Supporting information

Carbon nitride supported copper nanoparticles: A heterogeneous catalyst for the *N*-arylation of hetero-aromatic compounds

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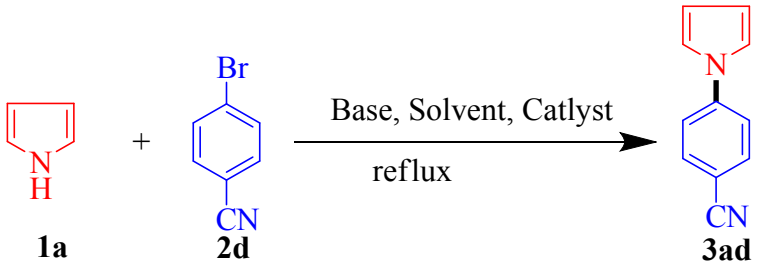
General Considerations:

Solvents were distilled from appropriate drying agent prior to use. Commercially available reagents were used without further purification unless otherwise stated. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE^{III}-400 spectrometer.^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) were registered in $CDCl_3$ or DMSO-d_6 as solvent and tetramethylsilane (TMS) as an internal standard. Chemical shifts are reported in δ units (ppm). All coupling constants (*J*) are reported in hertz (Hz).

Table S1: Optimization table of *N*-arylation reaction. [a, b]



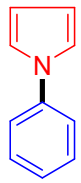
1a **2d** **3ad**

Entry	Catalyst (wt%)	Solvent	Base	T (^{0}C)	Time	Yield (%)[b]
1	Cu-*g*CN(10)	Xylene	Na_2CO_3	100	18	67
2	Cu-*g*CN(10)	Toluene	K_2CO_3	100	18	66
3	Cu-*g*CN(10)	Toluene	Cs_2CO_3	100	12	92
4	Cu-*g*CN(10)	Toluene	-	100	12	c
5	**Cu-*g*CN(5)**	**Toluene**	**Cs_2CO_3**	**100**	**12**	**92**
6	Cu-*g*CN(5)	Toluene	K_3PO_4	100	12	75
7	Cu-*g*CN(5)	Toluene	KO^{t}Bu	100	12	47
8	Cu-*g*CN(5)	Toluene	Cs_2CO_3	80	12	0
9	Cu-*g*CN(5)	Toluene	KOAc	100	12	66
10	Cu-*g*CN(5)	DMAc	Cs_2CO_3	100	22	75
11	Cu-*g*CN(5)	NMP	Cs_2CO_3	100	20	70
12	Cu-*g*CN(5)	DMF	Cs_2CO_3	100	20	32
13	Cu-*g*CN(5)	THF	Cs_2CO_3	100	20	38

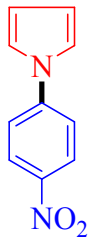
(a) Reaction condition: Pyrrole **1a** (0.07mL, 1.0 mmol), 4-bromobenzonitrile **2d** (216 mg, 1.2 mmol), Base (2.0 mmol) and Cu-*g*CN catalyst (5 mg) and solvent (4 mL). (b) Isolated yield, (c) Homocoupling product of aryl halide.

Characterization of N-arylated products:

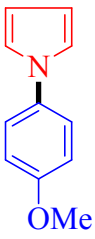
1-phenyl-1*H*-pyrrole (**3aa**):[1] White solid, (112 mg; 78% yield) mp: 59-59°C. Synthesized following the general procedure from pyrrole **1a** (0.07mL, 1.0 mmol), bromobenzene **2a** (0.126 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.35 (s, 2H), 7.09 (d, J=2 Hz, 2H), 7.22-7.26 (m, 1H), 7.38-7.44 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 110.4 (2C), 119.3 (2C), 120.5 (2C), 125.6, 129.5 (2C), 140.7.



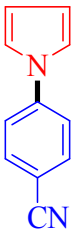
1-(4-nitrophenyl)-1*H*-pyrrole (**3ab**):[1] White solid, (165 mg; 88% yield) mp: 185-186°C. Synthesized following the general procedure from pyrrole **1a** (0.07mL, 1.0 mmol), 4-nitrobromobenzene **2b** (242 mg, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.41 (d, *J*=2.0 Hz, 2H), 7.16 (t, *J*=2 Hz, 2H), 7.50 (d, *J*=9.2 Hz, 2H), 8.30 (d, *J*=9.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 112.5 (2C), 119.0 (2C), 119.4 (2C), 125.6 (2C), 114.6, 145.2.



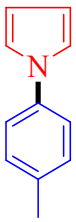
1-(4-methoxyphenyl)-1*H*-pyrrole (**3ac**):[1] White solid, (142 mg; 82% yield) mp: 112-113°C. Synthesized following the general procedure from pyrrole **1a** (0.07mL, 1.0 mmol), 4-methoxybromobenzene **2c** (0.15 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.82 (s, 3H), 6.30 (s, 2H), 6.93 (d, *J*=8.8 Hz, 2H), 6.98 (s, 2H), 7.29 (d, *J*=8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.2, 109.8 (2C), 114.5 (2C), 116.3 (2C), 122.1 (2C), 138.1, 159.4.



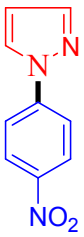
4-(1*H*-pyrrol-1-yl)benzonitrile (**3ad**):[2] White solid, (cycle: 1, 1.55 g; 92%, cycle: 2, 1.46 g; 87%, cycle: 3, 1.43 g; 85%, cycle: 4, 1.41 g; 84%, cycle: 5, 1.39 g; 83% and cycle: 6, 1.34 g; 80% yield) mp: 104-105°C. Synthesized following the general procedure from pyrrole **1a** (0.07mL, 1.0 mmol), 4-bromobenzonitrile **2d** (218 mg, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.39 (t, *J*=2.2 Hz, 2H), 7.12 (t, *J*=2.2 Hz, 2H), 7.46 (td, *J*=9.2, 2 Hz, 2H), 7.69 (td, *J*=9.0, 2.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 108.5, 112.1 (2C), 118.5, 118.8 (2C), 119.9 (2C), 133.7 (2C), 143.6.



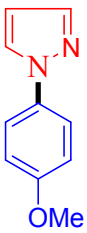
1-*p*-tolyl-1*H*-pyrrole (3ae):[2] White solid, (134 mg; 85% yield) mp: 84-85°C. Synthesized following the general procedure from pyrrole **1a** (0.07mL, 1.0 mmol), *p*-bromotoluene **2e** (0.148 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (s, 3H), 6.31 (t, *J*=2.0 Hz, 2H), 7.04 (t, *J*=2.0 Hz, 2H), 7.20 (d, *J*=8.4, Hz, 2H), 7.27 (d, *J*=8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.8, 110.0 (2C), 119.4 (2C), 120.5 (2C), 130.0 (2C), 135.4, 137.7.



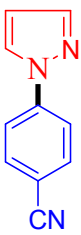
1-(4-nitrophenyl)-1*H*-pyrazole (3bb):[3] White solid (181 mg, 85% yield), mp: 170-172^{0}C, synthesized following the general procedure from pyrazole **1b** (68 mg, 1 mmol), 4-nitrobromobenzene **2b** (242 mg, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 6.54 (d, *J*= 1.2 Hz, 1H), 6.78 (d, *J*= 1.2 Hz, 1H), 7.87 (td, *J*= 10, 2.6 Hz, 2H), 8.01 (d, *J*= 2.4 Hz, 1H), 8.31 (t, *J*= 2.4 Hz, 2H),; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 109.3, 118.6 (2C), 125.4 (2C), 127.0, 142.8, 144.4, 145.4.



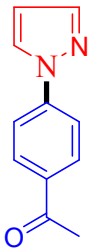
1-(4-methoxyphenyl)-1*H*-pyrazole (3bc):[3] light yellow viscous mass (162 mg, 93% yield). Synthesized following the general procedure from pyrazole **1b** (68 mg, 1 mmol), 4-methoxybromobenzene **2c** (0.15 mL, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 3.82 (s, 3H), 6.42 (t, *J*= 2.0 Hz, 1H), 6.95 (dd, *J*= 6.8, 2.0 Hz, 2H), 7.57 (dd, *J*= 6.8, 2.0 Hz, 2H), 7.68 (d, *J*= 1.2 Hz, 1H), 7.85 (d, *J*= 2.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 55.6, 107.2, 114.5 (2C), 120.9 (2C), 126.9, 133.9, 140.6, 158.2.



4-(1*H*-pyrazol-1-yl)benzonitrile (3bd):[4] White solid (161 mg, 95% yield), mp: 86-87^{0}C, synthesized following the general procedure from pyrazole **1b** (68 mg, 1 mmol), 4-bromobenzonitrile **2d** (218 mg, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 6.48 (t, *J*= 2.0 Hz, 1H), 7.68 (dd, *J*= 7.0, 1.8 Hz, 2H), 7.72 (d, *J*= 1.6, Hz, 1H), 7.76-7.78 (m, 1H), 7.95 (d, *J*= 2.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 108.6, 109.2, 118.2, 118.7 (2C), 126.7, 133.4 (2C) 142.5, 142.7.

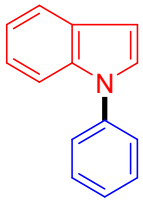


1-(4-(1H-pyrazol-1-yl)phenyl)ethanone (3bg):[5] White solid (167 mg, 90% yield), mp: 107-108^{0}C, synthesized following the general procedure from pyrazole **1b** (68 mg,

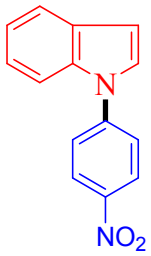


1 mmol), 1-(4-bromophenyl)ethanone **2g** (236 mg, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 2.57 (s, 3H), 6.47 (t, *J*= 2.0 Hz, 1H), 7.20 (s, 1H), 7.76 (d, *J*=8.4 Hz, 2H), 7.96 (d, *J*=2.8 Hz, 1H), 8.01 (d, *J*=8.4 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 26.6, 108.5, 118.3 (2C), 126.8, 130.0 (2C), 134.7, 142.0, 143.2, 196.8.

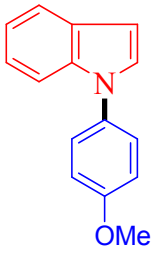
1-phenyl-1*H*-indole (**3ca**):[6] Colourless liquid, (154 mg; 80% yield). Synthesized following the general procedure from indole **1c** (117 mg, 1.0 mmol), bromobenzene **2a** (0.126 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.78 (dd, *J*=3.2, 0.8 Hz, 1H), 7.25-7.34 (m, 4H), 7.41-7.65 (m, 4H), 7.73 (d, *J*=3.2 Hz, 1H), 7.79 (d, *J*=6.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 103.5, 110.5, 120.3, 121.1, 122.3, 124.3 (2C), 126.4, 127.9, 129.3, 129.5 (2C), 135.8, 139.8.



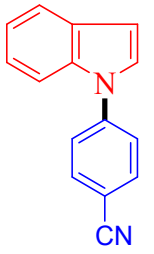
1-(4-nitrophenyl)-1*H*-indole (**3cb**):[7] Yellow solid (203 mg, 85% yield), mp: 131-132°C, Ssynthesized following the general procedure from indole **1c** (117 mg, 1.0 mmol), 4-nitrobromobenzene **2b** (242 mg, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 6.76-6.75 (m, 1H), 7.21-7.20 (m, 1H), 7.30-7.26 (m, 1H), 7.36 (d, *J*= 3.2 Hz, 1H), 7.69-7.62 (m, 4H), 8.39-3.80 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 110.2, 115.5, 117.1, 120.9, 123.0, 122.7, 125.8, 126.1, 126.2, 127.6, 130.3, 137.3, 145.5, 146.0.



1-(4-methoxyphenyl)-1*H*-indole (**3cc**):[8] White solid (186 mg, 80% yield), mp: 60-61°C, Ssynthesized following the general procedure from indole **1c** (117 mg, 1.0 mmol), 4-methoxybromobenzene **2c** (0.15 mL, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 3.87 (s, 3H), 6.65-6.80 (m, 1H), 7.02 (d, *J*=8.8 Hz, 2H), 7.12-7.18 (m, 1H), 7.27 (d, *J*= 3.2 Hz, 1H), 7.39 7.02 (d, *J*=8.8 Hz, 2H), 7.43-7.66 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 55.6, 102.9, 110.4, 114.7 (2C), 116.4, 120.1, 121.0, 122.1, 125.9 (2C), 128.3, 128.9, 138.2, 158.2.

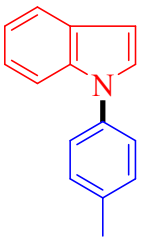


4-(1*H*-indol-1-yl)benzonitrile (**3cd**):[9] White solid (200 mg, 92% yield), mp: 94-95°C, Ssynthesized following the general procedure from indole **1c** (117 mg, 1.0 mmol), 4-bromobenzonitrile **2d** (218 mg, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 6.76-6.77

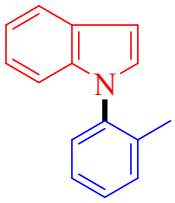


(m, 1H), 7.22-7.31 (m, 2H), 7.34 (d, *J*=3.6 Hz, 1H), 7.58-7.62 (m, 3H), 7.70-7.72 (m, 1H), 7.78 (d, J=8.4 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 105.6, 109.1, 110.3, 118.4, 121.3, 121.5, 123.1, 123.7 (2C), 127.0, 129.8, 133.7 (2C), 135.0, 143.4.

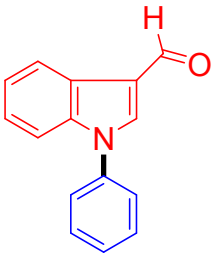
1-*p*-tolyl-1*H*-indole (**3ce**):[10] Colorless liquid (180 mg, 86% yield). Ssynthesized following the general procedure from indole **1c** (117 mg, 1.0 mmol), *p*-bromotoluene **2e** (0.148 mL, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 2.42 (s, 3H) 6.65-6.66 (m, 1H), 7.14-7.19 (m, 2H), 7.28-7.30 (m, 3H), 7.36-7.50 (m, 3H), 7.51 (d, *J*=7.6, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.1, 103.2, 110.5, 120.2, 121.0, 122.2, 124.3 (2C), 128.1, 129.1, 130.1 (2C), 135.1, 136.3, 137.3.



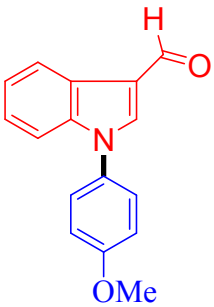
1-*o*-tolyl-1*H*-indole (**3cf**):[11] Colorless liquid (162 mg, 78% yield). Ssynthesized following the general procedure from indole **1c** (117 mg, 1.0 mmol), *o*-bromotoluene **2f** (0.144 mL, 1.2 mmol). ^{1}H NMR ($CDCl_3$, 400MHz): δ 2.06n (s, 3H) 6.66 (d, *J*=2.8 Hz, 1H), 7.01-7.13 (m, 1H), 7.13-7.18 (m, 3H), 7.29-7.37 (m, 3H), 7.56 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 17.6, 102.4, 110.5, 119.8, 120.8, 121.9, 126.7, 128.1, 128.2, 128.3, 128.6, 131.2, 135.8, 136.9, 138.3.



1-phenyl-1*H*-indole-3-carbaldehyde (**3da**):[12] White solid, (181 mg; 82% yield) mp: 79-80^{0}C. Synthesized following the general procedure from 1*H*-indole-3-carbaldehyde **1d** (145 mg, 1.0 mmol), bromobenzene **2a** (0.126 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35-7.31 (m, 2H), 7.46-7.56 (m, 6H), 7.90 (s, 1H), 8.36 (d, *J*=6.8 Hz, 1H), 10.09 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 111.1, 118.3, 119.7, 122.4, 123.5, 124.6, 124.9 (2C), 128.3, 129.9 (3C), 137.3, 138.1, 184.9.

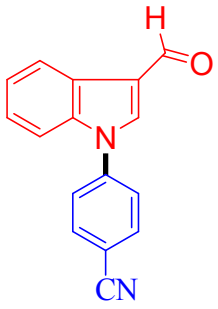


1-(4-methoxyphenyl)-1*H*-indole-3-carbaldehyde (**3dc**):[13] Light orange solid, (211 mg; 84% yield) mp: 126-128°C. Synthesized following the general procedure from 1*H*-indole-3-carbaldehyde **1d** (145 mg, 1.0 mmol), 4-methoxybromobenzene **2c** (0.15 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.88 (s, 3H), 7.06 (d,



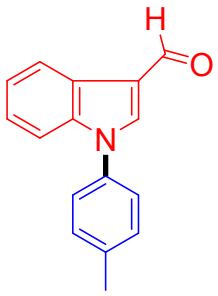
J=8.8 Hz, 2H), 7.30 (s, 1H), 7.32-7.42 (m, 4H), 7.85 (s, 1H), 8.35 (dd, *J*=6.8, 1.6 Hz, 1H), 10.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.6, 111.1, 119.4, 122.1, 123.3, 124.4, 124.7 (2C), 125.4, 130.4 (2C), 137.6, 138.2, 138.3, 158.4, 184.8.

4-(3-formyl-1H-indol-1-yl)benzonitrile (**3dd**): White solid, (219 mg; 89% yield) mp: 162-163°C.



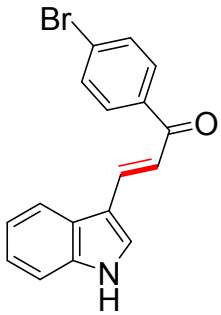
Synthesized following the general procedure from 1*H*-indole-3-carbaldehyde **1d** (145 mg, 1.0 mmol) 4-bromobenzonitrile **2d** (218 mg, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.39 (m, 2H), 7.50-7.52 (m, 1H), 7.68 (td, J=8.8, 2 Hz, 2H), 7.86-7.89 (m, 2H), 7.92 (s, 1H), 10.11 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 110.6, 111.6, 117.8, 120.8, 122.6, 124.1, 124.9 (2C), 125.2, 125.8, 134.1 (2C), 136.6, 137.1, 141.9, 184.9.

1-*p*-tolyl-1*H*-indole-3-carbaldehyde (**3de**):[14] Brown viscous mass, (200 mg; 85% yield).

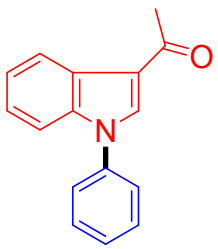


Synthesized following the general procedure from 1*H*-indole-3-carbaldehyde **1d** (145 mg, 1.0 mmol), *p*-bromotoluene **2e** (0.148 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.46 (s, 3H), 7.31-7.45 (m, 7H), 7.87 (s, 1H), 8.37 (d, J=7.6, 2 Hz, 1H), 7.86-7.89 (m, 2H), 7.92 (s, 1H),10.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.1, 111.1, 119.4, 122.1, 123.3, 124.4, 124.7 (2C), 125.4, 130.4 (2C), 135.5, 137.6, 138.2, 138.3, 184.8.

(*E*)-1-(4-bromophenyl)-3-(1H-indol-3-yl)prop-2-en-1-one (**3dg**):[15] White solid, (293 mg; 90% yield) mp: 201-202°C. Synthesized following the general procedure from 1*H*-indole-3-carbaldehyde **1d** (145 mg, 1.0 mmol), 1-(4-bromophenyl)ethanone **2g** (236 mg, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21-7.26 (m, 2H), 7.50 (d, *J*=8.4 Hz, 1H), 7.61 (d, *J*=15.2 Hz,, 1H), 7.74 (d, *J*=8.4 Hz,, 2H), 8.04-8.13 (m, 5H), 11.95 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 112.9, 113.3, 115.4, 120.9, 121.7, 123.4, 125.6, 126.8, 130.7 (2C), 132.2 (2C), 134.1, 137.9, 138.0, 140.1, 188.3.



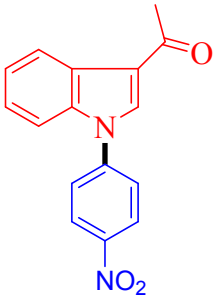
1-(1-phenyl-1*H*-indol-3-yl)ethanone (**3ea**):[16] White solid, (186 mg; 79% yield) mp: 144-145°C.



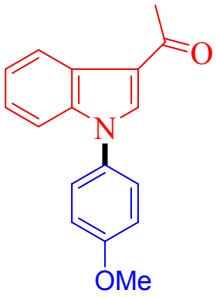
Synthesized following the general procedure from 1-(1H-indol-3-yl)ethanone **1e** (159 mg, 1.0 mmol), bromobenzene **2a** (0.126 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.567 (s, 3H), 7.26-7.35 (m, 4H), 7.43-7.52 (m, 4H), 7.92 (s, 1H), 8.45 (d, *J*=8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.7,

110.8, 118.7, 122.8, 123.1, 123.9, 124.9 (2C), 126.5, 128.0, 129.9 (2C), 134.6, 137.1, 138.4, 193.3.

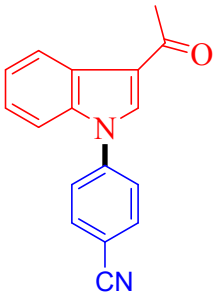
1-(1-(4-nitrophenyl)-1*H*-indol-3-yl)ethanone (**3eb**):[17] White solid, (232 mg; 83% yield) mp: 193-194°C. Synthesized following the general procedure from 1-(1H-indol-3-yl)ethanone **1e** (159 mg, 1.0 mmol), 4-nitrobromobenzene **2b** (242 mg, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.58 (s, 3H) 7.34-7.38 (m, 2H), 7.51-7.53 (m, 1H), 7.71-7.73 (m, 2H), 7.95-7.98 (m, 1H), 7.42-8.44 (m, 3H; ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.8, 110.4, 120.2, 123.2, 123.9, 124.7, 124.8 (2C), 125.6 (2C), 133.5, 136.0, 143.8, 146.4, 193.2.



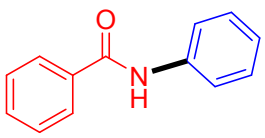
1-(1-(4-methoxyphenyl)-1H-indol-3-yl)ethanone (**3ec**) : White solid, (200 mg; 75% yield) mp: 115-1116°C.. Synthesized following the general procedure from 1-(1H-indol-3-yl)ethanone **1e** (159 mg, 1.0 mmol), 4-methoxybromobenzene **2c** (0.15 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.55 (s, 3H), 3.88 (s, 3H), 7.07 (d, *J*=8.8 Hz, 2H), 7.30 (s, 1H), 7.31-7.42 (m, 4H), 7.85 (s, 1H), 8.35 (dd, *J*=6.8, 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.8, 55.2, 110.5, 120.5, 120.2, 123.2, 123.9 (2C), 124.7, 124.8, 125.6 (2C), 127.0, 133.5, 136.6, 143.8, 159.5, 193.2.



4-(3-acetyl-1H-indol-1-yl)benzonitrile (**3ed**): White solid, (220 mg; 85% yield) mp: 131-132°C. Synthesized following the general procedure from 1-(1H-indol-3-yl)ethanone **1e** (159 mg, 1.0 mmol), 4-bromobenzonitrile **2d** (218 mg, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.57 (s, 3H) 7.31-7.37 (m, 2H), 7.84-7.50 (m, 1H), 7.67 (dd, *J*=6.8, 2.0 Hz, 2H), 7.89 (dd, *J*=6.8, 1.6 Hz, 2H), 7.92 (s, 1H), 8.44-8.43 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 27.8, 110.4, 111.3, 117.9, 119.9, 123.1, 123.7, 124.6, 124.9 (2C), 126.9, 133.5, 133.9 (2C), 136.2, 142.2, 193.3.

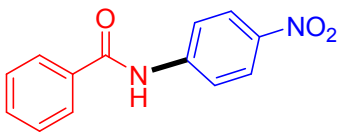


***N*-phenylbenzamide** (**5a**):[18] White solid, (168 mg; 85% yield) mp: 163-164°C. Synthesized following the general procedure from benzamide **4** (121 mg, 1.0 mmol), bromobenzene **2a** (0.126 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.13 (t, *J*=7.4, 1H), 7.35 (t, *J*=7.6, 2H), 7.43-7.67 (m, 2H), 7.50-7.54 (m,



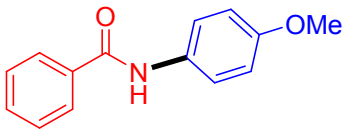
3H), 7.84 (d, *J*=9.2, 2H), 7.92 (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 120.2 (2C), 125.6, 1127.0 (2C), 128.8 (2C), 129.1 (2C), 131.8, 134.9, 137.9, 165.8.

***N*-(4-nitrophenyl)benzamide** (**5b**):[19] White solid, (228 mg; 94% yield) mp: 203-204°C.



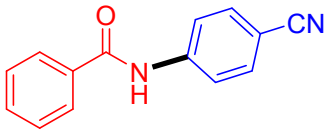
Synthesized following the general procedure from benzamide **4** (121 mg, 1.0 mmol), 4-nitrobromobenzene **2b** (242 mg, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43-7.47 (m, 4H), 7.56 (t, *J*=7.4, 2H), 7.82-7.84 (m, 3H), 9.19 (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.9 (2C), 124.9 (2C), 128.0 (2C), 128.6 (2C), 132.3, 134.3, 142.6, 145.6, 166.4.

***N*-(4-methoxyphenyl)benzamide** (**5c**):[20] White solid, (202 mg; 89% yield) mp: 145-146°C.



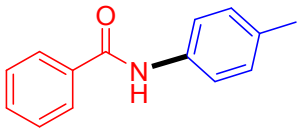
Synthesized following the general procedure from benzamide **4** (121 mg, 1.0 mmol), 4-methoxybromobenzene **2c** (0.15 mL, 1.2 mmol).^{1}H NMR (400 MHz, $CDCl_3$): δ 3.79 (s, 3H), 6.88 (d, *J*=8.8, 2H), 7.42-7.52 (m, 5H), 7.80 (brs, 1H), 7.82 (d, *J*=7.8, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.5, 114.2 (2C), 122.1 (2C), 126.9 (2C), 128.7 (2C), 131.0, 131.7, 135.0, 156.6, 165.6.

***N*-(4-cyanophenyl)benzamide** (**5d**):[21] White solid, (207 mg; 93% yield) mp: 165-166°C.



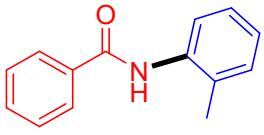
Synthesized following the general procedure from benzamide **4** (121 mg, 1.0 mmol), 4-bromobenzonitrile **2d** (218 mg, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.51 (m, 3H), 7.56-7.59 (m, 2H), 7.80-7.85 (m, 4H), 8.50 (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 107.1, 120.0, 127.2, 127.8 (2C), 128.8, 128.9 (2C), 132.3, 133.2 (2C), 134.1, 142.3, 166.3.

***N*-*p*-tolylbenzamide** (**5e**):[22] White solid, (190 mg; 90% yield) mp: 155-156°C. Synthesized



following the general procedure from benzamide **4** (121 mg, 1.0 mmol), *p*-bromotoluene **2e** (0.148 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.31 (s, 3H), 7.12 (d, *J*=8.4, 2H), 7.41 (t, *J*=7.6, 2H), 7.47-7.51 (m, 3H), 7.82 (d, *J*=7.6, 2H), 8.02 (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.9, 120.4, 126.9 (2C), 128.6 (2C), 129.5 (2C), 131.6 (2C), 134.1, 134.9, 135.3, 165.8.

***N*-*o*-tolylbenzamide** (**5f**):[20] White solid, (177 mg; 84% yield) mp: 142-143°C. Synthesized



following the general procedure from benzamide **4** (121 mg, 1.0 mmol), 4 *o*-bromotoluene **2f** (0.144 mL, 1.2 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.29 (s, 3H) 7.084-7.12 (m, 1H), 7.19-7.24 (m, 2H), 7.44-7.48 (m, 2H),

7.51-7.54 (m, 1H), 7.86 (d, *J*=7.6, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 17.8, 123.3, 125.4, 126.8, 127.0 (2C), 128.7 (2C), 129.5, 130.5, 131.7, 134.9, 135.7, 165.7.

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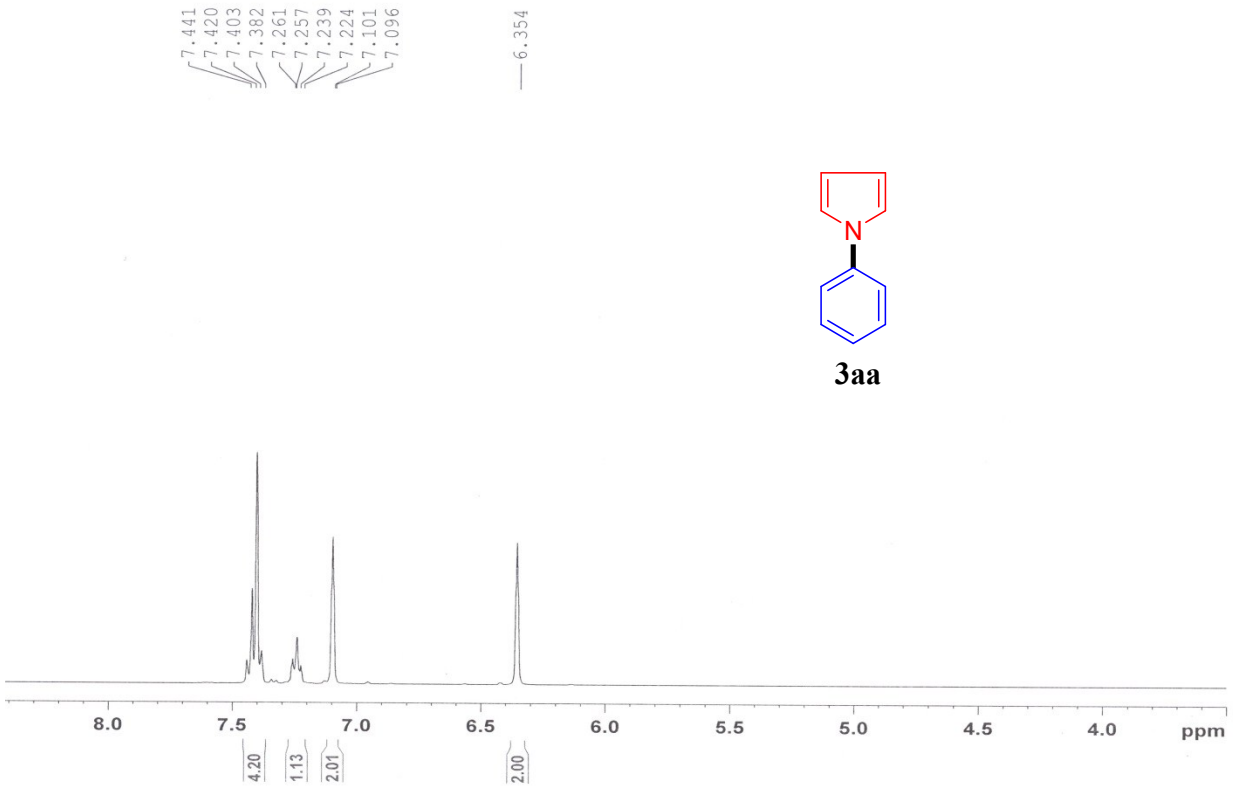

Figure S1. ^{1}H NMR spectrum of **3aa** in $CDCl_3$

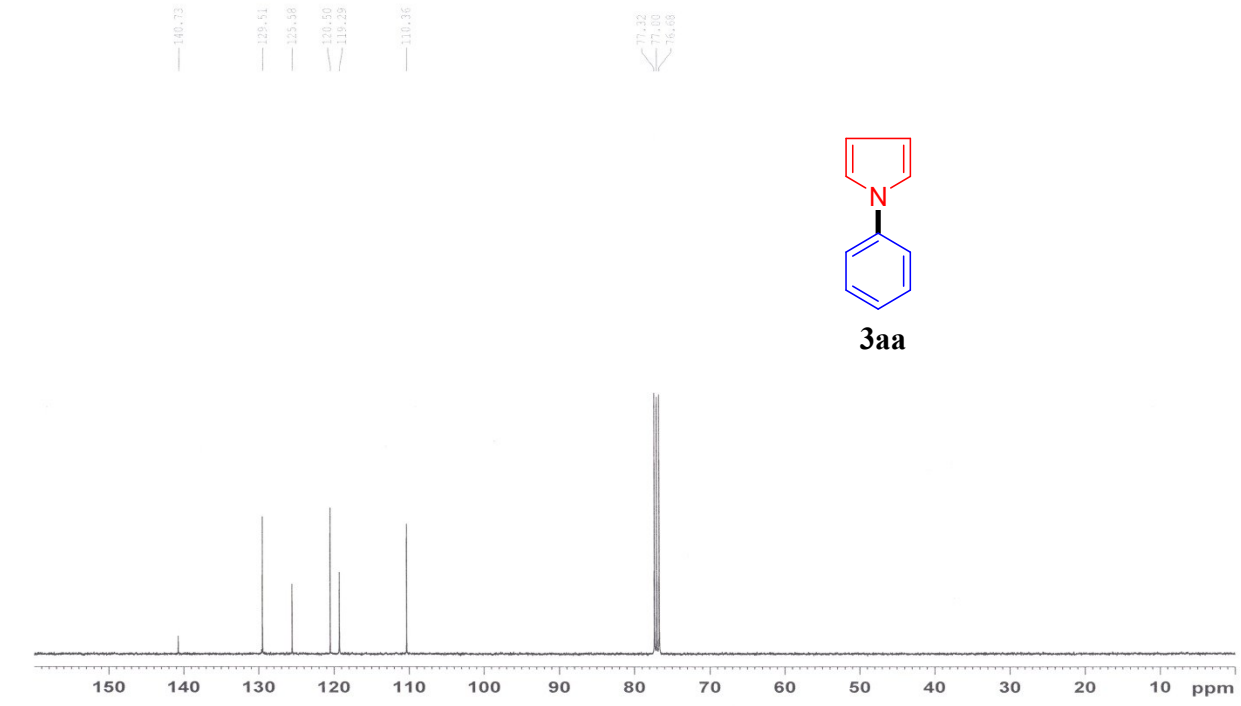

Figure S2. ^{13}C NMR spectrum of **3aa** in $CDCl_3$

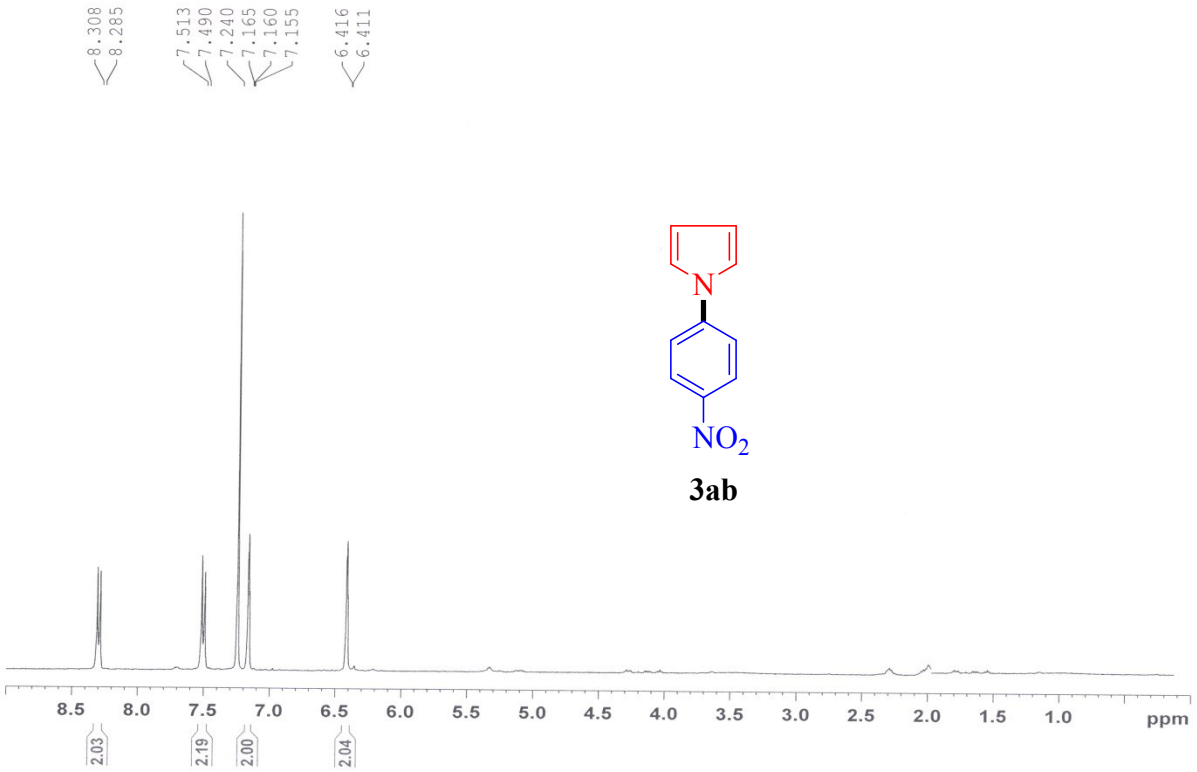

Figure S3. ^{1}H NMR spectrum of **3ab** in $CDCl_3$

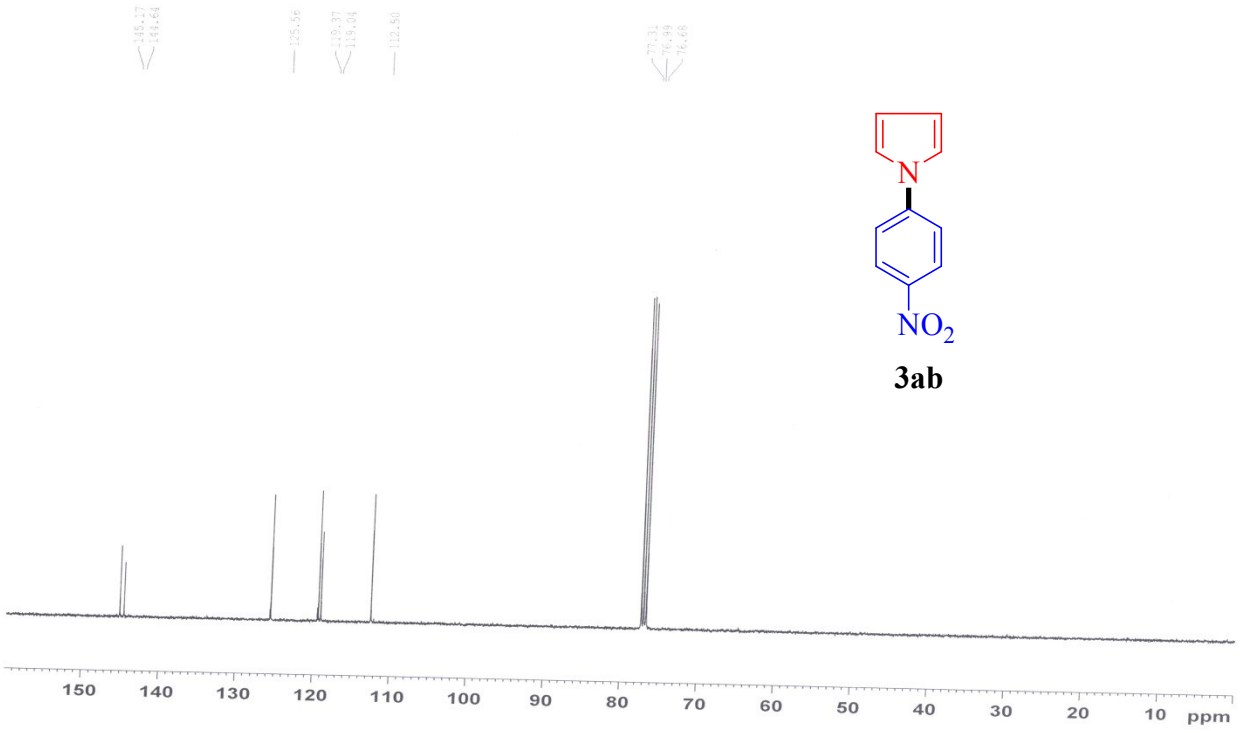

Figure S4. ^{13}C NMR spectrum of **3ab** in $CDCl_3$

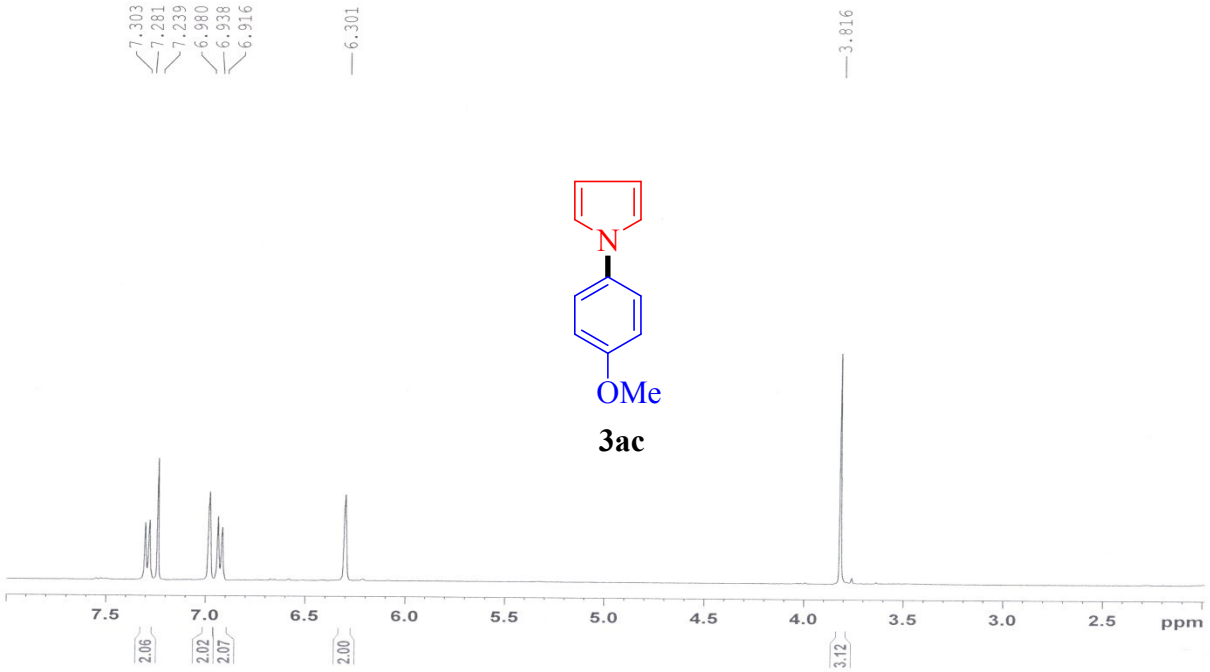

Figure S5. ^{1}H NMR spectrum of **3ac** in $CDCl_3$

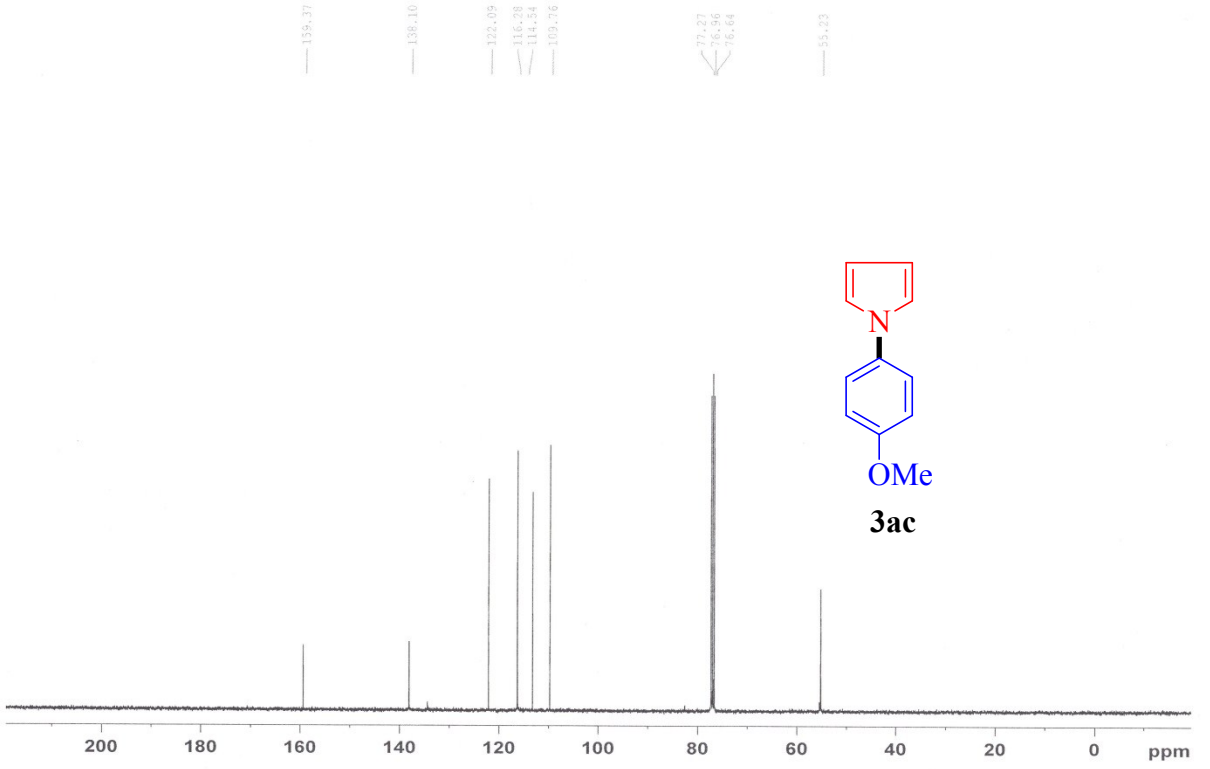

Figure S6. ^{1}H NMR spectrum of **3ac** in $CDCl_3$

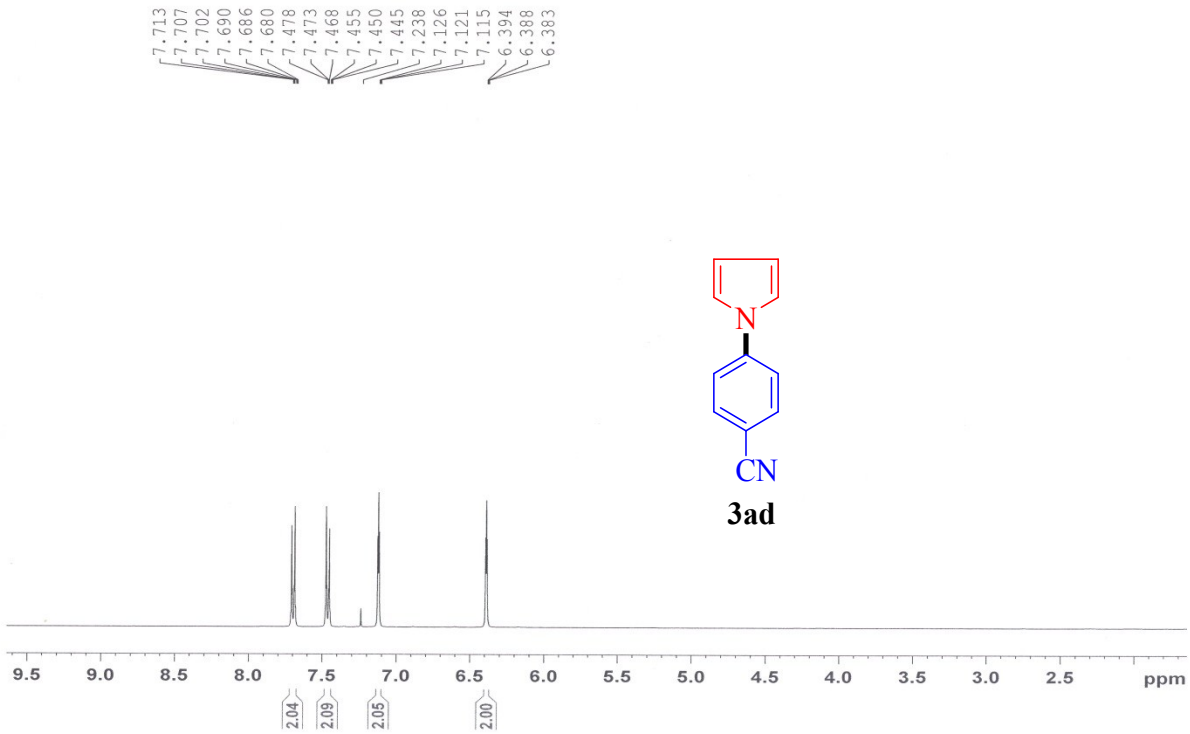

Figure S7. ^{1}H NMR spectrum of **3ad** in $CDCl_3$

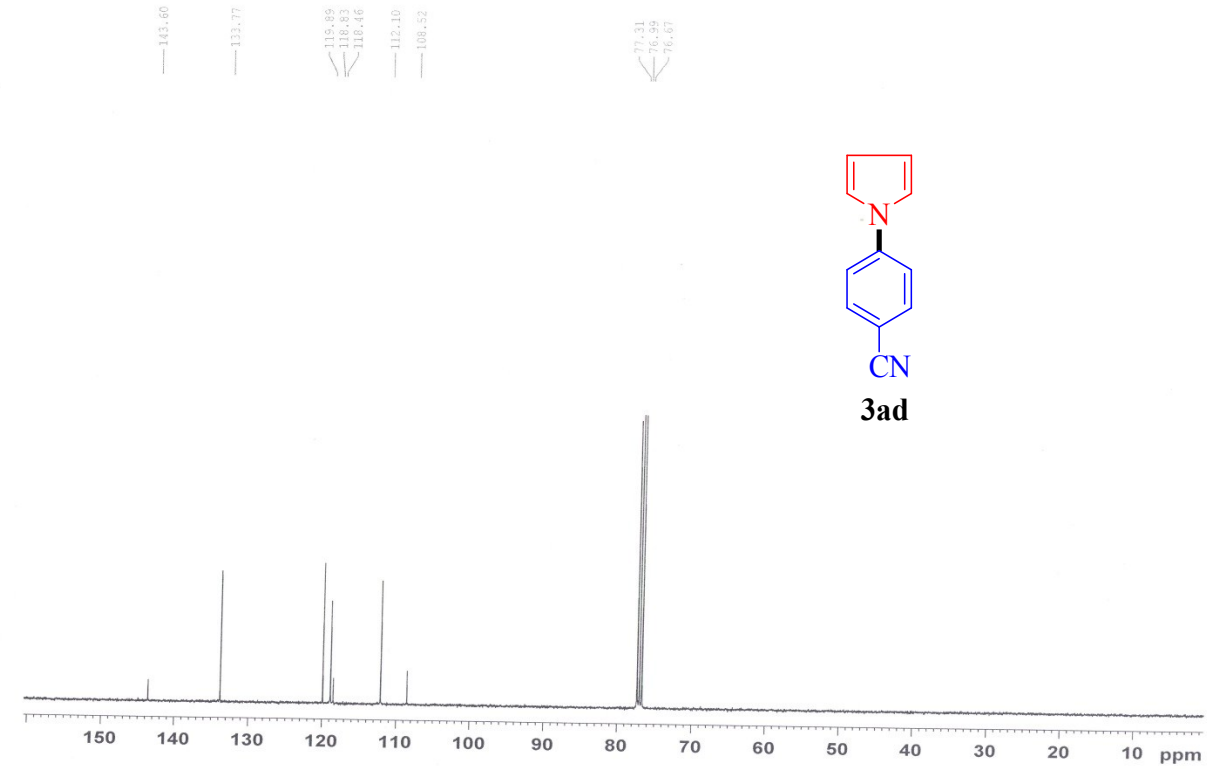

Figure S8. ^{13}C NMR spectrum of **3ad** in $CDCl_3$

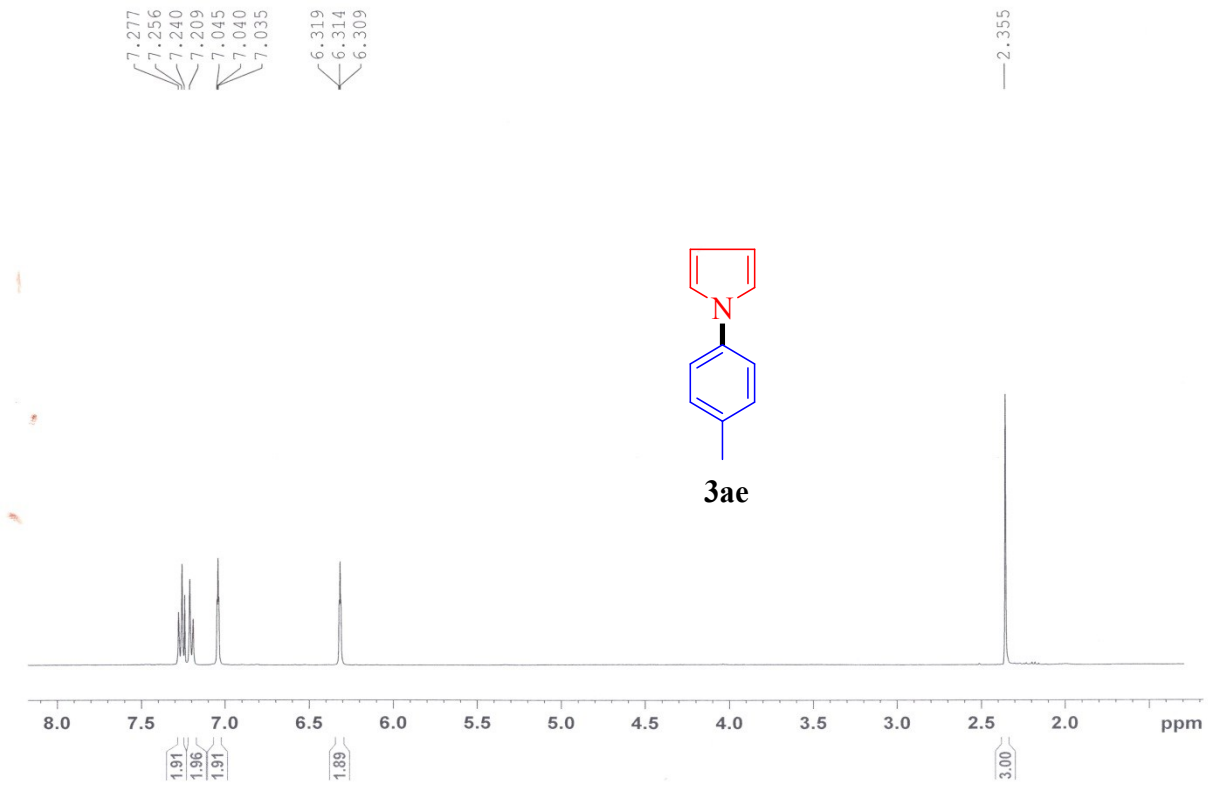

Figure S9. ^{1}H NMR spectrum of **3ae** in $CDCl_3$

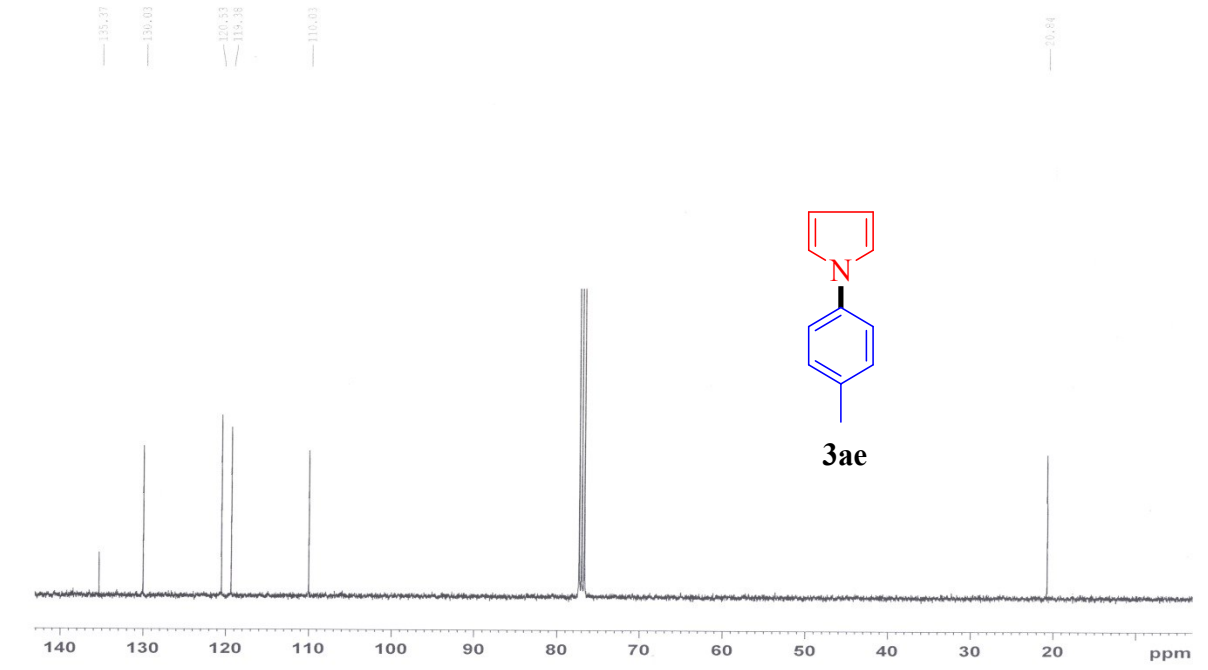

Figure S10. ^{13}C NMR spectrum of **3ae** in $CDCl_3$

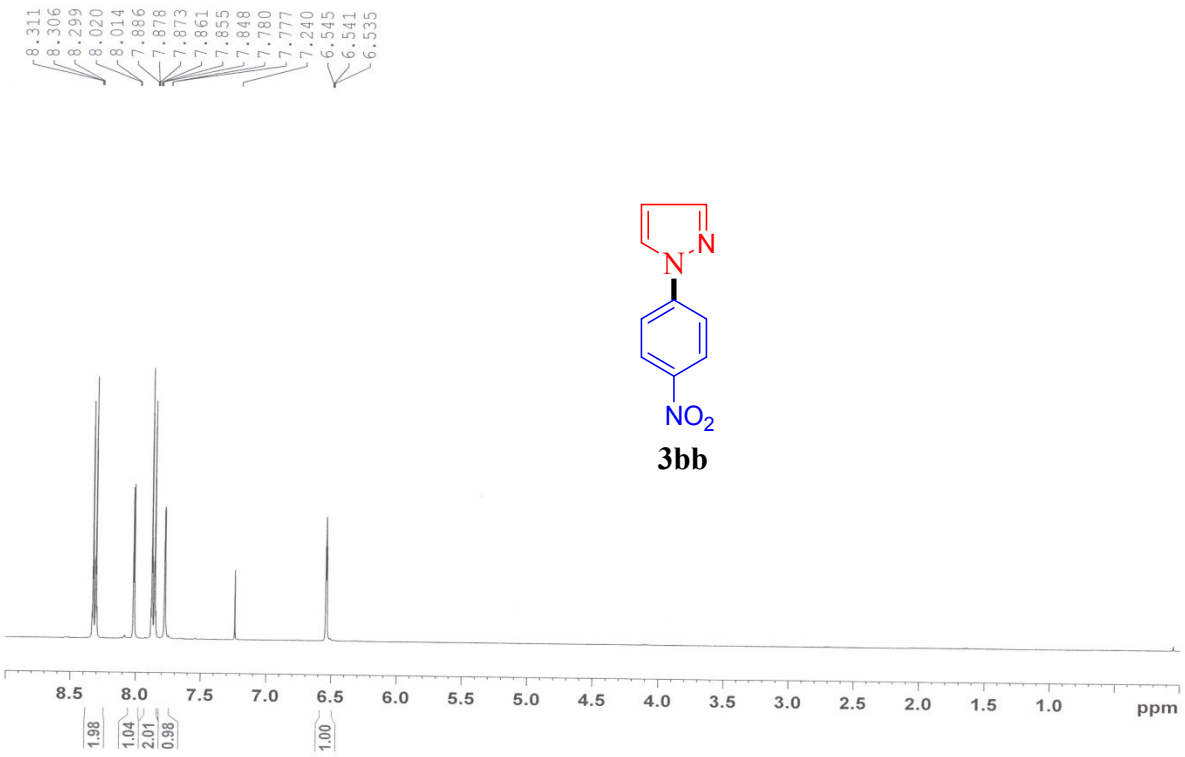

Figure S11. ^{1}H NMR spectrum of **3bb** in $CDCl_3$

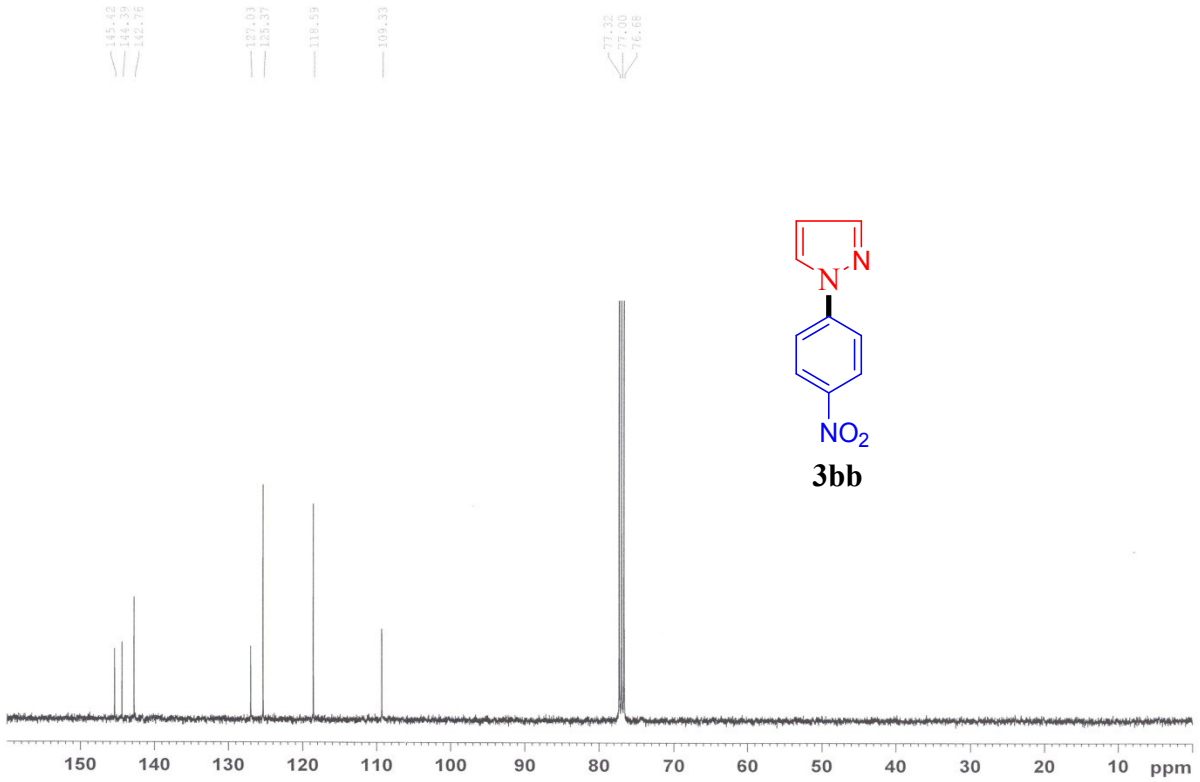

Figure S12. ^{13}C NMR spectrum of **3bb** in $CDCl_3$

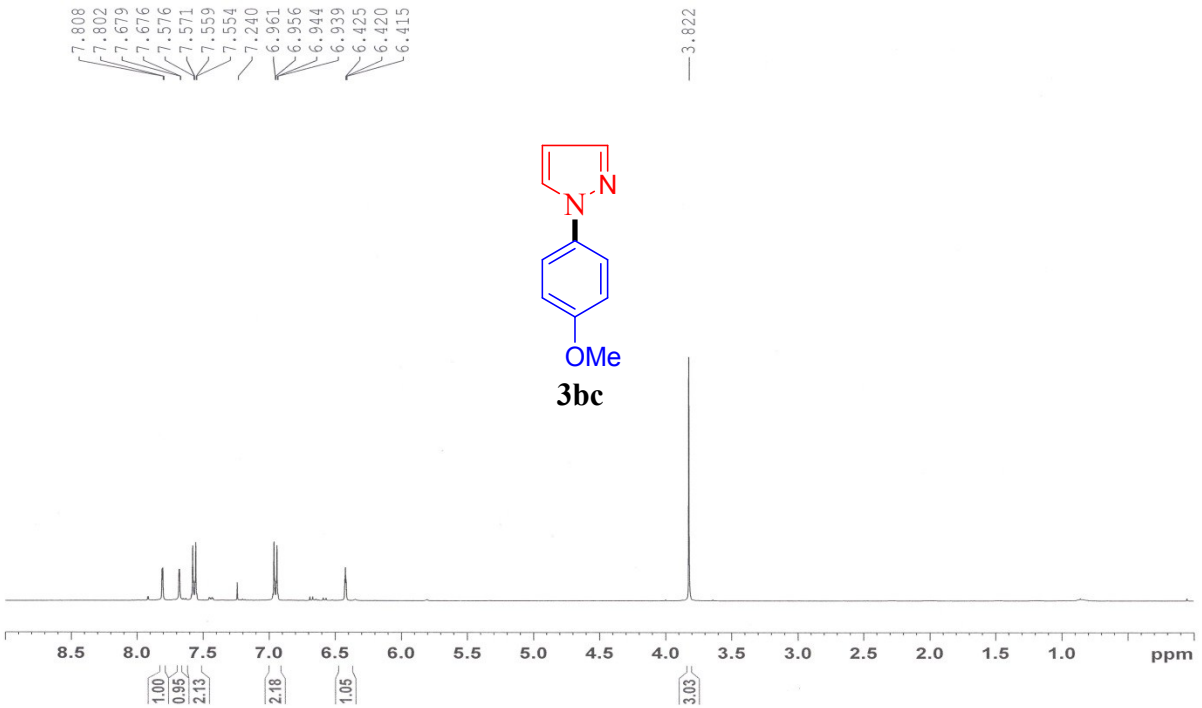

Figure S13. ^{1}H NMR spectrum of **3bc** in $CDCl_3$

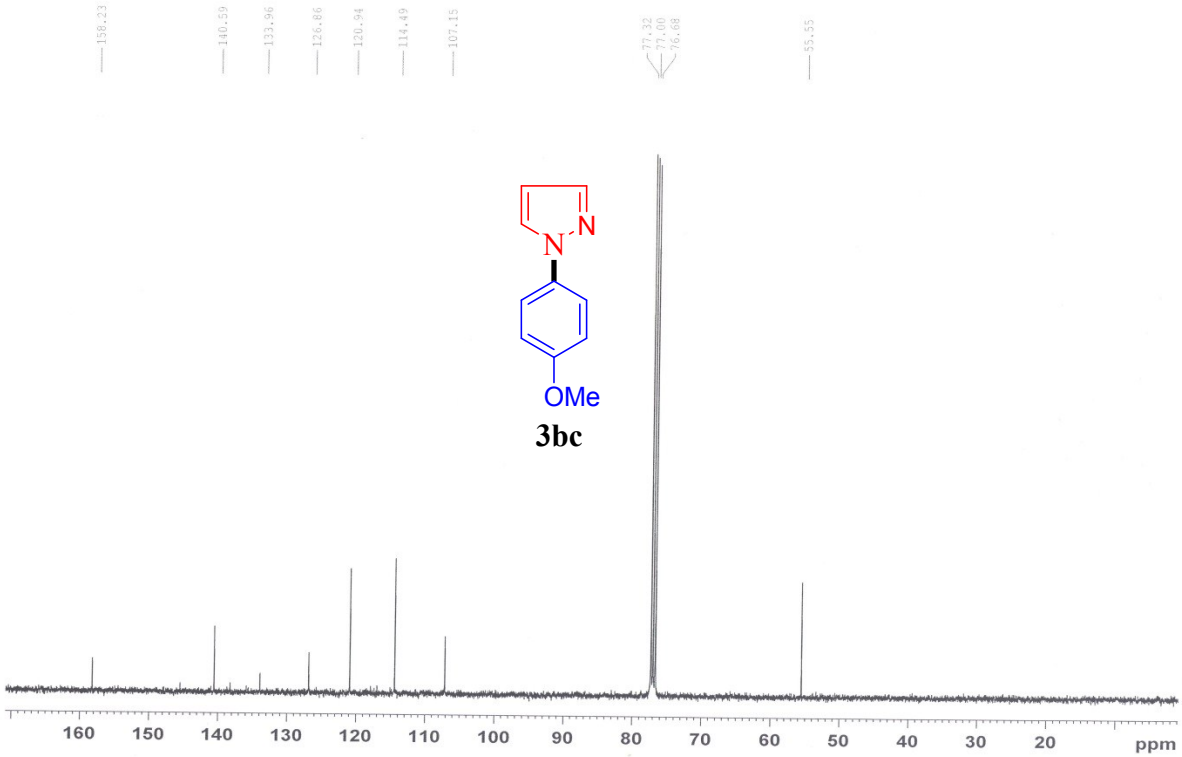

Figure S14. ^{1}H NMR spectrum of **3bc** in $CDCl_3$

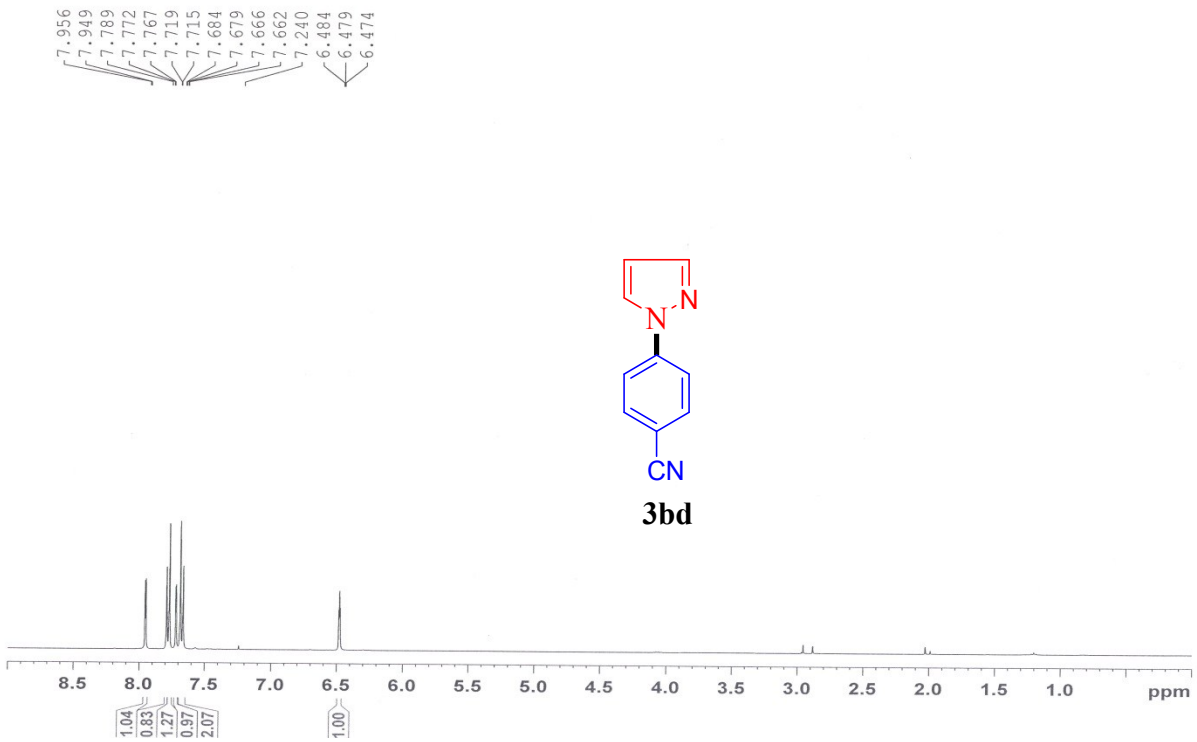

Figure S15. ^{1}H NMR spectrum of **3bd** in $CDCl_3$

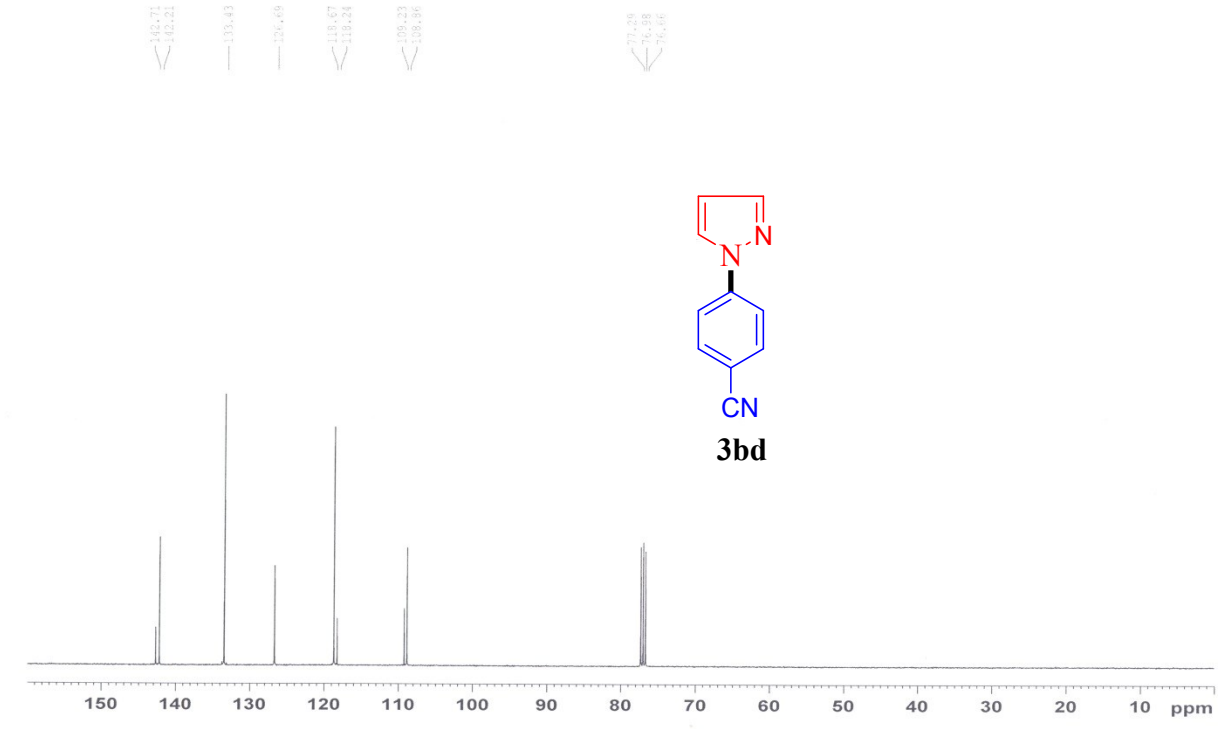

Figure S16. ^{1}H NMR spectrum of **3bd** in $CDCl_3$

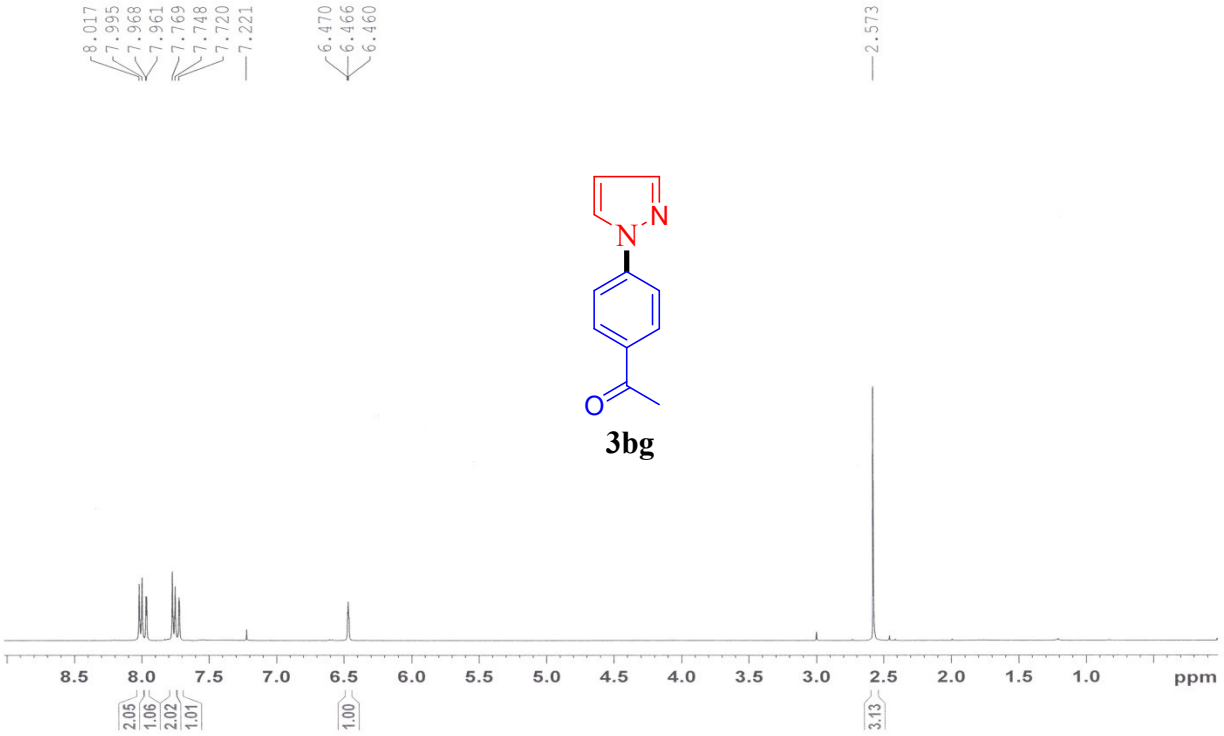

Figure S17. ^{1}H NMR spectrum of 3**bg** in $CDCl_3$

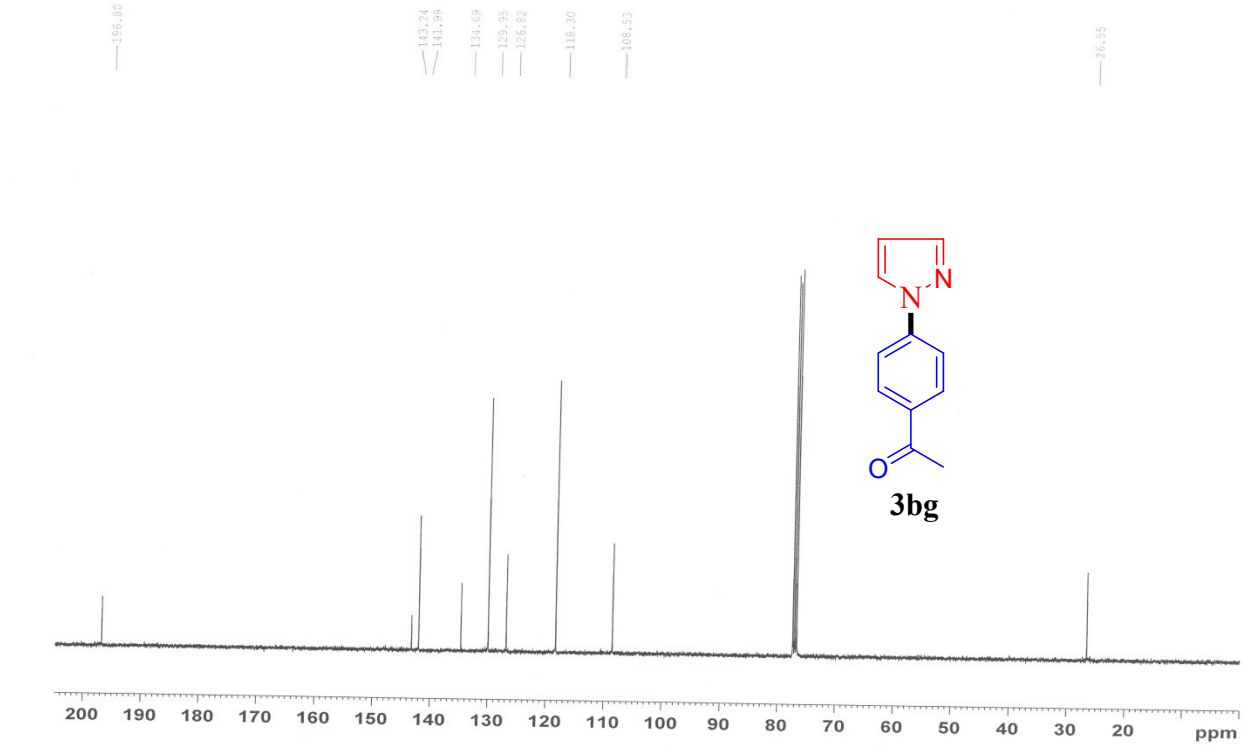

Figure S18. ^{1}H NMR spectrum of **3bg** in $CDCl_3$

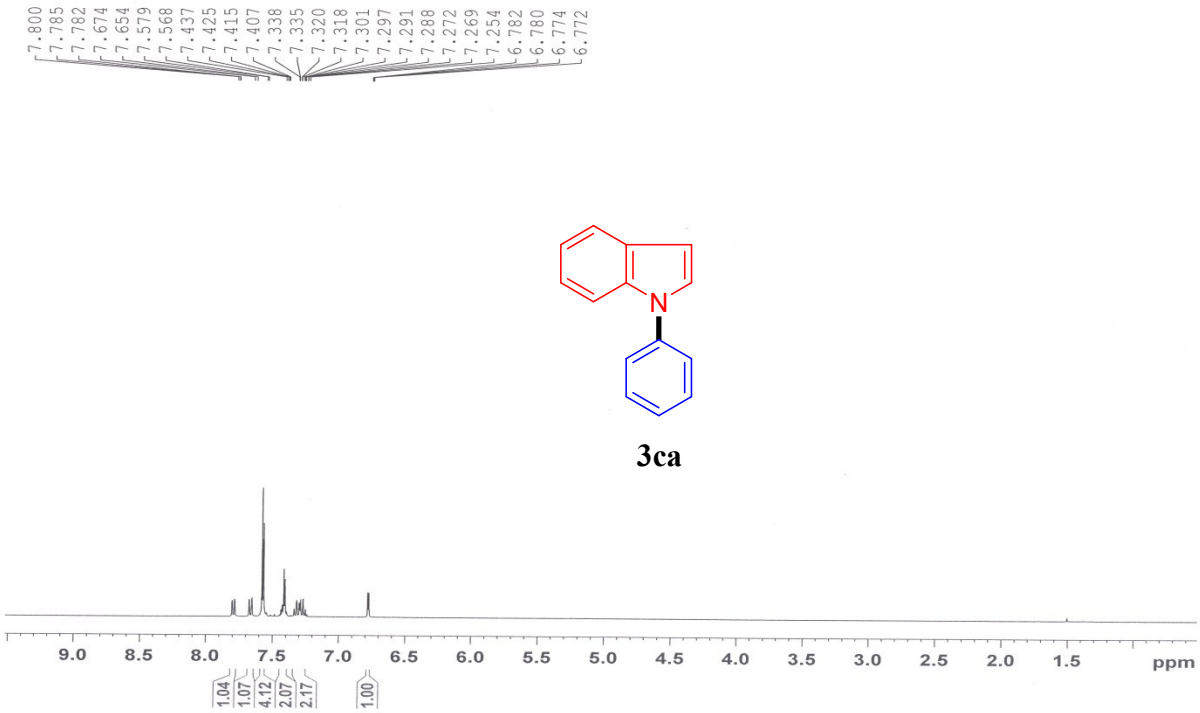

Figure S19. ^{1}H NMR spectrum of **3ca** in $CDCl_3$

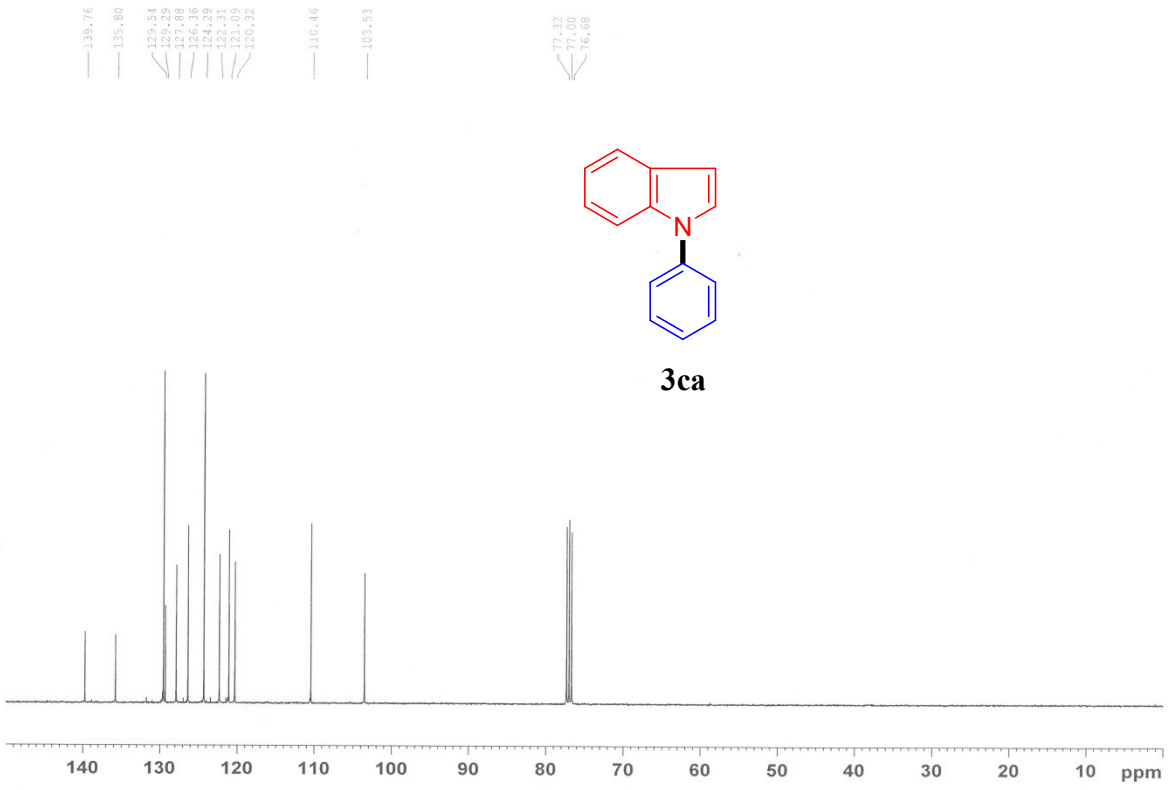

Figure S20. ^{1}H NMR spectrum of **3ca** in $CDCl_3$

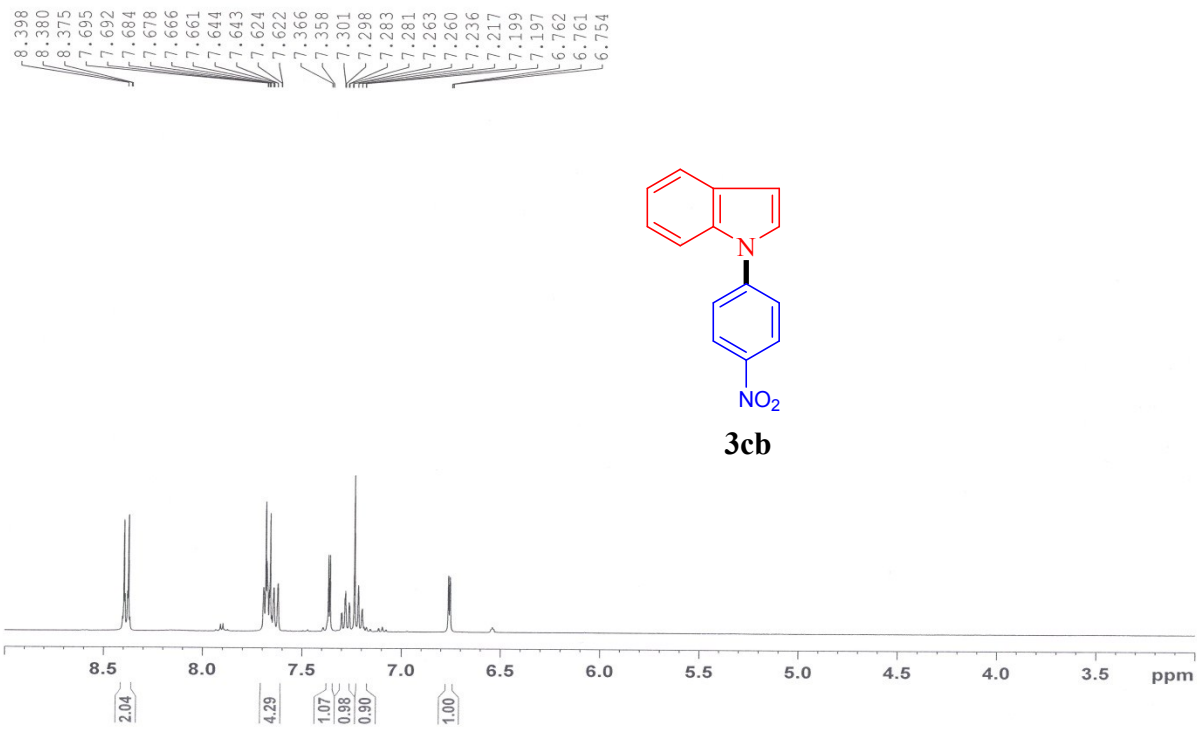

Figure S21. ^{1}H NMR spectrum of **3cb** in $CDCl_3$

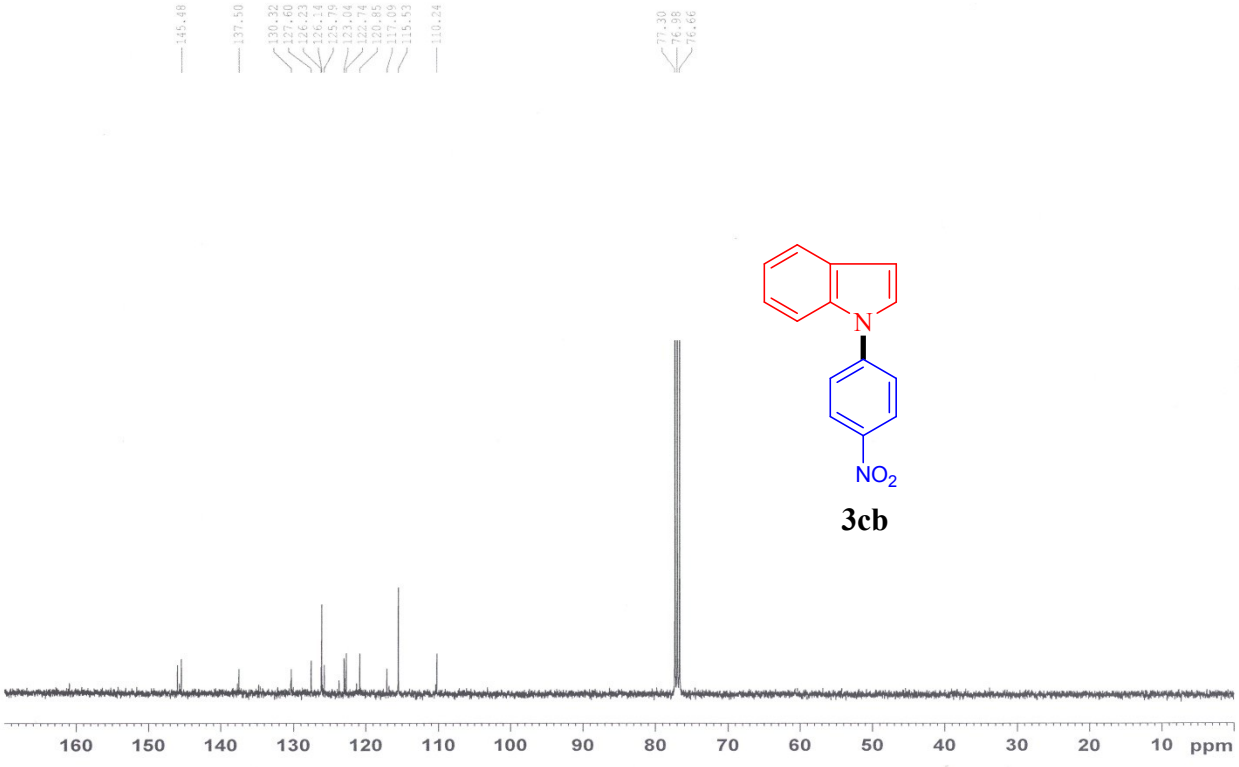

Figure S22. ^{13}C NMR spectrum of **3cb** in $CDCl_3$

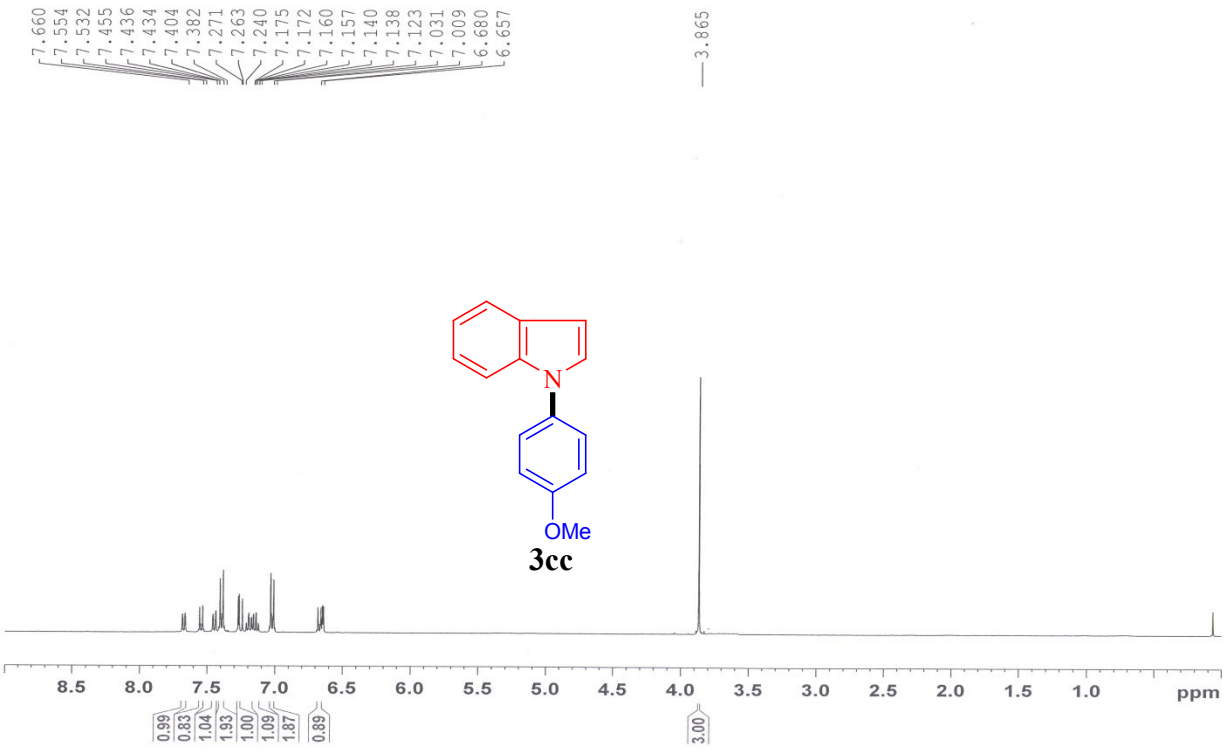

Figure S23. ^{1}H NMR spectrum of **3cc** in $CDCl_3$

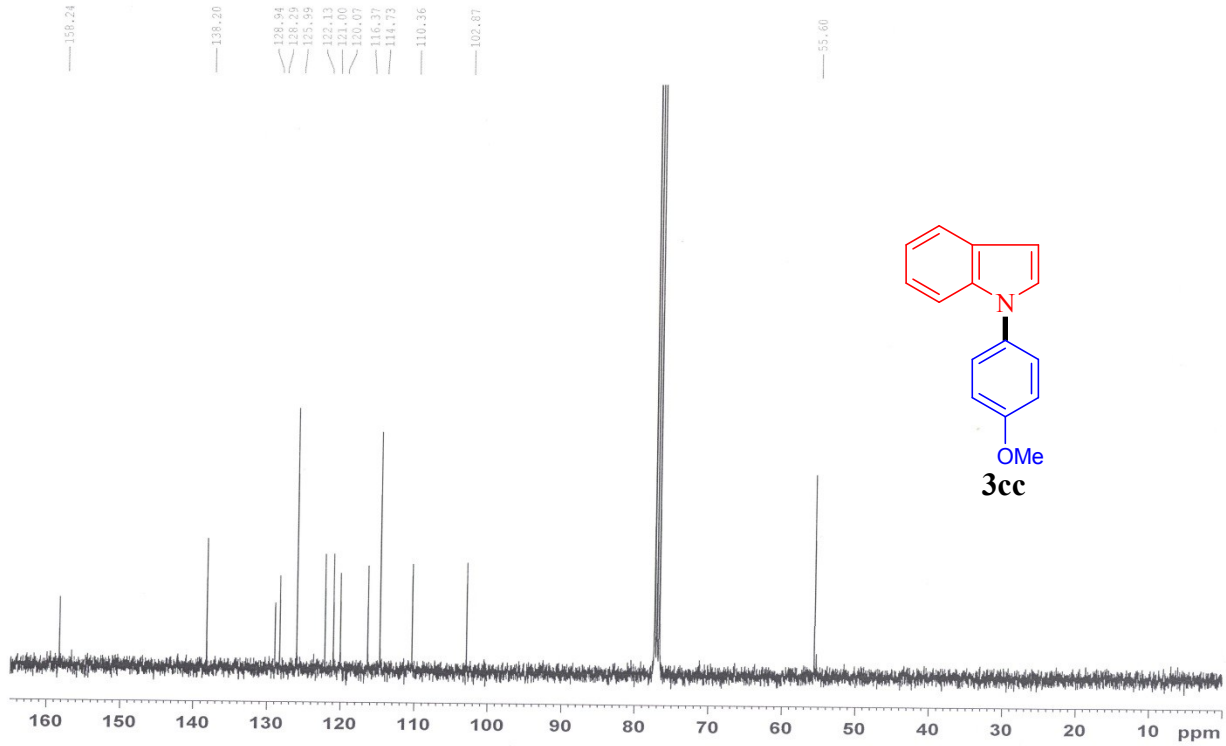

Figure S24. ^{13}C NMR spectrum of **3cc** in $CDCl_3$

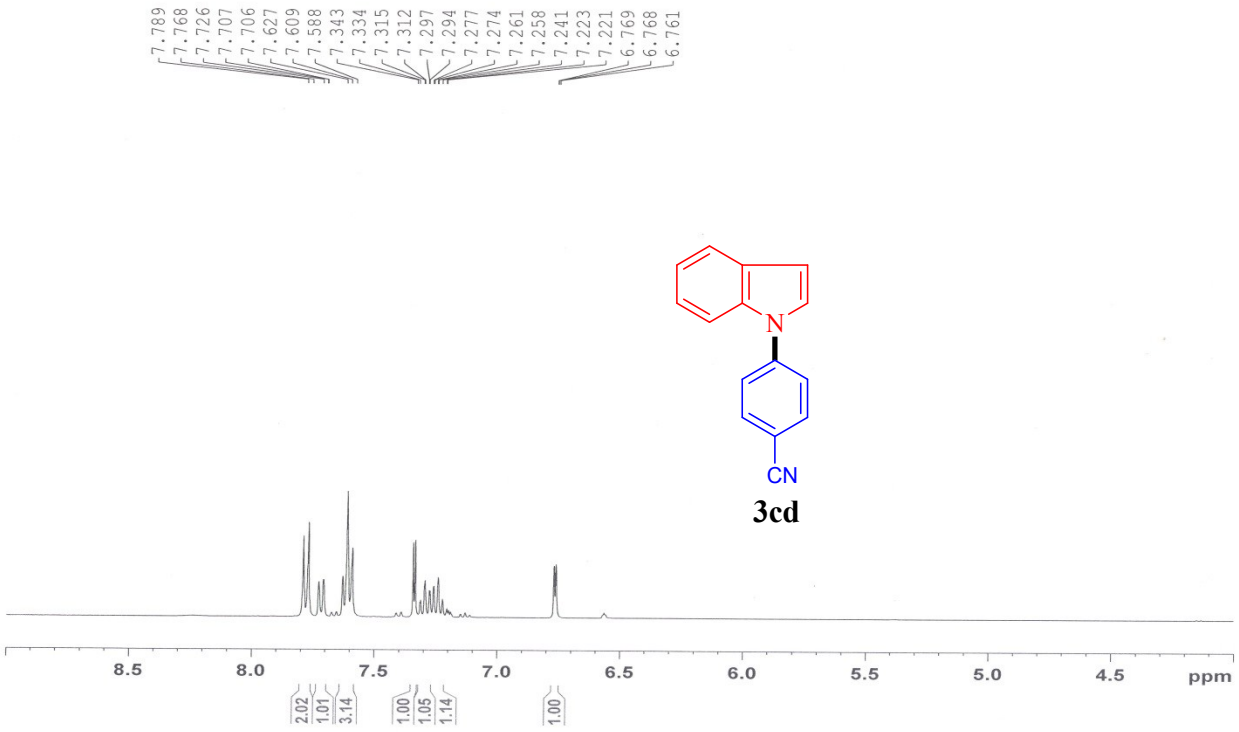

Figure S25. ^{1}H NMR spectrum of **3cd** in $CDCl_3$

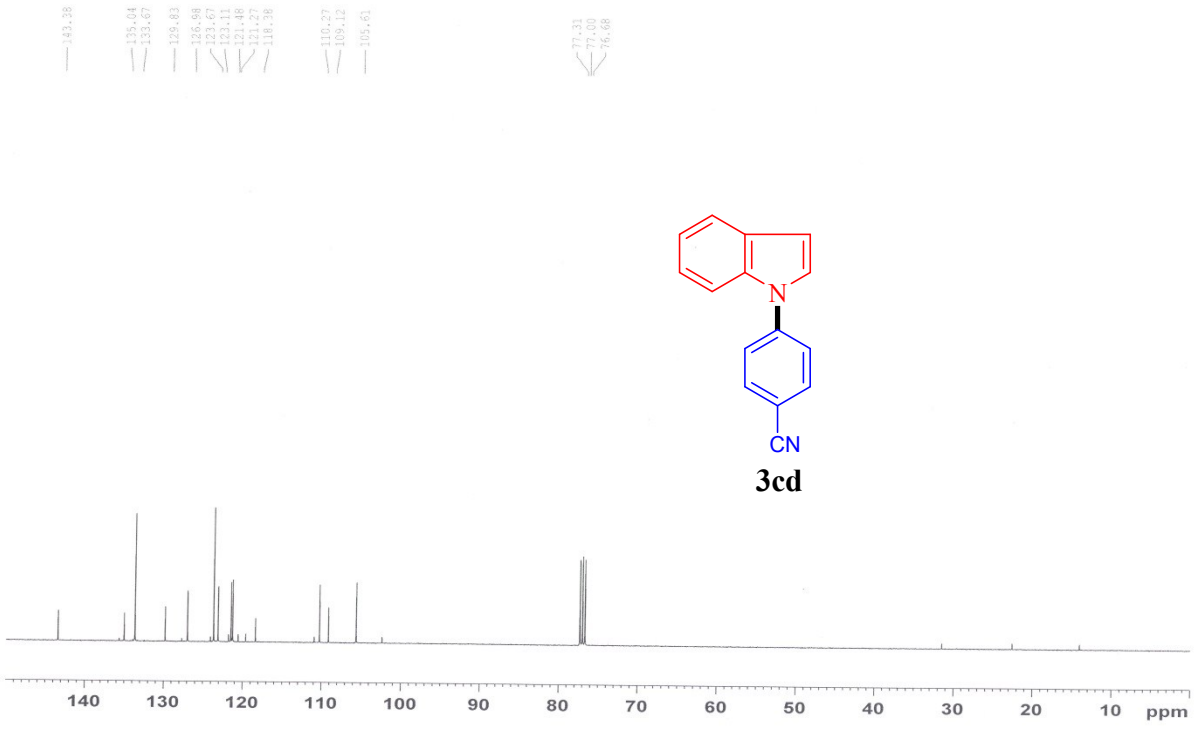

Figure S26. ^{13}C NMR spectrum of **3cd** in $CDCl_3$

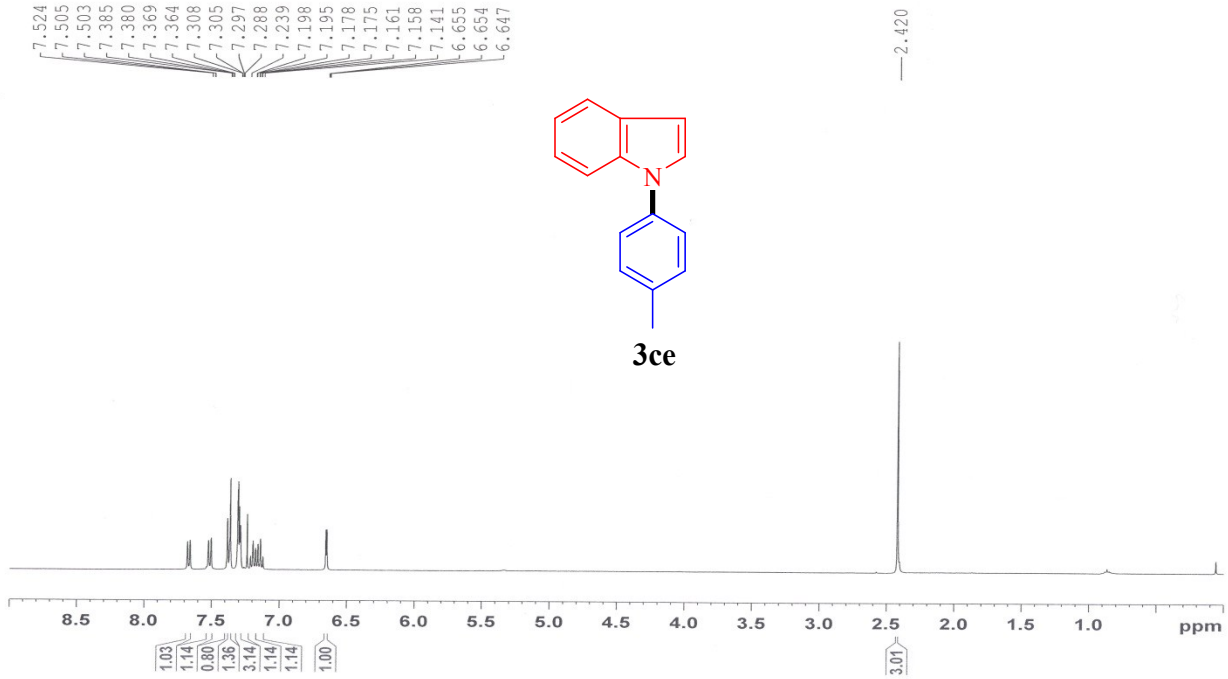

Figure S27. ^{1}H NMR spectrum of **3ce** in $CDCl_3$

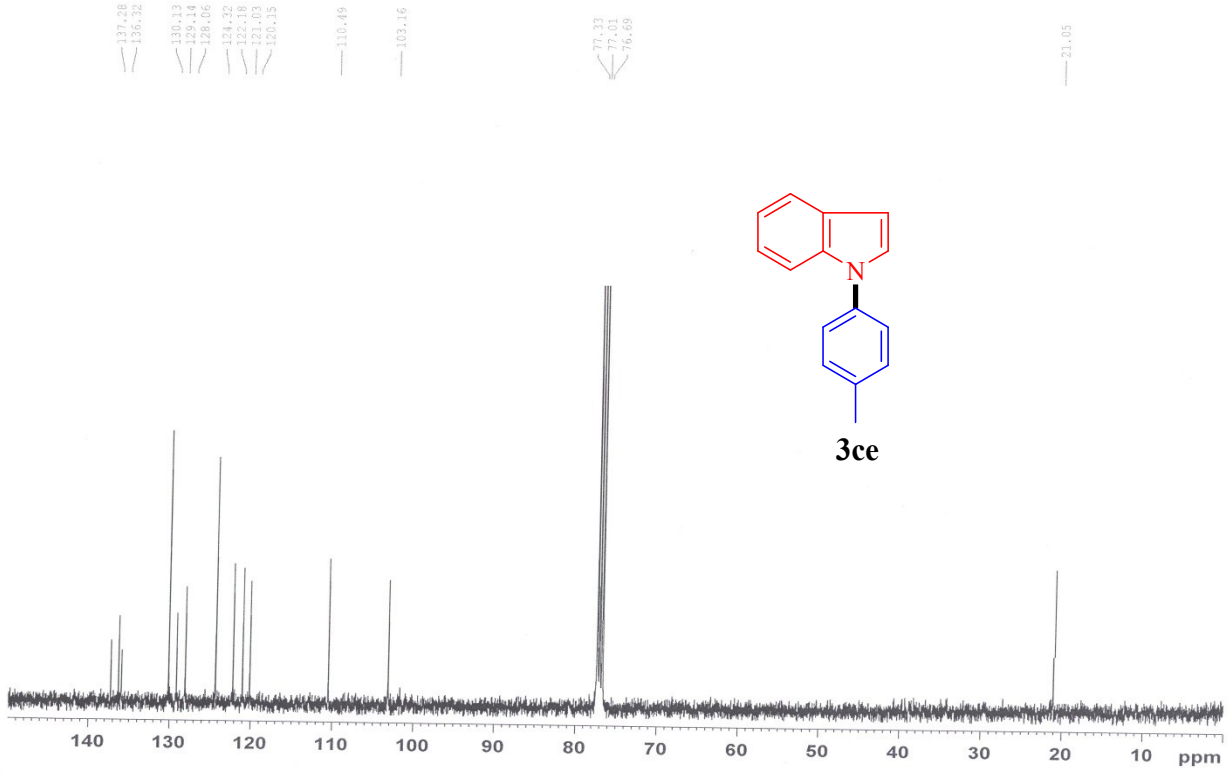

Figure S28. ^{13}C NMR spectrum of **3ce** in $CDCl_3$

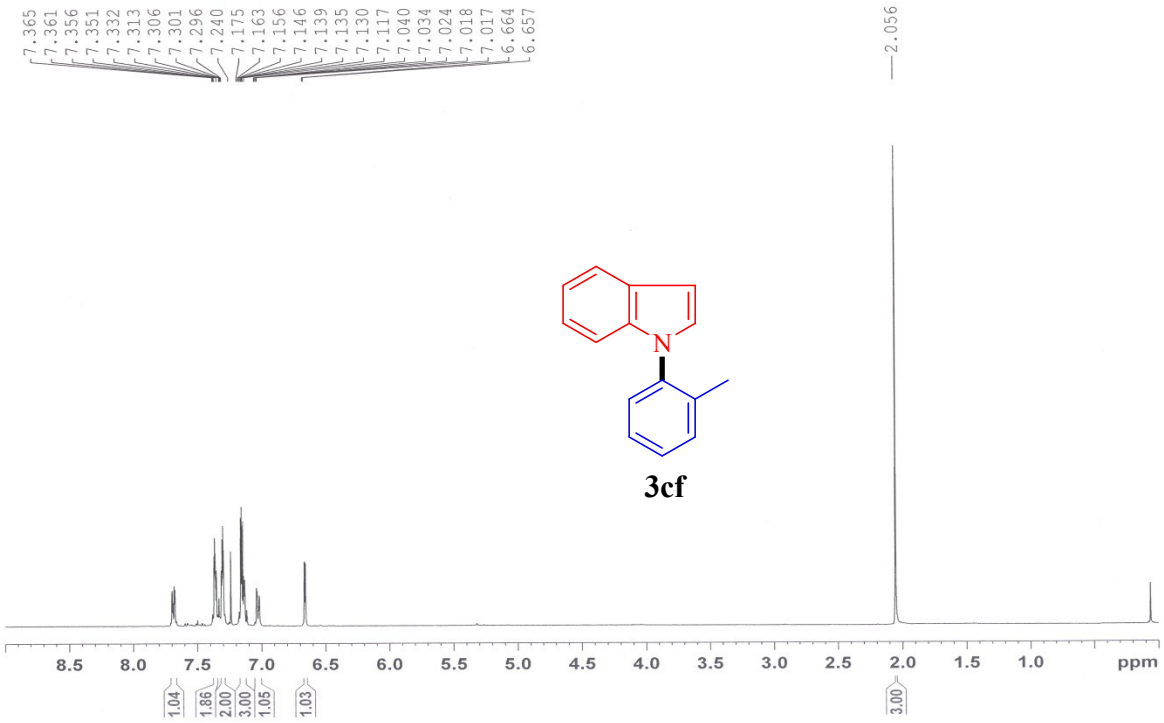

Figure S29. ^{1}H NMR spectrum of **3cf** in $CDCl_3$

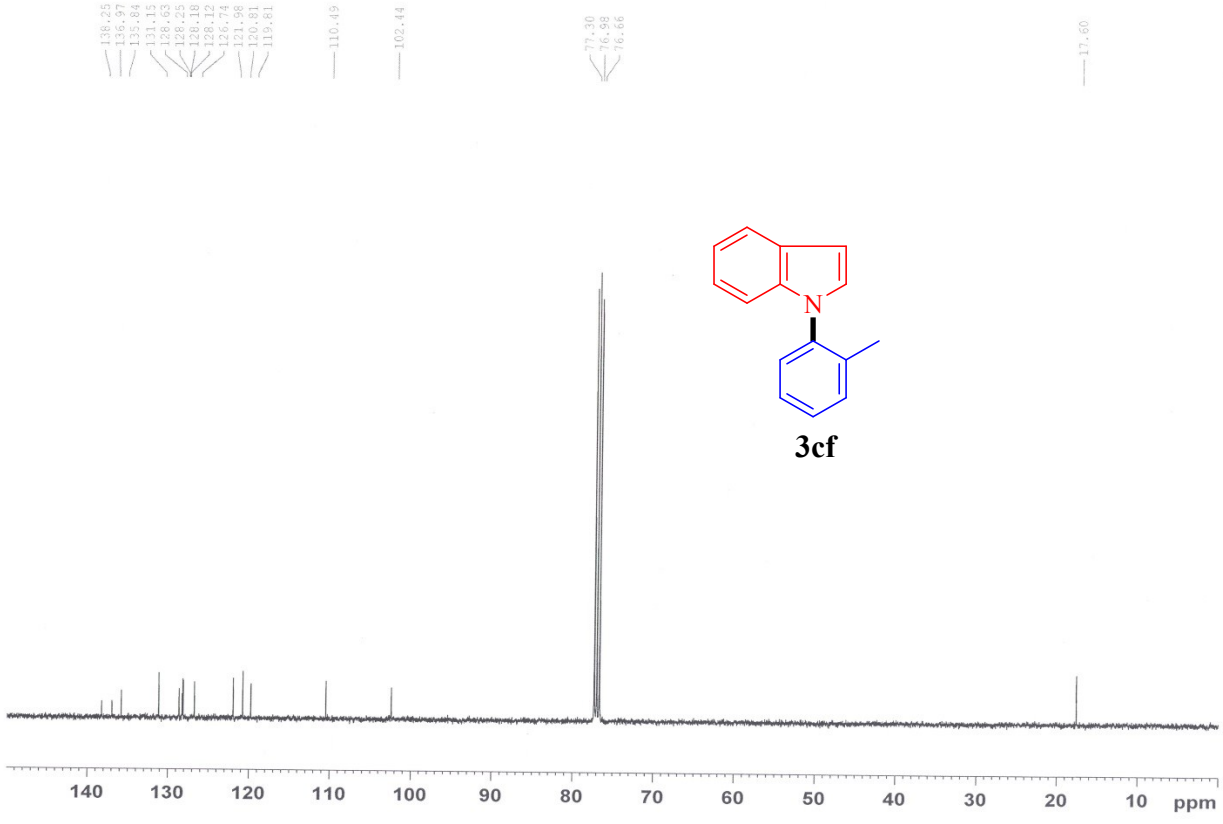

Figure S30. ^{13}C NMR spectrum of **3cf** in $CDCl_3$

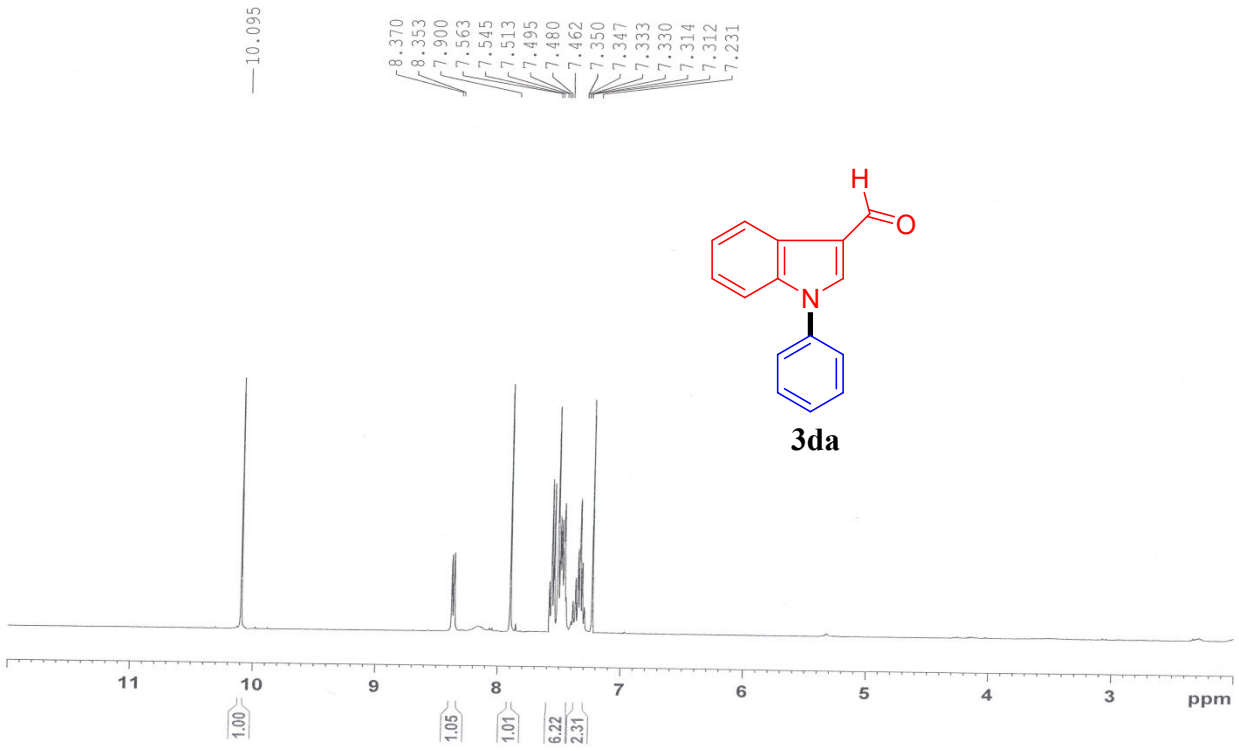

Figure S31. ^{1}H NMR spectrum of **3da** in $CDCl_3$

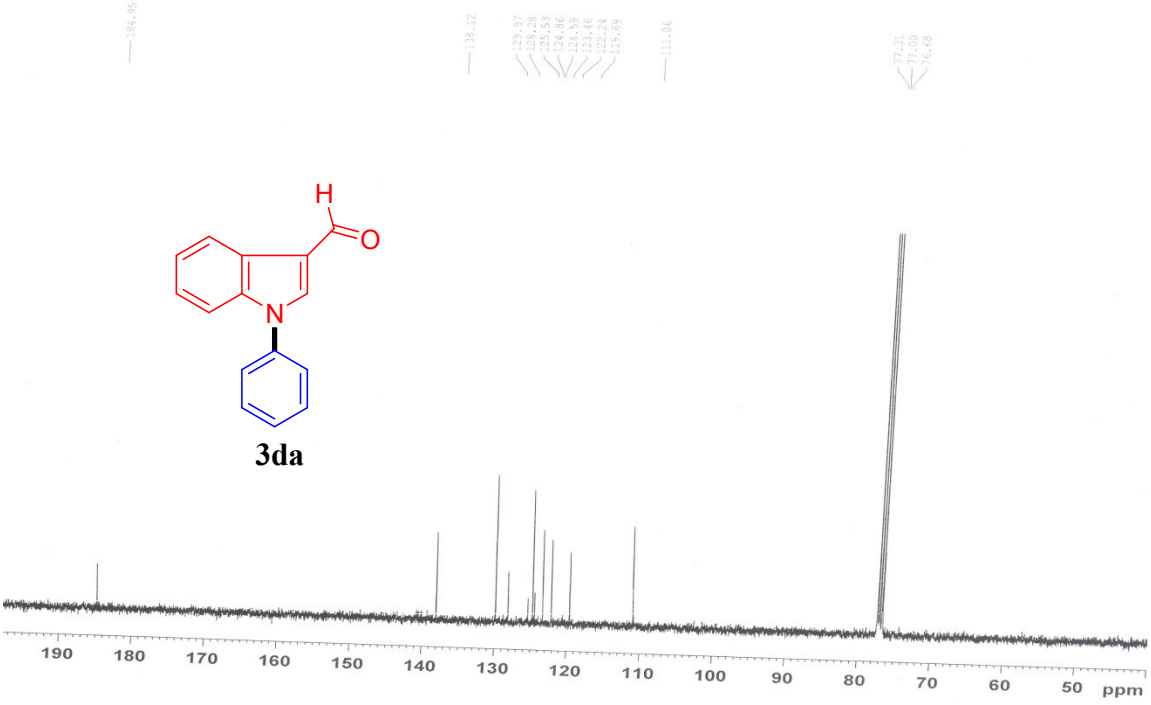

Figure S32. ^{13}C NMR spectrum of **3da** in $CDCl_3$

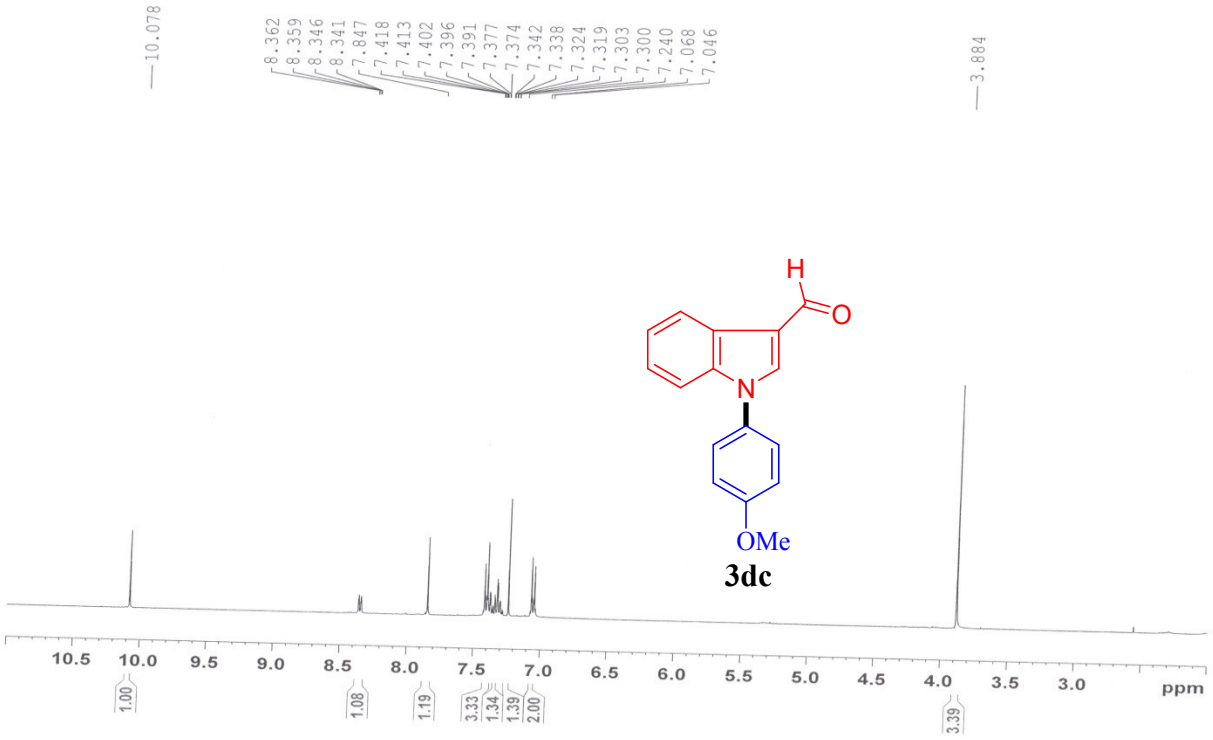

Figure S33. ^{1}H NMR spectrum of **3dc** in $CDCl_3$

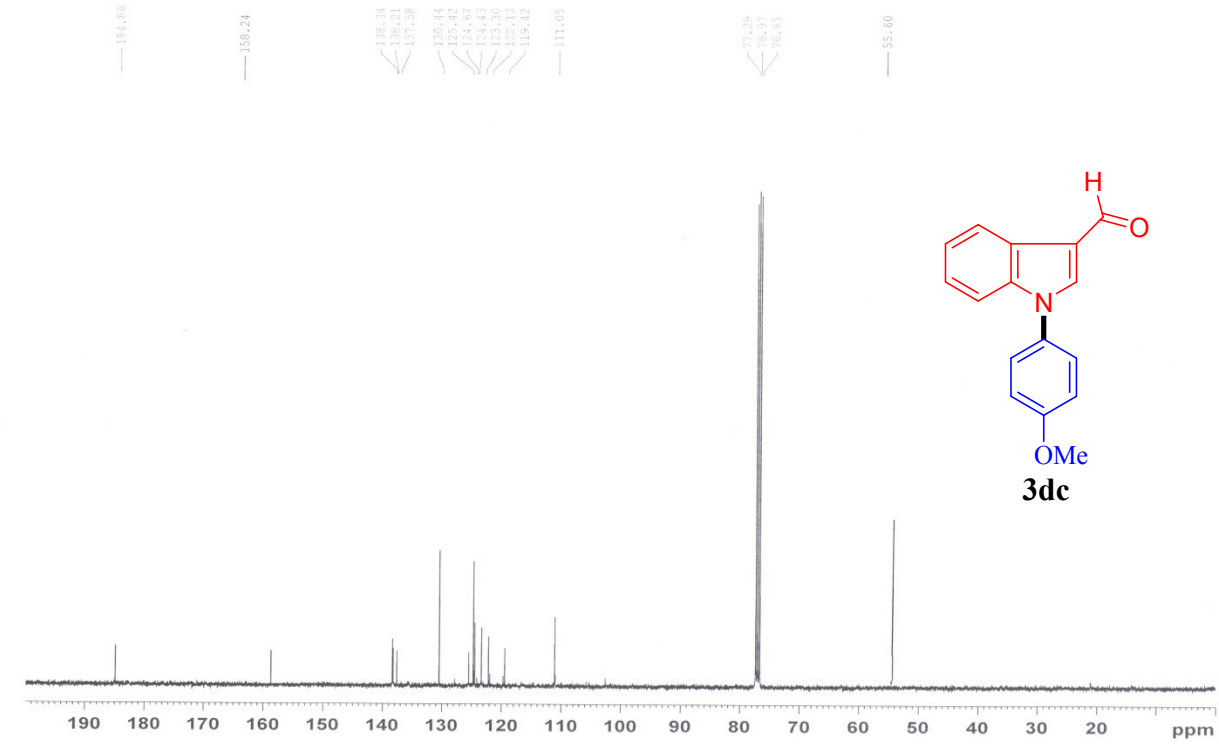

Figure S34. ^{13}C NMR spectrum of **3dc** in $CDCl_3$

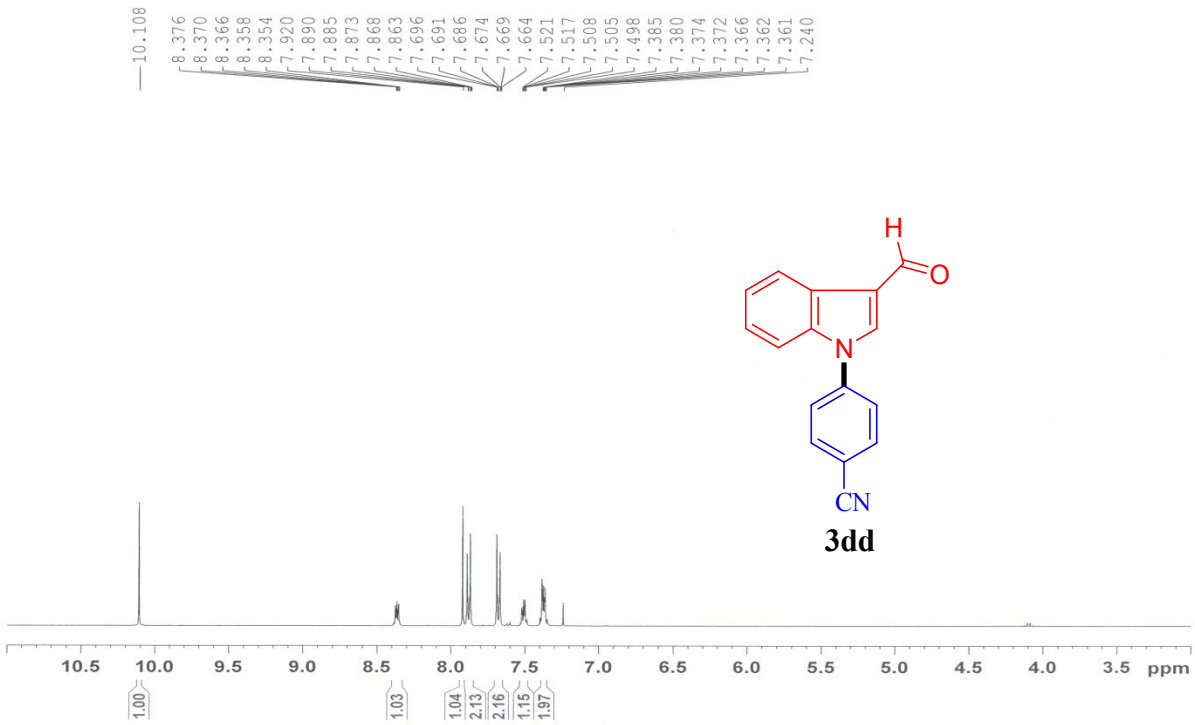

Figure S35. ^{1}H NMR spectrum of **3dd** in $CDCl_3$

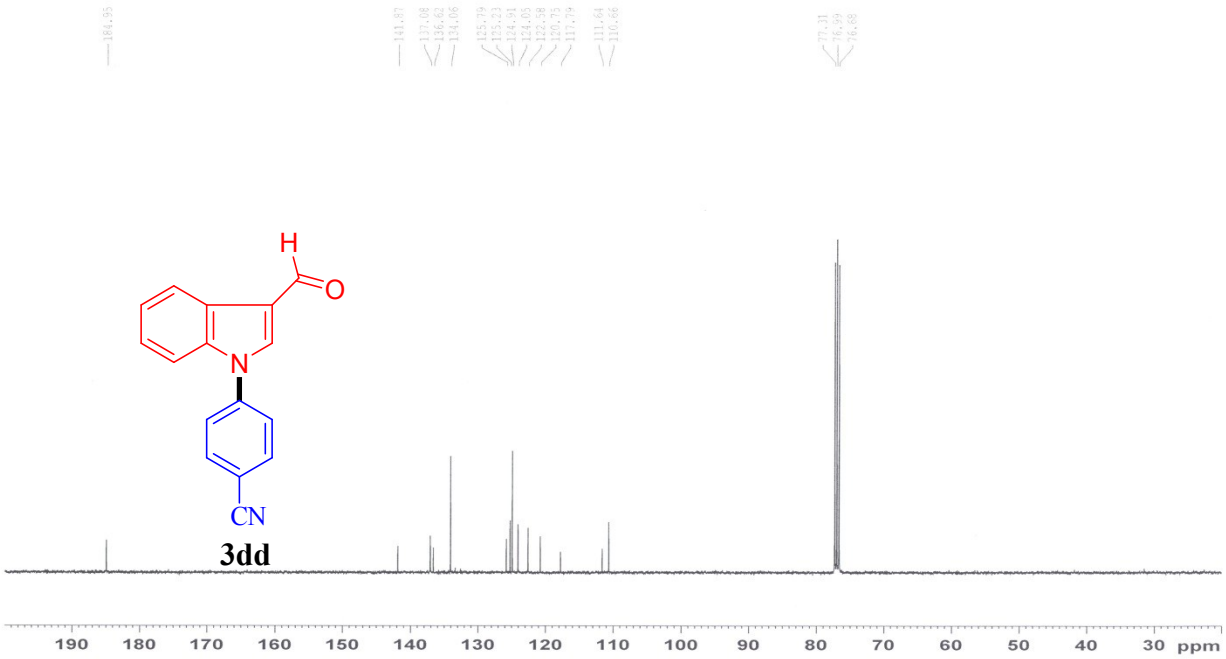

Figure S36. ^{13}C NMR spectrum of **3dd** in $CDCl_3$

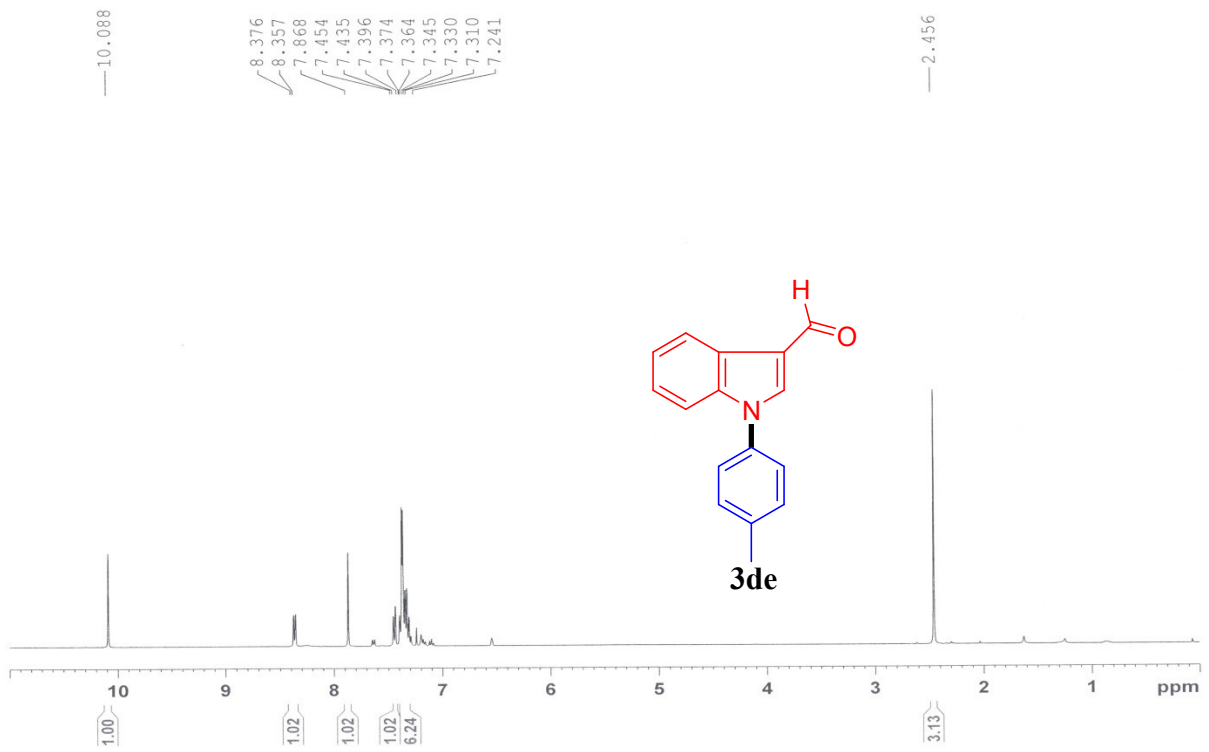

Figure S367. ^{1}H NMR spectrum of **3de** in $CDCl_3$

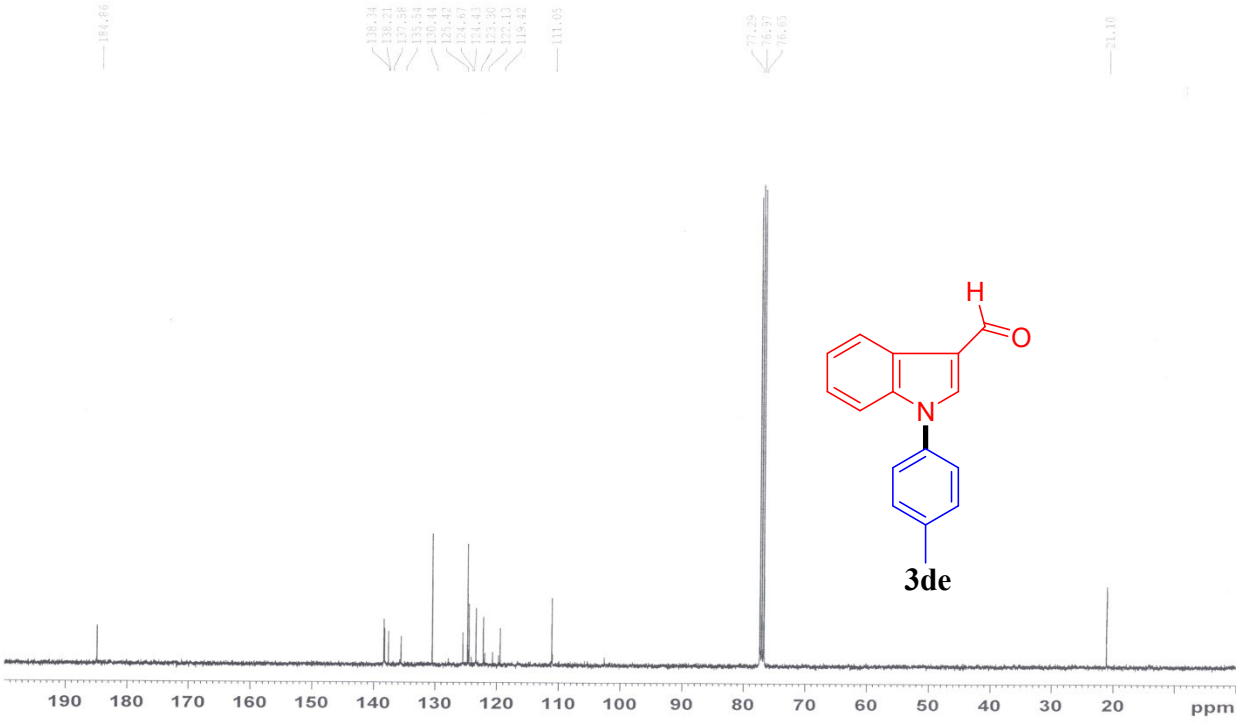

Figure S38. ^{13}C NMR spectrum of **3de** in $CDCl_3$

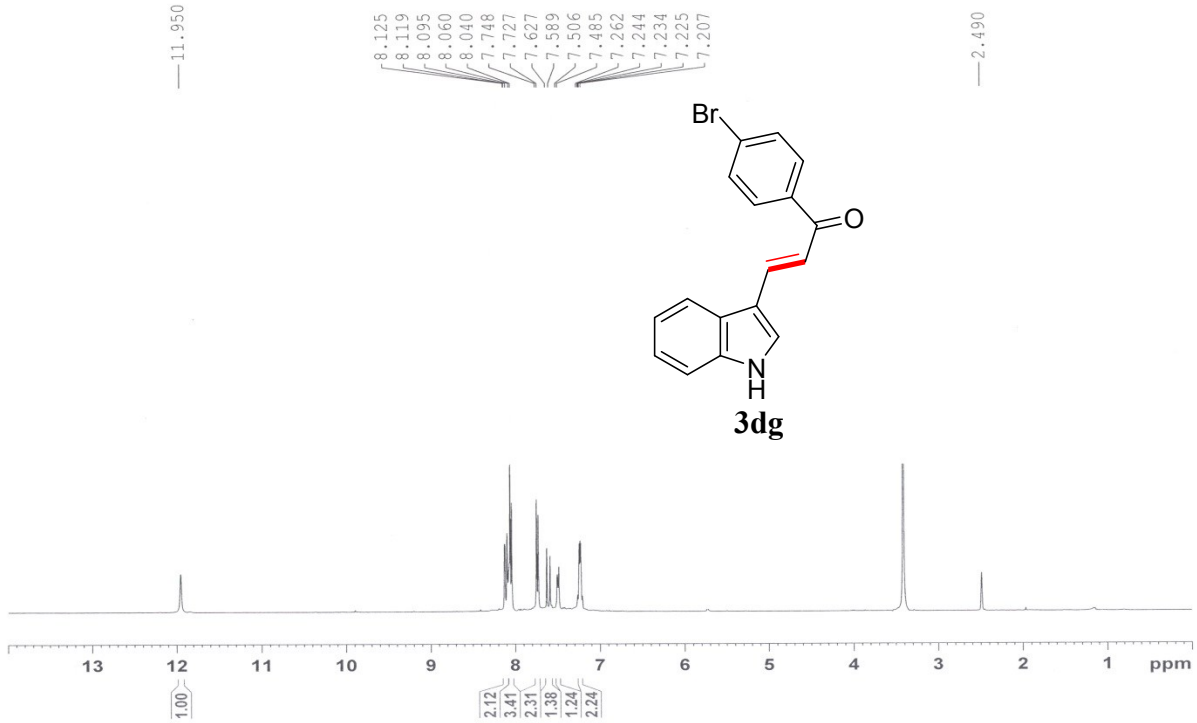

Figure S39. ^{1}H NMR spectrum of **3dg** in DMSO-d_6

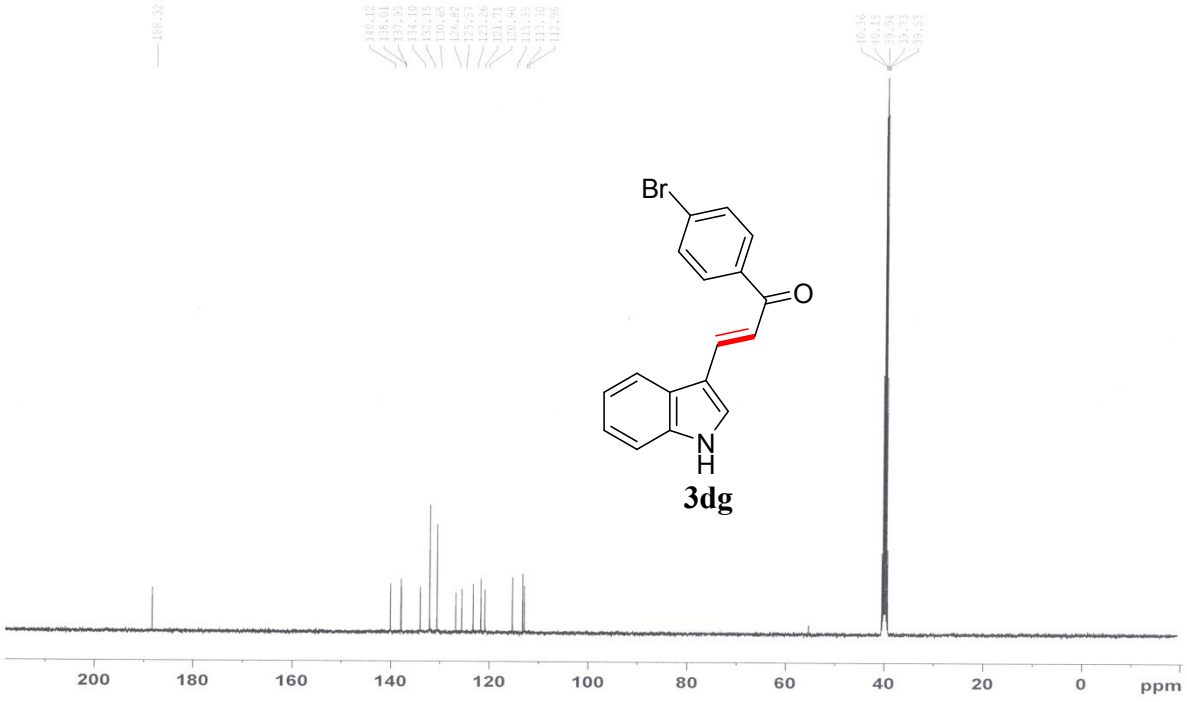

Figure S40. ^{13}C NMR spectrum of **3dg** in DMSO-d_6

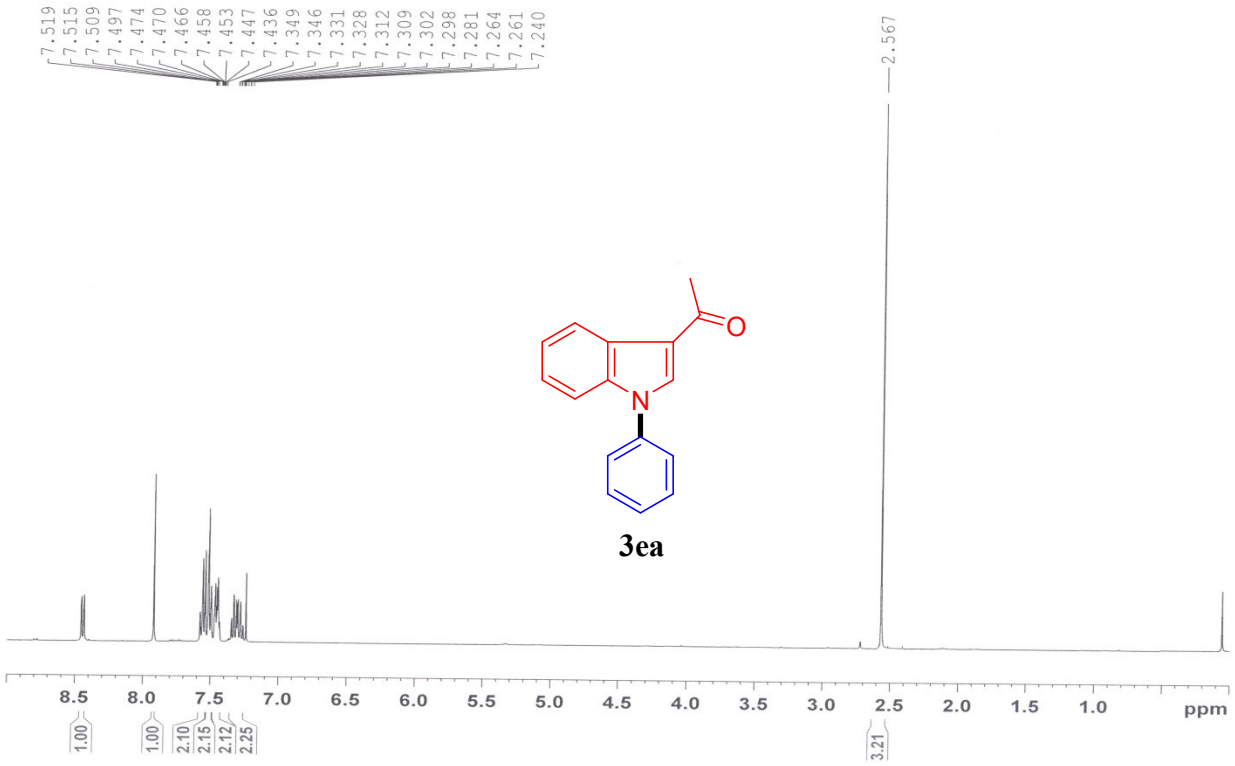

Figure S41. ^{1}H NMR spectrum of **3ea** in $CDCl_3$

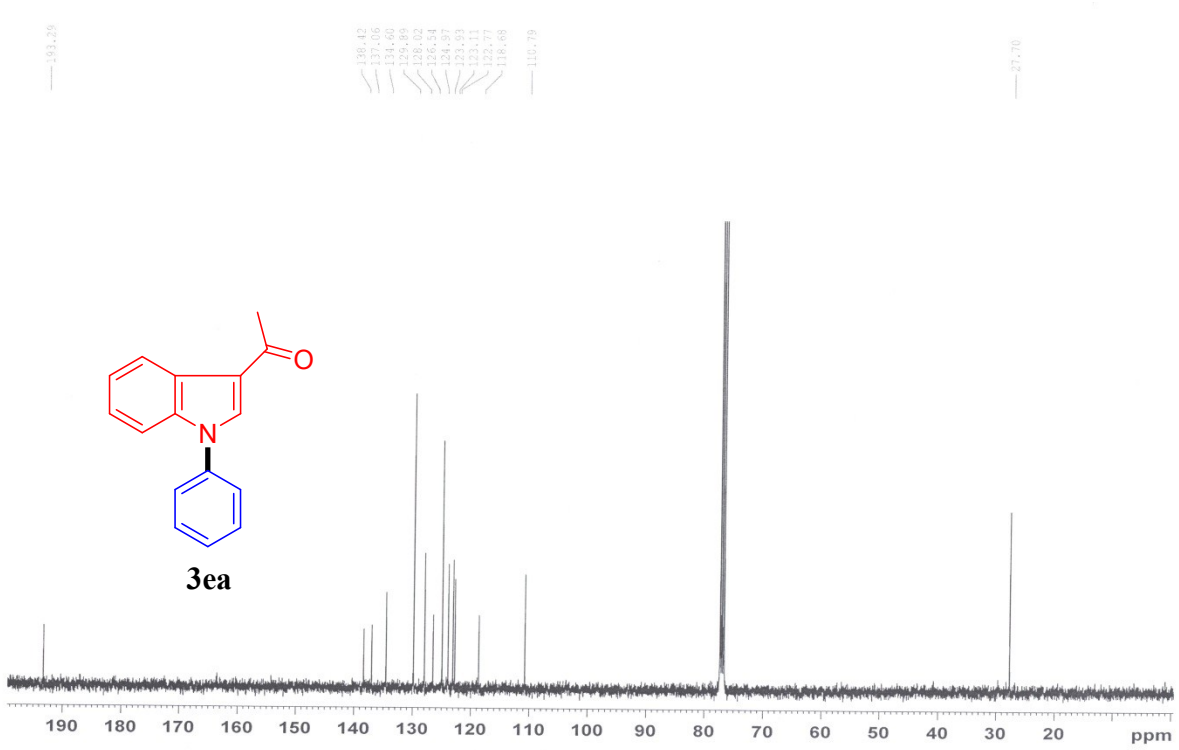

Figure S42. ^{13}C NMR spectrum of **3ea** in $CDCl_3$

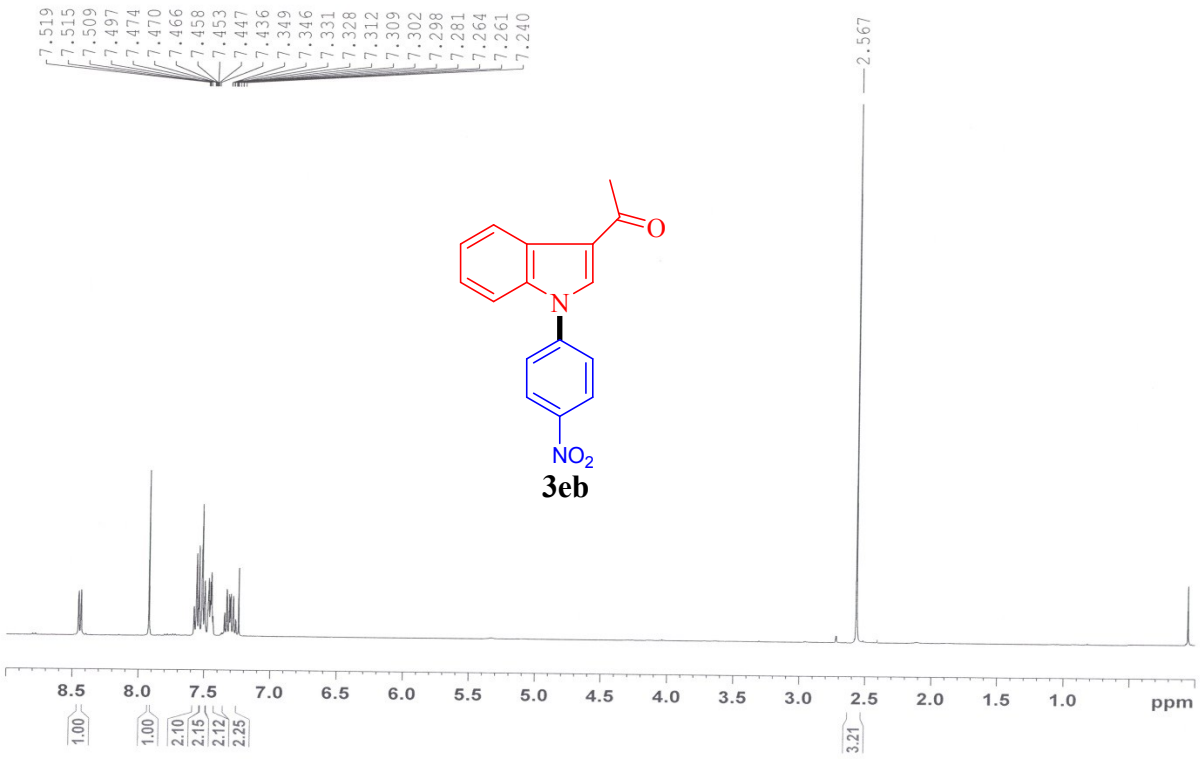

Figure S43. ^{1}H NMR spectrum of **3eb** in $CDCl_3$

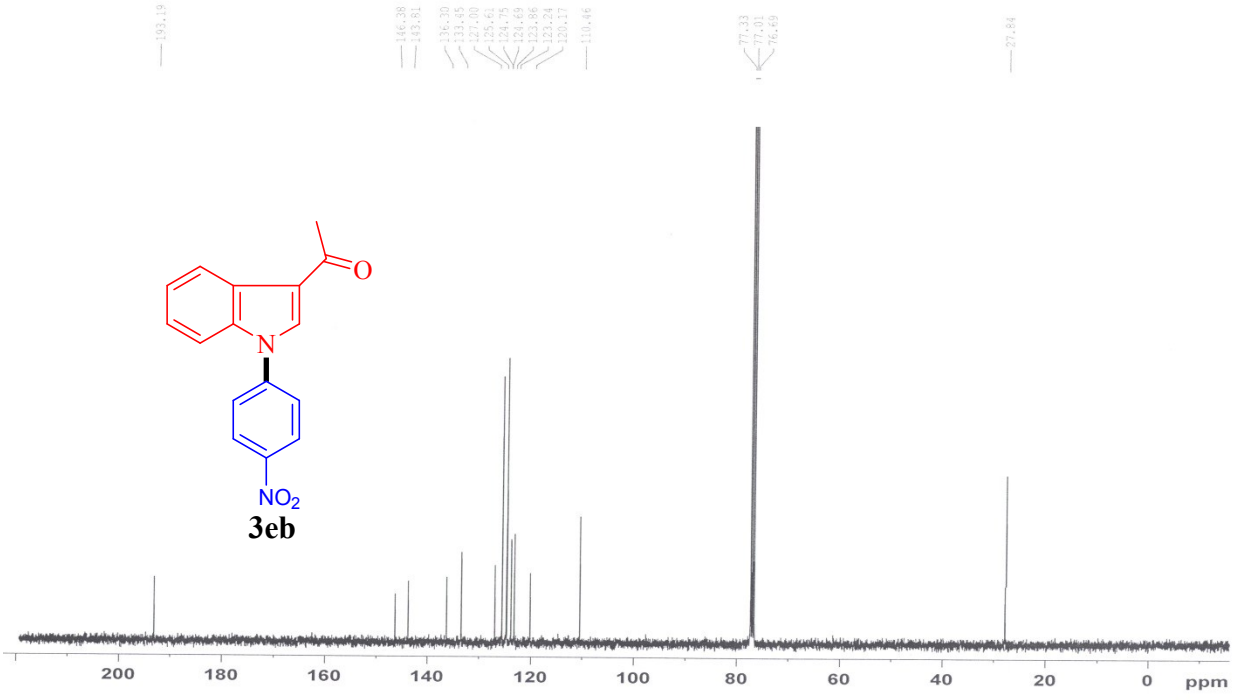

Figure S44. ^{13}C NMR spectrum of **3eb** in $CDCl_3$

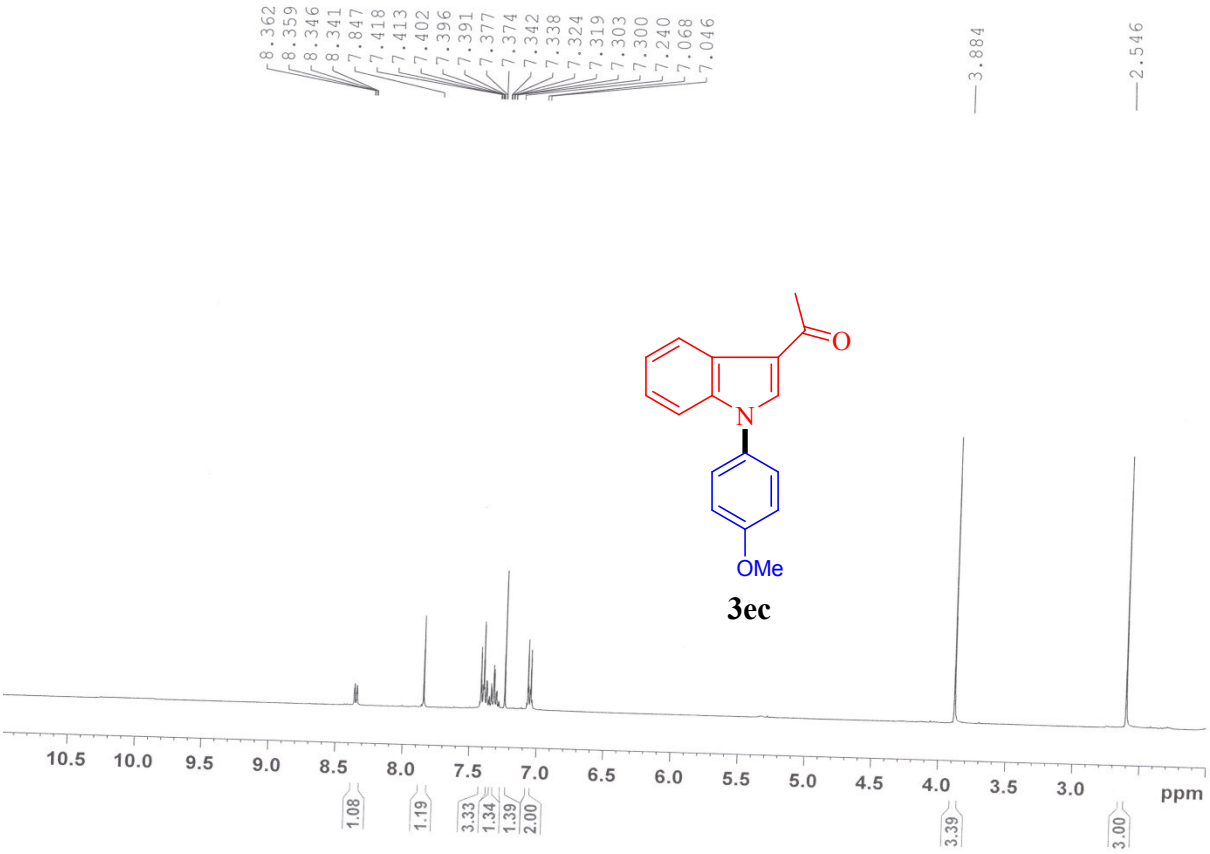

Figure S45. ^{1}H NMR spectrum of **3ec** in $CDCl_3$

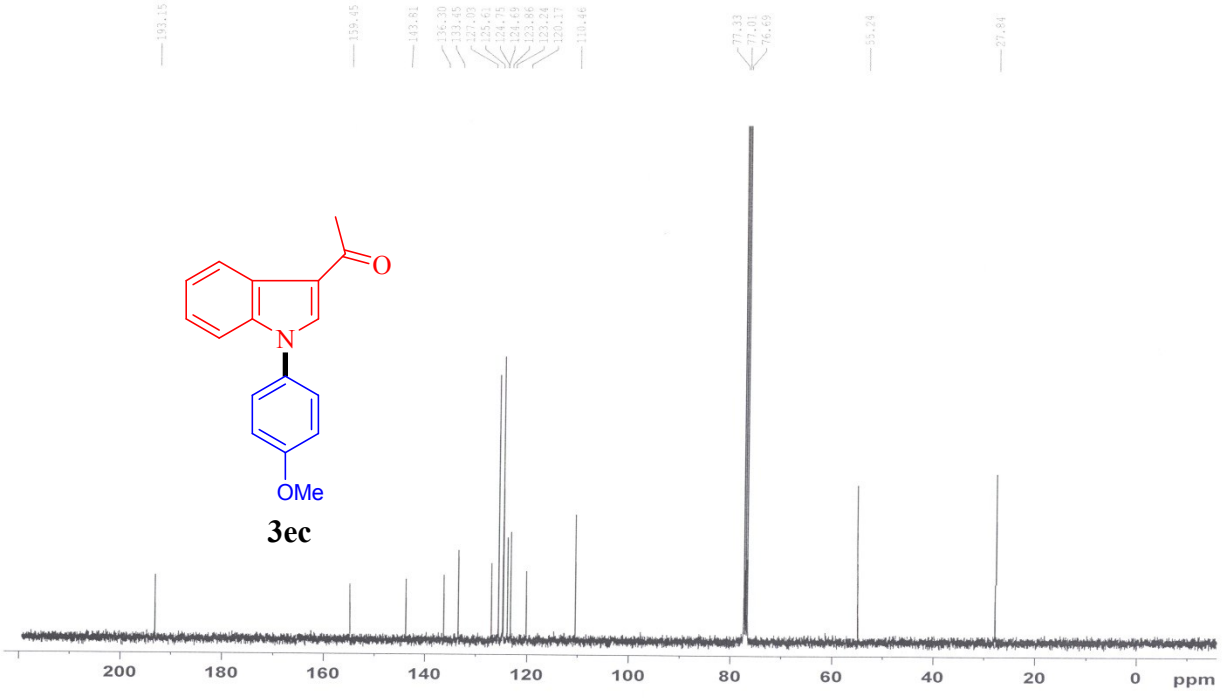

Figure S46. ^{13}C NMR spectrum of **3ec** in $CDCl_3$

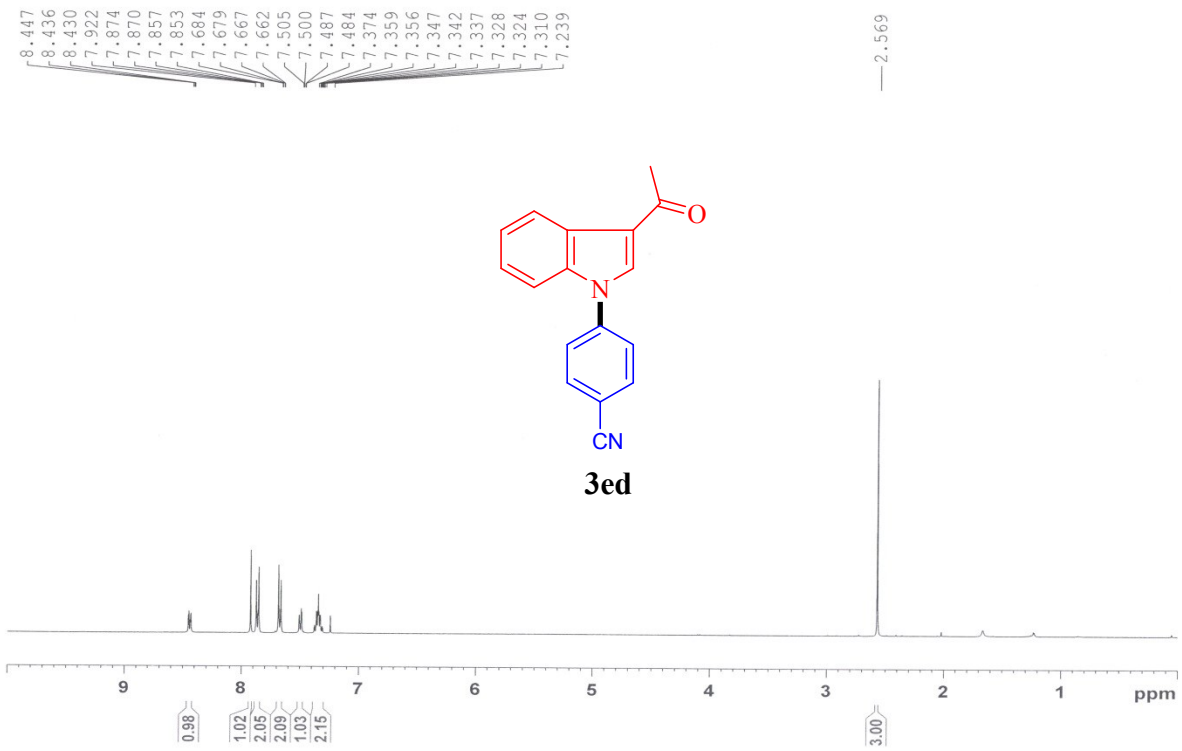

Figure S47. ^{1}H NMR spectrum of **3ed** in $CDCl_3$

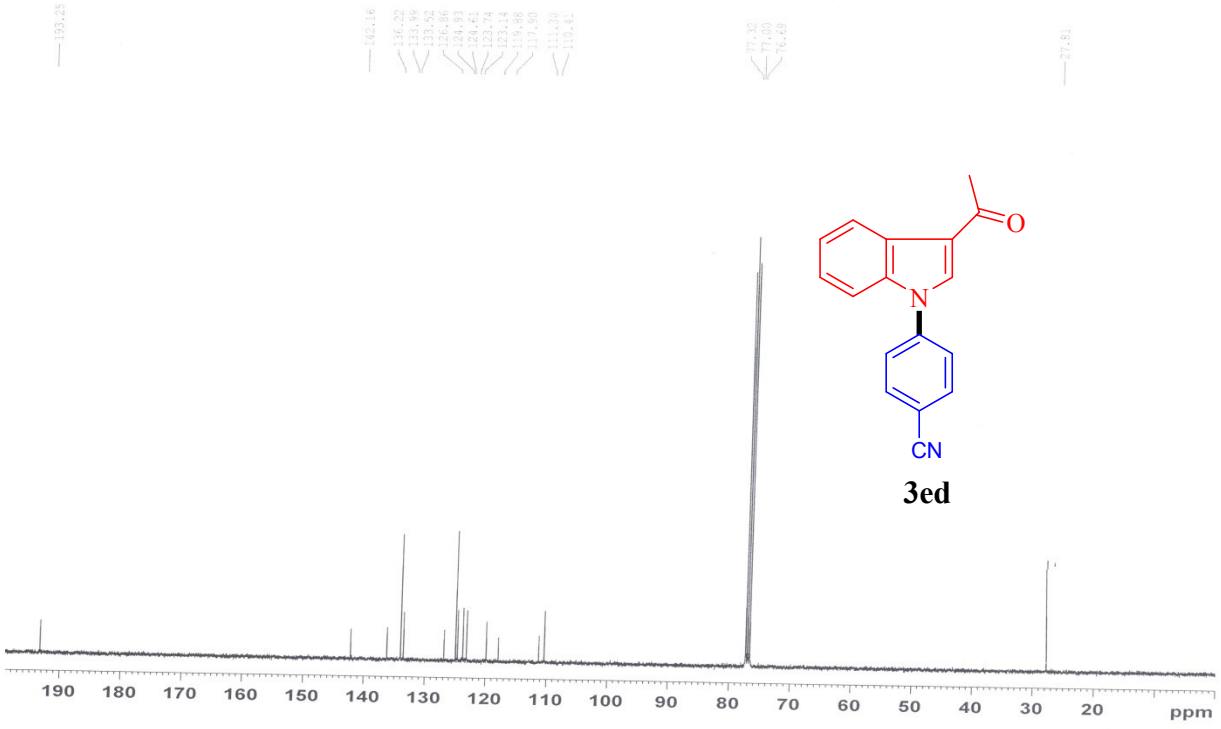

Figure S48. ^{13}C NMR spectrum of **3ed** in $CDCl_3$

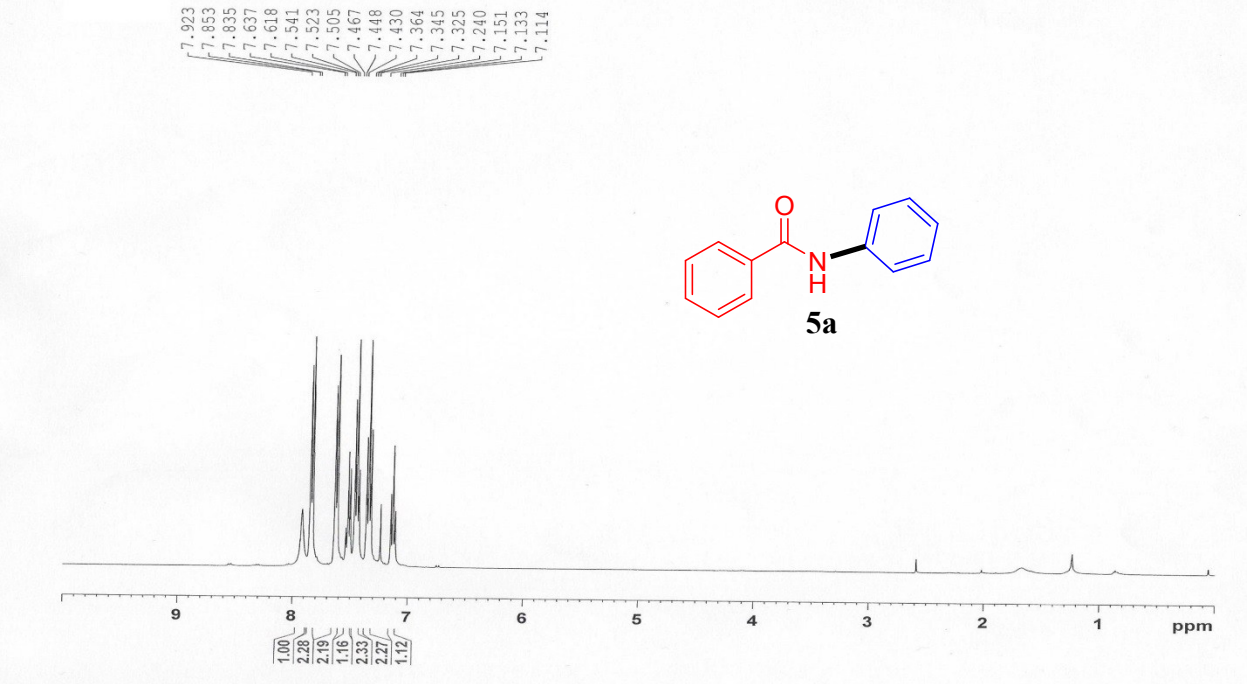

Figure S49. ^{1}H NMR spectrum of **5a** in $CDCl_3$

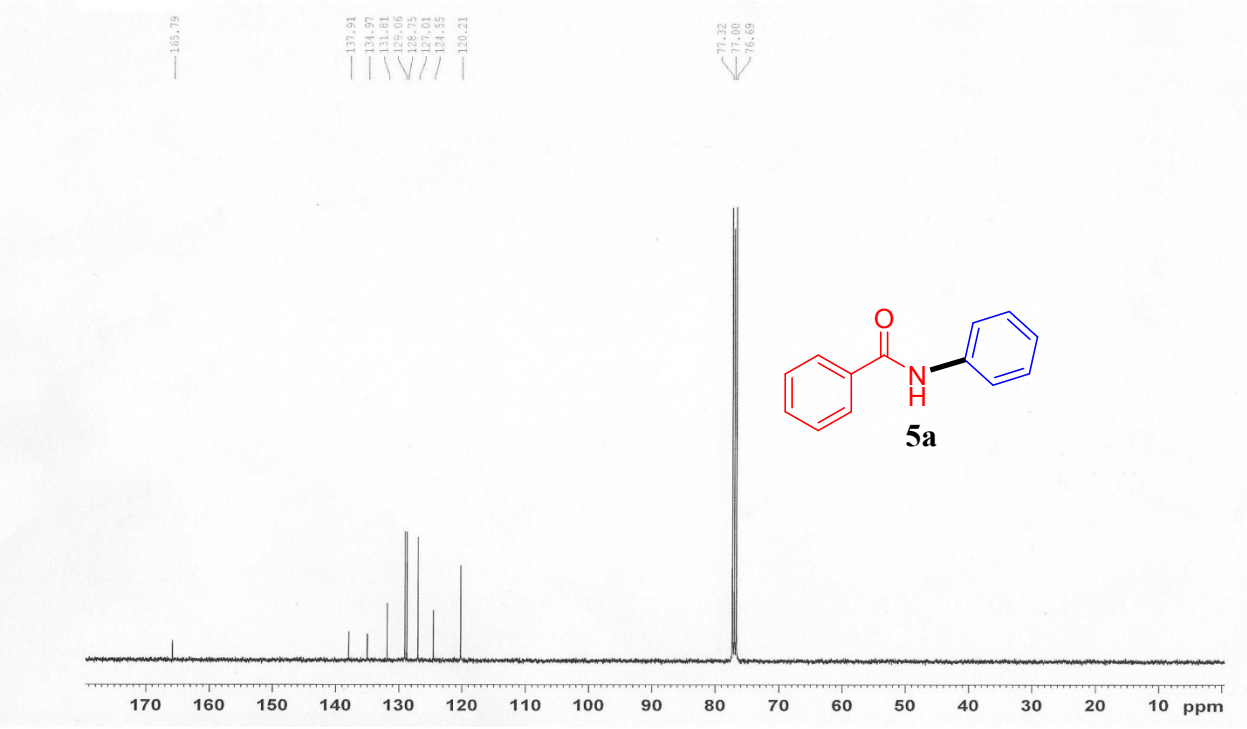

Figure S50. ^{13}C NMR spectrum of **5a** in $CDCl_3$

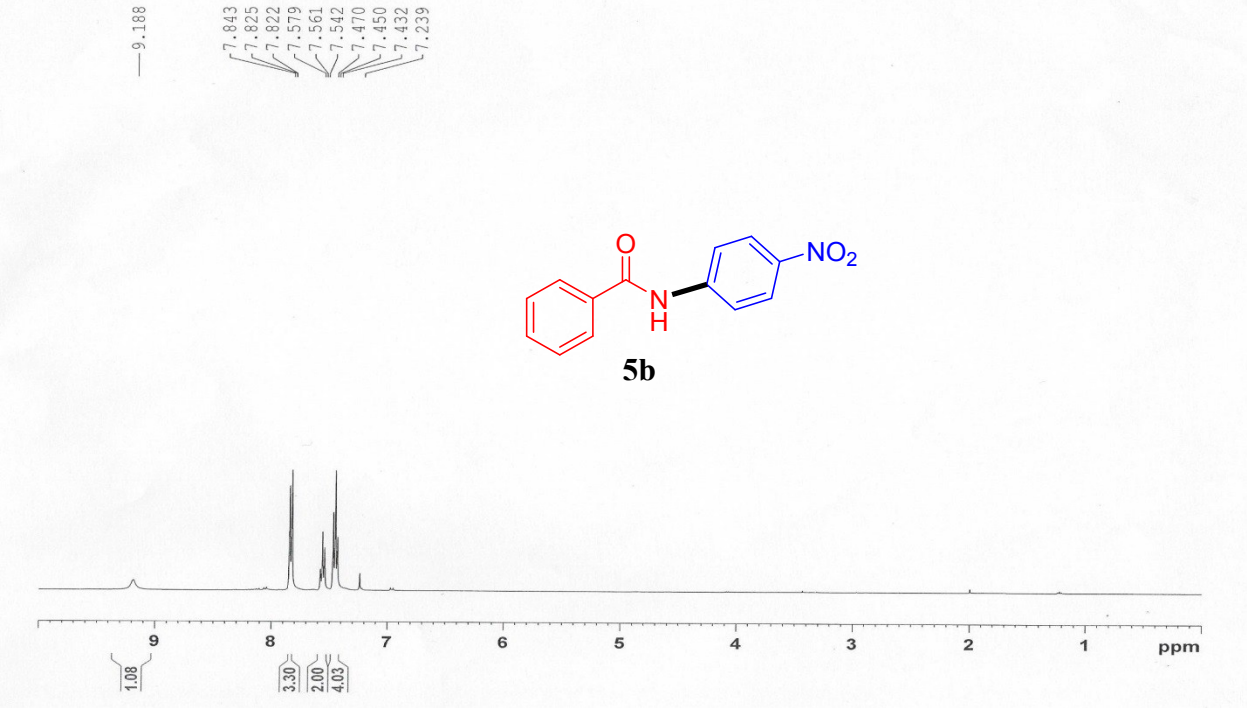

Figure S51. ^{1}H NMR spectrum of **5b** in $CDCl_3$

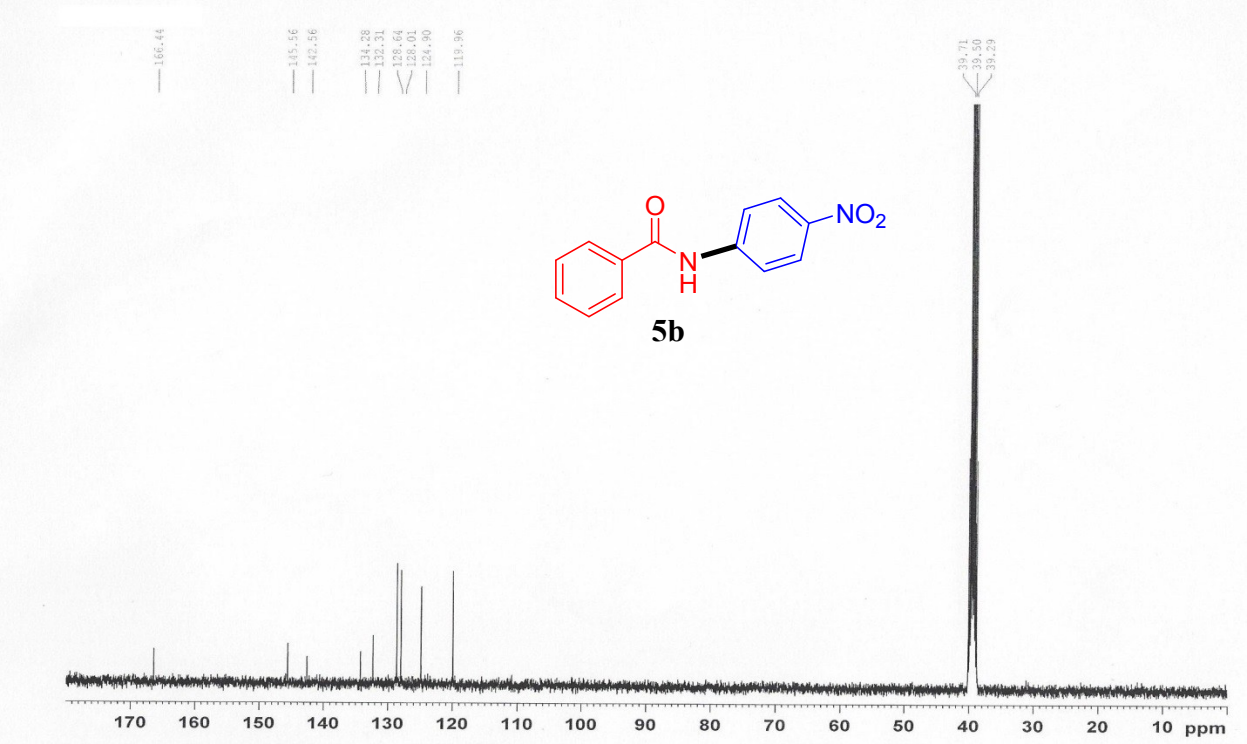

Figure S52. ^{13}C NMR spectrum of **5a** in DMSO-d_6

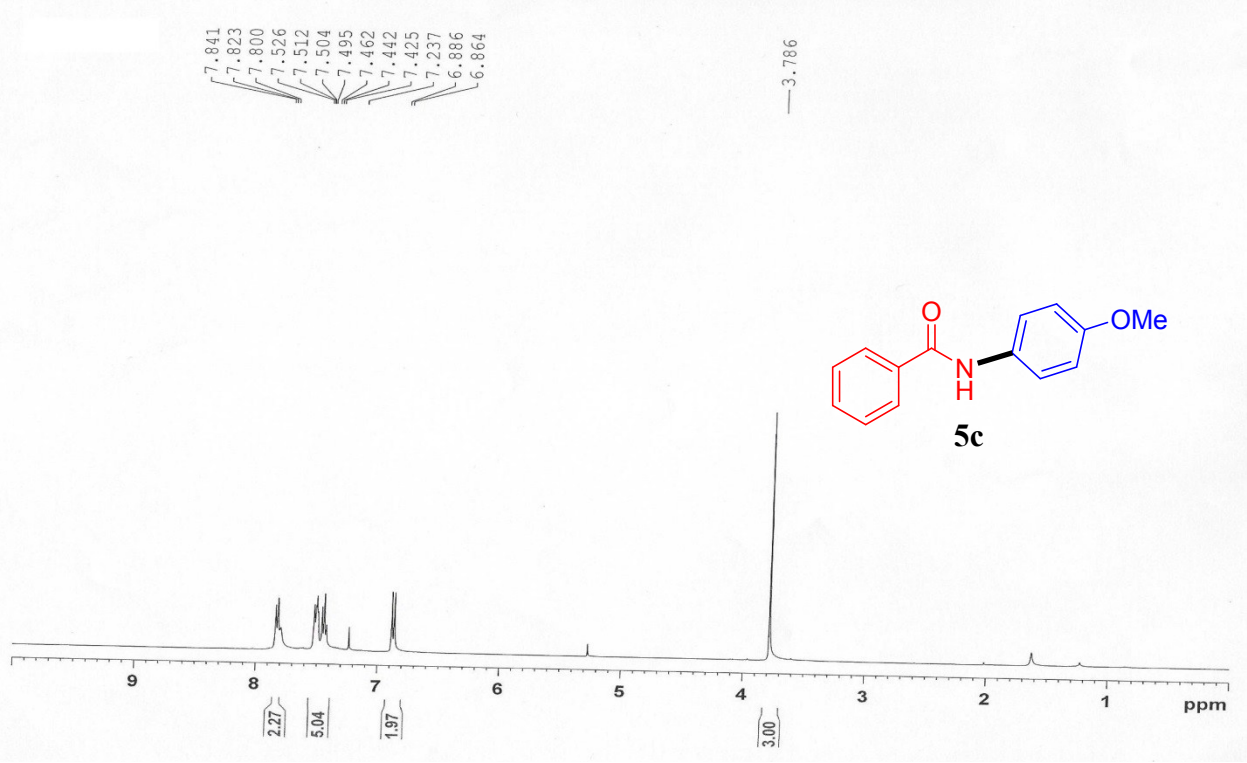

Figure S53. ^{1}H NMR spectrum of **5c** in $CDCl_3$

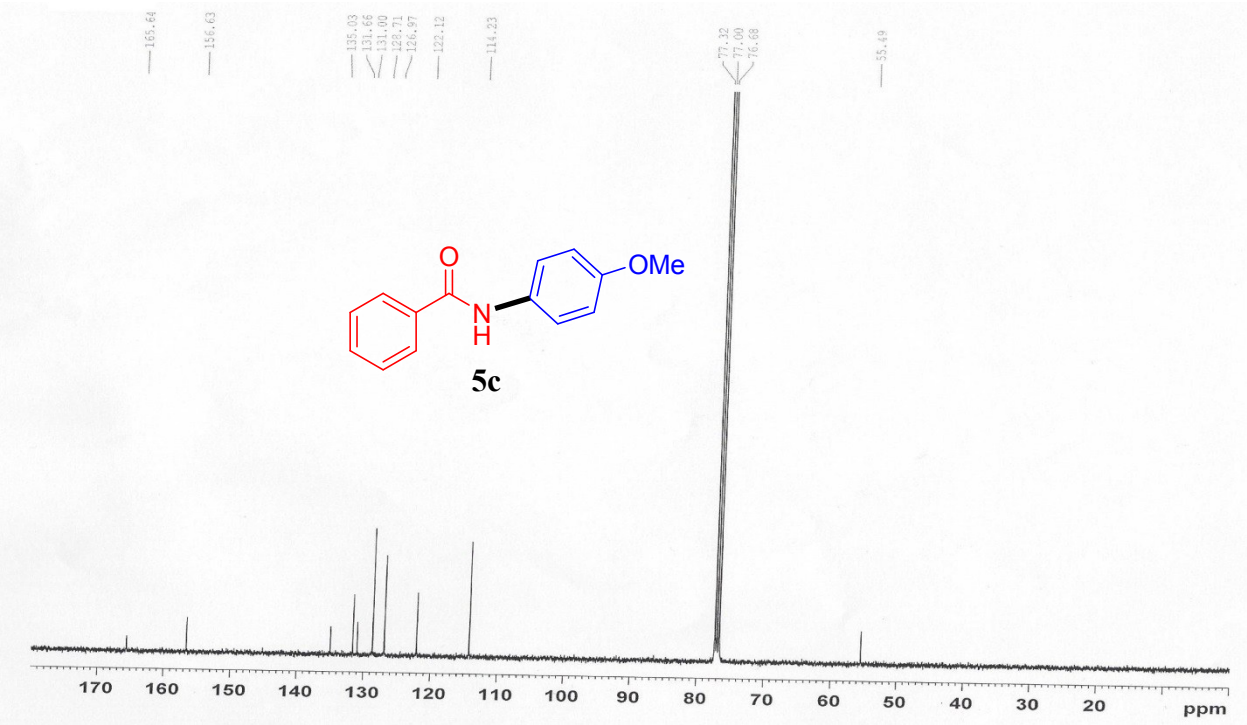

Figure S54. ^{13}C NMR spectrum of **5c** in $CDCl_3$

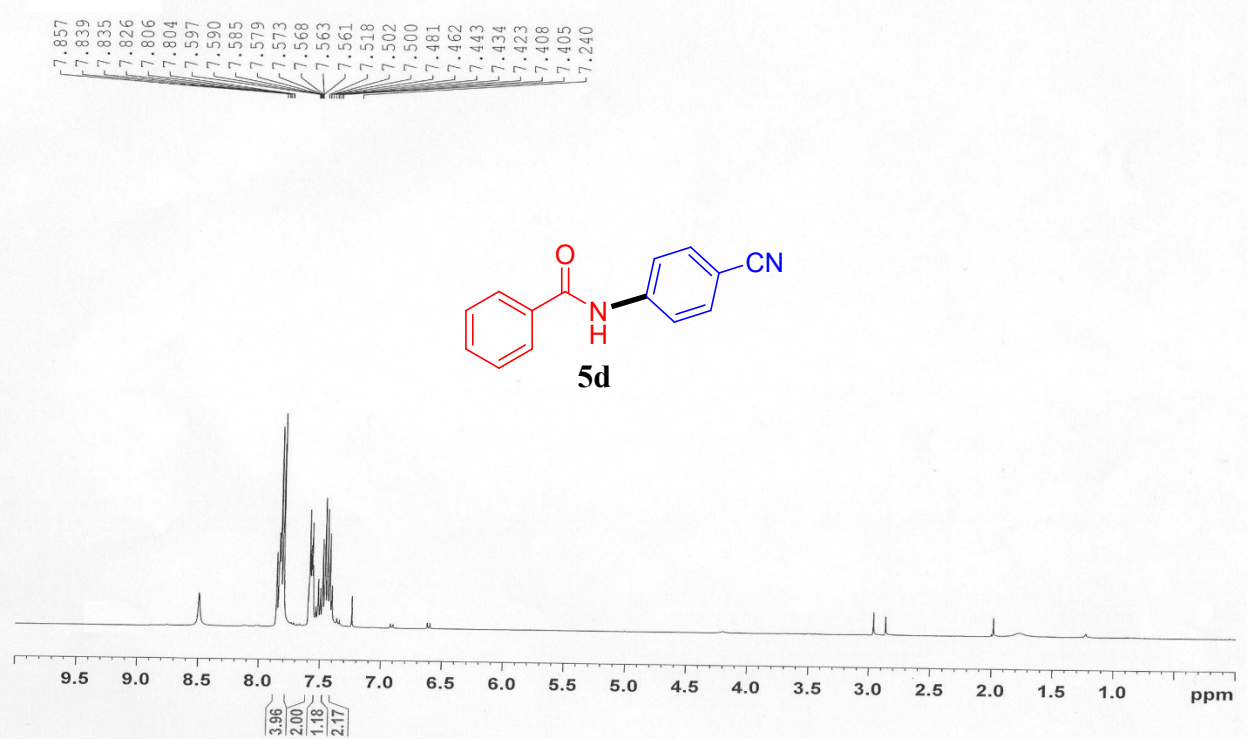

Figure S55. ^{1}H NMR spectrum of **5d** in $CDCl_3$

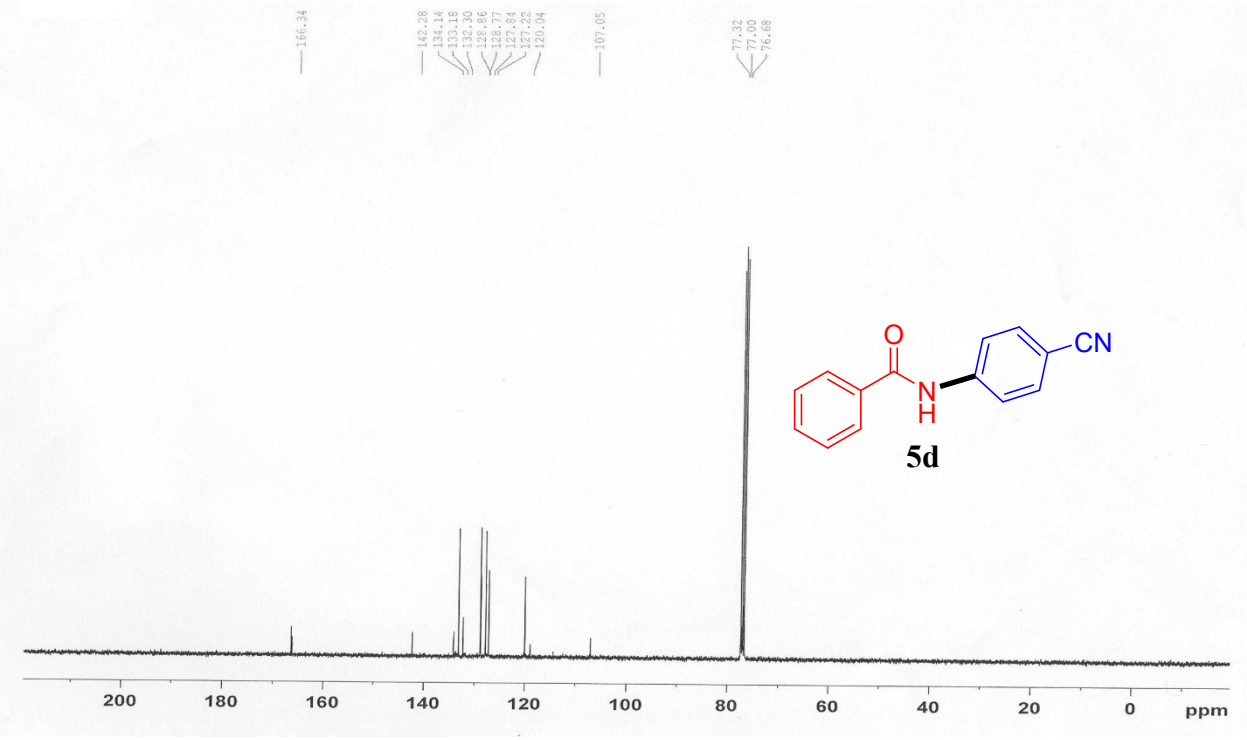

Figure S56. ^{13}C NMR spectrum of **5d** in $CDCl_3$

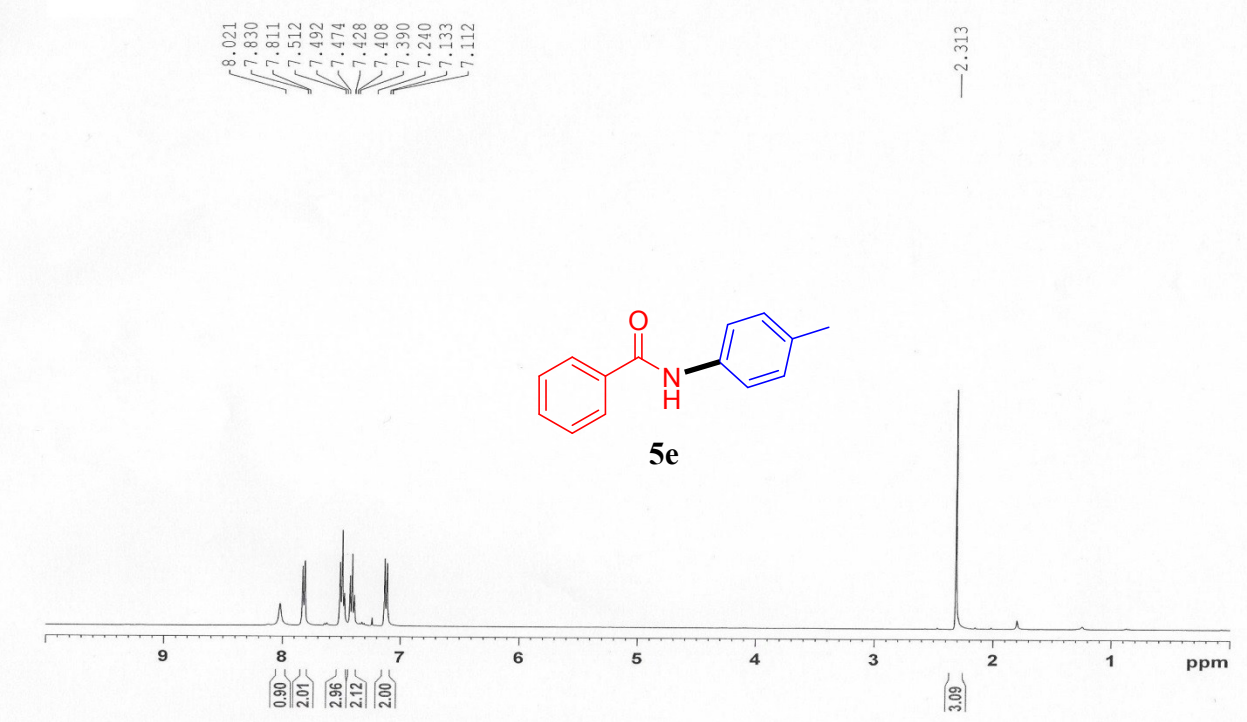

Figure S57. ^{1}H NMR spectrum of **5e** in $CDCl_3$

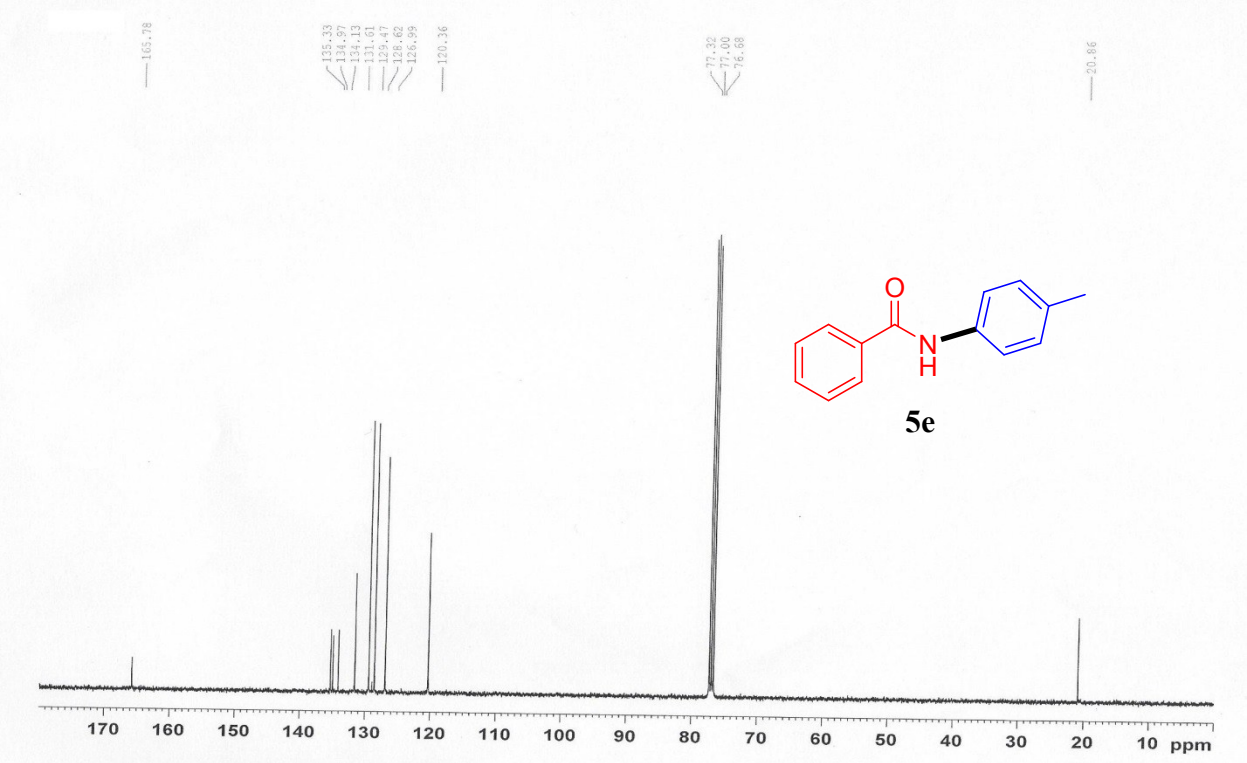

Figure S58. ^{13}C NMR spectrum of **5e** in $CDCl_3$

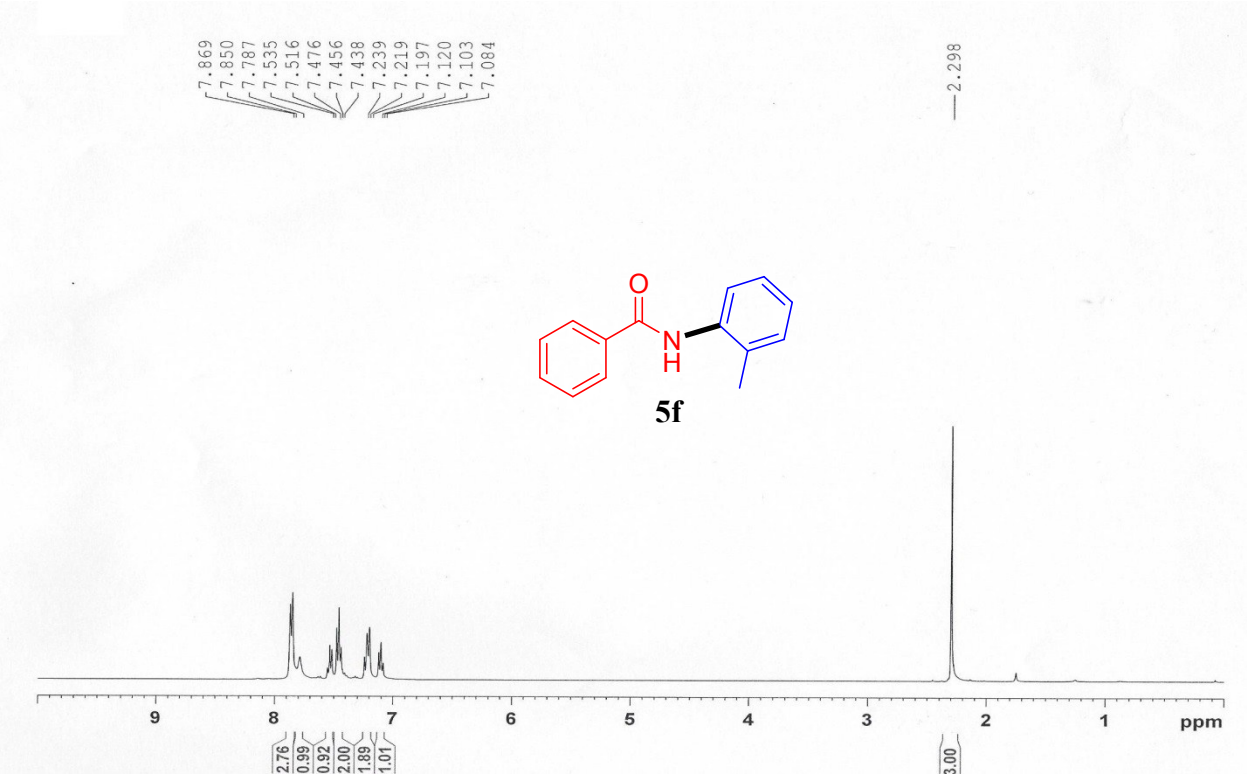

Figure S59. ^{1}H NMR spectrum of **5f** in $CDCl_3$

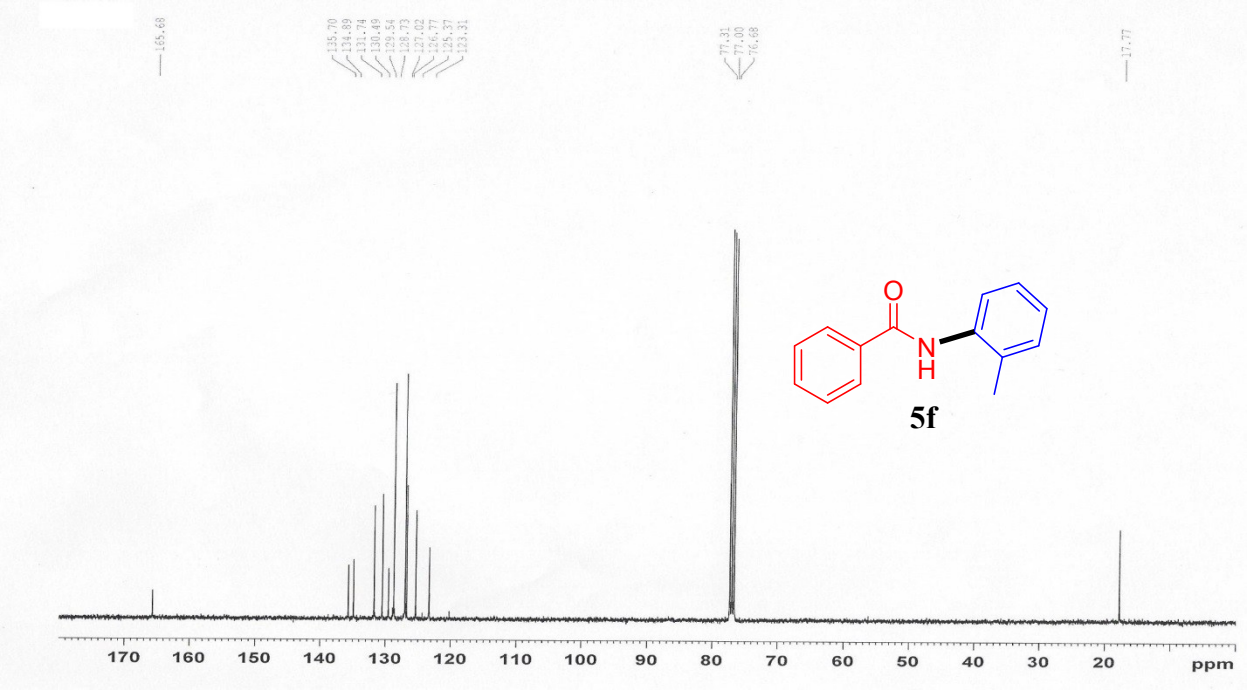

Figure S60. ^{13}C NMR spectrum of **5f** in $CDCl_3$