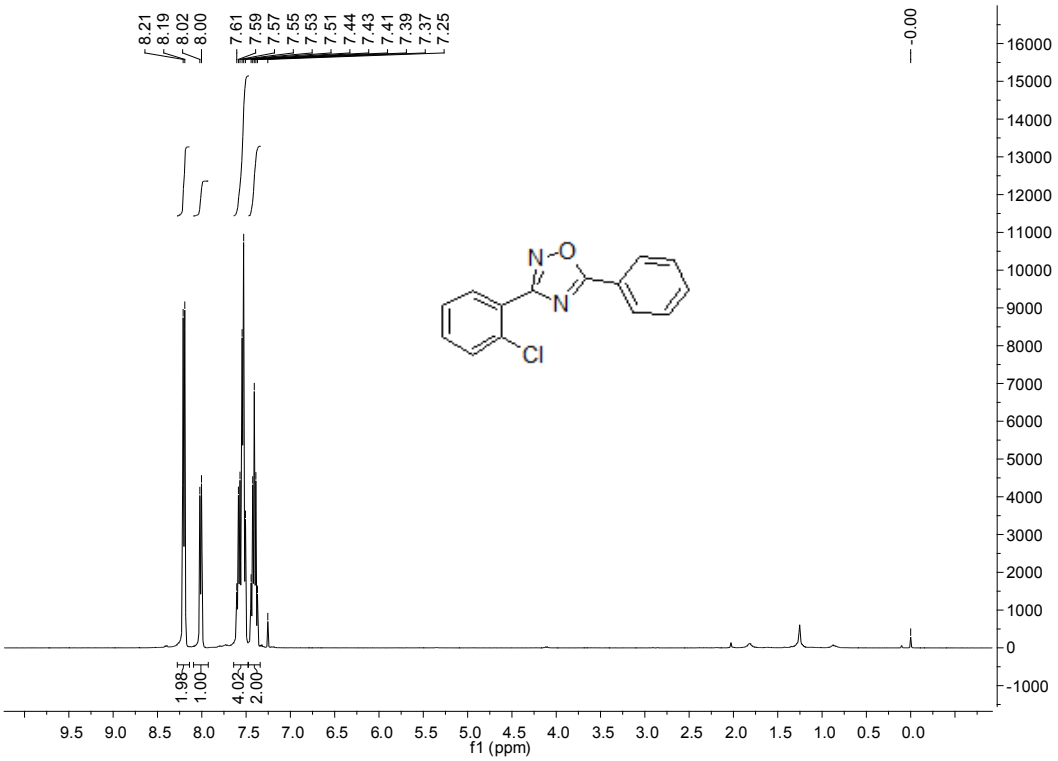
^{13}C NMR of **3ia**



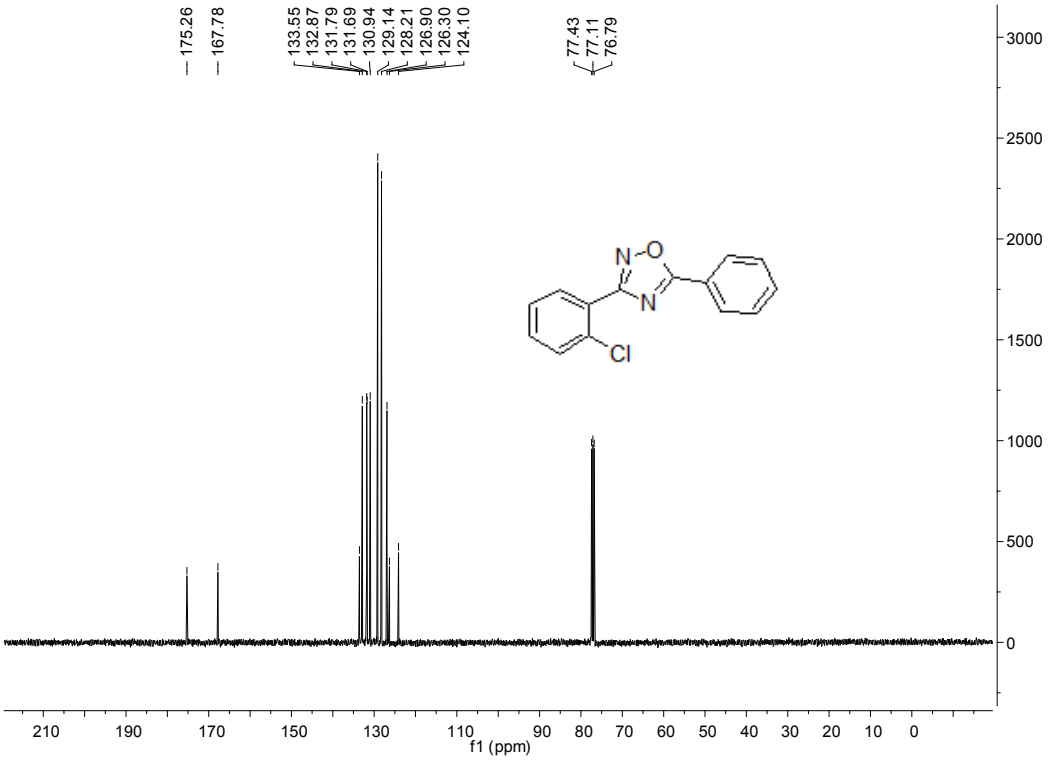
^{1}H NMR of **3ja**



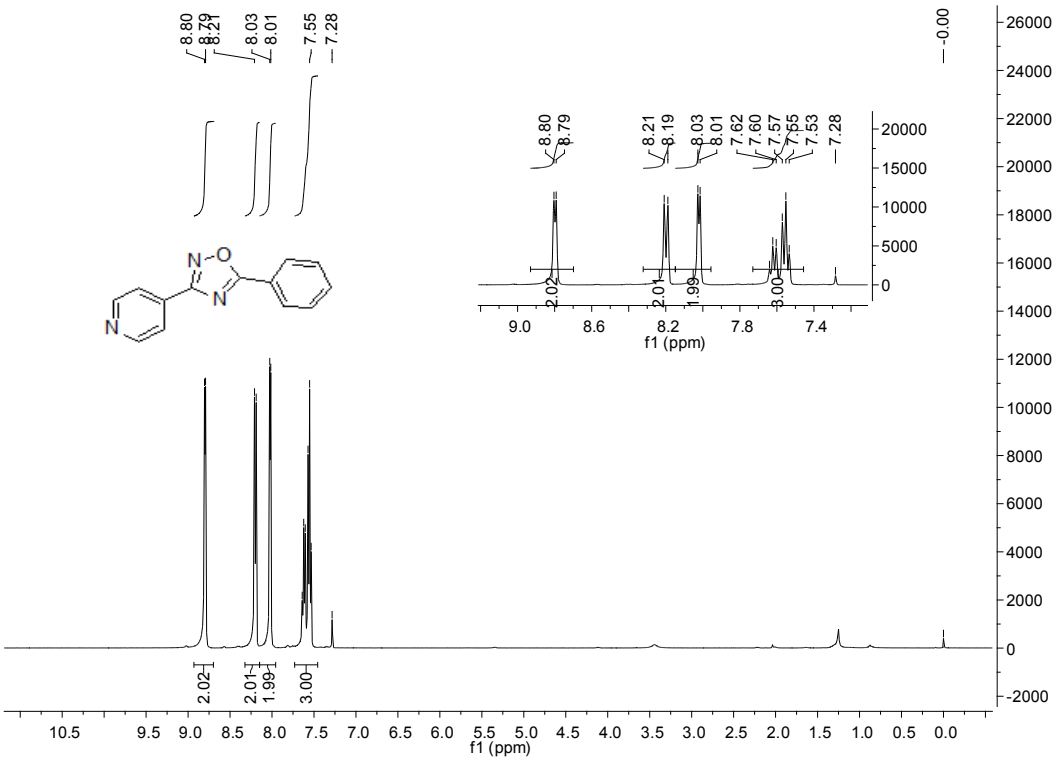
^{13}C NMR of **3ja**



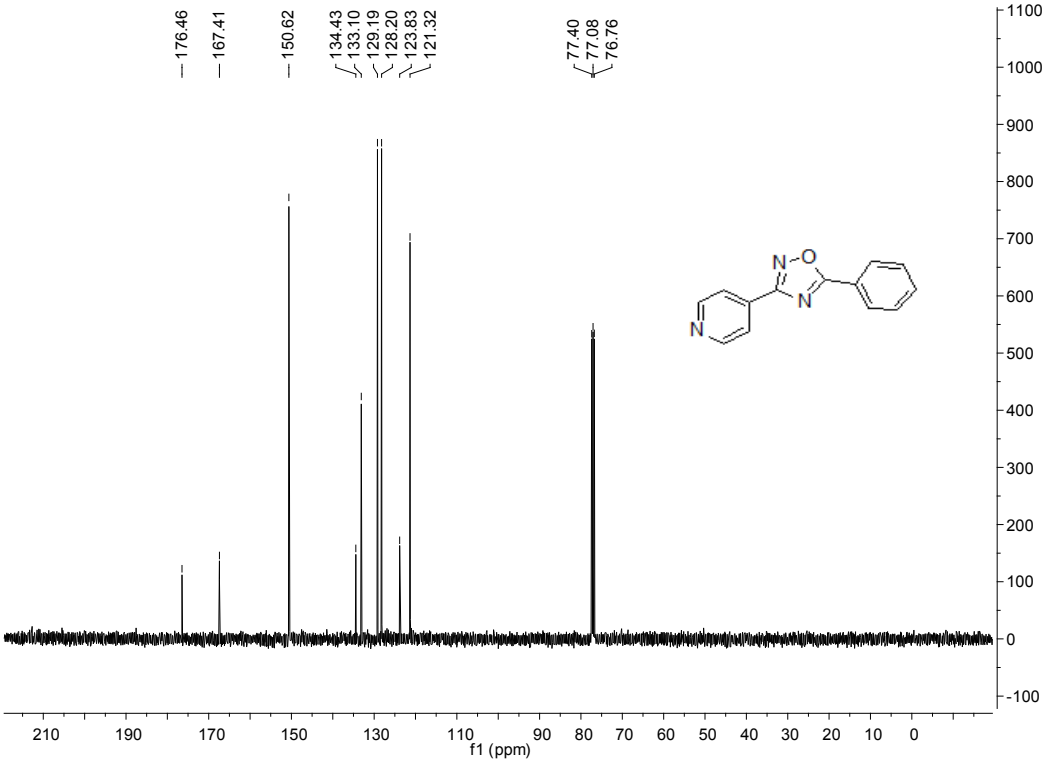
^{1}H NMR of **3ka**



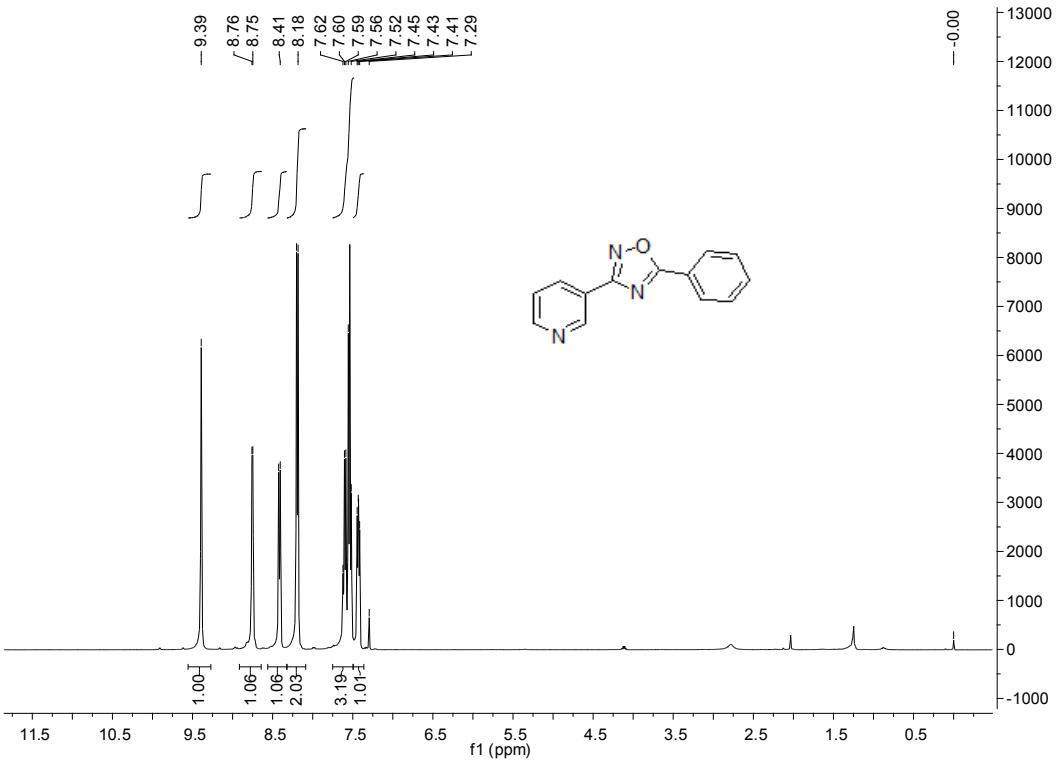
^{13}C NMR of **3ka**



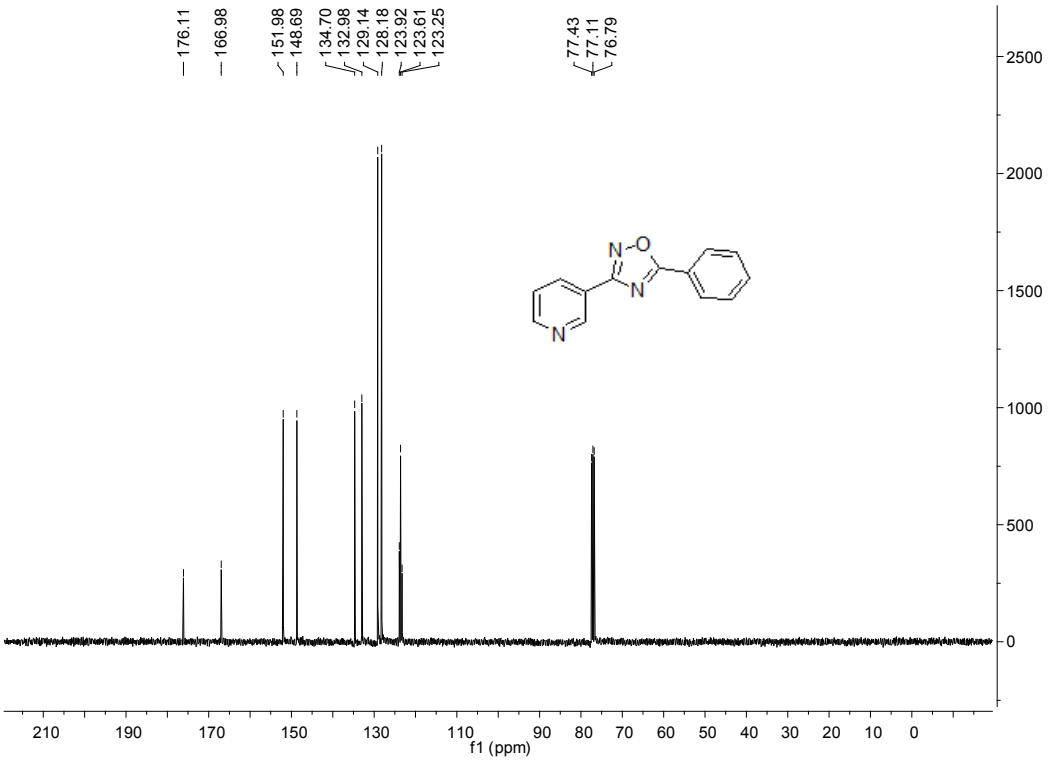
^{1}H NMR of **3la**



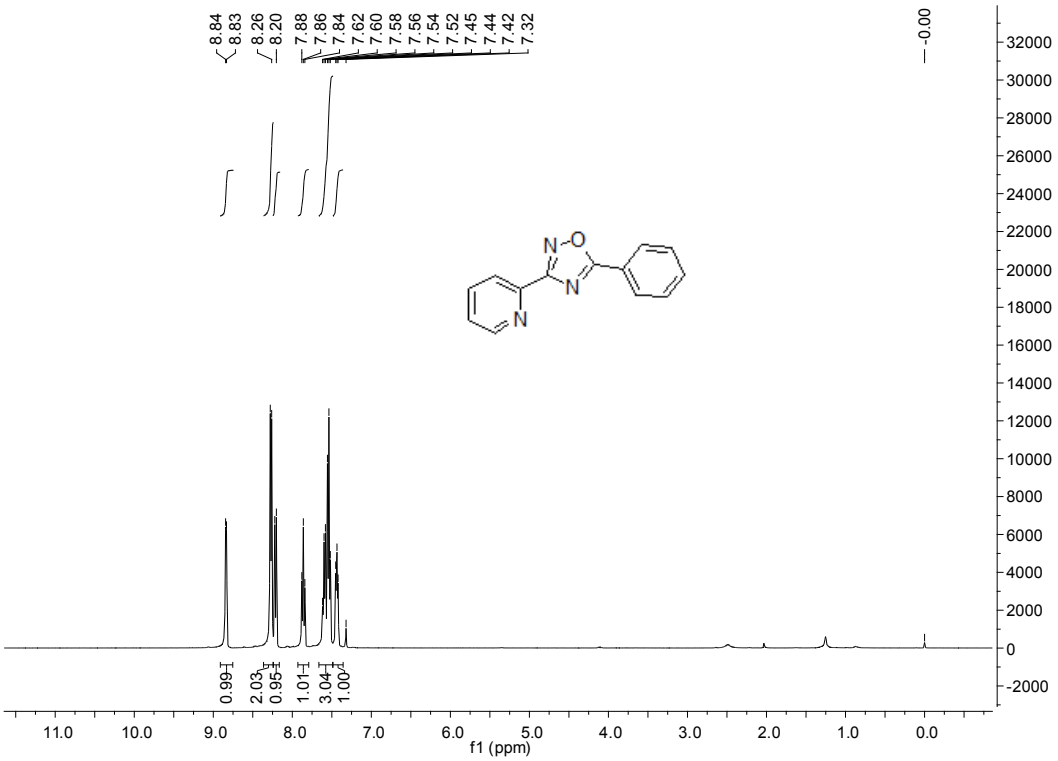
^{13}C NMR of **3la**



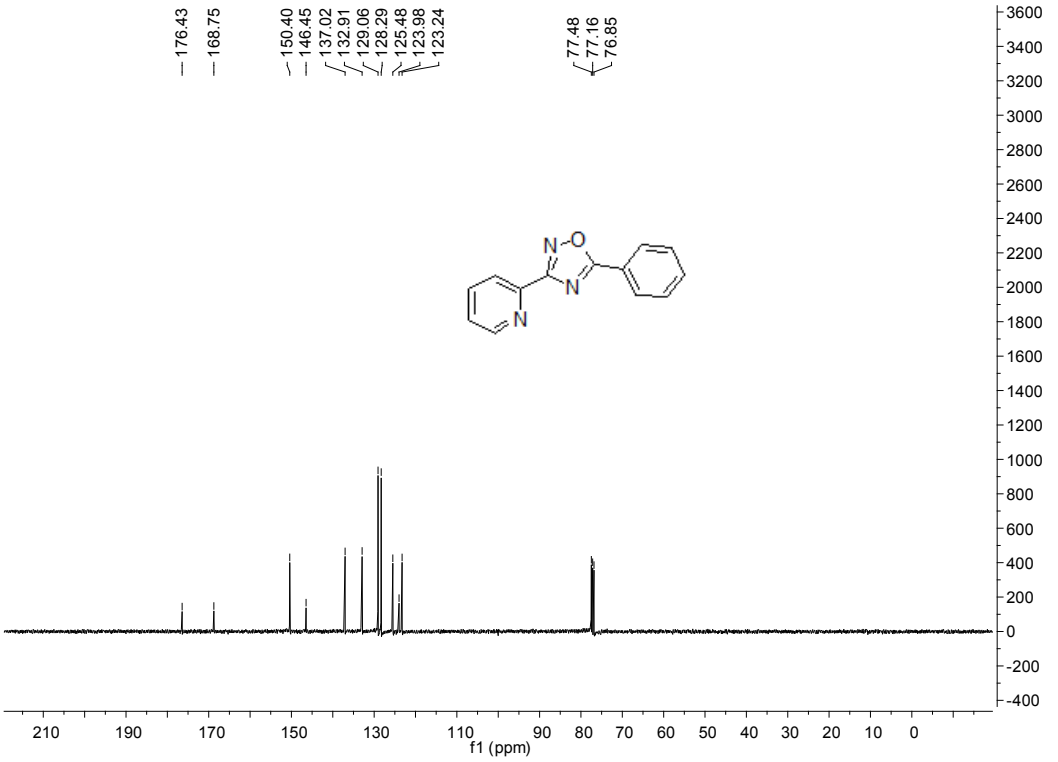
^{1}H NMR of **3ma**



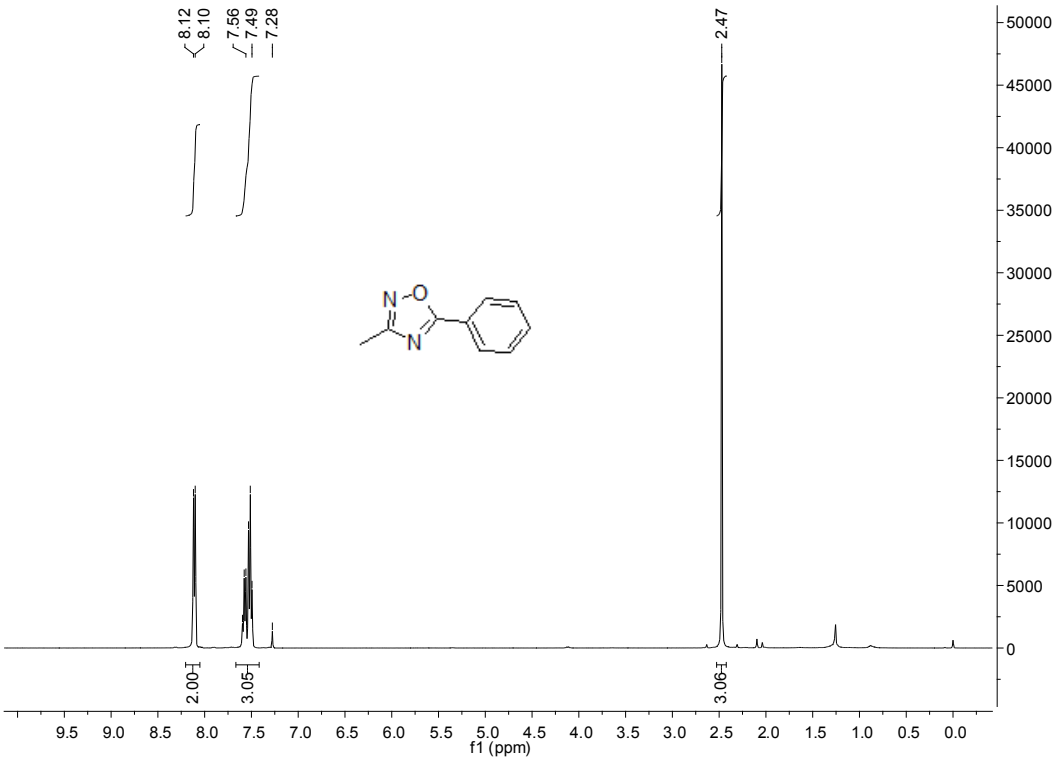
^{13}C NMR of **3ma**



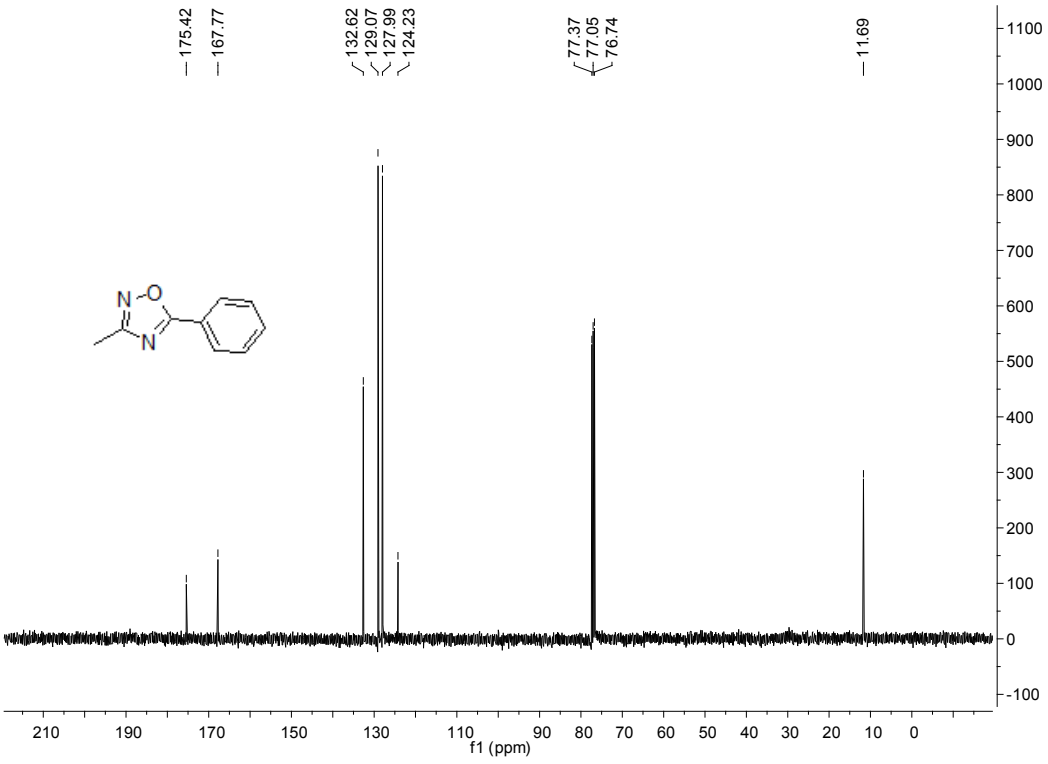
^{1}H NMR of **3na**



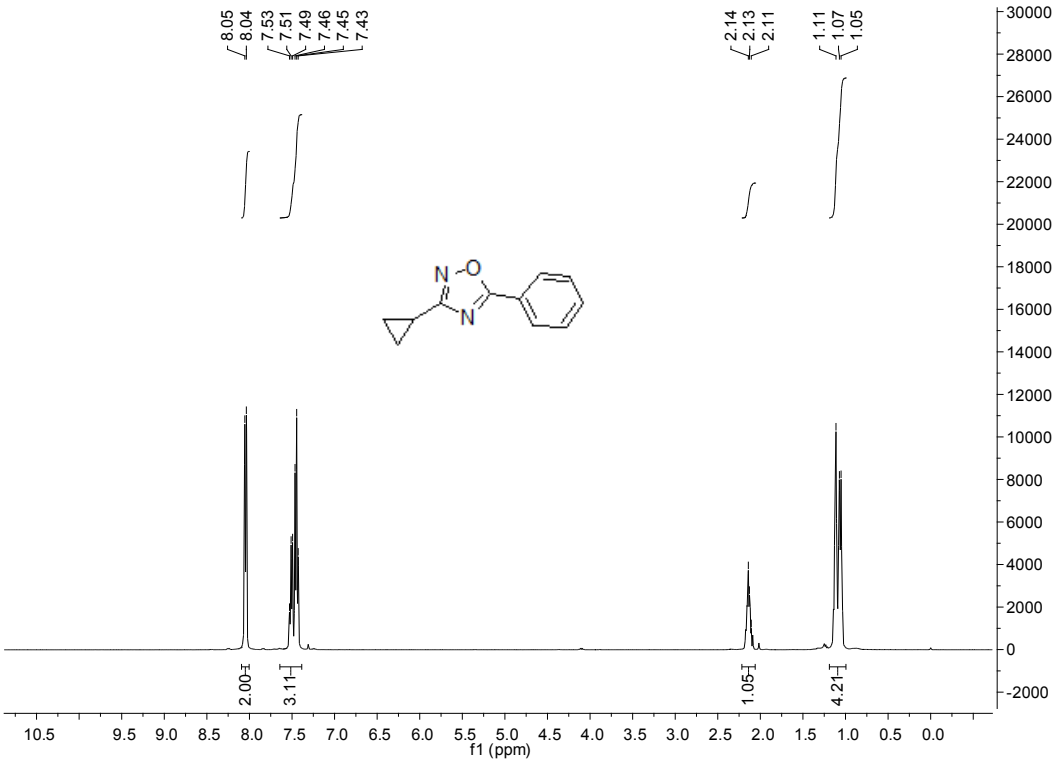
^{13}C NMR of **3na**



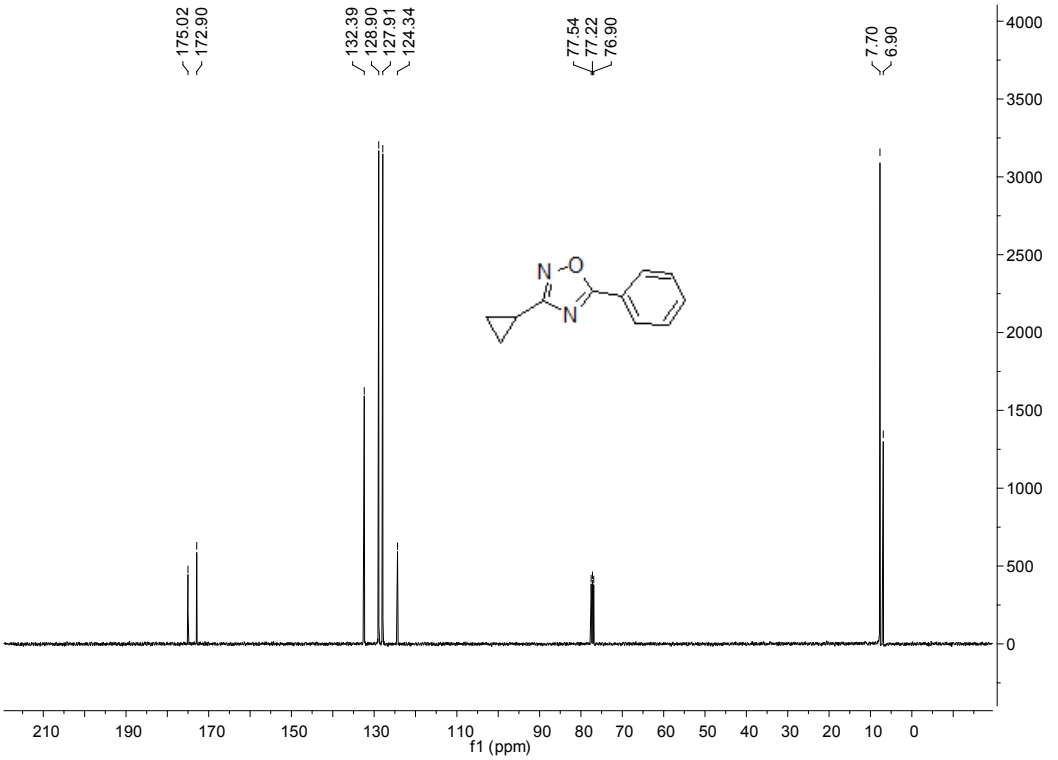
^{1}H NMR of **3oa**



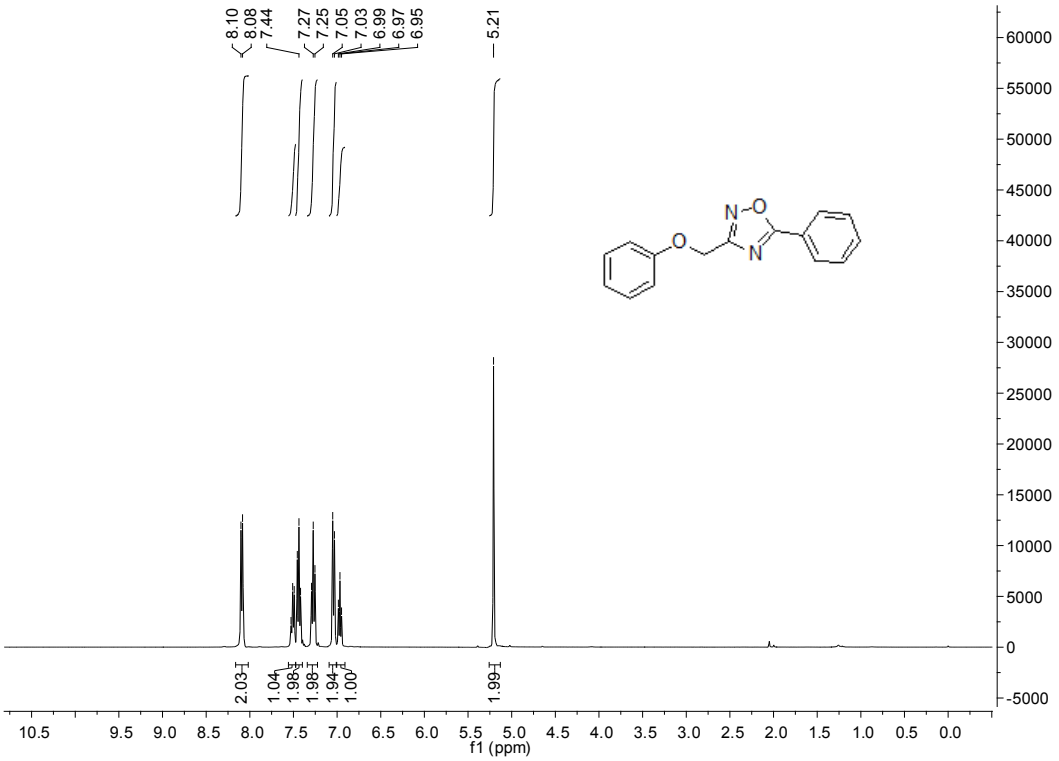
^{13}C NMR of **3oa**



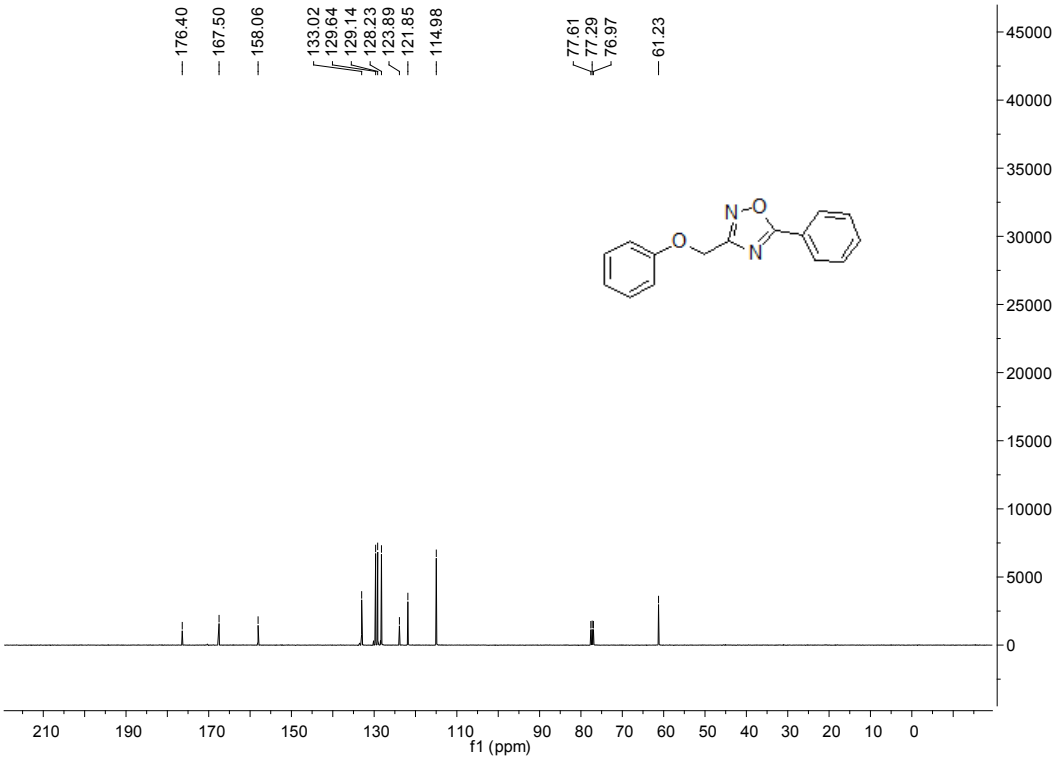
^{1}H NMR of **3pa**



^{13}C NMR of **3pa**



^{1}H NMR of **3qa**



^{13}C NMR of **3qa**