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Supporting Information

Copper-Catalyzed Aerobic Oxidative C–O Bond Formation for the Synthesis of 3,5-Disubstituted Isoxazoles from Enone Oximes

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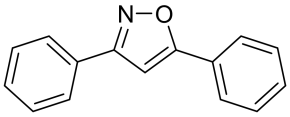
I. General method

Melting points were measured with a melting point instrument and were uncorrected. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker Avance (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform signals. High-resolution mass spectra were obtained with a LCMS-IT-TOF mass spectrometer. Column chromatography was performed on silica gel (100−200) mesh using ethyl acetate and petroleum ether as eluent in different ratios.

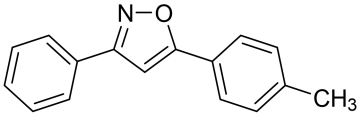
II. Typical procedure

To a dried Schlenk tube was added successively a mixture of enone oxime (0.2 mmol), $Cu(OAc)_2$ (3 mg, 10 mol %), DABCO (6 mg, 30 mol %) and 2 mL of DMSO. The mixture was stirred at 100 °C for 12 h under 1 atm of O_2. After the reaction was completed, the reaction mixture was washed with brine and extracted with ethyl acetate. The organic layer layers was dried over $MgSO_4$ and concentrated in vacuum. The residue was separated by column chromatography to give the desired products.

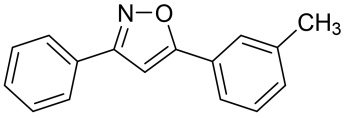
III. Analytical data for compounds 2,3,4,5



3,5-diphenylisoxazole (2aa):[1] white solid (37.6 mg, 85%); mp 141–142 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91–7.81 (m, 4H, ArH), 7.53–7.43 (m, 6H, ArH), 6.84 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 162.9, 130.1, 129.9, 129.0, 128.9, 128.8, 127.4, 126.7, 125.7, 97.4.

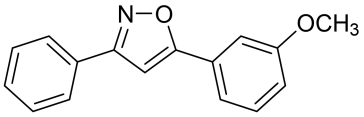


3-phenyl-5-(p-tolyl)isoxazole (2ab):[1] white solid (37.2 mg, 79%); mp 136–137 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (dt, J = 3.9, 2.2 Hz, 2H, ArH), 7.73 (d, J = 8.2 Hz, 2H, ArH), 7.53–7.39 (m, 3H, ArH), 7.28 (d, J = 7.9 Hz, 2H, ArH), 6.77 (s, 1H, isoxazole-H), 2.40 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 162.8, 140.4, 129.8, 129.6, 129.1, 128.8, 126.7, 125.6, 124.6, 96.8, 21.4.

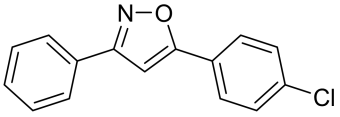


3-phenyl-5-(m-tolyl)isoxazole (2ac):[2] white solid (37.6 mg, 80%); mp 106–108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89–7.84

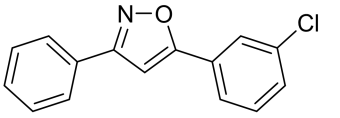
(m, 2H, ArH), 7.67–7.64 (m, 2H, ArH), 7.51–7.44 (m, 3H, ArH), 7.40–7.35 (m, 1H, ArH), 7.28–7.26 (m, 1H, ArH), 6.82 (s, 1H, isoxazole-H), 2.43 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 162.8, 138.7, 130.9, 129.9, 129.0, 128.8, 128.8, 127.2, 126.7, 126.3, 122.9, 97.3, 21.3.



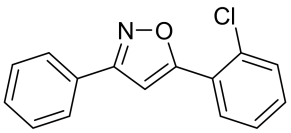
5-(3-methoxyphenyl)-3-phenylisoxazole (2ad):[3] white solid (38.7 mg, 77%); mp 70–71 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.89–7.82 (m, 2H, ArH), 7.53–7.33 (m, 6H, ArH), 7.53–6.97 (m, 1H, ArH), 6.81 (s, 1H, isoxazole-H), 3.86 (s, 3H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 162.8, 159.8, 130.4, 129.9, 129.0, 128.8, 128.5, 126.7, 118.2, 116.0, 110.8, 97.6, 55.3.



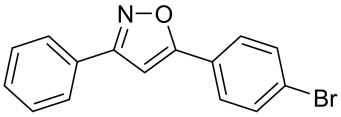
5-(4-chlorophenyl)-3-phenylisoxazole (2ae):[2] white solid (45.0 mg, 88%); mp 178–179 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.87–7.83 (m, 2H, ArH), 7.79–7.75 (m, 2H, ArH), 7.50–7.44 (m, 5H, ArH), 6.81 (s, 1H, isoxazole-H); ^{13}C NMR (100MHz, $CDCl_3$) δ 169.2, 163.0, 136.3, 130.1, 129.3, 128.9, 128.9, 127.1, 126.8, 125.9, 97.8.



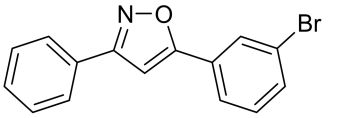
5-(3-chlorophenyl)-3-phenylisoxazole (2af):[1] white solid (44.0 mg, 86%); mp 134–136 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.87–7.81 (m, 3H, ArH), 7.74–7.69 (m, 1H, ArH), 7.51–7.46 (m, 3H, ArH), 7.44–7.41 (m, 2H, ArH), 6.84 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.9, 163.0, 135.1, 130.3, 130.1, 130.1, 129.0, 128.9, 128.8, 126.8, 125.8, 123.8, 98.2.



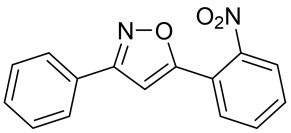
5-(2-chlorophenyl)-3-phenylisoxazole (2ag):[4] white solid (44.5 mg, 87%); mp 129–131 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.86–7.81 (m, 3H, ArH), 7.71 (t, J = 3.9 Hz, 1H, ArH), 7.48–7.40 (m, 5H, ArH), 6.84 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 163.0, 135.0, 130.3, 130.1, 130.1, 128.9, 128.7, 126.7, 125.8, 123.8, 123.8, 98.2.



5-(4-bromophenyl)-3-phenylisoxazole (2ah):[1] white solid (51.6 mg, 86%); mp 184–185 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.87–7.84 (m, 2H, ArH), 7.73–7.69 (m, 2H, ArH), 7.64–7.61 (m, 2H, ArH), 7.51–7.46 (m, 3H, ArH), 6.83 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 163.0, 132.2, 130.1, 128.9, 128.8, 127.2, 126.8, 126.3, 124.5, 97.8.

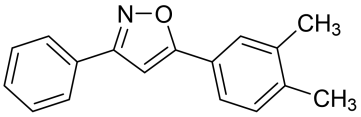


5-(3-bromophenyl)-3-phenylisoxazole (2ai):[5] white solid (51.0 mg, 85%); mp 178–180 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (t, J = 1.8 Hz, 1H, ArH), 7.88–7.84 (m, 2H, ArH), 7.78–7.76 (m, 1H, ArH), 7.59–7.57 (m, 1H, ArH), 7.51–7.46 (m, 3H, ArH), 7.36 (t, J = 7.9 Hz, 1H, ArH), 6.85 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 163.0, 133.0, 130.5, 130.1, 129.2, 128.9, 128.7, 128.7, 126.7, 124.3, 123.0, 98.2.

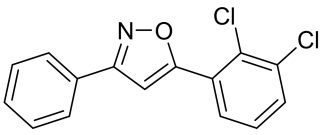


5-(2-nitrophenyl)-3-phenylisoxazole (2aj):[6] white solid (49.5 mg, 93%); mp 53–55 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.90 (dd, J = 8.1,

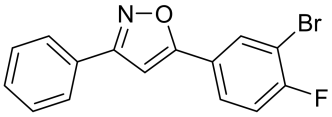
1.3 Hz, 1H, ArH), 7.85–7.82 (m, 3H, ArH), 7.73–7.69 (m, 1H, ArH), 7.64–7.60 (m, 1H, ArH), 7.48–7.45 (m, 3H, ArH), 6.80 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 162.9, 148.0, 132.6, 131.0, 130.4, 130.2, 128.9, 128.4, 126.8, 124.3, 121.5, 101.8.



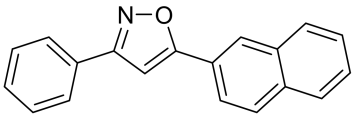
5-(3,4-dimethylphenyl)-3-phenylisoxazole (2ak): white solid (37.9 mg, 76%); mp 119–120 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89–7.87 (m, 2H, ArH), 7.62 (s, 1H, ArH), 7.58 (dd, *J* = 7.9, 1.3 Hz, 1H, ArH), 7.51–7.45 (m, 3H, ArH), 7.23 (d, *J* = 7.8 Hz, 1H, ArH), 6.77 (s, 1H, isoxazole-H), 2.34 (s, 3H, CH_3), 2.32 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 162.8, 139.1, 137.2, 130.1, 129.8, 129.2, 128.8, 126.8, 126.7, 125.0, 123.2, 96.7, 19.7, 19.7; HRMS-ESI (m/z): calcd for $C_{17}H_{16}NO$, $[M+H]^+$:250.1226; found, 250.1222.



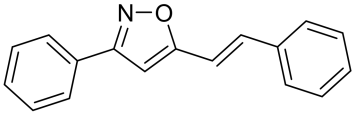
5-(2,3-dichlorophenyl)-3-phenylisoxazole (2al): white solid (51.6 mg, 89%); mp 132–134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93–7.87 (m, 3H, ArH), 7.58 (dd, *J* = 8.0, 1.6 Hz, 1H, ArH), 7.50–7.47 (m, 3H, ArH), 7.37 (t, *J* = 8.0 Hz, 1H, ArH), 7.27 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 162.9, 134.6, 131.6, 130.1, 130.1, 128.9, 128.8, 128.4, 127.7, 127.6, 126.8, 103.1; HRMS-ESI (m/z): calcd for $C_{15}H_{10}Cl_2NO$, $[M+H]^+$: 290.0134; found, 290.0129.



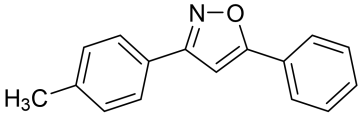
5-(3-bromo-4-fluorophenyl)-3-phenylisoxazole (2am): white solid (56.0 mg, 88%); mp 165–166 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 6.4, 2.2 Hz, 1H, ArH), 7.86–7.83 (m, 2H, ArH), 7.78–7.74 (m, 1H, ArH), 7.50–7.45 (m, 3H, ArH), 7.23 (t, *J* = 8.4 Hz, 1H, ArH), 6.79 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 163.1, 160.0 (d, *J* = 252.2 Hz), 131.1, 130.1, 128.9, 128.7, 126.7, 126.5 (d, *J* = 7.8 Hz), 125.1 (d, *J* = 4.0 Hz), 117.1 (d, *J* = 23.1 Hz), 110.0 (d, *J* = 21.8 Hz), 97.9 (d, *J* = 0.8 Hz); HRMS-ESI (m/z): calcd for $C_{15}H_{10}BrFNO$, $[M+H]^+$: 317.9924; found, 317.9922.



5-(naphthalen-2-yl)-3-phenylisoxazole (2an):[1] white solid (46.1 mg, 85%); mp 167–169 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H, ArH), 7.96–7.87 (m, 6H, ArH), 7.58–7.49 (m, 5H, ArH), 6.95 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 163.0, 133.9, 133.1, 130.0, 129.1, 128.9, 128.8, 128.6, 127.8, 127.3, 126.9, 126.8, 125.5, 124.7, 122.9, 97.8.

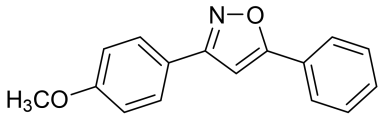


(*E*)-3-phenyl-5-styrylisoxazole (2ao):[1] white solid (41.1 mg, 83%); mp 135–137 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86–7.81 (m, 2H, ArH), 7.57–7.52 (m, 2H, ArH), 7.46–7.44 (m, 3H, ArH), 7.41–7.32 (m, 4H, ArH + C*H*=CH), 7.01 (d, *J* = 16.5 Hz, 1H, CH=C*H*), 6.57 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.9, 162.7, 135.5, 134.9, 129.9, 129.1, 129.0, 128.8, 128.8, 127.1, 126.7, 113.0, 99.4.

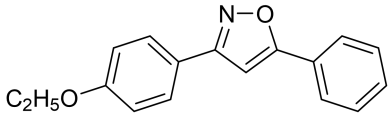


5-phenyl-3-(p-tolyl)isoxazole (2ba):[1] white solid (47.9 mg, 84%); mp 130–131°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85–7.82

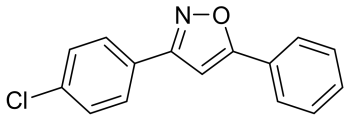
(m, 2H, ArH), 7.77 (d, J = 8.2 Hz, 2H, ArH), 7.51–7.42 (m, 3H, ArH), 7.29 (d, J = 7.9 Hz, 2H, ArH), 6.81 (s, 1H, isoxazole-H), 2.39 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 162.8, 140.0, 130.1, 129.5, 128.9, 127.4, 126.6, 126.2, 125.7, 97.3, 21.3.



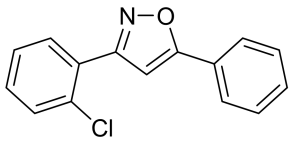
3-(4-methoxyphenyl)-5-phenylisoxazole (2ca):[1] white solid (41.7 mg, 83%); mp 120–121 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.83–7.78 (m, 4H, ArH), 7.49–7.41 (m, 3H, ArH), 7.00–6.96 (m, 2H, ArH), 6.76 (s, 1H, isoxazole-H), 3.84 (s, 3H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 162.5, 160.9, 130.0, 128.9, 128.1, 127.4, 125.7, 121.5, 114.2, 97.2, 55.2.



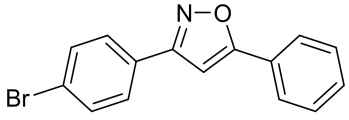
3-(4-ethoxyphenyl)-5-phenylisoxazole (2da):[7] white solid (45.6 mg, 86%); mp 129–130 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84–7.78 (m, 4H, ArH), 7.50–7.44 (m, 3H, ArH), 7.00–6.97 (m, 2H, ArH), 6.77 (s, 1H, isoxazole-H), 4.08 (q, J = 7.0 Hz, 2H, CH_2), 1.44 (t, J = 7.0 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 162.5, 160.3, 130.0, 128.9, 128.1, 127.5, 125.7, 121.3, 114.7, 97.2, 63.5, 14.7.



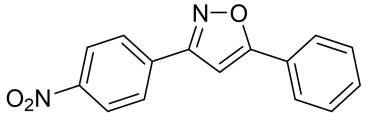
3-(4-chlorophenyl)-5-phenylisoxazole (2ea):[8] white solid (43.5 mg, 85%); mp 179–180 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85–7.79 (m, 4H, ArH), 7.52–7.45 (m, 5H, ArH), 6.80 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 161.9, 136.0, 130.3, 129.2, 129.0, 128.0, 127.6, 127.2, 125.8, 97.2.



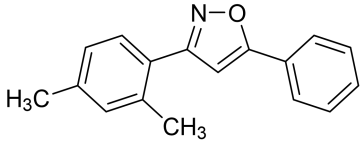
3-(2-chlorophenyl)-5-phenylisoxazole (2fa):[9] white solid (44.0 mg, 86%); mp 74–75 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.86–7.79 (m, 3H, ArH), 7.52–7.44 (m, 4H, ArH), 7.41–7.34 (m, 2H, ArH), 6.99 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.5, 161.4, 132.7, 130.8, 130.7, 130.3, 130.1, 128.8, 128.2, 127.2, 127.0, 125.7, 100.6.



3-(4-bromophenyl)-5-phenylisoxazole (2ga):[10] white solid (50.4 mg, 84%); mp 180–181 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84–7.82 (m, 2H, ArH), 7.74 (d, J = 8.5 Hz, 2H, ArH), 7.61 (d, J = 8.5 Hz, 2H, ArH), 7.51–7.46 (m, 3H, ArH), 6.80 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 162.0, 132.1, 130.3, 129.0, 128.2, 128.0, 127.2, 125.8, 124.3, 97.2.

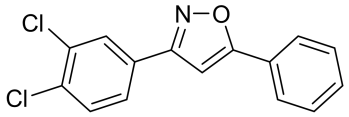


3-(4-nitrophenyl)-5-phenylisoxazole (2ha):[11] white solid (43.7 mg, 82%); mp 222–223 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.38–8.34 (m, 2H, ArH), 8.08–8.05 (m, 2H, ArH), 7.88–7.84 (m, 2H, ArH), 7.54–7.49 (m, 3H, ArH), 6.91 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 161.1, 148.6, 135.2, 130.6, 129.1, 127.6, 126.9, 125.9, 124.2, 97.4.

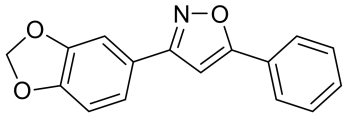


3-(2,4-dimethylphenyl)-5-phenylisoxazole (2ia):[12] white solid (43.9 mg, 88%); mp 63–64 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.87–7.84 (m, 2H, ArH), 7.52–7.43 (m, 4H, ArH), 7.16–7.11 (m,

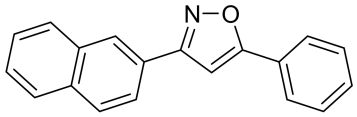
2H, ArH), 6.70 (s, 1H, isoxazole-H), 2.54 (s, 3H, CH_3), 2.39 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 163.5, 139.3, 136.6, 131.8, 129.9, 129.2, 128.8, 127.4, 126.6, 125.8, 125.6, 100.0, 21.1, 21.0.



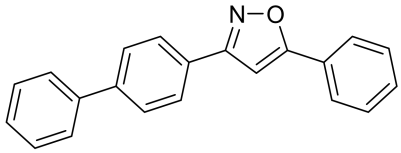
3-(3,4-dichlorophenyl)-5-phenylisoxazole (2ja):[1] white solid (47.6 mg, 82%); mp 159–160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 2.0 Hz, 1H, ArH), 7.83–7.81 (m, 2H, ArH), 7.70 (dd, *J* = 8.3, 2.0 Hz, 1H, ArH), 7.57–7.46 (m, 4H, ArH), 6.79 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 161.0, 134.1, 133.2, 130.9, 130.9, 130.5, 129.0, 128.6, 127.0, 125.8, 125.8, 97.1.



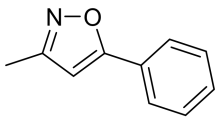
3-(benzo[d][1,3]dioxol-5-yl)-5-phenylisoxazole (2ka):[13] white solid (44.0 mg, 83%); mp 134–135 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83–7.79 (m, 2H, ArH), 7.48–7.43 (m, 3H, ArH), 7.38–7.36 (m, 1H, ArH), 7.32 (dd, *J* = 8.0, 1.7 Hz, 1H, ArH), 6.88 (d, *J* = 8.4 Hz, 1H, ArH), 6.73 (s, 1H, isoxazole-H), 6.01 (s, 2H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.1, 162.5, 149.0, 148.1, 130.1, 128.9, 127.4, 125.7, 123.0, 121.0, 108.5, 106.9, 101.4, 97.2.



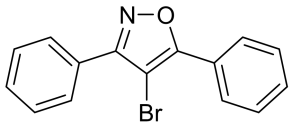
3-(naphthalen-2-yl)-5-phenylisoxazole (2la):[14] white solid (43.9 mg, 81%); mp 146–148 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48–8.46 (m, 1H, ArH), 7.98–7.88 (m, 4H, ArH), 7.77 (dd, *J* = 7.1, 1.1 Hz, 1H, ArH), 7.60–7.47 (m, 6H, ArH), 6.84 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 163.0, 133.7, 130.9, 130.1, 130.1, 128.9, 128.4, 127.6, 127.3, 126.9, 126.8, 126.2, 125.8, 125.5, 125.1, 100.8.



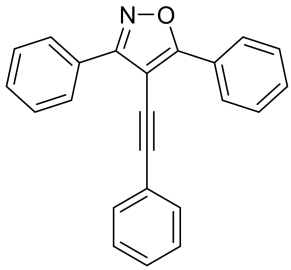
3-([1,1'-biphenyl]-4-yl)-5-phenylisoxazole (2ma):[1] white solid (47.5 mg, 80%); mp 198–199 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97–7.94 (m, 2H, ArH), 7.88–7.85 (m, 2H, ArH), 7.74–7.71 (m, 2H, ArH), 7.67–7.64 (m, 2H, ArH), 7.53 – 7.45 (m, 5H, ArH), 7.42 – 7.37 (m, 1H, ArH), 6.88 (s, 1H, isoxazole-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 162.6, 142.7, 140.2, 130.2, 129.0, 128.8, 127.9, 127.7, 127.5, 127.4, 127.2, 127.0, 125.8, 97.4.



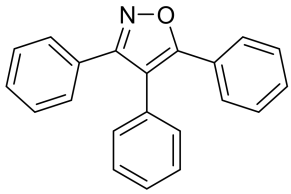
3-methyl-5-phenylisoxazole (2na):[15] white solid (24.8 mg, 78%); mp 63–64 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 – 7.70 (m, 2H, ArH), 7.46 – 7.37 (m, 3H, ArH), 6.33 (s, 1H, isoxazole-H), 2.33 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 160.2, 129.8, 128.7, 127.4, 125.5, 100.0, 11.40.



4-bromo-3,5-diphenylisoxazole (3):[16] white solid (97.5 mg, 65%); mp 131–132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12–8.08 (m, 2H, ArH), 7.89–7.85 (m, 2H, ArH), 7.57–7.51 (m, 6H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 162.0, 130.6, 130.1, 128.8, 128.6, 128.5, 127.8, 127.0, 126.7, 89.4.



3,5-diphenyl-4-(phenylethynyl)isoxazole (4): yellow solid (61.1 mg, 76%); mp 90–92 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29–8.26 (m, 2H, ArH), 8.16–8.13 (m, 2H, ArH), 7.57–7.51 (m, 8H, ArH), 7.40–7.37 (m, 3H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 162.5, 131.3, 130.7, 130.2, 128.8, 128.8, 128.6, 128.5, 128.4, 127.8, 127.3, 126.4, 122.7, 97.3, 96.4, 79.7; HRMS-ESI (m/z): calcd for $C_{23}H_{16}NO$, $[M+H]^+$: 322.1226; found, 322.1223.



3,4,5-triphenylisoxazole (5):[17] white solid (63.2 mg, 85%); mp 212–214 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58–7.55 (m, 2H, ArH), 7.45–7.43 (m, 2H, ArH), 7.42–7.34 (m, 6H, ArH), 7.33–7.30 (m, 3H, ArH), 7.29–7.26 (m, 2H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 162.1, 130.5, 130.4, 129.7, 129.3, 129.0, 128.9, 128.6, 128.4, 128.4, 128.2, 127.8, 126.9, 115.2.

IV. References

(1) Kumar, G. R.; Kumar, Y. K.; Reddy, M. S. *Chem. Commun*. **2016**, *52*, 6589–6592.

(2) Harigae, R.; Moriyama, K.; Togo, H. *J. Org. Chem*. **2014**, *79*, 2049–2058.

(3) Praveen, C.; Kalyanasundaram, A.; Perumal, P. T. *Synlett* **2010**, 777–781.

(4) Goergen, C.; Mueller, T. J. J. *Chem. Heterocycl. Compd*. **2017**, *53*, 422–429.

(5) Wei, X.; Fang, J.; Hu, Y.; Hu, H. *Synthesis* **1992**, 1205–1206.

(6) Bandiera, T.; Grunanger, P.; Albini, F. M. *J. Heterocycl. Chem.* **1992**, *29*, 1423–1428.

(7) Chrisope, D. R. ; Keel, R. A. ; Baumstark, A. L. ; Boykin, D. W. *J. Heterocycl. Chem.* **1981***, 18,* 795–798.

(8) Yoshimura, A.; Middleton, K. R.; Todora, A. D.; Kastern, B. J.; Koski, S. R.; Maskaev, A. V.; Zhdankin, V. V. *Org. Lett*. **2013**, *15*, 4010–4013.

(9) Das, B.; Holla, H.; Srinivas, Y.; Tirupathi, P.; Venkateswarlu, K. *Indian J. Heterocycl. Chem.* **2007**, *17*, 173–176.

(10) Tang, S.; He, J.; Sun, Y.; He, L.; She, X. *Org. Lett*. **2009**, *11*, 3982–3985.

(11) Jawalekar, A. M.; Reubsaet, E.; Rutjes, F. P. J. T.; Van Delft, F. L. *Chem. Commun*. **2011**, *47*, 3198–3200.

(12) Sammour, A.; Afify, A. A.; Hassan, M. A.; Abdel-Ghany, A. R. *Egypt. J. Chem*. **1978**, *19*, 601–620.

(13) Rosa, R. D.; Moraes, H. D. M.; Zimmermann, L. A.; Schenkel, E. P.; Steindel, M.; Bernardes, L. S. C. *Eur. J. Med. Chem*. **2017**, *128*, 25–35.

(14) Pusch, S.; Kowalczyk, D.; Opatz, T. *J. Org. Chem*. **2016**, *81*, 4170–4178.

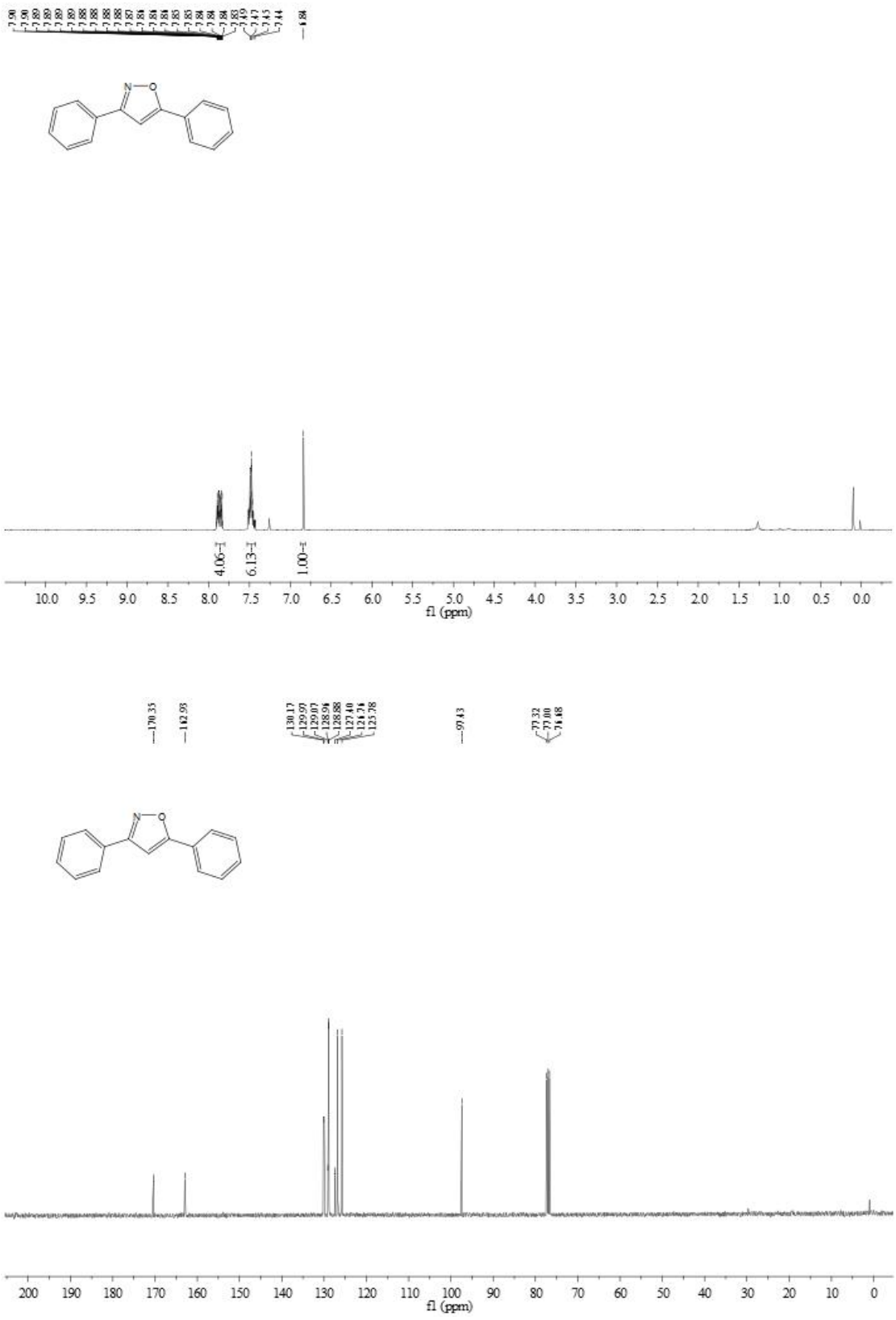
(15) Pusch S.; Opatz T. *Org. Lett*. **2014**, *16*, 5430–5433.

(16) Waldo, J. P.; Larock, R. C. *J. Org. Chem.* **2007**, *72*, 9643–9647.

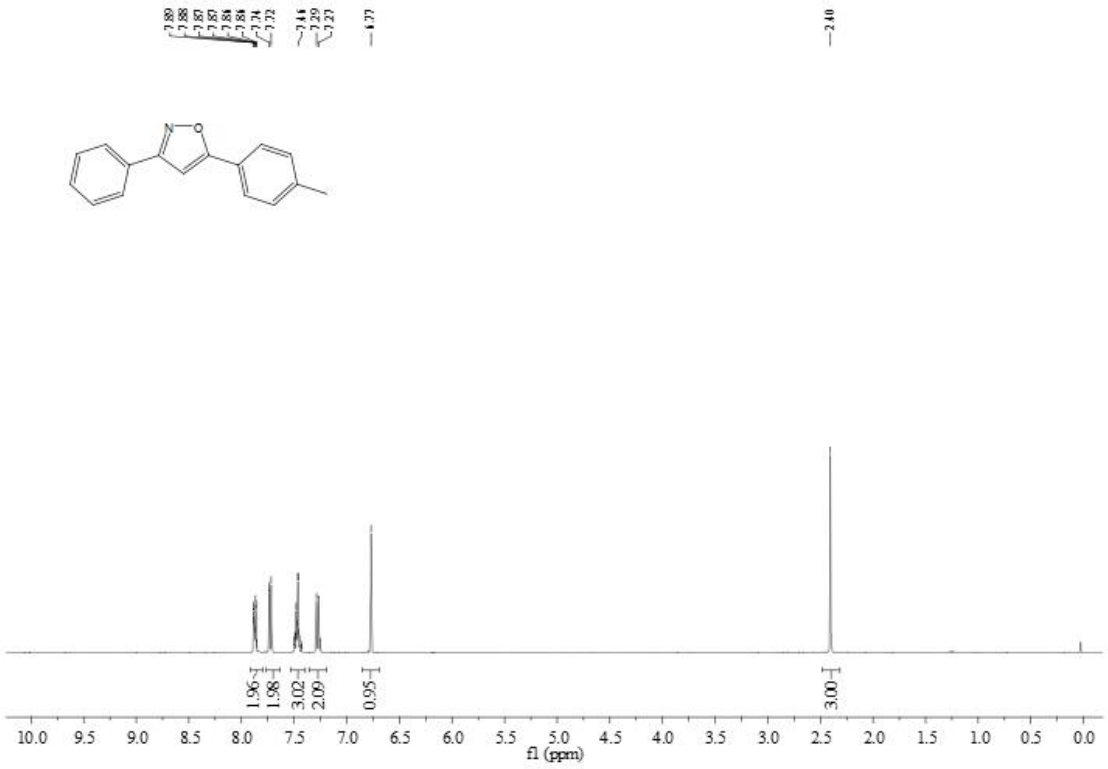
(17) Zhu, X.; Wang, Y. F.; Ren, W.; Zhang, F. L.; Chiba, S. *Org. Lett*. **2013**, *15*, 3214–3217.

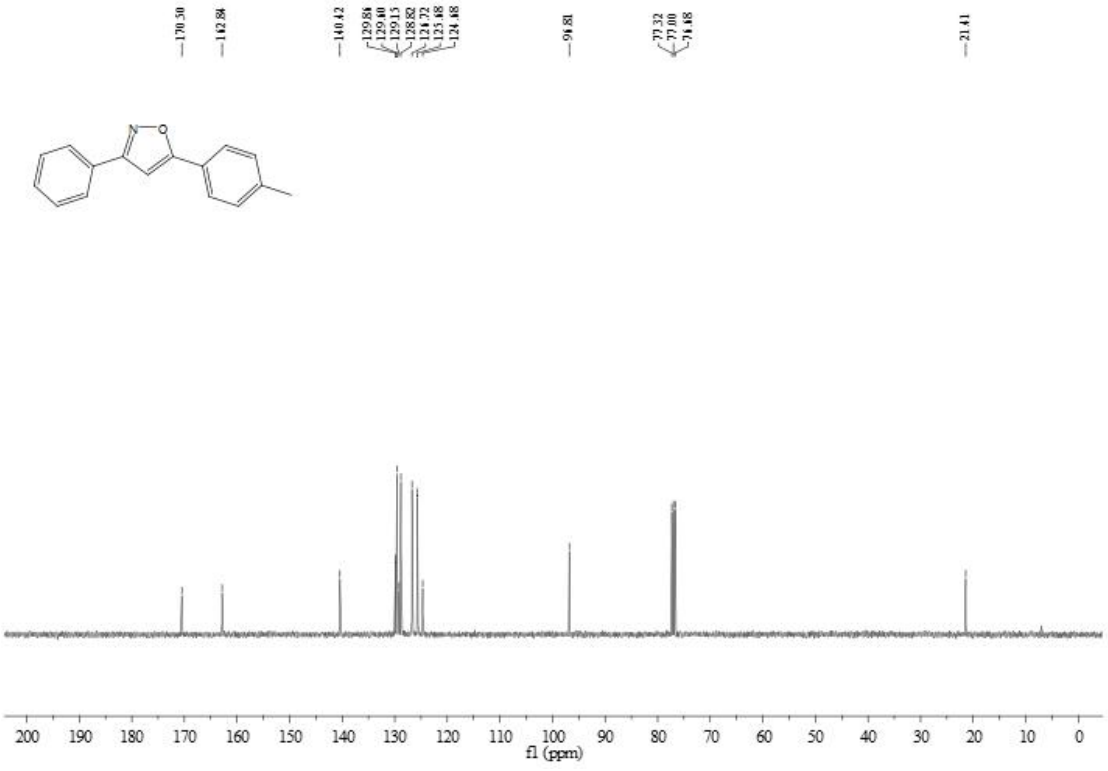
V. ^{1}H and ^{13}C NMR spectra of compounds 2,3,4,5

^{1}H and ^{13}C NMR spectra of compound 2aa



^{1}H and ^{13}C NMR spectra of compound 2ab





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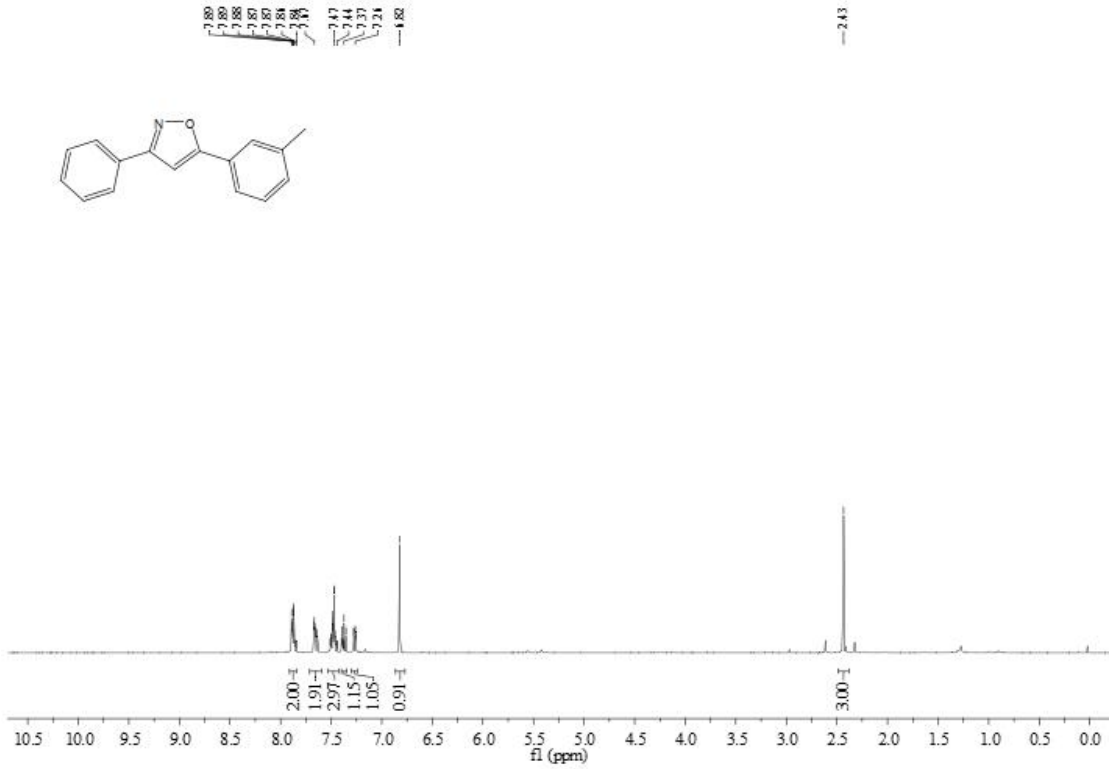
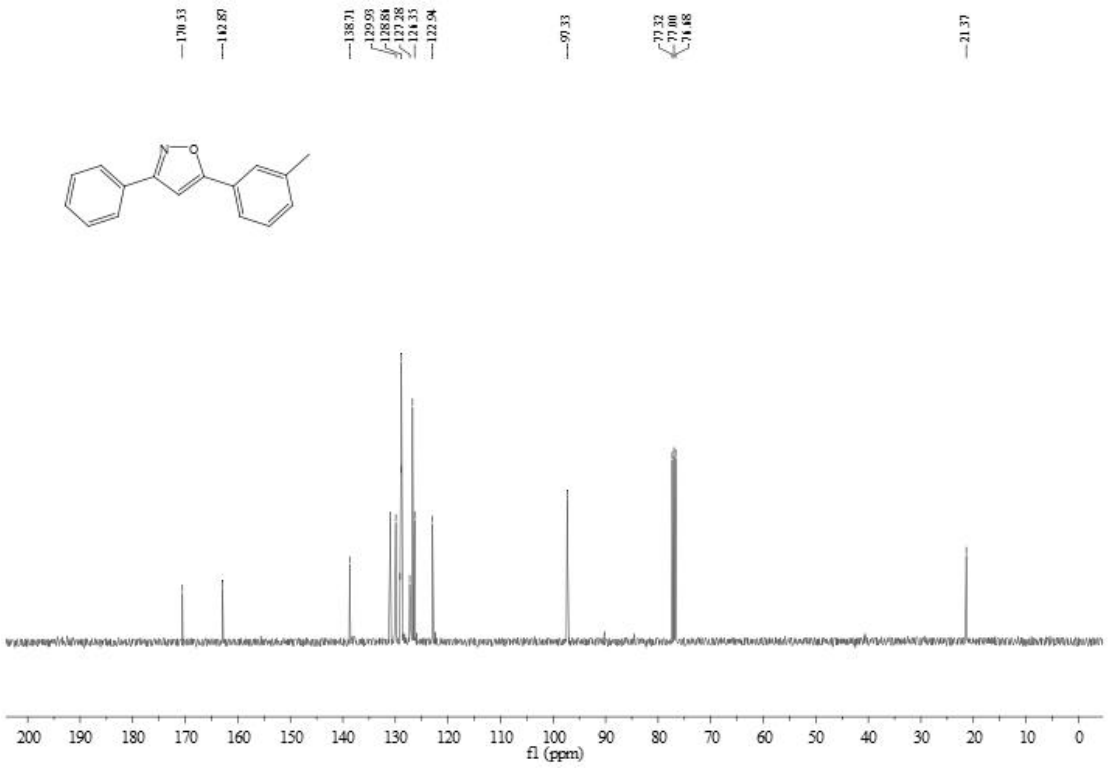
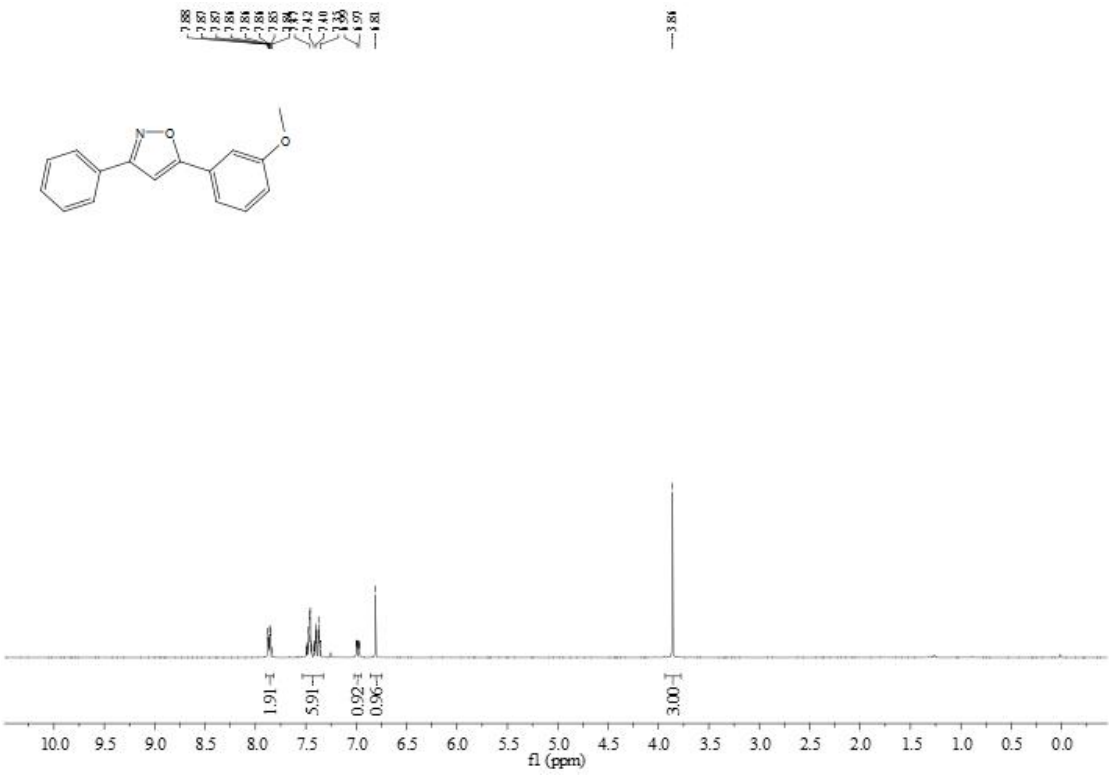
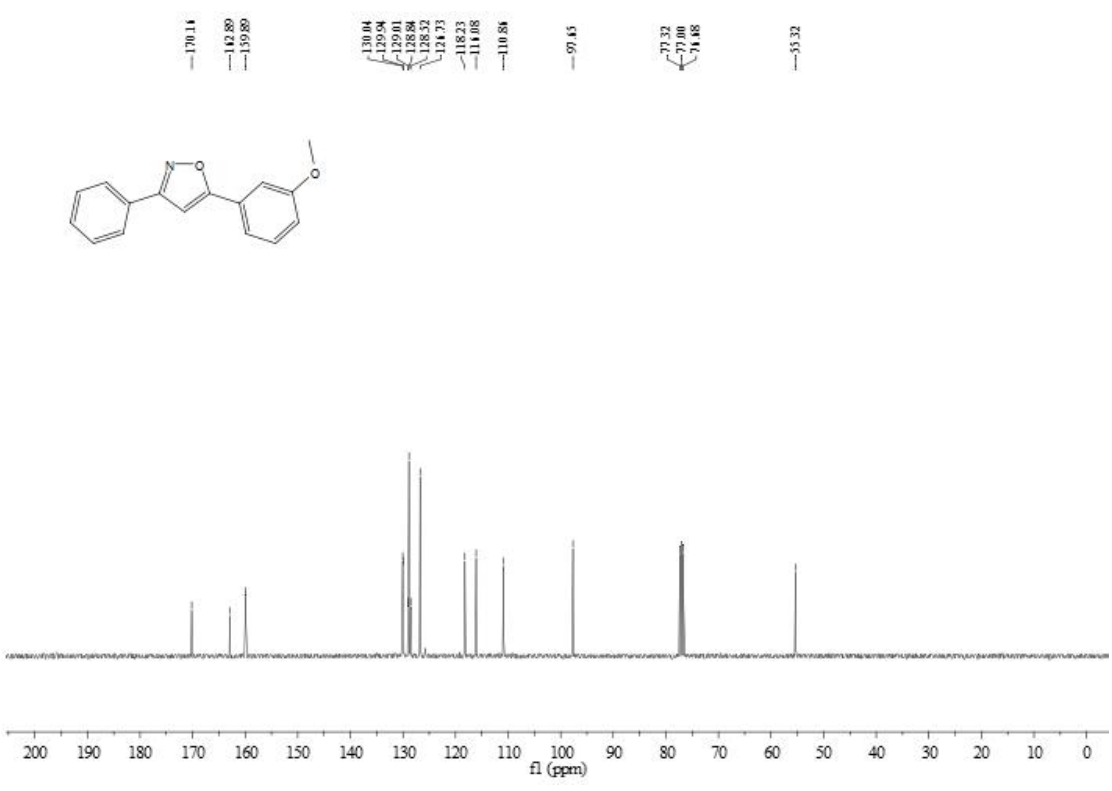




^{1}H and ^{13}C NMR spectra of compound 2ad





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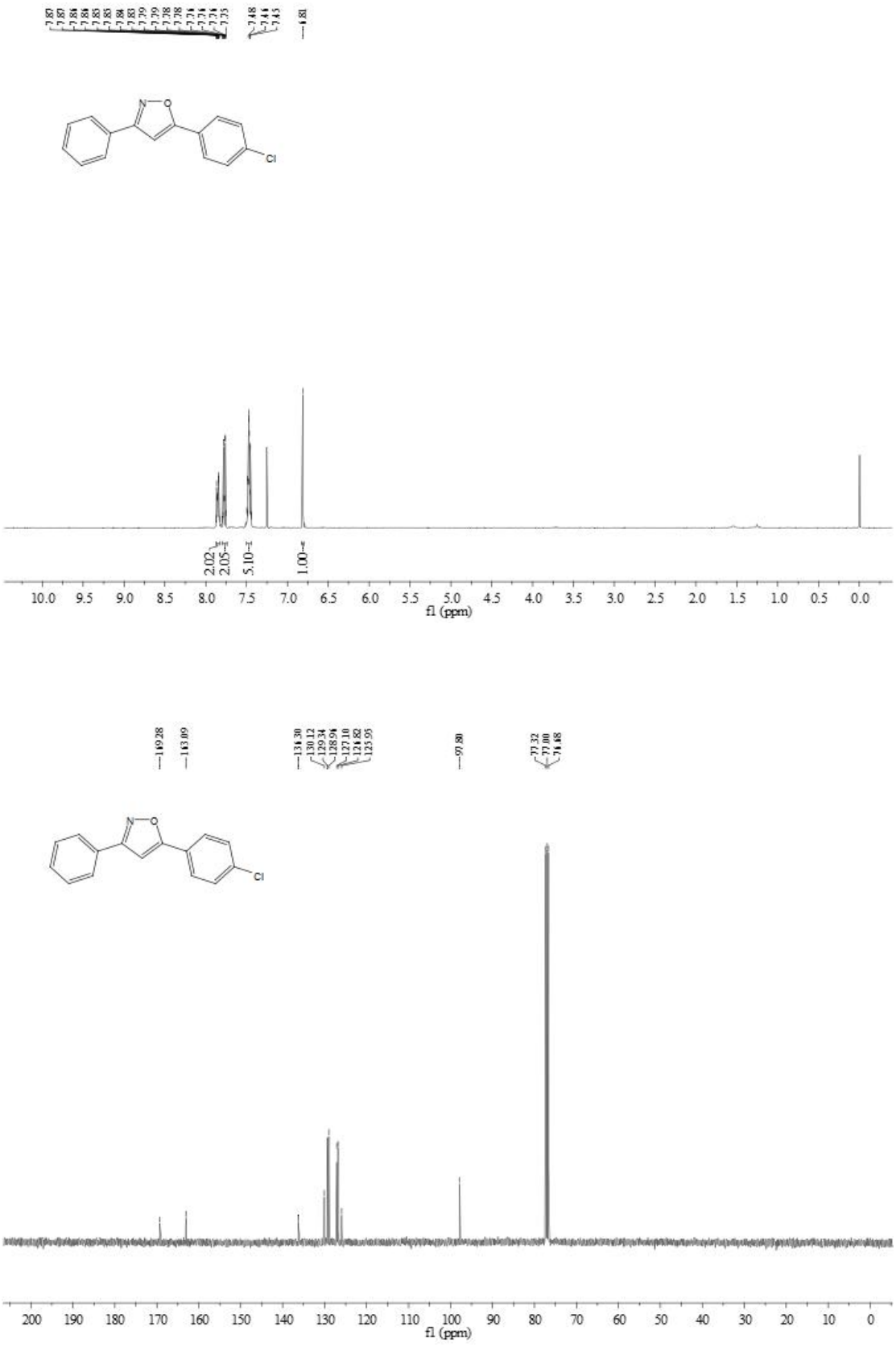
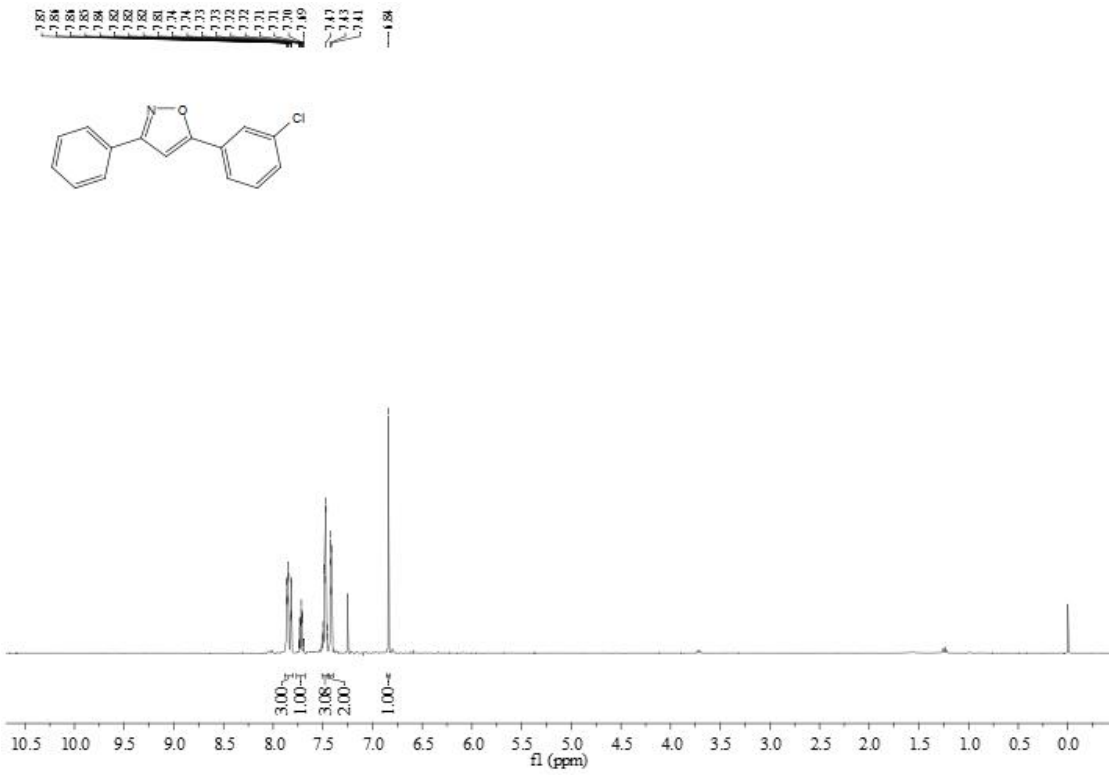
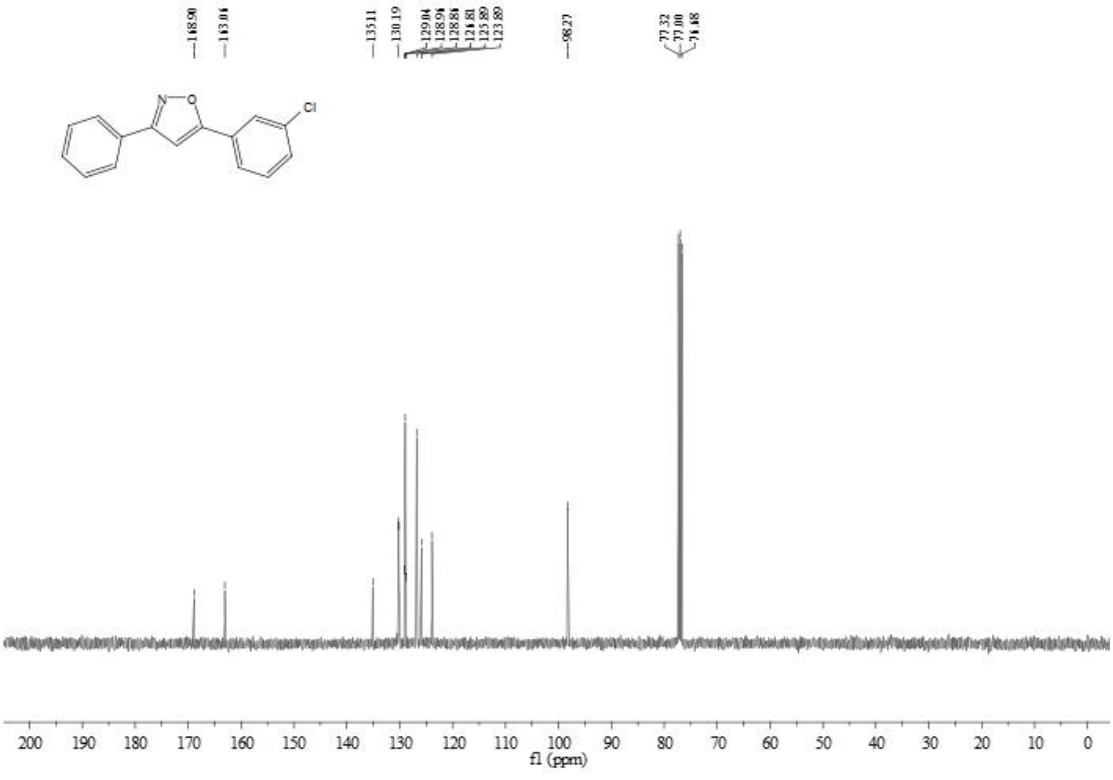
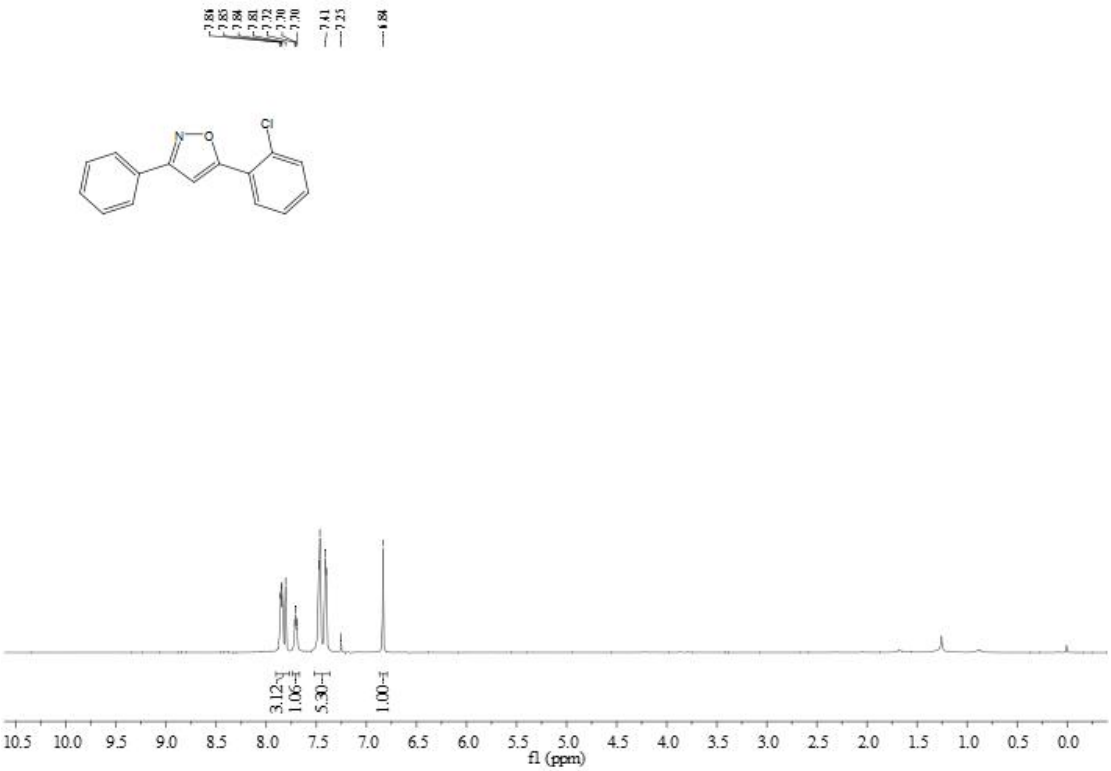


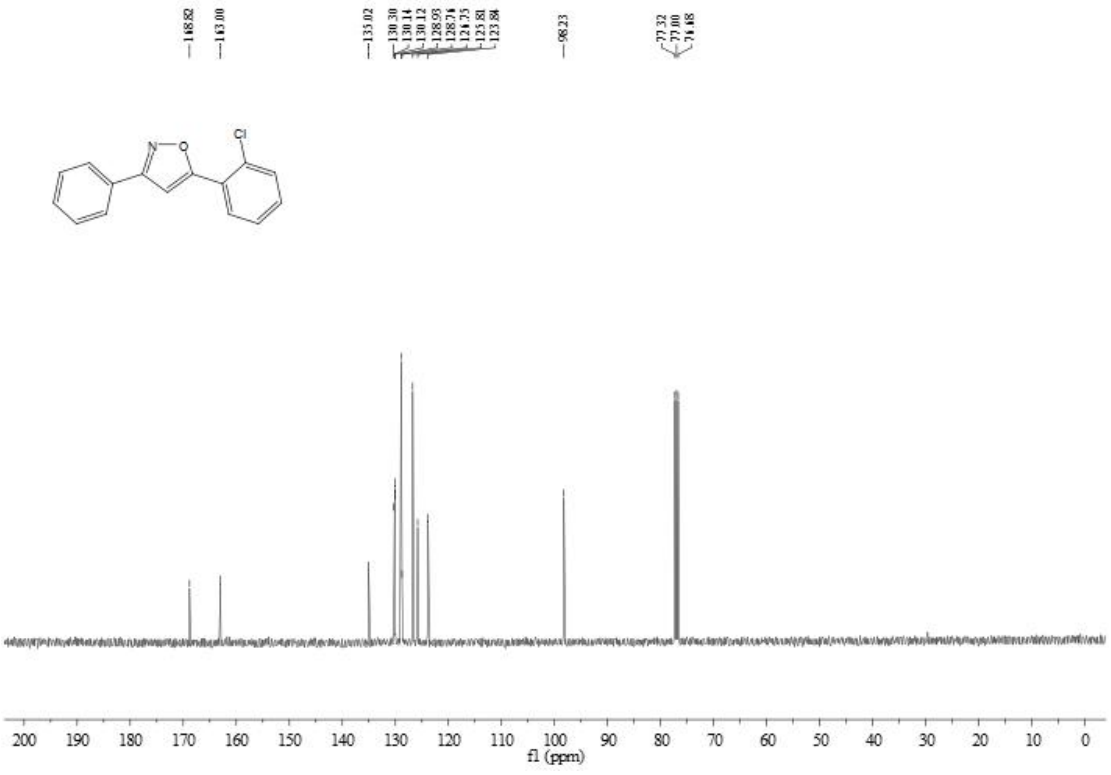
^{1}H and ^{13}C NMR spectra of compound 2af



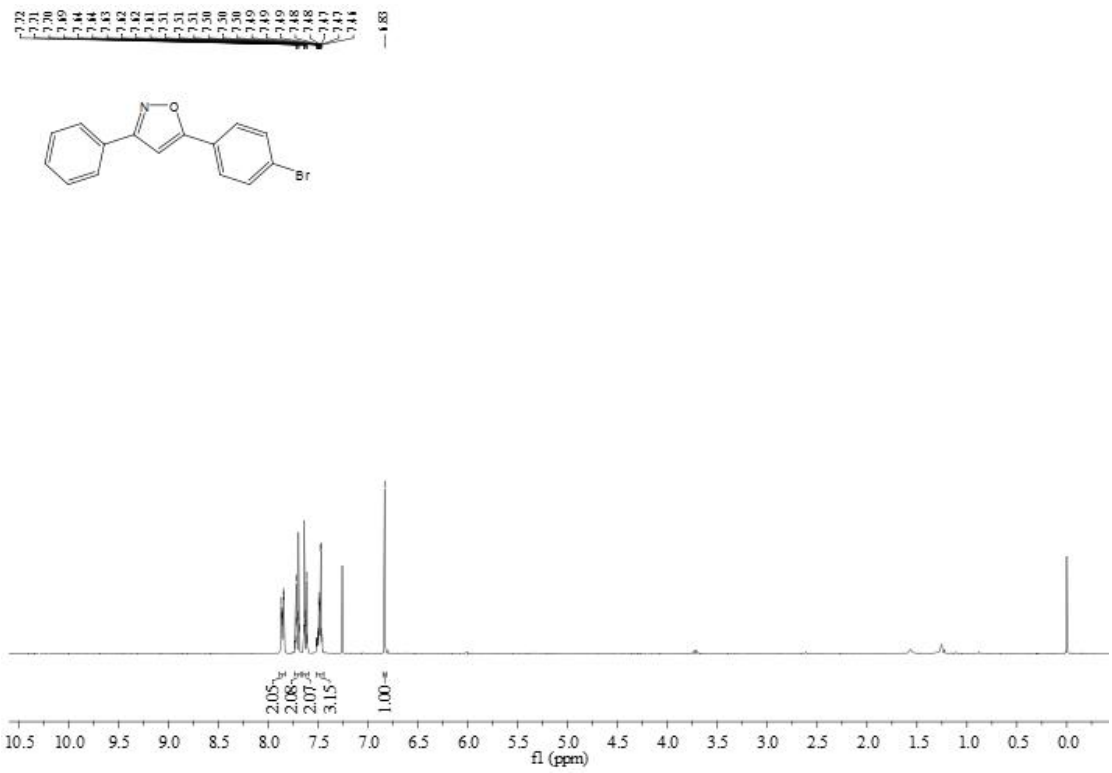


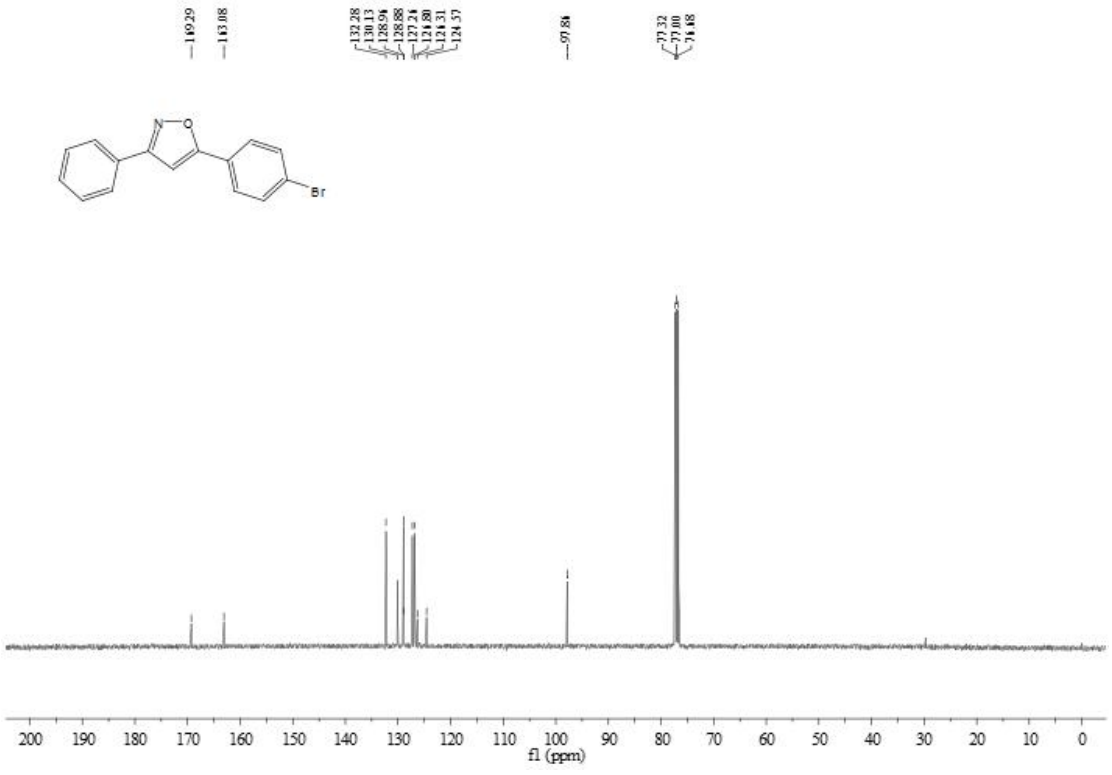
^{1}H and ^{13}C NMR spectra of compound 2ag



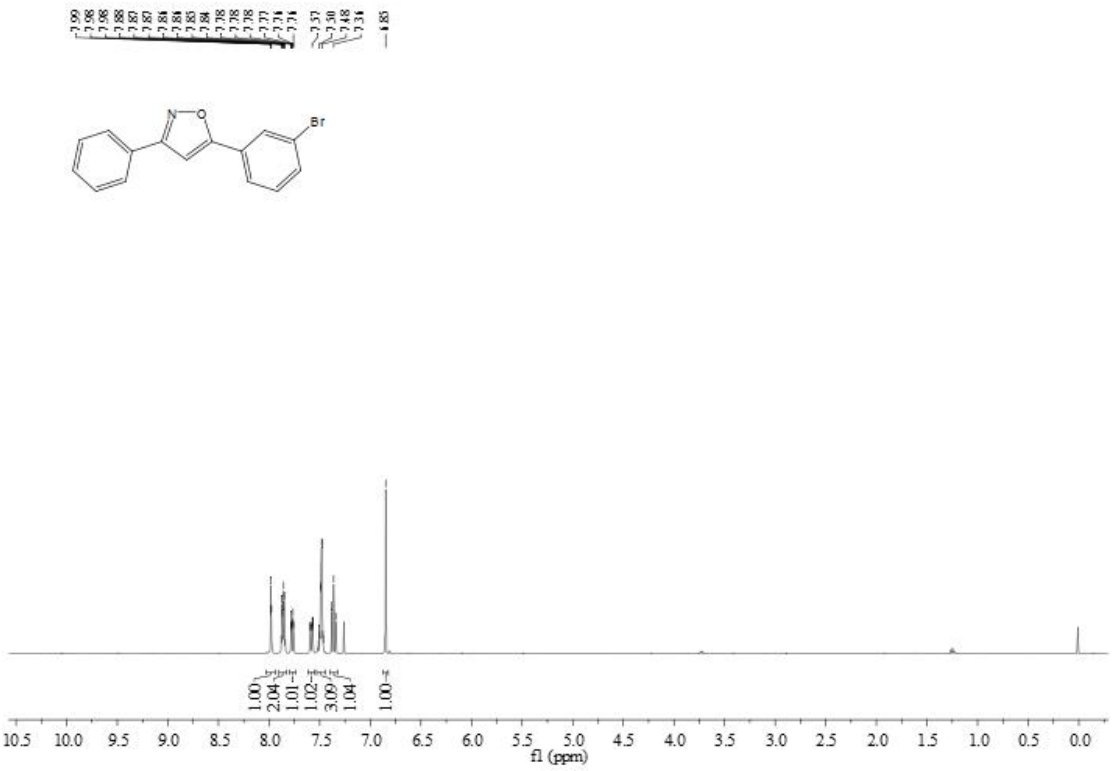


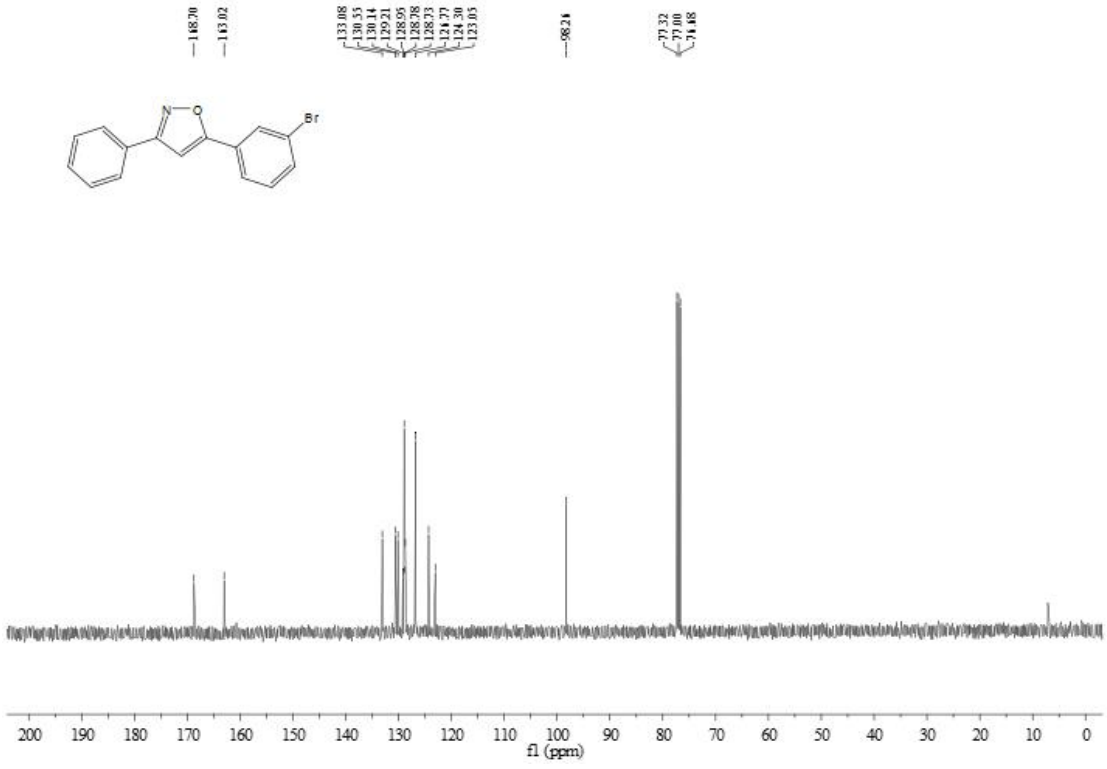
^{1}H and ^{13}C NMR spectra of compound 2ah



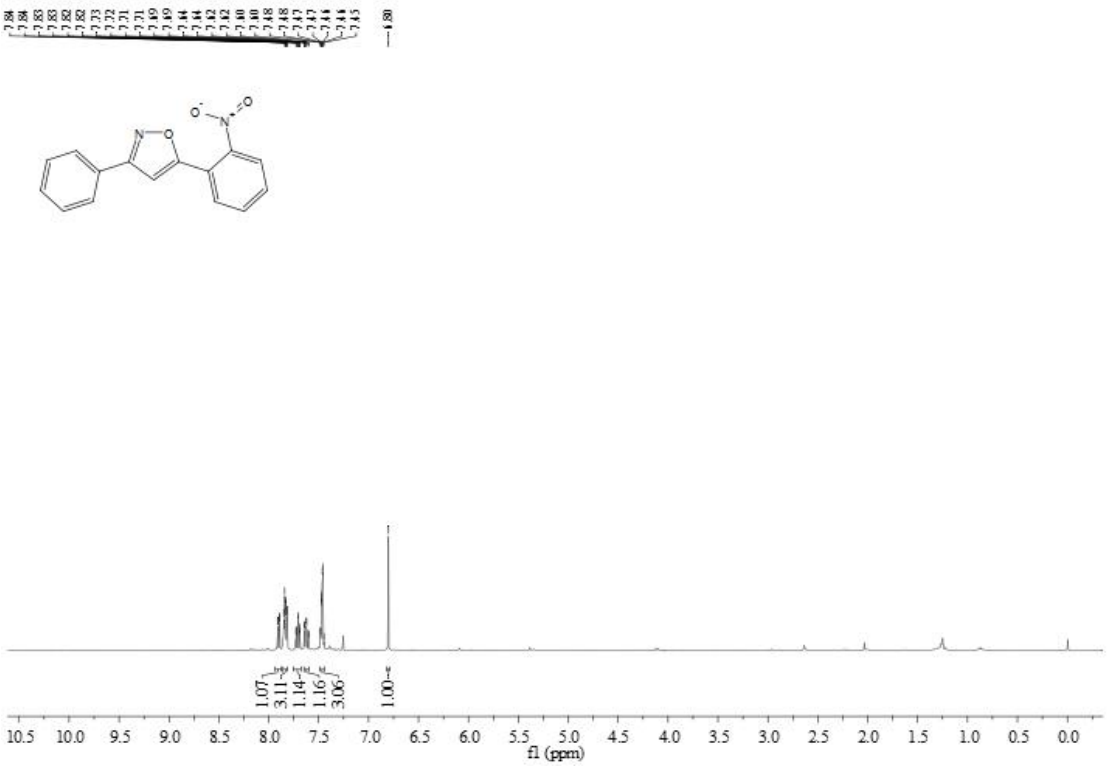


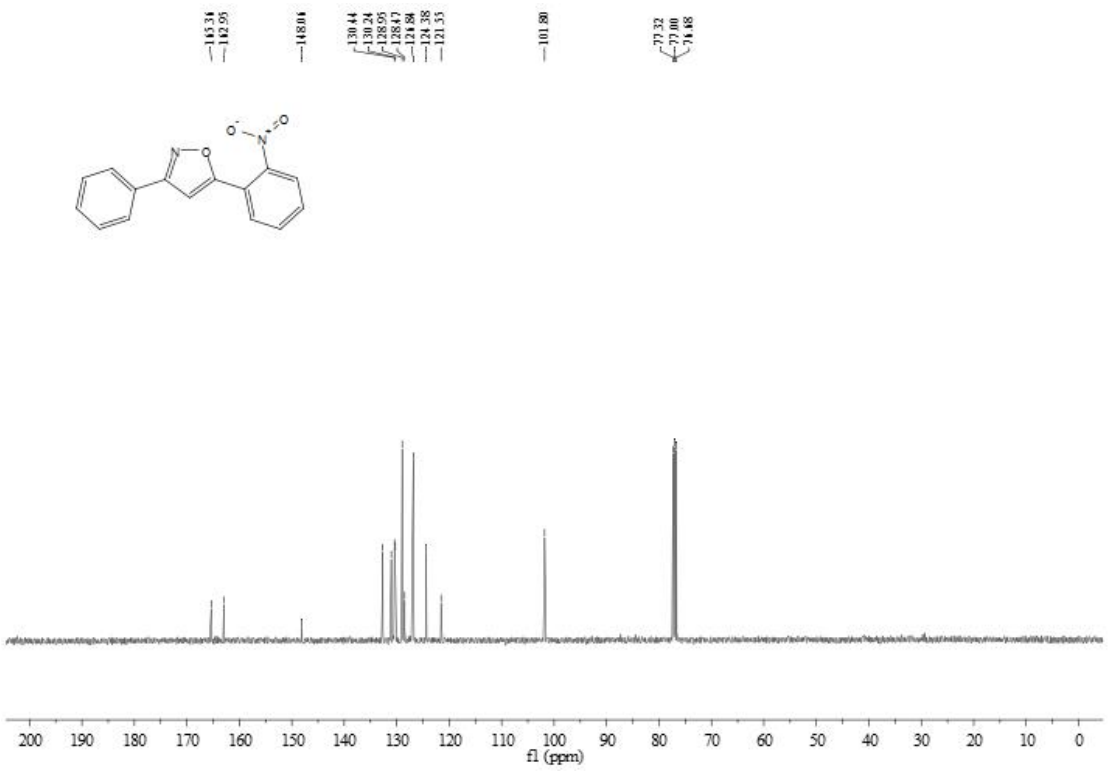
^{1}H and ^{13}C NMR spectra of compound 2ai



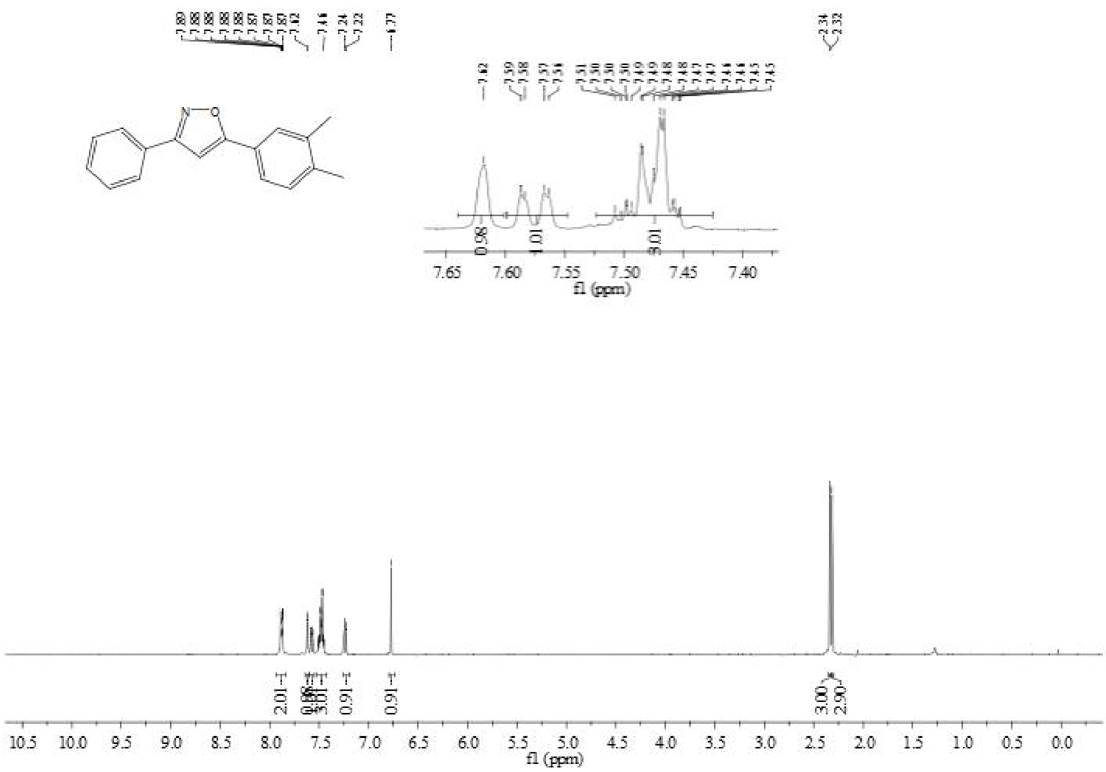


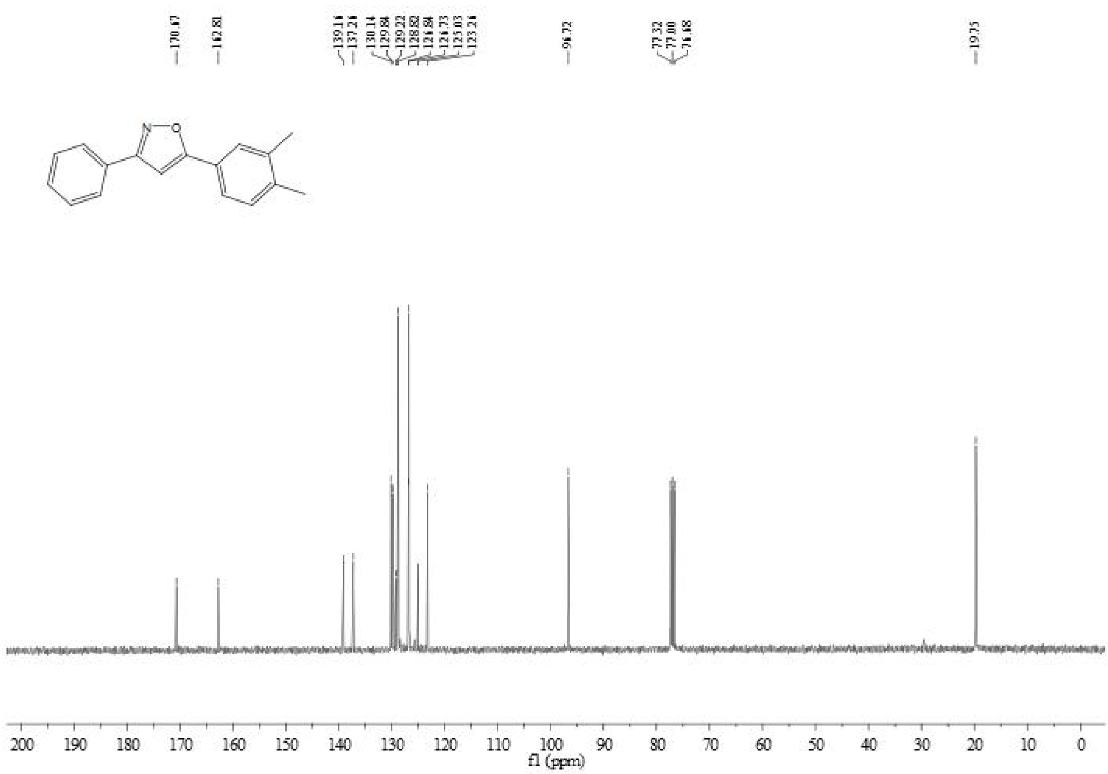
^{1}H and ^{13}C NMR spectra of compound 2aj



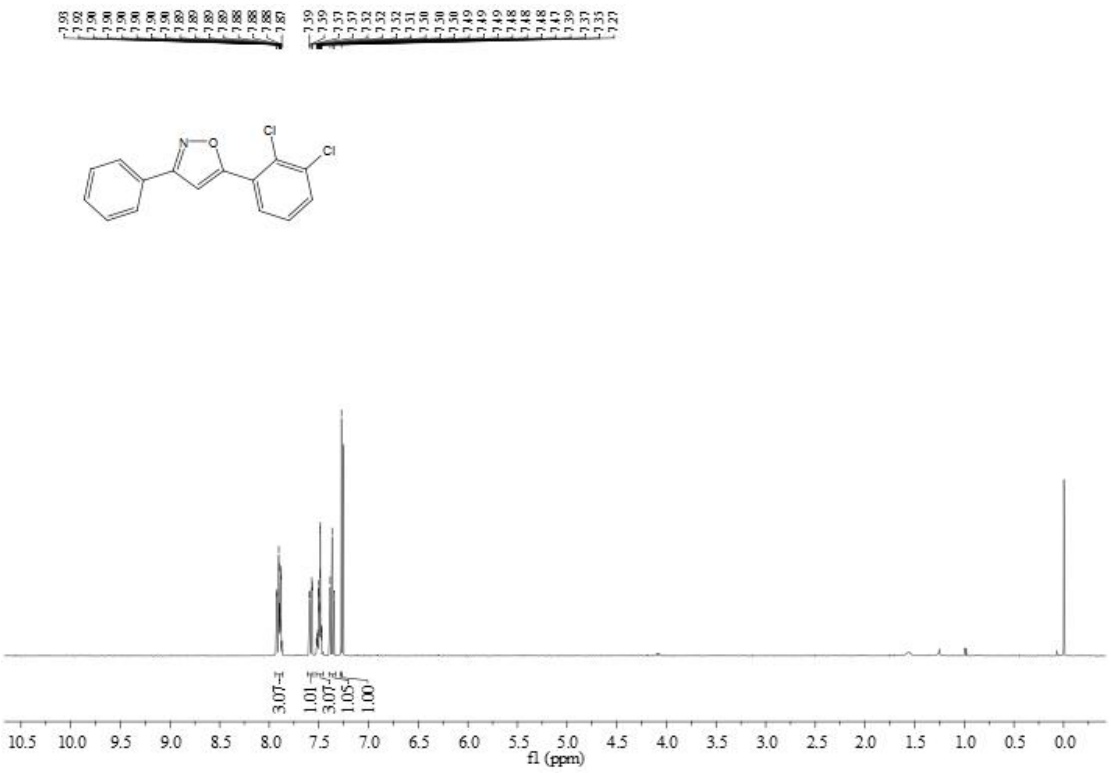


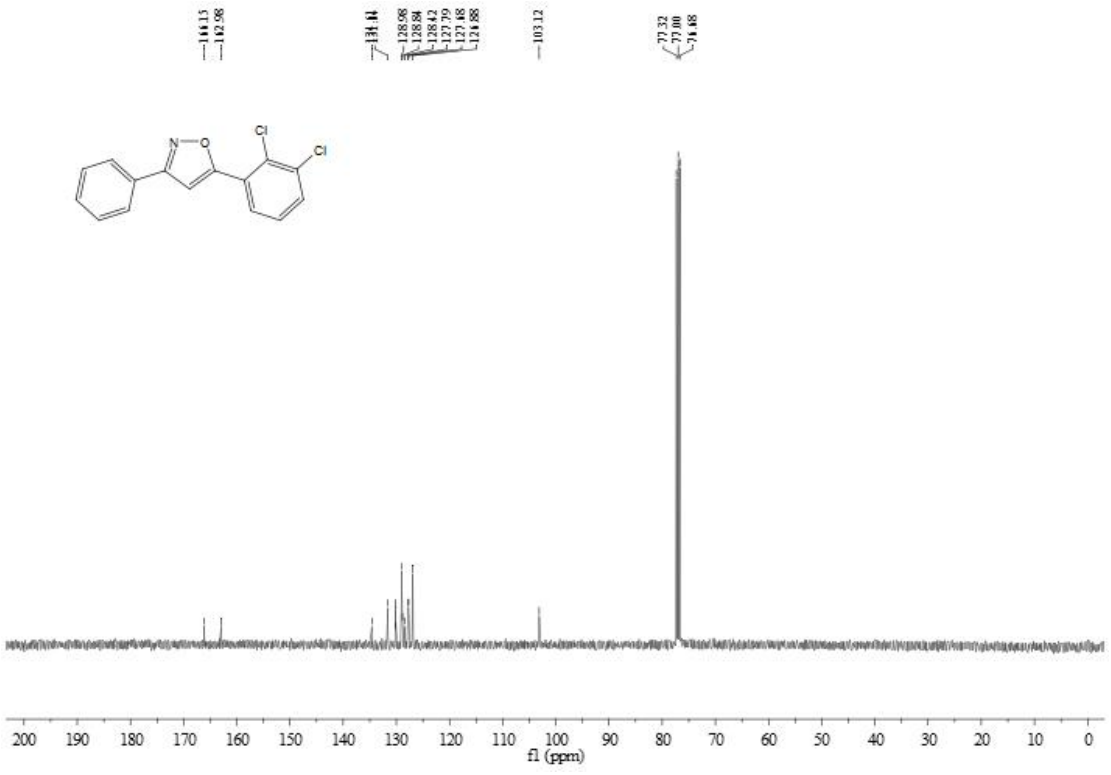
^{1}H and ^{13}C NMR spectra of compound 2ak



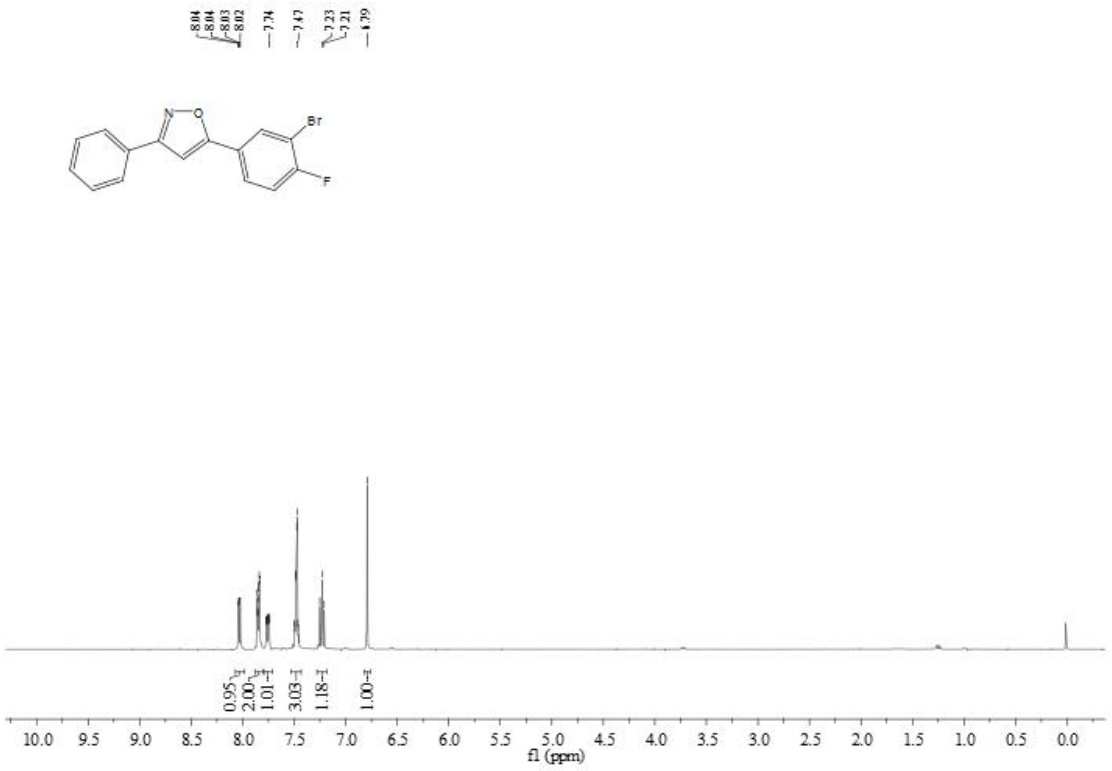


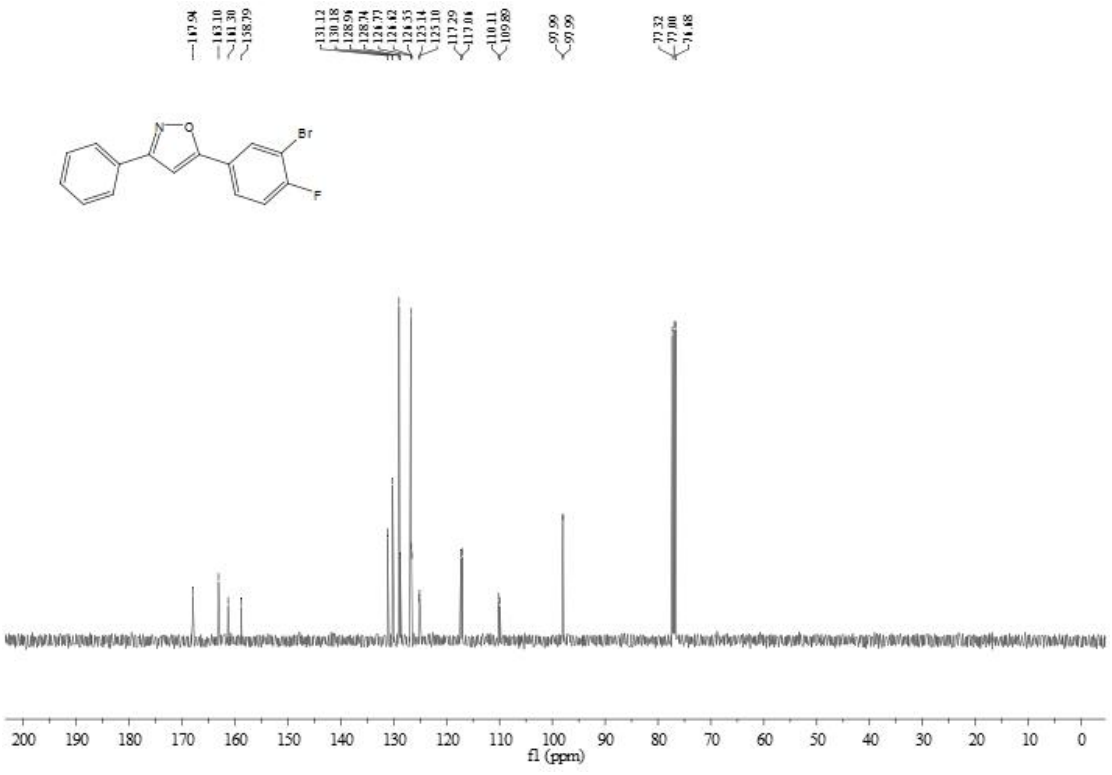
^{1}H and ^{13}C NMR spectra of compound 2al



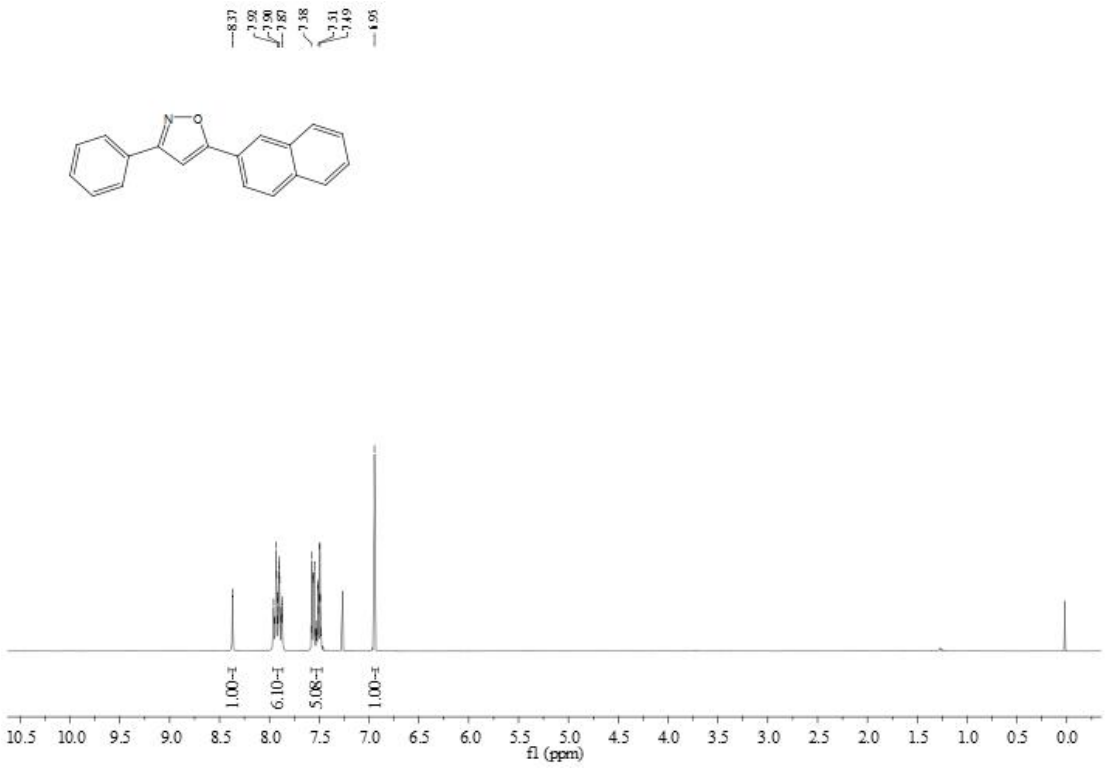


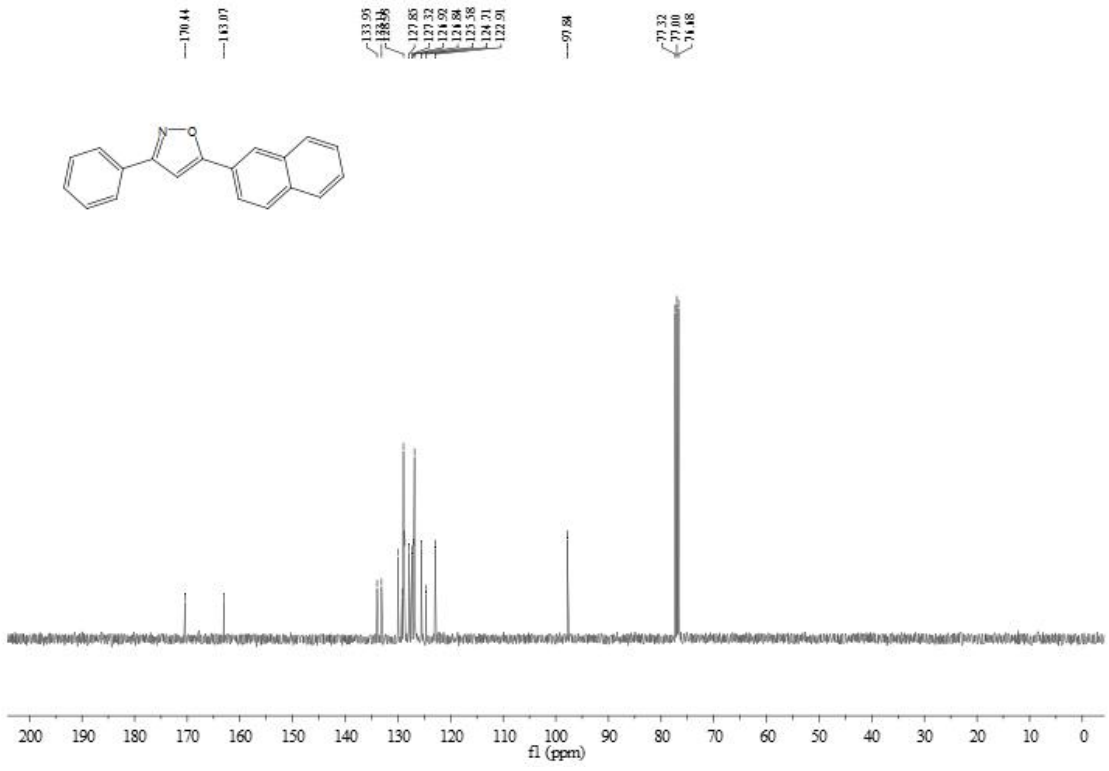
^{1}H and ^{13}C NMR spectra of compound 2am



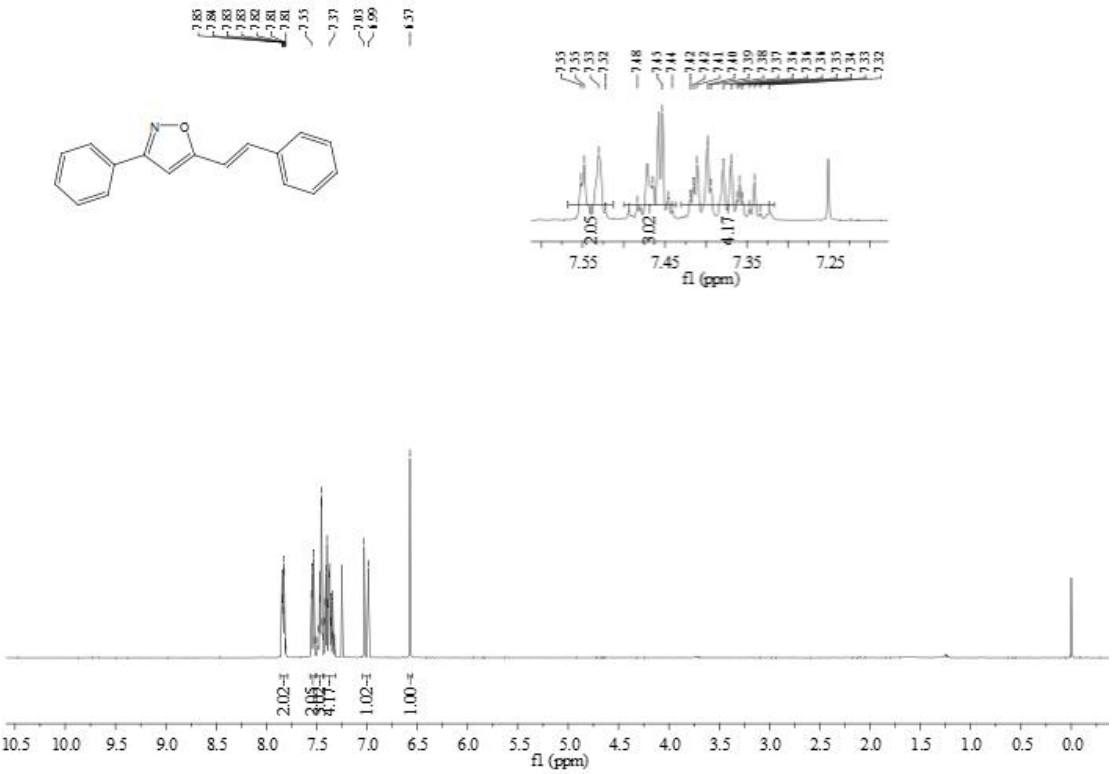


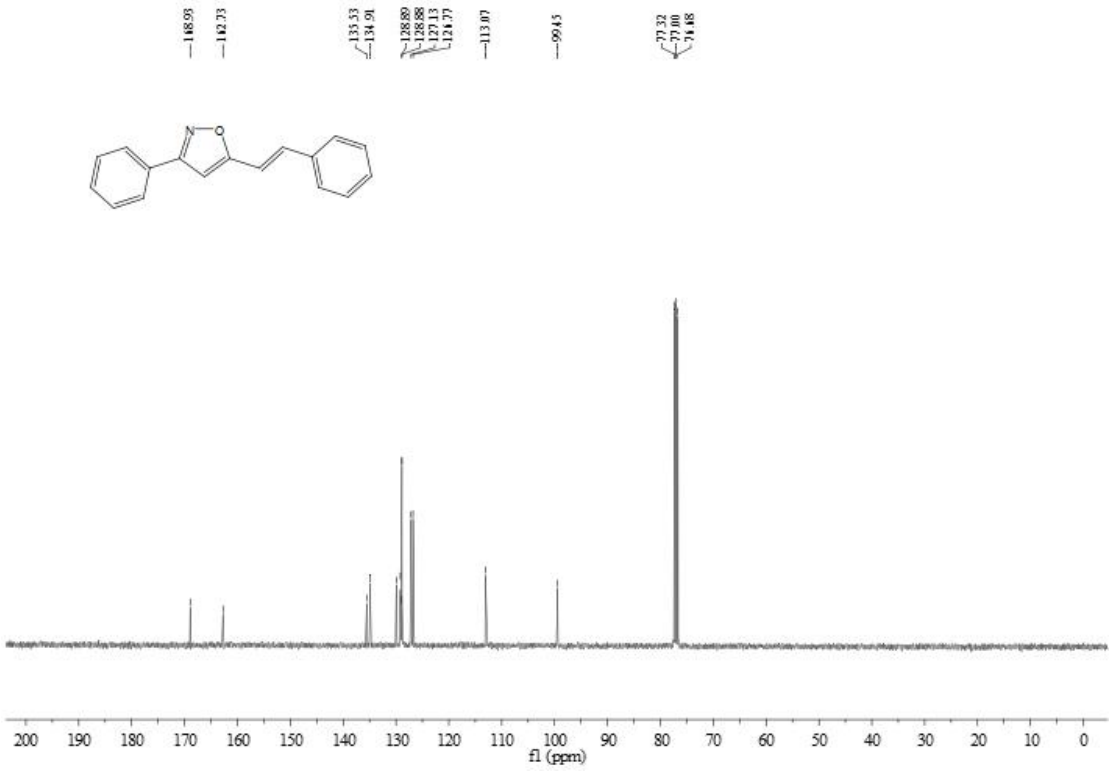
^{1}H and ^{13}C NMR spectra of compound 2an



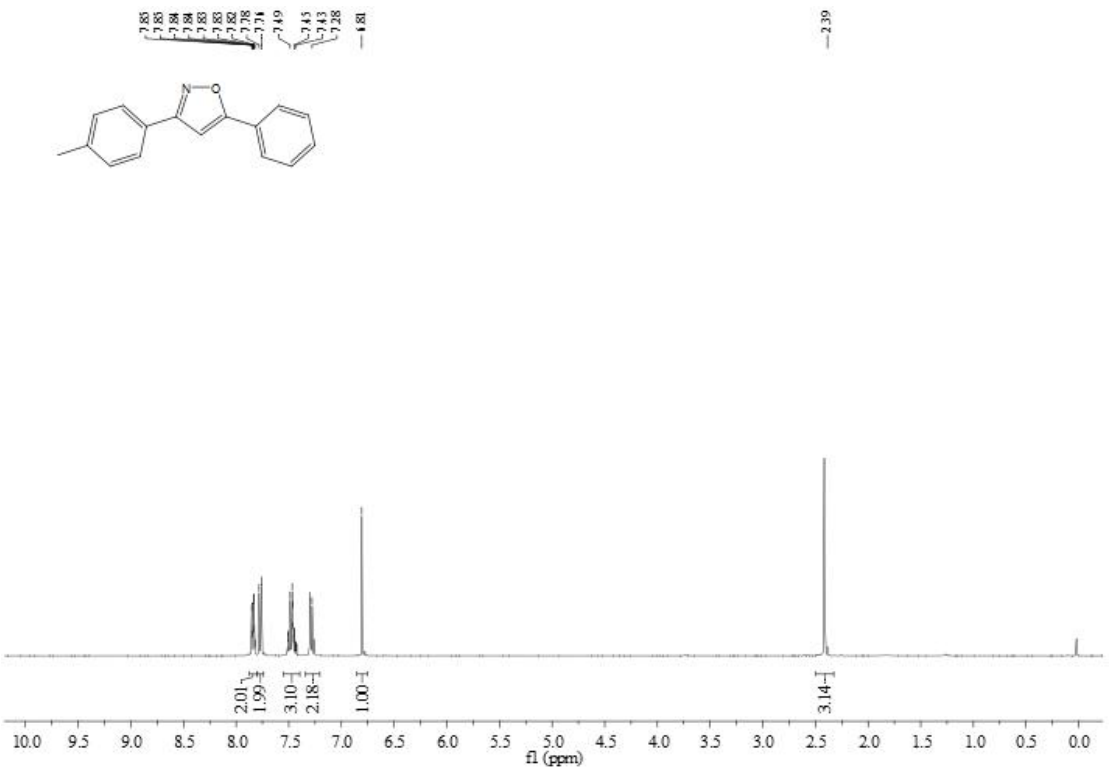


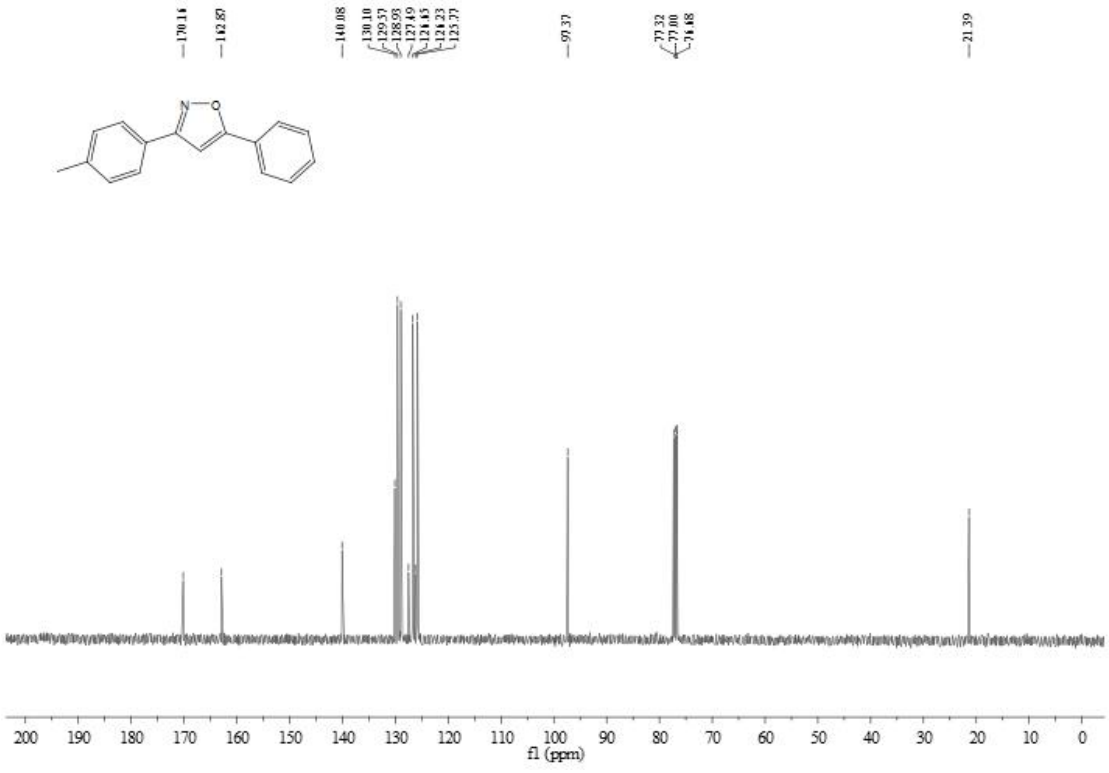
^{1}H and ^{13}C NMR spectra of compound 2ao



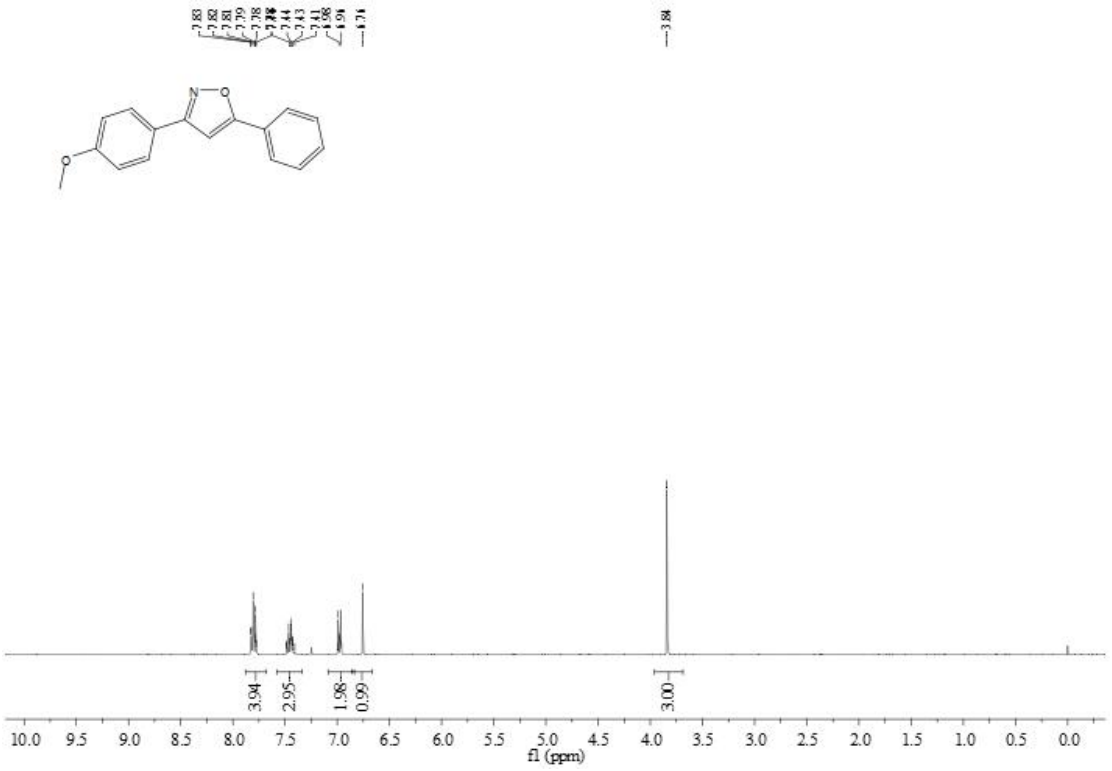


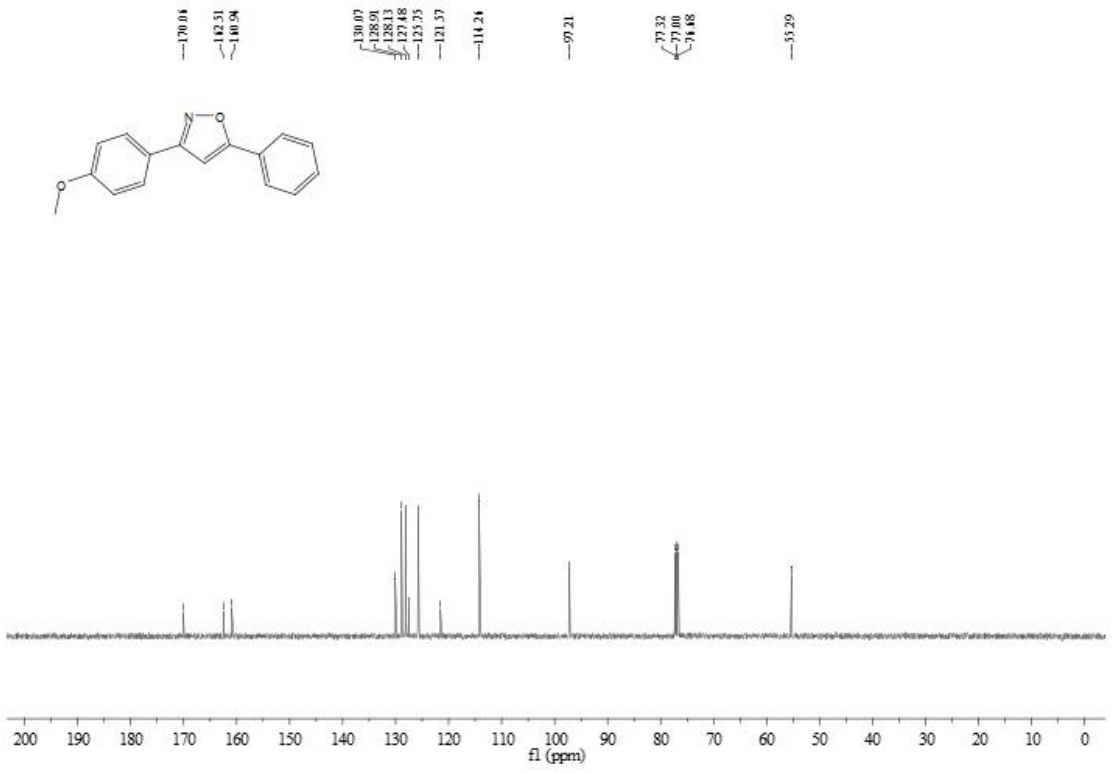
^{1}H and ^{13}C NMR spectra of compound 2ba



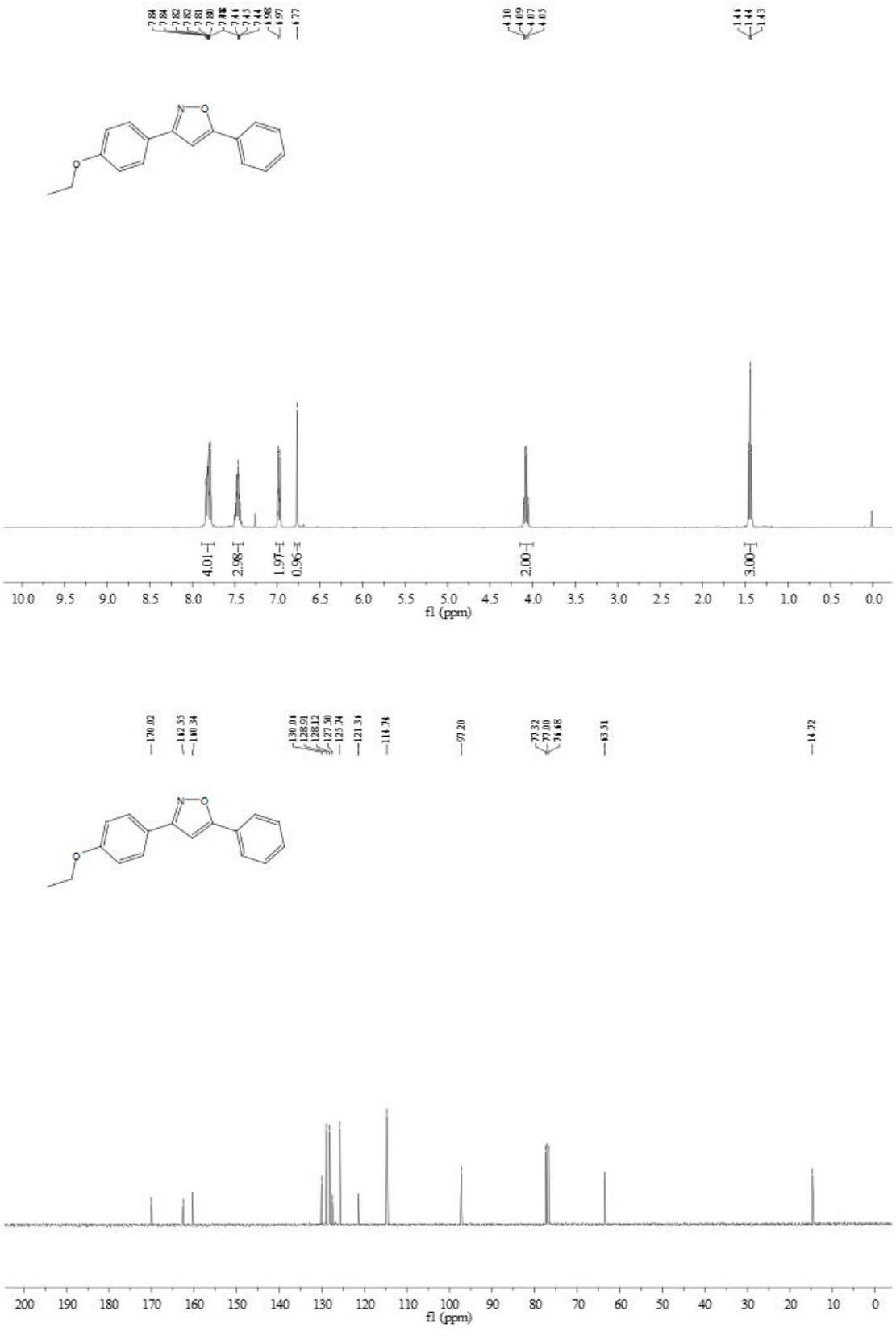


^{1}H and ^{13}C NMR spectra of compound 2ca

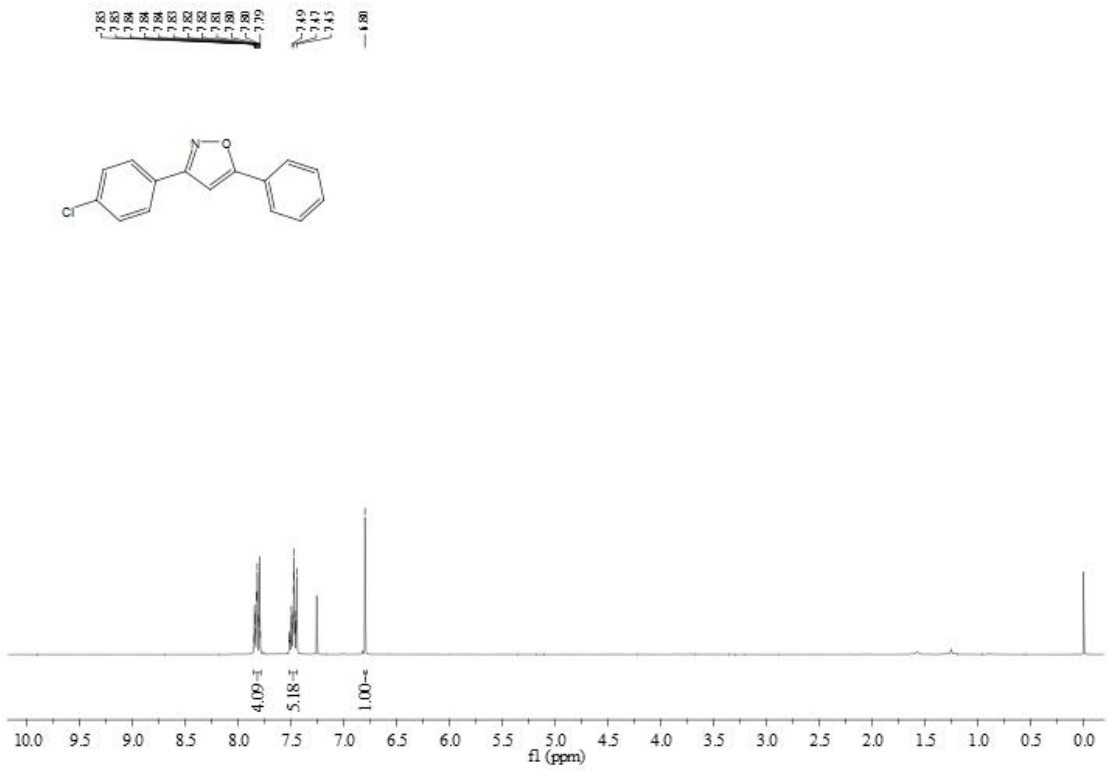


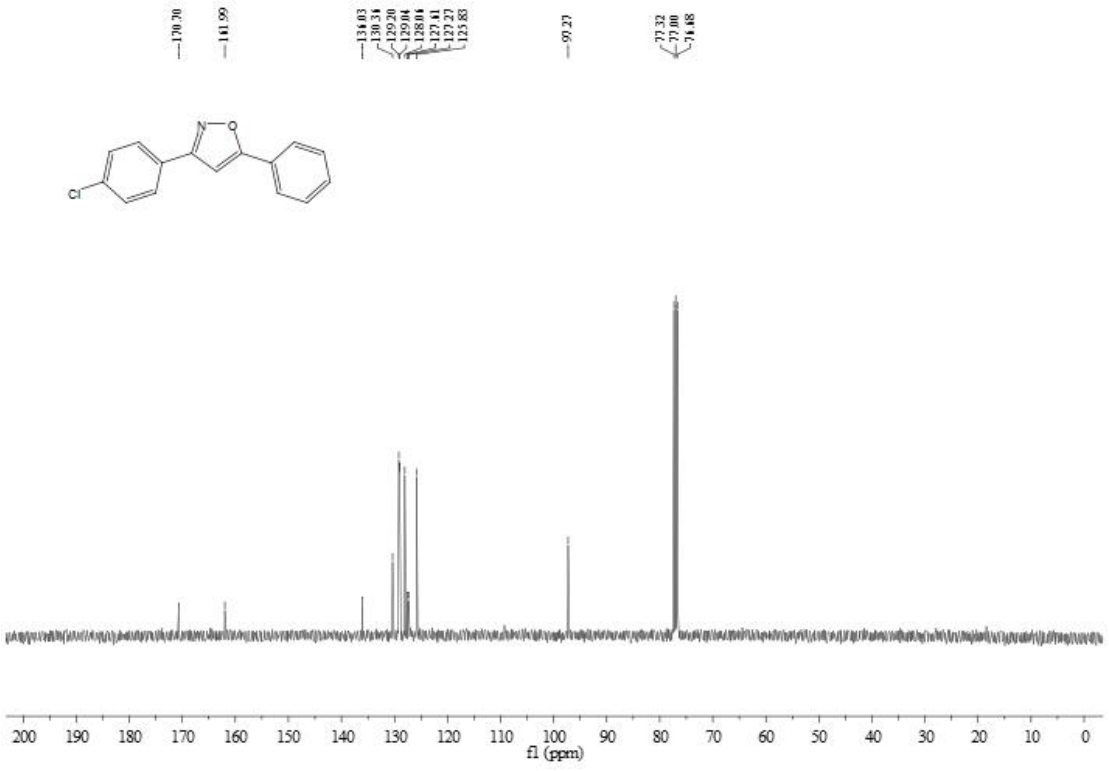


^{1}H and ^{13}C NMR spectra of compound 2da

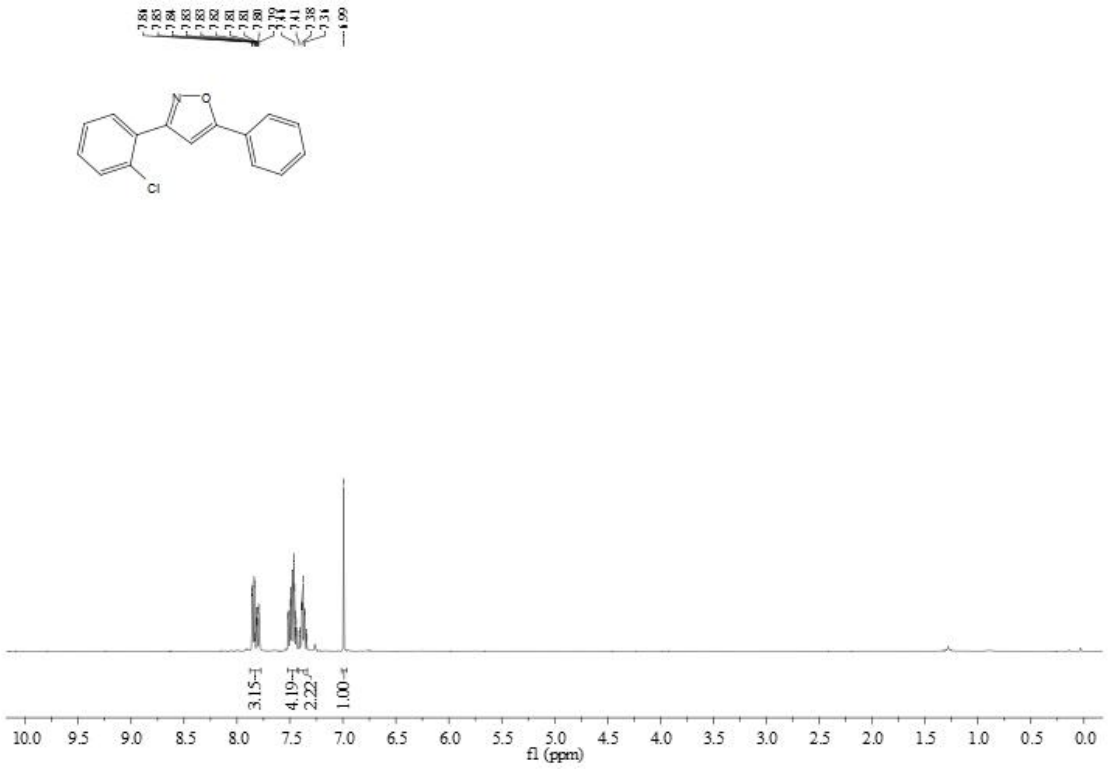


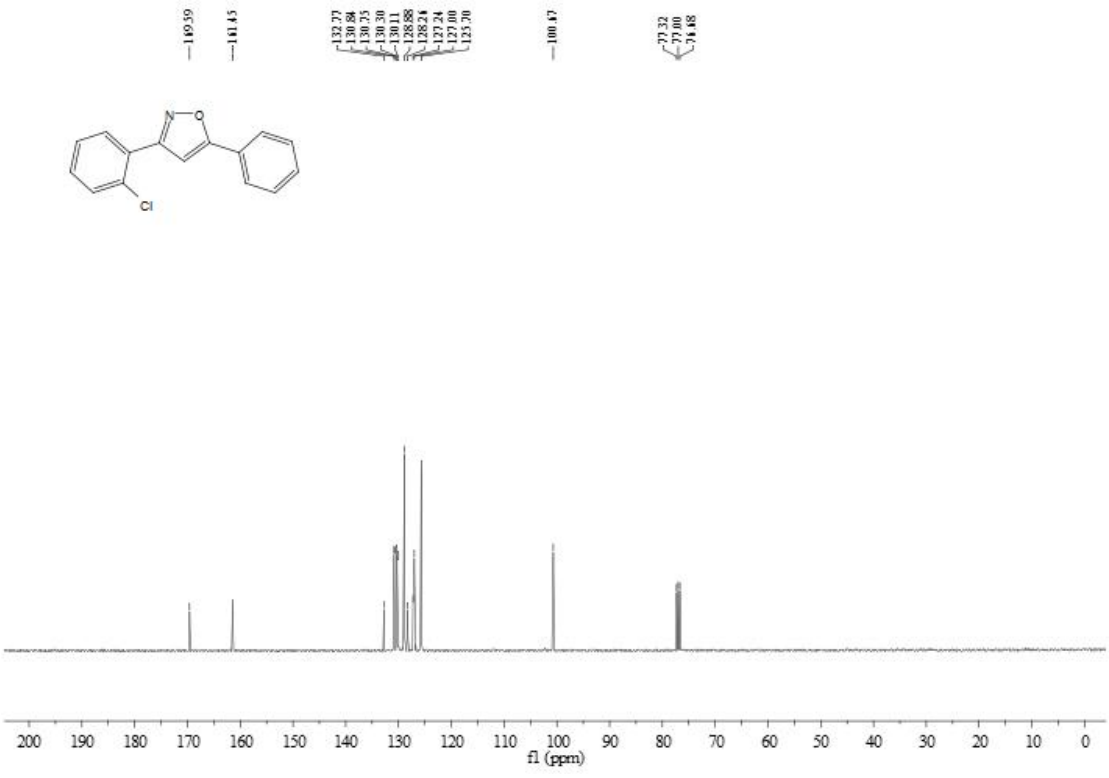
^{1}H and ^{13}C NMR spectra of compound 2ea



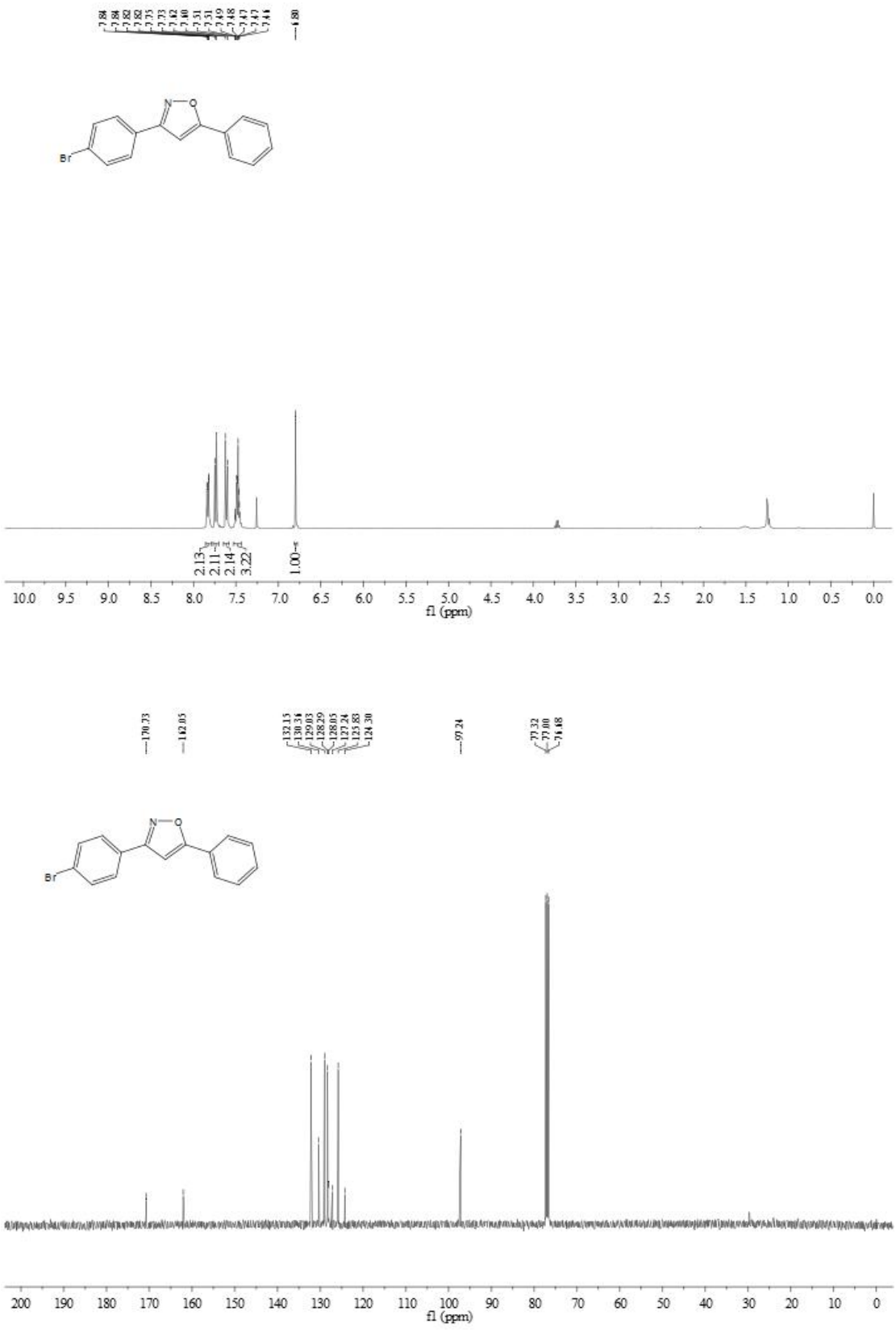


^{1}H and ^{13}C NMR spectra of compound 2fa

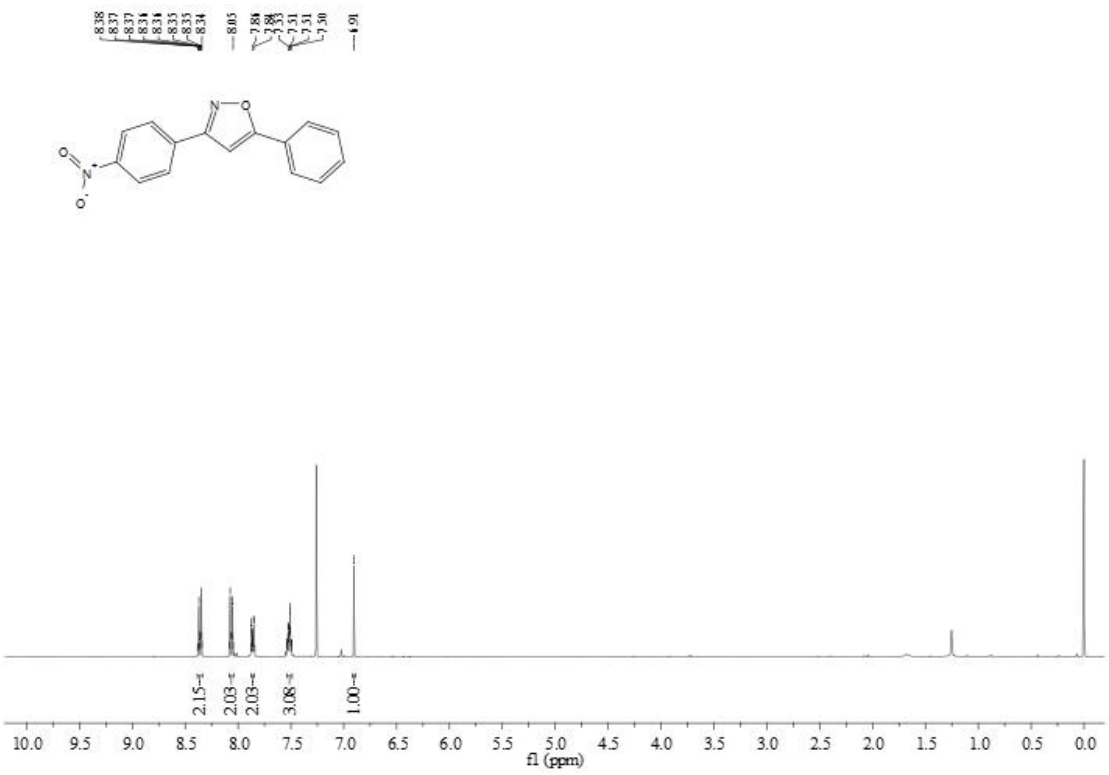


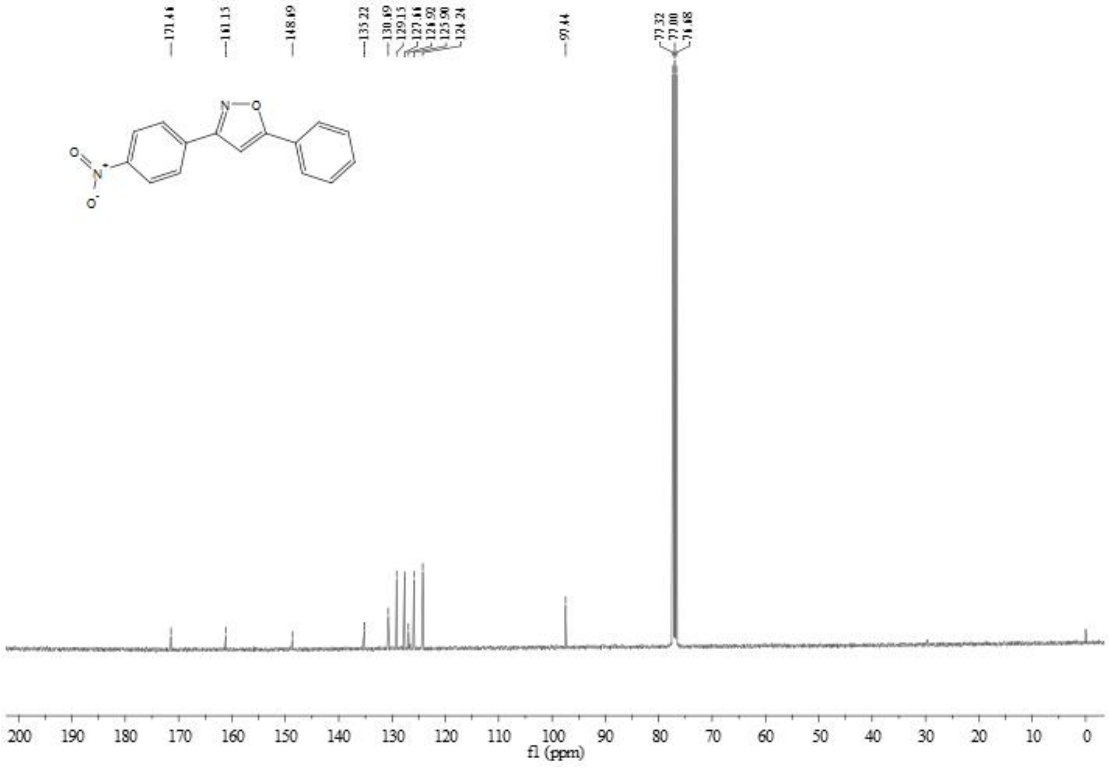


^{1}H and ^{13}C NMR spectra of compound 2ga

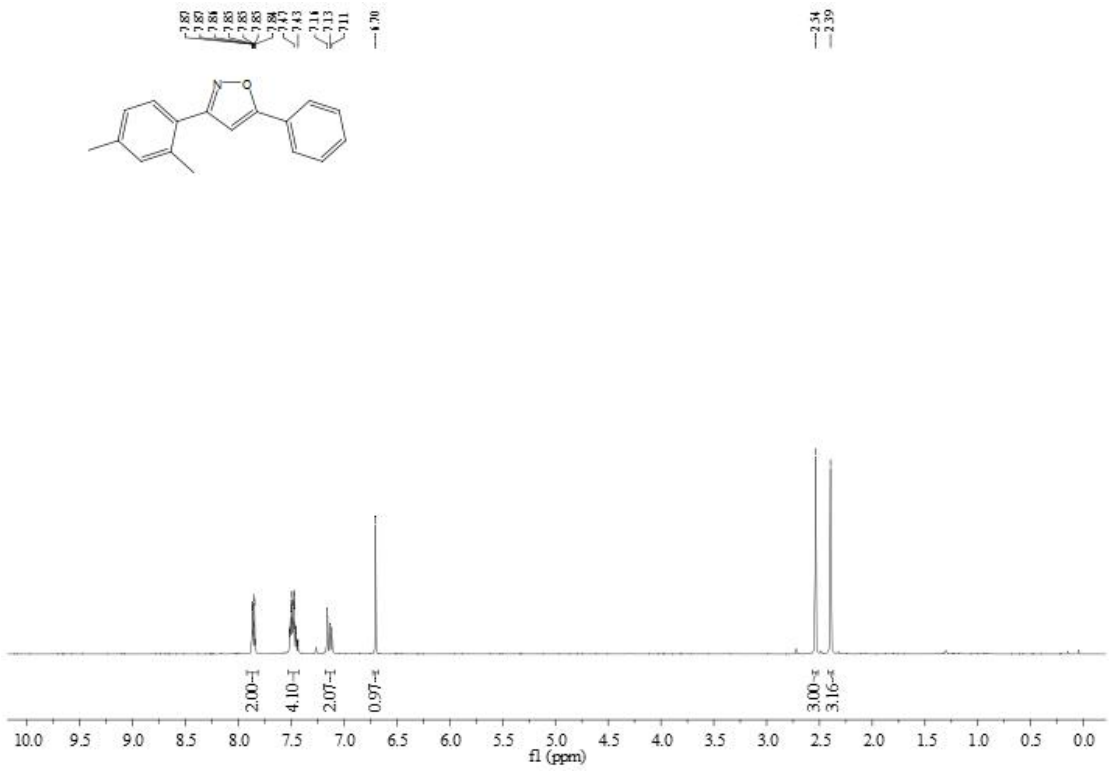


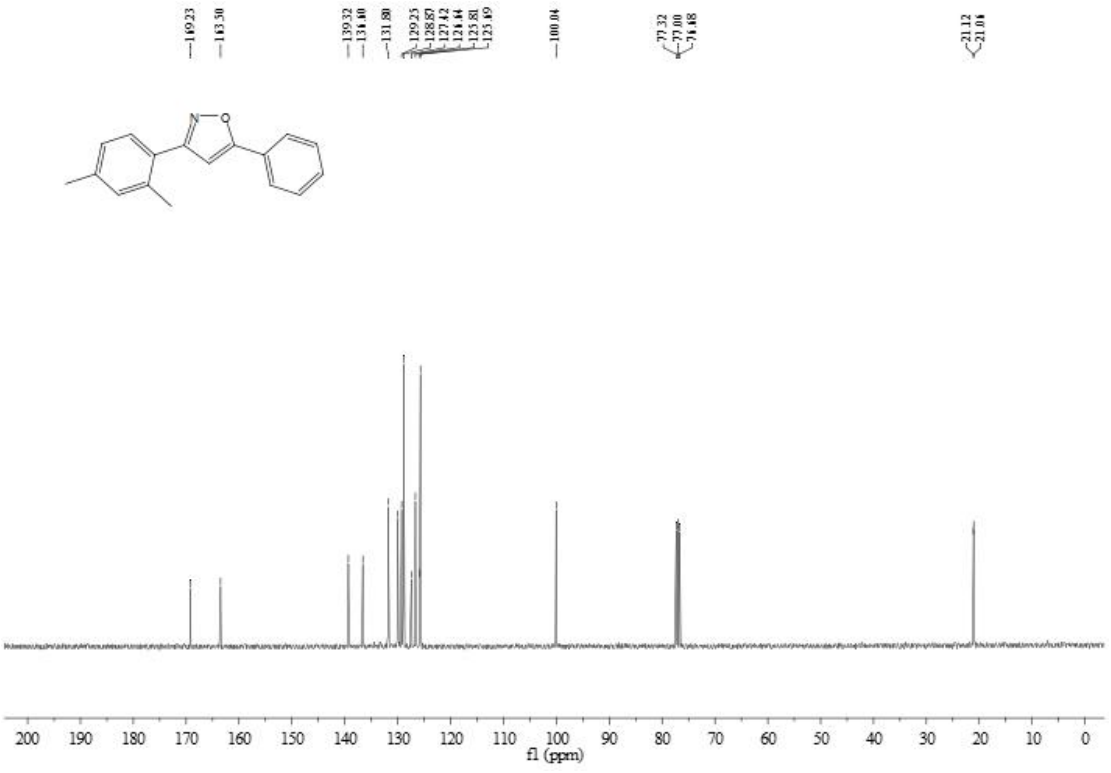
^{1}H and ^{13}C NMR spectra of compound 2ha



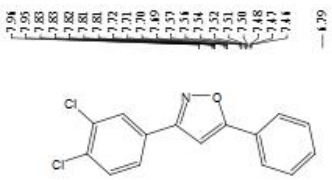


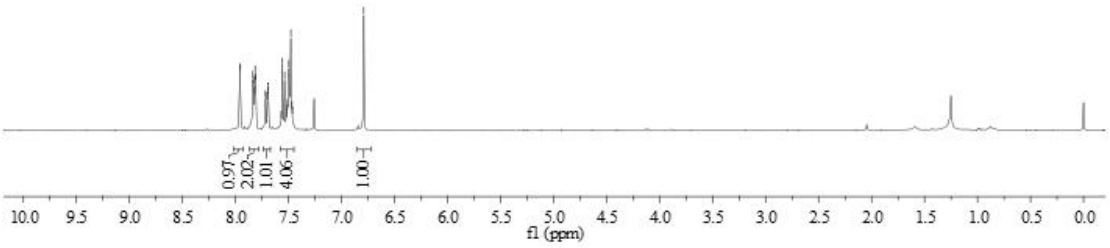
^{1}H and ^{13}C NMR spectra of compound 2ia

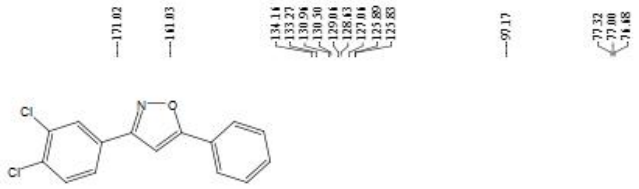


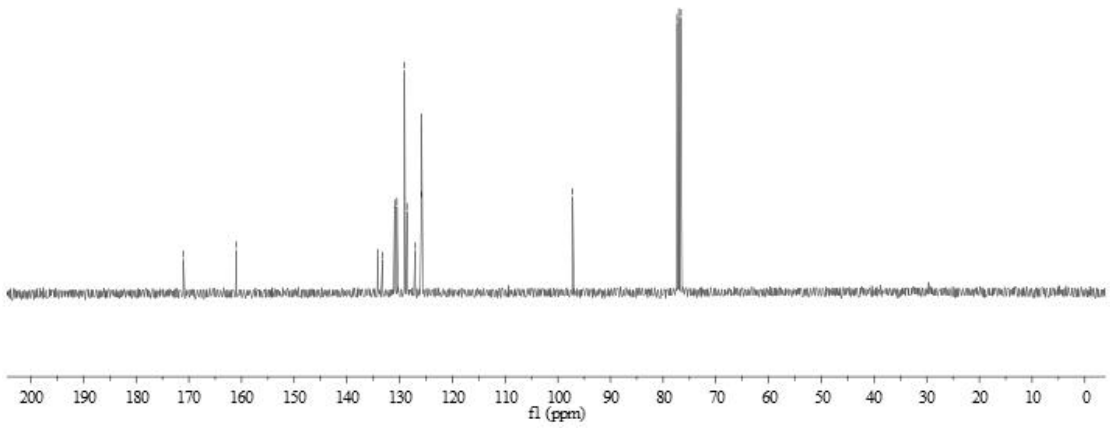


^{1}H and ^{13}C NMR spectra of compound 2ja

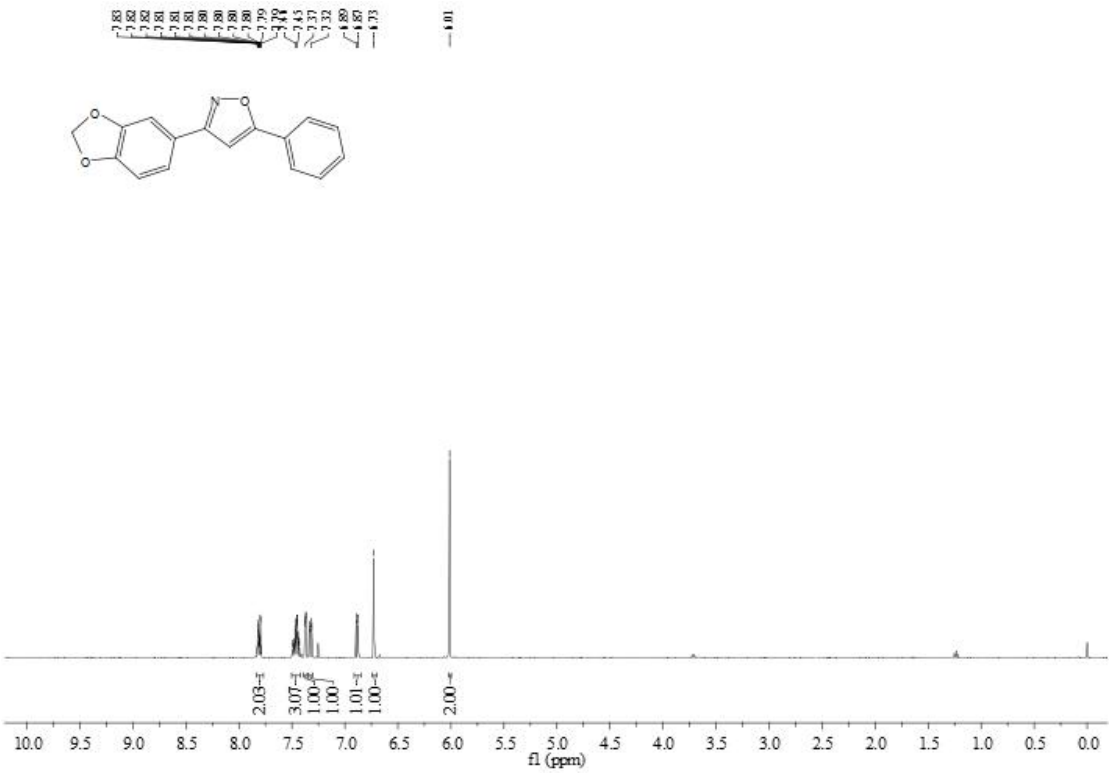


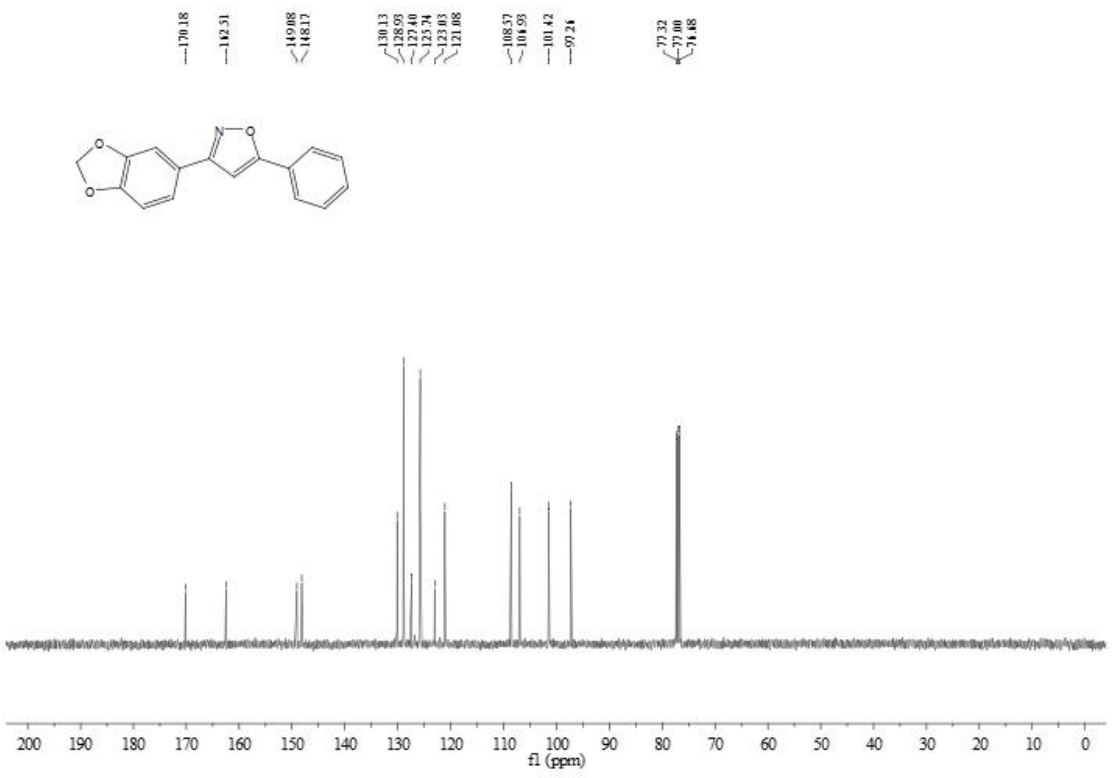




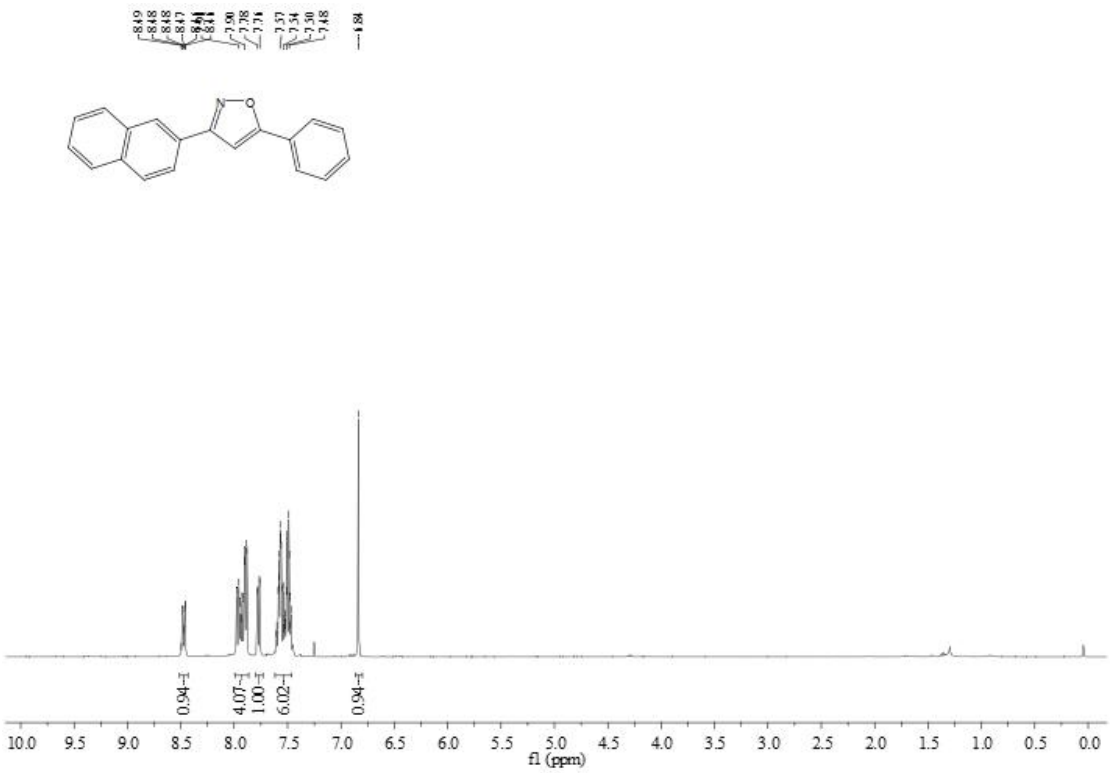


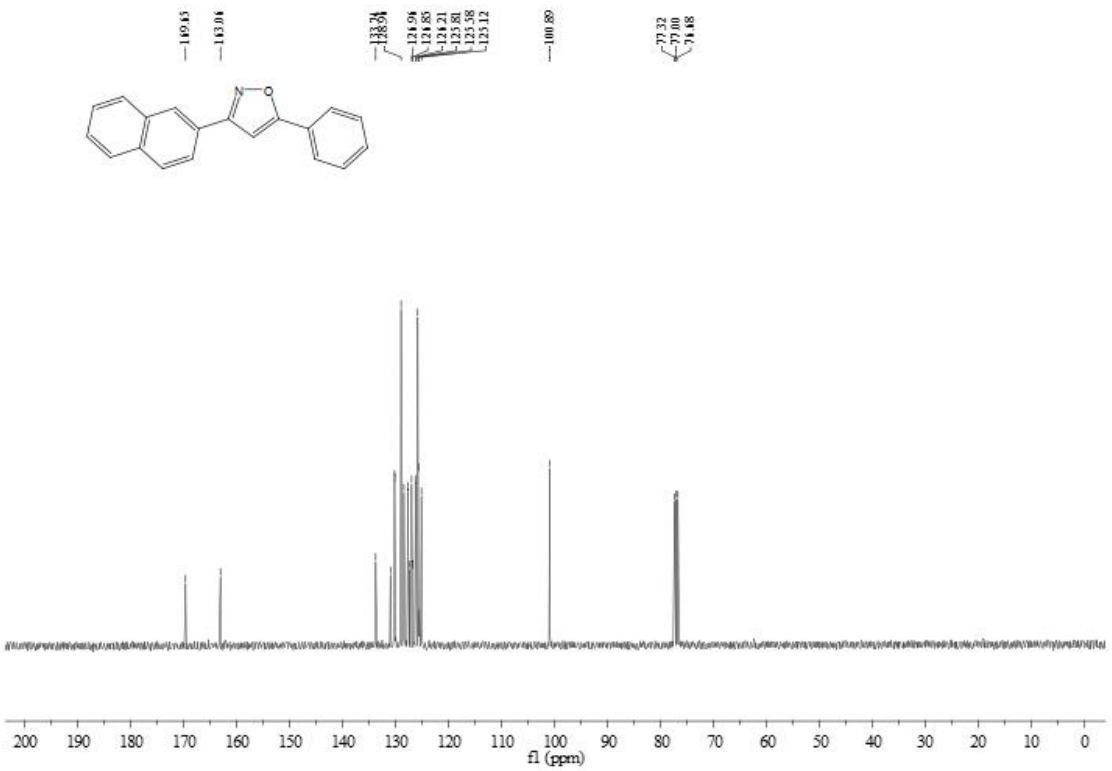
^{1}H and ^{13}C NMR spectra of compound 2ka



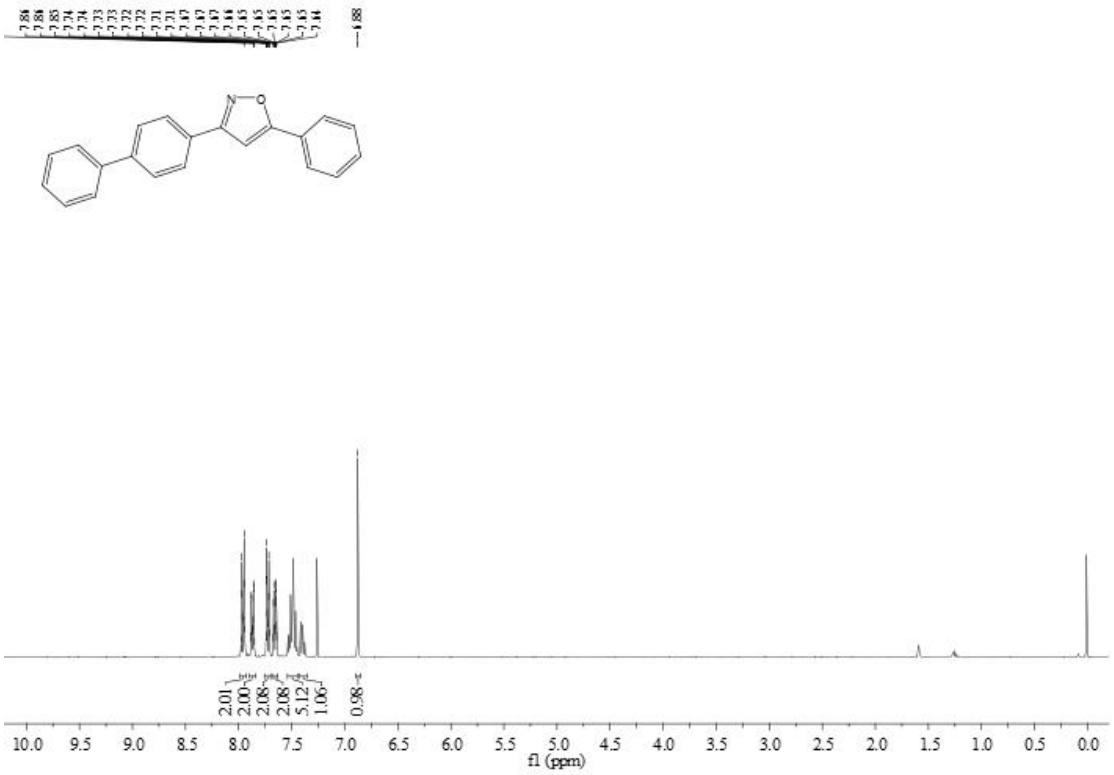


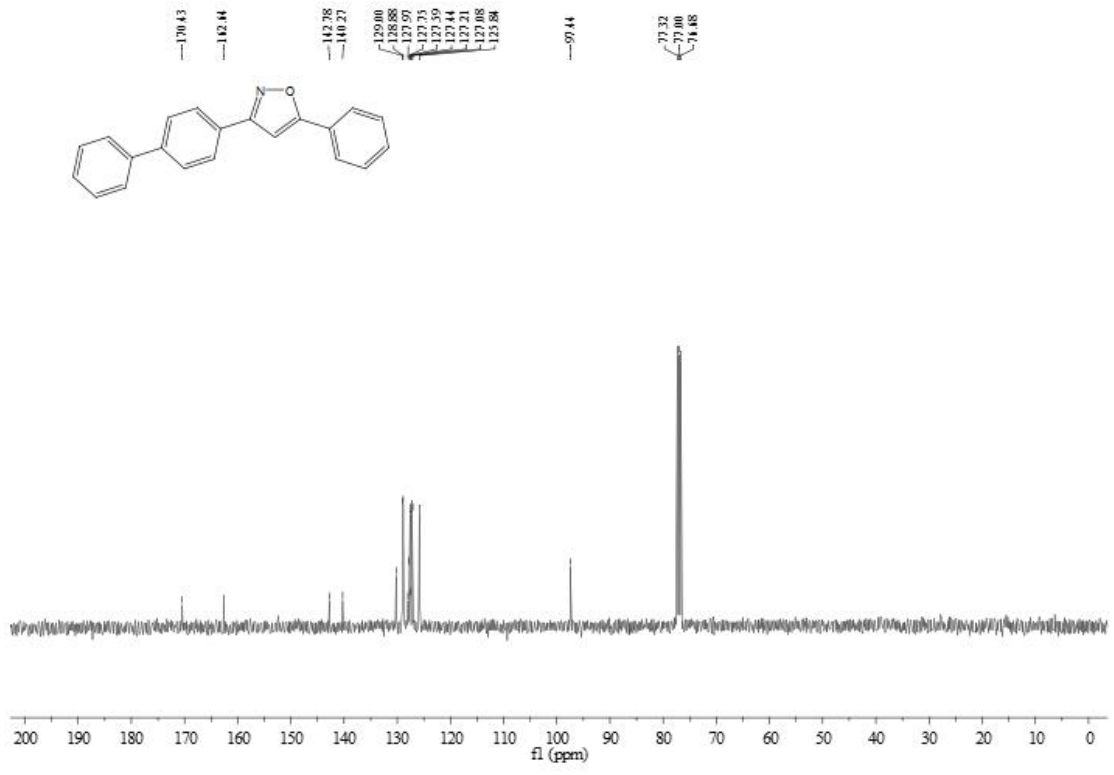
^{1}H and ^{13}C NMR spectra of compound 2la



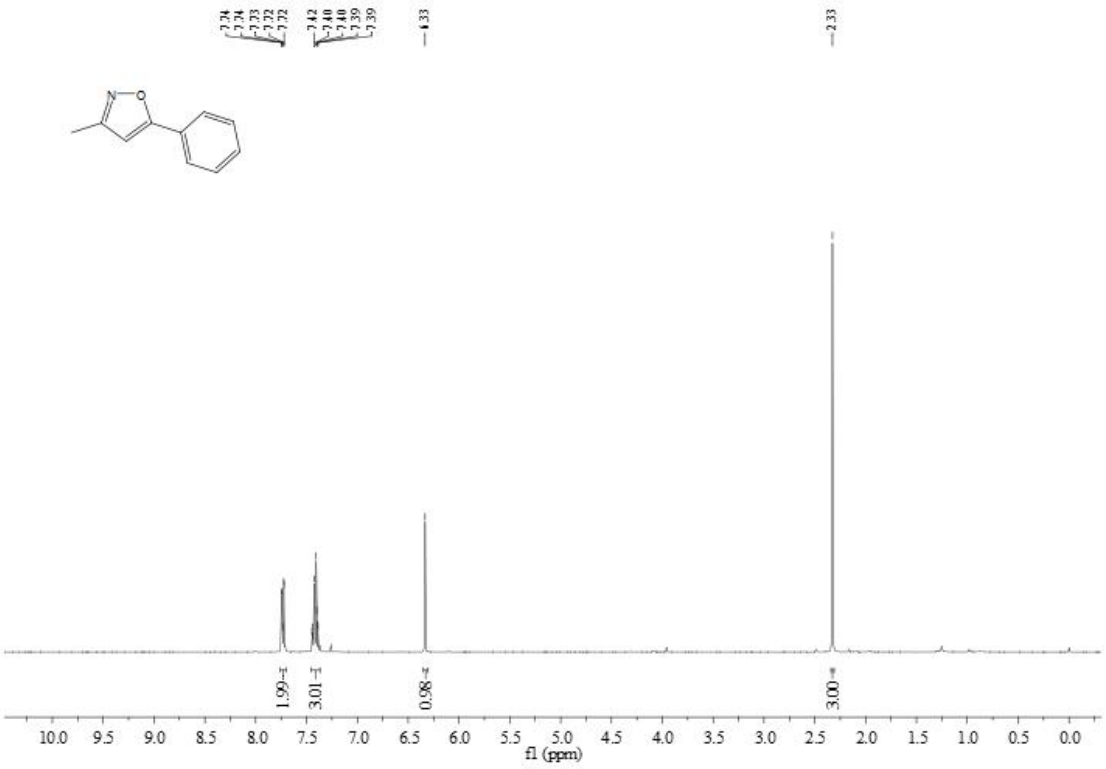


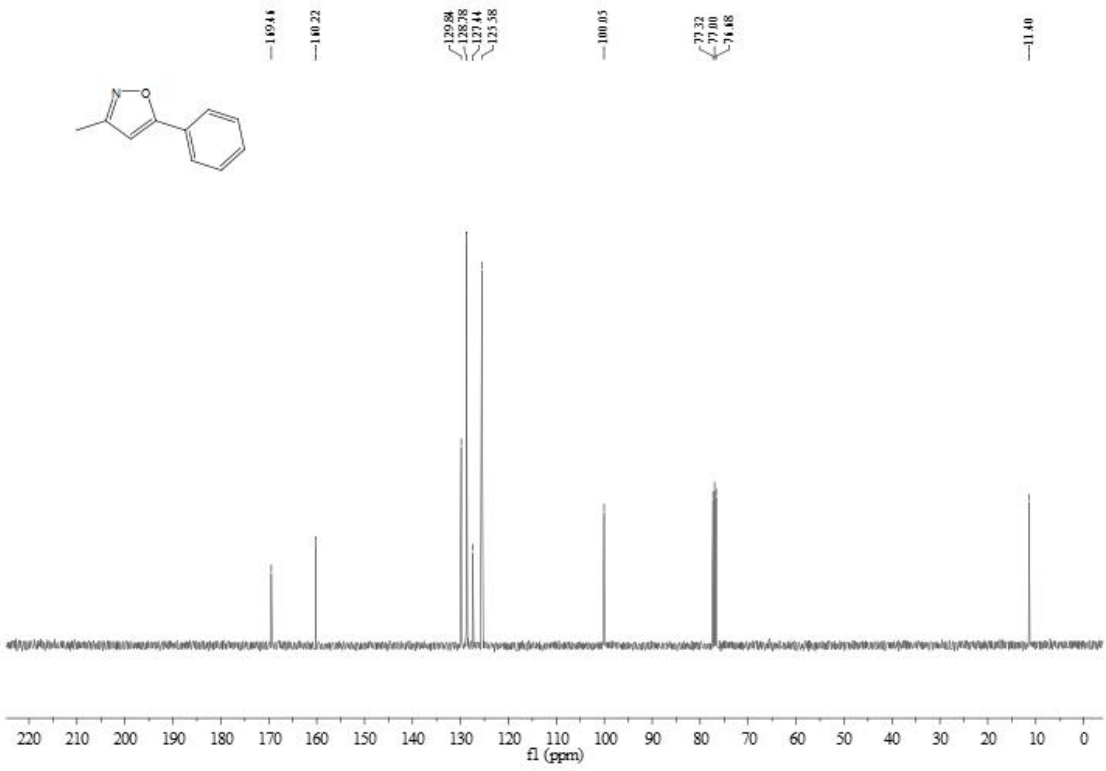
^{1}H and ^{13}C NMR spectra of compound 2ma



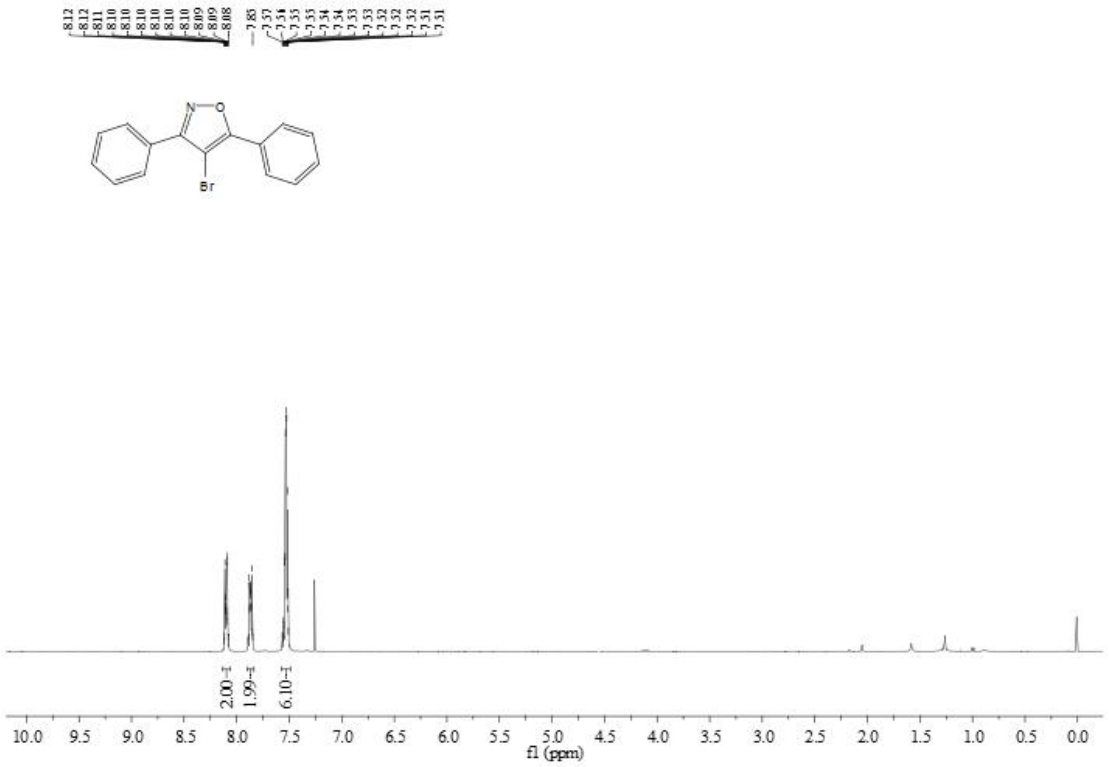


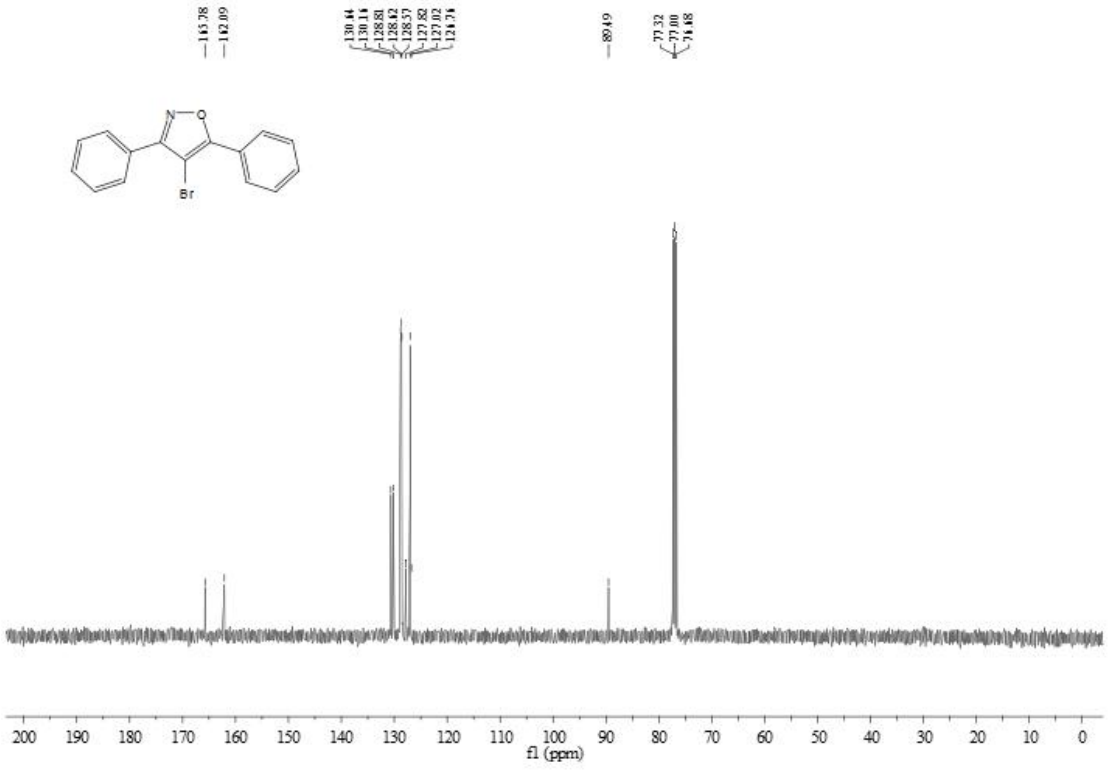
^{1}H and ^{13}C NMR spectra of compound 2na



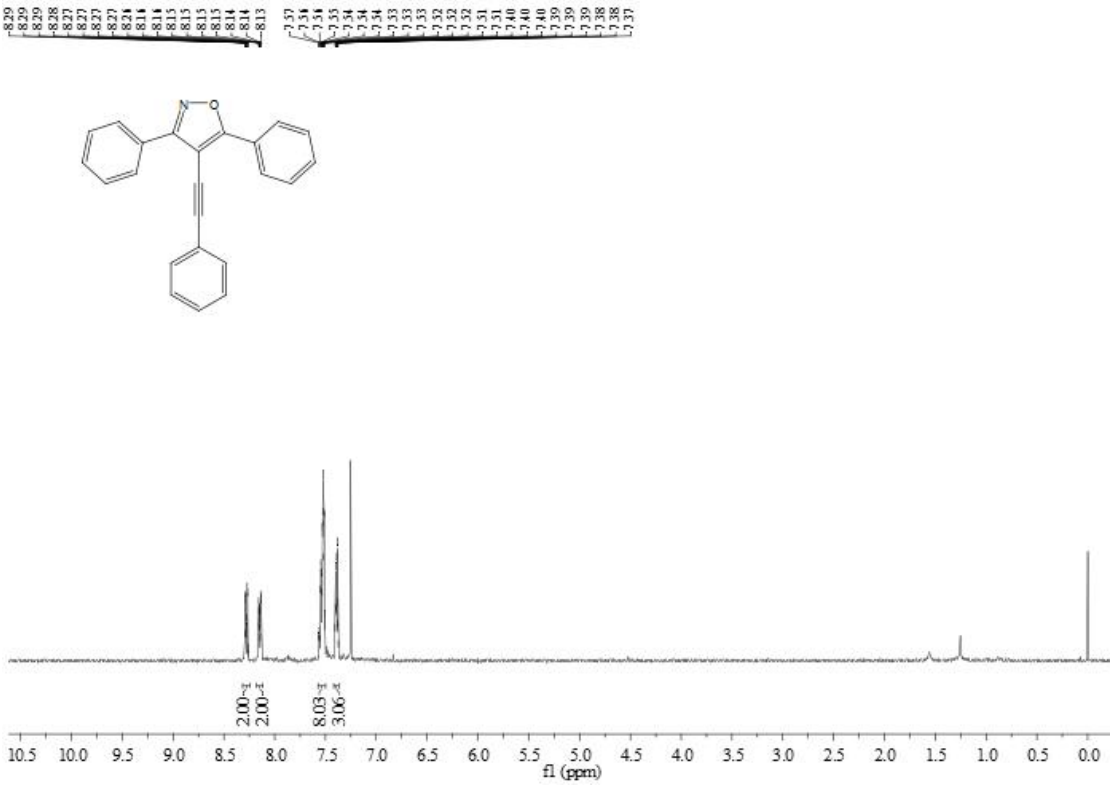


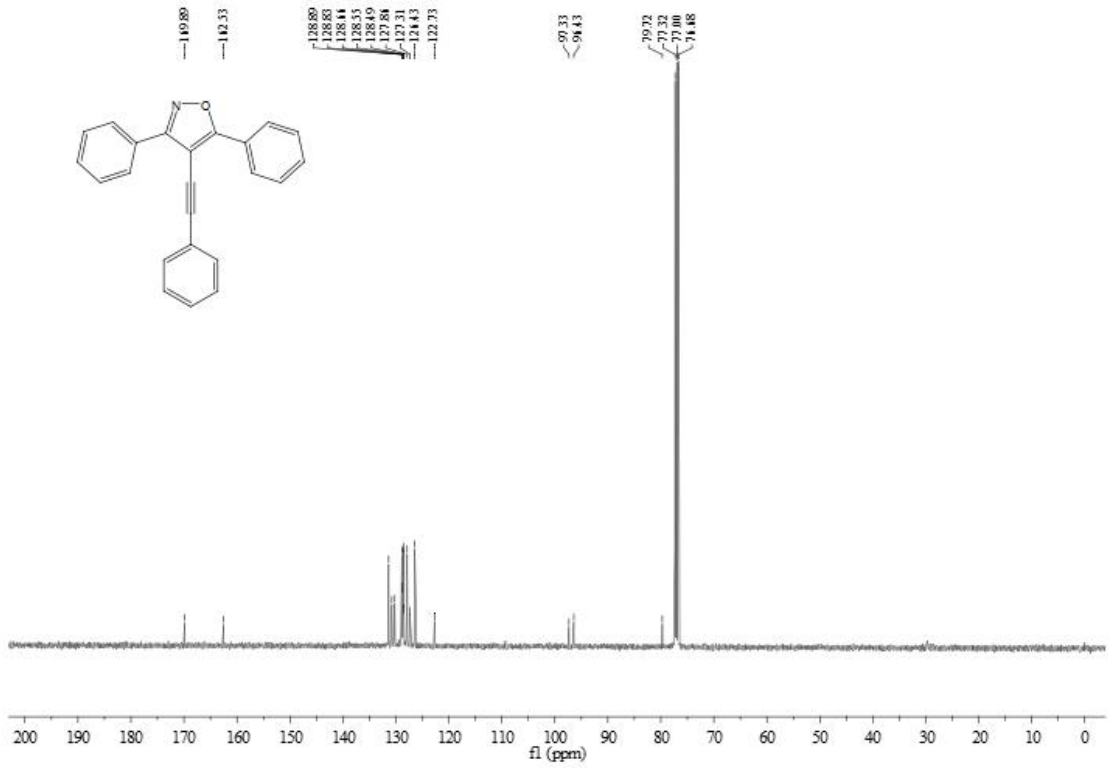
^{1}H and ^{13}C NMR spectra of compound 3



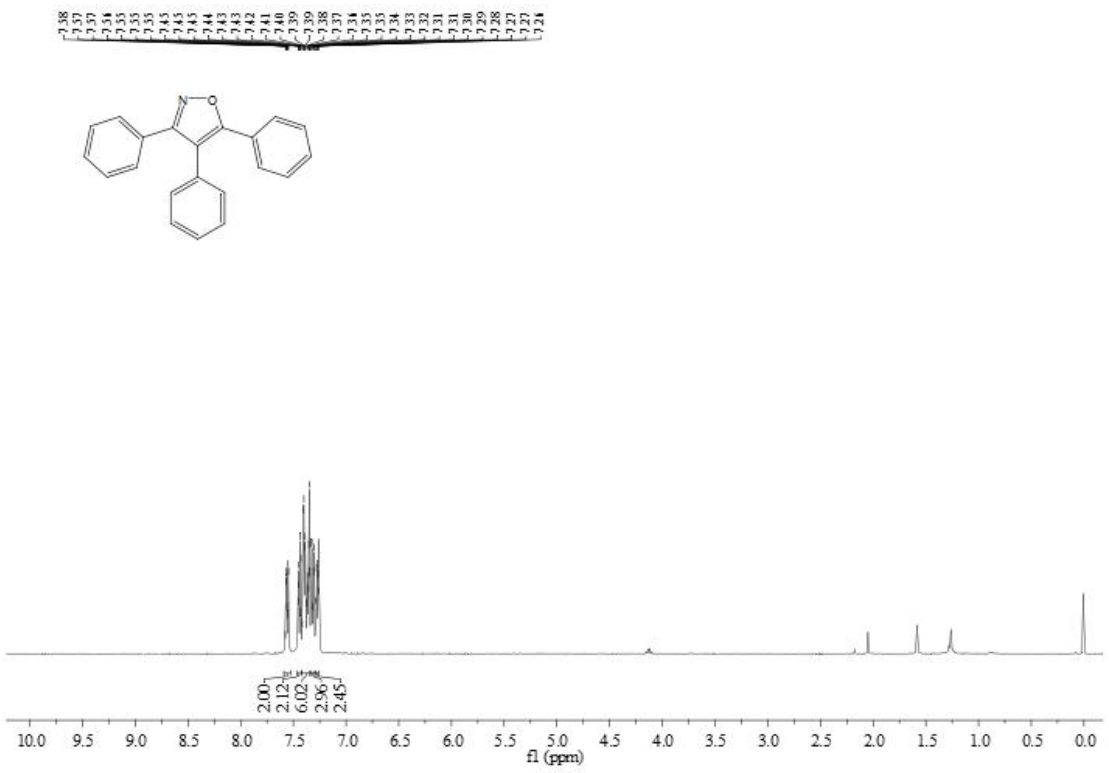


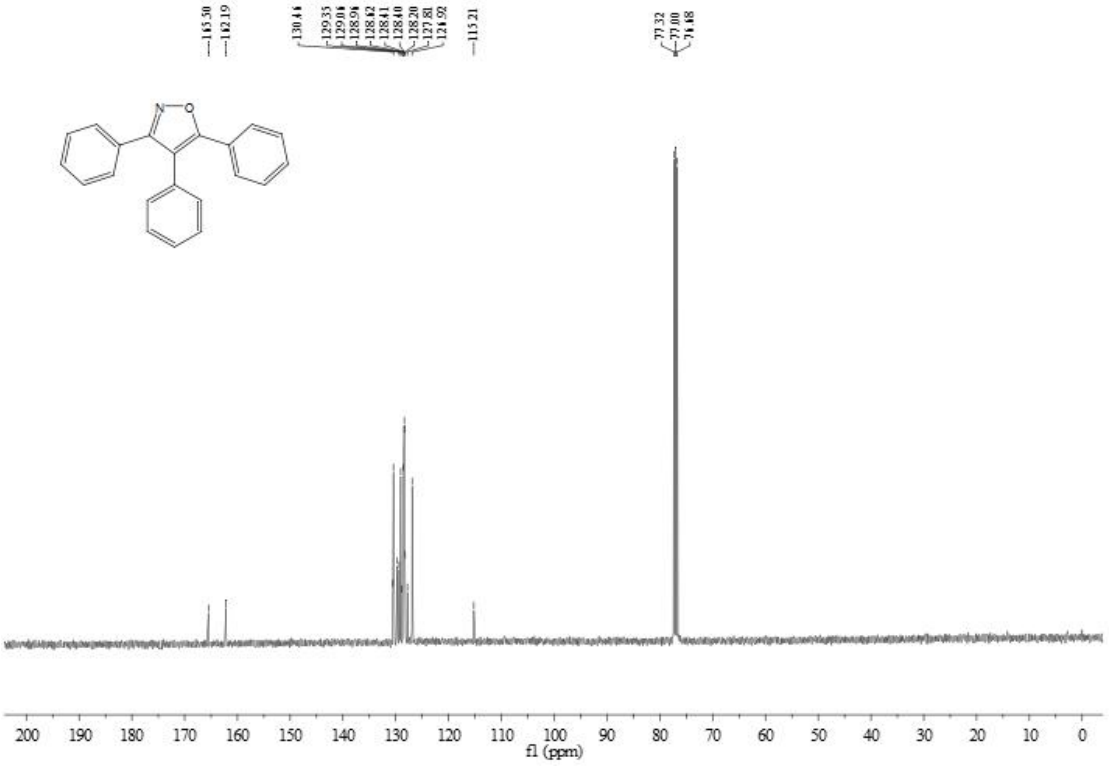
^{1}H and ^{13}C NMR spectra of compound 4





^{1}H and ^{13}C NMR spectra of compound 5

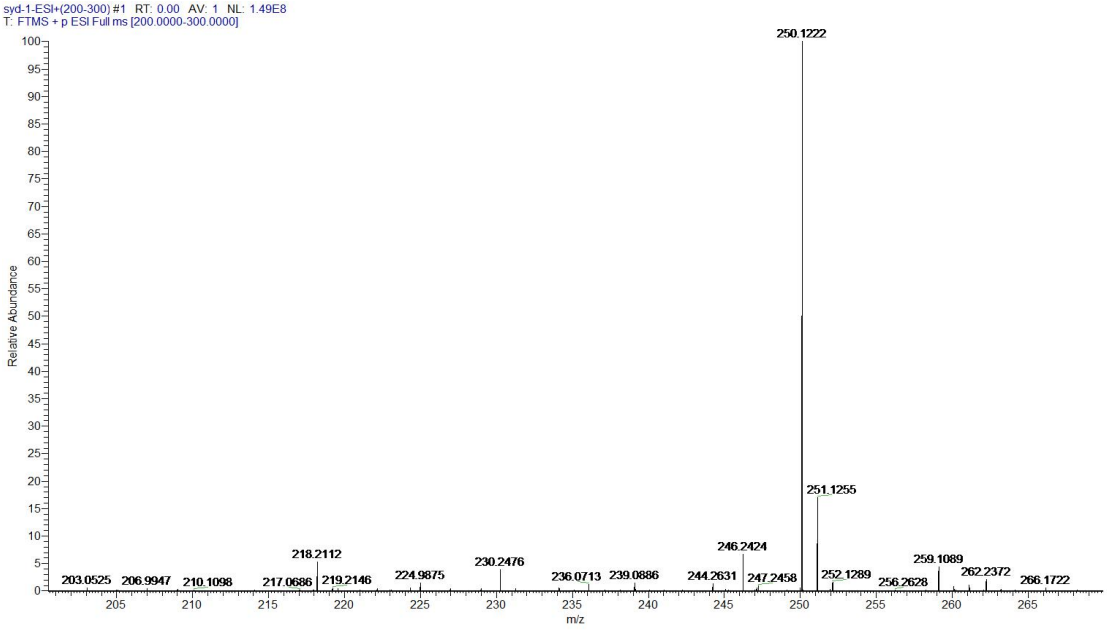




VI. HR-MS spectra of new compounds

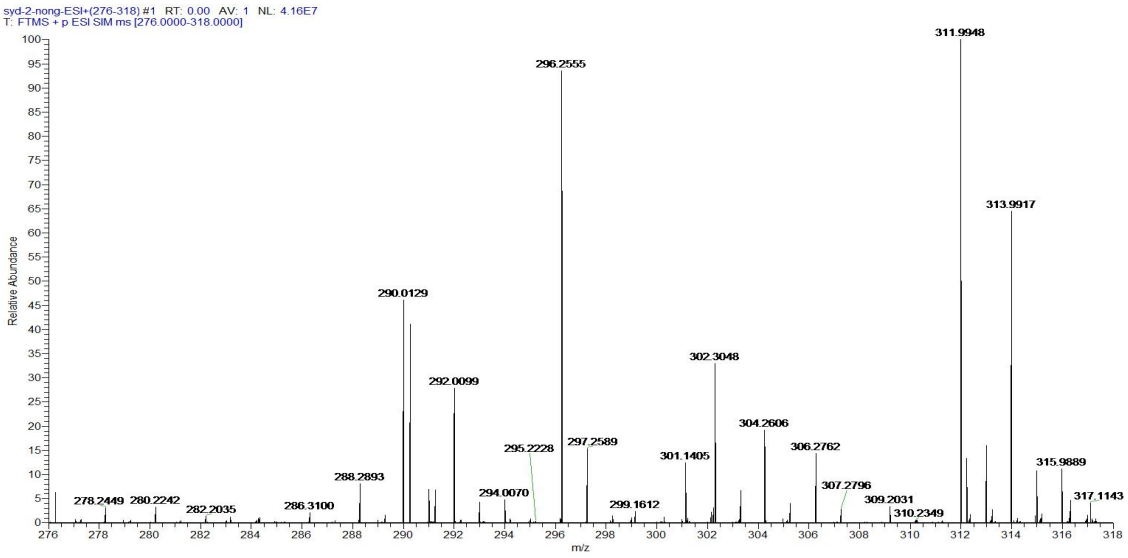
HR-MS spectra of compound 2ak

Formula: $C_{17}H_{15}NO$ $M+H^+$: 250.1226



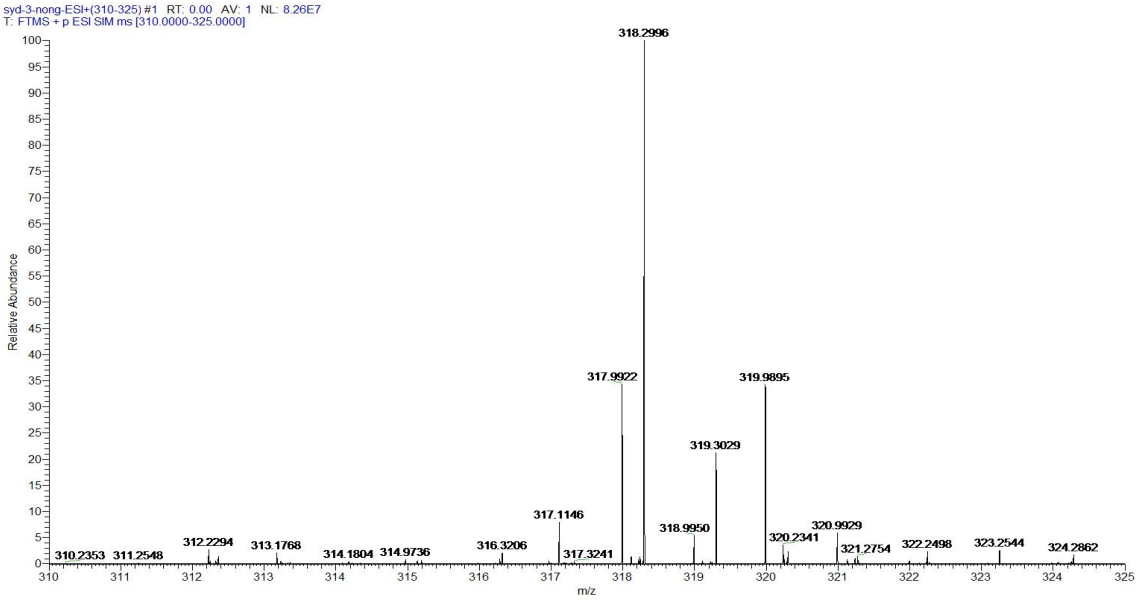
HR-MS spectra of compound 2al

Formula: $C_{15}H_9Cl_2NO$ $M+H^+$: 290.0134



HR-MS spectra of compound 2am

Formula: $C_{15}H_9BrFNO$ M+H$^+$: 317.9924



HR-MS spectra of compound 4

Formula: $C_{23}H_{15}NO$ M+H$^+$: 322.1226