Supporting Information

DMSO Promoted Catalyst-free Oxidative C-N/C-O Couplings towards Synthesis of Imidazoles and Oxazoles

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General experimental methods

^{1}H NMR and ^{13}C NMR spectra were obtained on Bruker 400 MHz or 300 MHz instrument at 400 MHz and 100 MHz or 300 MHz and 75 MHz respectively. Chemical shifts are reported in parts per million (ppm) downfield from an internal TMS (tetramethylsilane) reference. Coupling constants (*J*) are reported in hertz (Hz), and spin multiplicities are represented by the symbols s (singlet), brs (broad singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). X-ray diffraction was done on a Bruker SMART diffractometer equipped with a graphite monochromator and Mo-Kα (λ = 0.71073 Å) radiation. The progress of the reaction was checked by TLC using 300-400 mesh silica gel. Column chromatography was performed using 60-120 mesh silica gel. All the available reagents were purchased from commercial sources and used without purification. The solvents used during reactions were distilled for purity.

Experimental and characterization data

General synthesis of 1,2,4,5 tetra substitutedimidazole **(3aa-3ap):**

In an oven dried R.B 1,2- diketone (1 mmol), the primary amine that contain -CH_2-NH_2 (2 mmol) were taken in 1 ml DMSO and stirred at 110 ^{O}C for 5 hours in an oil bath under open air. The reaction progress was monitored by TLC. Finally after the completion of the reaction the reaction mixture was cooled to 0 ^{O}C and diluted with EtOAc and washed with brine (20 ml). The combined organic extract were repeatedly washed with brine solution and dried over anhydrous sodium sulphate and concentrated under reduced pressure to give crude product which were purified by column chromatography[silica gel (100-200 mesh)] using Petroleum ether: ethyl acetate (19:1) as eluent to obtained desire product.

General synthesis of 1,2,4,5 tetra substitutedimidazole **(5a-5x):**

In an oven dried R.B 1,2- diketone (1 mmol), primary amine that contain -CH_2-NH_2 (1 mmol) and amine having aryl-NH_2 (1 mmol) were taken in 1 ml DMSO and stirred at 110 ^{O}C for 5 hours in an oil bath under open air. The reaction progress was monitored by TLC. Finally after the completion of the reaction the reaction mixture was cooled to 0 ^{O}C and diluted with EtOAc and washed with brine (20 ml). The combined organic extract were repeatedly washed with brine solution and dried over anhydrous sodium sulphate and concentrated under reduced pressure to give crude product which were purified by column chromatography[silica gel (100-200 mesh)] using Petroleum ether: ethyl acetate (19:1) as eluent to obtained desire product

General synthesis of 2,4,5 tri substituted oxazole **(6aa-6co):**

In an oven dried R.B 1,2- diketone (1 mmol), primary amine that contain -CH_2-NH_2 (1 mmol) were taken in 1 ml DMSO and stirred at 110 ^{O}C for 5 hours in an oil bath under open air. The reaction progress was monitored by TLC. Finally after the completion of the reaction the reaction mixture was cooled to 0 ^{O}C and diluted with EtOAc and washed with brine (20 ml).

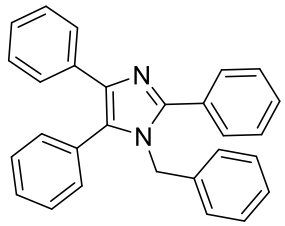
The combined organic extract were repeatedly washed with brine solution and dried over anhydrous sodium sulphate and concentrated under reduced pressure to give crude product which were purified by column chromatography [silica gel (100-200 mesh)] using Petroleum ether: ethyl acetate (97:3) as eluent to obtained desire product.

Procedure for synthesis of crossover product **(3ah, 3ac, 3X, 3Y):**

In an oven dried R.B Benzil (1 mmol), 4-methoxy benzylamine (1 mmol) and 4-Cyano benzylamine (1 mmol) were taken in 1 ml DMSO and stirred at 110 ^{O}C for 5 hours in an oil bath under open air. The reaction progress was monitored by TLC. Finally after the completion of the reaction the reaction mixture was cooled to 0 ^{O}C and diluted with EtOAc and washed with brine (20 ml). The combined organic extract were repeatedly washed with brine solution and dried over anhydrous sodium sulphate and concentrated under reduced pressure to give crude product which were purified by column chromatography[silica gel (100-200 mesh)] using Petroleum ether: ethyl acetate (19:1) as eluent to obtained desire product.

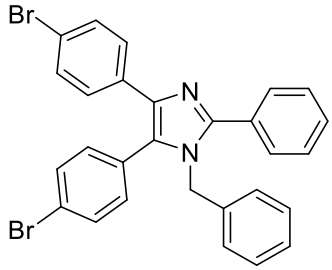
Characterization data:

1-benzyl-2,4,5-triphenyl-1H-imidazole (**3aa**)



Yield : 85 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.68-7.65 (m, 2H) , 7.60-7.57 (m, 2H) , 7.42-7.39 (m, 3H) , 7.35-7.28 (m, 3H) , 7.23-7.14 (m, 8H) , 6.81-6.78 (m, 2H) , 5.12 (s, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 148.1, 138.0, 137.5, 134.3, 131.2, 131.0, 130.8, 130.1, 129.1, 128.9, 128.8, 128.7, 128.7, 128.2, 127.5, 126.9, 126.5, 126.1, 48.5 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{23}N_2$ [M + H]+ : 387.1861 , found : 387.1865 .

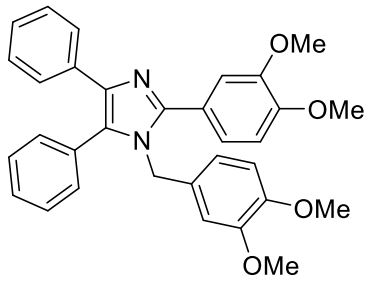
1-benzyl-4,5-bis(4-bromophenyl)-2-phenyl-1H-imidazole (**3ba**)



Yield : 80 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.67-7.64 (m, 2H) , 7.49-7.35 (m, 10H) , 7.26-7.23 (m , 2H) , 7.08-7.05 (m, 2H) , 6.83- 6.81 (m, 2H) , 5.11 (s, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 148.7, 137.5, 137.2, 133.1, 132.5, 132.2, 131.3, 130.5,

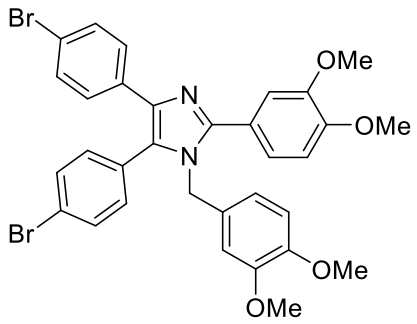
129.7, 129.2, 129.0, 128.8, 128.7, 128.4, 127.6, 125.9, 123.3, 120.5, 48.4 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{20}Br_2N_2$ [M + H]+ : 543.0071 , found : 543.0075 .

1-(3,4-dimethoxybenzyl)-2-(3,4-dimethoxyphenyl)-4,5-diphenyl-1H-imidazole (**3ab**)



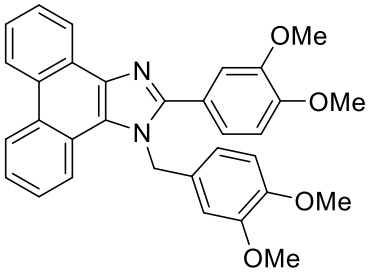
Yield : 70 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.62-7.37 (m , 5H) , 7.30-7.15 (m, 7H) , 6.87 (d, *J* = 9 Hz, 1H) , 6.73 (d, *J* = 3 Hz , 1H) , 6.39 (m, 1H) , 6.31 (s, 1H) , 5.05 (s, 2H) , 3.89 (s, 3H) , 3.83 (s, 3H) , 3.74 (m, 3H) , 3.70 (m, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 149.7, 149.0, 148.9, 148.3, 148.0, 134.4, 131.1, 130.2, 129.9, 128.9, 128.7, 128.4, 128.1, 128.0, 127.2, 126.9, 126.5, 123.4, 121.6, 118.5, 112.4, 111.2, 111.0, 109.4, 47.9 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{30}N_2O_4$ [M + H]+ : 507.2284 , found : 507.2274 .

4,5-bis(4-bromophenyl)-1-(3,4-dimethoxybenzyl)-2-(3,4-dimethoxyphenyl)-1H-imidazole (**3bb**)



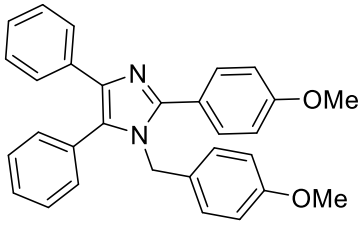
Yield : 72 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.51 (d, *J* = 9 Hz, 2H) , 7.42-7.43 (d, *J* = 9 Hz, 2H) , 7.36 (d, *J* = 6 Hz, 2H) , 7.22-7.19 (m, 2H), 7.11 (d, *J* = 6 Hz , 2H) , 6.92 (d, *J* = 9 Hz, 1H), 6.76 (d, *J* = 9 Hz, 1H) , 6.41 (d, *J* = 9 Hz, 1H) , 6.32 (d, *J* = 3 Hz, 1H) , 5.04 (s, 2H) , 3.92 (s, 3H) , 3.86 (s, 3H) , 3.80 (s, 3H) , 3.73 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 150.4, 149.7, 149.5, 149.0, 148.9, 133.6, 133.0, 132.8, 131.8, 130.3, 129.3, 128.9, 123.8, 123.6, 122.1, 118.9, 112.8, 111.8, 111.6, 109.7, 56.5, 56.4, 48.6 ppm ; HRMS-ESI (m/z): calcd for $C_{32}H_{29}Br_2N_2O_4$ [M + H]+ : 663.0494 , found : 663.0492 .

1-(3,4-dimethoxybenzyl)-2-(3,4-dimethoxyphenyl)-1H-phenanthro[9,10-d]imidazole (**3cb**)



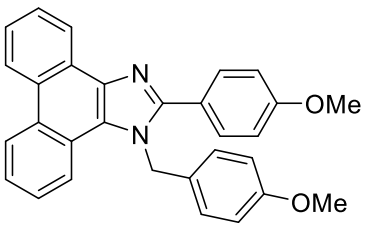
Yield : 69 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.84 (d, *J* = 8 Hz, 1H) , 8.80 (d, *J* = 8 Hz, 1H) , 8.71 (d, *J* = 8 Hz, 1H) , 8.01 (d, *J* = 8 Hz, 1H) , 7.72 (t, *J* = 8 Hz, 1H) , 7.65 (d, *J* = 8 Hz, 1H) , 7.57-7.49 (m, 1H) , 7.45 (d, *J* = 8 Hz, 1H) , 7.42-7.25 (m, 2H) , 6.95 (d, *J* = 8 Hz, 1H) , 6.84 (d, *J* = 8 Hz, 2H) , 6.72-6.75 (m, 1H) , 5.78 (s, 2H) , 3.92 (s, 3H) , 3.84 (s, 3H) , 3.78 (s, 3H) , 3.69 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 152.6, 149.8, 149.3, 148.4, 148.1, 129.1, 128.5, 127.7, 126.8, 126.7, 126.7, 126.5, 125.2, 124.5, 123.7, 122.7, 122.4, 122.2, 121.8, 120.7, 117.5, 112.0, 111.4, 110.8, 108.3, 55.6, 55.5, 55.2, 50.2 ppm ; HRMS-ESI (m/z): calcd for $C_{32}H_{28}N_2O_4$ [M + H]+ : 505.2127 , found : 505.2122 .

1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole (**3ac**)



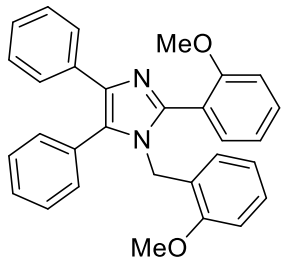
Yield : 78 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.60-7.54 (m, 4H) , 7.35-7.32 (m, 3H) , 7.23-7.13 (m, 5H) , 6.94 (d, *J* = 1.8 Hz , 2H) , 6.91-6.71 (m , 4H) , 5.02 (s , 2H) , 3.83 (s, 3H) , 3.75 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 160.6, 159.3, 148.5, 131.8, 131.6, 131.0, 130.2, 129.3, 129.1, 128.6, 127.8, 127.3, 114.6, 114.5, 55.9, 55.8, 48.2 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{21}N_2Cl_2$ [M + H]+ : 447.2073 , found : 447.2071 .

1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-1H-phenanthro[9,10-d]imidazole (**3cc**)



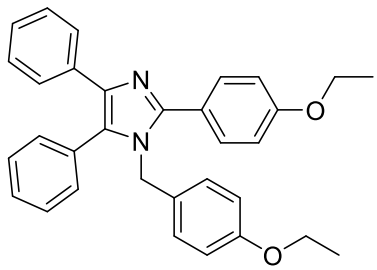
Yield : 76 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.88 (d, *J* = 6 Hz, 1H) , 8.81 (d, *J* = 9 Hz, 1H) , 8.72 (d, *J* = 9 Hz, 1H) , 8.00 (d, *J* = 9 Hz, 1H) , 7.77-7.40 (m, 6H) , 7.14 (d, *J* = 9 Hz, 2H) , 6.98 (d, *J* = 6 Hz, 2H) , 6.91 (d, *J* = 9 Hz, 2H) , 5.76 (s, 2H) , 3.86 (s, 3H) , 3.80 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 160.7, 159.1, 153.0, 137.7, 131.0, 129.1, 129.0, 128.2, 127.3, 127.0, 126.9, 126.7, 125.5, 124.7, 124.2, 123.1, 123.0, 122.7, 121.1, 114.7, 114.2, 55.4, 55.3, 50.3 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{24}N_2O_2$ [M + H]+ : 445.1916 , found : 445.1916 .

1-(2-methoxybenzyl)-2-(2-methoxyphenyl)-4,5-diphenyl-1H-imidazole (**3ad**)



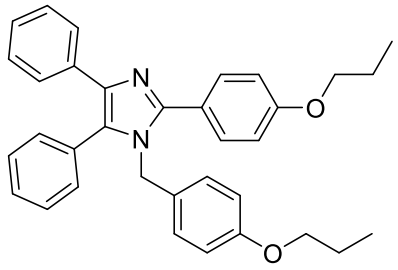
Yield : 73 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 7.62 (d, *J* = 8 Hz, 2H) , 7.51 (d, *J* = 4 Hz, 1H) , 7.38-7.27 (m, 6H) , 7.22 (t, *J* = 8 Hz, 2H) , 7.16-7.08 (m, 2H) , 6.99 (t, *J* = 8 Hz, 1H) , 6.78-6.75 (m, 1H) , 6.65-6.60 (m, 2H) , 4.98 (s, 2H) , 3.79 (s, 3H) , 3.55 (s, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 157.6, 155.9, 145.9, 137.6, 134.7, 132.7, 131.4, 131.0, 130.8, 129.7, 128.6, 128.3, 128.0, 127.5, 126.9, 126.1, 125.9, 120.8, 120.4, 120.2, 110.8, 109.7, 55.4, 55.1, 43.1 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{26}N_2O_2$ [M + H]+ : 447.2073 , found : 447.2065 .

1-(4-ethoxybenzyl)-2-(4-ethoxyphenyl)-4,5-diphenyl-1H-imidazole (**3ae**)



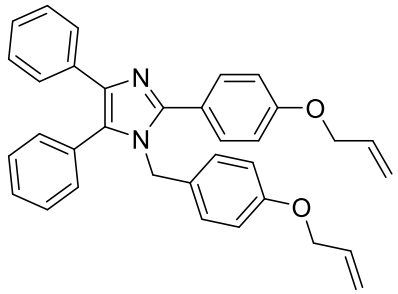
Yield : 74 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.59-7.56 (m, 4H) , 7.37-7.34 (m, 4H) , 7.25-7.19 (m, 5H), 6.94 (s, 2H) , 6.72 (d, J = 3 Hz , 3H) , 5.03 (s, 2H) , 4.12-4.06 (m, 2H) , 4.04-3.95 (m , 2H) , 1.47-1.38 (m, 6H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 159.5, 158.1, 148.0, 137.7, 134.6, 131.3, 131.1, 130.5, 129.7, 129.6, 128.8, 128.5, 128.1, 127.8, 127.3, 126.8, 126.3, 123.3, 114.8, 114.5, 63.5, 63.4, 47.7, 14.8 ppm ; HRMS-ESI (m/z): calcd for $C_{32}H_{30}N_2O_2$ [M + H]+ : 475.2386 , found : 475.2384 .

4,5-diphenyl-1-(4-propoxybenzyl)-2-(4-propoxyphenyl)-1H-imidazole (**3af**)



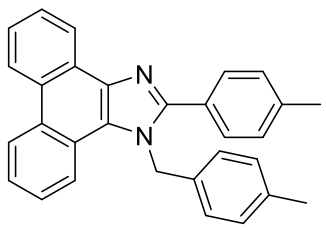
Yield : 72 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.61-7.57 (m, 4H) , 7.37-7.32 (m, 3H) , 7.26-7.15 (m, 5H) , 6.94 (d, *J* = 9 Hz, 2H) , 6.77-6.71 (m , 4H), 5.04 (s, 2H) , 3.96 (t, *J* = 6 Hz, 2H) , 3.88 (t, *J* = 6 Hz, 2H) , 1.87-1.77 (m, 4H) , 1.09-1.02 (m, 6H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 159.7, 158.3, 148.0, 137.8, 134.7, 131.3, 131.1, 130.4, 129.7, 129.5, 128.8, 128.5, 128.1, 127.2, 126.8, 126.2, 123.3, 114.6, 114.5, 69.6, 69.5, 47.7, 22.6, 22.5, 10.5 ppm ; HRMS-ESI (m/z): calcd for $C_{34}H_{34}N_2O_2$ [M + H]+ : 503.2699 , found : 503.2695 .

1-(4-(allyloxy)benzyl)-2-(4-(allyloxy)phenyl)-4,5-diphenyl-1H-imidazole (**3ag**)



Yield : 73 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.61-7.56 (m, 4H) , 7.37-7.34 (m, 3H) , 7.25-7.15 (m, 5H) , 6.97 (d, *J* = 9 Hz, 2H) , 6.78-6.69 (m, 4H) , 6.09-6.03 (m, 2H) , 5.47-5.28 (m, 4H) , 5.04 (s, 2H) , 4.58 (d, *J* = 6 Hz, 2H) , 4.49 (d, *J* = 6 Hz, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 159.1, 157.8, 147.9, 137.8, 134.6, 133.1, 133.0, 131.2, 131.1, 130.5, 129.9, 129.7, 128.8, 128.5, 128.1, 127.3, 126.8, 126.3, 123.7, 117.9, 117.8, 114.8, 68.8, 47.7 ppm ; HRMS-ESI (m/z): calcd for $C_{34}H_{30}N_2O_2$ [M + H]+ : 499.2386 , found : 499.2381 .

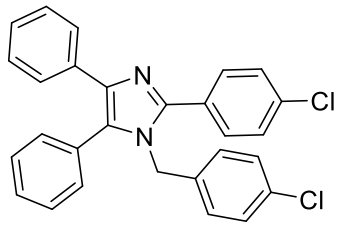
1-(4-methylbenzyl)-2-(p-tolyl)-1H-phenanthro[9,10-d]imidazole (**3ch**)



Yield : 81 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.87 (d, *J* = 7.8 Hz, 1H) , 8.79 (d, *J* = 8.4Hz, 1H) , 8.70 (d, *J* = 8.1 Hz, 1H) , 7.98 (d, *J* = 8.1 Hz, 1H) , 7.73 (t, *J* = 7.5 Hz, 1H) , 7.64-7.53 (m, 4H) , 7.40 (t, *J* = 8.1 Hz, 1H) , 7.25 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.09 (d, *J* = 8.1 Hz, 2H) , 5.78 (s, 2H) , 2.40 (s, 3H), 2.34 (s, 3H) ; ^{13}C NMR (

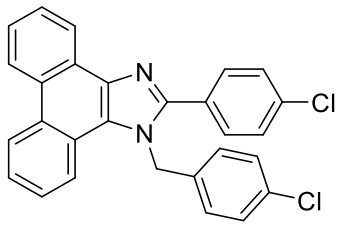
75 MHz, $CDCl_3$) = 153.8, 140.3, 138.3, 138.0, 134.6, 130.6, 130.0, 129.7, 128.8, 127.9, 127.8, 127.6, 127.2, 126.1, 125.2, 124.7, 123.6, 123.2, 121.7, 51.1, 22.0, 21.7 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{24}N_2$ [M + H]+ : 413.2018 , found : 413.2015 .

1-(4-chlorobenzyl)-2-(4-chlorophenyl)-4,5-diphenyl-1H-imidazole (**3ai**)



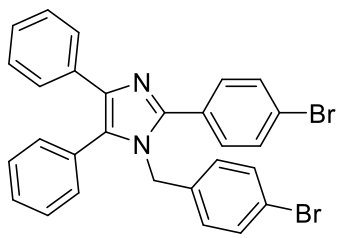
Yield : 84 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.58-7.53 (m, 4H) , 7.39-7.31 (m, 5H) , 7.23-7.15 (m, 7H), 6.72 (d, *J* = 8.4 Hz, 2H) , 5.05 (s, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 147.0, 138.6, 135.9, 135.3, 134.2, 133.6, 131.1, 130.8, 130.3, 129.3, 129.1, 129.0, 128.3, 127.4, 126.9, 126.8, 47.8 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{21}Cl_2N_2$ [M + H]+ : 455.1082 , found : 455.1082 .

1-(4-chlorobenzyl)-2-(4-chlorophenyl)-1H-phenanthro[9,10-d]imidazole (**3ci**)



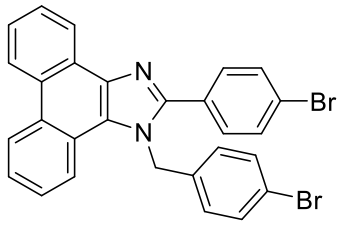
Yield : 82 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 9.00 (s, 1H) , 8.82 (d, *J* = 8 Hz, 1H) , 8.71 (d, *J* = 8 Hz, 1H) , 8.33 (d, *J* = 8 Hz, 1H) , 7.91 (d, *J* = 8 Hz, 1H) , 7.77 (t, *J* = 8 Hz, 1H) , 7.73-7.54 (m, 4H) , 7.47 (d, *J* = 8 Hz, 2H) , 7.38 (d, *J* = 8 Hz, 2H) , 7.15 (d, *J* = 8 Hz, 2H) , 5.83 (s, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 145.6, 132.7, 131.4, 129.8, 129.1, 127.7, 127.5, 127.1, 126.6, 125.9, 123.9, 123.6, 123.0, 121.1, 118.4, 114.0, 52.1 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{19}Cl_2N_2$ [M + H]+ : 453.0925 , found : 453.0929 .

1-(4-bromobenzyl)-2-(4-bromophenyl)-4,5-diphenyl-1H-imidazole (**3aj**)



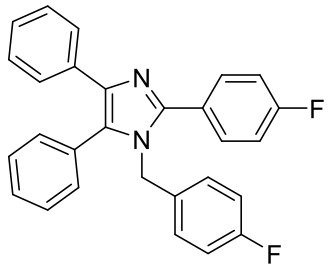
Yield : 81 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 7.67-7.65 (m, 1H) , 7.58-7.53 (m, 4H) , 7.42-7.34 (m, 6H) , 7.26-7.21 (m, 5H) , 6.83-6.80 (m, 1H) , 6.69 (d, *J* = 9 Hz, 1H) , 5.05 (s, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 146.9, 136.3, 131.9, 131.9, 131.1, 131.0, 130.4, 129.1, 129.0, 128.8, 128.6, 128.2, 128.1, 127.6, 126.8, 126.0, 123.5, 121.5, 47.8 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{20}Br_2N_2$ [M + H]+ : 543.0071 , found : 543.0079 .

1-(4-bromobenzyl)-2-(4-bromophenyl)-1H-phenanthro[9,10-d]imidazole (**3cj**)



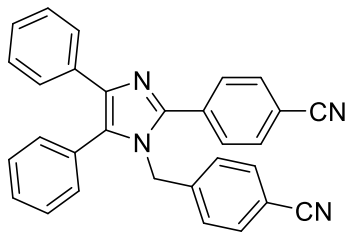
Yield : 80 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.55-8.44 (m, 3H) , 8.13 (s, 1H) , 7.65 (d, *J* = 8 Hz, 1H) , 7.47-7.39 (m, 4H) , 7.34 (d, *J* = 8 Hz, 2H) , 7.29-7.19 (m, 3H) , 6.83 (d, *J* = 8 Hz, 2H) , 5.55 (s, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 148.1, 129.1, 128.5, 127.7, 126.7, 126.5, 125.2, 124.5, 123.7, 122.7, 122.4, 121.8, 50.2 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{19}Br_2N_2$ [M + H]+ : 540.9915 , found : 540.9920 .

1-(4-fluorobenzyl)-2-(4-fluorophenyl)-4,5-diphenyl-1H-imidazole (**3ak**)



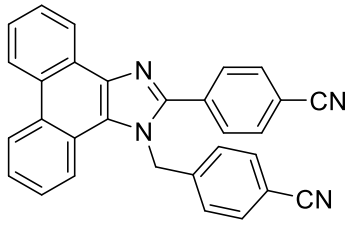
Yield : 88 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.64-7.53 (m, 4H) , 7.36-7.34 (m, 3H) , 7.23-7.07 (m, 7H) , 6.91-6.85 (m, 2H) , 6.74- 6.70 (m, 2H) , 5.04 (s, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 164.9, 163.7, 161.6, 160.4, 147.1, 138.2, 134.1, 133.0, 132.9, 131.1, 131.0, 131.0, 130.8, 130.0, 129.0, 128.8, 128.3, 128.2, 127.8, 127.7, 127.0, 127.0, 126.8, 126.6, 115.9, 115.8, 115.6, 115.5, 47.7 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{20}F_2N_2$ [M + H]+ : 423.1673 , found : 423.1671 .

4-(1-(4-cyanobenzyl)-4,5-diphenyl-1H-imidazol-2-yl)benzonitrile (**3al**)



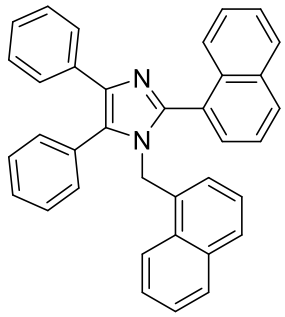
Yield : 92 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 7.77 (d, *J* = 8 Hz, 2H) , 7.69 (d, *J* = 8Hz, 2H) , 7.55-7.51 (m, 4H) , 7.41-7.34 (m, 3H) , 7.24-7.18 (m, 5H) , 6.90 (d, *J* = 8 Hz , 2H) , 5.19 (s, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 145.8, 142.0, 139.2, 134.6, 133.4, 132.7, 132.6, 131.1, 130.8, 129.9, 129.4, 129.3, 129.2, 128.3, 127.1, 126.8, 126.6, 118.3, 118.2, 112.7, 111.9, 48.3 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{21}N_4$ [M + H]+ : 437.1766 , found : 437.1759 .

4-(1-(4-cyanobenzyl)-1H-phenanthro[9,10-d]imidazol-2-yl)benzonitrile (**3cl**)



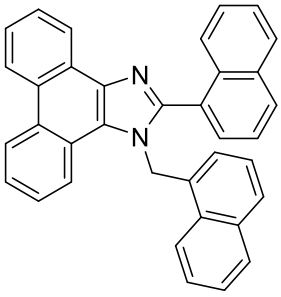
Yield : 88 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 9.0 (s, 1H) , 8.82 (d, *J* = 8 Hz, 1H) , 8.71 (d, *J* = Hz, 1H) , 8.33 (d, *J* = 8 Hz, 1H) , 7.91 (d, *J* = 8 Hz, 1H) , 7.77 (t, *J* = 8 Hz, 1H) , 7.73-7.54 (m, 4H) , 7.47 (d, *J* = 8 Hz, 2H) , 7.38 (d, *J* = 8 Hz, 2H) , 7.15 (d, *J* = 8 Hz, 2H) , 5.83 (s, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 145.6, 132.7, 131.4, 129.8, 129.1, 127.7, 127.5, 127.5, 127.1, 126.6, 125.9, 123.9, 123.6, 123.0, 121.1, 120.8, 118.4, 114.0, 52.1 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{19}N_4$ [M + H]+ : 435.1610 , found : 435.1618

2-(naphthalen-1-yl)-1-(naphthalen-1-ylmethyl)-4,5-diphenyl-1H-imidazole (**3am**)



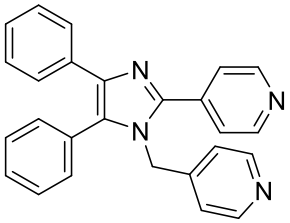
Yield : 81 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.04 (d, *J* = 9 Hz, 1H) , 7.87-7.81 (m, 2H) , 7.76 (d, *J* = 6 Hz, 1H) , 7.72-7.64 (m, 3H) , 7.58-7.51 (m, 3H) , 7.44-7.20 (m, 13H) , 6.85 (d, *J* = 6 Hz, 1H) , 5.38 (s, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 146.9, 138.2, 134.6, 133.7, 133.2, 133.0, 132.7, 131.0, 130.9, 129.8, 129.7, 128.9, 128.7, 128.3, 128.2, 127.9, 126.9, 126.5, 126.2, 126.1, 125.7, 125.6, 125.2, 125.0, 123.8, 122.0, 46.1 ppm ; HRMS-ESI (m/z): calcd for $C_{36}H_{26}N_2$ [M + H]+ : 487.2174 , found : 487.2170 .

2-(naphthalen-1-yl)-1-(naphthalen-1-ylmethyl)-1H-phenanthro[9,10-d]imidazole (**3cm**)



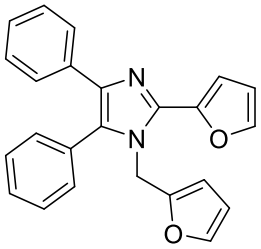
Yield : 79 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.97 (s, 1H) , 8.85 (d, *J* = 8 Hz, 1H) , 8.78 (d, *J* = 8Hz, 1H) , 7.96-7.92 (m, 4H) , 7.84-7.72 (m, 6H) , 7.64 (d, *J* = 8 Hz, 1H) , 7.61-7.39 (m, 5 H), 7.27-7.25 (m, 1H) , 6.98 (s, 1H) , 6.12 (s, 2H) , ^{13}C NMR (100 MHz, $CDCl_3$) = 149.7, 133.7, 129.6, 129.2, 128.4, 127.5, 126.8, 126.2, 125.8, 125.0, 124.2, 123.2, 121.8, 121.0, 48.6 ppm ; HRMS-ESI (m/z): calcd for $C_{36}H_{25}N_2$ [M + H]+ : 485.2018 , found : 485.2011 .

4-(4,5-diphenyl-1-(pyridin-4-ylmethyl)-1H-imidazol-2-yl)pyridine (**3an**)



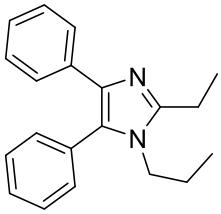
Yield : 75 % ; White solid ; ^{1}H NMR (300 MHz, DMSO(d_6)): δ (ppm) = 8.67 (d, *J* = 6 Hz , 2H) , 8.01 (d, *J* = 6 Hz , 2H) , 7.57-7.40 (m, 10H) , 7.35-7.25 (m, 4H) , 5.76 (s, 2H) ; ^{13}C NMR (75 MHz, DMSO(d_6)) = 150.7, 138.5, 137.4, 135.1, 131.1, 130.1, 129.2, 129.1, 128.7, 128.7, 127.6, 127.3, 119.5, 45.8 ppm ; HRMS-ESI (m/z): calcd for $C_{26}H_{21}N_4$ [M + H]+ : 389.1766 , found : 389.1761 .

2-(furan-2-yl)-1-(furan-2-ylmethyl)-4,5-diphenyl-1H-imidazole (**3ao**)



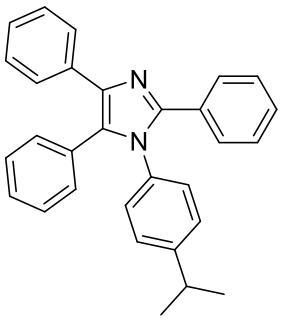
Yield : 78 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.55-7.16 (m, 12H) , 6.97 (s, 1H) , 6.53 (d, *J* = 1.5 Hz, 1H) , 6.21 (d, *J* = 1.2 Hz, 1H) , 5.84 (d, *J* = 2.7 Hz, 1H) , 5.22 (s, 2H) ; ^{13}C NMR (75 MHz, DMSO(d_6)) = 149.8, 143.0, 142.3, 138.8, 133.6, 131.3, 130.1, 129.1, 129.0, 128.1, 127.0, 126.7, 111.7, 110.9, 110.5, 108.0, 42.1 ppm ; HRMS-ESI (m/z): calcd for $C_{24}H_{18}N_2O_2$ [M + H]+ : 367.1447 , found : 367.1445 .

2-ethyl-4,5-diphenyl-1-propyl-1H-imidazole (**3ap**)



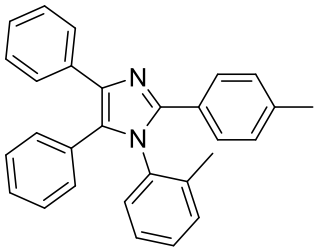
Yield : 60 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.44-7.41 (m, 5H) , 7.34-7.30 (m, 2H) ,7.19-7.09 (m, 3H) , 3.68 (t, *J* = 7.8 Hz, 2H) , 2.80 (q, *J* = 7.8 Hz, 2H) , 1.55-1.41 (m, 5H) , 0.76 (t, *J* = 7.2 Hz, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 149.5, 136.9, 135.4, 132.3, 131.6, 129.5, 128.9, 128.7, 128.6, 127.2, 126.5, 45.8, 24.7, 21.3, 13.4, 11.7 ppm ; HRMS-ESI (m/z): calcd for $C_{20}H_{22}N_2$ [M + H]+ : 291.1861 , found : 291.1863 .

1-(4-isopropylphenyl)-2,4,5-triphenyl-1H-imidazole (**5a**)



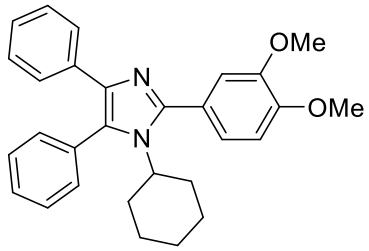
Yield : 82 % ; White solid ; ^{1}H NMR (300 MHz, DMSO(d_6)) : δ (ppm) = 7.48 (d, *J* = 6 Hz , 2H) , 7.39-7.36 (m, 2H) , 7.32-7.22 (m, 11H) ,7.20-7.14 (m, 4H) , 2.91-2.82 (m, 1H) , 1.15 (s, 3H) , 1.13 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 149.3, 146.6, 137.3, 135.0, 134.8, 131.8, 131.6, 130.9, 129.0, 128.9, 128.7, 128.6, 127.4, 126.9, 33.4, 24.1 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{26}N_2$ [M + H]+ : 415.2174 , found : 415.2172

4,5-diphenyl-1-(o-tolyl)-2-(p-tolyl)-1H-imidazole (**5b**)



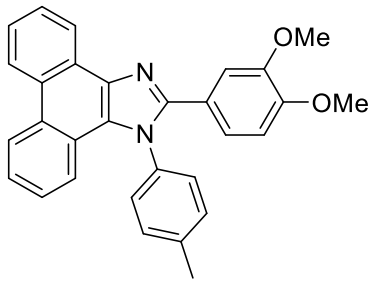
Yield : 83 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.61 (d, *J* = 7.2 Hz, 2H) , 7.32 (d, *J* = 8.1 Hz, 2H) , 7.26-7.09 (m, 12H) , 7.00 (d, *J* = 8.1 Hz, 2H) , 2.27 (s, 3H) , 1.87 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 147.0, 138.4, 136.4, 136.2, 134.6, 131.0, 130.8, 130.8, 130.7, 129.5, 129.1, 129.0, 128.4, 128.3, 128.1, 128.0, 127.5, 126.7, 21.4, 17.8 ppm ; HRMS-ESI (m/z): calcd for $C_{29}H_{24}N_2$ [M + H]+ : 401.2018 , found : 401.2015 .

1-cyclohexyl-2-(3,4-dimethoxyphenyl)-4,5-diphenyl-1H-imidazole (**5c**)



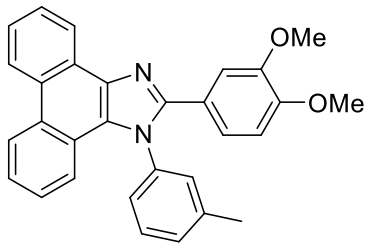
Yield : 79 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.50-7.43 (m, 7H) , 7.19-7.10 (m, 5H) , 6.98 (d, *J* = 9 Hz, 1H) , 3.97 (s, 3H) , 3.96 (s, 3H) , 1.88-1.84 (m, 2H) , 1.68-1.46 (m, 5H) , 1.14-1.01 (m, 2H) , 0.84-0.71 (m, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 149.6, 148.7, 147.6, 134.6, 132.6, 129.0, 128.8, 128.7, 127.9, 126.7, 126.0, 124.8, 122.6, 113.3, 110.8, 58.3, 56.0, 33.6, 26.2, 25.1 ppm ; HRMS-ESI (m/z): calcd for $C_{29}H_{30}N_2O_2$ [M + H]+ : 438.2307 , found : 438.2315 .

2-(3,4-dimethoxyphenyl)-1-(p-tolyl)-1H-phenanthro[9,10-d]imidazole (**5d**)



Yield : 77 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.95 (d, *J* = 9 Hz, 1H) , 8.75 (d, *J* = 9 Hz, 1H) , 8.70 (d, *J* = 9 Hz, 1H) , 7.79-7.74 (m, 1H) , 7.67-7.53 (m, 1H) , 7.51-7.42 (m, 3H) , 7.37-7.18 (m, 6H) , 6.79 (d, *J* = 9 Hz, 1H) , 3.86 (s, 3H) , 3.74 (s, 3H) , 2.44 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 150.6, 149.5, 148.3, 140.5, 139.0, 137.1, 130.5, 130.0, 129.6, 129.1, 128.3, 128.1, 127.3, 127.2, 126.3, 126.2, 125.6, 124.8, 124.1, 123.2, 123.1, 122.8, 122.4, 120.9, 112.3, 110.8, 55.8, 55.7, 21.4 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{24}N_2O_2$ [M + H]+ : 445.1916 , found : 445.1012 .

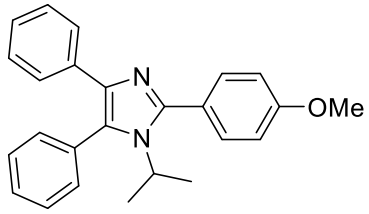
2-(3,4-dimethoxyphenyl)-1-(m-tolyl)-1H-phenanthro[9,10-d]imidazole (**5e**)



Yield : 78 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.89 (d, *J* = 7.8 Hz, 1H) , 8.75 (d, *J* = 8.4 Hz , 1H) , 8.71 (d, *J* = 2.4 Hz, 1H) 7.73 (t, *J* = 7.5, 1H) , 7.64 (t, *J* = 8.1 Hz, 1H) , 7.44-7.32 (m, 3H) , 7.33-7.17 (m, 6H) , 6.78 (d, *J* = 8.4 Hz, 1H) , 3.86 (s, 3H) , 3.73 (s, 3H) , 2.43 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 150.8, 149.7, 148.5, 140.6, 139.2,

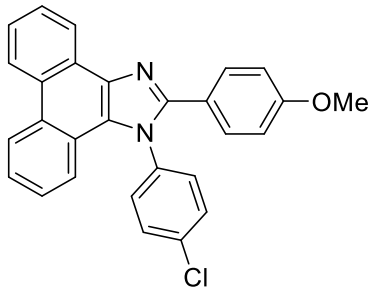
137.3, 126.4, 123.3, 122.9, 122.5, 112.5, 110.9, 56.0, 55.9, 21.6 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{24}N_2O_2$ [M + H]+ : 445.1916 , found : 445.1912 .

1-isopropyl-2-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole (**5f**)



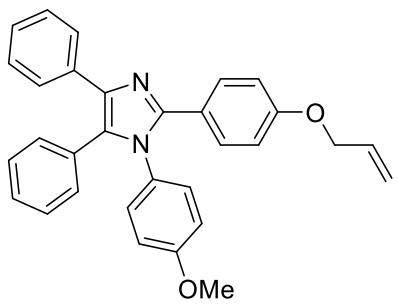
Yield : 80 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.67 (d, *J* = 1.8 Hz, 2H) , 7.65-7.43 (m, 7H) , 7.18-7.08 (m, 3H) , 7.01 (d, *J* = 2.1 Hz, 2H) , 4.46-4.42 (m, 1H) , 3.86 (s, 3H) , 1.25 (s, 3H) , 1,22 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 160.7, 147.9, 133.0, 132.7, 131.9, 129.3, 129.3, 128.4, 127.2, 126.6, 114.3, 55.9, 49.9, 23.8 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{26}N_2O_2$ [M + H]+ : 369.1967 , found : 369.1963 .

1-(4-chlorophenyl)-2-(4-methoxyphenyl)-1H-phenanthro[9,10-d]imidazole (**5g**)



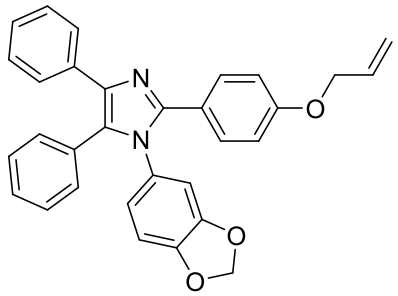
Yield : 78 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.91 (d, *J* = 8 Hz, 1H) , 8.78 (d, *J* = 12 Hz, 1H) , 8.71 (d, *J* = 8 Hz, 1H) , 7.76 (t, *J* = 8 Hz, 1H) , 7.67 (t, *J* = 8 Hz, 1H) , 7.59 (d, *J* = 8 Hz, 2H) , 7.54 (d, *J* = 8 Hz, 1H) , 7.50 (d, *J* = 8 Hz, 2H) , 7.45 (d, *J* = 8 Hz, 2H) , 7.34-7.31 (m, 1H) , 7.21 (d, *J* = 8 Hz, 1H) , 6.86 (d, *J* = 8 Hz, 2H) , 3.82 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 160.3, 150.9, 137.3, 135.7, 131.0, 130.5, 130.4, 129.2, 128.3, 127.7, 127.4, 126.9, 126.4, 125.8, 125.0, 124.2, 123.1, 123.0, 122.8, 120.6, 113.9, 55.3 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{19}ClN_2O$ [M + H]+ : 435.1264 , found : 435.1261 .

2-(4-(allyloxy)phenyl)-1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole (**5h**)



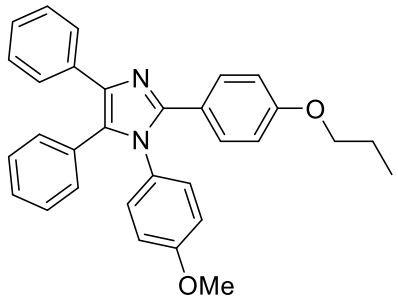
Yield : 75 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.61 (d, *J* = 9 Hz, 2H) , 7.40 (d, *J* = 9 Hz, 2H) , 7.29-7.15 (m, 8H) , 6.98 (d, *J* = 9 Hz, 2H) , 6.83-6.79 (m, 4H) , 6.12-5.99 (m, 1H) , 5.45-5.38 (m, 1H) , 5.32-5.28 (m, 1H) , 4.53 (d, *J* = 6 Hz, 2H) , 3.79 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 159.1, 158.6, 147.0, 137.9, 134.6, 133.0, 131.2, 130.9, 130.7, 130.3, 130.0, 129.5, 128.3, 128.1, 127.8, 127.4, 126.5, 123.4, 117.8, 114.3, 114.2, 68.7, 55.4 ppm ; HRMS-ESI (m/z): calcd for $C_{31}H_{26}N_2O_2$ [M + H]+ : 459.2073 , found : 459.2077 .

2-(4-(allyloxy)phenyl)-1-(benzo[d][1,3]dioxol-5-yl)-4,5-diphenyl-1H-imidazole (**5i**)



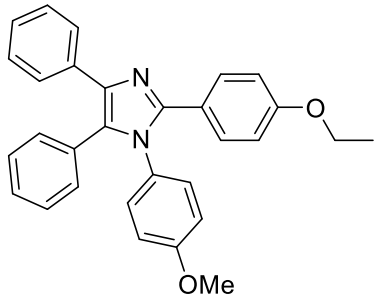
Yield : 76 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.61 (d, *J* = 6 Hz, 2H) , 7.46 (d, *J* = 9 Hz, 2H) , 7.30-7.16 (m, 8H) , 6.86 (d, *J* = 9 Hz, 2H) , 6.69 (d, *J* = 9 Hz, 1H) , 6.58-6.54 (m, 2H) , 6.11-6.02 (m, 1H) , 6.00 (s, 2H) , 5.46-5.39 (m, 1H) , 5.33-5.28 (m, 1H) , 4.55 (d, *J* = 3 Hz, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 148.0, 147.5, 146.9, 133.0, 131.1, 130.7, 130.4, 128.5, 128.2, 128.1, 127.5, 126.7, 122.3, 117.8, 114.4, 109.3, 108.1, 101.9, 68.8 ppm ; HRMS-ESI (m/z): calcd for $C_{31}H_{24}N_2O_2$ [M + H]+ : 473.1865 , found : 473.1671 .

1-(4-methoxyphenyl)-4,5-diphenyl-2-(4-propoxyphenyl)-1H-imidazole (**5j**)



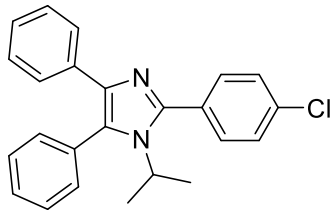
Yield : 77 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.60 (d, *J* = 7.2 Hz, 2H) , 7.39-7.15 (m, 10 H) , 6.97 (d, *J* = 8.4 Hz, 2H) , 6.78 (m, 4H) , 4.02 (d, *J* = 8.7 Hz, 2H) , 3.79 (s, 3H) , 1.81 (s, 2H) , 1.41 (t, *J* = 6.9 Hz, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 159.0, 158.9, 147.1, 137.8, 134.6, 131.2, 130.9, 130.7, 130.3, 130.0, 129.5, 128.3, 128.1, 127.8, 127.4, 126.5, 123.1, 114.2, 114.1, 63.4, 55.4, 24.7, 14.8 ppm ; HRMS-ESI (m/z): calcd for $C_{31}H_{28}N_2O_2$ [M + H]+ : 461.2229 , found : 461.2226 .

2-(4-ethoxyphenyl)-1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole (**5k**)



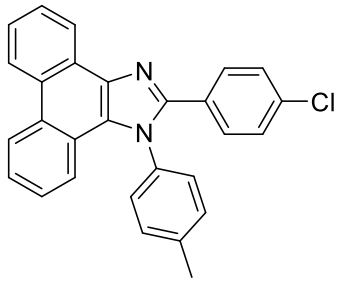
Yield : 79 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.60 (d, *J* = 6 Hz, 2H) , 7.39-7.15 (m, 10 H) , 6.97 (d, *J* = 6 Hz, 2H) , 6.78 (s, 4H) , 4.03 (t, *J* = 6 Hz, 2H) , 3.79 (s, 3H) , 1.41 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 159.0, 158.9, 147.1, 137.9, 134.6, 131.2, 130.9, 130.7, 130.3, 130.0, 129.5, 128.3, 128.1, 127.8, 127.4, 126.5, 123.1, 114.2, 114.1, 63.4, 55.4, 24.7, 14.8 ppm ; HRMS-ESI (m/z): calcd for $C_{30}H_{26}N_2O_2$ [M + H]+ : 447.2073 , found : 447.2076 .

2-(4-chlorophenyl)-1-isopropyl-4,5-diphenyl-1H-imidazole (**5l**)



Yield : 86 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.57 (d, *J* = 8.4 Hz , 2H) , 7.47-7.46 (m, 6H) , 7.44-7.42 (m, 2H) , 7.40-7.39 (m, 1H) , 7.27-7.09 (m, 3H), 4.46-4.37 (m, 1H) , 1.25 (s, 3H) , 1.23 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 146.4, 138.2, 135.3, 134.5, 132.3, 132.2, 131.5, 130.9, 129.4, 129.1, 128.9, 128.8, 128.1, 126.8, 126.4, 49.6, 23.4 ppm ; HRMS-ESI (m/z): calcd for $C_{24}H_{21}ClN_2$ [M + H]+ : 373.1472 , found : 373.1474 .

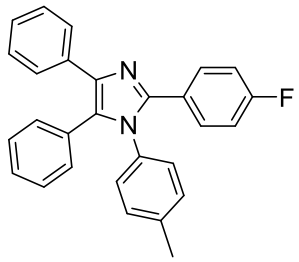
2-(4-chlorophenyl)-1-(p-tolyl)-1H-phenanthro[9,10-d]imidazole (**5m**)



Yield : 84 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.89 (d, *J* = 9 Hz, 1H) , 8.78 (d, *J* = 9 Hz, 1H) , 8.71 (d, *J* = 9 Hz, 1H) , 7.76-7.64 (m, 4H) , 7.55-7.50 (m, 1H) , 7.45 (d, *J* = 9 Hz, 2H) , 7.38 (d, *J* = 9 Hz, 2H) , 7.33-7.23 (m, 1H) , 7.22 (d, *J* = 9 Hz, 1H) , 7.15 (d, *J* = 9 Hz, 1H) , 2.36 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 151.1, 139.2, 137.9, 133.4, 130.8, 129.4, 129.3, 129.1, 128.3, 127.8, 127.4, 127.1, 126.4, 125.7, 125.0, 124.2,

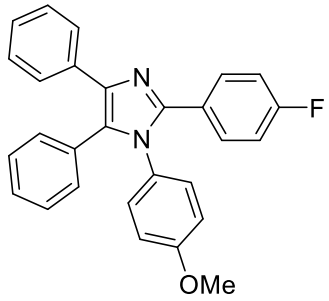
123.7, 123.1, 122.8, 120.6, 21.4 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{19}ClN_2$ [M + H]+ : 419.1315 , found : 419.1319 .

2-(4-fluorophenyl)-4,5-diphenyl-1-(p-tolyl)-1H-imidazole (**5n**)



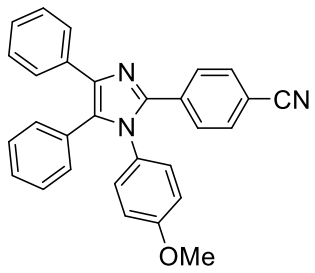
Yield : 91 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 7.58 (d, *J* = 6 Hz, 2H) , 7.46-7.49 (m, 3H) , 7.35-7.39 (m, 2H) , 7.29-7.23 (m, 2H) , 7.13-7.16 (m, 2H) , 7.03-7.09 (m, 3H) , 6.92 (t, *J* = 9Hz, 4H) , 2.34 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 164.3, 146.2, 145.1, 138.4, 138.1, 134.3, 134.2, 131.1, 131.0, 130.9, 130.7, 130.5, 129.8, 128.5, 128.4, 128.2, 128.1, 128.0, 127.6, 127.4, 126.7, 116.0, 115.7, 115.3, 115.0, 21.2 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{21}FN_2$ [M + H]+ : 405.1767 , found : 405.1761 .

2-(4-fluorophenyl)-1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole (**5o**)



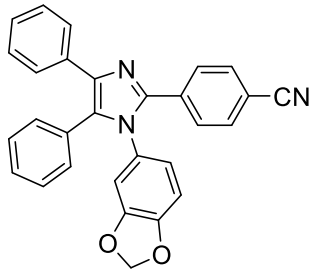
Yield : 89 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 7.59 (d, *J* = 8 Hz, 2H) , 7.48 (d, J = 8 Hz, 3H), 7.46-7.38 (m, 2H), 7.37-7.29 (m, 2H), 7.27-7.23 (m, 2H) , 7.16-7.03 (m, 3H) , 6.95-6.89 (m, 4H) , 2.34 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 164.3, 161.4, 159.2, 146.2, 144.9, 138.0, 134.3, 131.1, 130.8, 130.7, 130.5, 129.6, 129.4, 128.5, 128.4, 128.3, 128.1, 128.0, 127.8, 127.4, 126.7, 126.7, 116.0, 115.7, 115.3, 115.1, 114.3, 55.4 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{21}FN_2O$ [M + H]+ : 421.1716 , found : 421.1710 .

4-(1-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazol-2-yl)benzonitrile (**5p**)



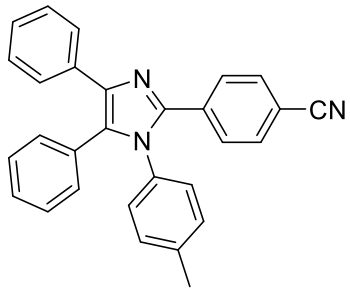
Yield : 92 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 7.62-7.59 (m, 4H) , 7.56 (d, *J* = 12 Hz, 2H) , 7.31-7.23 (m, 6H) , 7.16 (d, *J* = 8 Hz, 2H) , 7.01 (d, *J* = 8 Hz, 2H) , 6.83 (d, *J* = 8 Hz, 2H) , 3.82 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 159.6, 144.7, 138.7, 134.5, 133.7, 132.4, 132.0, 132.1, 130.0, 129.3, 129.1, 129.0, 128.5, 128.4, 128.3, 127.4, 127.1, 118.7, 114.6, 111.5, 55.5 ppm ; HRMS-ESI (m/z): calcd for $C_{29}H_{21}N_3O$ [M + H]+ : 428.1763 , found : 428.1761 .

4-(1-(benzo[d][1,3]dioxol-5-yl)-4,5-diphenyl-1H-imidazol-2-yl)benzonitrile (**5q**)



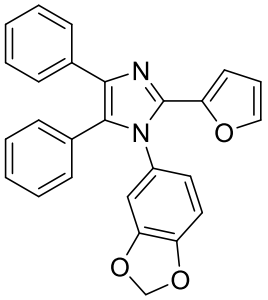
Yield : 90 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 7.64-7.55 (m, 6H) , 7.32-7.17 (m, 9H) , 6.73 (d, *J* = 9 Hz, 1H) , 6.60-6.55 (m, 2H) , 6.03 (s, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 148.3, 148.0, 144.8, 139.0, 134.6, 133.9, 132.4, 132.0, 131.0, 130.2, 130.0, 128.8, 128.6, 128.5, 128.5, 128.3, 128.2, 127.3, 127.0, 122.1, 118.7, 109.0, 108.4, 102.1 ppm ; HRMS-ESI (m/z): calcd for $C_{29}H_{19}N_3O_2$ [M + H]+ : 442.1556 , found : 442.1551 .

4-(4,5-diphenyl-1-(p-tolyl)-1H-imidazol-2-yl)benzonitrile (**5r**)



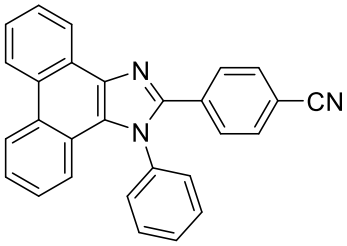
Yield : 91 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.63-7.58 (m, 4H) , 7.54 (d, *J* = 9 Hz, 2H) , 7.30-7.22 (m, 6H) , 7.18-7.11 (m, 4H) , 6.97 (d, *J* = 9 Hz, 2H) , 2.37 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 144.7, 139.0, 139.0, 134.8, 134.0, 132.3, 131.9, 131.1, 130.2, 130.1, 129.0, 128.5, 128.3, 128.3, 128.0, 127.3, 127.0, 118.8, 111.4, 21.3 ppm ; HRMS-ESI (m/z): calcd for $C_{29}H_{21}N_3$ [M + H]+ : 412.1814 , found : 412.1809

1-(benzo[d][1,3]dioxol-5-yl)-2-(furan-2-yl)-4,5-diphenyl-1H-imidazole (**5s**)



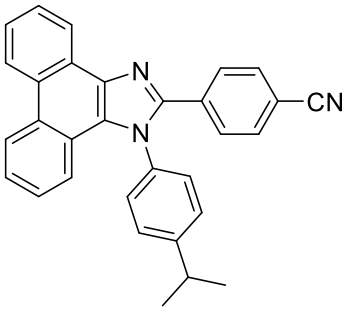
Yield : 88 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.62 (d, *J* = 9 Hz, 2H) , 7.47 (s, 1H) , 7.24-7.19 (m, 8H) , 6.77-6.68 (m, 3H) , 6.36 (s, 1H) , 6.18 (s, 1H) , 6.05 (s, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 148.2, 143.4, 131.0, 128.6, 128.4, 128.2, 127.6, 127.1, 122.4, 116.9, 111.3, 109.4, 108.2, 102.1 ppm ; HRMS-ESI (m/z): calcd for $C_{26}H_{19}N_2O_3$ [M + H]+ : 407.1396 , found : 407.1391.

4-(1-phenyl-1H-phenanthro[9,10-d]imidazol-2-yl)benzonitrile (**5t**)



Yield : 78 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.86 (d, *J* = 9 Hz, 1H) , 8.78 (d, *J* = 9 Hz, 1H) , 8.71 (d, *J* = 6 Hz, 1H) , 7.79 (d, *J* = 9 Hz, 1H) , 7.75-7.63 (m, 6H) , 7.57-7.50 (m, 5H) , 7.31-7.26 (m, 1H) , 7.17 (d, *J* = 9 Hz, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 148.3, 138.3, 137.7, 134.7, 131.9, 130.6, 130.4, 129.7, 129.4, 128.9, 128.8, 128.5, 127.5, 127.0, 126.5, 126.1, 125.5, 124.2, 123.2, 122.8, 122.7, 121.0, 118.6, 112.0 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{17}N_3$ [M + H]+ : 396.1501 , found : 396.1506 .

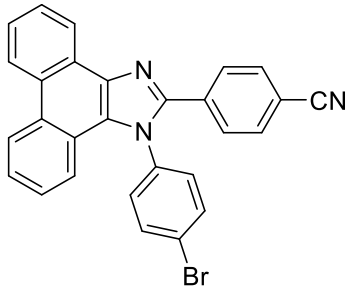
4-(1-(4-isopropylphenyl)-1H-phenanthro[9,10-d]imidazol-2-yl)benzonitrile (**5u**)



Yield : 91 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.87 (d, *J* = 9 Hz, 1H) , 8.78 (d, *J* = 6 Hz, 1H) , 8.72 (d, *J* = 9 Hz, 1H) , 7.80-7.66 (m, 4H) , 7.58-7.42 (m, 7H) , 7.30-7.27 (m, 1H) , 7.21 (d, *J* = 6 Hz, 1H) , 3.19-3.10 (m, 1H) , 1.43 (s, 3H) , 1.41 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 151.6, 148.4, 137.5, 135.7, 134.8, 131.9, 129.6, 129.5, 128.9, 128.6, 128.5, 128.5, 127.5, 127.0, 126.5, 126.0, 125.4, 124.2, 123.2, 122.9, 122.7, 121.1,

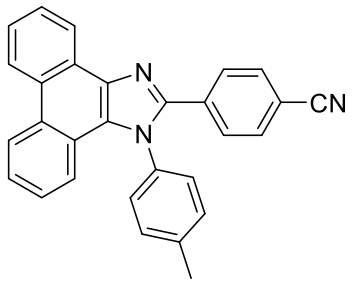
118.6, 112.0, 34.0, 24.0 ppm ; HRMS-ESI (m/z): calcd for $C_{31}H_{23}N_3$ [M + H]+ : 438.1970 , found : 438.1965 .

4-(1-(4-bromophenyl)-1H-phenanthro[9,10-d]imidazol-2-yl)benzonitrile (**5v**)



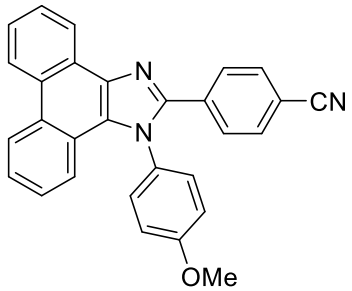
Yield : 88 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.83 (d, *J* = 6 Hz, 1H) , 8.78 (d, *J* = 9 Hz, 1H) , 8.70 (d, *J* = 9 Hz, 1H) , 7.79-7.69 (m, 3H) , 7.66-7.52 (m, 6H) , 7.41-7.28 (m, 3H) , 7.18 (d, *J* = 9 Hz, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 148.3, 137.7, 137.2, 134.3, 133.8, 132.1, 130.5, 129.7, 129.5, 128.5, 128.5, 127.6, 126.8, 126.7, 126.3, 125.7, 124.5, 124.4, 123.2, 122.7, 122.5, 120.8, 118.4, 112.3 ppm ; HRMS-ESI (m/z): calcd for $C_{28}H_{16}BrN_3$ [M + H]+ : 474.0606 , found : 474.0615 .

4-(1-(p-tolyl)-1H-phenanthro[9,10-d]imidazol-2-yl)benzonitrile (**5w**)



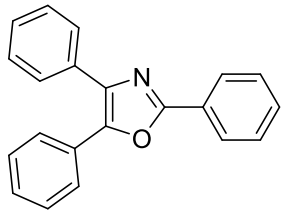
Yield : 86 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.87 (d, *J* = 9 Hz, 1H) , 8.77 (d, *J* = 9 Hz , 1H) , 8.70 (d, *J* = 6 Hz, 1H) , 7.79-7.74 (m, 4H) , 7.70-7.65 (m, 3H) , 7.54-7.38 (m, 4H) , 7.30 (d, *J* = 9 Hz, 1H) , 7.22 (d, *J* = 6 Hz, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 148.4, 140.6, 137.5, 135.5, 134.7, 131.9, 131.2, 129.6, 129.4, 128.8, 128.5, 128.5, 127.5, 126.9, 126.5, 126.0, 125.5, 124.2, 123.2, 122.8, 122.7, 121.0, 118.6, 112.0, 21.6 ppm ; HRMS-ESI (m/z): calcd for $C_{29}H_{19}N_3$ [M + H]+ : 410.1657 , found : 410.1651 .

4-(1-(4-methoxyphenyl)-1H-phenanthro[9,10-d]imidazol-2-yl)benzonitrile (**5x**)



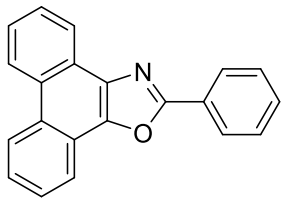
Yield : 87 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.87 (d, *J* = 9 Hz, 1H) , 8.79 (d, *J* = 9 Hz, 1H) , 8.72 (d, *J* = 9 Hz, 1H) , 7.80-7.66 (m, 4H) , 7.57 (t, *J* = 9 Hz, 3H) , 7.44 (d, *J* = 9 Hz, 2H) , 7.36-7.24 (m, 2H) , 7.14 (d, *J* = 6 Hz, 2H) , 3.99 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 160.7, 148.5, 137.4, 134.7, 132.0, 130.6, 130.0, 129.7, 129.5, 129.0, 128.5, 127.5, 126.9, 126.5, 126.0, 125.5, 124.2, 123.2, 122.9, 122.7, 121.0, 118.6, 115.6, 112.1, 55.7 ppm ; HRMS-ESI (m/z): calcd for $C_{29}H_{19}N_3O$ [M + H]+ : 426.1606 , found : 426.1610 .

2,4,5-triphenyloxazole (**6aa**)



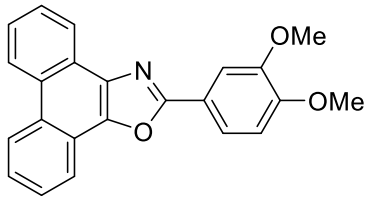
Yield : 80 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.22-8.18 (m, 1H) , 7.94 (d, *J* = 9 Hz, 2H) , 7.76 (d, *J* = 6 Hz, 1H) , 7.73-7.66 (m, 2H) , 7.63-7.58 (m, 1H) , 7.54-7.34 (m, 8H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 160.2, 148.4, 145.6 , 133.7, 133.1, 132.5, 130.4, 129.9, 129.4, 129.1, 129.0, 128.8, 128.7, 128.7, 128.6, 128.3, 128.3, 128.2, 127.3, 126.6, 126.5 ppm ; HRMS-ESI (m/z): calcd for $C_{21}H_{15}NO$ [M + H]+ : 298.1232 , found : 298.1236 .

2-phenylphenanthro[9,10-d]oxazole (**6ca**)



Yield : 82 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.74 (t, *J* = 8 Hz, 2H) , 8.63 (d, *J* = 8 Hz, 1H) , 8.40 (d, *J* = 8 Hz, 2H) , 8.34 (d, *J* = 8 Hz, 1H) , 7.79-7.67 (m, 4H) , 7.59 (d, *J* = 8 Hz, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 162.2, 144.9, 135.5, 131.0, 129.3, 129.0, 128.9, 127.6, 127.5, 127.3, 127.2, 126.4, 126.2, 123.8, 123.4, 123.0, 121.1, 120.9 ppm ; HRMS-ESI (m/z): calcd for $C_{21}H_{13}NO$ [M + H]+ : 296.1075 , found : 296.1071 .

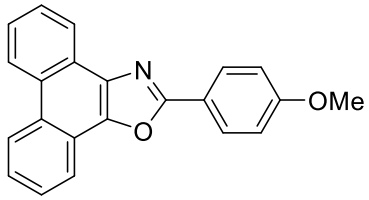
2-(3,4-dimethoxyphenyl)phenanthro[9,10-d]oxazole (**6cb**)



Yield : 71 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.72-8.69 (m, 2H) , 8.63 (d, *J* = 8 Hz, 1H) , 8.29 (d, *J* = 8 Hz, 1H) , 7.92 (d, *J* = 8 Hz, 1H) , 7.85 (s, 1H) , 7.77-

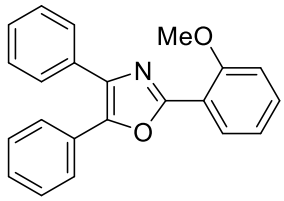
7.64 (m, 4H) , 6.99 (d, *J* = 8 Hz, 1H) , 4.08 (s, 3H) , 3.98 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 162.2, 151.5, 149.2, 144.6, 135.3, 129.1, 128.8, 127.4, 127.2, 126.2, 126.1, 126.0, 123.7, 123.4, 123.0, 121.0, 120.7, 120.6, 120.1, 111.0, 109.8, 56.2, 56.0 ppm ; HRMS-ESI (m/z): calcd for $C_{23}H_{17}NO_3$ [M + H]+ : 356.1287 , found : 356.1281 .

2-(4-methoxyphenyl)phenanthro[9,10-d]oxazole (**6cc**)



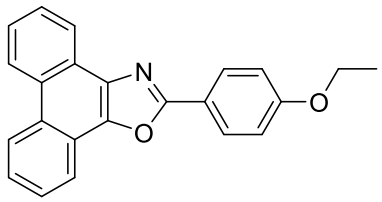
Yield : 75 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.75 (t, *J* = 6 Hz, 2H) , 8.64 (d, *J* = 6 Hz, 1H) , 8.34 (d, *J* = 9 Hz, 3H) , 7.79-7.66 (m, 4H) , 7.09 (d, *J* = 9 Hz, 2H) , 3.93 (s, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 162.4, 161.9, 144.6, 135.5, 129.1, 128.9, 128.9, 127.4, 127.2, 126.2, 126.0, 123.7, 123.4, 122.9, 121.1, 120.7, 120.2, 114.4, 55.5 ppm ; HRMS-ESI (m/z): calcd for $C_{22}H_{15}NO_2$ [M + H]+ : 326.1181 , found : 326.1186 .

2-(2-methoxyphenyl)-4,5-diphenyloxazole (**6ad**)



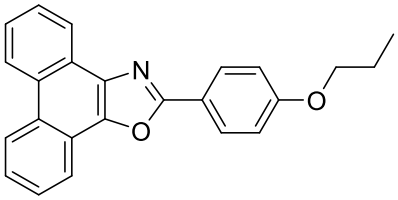
Yield : 76 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.52 (d, *J* = 9 Hz, 1H) , 7.71-7.33 (m, 11H) , 7.17-7.12 (m, 1H) , 7.06 (d, *J* = 9 Hz, 1H) , 4.06 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 155.7, 144.1, 129.5, 128.7, 127.8, 121.7, 118.2, 111.2, 55.9 ppm ; HRMS-ESI (m/z): calcd for $C_{21}H_{13}NO$ [M + H]+ : 328.1338 , found : 328.1339 .

2-(4-ethoxyphenyl)phenanthro[9,10-d]oxazole (**6ce**)



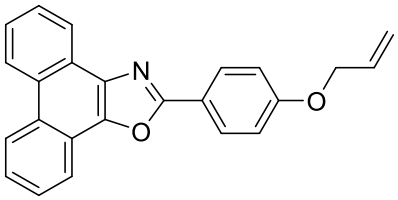
Yield : 79 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.75-8.61 (m, 3H) , 8.32-8.29 (m, 3H) , 7.85-7.64 (m, 4H) , 7.07-6.97 (m, 2H) , 4.14 (q, *J* = 9 Hz, 2H) , 1.49 (t, *J* = 6 Hz, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 162.4, 161.3, 135.5, 132.0, 129.0, 128.9, 128.8, 127.3, 127.2, 126.2, 126.1, 126.0, 123.7, 123.4, 122.9, 121.1, 120.7, 120.0, 114.8, 114.7, 63.7, 14.8 ppm ; HRMS-ESI (m/z): calcd for $C_{23}H_{17}NO_2$ [M + H]+ : 340.1338 , found : 340.1335 .

2-(4-propoxyphenyl)phenanthro[9,10-d]oxazole (**6cf**)



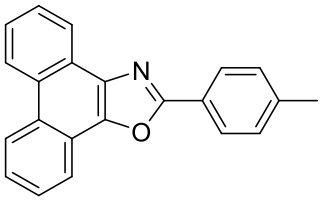
Yield : 78 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.75 (t, *J* = 8 Hz, 2H) , 8.64 (d, *J* = 8 Hz, 1H) , 8.34-8.30 (m, 3H) , 7.79-7.66 (m, 4H) , 7.08 (d, *J* = 8 Hz, 2H) , 4.04 (t, *J* = 8 Hz, 2H) , 1.94-1.85 (m, 2H) , 1.11 (t, *J* = 8 Hz, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 162.5, 161.5, 135.6, 129.0, 128.9, 128.9, 127.3, 127.2, 126.2, 126.1, 126.0, 123.7, 123.4, 122.9, 121.2, 120.7, 120.0, 114.8, 69.7, 22.6, 10.6 ppm ; HRMS-ESI (m/z): calcd for $C_{24}H_{19}NO_2$ [M + H]+ : 354.1494 , found : 354.1490 .

2-(4-(allyloxy)phenyl)phenanthro[9,10-d]oxazole (**6cg**)



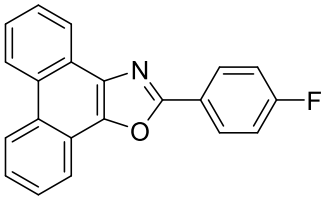
Yield : 76 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.75 (t, *J* = 8 Hz, 2H) , 8.63 (d, *J* = 8 Hz, 1H) , 8.32 (d, *J* = 8 Hz, 3H) , 7.78-7.66 (m, 4H) , 7.10 (d, *J* = 8 Hz, 2H) , 6.17-6.08 (m, 1H) , 5.50 (d, *J* = 16 Hz, 1H) , 5.38 (d, *J* = 12 Hz, 1H) , 4.66 (d, *J* = 8 Hz, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 162.3, 160.9, 144.6, 135.5, 132.8, 129.1, 128.9, 128.9, 127.4, 127.2, 126.2, 126.2, 126.0, 123.7, 123.4, 122.9, 121.1, 120.7, 120.4, 118.2, 115.1, 115.0, 68.9 ppm ; HRMS-ESI (m/z): calcd for $C_{24}H_{17}NO_2$ [M + H]+ : 352.1338 , found : 352.1331 .

2-(p-tolyl)phenanthro[9,10-d]oxazole (**6ch**)



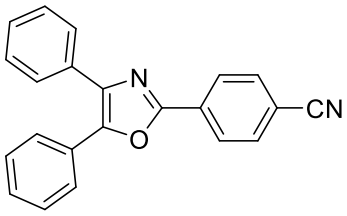
Yield : 80 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.76 (t, *J* = 8 Hz, 2H) , 8.66 (d, *J* = 8 Hz, 1H) , 8.36 (d, *J* = 8Hz, 1H) , 8.30 (d, *J* = 8 Hz, 2H) , 7.80-7.68 (m, 4H) , 7.40 (d, *J* = 8 Hz, 2H) , 2.49 (s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 162.5, 144.7, 141.4, 135.5, 129.7, 129.2, 128.9, 127.4, 127.3, 127.2, 126.3, 126.2, 126.1, 124.8, 123.8, 123.4, 123.0, 121.1, 120.8, 21.7 6 ppm ; HRMS-ESI (m/z): calcd for $C_{22}H_{15}NO$ [M + H]+ : 310.1232 , found : 310.1232 .

2-(4-fluorophenyl)phenanthro[9,10-d]oxazole (**6ck**)



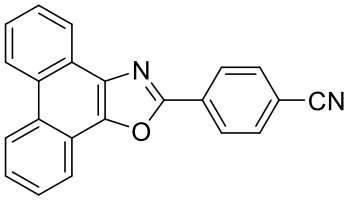
Yield : 84 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.78-8.73 (m, 2H) , 8.63 (d, *J* = 9 Hz, 1H) , 8.41-8.32 (m, 3H) , 7.80-7.68 (m, 4H) , 7.30-7.24 (m, 2H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 162.8, 161.4, 144.9, 129.4, 129.3, 129.3, 128.9, 127.5, 127.3, 126.5, 126.2, 126.1, 124.0, 123.8, 123.5, 122.9, 121.0, 120.8, 116.3, 116.0 ppm ; HRMS-ESI (m/z): calcd for $C_{21}H_{12}FNO$ [M + H]+ : 314.0981 , found : 314.0975 .

4-(4,5-diphenyloxazol-2-yl)benzonitrile (**6al**)



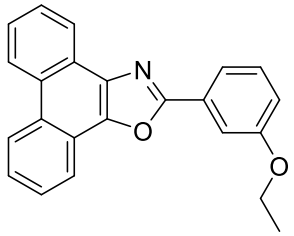
Yield : 82 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.77 (d, *J* = 9 Hz, 3H) , 7.69-7.64 (m, 6H) , 7.42-7.34 (m, 4H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 162.7, 149.7, 146.4, 142.2, 137.5, 132.3, 130.5, 129.8, 129.4, 128.5, 118.4, 112.8 ppm ; HRMS-ESI (m/z): calcd for $C_{22}H_{14}N_2O$ [M + H]+ : 323.1184 , found : 323.1181 .

4-(phenanthro[9,10-d]oxazol-2-yl)benzonitrile (**6cl**)



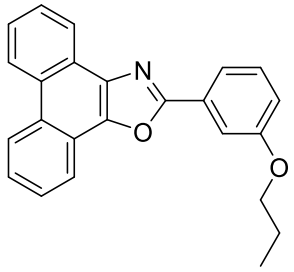
Yield : 80 % ; White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 8.80-8.75 (m, 2H) , 8.63 (d, *J* = 8 Hz, 1H) , 8.47 (d, *J* = 8Hz, 2H) , 8.37-8.34 (m, 1H) , 7.86 (d, *J* = 8 Hz, 2H) , 7.81-7.73 (m, 4H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 160.0, 135.8, 145.6, 132.7, 131.4, 129.8, 129.1, 127.7, 127.5, 127.4, 127.1, 126.6, 125.9, 123.9, 123.5, 123.0, 121.1, 120.8, 118.4, 114.0 ppm ; HRMS-ESI (m/z): calcd for $C_{22}H_{12}N_2O$ [M + H]+ : 321.1028 , found : 321.1021.

2-(3-ethoxyphenyl)phenanthro[9,10-d]oxazole (**6cq**)



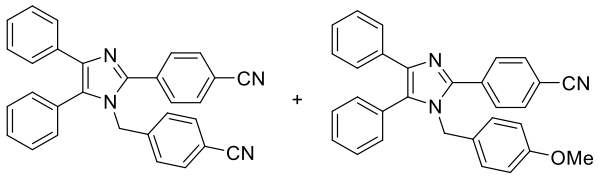
Yield : 78 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.73 (t, *J* = 6 Hz, 2H) , 8.64 (d, *J* = 9 Hz, 1H) , 8.33 (d, *J* = 9 Hz, 1H) , 7.97-7.90 (m, 2H) , 7.79-7.66 (m, 4H) , 7.50-7.45 (m, 1H) , 7.09 (d, *J* = 9 Hz, 1H) , 4.25-4.18 (m, 2H) , 1.53 (t, *J* = 6 Hz, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 162.1, 159.4, 144.9, 135.5, 130.0, 129.3, 128.9, 128.7, 127.4, 127.3, 126.4, 126.2, 126.1, 123.7, 123.4, 123.0, 121.1, 120.9, 119.6, 117.8, 112.5, 63.8, 14.9 ppm ; HRMS-ESI (m/z): calcd for $C_{23}H_{17}NO_2$ [M + H]+ : 340.1338 , found : 340.1331 .

2-(3-propoxyphenyl)phenanthro[9,10-d]oxazole (**6cr**)



Yield : 75 % ; White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 8.79-8.74 (m, 2H) , 8,67 (d, *J* = 9 Hz, 1H) , 8.38 (d, *J* = 9 Hz, 1H) , 7.99 (d, *J* = 9 Hz, 1H) , 7.94 (d, *J* = 3 Hz, 1H) , 7.81-7.68 (m, 4H) , 7.49 (t, *J* = 9 Hz, 1H) , 7.11 (d, *J* = 6 Hz, 1H) , 4.12 (t, *J* = 6 Hz, 2H) , 1.96-1.87 (m, 2H) , 1.14 (t, *J* = 6Hz, 3H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 162.2, 159.6, 144.9, 135.5, 130.0, 129.3, 128.9, 128.7 , 127.5, 127.3, 126.5, 126.2, 126.2, 123.8, 123.5, 123.0, 121.1, 120.9, 119.5, 117.9, 112.6, 69.8, 22.7, 10.6 ppm ; HRMS-ESI (m/z): calcd for $C_{24}H_{19}NO_2$ [M + H]+ : 354.1494 , found : 354.1498 .

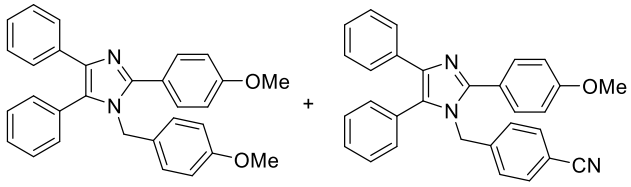
4-(1-(4-cyanobenzyl)-4,5-diphenyl-1H-imidazol-2-yl)benzonitrile(3ah) + 4-(1-(4-methoxybenzyl)-4,5-diphenyl-1H-imidazol-2-yl)benzonitrile (**3Y**)



White solid ; ^{1}H NMR (300 MHz, $CDCl_3$) : δ (ppm) = 7.89 (d, *J* = 9 Hz, 4H) , 7.71 (d, *J* = 6 Hz) , 7.75-7.45(m, 14 H), 7.43-7.32 (m, 9H) , 7.27-7.16 (m, 15H) , 6.96-6.86 (m, 8H) ; ^{13}C NMR (75 MHz, $CDCl_3$) = 160.4, 148.1, 145.9, 142.8, 142.1, 139.4, 134.8, 134.1, 133.6, 132.7, 132.6, 132.4, 131.1, 130.9, 130.8, 130.4, 130.0, 129.5, 129.3, 129.2, 129.1, 129.0,

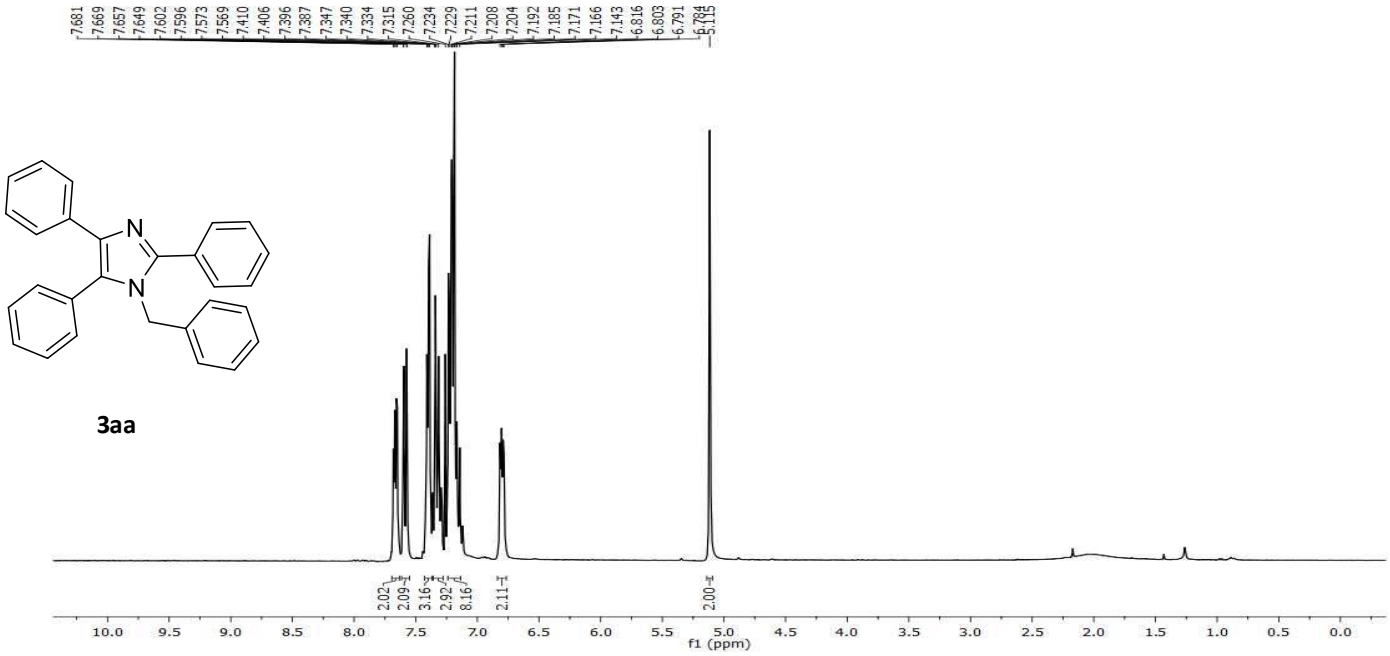
128.9, 128.3, 128.1, 127.1, 126.8, 126.6, 122.8, 118.5, 118.4, 118.2, 114.3, 112.6, 111.9, 111.4, 55.4, 48.3, 48.0 ppm

1-(4-methoxybenzyl)-2-(4-methoxyphenyl)-4,5-diphenyl-1H-imidazole (3ac) + 4-((2-(4-*methoxyphenyl)-4,5-diphenyl-1H-imidazol-1-yl)methyl)benzonitrile* (**3X**)



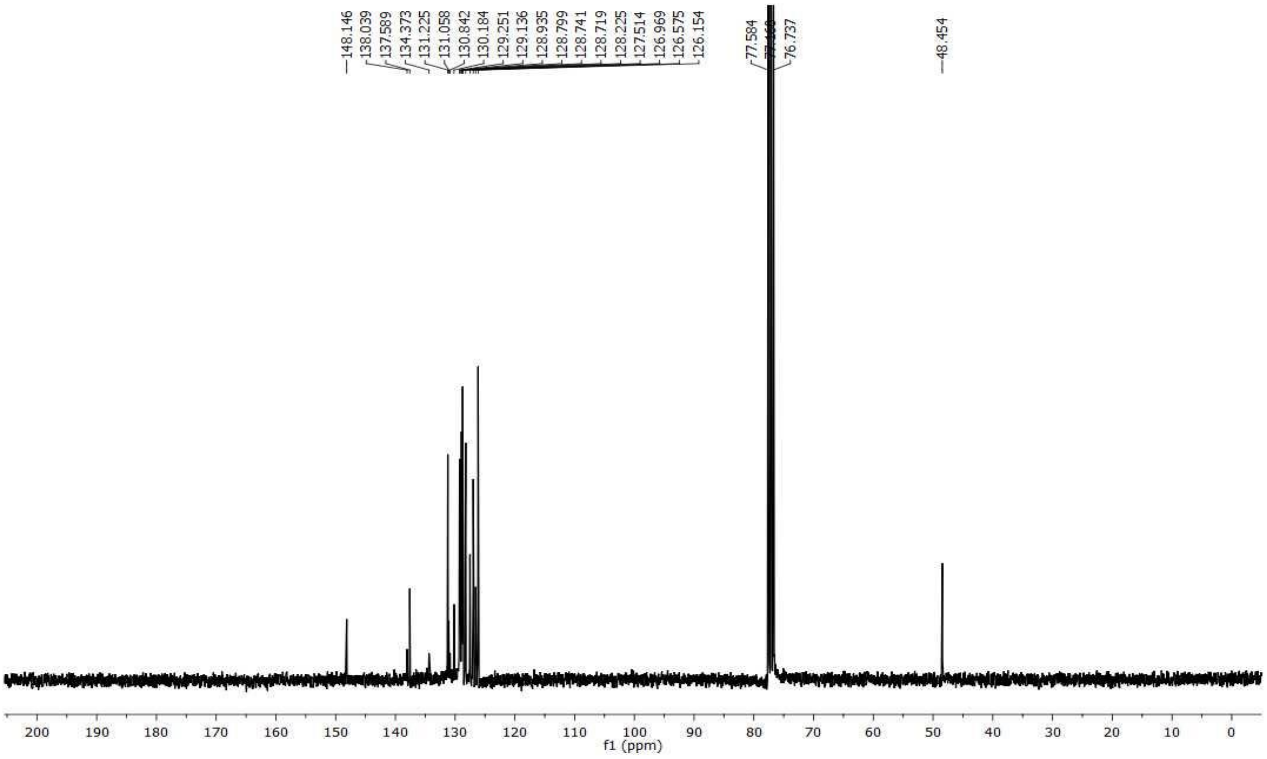
White solid ; ^{1}H NMR (400 MHz, $CDCl_3$) : δ (ppm) = 7.34 (d, *J* = 8.4 Hz, 2H) , 7.57-7.53 (m, 3H) , 7.43-7.35 (m, 10H) , 7.27-7.14 (m, 11 H) , 6.90-6.84 (m, 2H) , 6.79-6.71 (m, 6H) , 6.67-6.64 (m, 2H), 5.07 (s, 2H), 5,00(s, 2H) , 3.81 (s, 3H), 3.79 (s, 3H), 3.78(s, 3H) ; ^{13}C NMR (100 MHz, $CDCl_3$) = 160.2, 159.1, 158.8, 148.1, 144.1, 139.0, 137.7, 134.3, 134.1, 133.9, 131.4, 131.1, 131.0, 130.4, 130.3, 129.8, 129.4, 129.1, 129.0,128.9, 128.7, 128.3, 128.2, 127.3, 126.9, 122.9, 118.9, 114.0, 112.2, 111.1, 55.3, 48.0, 47.7 ppm

^{1}H and ^{13}C NMR spectra of compounds

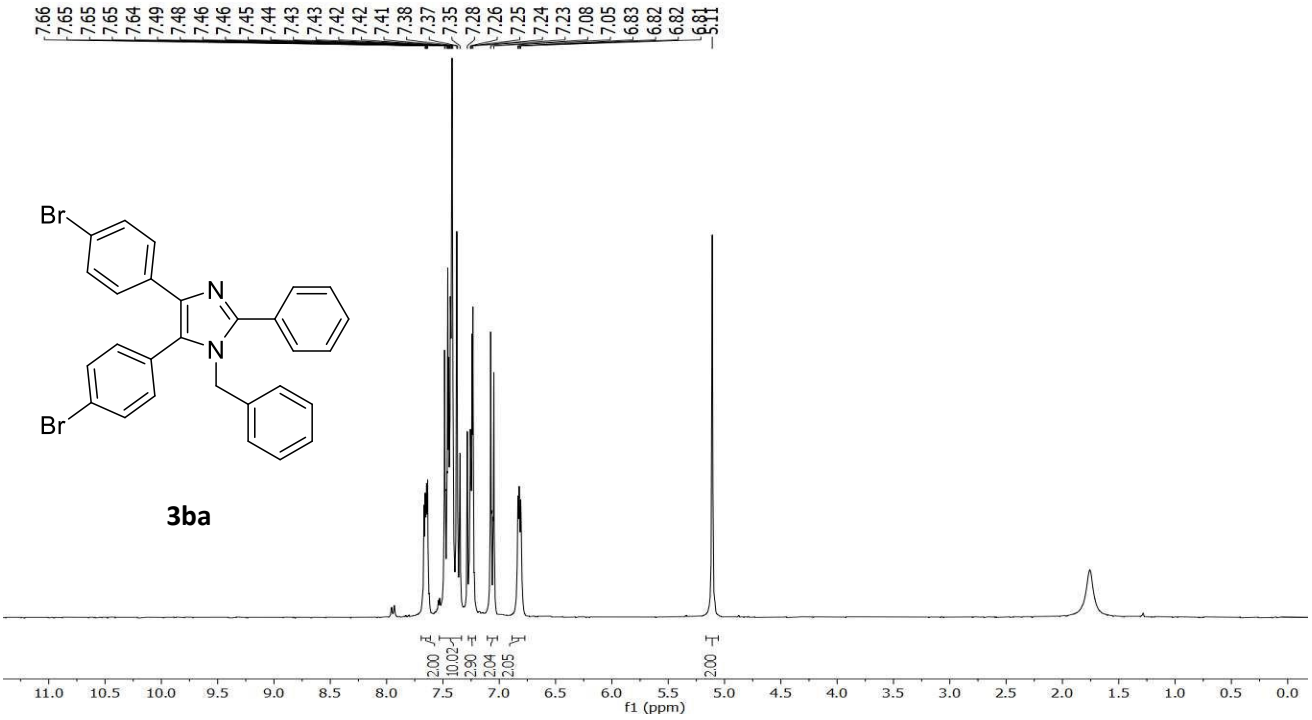


3aa

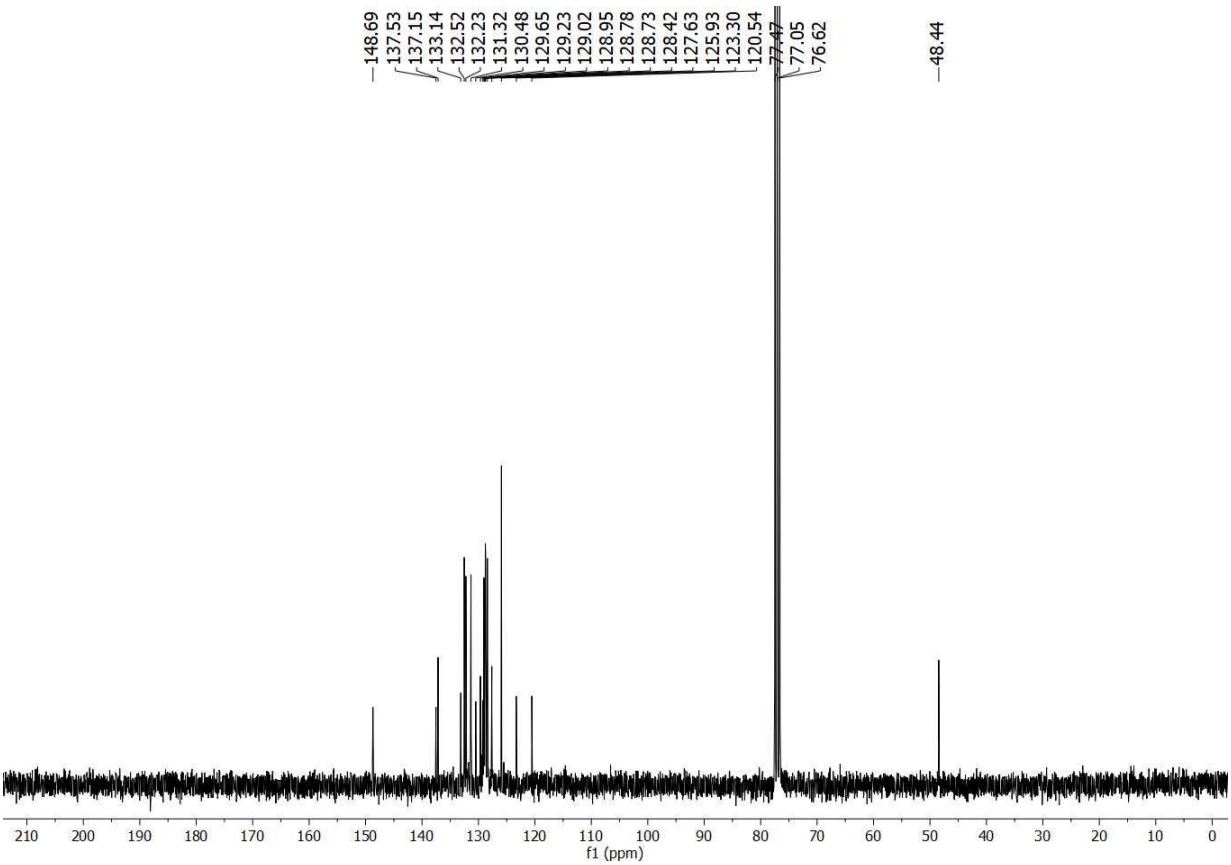
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3aa



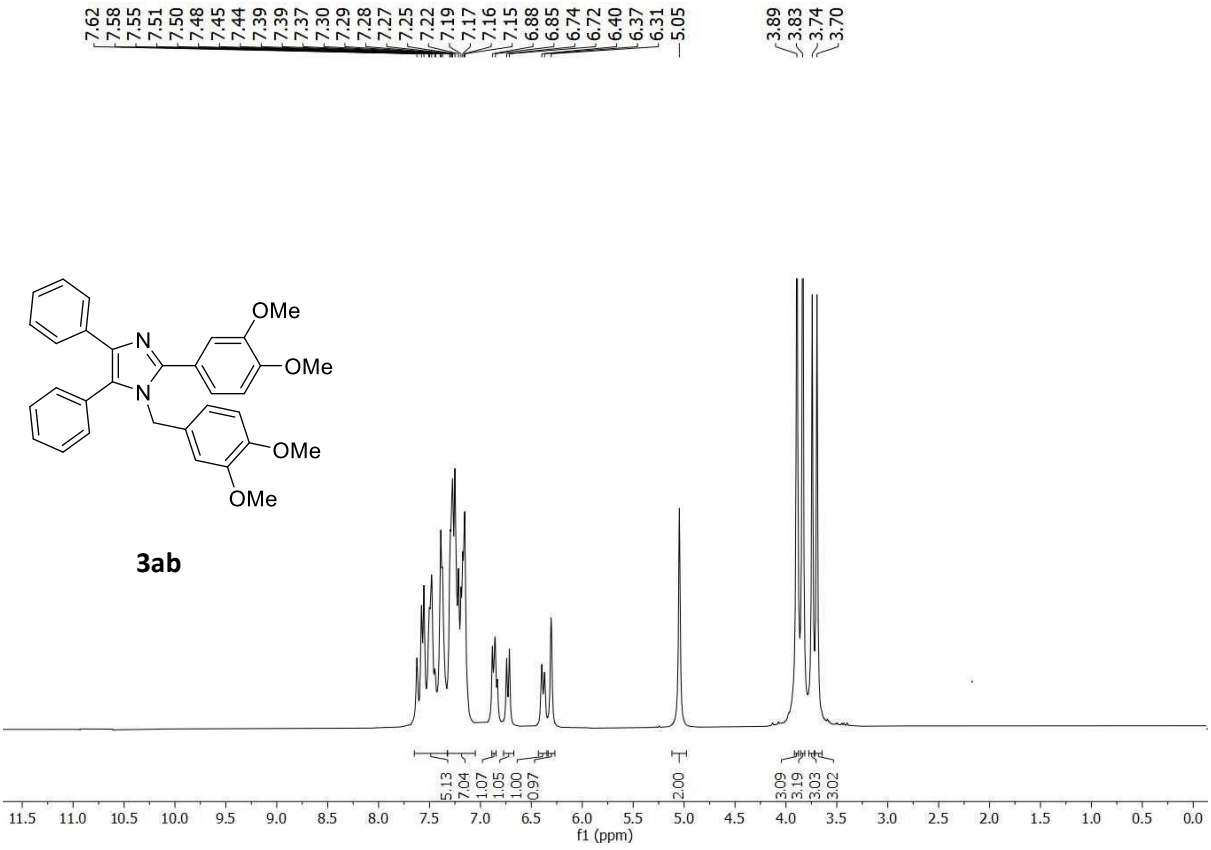
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3aa



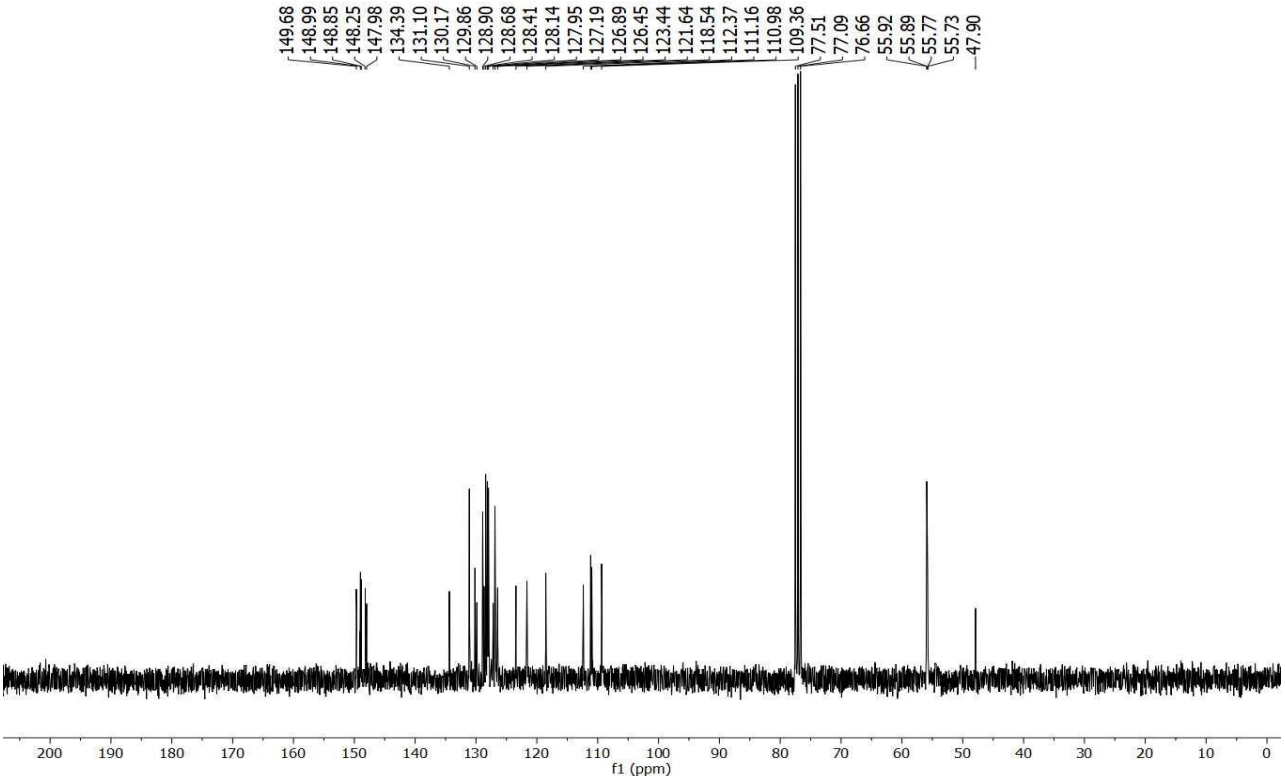
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ba



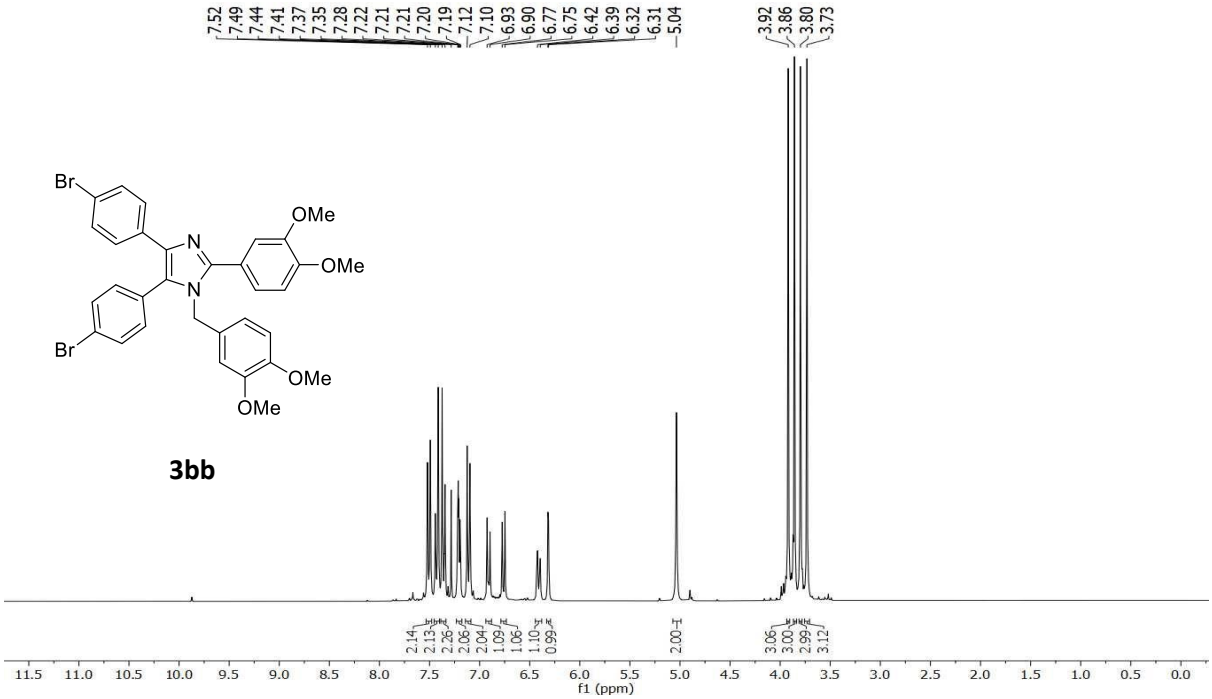
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ba



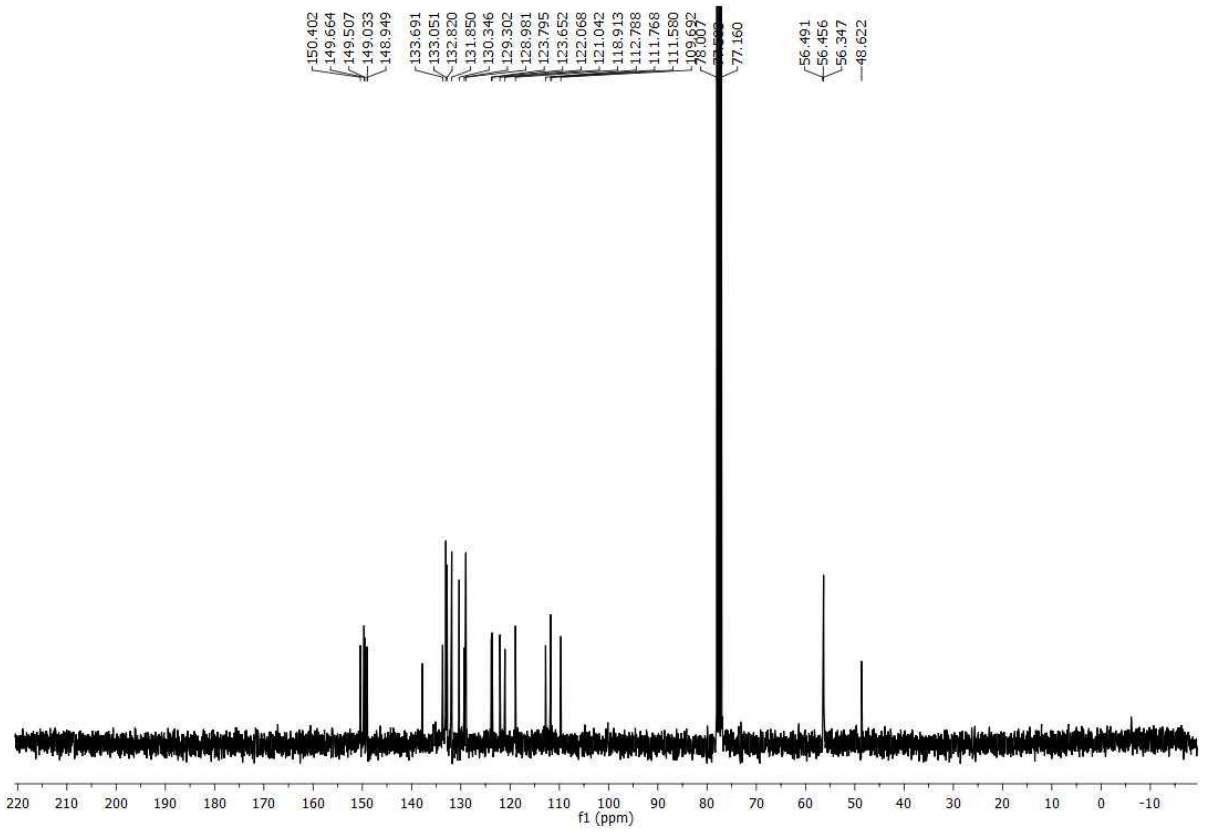
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ab



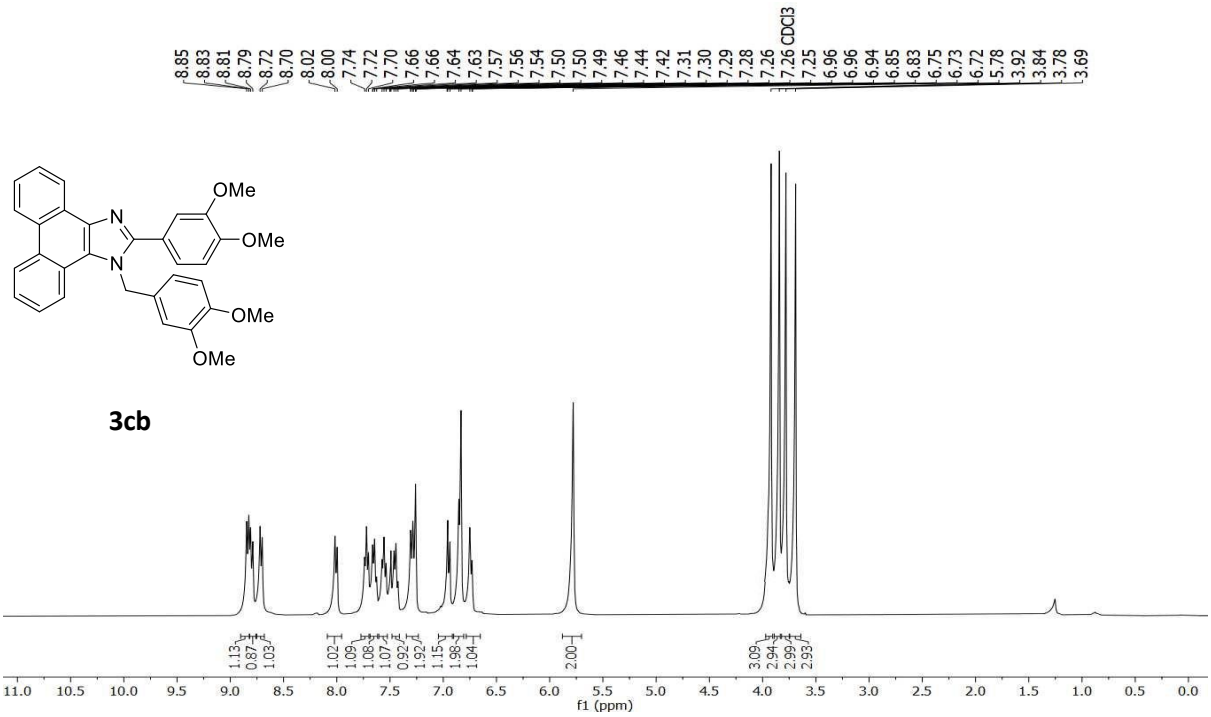
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ab



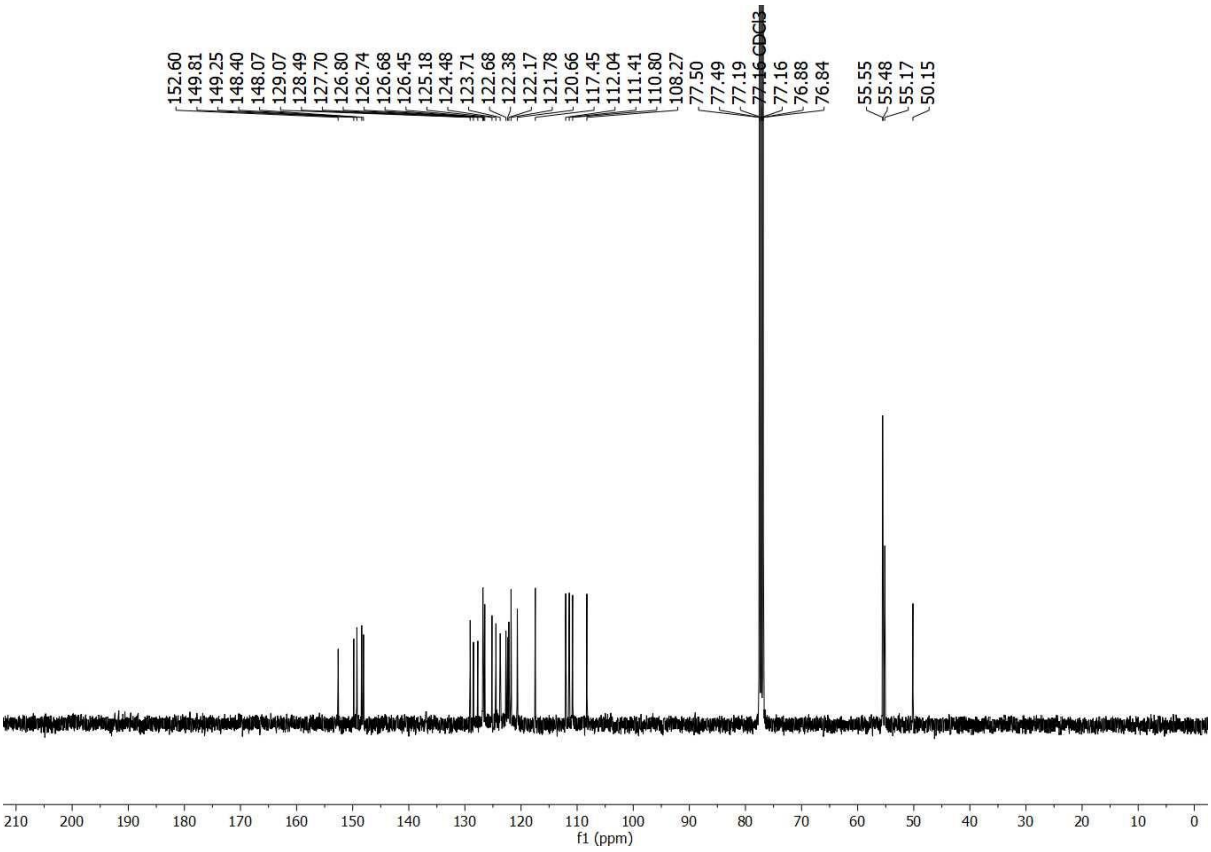
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3bb



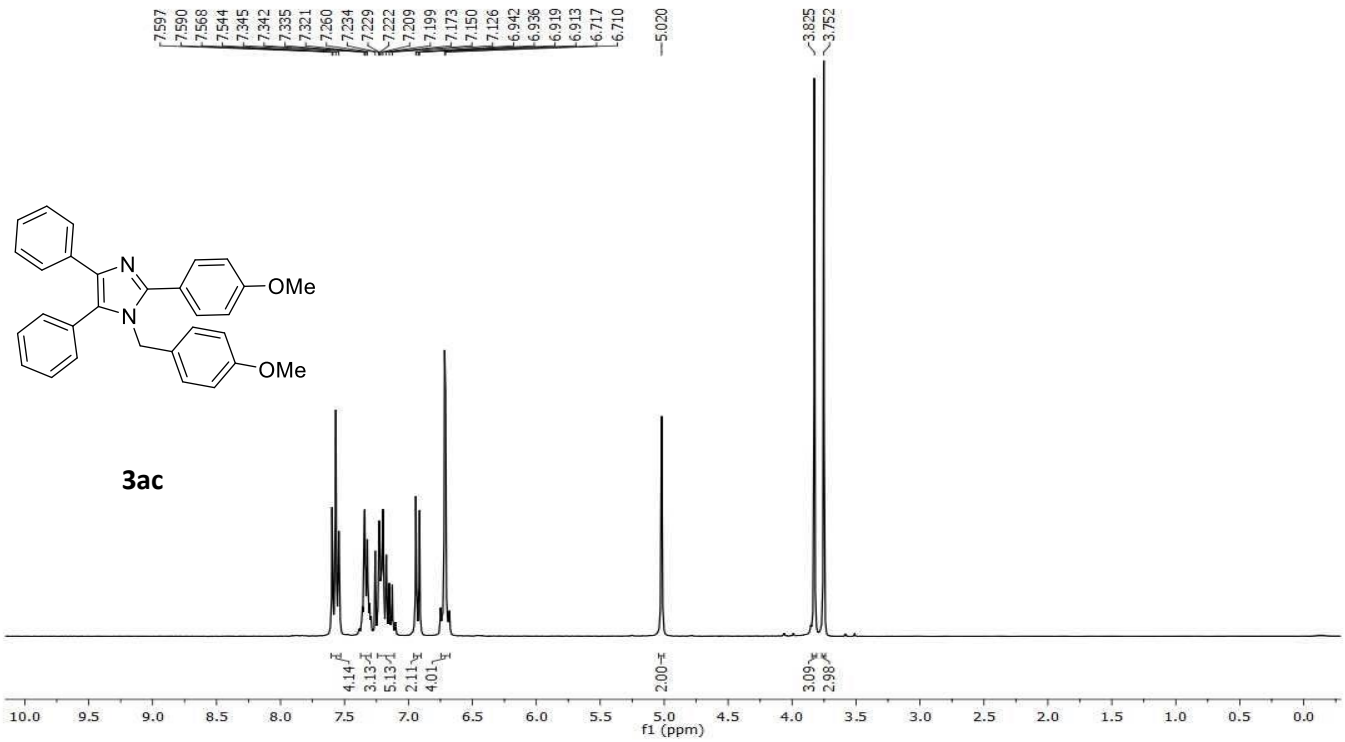
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3bb



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3cb

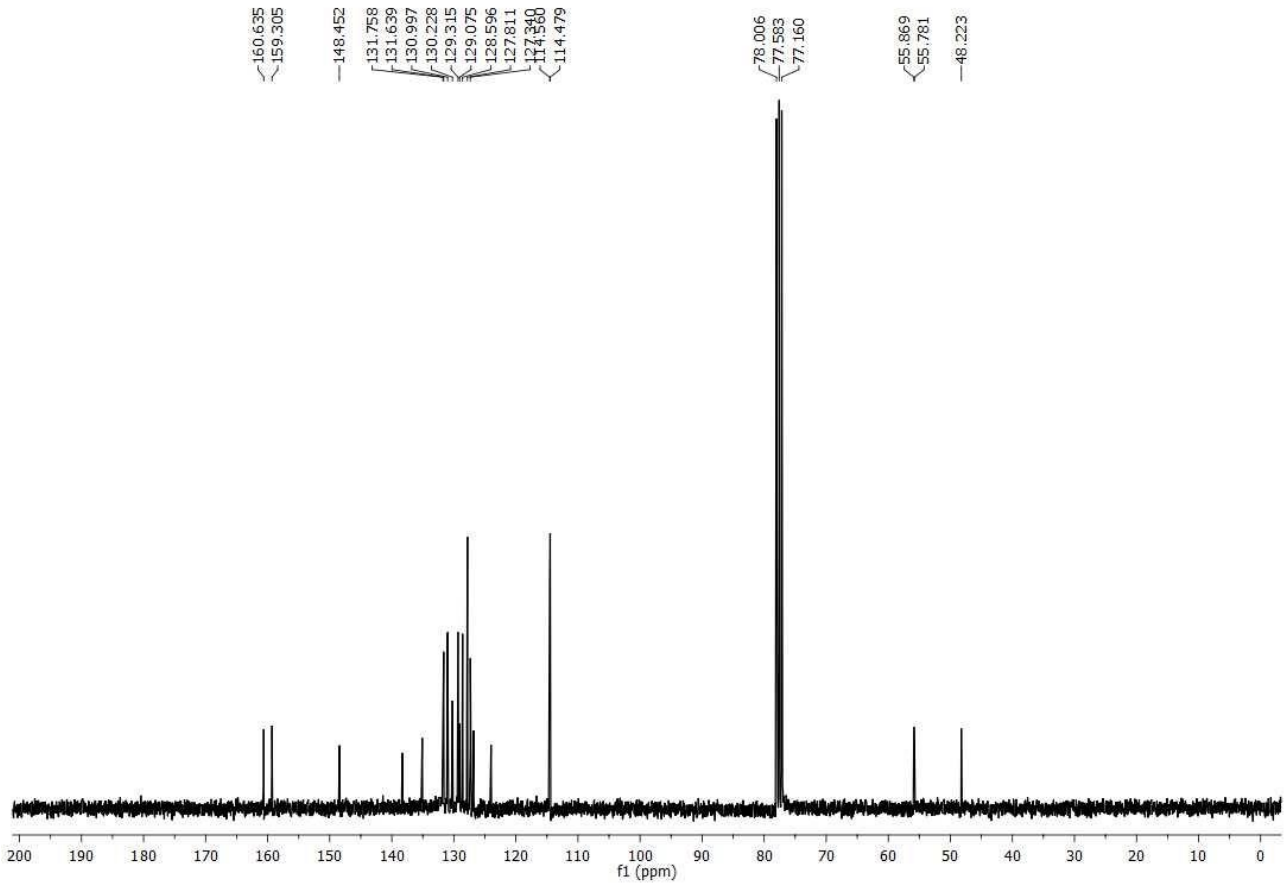


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3cb

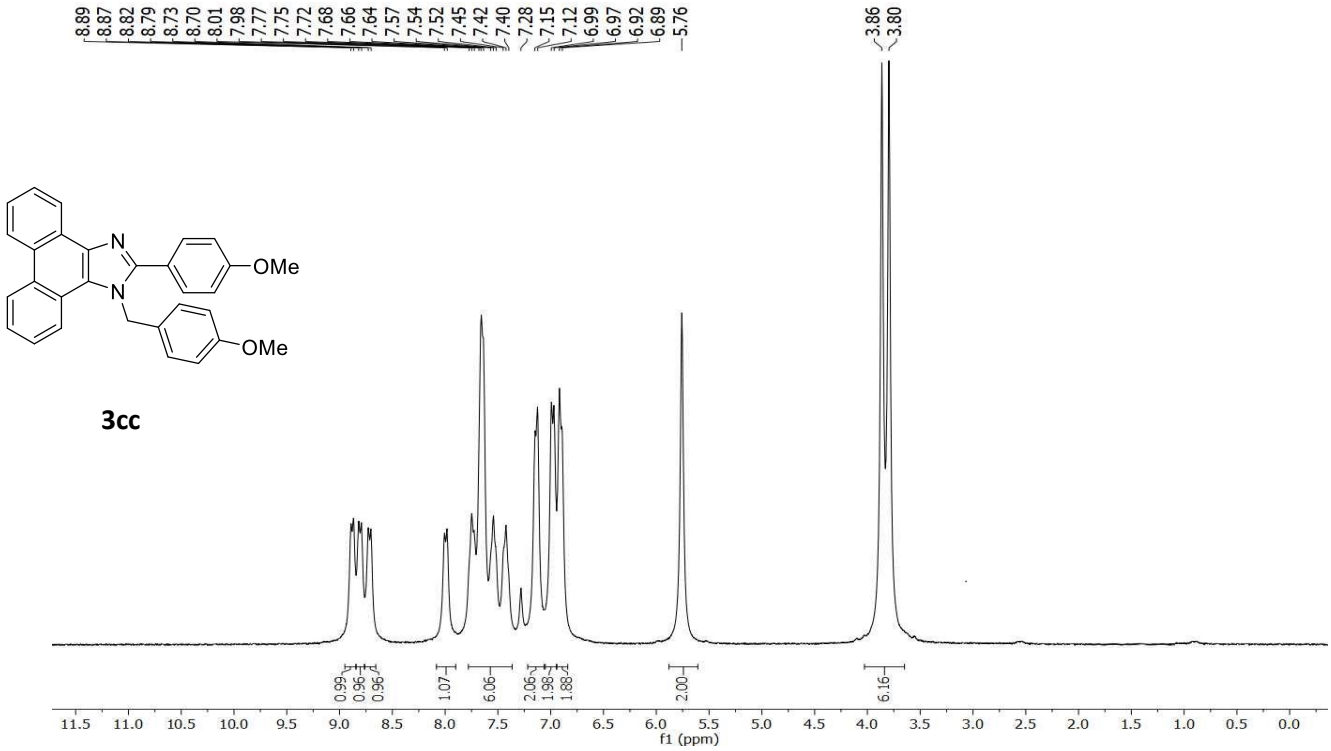


3ac

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ac

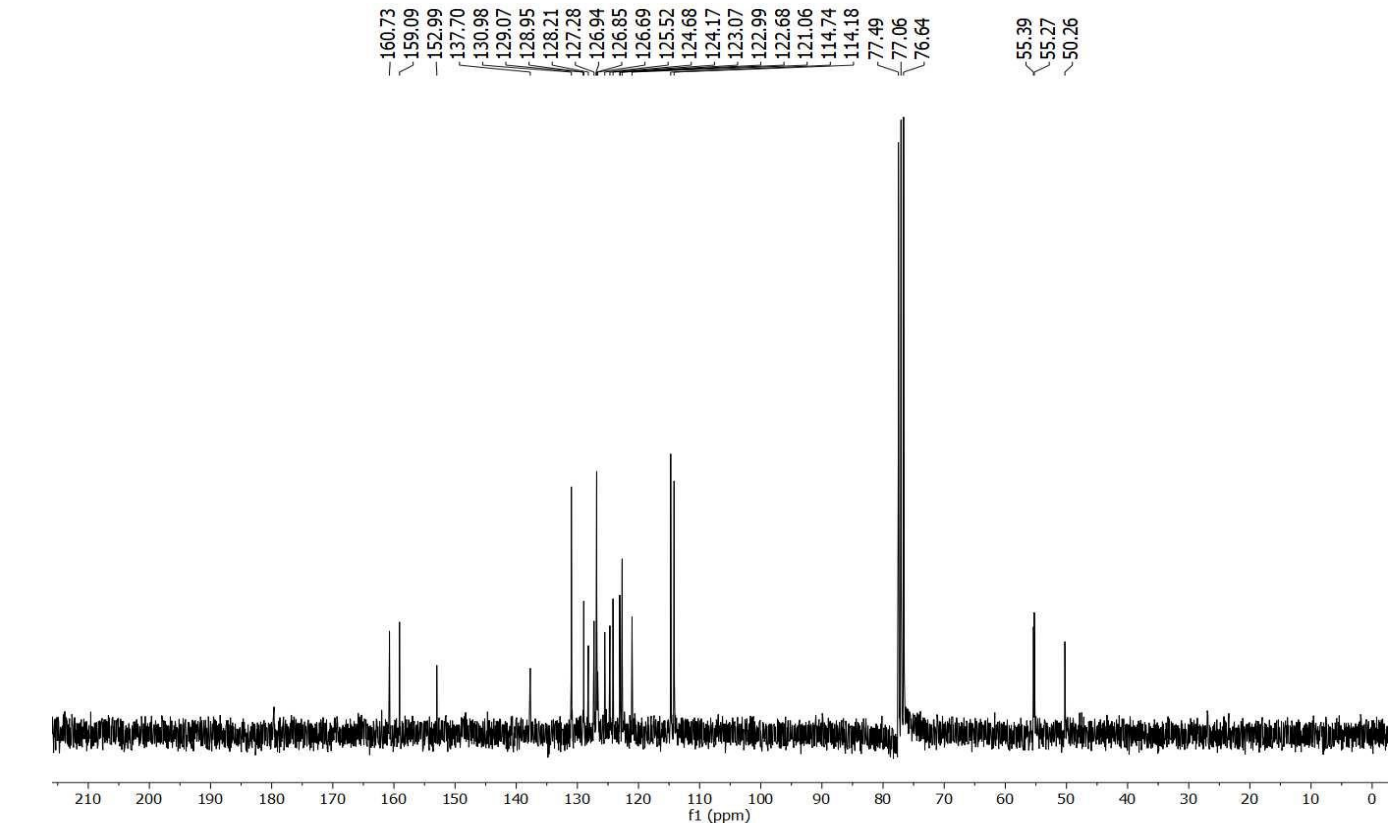


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ac

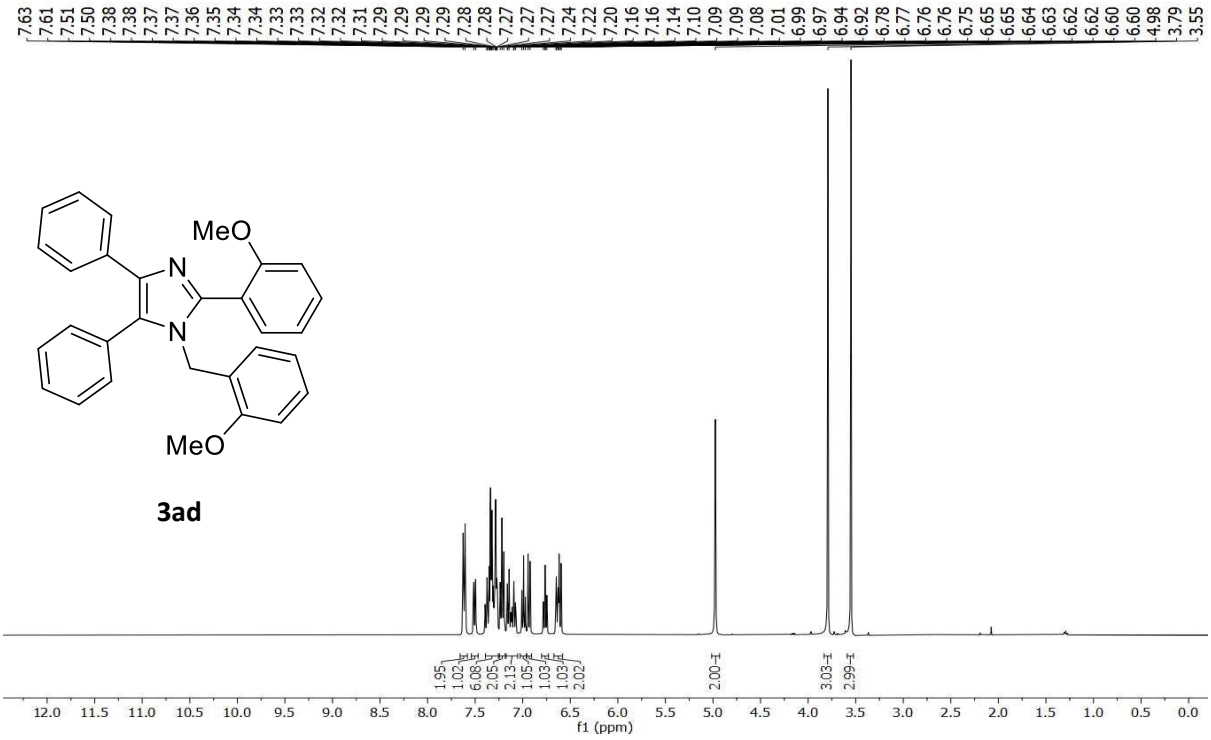


3cc

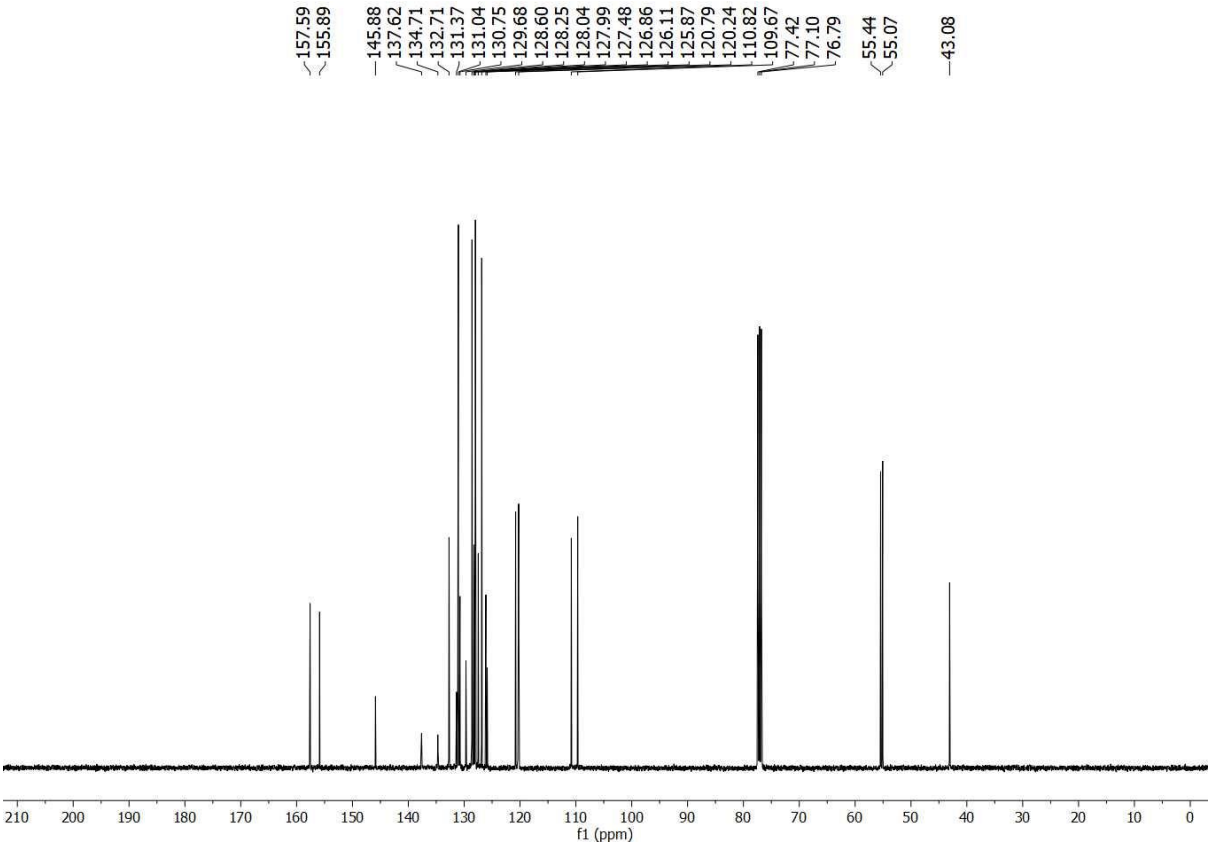
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3cc



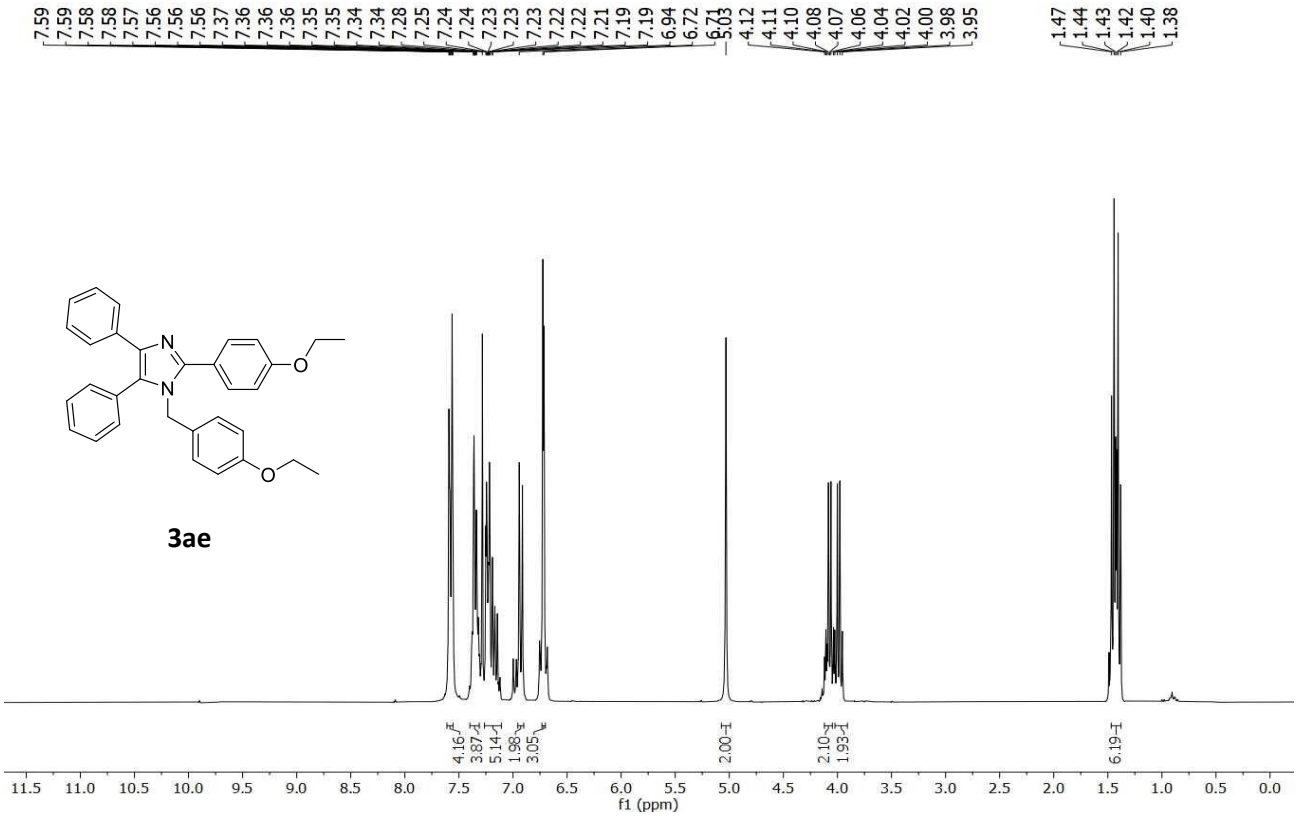
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3cc



^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3ad

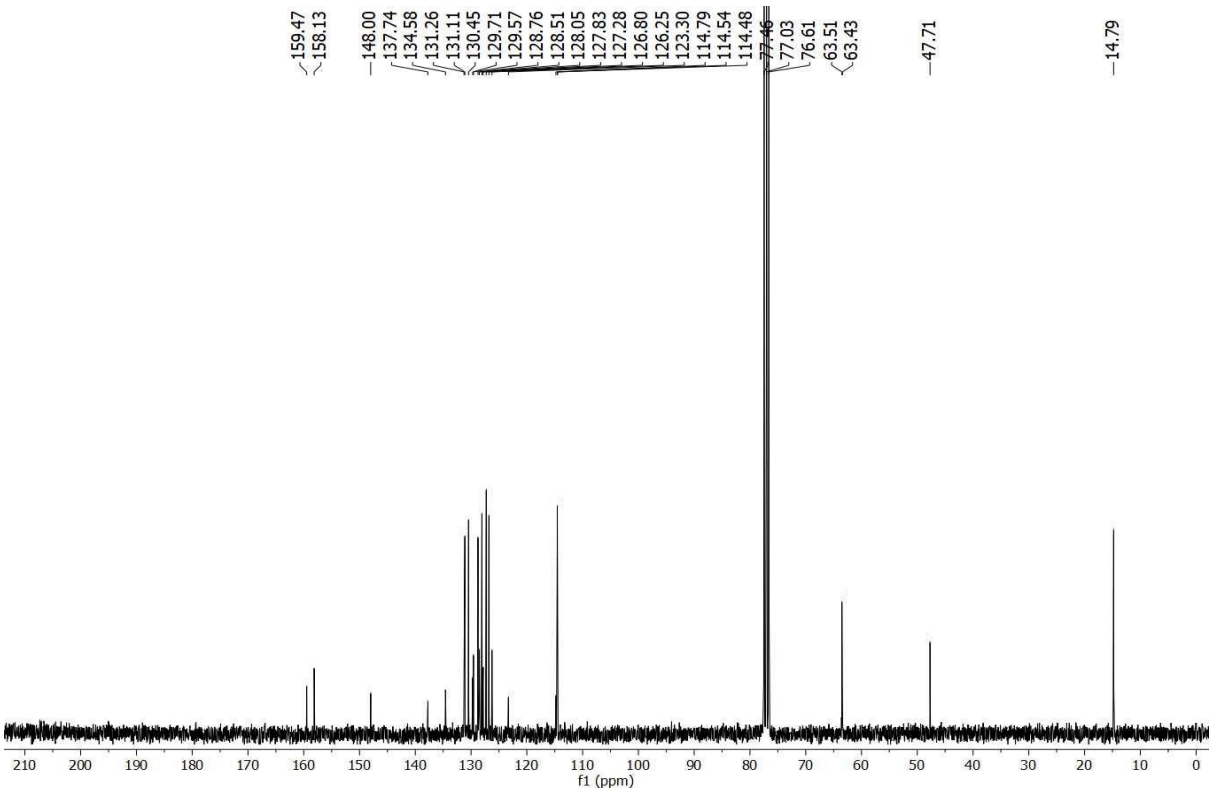


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3ad

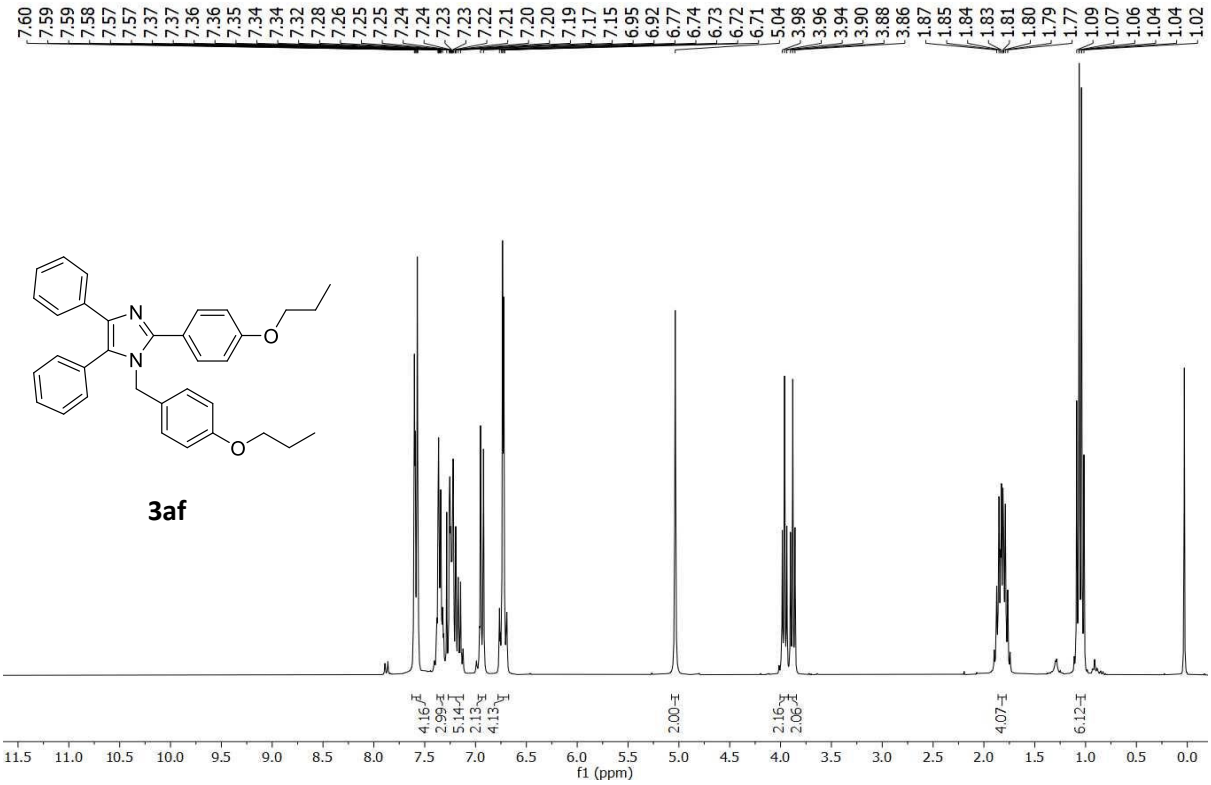


3ae

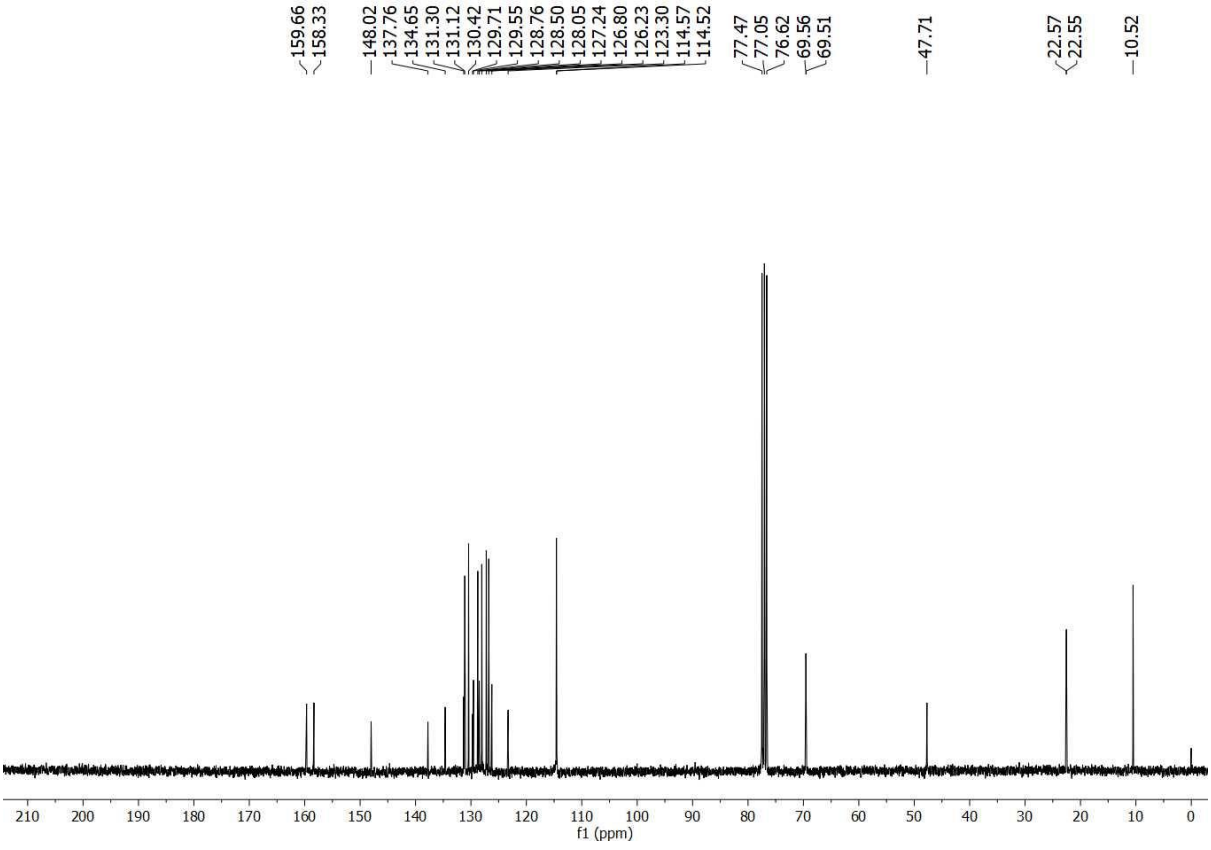
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ae



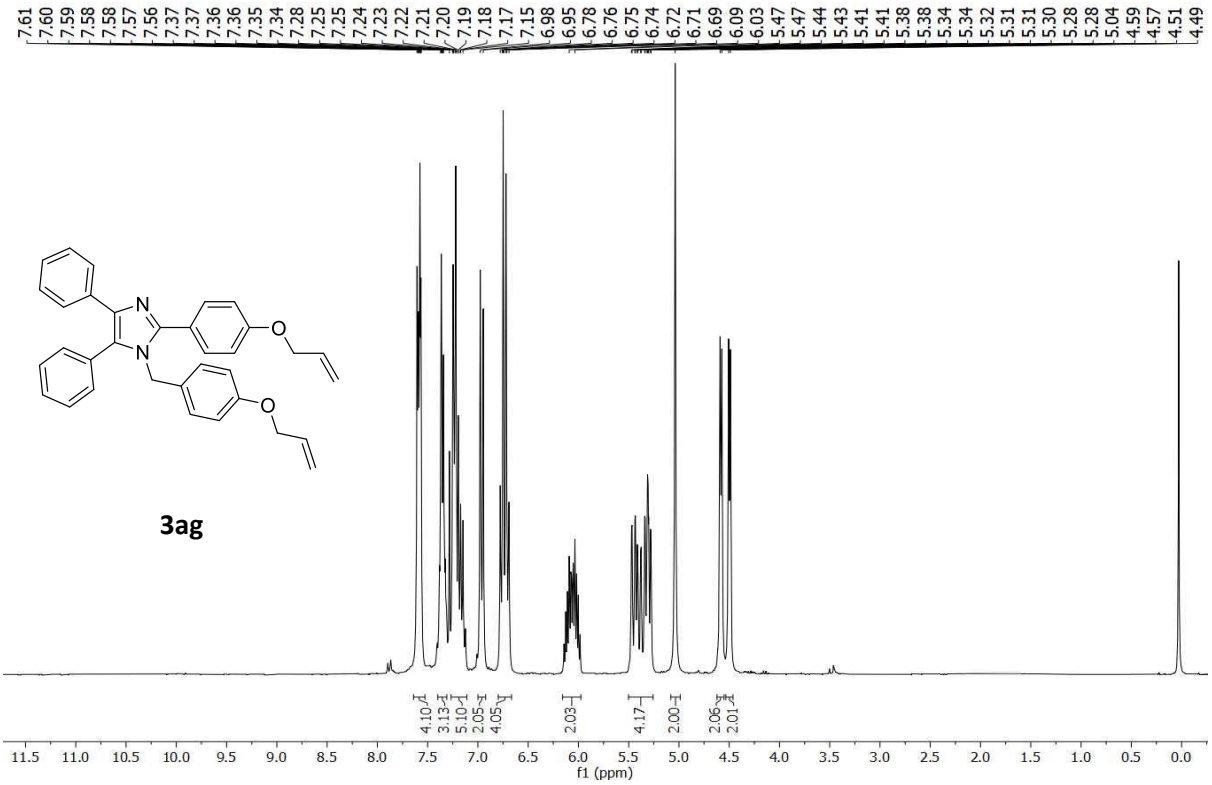
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ae



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3af

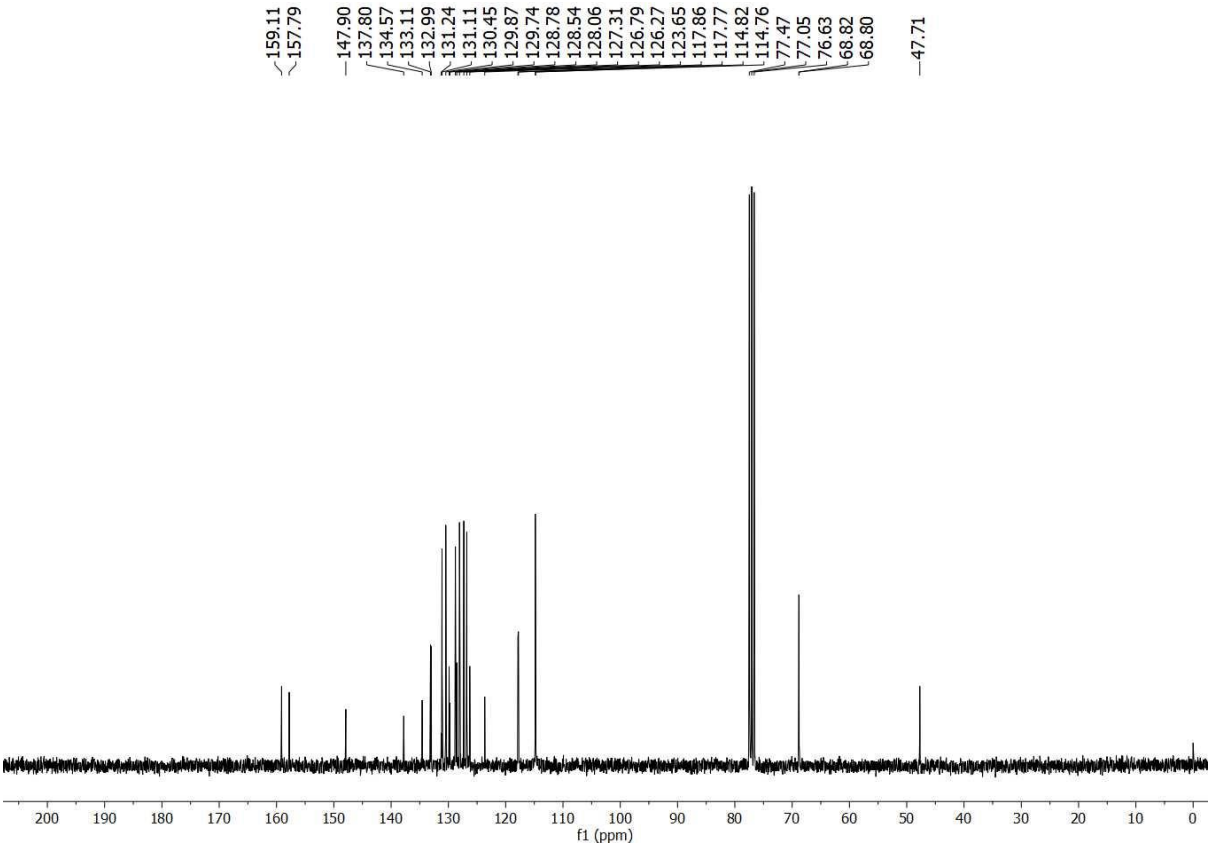


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3af

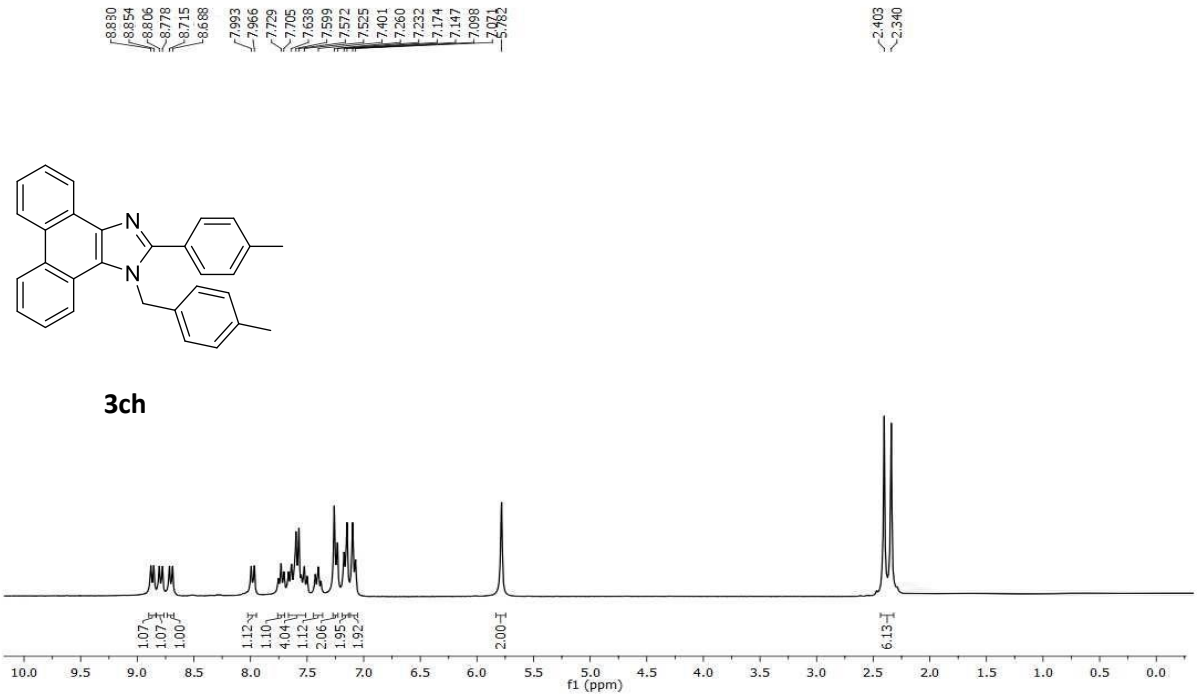


3ag

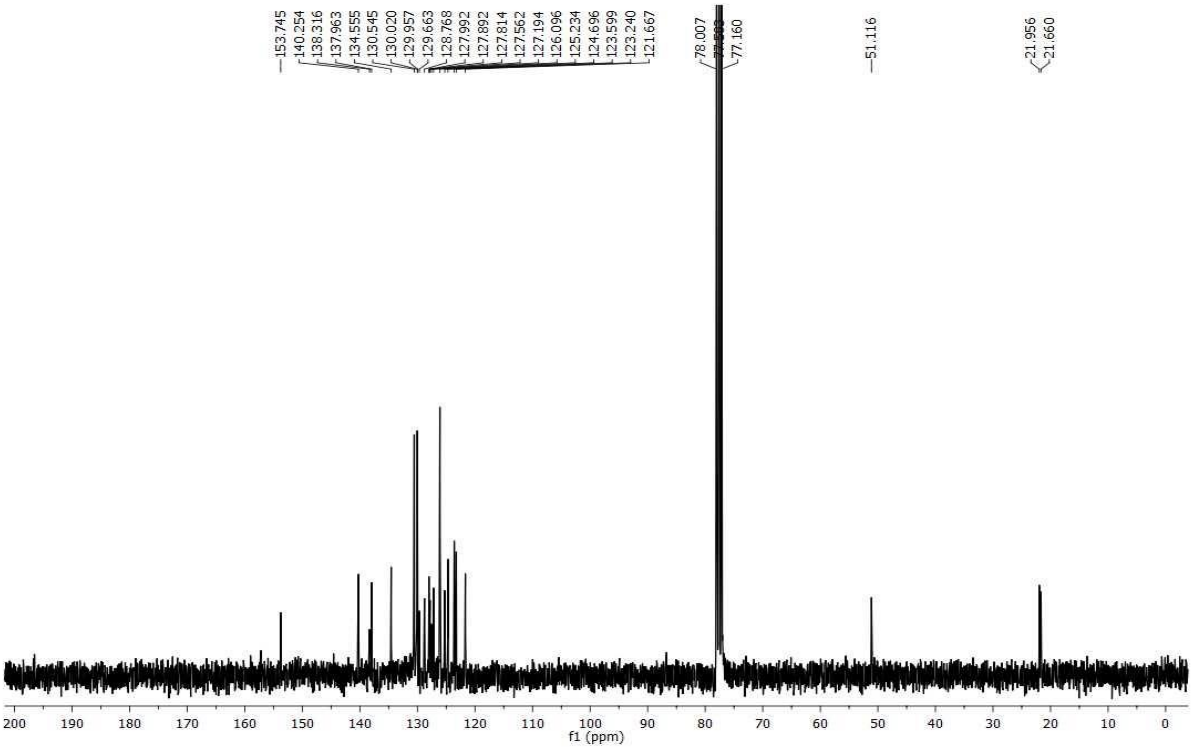
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ag



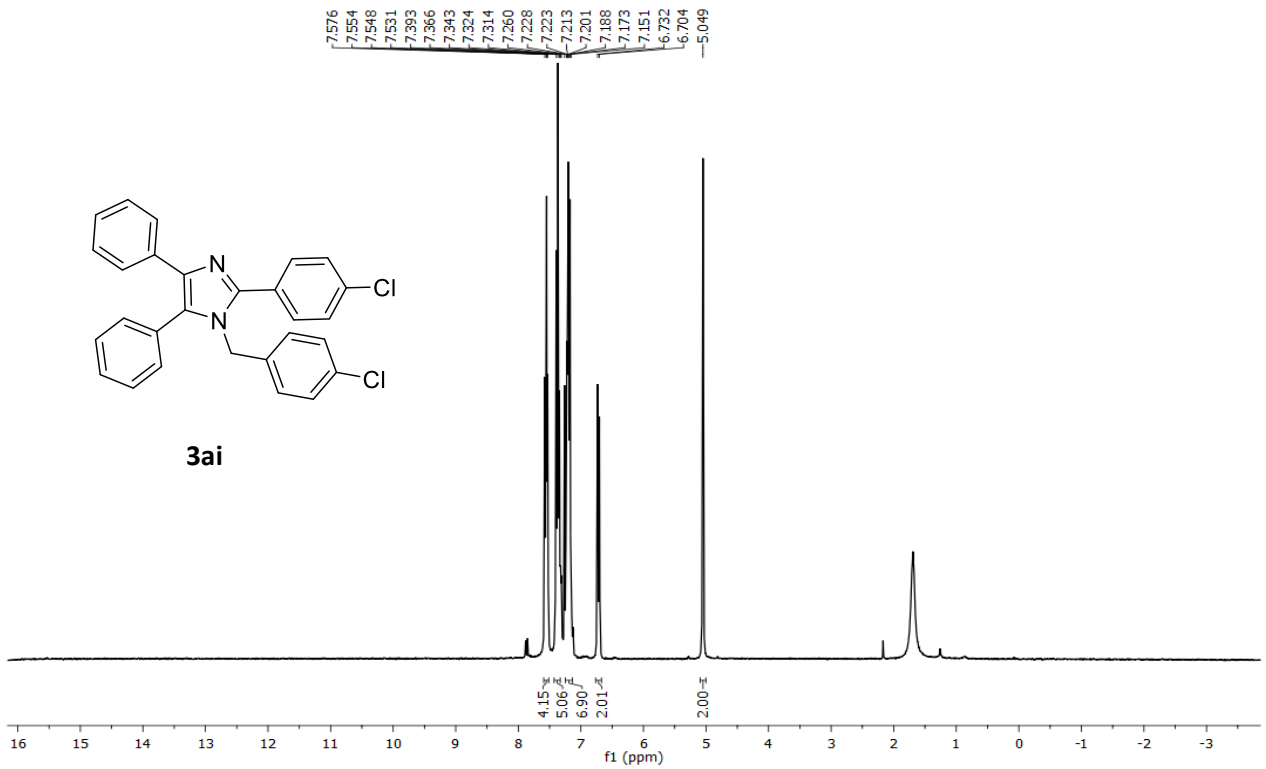
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ag



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ch

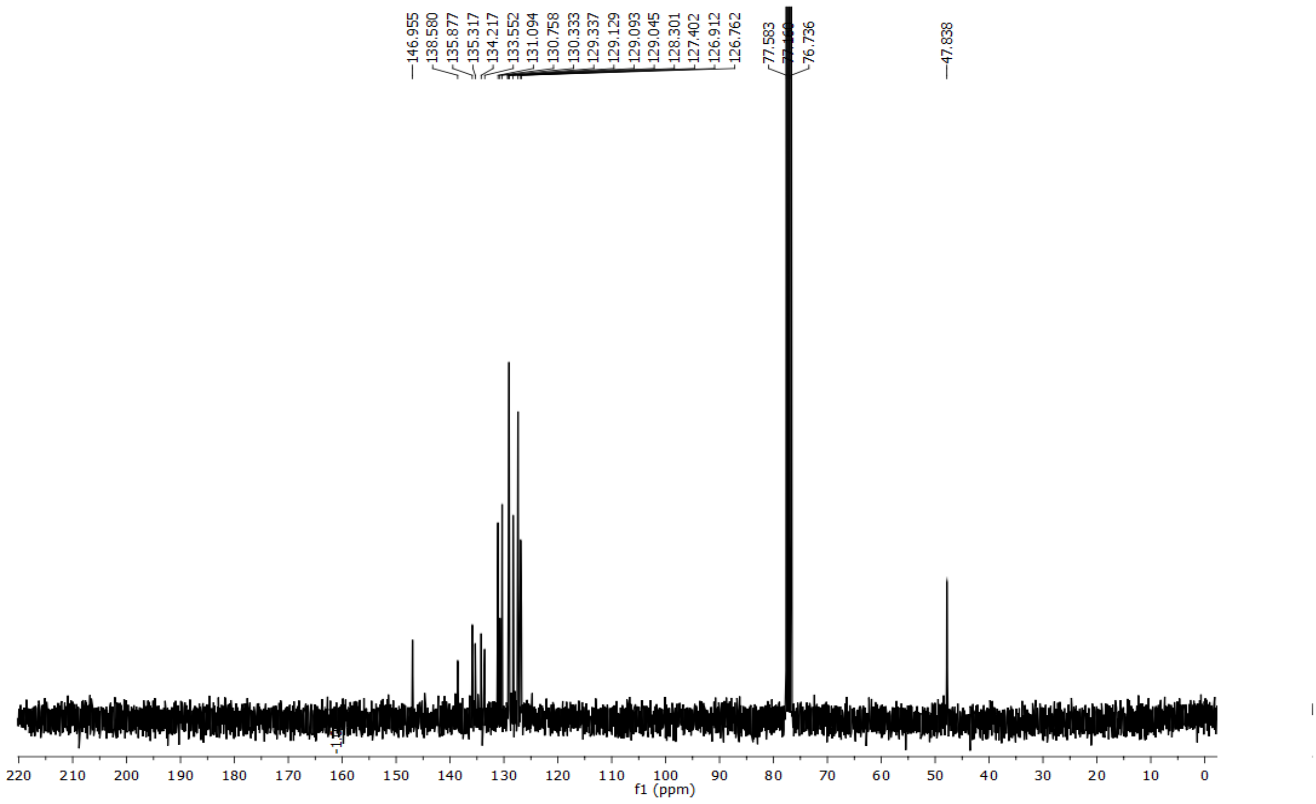


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ch

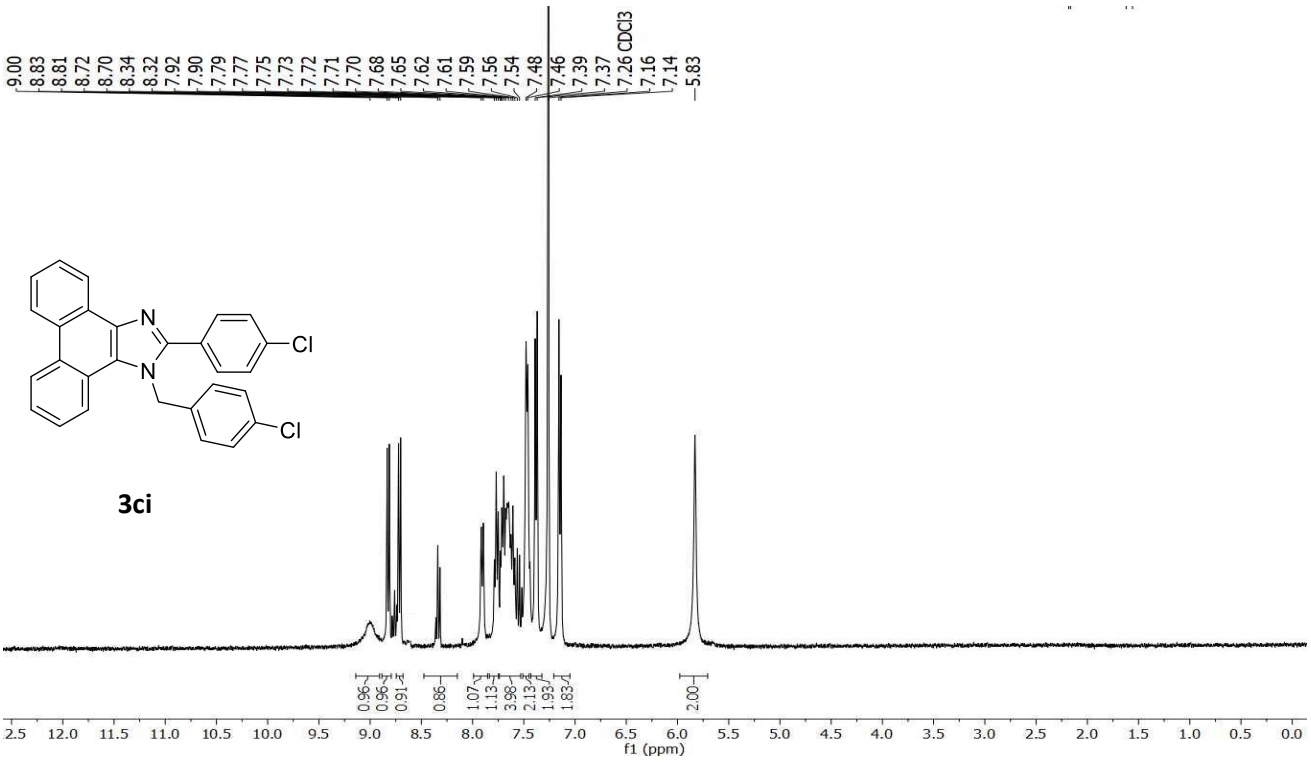


3ai

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ai

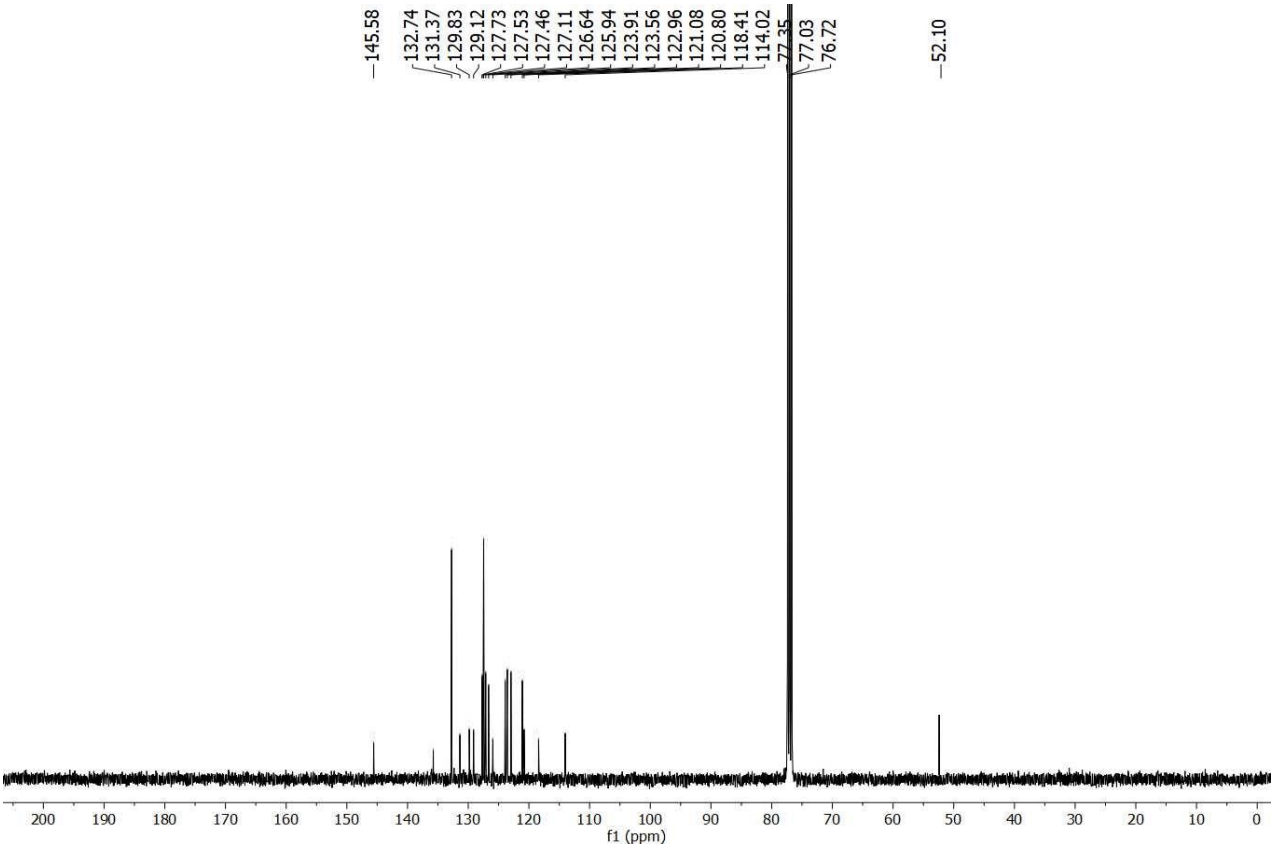


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ai

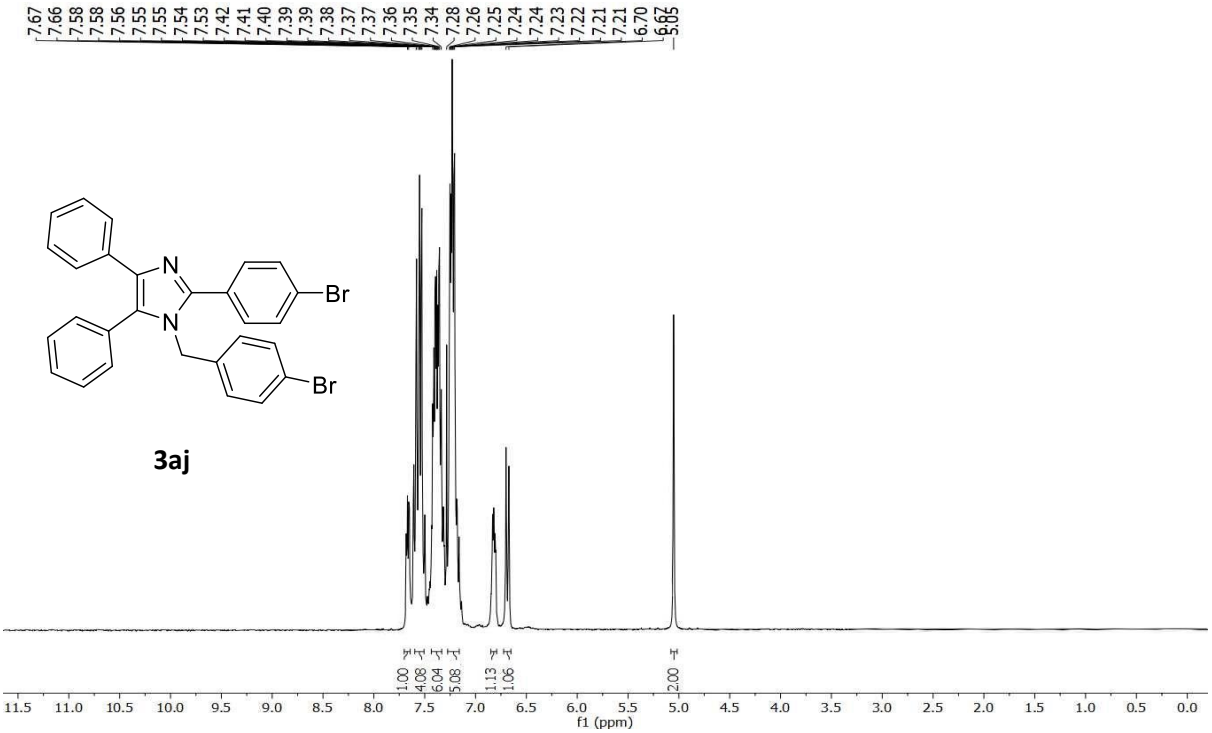


3ci

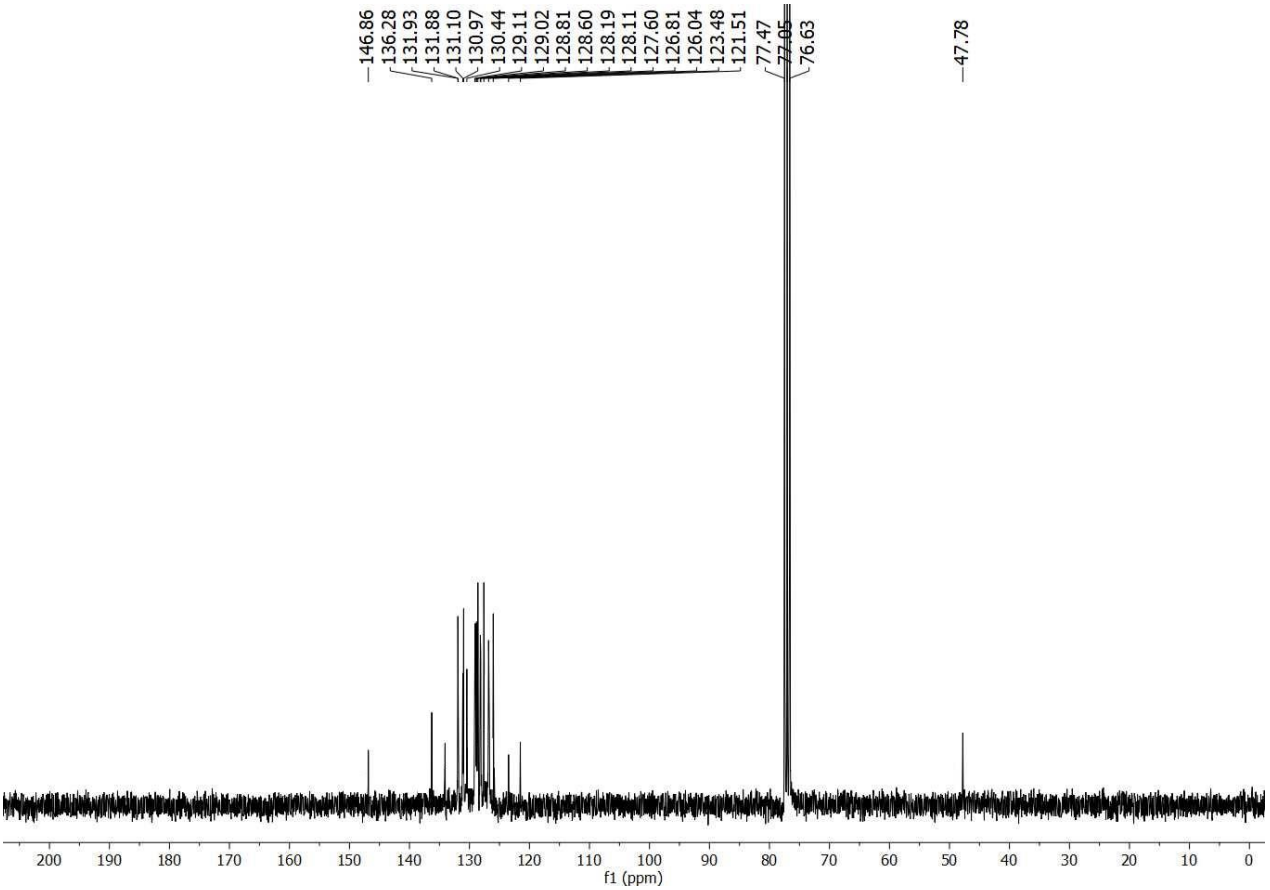
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3ci



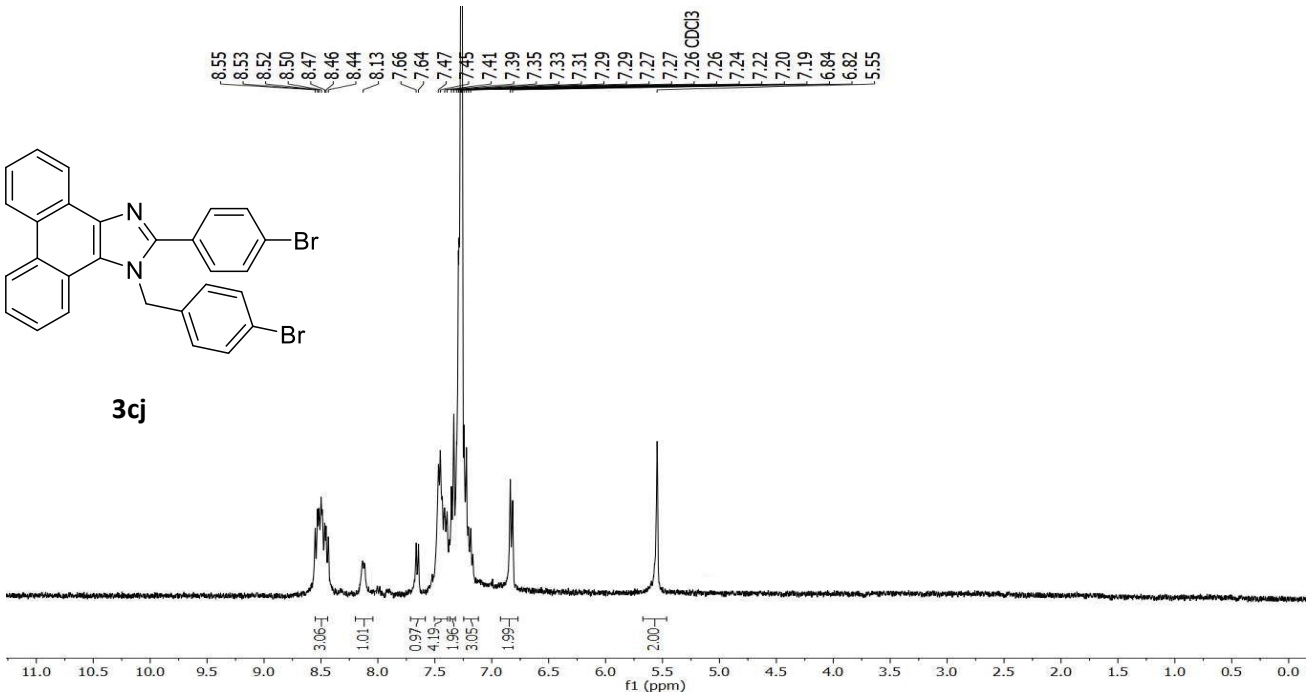
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3ai



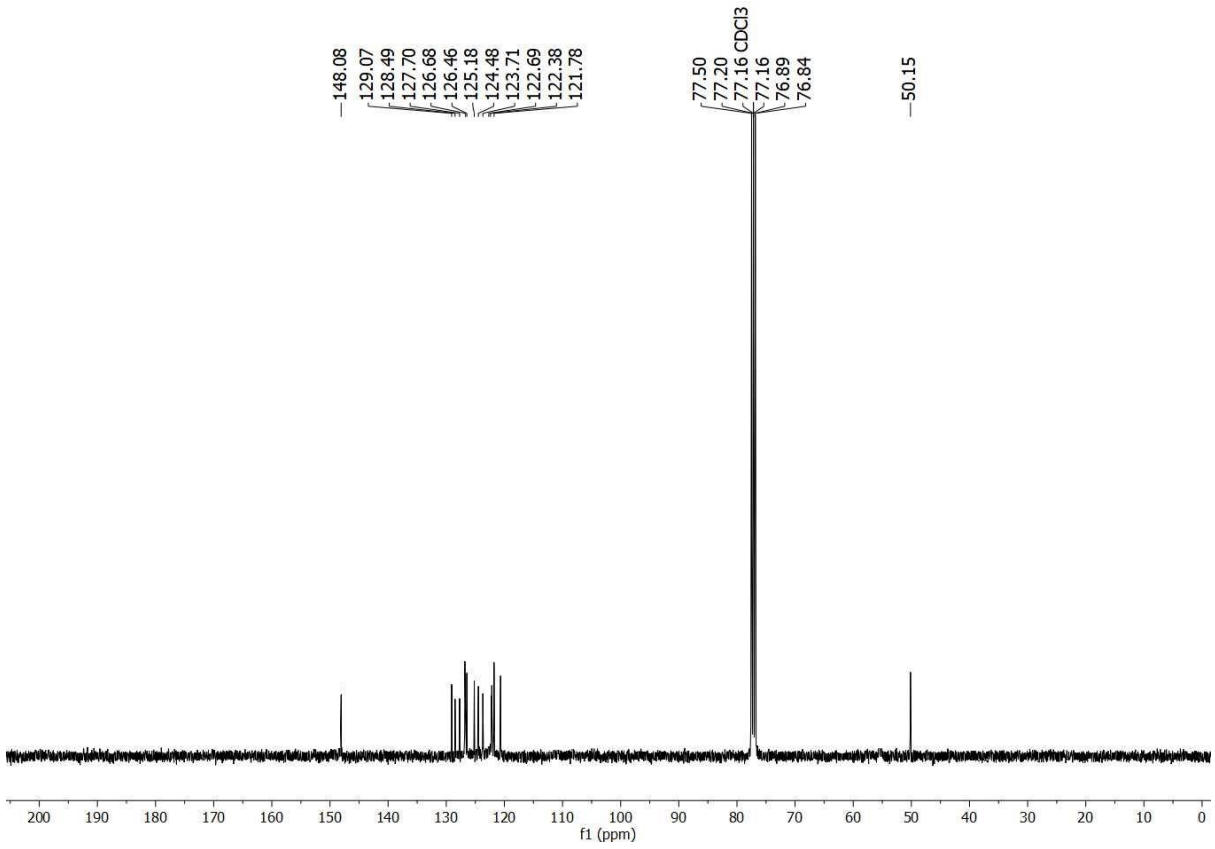
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3aj



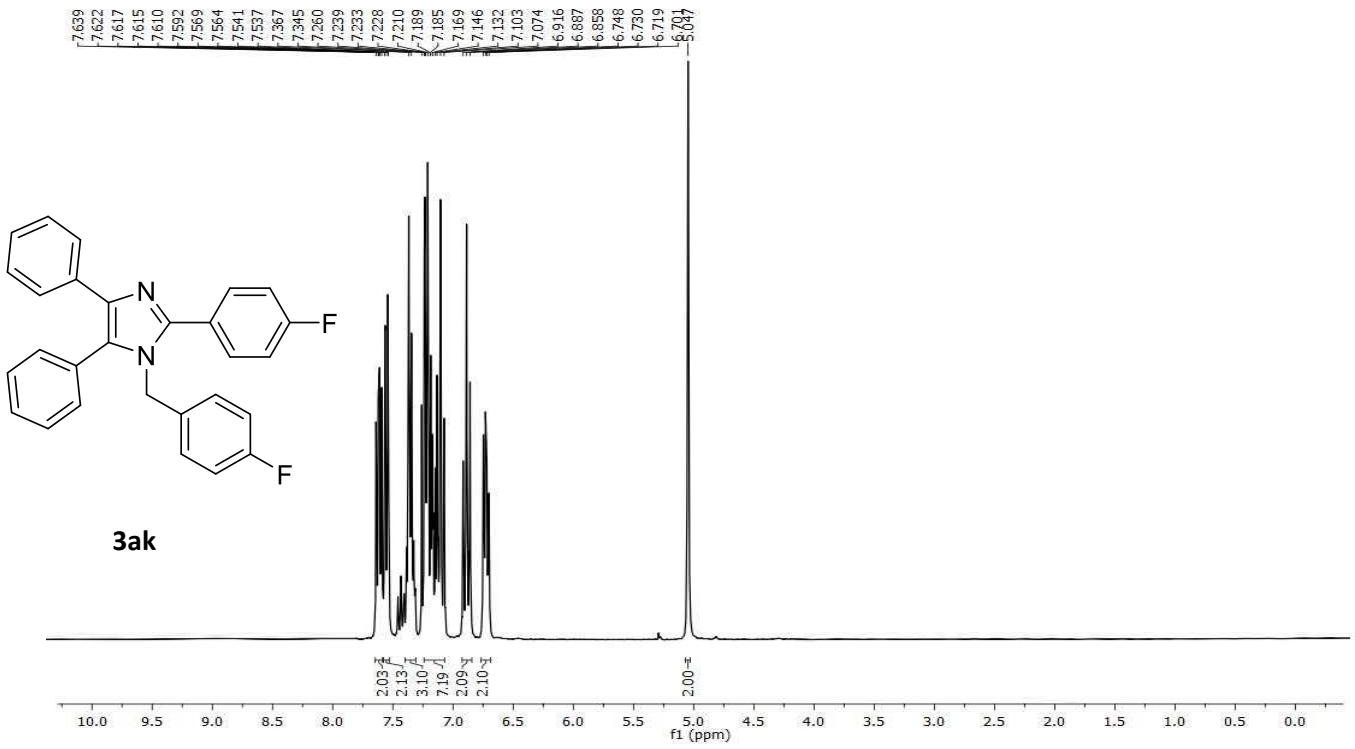
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3aj



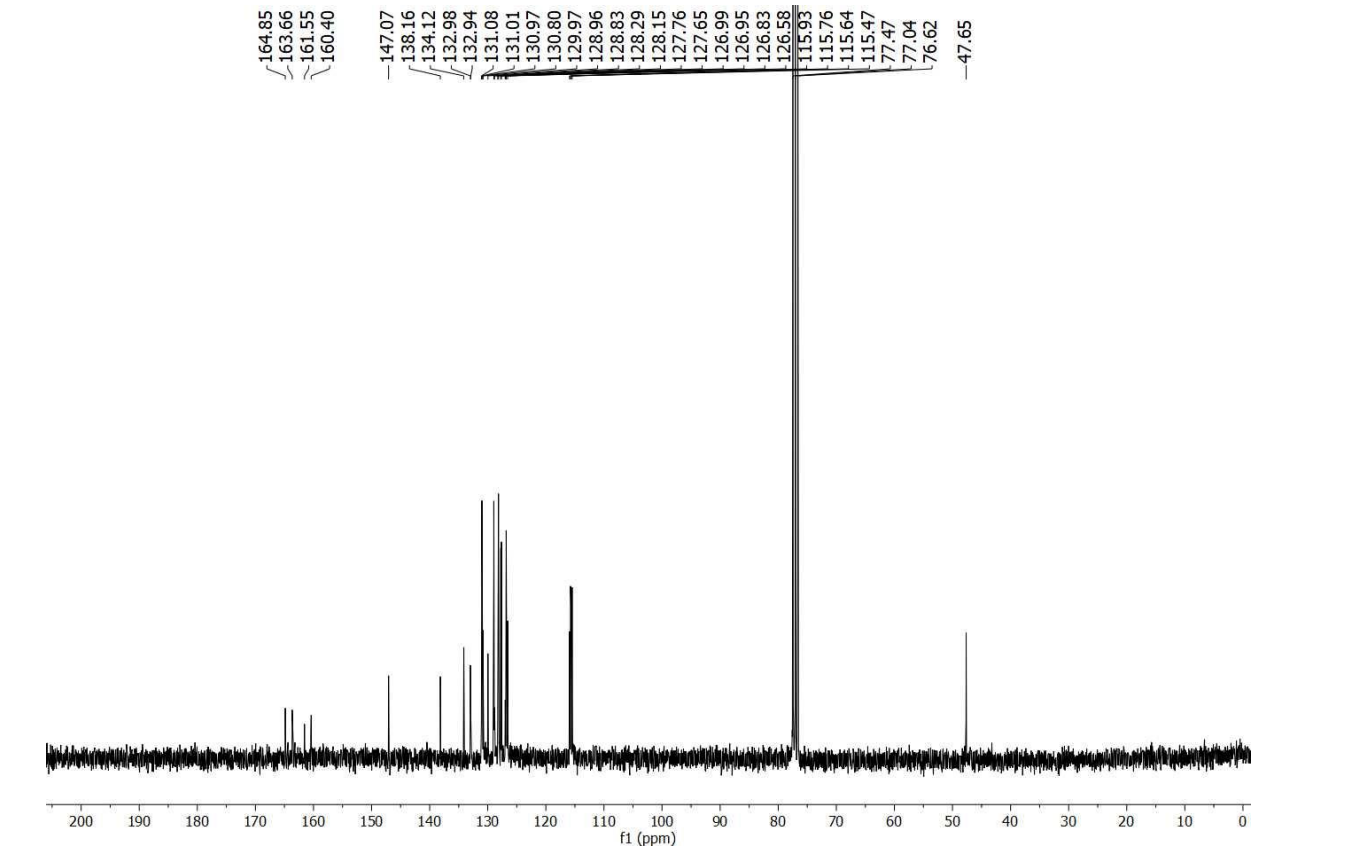
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3cj



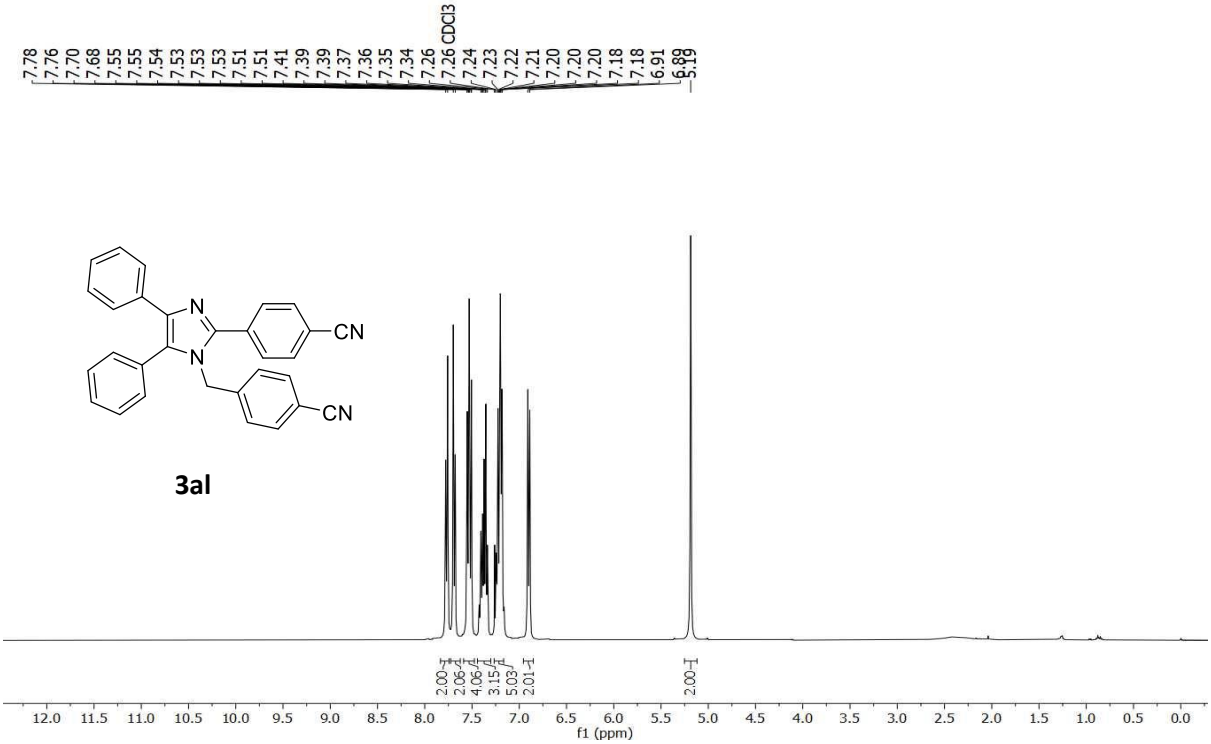
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3cj



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ak

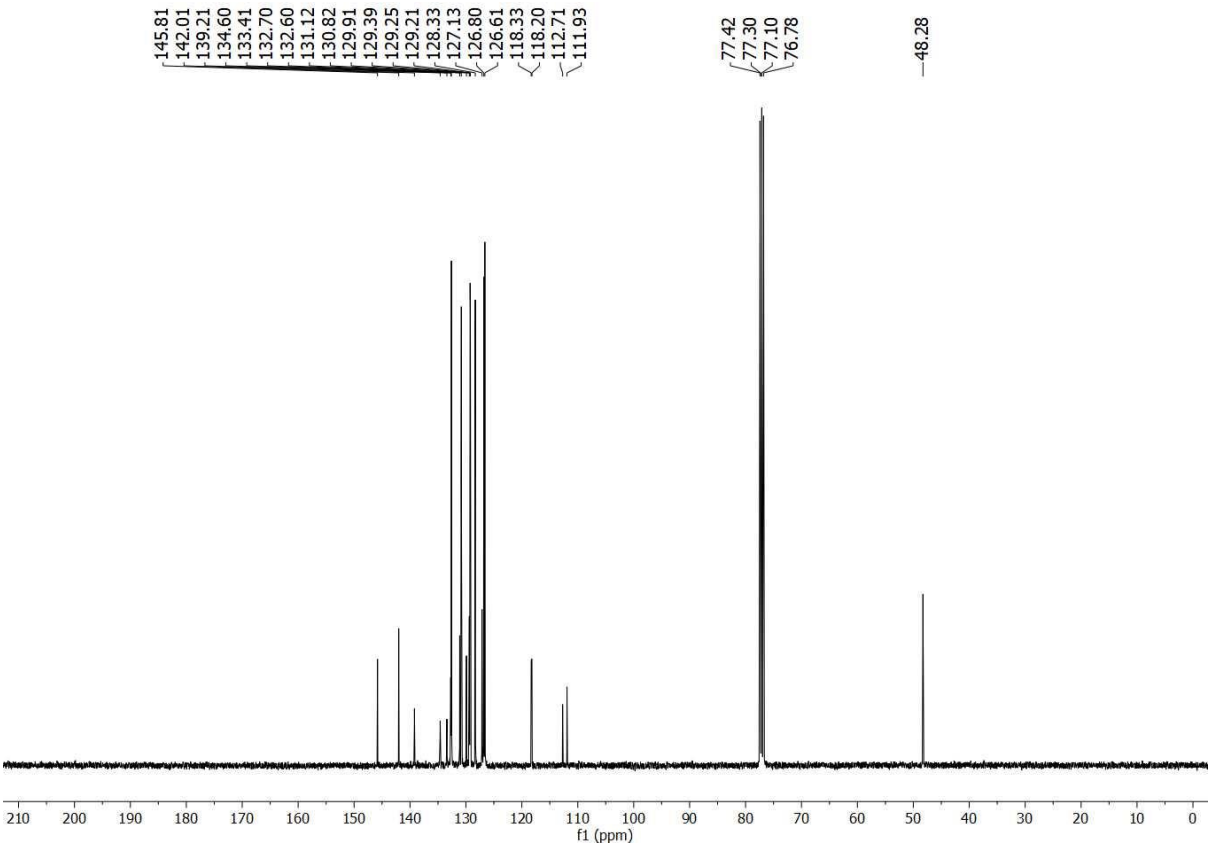


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ak

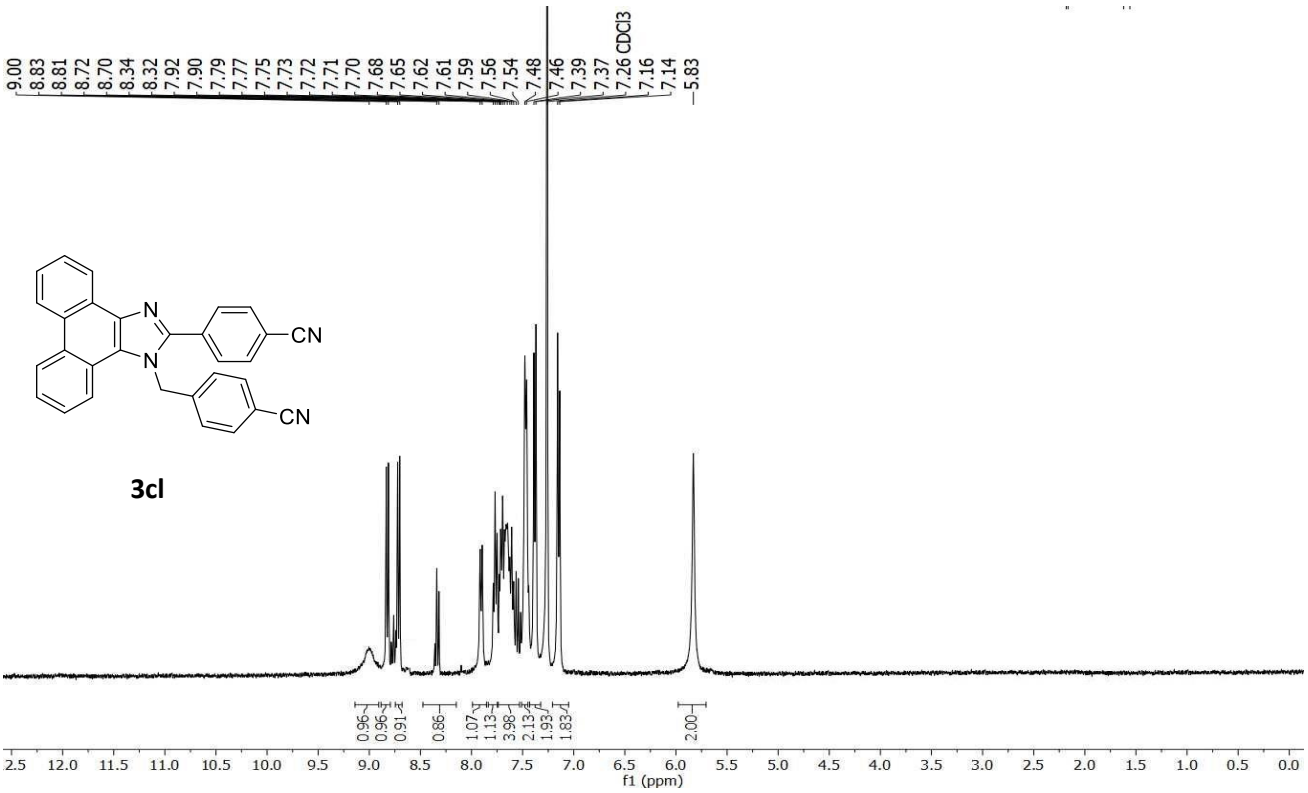


3al

^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3al

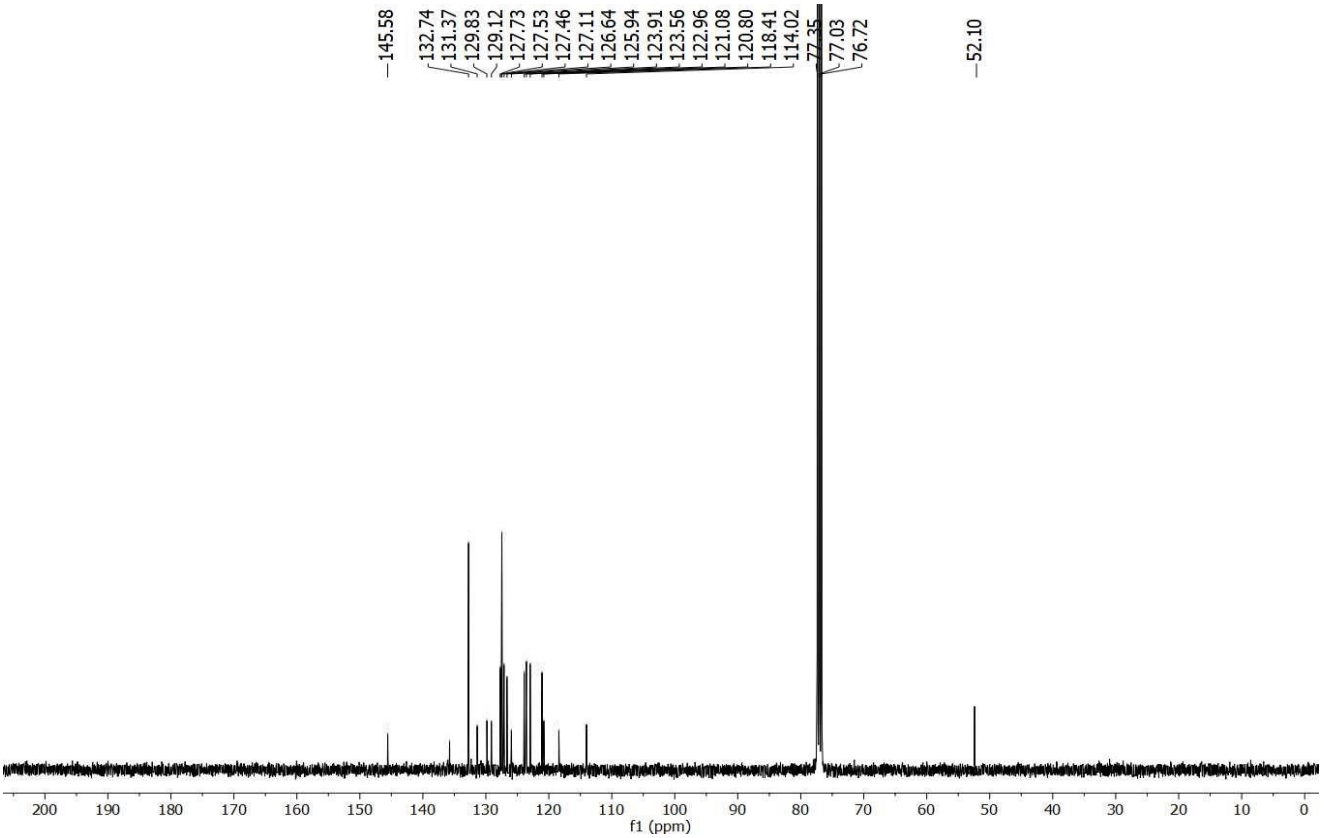


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3al

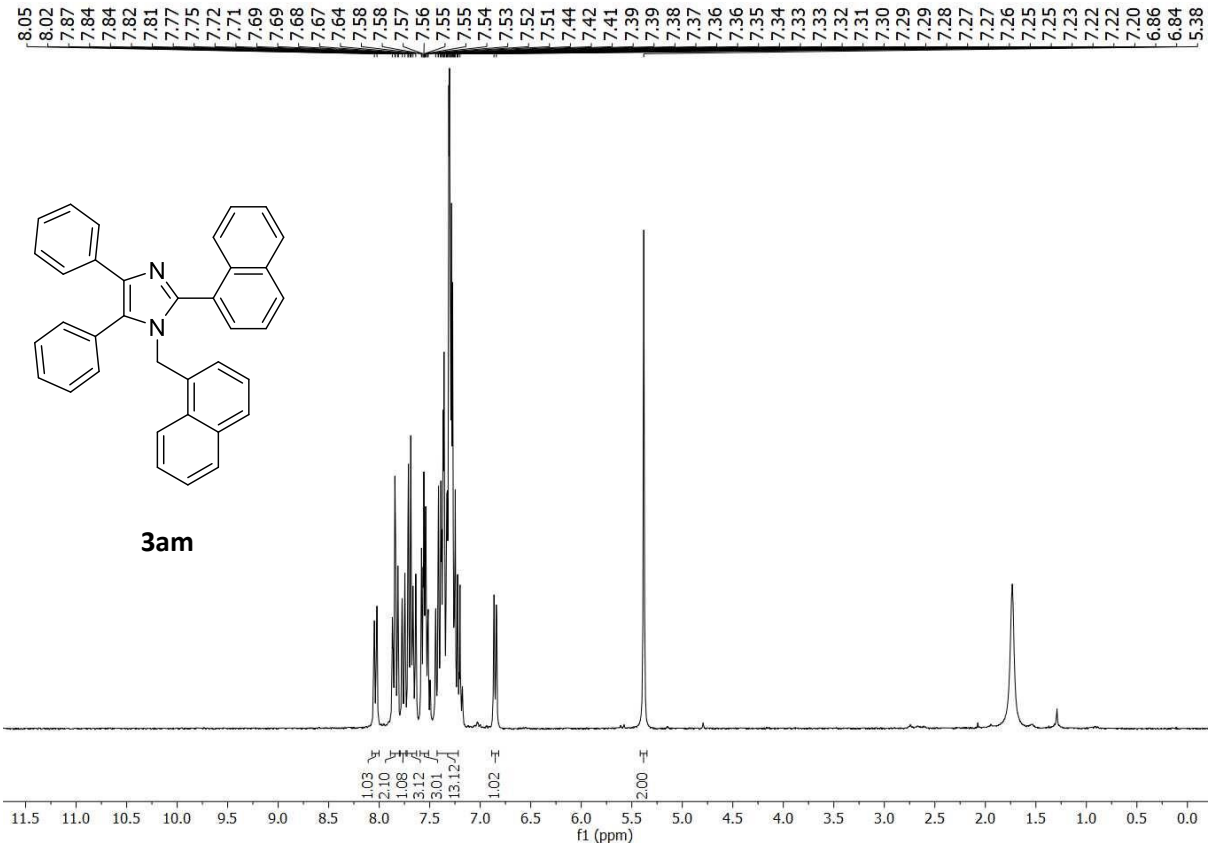


3cl

^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3cl

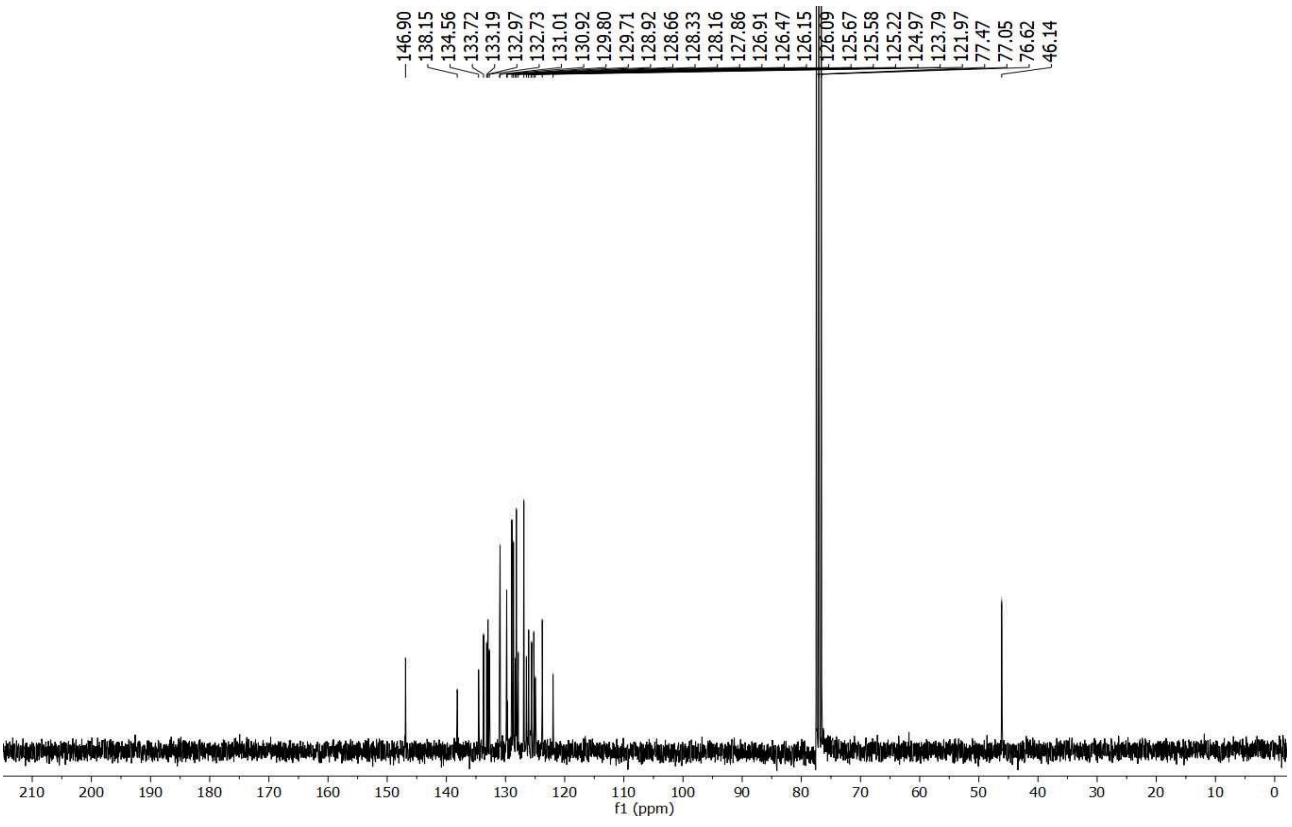


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3cl

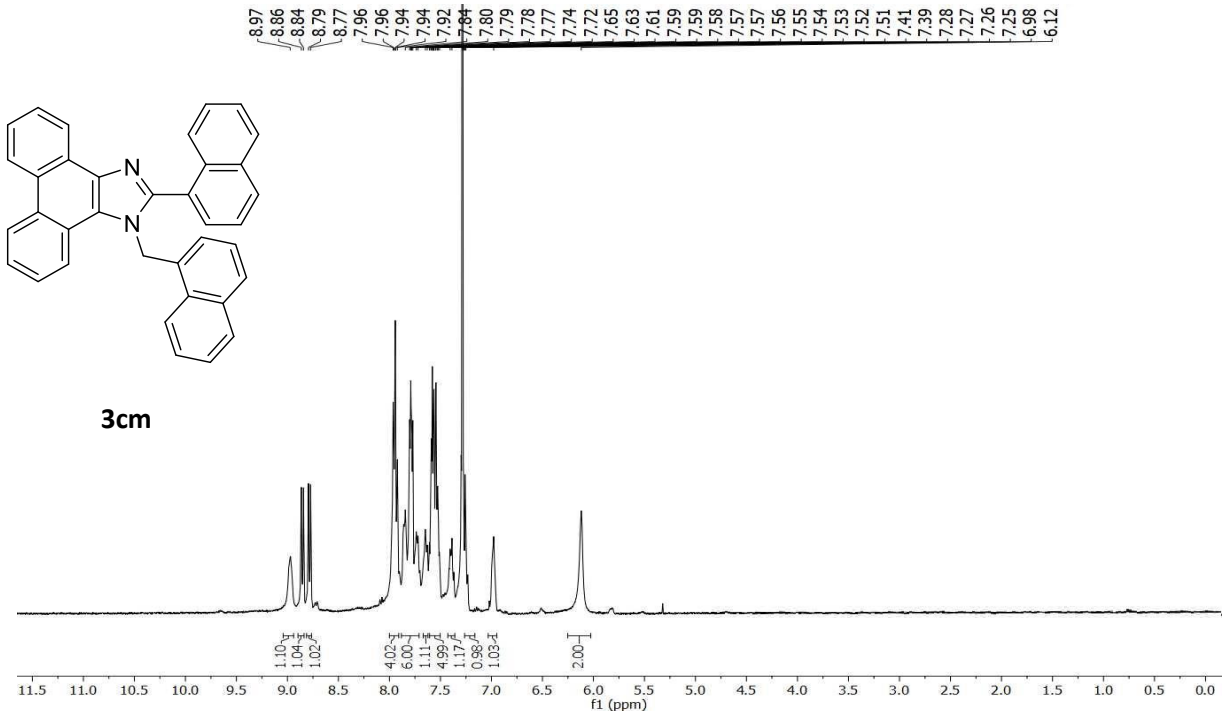


3am

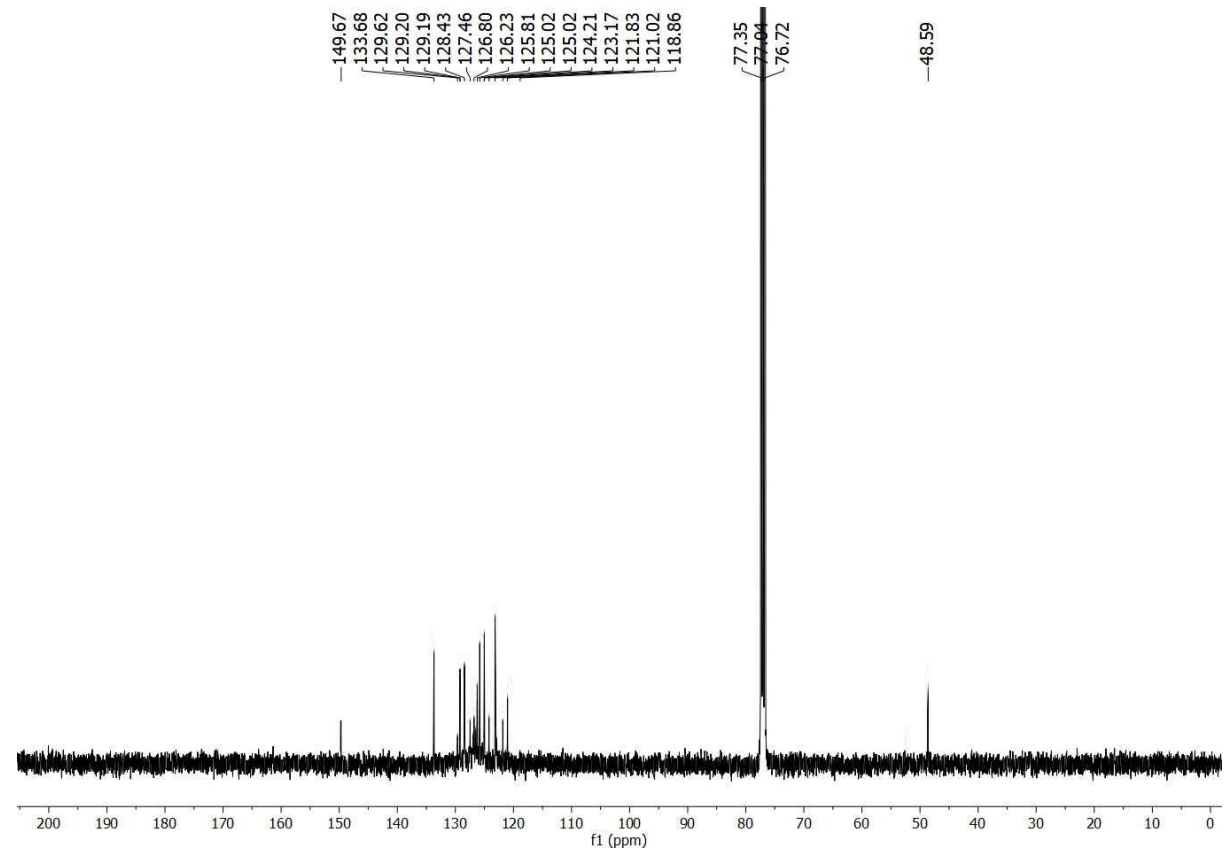
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3am



^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3am

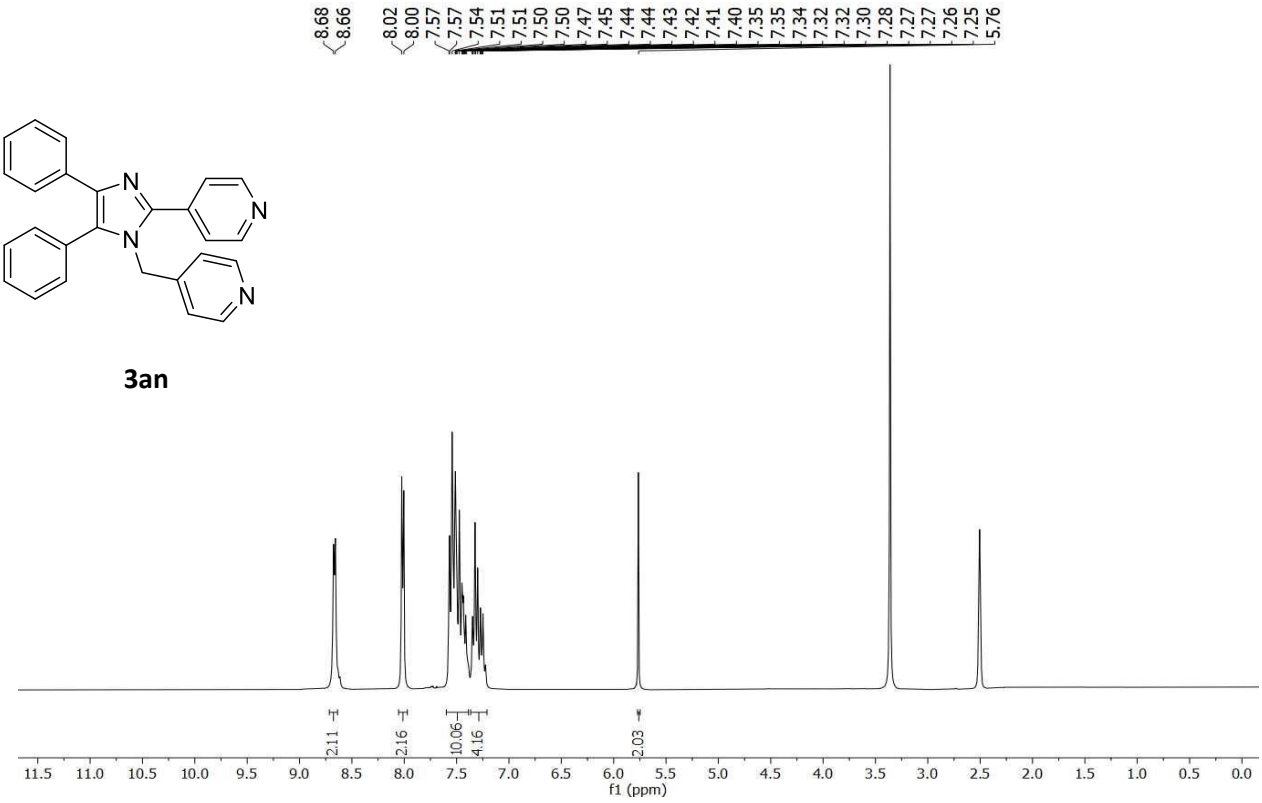


^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 3cm

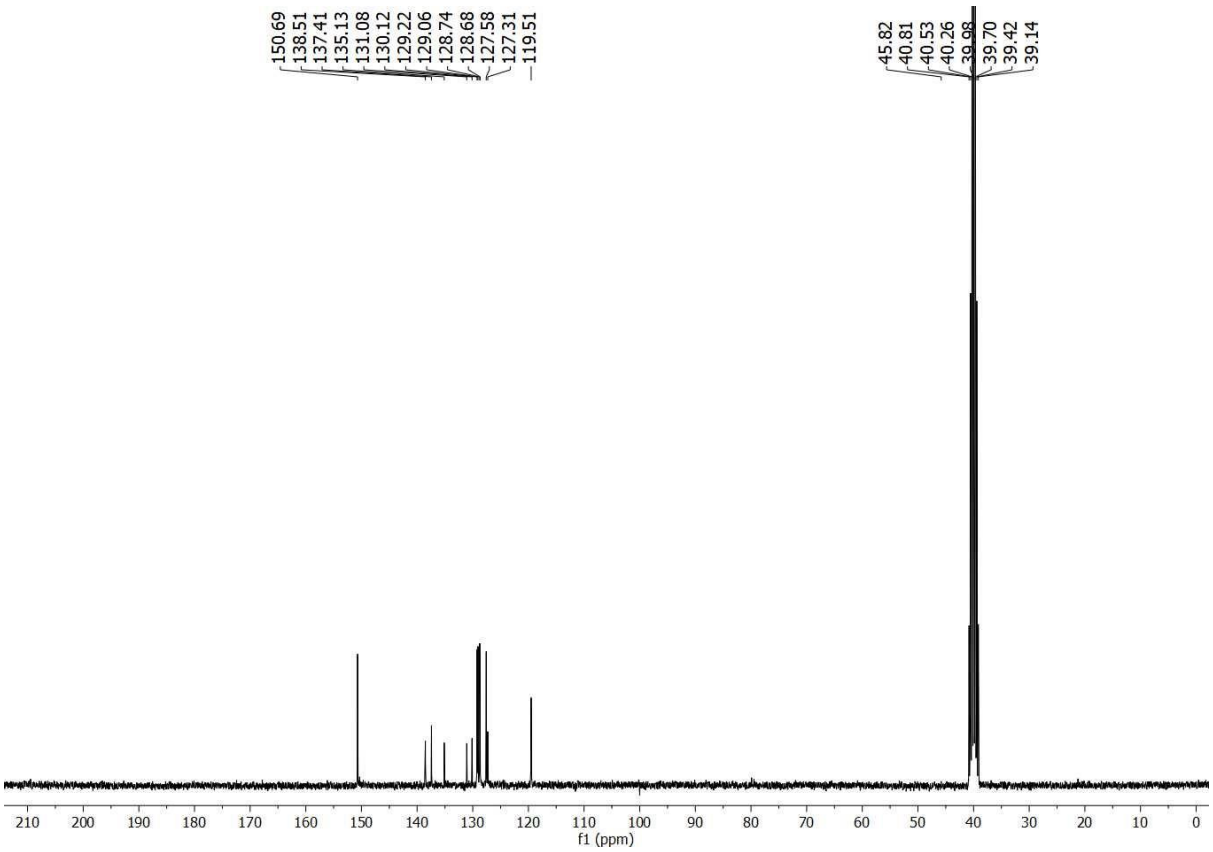


^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 3cm

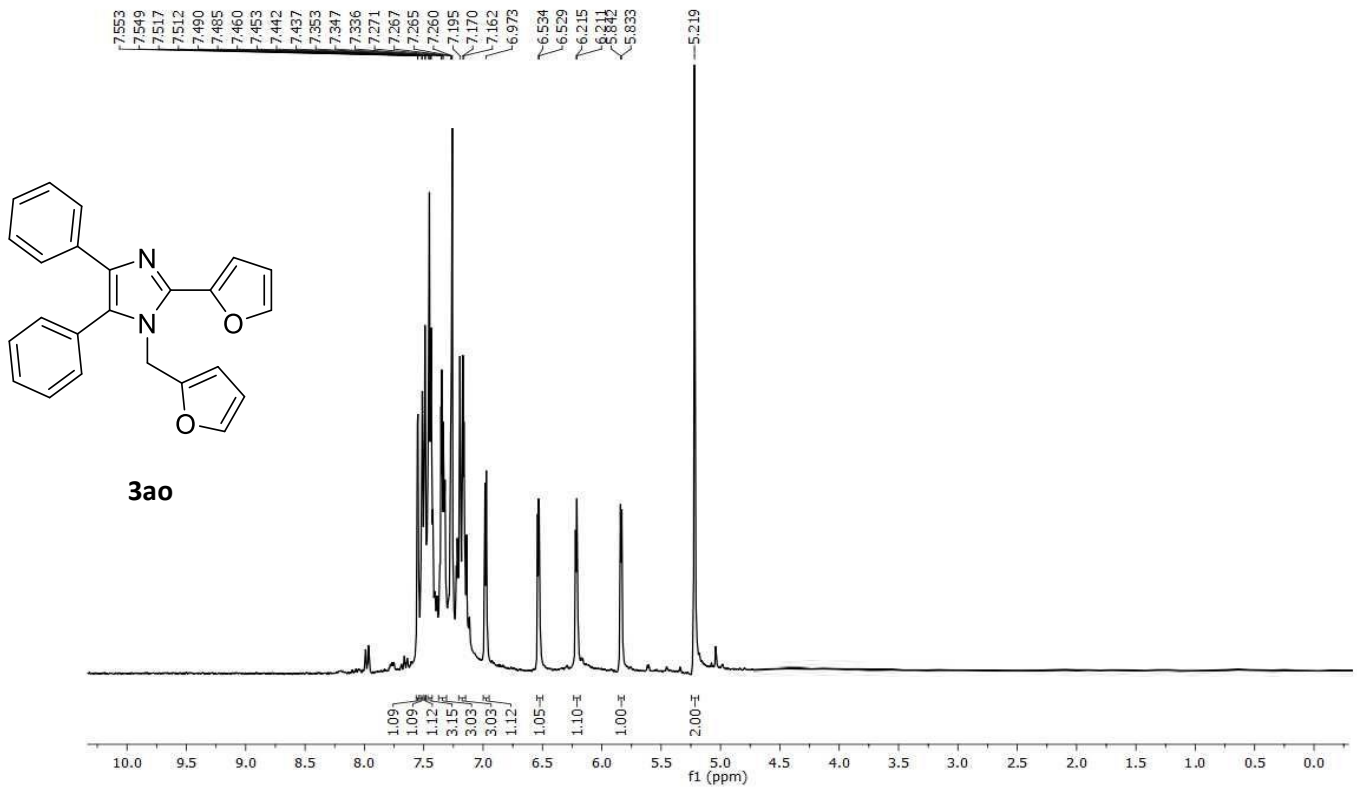
3an



^{1}H NMR (300 MHz, DMSO-d6) spectrum of compound 3an

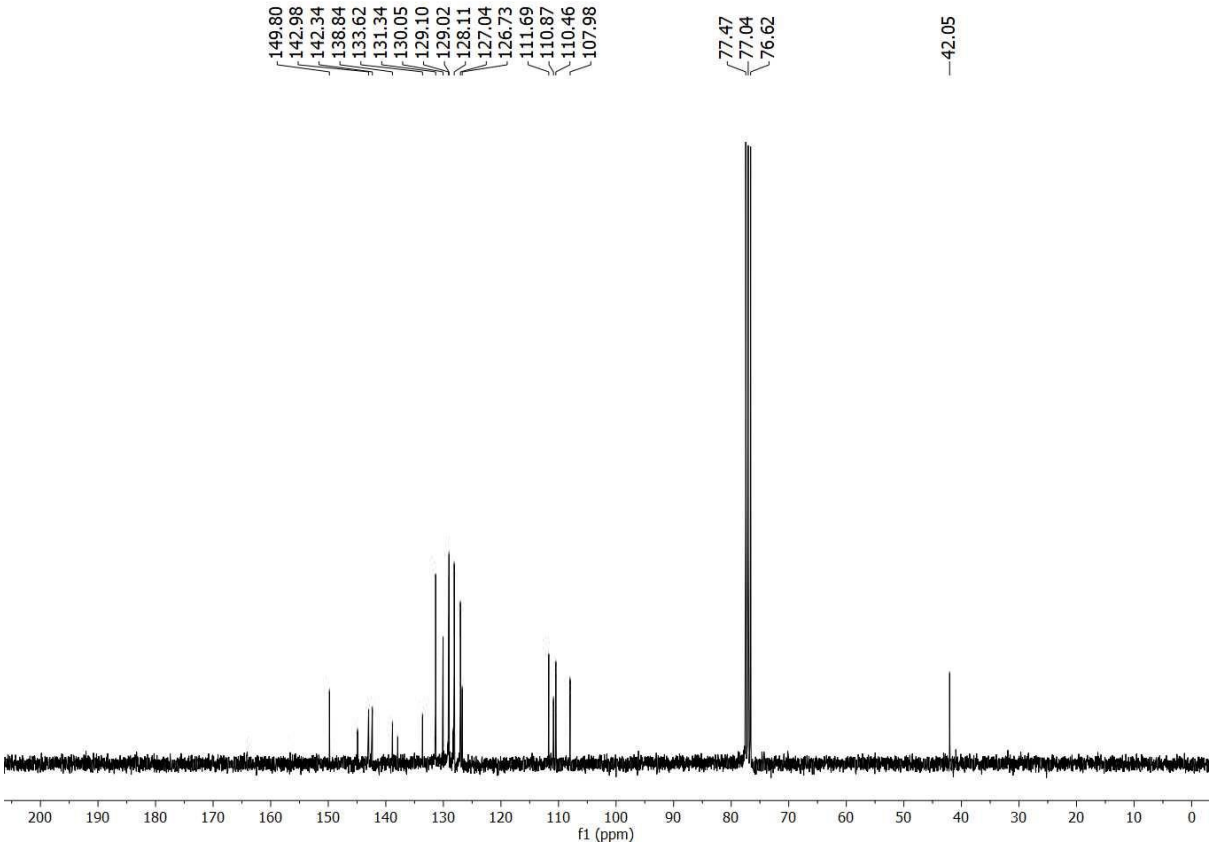


^{13}C NMR (75 MHz, DMSO-d6) spectrum of compound 3an

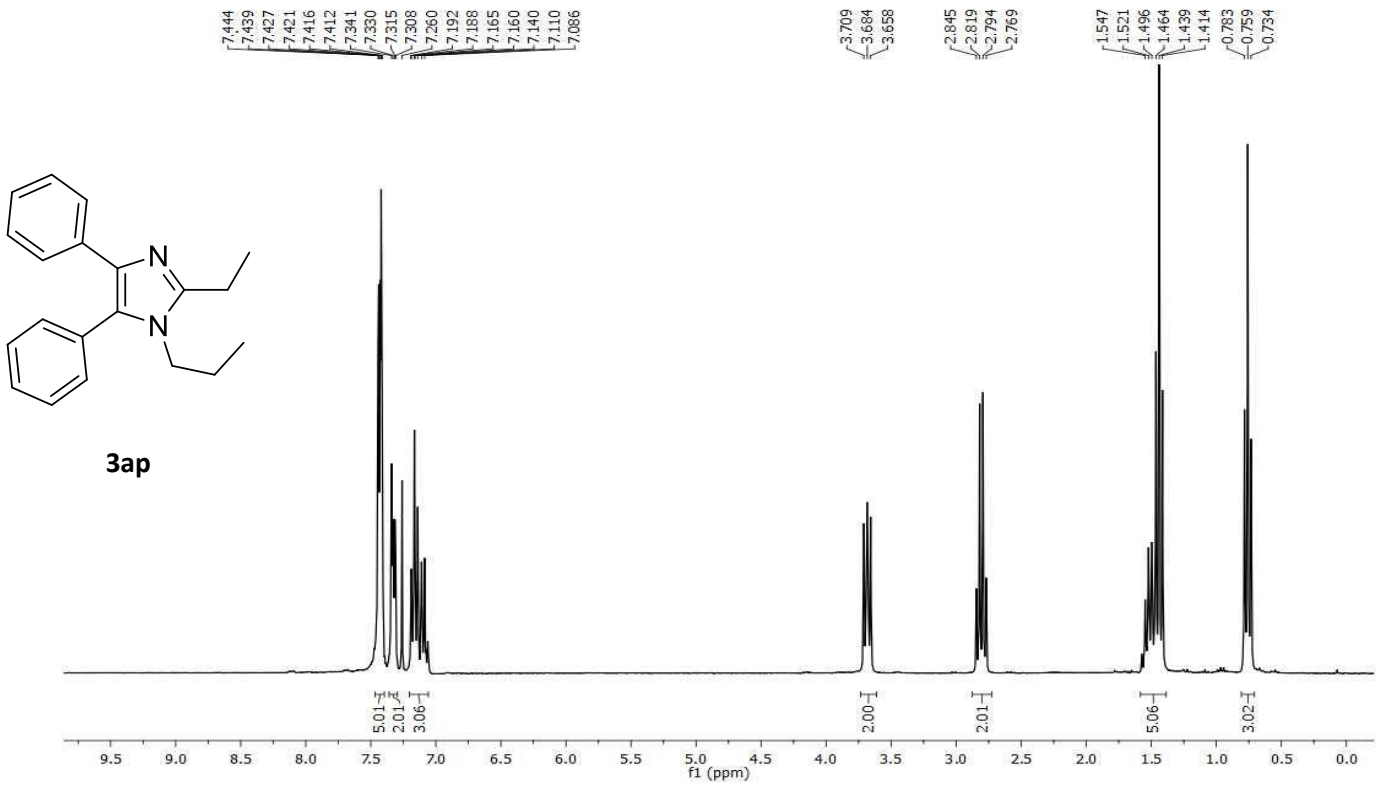


3ao

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ao

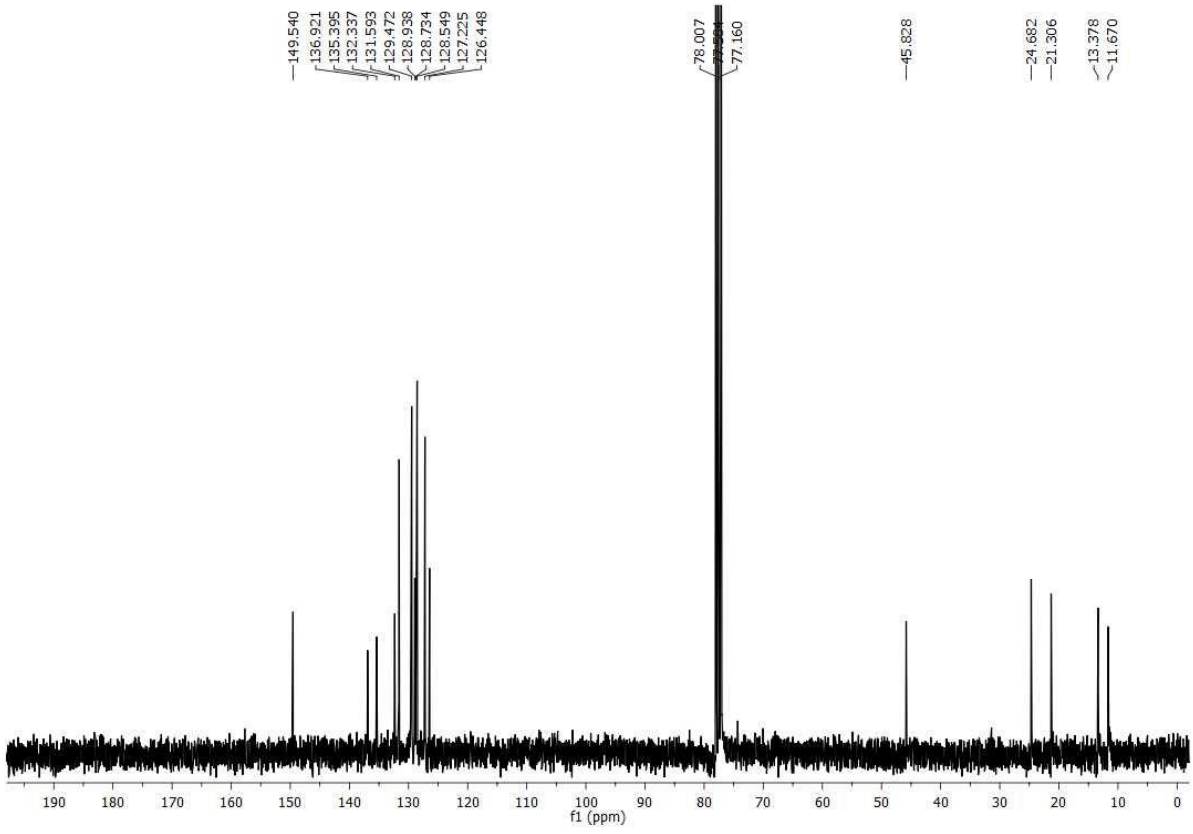


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ao

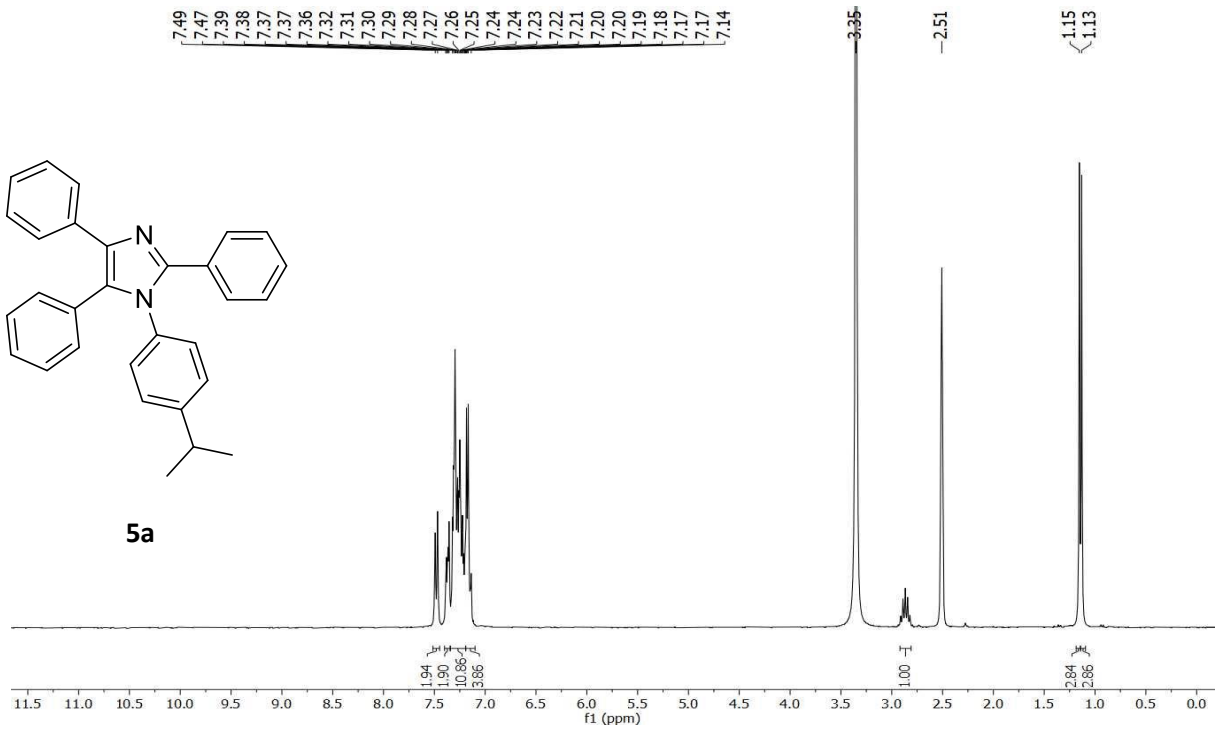


3ap

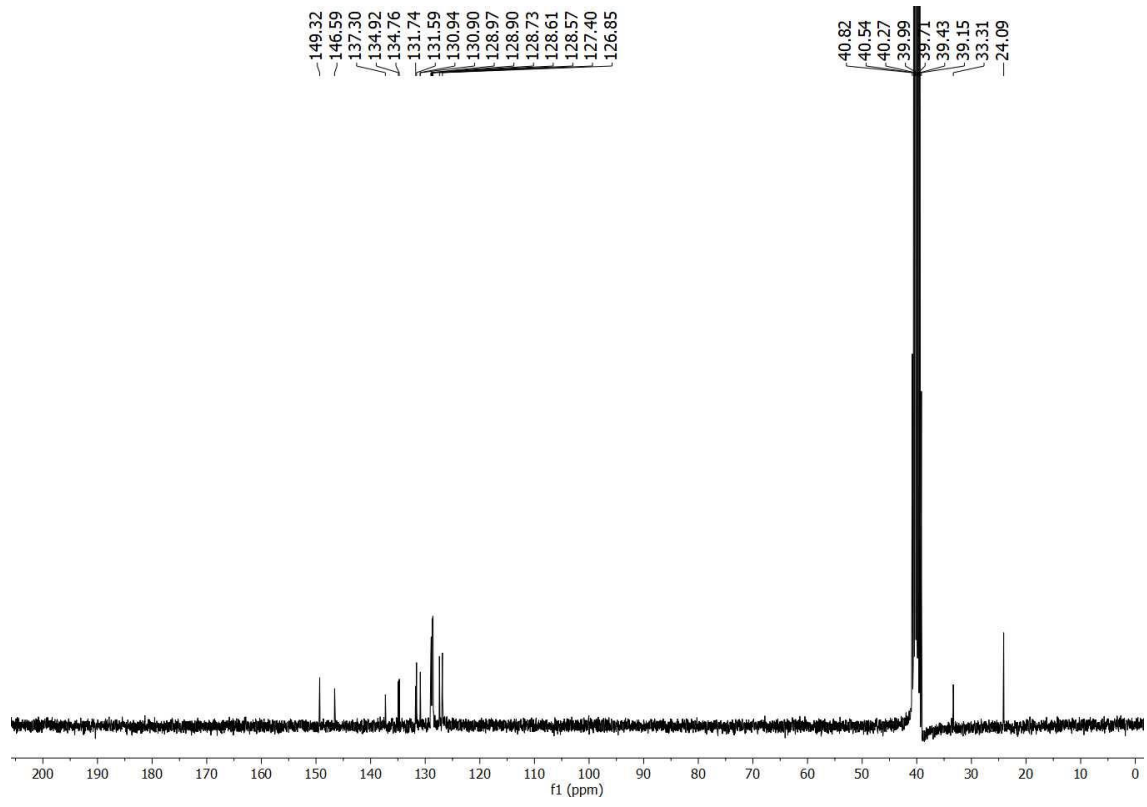
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ap



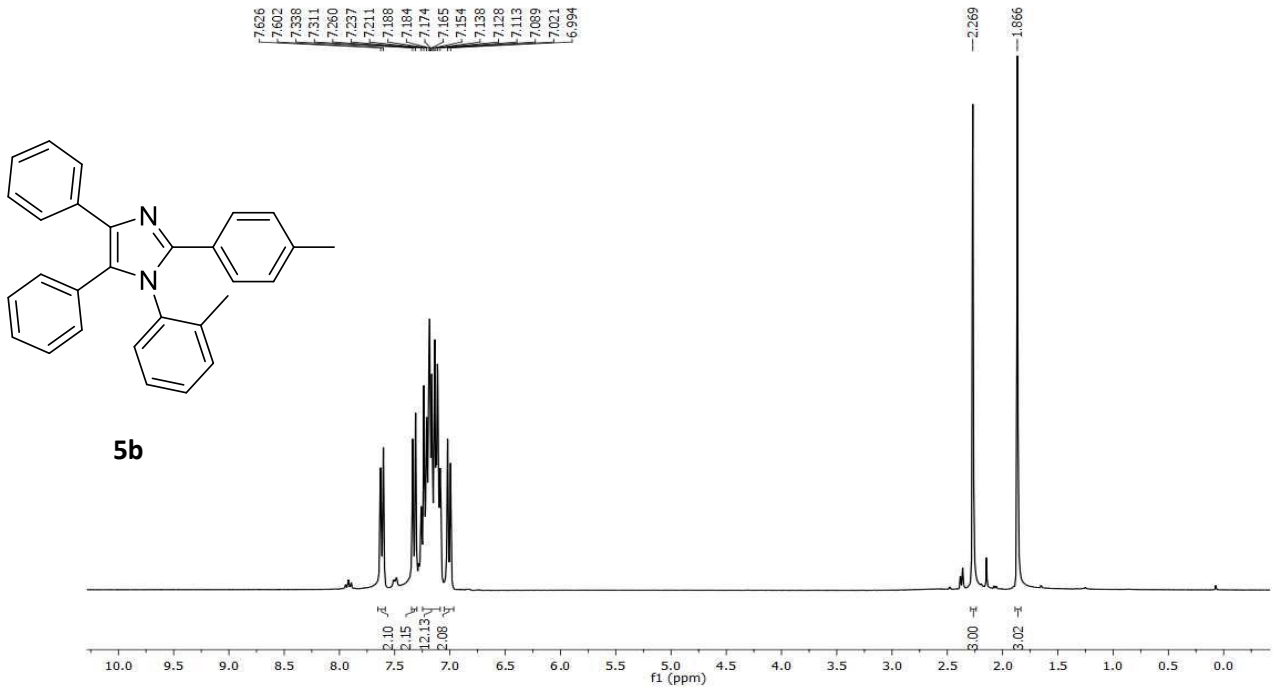
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ap



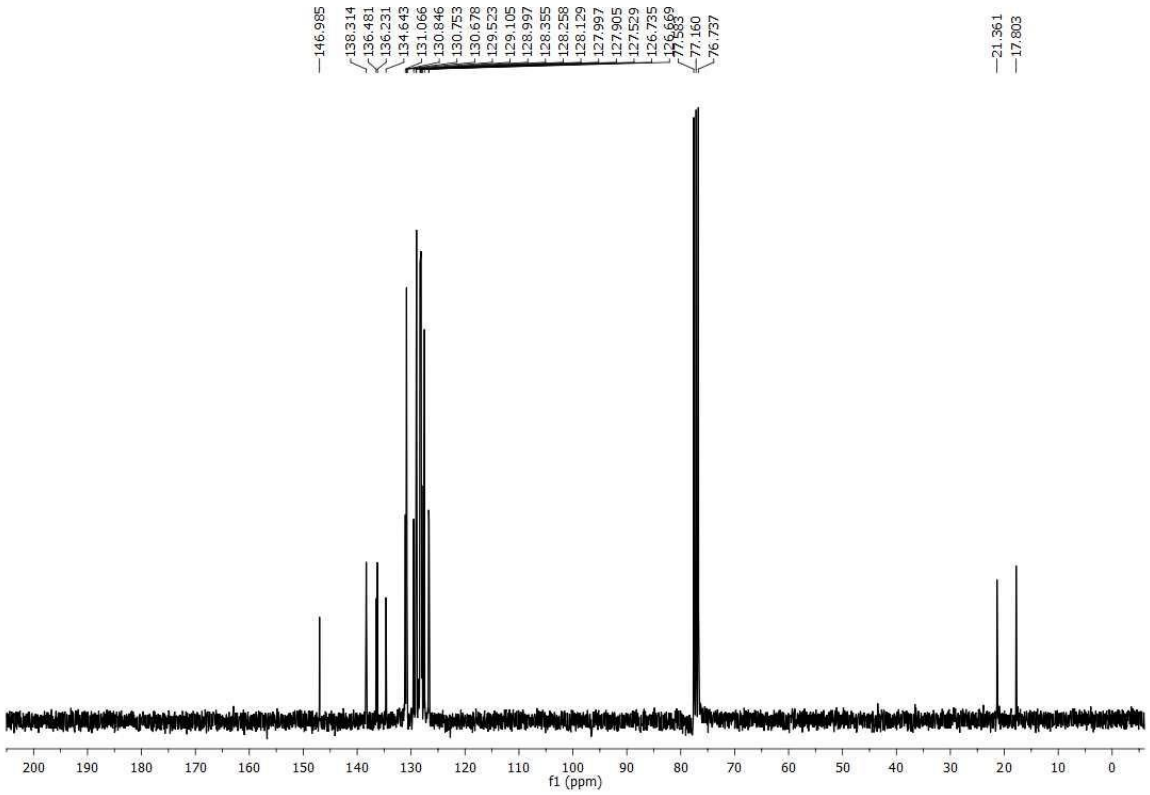
^{1}H NMR (300 MHz, DMSO-d6) spectrum of compound 5a



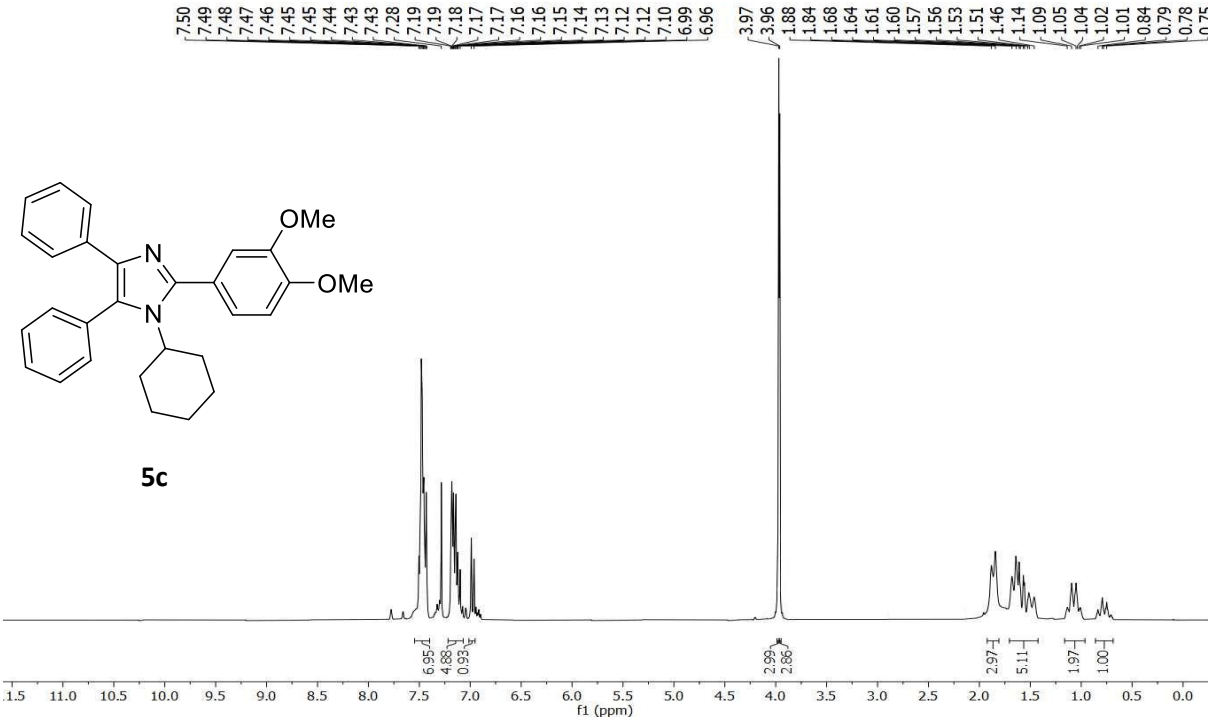
^{13}C NMR (75 MHz, DMSO-d6) spectrum of compound 5a



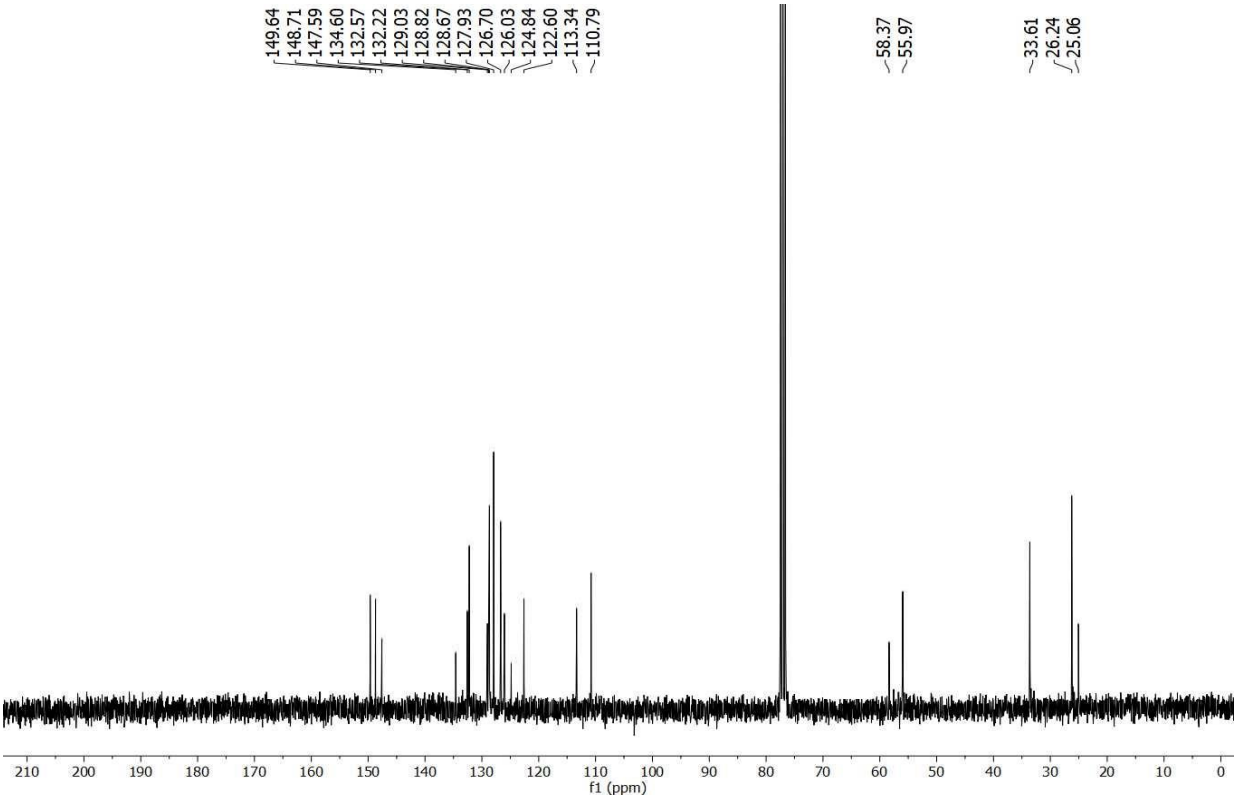
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5b



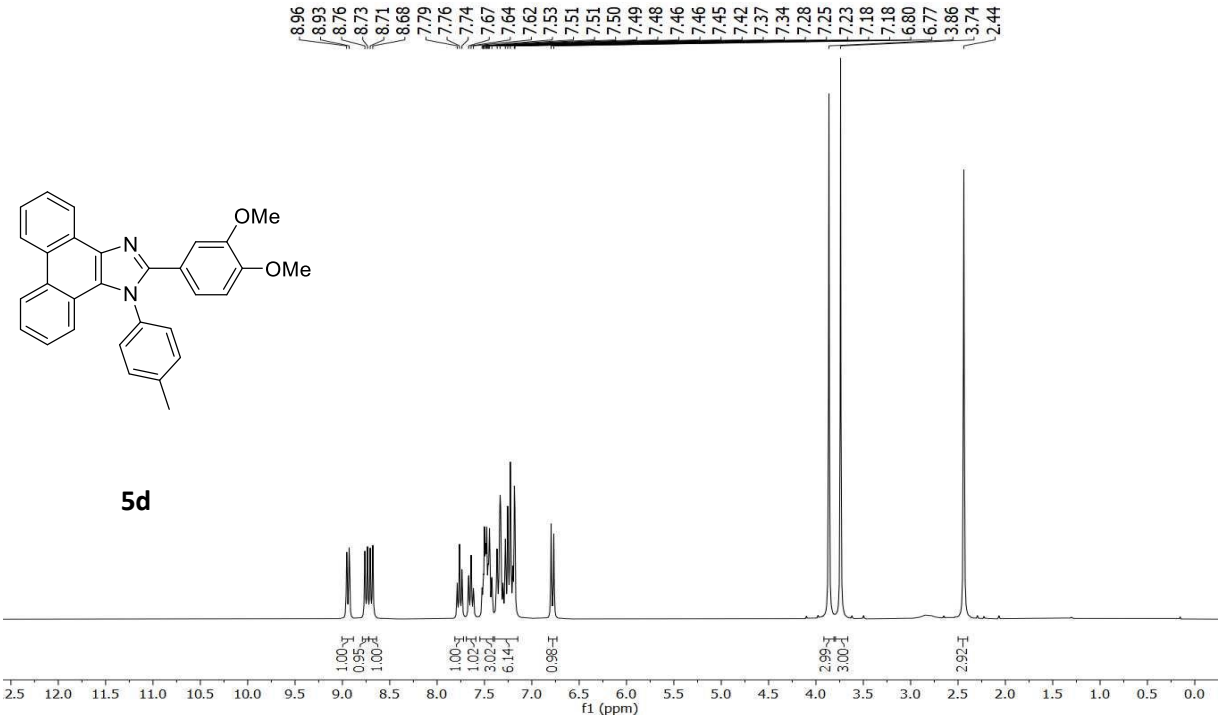
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5b



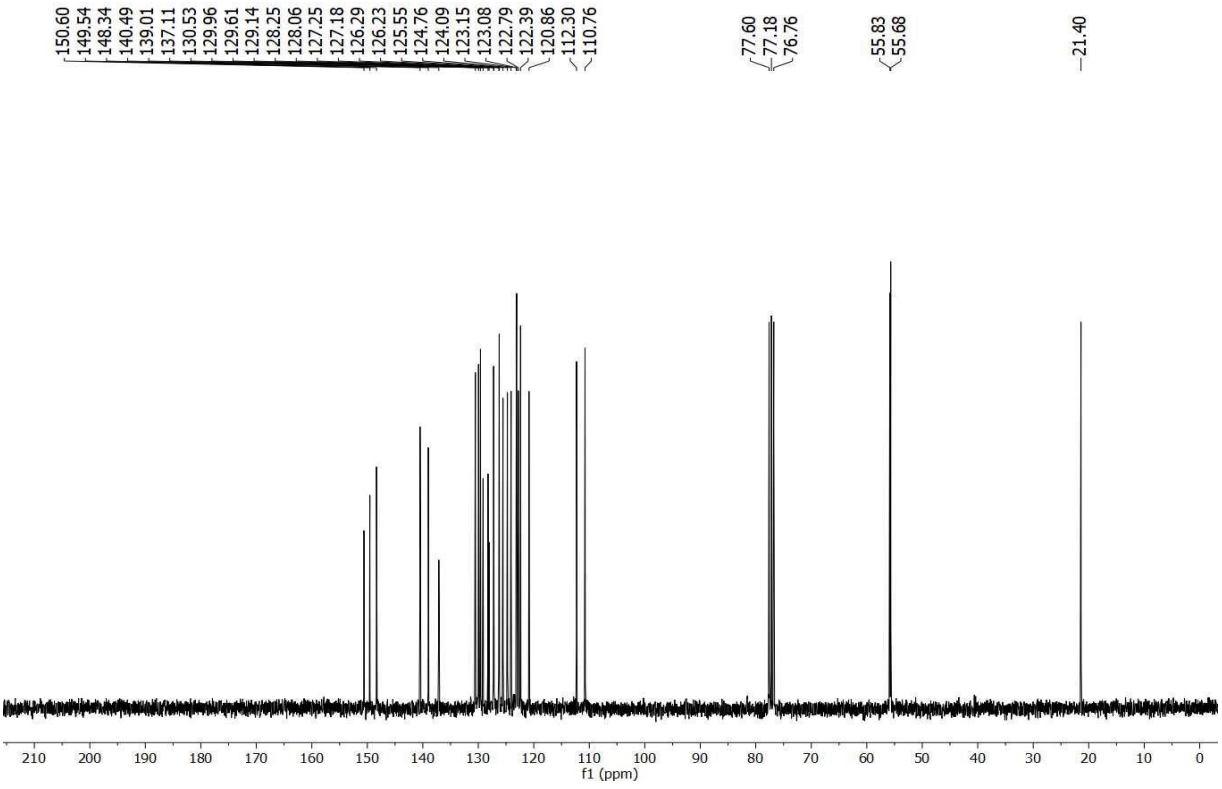
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5c



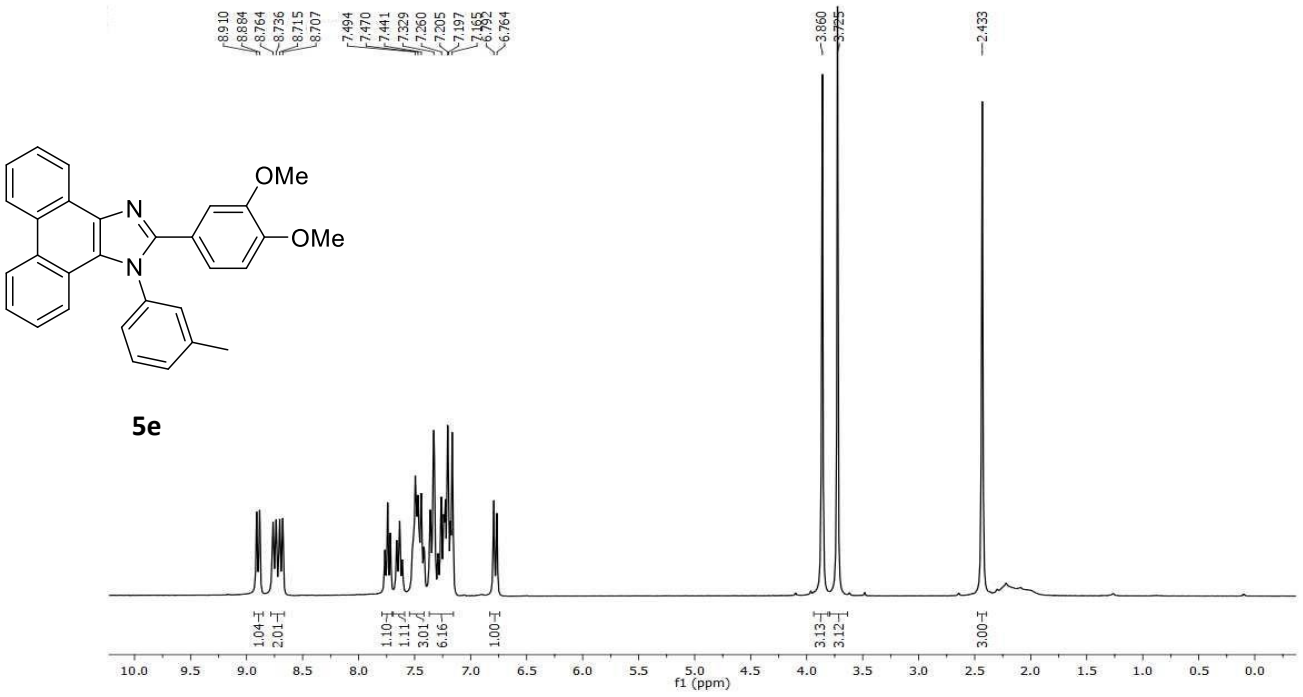
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5c



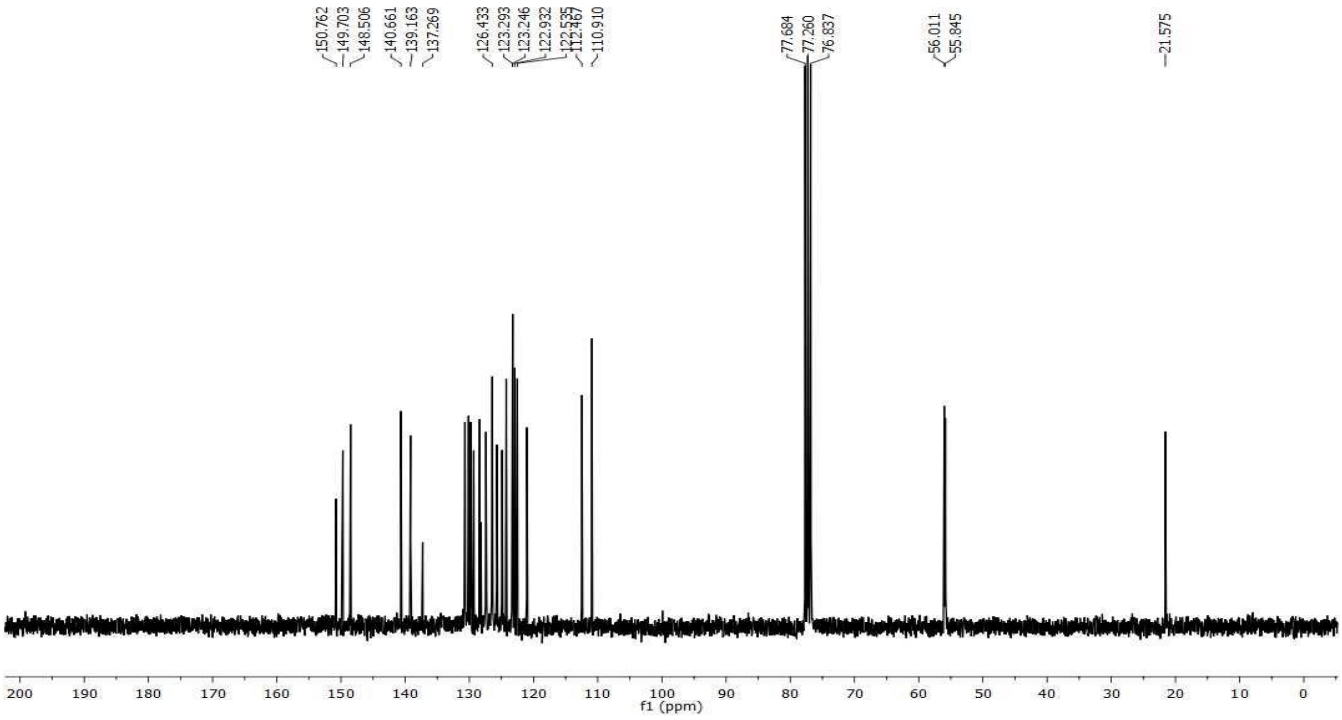
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5d



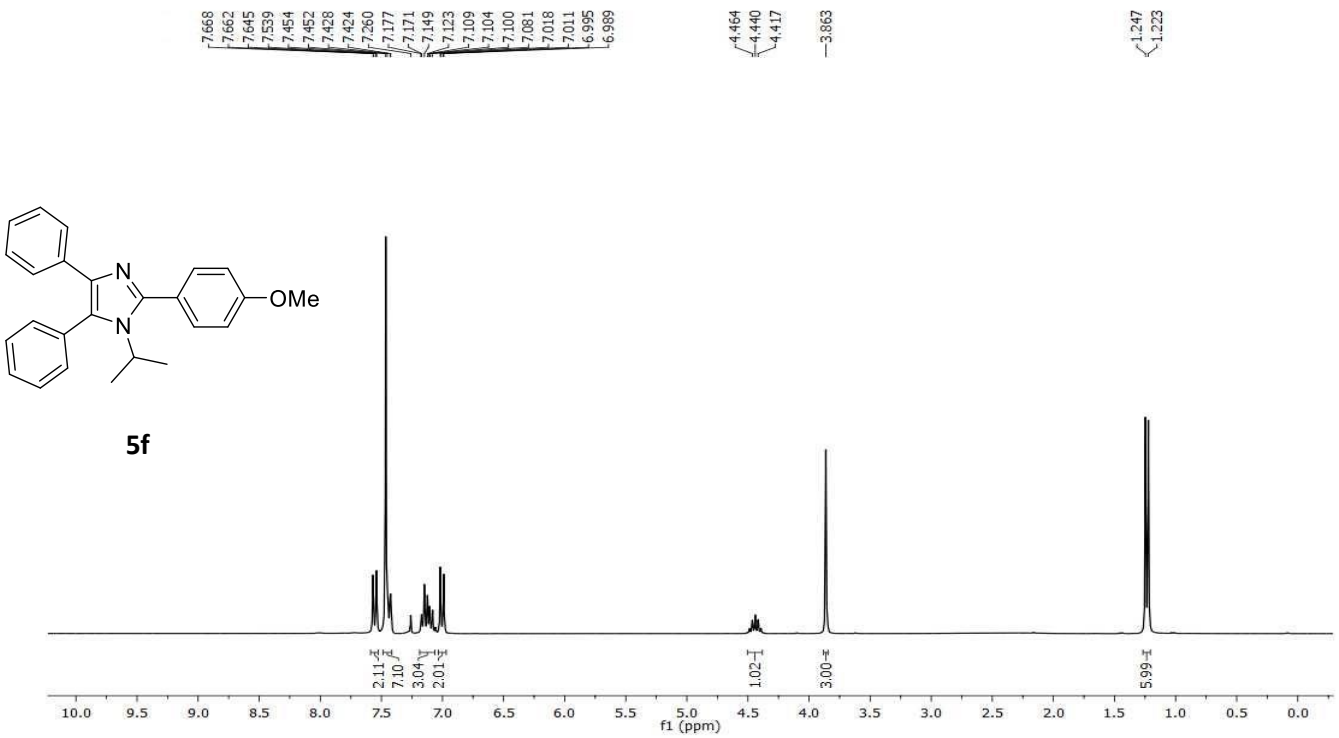
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5c



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5e

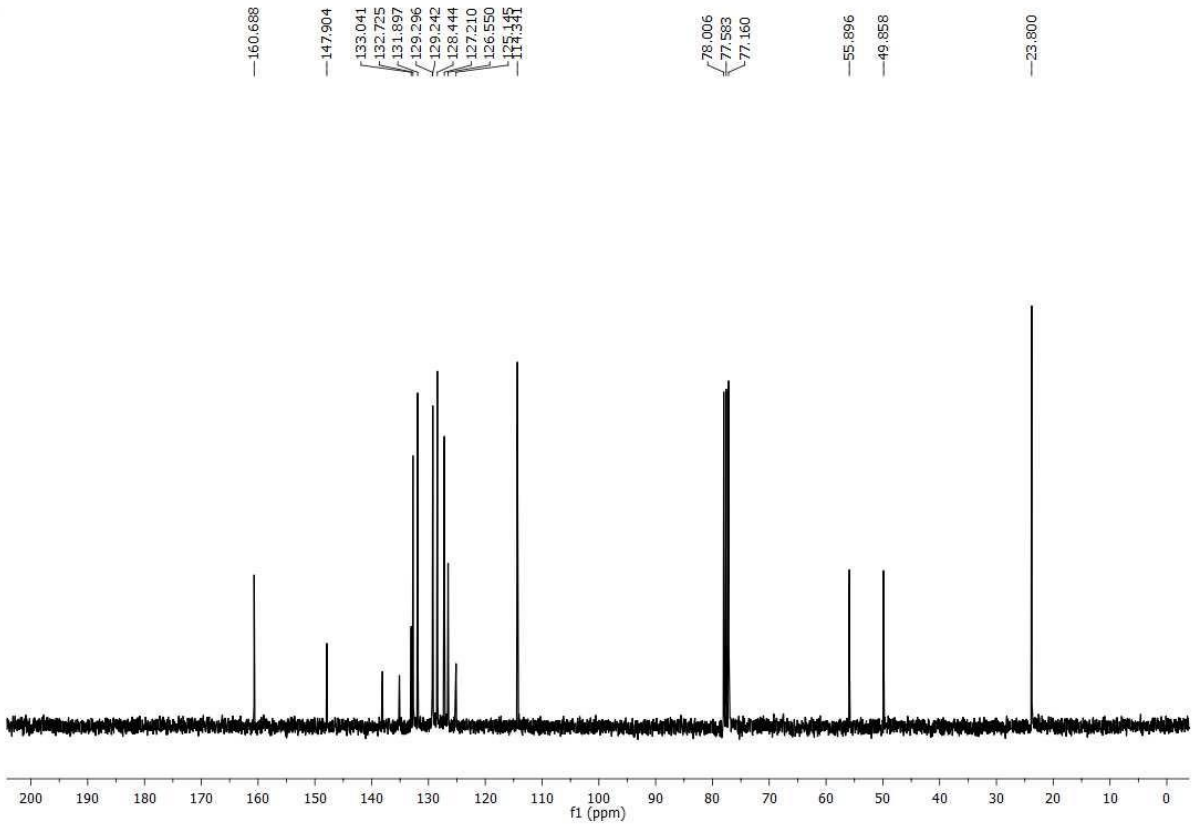


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5e

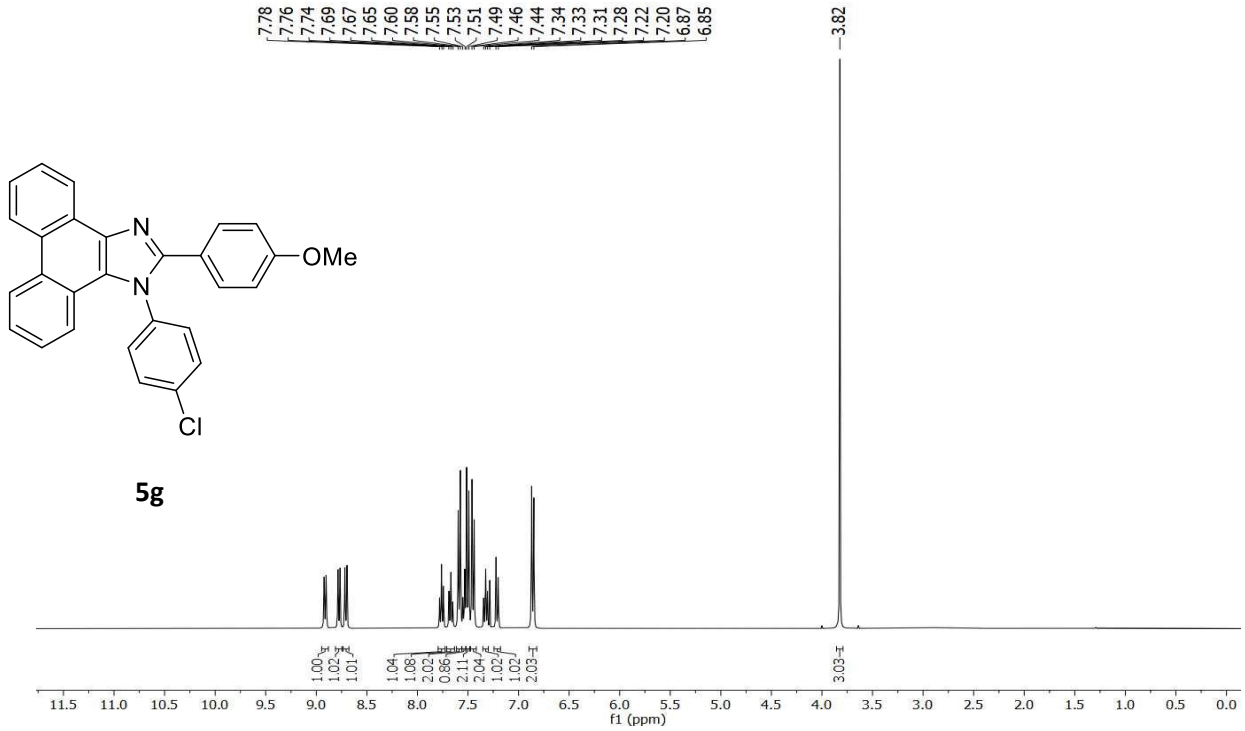


5f

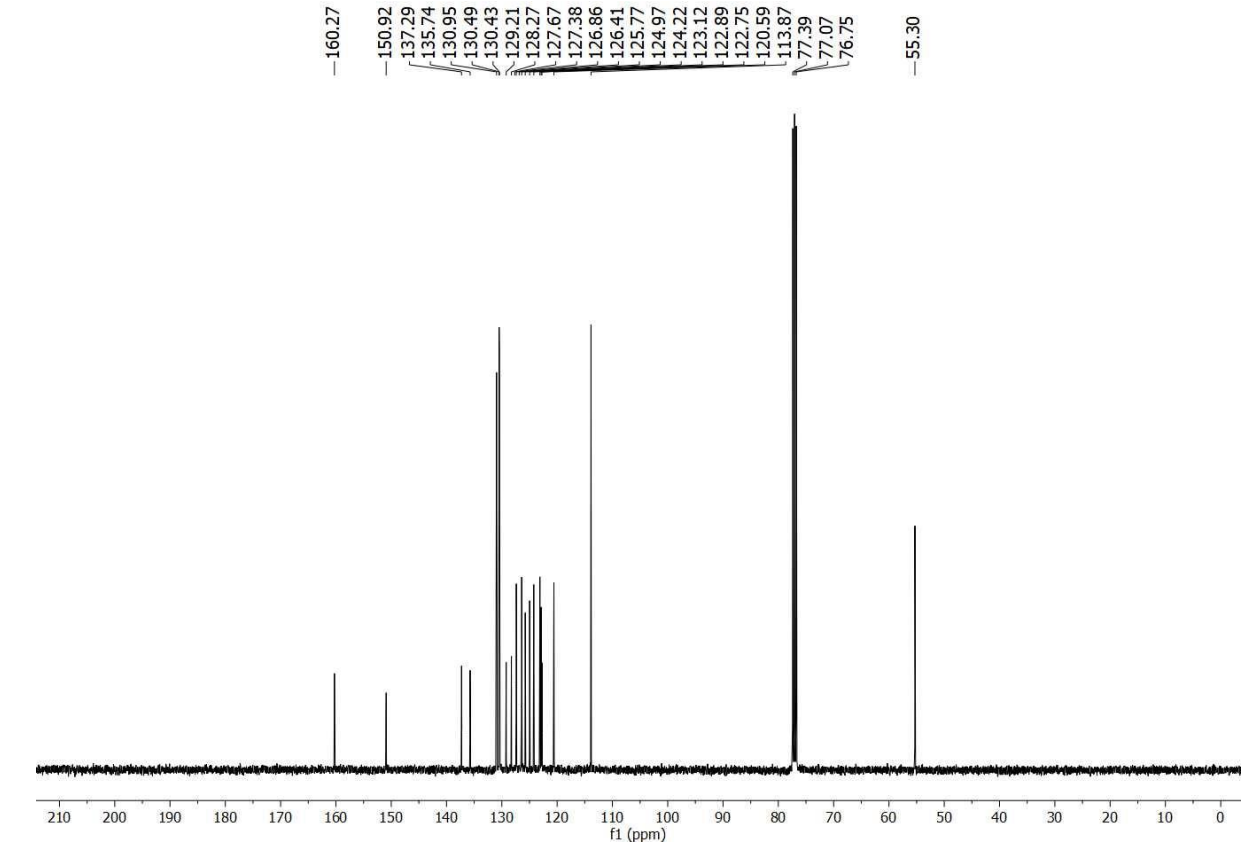
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5e



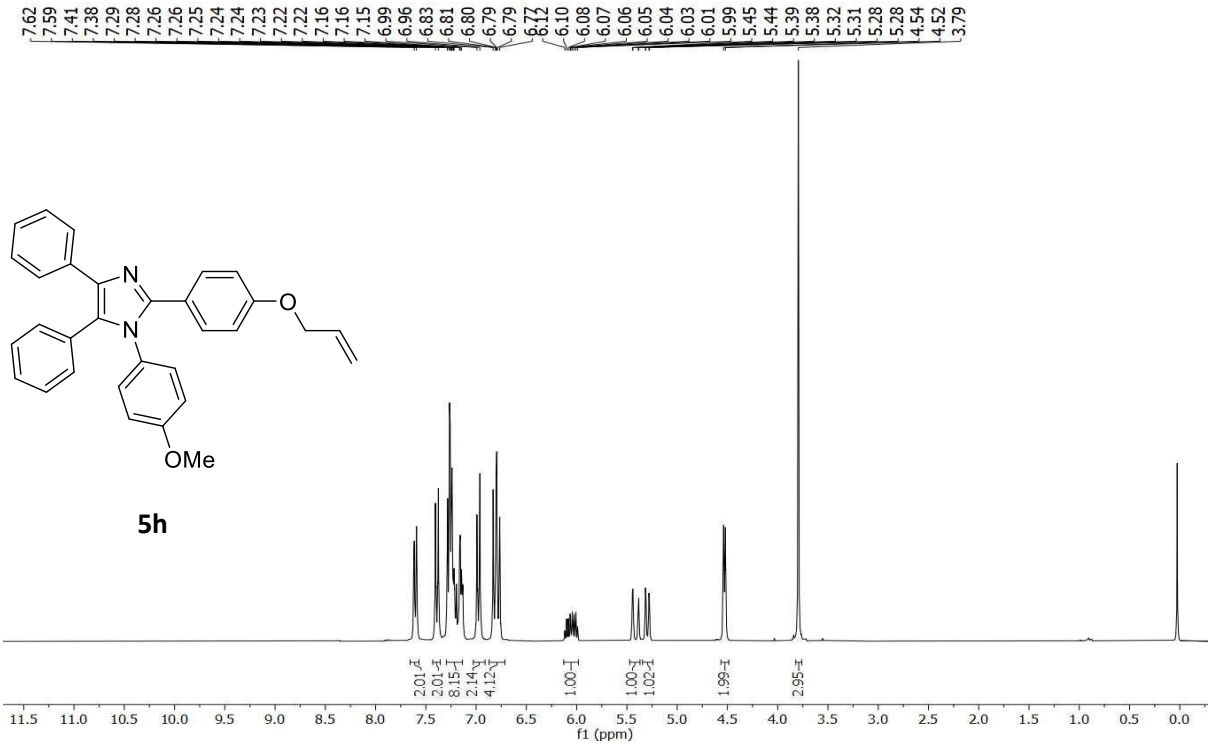
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5f



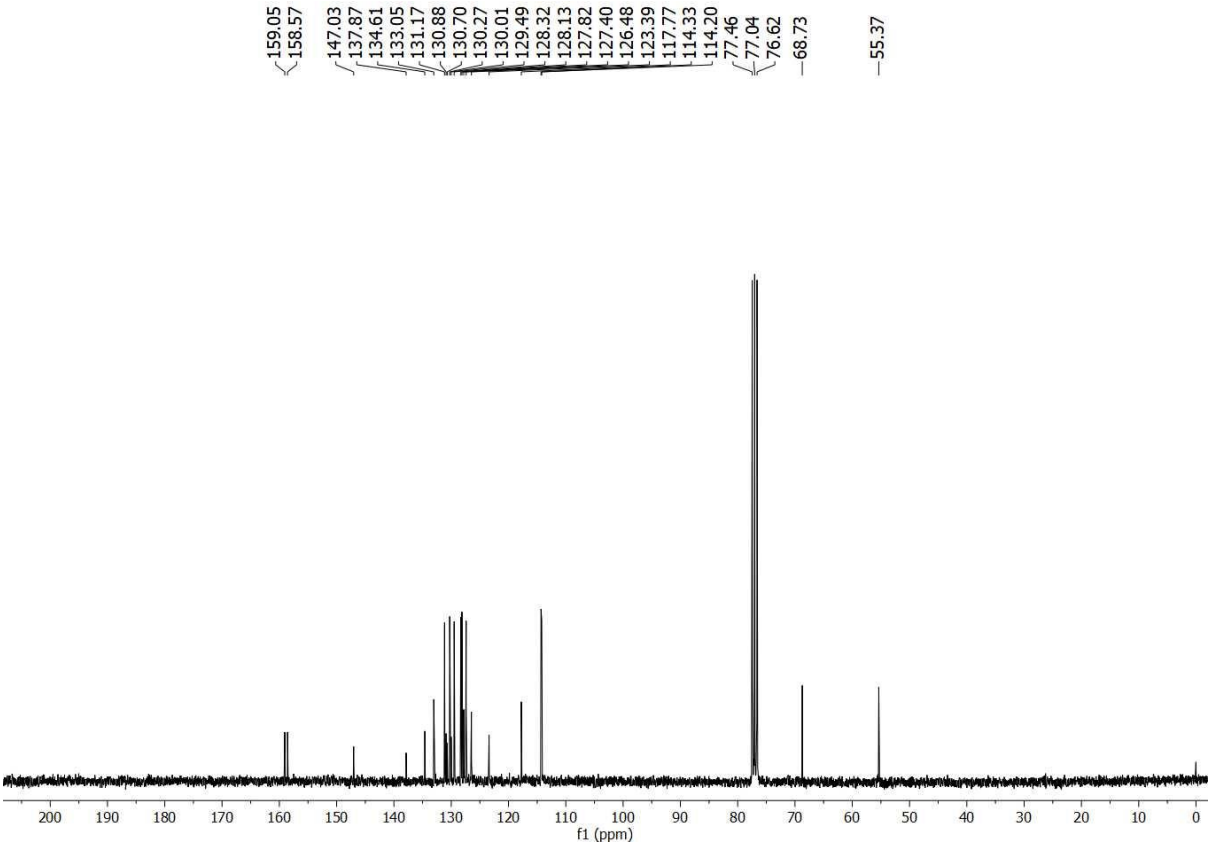
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound 5g



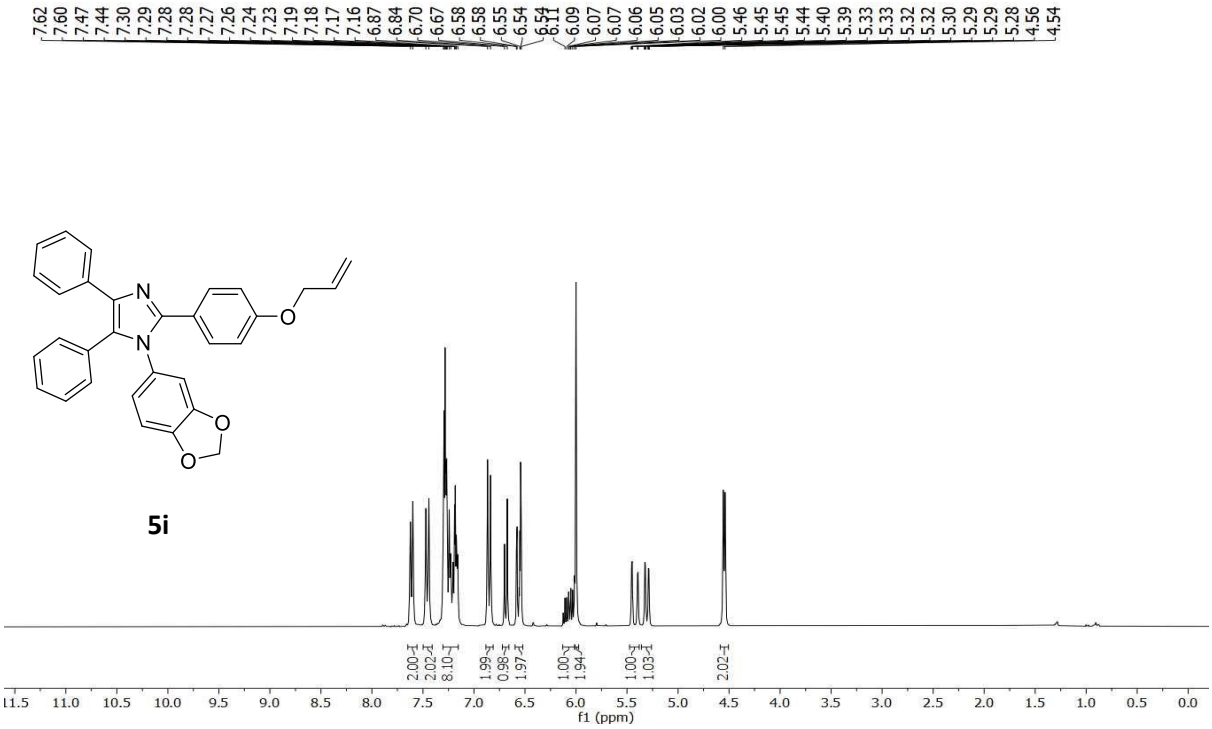
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound 5g



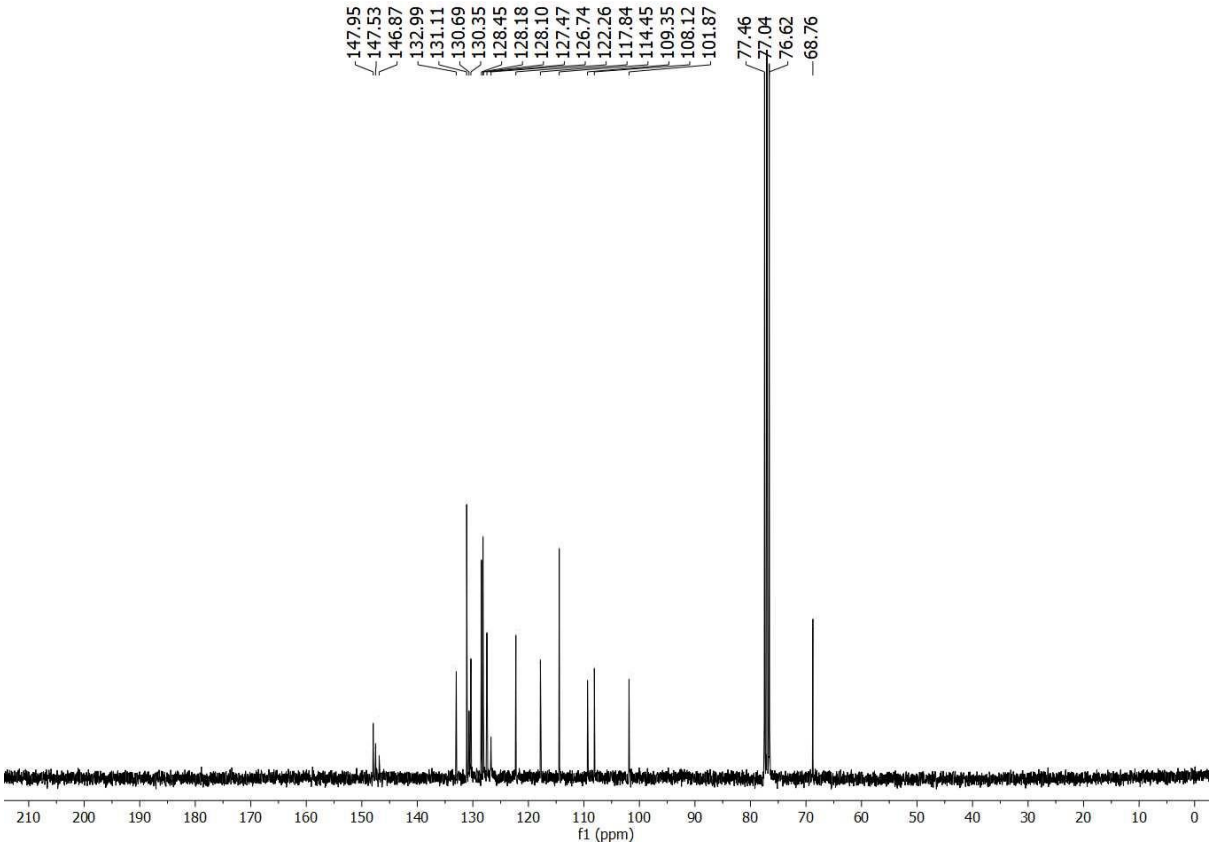
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5h



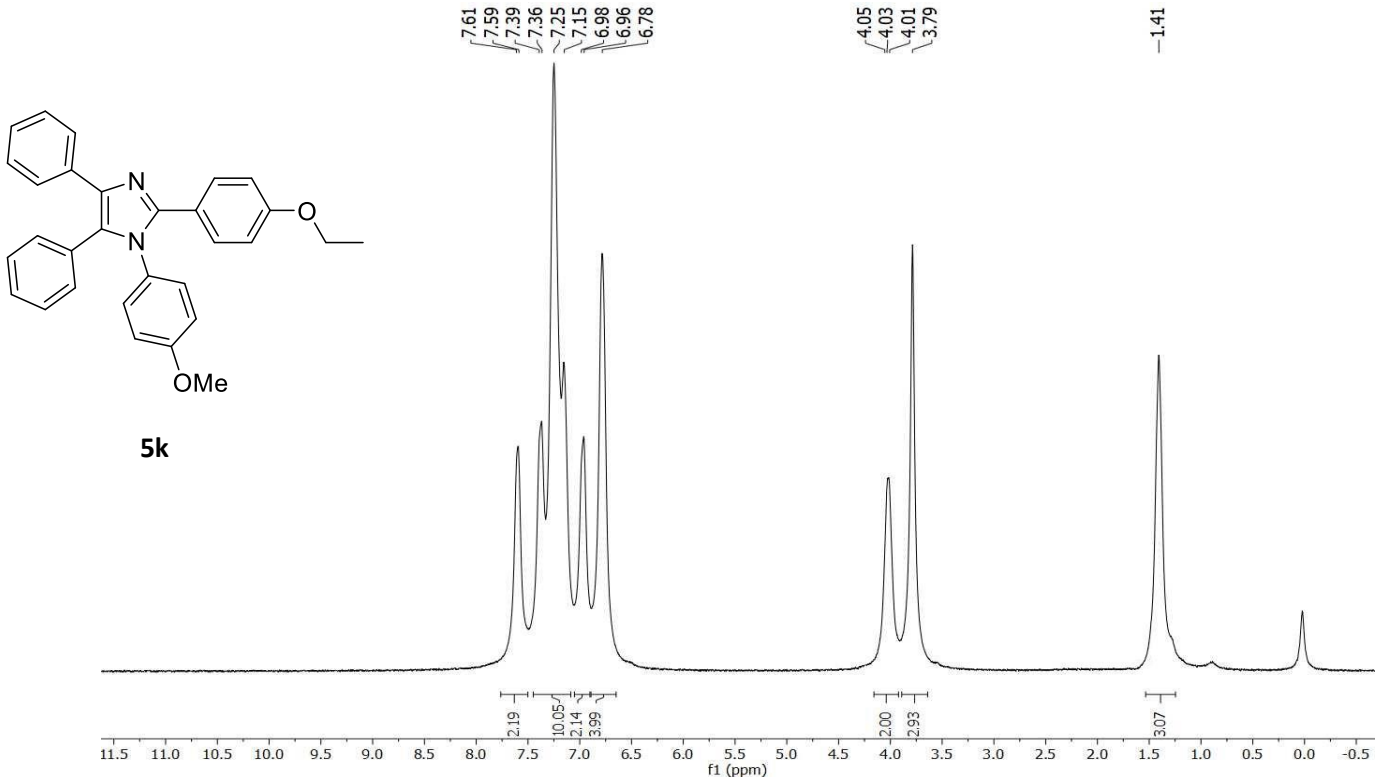
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5h



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5i

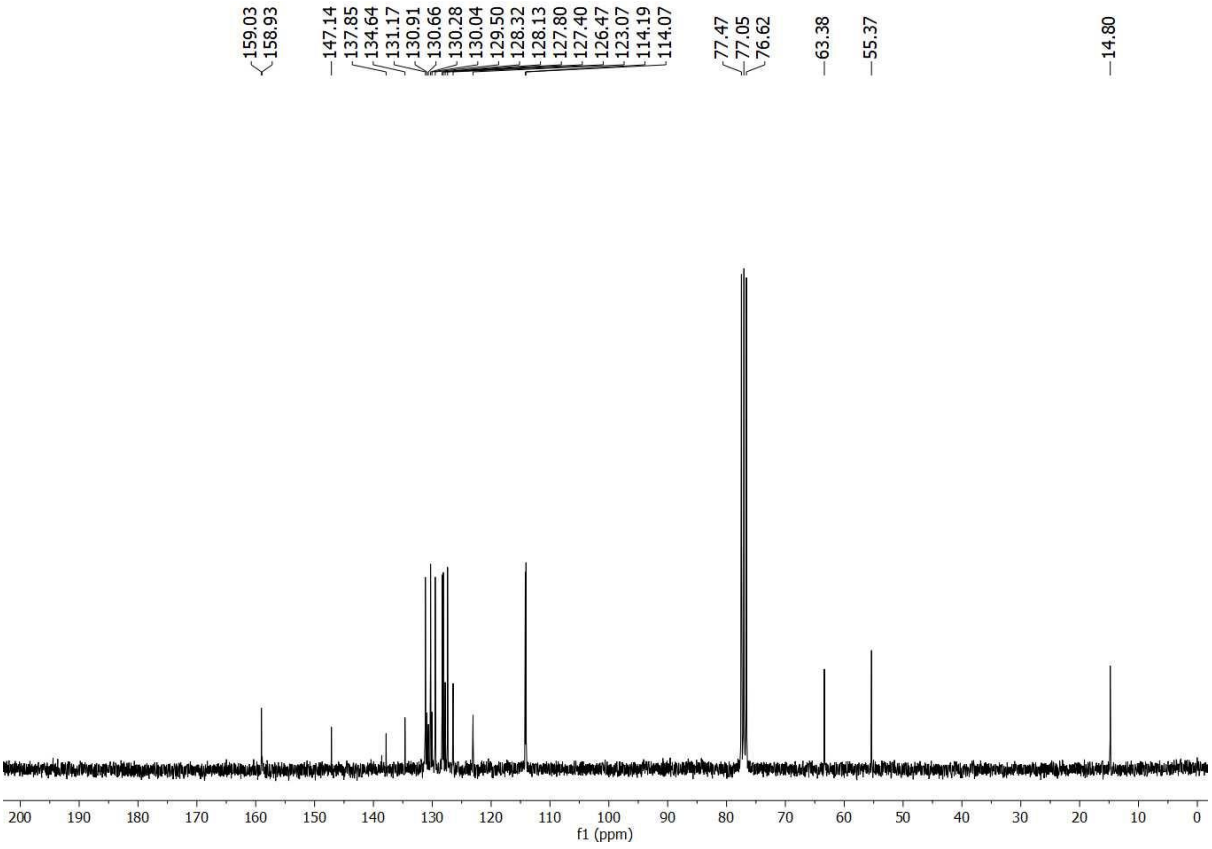


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5i

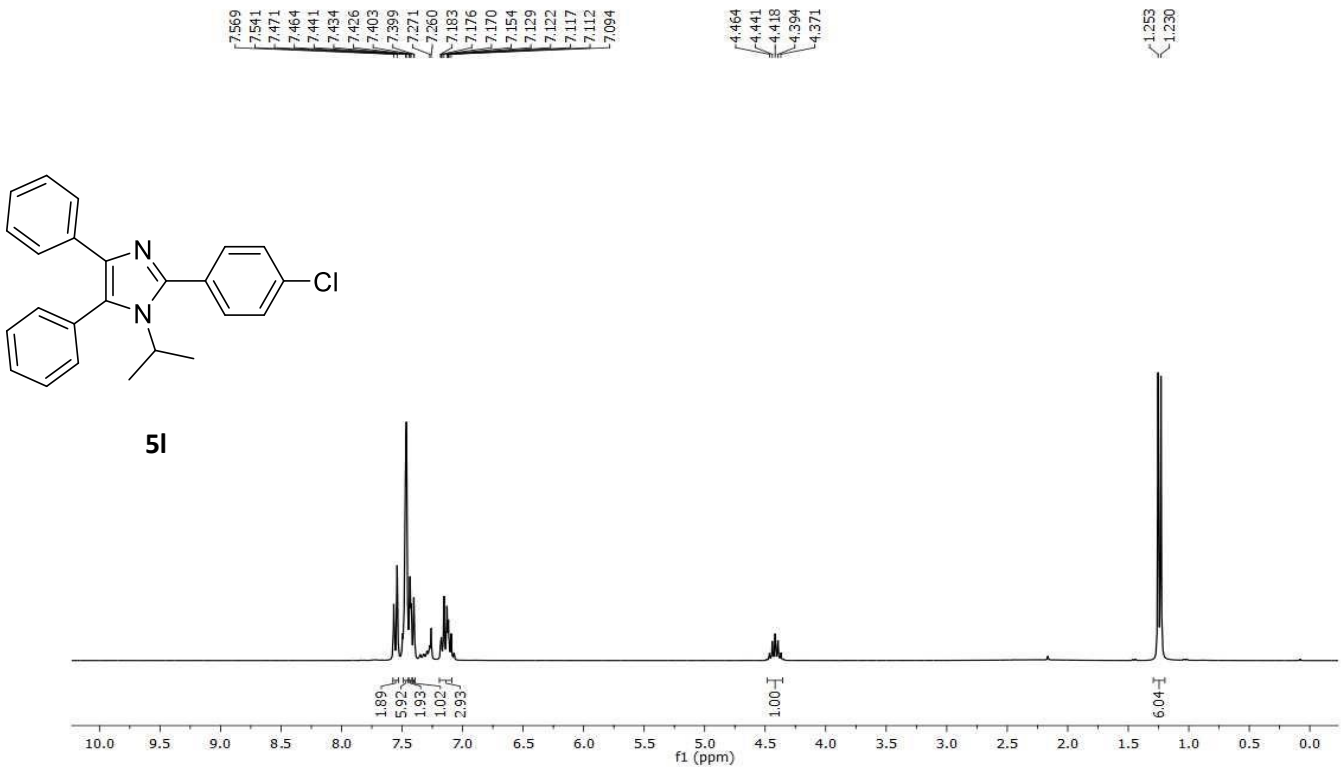


5k

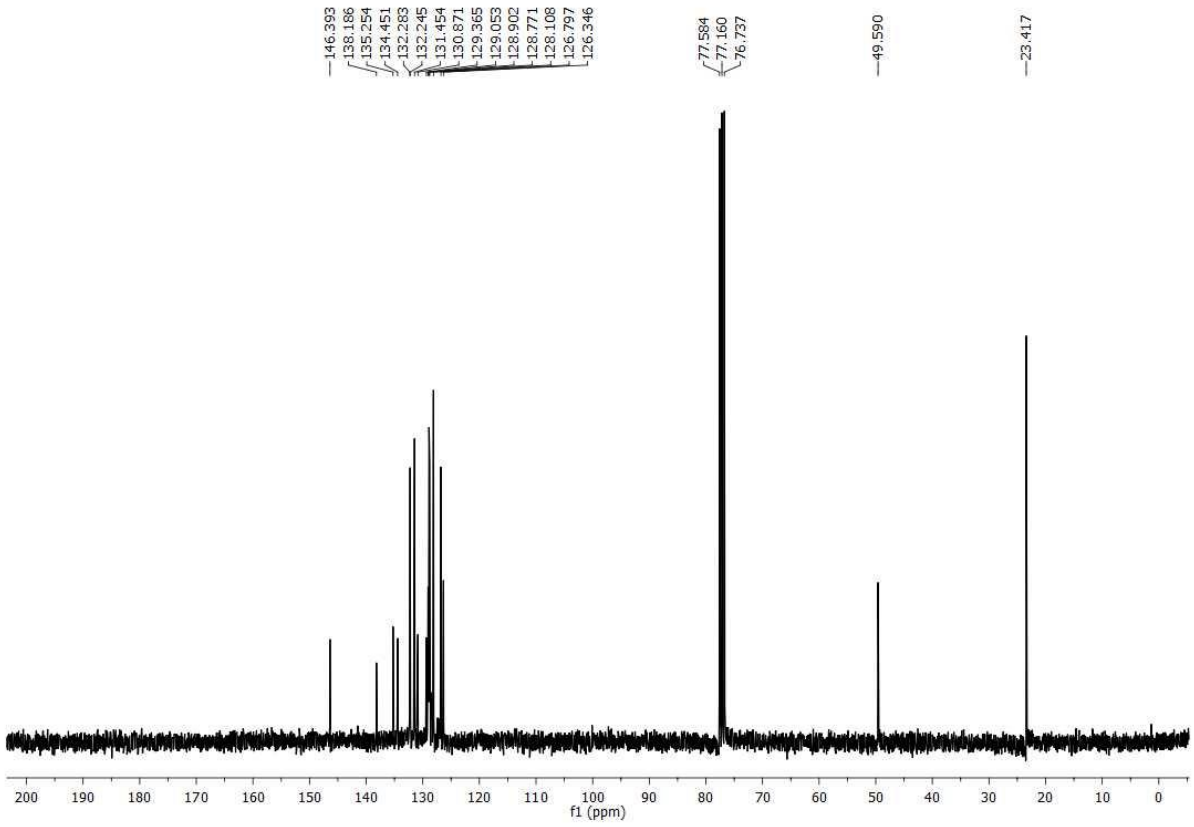
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5k



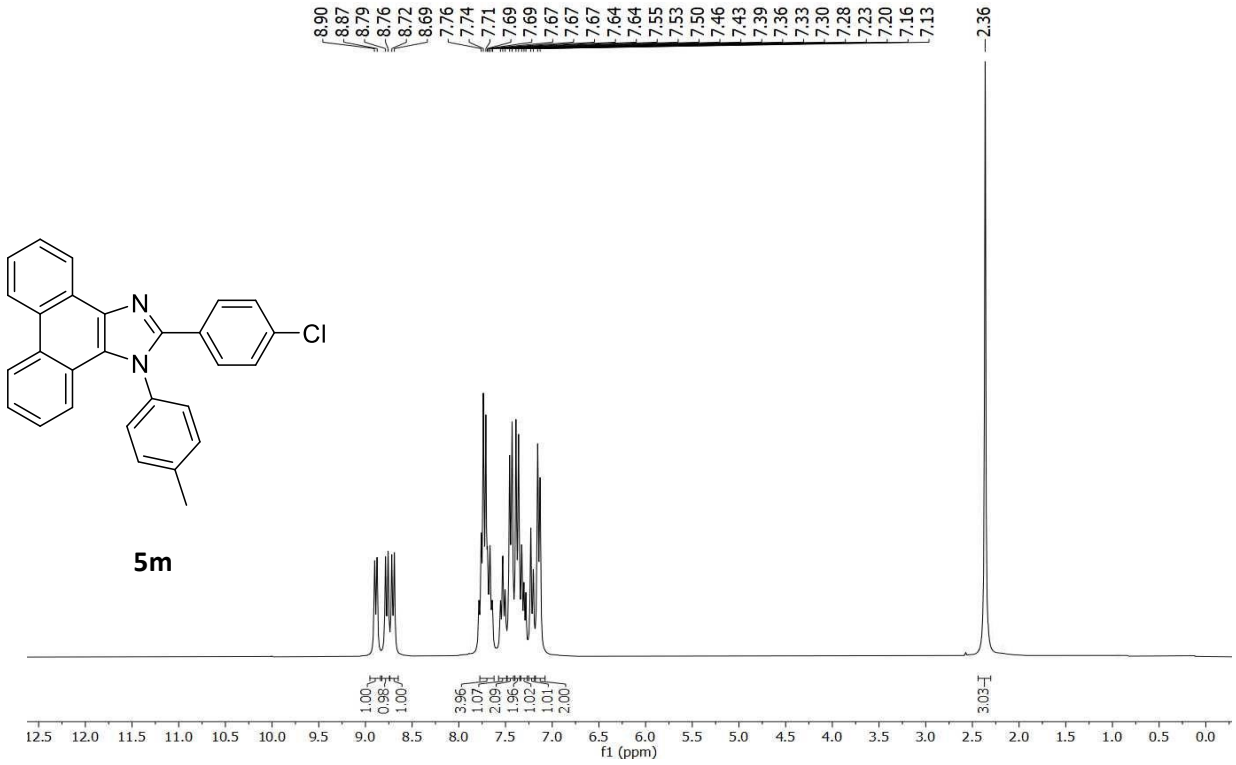
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5k



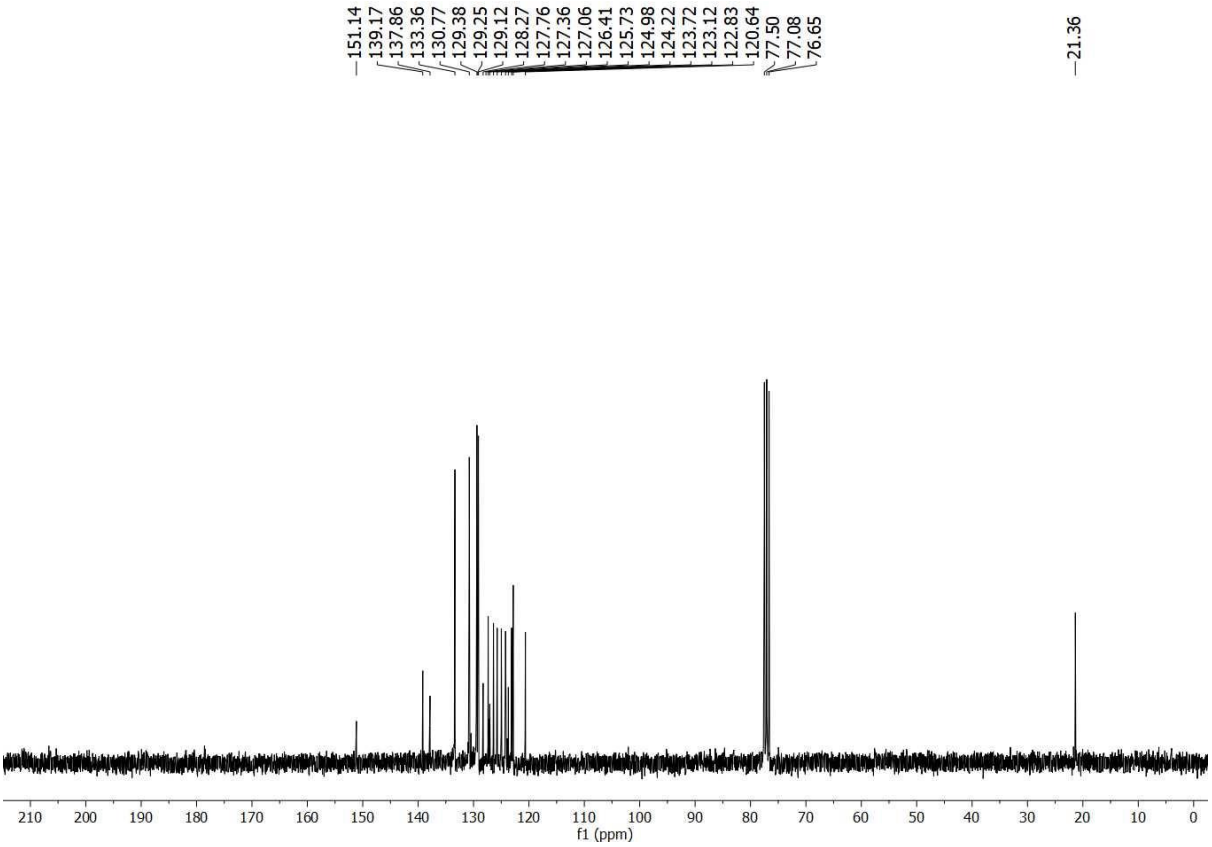
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5l



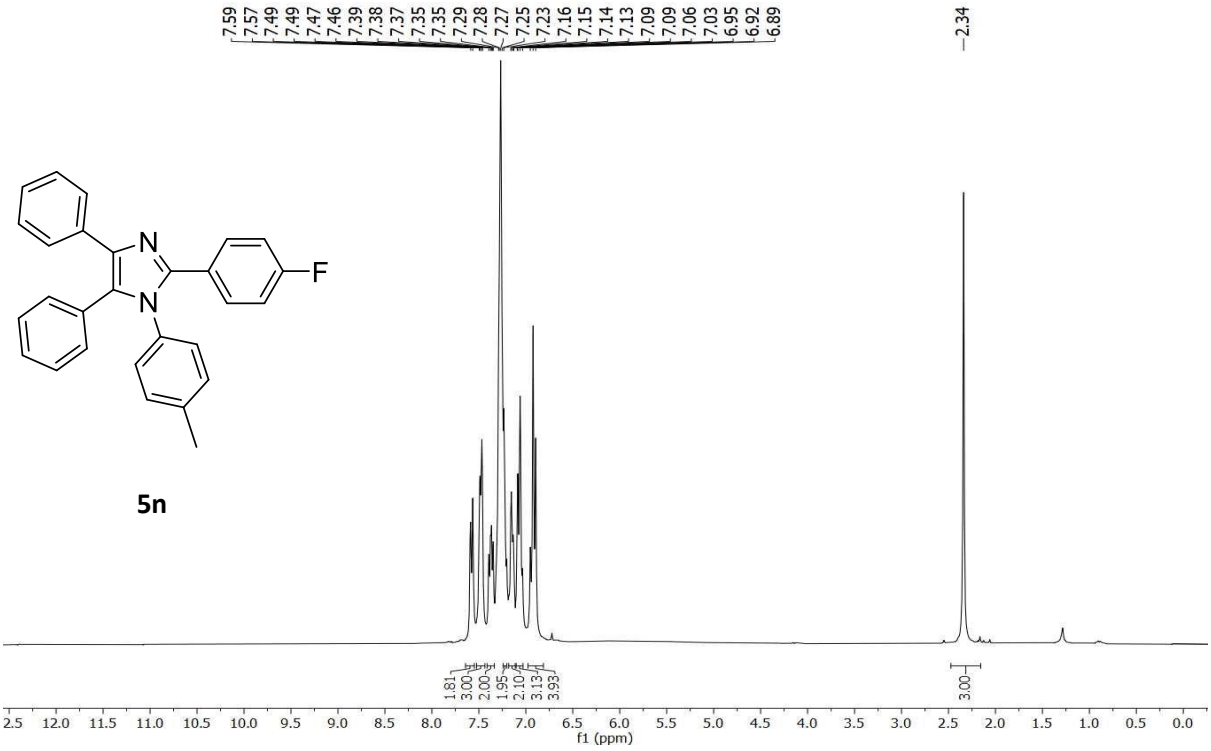
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5l



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5m

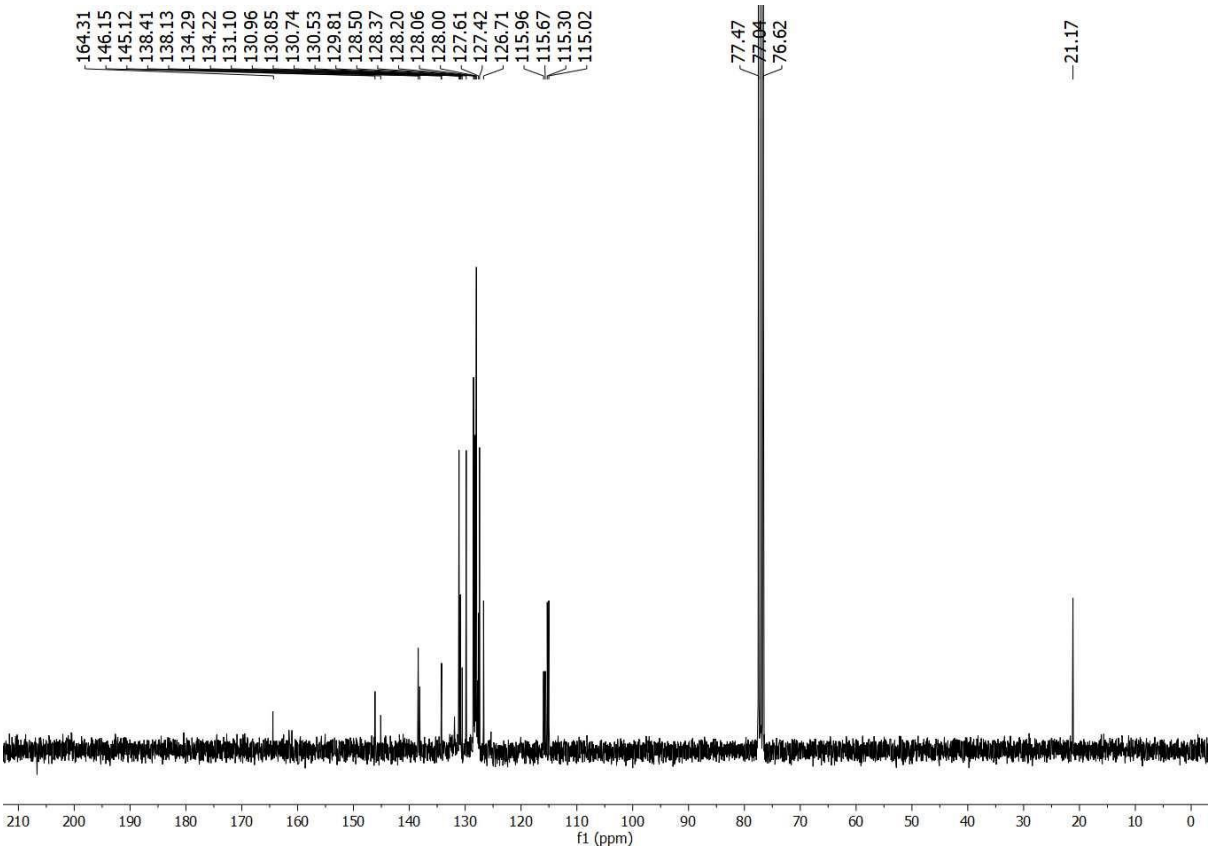


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5m

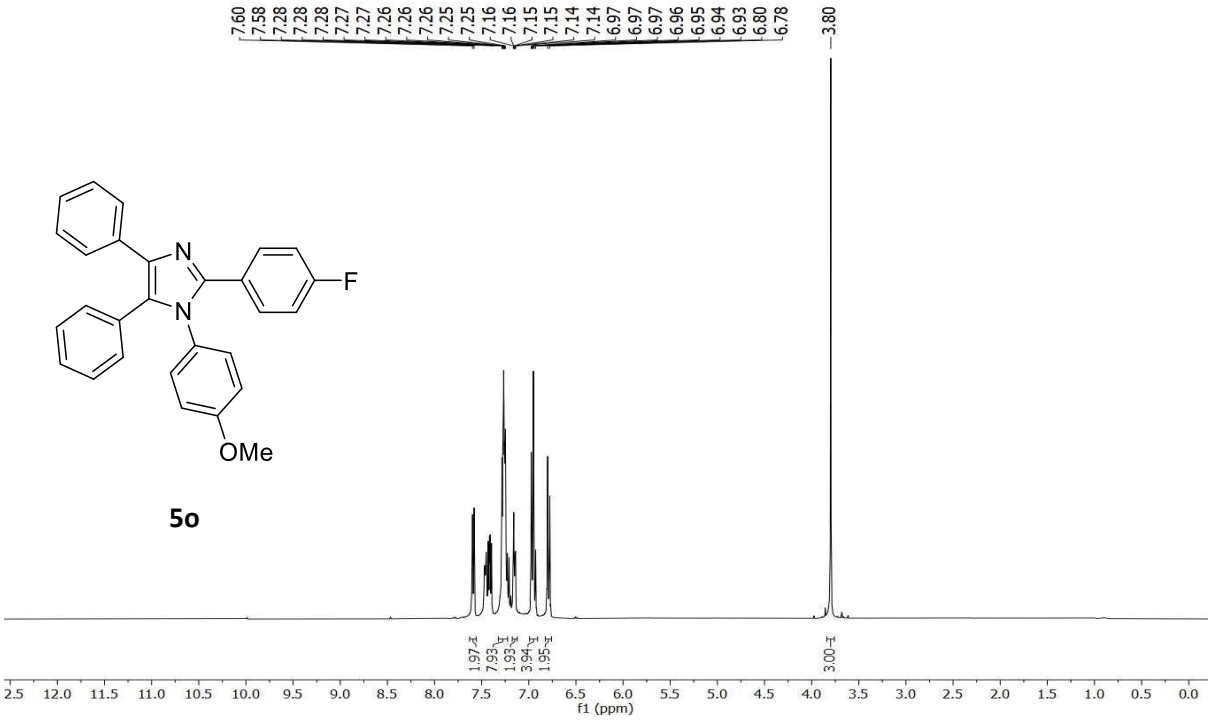


5n

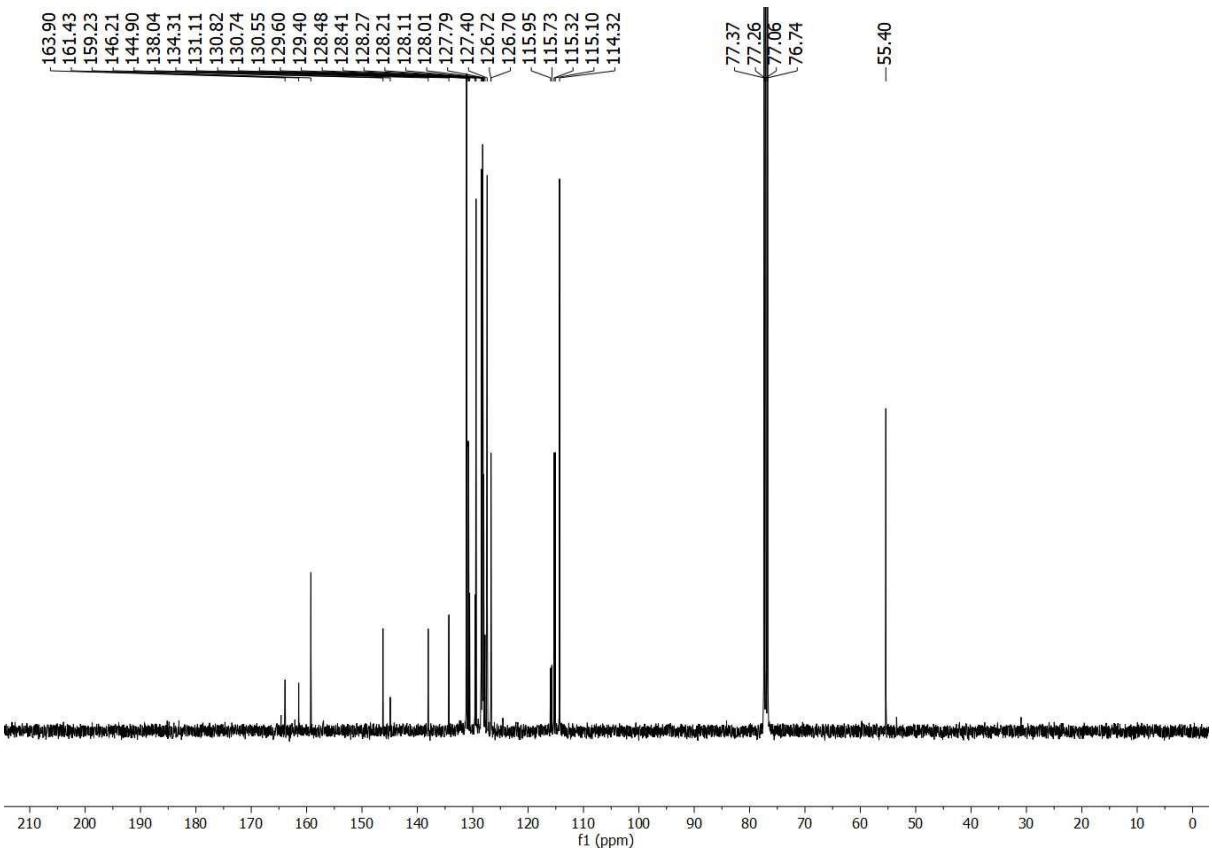
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5n



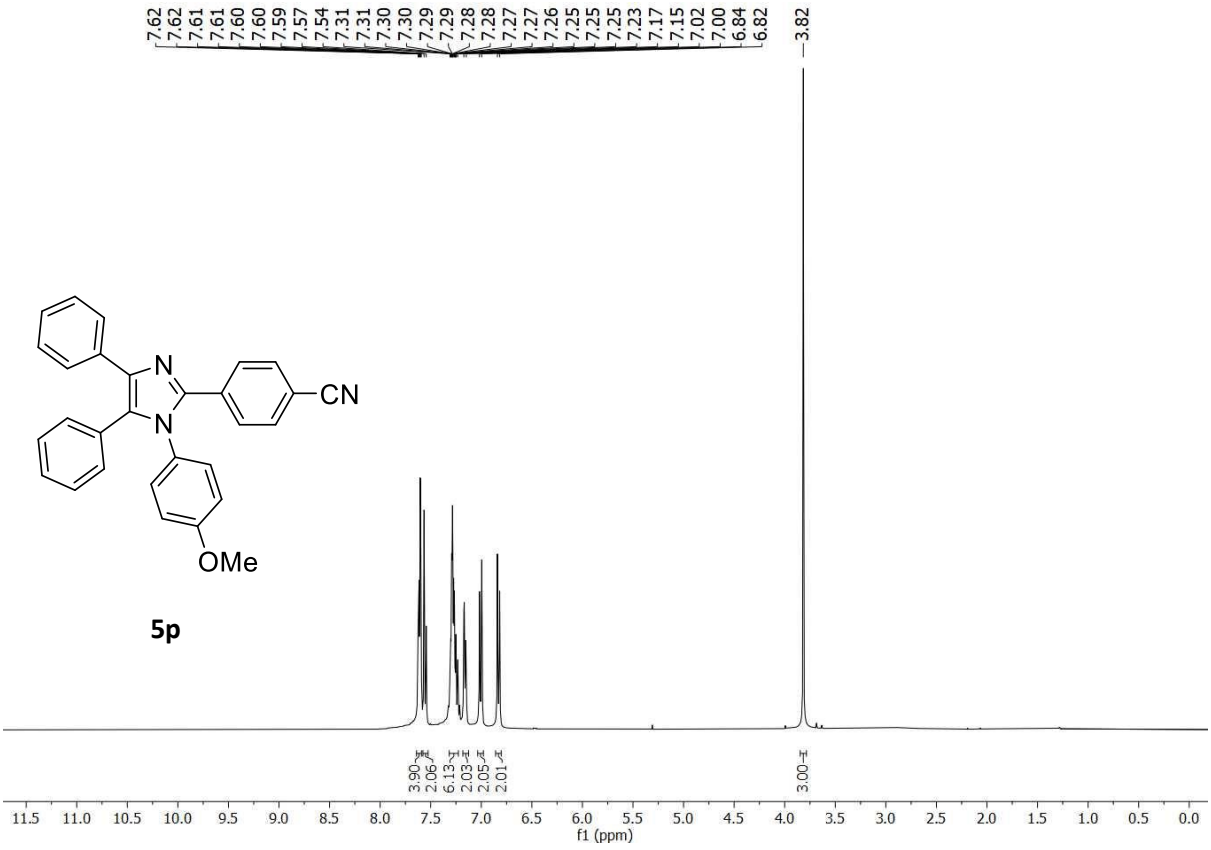
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5n



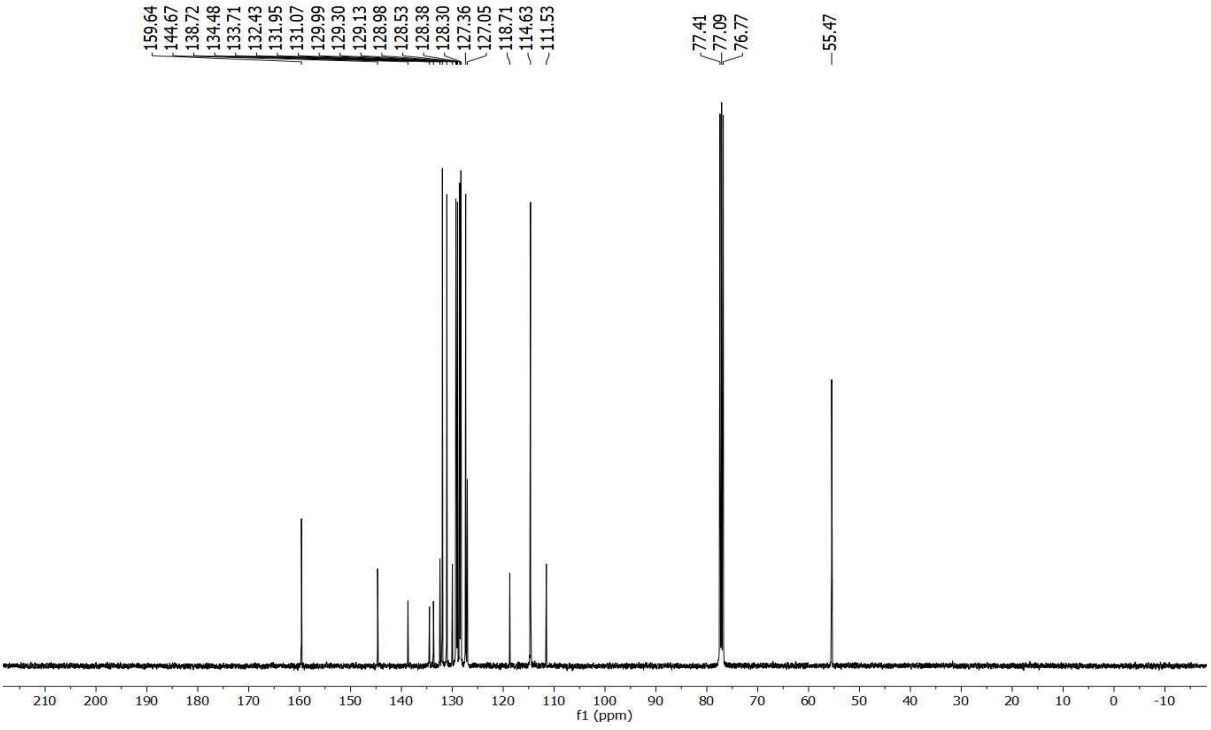
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5o



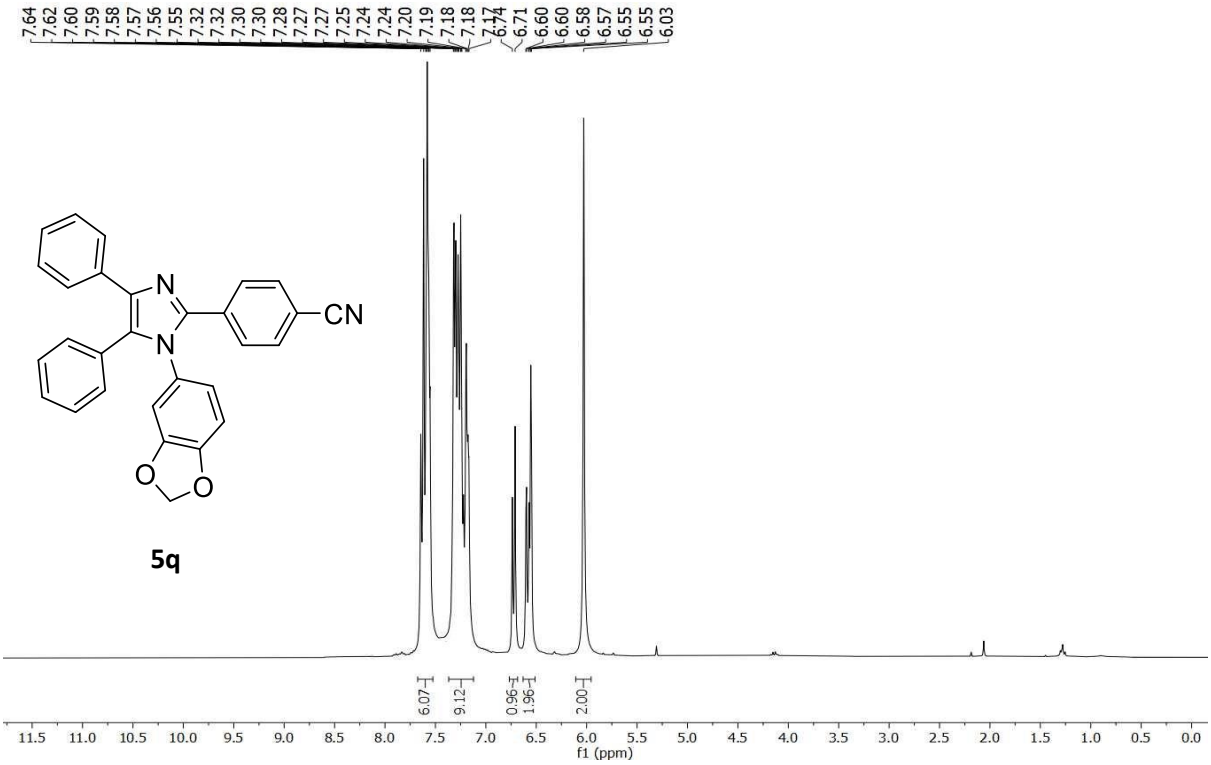
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5o



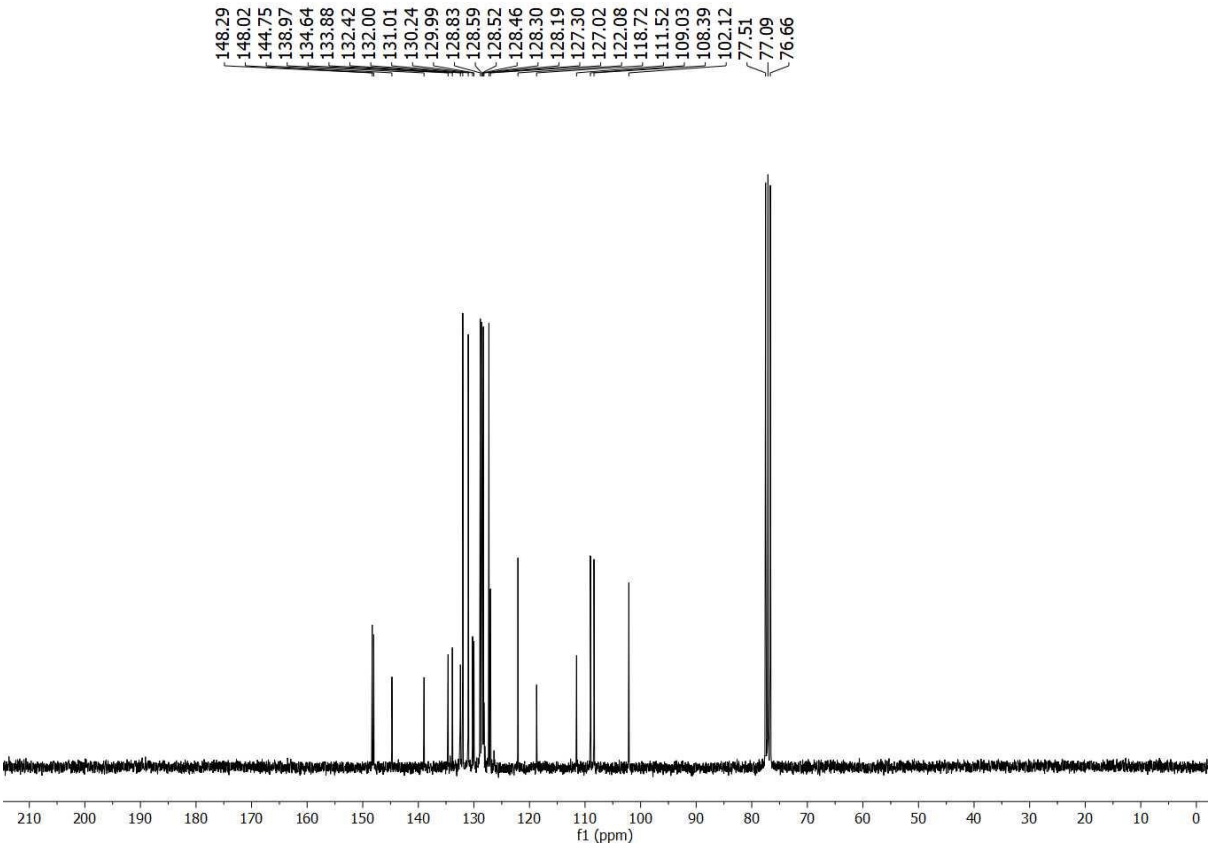
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5p



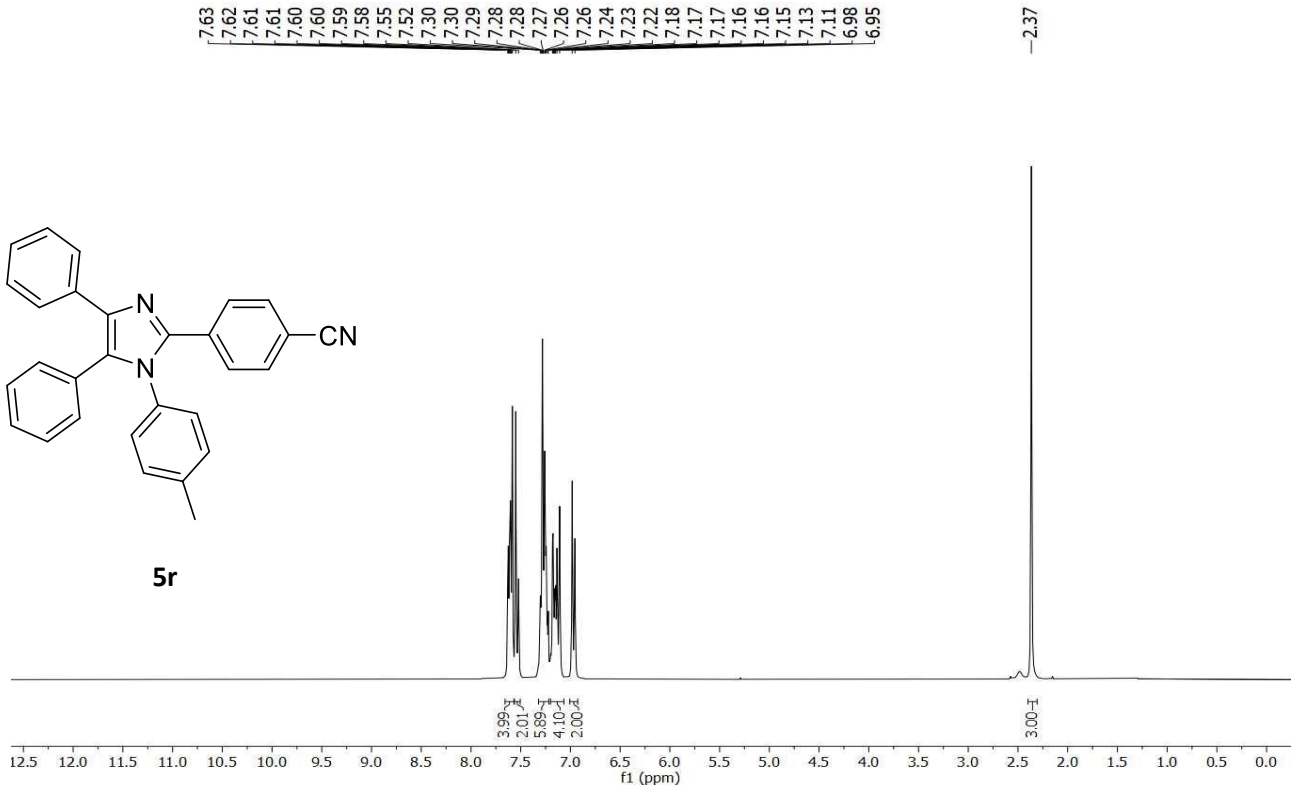
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5p



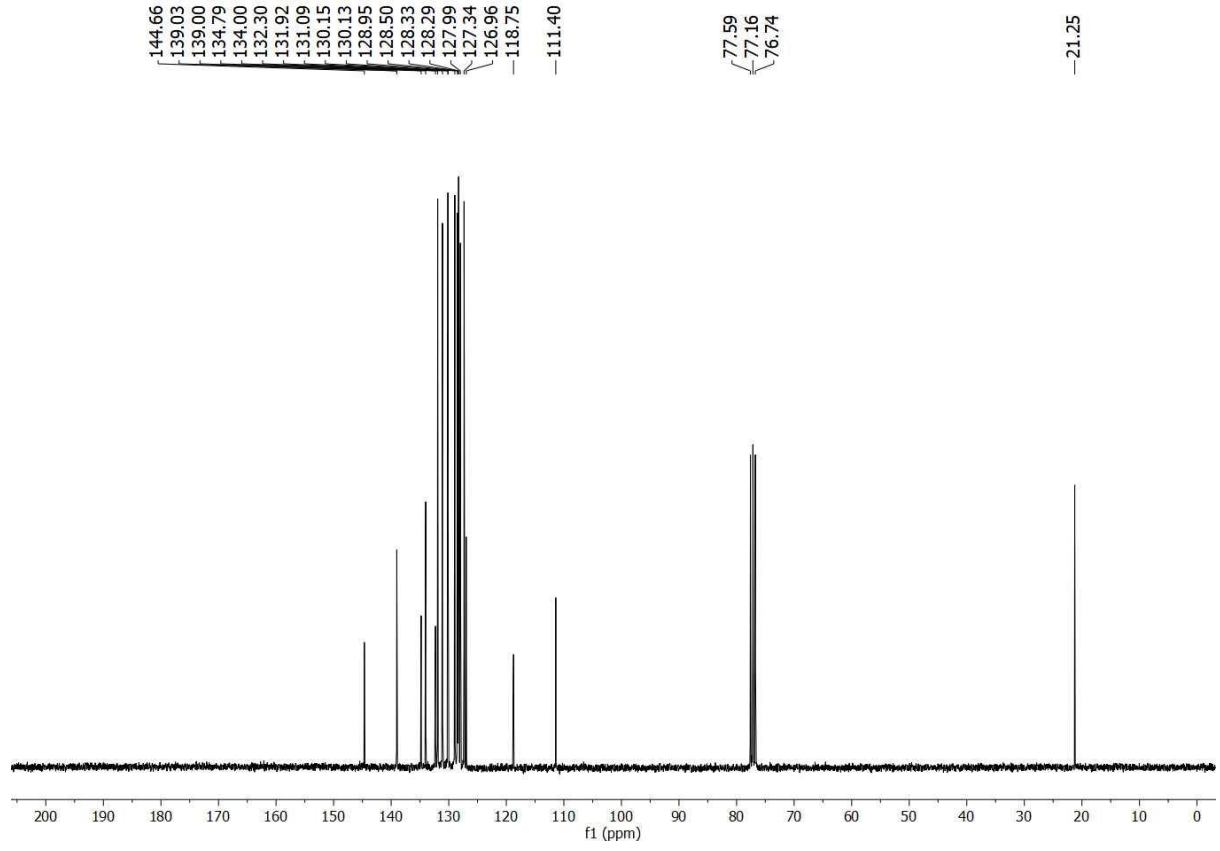
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5q



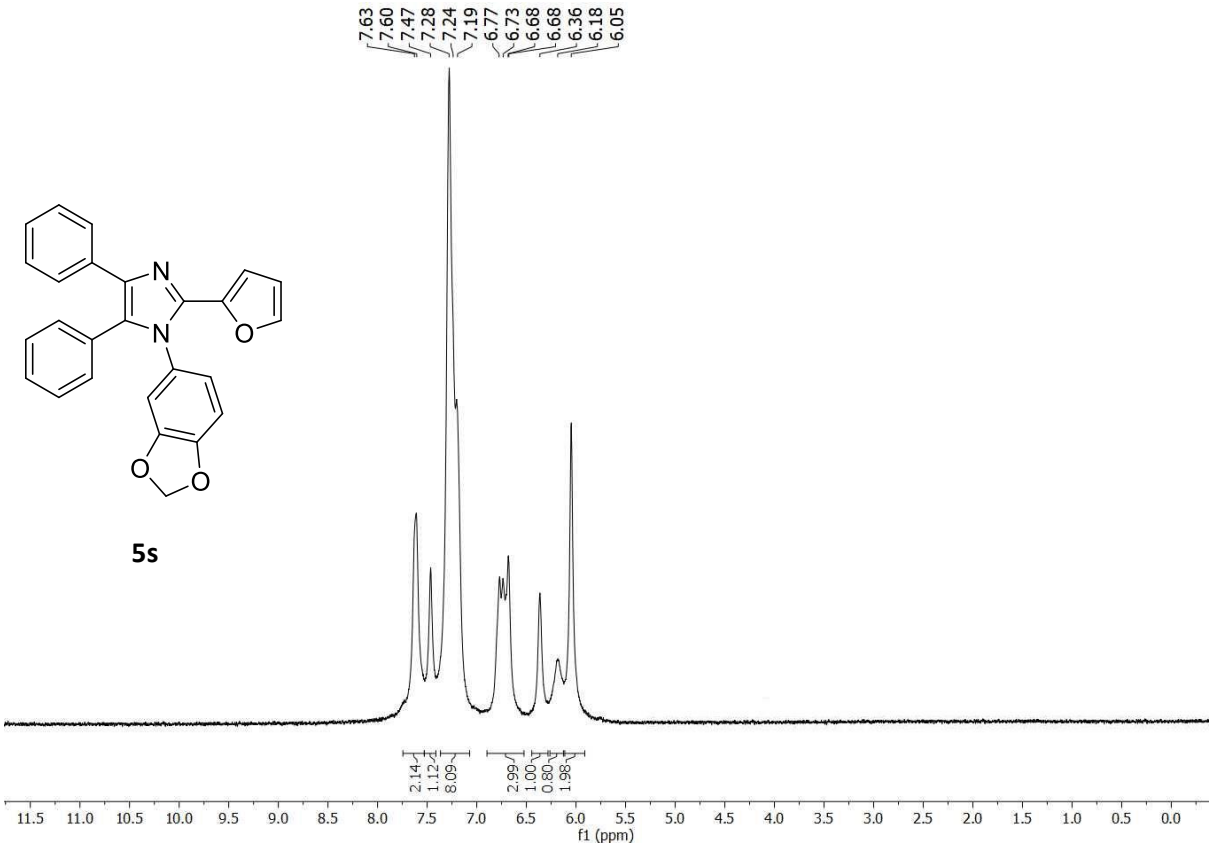
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5q



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5r

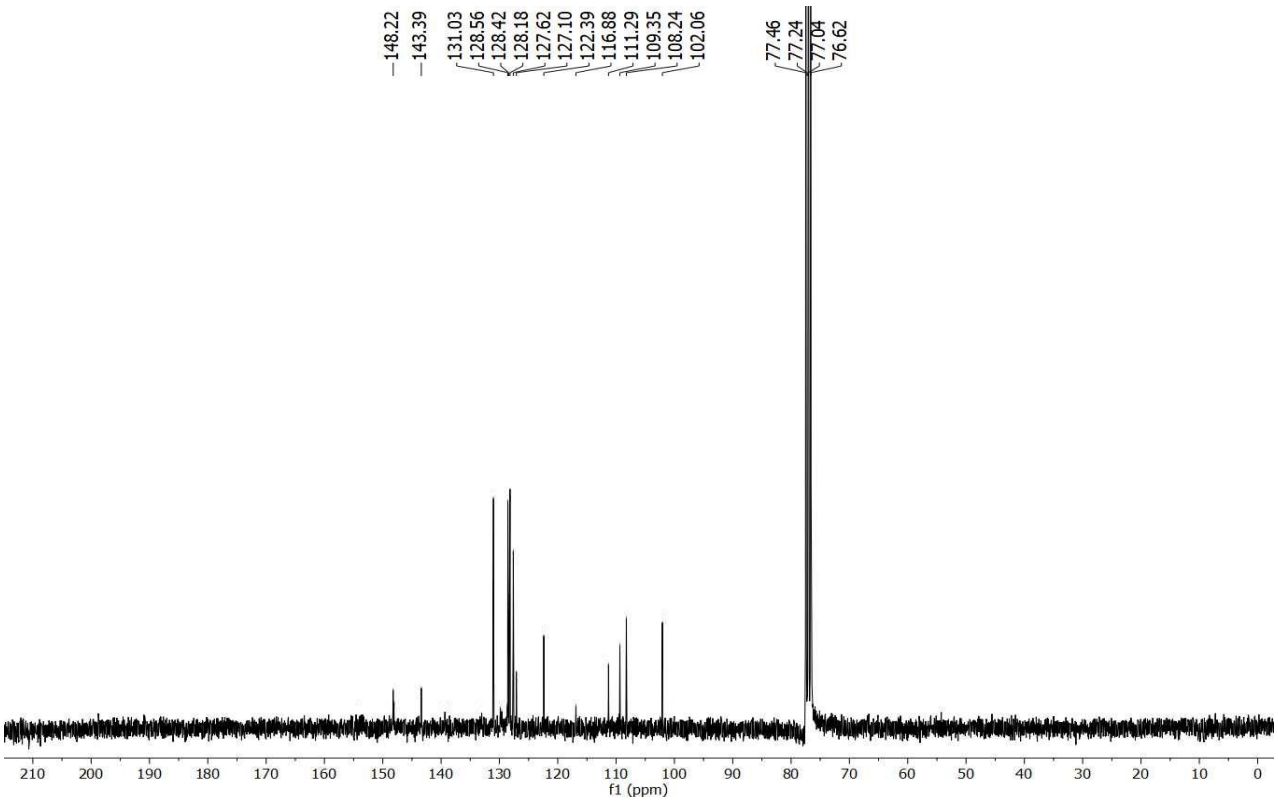


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5r

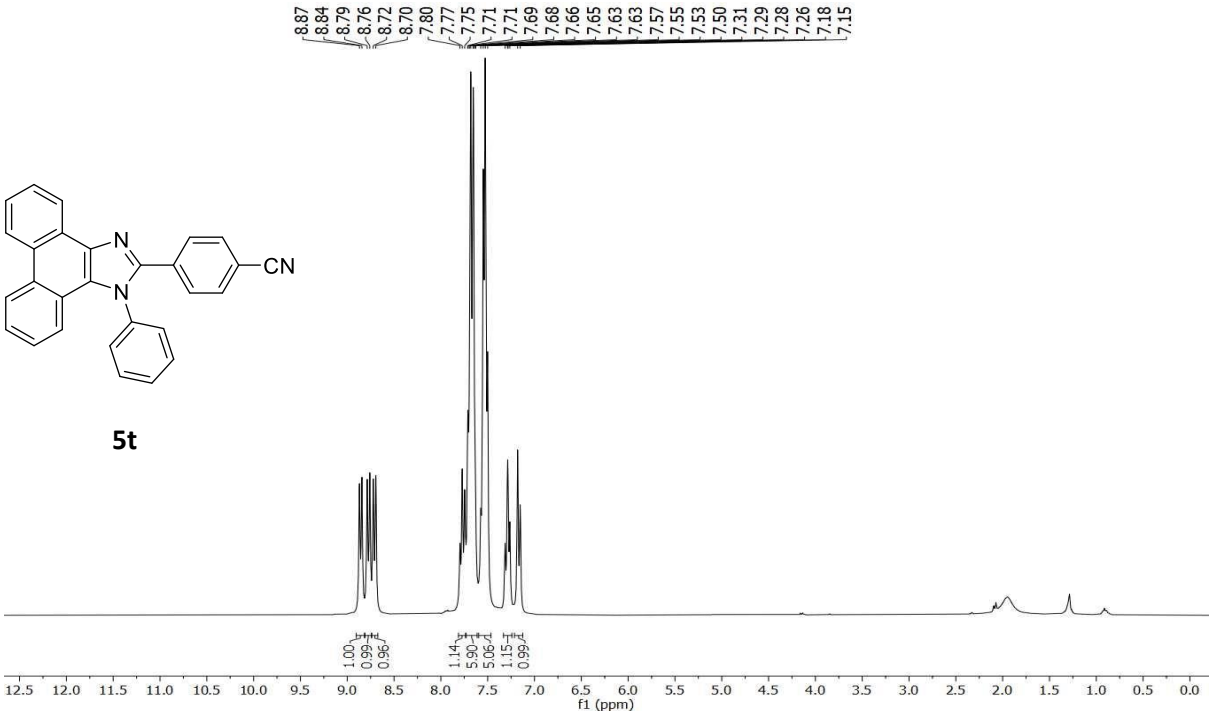


5s

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5t

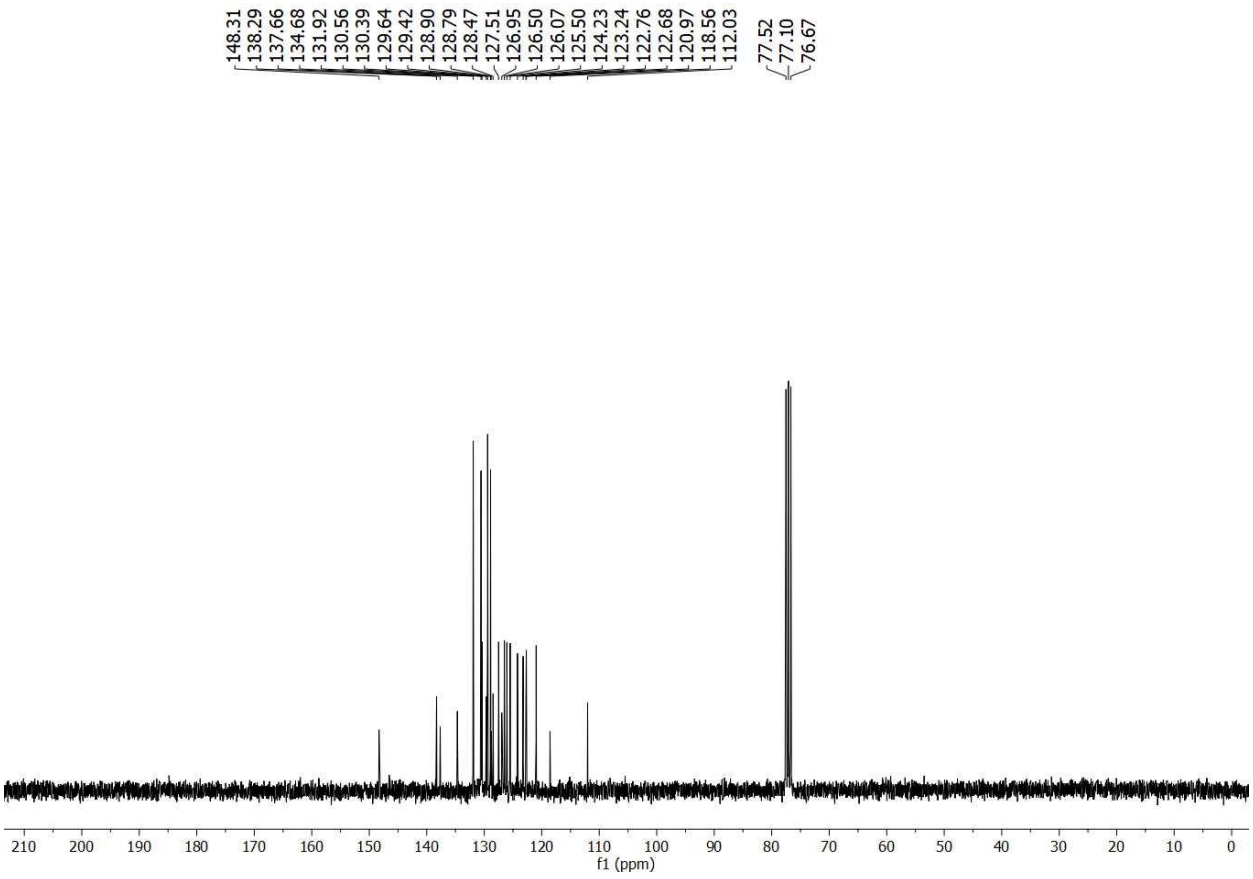


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5t

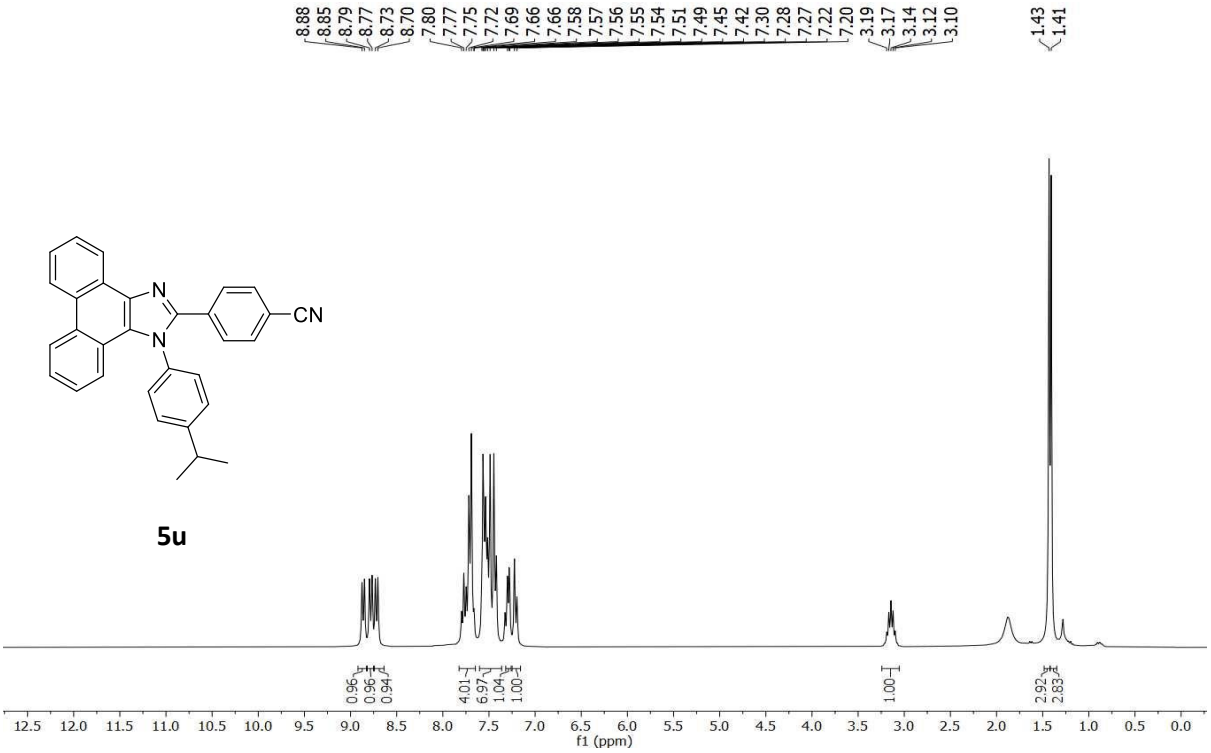


5t

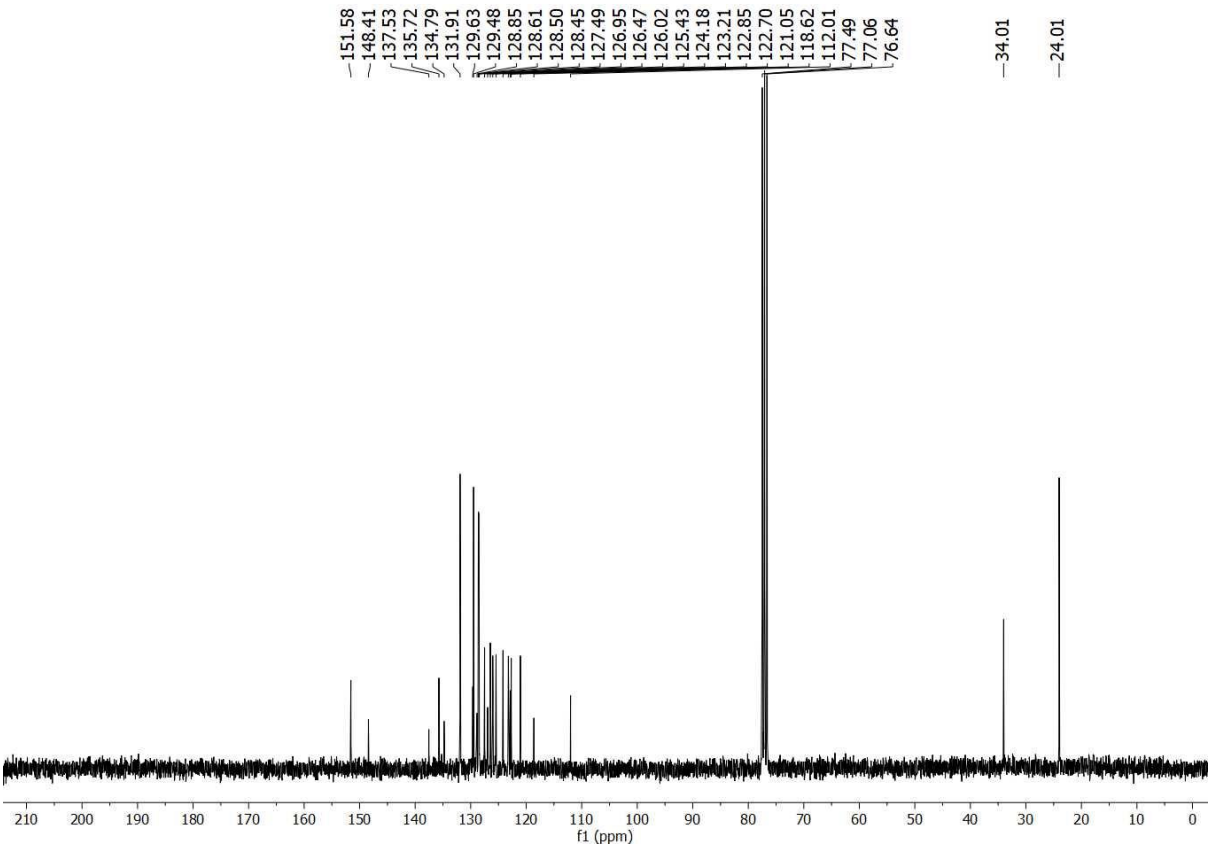
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5u



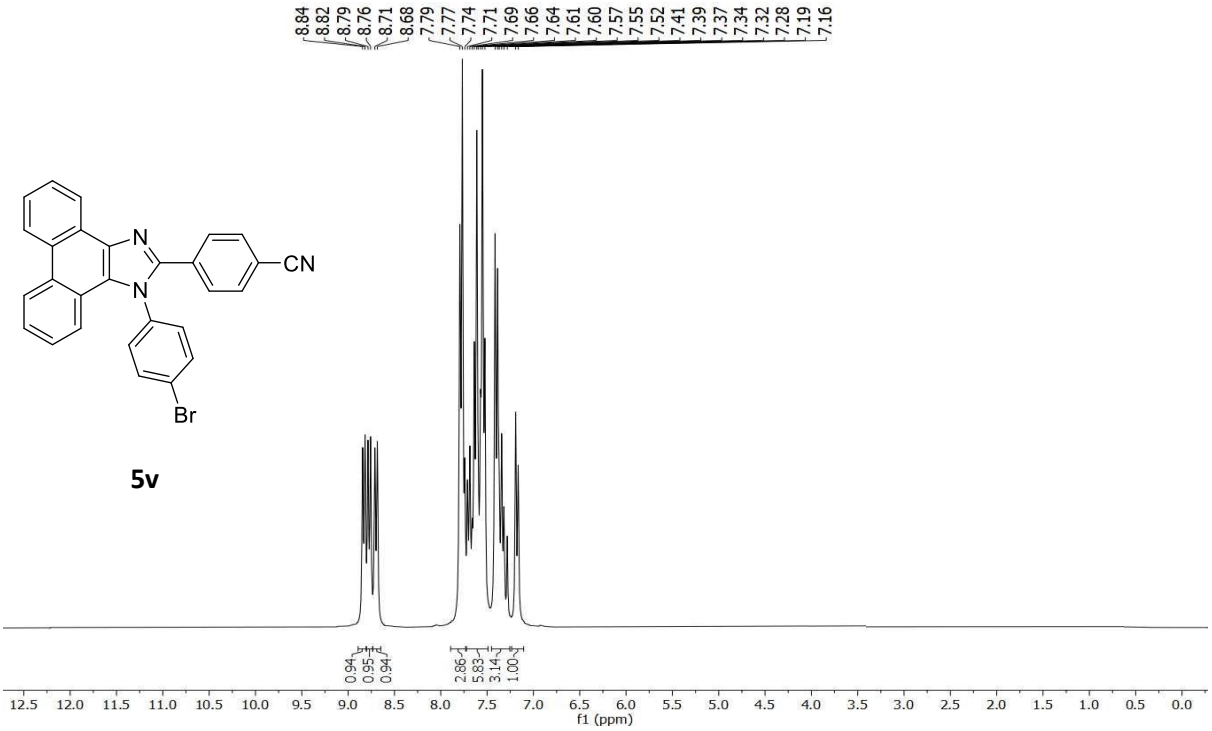
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5u



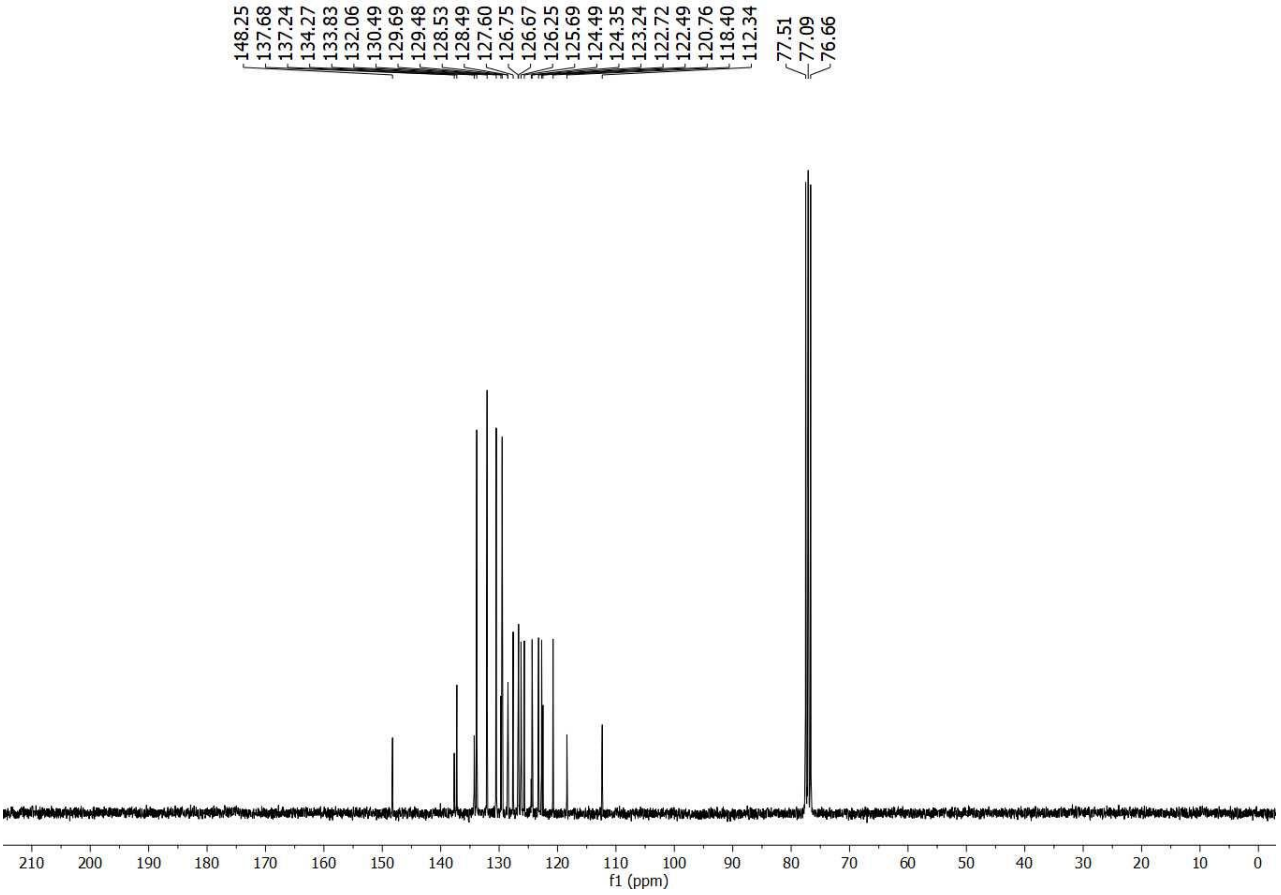
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5v



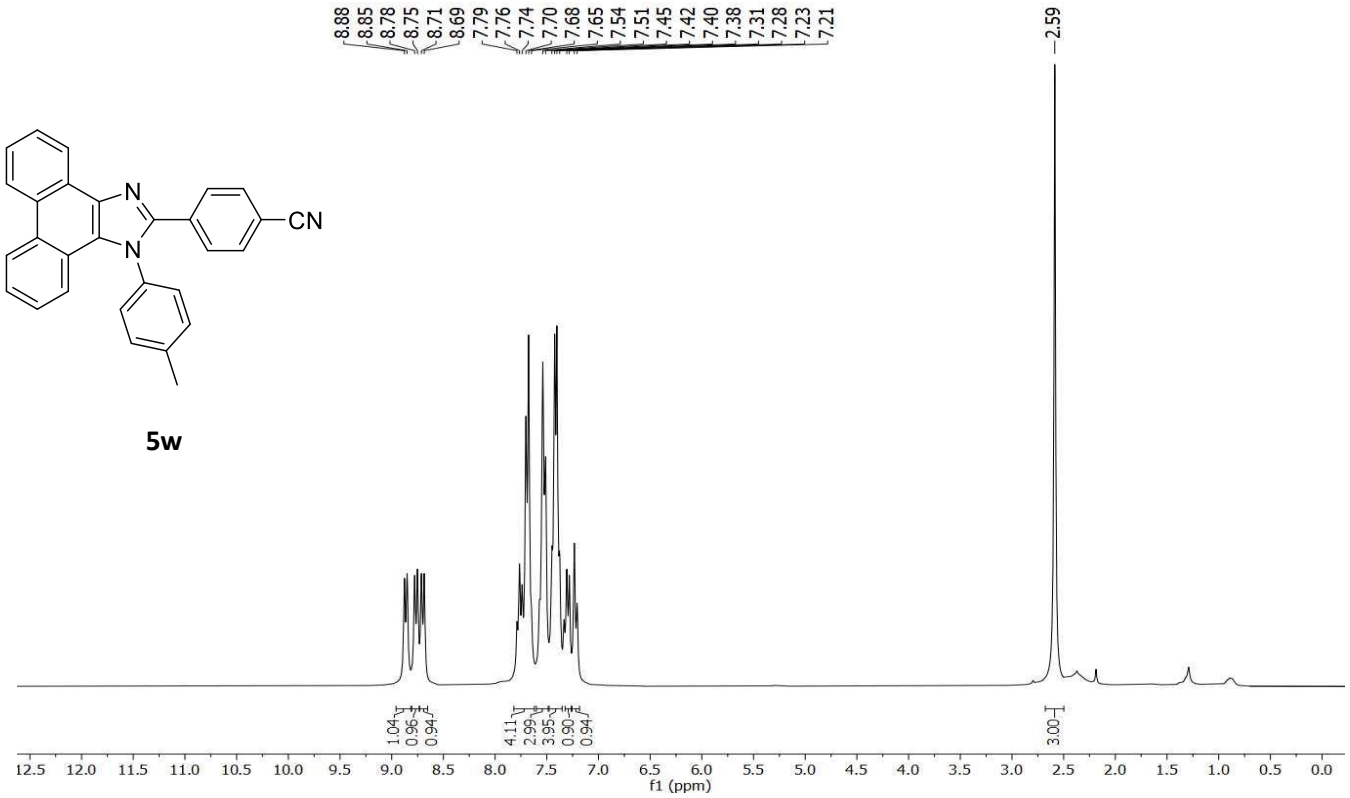
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5v



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5w

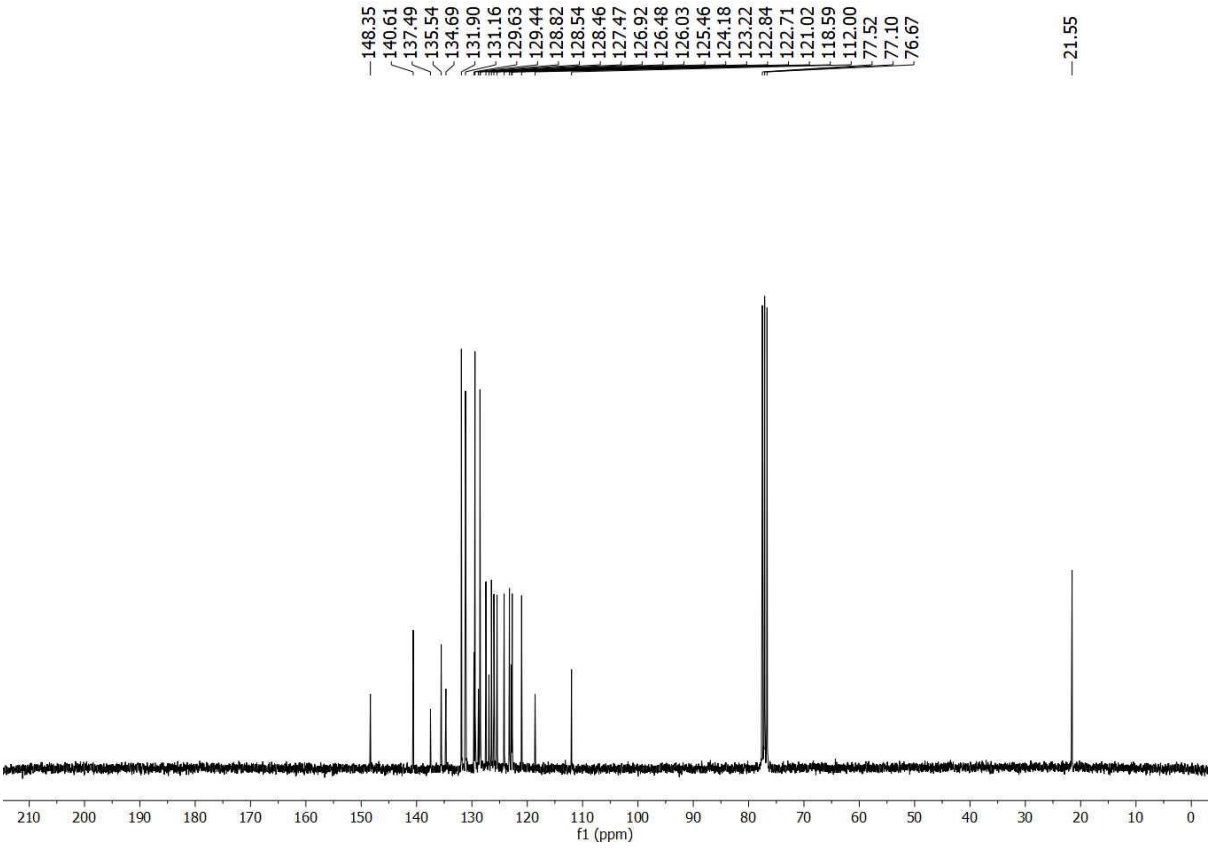


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5w

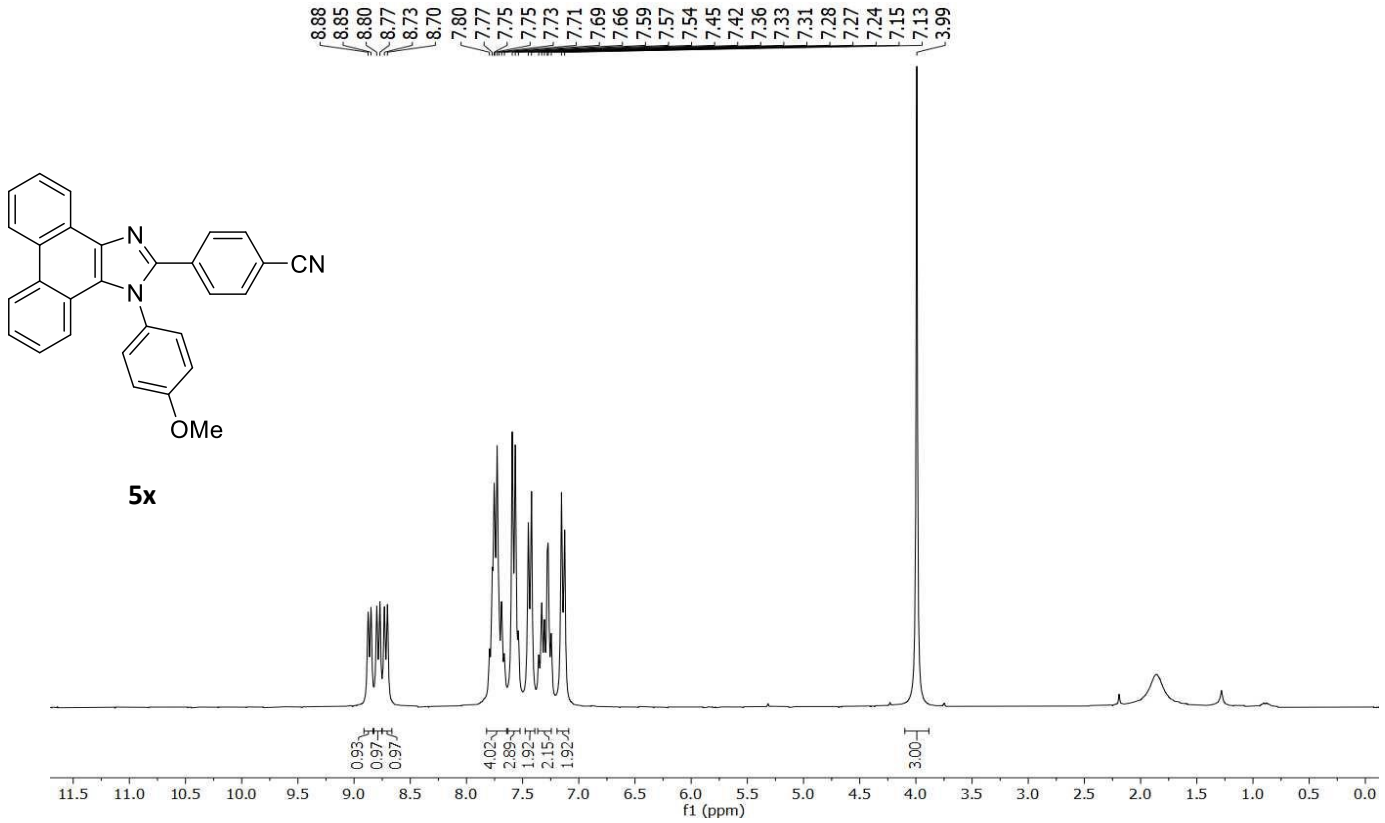


5w

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 5x

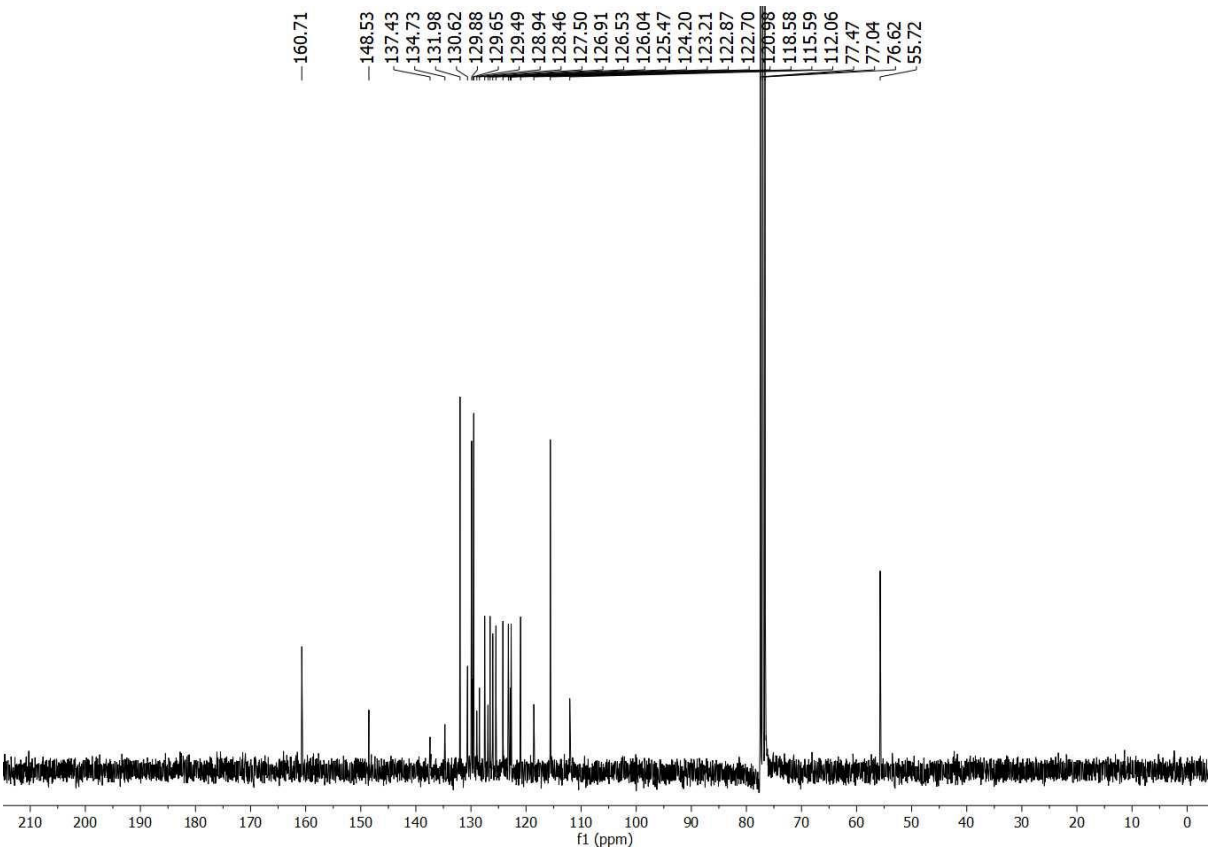


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 5x

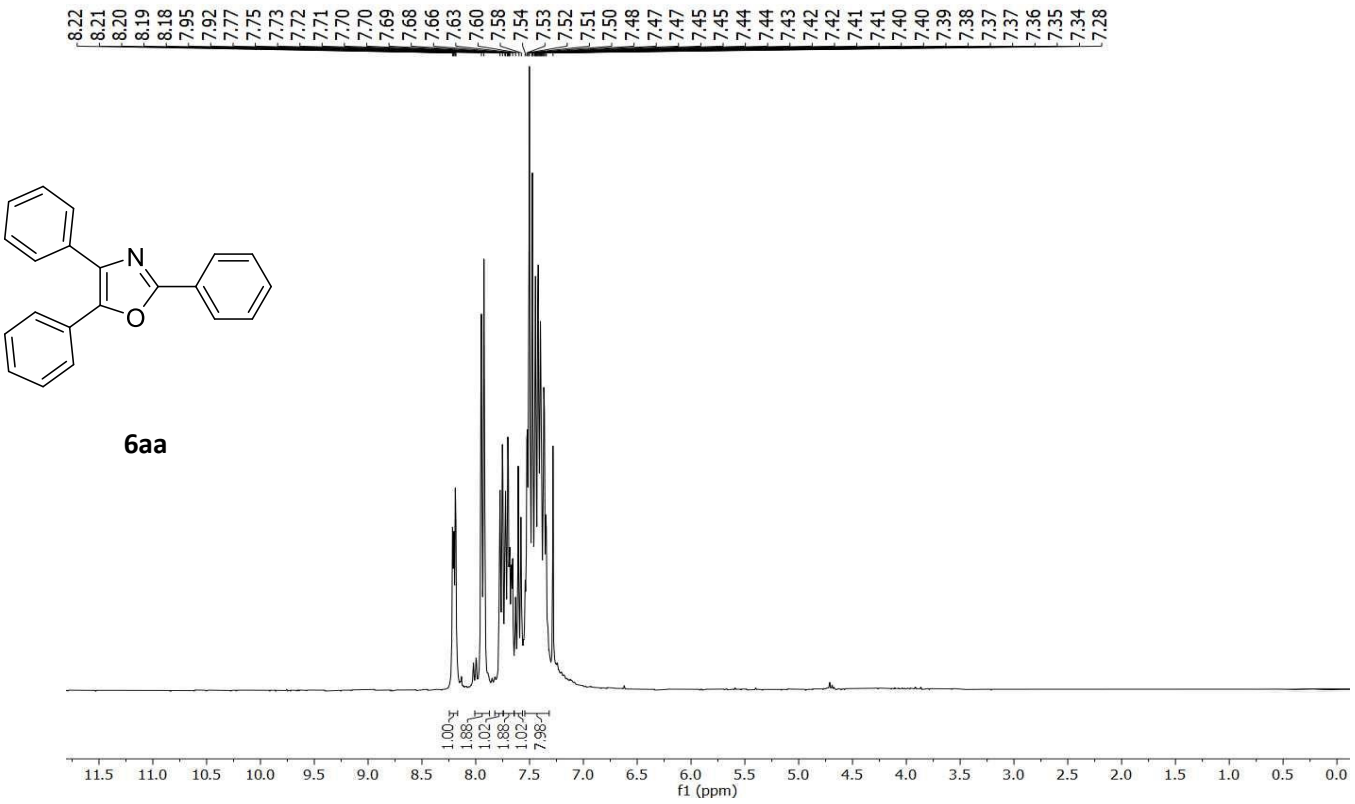


5x

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 4aa

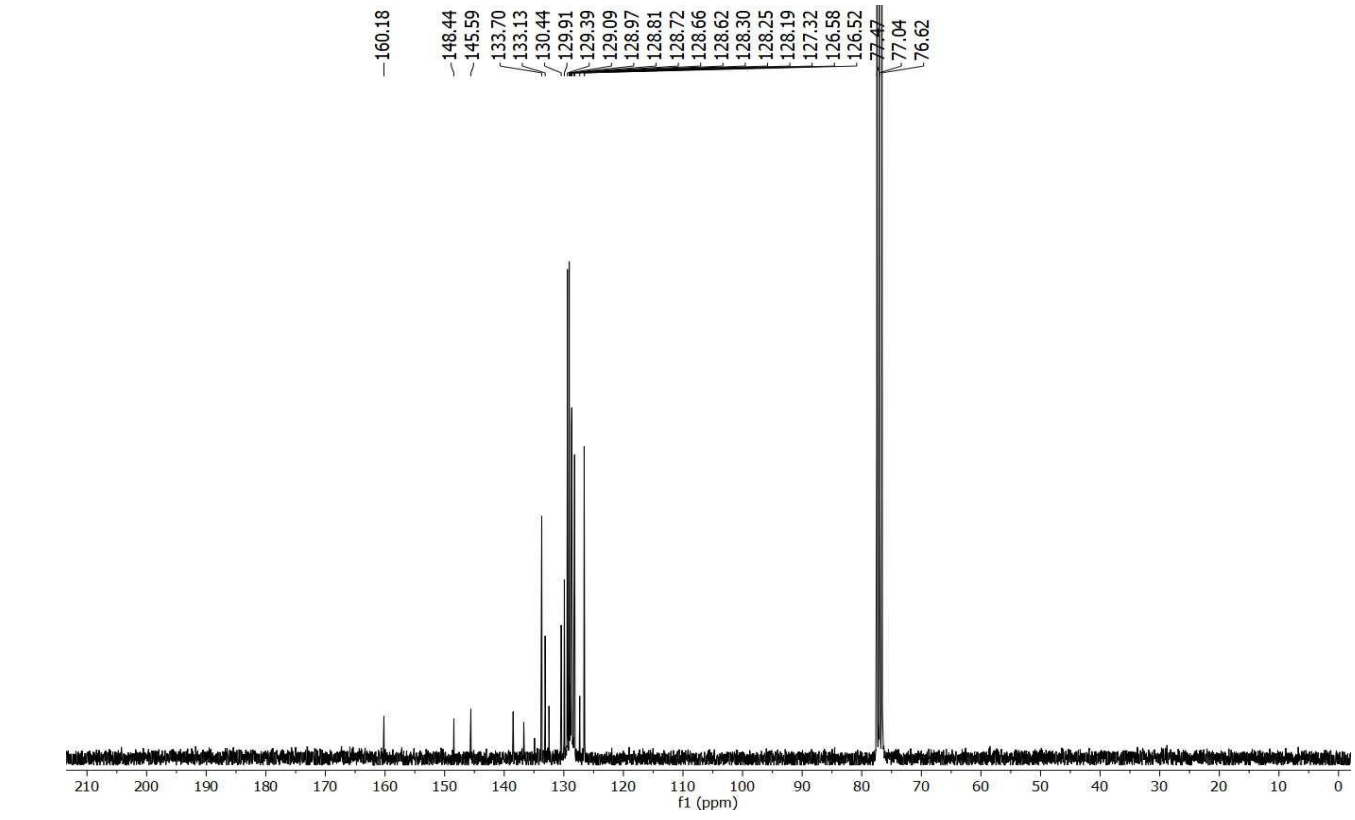


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 4aa

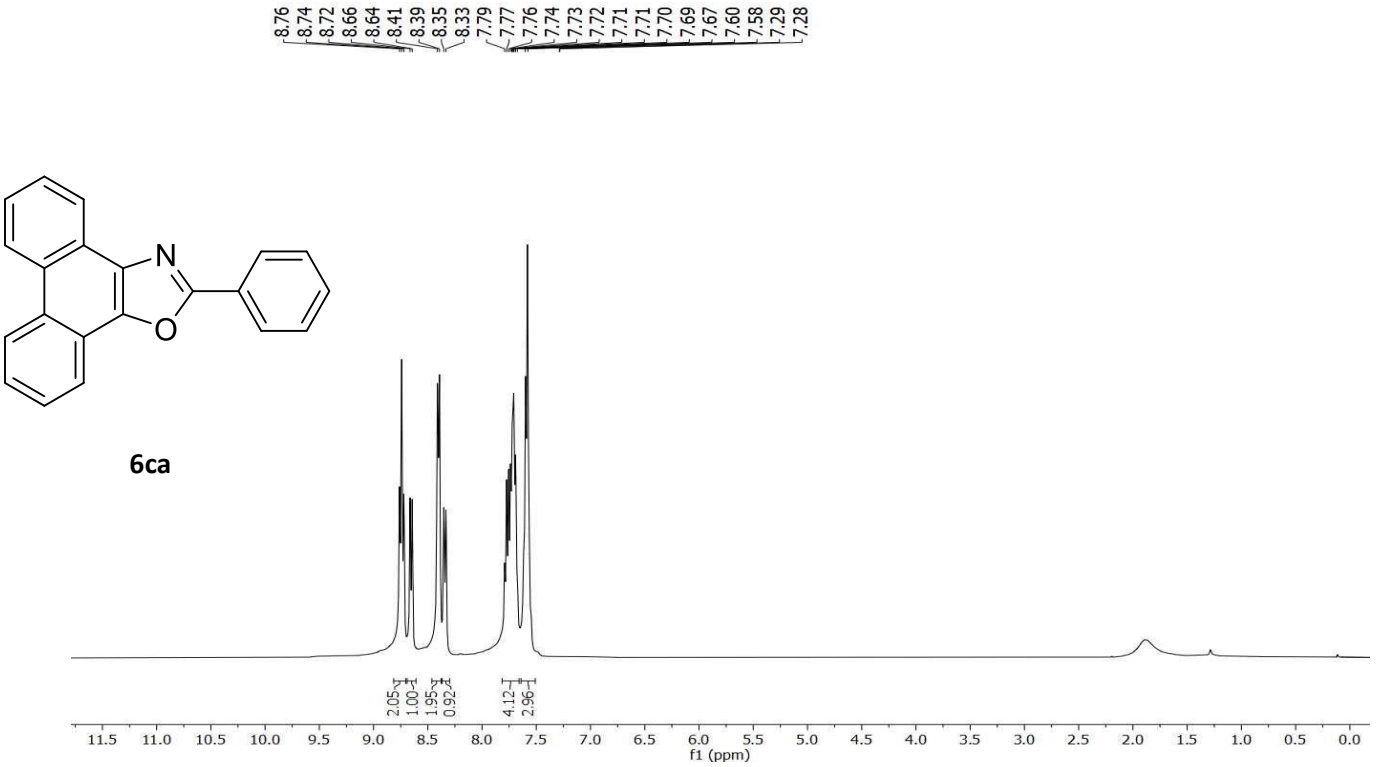


6aa

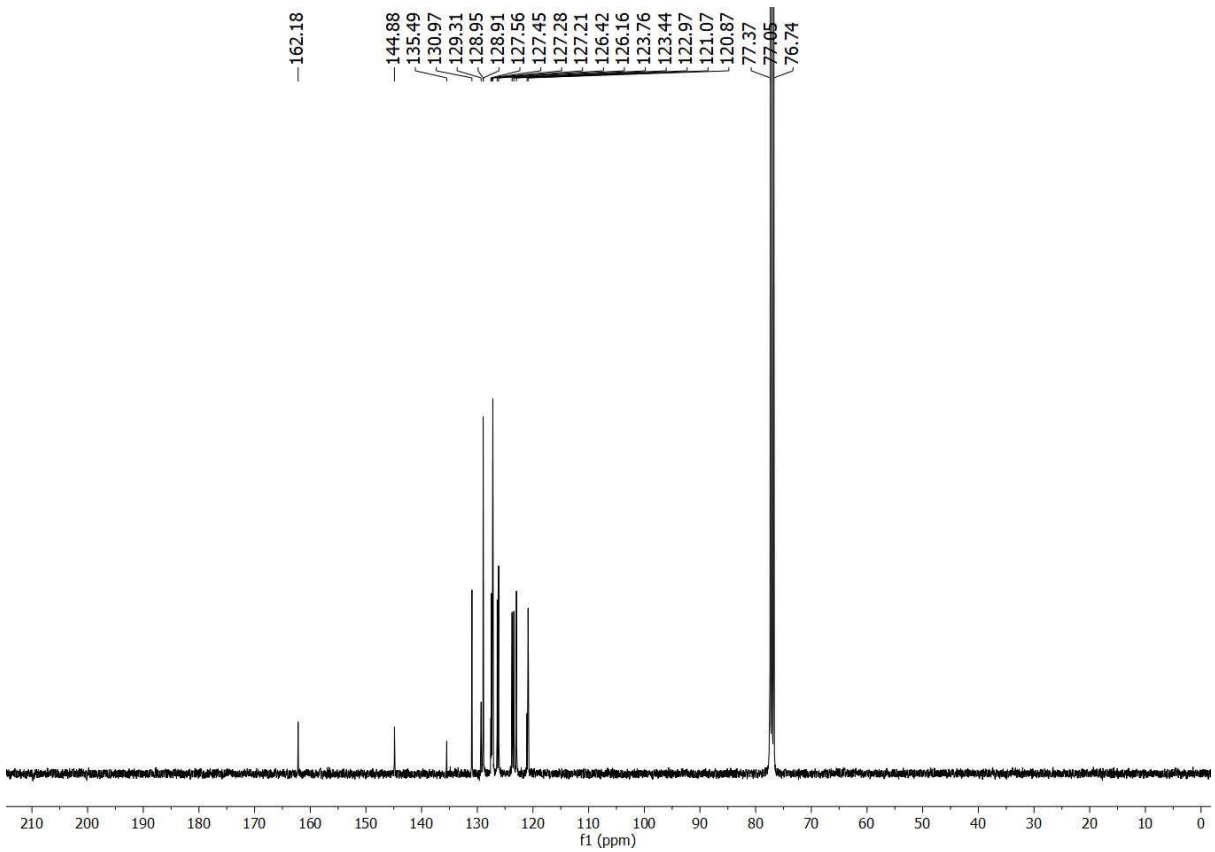
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6aa



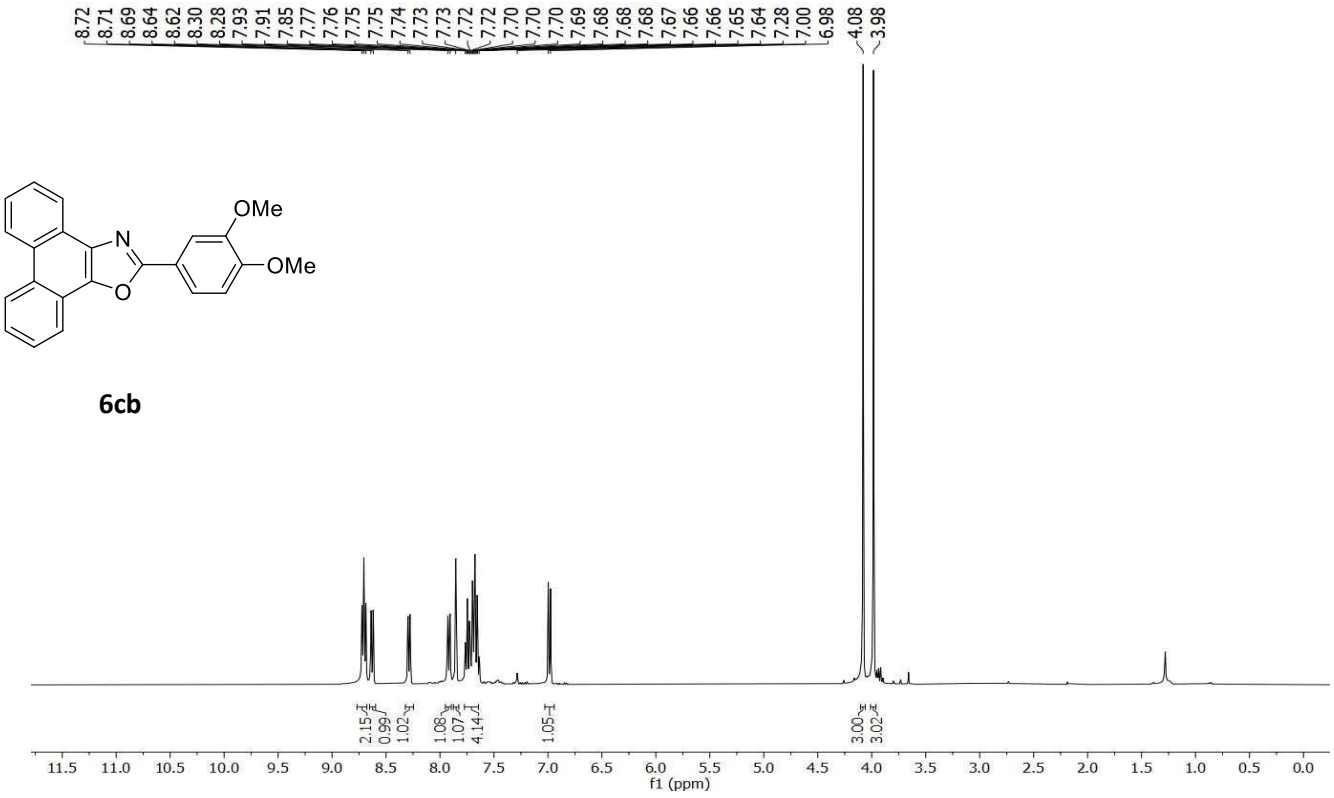
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6aa



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6ca

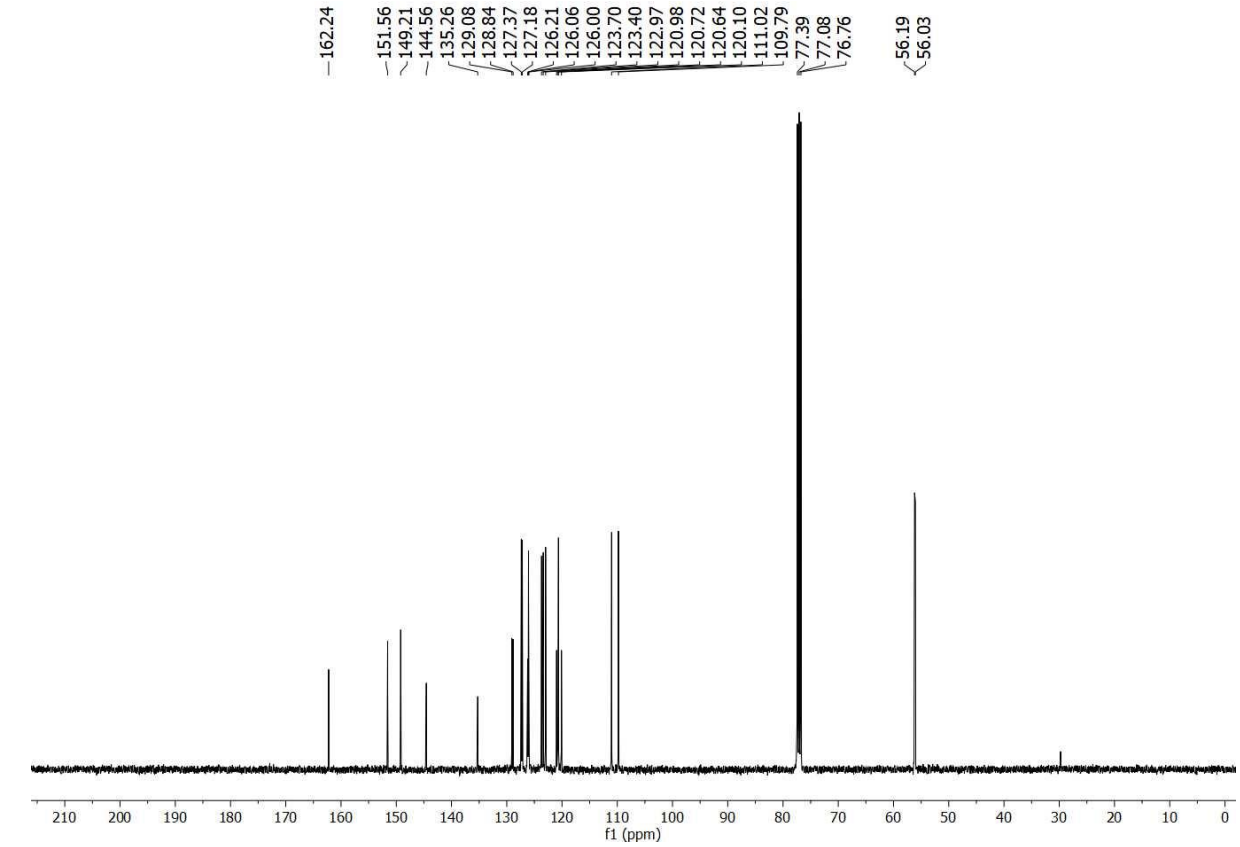


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6ca

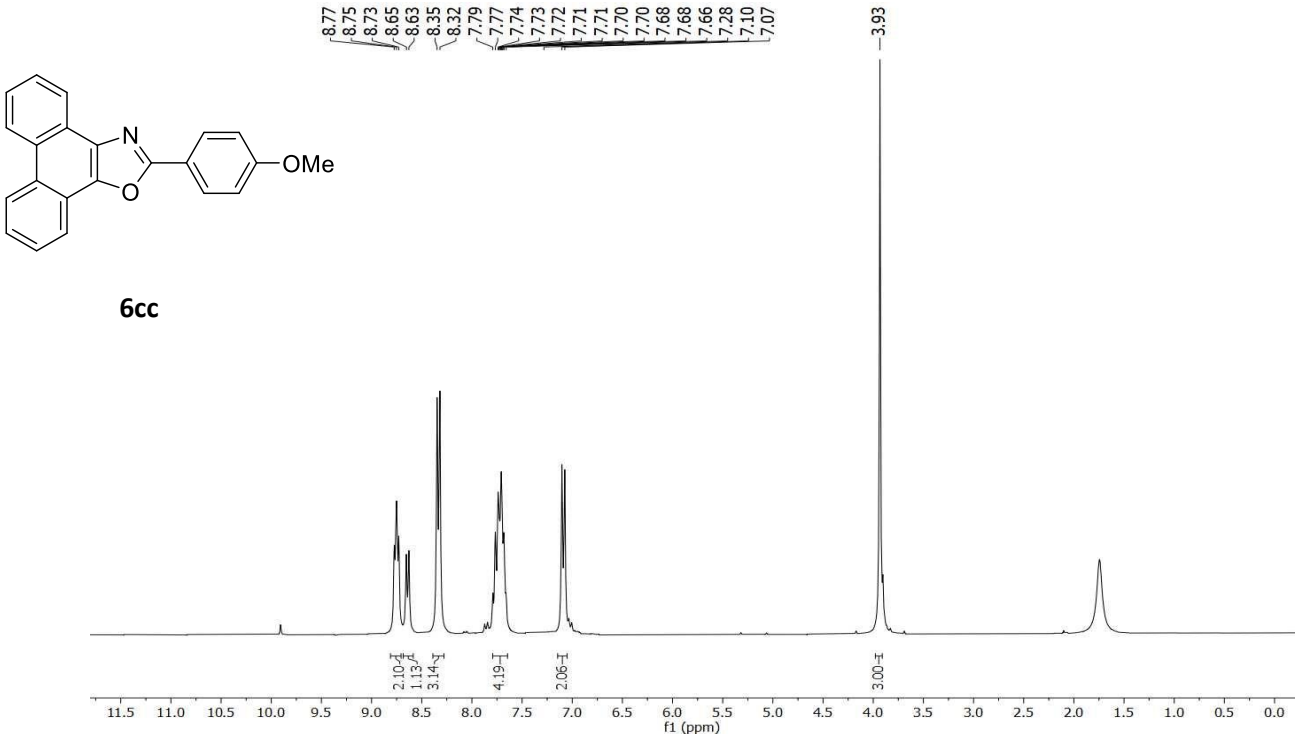


6cb

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6cb

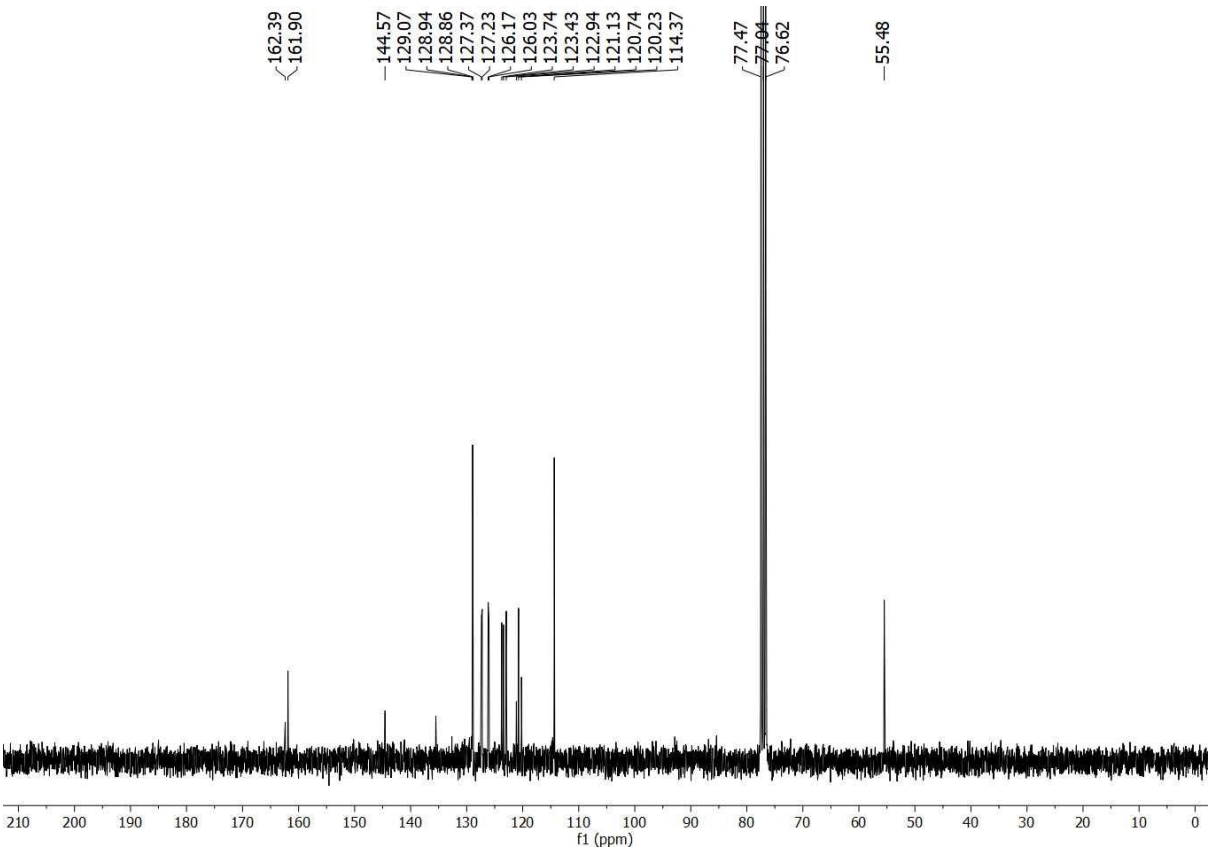


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6cb

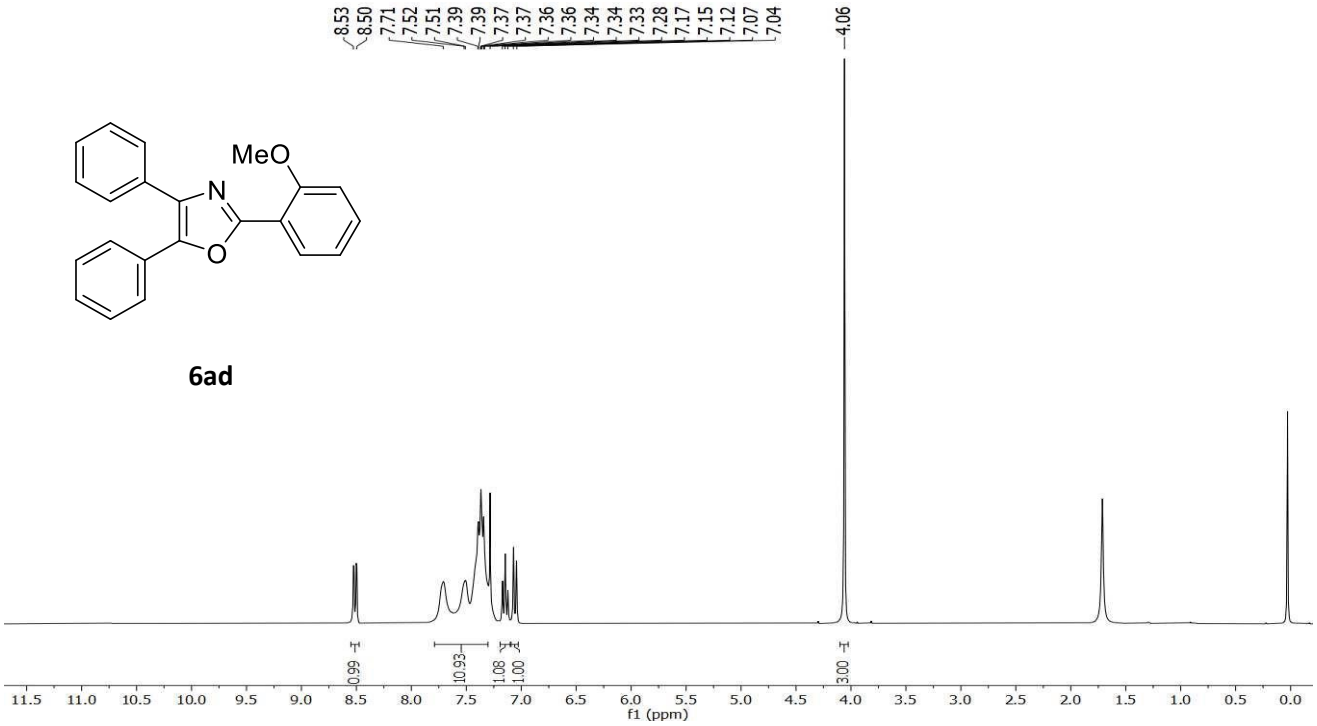


6cc

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6cc

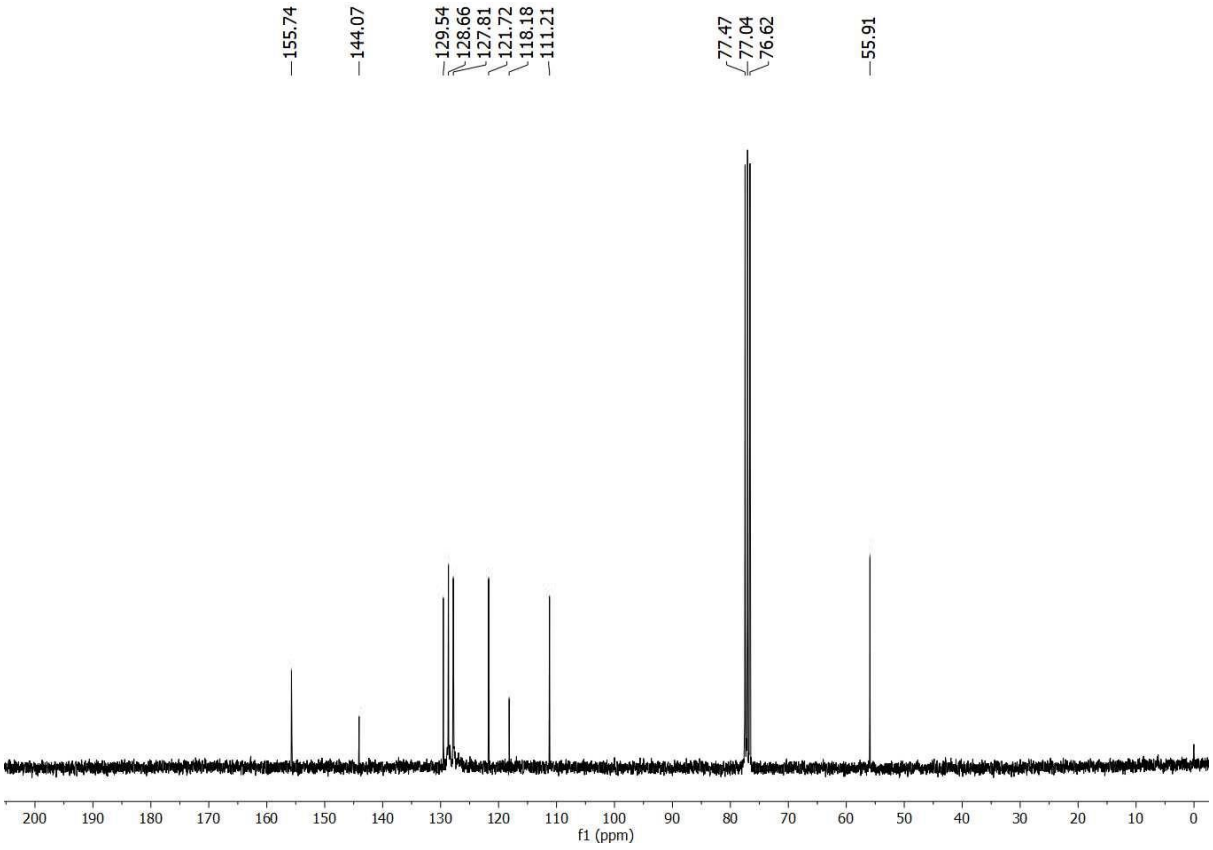


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6cc

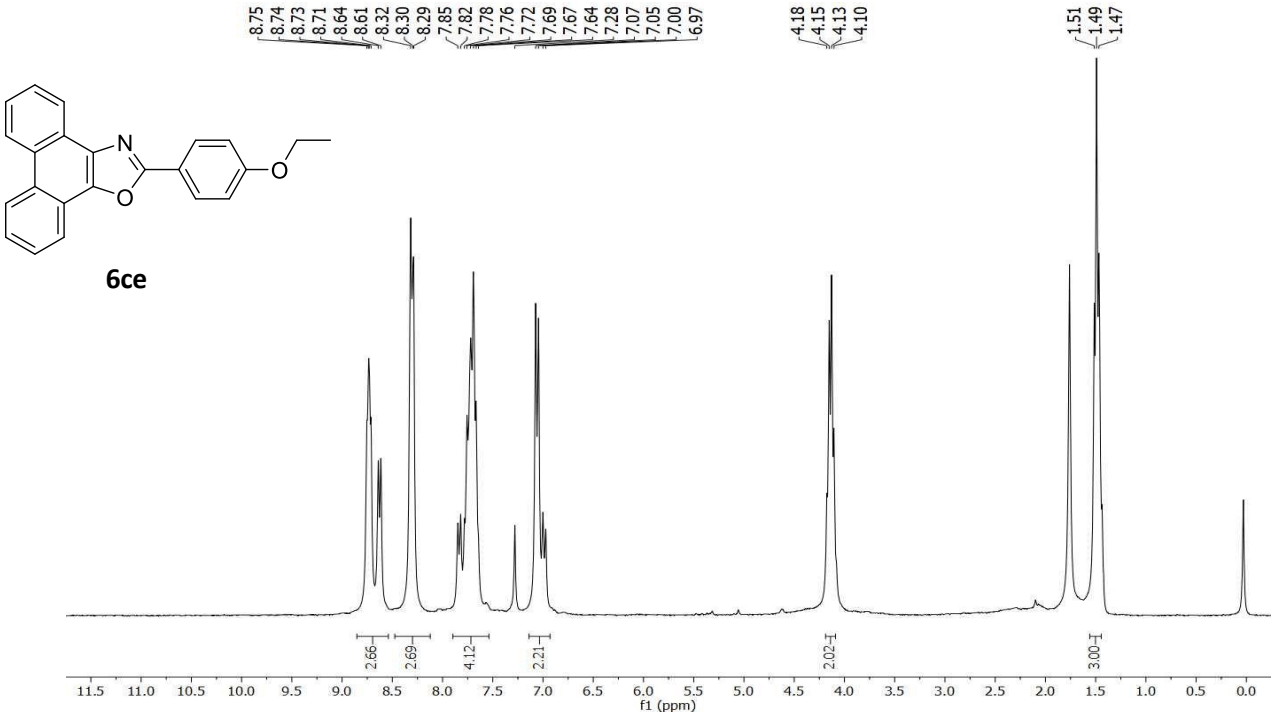


6ad

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6ad

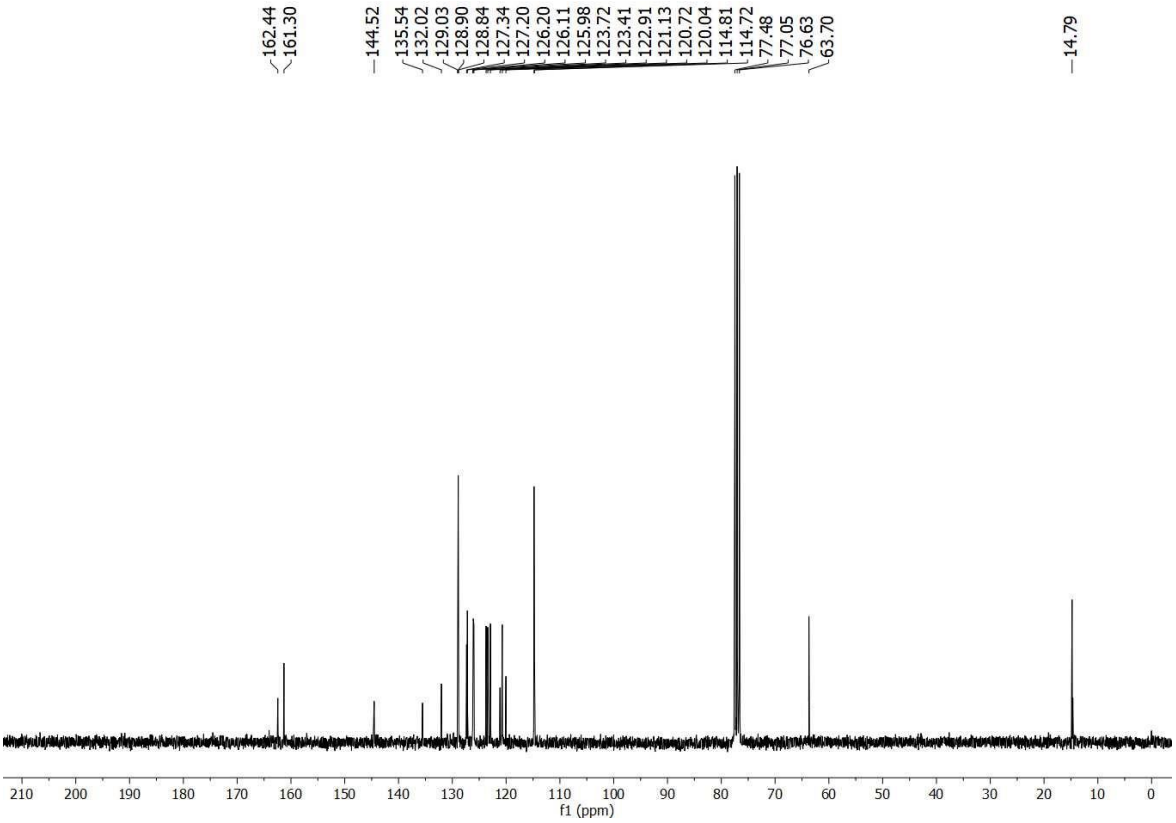


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6ad

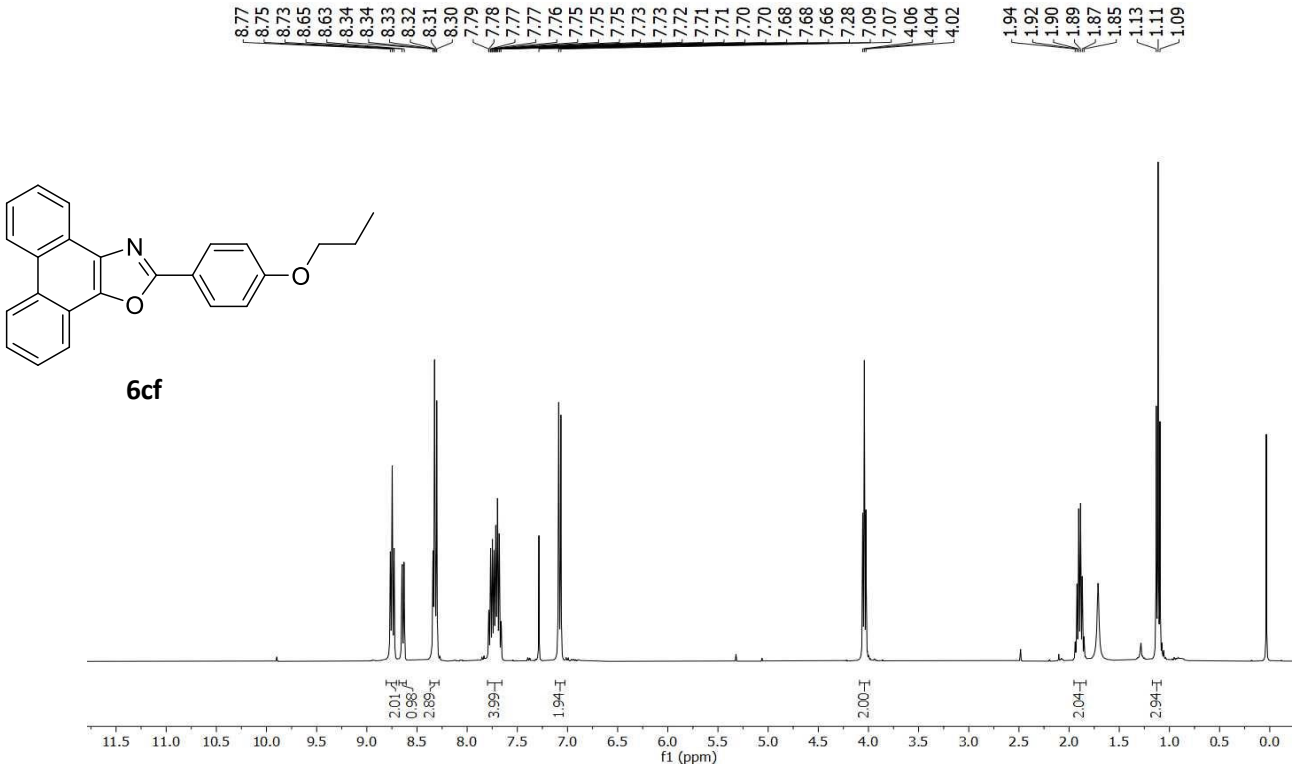


6ce

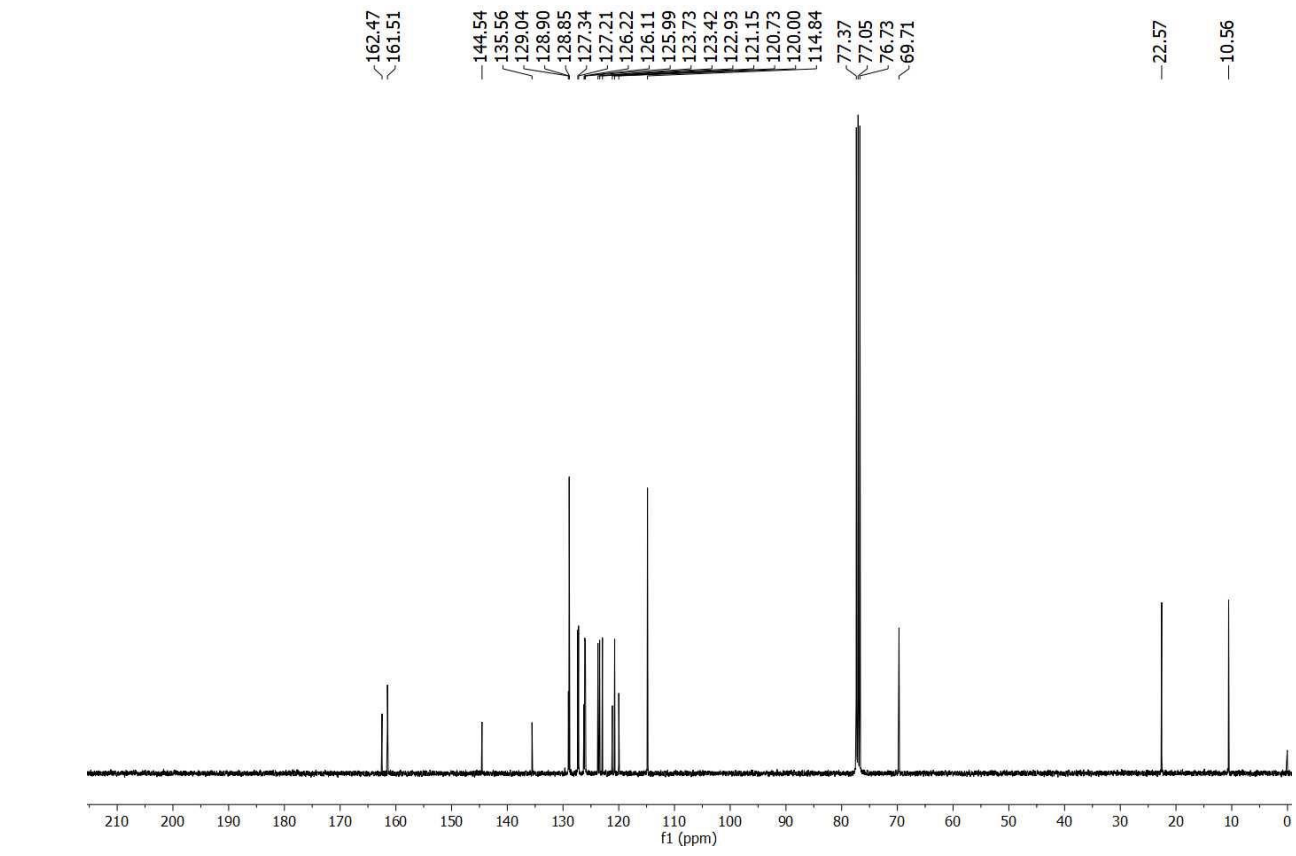
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6ce



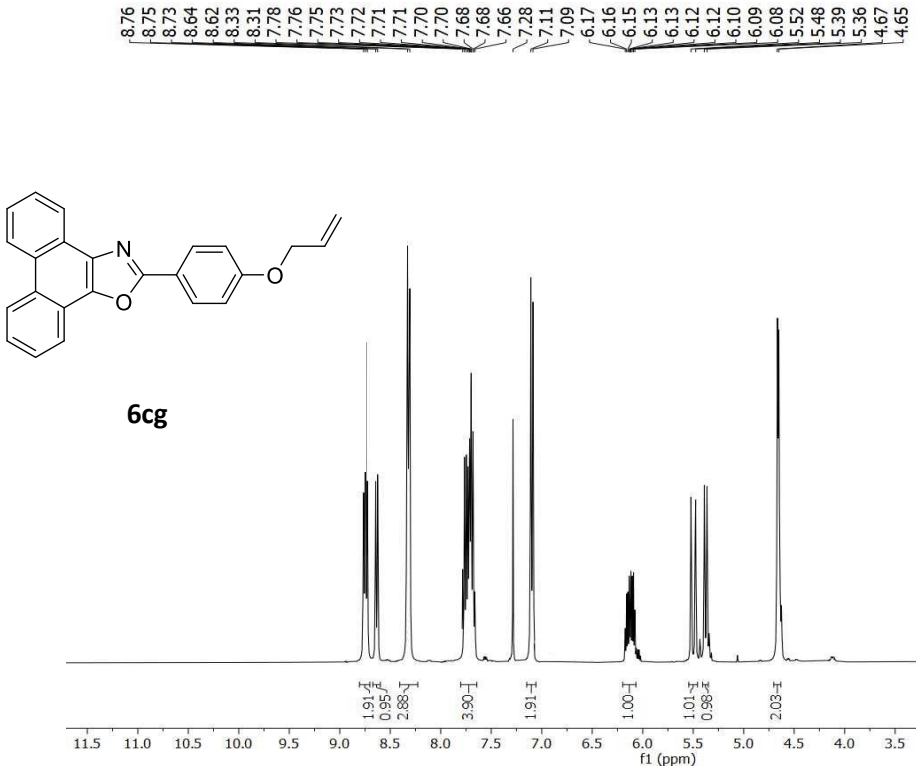
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6ce



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6cf

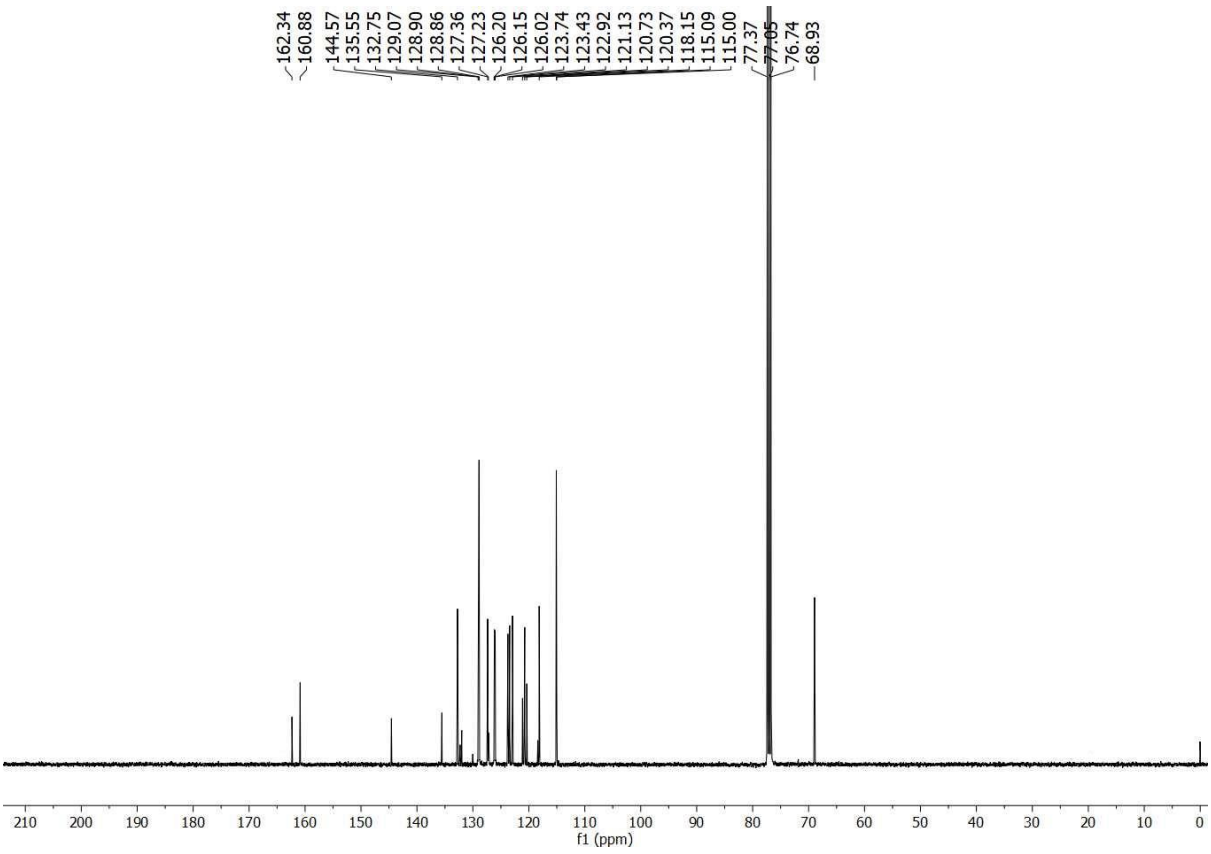


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6cf

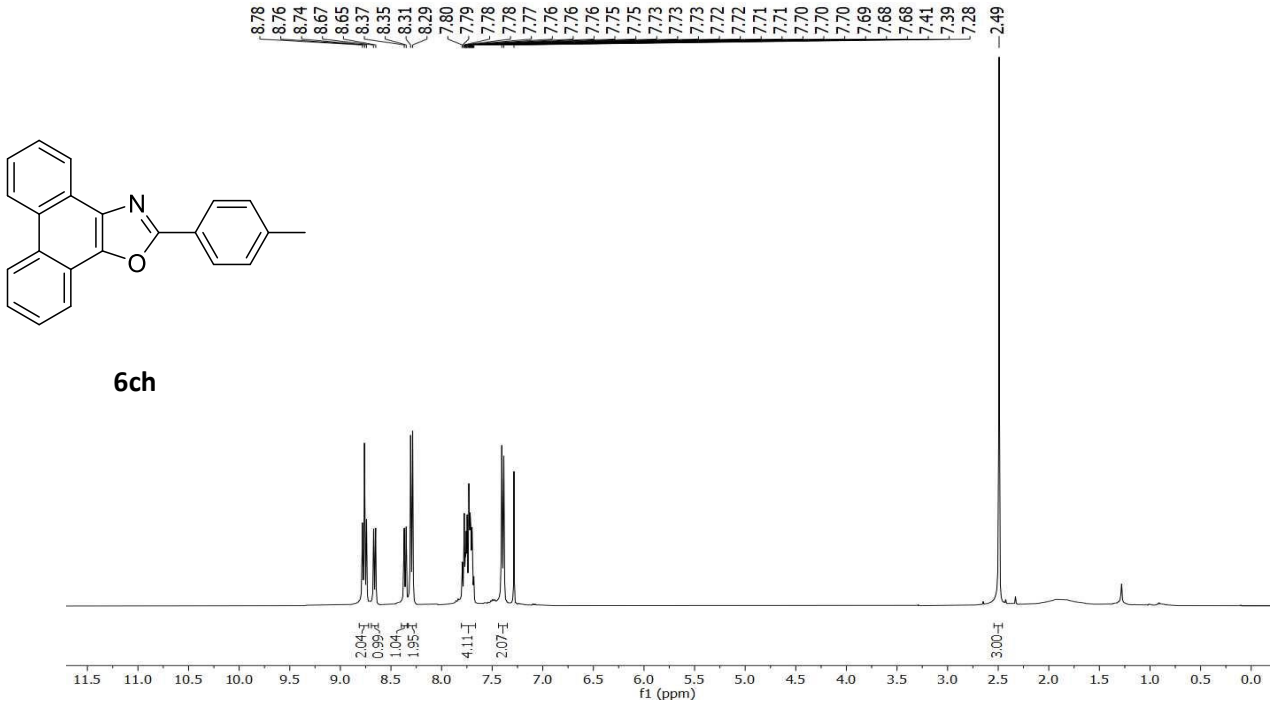


6cg

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6cg

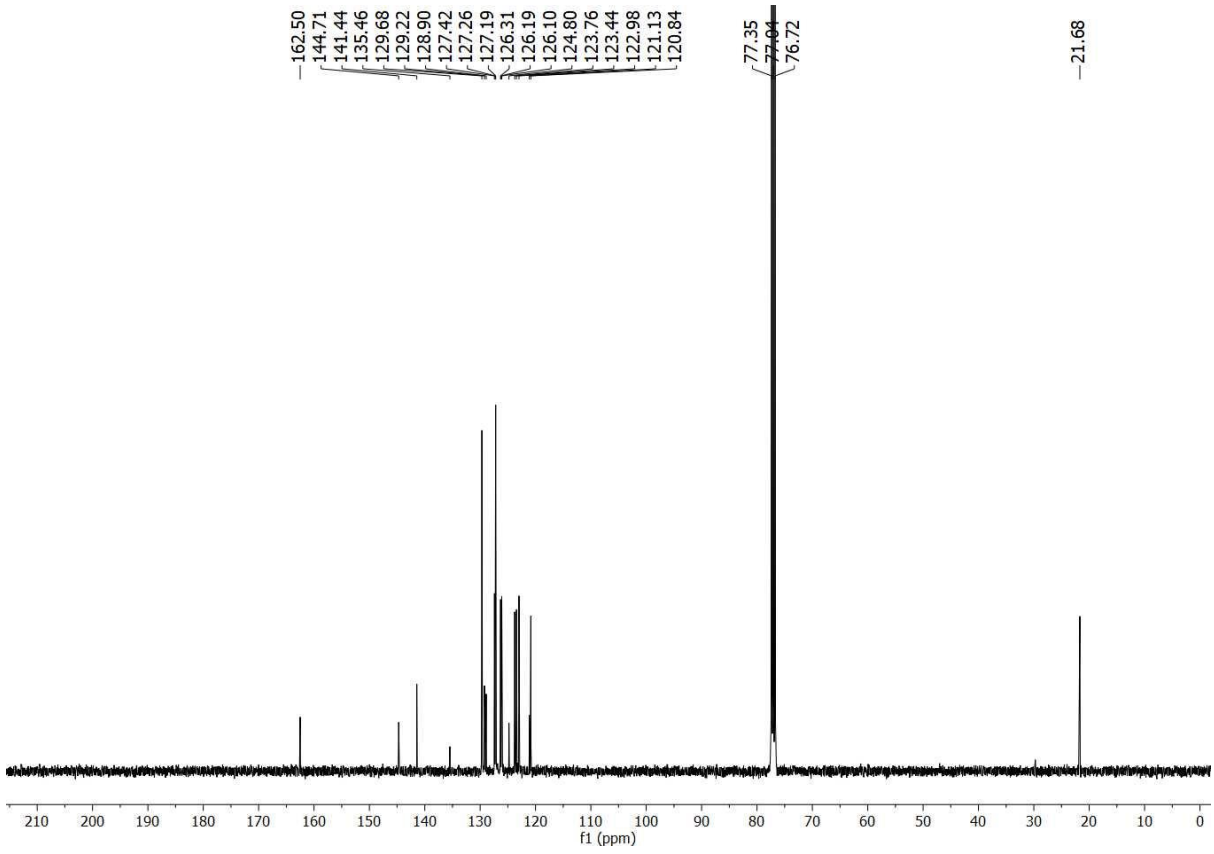


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6cg

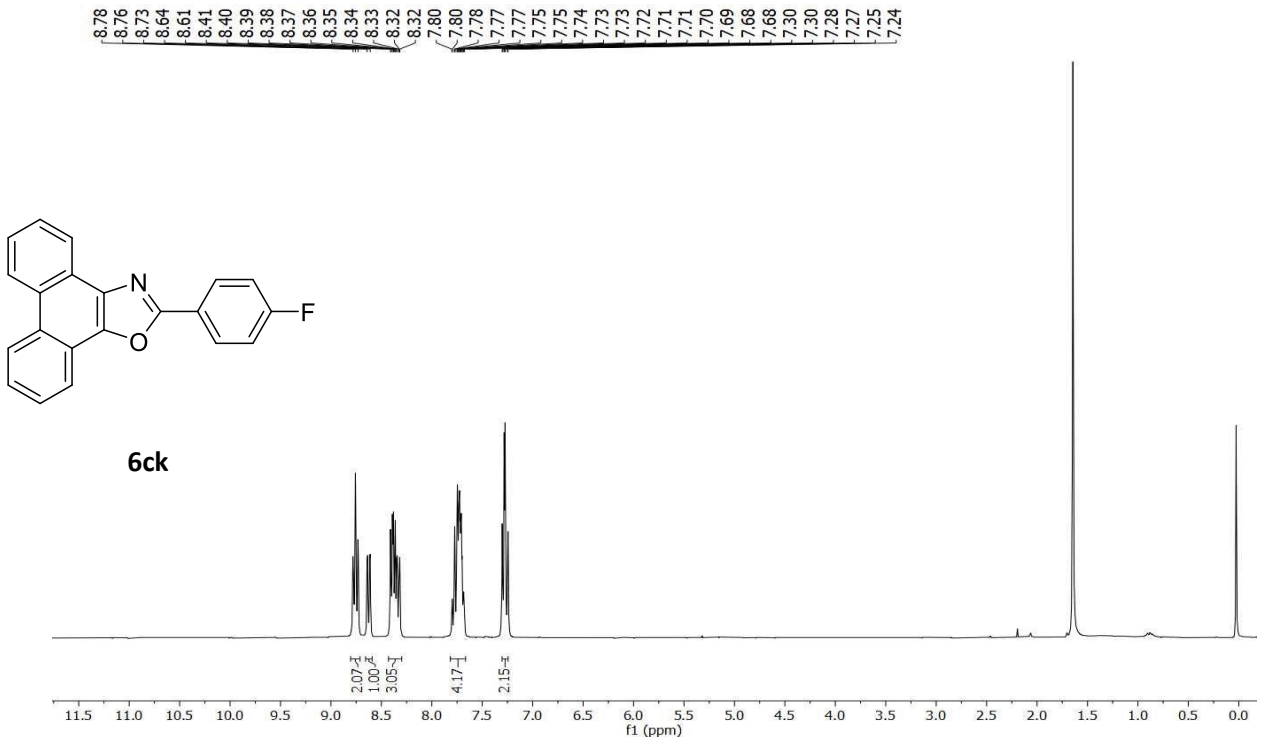


6ch

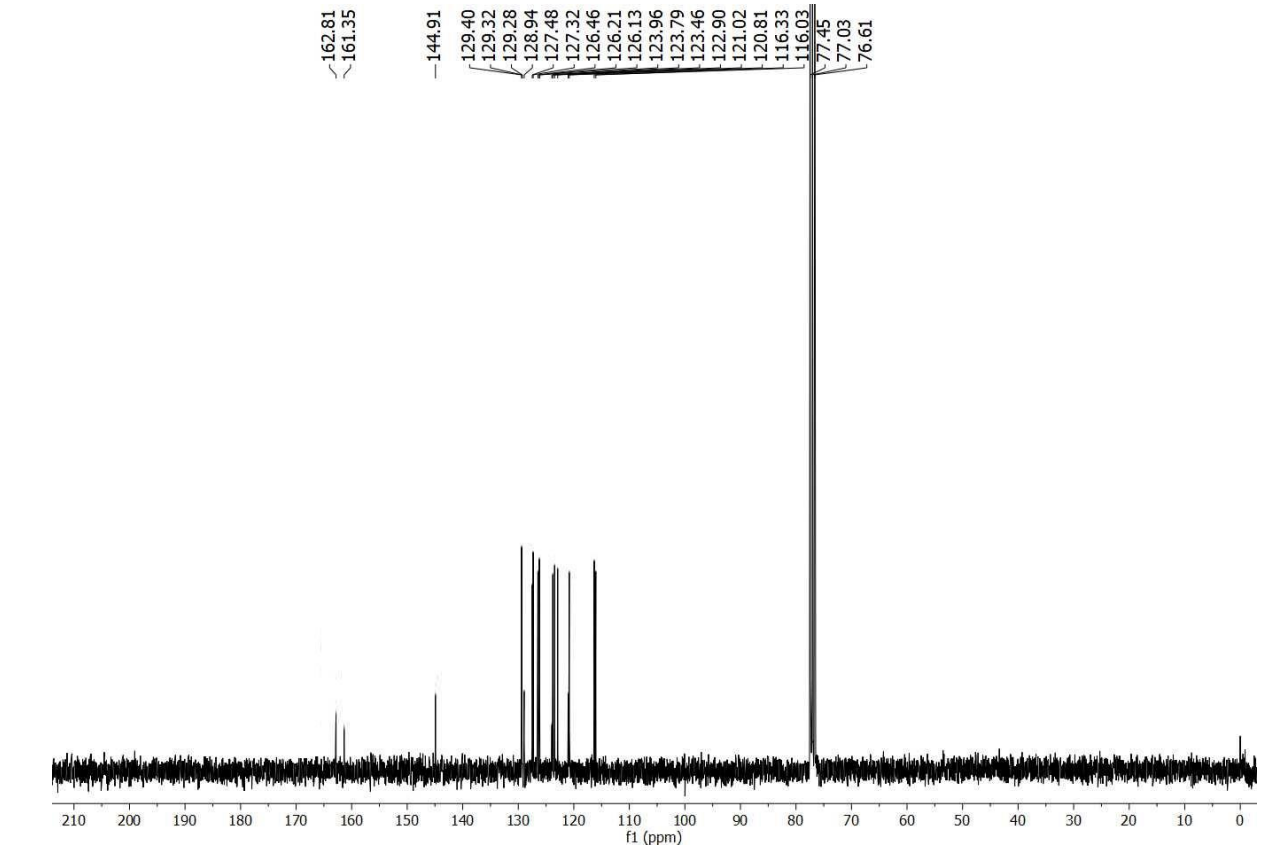
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6ch



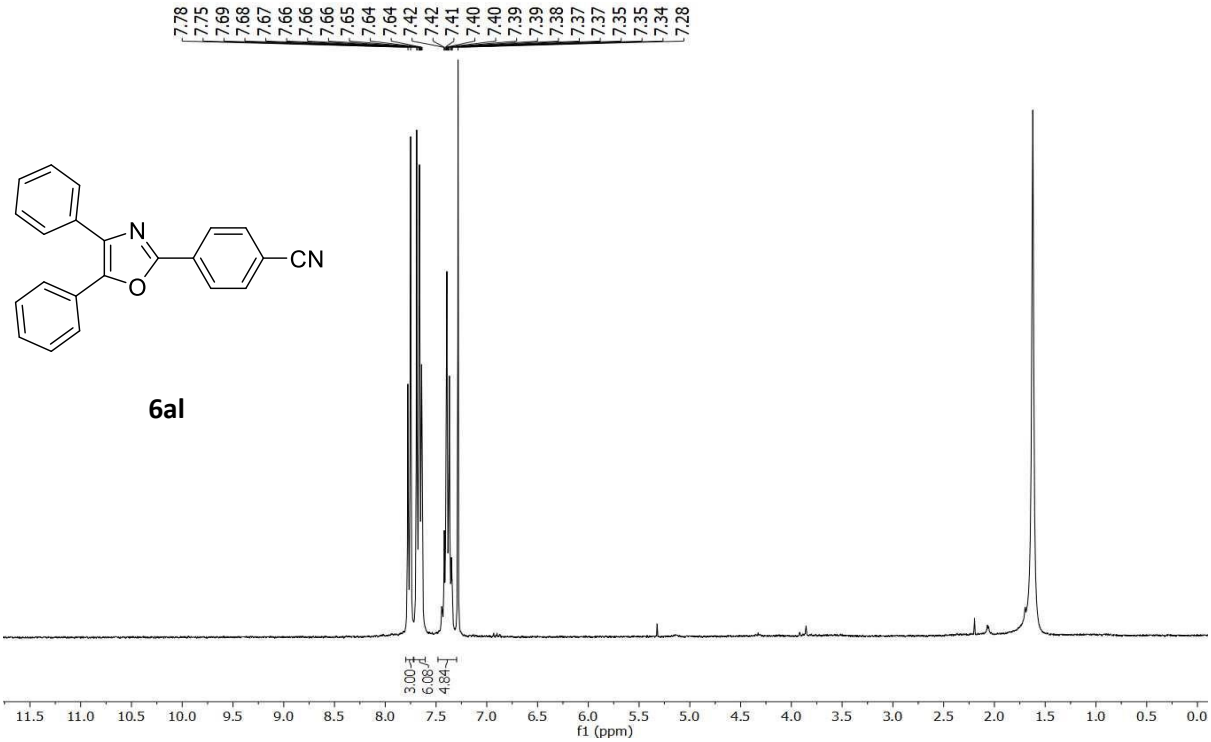
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6ch



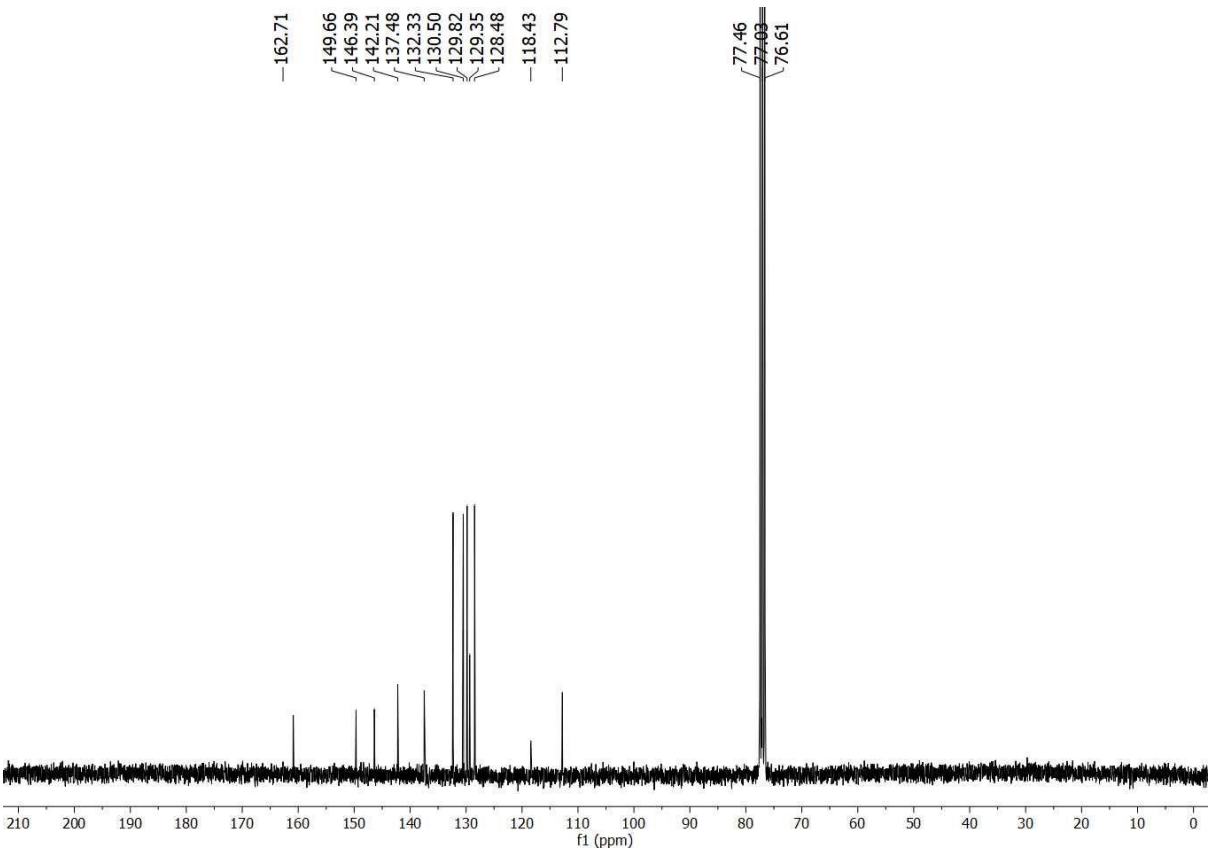
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6ck



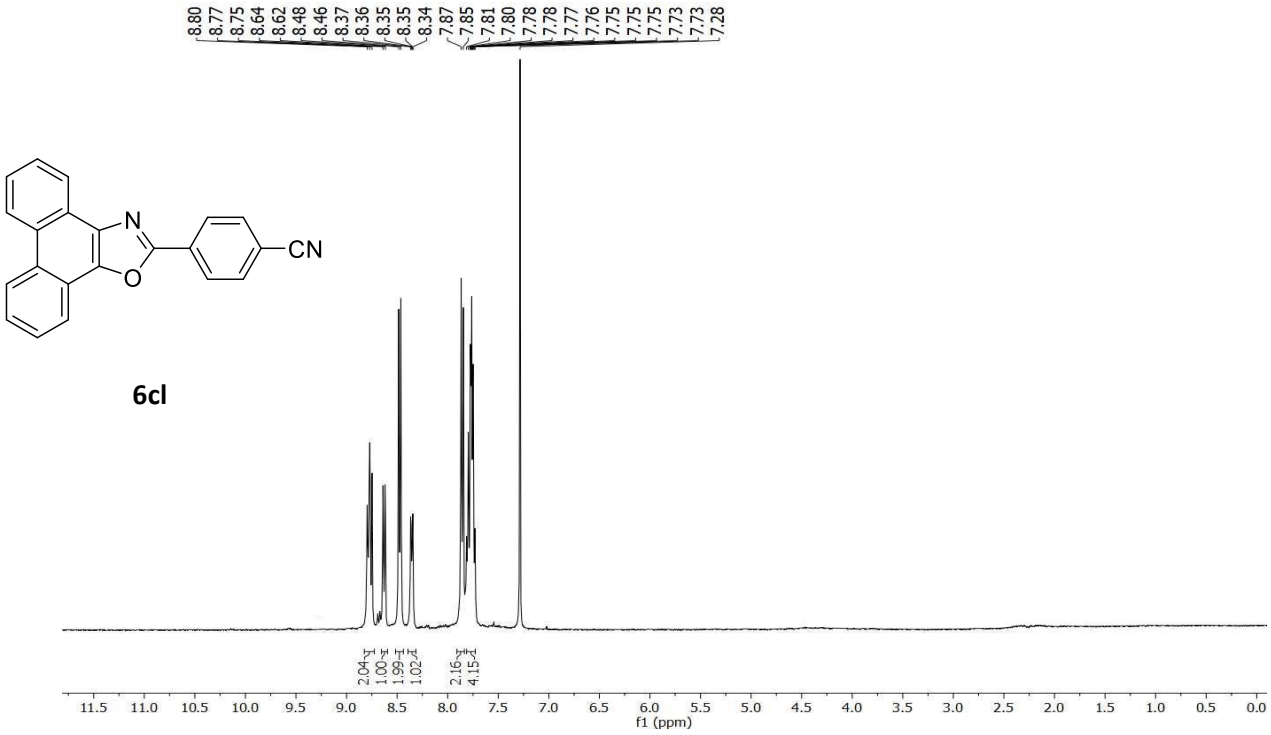
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6ck



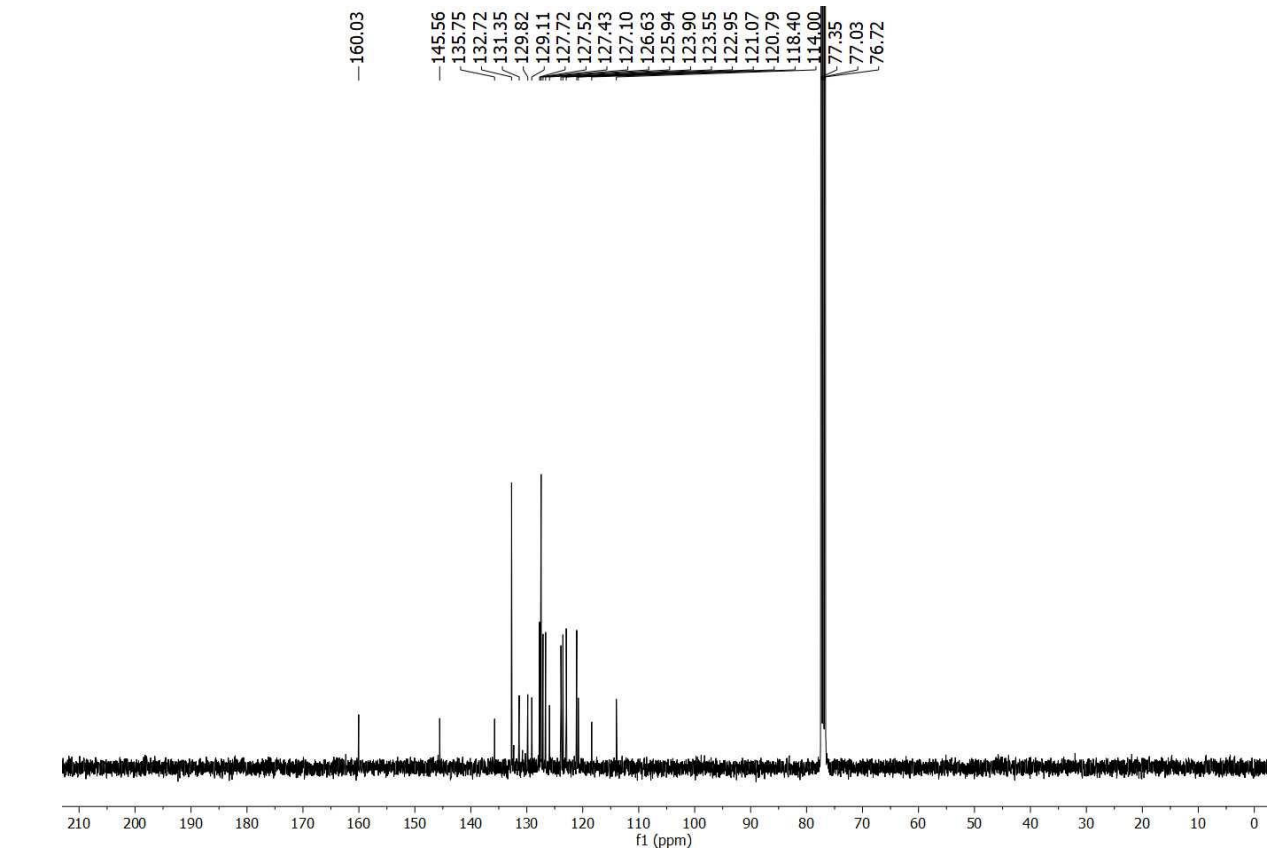
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6al



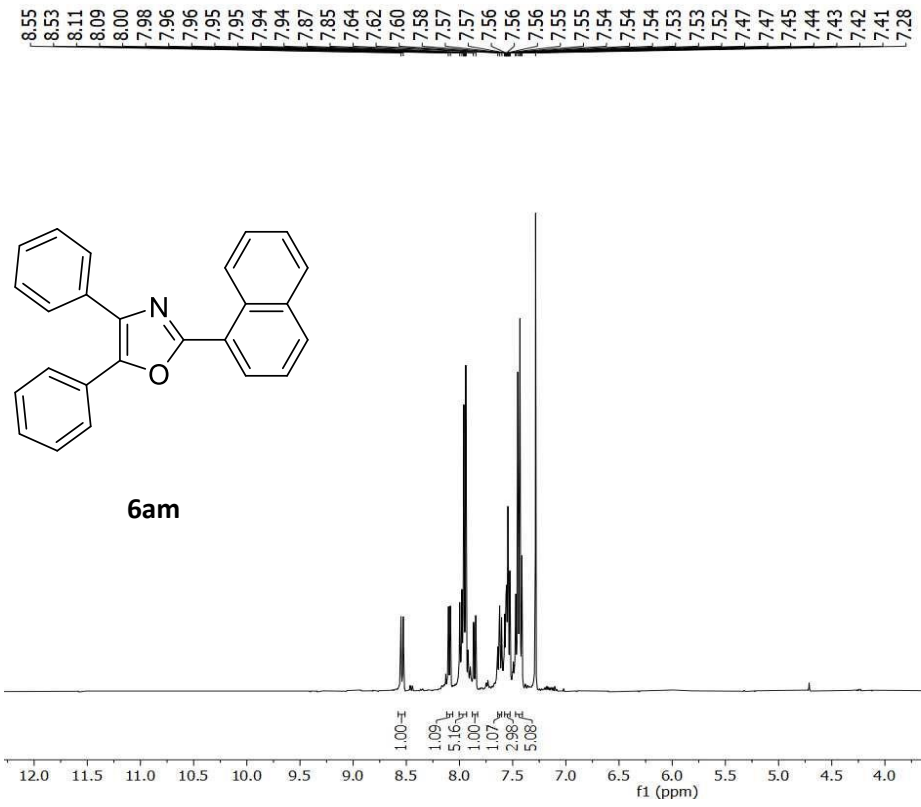
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6al



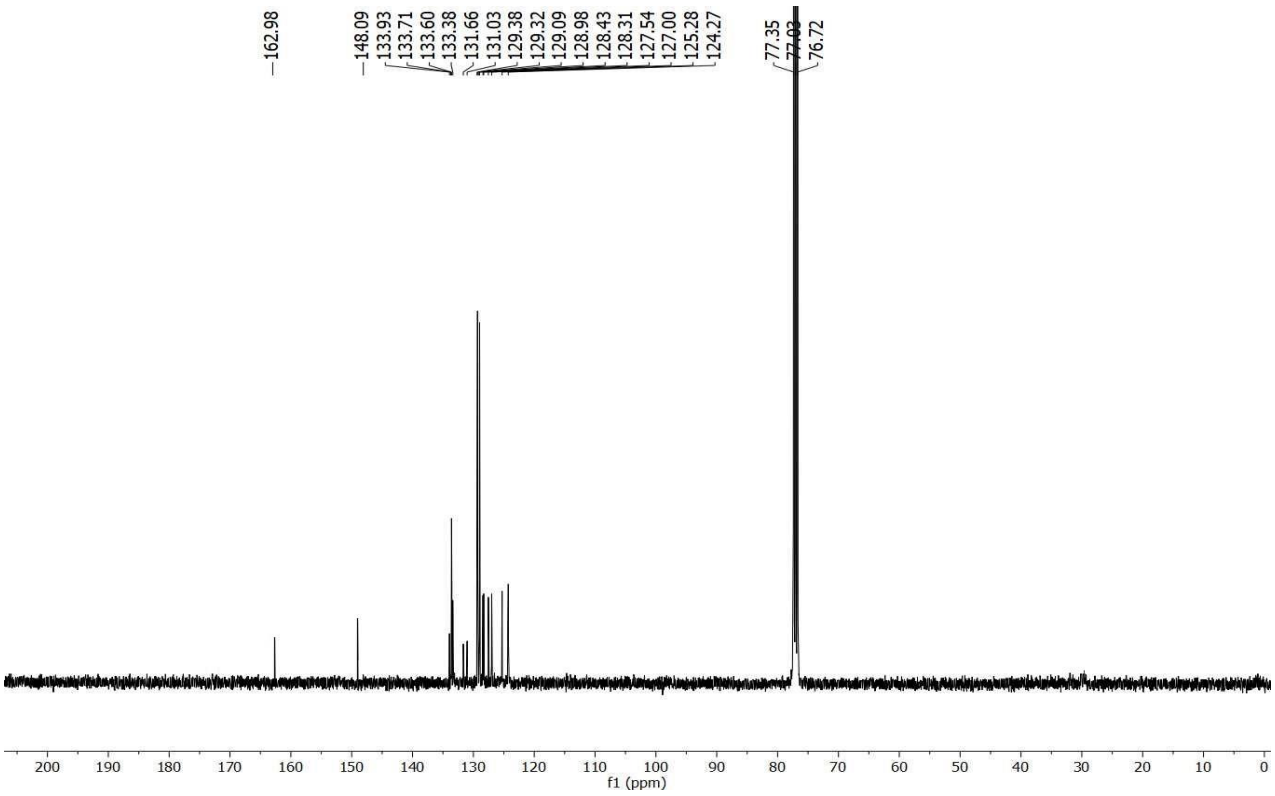
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6cl



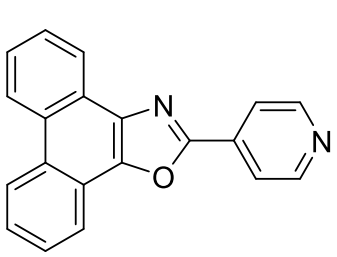
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6cl



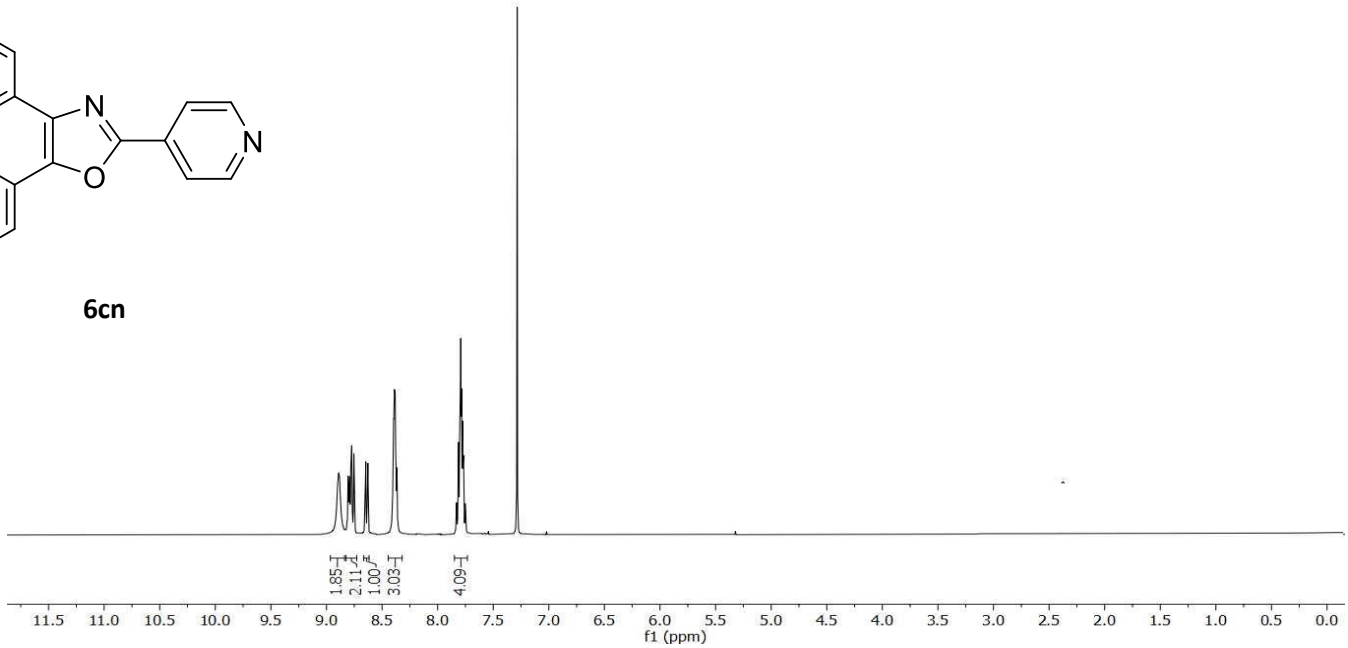
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6am



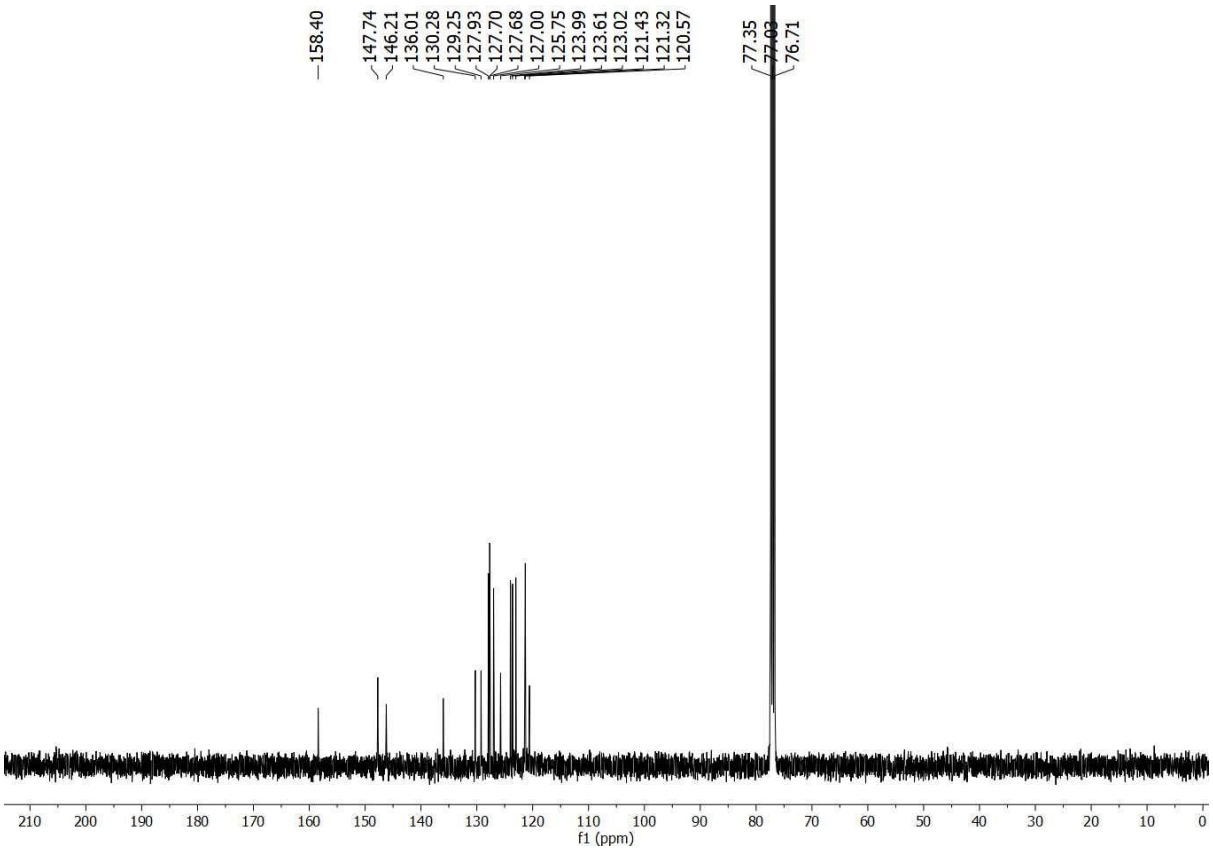
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6am



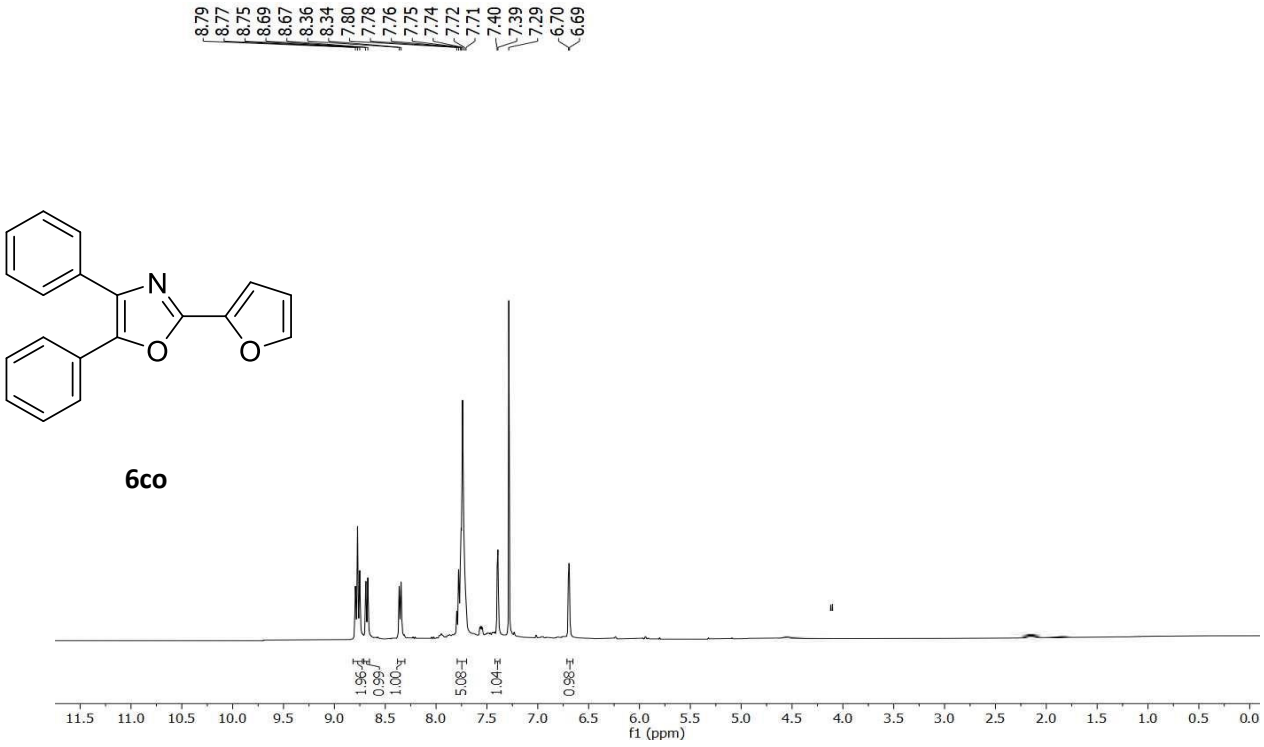
6cn



^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6cn

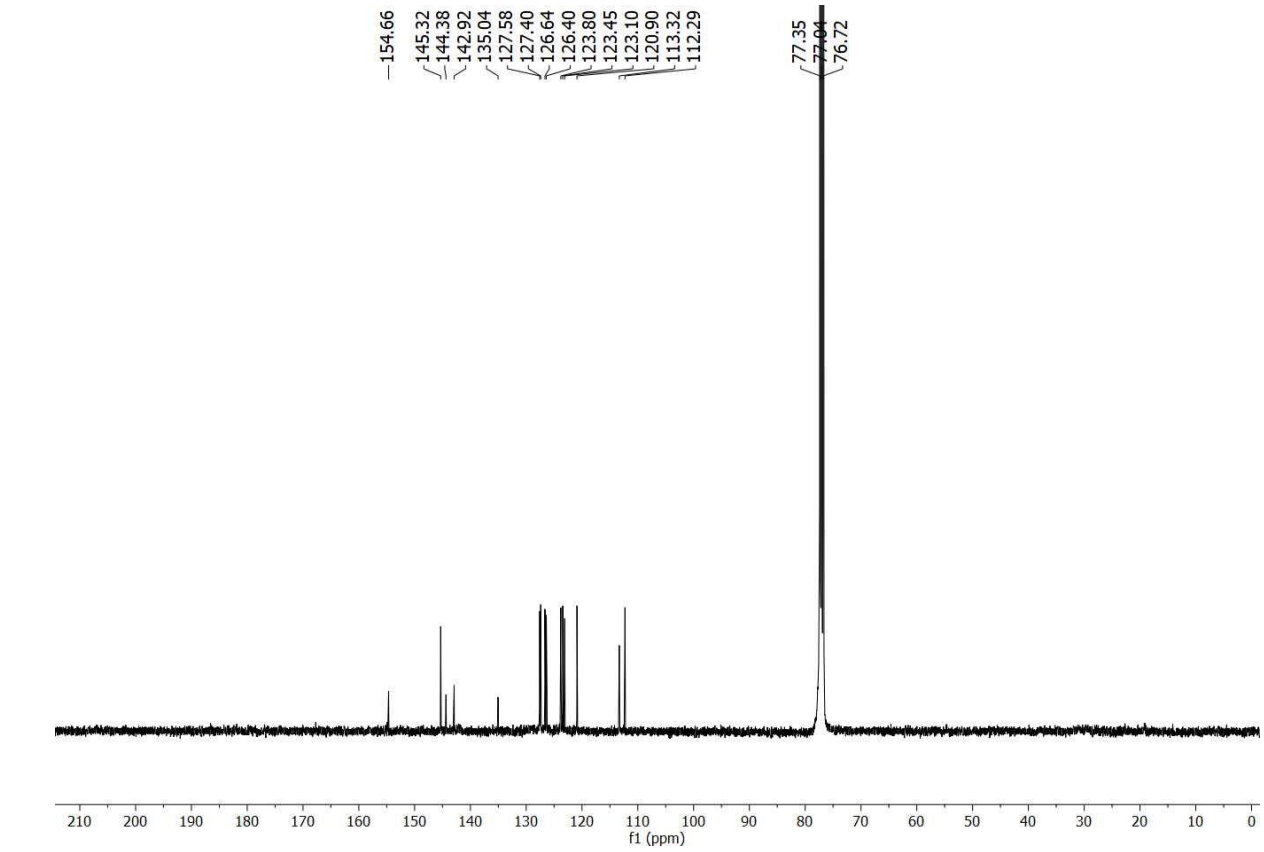


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6cn

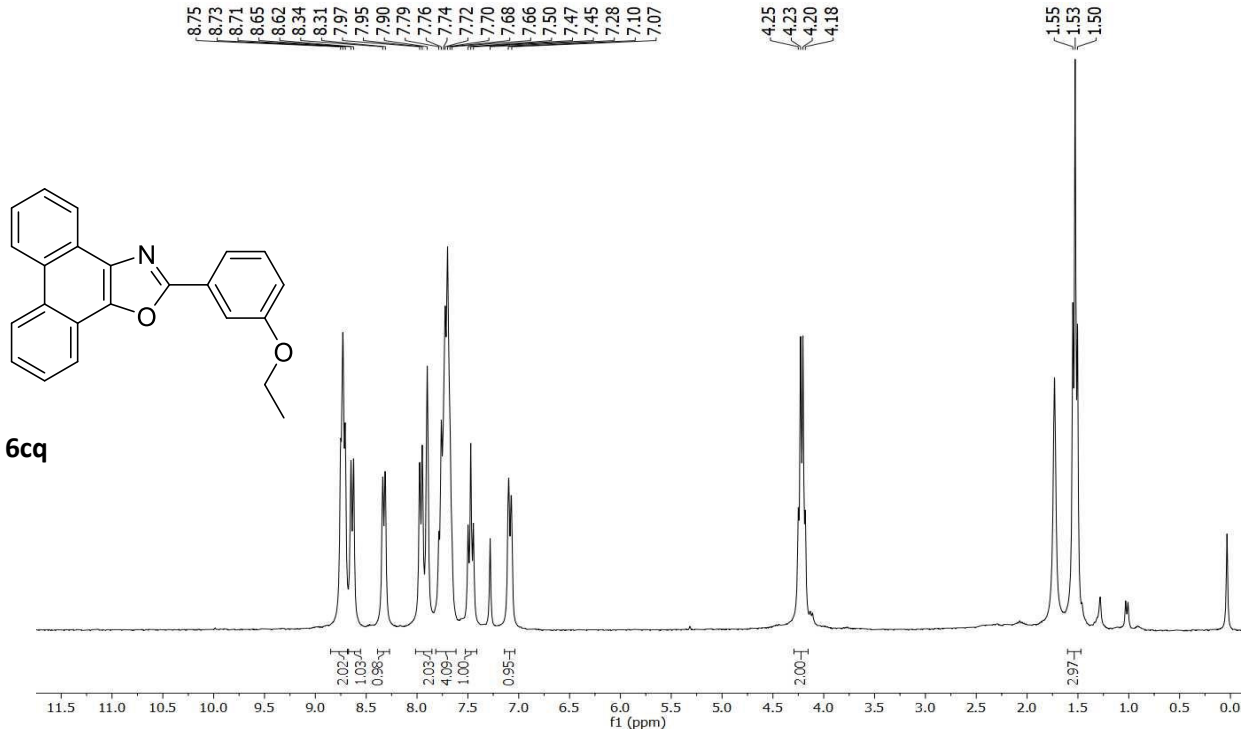


6co

^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6co

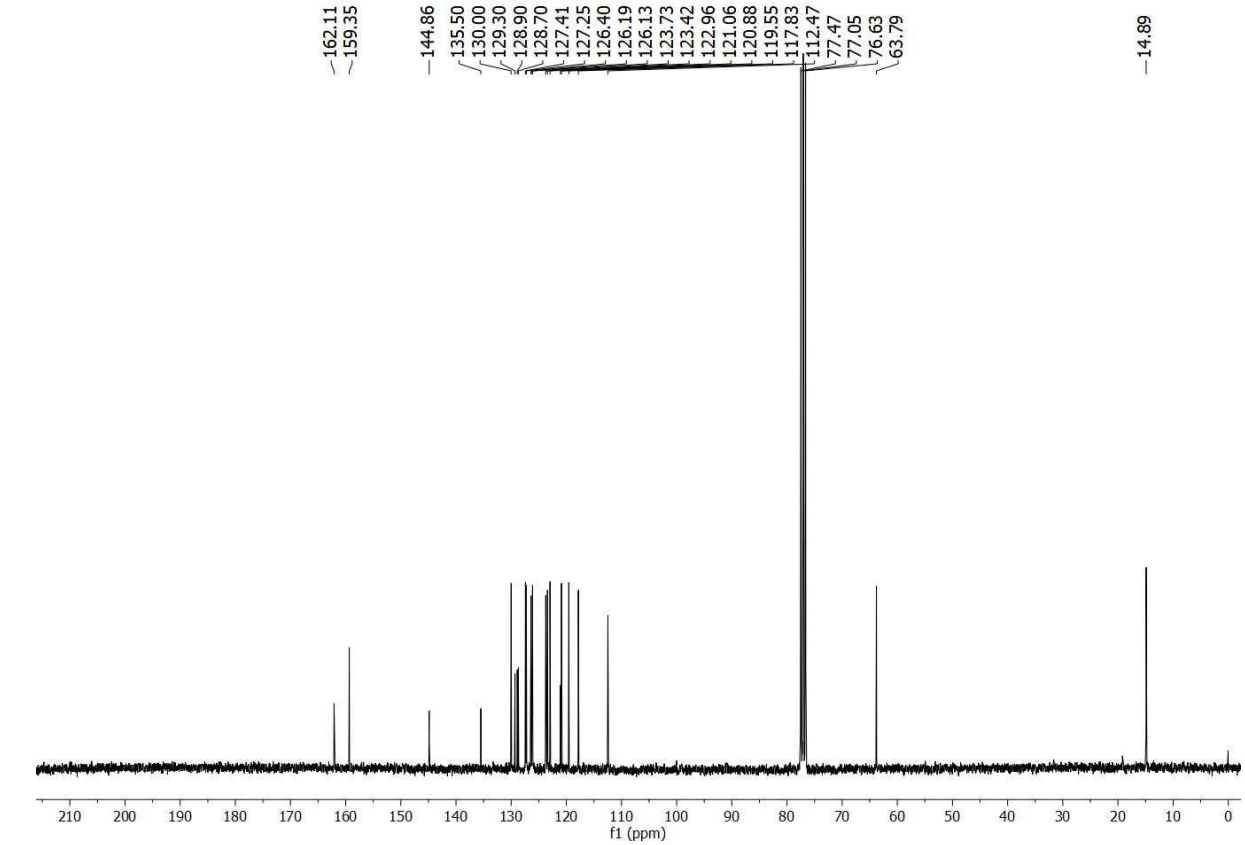


^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6co

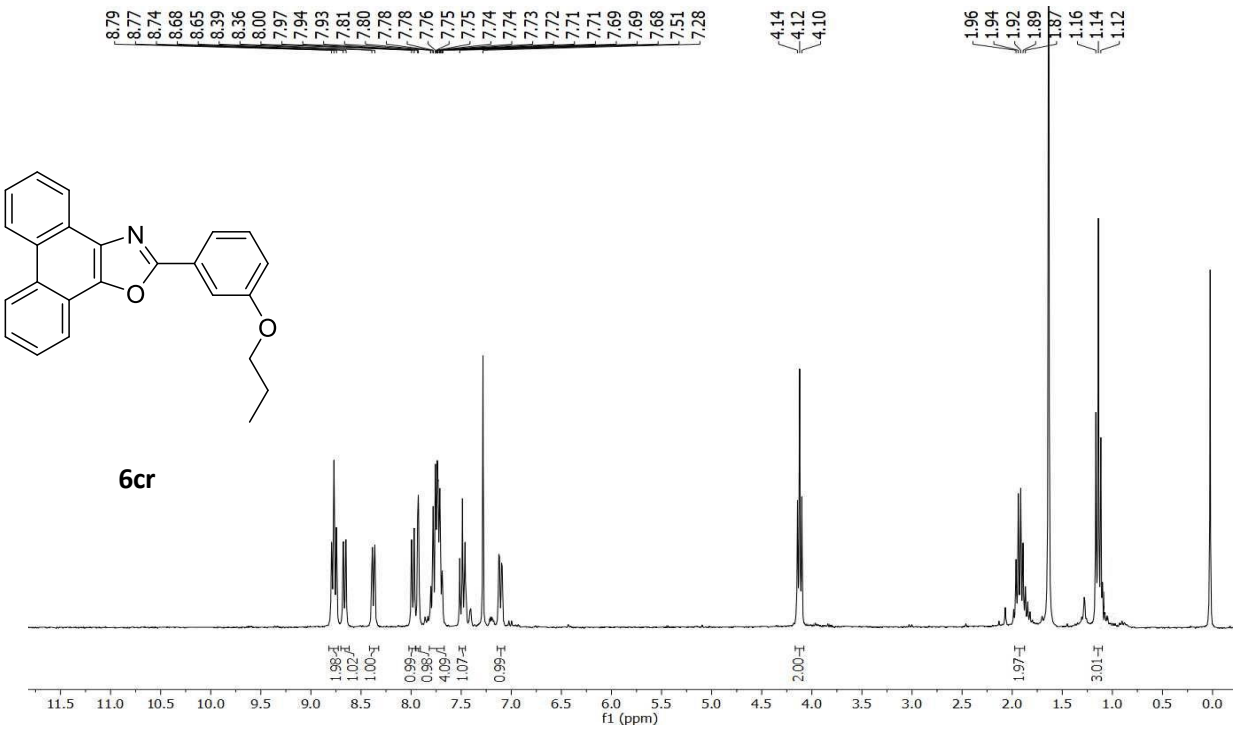


6cq

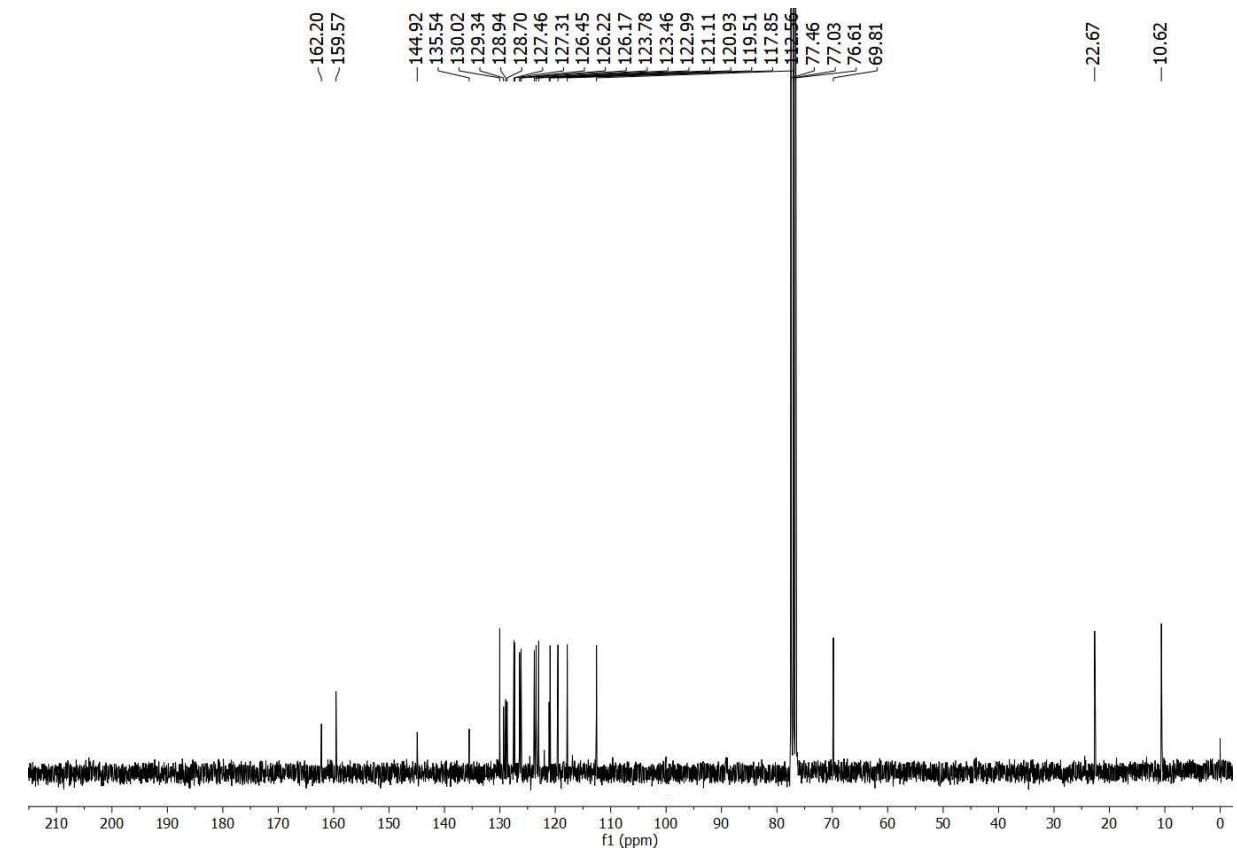
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6cq



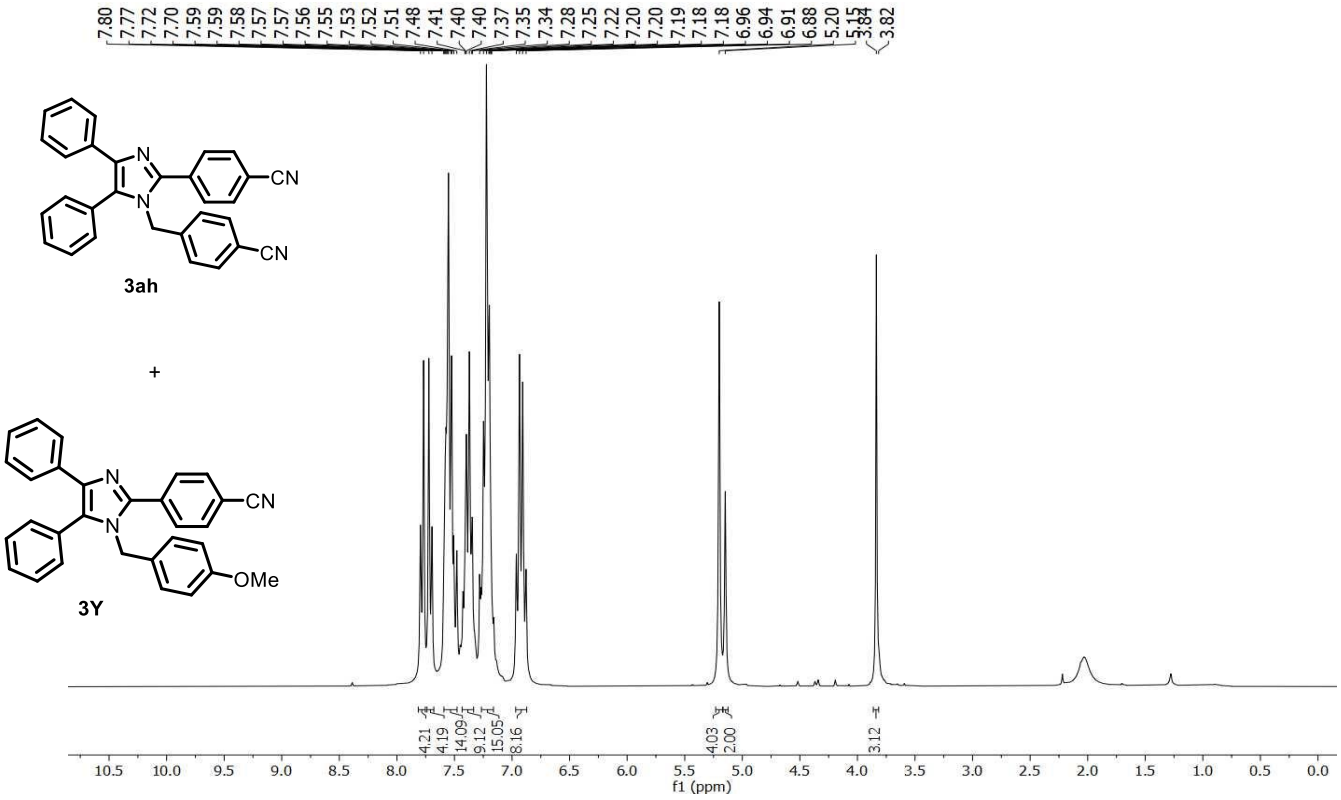
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6cq



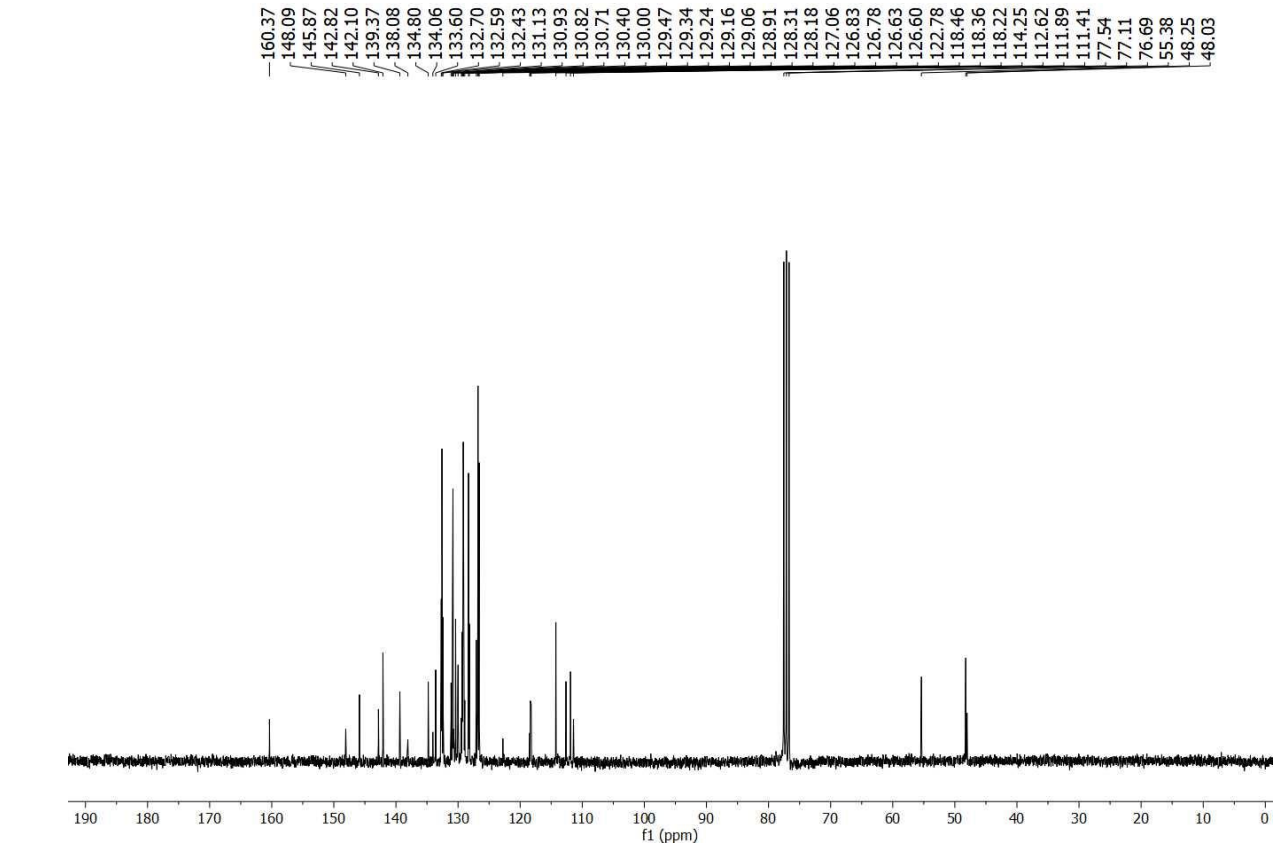
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 6cr



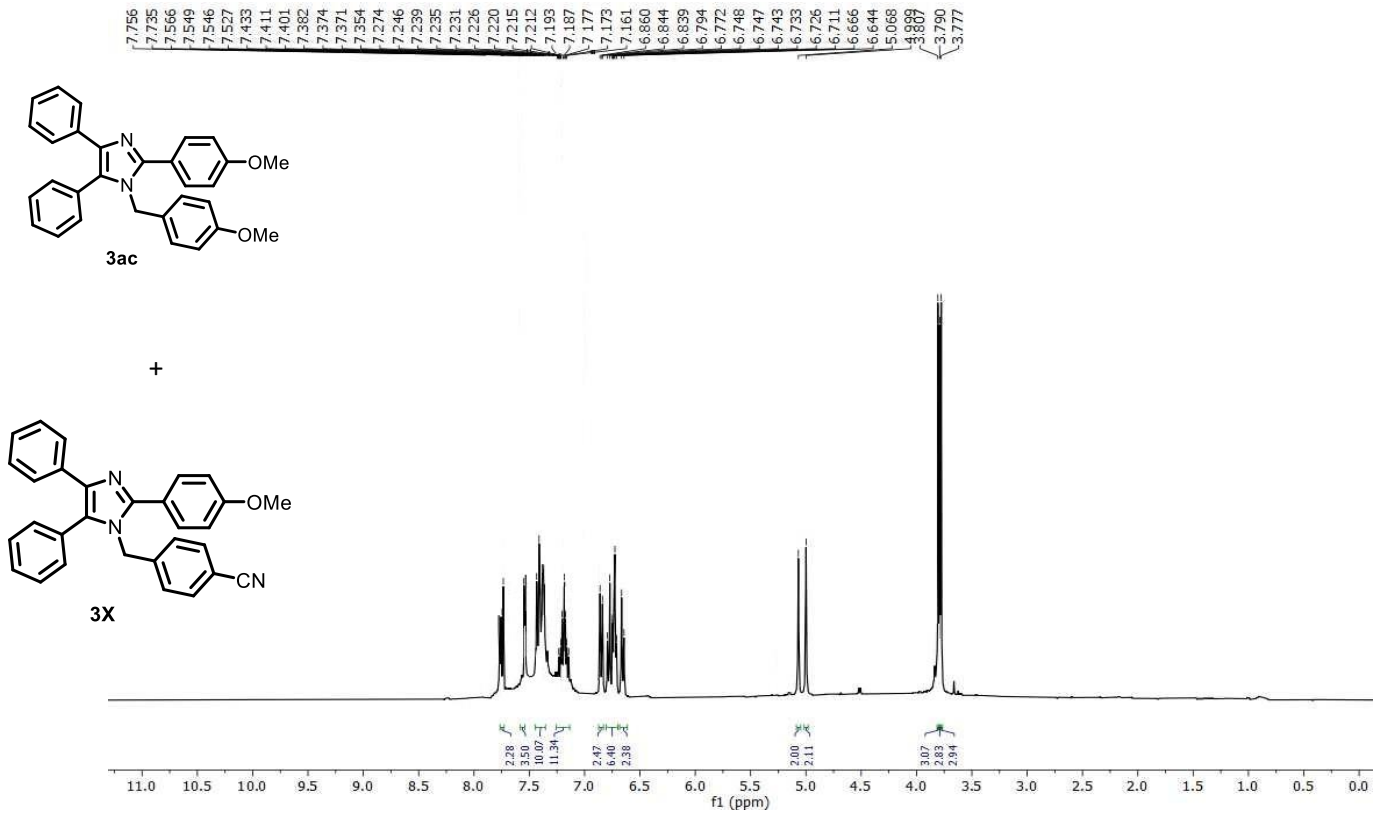
^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 6cr



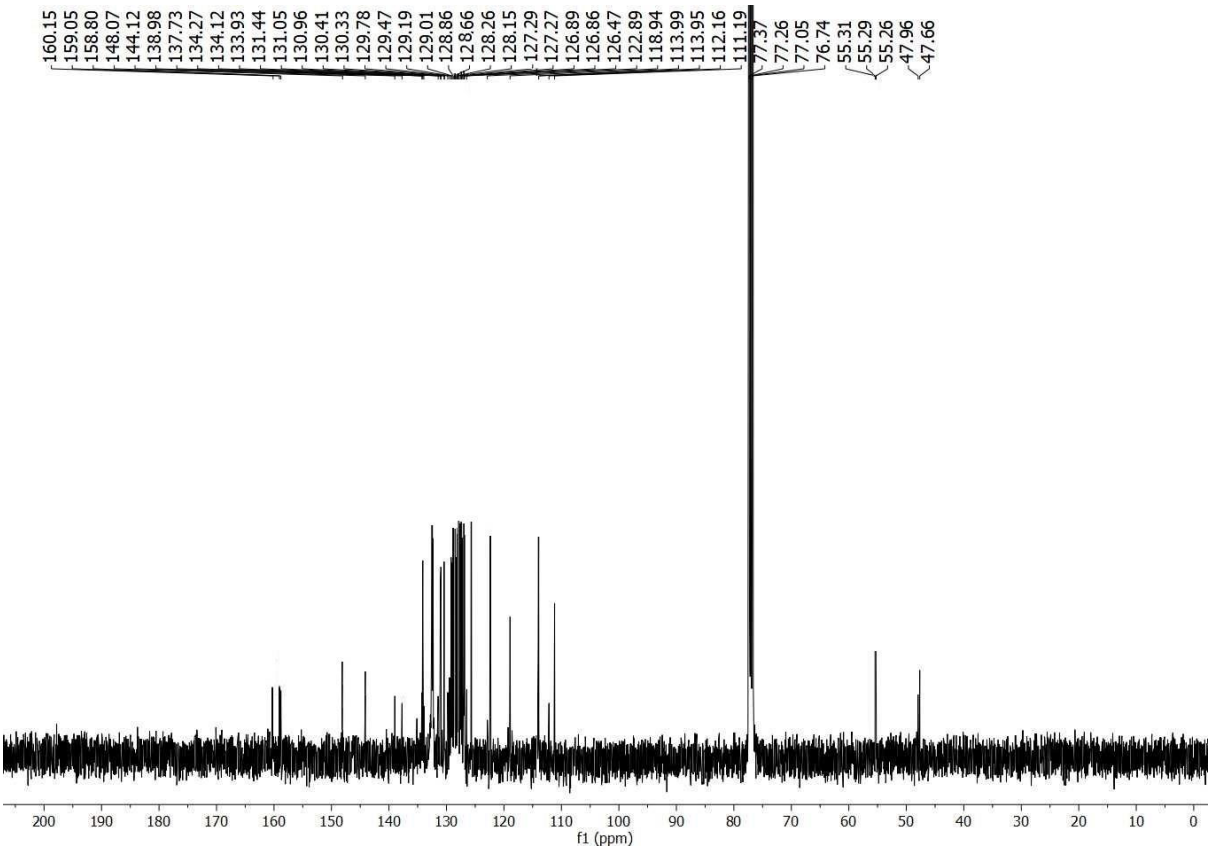
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ah +3y



^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ah+3y

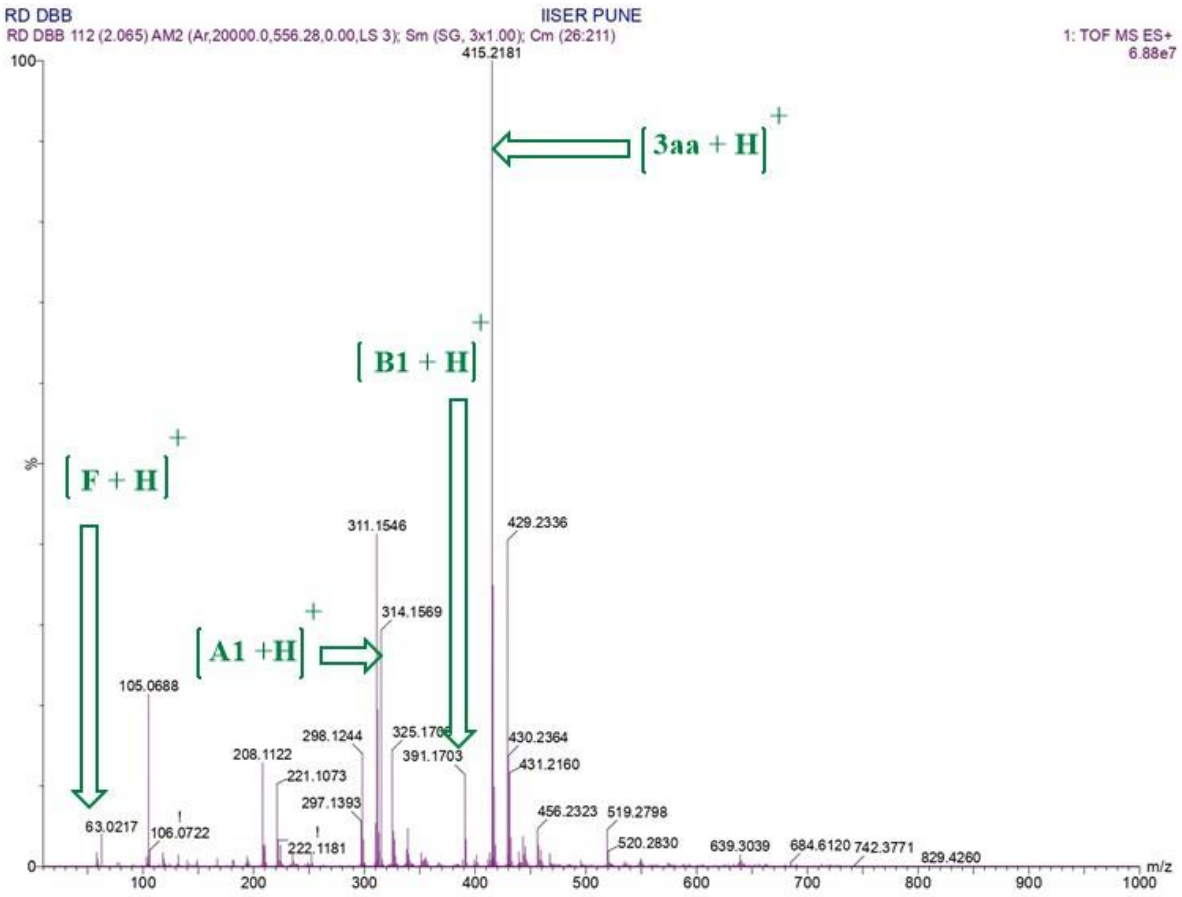


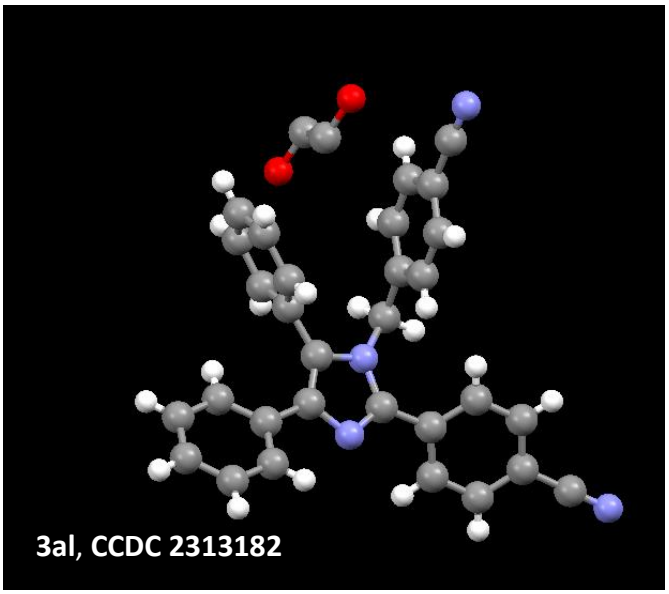
^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound 3ac+3x



^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound 3ac+3x

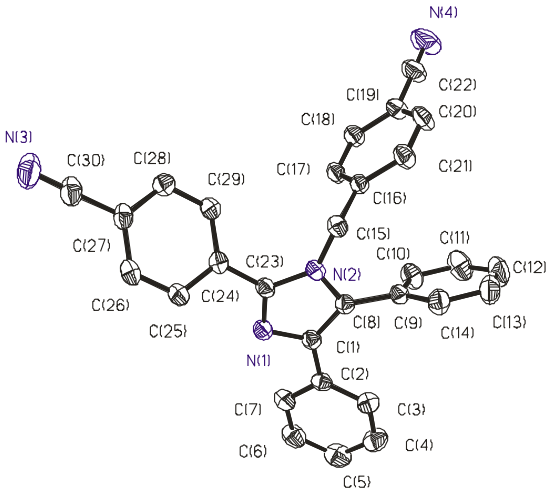
Figure 2 : Mass spectrum of crude reaction mixture after 2.5 hour





X-ray structures of **3al**

Crystallographic table



Molecular geometries of (a) **2286.½CH_3OH**

Crystallographic table

Complexes	**2286.½CH_3OH**
CCDC	2313182
formula	$C_{61}H_{40}N_8O$
fw	901.01
crystal color	White
crystal system	triclinic
space group	*P* -1
a (Å)	9.5461(5)
b (Å)	11.3648(6)
c(Å)	13.2742(8)
α (°)	66.284(2)
β (°)	72.713(2)
γ (°)	85.367(2)
V (Å^3)	1257.70(12)
Z	1
T (K)	273(2)
2θ	51.780
calcd (g cm^{-3})	1.190
Reflections collected	19602
Unique reflections	4933
reflection (I>2*σ*(I))	3804
λ (Å)/*μ* (mm^{-1})	0.71073 /0.073
F(000)	470

observation criterion: [a]R1 = $\Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b]GOF = $\{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$, [c]*w*R2 = $[\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$ where $w = 1/[\sigma^2(F_o^2)+(aP)^2+bP]$, $P = (F_o^2+2F_c^2)/3$.