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Supporting Information

Palladium Catalyzed Amide-oxazoline Directed C-H Acetoxylation of Arenes

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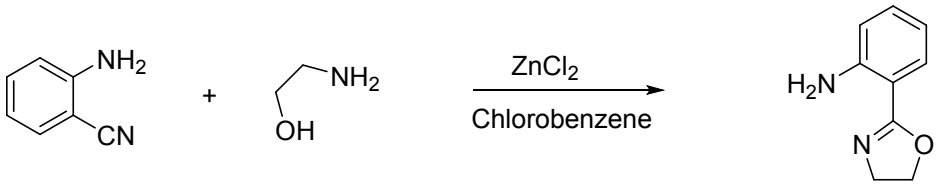
Materials and Methods

Unless otherwise stated, starting materials were purchased from Alfa Aesar, TCI, Energy or Arcos and used without purification. All of the reactions were monitored by thin layer chromatography (TLC) on GF254 silica gel plates. ^{1}H NMR spectra and ^{13}C NMR spectra were recorded on a Bruker AVANCE III 400 (400 MHz) spectrometer in needful D-reagents ($CDCl_3$) with tetramethylsilane (TMS) as an internal reference. HRMS of additional products were carried out on Brucker Apex IV FTMS. Melting points were determined on X5A made by Beijing Fukai Company as uncorrected values.

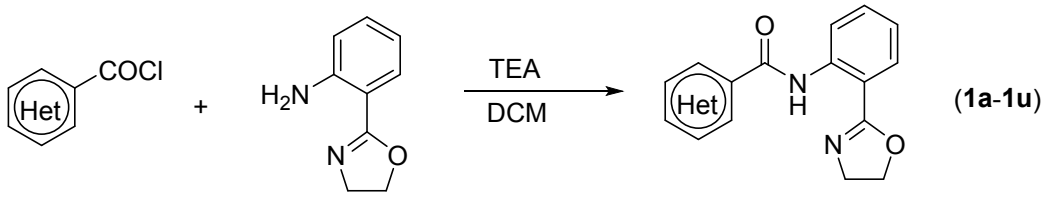
Preparation of Substrates of 1a-1u

1. Synthesis of 2-(4,5-dihydrooxazol-2-yl)aniline[1]



In a three-necked flask (50 mL), 2-aminobenzonitrile (20 mmol, 2.3 g), $ZnCl_2$ (2 mmol, 273 mg) and 2-aminoethan-1-ol (60 mmol, 3.7 mL) were added and then dissolved in chlorobenzene (12 mL) under Argon. The mixture was heated to reflux for 36 h. After that, the solvent was removed under reduced pressure. The crude product was purified by flash chromatography on silica gel (P : E=4 : 1) and further recrystallized from EtOAc/PET to give colorless crystals of the compound 2-(4,5-dihydrooxazol-2-yl)aniline (81 %).

2. Preparation of Substrates[2]

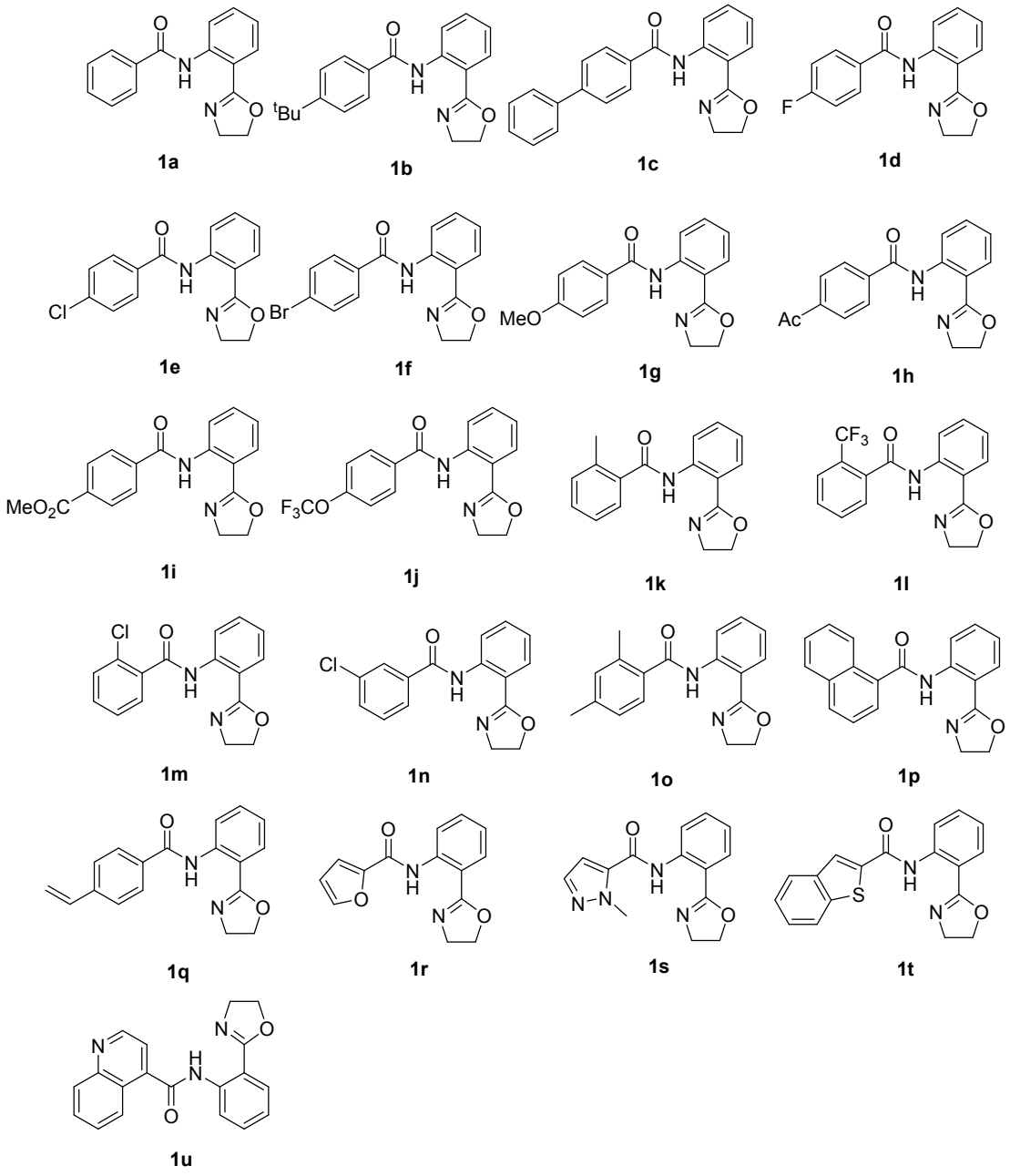


(**1a**-**1u**)

2-(4,5-dihydrooxazol-2-yl)aniline (3 mmol) and TEA (1.2 eq) were added to a 50 mL flask and then dissolved in CH_2Cl_2 (20 mL). Acid chloride (1.1 eq) was added to the solution and stirred at room temperature for 10 h and quenched with saturated $NaHCO_3$. And then the mixture was extracted with EtOAc. Combined organic phase was washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude product was further recrystallized from EtOAc/PET or EtOH to give colorless crystals of the product. And all the substrates were

[1] R. Giri, N. L. Maugel, B. M. Foxman and J.-Q. Yu, *Organometallics*, 2008, **27**, 1667.
[2] M. Shang, S.-Z. Sun, H.-X. Dai and J.-Q. Yu, *J. Am. Chem. Soc*., 2014, **136**, 3354.

known compounds except for **1i**, **1j**, **1t**.

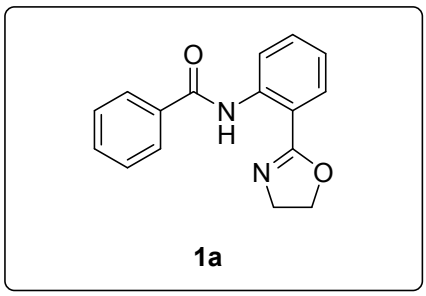


General Procedure for the Pd-Catalyzed Acetoxylation of Arlys

To a 15 mL sealed tube was added **1a** (0.2 mmol), PIDA (0.5 mmol, 162mg), $Pd(TFA)_2$ (0.02 mmol, 6.7 mg), $AcOH/Ac_2O$ (12 mg/40 mg) and DCE (3 mL). The reaction mixture was vigorously stirred at 130 °C for 10 h. And then the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatography on silica gel to afford the desired products.

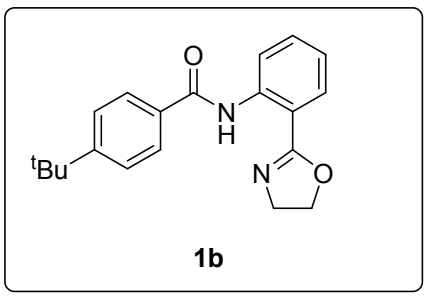
Analytical Data

1. Substrates (1a-1u)



1a

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)benzamide (1a)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.03 (s, 1H), 8.97 (dd, J = 8.5, 0.8 Hz, 1H), 8.28 – 7.98 (m, 2H), 7.89 (dd, J = 7.9, 1.6 Hz, 1H), 7.71 – 7.38 (m, 4H), 7.11 (td, J = 7.9, 1.1 Hz, 1H), 4.41 (dd, J = 14.3, 5.0 Hz, 2H), 4.18 (dd, J = 14.4, 5.1 Hz, 2H). ^{13}C NMR (100 MHz, CDC_{l3}) δ 166.11, 164.96, 140.21, 135.34, 132.67, 131.67, 129.31, 128.59, 127.76, 122.42, 119.90, 113.57, 66.28, 54.70**.**

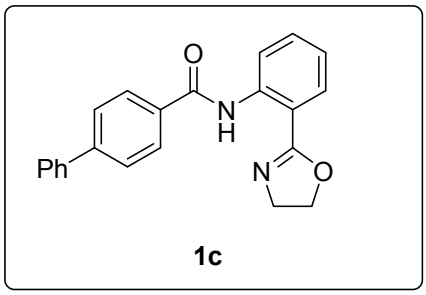


1b

4-(t-Butyl)-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (1b)[3]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.98 (s, 1H), 8.98 (d, J = 8.4 Hz, 1H), 8.04 (d, J = 8.4 Hz, 2H), 8.03 – 7.79 (m, 1H), 7.50 (dd, J = 15.3, 8.7 Hz, 3H), 7.10 (t, J = 7.5 Hz, 1H), 4.41 (t, J = 9.4 Hz, 2H), 4.21 (t, J = 9.4 Hz, 2H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.08, 164.95, 155.15, 140.34, 132.65, 132.45, 129.28, 127.62, 125.56, 122.25, 119.90, 113.49, 66.25, 54.76, 34.98, 31.21.

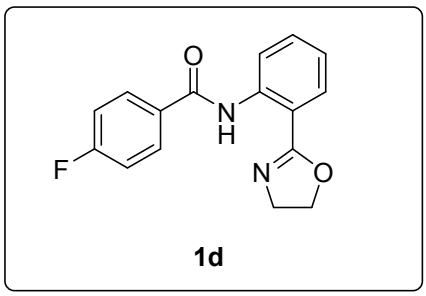
N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-[1,1'-biphenyl]-

[3] M. Shang, H.-L. Wang, S.-Z. Sun, H.-X. Dai and J.-Q. Yu, *J. Am. Chem. Soc*., 2014, **136**, 11590.



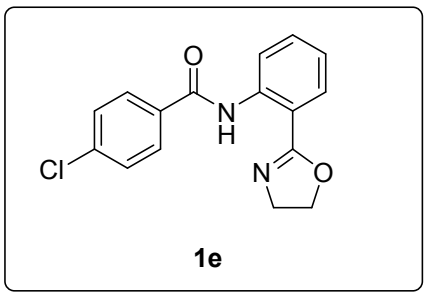
1c

4-carboxamide (1c)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.07 (s, 1H), 8.99 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 8.3 Hz, 2H), 7.91 (dd, J = 7.9, 1.1 Hz, 1H), 7.72 (d, J = 8.3 Hz, 2H), 7.65 (d, J = 7.3 Hz, 2H), 7.58 – 7.34 (m, 4H), 7.11 (t, J = 7.6 Hz, 1H), 4.41 (t, J = 9.6 Hz, 2H), 4.21 (t, J = 9.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.84, 165.02, 144.39, 140.26, 140.13, 134.06, 132.70, 129.33, 128.92, 128.30, 127.99, 127.27, 127.25, 122.41, 119.91, 113.54, 66.29, 54.73.



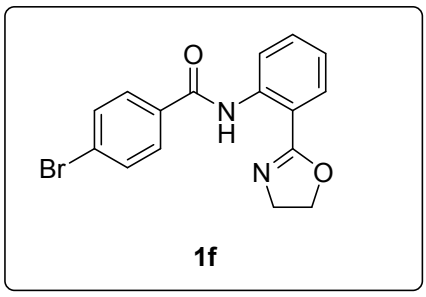
1d

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-4-fluorobenzamide (1d)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.01 (s, 1H), 8.93 (d, J = 8.0 Hz, 1H), 8.27 – 7.98 (m, 2H), 7.91 (dd, J = 7.9, 1.4 Hz, 1H), 7.72 – 7.36 (m, 1H), 7.14 (ddd, J = 15.3, 12.8, 4.8 Hz, 3H), 4.43 (dd, J = 14.4, 5.0 Hz, 2H), 4.20 (dd, J = 14.3, 5.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.09, 164.97 (d $J_{C\text{-}F}$ = 251 Hz), 164.96, 140.12, 132.73, 131.53 (d $J_{C\text{-}F}$ = 3.0 Hz), 130.10 (d $J_{C\text{-}F}$ = 9.0 Hz), 129.33, 122.50, 119.83, 115.60 (d $J_{C\text{-}F}$ = 22 Hz), 113.51, 66.30, 54.67.



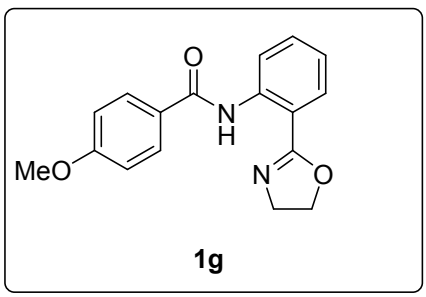
1e

4-Chloro-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (1e)[3]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.06 (s, 1H), 8.95 (d, J = 8.4 Hz, 1H), 8.07 (dd, J = 15.6, 8.6 Hz, 2H), 7.92 (dd, J = 7.9, 1.4 Hz, 1H), 7.62 – 7.43 (m, 3H), 7.22 – 7.03 (m, 1H), 4.44 (t, J = 9.7 Hz, 2H), 4.22 (t, J = 9.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.07, 164.96, 140.01, 137.93, 133.77, 132.74, 129.34, 129.17, 128.85, 122.60, 119.85, 113.54, 66.31, 54.65.



1f

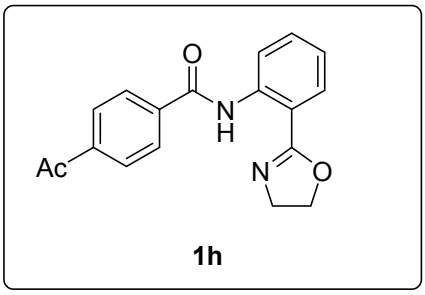
4-Bromo-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (1f)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.05 (s, 1H), 8.92 (d, J = 8.5 Hz, 1H), 7.96 (d, J = 8.5 Hz, 2H), 7.94 – 7.86 (m, 1H), 7.64 (d, J = 8.5 Hz, 2H), 7.52 (t, J = 7.3 Hz, 1H), 7.13 (t, J = 7.6 Hz, 1H), 4.43 (t, J = 9.4 Hz, 2H), 4.19 (t, J = 9.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.12, 165.08, 139.99, 134.24, 132.75, 131.83, 129.36, 126.47, 122.63, 119.86, 113.55, 66.32, 54.65.



1g

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-4-methoxybenzamide (1g)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.91 (s, 1H), 8.95 (d, J = 8.5 Hz, 1H), 8.07 (d, J = 8.7 Hz, 2H), 7.89 (d, J = 7.9 Hz, 1H), 7.51 (t,

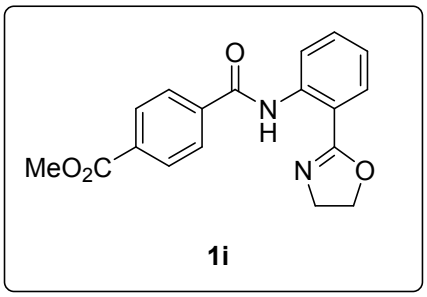
J = 7.9 Hz, 1H), 7.09 (t, J = 7.6 Hz, 1H), 7.03 (dd, J = 38.2, 8.2 Hz, 2H), 4.41 (t, J = 9.3 Hz, 2H), 4.21 (t, J = 9.5 Hz, 2H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.71, 165.02, 162.39, 140.42, 132.65, 129.63, 129.28, 127.70, 122.13, 119.82, 113.80, 113.39, 66.24, 55.43, 54.72.



1h

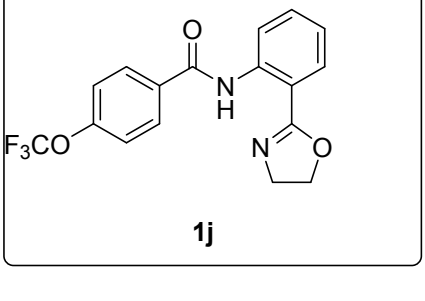
4-Acetyl-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (1h)[4]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.17 (s, 1H), 8.95 (d, J = 8.4 Hz, 1H), 8.12 (dd, J = 41.6, 8.2 Hz, 4H), 7.91 (d, J = 7.9 Hz, 1H), 7.54 (t, J = 7.9 Hz, 1H), 7.14 (t, J = 7.6 Hz, 1H), 4.43 (t, J = 9.4 Hz, 2H), 4.21 (t, J = 9.5 Hz, 2H), 2.66 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.61, 165.06, 164.99, 139.88, 139.24, 139.21, 132.76, 129.37, 128.53, 128.01, 122.81, 119.90, 113.66, 66.36, 54.64, 26.85.

Methyl 4-((2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)benzoate (1i): White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.16 (s, 1H), 8.95 (d, J = 8.5 Hz, 1H), 8.27 – 8.07 (m, 4H), 7.91 (d, J = 7.9 Hz, 1H), 7.53 (t, J = 7.9 Hz, 1H), 7.14 (t, J = 7.6 Hz, 1H), 4.43 (t, J = 9.5 Hz, 2H), 4.20 (t, J = 9.5 Hz, 2H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.45, 165.08, 165.03, 139.90, 139.24, 132.74, 129.84, 129.35, 127.75, 122.77, 119.89, 113.64, 110.00, 66.35, 54.63, 52.38. HRMS calcd for $C_{18}H_{17}N_2O_4$ $[M+H]^+$ 425.1183, found 325.1191.



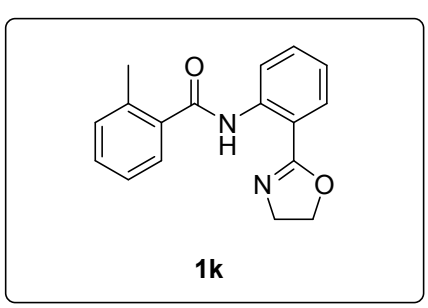
1i

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-4-(trifluoromethoxy)benzamide (1j): White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.07 (s, 1H), 8.93 (d, J = 8.5 Hz, 1H), 8.13 (d, J = 8.7 Hz, 2H), 7.90 (d, J = 7.9 Hz, 1H), 7.52 (t, J = 7.9 Hz, 1H), 7.32 (d, J = 8.4 Hz, 2H), 7.12 (t, J = 7.6 Hz, 1H), 4.42 (t, J = 9.4 Hz, 2H), 4.19 (t, J = 9.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.09, 164.59, 151.64, 139.98, 133.72, 132.73, 129.62, 129.35, 122.64, 120.53, 120.28 (q, J_{C-F} = 257 Hz), 119.83, 113.56, 66.31, 54.64. HRMS calcd for $C_{17}H_{14}F_3N_2O_3$ $[M+H]^+$ 351.0951, found 351.0962.



1j

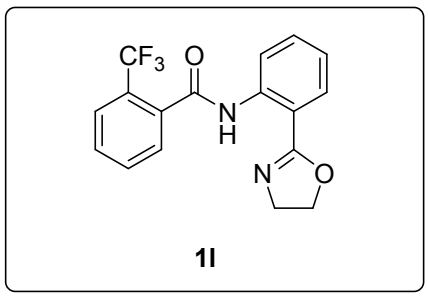
N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-2-methylbenzamide (1k)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.61 (s, 1H), 8.97 (d, J = 8.4 Hz, 1H), 7.92 (dd, J = 7.9, 1.3 Hz, 1H), 7.66 (d, J = 7.2 Hz, 1H), 7.59 – 7.50 (m, 1H), 7.39 (t, J = 7.0 Hz, 1H), 7.34 – 7.26 (m, 2H), 7.14 (t, J = 7.6 Hz, 1H), 4.38 (t, J = 9.5 Hz, 2H), 4.08 (t, J = 9.5 Hz, 2H), 2.60 (s, 3H). ^{13}C NMR (100



1k

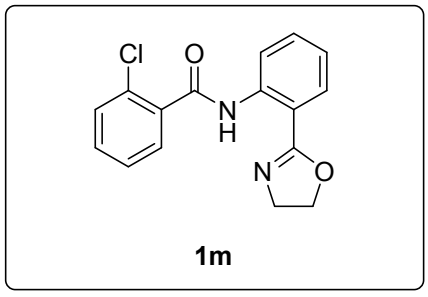
[4] M. Shang, S.-Z. Sun, H.-L. Wang, B. N. Laforteza, H.-X. Dai and J.-Q. Yu, *Angew. Chem. Int. Ed.*, 2014, **53**, 10439.

MHz, $CDCl_3$) δ 168.71, 164.64, 140.15, 137.19, 136.77, 132.59, 131.36, 130.12, 129.25, 127.55, 125.77, 122.44, 119.76, 113.48, 66.19, 54.70, 20.36.



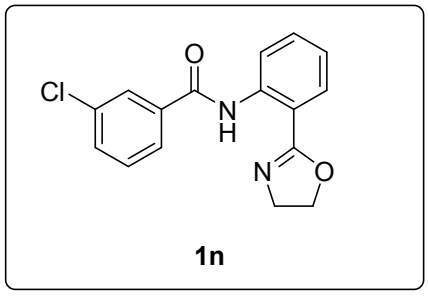
1l

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-2-(trifluoromethyl)benzamide (1l)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.67 (s, 1H), 8.89 (d, J = 8.4 Hz, 1H), 7.89 (dd, J = 7.9, 1.5 Hz, 1H), 7.76 (d, J = 7.6 Hz, 1H), 7.74 – 7.45 (m, 4H), 7.21 – 7.08 (m, 1H), 4.34 (t, J = 9.5 Hz, 2H), 3.99 (t, J = 9.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.42, 164.56, 139.64, 136.63, 132.66, 131.93, 129.93, 129.20, 128.31, 127.90 (q, $J_{C\text{-}F}$ = 32 Hz), 126.78 (CF_3, q, $J_{C\text{-}F}$ = 15 Hz), 123.65 (q, $J_{C\text{-}F}$ = 295 Hz), 122.96, 120.01, 113.63, 66.23, 54.59.



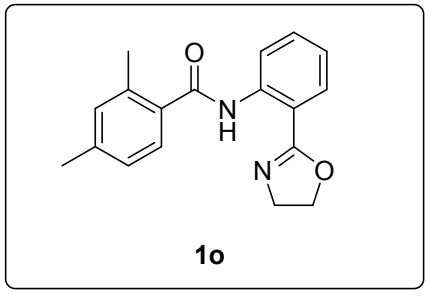
1m

2-Chloro-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (1m)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.73 (s, 1H), 8.95 (d, J = 8.4 Hz, 1H), 7.91 (dd, J = 7.9, 1.5 Hz, 1H), 7.67 (dd, J = 7.4, 1.8 Hz, 1H), 7.60 – 7.52 (m, 1H), 7.49 (dd, J = 7.8, 1.3 Hz, 1H), 7.39 (dtd, J = 16.4, 7.4, 1.6 Hz, 2H), 7.23 – 7.09 (m, 1H), 4.38 (t, J = 9.6 Hz, 2H), 4.06 (t, J = 9.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.72, 164.51, 139.66, 136.65, 132.62, 131.56, 131.09, 130.55, 129.32, 129.22, 126.86, 122.85, 120.01, 113.68, 66.24, 54.64.



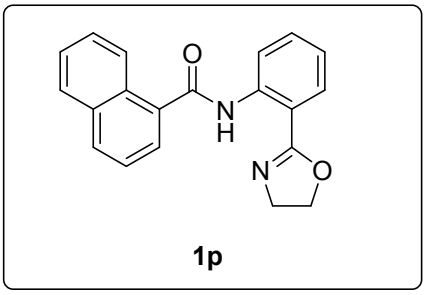
1n

3-Chloro-N-(2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (1n)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.11 (s, 1H), 8.92 (d, J = 8.4 Hz, 1H), 8.11 (s, 1H), 7.97 (d, J = 7.7 Hz, 1H), 7.90 (dd, J = 7.9, 1.2 Hz, 1H), 7.53 (dd, J = 13.8, 6.3 Hz, 2H), 7.43 (t, J = 7.8 Hz, 1H), 7.13 (t, J = 7.6 Hz, 1H), 4.43 (t, J = 9.4 Hz, 2H), 4.22 (t, J = 9.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.04, 164.58, 139.91, 137.09, 134.73, 132.75, 131.62, 129.88, 129.33, 128.17, 125.87, 122.70, 119.85, 113.61, 66.37, 54.54.



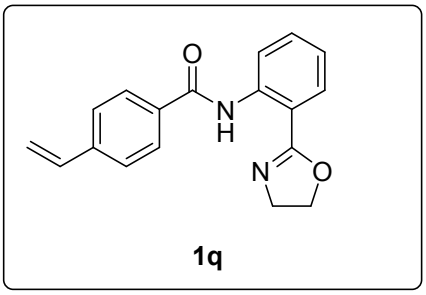
1o

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-2,4-dimethylbenzamide (1o)[4]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.57 (s, 1H), 8.97 (d, J = 8.4 Hz, 1H), 7.91 (dd, J = 7.9, 1.2 Hz, 1H), 7.66 – 7.43 (m, 2H), 7.12 (q, J = 7.5 Hz, 3H), 4.37 (d, J = 9.4 Hz, 2H), 4.10 (d, J = 9.4 Hz, 2H), 2.57 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.72, 164.65, 140.29, 140.21, 137.43, 133.82, 132.56, 132.24, 129.23, 127.74, 126.42, 122.28, 119.72, 113.41, 66.16, 54.72, 21.30, 20.42.



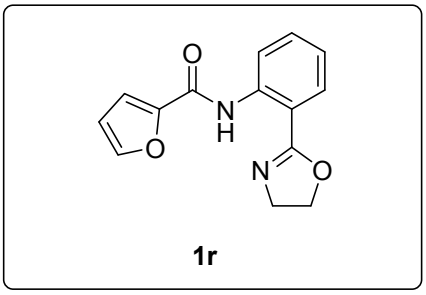
1p

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-1-naphthamide (1p)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.84 (s, 1H), 9.05 (d, J = 8.1 Hz, 1H), 8.57 (d, J = 8.0 Hz, 1H), 8.12 – 7.75 (m, 4H), 7.72 – 7.45 (m, 4H), 7.20 – 7.03 (m, 1H), 4.33 (t, J = 9.5 Hz, 2H), 3.97 (t, J = 9.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.26, 164.61, 140.22, 134.87, 133.93, 132.64, 131.05, 130.59, 129.27, 128.25, 127.04, 126.35, 125.90, 125.87, 124.77, 122.62, 119.94, 113.62, 66.20, 54.63.



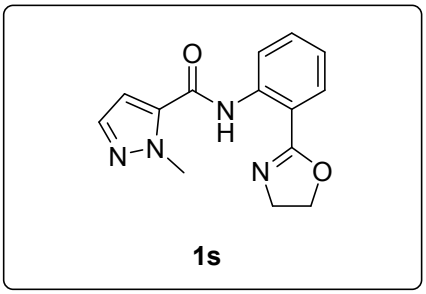
1q

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-4-vinylbenzamide (1q)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.02 (s, 1H), 9.16 – 8.85 (m, 1H), 8.06 (d, J = 8.4 Hz, 2H), 7.90 (dd, J = 7.9, 1.6 Hz, 1H), 7.51 (dd, J = 10.8, 5.0 Hz, 3H), 7.23 – 6.99 (m, 1H), 6.77 (dd, J = 17.6, 10.9 Hz, 1H), 5.87 (d, J = 17.6 Hz, 1H), 5.37 (d, J = 10.9 Hz, 1H), 4.42 (dd, J = 14.3, 5.0 Hz, 2H), 4.20 (dd, J = 14.4, 5.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.74, 165.00, 140.74, 140.24, 136.09, 134.48, 132.69, 129.31, 128.08, 126.37, 122.39, 119.89, 115.96, 113.52, 66.27, 54.71.



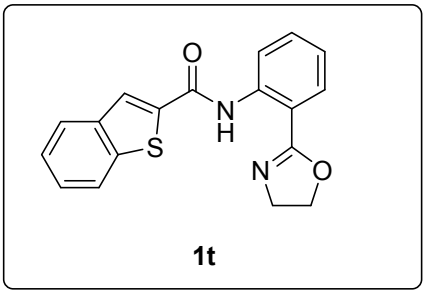
1r

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)furan-2-carboxamide (1r)[2]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.01 (s, 1H), 8.88 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 7.9 Hz, 1H), 7.58 (s, 1H), 7.50 (t, J = 7.9 Hz, 1H), 7.23 (d, J = 3.4 Hz, 1H), 7.11 (t, J = 7.6 Hz, 1H), 6.54 (dd, J = 3.3, 1.6 Hz, 1H), 4.42 (t, J = 9.5 Hz, 2H), 4.23 (t, J = 9.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.74, 157.09, 148.73, 144.73, 139.66, 132.56, 129.24, 122.47, 119.99, 114.68, 113.56, 112.05, 66.29, 54.76.



1s

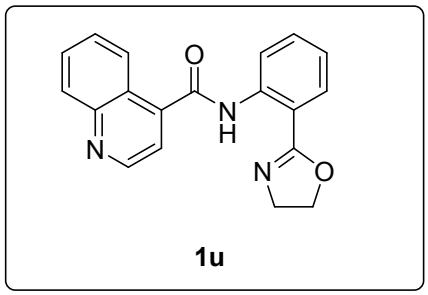
N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)-1-methyl-1H-pyrazole-5-carboxamide (1s)[3]: White Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.97 (s, 1H), 8.81 (d, J = 8.4 Hz, 1H), 7.90 (dd, J = 7.9, 1.5 Hz, 1H), 7.67 – 7.38 (m, 2H), 7.19 – 7.05 (m, 1H), 6.92 (d, J = 2.1 Hz, 1H), 4.43 (dd, J = 14.5, 5.1 Hz, 2H), 4.27 (s, 3H), 4.20 (dd, J = 14.3, 5.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.92, 158.56, 139.70, 137.62, 136.13, 132.67, 129.38, 122.70, 119.58, 113.43, 107.65, 66.34, 54.63, 39.62.



1t

N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)benzo[b]thiophene-2-carboxamide (1t):

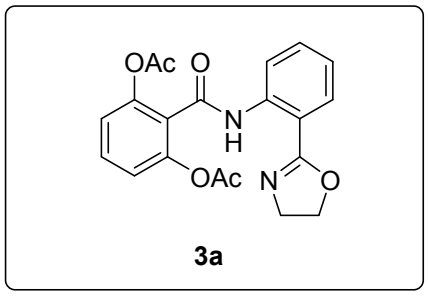
Yellow Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.24 (s, 1H), 8.87 (d, J = 8.4 Hz, 1H), 8.00 (s, 1H), 7.88 (ddd, J = 6.2, 3.9, 1.6 Hz, 3H), 7.57 – 7.46 (m, 1H), 7.45 – 7.36 (m, 2H), 7.19 – 7.06 (m, 1H), 4.44 (dd, J = 14.4, 5.1 Hz, 2H), 4.25 (dd, J = 14.3, 5.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.05, 161.17, 141.48, 140.80, 139.81, 139.30, 132.74, 129.32, 126.31, 125.60, 125.24, 124.78, 122.77, 122.61, 119.79, 113.36, 66.37, 54.63. HRMS calcd for $C_{18}H_{15}N_2O_2S$ $[M+H]^+$ 323.0849, found 323.0855.



1u

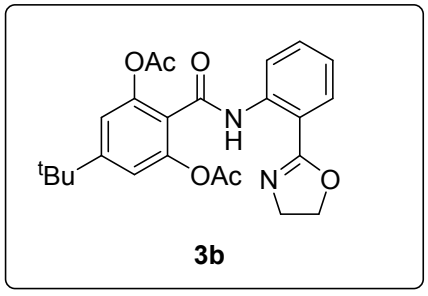
N-(2-(4,5-Dihydrooxazol-2-yl)phenyl)quinoline-4-carboxamide (1u)[3]: Yellow Solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 13.06 (s, 1H), 9.02 (dd, J = 14.0, 6.4 Hz, 2H), 8.50 (d, J = 8.4 Hz, 1H), 8.18 (d, J = 8.4 Hz, 1H), 7.93 (dd, J = 7.9, 1.3 Hz, 1H), 7.86 – 7.74 (m, 1H), 7.66 (dd, J = 18.7, 2.6 Hz, 1H), 7.67 – 7.51 (m, 2H), 7.19 (dd, J = 11.2, 4.1 Hz, 1H), 4.35 (t, J = 9.6 Hz, 2H), 3.98 (t, J = 9.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.97, 164.71, 149.98, 149.02, 142.14, 139.61, 132.75, 129.92, 129.83, 129.35, 127.57, 125.77, 124.78, 123.23, 119.99, 118.94, 113.75, 66.32, 54.54.

1. Products (3a-3u)



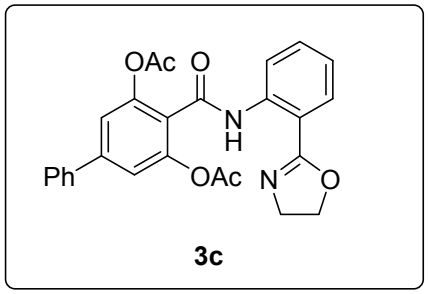
3a

2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-1,3-phenylene diacetate (3a): White solid. Melting point: 120.8 ~ 122.3 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.54 (s, 1H), 8.89 (d, J = 8.4 Hz, 1H), 7.87 (dd, J = 7.9, 1.5 Hz, 1H), 7.62 – 7.39 (m, 2H), 7.14 (dd, J = 9.5, 4.7 Hz, 3H), 4.34 (t, J = 9.6 Hz, 2H), 4.01 (t, J = 9.5 Hz, 2H), 2.18 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.72, 164.20, 161.65, 148.33, 139.50, 132.63, 130.33, 129.17, 124.32, 122.87, 120.53, 119.90, 113.39, 66.36, 54.50, 20.98. HRMS calcd for $C_{20}H_{19}N_2O_6$ $[M+H]^+$ 383.1238, found 383.1237.



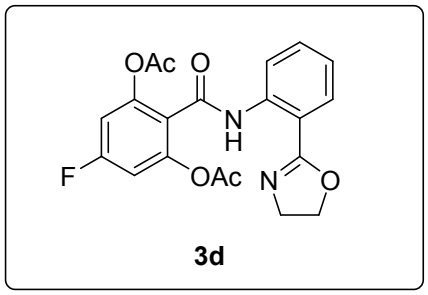
3b

5-(t-Butyl)-2-((2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)-1,3-phenylene diacetate (3b): White solid. Melting point: 171.2 ~ 172.4 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.46 (s, 1H), 8.89 (d, J = 8.4 Hz, 1H), 7.86 (dd, J = 7.9, 1.3 Hz, 1H), 7.49 (s, 1H), 7.18 – 7.04 (m, 3H), 4.64 – 4.21 (m, 2H), 4.18 – 3.91 (m, 2H), 2.18 (s, 6H), 1.33 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.80, 164.17, 161.91, 154.70, 148.14, 139.64, 132.57, 129.14, 122.70, 121.30, 119.96, 117.77, 113.38, 66.32, 54.59, 35.13, 30.96, 21.00. HRMS calcd for $C_{24}H_{27}N_2O_6$ $[M+H]^+$ 439.1864, found 439.1857.



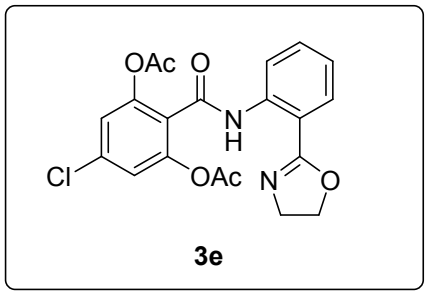
3c

4-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-[1,1'-biphenyl]-3,5-diyl diacetate (3c): White solid. Melting point: 166.8 ~ 167.9 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.58 (s, 1H), 8.91 (d, J = 8.4 Hz, 1H), 7.88 (dd, J = 7.9, 1.5 Hz, 1H), 7.65 – 7.56 (m, 2H), 7.56 – 7.48 (m, 1H), 7.48 – 7.36 (m, 3H), 7.35 (s, 2H), 7.19 – 7.06 (m, 1H), 4.34 (t, J = 9.5 Hz, 2H), 4.03 (t, J = 9.6 Hz, 2H), 2.20 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.70, 164.25, 161.61, 148.68, 143.86, 139.58, 138.74, 132.63, 129.18, 128.92, 128.44, 127.24, 122.84, 122.72, 119.94, 119.18, 113.40, 66.37, 54.55, 21.00. HRMS calcd for $C_{26}H_{23}N_2O_6$ $[M+H]^+$ 459.1551, found 459.1542.



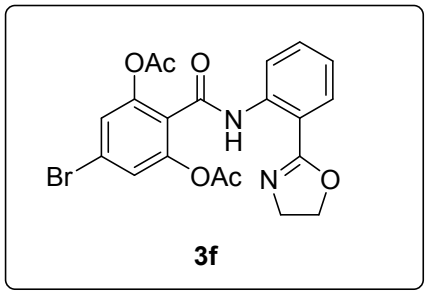
3d

2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-5-fluoro-1,3-phenylene diacetate (3d): White solid. Melting point: 157.1 ~ 159.2 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.54 (s, 1H), 8.86 (d, J = 8.4 Hz, 1H), 7.88 (dd, J = 7.9, 1.2 Hz, 1H), 7.51 (t, J = 7.4 Hz, 1H), 7.14 (t, J = 7.6 Hz, 1H), 6.91 (d, J = 9.0 Hz, 2H), 4.35 (t, J = 9.5 Hz, 2H), 4.01 (t, J = 9.5 Hz, 2H), 2.18 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.24, 164.33, 162.46 (d, $J_{C\text{-}F}$ = 250 Hz), 160.95, 149.22 (d, $J_{C\text{-}F}$ = 13 Hz), 139.43, 132.68, 129.22, 122.96, 120.76 (d, $J_{C\text{-}F}$ = 4.0 Hz), 119.83, 113.34, 108.77 (d, $J_{C\text{-}F}$ = 25 Hz), 66.39, 54.45, 20.90. HRMS calcd for $C_{20}H_{18}FN_2O_6$ $[M+H]^+$ 401.1143, found 401.1136.



3e

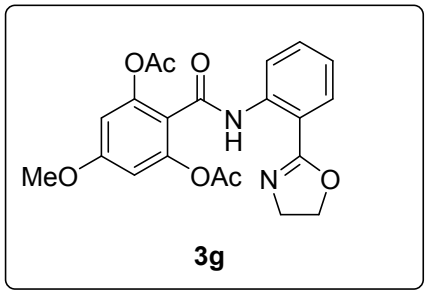
5-Chloro-2-((2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)-1,3-phenylene diacetate (3e): White solid. Melting point: 147.2 ~ 149.0 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.69 (s, 1H), 8.97 (d, J = 8.4 Hz, 1H), 7.99 (dd, J = 7.9, 1.3 Hz, 1H), 7.62 (t, J = 7.3 Hz, 1H), 7.34 – 7.18 (m, 3H), 4.46 (t, J = 9.6 Hz, 2H), 4.13 (t, J = 9.5 Hz, 2H), 2.29 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.27, 164.30, 160.81, 148.65, 139.38, 135.62, 132.68, 129.21, 123.01, 121.24, 119.85, 113.36, 66.39, 54.47, 20.89. HRMS calcd for $C_{20}H_{18}ClN_2O_6$ $[M+H]^+$ 417.0848, found 417.0839.



3f

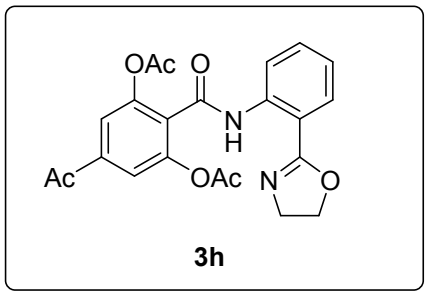
5-Bromo-2-((2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)-1,3-phenylene diacetate (3f): White solid. Melting point: 127.8 ~ 129.5 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.59 (s, 1H), 8.88 (d, J = 8.3 Hz, 1H), 7.90 (dd, J = 7.9, 1.4 Hz, 1H), 7.57 – 7.49 (m, 1H), 7.34 (s, 2H), 7.21 – 7.09 (m, 1H), 4.37 (t, J = 9.6 Hz, 2H), 4.04 (t, J = 9.5 Hz, 2H), 2.20 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.25, 164.30, 160.85, 148.66, 139.36, 132.68, 129.21, 124.06, 123.48, 123.03, 123.01, 119.86, 113.37, 66.39, 54.48, 20.87. HRMS calcd

for $C_{20}H_{18}BrN_2O_6$ $[M+H]^+$ 461.0343, found 461.0334.



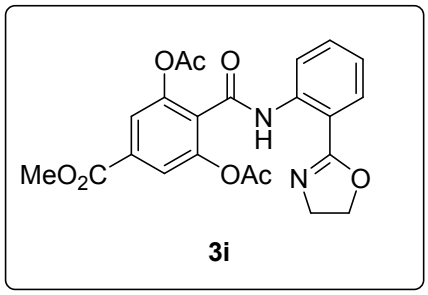
3g

2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-5-methoxy-1,3-phenylene diacetate (3g): White solid. Melting point: 153.3 ~ 155.0 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.44 (s, 1H), 8.88 (d, J = 8.4 Hz, 1H), 7.86 (dd, J = 7.9, 1.4 Hz, 1H), 7.51 (ddd, J = 15.8, 7.2, 2.3 Hz, 1H), 7.21 – 6.92 (m, 1H), 6.66 (s, 2H), 4.34 (t, J = 9.6 Hz, 2H), 4.03 (t, J = 9.5 Hz, 2H), 3.83 (s, 3H), 2.17 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.62, 164.23, 161.68, 160.91, 149.47, 139.73, 132.59, 129.14, 122.62, 119.83, 116.93, 113.26, 106.72, 66.31, 55.75, 54.55, 21.01. HRMS calcd for $C_{21}H_{21}N_2O_7$ $[M+H]^+$ 413.1343, found 413.1338.



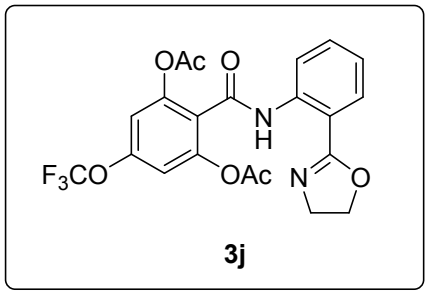
3h

5-Acetyl-2-((2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)-1,3-phenylene diacetate (3h): White solid. Melting point: 145.1 ~ 146.9 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.65 (s, 1H), 8.86 (d, J = 8.4 Hz, 1H), 8.07 – 7.83 (m, 1H), 7.69 (s, 2H), 7.52 (t, J = 7.8 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 4.34 (t, J = 9.5 Hz, 2H), 4.00 (t, J = 9.5 Hz, 2H), 2.61 (s, 3H), 2.20 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.52, 168.46, 164.28, 160.77, 148.54, 139.26, 138.65, 132.67, 129.22, 128.21, 123.13, 120.46, 119.92, 113.46, 66.40, 54.45, 26.68, 20.85. HRMS calcd for $C_{22}H_{21}N_2O_7$ $[M+H]^+$ 425.1343, found 425.1333.



3i

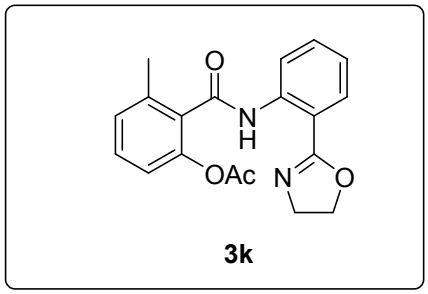
2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-5-(methoxycarbonyl)-1,3-phenylene diacetate (3i): White solid. Melting point: 144.9 ~ 146.2 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.66 (s, 1H), 8.87 (d, J = 8.4 Hz, 1H), 7.88 (dd, J = 7.9, 1.2 Hz, 1H), 7.80 (s, 2H), 7.52 (t, J = 7.9 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 4.34 (t, J = 9.6 Hz, 2H), 4.00 (t, J = 9.6 Hz, 2H), 3.93 (s, 3H), 2.20 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.43, 164.95, 164.25, 160.85, 148.24, 139.26, 132.67, 132.27, 129.21, 128.21, 123.13, 121.82, 119.91, 113.44, 66.41, 54.44, 52.66, 20.86. HRMS calcd for $C_{22}H_{21}N_2O_8$ $[M+H]^+$ 441.1292, found 441.1282.



3j

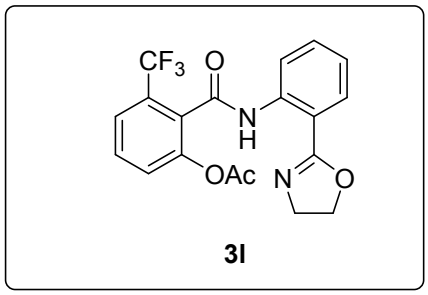
2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-5-(trifluoromethoxy)-1,3-phenylene diacetate (3j): White solid. Melting point: 119.6 ~ 121.3 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.62 (s, 1H), 8.88 (d, J = 8.4 Hz, 1H), 7.90 (d, J = 7.9 Hz, 1H), 7.53 (t, J = 7.4 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 7.06 (s, 2H), 4.37 (t, J = 9.6 Hz, 2H), 4.04 (t, J = 9.5 Hz, 2H), 2.21 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.13, 164.33, 160.63, 149.53, 149.02, 139.35, 132.69, 129.23, 123.06, 122.85, 120.23 (CF_3O, q, $J_{C\text{-}F}$ = 258 Hz), 119.87, 113.39, 113.25,

66.40, 54.46, 20.87. HRMS calcd for $C_{21}H_{18}F_3N_2O_7$ $[M+H]^+$ 467.1061, found 467.1051.



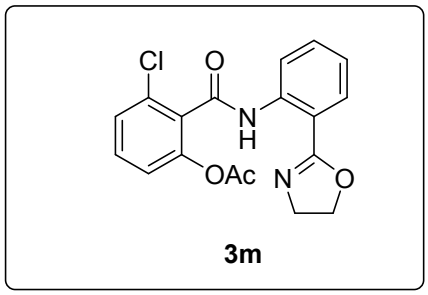
3k

2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-3-methylphenyl acetate (3k): White solid. Melting point: 100.2 ~ 101.8 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.41 (s, 1H), 8.95 (d, J = 8.3 Hz, 1H), 7.90 (dd, J = 7.9, 1.4 Hz, 1H), 7.61 – 7.50 (m, 1H), 7.35 (t, J = 7.9 Hz, 1H), 7.16 (dd, J = 10.6, 4.2 Hz, 2H), 7.07 (d, J = 8.1 Hz, 1H), 4.35 (t, J = 9.5 Hz, 2H), 4.01 (t, J = 9.5 Hz, 2H), 2.47 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.07, 165.38, 164.23, 147.29, 139.51, 137.01, 132.58, 130.98, 129.66, 129.20, 127.89, 122.81, 120.20, 120.03, 113.52, 66.26, 54.62, 20.96, 19.48. HRMS calcd for $C_{19}H_{19}N_2O_4$ $[M+H]^+$ 339.1339, found 339.1349.



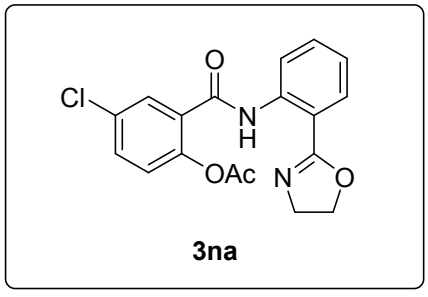
3l

2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-3-(trifluoromethyl)phenyl acetate (3l): White solid. Melting point: 137.2 ~ 138.6 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.57 (s, 1H), 8.89 (dd, J = 43.4, 39.3 Hz, 1H), 7.88 (dd, J = 7.9, 1.3 Hz, 1H), 7.69 – 7.41 (m, 4H), 7.15 (dd, J = 14.7, 7.3 Hz, 1H), 4.33 (t, J = 9.6 Hz, 2H), 3.96 (t, J = 9.5 Hz, 2H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.62, 164.16, 162.47, 147.83, 139.19, 137.98 (d, $J_{C\text{-}F}$ = 49 Hz), 132.62, 130.09, 129.14, 128.08 (q, $J_{C\text{-}F}$ = 207 Hz), 126.98, 123.77 (CF_3, q, $J_{C\text{-}F}$ = 140 Hz), 123.14, 121.31 (d, $J_{C\text{-}F}$ = 102 Hz), 120.16, 113.66, 66.31, 54.48, 20.79. HRMS calcd for $C_{19}H_{16}F_3N_2O_4$ $[M+H]^+$ 393.1057, found 393.1046.



3m

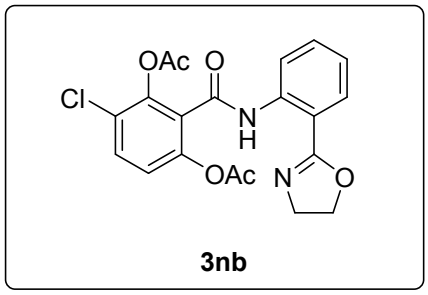
3-Chloro-2-((2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)phenyl acetate (3m): White solid. Melting point: 150.3 ~ 153.3 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.61 (s, 1H), 8.91 (d, J = 8.3 Hz, 1H), 7.90 (dd, J = 7.9, 1.4 Hz, 1H), 7.55 (dd, J = 11.4, 4.3 Hz, 1H), 7.44 – 7.34 (m, 2H), 7.23 – 7.12 (m, 2H), 4.36 (t, J = 9.6 Hz, 2H), 4.02 (t, J = 9.5 Hz, 2H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.66, 164.21, 162.34, 148.24, 139.26, 132.59, 131.97, 130.80, 130.36, 129.17, 127.24, 123.08, 121.66, 120.16, 113.70, 66.31, 54.57, 20.87. HRMS calcd for $C_{18}H_{16}ClN_2O_4$ $[M+H]^+$ 359.0793, found 359.0782.



3na

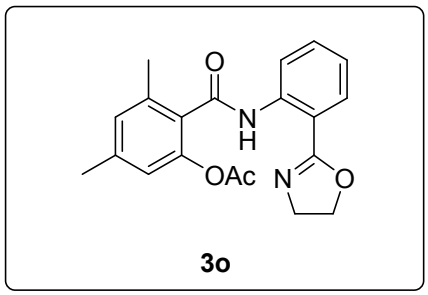
4-Chloro-2-((2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)phenyl acetate (3na): White solid. Melting point: 145.9 ~ 146.3 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.81 (s, 1H), 8.82 (d, J = 8.4 Hz, 1H), 8.03 – 7.80 (m, 2H), 7.65 – 7.43 (m, 2H), 7.14 (dd, J = 7.7, 5.7 Hz, 2H), 4.40 (t, J = 9.5 Hz, 2H), 4.12 (t, J = 9.5 Hz, 2H), 2.29 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.22,

164.70, 163.25, 147.30, 139.59, 132.64, 131.66, 131.47, 130.66, 129.50, 129.23, 125.00, 122.91, 120.04, 113.66, 66.38, 54.51, 21.07. HRMS calcd for $C_{18}H_{16}ClN_2O_4$ $[M+H]^+$ 359.0793, found 359.0793.



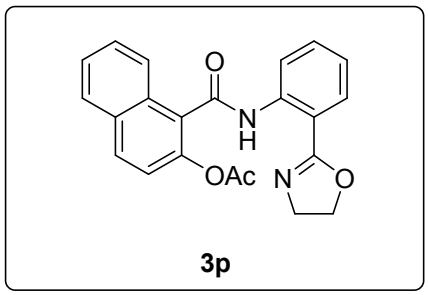
3nb

4-Chloro-2-((2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)-1,3-phenylene diacetate (3nb): colorless oil, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.59 (s, 1H), 8.85 (d, J = 8.3 Hz, 1H), 7.87 (dd, J = 7.8, 1.1 Hz, 1H), 7.51 (t, J = 6.5 Hz, 2H), 7.15 (t, J = 7.3 Hz, 2H), 4.34 (t, J = 9.5 Hz, 2H), 4.02 (t, J = 9.5 Hz, 2H), 2.25 (s, 3H), 2.15 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.35, 167.45, 164.10, 160.72, 146.40, 145.18, 139.25, 132.60, 130.88, 129.17, 126.49, 125.38, 123.11, 121.69, 119.99, 113.56, 66.41, 54.49, 20.92, 20.35. HRMS calcd for $C_{20}H_{18}ClN_2O_6$ $[M+H]^+$ 417.0848, found 417.0838.



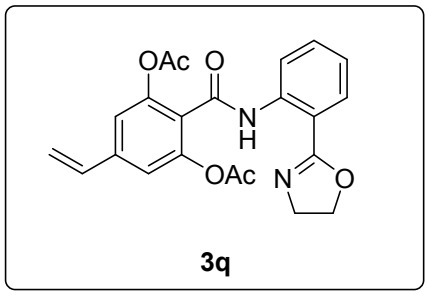
3o

2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-3,5-dimethylphenyl acetate (3o): White solid. Melting point: 123.5 ~ 126.1 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.34 (s, 1H), 8.92 (d, J = 8.4 Hz, 1H), 7.87 (d, J = 7.0 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.13 (dd, J = 13.9, 6.3 Hz, 1H), 6.94 (s, 1H), 6.85 (s, 1H), 4.33 (t, J = 9.5 Hz, 2H), 4.00 (t, J = 9.5 Hz, 2H), 2.40 (s, 3H), 2.35 (s, 3H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.19, 165.55, 164.21, 147.31, 140.03, 139.61, 136.74, 132.56, 129.18, 128.84, 128.19, 122.68, 120.69, 119.99, 113.46, 66.23, 54.66, 21.30, 20.97, 19.51. HRMS calcd for $C_{20}H_{21}N_2O_4$ $[M+H]^+$ 353.1496, found 353.1494.



3p

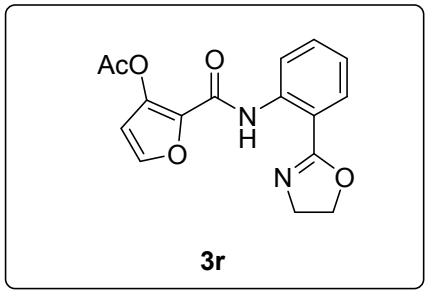
1-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)naphthalen-2-yl acetate (3p): White solid. Melting point: 151.8 ~ 152.3 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.69 (s, 1H), 9.07 (d, J = 8.4 Hz, 1H), 8.08 (d, J = 8.0 Hz, 1H), 7.96 – 7.81 (m, 3H), 7.63 – 7.45 (m, 3H), 7.35 (d, J = 8.9 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 4.28 (t, J = 9.5 Hz, 2H), 3.85 (t, J = 9.5 Hz, 2H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.13, 164.85, 164.12, 144.97, 139.61, 132.65, 131.59, 130.93, 130.68, 129.21, 128.11, 127.37, 126.54, 126.09, 125.42, 122.98, 121.57, 120.15, 113.58, 66.29, 54.45, 21.05. HRMS calcd for $C_{22}H_{19}N_2O_4$ $[M+H]^+$ 375.1339, found 375.1341.



3q

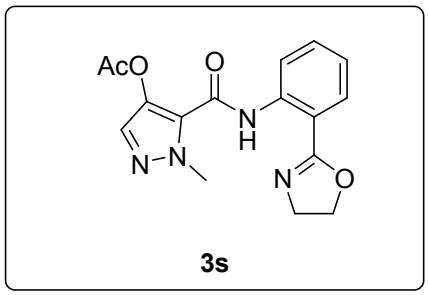
2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-5-vinyl-1,3-phenylene diacetate (3q): White solid. Melting point: 129.5 ~ 131.2 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.53 (s, 1H), 8.89 (d, J = 8.4 Hz, 1H), 7.87 (dd, J = 7.9, 1.5 Hz, 1H), 7.76 – 7.46 (m, 1H), 7.19 – 7.04 (m,

3H), 6.67 (dd, *J* = 17.5, 10.9 Hz, 1H), 5.80 (d, *J* = 17.5 Hz, 1H), 5.39 (d, *J* = 10.9 Hz, 1H), 4.34 (t, *J* = 9.6 Hz, 2H), 4.02 (t, *J* = 9.5 Hz, 2H), 2.18 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.69, 164.22, 161.52, 148.57, 140.31, 139.55, 134.95, 132.62, 129.16, 123.19, 122.82, 119.90, 118.22, 117.06, 113.36, 66.35, 54.53, 20.99. HRMS calcd for $C_{22}H_{21}N_2O_6$ $[M+H]^+$ 409.1394, found 409.1384.



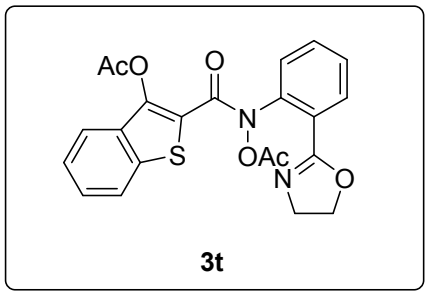
3r

2-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)furan-3-yl acetate (3r): White solid. Melting point: 137.4 ~ 139.2 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.85 (s, 1H), 8.78 (d, *J* = 8.4 Hz, 1H), 7.88 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.61 – 7.35 (m, 2H), 7.24 – 6.97 (m, 1H), 6.61 (d, *J* = 2.0 Hz, 1H), 4.41 (t, *J* = 9.1 Hz, 2H), 4.19 (t, *J* = 9.3 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.94, 164.55, 156.36, 142.67, 142.21, 139.28, 135.72, 132.41, 129.22, 122.63, 120.32, 113.86, 109.17, 66.28, 54.79, 20.93. HRMS calcd for $C_{16}H_{15}N_2O_5$ $[M+H]^+$ 315.0976, found 315.0974.



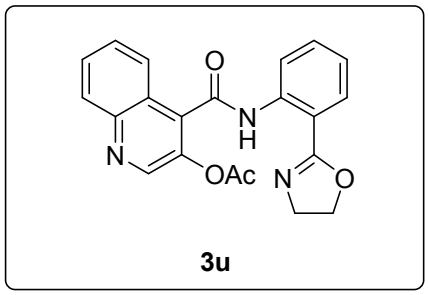
3s

5-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)-1-methyl-1H-pyrazol-4-yl acetate (3s): colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.43 (s, 1H), 8.62 (d, *J* = 8.4 Hz, 1H), 7.90 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.62 (s, 1H), 7.58 – 7.46 (m, 1H), 7.23 – 7.11 (m, 1H), 4.39 (t, *J* = 9.6 Hz, 2H), 4.14 (s, 3H), 4.06 (t, *J* = 9.5 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.63, 164.43, 157.27, 138.81, 134.39, 132.40, 130.03, 129.38, 125.96, 123.27, 121.10, 114.45, 66.33, 54.73, 40.15, 20.96. HRMS calcd for $C_{16}H_{17}N_4O_4$ $[M+H]^+$ 329.1244, found 329.1239.



3t

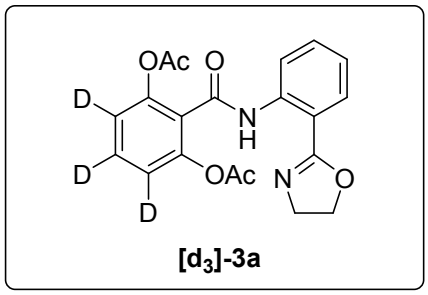
2-(Acetoxy(2-(4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)benzo[b]thiophen-3-yl acetate (3t): colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.22 (m, 1H), 7.88 – 7.74 (m, 3H), 7.65 (dd, *J* = 6.6, 2.2 Hz, 1H), 7.59 – 7.44 (m, 3H), 4.52 (t, *J* = 5.6 Hz, 2H), 4.36 (t, *J* = 5.5 Hz, 2H), 2.30 (s, 3H), 1.97 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.56, 169.21, 167.67, 162.14, 147.94, 147.05, 140.15, 136.84, 134.70, 131.71, 127.88, 126.92, 126.87, 125.33, 122.81, 122.06, 121.67, 120.90, 61.35, 44.90, 20.85, 20.50. HRMS calcd for $C_{22}H_{19}N_2O_5S$ $[M+H]^+$ 423.1009, found 423.0995.



3u

4-((2-(4,5-Dihydrooxazol-2-yl)phenyl)carbamoyl)quinolin-3-yl acetate (3u): White solid. Melting point: 189.4 ~ 190.7 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.92 (s, 1H), 9.02 (d, *J* = 8.4 Hz, 1H), 8.87 (s, 1H), 8.18 (d, *J* = 8.4 Hz, 1H), 8.09 (dd, *J* = 8.4,

0.6 Hz, 1H), 7.91 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.75 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.66 – 7.52 (m, 2H), 7.24 – 7.17 (m, 1H), 4.31 (t, *J* = 9.6 Hz, 2H), 3.87 (t, *J* = 9.6 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.74, 164.30, 162.38, 146.66, 146.32, 139.85, 139.18, 133.01, 132.76, 129.71, 129.41, 129.29, 127.98, 125.41, 125.03, 123.43, 120.16, 113.65, 66.38, 54.37, 20.83. HRMS calcd for $C_{21}H_{18}N_3O_4$ $[M+H]^+$ 376.1292, found 376.1285.



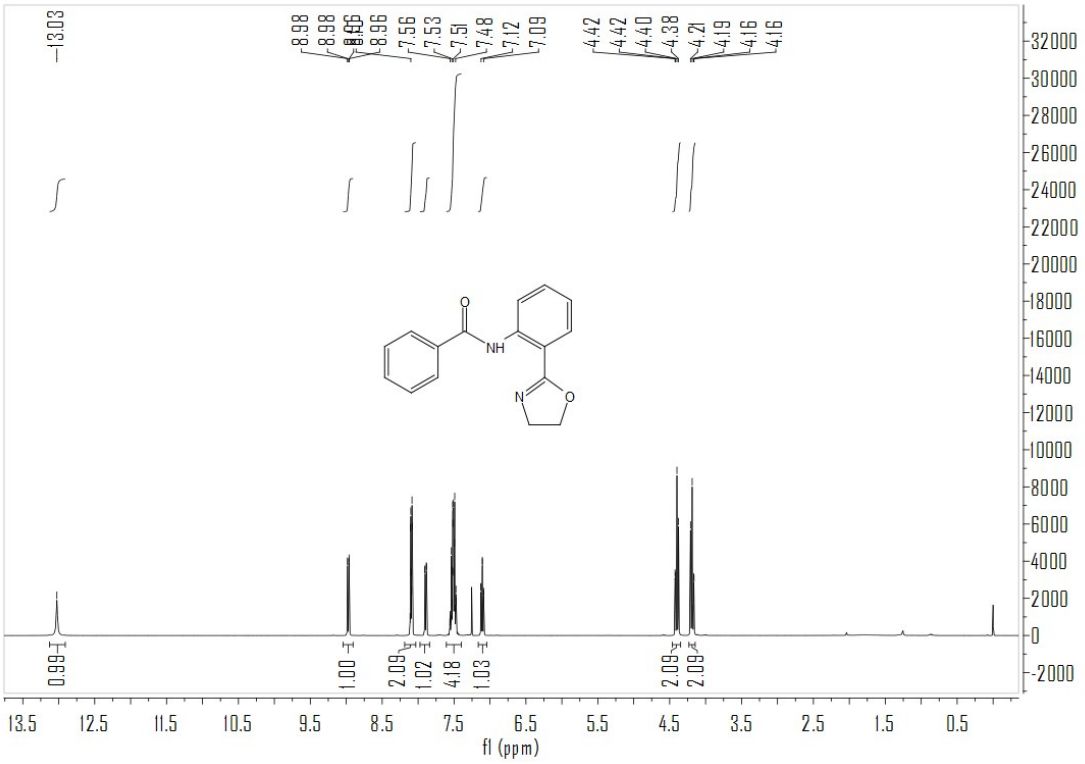
[d_3]-3a

(1:1 products). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.53 (s, 1H), 8.79 (dd, *J* = 83.6, 8.5 Hz, 1H), 7.87 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.56 – 7.48 (m, 1H), 7.45 (t, *J* = 8.3 Hz, **0.52H**), 7.20 – 7.07 (m, 2H), 4.62 – 4.22 (m, 2H), 4.19 – 3.73 (m, 2H), 2.44 – 2.10 (m, 6H).

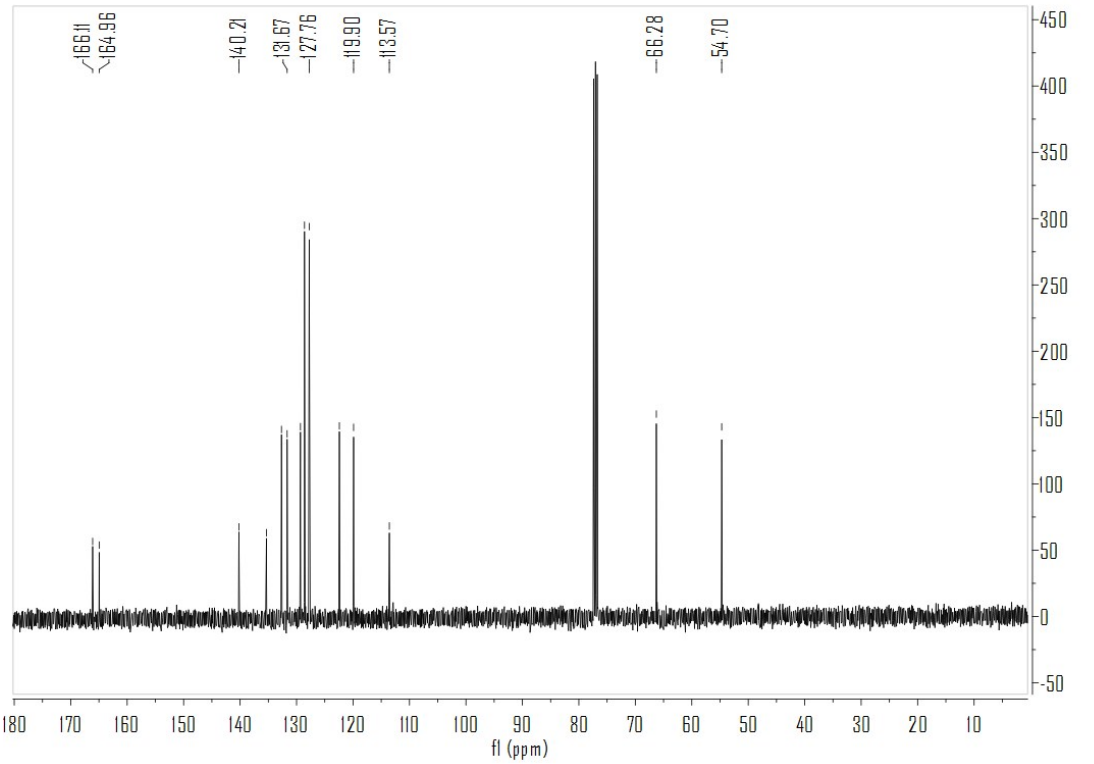
NMR Spectra

1. Substrates

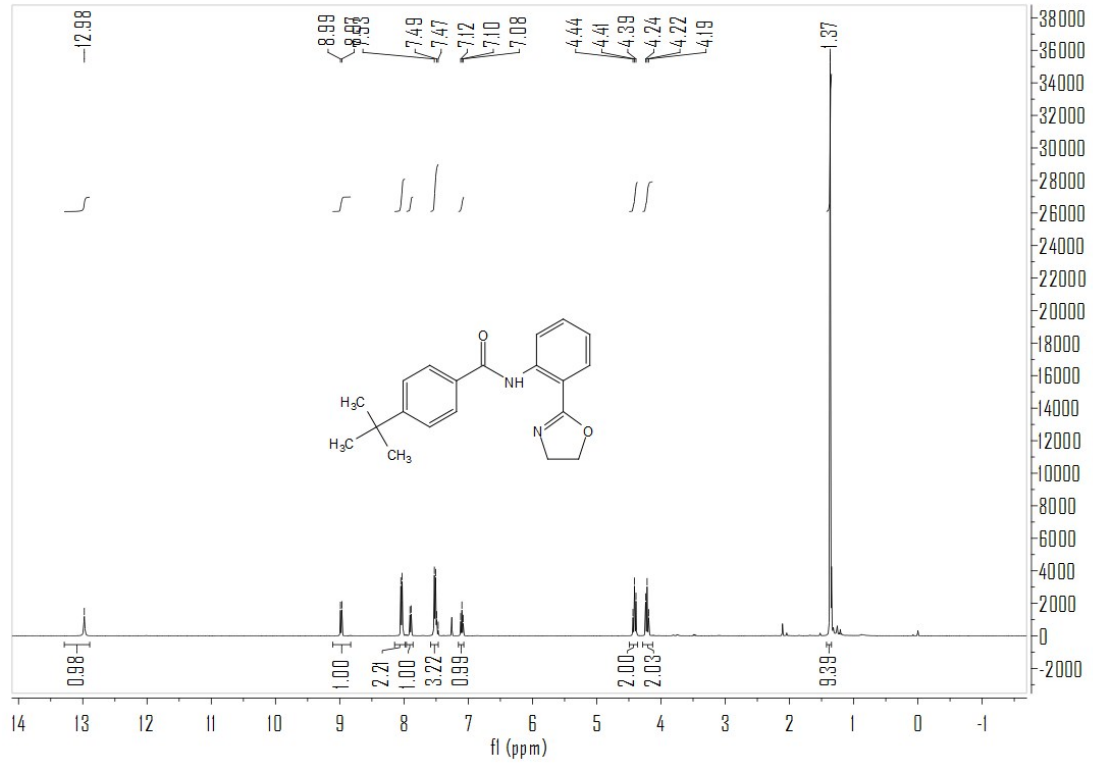
^{1}H NMR of 1a



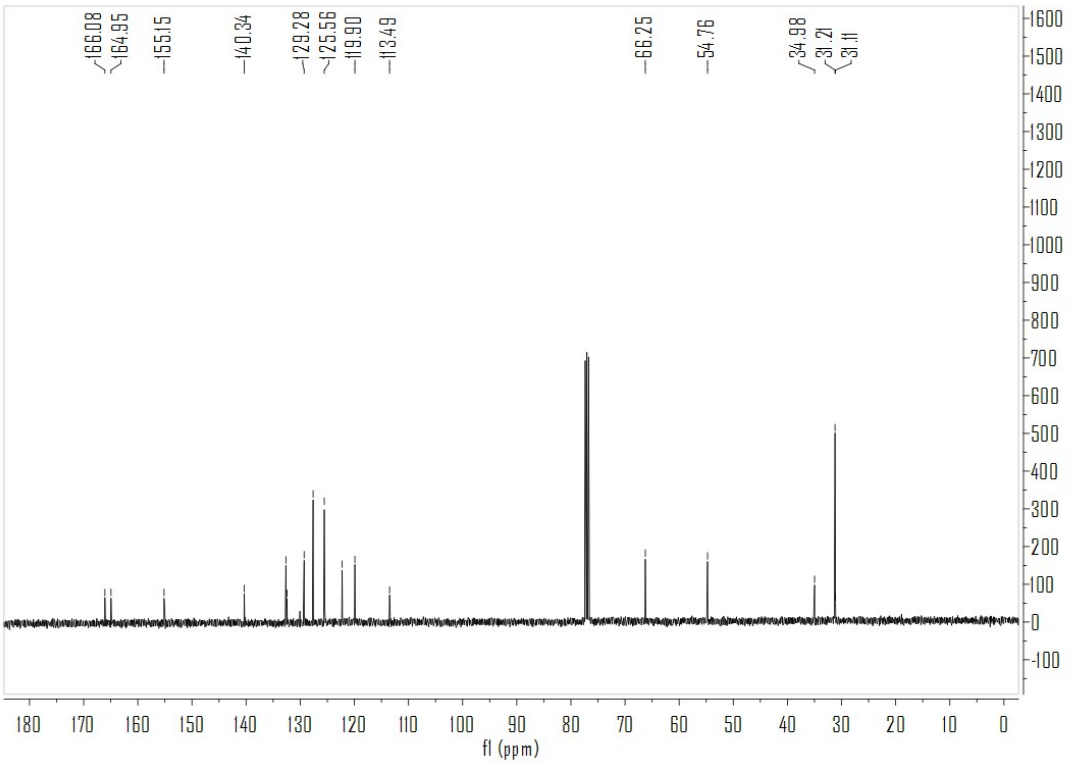
^{13}C NMR of 1a



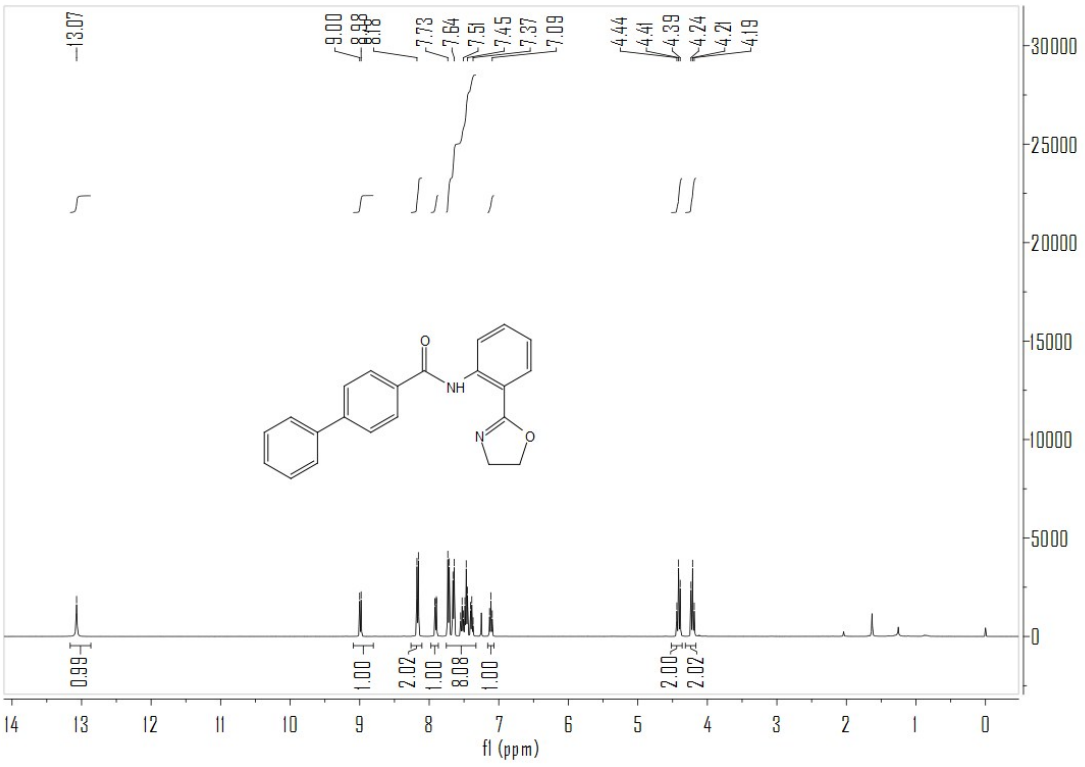
^{1}H NMR of 1b



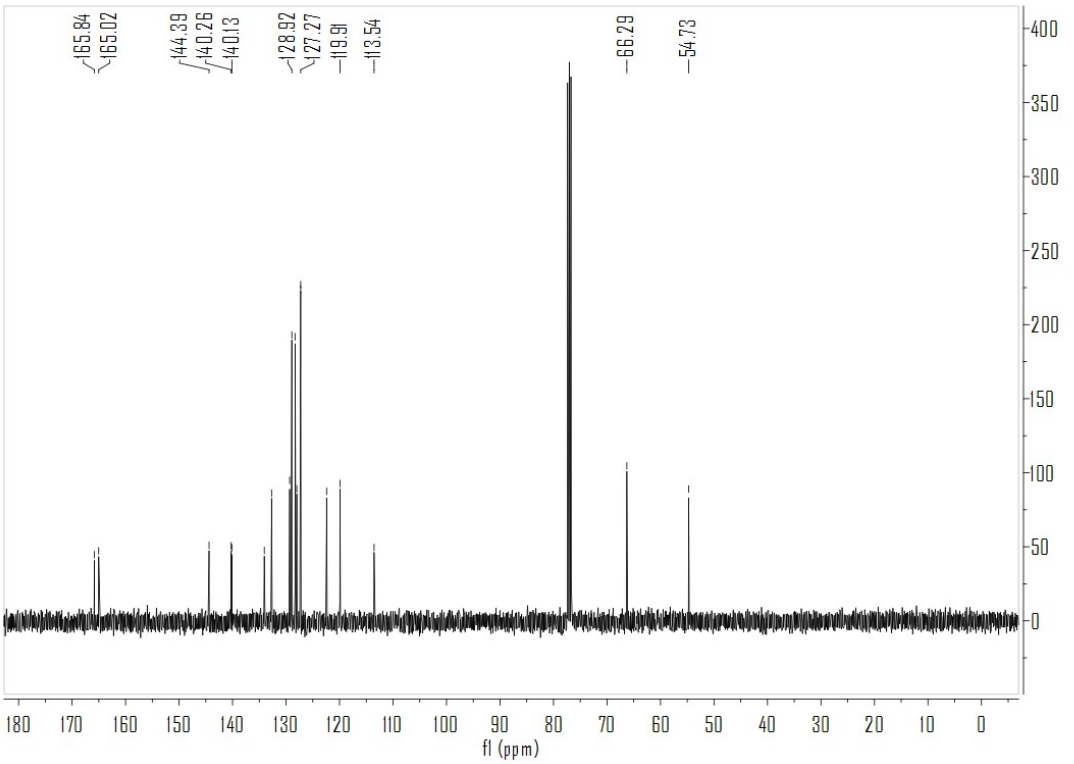
^{13}C NMR of 1b



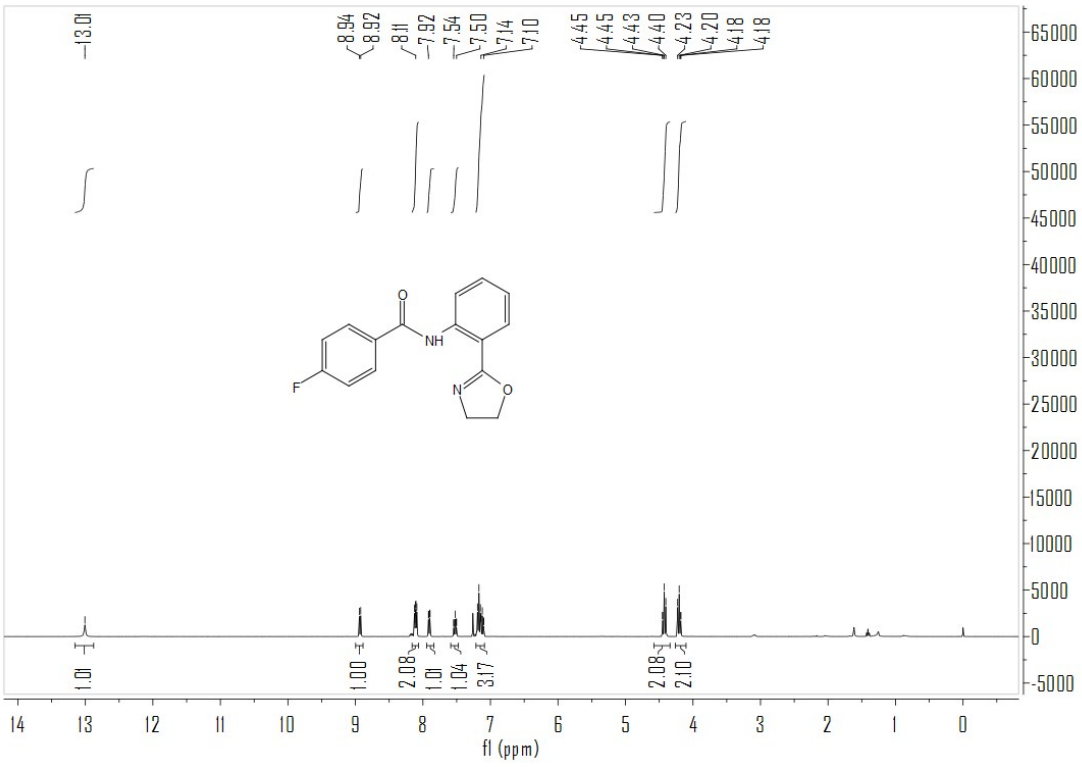
^{1}H NMR of 1c



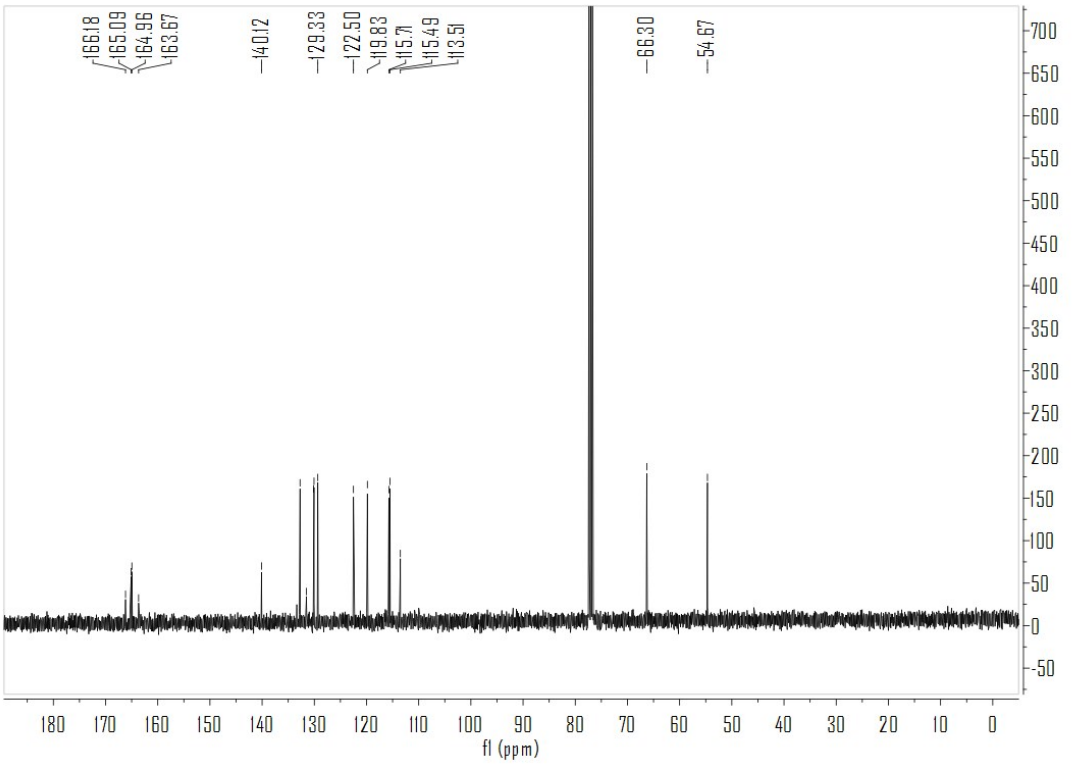
^{13}C NMR of 1c



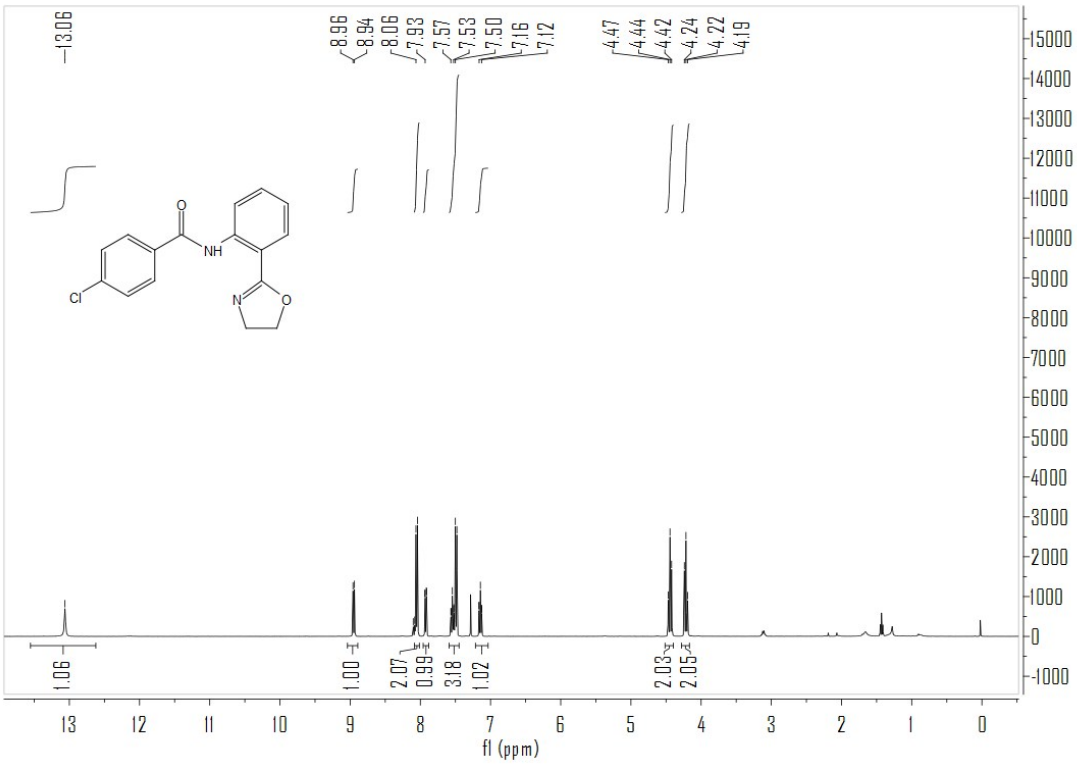
^{1}H NMR of 1d



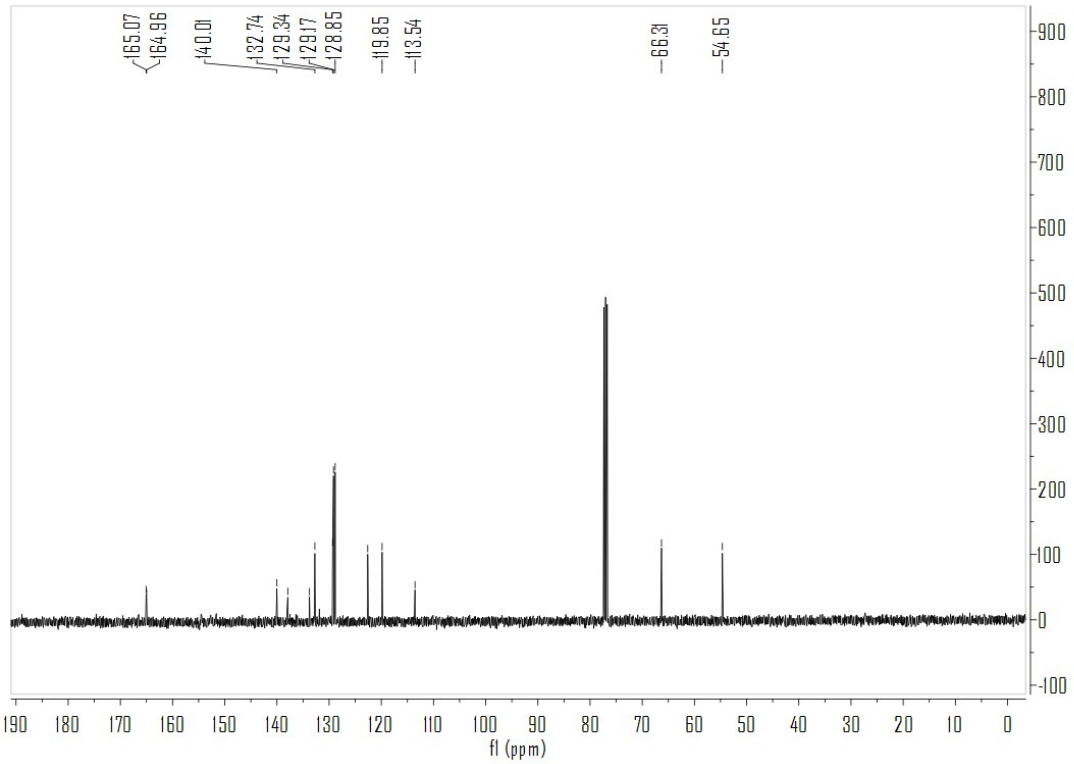
^{13}C NMR of 1d



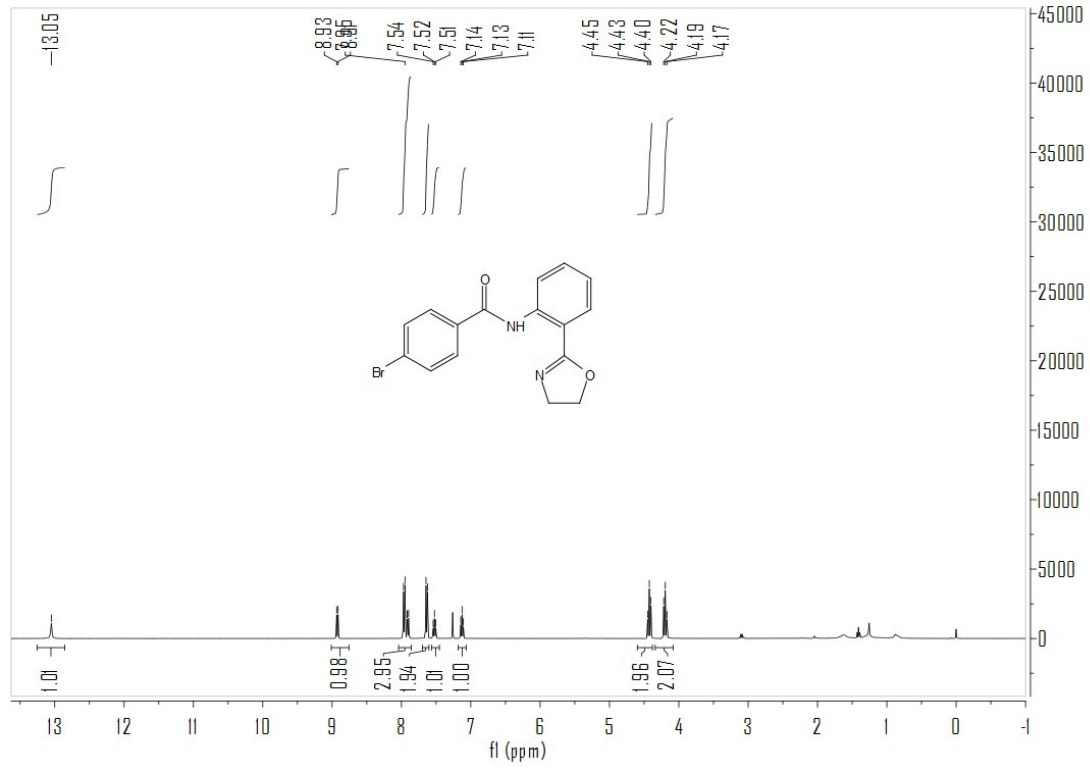
^{1}H NMR of 1e



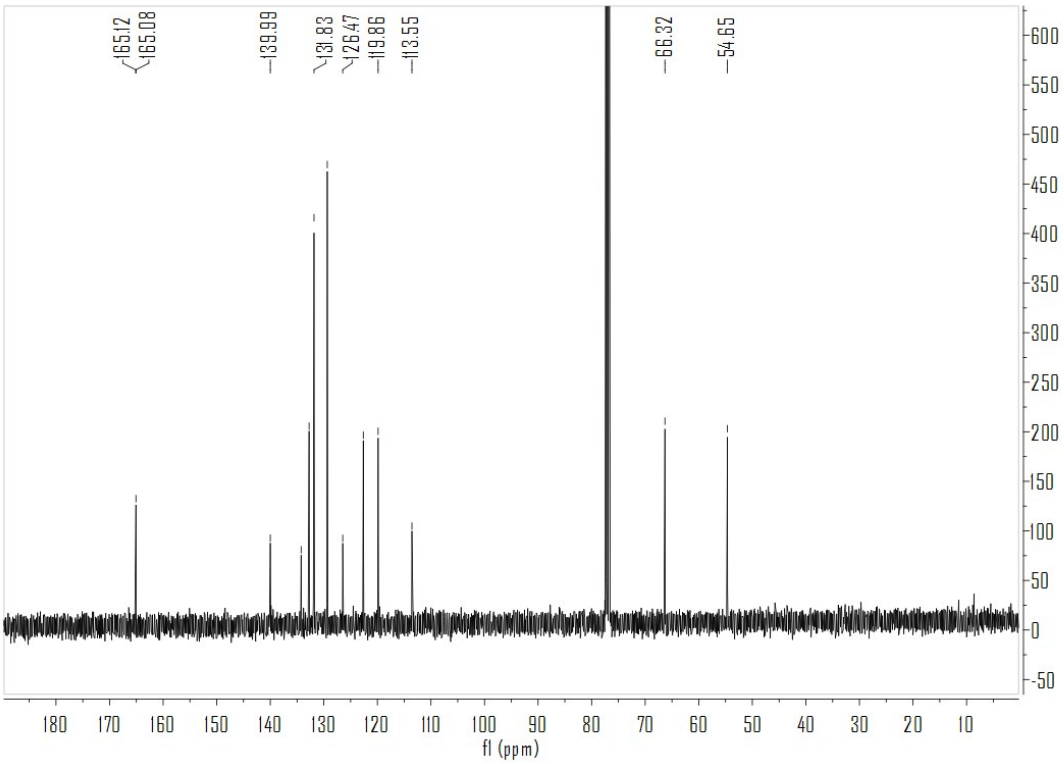
^{13}C NMR of 1e



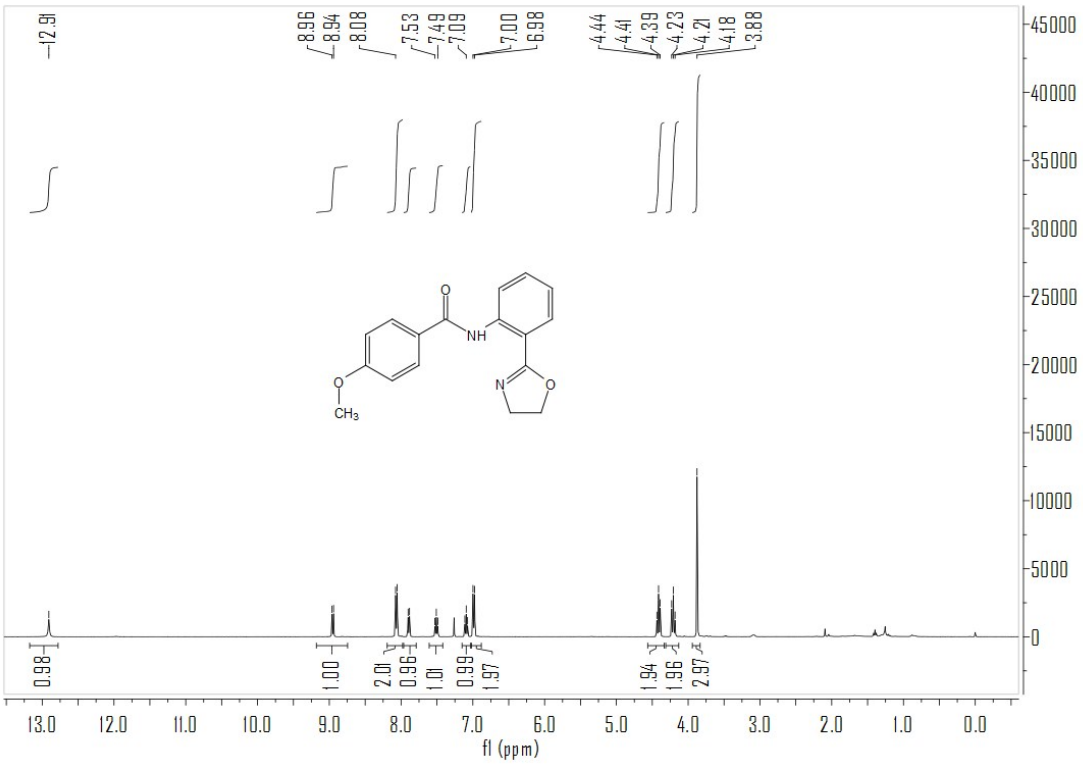
^{1}H NMR of 1f



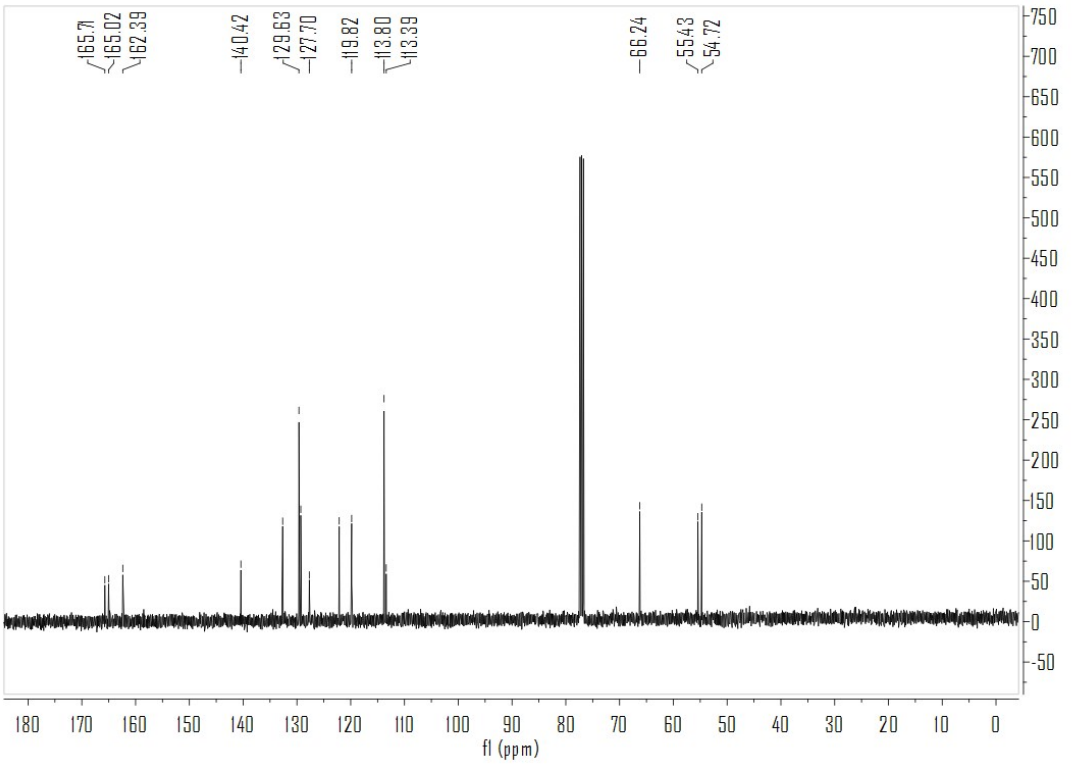
^{13}C NMR of 1f



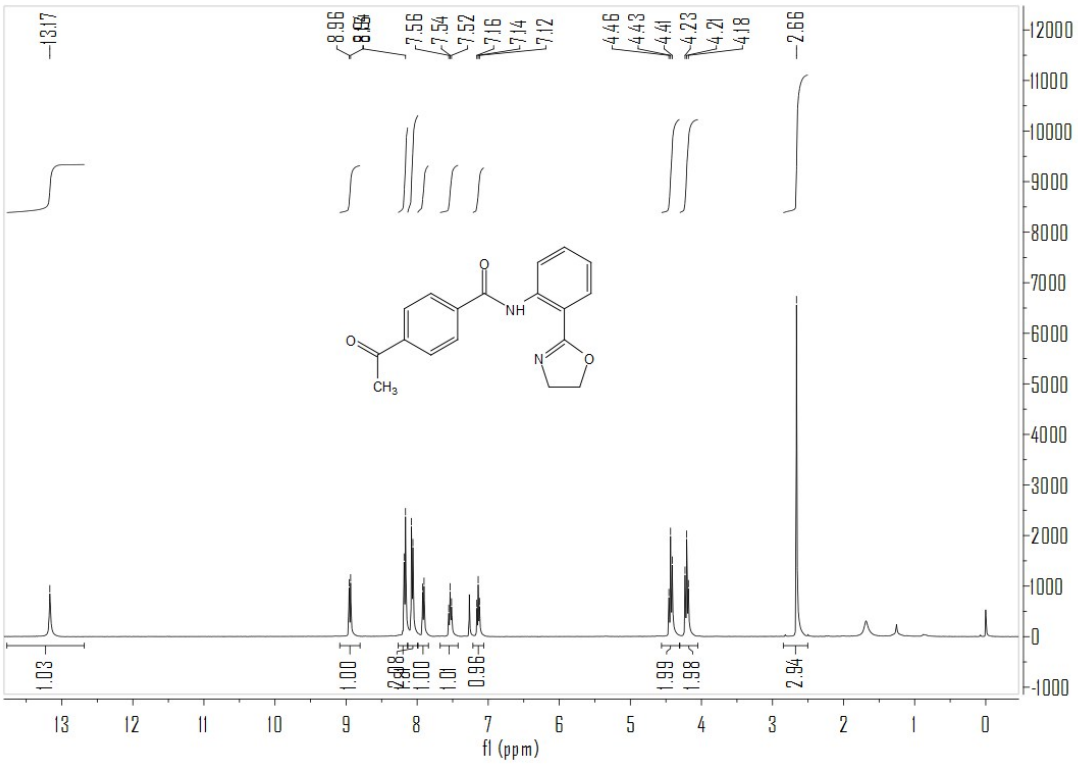
^{1}H NMR of 1g



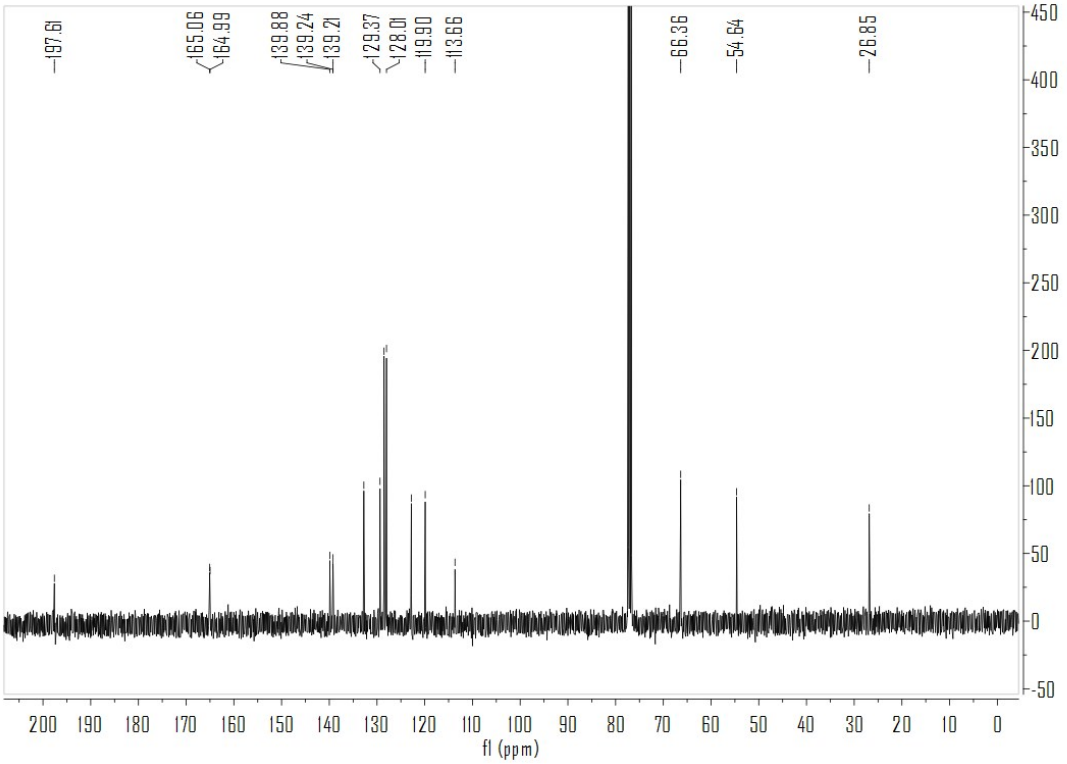
^{13}C NMR of 1g



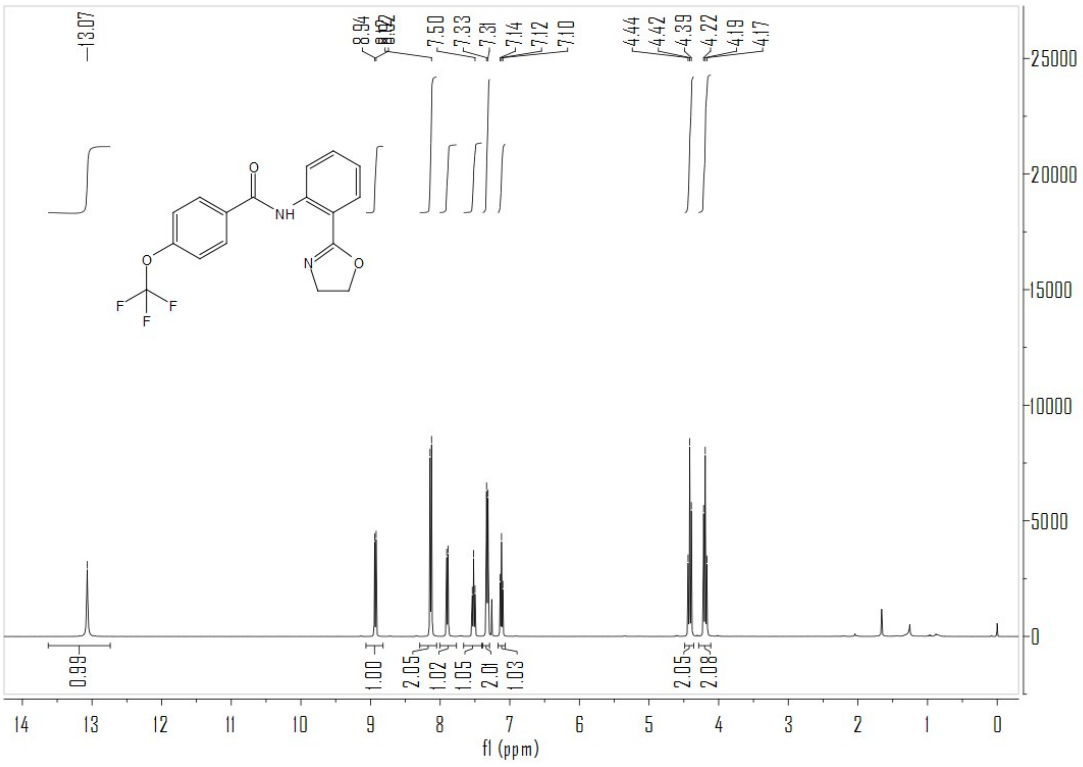
^{1}H NMR of 1h



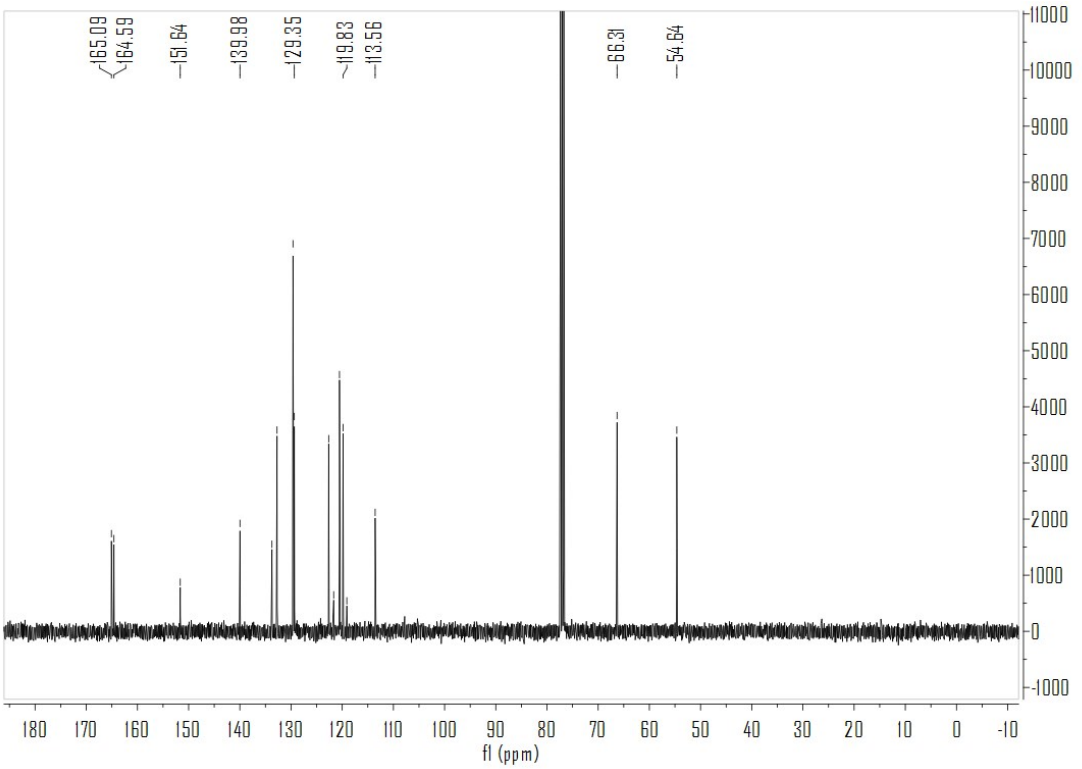
^{13}C NMR of 1h



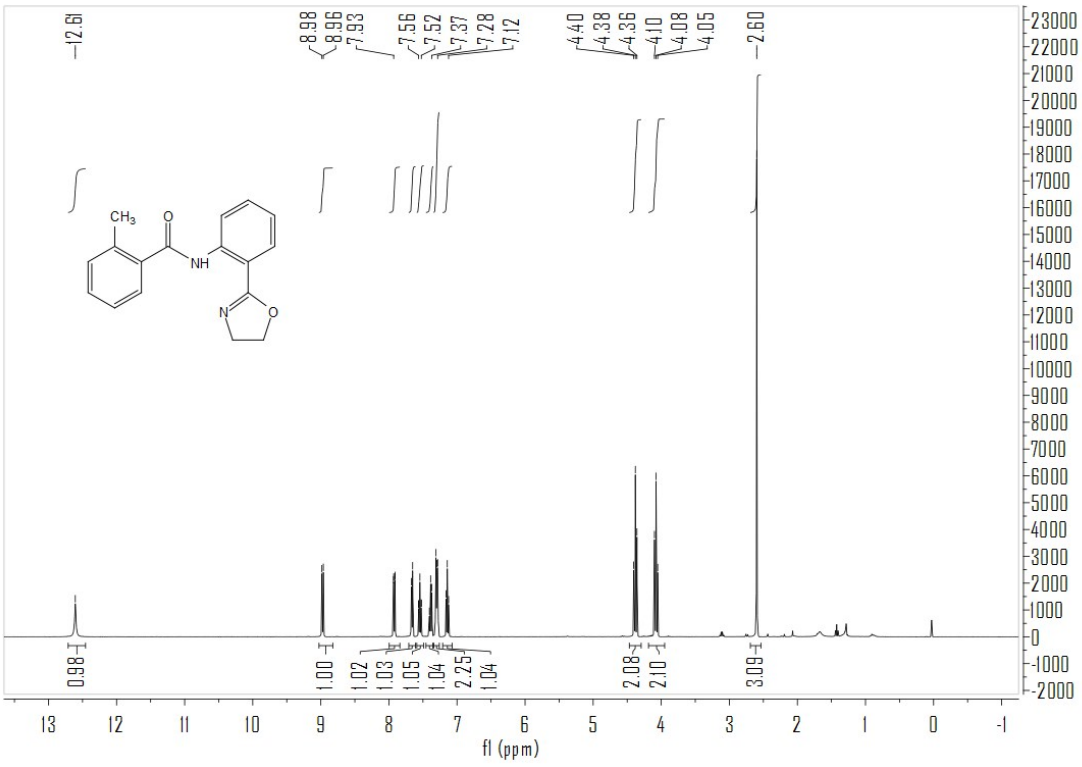
^{1}H NMR of 1j



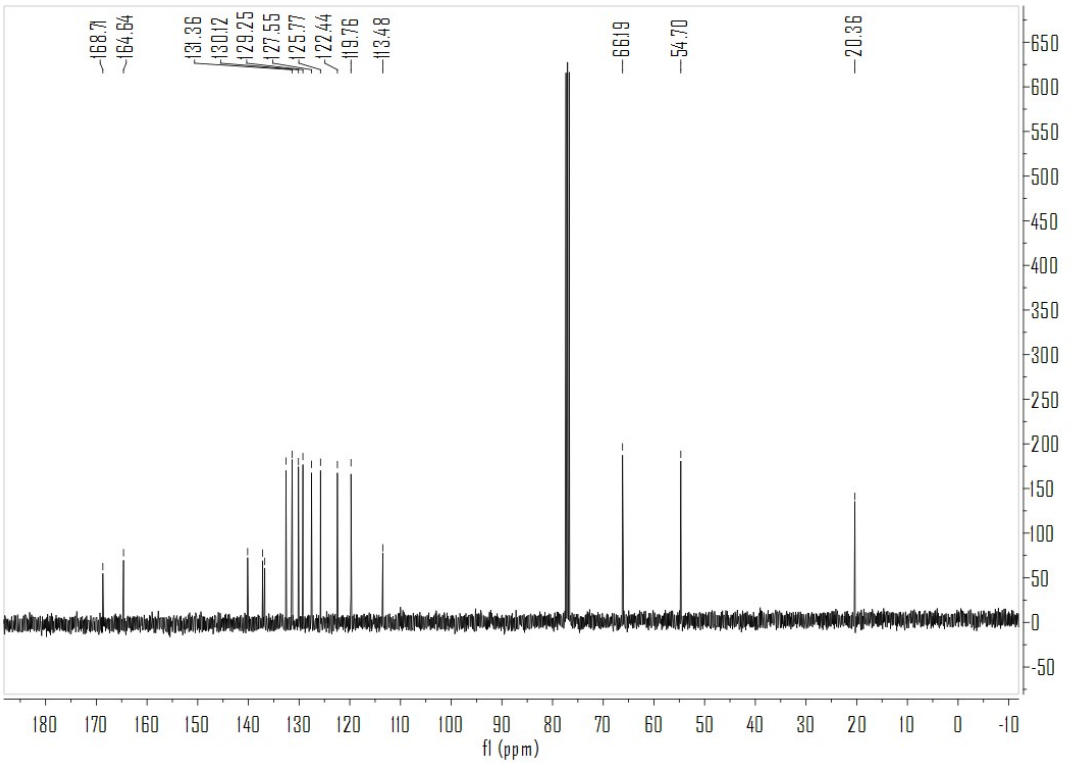
^{13}C NMR of 1j



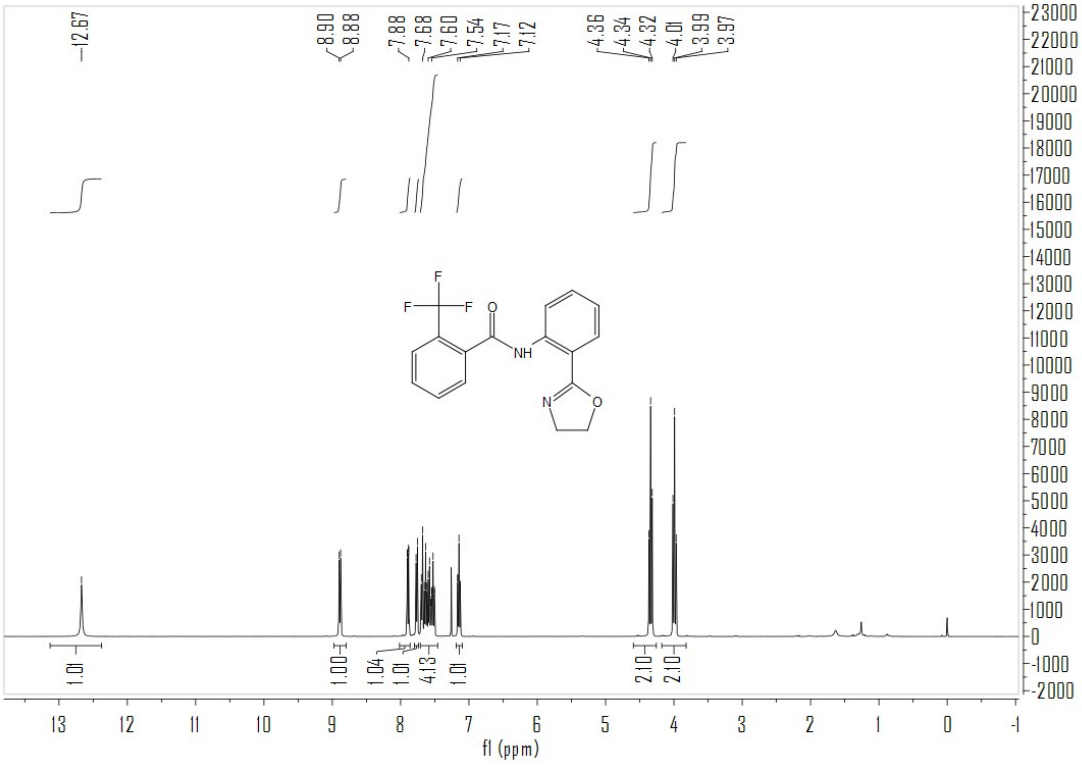
^{1}H NMR of 1k



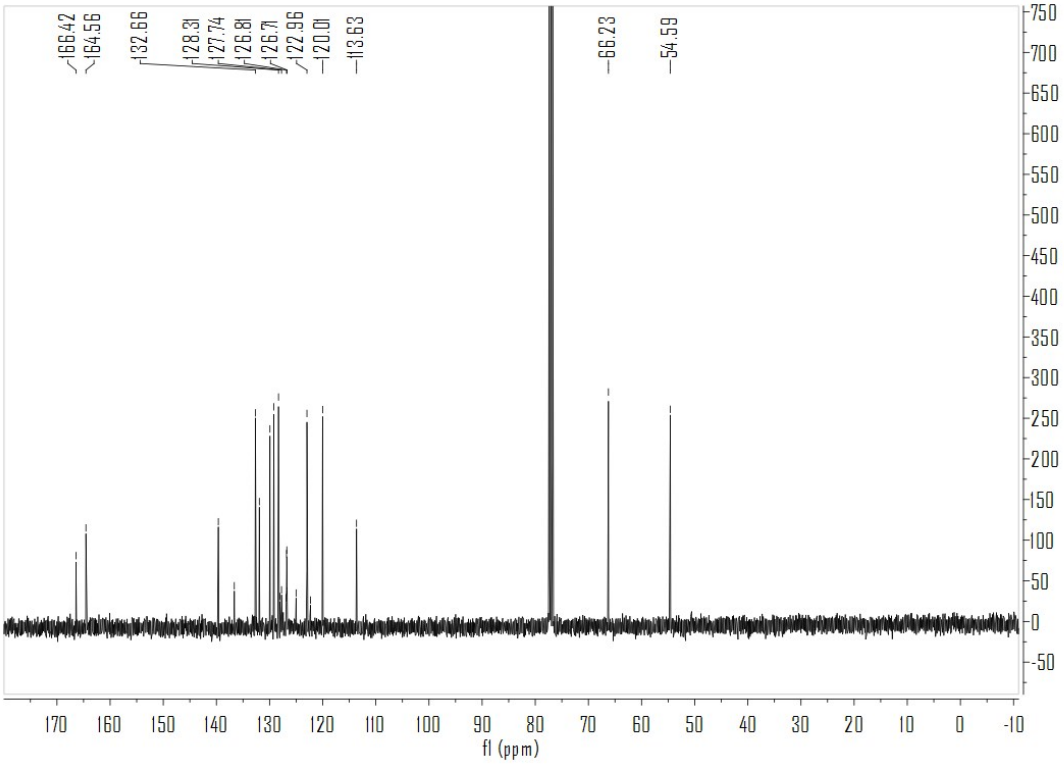
^{13}C NMR of 1k



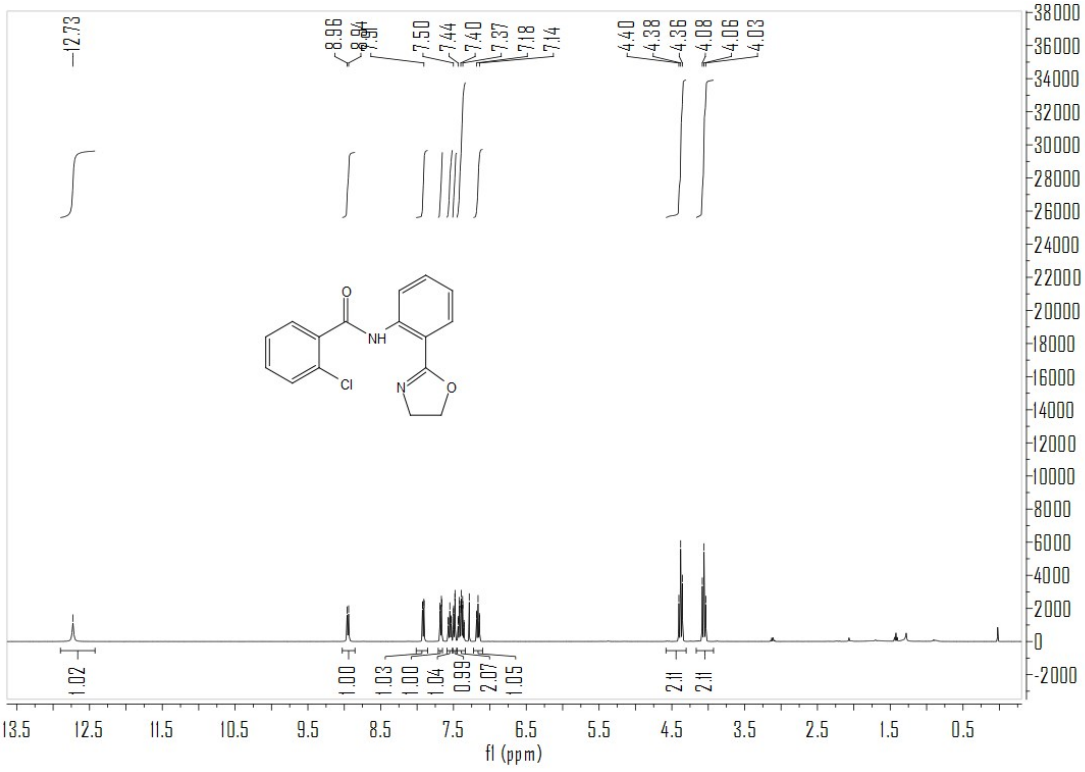
^{1}H NMR of 1l



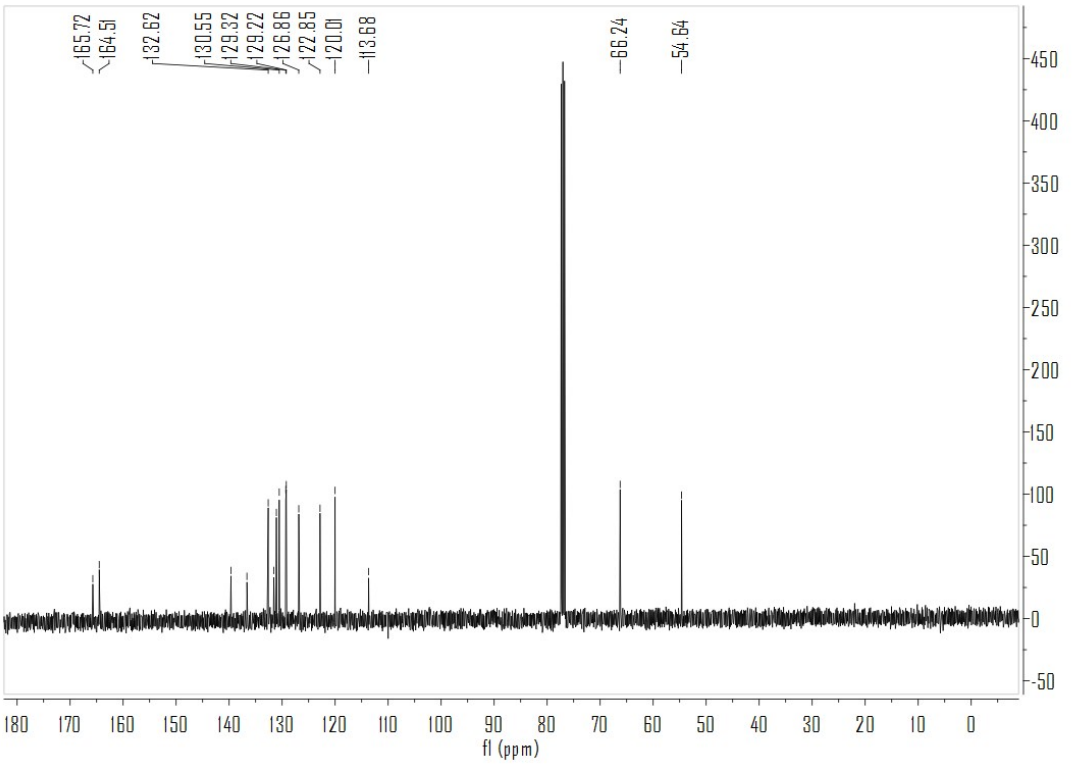
^{13}C NMR of 1l



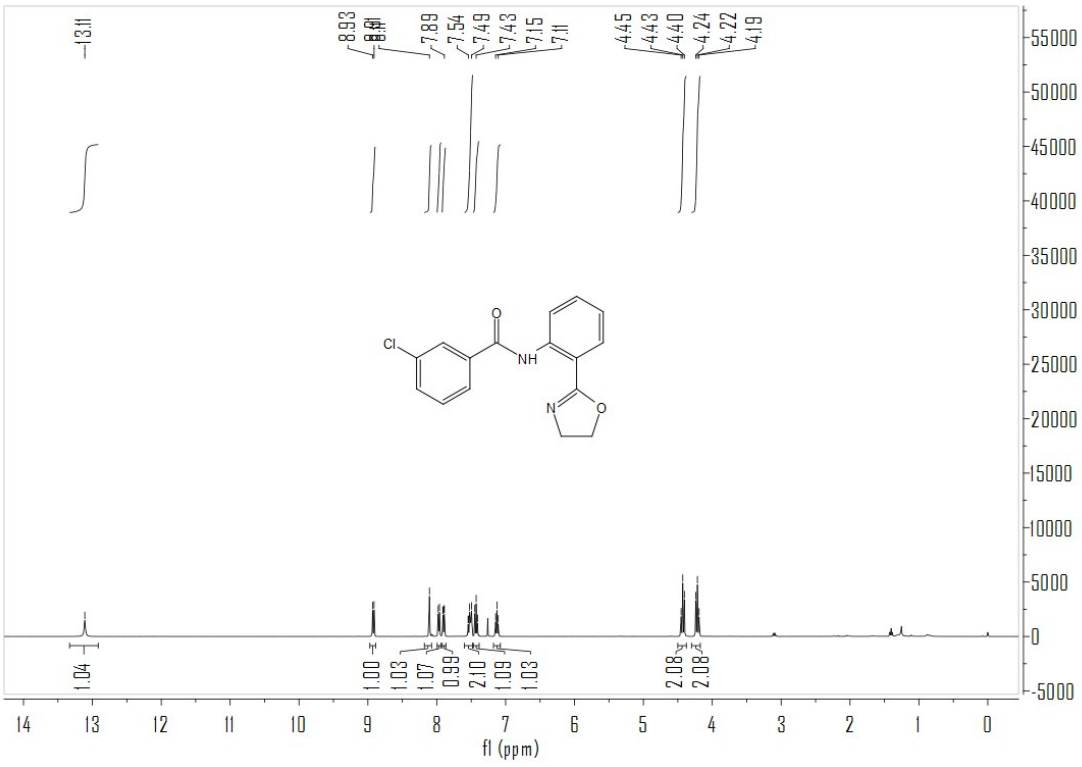
^{1}H NMR of 1m



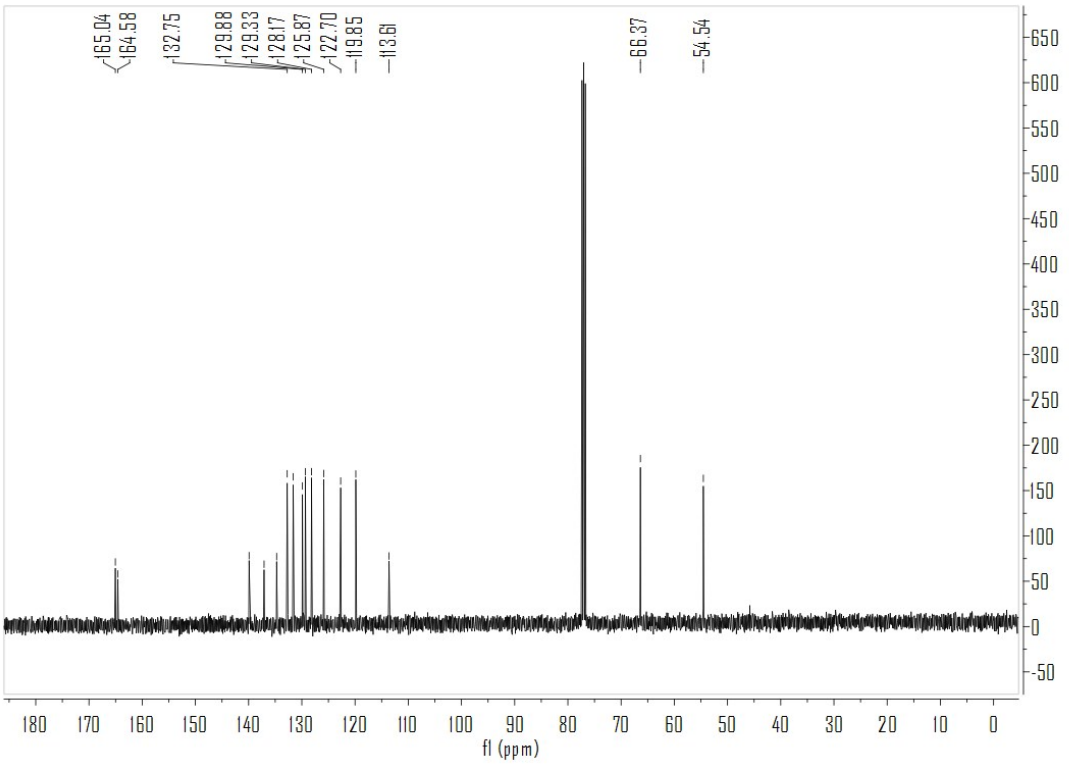
^{13}C NMR of 1m



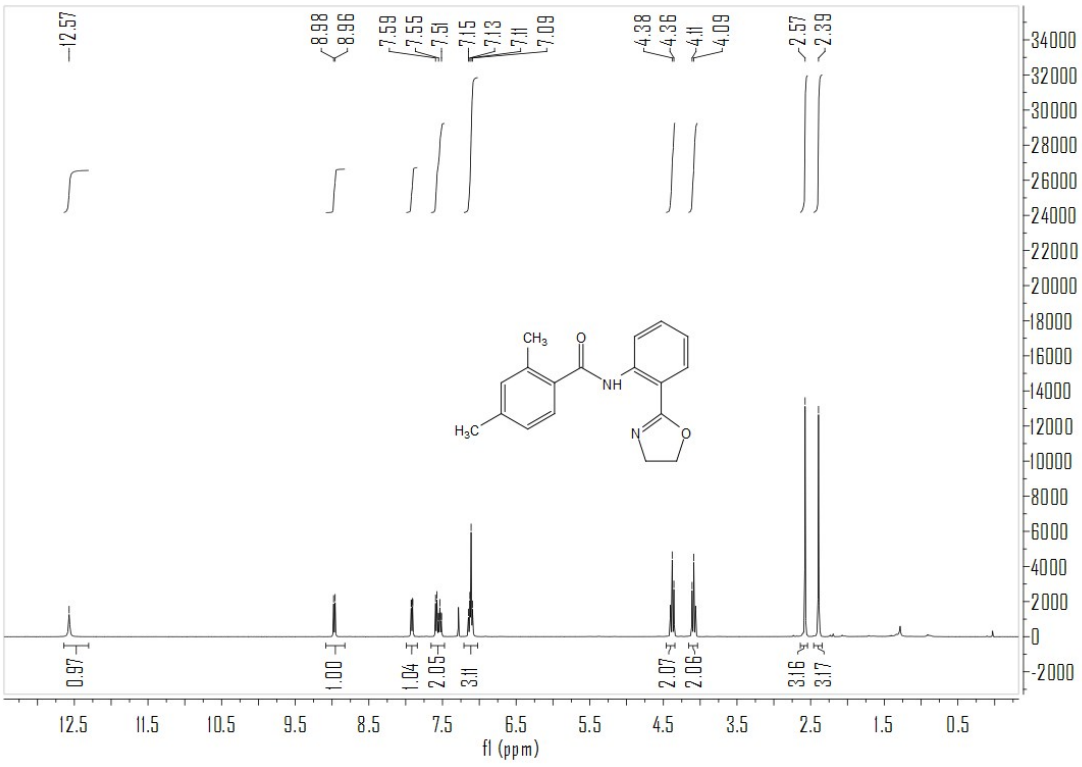
^{1}H NMR of 1n



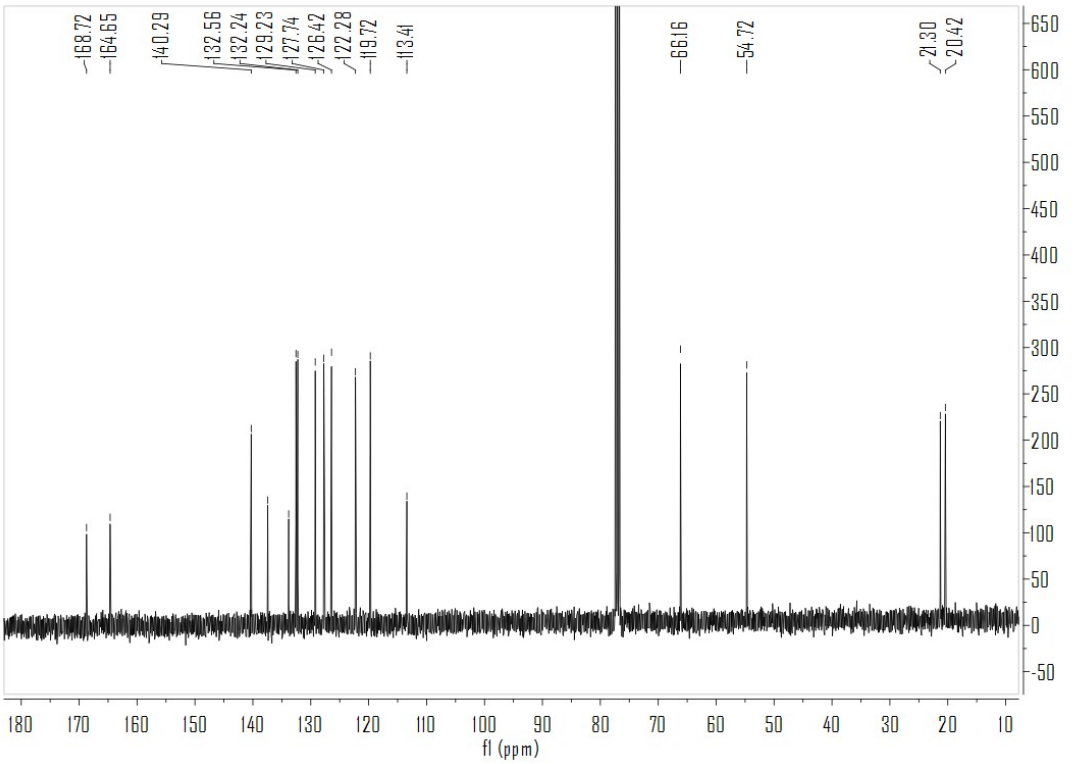
^{13}C NMR of 1n



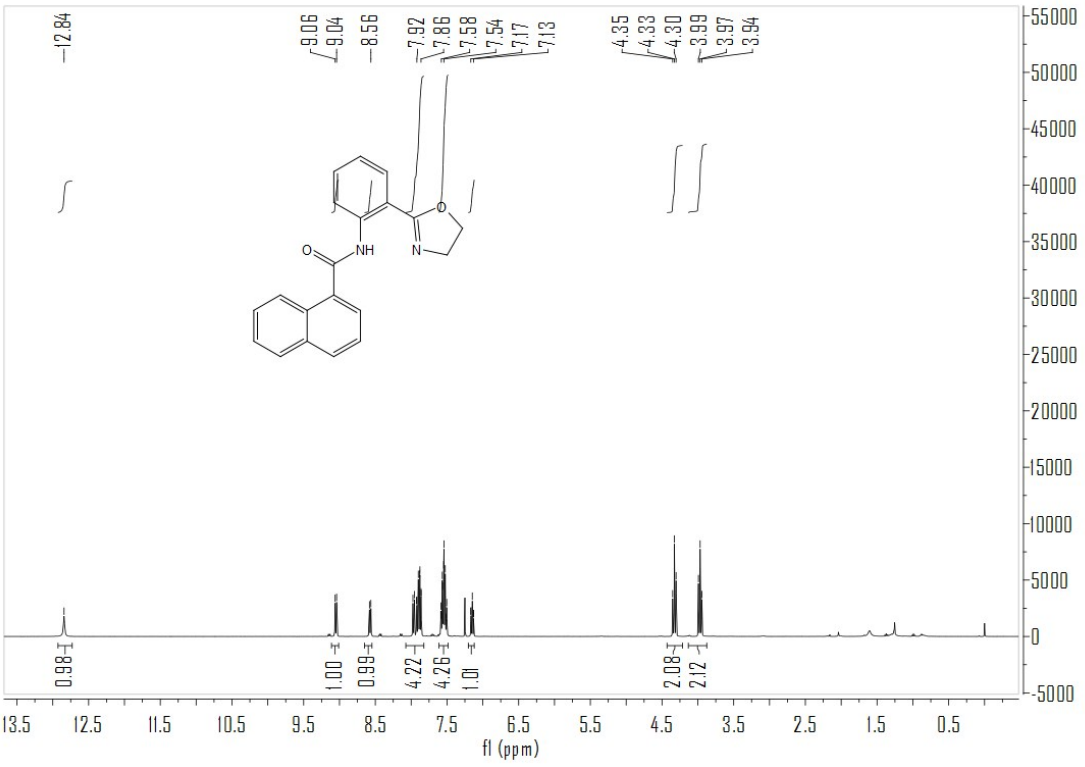
^{1}H NMR of 1o



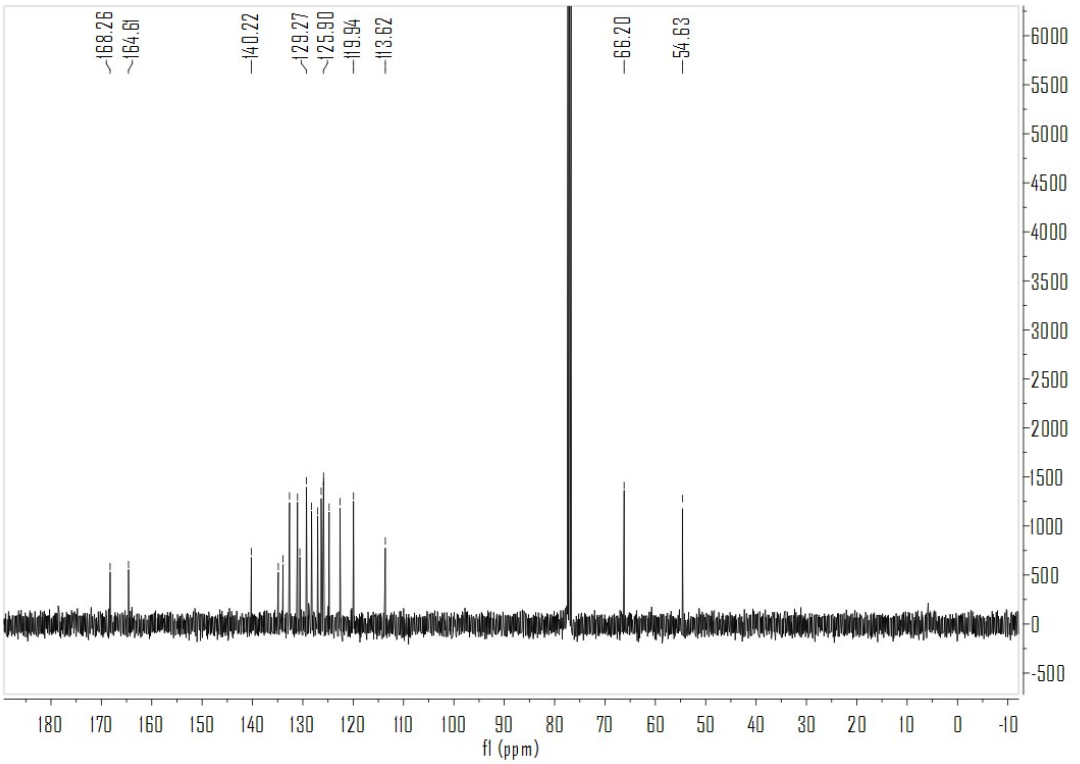
^{13}C NMR of 1o



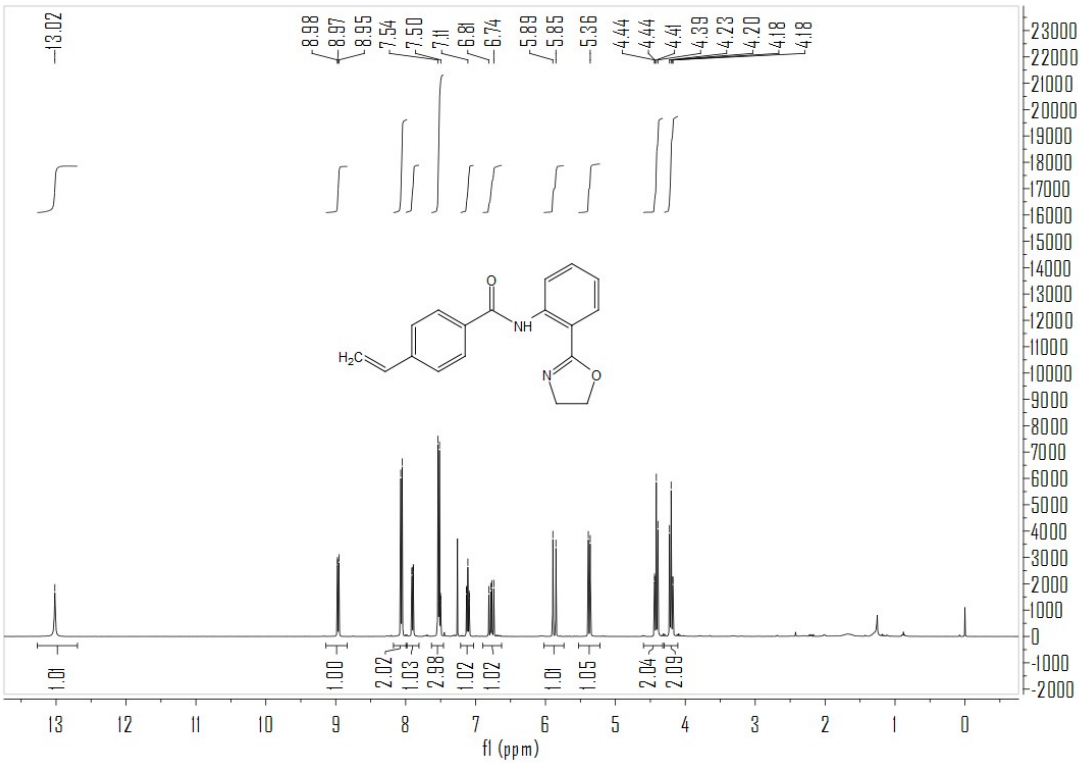
^{1}H NMR of 1p



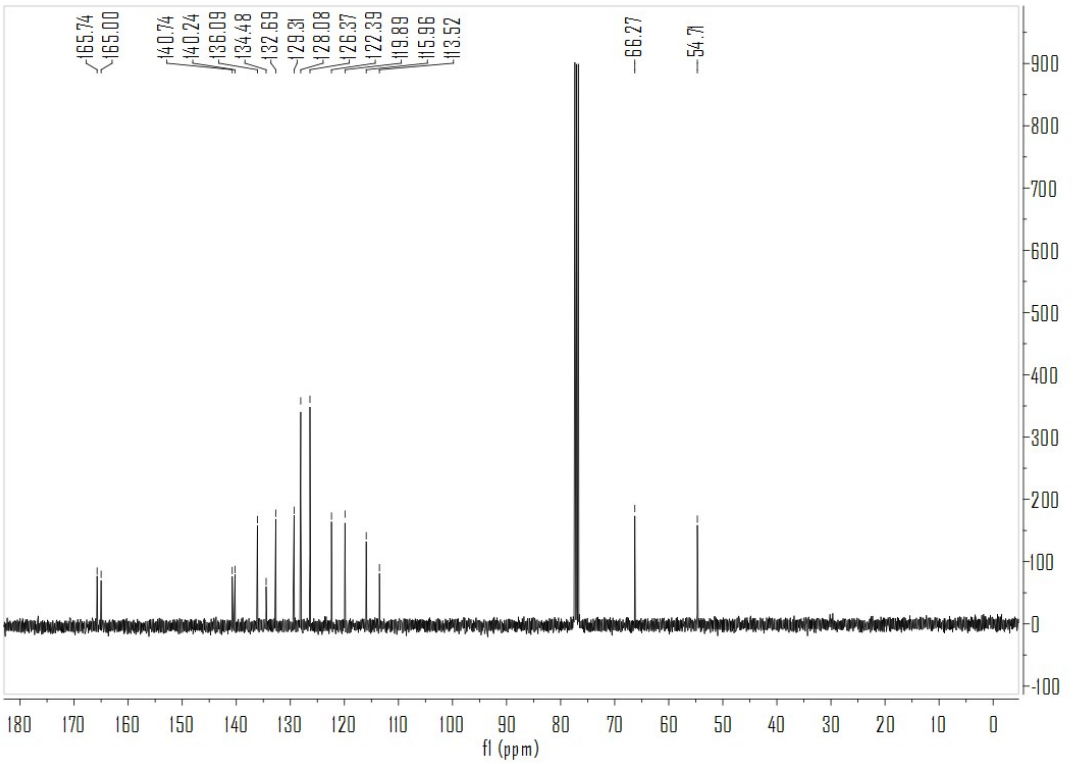
^{13}C NMR of 1p



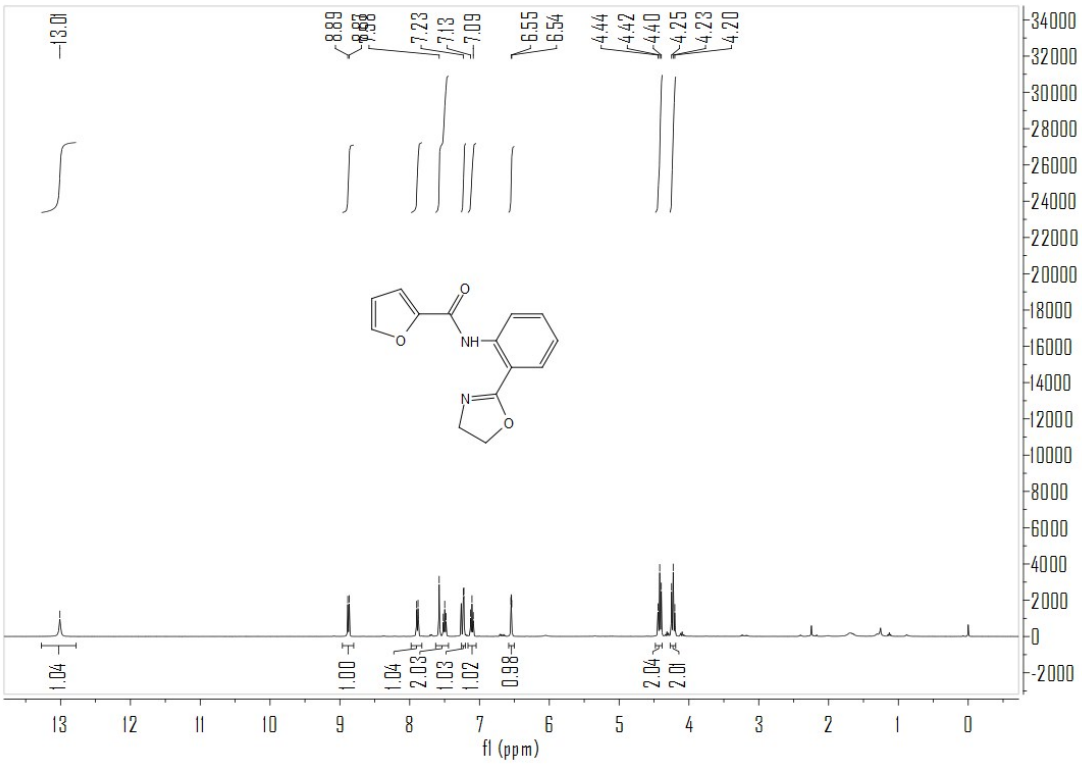
^{1}H NMR of 1q



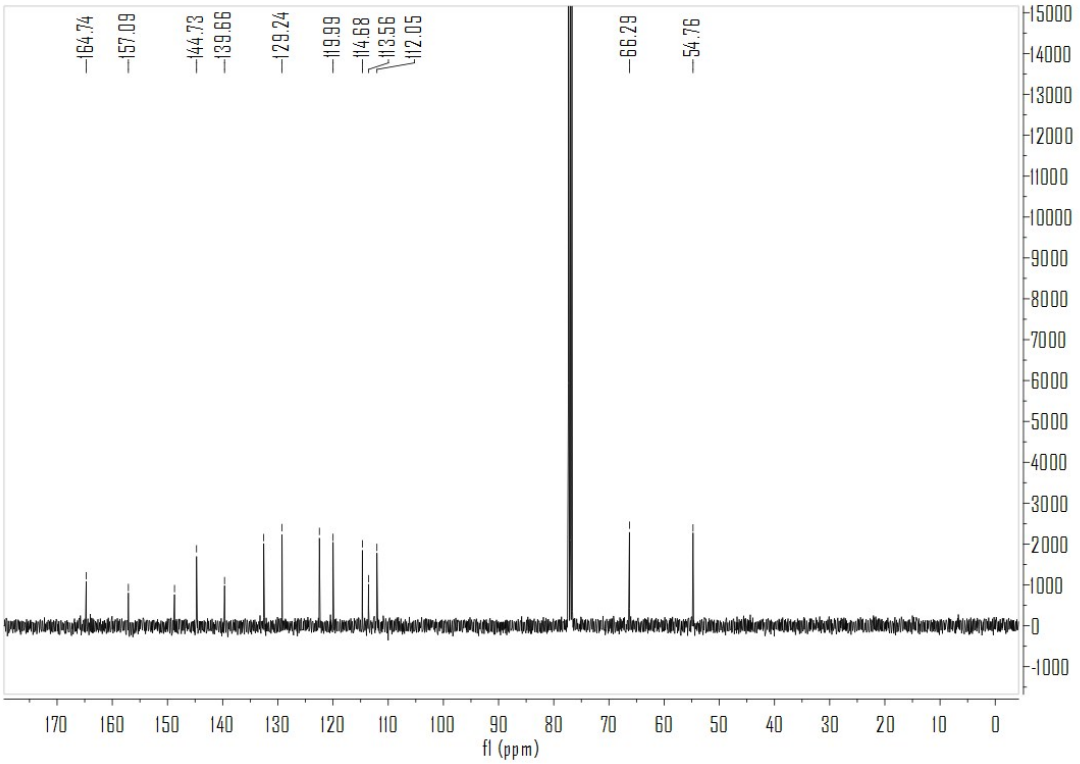
^{13}C NMR of 1q



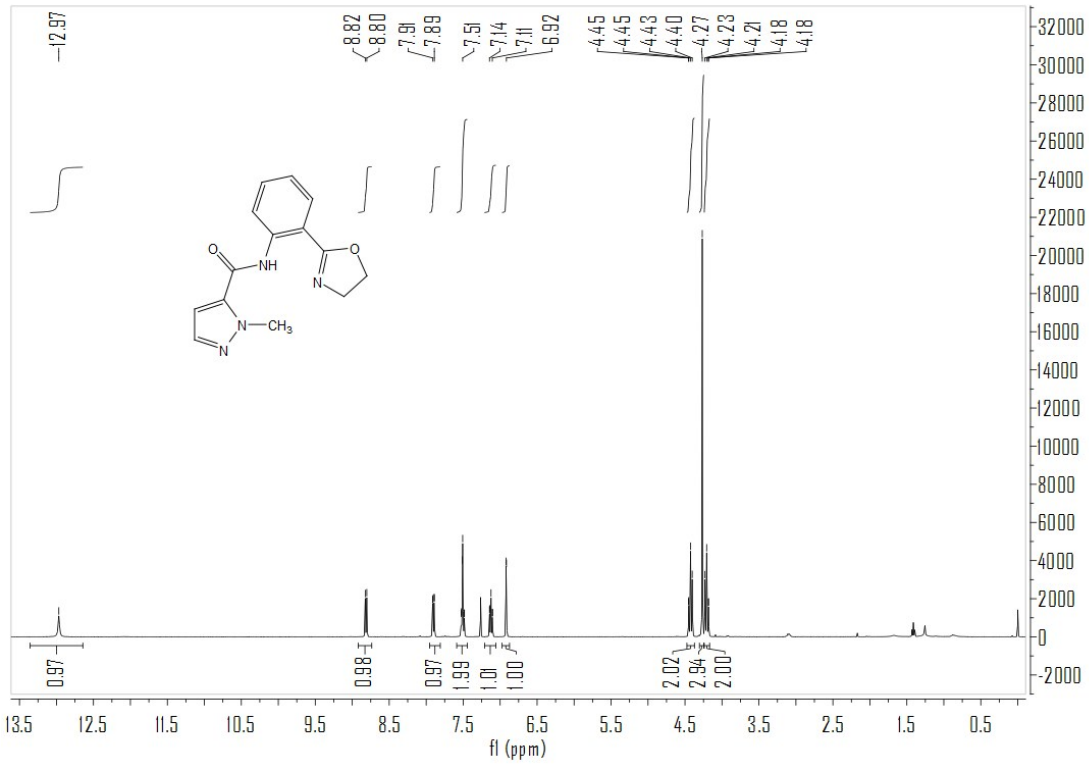
^{1}H NMR of 1r



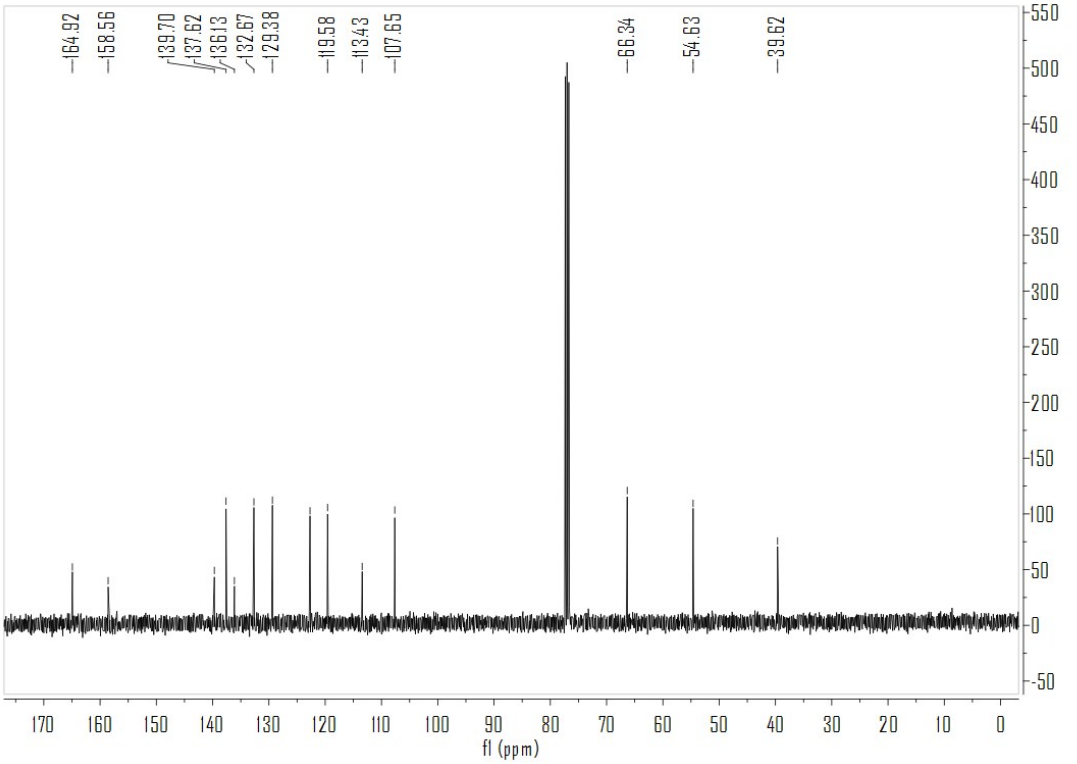
^{13}C NMR of 1r



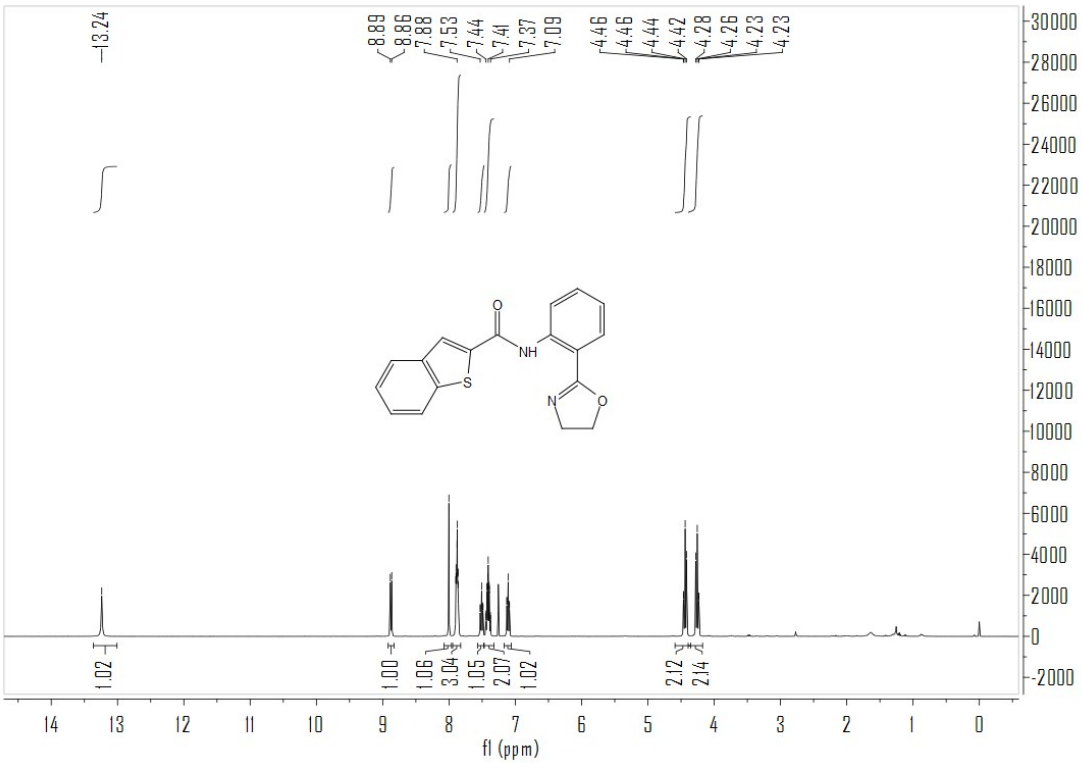
^{1}H NMR of 1s



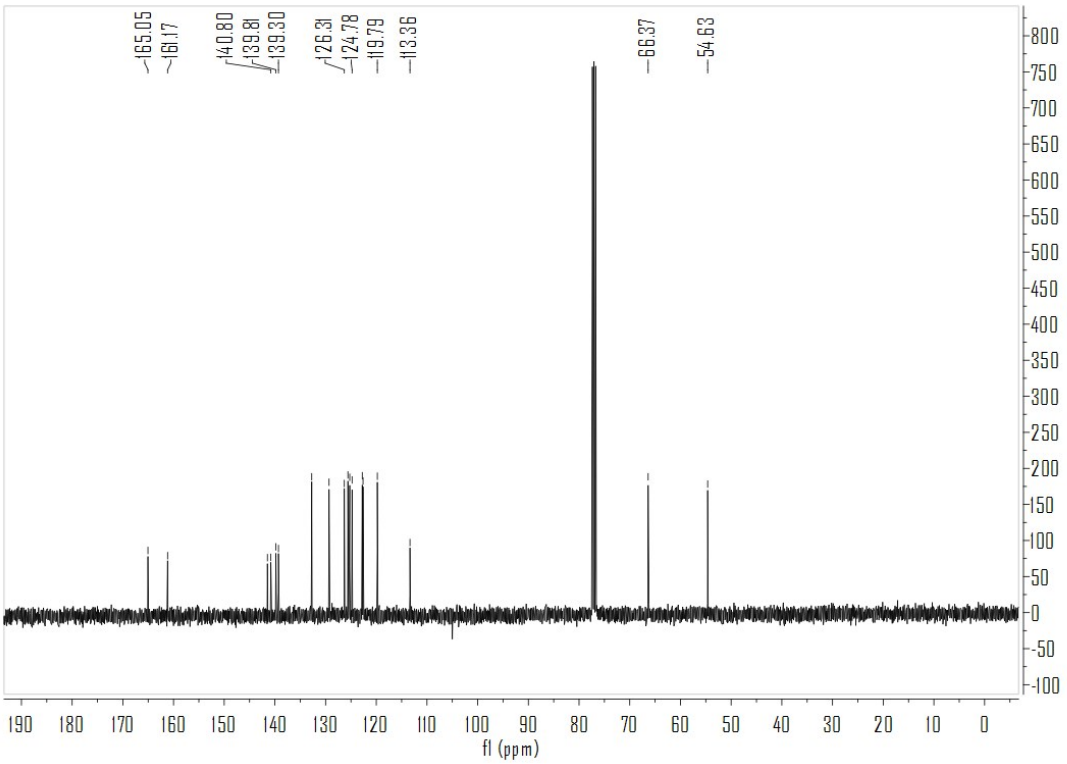
^{13}C NMR of 1s



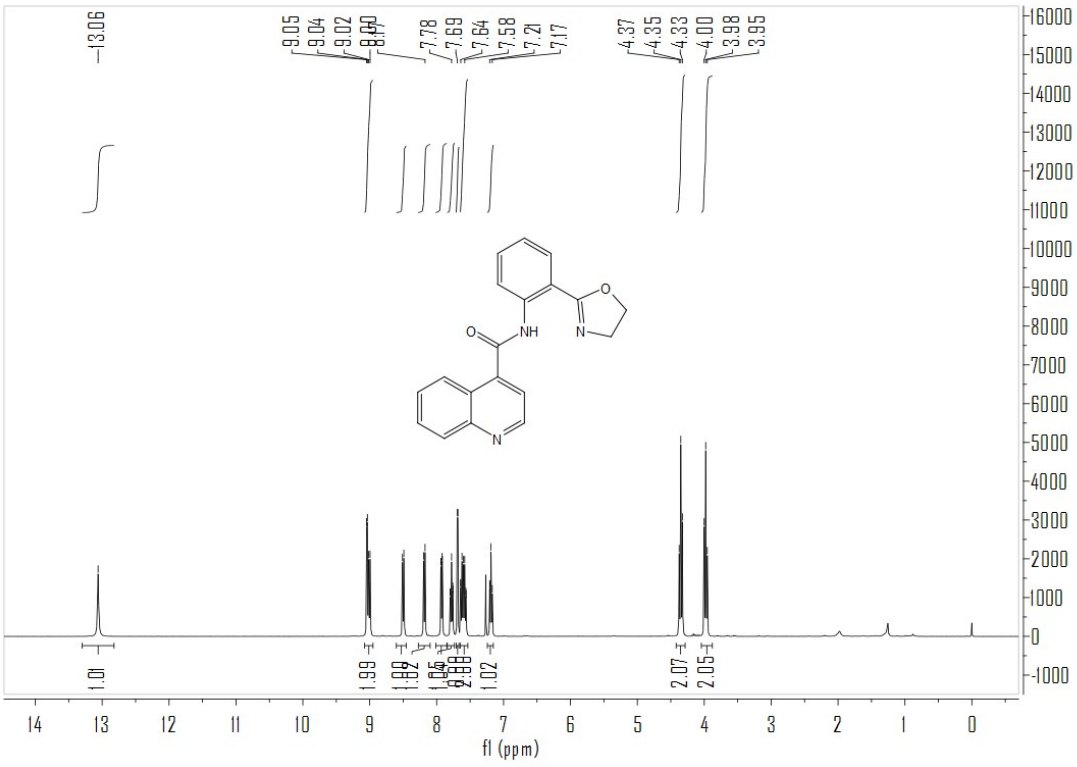
^{1}H NMR of 1t



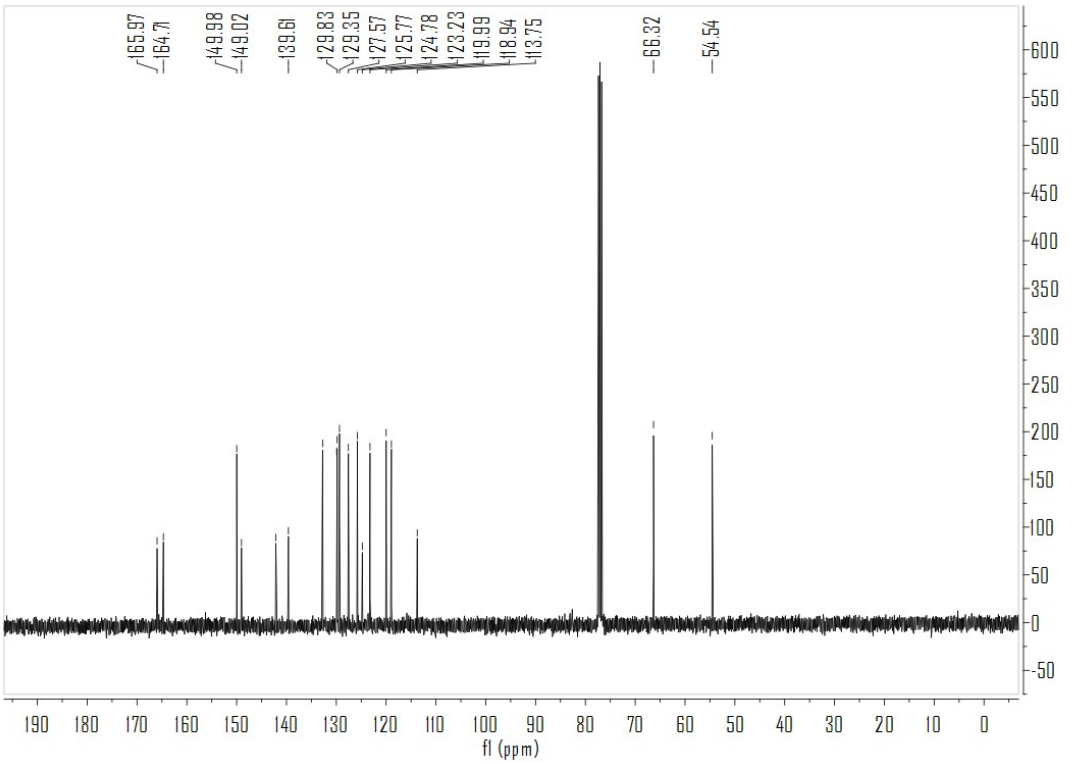
^{13}C NMR of 1t



^{1}H NMR of 1u

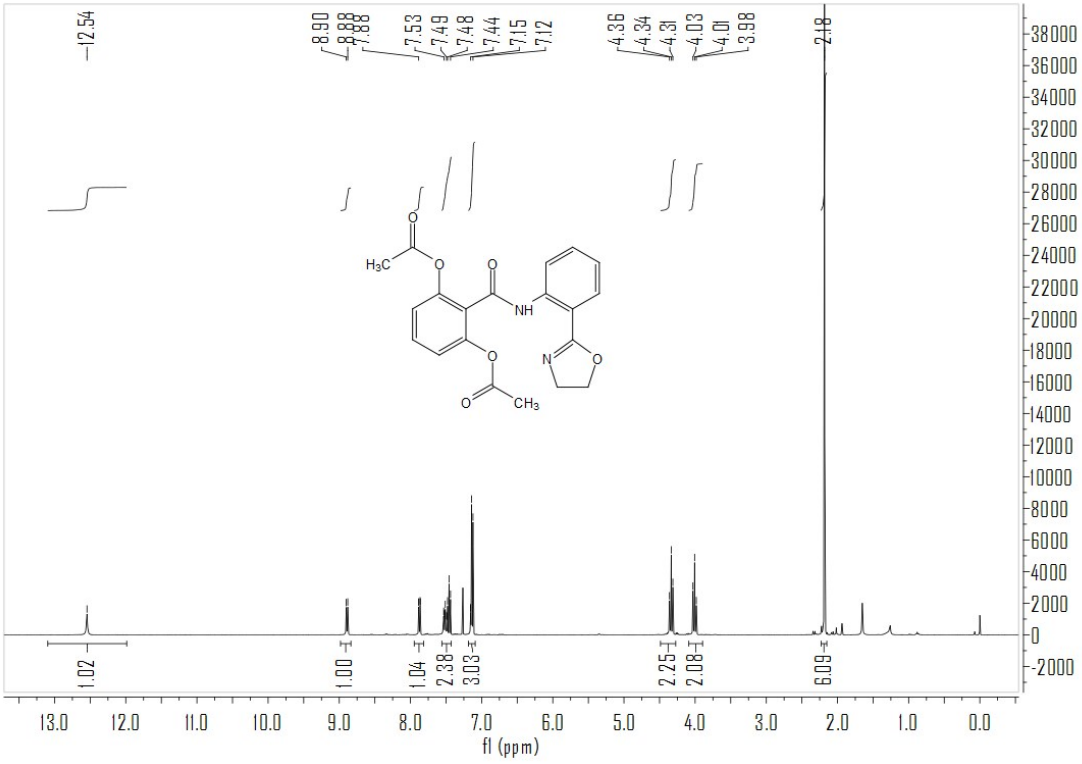


^{13}C NMR of 1u

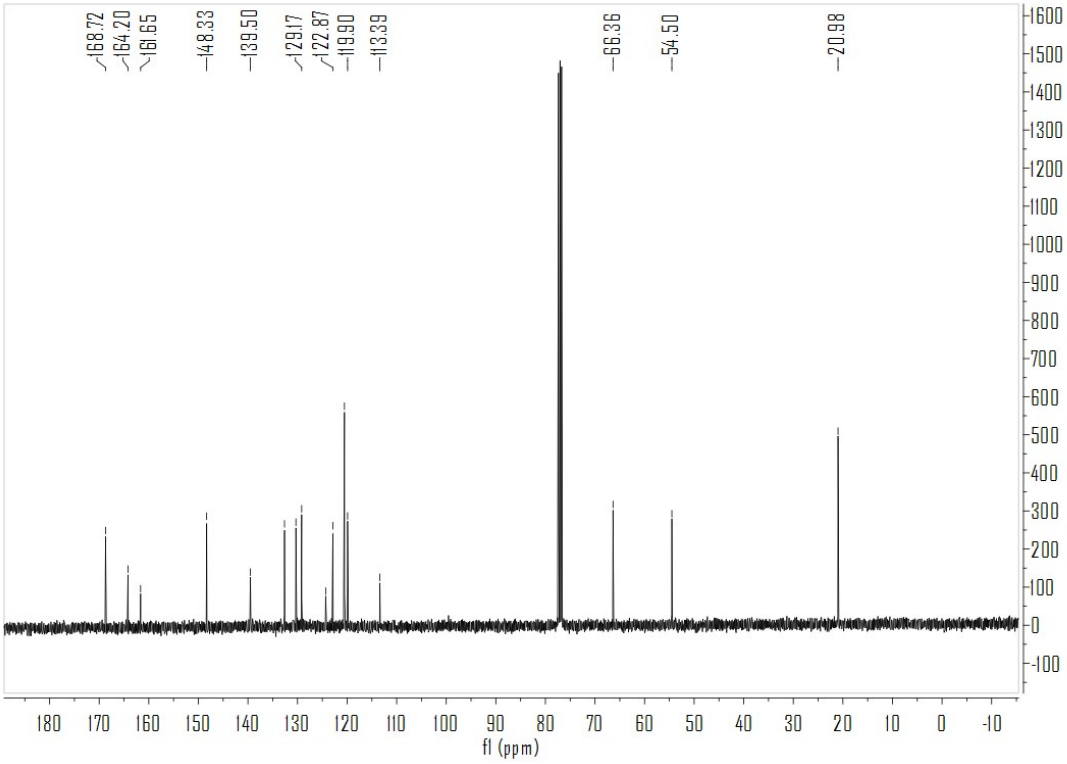


2. Products

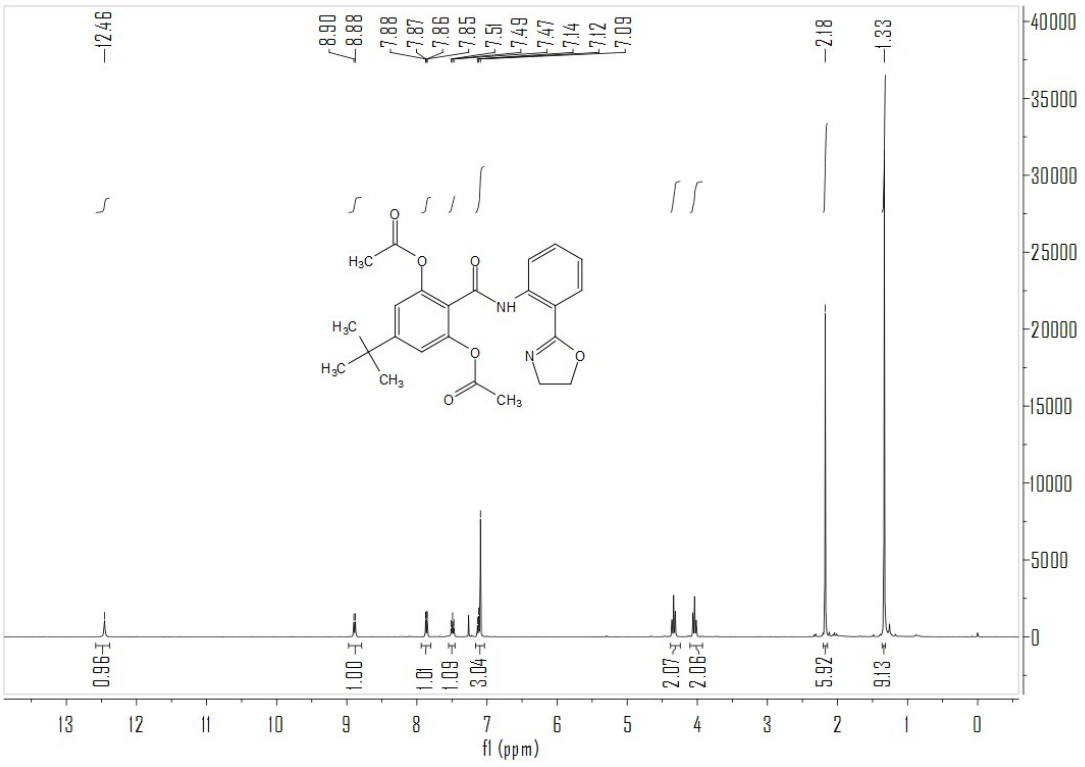
1H NMR of 3a



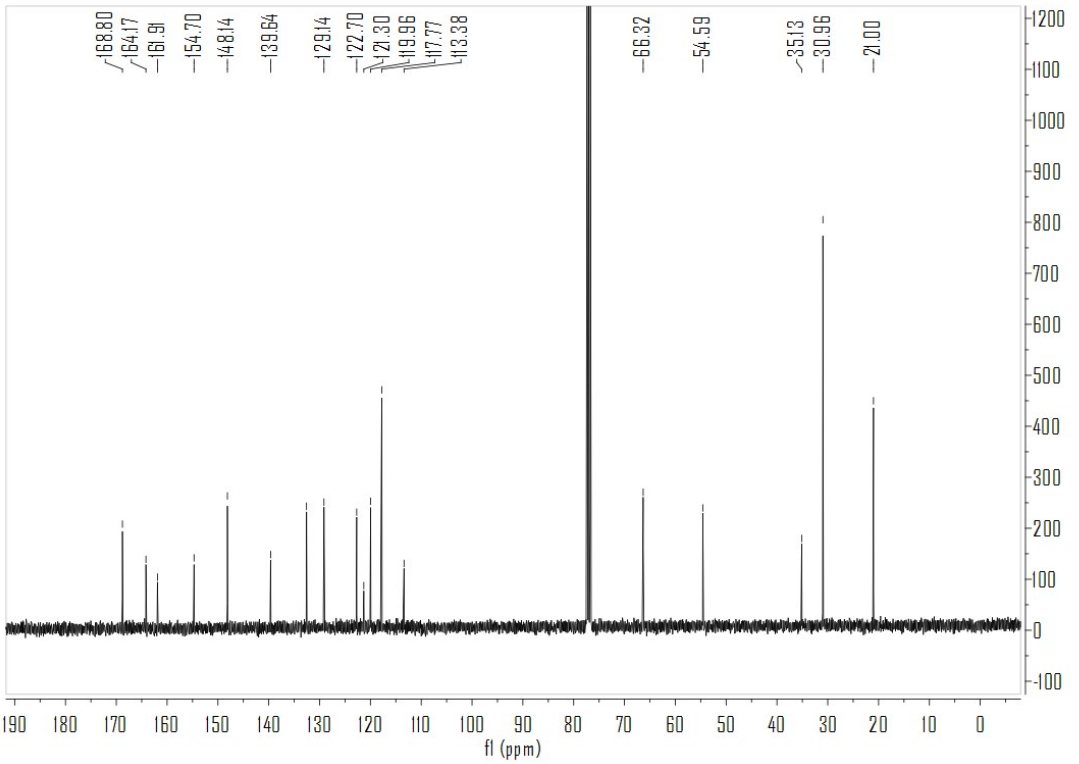
^{13}C NMR of 3a



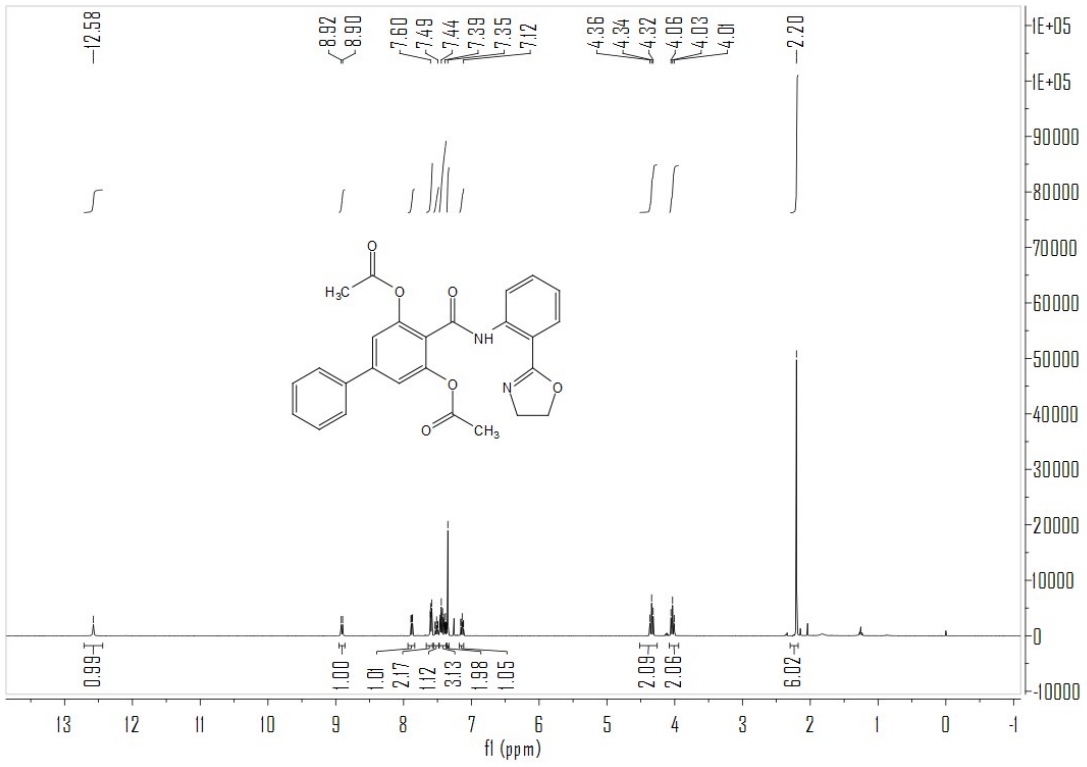
^{1}H NMR of 3b



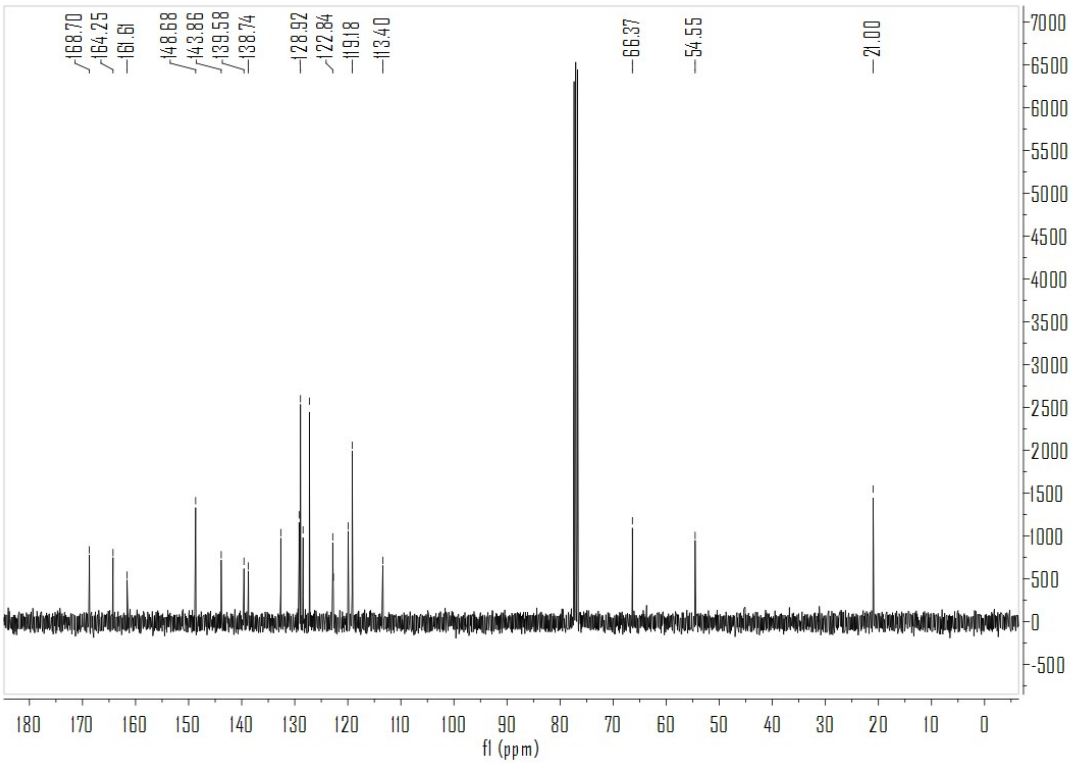
^{13}C NMR of 3b



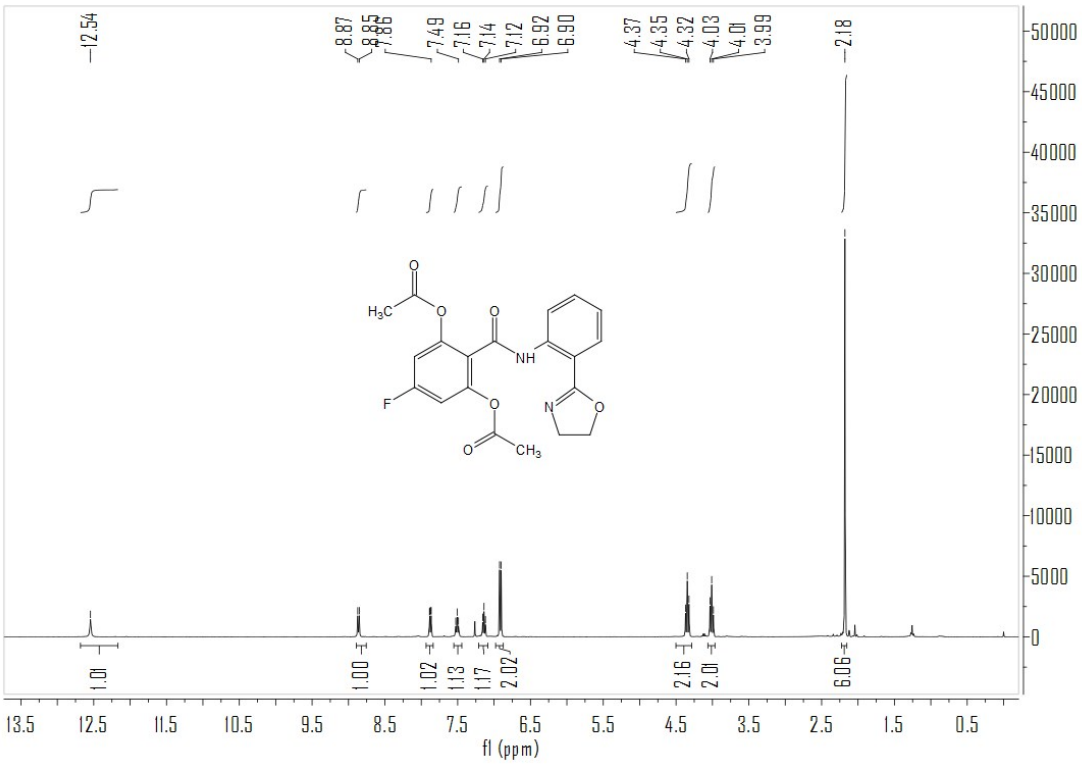
[1]H NMR of 3c



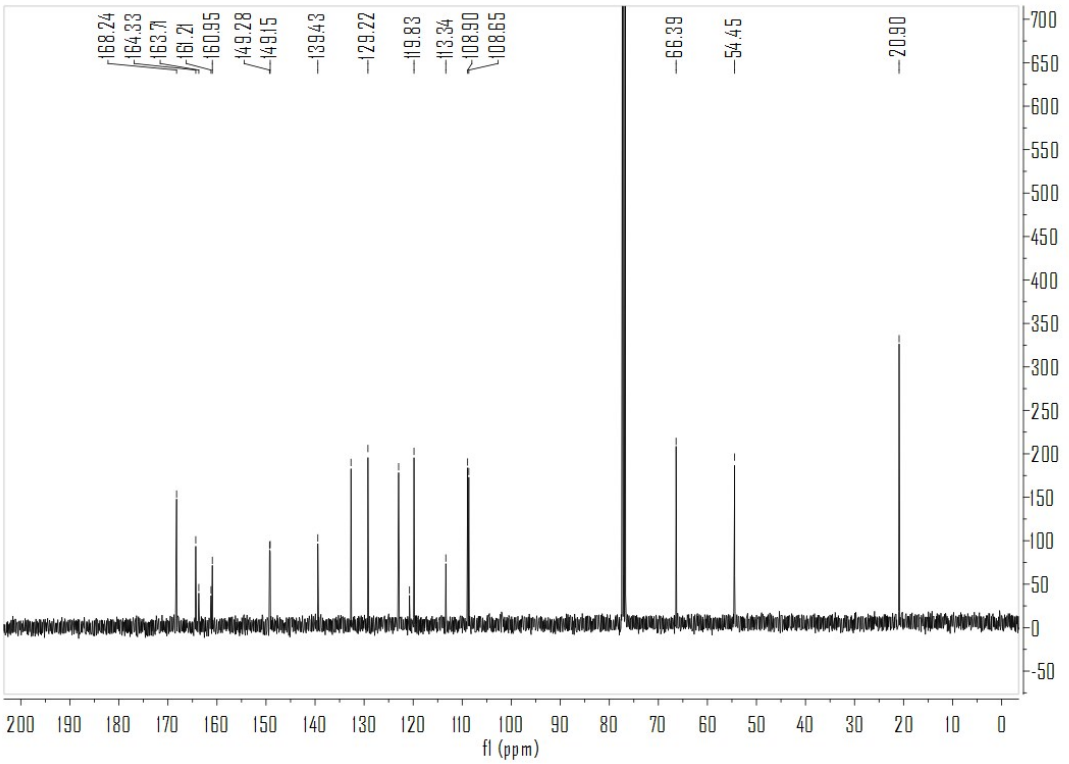
[13]C NMR of 3c



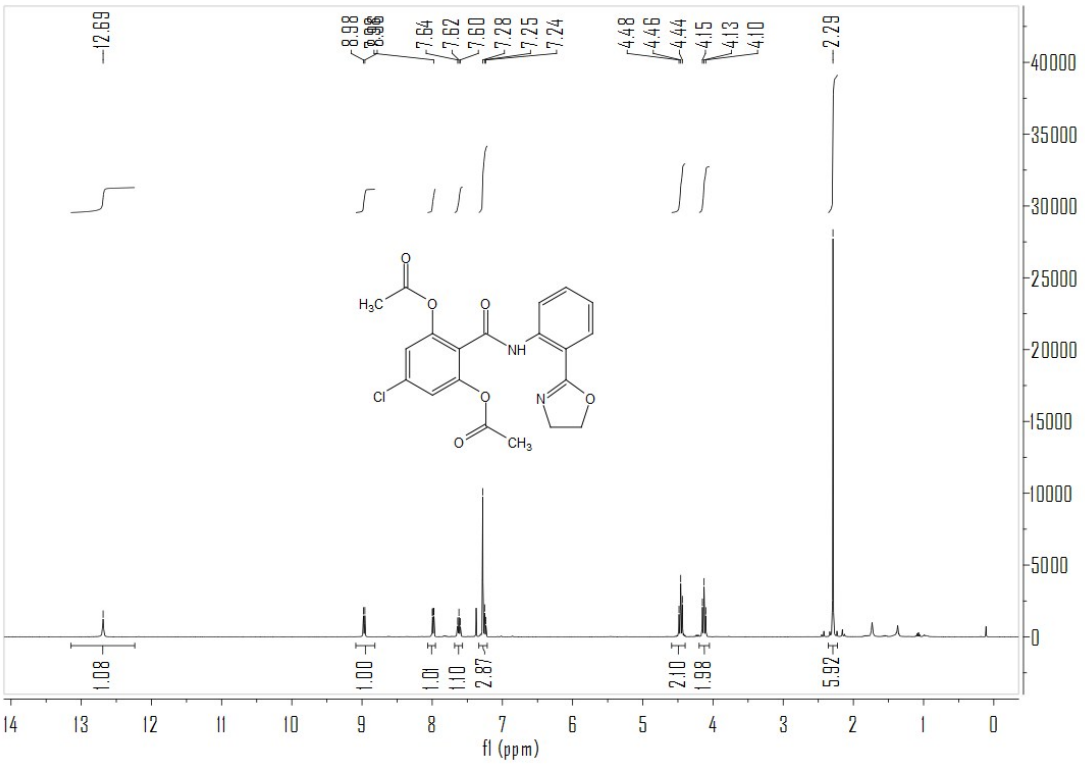
[1]H NMR of 3d



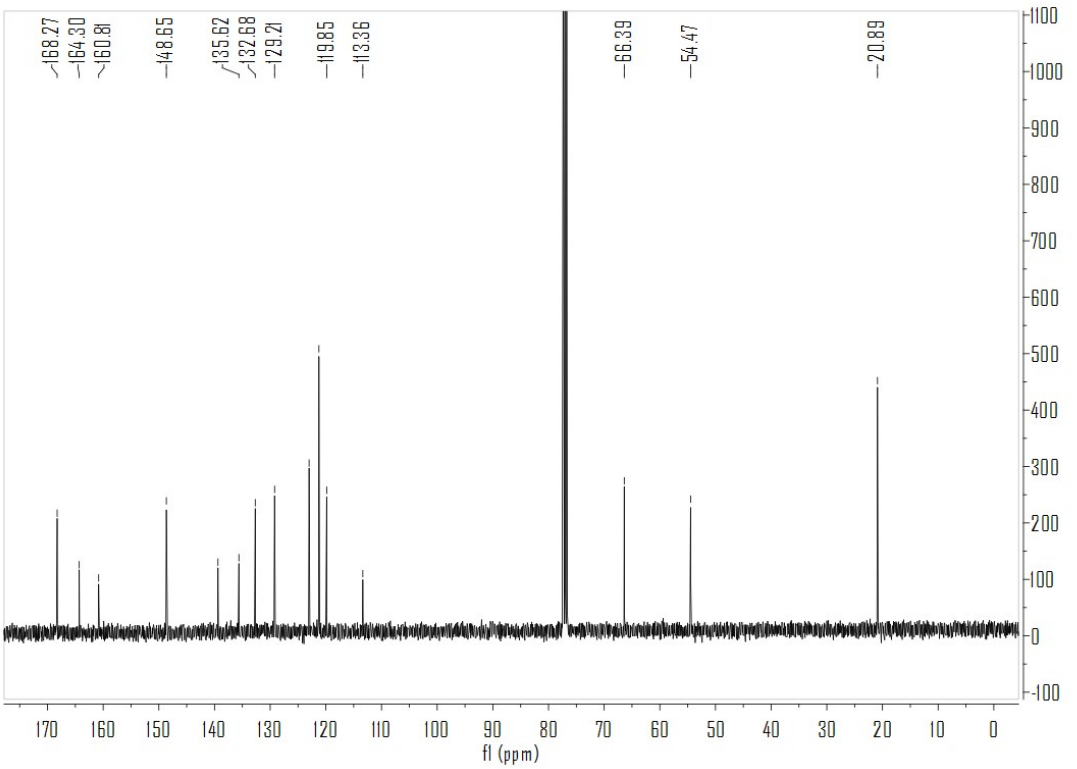
[13]C NMR of 3d



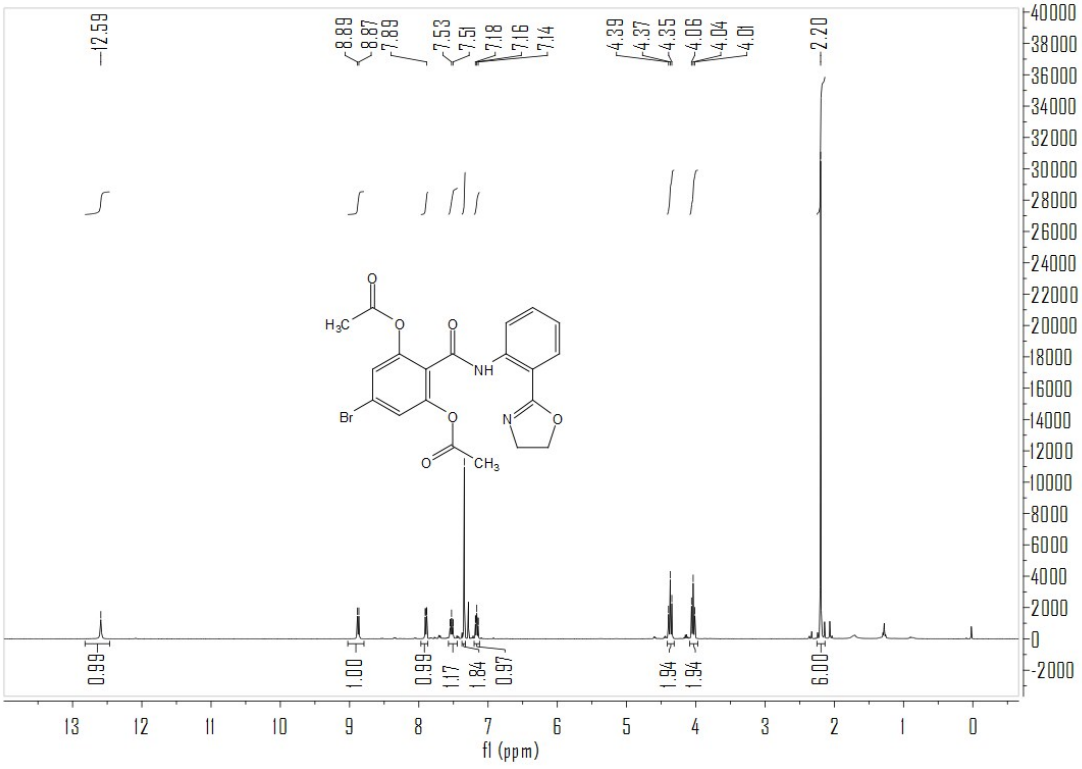
^{1}H NMR of 3e



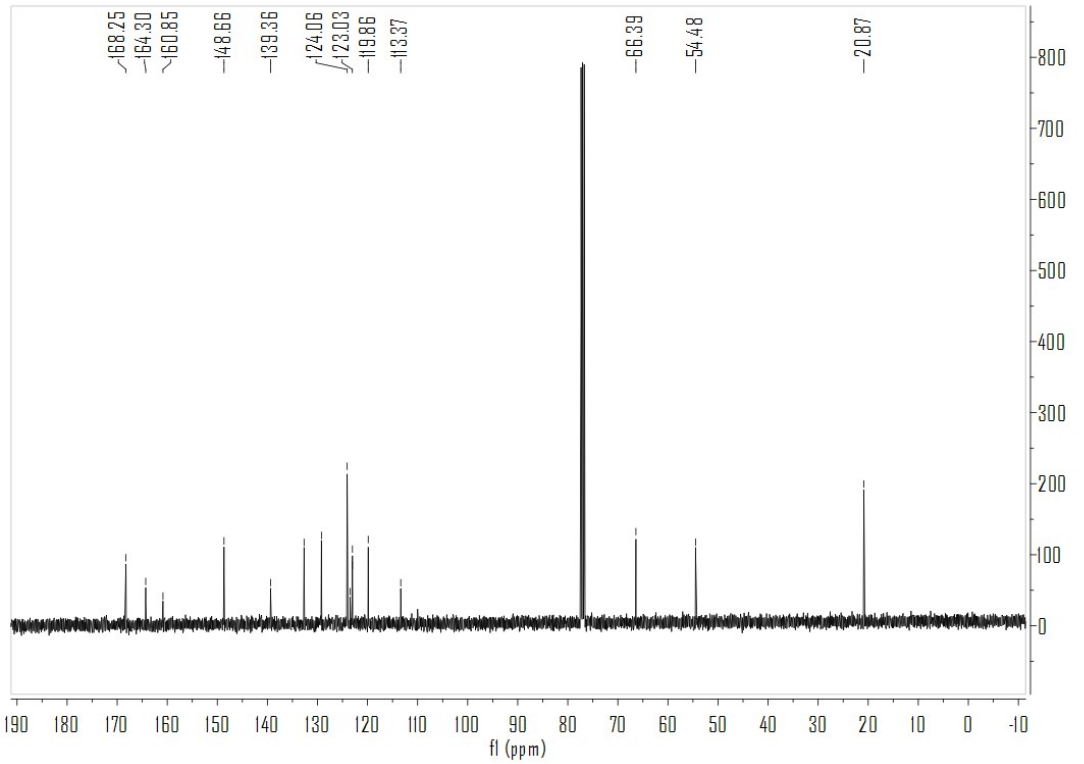
^{13}C NMR of 3e



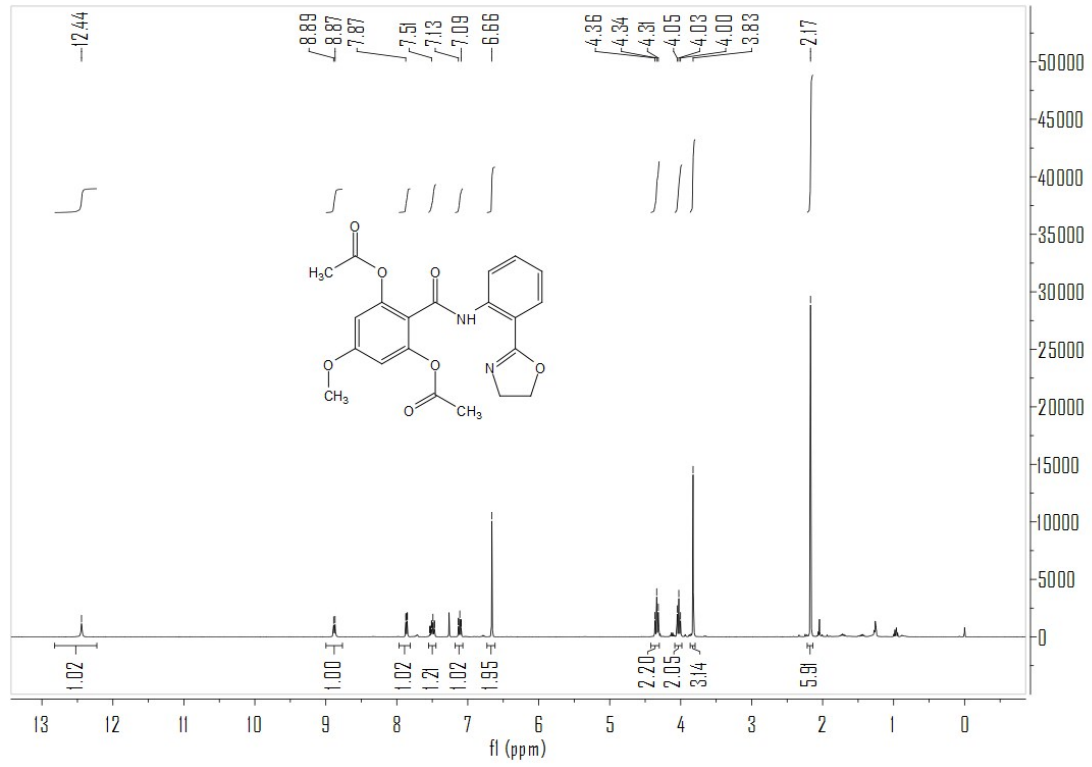
^{1}H NMR of 3f



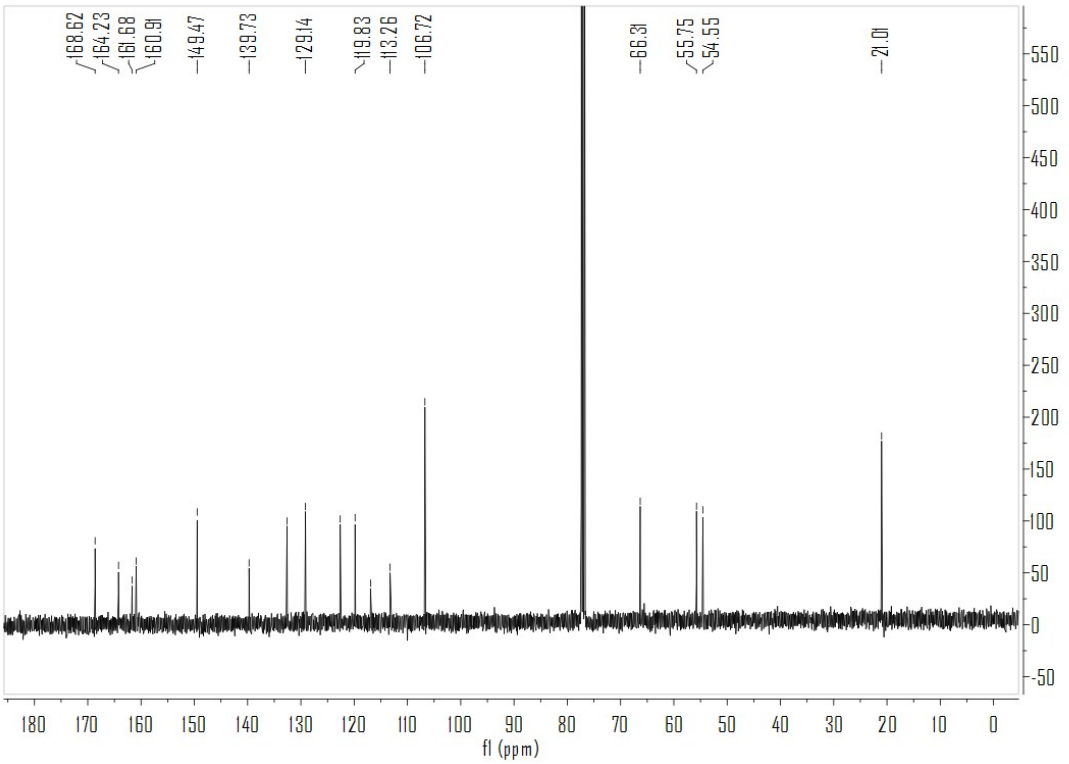
^{13}C NMR of 3f



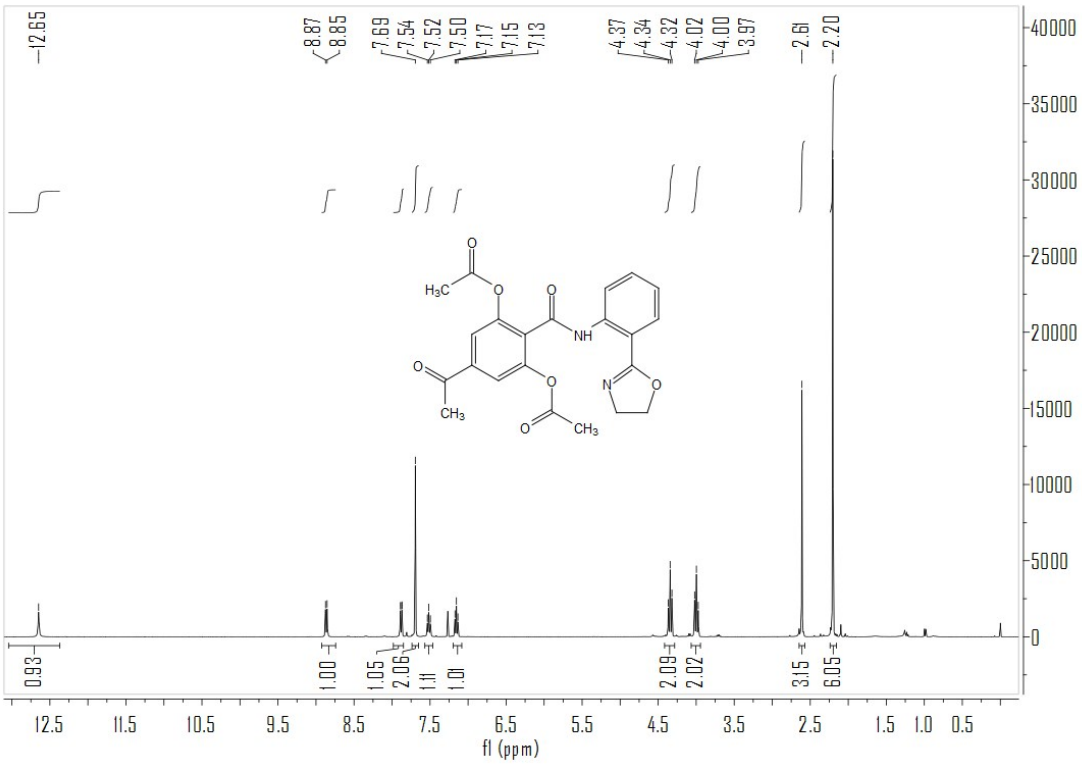
^{1}H NMR of 3g



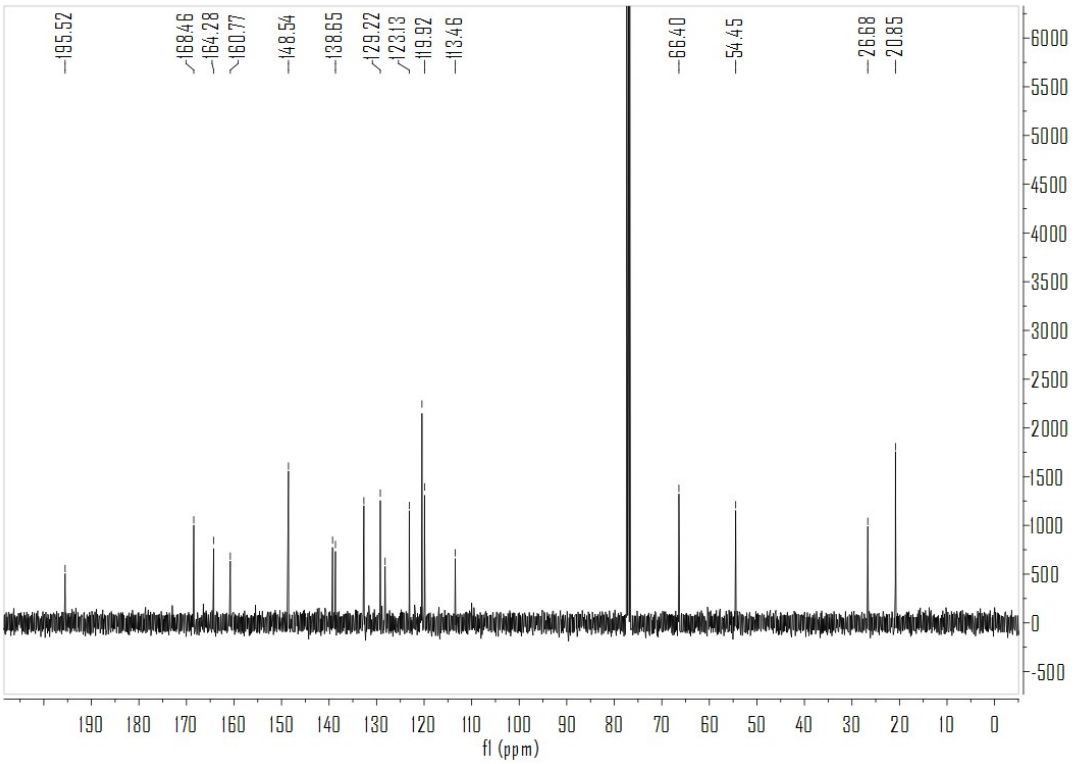
^{13}C NMR of 3g



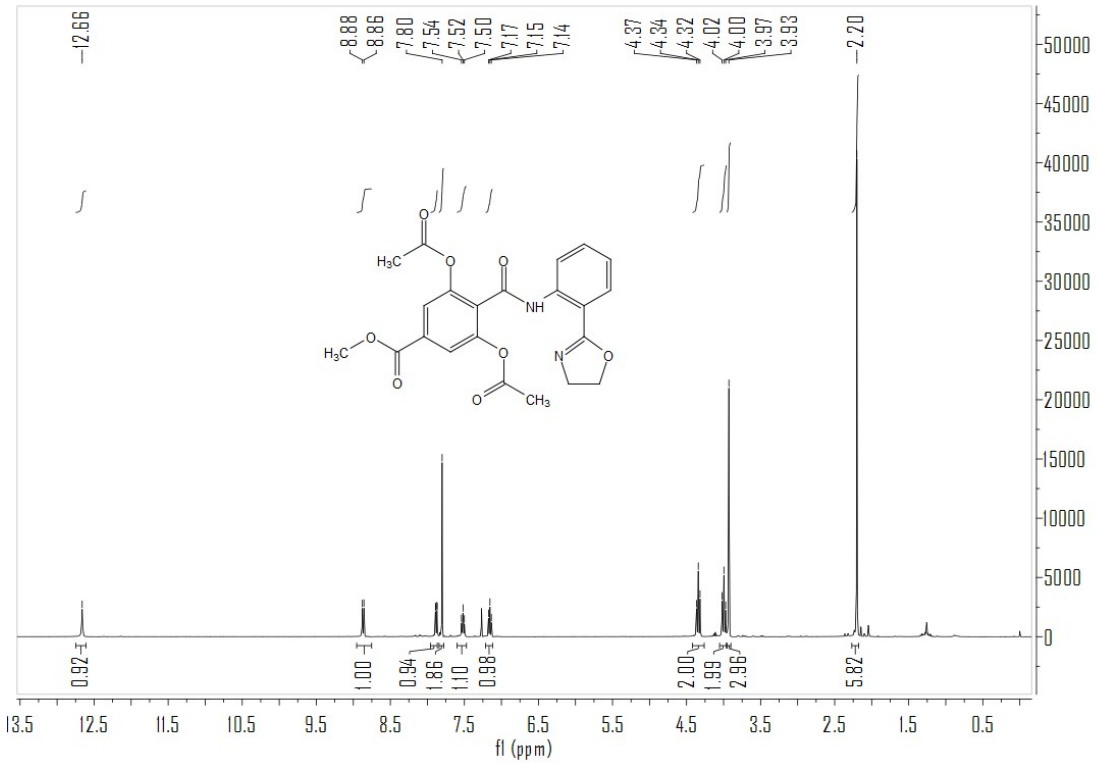
^{1}H NMR of 3h



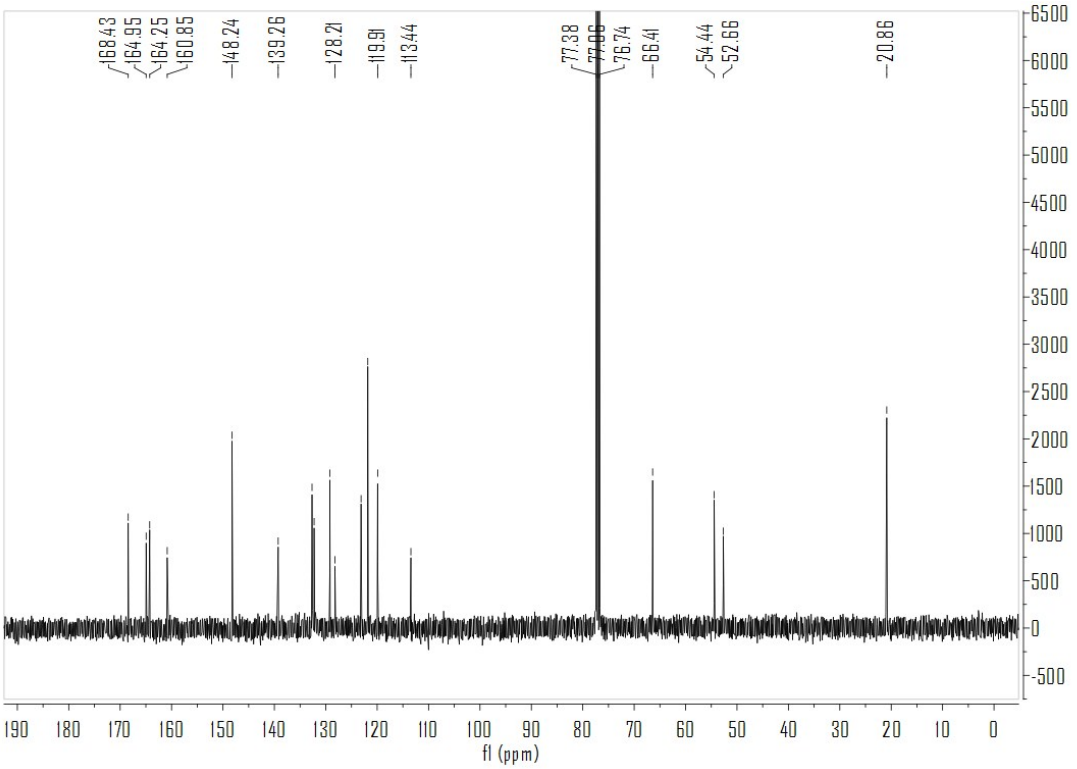
^{13}C NMR of 3h



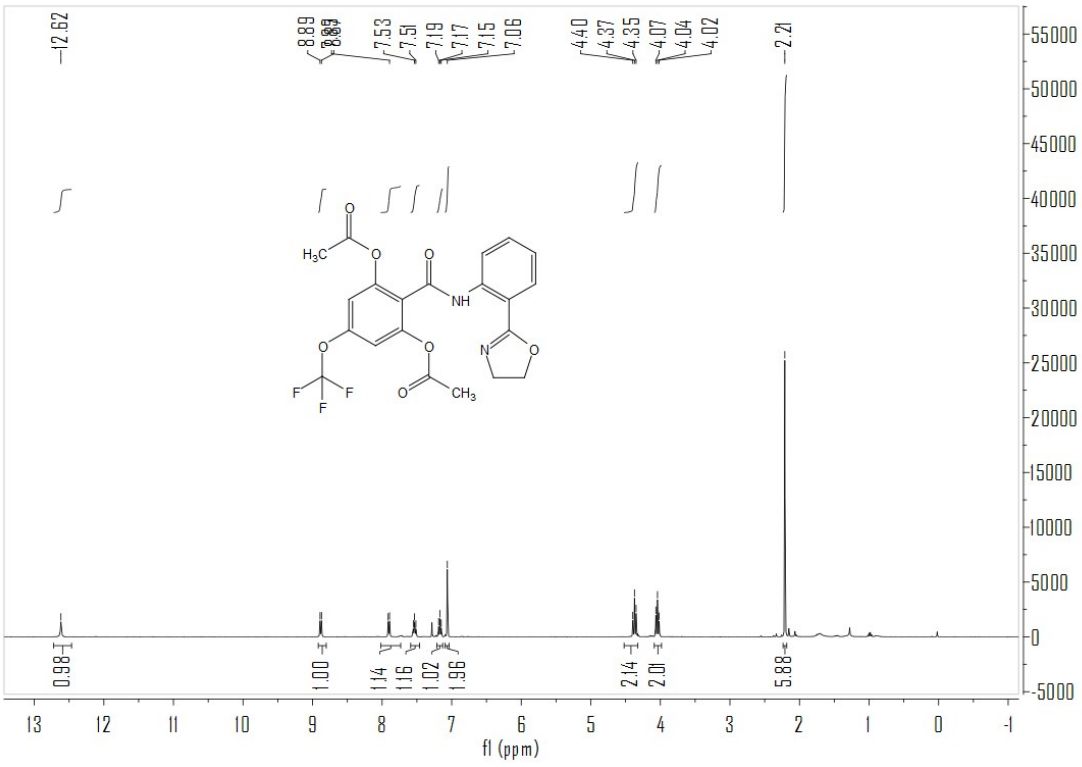
[1]H NMR of 3i



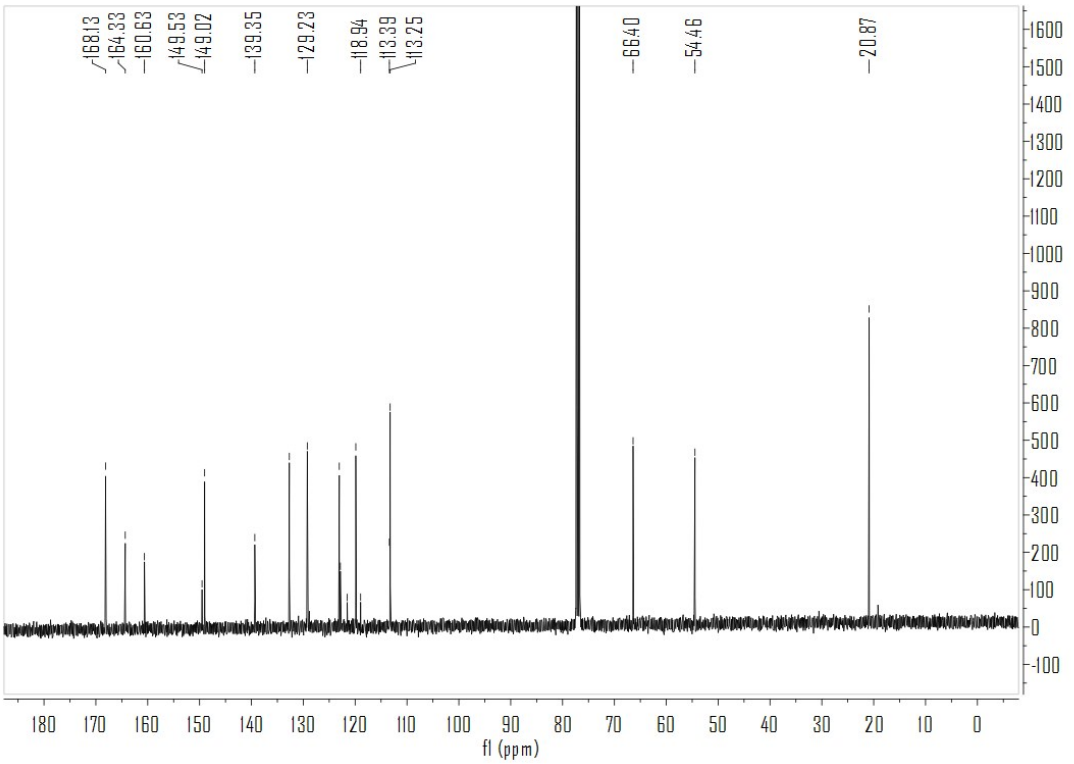
[13] C NMR of 3i



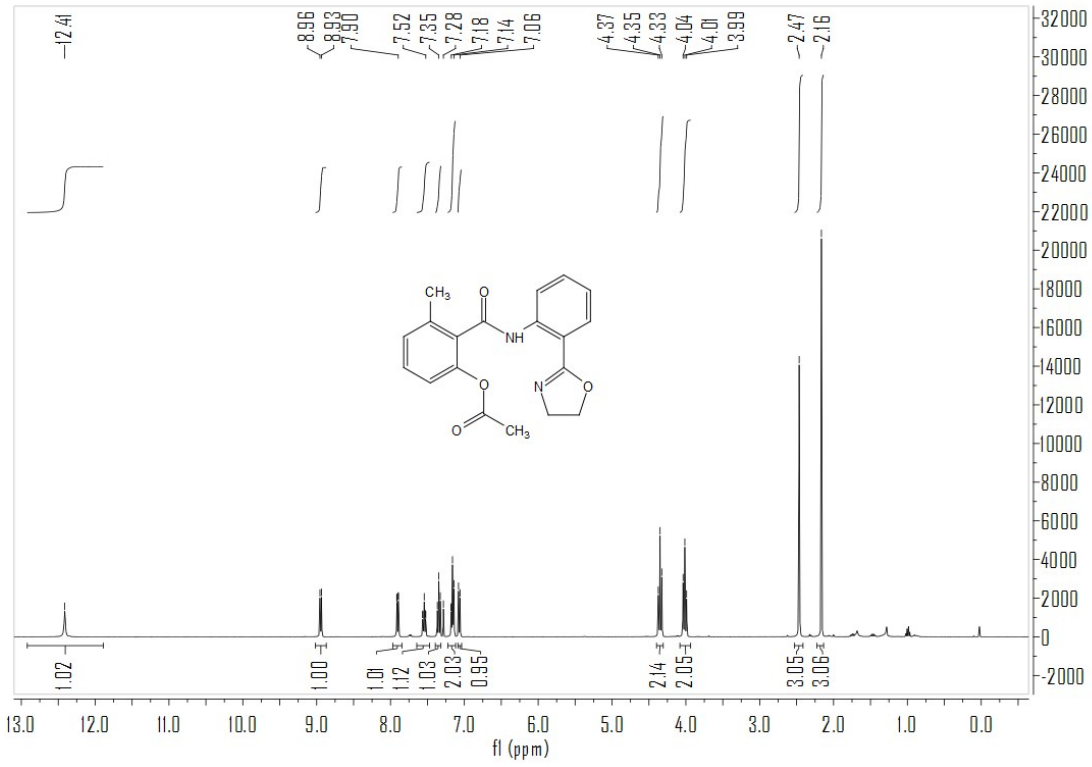
^{1}H NMR of 3j



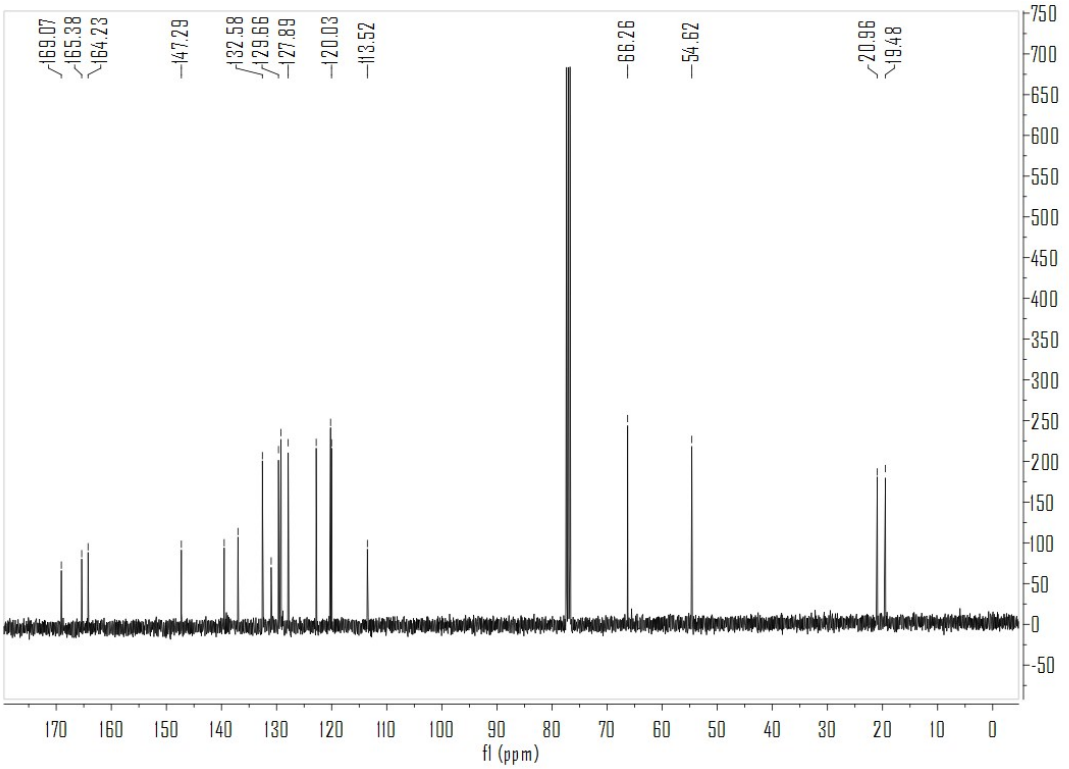
^{13}C NMR of 3j



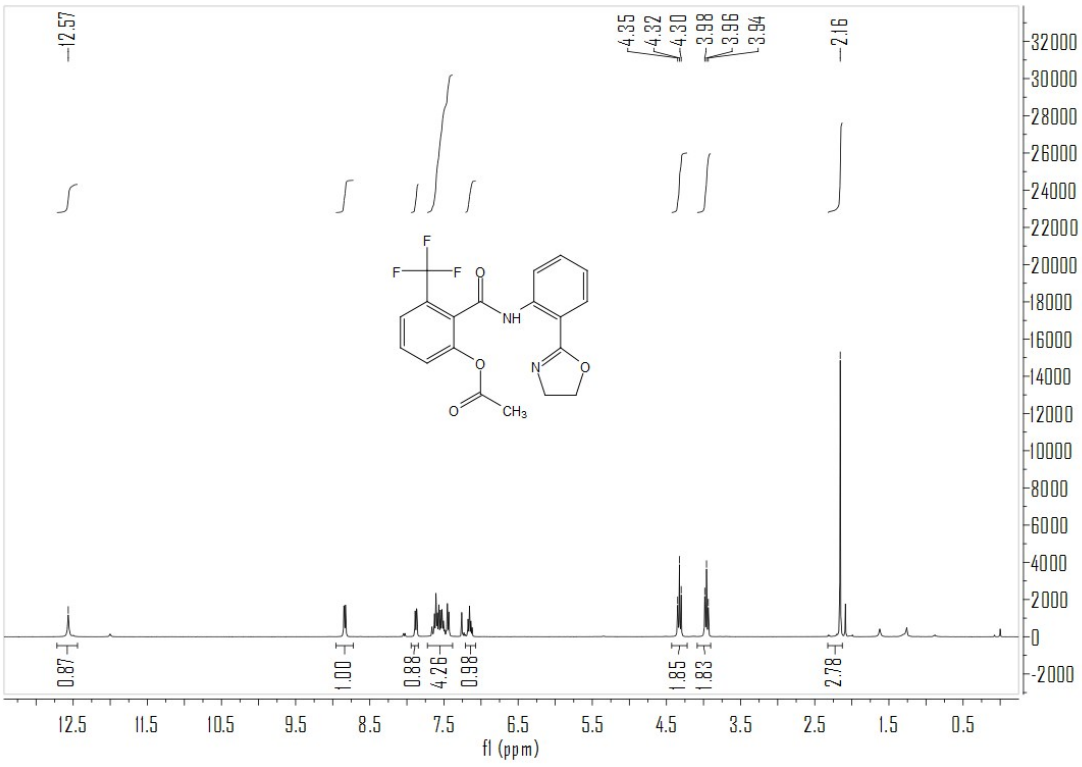
^{1}H NMR of 3k



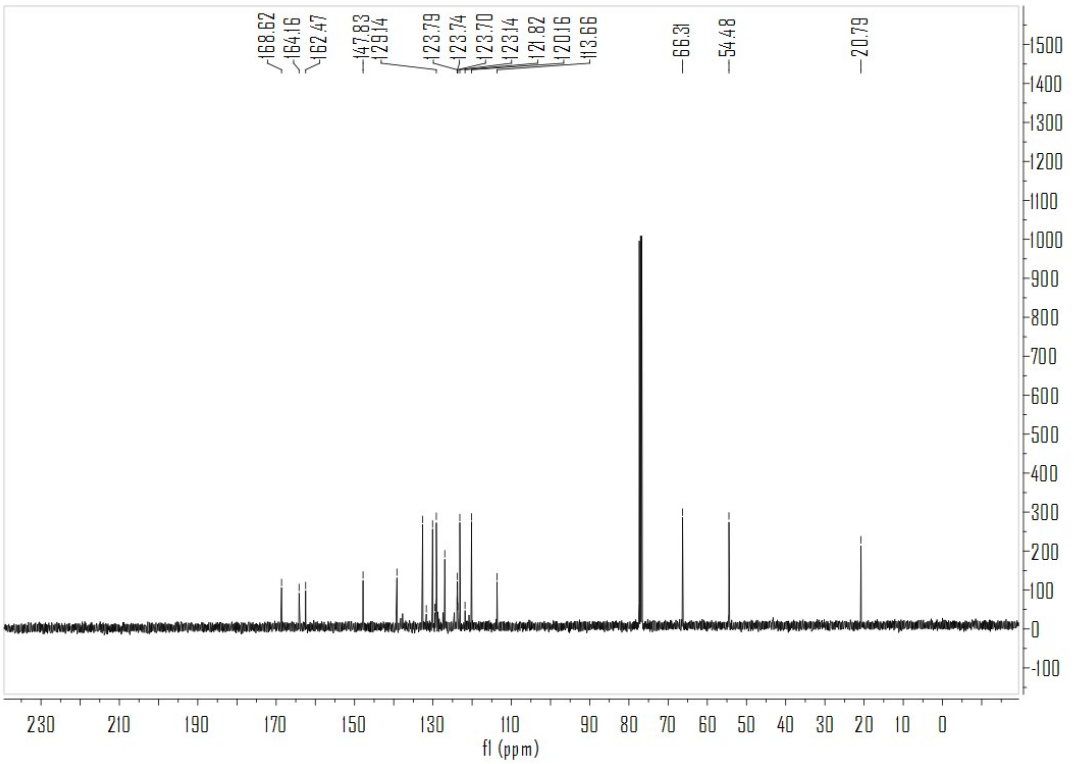
^{13}C NMR of 3k



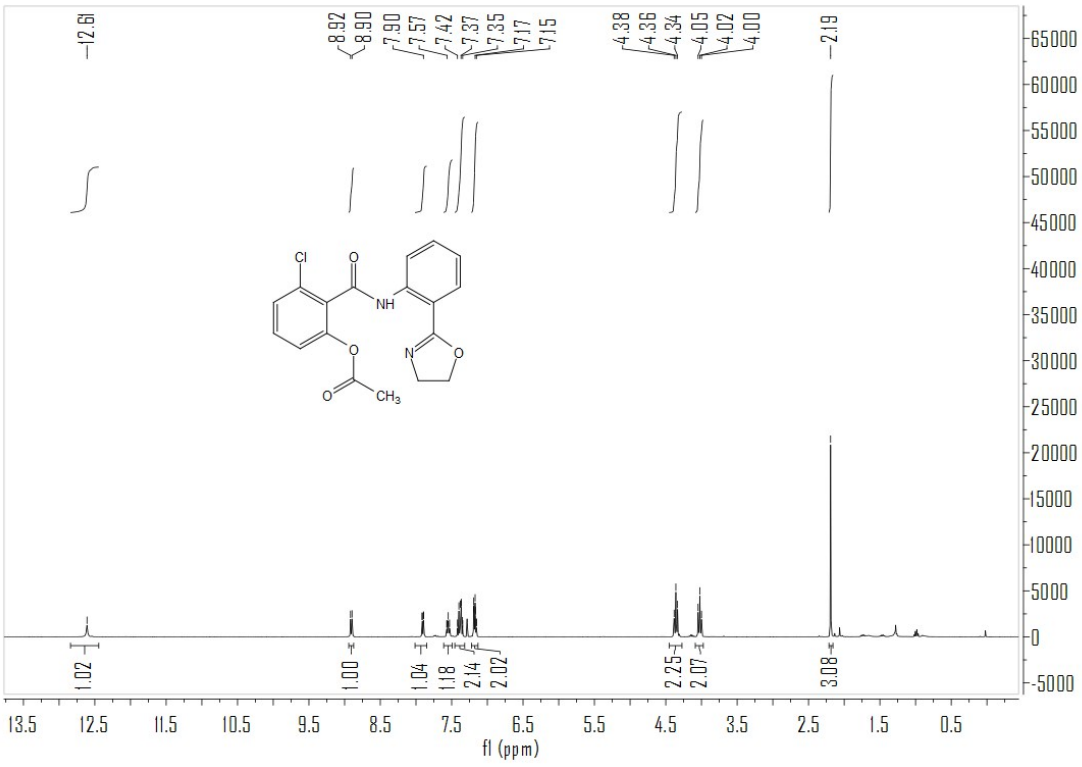
^{1}H NMR of 3l



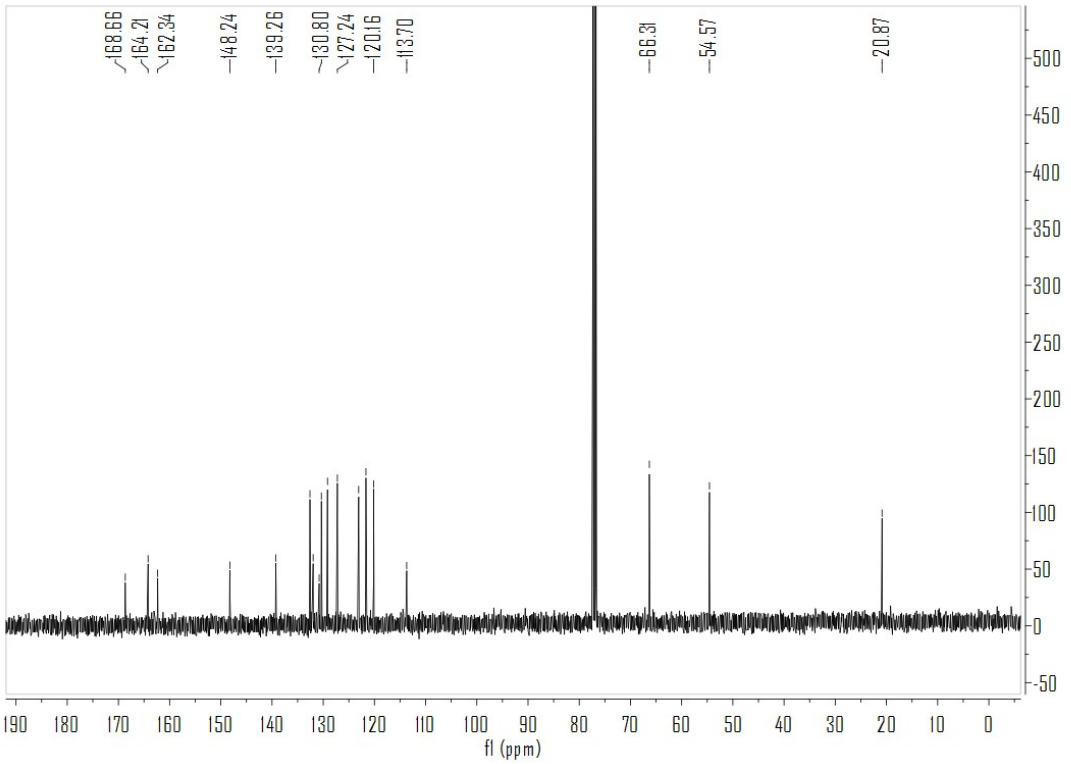
^{13}C NMR of 3l



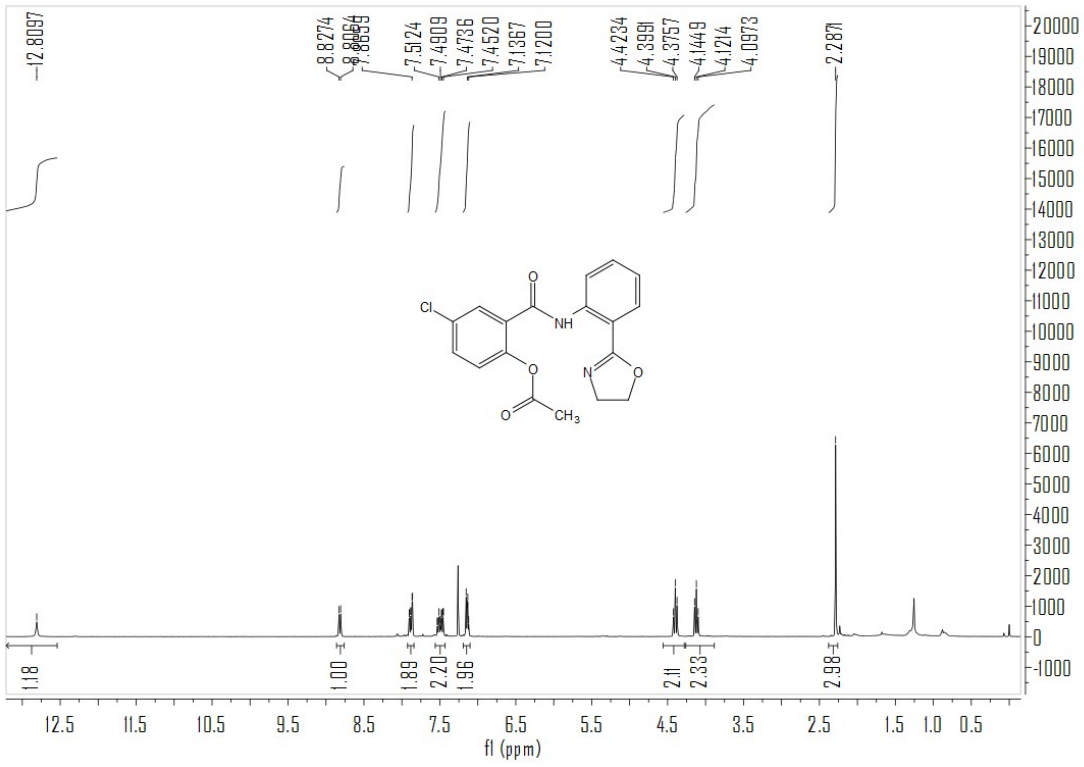
^{1}H NMR of 3m



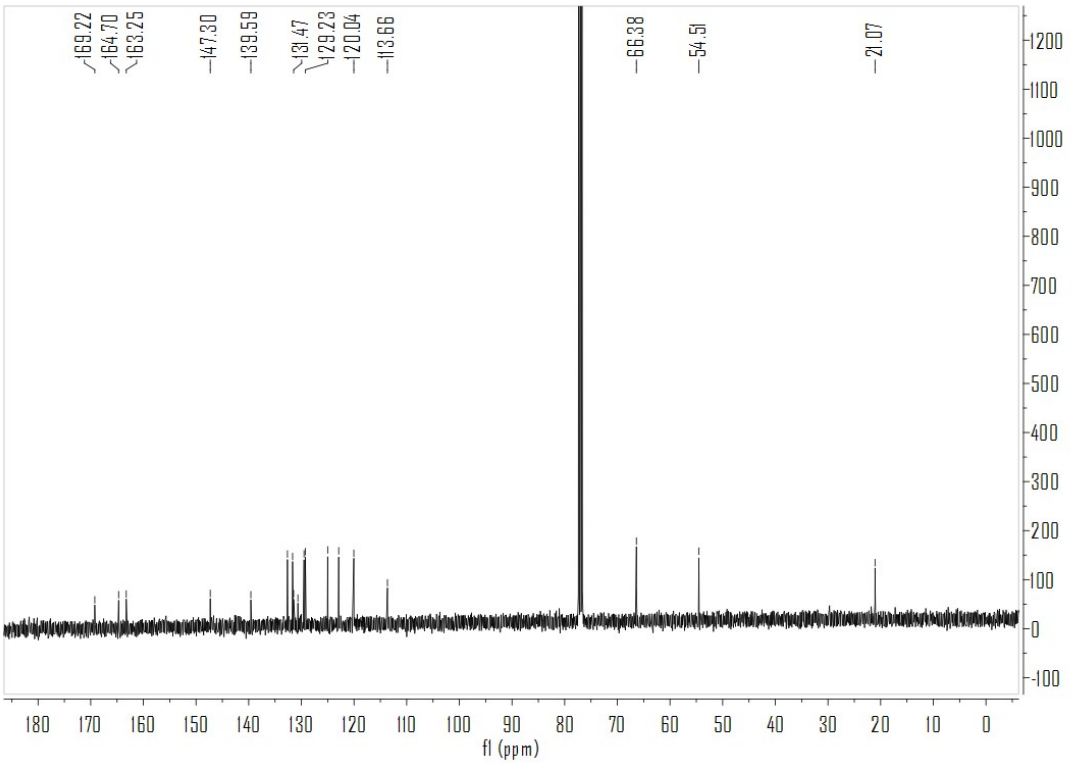
^{13}C NMR of 3m



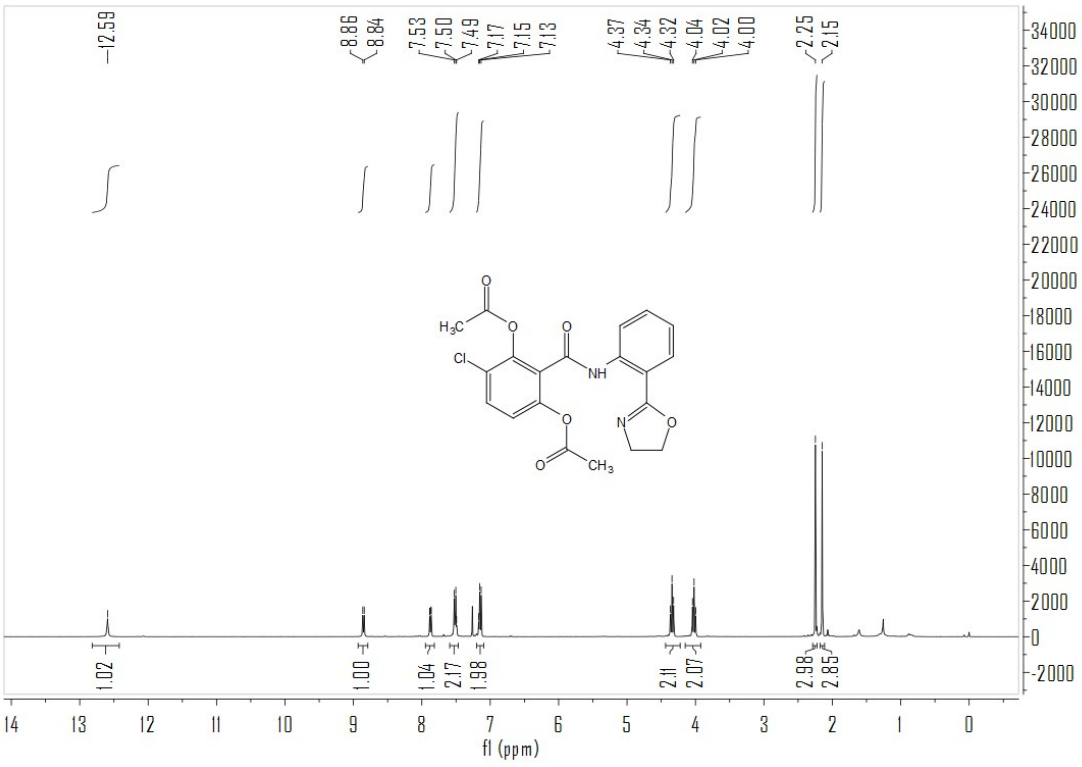
^{1}H NMR of 3na (mono)



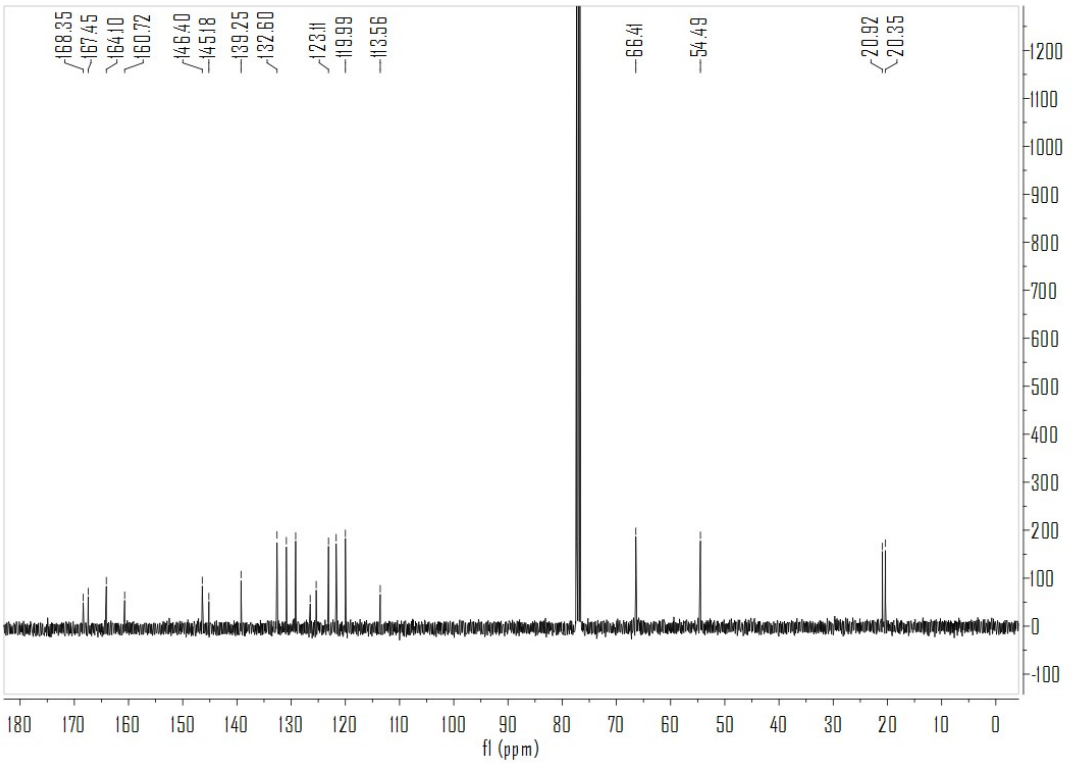
^{13}C NMR of 3na (mono)



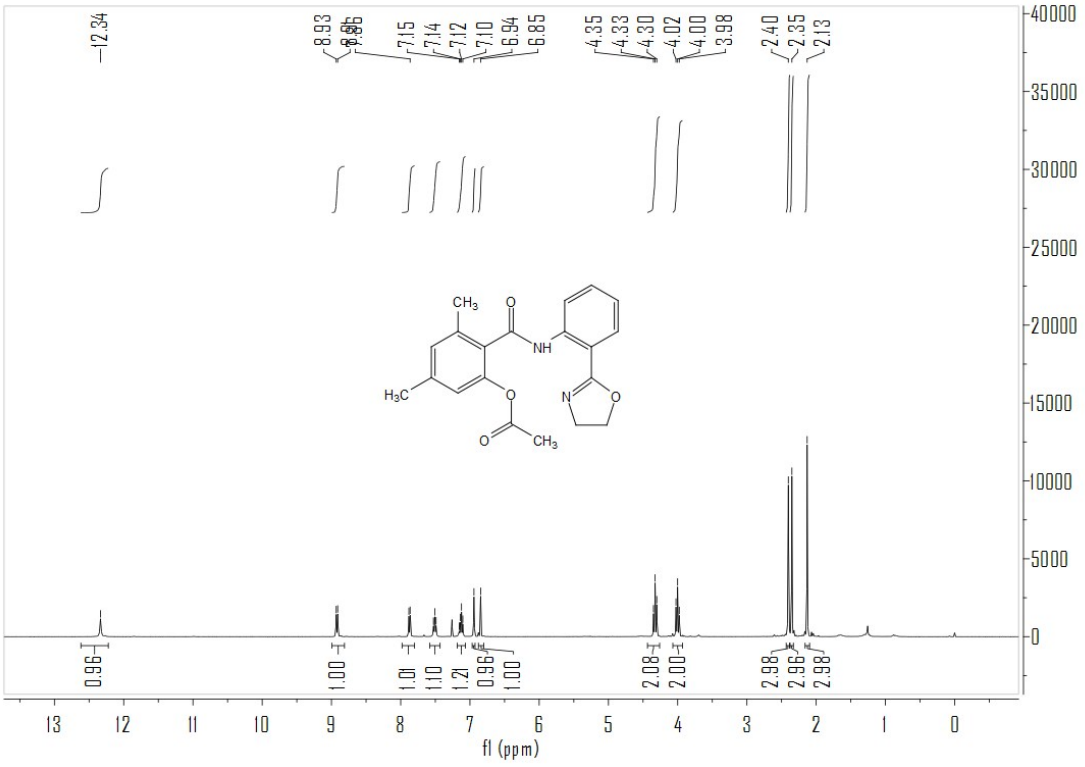
^{1}H NMR of 3nb



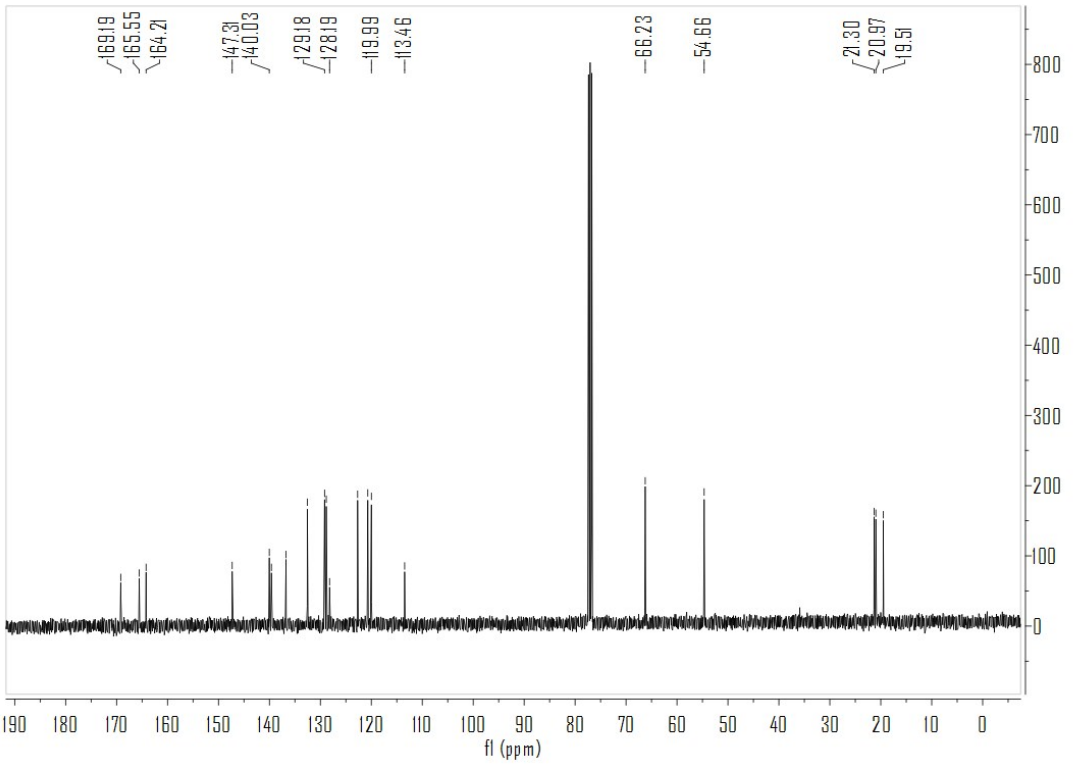
^{13}C NMR of 3nb



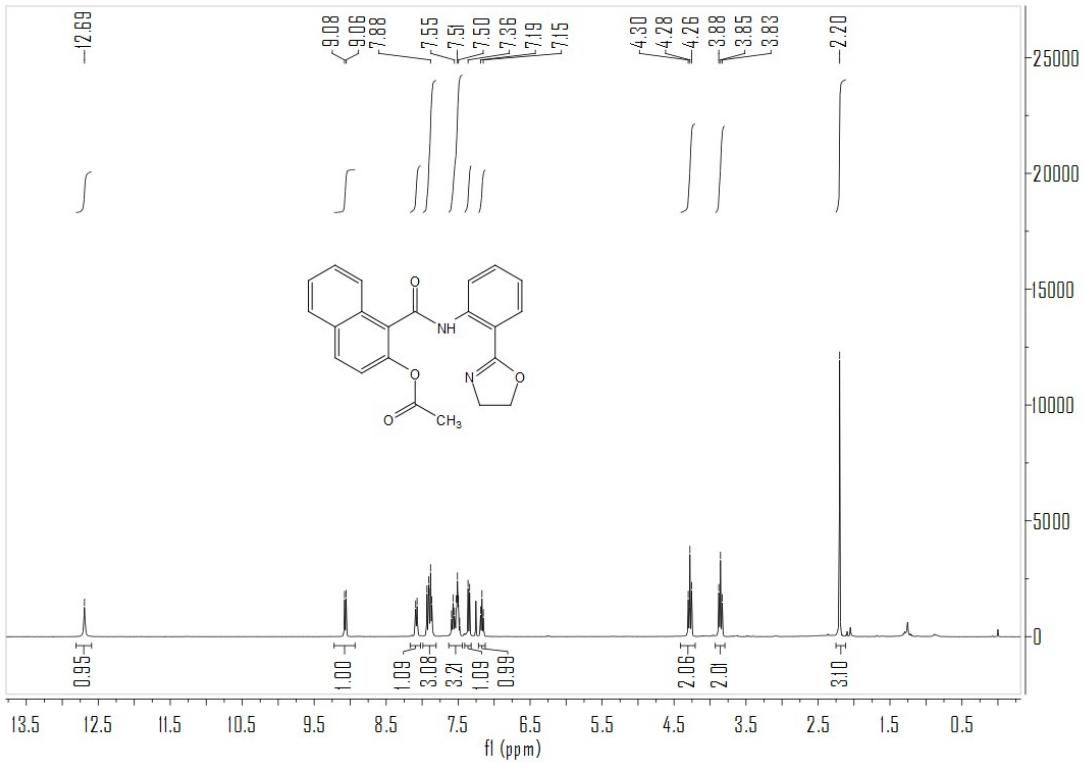
^{1}H NMR of 3o



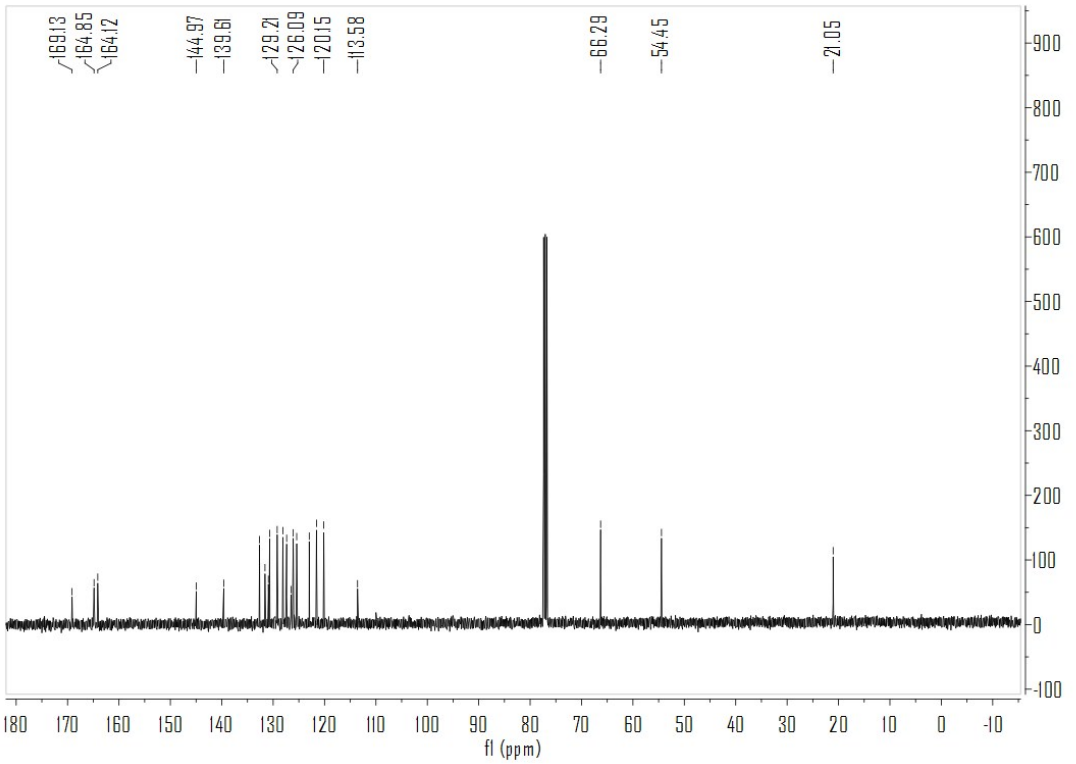
^{13}C NMR of 3o



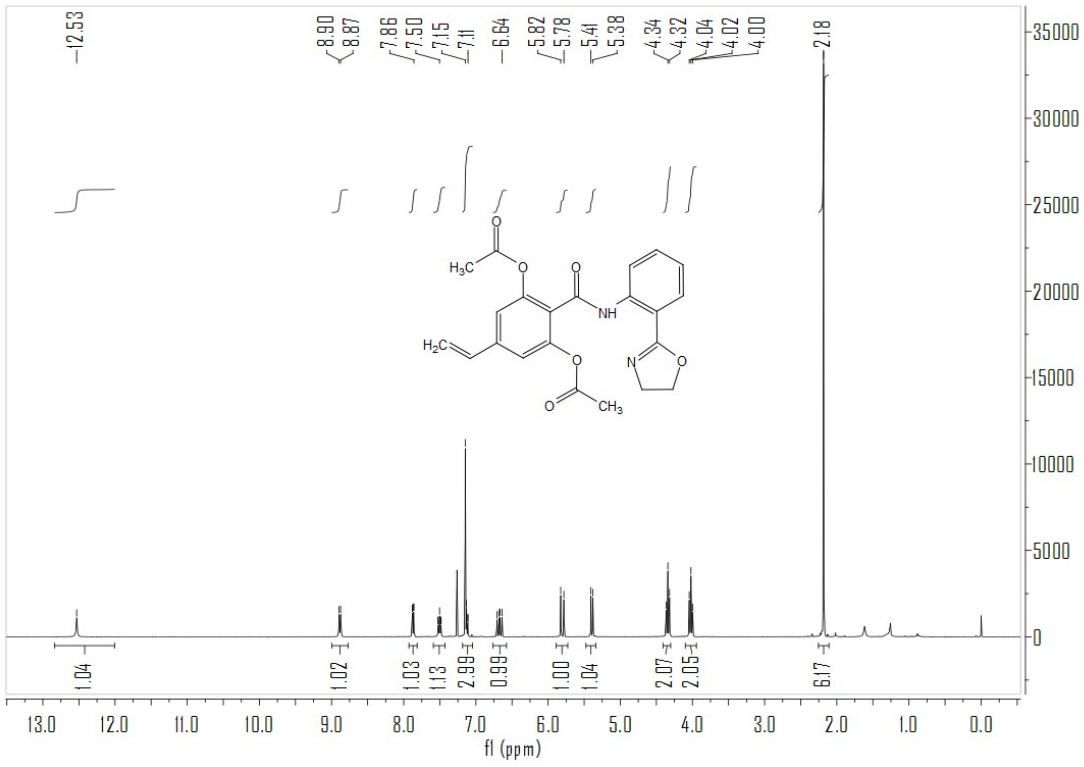
^{1}H NMR of 3p



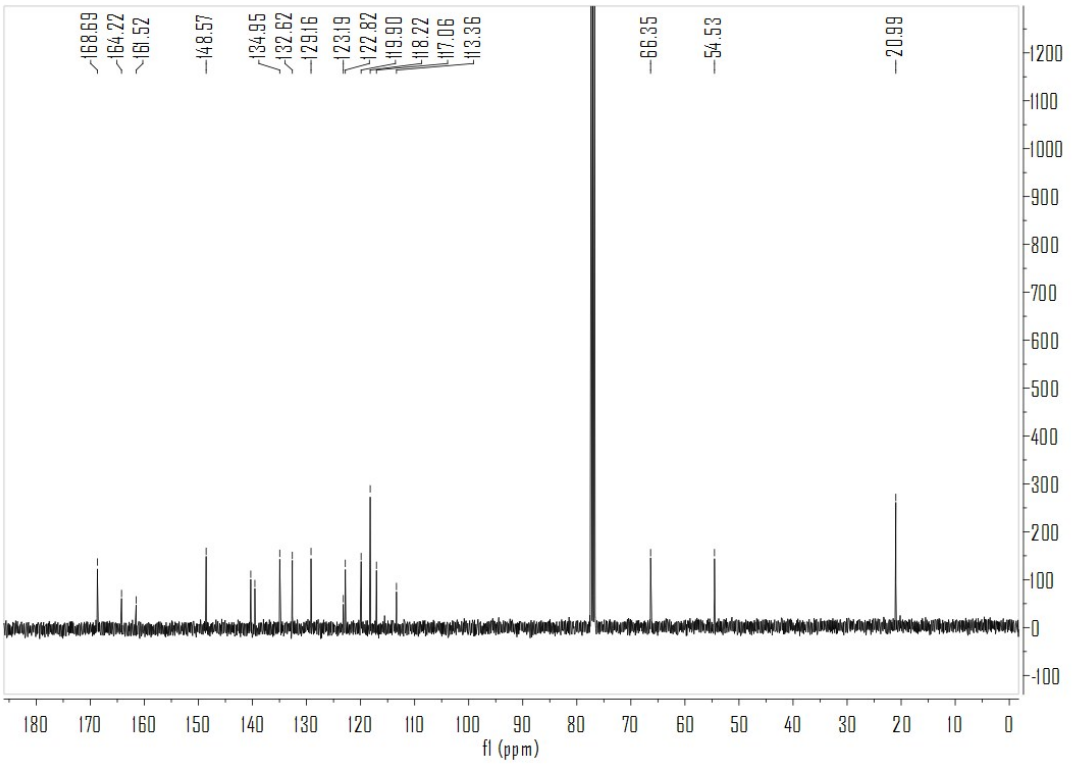
^{13}C NMR of 3p



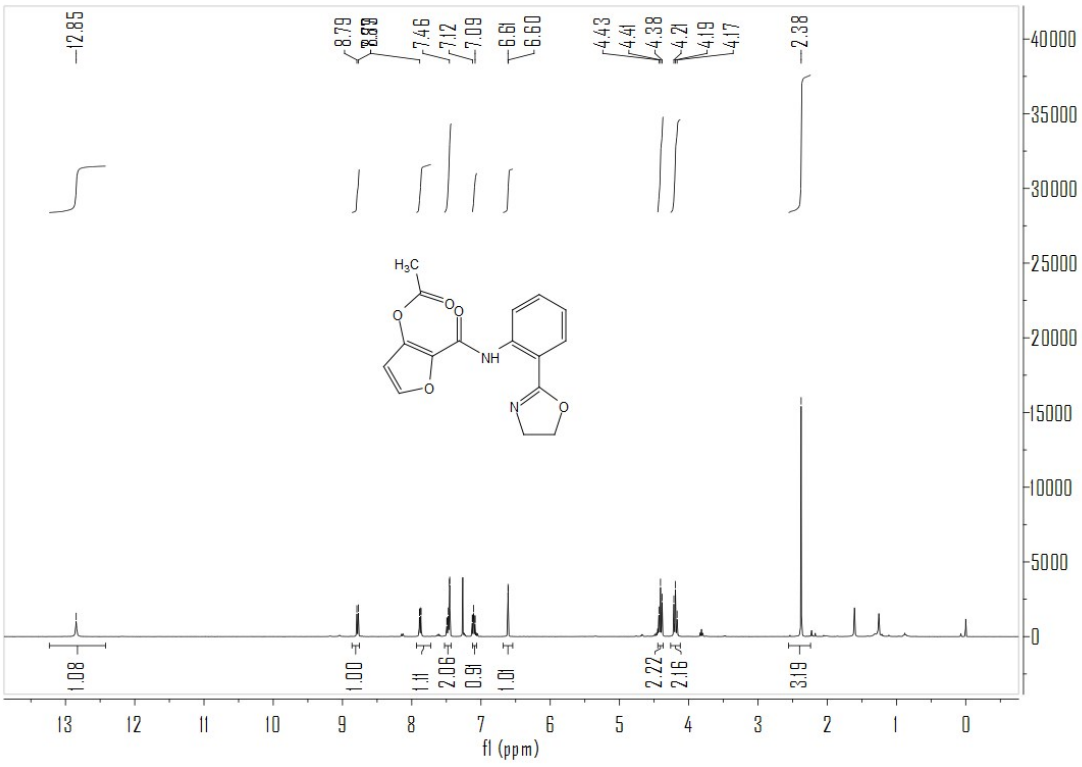
^{1}H NMR of 3q



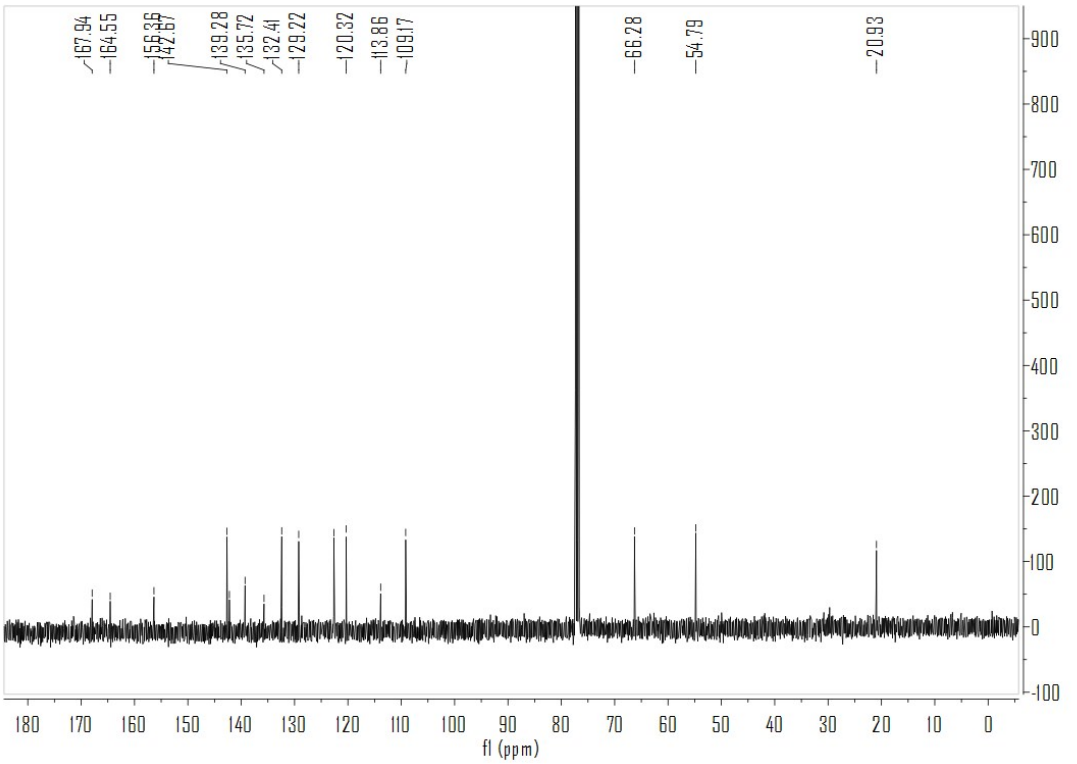
^{13}C NMR of 3q



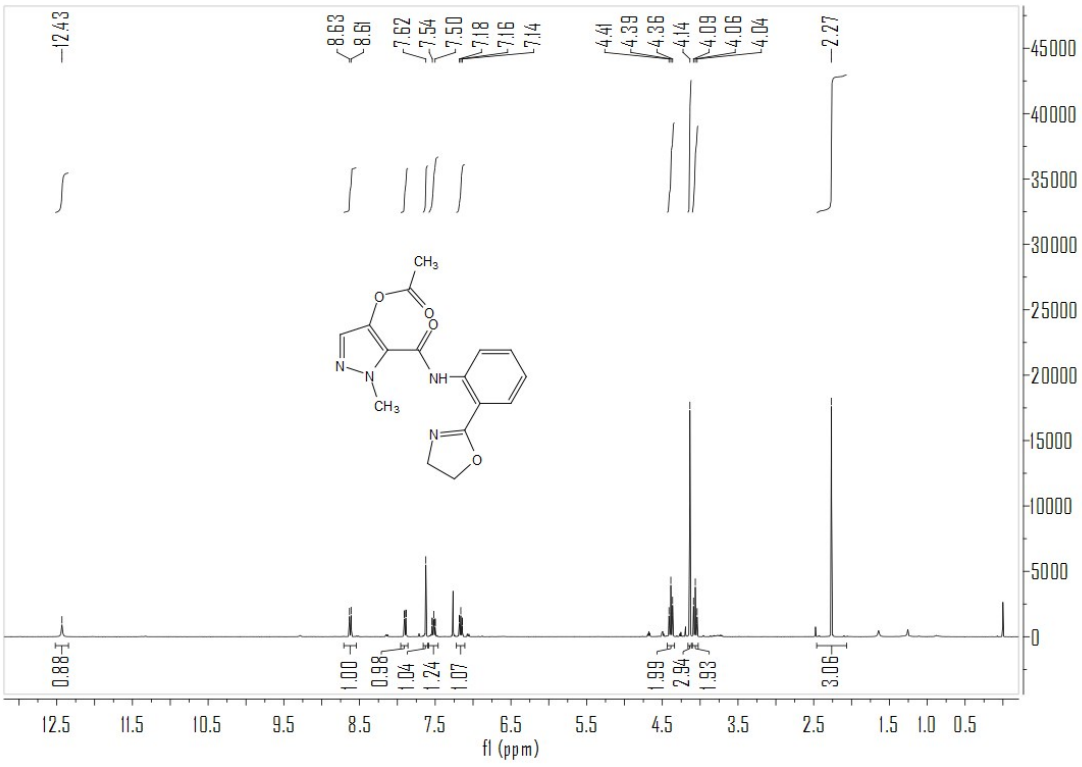
^{1}H NMR of 3r



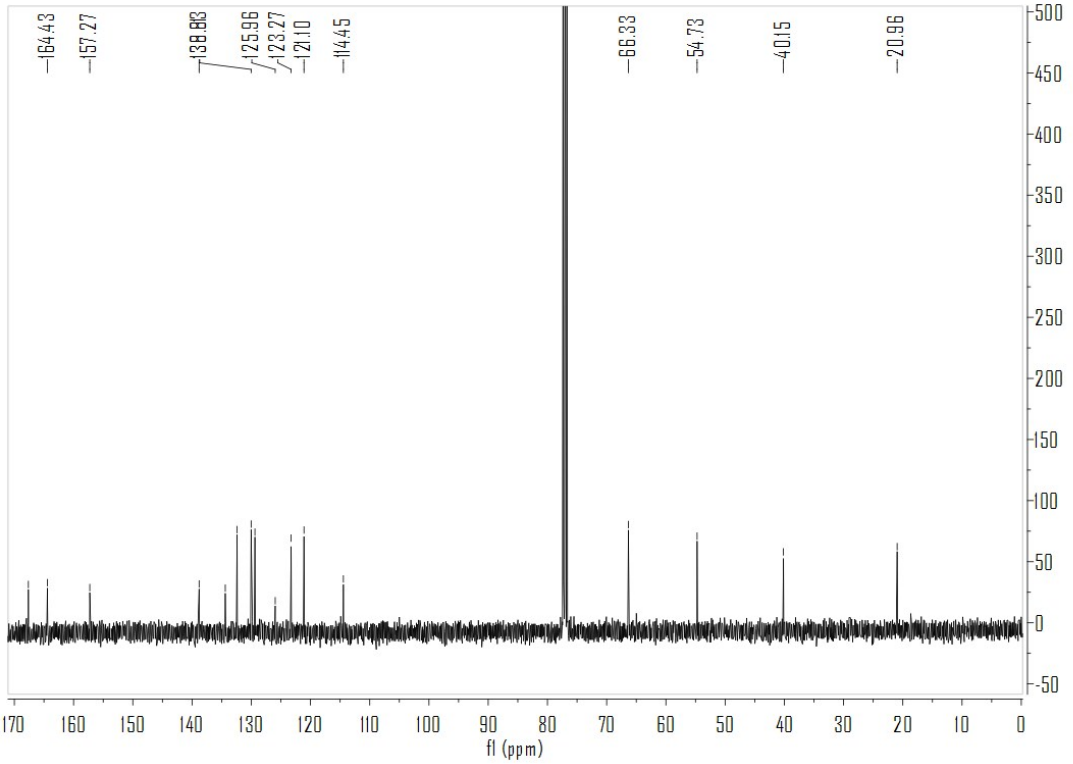
^{13}C NMR of 3r



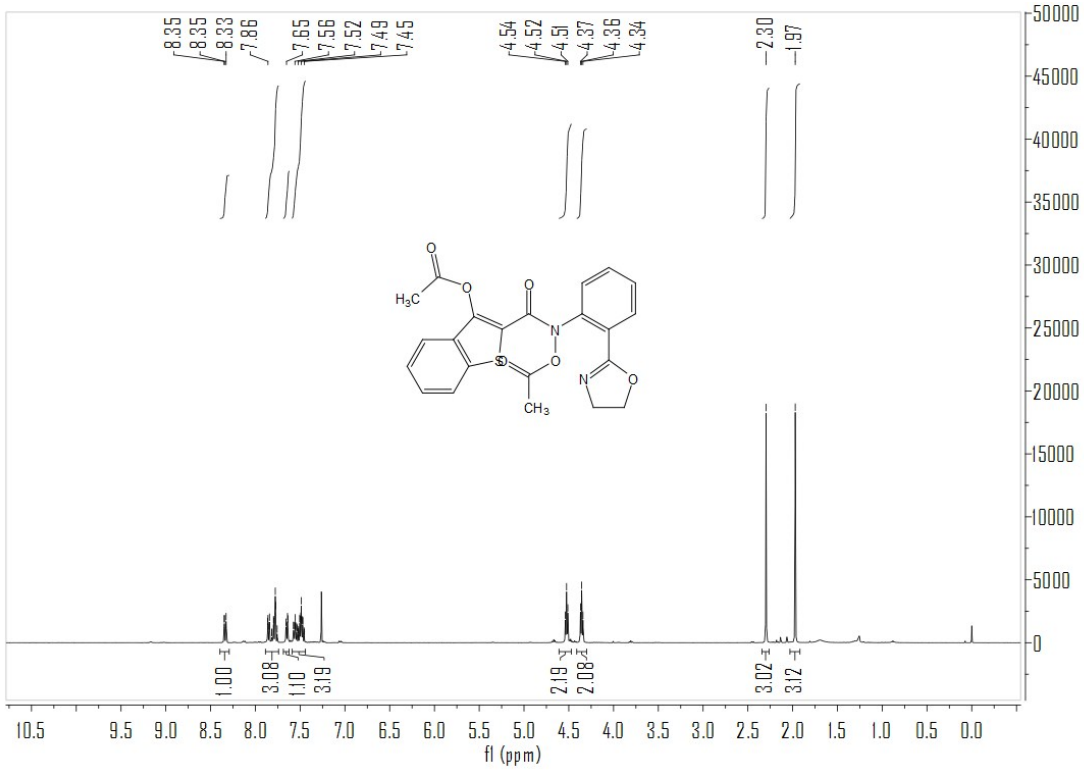
^{1}H NMR of 3s



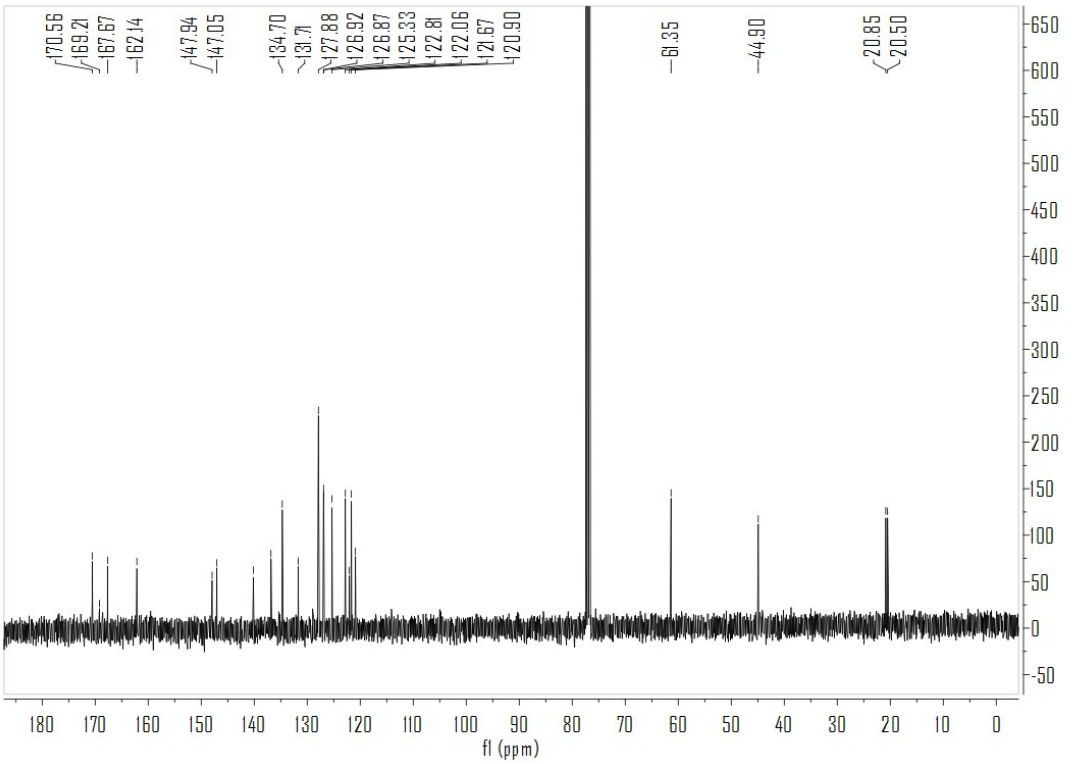
^{13}C NMR of 3s



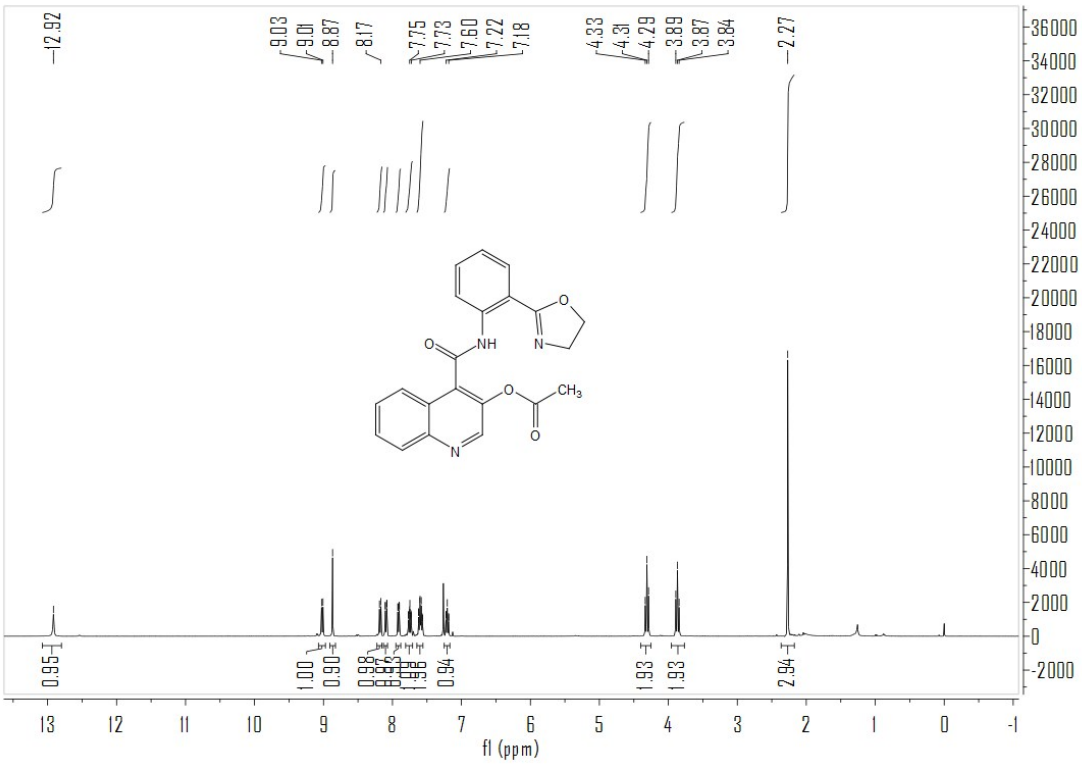
^{1}H NMR of 3t



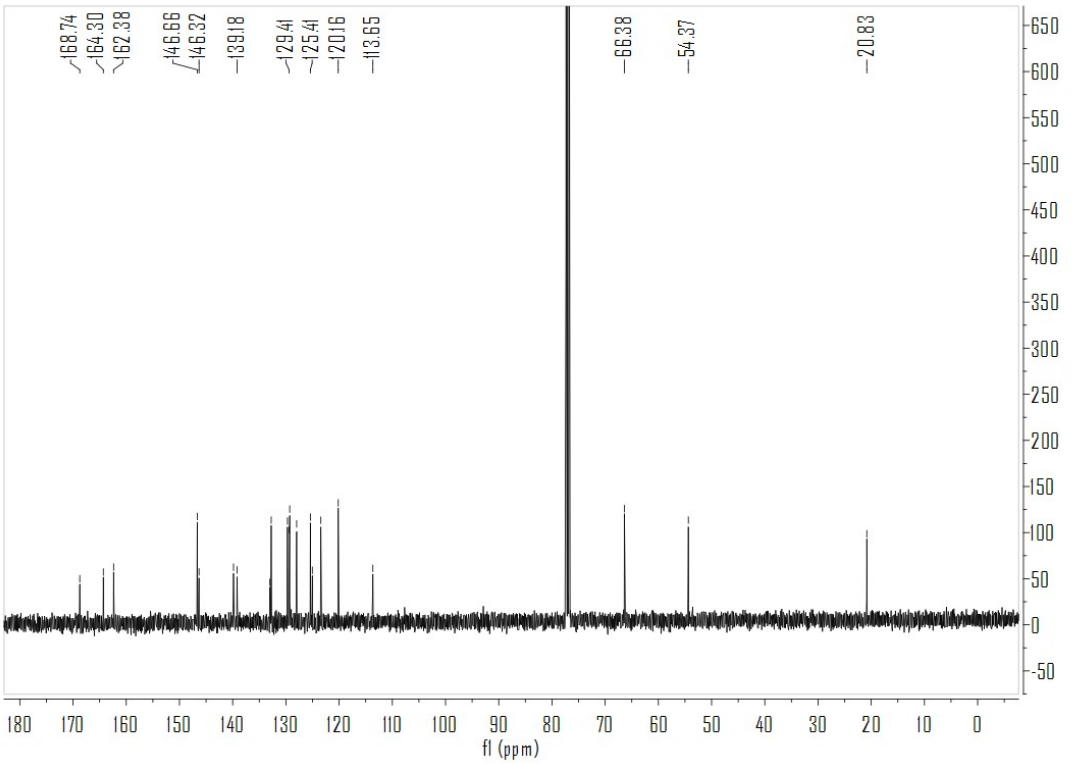
^{13}C NMR of 3t



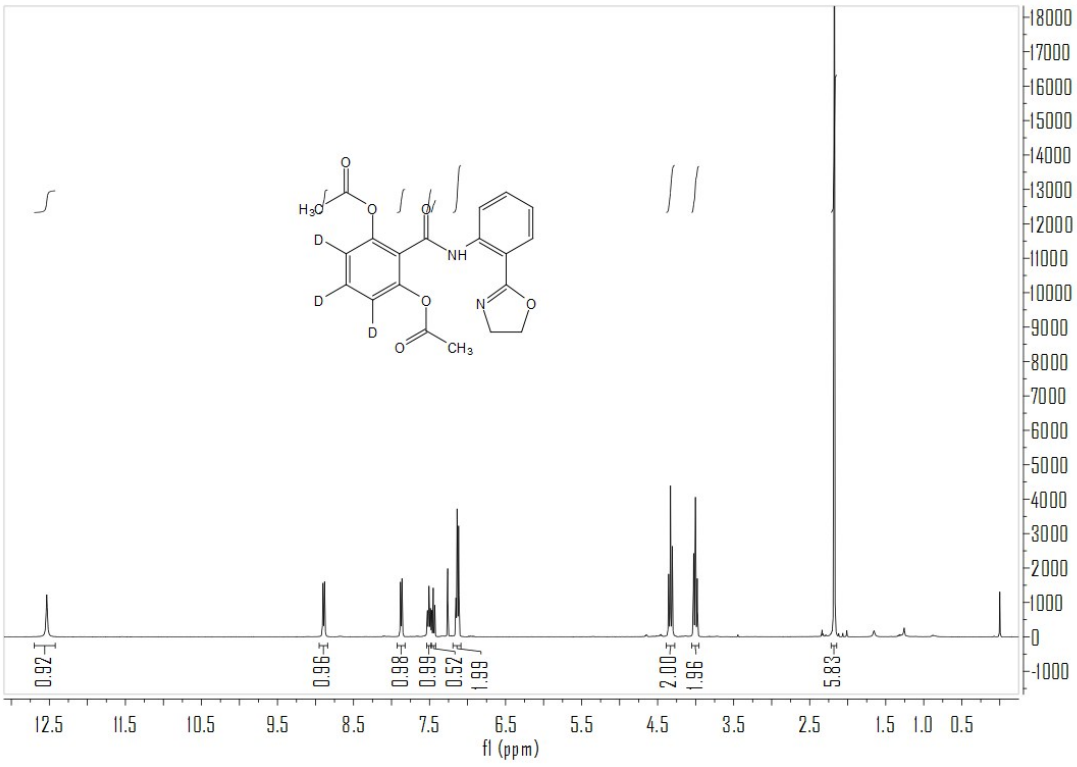
^{1}H NMR of 3u



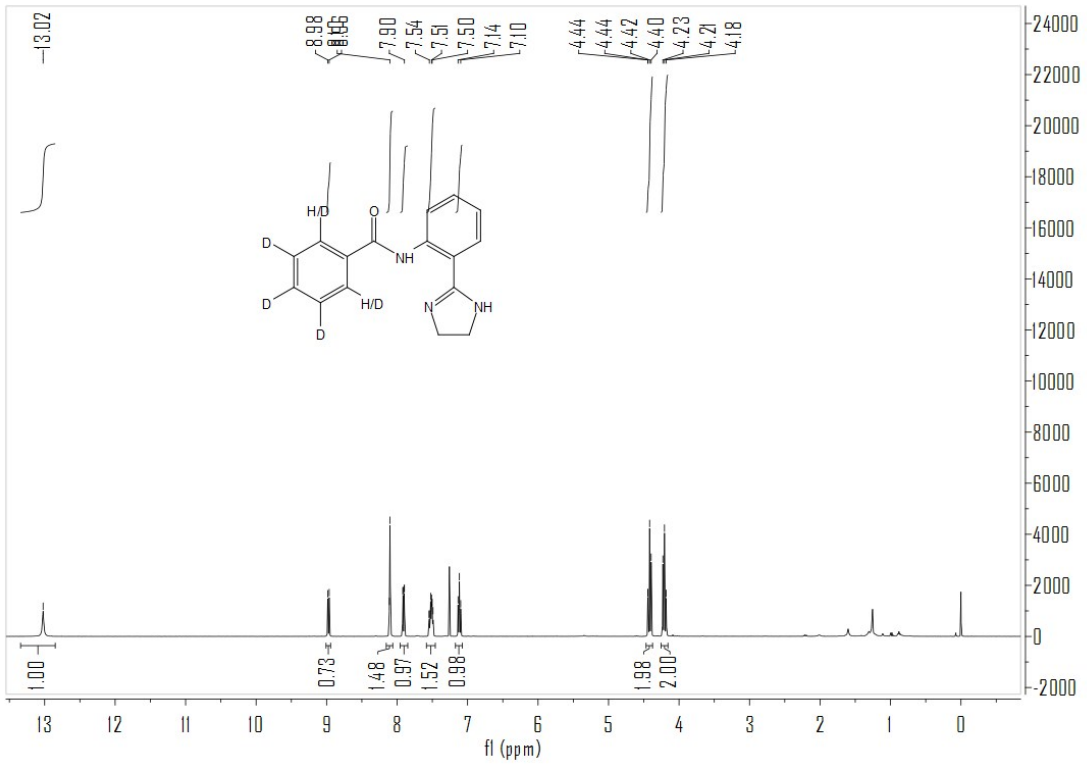
^{13}C NMR of 3u

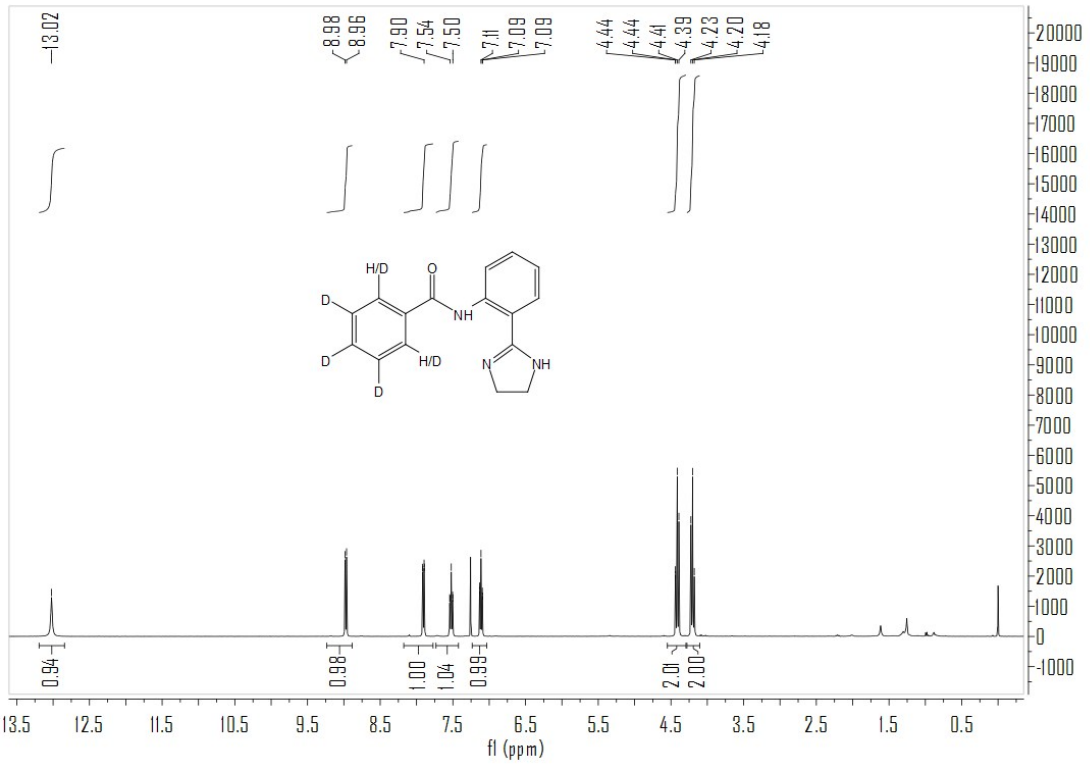


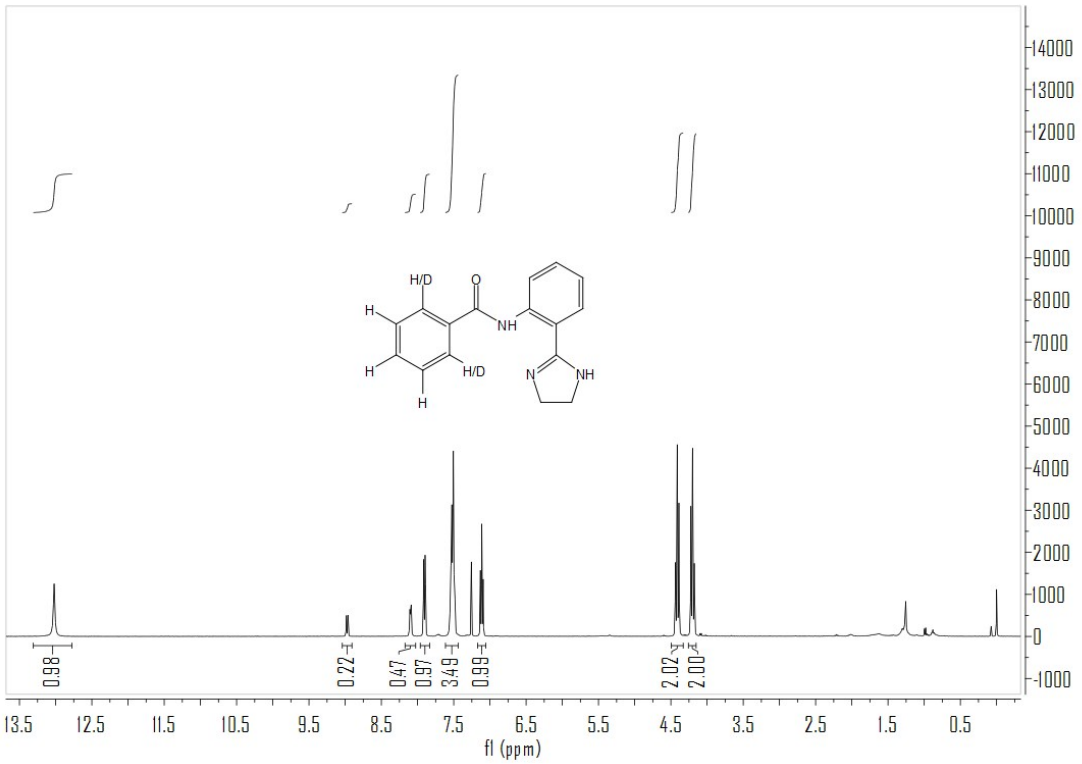
^{1}H NMR of [d_3]-3a and 3a



H/D exchange


13.02
8.98
8.96
7.90
7.54
7.51
7.50
7.14
7.10
4.44
4.44
4.42
4.40
4.23
4.21
4.18
H/D
O
NH
D
D
H/D
D
N
NH
1.00
0.73
1.48
0.97
1.52
0.98
1.98
2.00
f1 (ppm)


13.02
8.98
8.96
7.90
7.54
7.50
7.11
7.09
7.09
4.44
4.44
4.41
4.39
4.23
4.20
4.18
H/D
O
NH
D
D
H/D
D
N
NH
0.94
0.98
1.00
1.04
0.99
2.01
2.00
f1 (ppm)


H/D
O
NH
H
H
H/D
H
N
NH
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
0.98
0.22
0.47
0.97
3.49
0.99
2.02
2.00
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)