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An Electrochemical Oxidative Multicomponent Cascade Annulation of Ketones and Amines Used to Produce Imidazoles

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Supporting Information

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(A) Materials and equipment

All glassware was oven dried at 110 ℃ for hours and cooled down under vacuum. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. The instrument for electrolysis was dual display potentiostat (DJS-292B) (made in China, Figure S 1b). Both of the anode electrode and cathodic electrode were platinum plates (15 mm×15 mm×0.2 mm). Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200- 300 mesh silica gel in petroleum (bp. 60-90℃). ^{1}H and ^{13}C NMR data were recorded with Bruker Advance III (400 MHz) spectrometers with tetramethylsilane as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. All chemical shifts are reported relative to tetramethylsilane and d-solvent peaks (77.00 ppm, chloroform), respectively.

(B) **Typical experimental procedure**

In an oven-dried undivided three-necked bottle (15 mL) equipped with a stir bar, acetophenone (0.50 mmol), benzylamine (0.5 mmol), butan-1-amine (0.75 mmol), NH_4I (0.25 mmol), $LiClO_4$ (0.1 mmol) and CH_3CN (10 mL) were combined and added. The bottle was equipped with platinum plate (15 mm×15 mm×0.2 mm) as the anode and platinum plate (15 mm×15 mm×0.2 mm) as the cathode and was then charged with argon (Figure S1). The reaction mixture was stirred and electrolyzed at a constant current of 9 mA for 10 hours at room temperature. When the reaction was finished, 200 - 300 mesh silica gel (1 g) was added to the reaction mixture. Evaporation of MeCN

gave the residues. The residues were purified by flash column chromatography on silica gel (petroleum ether: ethyl ether = 8:1) to give the desired product.

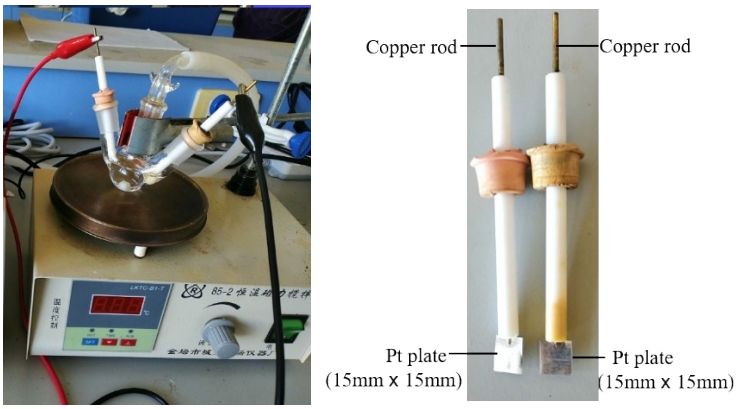


Figure S1 Electrolysis setup

(C) Large-scale experimental procedure

In an oven-dried undivided three-necked bottle (100 mL) equipped with a stir bar, acetophenone (5.0 mmol), benzylamine (5.0 mmol), butan-1-amine (7.5 mmol), NH_4I (2.5 mmol), $LiClO_4$ (0.1 M) and CH_3CN (65 mL) were combined and added. The bottle was equipped with platinum plate (20 mm x 20 cm x 0.2 mm) as the anode and platinum plate (20 mm x 20 cm x 0.2 mm) as the cathode and was then charged with argon. The reaction mixture was stirred and electrolyzed at a constant current of 9 mA for 20 hours at room temperature. When the reaction was finished, 200 - 300 mesh silica gel (3 g) was added to the reaction mixture. Evaporation of MeCN gave the residues. The residues were purified by flash column chromatography on silica gel (petroleum ether: ethyl ether = 8:1) to give the desired product

(D) **cyclic voltammetry experiments**

Cyclic voltammetry was performed in a three-electrode cell connected to a schlenk line under nitrogen at room temperature. The working electrode was a steady glassy

carbon disk electrode, the counter electrode a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. 10 mL of CH_3CN containing 0.1 M $KClO_4$ were poured into the electrochemical cell in all experiments. The scan rate is 0.1 V/s, ranging from 0 V to 2.0 V.

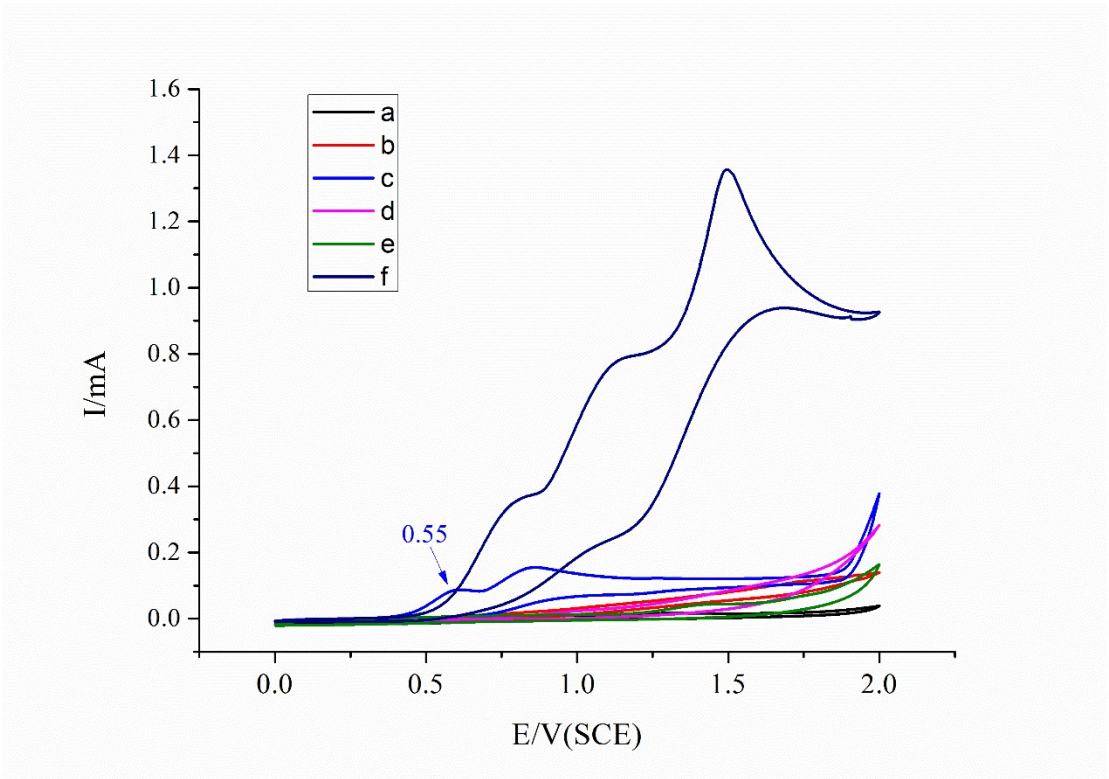
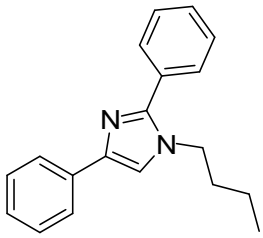


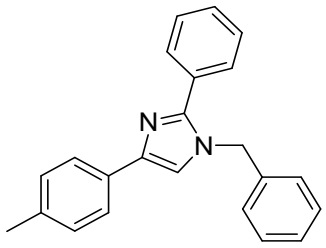
Figure S2. Cyclic voltammograms of 0.1mol L^{-1} of $LiClO_4$ in acetonitrile (10 mL) solution containing different compounds: (a) blank experiment; (b) only n-butyl amine (0.75mmol); (c) only ammonium iodide (0.25 mmol); (d) only benzyl amine (0.5 mmol); (e) only acetophenone (0.5 mmol); (f) n-butyl amine (0.75mmol), ammonium iodide (0.25 mmol), benzyl amine (0.5 mmol), acetophenone (0.5 mmol); with a GC disk working electrode, Pt counter electrode, and SCE reference electrode at 0.1 V/s scan rate.

(E) **Analytical data**



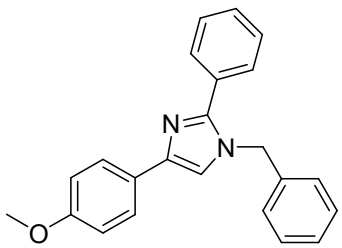
4aa

1-butyl-2,4-diphenyl-1H-imidazole (4aa) [1]: Yellow oil, 85% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.85 (d, J = 7.2 Hz, 2H), 7.63 (dd, J = 1.6 Hz, J = 1.2 Hz, 2H), 7.49-7.42 (m, 3H), 7.39 (t, J = 7.8 Hz, 2H), 7.30 (s, 1H), 7.23 (d, J = 7.2 Hz, 1H), 4.01 (t, J = 7.4 Hz, 2H), 1.79-1.71 (m, 2H), 1.34-1.27 (m, 2H), 0.90 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.1, 141.1, 134.2,130.9, 129.1, 128.8, 128.52, 128.47, 126.6, 124.8, 116.0, 46.6, 33.1, 19.7, 13.5; LRMS (EI 70 ev) m/z (%): 276 (M^+, 100); HRMS m/z (ESI) calcd for $C_{19}H_{21}N_2$ $(M+H)^+$ 277.1699, found 277.1690.



4ab

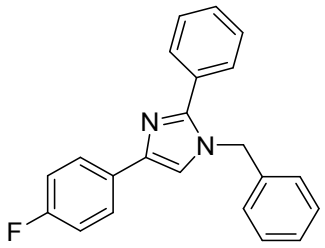
1-benzyl-2-phenyl-4-p-tolyl-1H-imidazole (4ab) [1]: yellow oil, 81% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.74 (d, J = 8.4 Hz, 2H), 7.62-7.60 (m, 2H), 7.42-7.40 (m, 3H), 7.38-7.28 (m, 3H), 7.21(s, 1H), 7.19-7.13 (m, 4H), 5.22 (s, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.5, 141.6, 136.9, 136.4, 131.3, 130.5, 129.2, 129.0, 129.0, 129.0, 128.6, 128.0, 126.7, 124.9, 116.4, 50.5, 21.2; LRMS (EI 70 ev) m/z (%): 324 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{23}H_{21}N_2$ $(M+H)^+$ 325.1700, found 325.1708.



4ac

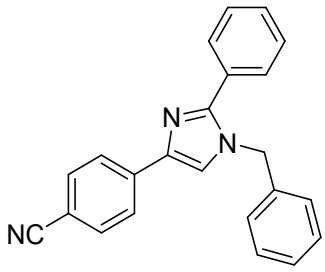
1-benzyl-4-(4-methoxyphenyl)-2-phenyl-1H-imidazole (4ac) [1]: yellow oil, 76%

yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.75 (d, J = 8.8 Hz, 2H), 7.60-7.58 (m, 2H), 7.40-7.39 (m, 3H), 7.33-7.29 (m, 3H), 7.24 (s, 1H), 7.13 (t, J = 1.6 Hz, 2H), 6.91 (d, J = 2.0 Hz, 2H), 5.18 (s, 2H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.7, 148.4, 141.4, 136.9, 130.4, 129.0, 128.94, 128.87, 127.9, 127.4, 126.6, 126.1, 115.8, 113.9, 55.2, 50.4; LRMS (EI 70 ev) m/z (%): 340 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{23}H_{21}N_2O$ $(M+H)^+$ 341.1649, found 341.1658.



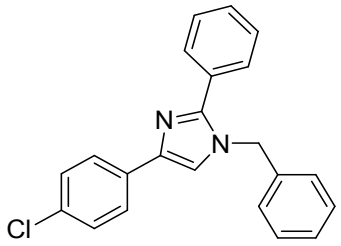
4ad

1-benzyl-4-(4-fluorophenyl)-2-phenyl-1H-imidazole (4ad) [1]: yellow oil, 69% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.81-7.77 (m, 2H), 7.61-7.59 (m, 2H), 7.44-7.41 (m, 3H), 7.37-7.32 (m, 3H), 7.19 (s, 1H), 7.17-7.13 (m, 2H), 7.05 (t, J = 8.0 Hz, 2H), 5.22 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.2 ($J_{C\text{-}F}$ = 243.8 Hz), 148.6, 140.7, 136.7, 130.3($J_{C\text{-}F}$ = 6.4 Hz), 130.2, 129.07, 129.03, 129.00, 128.6, 128.0, 126.6, 126.5 ($J_{C\text{-}F}$ = 7.5 Hz), 116.4, 115.4 ($J_{C\text{-}F}$ = 22.5 Hz), 50.5; LRMS (EI 70 ev) m/z (%): 328 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{22}H_{18}FN_2$ $(M+H)^+$ 329.1448, found 329.1458.



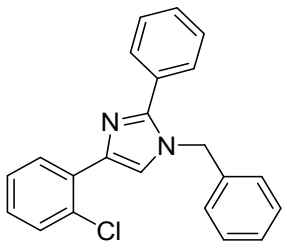
4ae

4-(1-benzyl-2-phenyl-1H-imidazol-4-yl)benzonitrile (4ae): yellow oil, 65% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91 (d, J = 8.4 Hz, 2H), 7.63-7.59 (m, 4H), 7.45-7.43 (m, 3H), 7.37-7.34 (m, 4H) 7.13 (d, J = 8.0 Hz, 2 H), 5.23 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.4, 139.7, 138.6, 136.4, 132.4, 130.0, 129.4, 129.2, 129.0, 128.7, 128.3, 126.8, 125.2, 119.3, 118.6, 109.8, 50.7; LRMS (EI 70 ev) m/z (%): 335 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{23}H_{18}N_3$ $(M+H)^+$ 336.1496, found 336.1488.



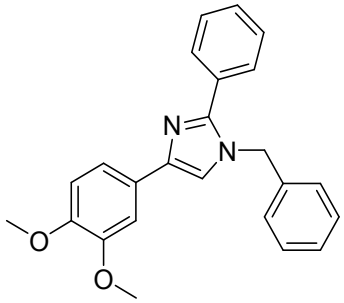
4af

1-benzyl-4-(4-chlorophenyl)-2-phenyl-1H-imidazole (4af) [1]: brown oil, 71% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.77 (dd, *J* = 2.0 Hz, *J* = 2.0 Hz, 2H), 7.61 (dd, *J* = 4.0 Hz, *J* = 2.0 Hz, 2H), 7.44-7.42 (m, 3H), 7.36-7.31 (m, 5H), 7.23 (s, 1H), 7.14 (d, *J* = 6.8 Hz, 2H), 5.22 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.8, 140.5, 136.7, 132.6, 132.3, 130.3, 129.1, 129.03, 129.00, 128.7, 128.6, 128.1, 126.7, 126.2, 116.9, 50.6; LRMS (EI 70 ev) m/z (%): 344 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{22}H_{18}ClN_2$ $(M+H)^+$ 345.1154, found 345.1146.



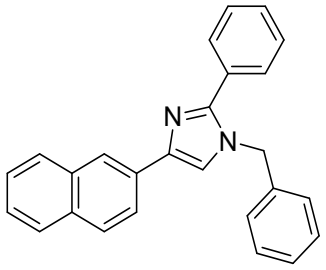
4ag

1-benzyl-4-(2-chlorophenyl)-2-phenyl-1H-imidazole (4ag) [2]: pale yellow solid, 62% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.33 (dd, *J* = 1.6, *J* = 1.6 Hz, 1H), 7.76 (s, 1H), 7.62-7.60 (m, 2H), 7.44-7.41 (m, 4H), 7.40-7.36 (m, 1H), 7.33-7.30 (m, 2H), 7.28-7.26 (m, 2H), 7.10 (d, *J* = 3.6, 2H), 5.27 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.5, 137.4, 136.7, 132.3, 130.7, 130.1, 129.6, 129.0, 128.9, 128.7, 128.5, 128.4, 127.9, 127.5, 127.0, 126.5, 121.6, 50.5; LRMS (EI 70 ev) m/z (%): 344 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{22}H_{18}ClN_2$ $(M+H)^+$ 345.1154, found 345.1146.



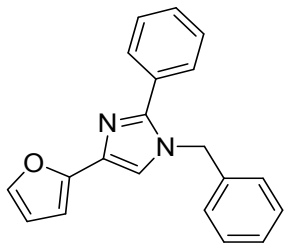
4ah

1-benzyl-4-(3,4-dimethoxyphenyl)-2-phenyl-1H-imidazole (4ah) [3]: yellow powder, 76% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.63-7.60 (m, 2H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.42-7.40 (m, 3H), 7.36-7.31 (m, 4H), 7.18 (s, 1H), 7.15 (d, *J* = 7.2 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 1H), 5.21 (s, 2H), 3.95 (s, 3H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.1, 148.4, 148.1, 141.4, 136.9, 130.4, 129.0, 128.9, 128.6, 127.9, 127.3, 126.6, 117.2, 116.0, 111.3, 108.4, 55.9, 55.9, 50.4; LRMS (EI 70 ev) m/z (%): 370 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{24}H_{23}N_2O_2$ $(M+H)^+$ 371.1755, found 371.1762.



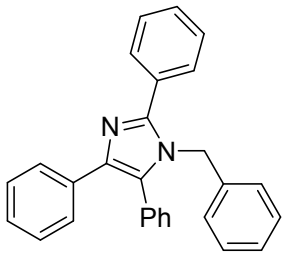
4ai

1-benzyl-4-(naphthalen-3-yl)-2-phenyl-1H-imidazole (4ai) [1]: brown oil, 62% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.30 (s, 1H), 7.81-7.70 (m, 4H), 7.57-7.45 (m, 2H), 7.37-7.32 (m, 4H), 7.32-7.26 (m, 3H), 7.26-7.20 (m, 2H), 7.09-7.03 (m, 2H), 5.13 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.9, 141.5, 136.8, 133.8, 132.6, 131.4, 130.4, 129.3, 129.1, 129.0, 128.6, 128.1, 128.04, 128.01, 127.6, 126.7, 126.0, 125.3, 123.7, 123.0, 117.3, 50.5; LRMS (EI 70 ev) m/z (%): 360 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{26}H_{21}N_2$ $(M+H)^+$ 361.1700, found 361.1691.



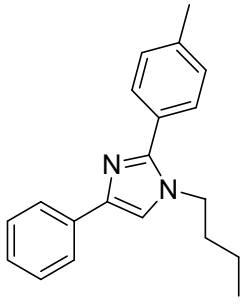
4aj

1-benzyl-4-(furan-2-yl)-2-phenyl-1H-imidazole (4aj): brown oil, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.59 (dd, *J* = 3.2 Hz, *J* = 2.8 Hz, 2H), 7.42 (t, *J* = 3.4 Hz, 3H), 7.37-7.32 (m, 5H), 7.19 (s, 1H), 7.13 (d, *J* = 6.4 Hz, 2H), 6.71 (d, *J* = 3.2 Hz, 1H), 5.20 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.9,148.7, 140.9, 136.6, 134.2, 129.1, 129.07, 129.00, 128.94, 128.6, 128.0, 126.7, 116.7, 111.2, 104.4, 50.5; LRMS (EI 70 ev) m/z (%): 300 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{20}H_{17}N_2O$ $(M+H)^+$ 301.1336, found 301.1329.



4ak

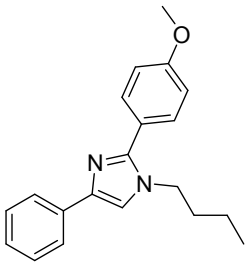
1-benzyl-2,4,5-triphenyl-1H-imidazole **(4ak)** [4]**:** white soild, 77% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.59-7.57 (m, 2H), 7.42 (t, *J* = 3.2 Hz, 3H), 7.37-7.31 (m, 6H), 7.24 (s, 2H), 7.19 (s, 2H), 7.13 (t, *J* = 4.0 Hz, 2H), 7.03 (d, *J* = 6.8 Hz, 1H), 6.71 (t, *J* = 2.8 Hz, 2H), 5.20 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 149.9, 148.7, 140.9, 136.6, 134.1, 130.1, 129.1, 129.07, 129.00, 128.9, 128.6, 128.0, 127.0, 126.7, 116.7, 111.2, 110.3, 104.4, 50.5; LRMS (EI 70 ev) m/z (%): 386 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{28}H_{23}N_2$ $(M+H)^+$ 387.1855, found 387.1865.



4ba

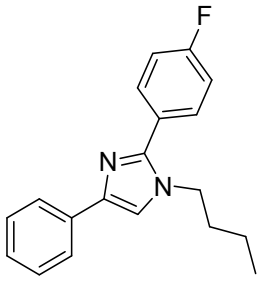
1-butyl-4-phenyl-2-p-tolyl-1H-imidazole (**4ba**): yellow oil, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 7.51 (d, *J* = 8.0 Hz, 3H), 7.39-7.35 (m, 3H), 7.28-7.26 (m, 2H), 7.23 (d, J = 8.0 Hz, 2H), 3.99 (t, *J* = 7.6 Hz, 2H), 1.83-1.72 (m, 2H), 1.33-1.26 (m, 2H), 0.88 (t, *J* = 8.0 Hz, 3H);^{13}C NMR (100 MHz, $CDCl_3$) *δ*: 148.4, 138.9, 129.7, 129.3, 129.0, 129.0, 128.5, 126.7, 126.6, 124.9, 115.9, 46.7, 33.2, 19.8, 13.6; LRMS (EI 70 ev) m/z (%): 290 (M^+, 100); HRMS m/z (ESI) calcd for $C_{20}H_{23}N_2$ $(M+H)^+$

291.1855, found 291.1846.



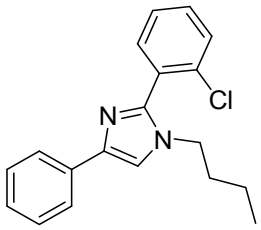
4ca

1-butyl-2-(4-methoxyphenyl)-4-phenyl-1H-imidazole (4ca): yellow oil, 82% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.83 (d, J = 7.2 Hz, 2H), 7.55 (d, J = 8.4 Hz, 2H), 7.37 (t, J = 8.0 Hz, 2H), 7.28 (s, 1H), 7.23 (t, J = 7.2 Hz, 1H), 3.97 (t, J = 7.6 Hz, 2H), 3.86 (s, 3H), 1.79-1.71 (m, 2H), 1.35-1.25 (m, 2H), 0.88 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 160.0, 148.0, 140.7, 134.1, 130.4, 128.5, 126.6, 124.8, 123.1, 115.7, 113.9, 55.3, 46.6, 33.1, 19.7, 13.5; LRMS (EI 70 ev) m/z (%): 306 (M^+, 100); HRMS m/z (ESI) calcd for $C_{20}H_{23}N_2O$ $(M+H)^+$ 307.1804, found 307.1813.



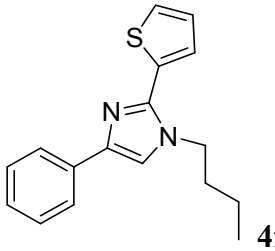
4da

1-butyl-2-(4-fluorophenyl)-4-phenyl-1H-imidazole (4da): yellow powder, 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.82 (d, J =7.2 Hz, 2H), 7.62-7.58 (m, 2H), 7.37 (t, J = 7.6, 2H), 7.29 (s, 1H), 7.23 (d, J = 8.4 Hz, 1H), 7.16 (t, J =8.8 Hz, 2H), 3.96 (t, J = 7.2 Hz, 2H), 1.78-1.71 (m, 2H), 1.33-1.27 (m, 2H), 0.88 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.3 ($J_{C\text{-}F}$ = 246 Hz), 147.1, 141.1, 136.8, 134.1, 133.1, 131.0 ($J_{C\text{-}F}$ = 8.3 Hz), 128.6 ($J_{C\text{-}F}$ = 7.2 Hz), 126.7, 124.8, 115.8 ($J_{C\text{-}F}$ = 22.1 Hz), 46.6, 33.1, 19.7, 13.5; LRMS (EI 70 ev) m/z (%): 294 (M^+, 100); HRMS m/z (ESI) calcd for $C_{19}H_{20}FN_2$ $(M+H)^+$ 295.1505, found 295.1513.



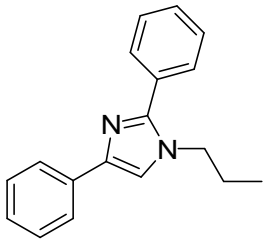
4ea

1-butyl-2-(2-chlorophenyl)-4-phenyl-1H-imidazole (4ea): yellow oil, 64% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.84 (dd, J = 1.2 Hz, J = 0.8 Hz, 2H), 7.52-7.47 (m, 2H), 7.38-7.32 (m, 4H), 7.25-7.20 (m, 2H), 3.80 (t, J = 7.4 Hz, 2H), 1.70-1.62 (m, 2H), 1.26-1.19 (m, 2H), 0.83 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 145.4, 141.2, 134.7, 134.1, 132.7, 130.8, 130.5, 129.6, 128.5, 126.9, 126.6, 124.8, 115.1, 46.3, 32.7, 19.6, 13.4; LRMS (EI 70 ev) m/z (%): 310 (M^+, 100); HRMS m/z (ESI) calcd for $C_{19}H_{20}ClN_2$ $(M+H)^+$ 311.1310, found 311.1318.



4fa

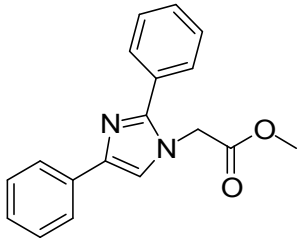
1-butyl-4-phenyl-2-(thiophen-2-yl)-1H-imidazole (4fa): brown powder, 75% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.83-7.81 (m, 2H), 7.41-33 (m, 4H), 7.26-7.21 (m, 2H), 7.13-7.11 (m, 1H), 4.10 (t, J = 8.0 Hz, 2H), 1.86-1.78 (m, 2H), 1.44-1.35 (m, 2H), 0.94 (t, J = 8.0 Hz, 3H);^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.9, 141.3, 134.0, 132.5, 128.5, 127.4, 126.8, 126.7, 126.6, 124.9, 116.8, 47.0, 33.0, 19.9, 13.6; LRMS (EI 70 ev) m/z (%): 285 (M^+, 100); HRMS m/z (ESI) calcd for $C_{17}H_{19}N_2S$ $(M+H)^+$ 286.1263, found 286.1269.



4ga

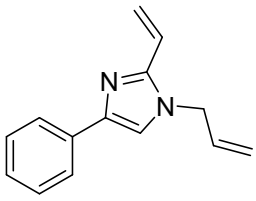
2,4-diphenyl-1-propyl-1H-imidazole (4ga) [1]: yellow oil, 72% yield; ^{1}H NMR (400

MHz, $CDCl_3$) δ: 7.85-7.83 (m, 2H), 7.64-7.61 (m, 2H), 7.47-7.43 (m, 3H), 7.38 (t, J = 7.8 Hz, 2H), 7.31 (s, 1H), 7.25-7.21(m, 1H), 3.97 (t, J = 7.6 Hz, 2H), 1.86-1.77 (m, 2H), 0.91 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.2, 141.1, 134.2, 131.0, 129.1, 128.8, 128.6, 128.5, 126.7, 124.9, 116.0, 48.5, 24.4, 11.1; LRMS (EI 70 ev) m/z (%): 262 (M^+, 100); HRMS m/z (ESI) calcd for $C_{18}H_{19}N_2$ $(M+H)^+$ 263.1542, found 263.1549.



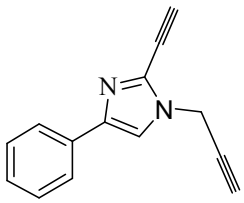
4ha

methyl 2-(2,4-diphenyl-1H-imidazol-1-yl)acetate (4ha): yellow oil, 55% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.75-7.73 (m, 2H), 7.46-7.42 (m, 4H), 7.38-7.34 (m, 2H), 7.32-7.26 (m, 3H), 4.71 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.9, 155.0, 148.8, 135.2, 134.0, 131.1, 129.8, 128.9, 128.3, 125.1, 124.9, 115.8, 53.1, 50.0; LRMS (EI 70 ev) m/z (%): 324 (M^+, 100); LRMS (EI 70 ev) m/z (%): 292 (M^+, 100); HRMS m/z (ESI) calcd for $C_{18}H_{17}N_2O_2$ $(M+H)^+$ 293.1285, found 293.1275.



4ia

1-allyl-4-phenyl-2-vinyl-1H-imidazole (4ia): yellow oil, 63% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.81 (t, J = 4.2, 2H), 7.38-7.36 (m, 2H), 7.24 (t, J = 7.4, 1H), 7.15 (s, 1H), 6.60 (dd, J = 11.2, J = 11.2, 1H), 6.29 (dd, J = 1.6, J = 1.6, 1H), 6.00-5.91 (m, 1H), 5.46 (dd, J = 1.6, J = 1.2, 1H), 5.28 (d, J = 10.0, 1H), 5.12 (d, J = 17.2, 1H), 4.59 (dt, J = 1.6, J = 1.8, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 145.3, 141.3, 134.0, 132.6, 128.5, 126.8, 124.9, 122.6, 118.8, 117.9, 116.3, 48.3; LRMS (EI 70 ev) m/z (%): 210 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{14}H_{15}N_2$ $(M+H)^+$ 211.1230, found 211.1221.



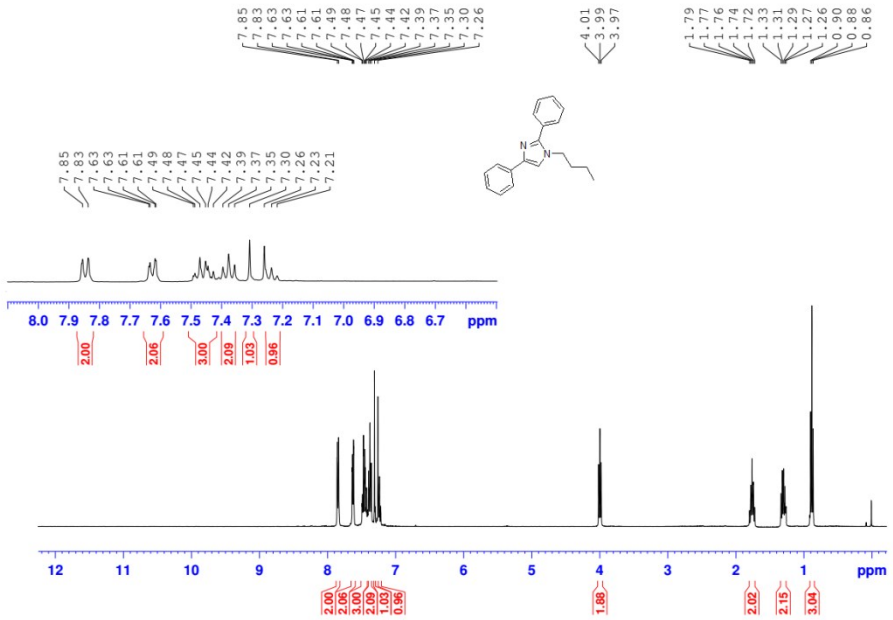
4ja

2-ethynyl-4-phenyl-1-(prop-2-ynyl)-1H-imidazole (4ja): yellow oil, 71% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79 (d, *J* = 8.4 Hz, 2H), 7.42 (s, 1H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.28 (t, *J* = 6.4 Hz, 1H), 4.85 (d, *J* = 2.8 Hz, 2H), 3.43 (s, 1H), 2.51 (t, J = 5.2, Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 142.5, 133.1, 130.5, 128.6, 127.4, 125.1, 115.7, 82.6, 76.2, 74.8, 72.5, 36.5; LRMS (EI 70 ev) m/z (%): 206 (M^+, 100); HRMS *m/z* (ESI) calcd for $C_{14}H_{11}N_2$ $(M+H)^+$ 207.0917, found 207.0927.

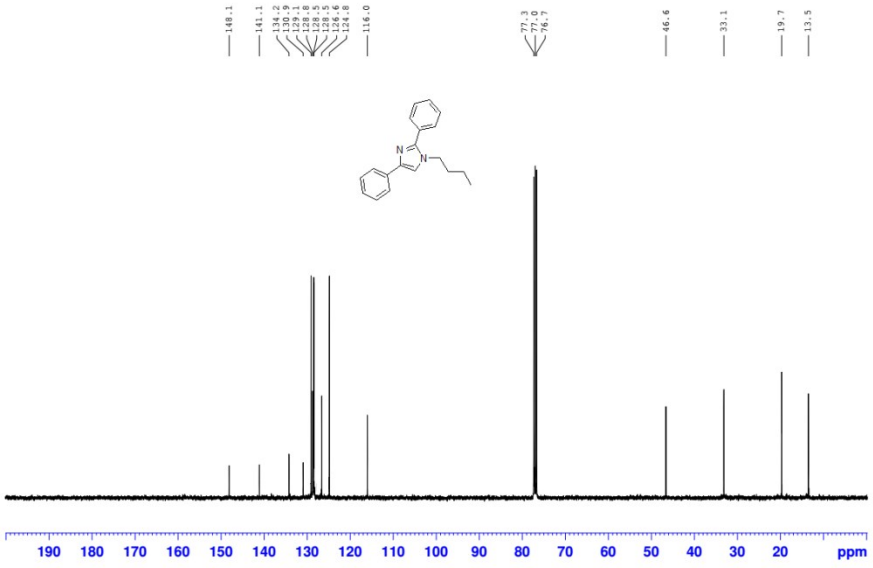
(F) Reference

1. H. Huang; X. Ji; W. Wu; H. Jiang, *Adv. Synth. Catal.,* 2013, **355**, 170-180.
2. L. Xiang; Y. Niu; X. Pang; X. Yang; R. Yan, *Chem. Commun.,* 2015, **51**, 6598-6600.
3. C. T. F. Salfeena; R. Jalaja; R. Davis; E. Suresh; S. B. Somappa, *ACS Omega,* 2018, **3**, 8074-8082.
4. R. Sarkar; C. Mukhopadhyay, *Eur. J. Org. Chem.,* 2015, **2015**, 1246-1256.

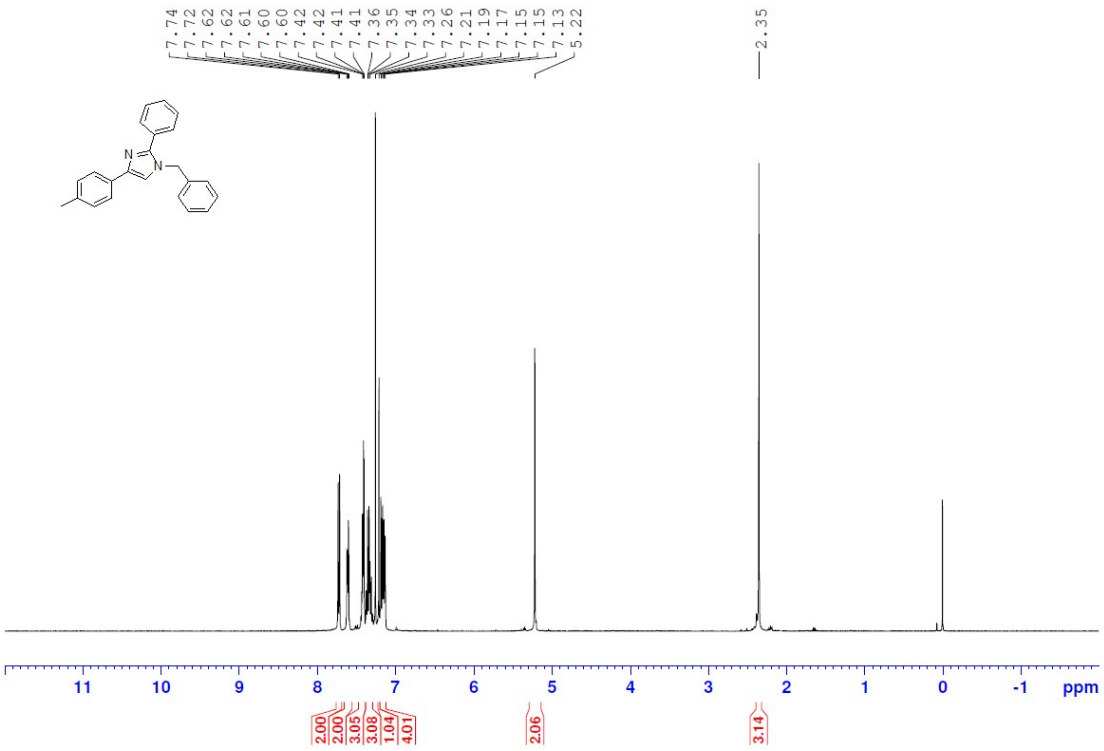
(G) Spectra



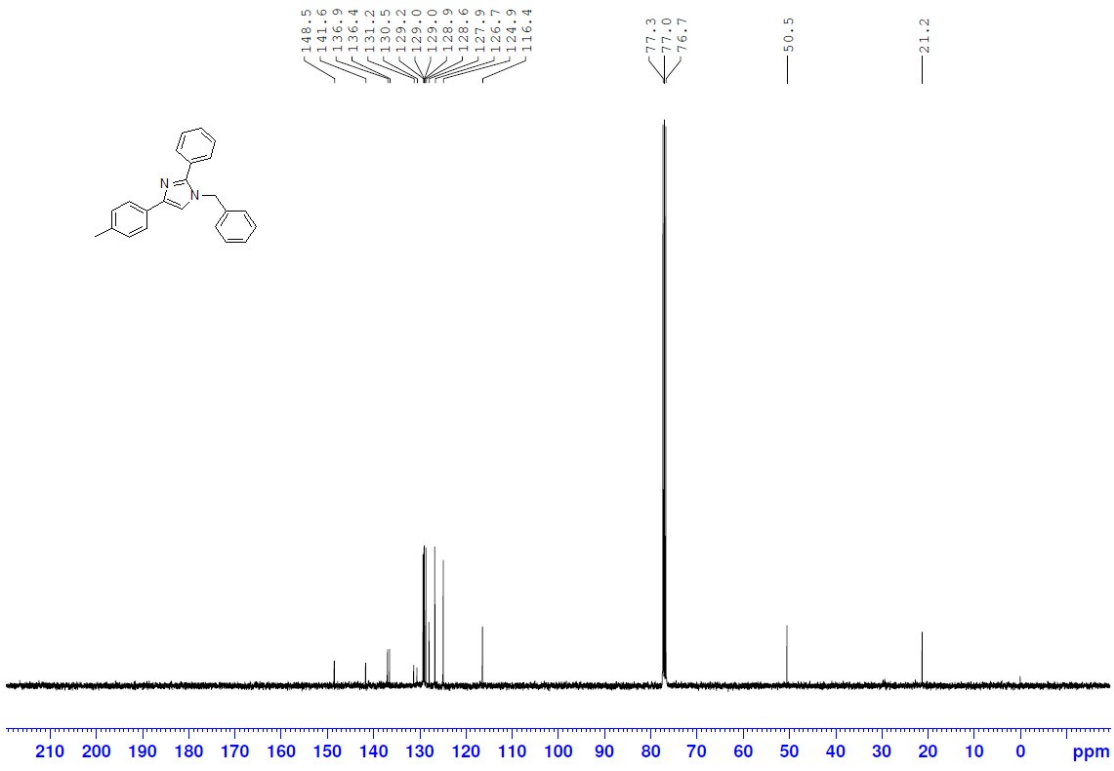
^{1}H NMR of **4aa**



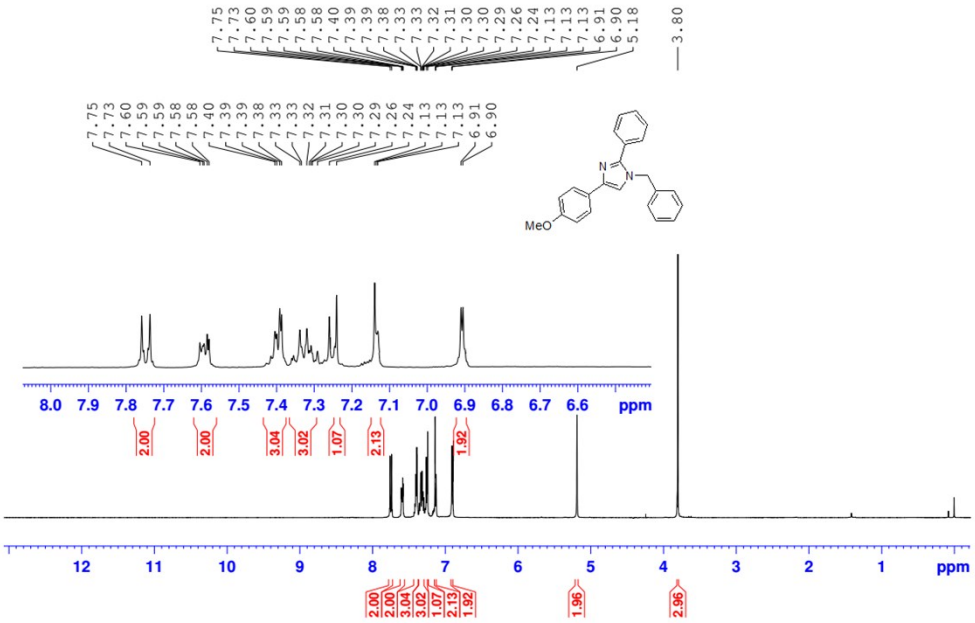
^{13}C NMR of **4aa**



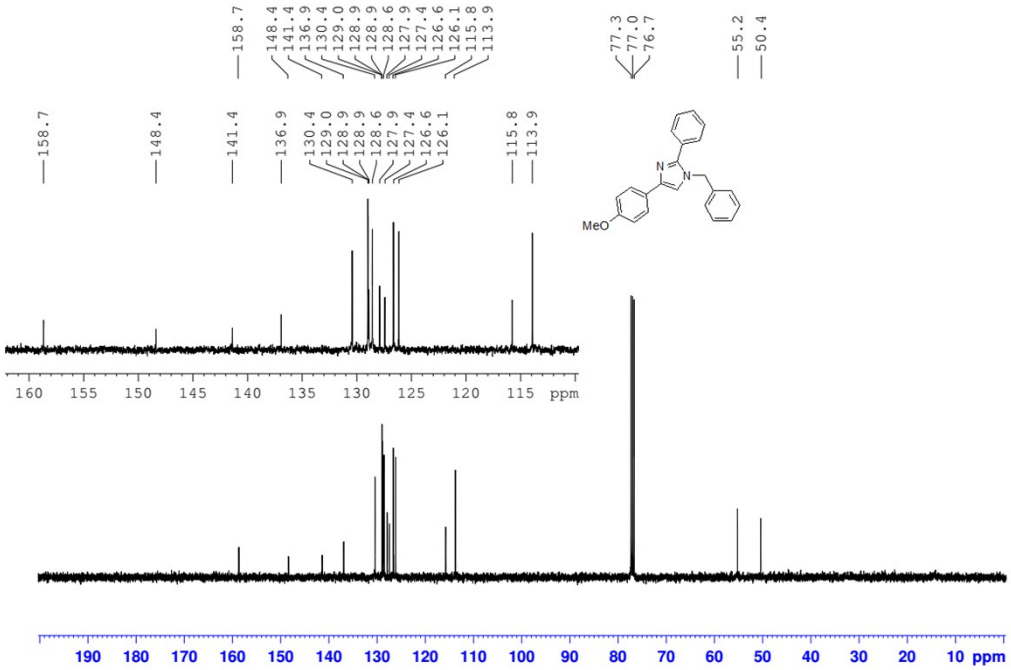
^{1}H NMR of **4ab**



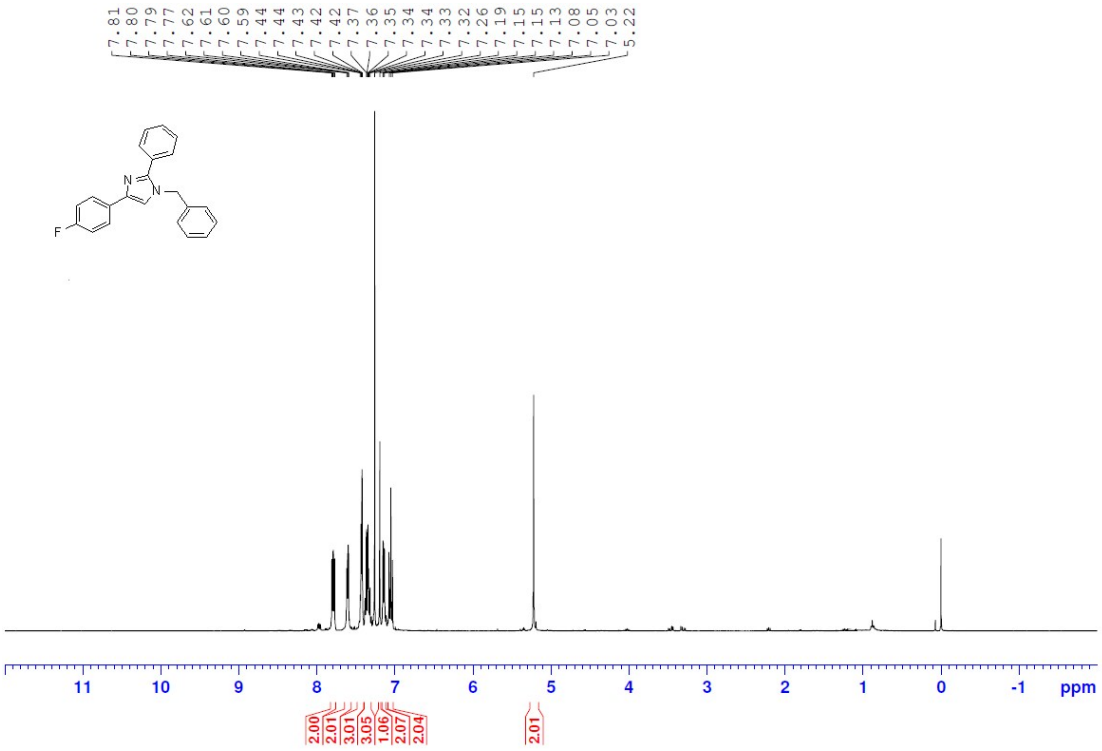
^{13}C NMR of **4ab**



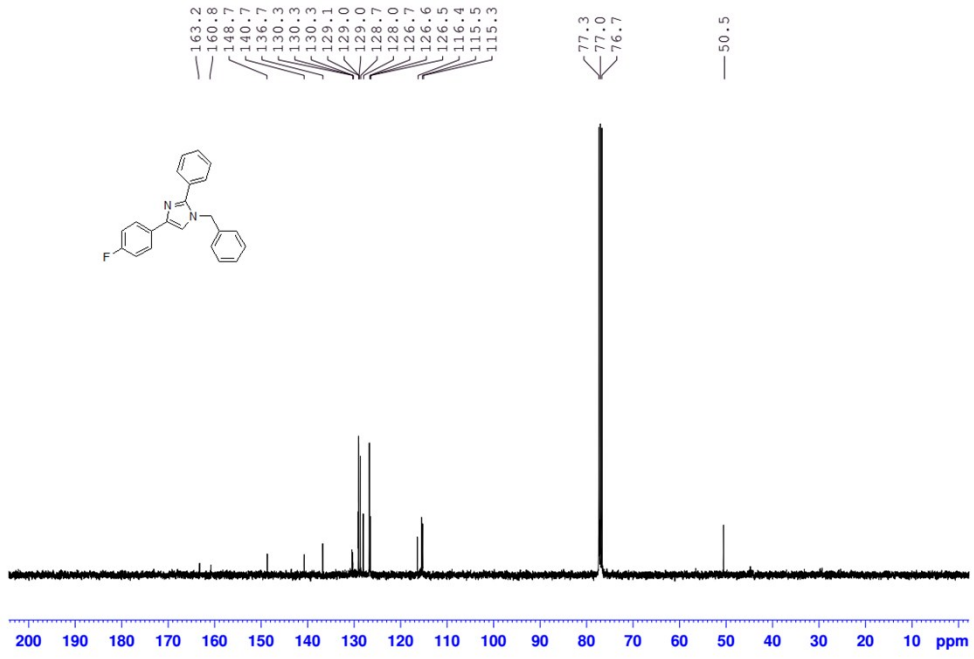
^{1}H NMR of **4ac**



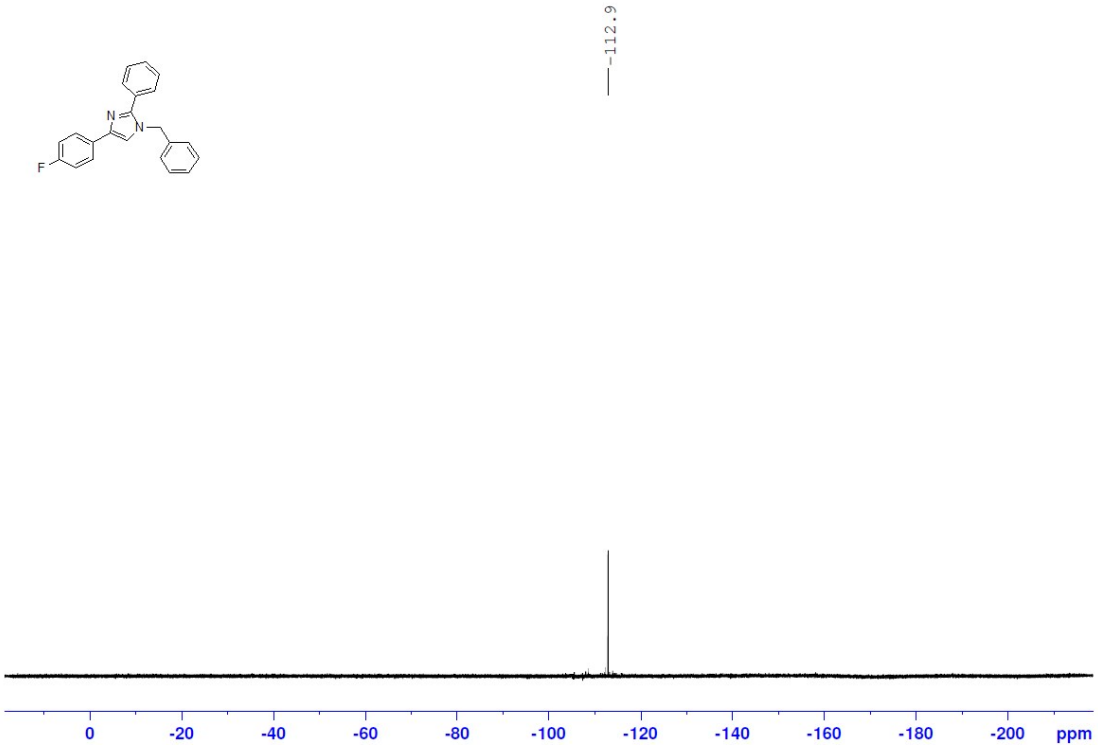
^{13}C NMR of **4ac**



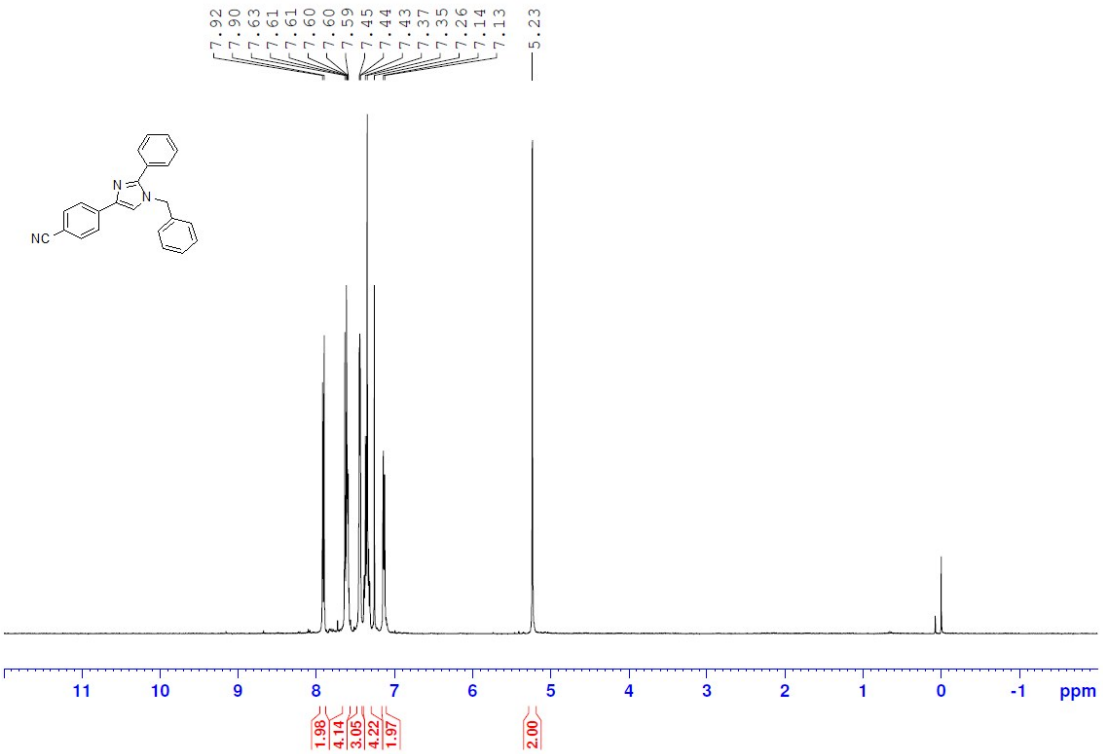
^{1}H NMR of **4ad**



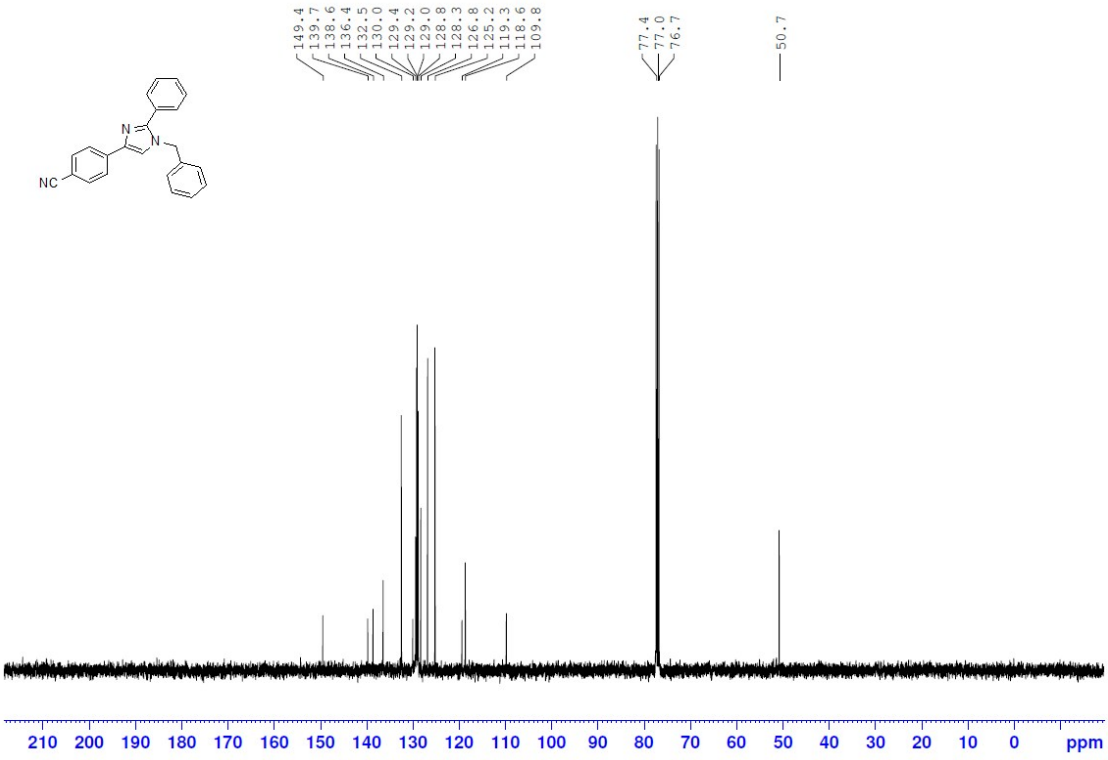
^{13}C NMR of **4ad**



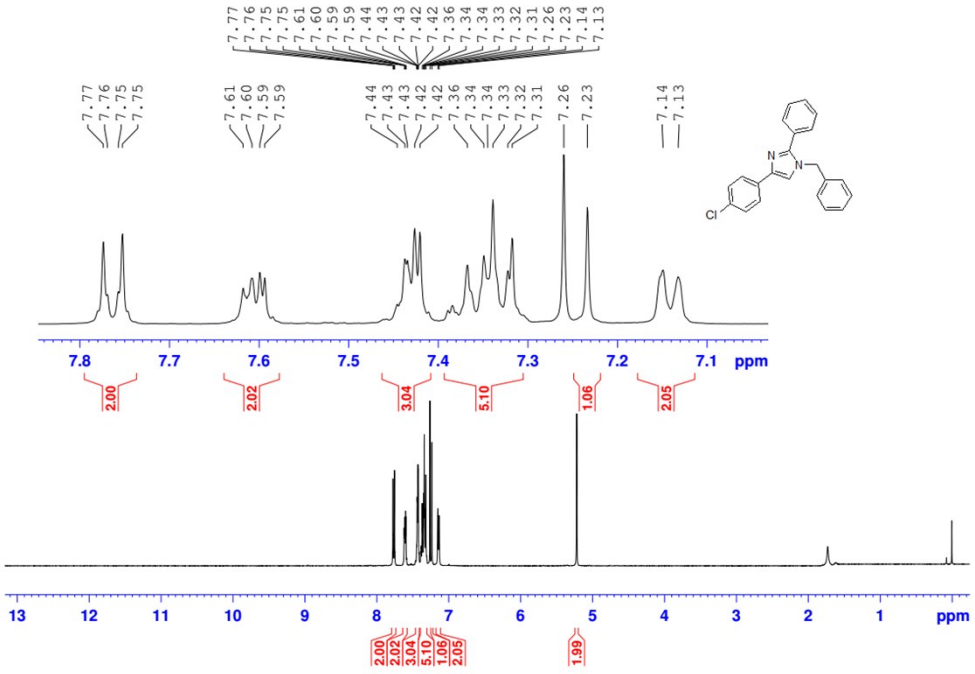
^{19}F NMR of **4ad**



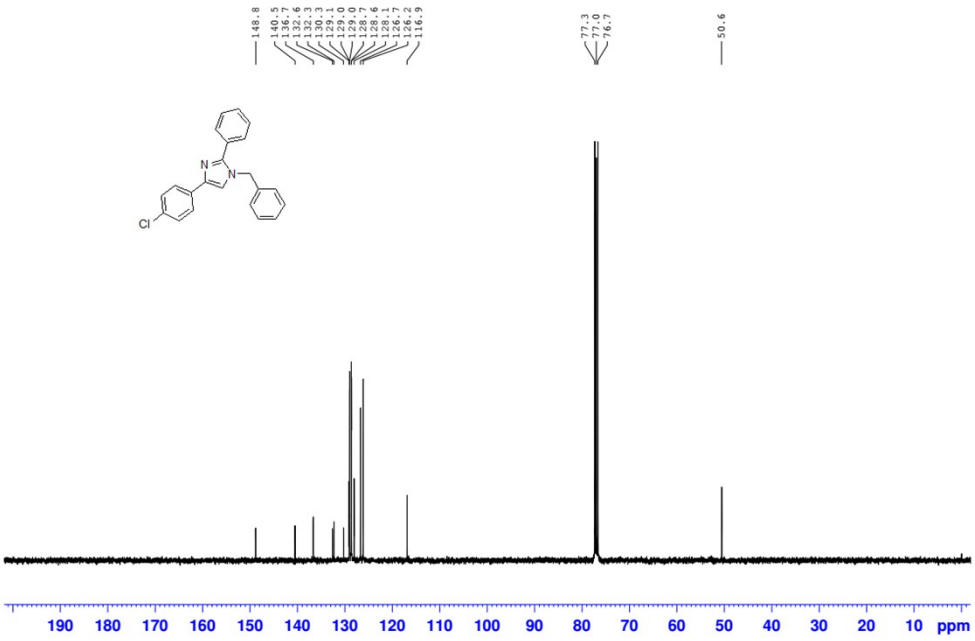
^{1}H NMR of **4ae**



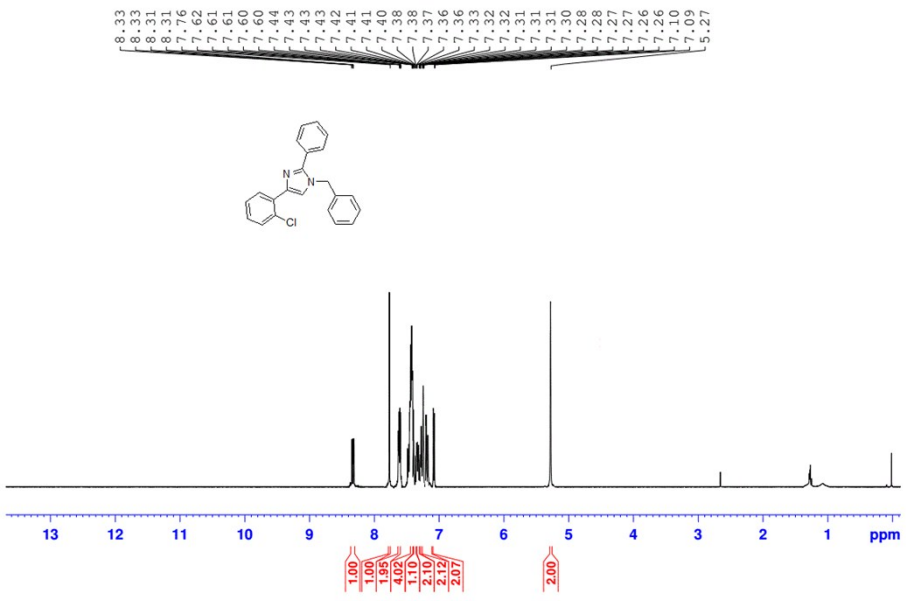
^{13}C NMR of **4ae**



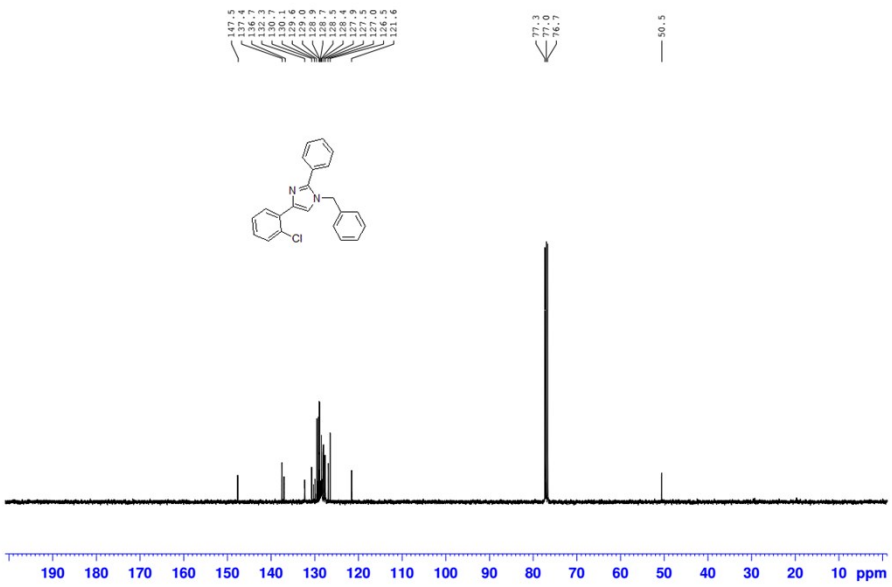
^{1}H NMR of **4af**



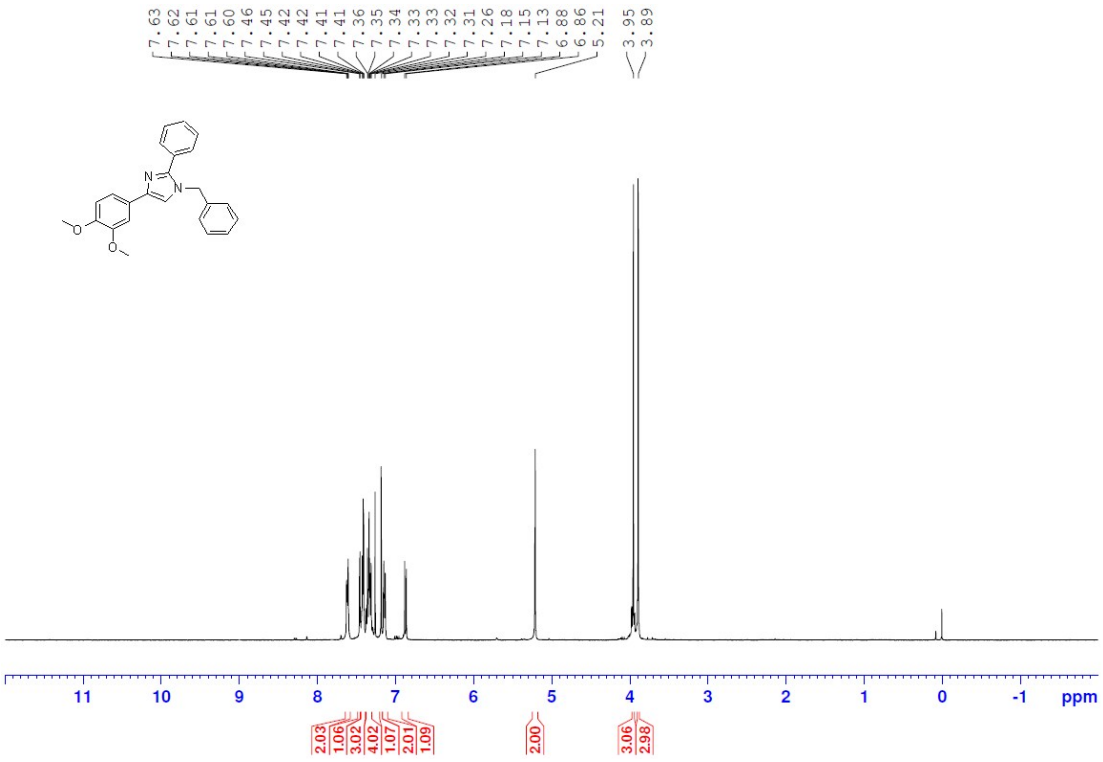
^{13}C NMR of **4af**



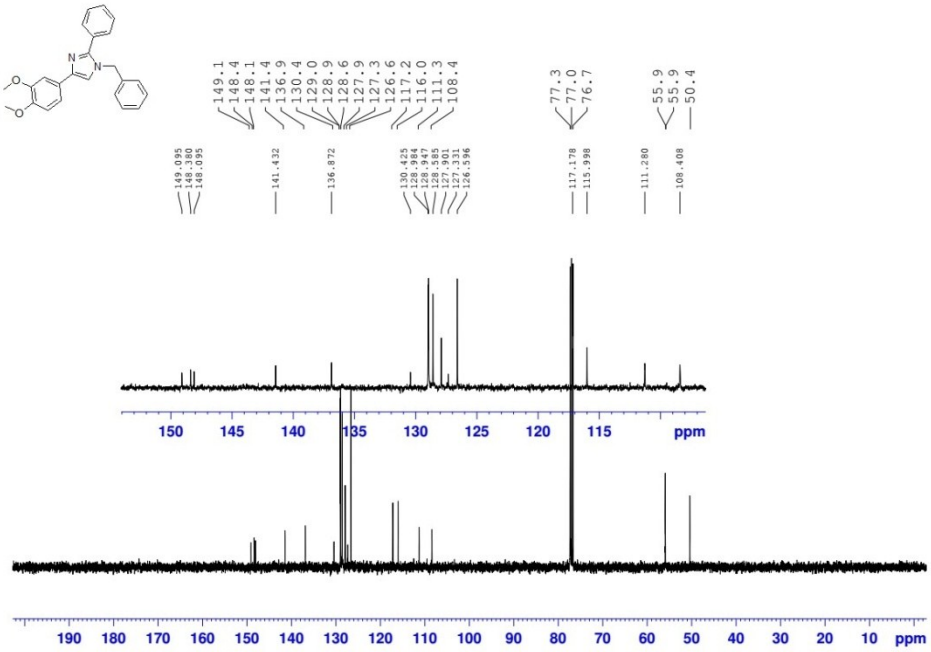
^{1}H NMR of **4ag**



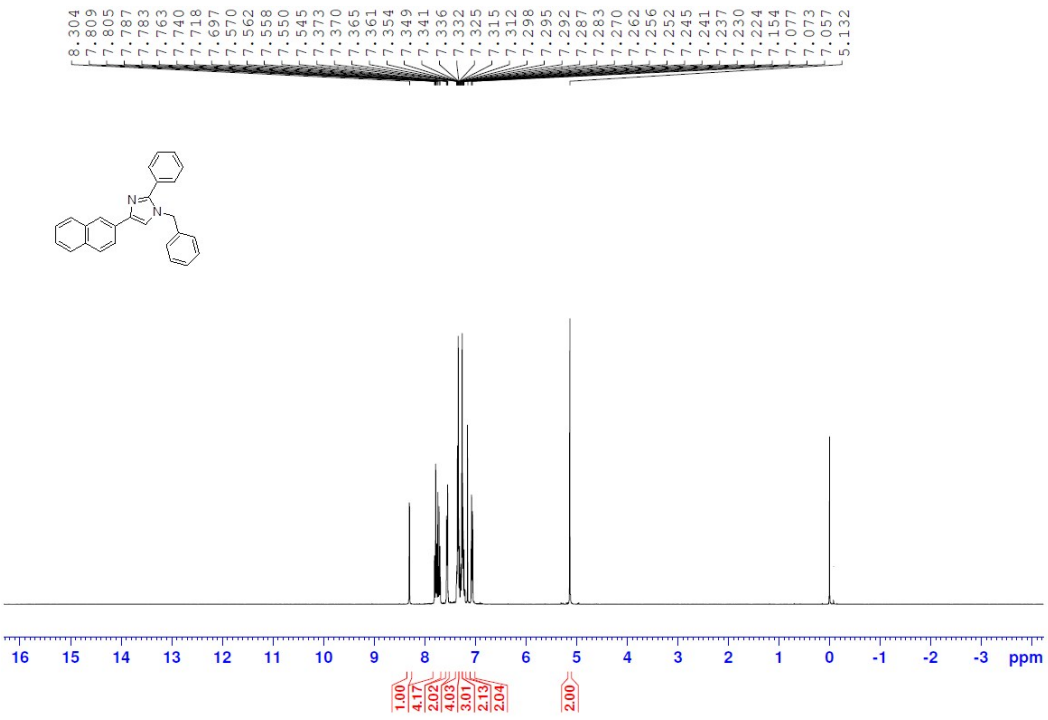
^{13}C NMR of **4ag**



^{1}H NMR of **4ah**



^{13}C NMR of **4ah**



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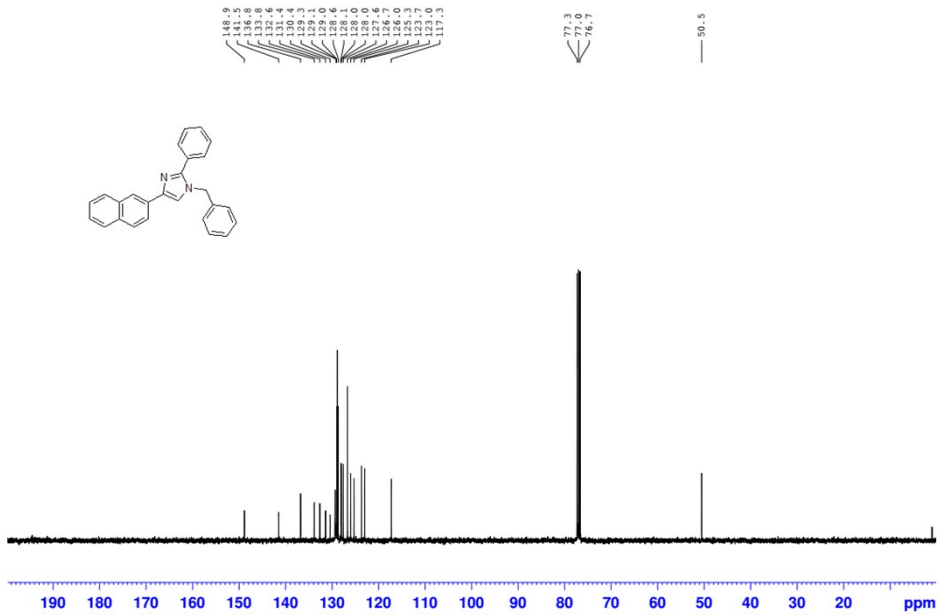
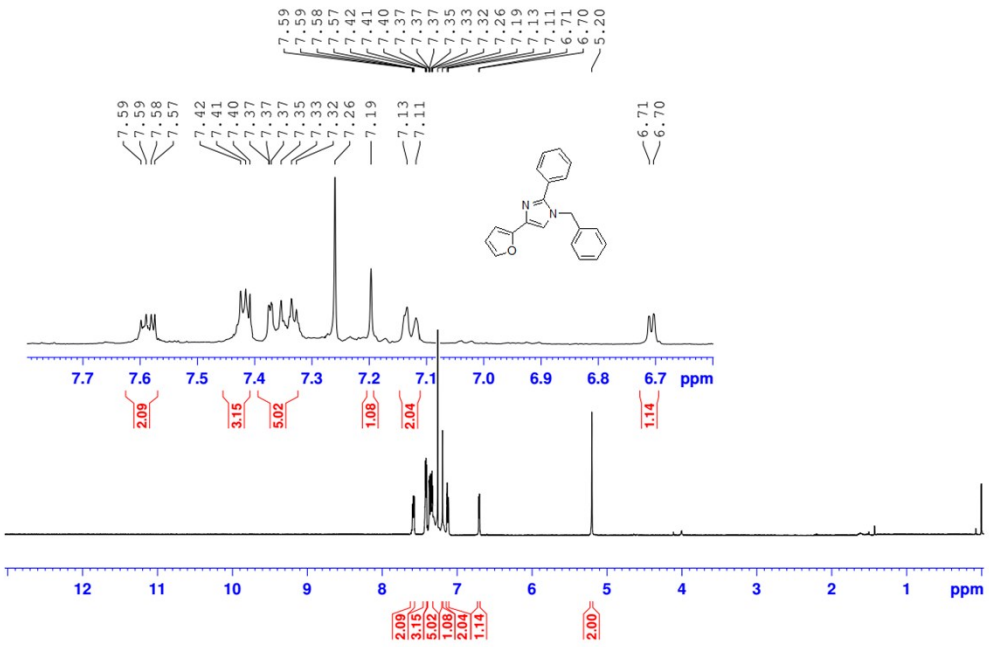
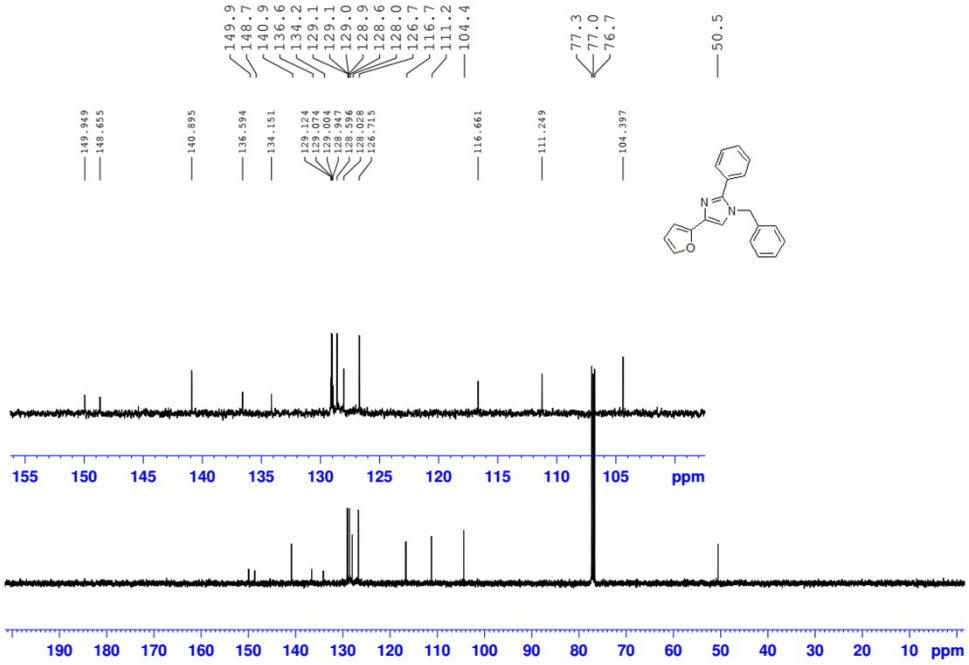


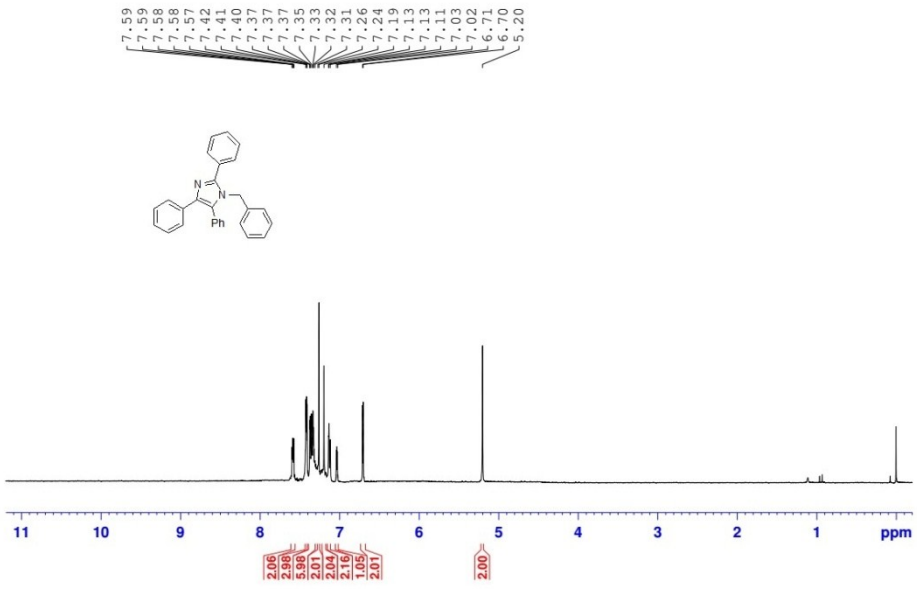
^{13}C NMR of **4ai**



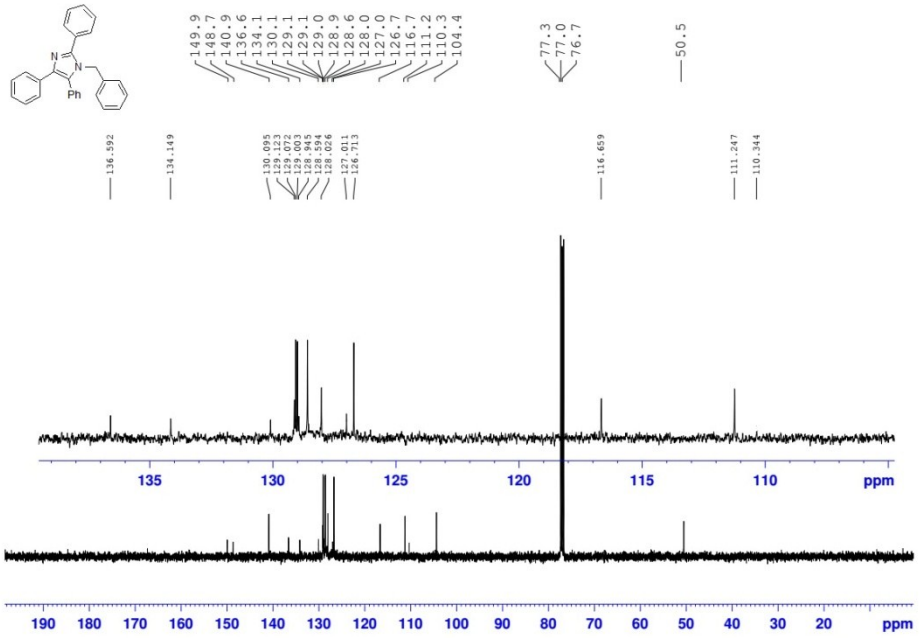
^{1}H NMR of **4aj**



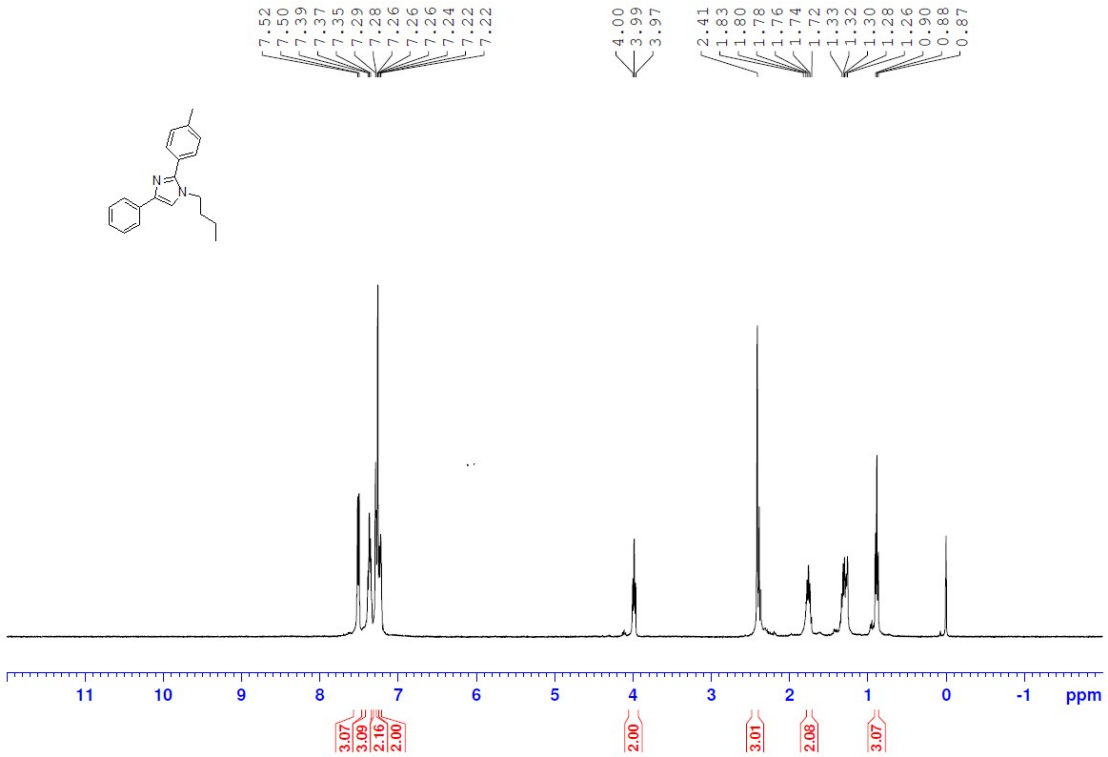
^{13}C NMR of **4aj**



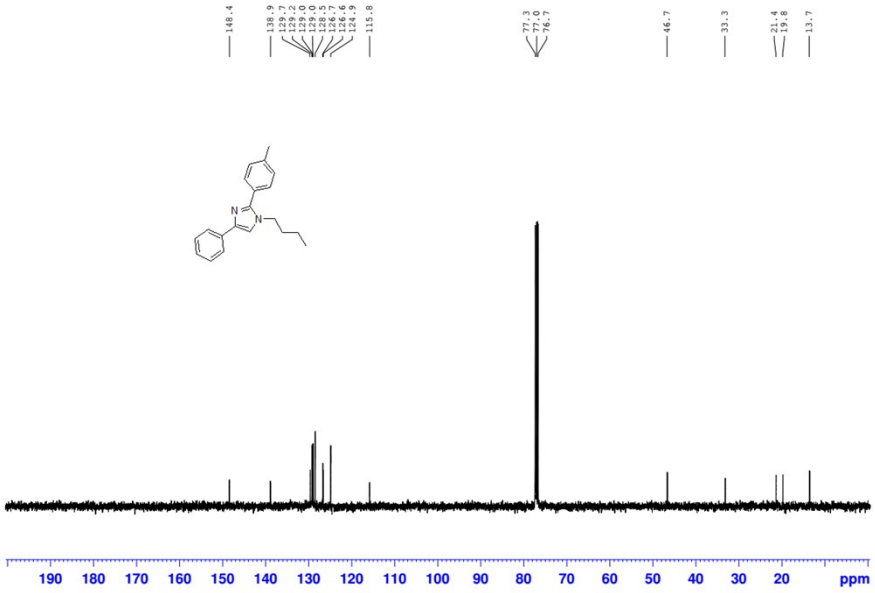
^{1}H NMR of **4ak**



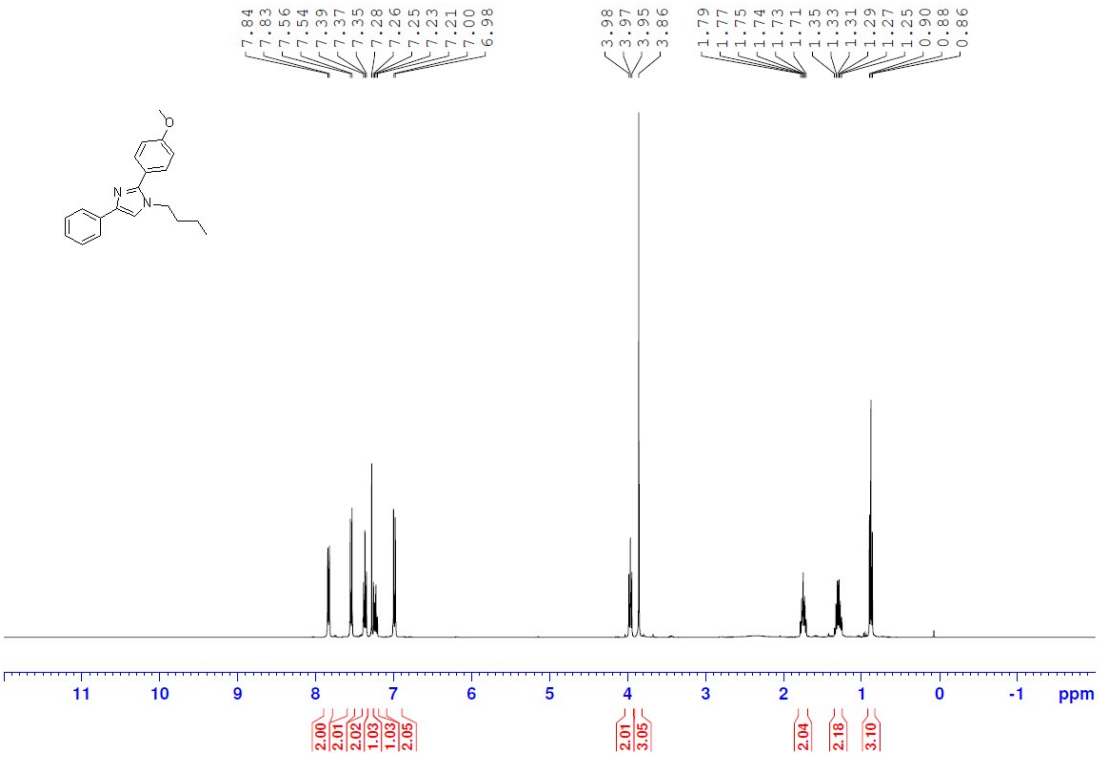
^{13}C NMR of **4ak**



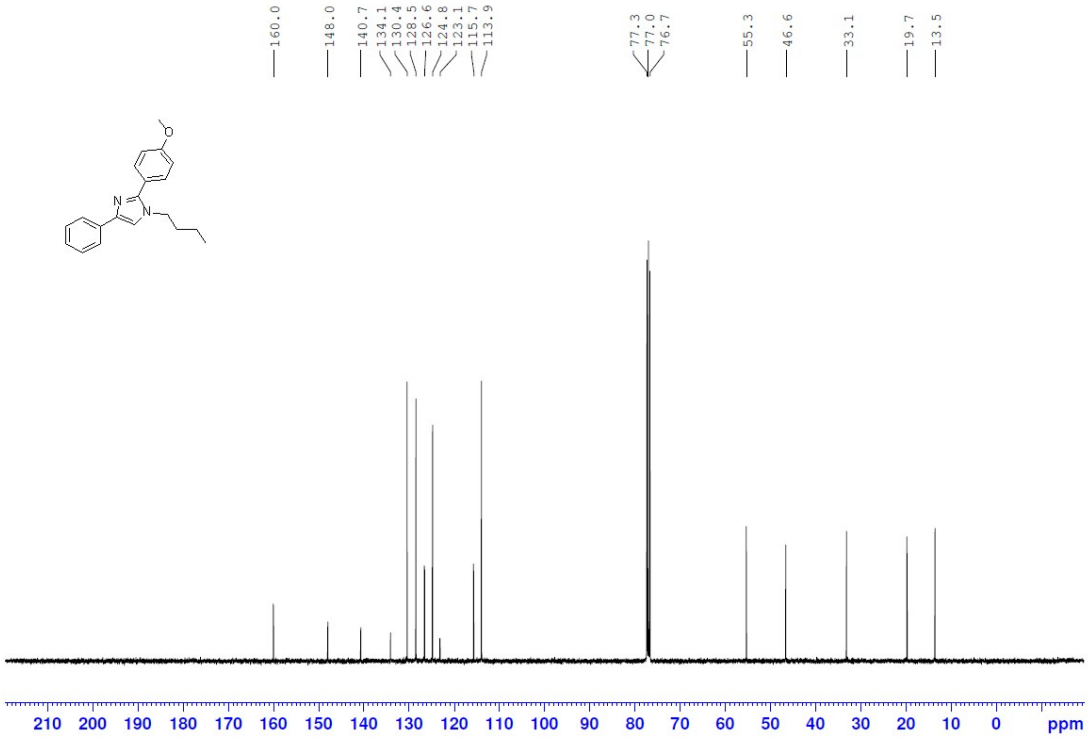
^{1}H NMR of **4ba**



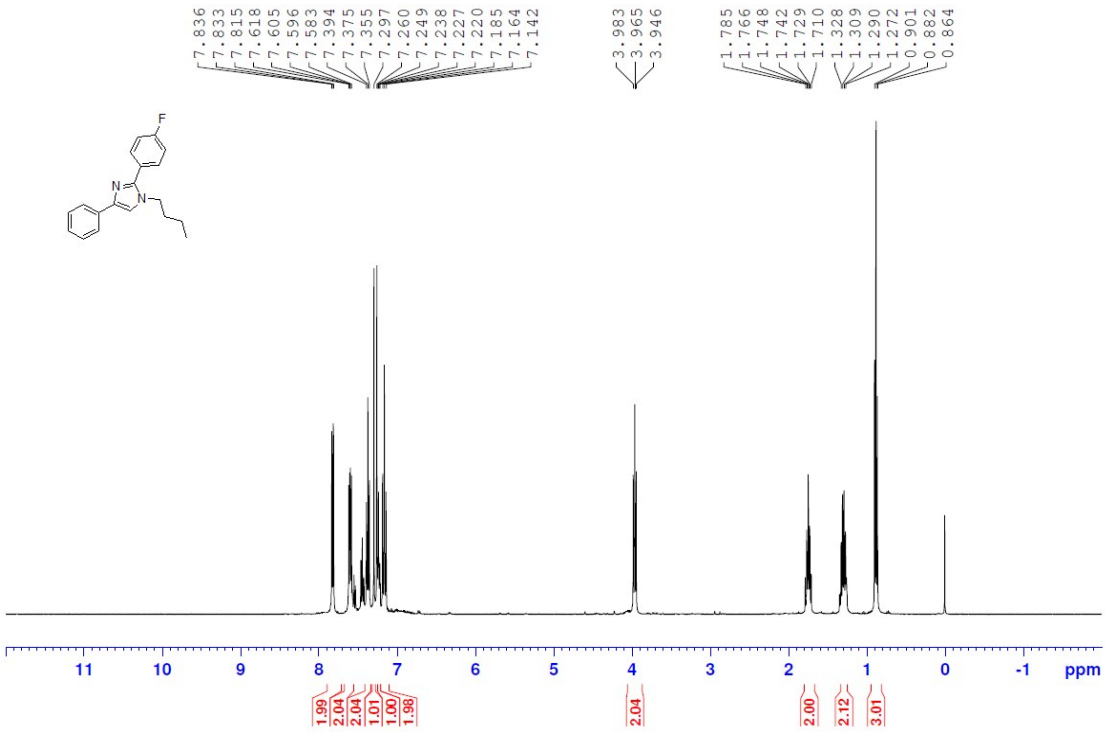
^{13}C NMR of **4ba**



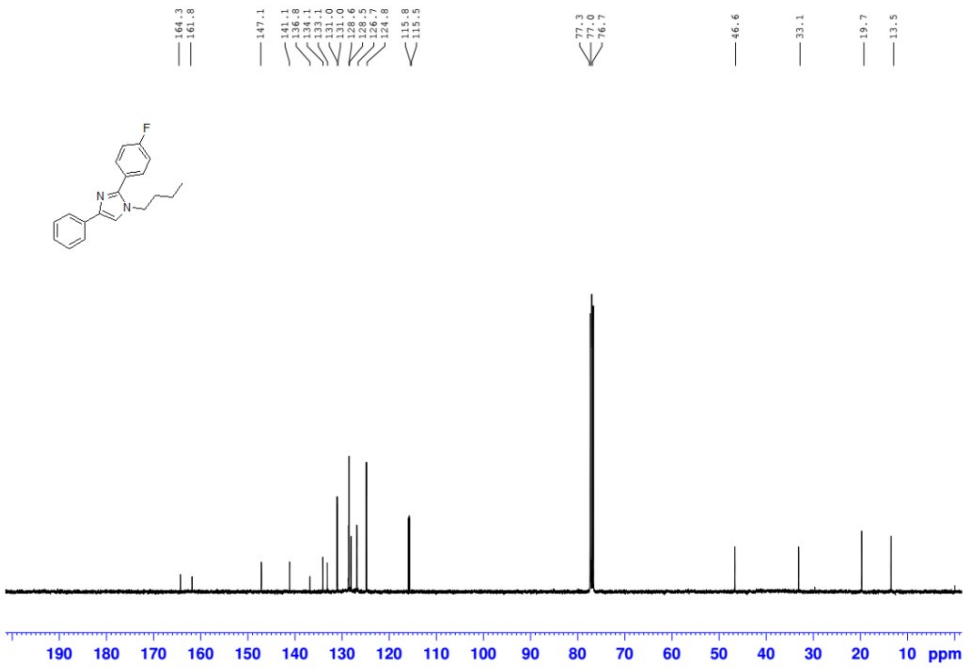
^{1}H NMR of **4ca**



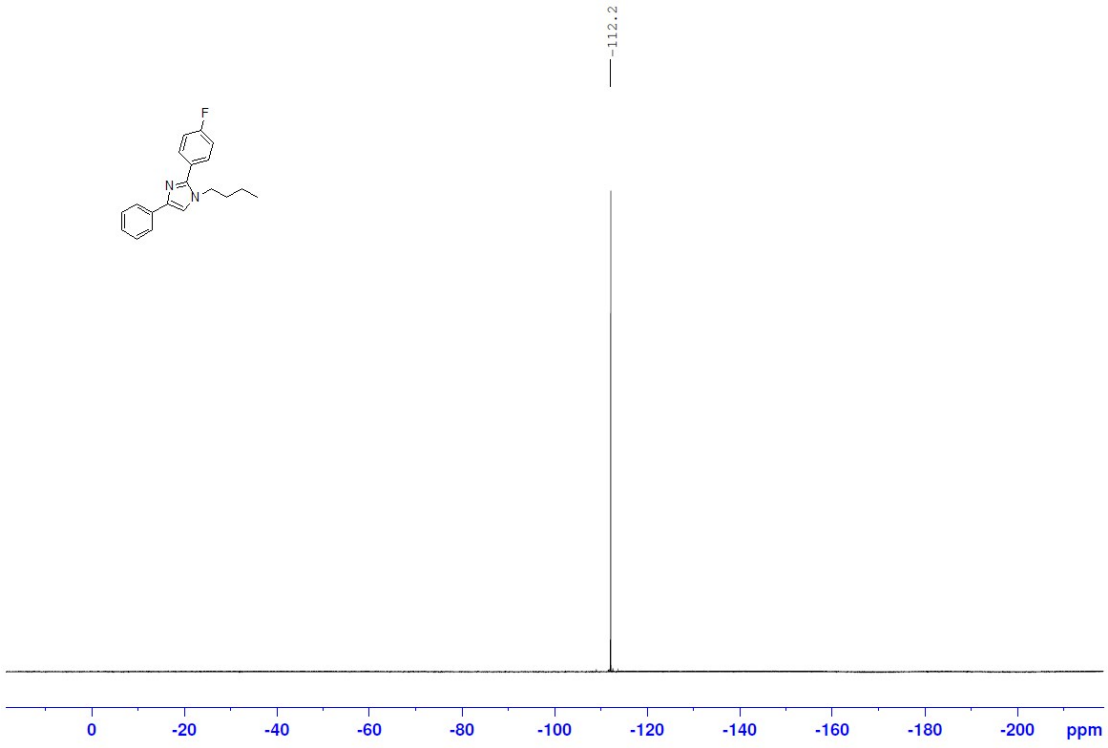
^{13}C NMR of **4ca**



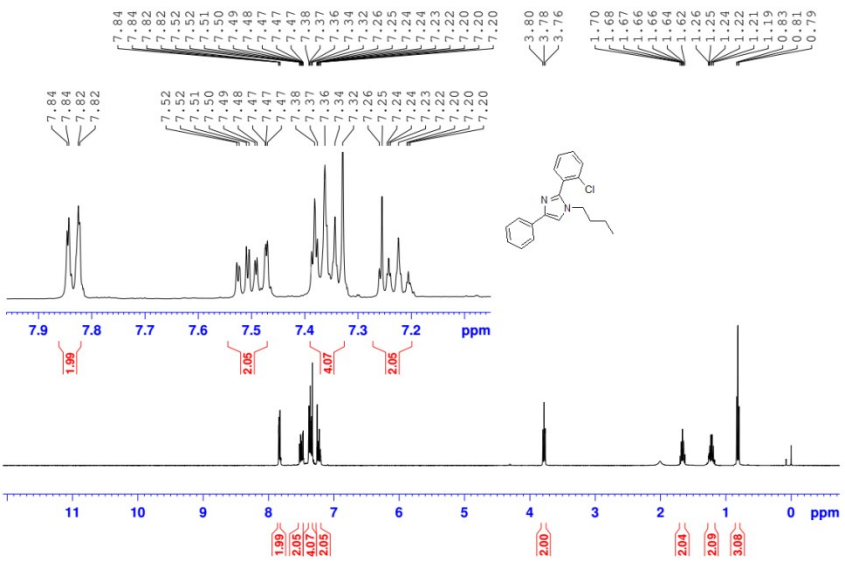
^{1}H NMR of **4da**



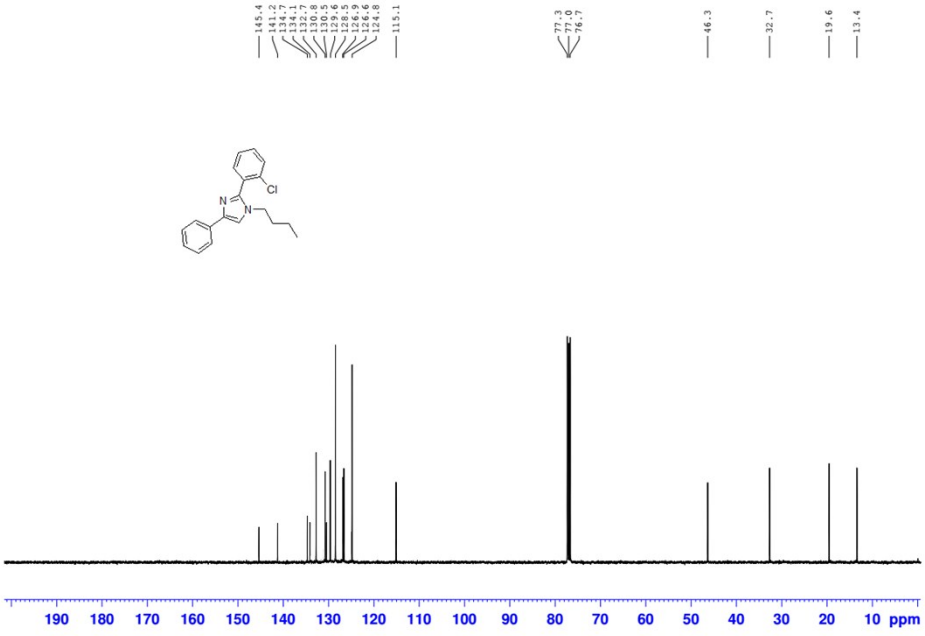
^{13}C NMR of **4da**



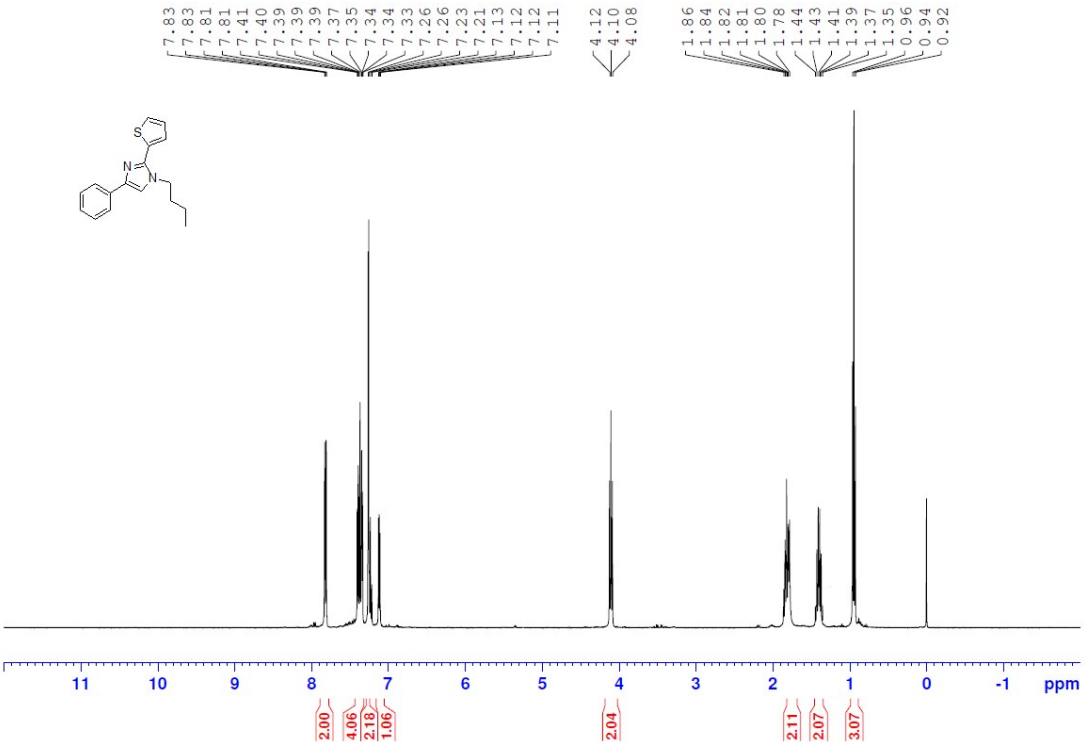
^{19}F NMR of **4da**



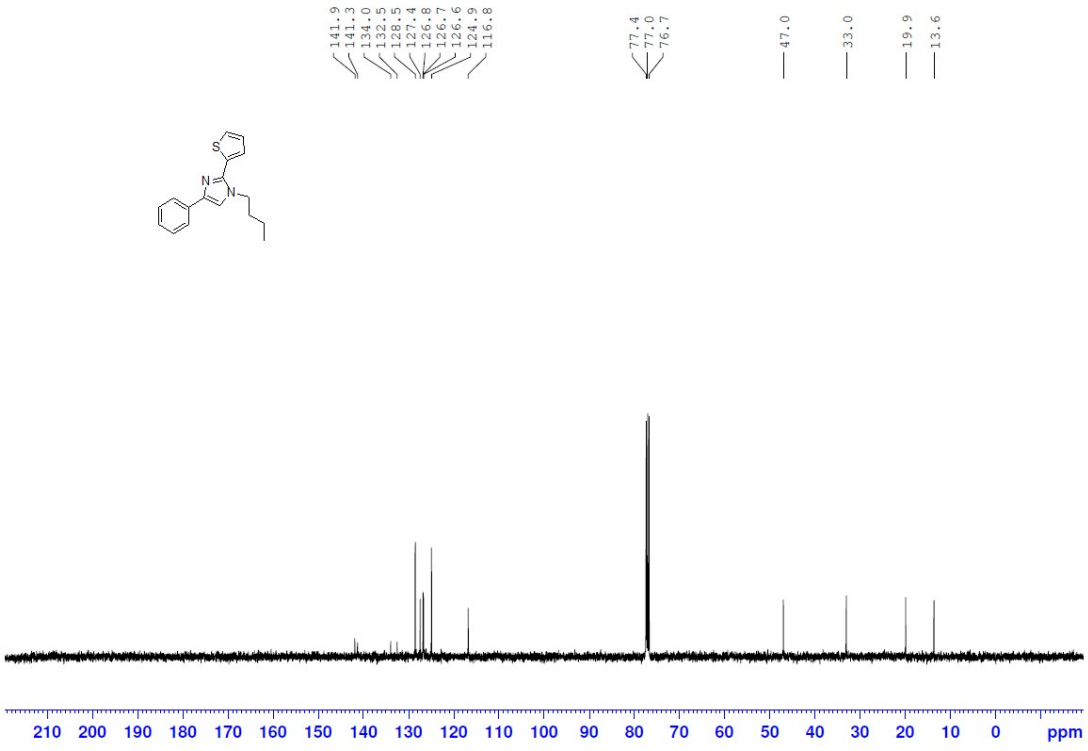
^{1}H NMR of **4ea**



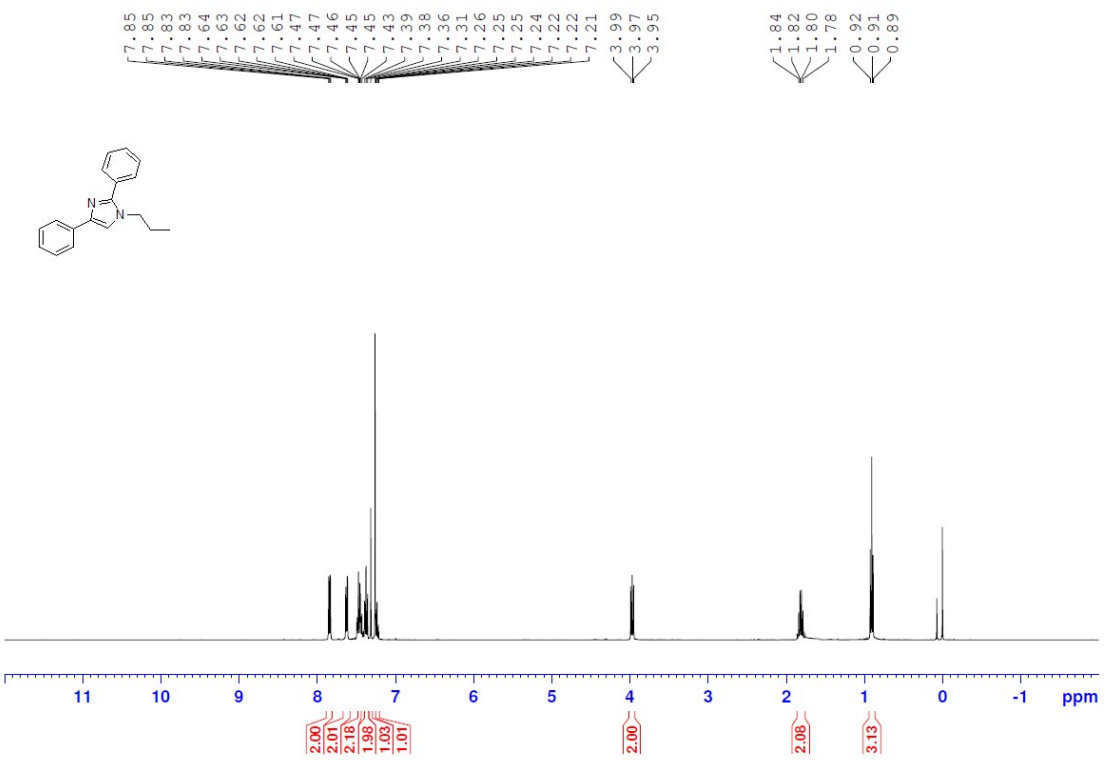
^{13}C NMR of **4ea**



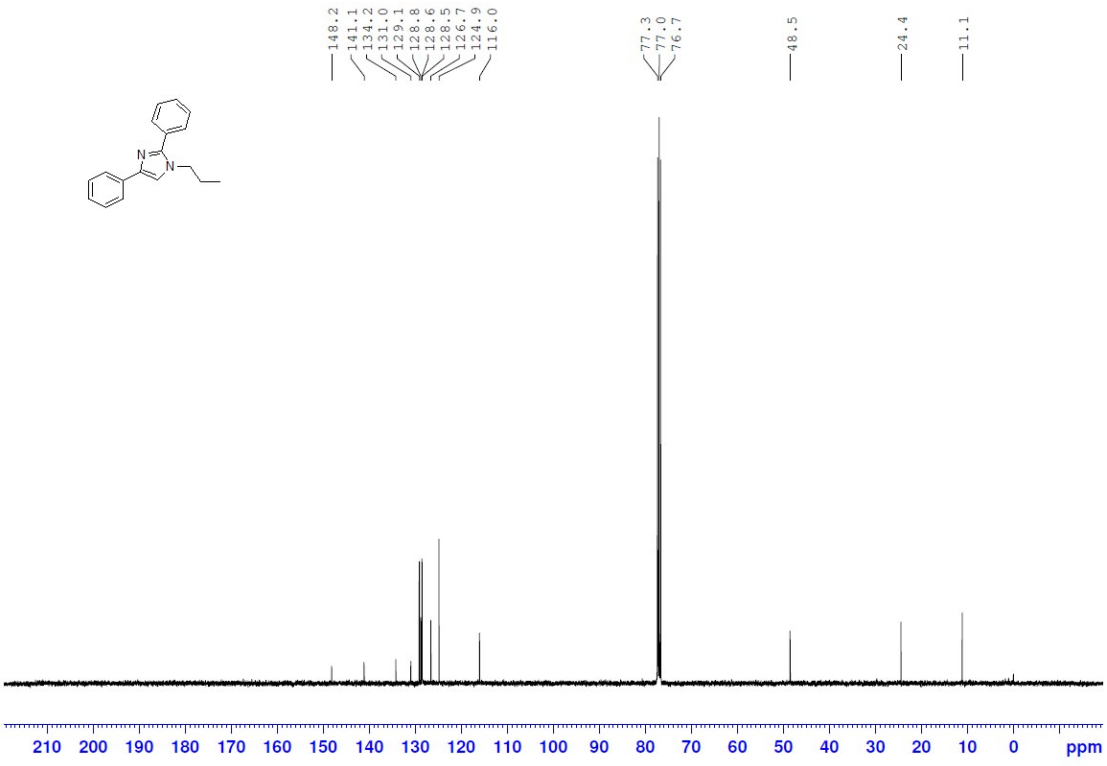
^{1}H NMR of **4fa**



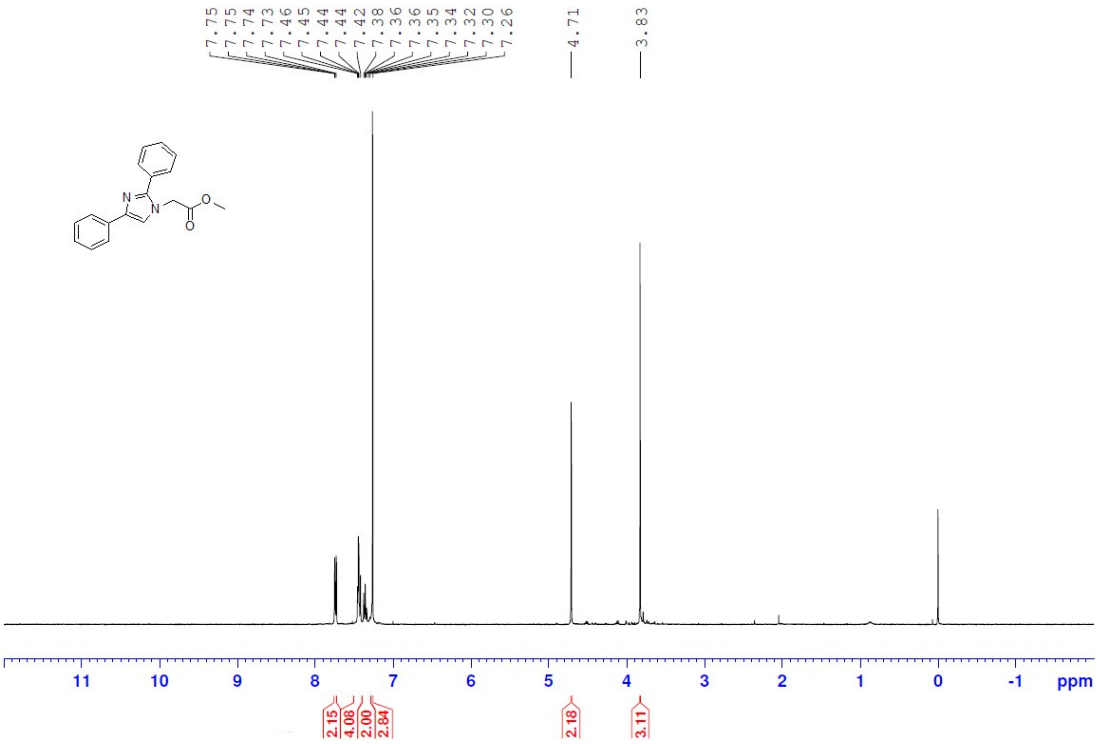
^{13}C NMR of **4fa**



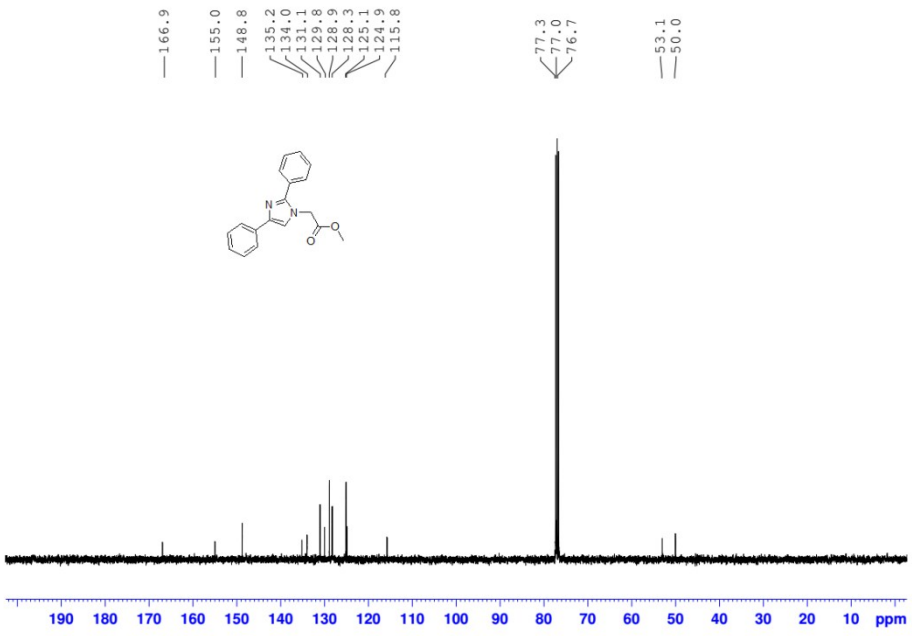
^{1}H NMR of **4ga**



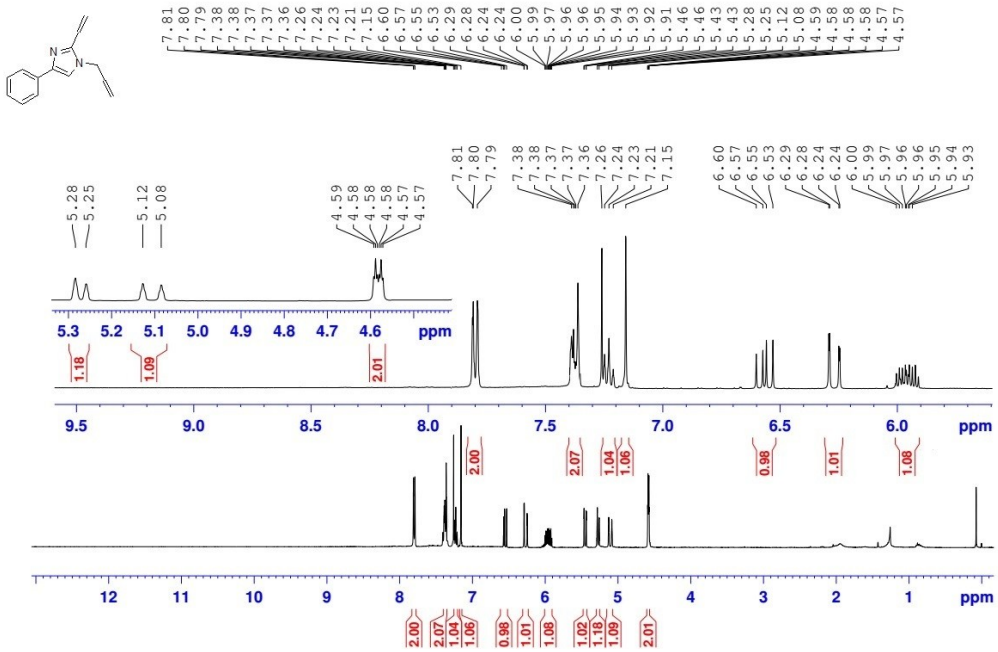
^{13}C NMR of **4ga**



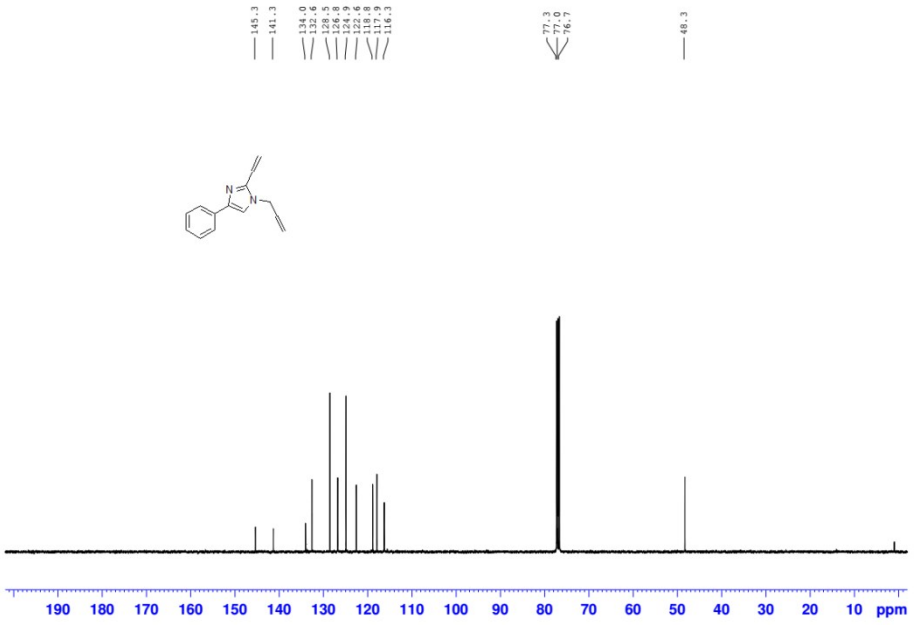
^{1}H NMR of **4ha**



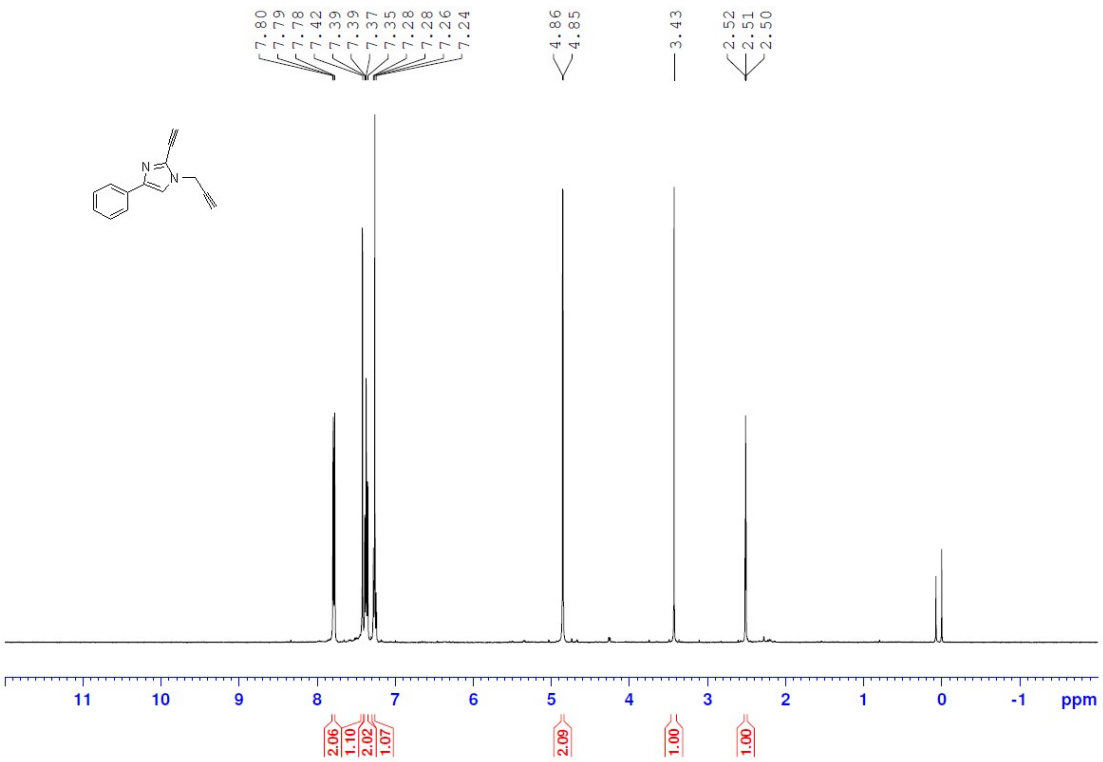
^{13}C NMR of **4ha**



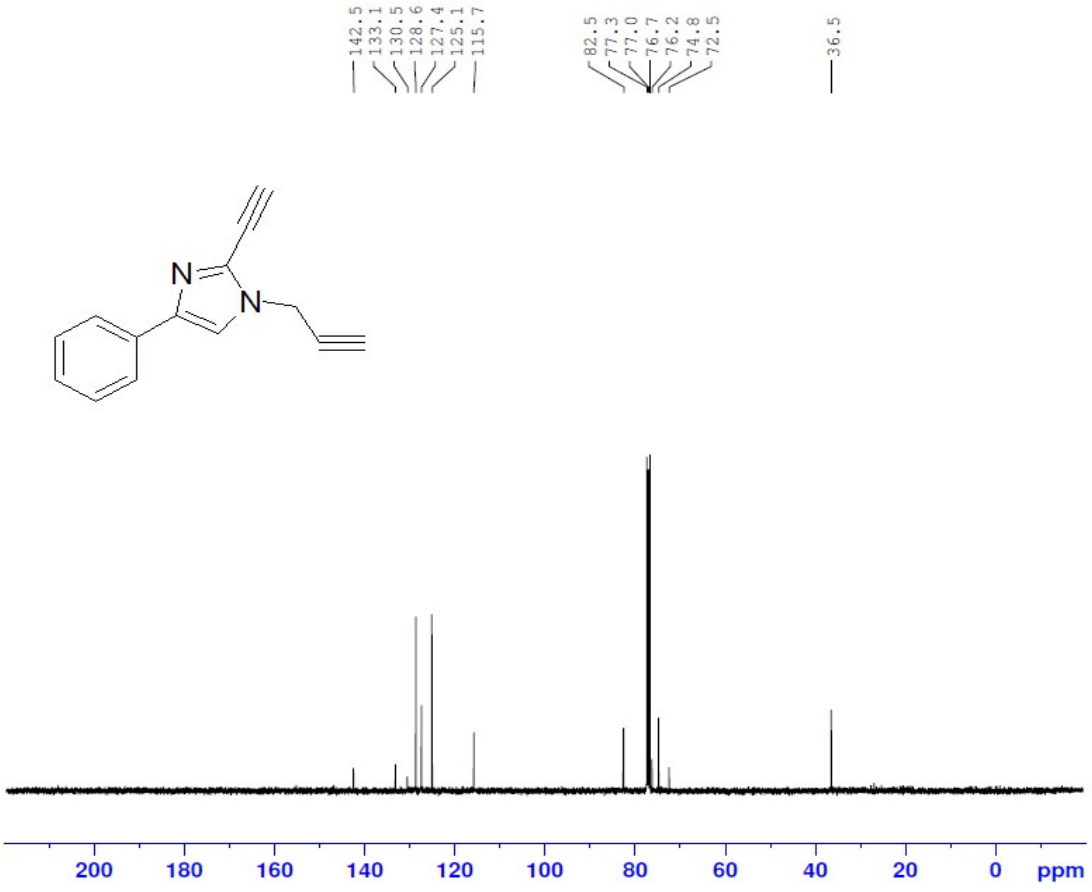
^{1}H NMR of **4ia**



^{13}C NMR of **4ia**



^{1}H NMR of **4ja**



^{13}C NMR of **4ja**