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Supporting Information

Iodine Catalyzed Intramolecular C(Sp3)-H Functionalization: Synthesis of 2, 5-disubstituted Oxazoles from N-arylethylamides

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Experimental Section:

General: All commercially available chemicals and reagents were used without any further purification unless otherwise indicated. . Acetonitrile was dried with CaH, distilled, and stored with molecular sieves. ^{1}H and ^{13}C NMR spectra were recorded at 500 and 125 MHz, respectively. The spectra were recorded in $CDCl_3$ as solvent. Multiplicity was indicated as follows: s (singlet); d (doublet); t (triplet); m (multiplet); dd (doublet of doublets), etc. and coupling constants (J) were given in Hz. Chemical shifts are reported in ppm relative to TMS as an internal standard. The peaks around delta values of ^{1}H NMR (7.26), and ^{13}C NMR (77.0) are corresponding to the solvent $CDCl_3$. All products were purified through column chromatography using silica gel 100-200 mesh size using ethyl acetate /hexane as an eluent.

General procedure for the preparation of starting corresponding amides 1a-r and 1v-ae:

1.0 mmol of 2-phenylethylamine, 1.2 mmol of triethylamine and catalytic amount (5 mol%) of DIMAP were dissolved in 5 mL DCM solvent and cooled in ice bath. Then 1.2 mmol of benzoyl chloride was added drop wise and after complete the addition, it was allowed to react at room temperature under stirring for 2 h. After completion of the reaction (monitored by TLC), water was added under stirring for 5 minutes. The DCM layer was separated, dried over anhydrous Na_2SO_4. Removal of solvent gives white solid N-phenethylbenzamide (**1a**) 95 % yield. Same procedure has been followed for other starting materials (**1b-r** and **1v-ae**).

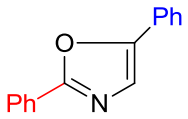
General procedure for the preparation of starting corresponding amides 1s-u[1]:

2 mmol of 2-phenylethylamine, 1.0 mmol of picolinamide and chitosan (20 wt. %; 24 mg) was stirred at 150°C temperature for 36 h. After the completion of the reaction (monitored by TLC), cooled to room temperature and the reaction mixture was dissolved with DCM (15 mL). After removal of solvent, the crude reaction mixture left out was purified by column chromatography (eluted with dichloromethane and ethyl acetate) using silica gel (200-400 mesh) to obtain 64% of N-phenethylpicolinamide (**1t**). Same procedure has been followed for other starting materials (**1t-u)**

A typical experimental procedure for the synthesis of 2, 5-disubstituted Oxazoles (2a):

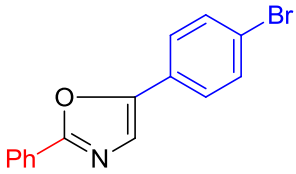
In a sealed tube, 45 mg (0.2 mmol) of N-phenethylbenzamide (1a), I2 (0.04 mmol) 10 mg were added in 1 mL of dry acetonitrile and the tube was closed with rubber septum. initially 120 µL (3 equiv) of TBHP (5 – 6M decane solution) was added through a syringe. Then the sealed tube was heated to 100°C under stirring and the rest of the 80 µL (2 equiv) of TBHP was added to the reaction mixture after 18 h. After complete addition of TBHP the reaction was continued another 18 h. After the completion of the reaction, reaction mixture was cooled to room temperature and added water, extracted the organic portion with DCM (2x10 mL) and dried with anhydrous sodium sulphate. After removing the solvent, the crude product left out was purified by column chromatography on silica gel (100-200 mesh) using ethyl acetate/ hexane mixture as eluent.

2,5-diphenyloxazole (**2a**)[2]:



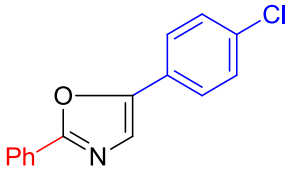
Yield (30.0 mg, 68%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.12 - 8.10 (m, 2H), 7.72 (d, *J* = 7.5 Hz, 2H), 7.50 – 7.42 (m, 6H), 7.35 (t, *J* = 7.5 Hz , 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 155.9, 146.0, 125.1, 123.7, 123.6, 123.2, 122.8, 121.1, 119.0, 118.2.

5-(4-bromophenyl)-2-phenyloxazole (**2b**)[3]:



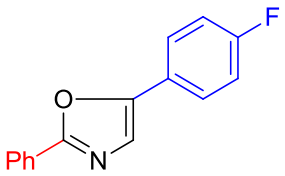
Yield (38 mg, 63%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 - 8.08 (m, 2H), 7.59 - 7.57 (m, 4H), 7.49 - 7.46 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): 161.4, 150.3, 132.5, 130.5,128.8, 127.1, 126.9, 126.3, 125.6, 123.9, 122.3.

5-(4-chlorophenyl)-2-phenyloxazole (**2c**)[2]:



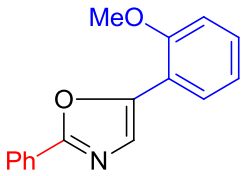
Yield (34 mg, 67%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 - 8.09 (m, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.49 - 7.48 (m, 3H), 7.45 (t, *J* = 8.5 Hz , 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.0, 150.2, 134.2, 130.5, 129.2, 128.8, 127.2, 126.4, 126.3, 125.4, 123.7.

5-(4-fluorophenyl)-2-phenyloxazole (**2d**)[4]:



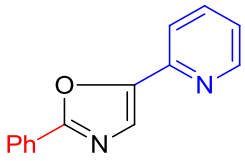
Yield (35 mg, 74%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 - 8.09 (m, 2H), 7.71 - 7.69 (m, 2H), 7.49 (d, *J* = 7.0 Hz, 3H), 7.39 (s, 1H), 7.16 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.6, 161.7, 161.1, 150.4, 130.4, 128.8, 127.2, 126.2, 126.1, 126.0, 124.3, 123.0, 116.2, 116.0.

5-(2-methoxyphenyl)-2-phenyloxazole (**2e**)[3]:



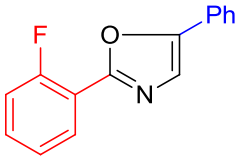
Yield (21 mg, 42%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.08 (s, 2H), 7.87 (d, *J* = 7.5 Hz, 1H), 7.73 (s, 1H), 7.44 (s, 3H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 1H), 3.99 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.1, 154.7, 146.8, 129.3, 128.2, 127.7, 126.3, 125.5, 124.7, 119.8, 109.9, 54.4.

2-phenyl-5-(pyridin-2-yl)oxazole (**2f**)[5]:



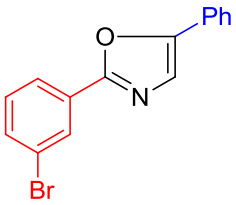
Yield (21 mg, 48%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.63 – 8.62 (m, 1H), 8.08 – 8.06 (m, 2H), 7.77 (s, 1H), 7.74 (t, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.41 – 7.40 (m, 3H), 7.19 – 7.17 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 162.0, 150.4, 149.7, 147.0, 137.1, 133.0, 130.7, 129.9, 128.8, 128.3, 127.0, 126.5, 122.9, 119.2.

2-(2-fluorophenyl)-5-phenyloxazole (**2g**)[6]:



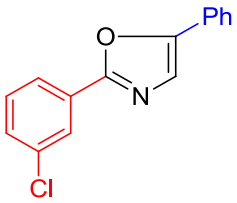
Yield (34.5 mg, 72%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.12 (t, *J* = 7.0 Hz, 1H), 7.75 (d, *J* = 7.5 Hz, 1H), 7.51 (s, 1H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.38 – 7.34 (m, 1H), 7.30 – 7.21 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): 161.6, 161.0, 158.9, 157.5, 157.4, 151.4, 131.9, 131.8, 129.8, 129.3, 128.9, 128.6, 128.3, 127.7, 124.3, 123.3, 116.9, 116.8.

2-(3-bromophenyl)-5-phenyloxazole (**2h**)[7]:



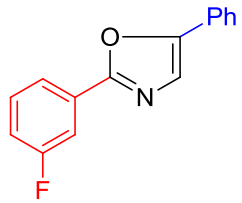
Yield (37 mg, 62%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (s, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 7.5 Hz, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.47 – 7.44 (m, 3H), 7.37 – 7.34 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 158.6, 150.7, 132.1, 129.3, 128.1, 127.9, 127.6, 126.7, 123.7, 123.2, 122.5, 121.9.

2-(3-chlorophenyl)-5-phenyloxazole (**2i**)[3]:



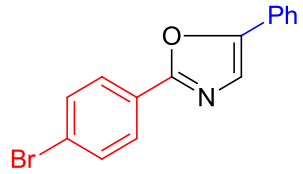
Yield (33 mg, 64%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.11 – 8.09 (m, 1H), 8.00 – 7.99 (m, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.42 (m, 5H), 7.38 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.7, 151.7, 134.9, 130.3, 130.1, 129.0, 128.7, 126.2, 124.3, 123.5.

2-(3-fluorophenyl)-5-phenyloxazole (**2j**)[7]:



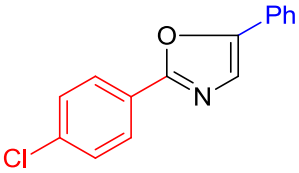
Yield (34.5 mg, 72%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.90 (d, *J* = 7.5 Hz, 1H), 7.80 – 7.78 (m, 1H), 7.73 (d, *J* = 7.5 Hz, 2H), 7.47 – 7.44 (m, 4H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.17 – 7.14 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 163.9, 161.9, 159.9, 151.6, 130.6, 130.5, 129.0, 128.7, 127.7, 124.2, 123.5, 121.9, 117.3, 117.2, 113.3, 113.1.

2-(4-bromophenyl)-5-phenyloxazole (**2k**)[8]:



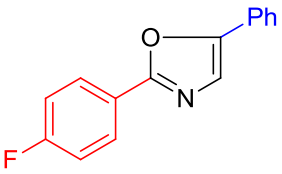
Yield (36 mg, 60%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.62 (d, *J* = 8.5 Hz, 2H), 7.46 – 7.43 (m, 3H), 7.37 (t, *J* = 7.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.2, 151.5, 132.0, 128.9, 128.6, 128.4, 127.8, 127.7, 124.7, 124.2, 123.5.

2-(4-chlorophenyl)-5-phenyloxazole (**2l**)[2]:



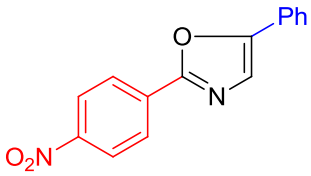
Yield (33 mg, 64%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.04 (d, *J* = 9.0 Hz, 2H), 7.71 (d, *J* = 7.5 Hz, 2H), 7.46 – 7.43 (m, 5H), 7.36 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.2, 151.5, 136.4, 129.1, 128.9, 128.6, 127.7, 127.5, 125.9, 124.2, 123.5.

2-(4-fluorophenyl)-5-phenyloxazole (**2m**)[2]:



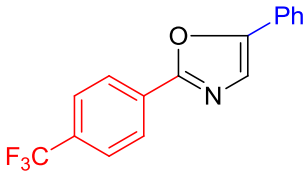
Yield (36 mg, 76%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.11 – 8.09 (m, 2H), 7.72 (d, *J* = 8.0 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 3H), 7.36 (t, *J* = 7.5 Hz, 1H), 7.19 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 165.0, 163.0, 160.3, 151.3, 128.9, 128.5, 128.4, 128.3, 127.8, 124.1, 123.3, 116.1, 115.9.

2-(4-nitrophenyl)-5-phenyloxazole (**2n**)[2]:



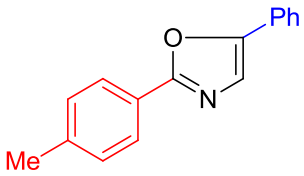
Yield (39 mg, 74%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.35 (d, *J* = 8.0 Hz, 2H), 8.27 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 7.5 Hz, 2H), 7.53 (s, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 158.9, 152.8, 148.5, 132.8, 129.2, 129.1, 127.3, 126.8, 124.5, 124.2.

5-phenyl-2-(4-(trifluoromethyl)phenyl)oxazole (**2o**)[2]:



Yield (40 mg, 69%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.22 (d, *J* = 8.0 Hz, 2H), 7.75 – 7.73 (m, 4H), 7.48 – 7.44 (m, 3H), 7.39 – 7.35 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.7, 152.1, 131.9, 131.7, 130.5, 129.8, 129.0, 128.8, 128.7, 128.5, 127.6, 127.4, 126.4, 125.8, 124.3, 123.7, 122.7.

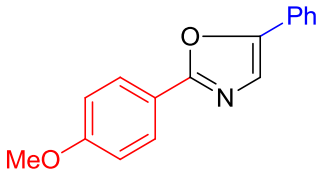
5-phenyl-2-(p-tolyl)oxazole (**2p**)[2]:



Yield (25 mg, 53%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.00 (d, *J* = 7.5 Hz, 2H), 7.72 (d, *J* = 7.5 Hz, 2H), 7.45 – 7.42 (m, 3H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 2.41 (s, 3H); ^{13}C

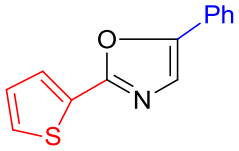
NMR (125 MHz, $CDCl_3$): 149.9, 139.6, 128.5, 127.8, 127.2, 127.0, 125.2, 123.7, 123.1, 122.2, 20.4.

2-(4-methoxyphenyl)-5-phenyloxazole (**2q**)[2]:



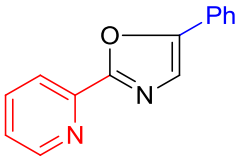
Yield (25.5 mg, 51%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.05 (d, *J* = 9.0 Hz, 2H), 7.71 (d, *J* = 7.0 Hz, 2H), 7.45 – 7.41 (m, 3H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.00 – 6.98 (m, 2H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.3, 160.2, 149.7, 127.8, 127.1, 126.9, 123.0, 122.1, 119.2, 113.2, 54.3.

5-phenyl-2-(thiophen-2-yl)oxazole (**2r**)[2]:



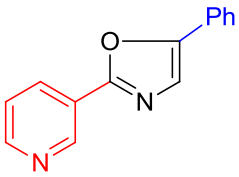
Yield (25 mg, 56%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.75 – 7.74 (m, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.45 – 7.42 (m, 3H), 7.39 (s, 1H), 7.35 – 7.32 (m, 1H), 7.15 – 7.13 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 157.4, 150.8, 130.0, 128.9, 128.6, 128.4, 128.2, 127.9, 127.7, 127.6, 124.1, 123.3.

5-phenyl-2-(pyridin-2-yl)oxazole (**2s**)[4]:



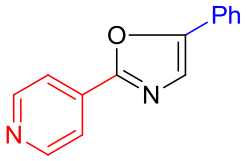
Yield (17.5 mg, 39%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.60 – 8.58 (m, 1H), 8.21 (d, *J* = 7.5 Hz, 1H), 7.88 – 7.81 (m, 3H), 7.53 (d, *J* = 6.5 Hz, 1H), 7.47 (d, *J* = 7.0 Hz, 3H), 7.40 (t, *J* = 6.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.1, 153.1, 149.4, 146.0, 137.3, 128.7, 128.6, 127.3, 126.5, 124.7, 124.6, 122.4.

5-phenyl-2-(pyridin-3-yl)oxazole (**2t**)[8]:



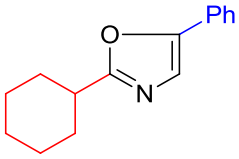
Yield (20.5 mg, 46%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.35 (s, 1H), 8.71 – 8.70 (m, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 7.74 (d, *J* = 8.5 Hz, 2H) 7.49 – 7.43 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): 158.6, 152.0, 150.7, 147.3, 133.5, 133.2, 130.0, 129.0, 128.8, 128.7, 128.3, 127.5, 124.3, 123.7, 123.6.

5-phenyl-2-(pyridin-4-yl)oxazole (**2u**)[9]:



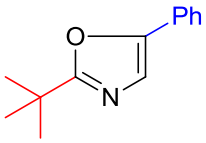
Yield (18 mg, 41%); ^{1}H NMR (500 MHz, CDCl3): δ 8.73 (d, *J* = 6.0 Hz, 2H), 7.91 (d, *J* = 6.0 Hz, 2H), 7.71 (d, *J* = 9.0 Hz, 2H), 7.49 (s, 1H), 7.43 – 7.41 (m, 2H), 7.36 (t, *J* = 7.5 Hz, 1H) ^{13}C NMR (125 MHz, $CDCl_3$): 161.4, 154.0, 150.5, 134.2, 132.4, 132.0, 130.8, 129.1, 129.0, 128.82, 128.8,128.7, 128.6, 127.3, 124.5, 124.0, 119.8.

2-cyclohexyl-5-phenyloxazole (**2v**)[2]:



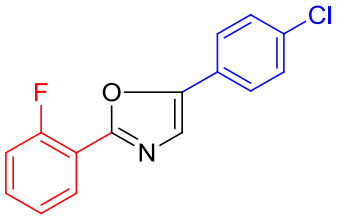
Yield (23.6 mg, 52%);^{1}H NMR (500 MHz, CDCl3): δ 7.58-7.53(m, 2H), 7.35 – 7.33 (m, 2H),7.25 – 7.23 (m, 1H), 7.19 (s, 1H), 2.81 – 2.75 (m,1H), 2.06 – 2.04 (m,2H), 1.79 – 1.76 (m, 2H), 1.58 – 1.52 (m, 3H), 1.36 – 1.30 (m, 3H); ^{13}C NMR (125 MHz, CDCl3): 168.3, 149.7, 129.2, 128.9, 128.6, 124.1, 121.9, 37.7, 30.7, 25.9, 25.7.

2-(tert-butyl)-5-phenyloxazole (**2w**)[2]:



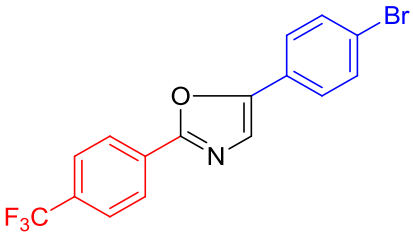
Yield (26 mg, 64%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.62 (d, *J* = 7.5 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.20 (s, 1H), 1.44 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): 170.8, 150.6, 128.7, 128.5, 128.4, 128.0, 123.9, 121.4, 33.8, 28.6.

5-(4-chlorophenyl)-2-(2-fluorophenyl)oxazole (**2x**):



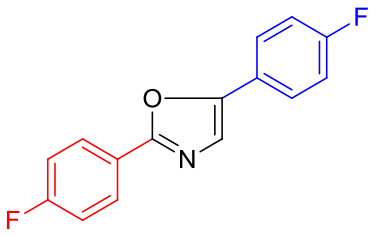
Yield (43 mg, 78%, White solid); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.11 – 8.07 (m, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.50 – 7.47 (m, 1H), 7.43 (d, *J* = 8.5 Hz, 1H), 7.29 – 7.22 (m, 4H), 7.12 – 7.08 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 161.7, 161.0, 159.7, 159.0, 157.7, 150.5, 134.0, 133.7, 133.6, 132.2, 131.1, 129.3, 129.2, 128.5, 125.5, 123.7, 117.0, 116.8, 116.2, 116.0. HRMS-calculated for $C_{15}H_{10}NOFCl$= 274.0435; found 274.0429.

5-(4-bromophenyl)-2-(4-(trifluoromethyl)phenyl)oxazole (**2y**):



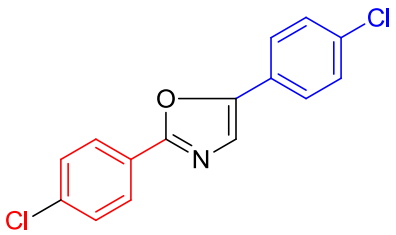
Yield (48 mg, 65%, White solid); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.20 (d, *J* = 8.5 Hz, 2H), 7.74 (d, *J* = 8.5 Hz, 2H), 7.58 (s, 4H), 7.48 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): 154.7, 154.9, 127.2, 127.0, 126.9, 126.6, 125.1, 121.3, 120.7, 120.5, 119.7, 119.0, 117.6, 117.5. HRMS-calculated for $C_{16}H_{10}NOF_3Br$= 367.9898; found 367.9887.

2,5-bis(4-fluorophenyl)oxazole (**2z**)[4]:



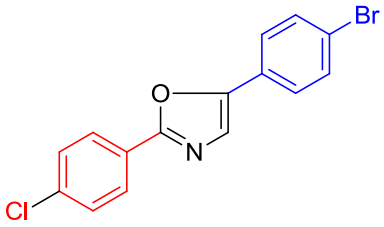
Yield (36 mg, 70%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 – 8.07 (m, 2H), 7.70 – 7.67 (m, 2H), 7.37 (s, 1H), 7.19 – 7.13 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): 165.0, 163.6, 163.0, 161.7, 160.3, 150.5, 128.4, 128.3, 126.1, 126.0, 124.2, 123.6, 123.0, 116.2, 116.1, 116.0, 115.9.

2,5-bis(4-chlorophenyl)oxazole (**2aa**)[10]:



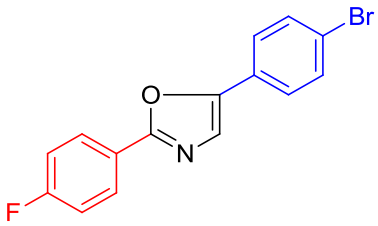
Yield (39.5 mg, 68%, White solid); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.5 Hz, 2H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.46 – 7.41 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.4, 150.5, 136.6, 134.4, 129.3, 129.2, 127.5, 126.2, 125.4, 123.8. HRMS- calculated for $C_{15}H_{10}NOCl_2$ = 290.0139; found 290.0139.

5-(4-bromophenyl)-2-(4-chlorophenyl)oxazole (**2ab**)[9]:



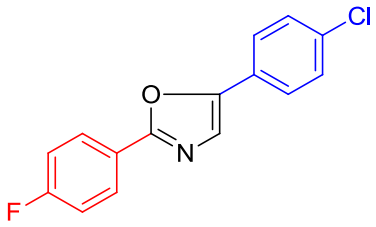
Yield (43.5 mg, 65%, Yellow solid); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.03 (d, *J* = 7.5 Hz, 2H), 7.61 – 7.57 (m, 4H), 7.46 – 7.45 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.4, 150.5, 136.6, 132.2, 131.8, 131.6, 129.4, 129.3, 129.2, 127.5, 126.6, 125.6, 123.9, 122.5. HRMS- calculated for $C_{15}H_{10}NOClBr$ = 333.9634; found 333.9644

5-(4-bromophenyl)-2-(4-fluorophenyl)oxazole (**2ac**):



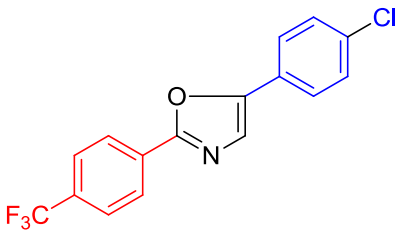
Yield (41 mg, 65%, White solid); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.09 – 8.07 (m, 2H), 7.60 – 7.56 (m, 4H), 7.42 (s, 1H), 7.18 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 165.1, 163.1, 160.5, 150.3, 132.1, 131.7, 128.5, 128.4, 126.8, 125.6, 123.8, 123.6, 122.3, 116.1, 116.0. HRMS- calculated for $C_{15}H_{10}NOFBr$ = 317.9930; found 317.9915.

5-(4-chlorophenyl)-2-(4-fluorophenyl)oxazole (**2ad**):



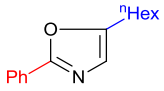
Yield (37 mg, 67%, White solid); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.10 – 8.07 (m, 2H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.43 – 7.41 (m, 3H), 7.19 (t, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 165.1, 163.1, 160.5, 150.3, 134.2, 130.5, 129.2, 128.5, 128.4, 126.3, 125.3, 123.7, 116.1. 116.0. HRMS- calculated for $C_{15}H_{10}NOFCl$ = 274.0435; found 274.0424

5-(4-chlorophenyl)-2-(4-(trifluoromethyl)phenyl)oxazole (**2ae**):



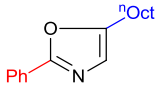
Yield (41.5 mg, 64%, Yellow solid); ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.5 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.48 (s, 1H), 7.44 (d, *J* = 8.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 159.9, 151.1, 134.6, 131.5, 130.3, 129.3, 128.8, 126.5, 126.1, 126.0, 125.9, 125.5, 124.1. HRMS- calculated for $C_{16}H_{10}NOF_3Cl$ = 324.0403; found 324.0406.

5-hexyl-2-phenyloxazole (**2af**)[11]:



Yield (13 mg, 28%); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99 (d, *J* = 6.5 Hz, 2H), 7.45 – 4.41(m, 3H), 6.83 (s, 1H), 2.71 (t, *J* = 7.5 Hz, 2H), 1.71– 1.66 (m, 2H) 1.41 – 1.37 (m, 2H), 1.33 – 1.32(m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.5, 153.2, 129.8, 128.6, 127.8, 125.9, 123.5, 31.4, 28.7, 27.5, 25.6, 22.5, 14.0.

5-octyl-2-phenyloxazole (**2ag**)[2]:



Yield (13 mg, 25%,); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.98 (d, *J* = 6.5 Hz, 2H), 7.43 – 4.39(m, 3H), 6.82 (s, 1H), 2.69 (t, *J* = 7.5 Hz, 2H), 1.71– 1.65 (m, 2H) 1.39 – 1.35 (m, 2H), 1.32 – 1.28 (m, 8H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 160.5, 153.2, 129.8, 128.6, 127.8, 125.9, 123.5, 31.4, 29.2, 29.1, 29.0,27.6, 25.6, 22.6, 14.0.

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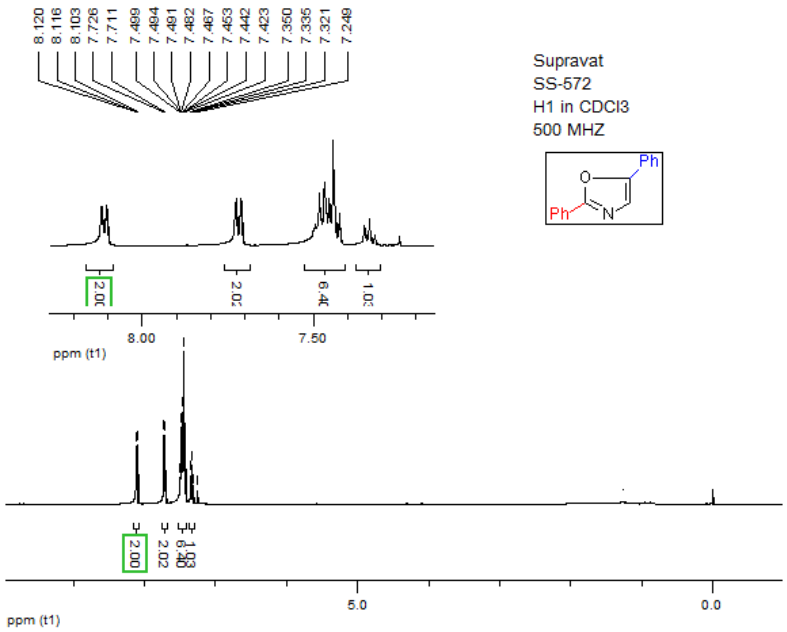
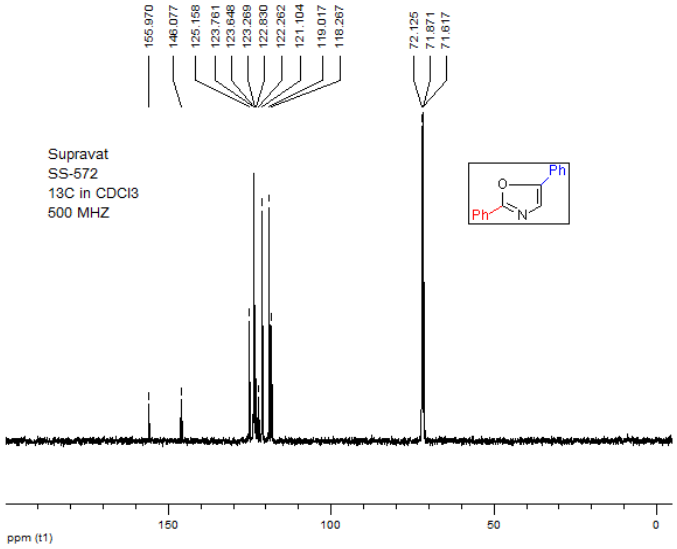
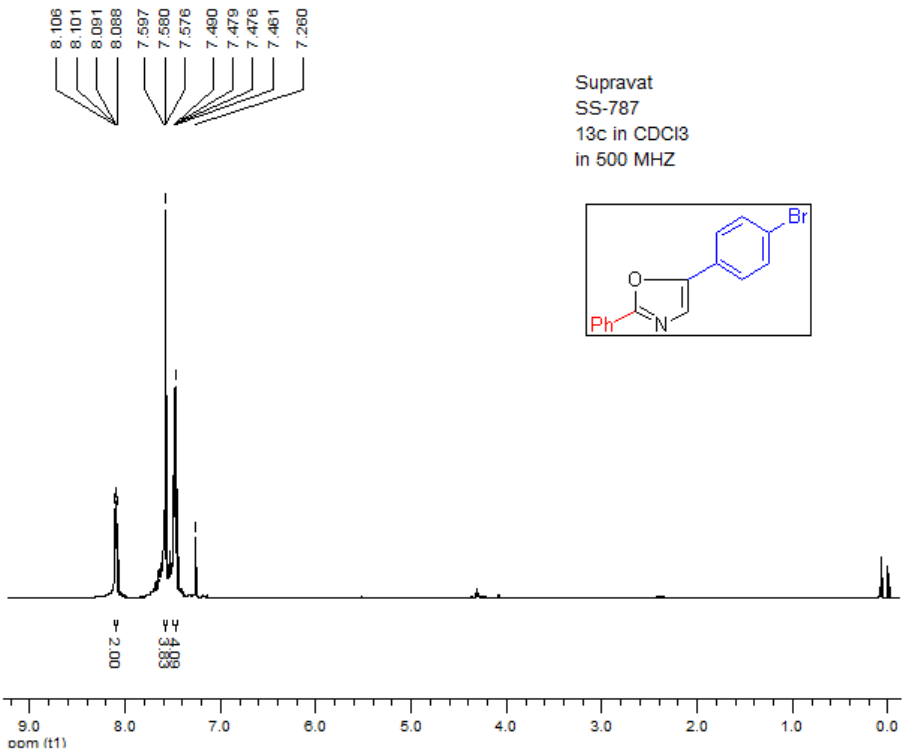
Copies of ^{1}H & ^{13}C- NMR



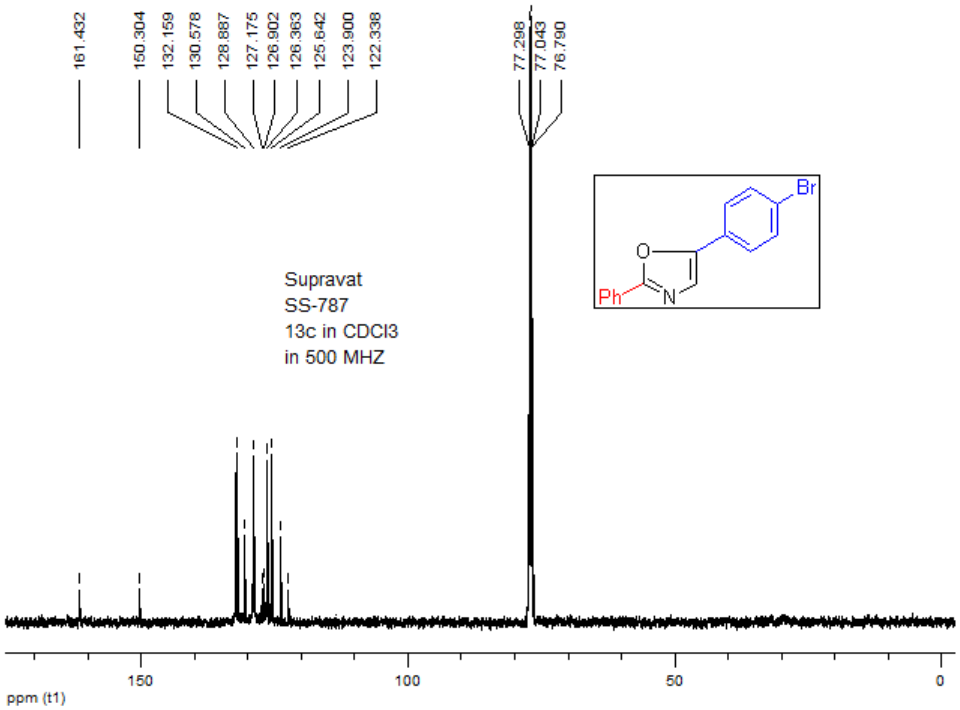
^{1}H NMR of 2a



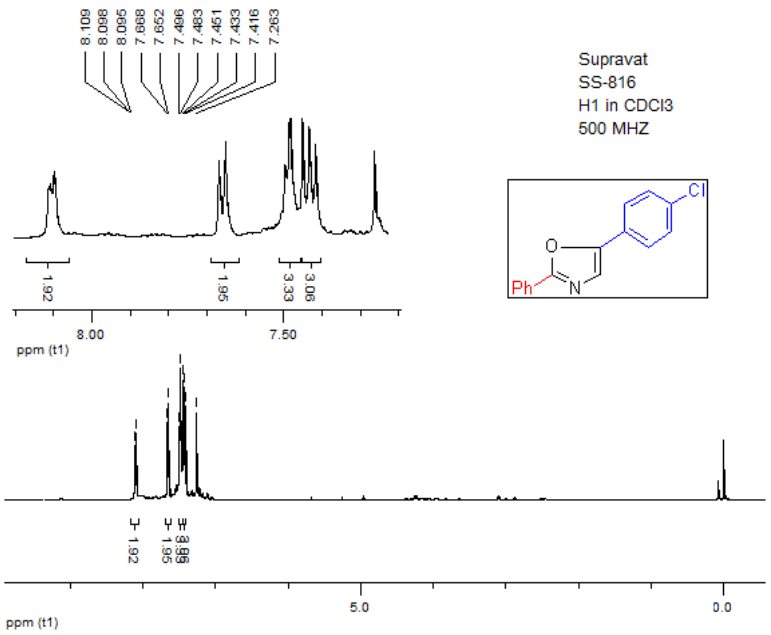
^{13}C NMR of 2a



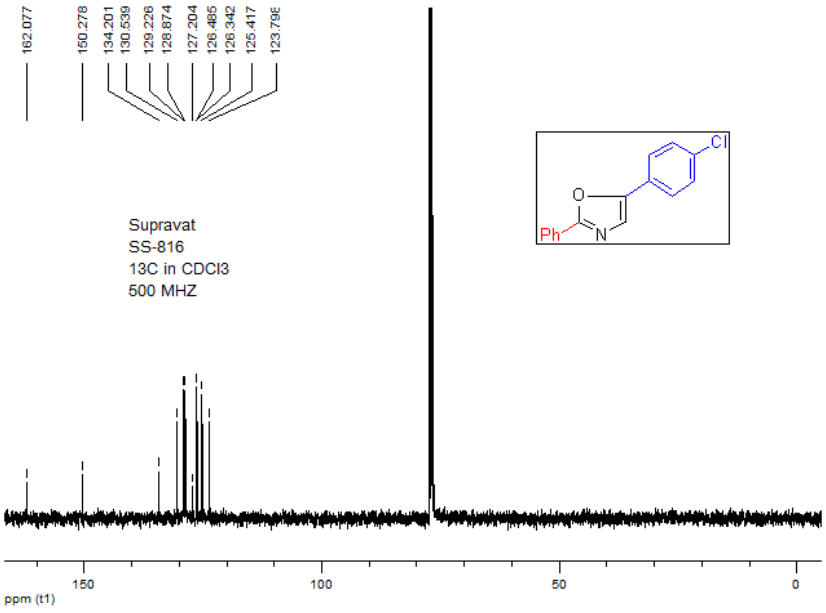
^{1}H NMR of 2b



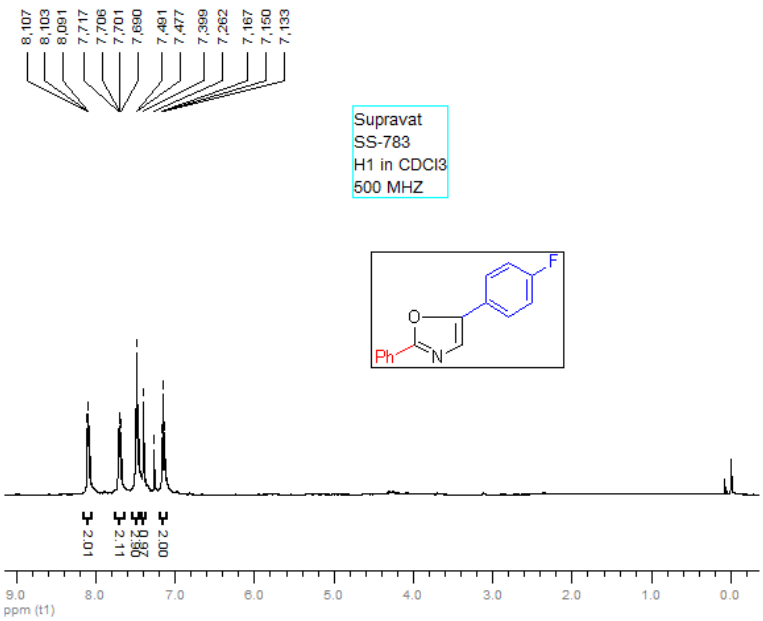
^{13}C NMR of 2b



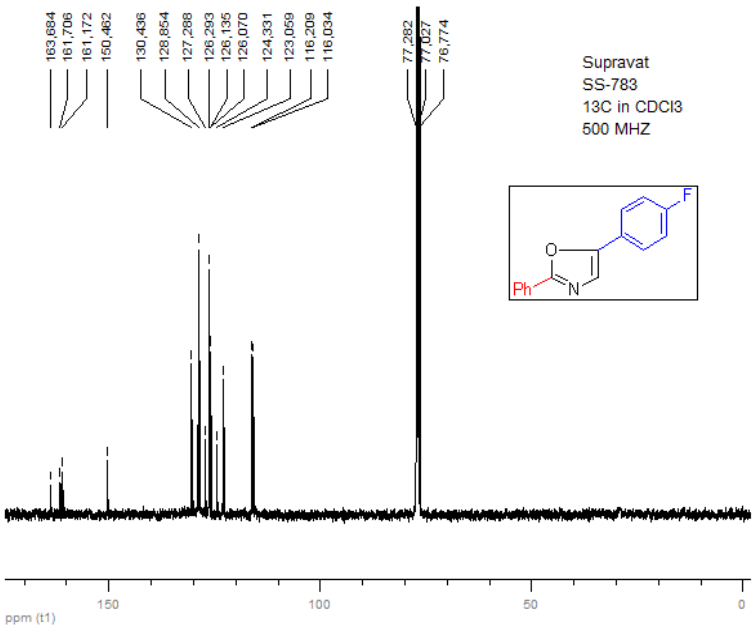
^{1}H NMR of 2c



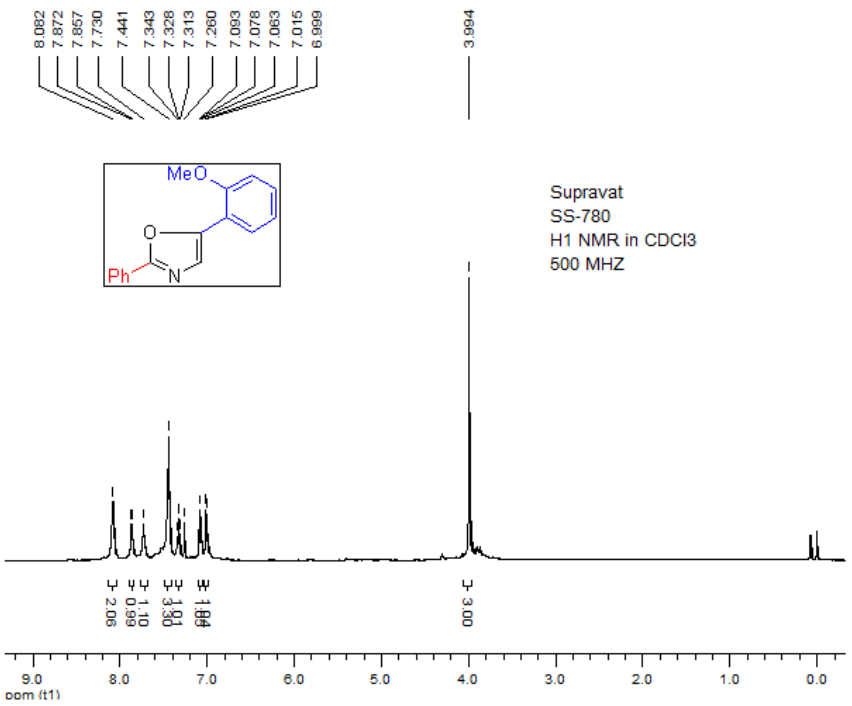
^{13}C NMR of 2c



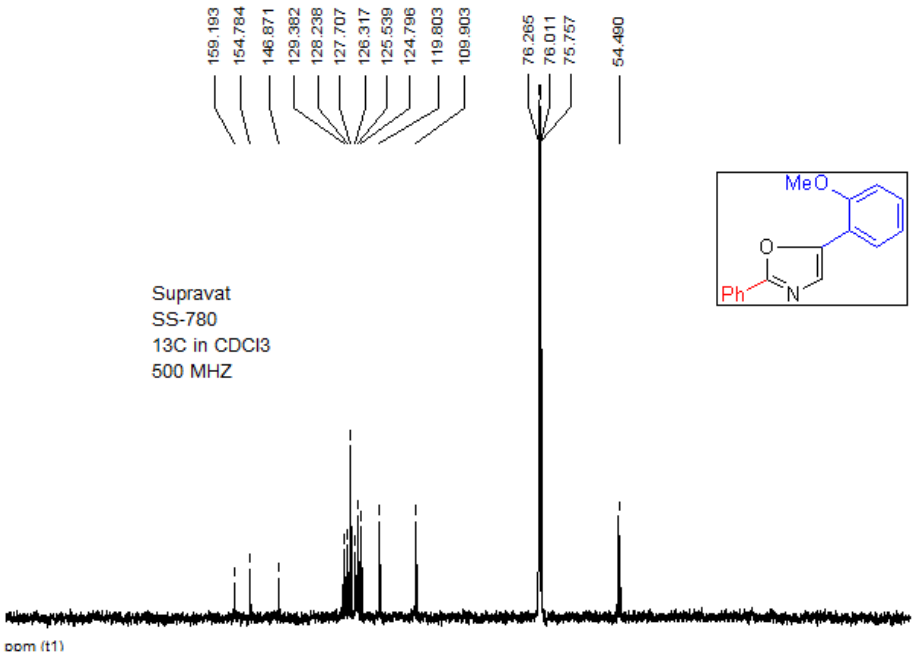
^{1}H NMR of 2d



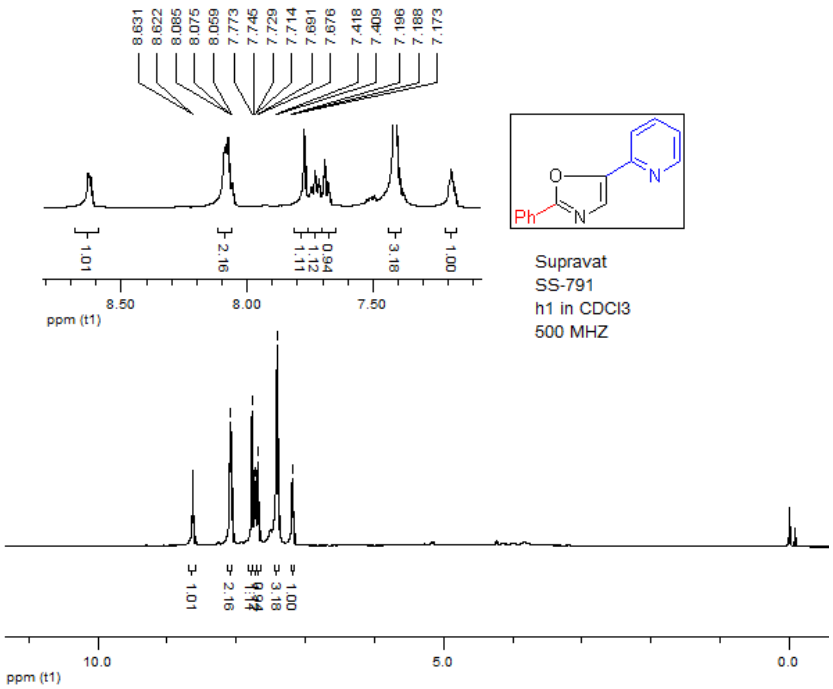
^{13}C NMR of 2d



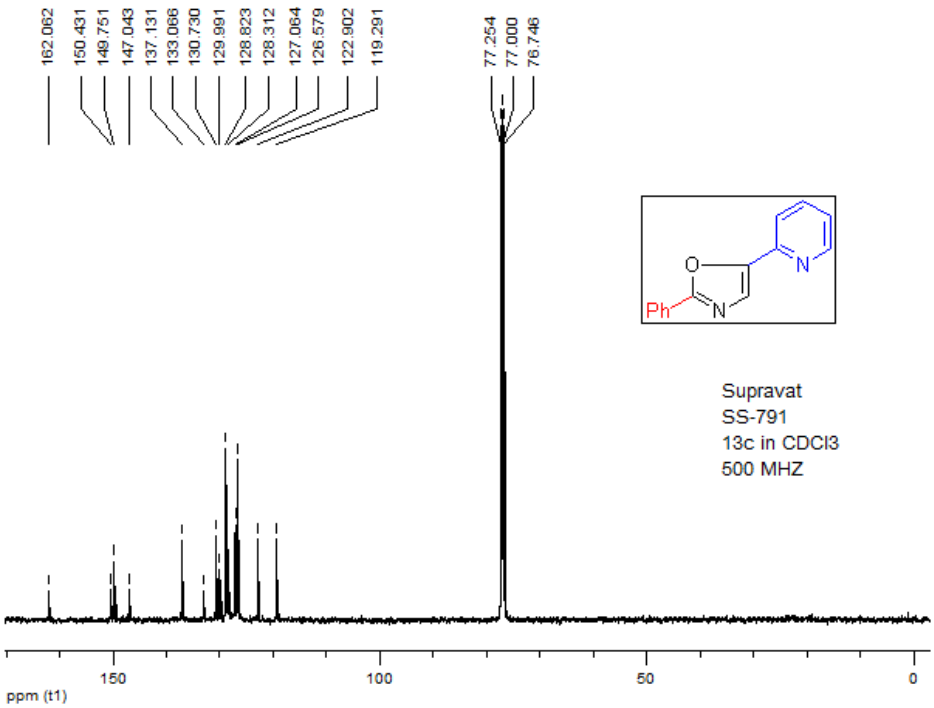
^{1}H NMR of 2e



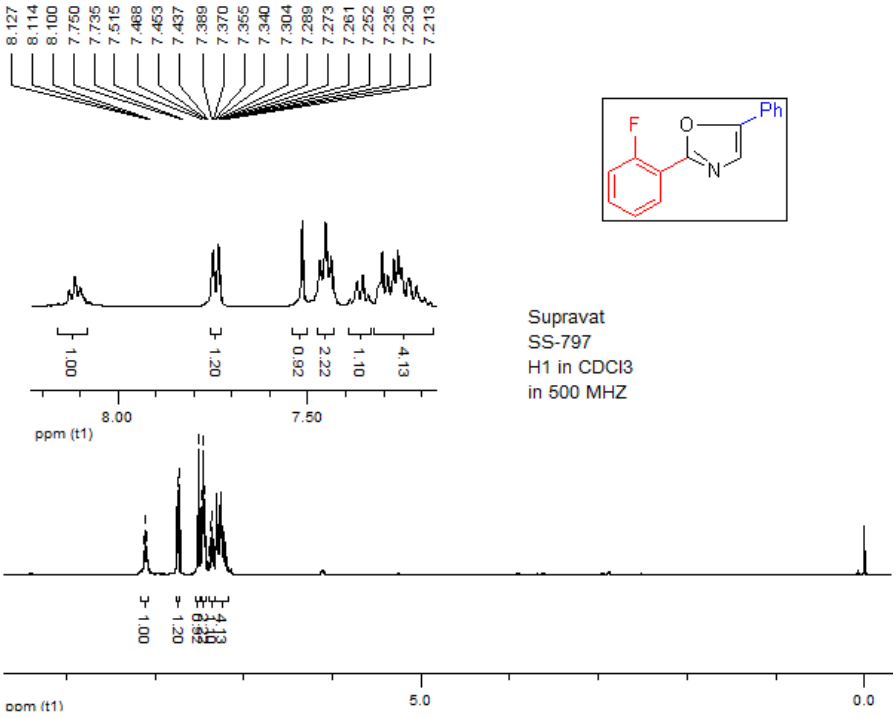
^{13}C NMR of 2e



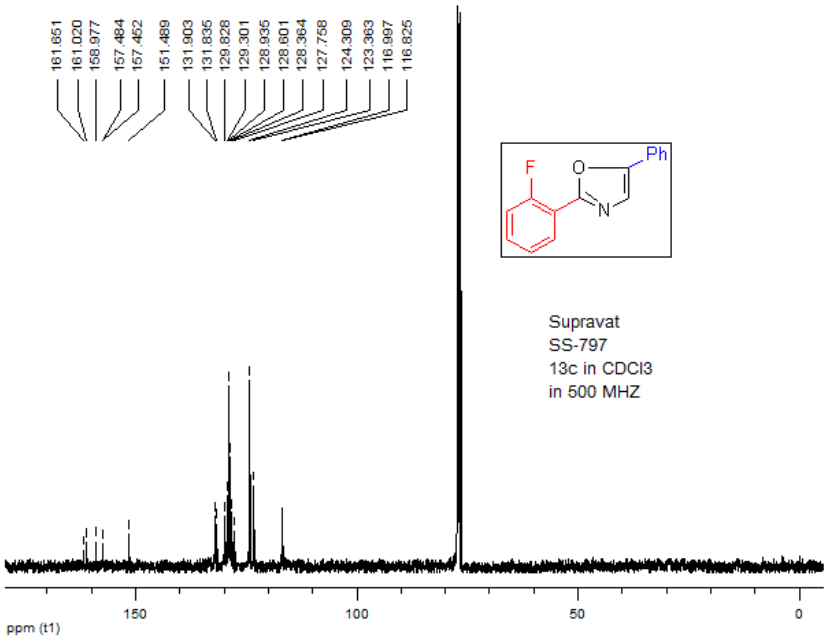
^{1}H NMR of 2f



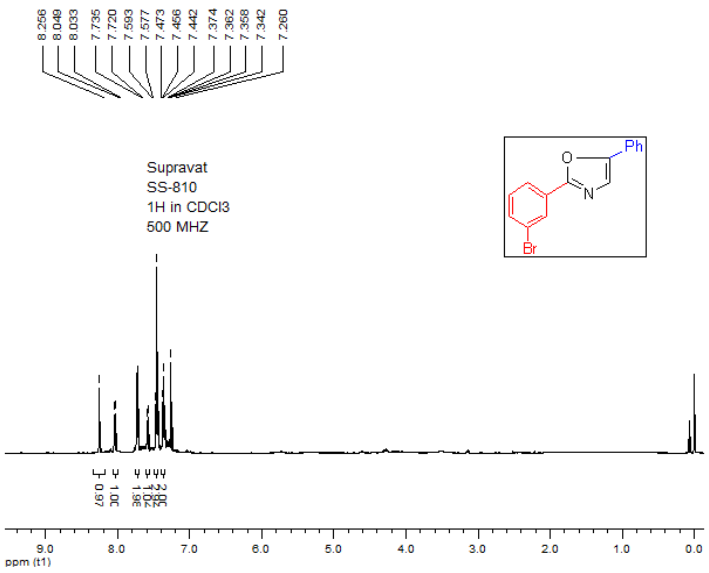
^{13}C NMR of 2f



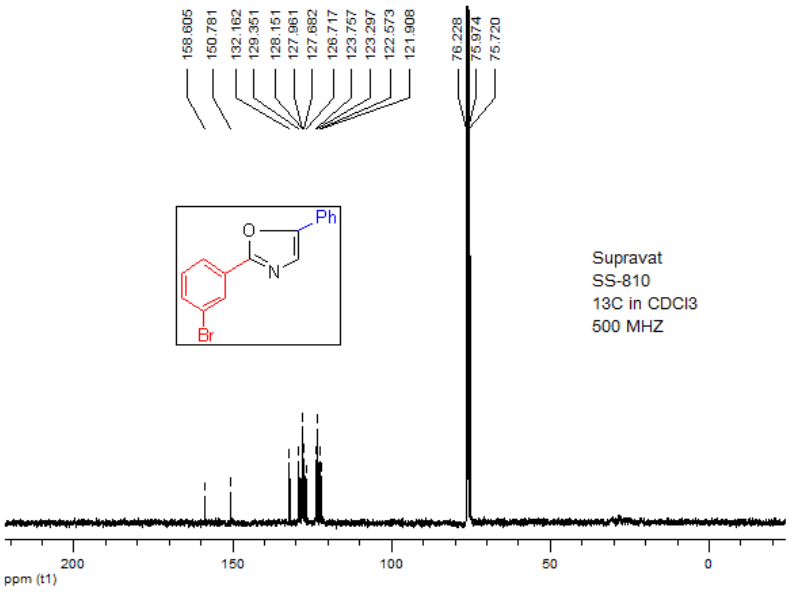
^{1}H NMR of 2g



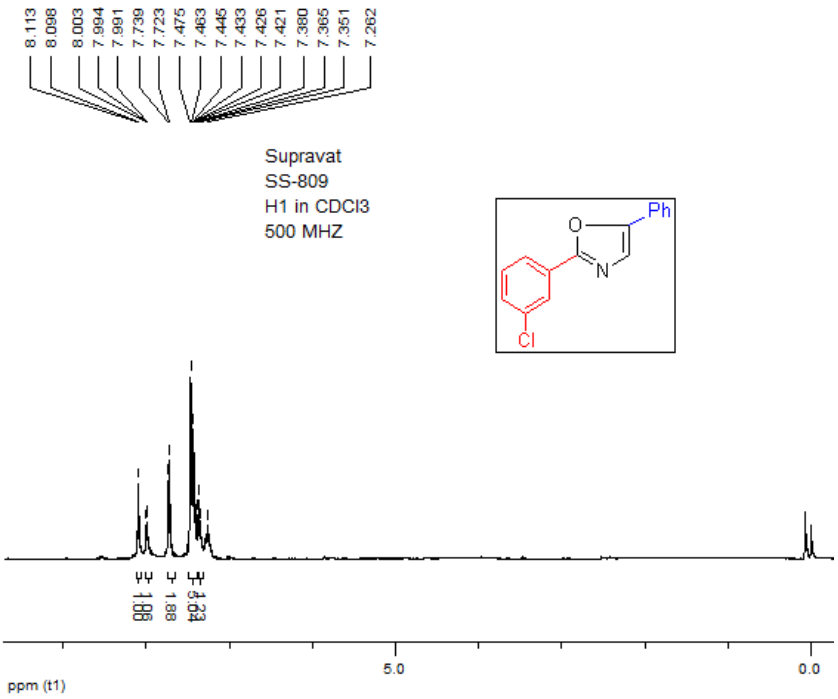
^{13}C NMR of 2g



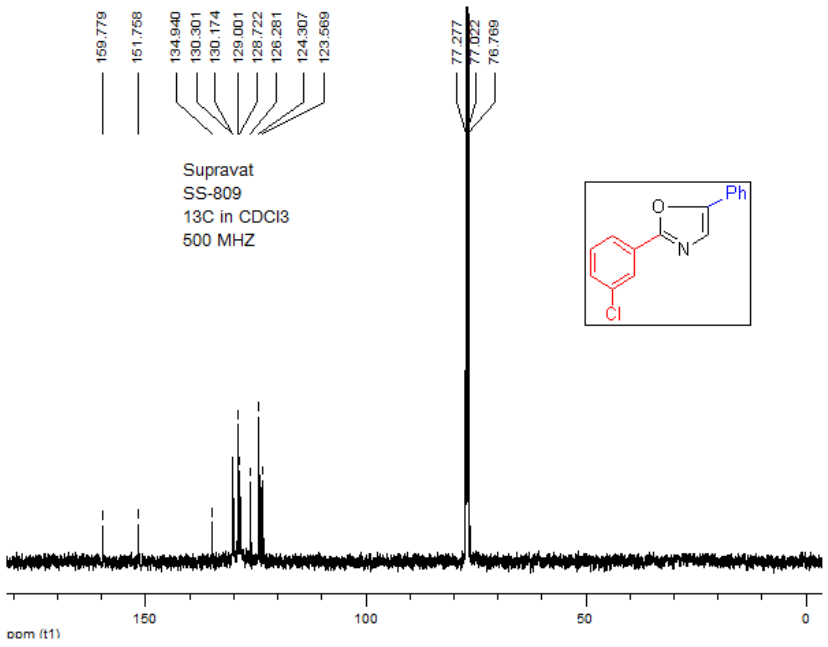
^{1}H NMR of 2h



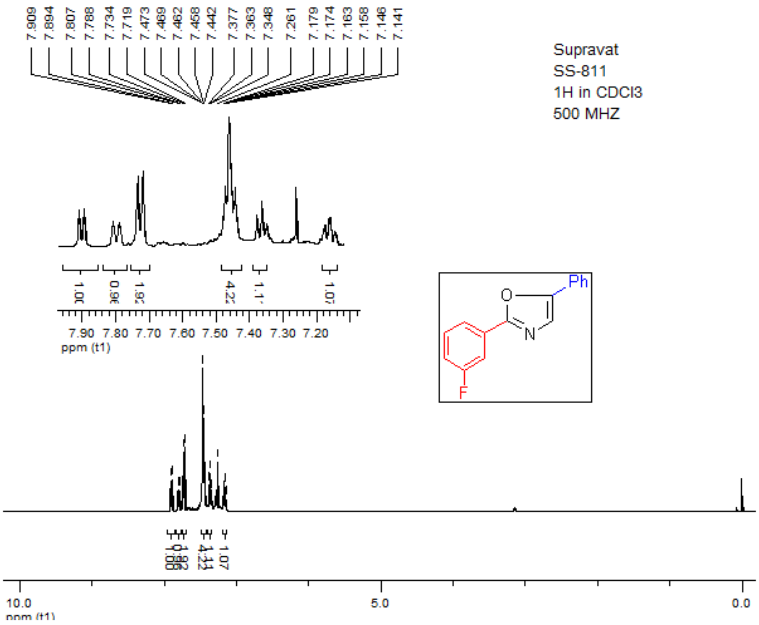
^{13}C NMR of 2h



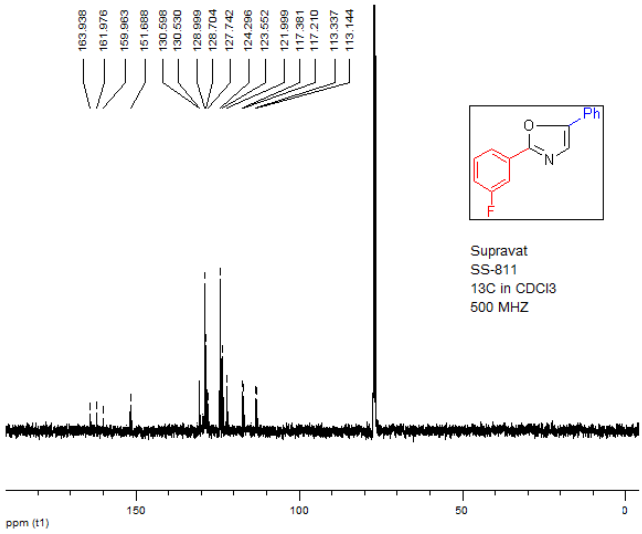
^{1}H NMR of 2i



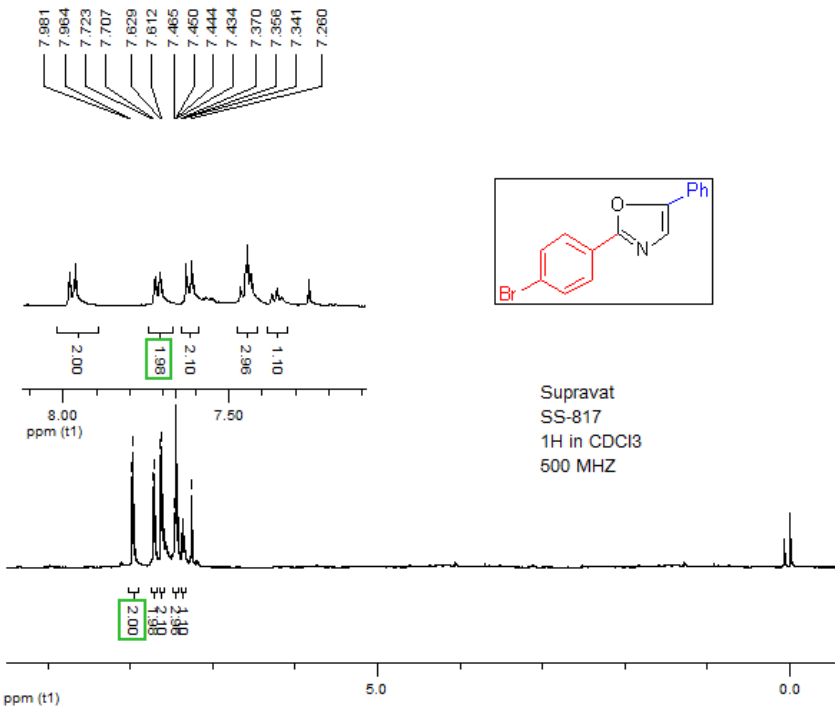
^{13}C NMR of 2i



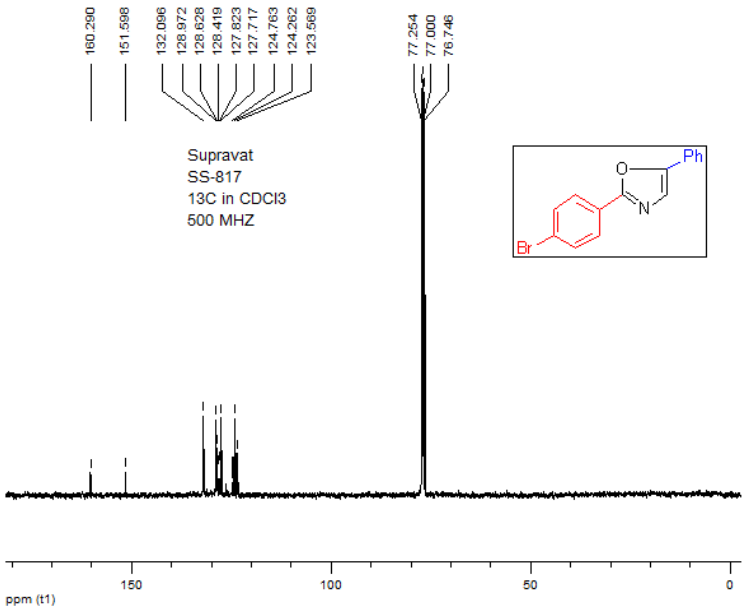
^{1}H NMR of 2j



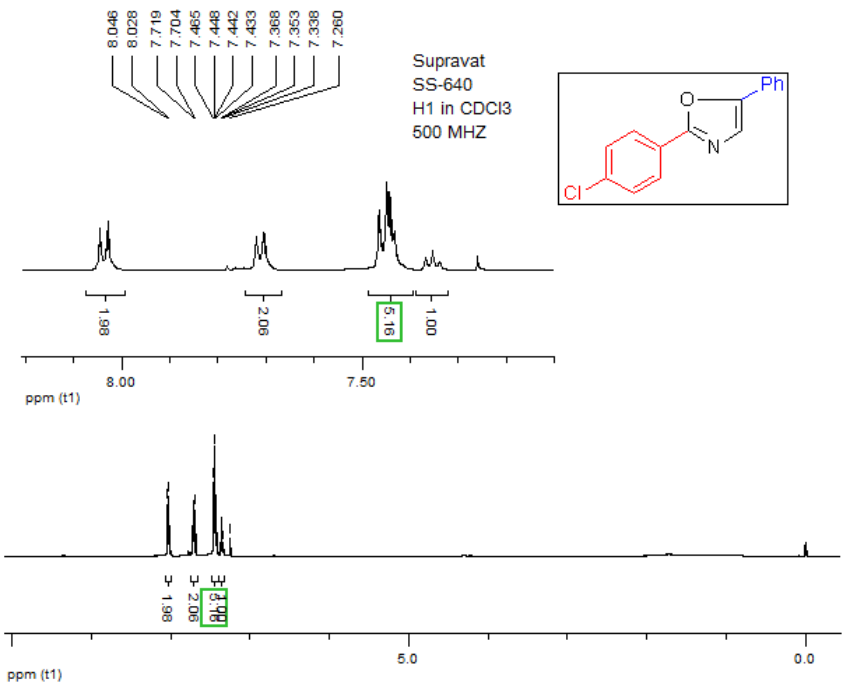
^{13}C NMR of 2j



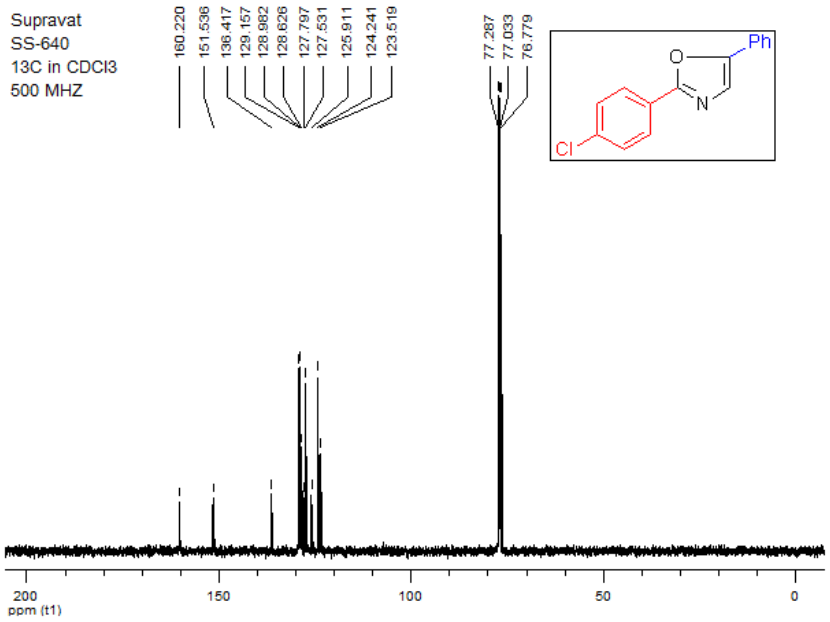
^{1}H NMR of 2k



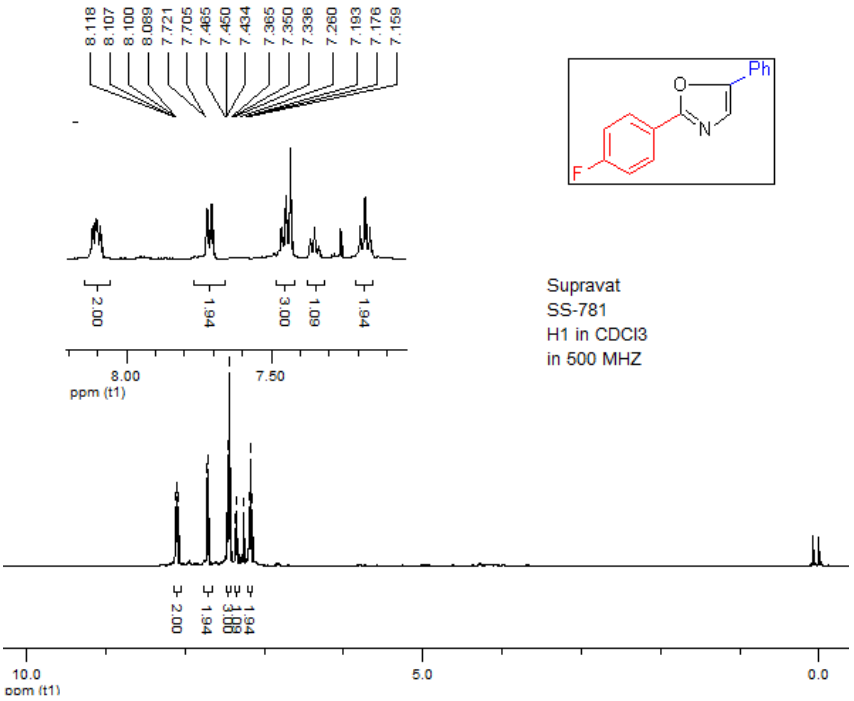
^{13}C NMR of 2k



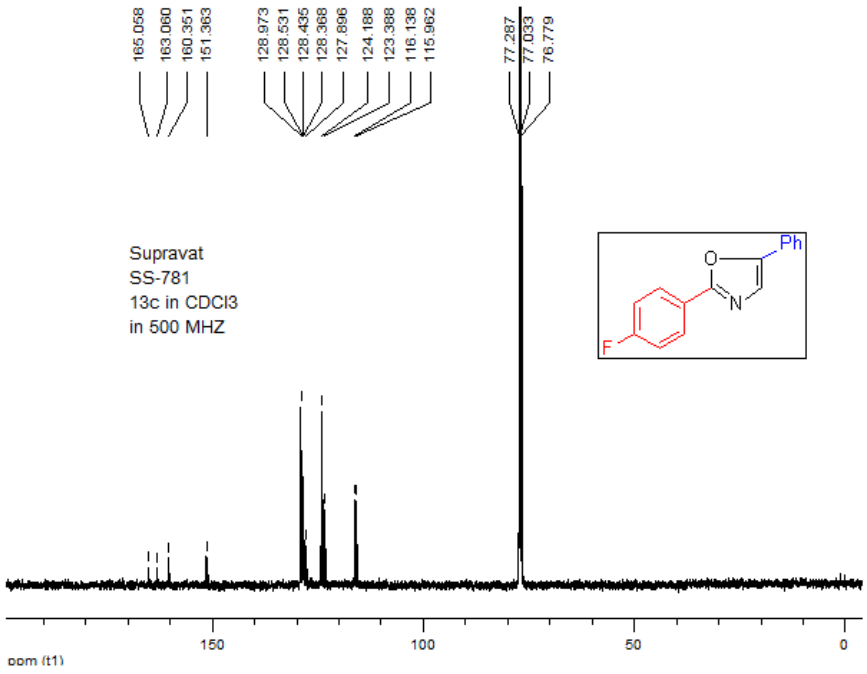
^{1}H NMR of 2l



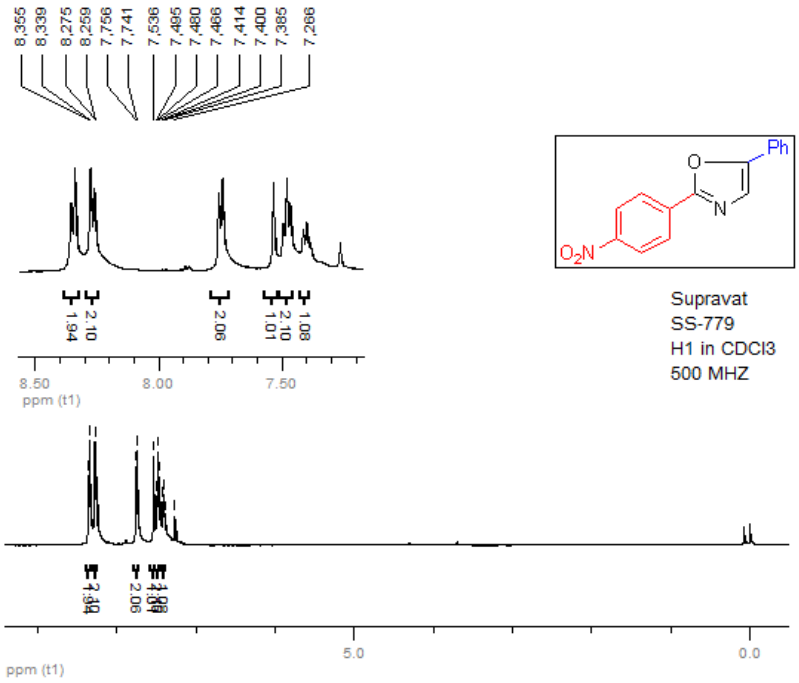
^{13}C NMR of 2l



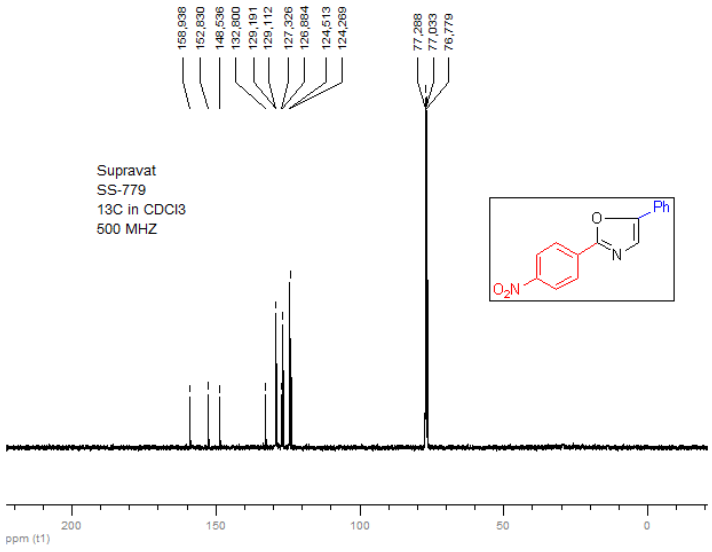
^{1}H NMR of 2m



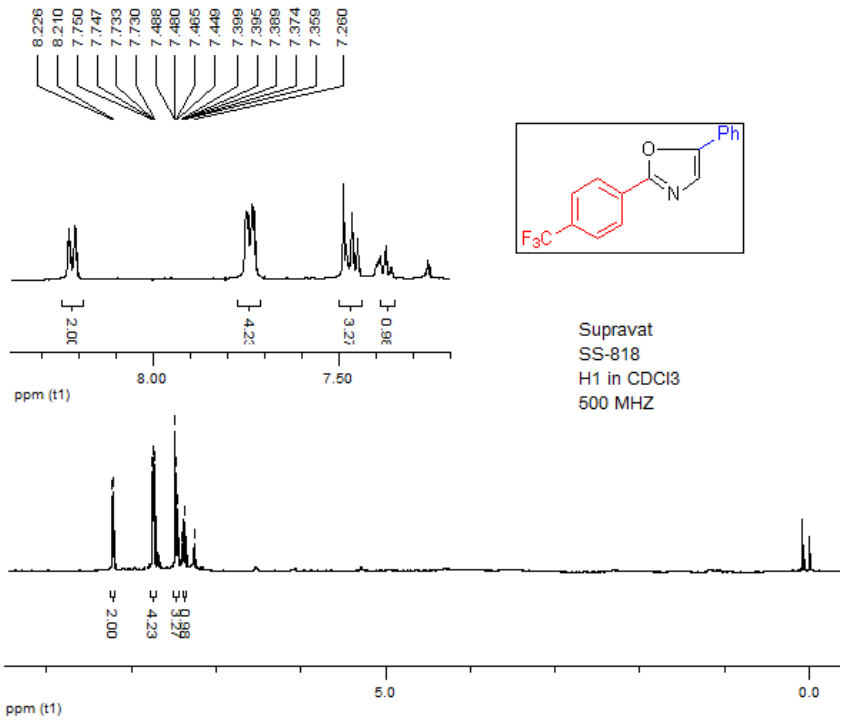
^{13}C NMR of 2m



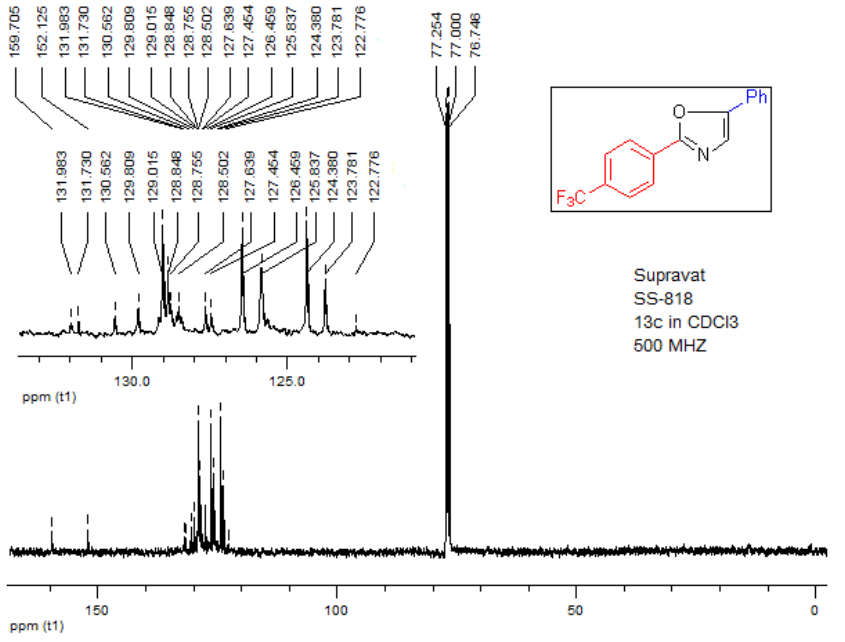
^{1}H NMR of 2n



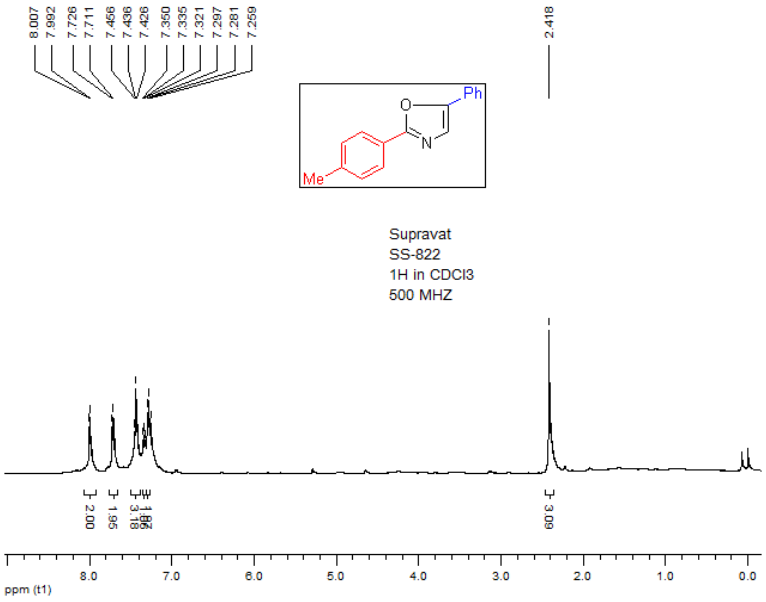
^{13}C NMR of 2n



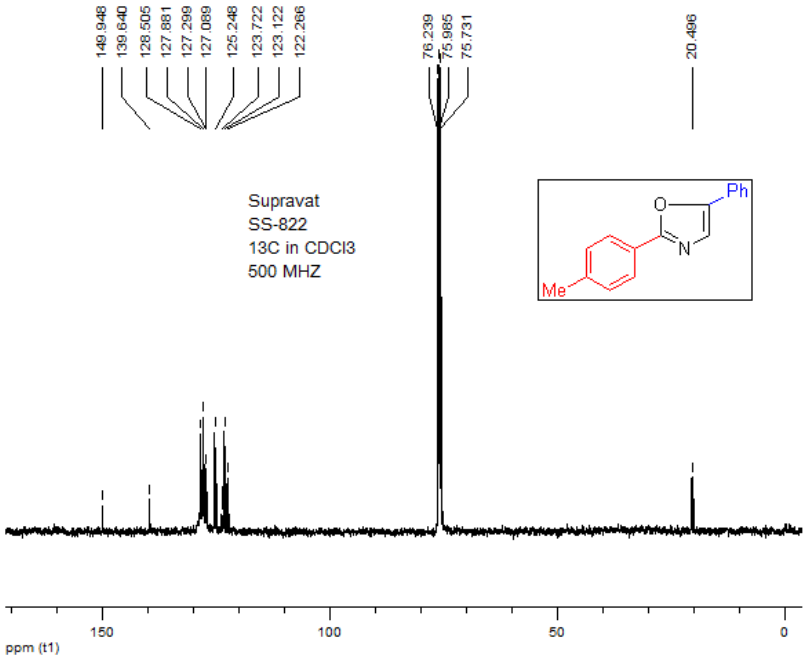
^{1}H NMR of 2o



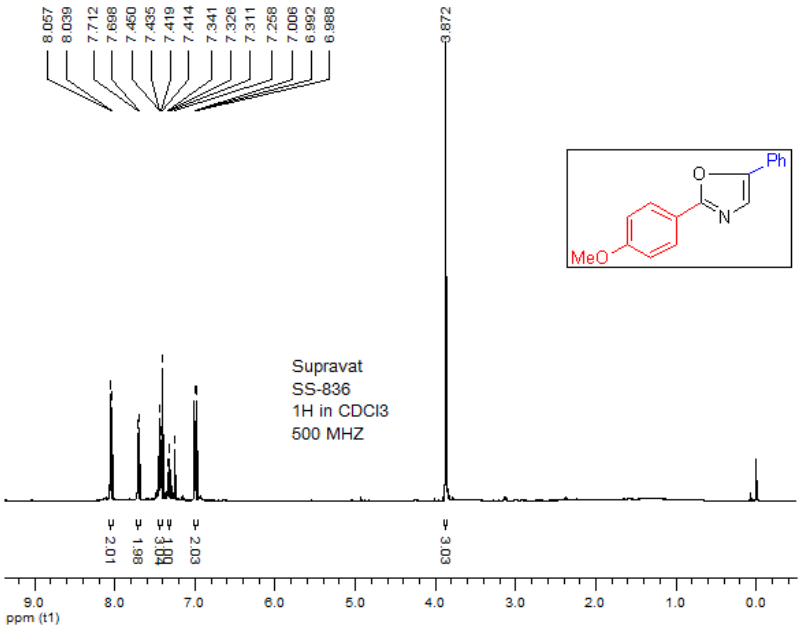
^{13}C NMR of 2o



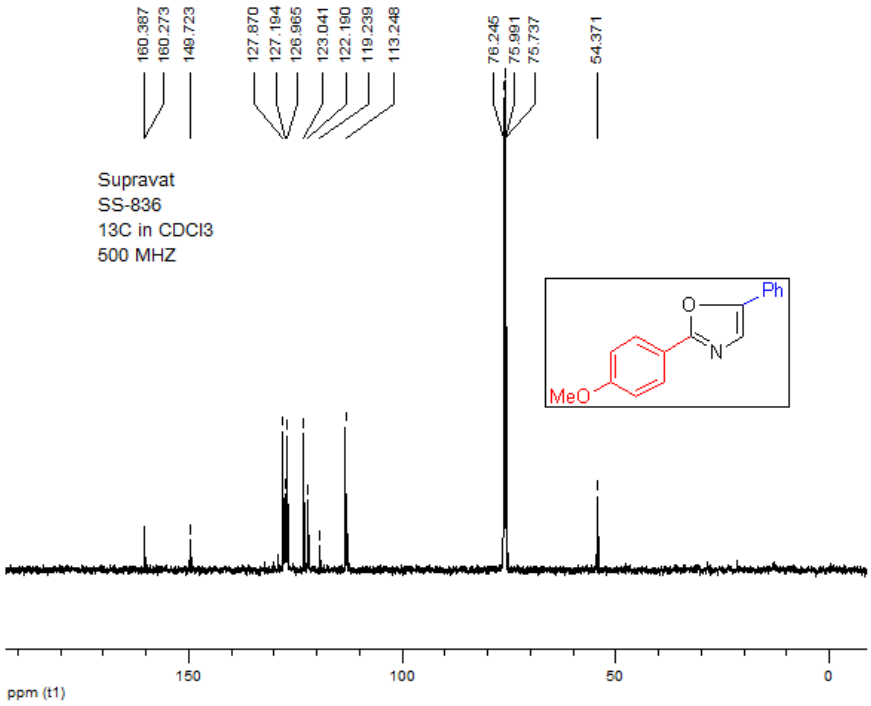
^{1}H NMR of 2p



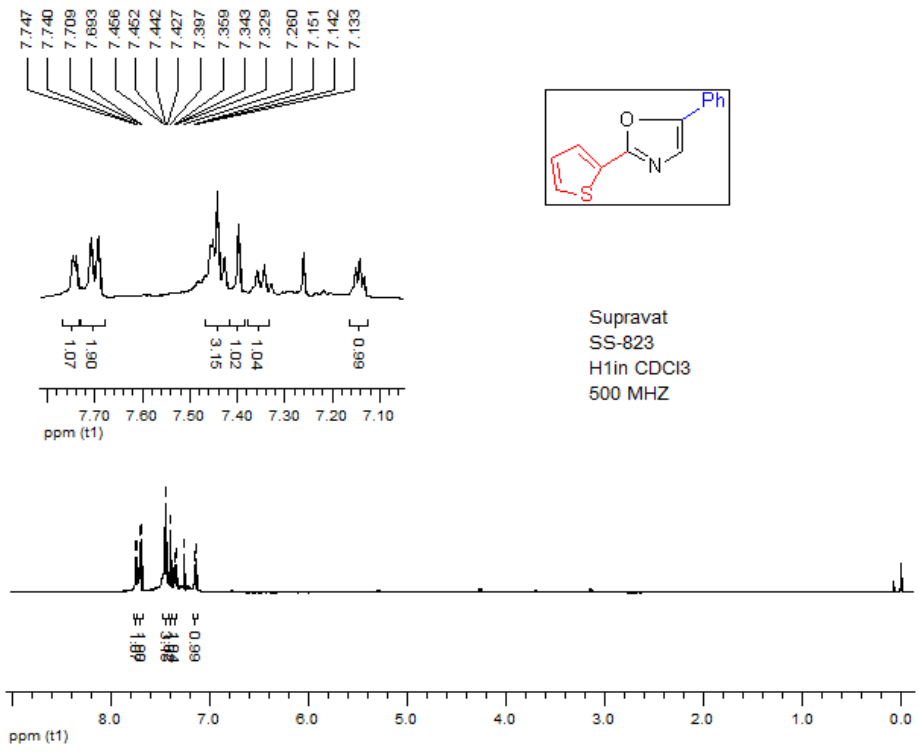
^{13}C NMR of 2p



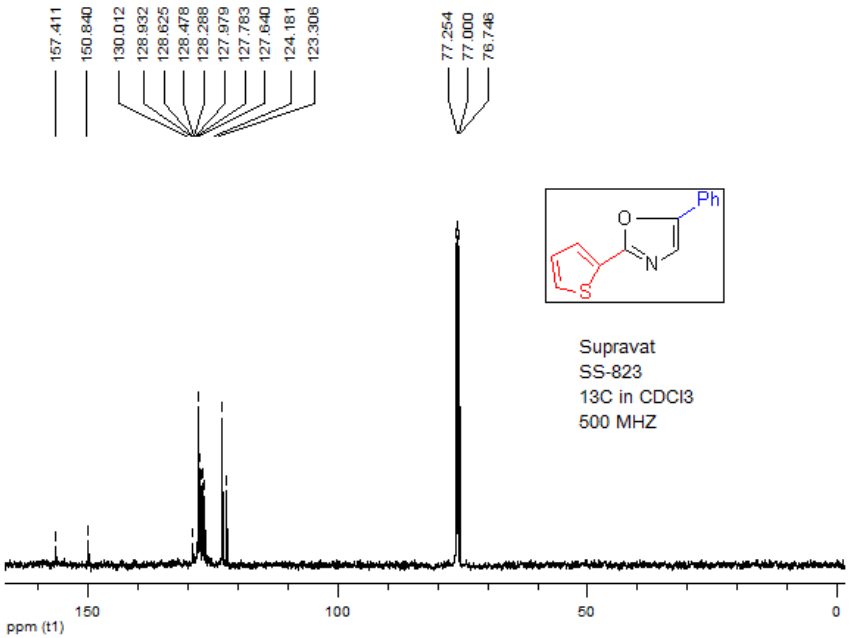
^{1}H NMR of 2q



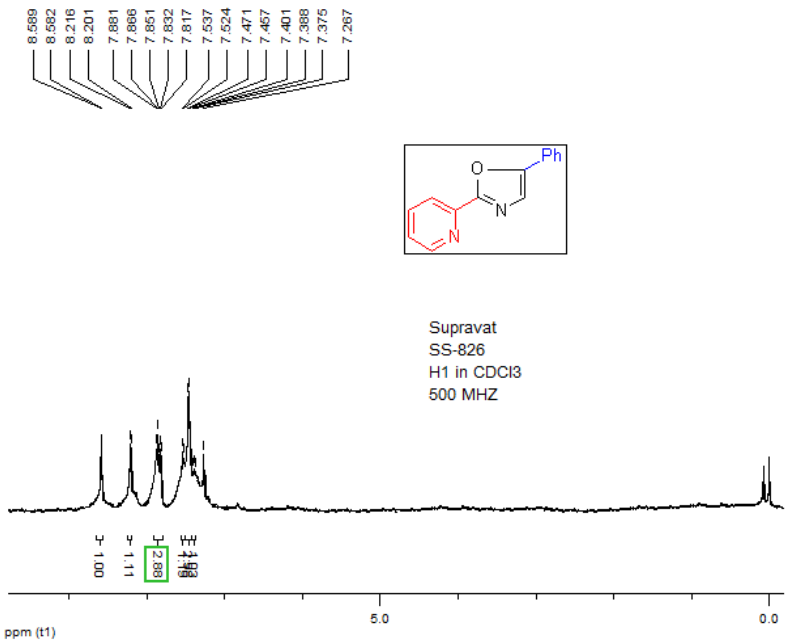
^{13}C NMR of 2q



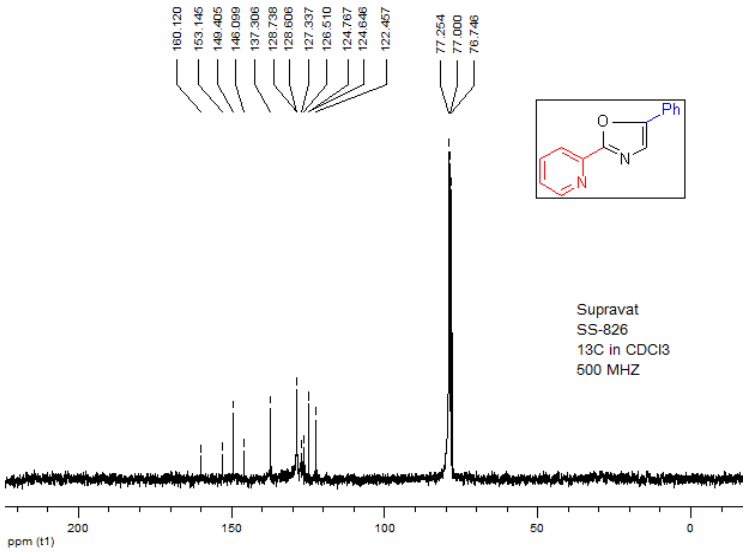
^{1}H NMR of 2r



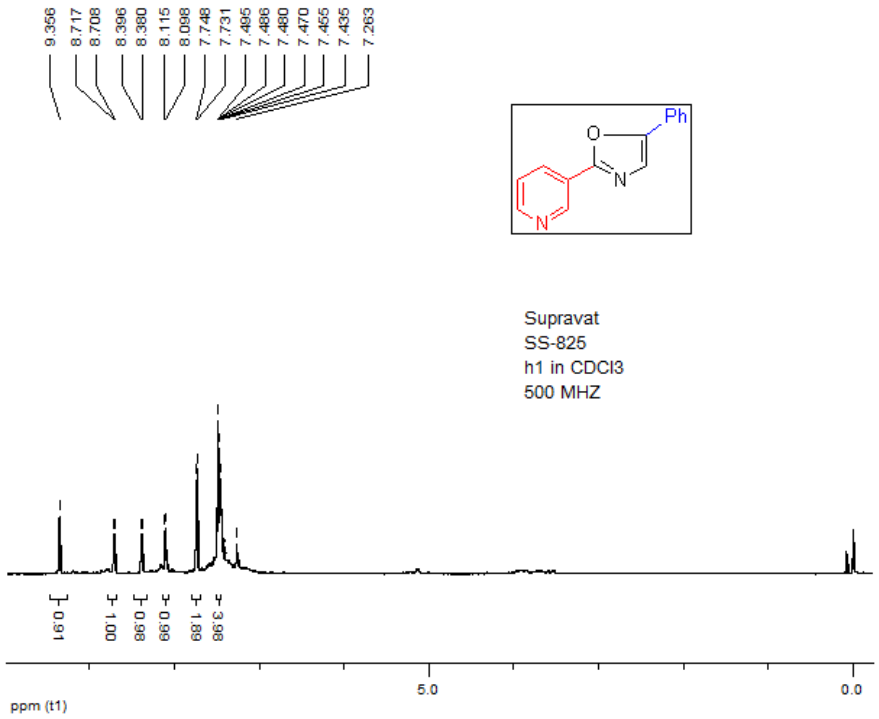
^{13}C NMR of 2r



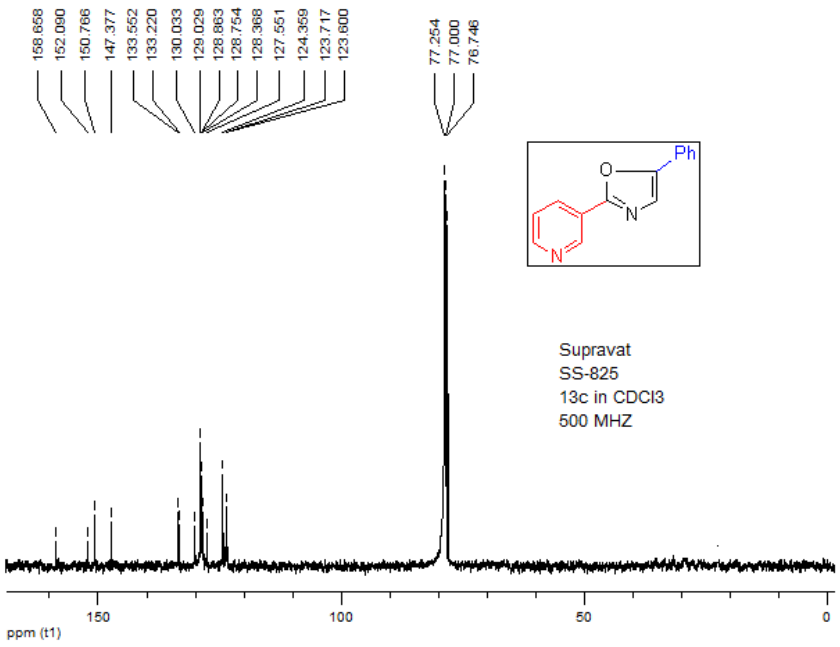
^{1}H NMR of 2s



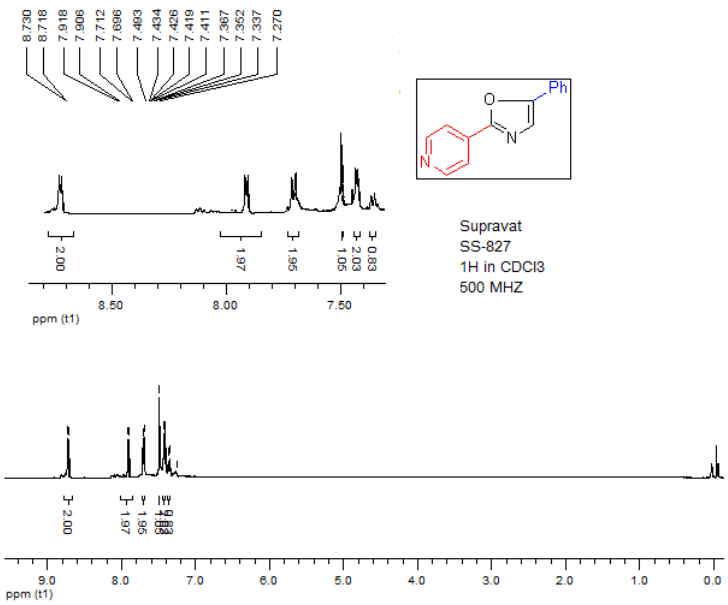
^{13}C NMR of 2s



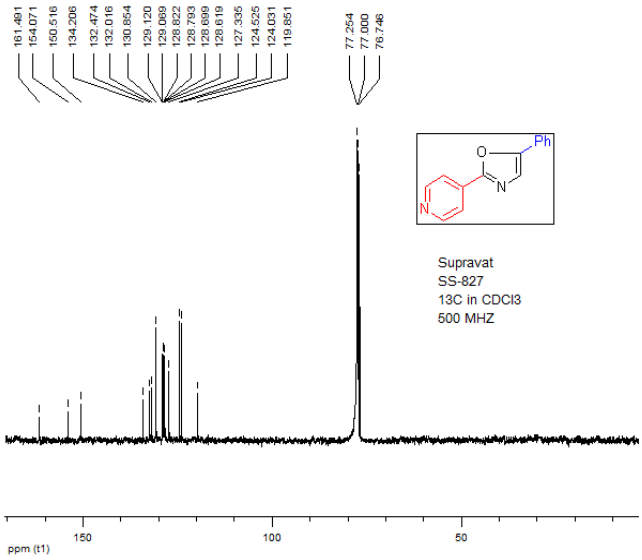
^{1}H NMR of 2t



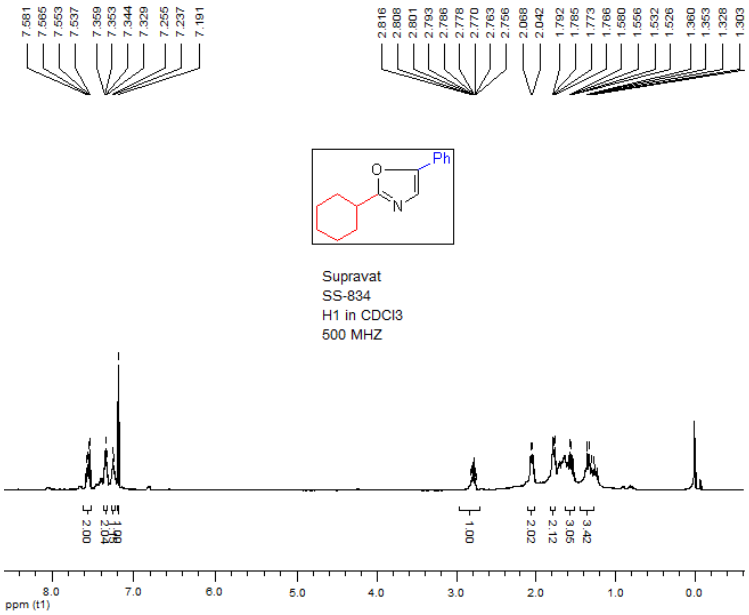
^{13}C NMR of 2t



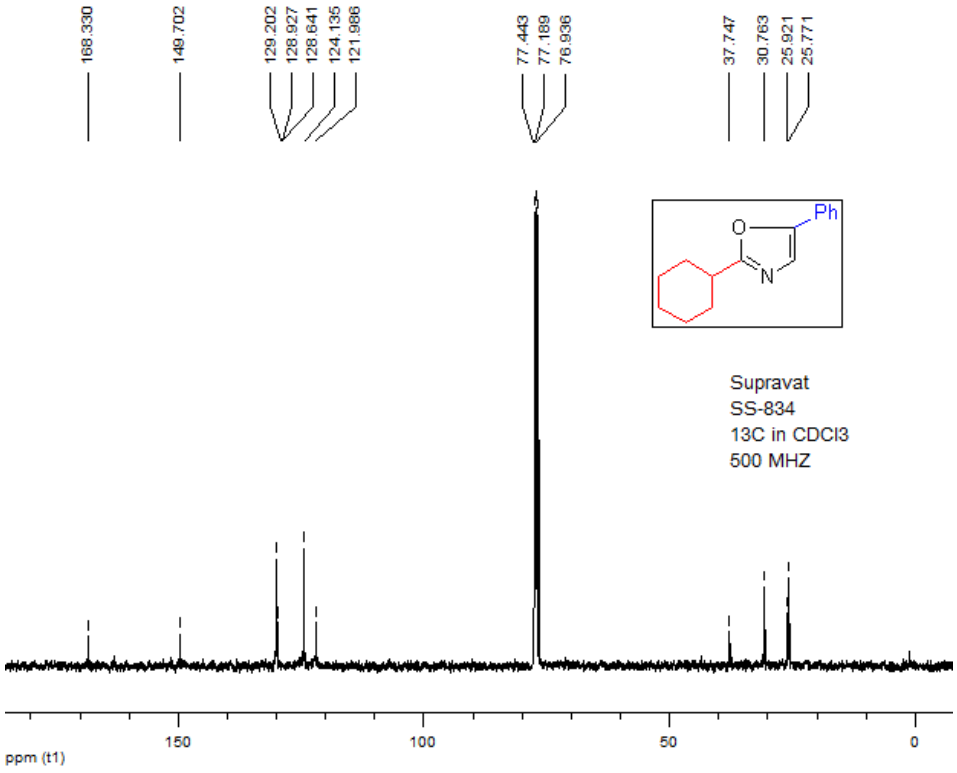
^{1}H NMR of 2u



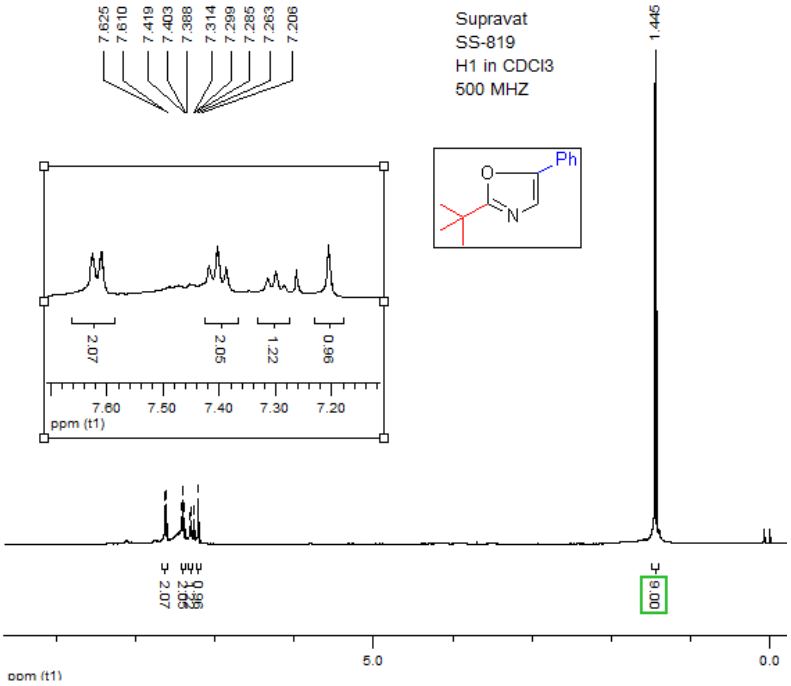
^{13}C NMR of 2u



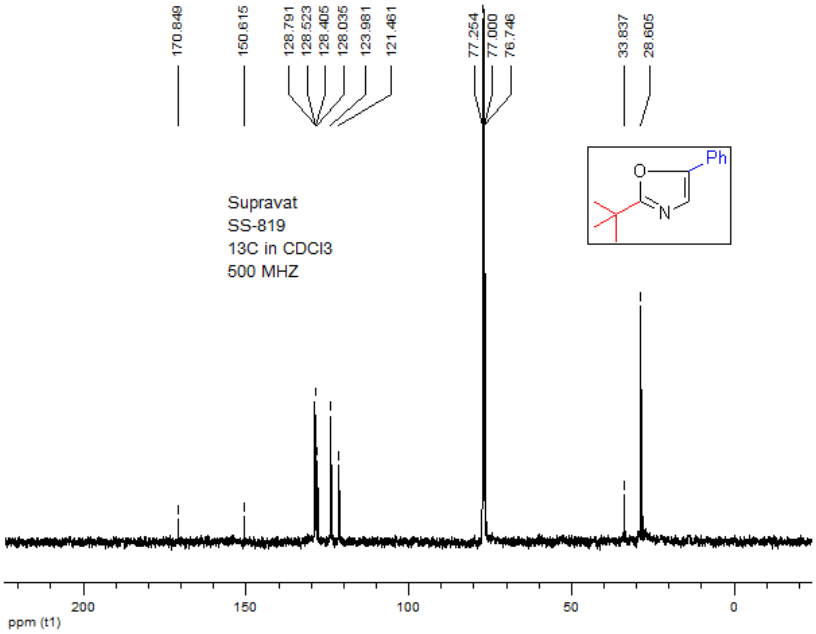
^{1}H NMR of 2v



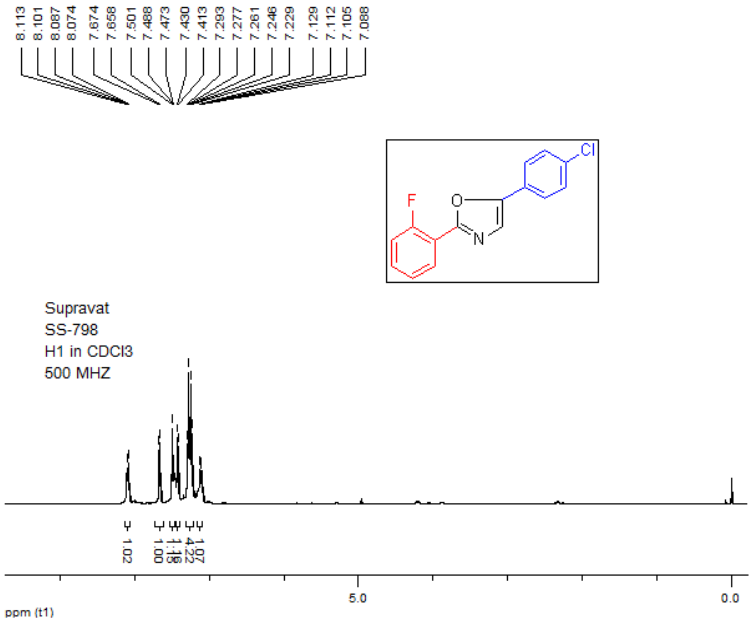
^{13}C NMR of 2v



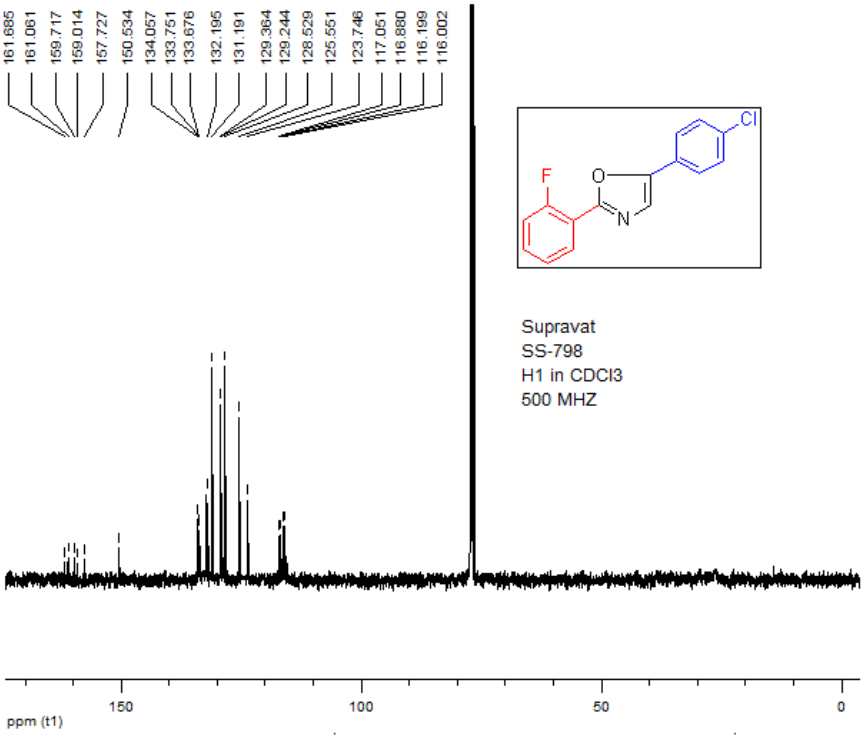
^{1}H NMR of 2w



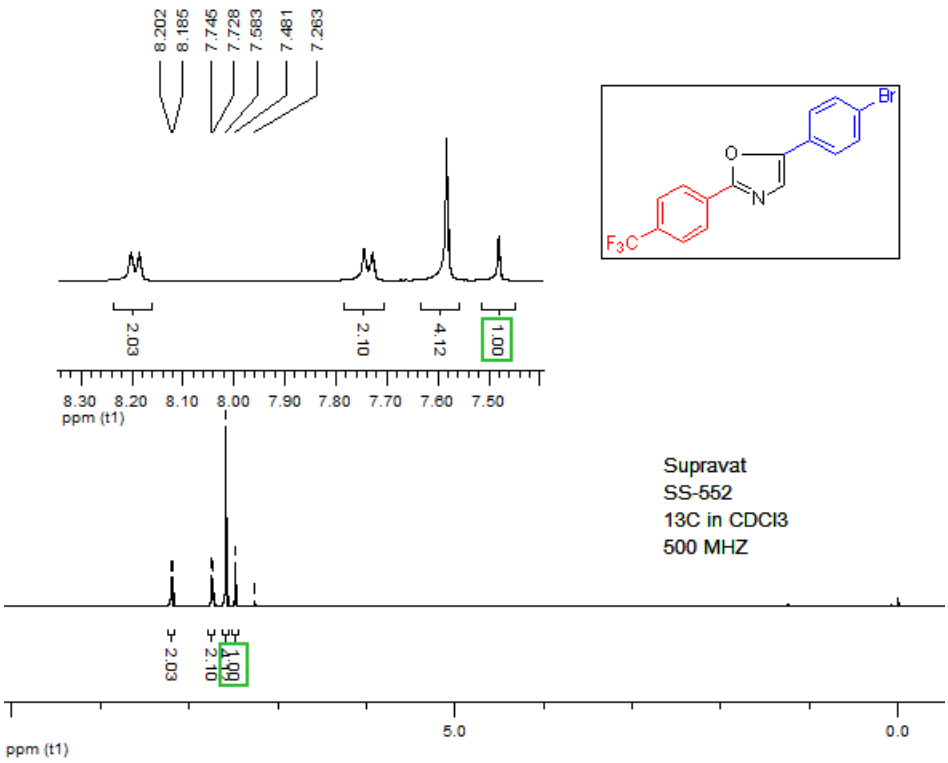
^{13}C NMR of 2w



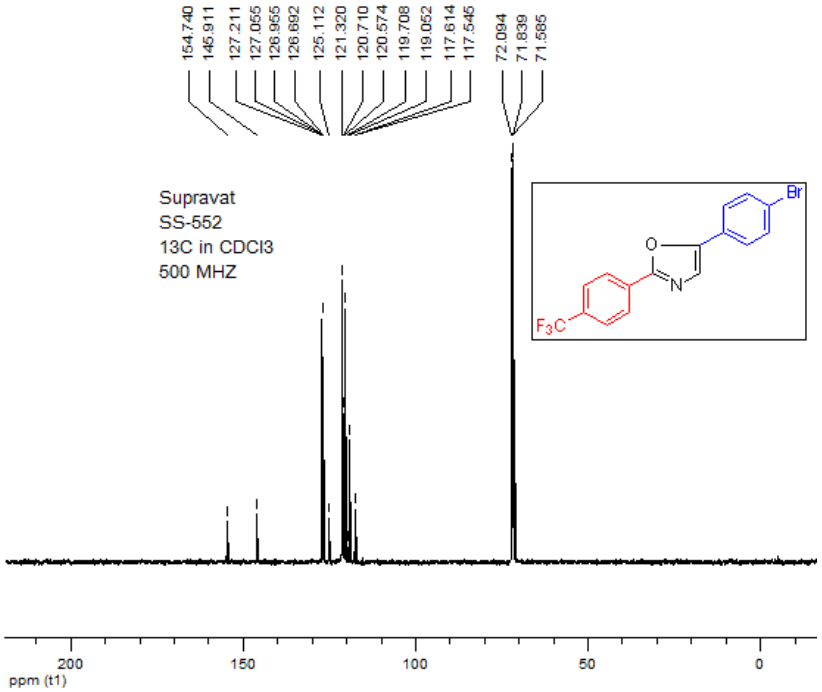
^{1}H NMR of 2x



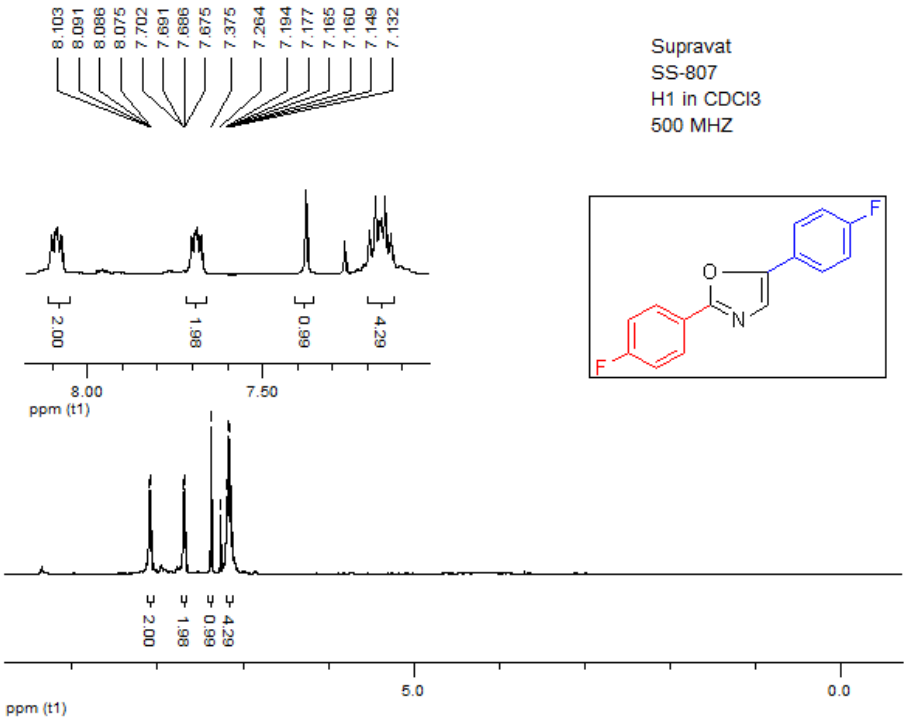
^{13}C NMR of 2x



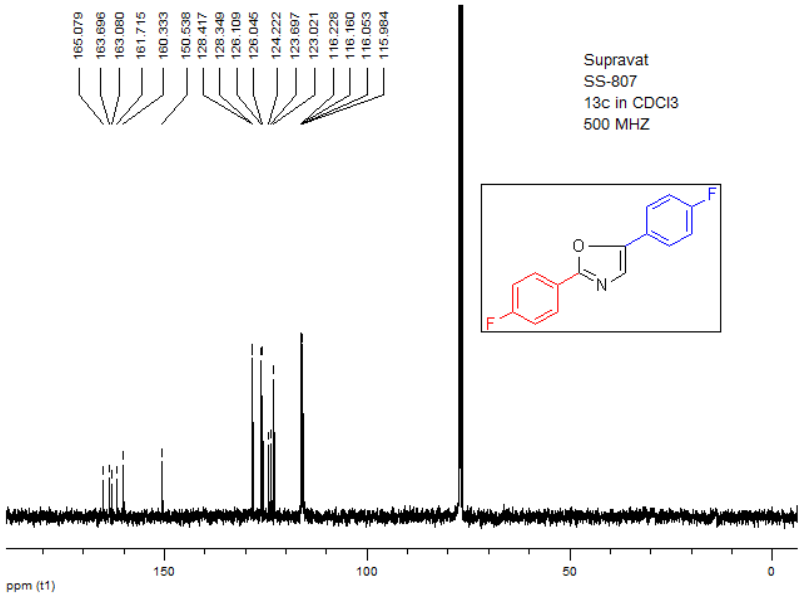
^{1}H NMR of 2y



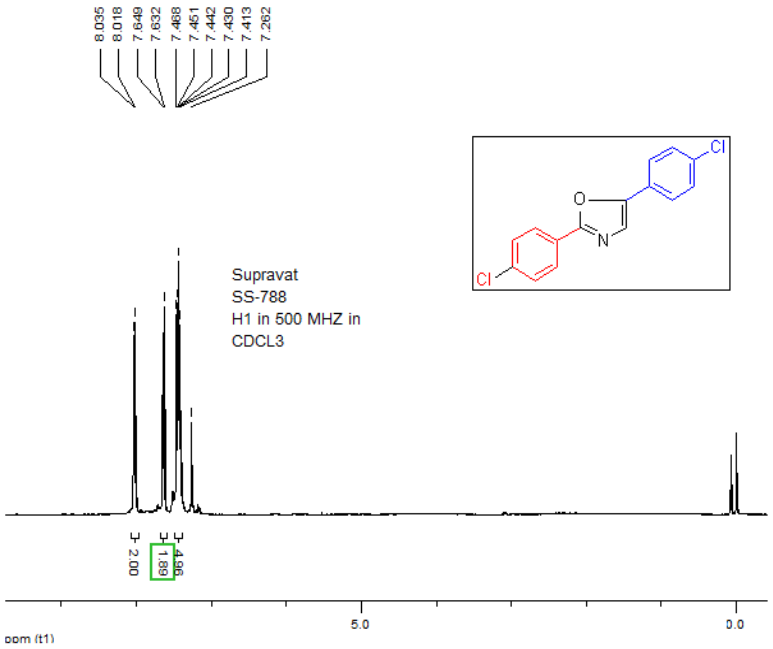
^{13}C NMR of 2y



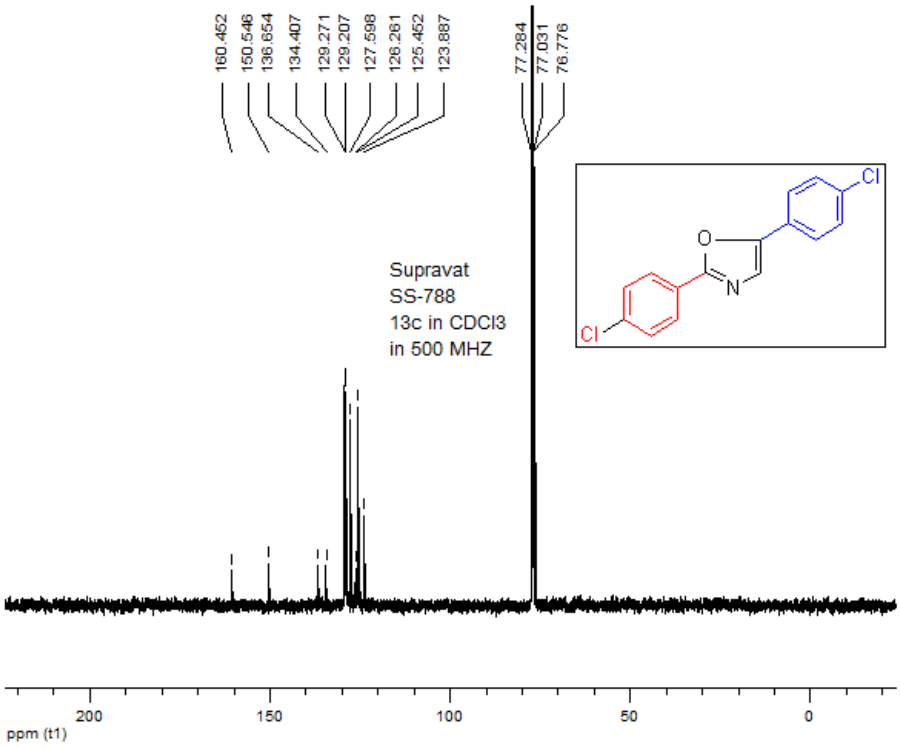
^{1}H NMR of 2z



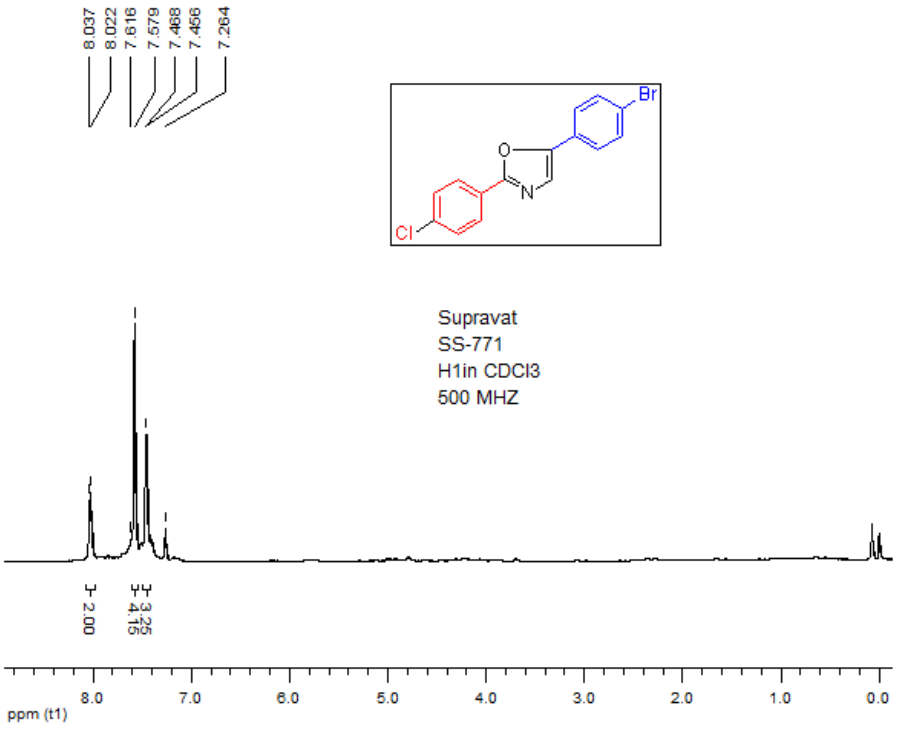
^{13}C NMR of 2z



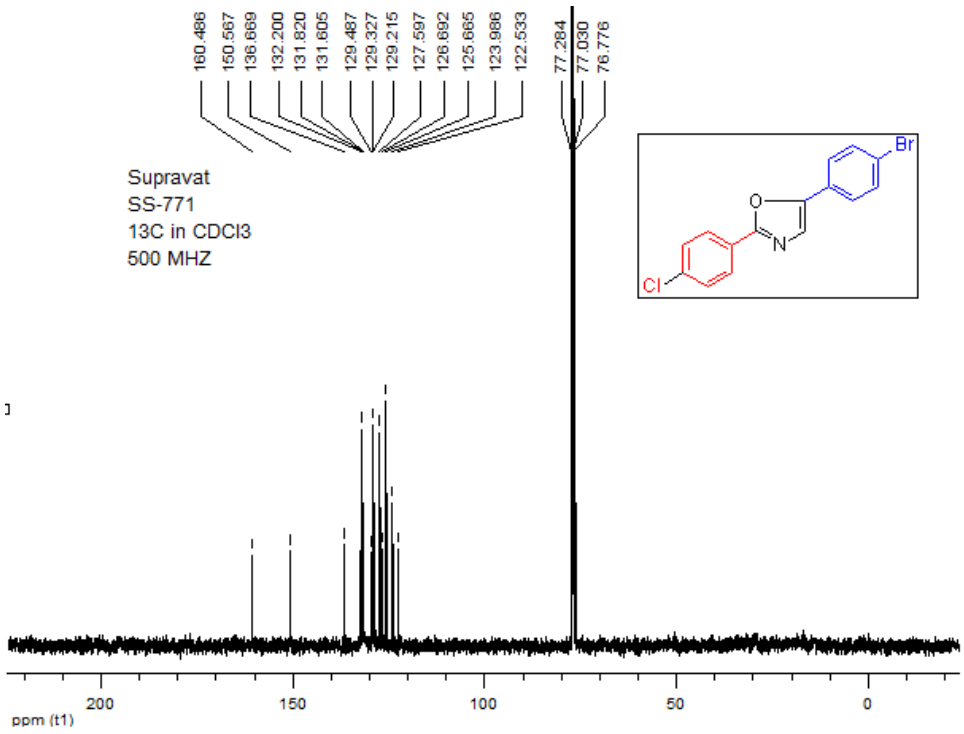
^{1}H NMR of 2aa



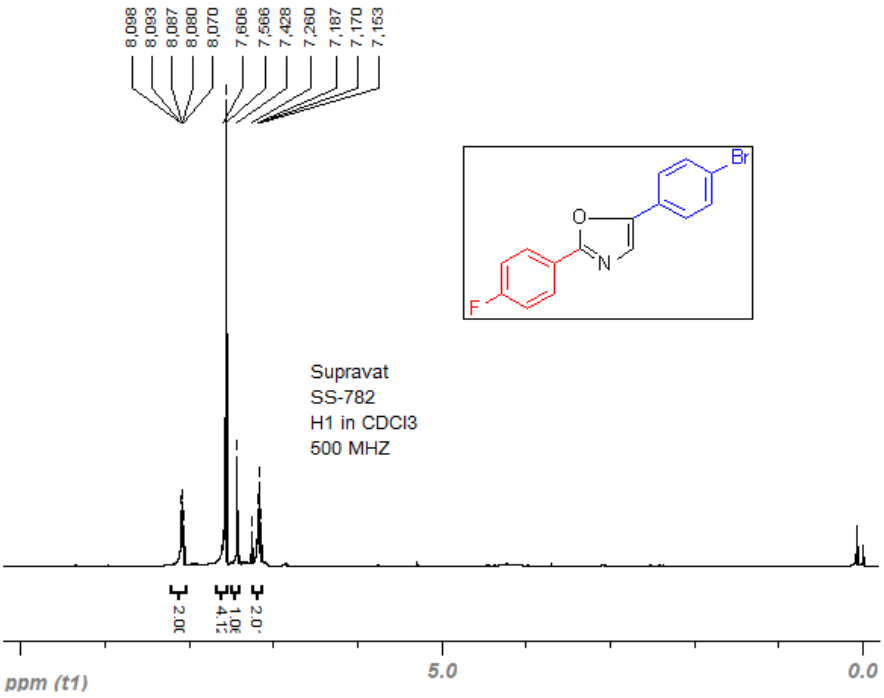
^{13}C NMR of 2aa



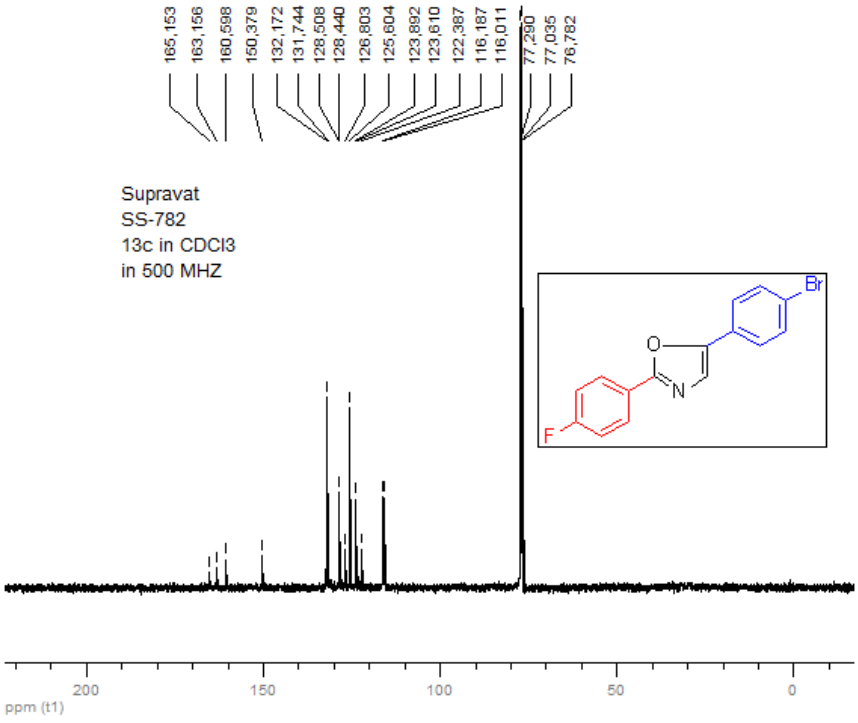
^{1}H NMR of 2ab



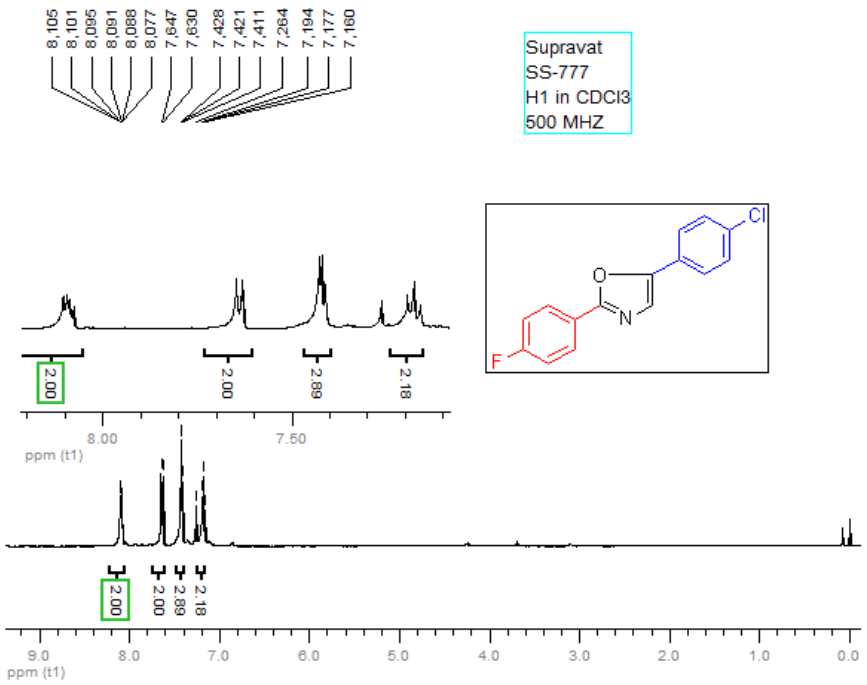
^{13}C NMR of 2ab



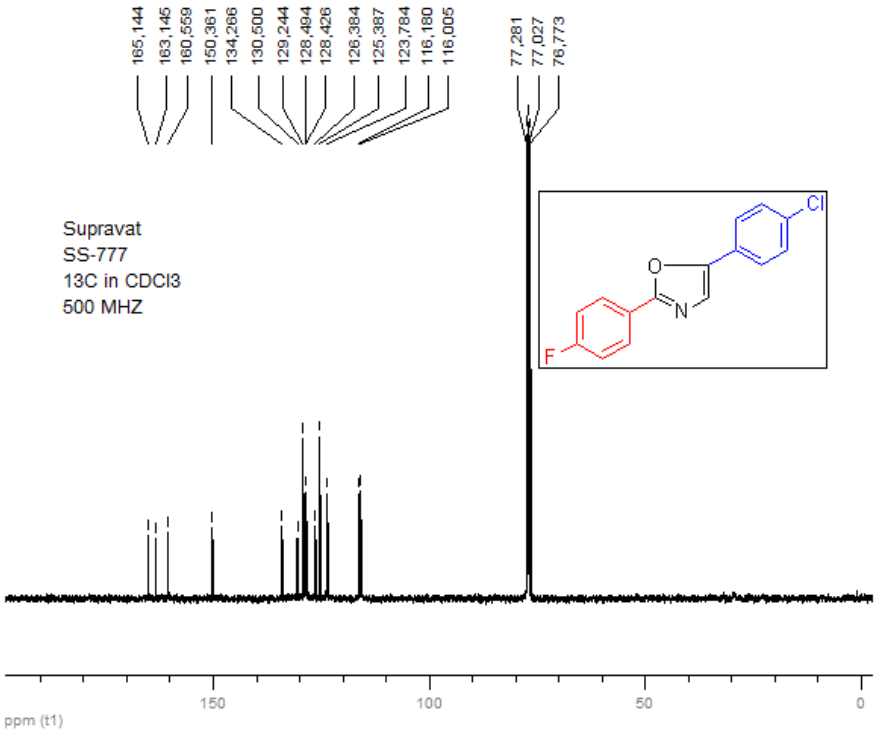
^{1}H NMR of 2ac



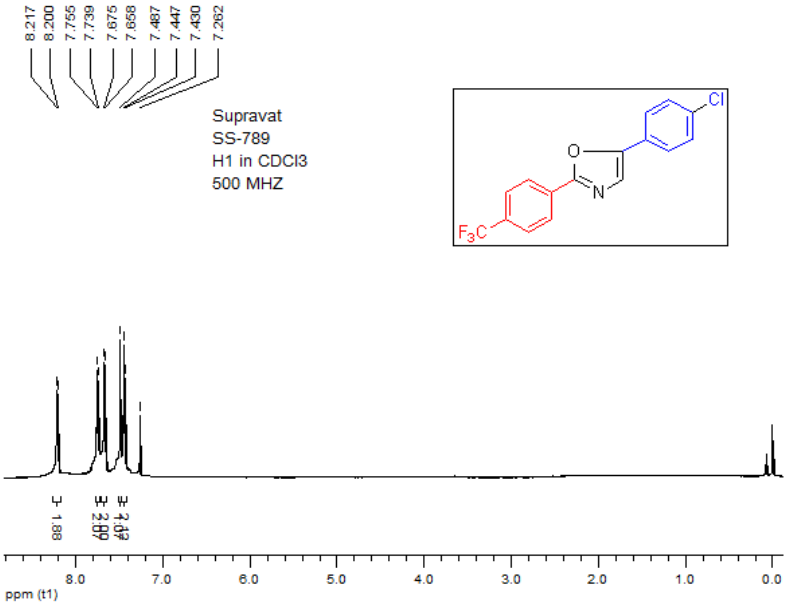
^{13}C NMR of 2ac



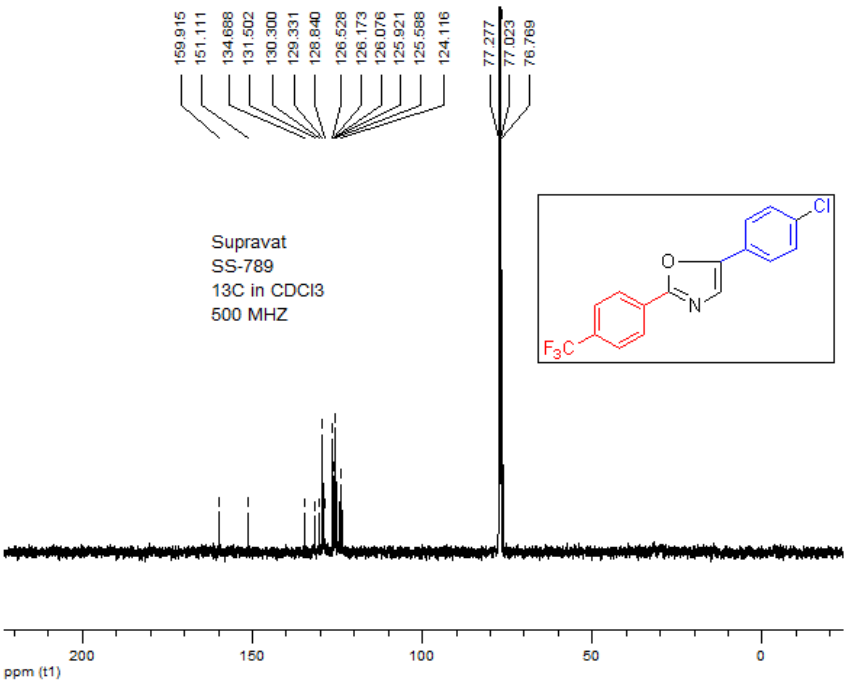
^{1}H NMR of 2ad



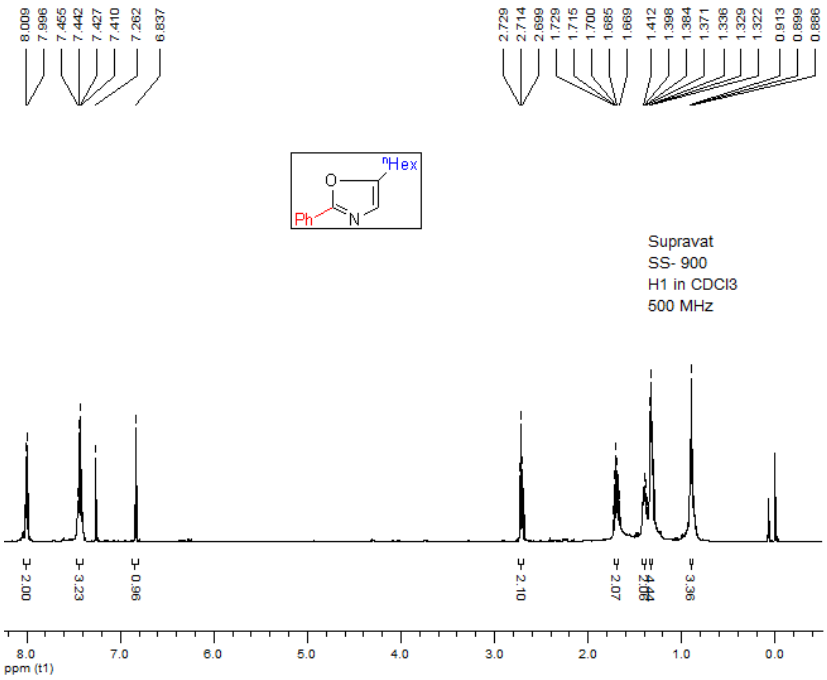
^{13}C NMR of 2ad



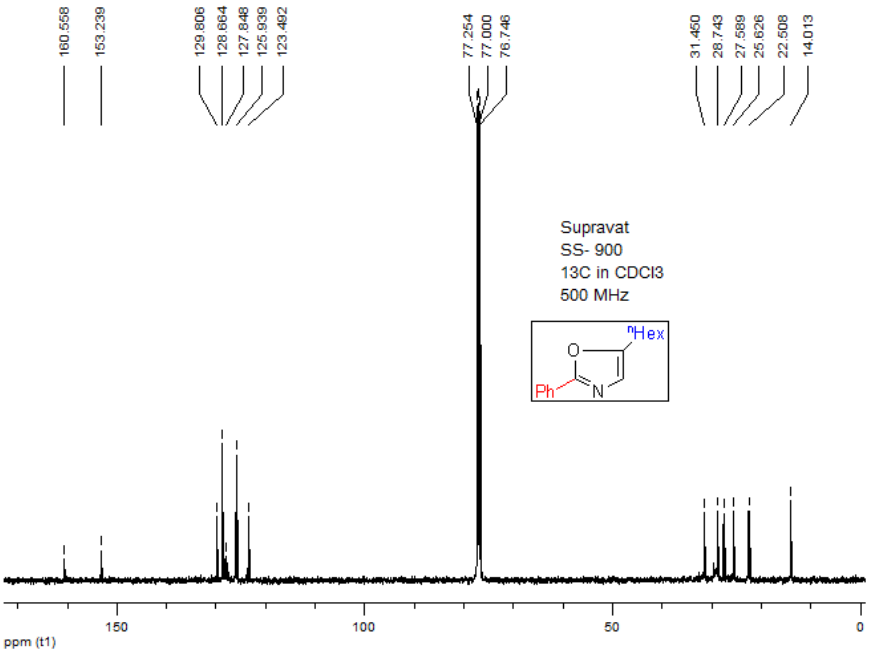
^{1}H NMR of 2ae



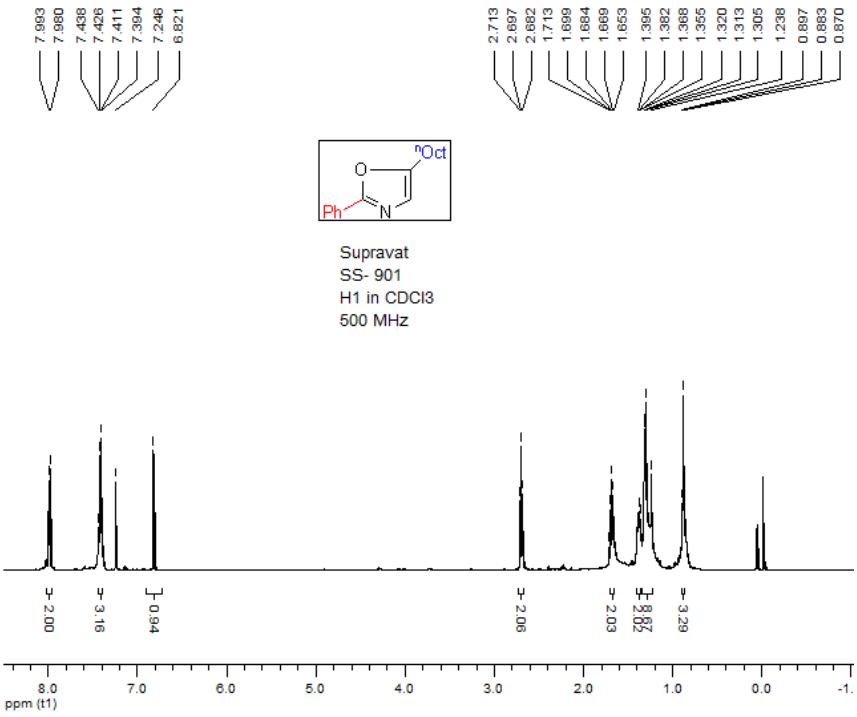
^{13}C NMR of 2ae



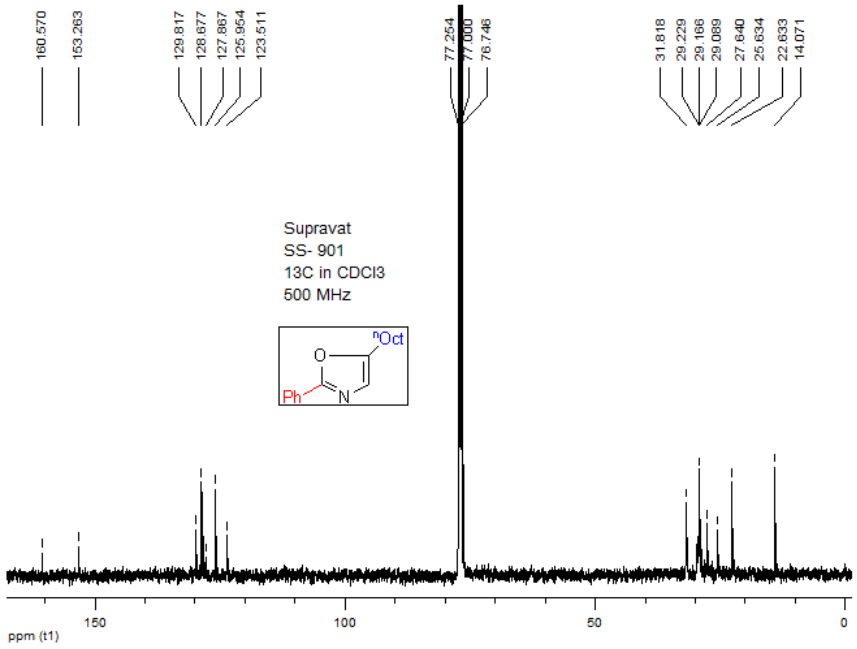
^{1}H NMR of 2af



^{13}C NMR of 2af



^{1}H NMR of 2ag



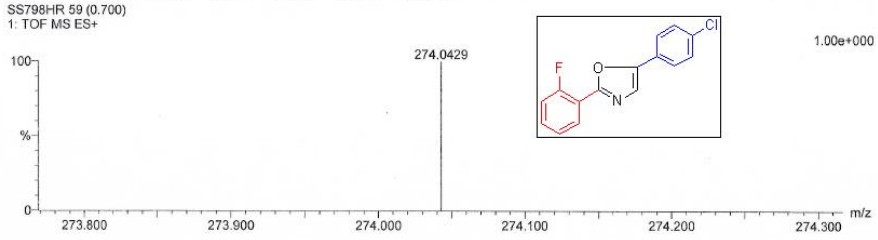
^{13}C NMR of 2ag

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-10 N: 0-1 O: 0-1 F: 0-1 Si: 0-1 Cl: 0-1

SS798HR 59 (0.700)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
274.0429	274.0435	-0.6	-2.2	10.5	n/a	C15 H10 N O F Cl

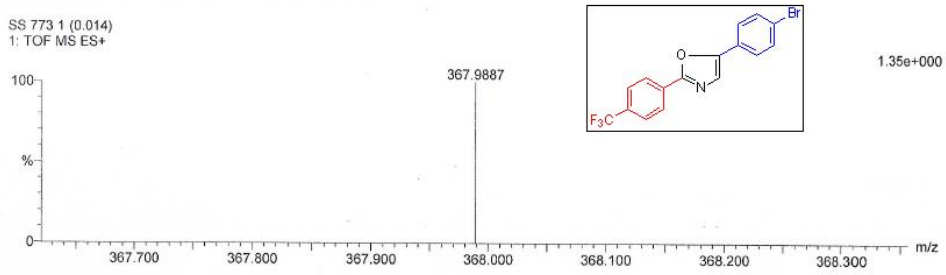
HRMS of **2x**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-17 H: 0-10 N: 0-1 O: 0-1 F: 0-3 Br: 0-1

SS 773 1 (0.014)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
367.9887	367.9898	-1.1	-3.0	10.5	n/a	C16 H10 N O F3 Br

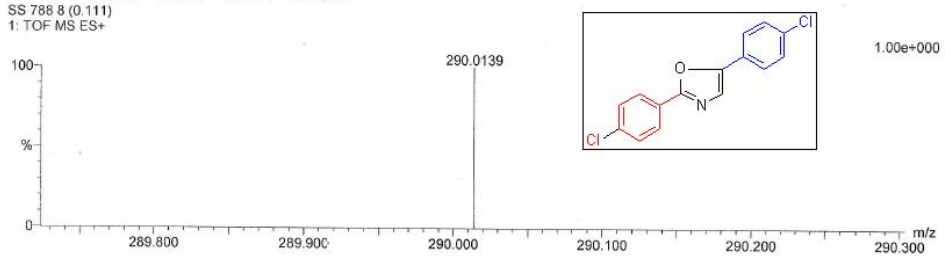
HRMS of **2y**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-10 N: 0-1 O: 0-1 Cl: 0-2

SS 788 8 (0.111)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.0139	290.0139	0.0	0.0	10.5	n/a	C15 H10 N O Cl2

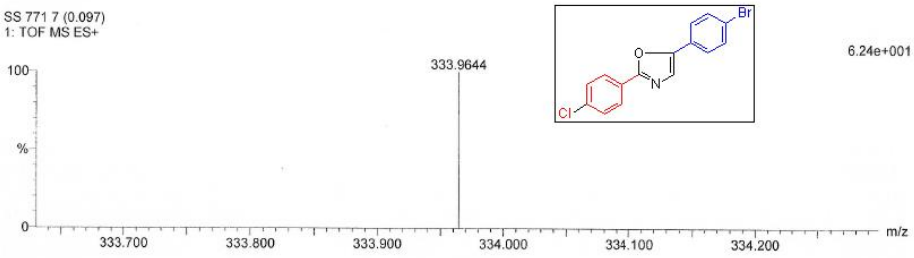
HRMS of **2aa**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-10 N: 0-1 O: 0-1 Cl: 0-1 Br: 0-1

SS 771 7 (0.097)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
333.9644	333.9634	1.0	3.0	10.5	n/a	C15 H10 N O Cl Br

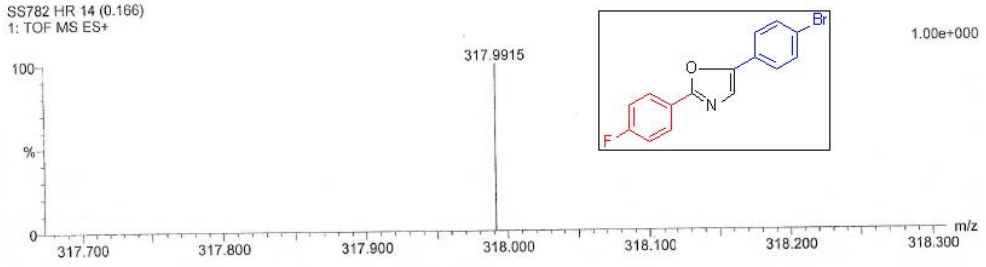
HRMS of **2ab**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-10 N: 0-1 O: 0-1 F: 0-1 Si: 0-1 Br: 0-1

SS782 HR 14 (0.166)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
317.9915	317.9930	-1.5	-4.7	10.5	n/a	C15 H10 N O F Br

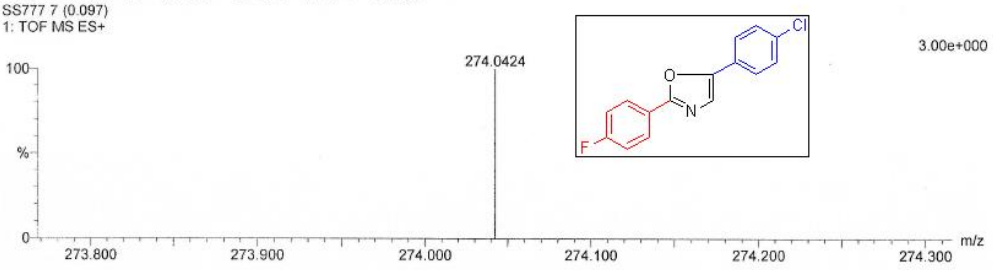
HRMS of **2ac**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

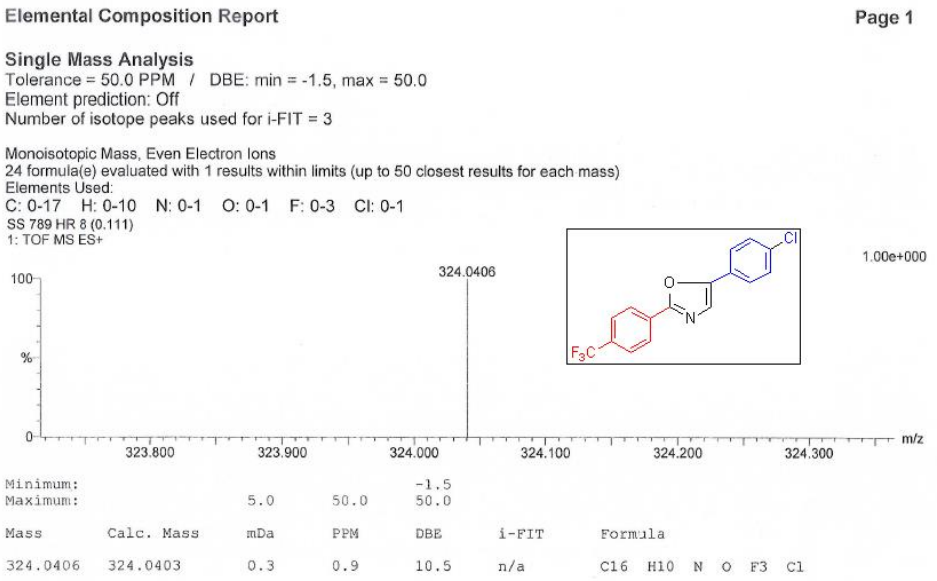
Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 0-16 H: 0-10 N: 0-1 O: 0-1 F: 0-1 Cl: 0-1

SS777 7 (0.097)
1: TOF MS ES+



Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
274.0424	274.0435	-1.1	-4.0	10.5	n/a	C15 H10 N O F Cl

HRMS of **2ad**



HRMS of **2ae**

HRMS of the reaction mixture using TEMPO (3):