Electronic Supplementary Material (ESI) for ChemComm.

Weakly Coordinating *tert*-Amide Assisted Rh(III)-Catalyzed C4-Cyanation of Indoles: Application in Photophysical Studies

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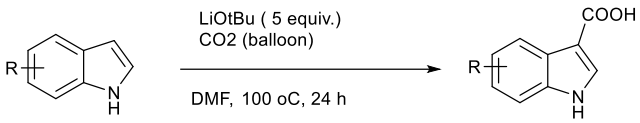
Experimental Section

General information: All commercially available compounds were used without further purification. Solvents for elution in column were distilled. Analytical thin layer chromatography (TLC) was performed on pre-coated silica gel 60 F254. Visualization on TLC was achieved using UV light (254 nm). Column chromatography was undertaken on silica gel (230-400 mesh). ^{1}H and ^{13}C NMR spectra were recorded on BRUKER ULTRA SHIELD and BRUKER ASCEND (400 MHz and 500 MHz) instruments. Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br= broad, s= singlet, d= doublet, t= triplet, q= quartet, dd= doublet of doublet, td= triplet of doublet, ddd= doublet of doublet of doublet, m= multiplet. Coupling constants, *J*, were reported in hertz unit (Hz). ^{13}C NMR spectra were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the centre of a triplet at 77.16 ppm of $CDCl_3$. Infrared (IR) spectra were recorded using Spectrum BX FTIR instrument from Perkin Elmer. Frequencies are given in reciprocal centimeters (cm^{-1}) and only selected absorbance peaks are reported. High-resolution mass spectra were obtained from Agilent AdvanceBio 6545XT LC/Q-TOF (1260 Infinity II). LC-MS were obtained from Agilent Technologies A6120BW (single quadruple mass analyzer). Materials were obtained from commercial suppliers or prepared according to standard procedures unless otherwise noted.

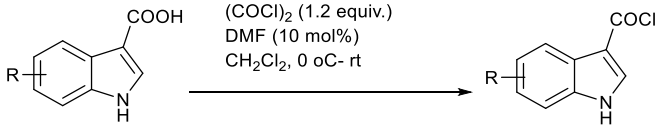
1. General procedure for the synthesis of starting materials:

1.1 General procedure for the synthesis of indole-3-carboxylicacid[1]

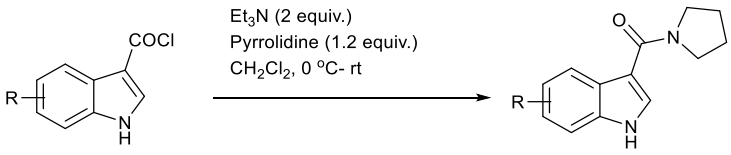


LiO^tBu (10 mmol, 5 equiv) and indole (2 mmol, 1 equiv) were taken in a dried two-necked round bottom flask. The reaction vessel was evacuated under high vacuum and the atmosphere was replaced with a balloon of CO_2. Then DMF (10 mL) was added and the mixture was stirred for 24 h at 100 °C in oil bath. The resulting mixture was cooled and carefully quenched with a solution of HCl (2 N) and extracted with EtOAc. The combined organic layers were washed with water (2 times), brine and dried over anhydrous Na_2SO_4. The dried organic layer was concentrated under reduce pressure and the residue was purified by column chromatography using 40 to 60 % acetone in hexane.

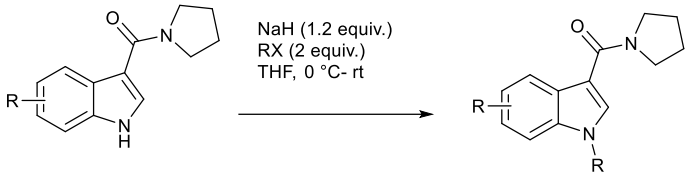
1.2 General procedure for the synthesis of indole-3-carboxamide[2]



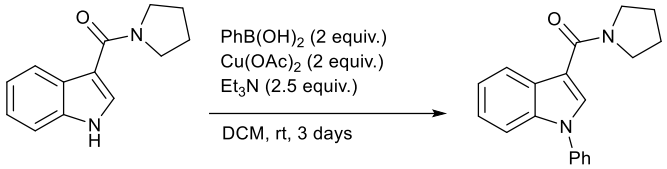
DMF (0.5 mmol) was added to a suspension solution of substituted indole-3-carboxylic acid (5 mmol) in CH_2Cl_2 at 0 °C. Next, oxalyl chloride (6 mmol) was added dropwise. The reaction mixture was allowed to warm to room temperature gradually and stirred for another 3 h. Afterward, the reaction mixture was evaporated and used directly to the next step without further purification.



The crude acid chloride (5 mmol) was dissolved in dry CH_2Cl_2. Then it was transferred with a cannula to a solution of triethylamine (10 mmol) and pyrrolidine (6 mmol) in dry CH_2Cl_2 at 0 $^{\circ}$C under a nitrogen atmosphere. The reaction mixture was allowed to warm to room temperature and stirred for overnight. Next, it was quenched with 50 ml 1(N) HCl, and the organic layer was extracted with CH_2Cl_2 two times, and dried over anhydrous Na_2SO_4. Next, the solvent was evaporated and used directly to the following step without further purification.

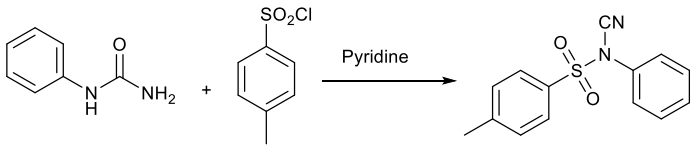


NaH (1.2 equiv.) was added to the above carboxamide (1 equiv.) in THF at 0 °C. The mixture was stirred for 30 min, followed by alkyl halide (2 equiv.) added at 0 °C. The mixture was further stirred at room temperature for 12 h, and saturated aq. NH_4Cl solution (50 mL) was added. The aqueous layer was extracted with CH_2Cl_2 (100 mL × 2). The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated and purified with column chromatography using 60 to 80 % ethyl acetate in hexane.



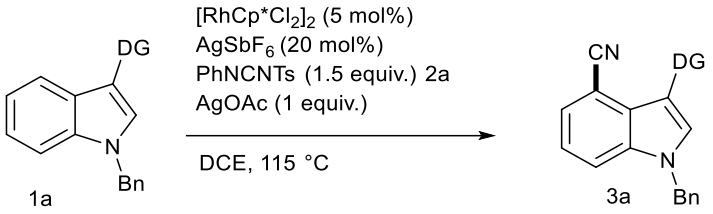
In an oven-dried sealed tube, indole-3-carboxamide (428 mg, 2 mmol) dissolved in 20 ml CH_2Cl_2, phenylboronic acid (488 mg, 4 mmol), anhydrous copper(II)acetate (725 mg, 4 mmol), and triethylamine (506 mg, 5 mmol) were added. The mixture was stirred at room temperature for 3 days, concentrated in vacuo, diluted with chloroform and water. The organic layer was separated, washed with brine, dried with anhydrous Na_2SO_4, concentrated, and purified by column chromatography using 60 to 80 % ethyl acetate in hexane to obtain pure product in yield 430 mg, 74%.

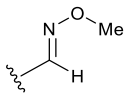
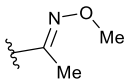
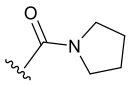
1.3 Synthesis of *N*-cyano-4-methyl-*N*-phenylbenzenesulfonamide:



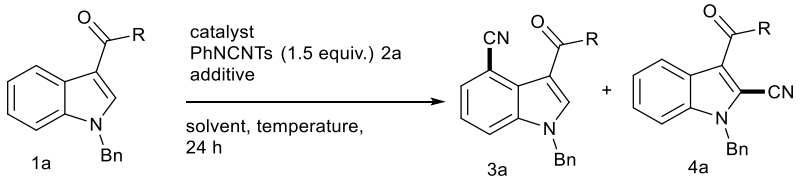
p-Toluenesulfonyl chloride (10.58 g) was added to a mixture of phenylurea (2.18 g) and pyridine (15 mL) over 3 minutes at room temperature. The reaction mixture was stirred at room temperature for 20 minutes. The reaction mixture was poured into ice-cooled water (100 ml) with vigorous stirring. The precipitate was filtered and washed with water. The product was purified through recrystallization in ethanol.

1.4 Tabel S1: Optimization for directing group



Sl No.	Directing Group (DG)	Yield of 3a (%)
1	-CHO	N.D.
2	-COMe	N.D.
3		N.D.
4		N.D.
5	-$COCF_3$	N.D.
6		11

1.5 Table S2. Detailed optimization table for Synthesis of synthesis of 1-benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile.

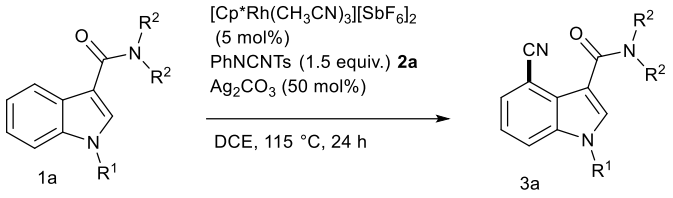


Sl. No	R	Catalyst (mol%)	Additive (mol%)	Solvent	Temp (˚C)	Yield (3a:4a)
1[a]	pyrrolidine	[Ru(*p*-cym)Cl_2]$_2$ (10)	AgOAc (100)	DCE	90	Trace:42
2[a]	pyrrolidine	[IrCp*Cl_2]$_2$ (5)	AgOAc (100)	DCE	90	-
3[a]	pyrrolidine	[RhCp*Cl_2]$_2$ (5)	AgOAc (100)	DCE	90	<5:trace
4[a]	pyrrolidine	[RhCp*Cl_2]$_2$ (5)	AgOAc (100)	DCE	110	11: trace
5	pyrrolidine	[Cp*Rh(ACN)$_3$][SbF_6]$_2$ (7)	AgOAc (100)	DCE	110	37:10
6	pyrrolidine	[Cp*Rh(ACN)$_3$][SbF_6]$_2$ (7)	NaOAc (100)	DCE	110	10: <5
7	pyrrolidine	[Cp*Rh(ACN)$_3$][SbF_6]$_2$ (7)	Ag_2CO_3 (20)	DCE	110	63: <5
8	pyrrolidine	[Cp*Rh(ACN)$_3$][SbF_6]$_2$ (7)	Ag_2CO_3 (50)	DCE	115	89: <5

9	**pyrrolidine**	**$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)**	**Ag_2CO_3 (50)**	**DCE**	**115**	**83: <5**
10	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	dioxane	115	51: <5
11	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	MeCN	115	17: <5
12	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	^{t}AmOH	115	23: <5
13	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	EtOH	115	trace
14	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	DME	115	21: <5
15	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	DMF	115	trace
16	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	DMSO	115	nr
17	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$(5)	$AgNO_3$ (50)	DCE	115	trace
18	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	K_2CO_3 (50)	DCE	115	trace
20	$CONMe_2$	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	DCE	115	86:<5
21	$CON(^iPr)_2$	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	DCE	115	58:14
22	piperidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	DCE	115	66:11
23	pyrrolidine	$[Cp^*Rh(ACN)_3][SbF_6]_2$ (5)	Ag_2CO_3 (50)	DCE	130	78: <5

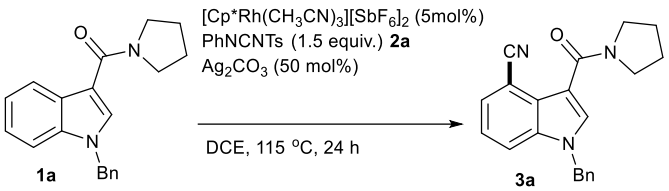
Reaction conditions: **1a** (0.1 mmol), **2** (0.15 mmol), Rh(III) catalyst (5 mol%), additive (50 mol%), solvent (0.1 M), 24 h, 110-115 °C. [a]$AgSbF_6$ was used as an additive in 20 mol%.

1.6.1 General procedure for Rh(III) catalyzed C-4 cyanation of indole-3-carboxamide derivatives:



In a 10 mL screw cap vial equipped with magnetic stirring bar indole-3-carboxamide derivatives (0.20 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (0.01 mmol, 5 mol%), PhNCNTs (0.3 mmol, 1.5 equiv.) and silver carbonate (0.1 mmol, 50 mol%) were taken in dry 1,2-dichloroethane (2 ml). The reaction mixture was stirred at 115 °C temperature in an oil bath for 24 h. After the completion, the reaction mixture was purified directly through silica gel column chromatography with 60 to 80 % ethyl acetate/hexane as eluent to give the desired product.

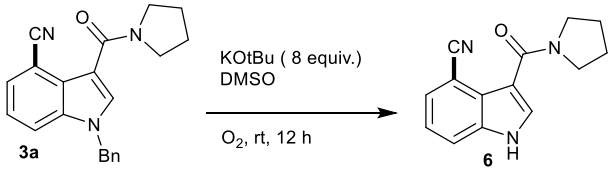
1.6.2 Scale up synthesis:



In a 10 mL screw cap vial equipped with magnetic stirring bar indole-3-carboxamide derivatives (4 mmol, 1.52 g), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (0.02 mmol, 5 mol%) PhNCNTs (6 mmol, 1.632 g, 1.5 equiv.) and silver carbonate (2 mmol, 0.551 g, 50 mol%) were taken in dry 1,2-dichloroethane (10 ml). The reaction mixture was stirred at 115 °C temperature in an oil bath for 24 h. After the completion, the reaction mixture was purified directly through silica gel column chromatography with 60 to 80 % ethyl acetate/hexane as eluent to give the desired product **3a** in 73% yield (1.2 g).

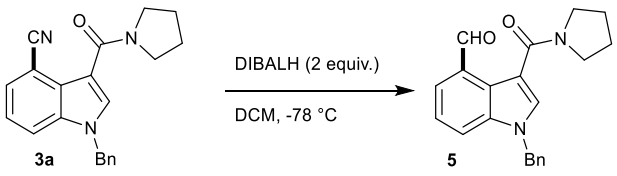
1.7 Product modifications

1.7.1 Deprotection of benzyl group[3]:



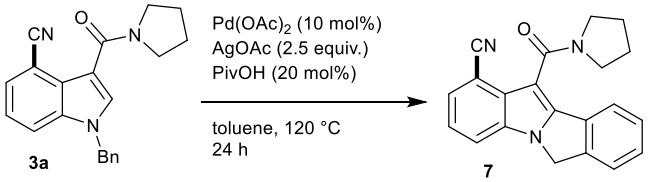
To a stirred solution of compound **3a** (65.8 mg, 0.2 mmol) dissolved in dry DMSO (3 mL), KO^{t}Bu (180 mg, 1.6 mmol) was added. Oxygen was then bubbled into the solution until complete consumption of starting material (as monitored by TLC). After completion, the reaction mixture was quenched by saturated solution of ammonium chloride and extracted with dichloromethane. The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to obtain pure product **6** (44 mg, 92%) as a yellow amorphous solid. The product was further characterized by analytical data.

1.7.2 Synthesis of 1-benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbaldehyde:



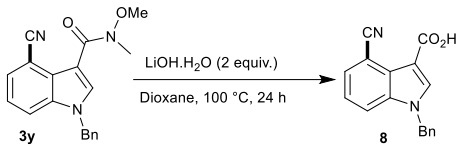
In a 50 mL three-necked flask fitted with a septum inlet, a low-temperature thermometer, and a septum outlet, **3a** (65.8 mg, 0.2 mmol) was dissolved in dry dichloromethane. The solution was cooled to -78 °C, where upon diisobutylaluminium hydride solution (0.4 mmol) was added dropwise by a syringe. The reaction mixture was stirred at this temperature for 30 minutes and allowed to warm to room temperature slowly. After that, the reaction was quenched by the addition of aqueous 1 N HCl (5 mL) at room temperature and extracted with dichloromethane (2 x 10 mL). Combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to obtain pure product **5** (57.8 mg, 87%) as a yellow gel.

1.7.3 Synthesis of 11-(pyrrolidine-1-carbonyl)-6*H*-isoindolo[2,1-a]indole-1-carbonitrile:



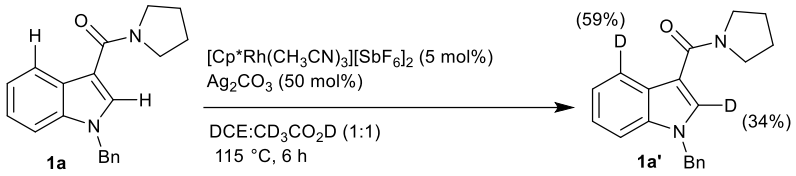
To an oven-dried 10 mL screw cap vial equipped with a magnetic stirring bar **3a** (0.2 mmol, 1 equiv) was taken in 1 ml toluene. Then palladium acetate (0.02 mmol, 10 mol%), silver acetate (0.5 mmol, 2.5 equiv.), and pivalic acid (0.04 mmol, 20 mol%) were added subsequently. Next, it was stirred for 24 hours at 120 °C in an oil bath. After cooling to room temperature, the reaction mixture was directly packed to the column and eluted using 50% to 70% ethyl acetate in hexane to obtain pure product **7** (47 mg, 72%).

1.7.4 Hydrolysis of amide group:



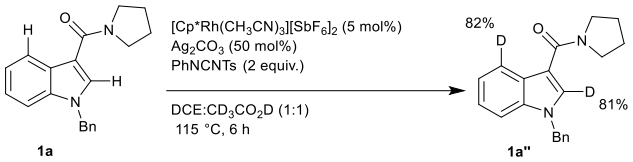
Compound **3y** (63.8 mg, 0.2 mmol) was taken in an oven-dried 10 mL screw cap vial equipped with a magnetic stirring bar. Then 0.5 ml dioxane and 0.5 ml aqueous solution lithium hydroxide (16.8 mg, 0.4 mmol) was added and the reaction mixture was stirred at 100 °C for 24 hours. After cooling to room temperature, the reaction mixture was diluted with 2 N HCl to adjust pH 2 and extracted with ethyl acetate. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography to obtain pure product **8** (49.2 mg, 89%).

1.8.1 Study of deuterium incorporation in the absence of PhNCNTS (2a):



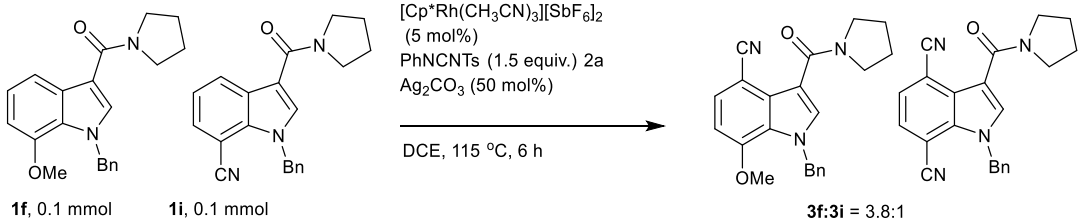
To an oven-dried 10 mL screw cap vial equipped with a magnetic stirring bar **1a** (0.1 mmol, 1 equiv) was taken in 1 ml DCE and 1 ml CD_3COOD. Then $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (0.005 mmol, 5 mol%) and silver carbonate (0.05 mmol, 13.5 mg, 50 mol%) were added subsequently. Next, it was stirred for 6 hours at 115 ˚C in an oil bath. After cooling to room temperature, the solvent was removed under reduced pressure, and the **1a** was isolated by column chromatography and deuterium incorporation was studied by ^1H NMR. The analysis showed that there is 59% deuterium incorporation at C4-position and 34% deuterium incorporation at C2-position.

1.8.2 Study of deuterium incorporation in the presence of PhNCNTS (2a):

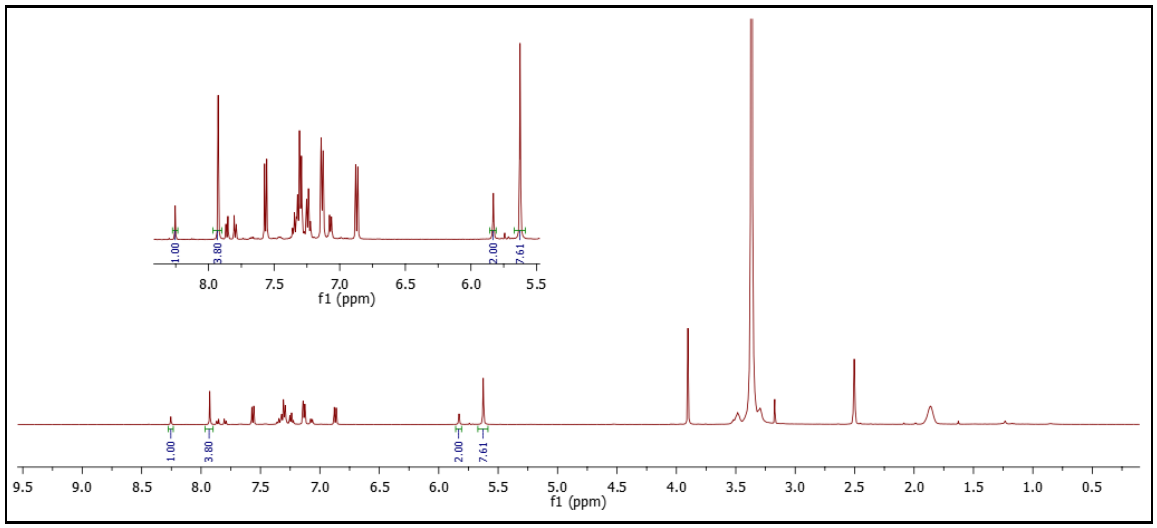


To an oven-dried 10 mL screw cap vial equipped with a magnetic stirring bar **1a** (0.1 mmol, 1 equiv) was taken in 1 ml DCE and 1 ml CD_3COOD. Then $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (0.005 mmol, 5 mol%) PhNCNTs (0.15 mmol, 41 mg, 1.5 equiv.) and silver carbonate (0.05 mmol, 13.5 mg, 50 mol%) were added subsequently. Next, it was stirred for 6 hours at 115 ˚C in an oil bath. After cooling to room temperature, the solvent was removed under reduced pressure, and the **1a** was isolated by column chromatography and deuterium incorporation was studied by ^1H NMR. The analysis showed that there is 82% deuterium incorporation at C4-position and 81% deuterium incorporation at C2-position.

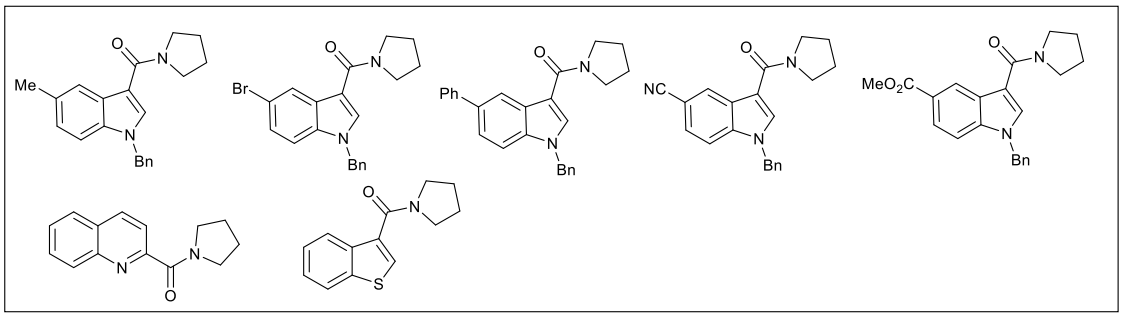
1.9 Kinetic experiments with electronically variable indole derivative



To an oven-dried 10 mL screw cap vial equipped with a magnetic stirring bar **1f** (33.4 mg, 0.1 mmol, 1 equiv) and **1i** (32.9 mg, 0.1 mmol, 1 equiv.) were taken in 2 ml DCE. Then $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (4.1 mg, 0.005 mmol, 5 mol%), PhNCNTs (0.15 mmol, 41 mg, 1.5 equiv.) and silver carbonate (0.05 mmol, 13.5 mg, 50 mol%) were added subsequently. Next it was stirred for 6 hours at 115 °C in oil bath. After cooling to room temperature, the solvent was removed under reduced pressure, and filtered through silica gel column chromatography using an 80% ethylacetate in hexane mixture as the eluent and product ratio was monitored via ^{1}H NMR spectroscopy of crude product mixture (**3f : 3i** = 3.8:1).



1.10 Unsuccessful Substrate scope.



2. Photophysical studies

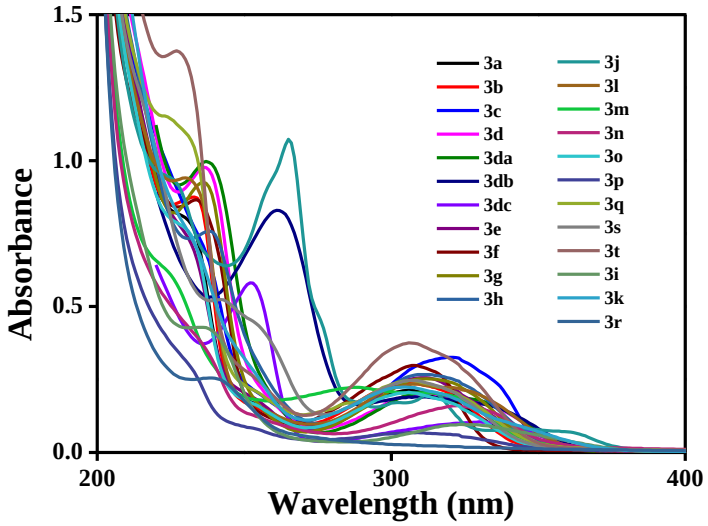


Figure S1: Absorbance spectra of **3a** to **3t** compounds

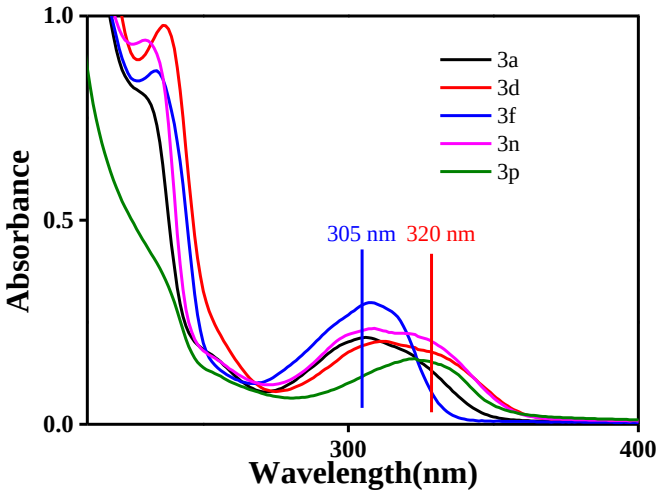


Figure S2: Absorbance spectra of **3a, 3d, 3f, 3n, 3p** compounds

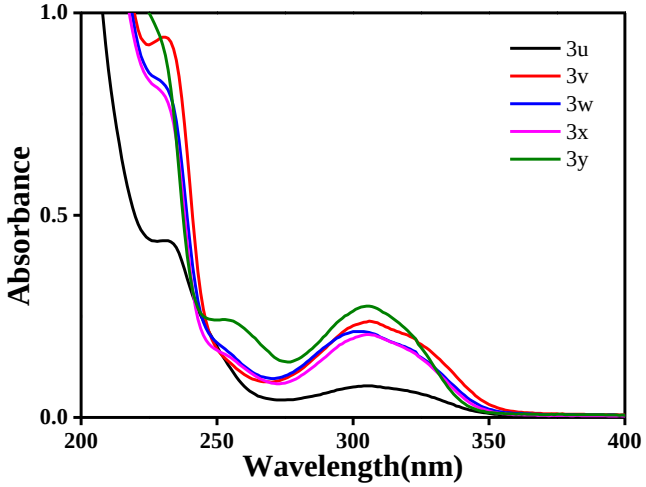


Figure S3: Absorbance spectra of **3u** to **3y** compounds

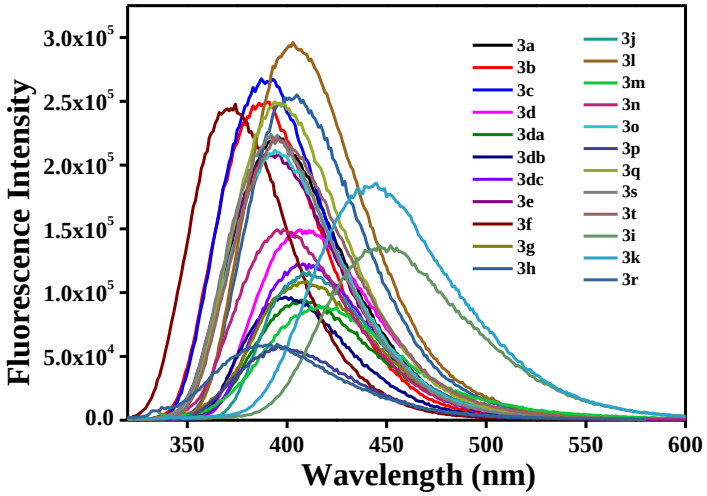


Figure S4: Emission spectra of **3a** to **3t** compounds

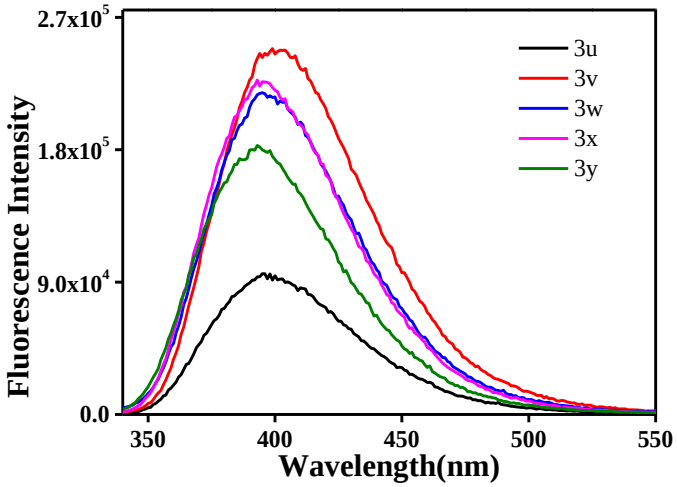


Figure S5: Fluorescence spectra of **3u** to **3y** compounds

Table S3. Photophysical parameters of all compounds

Molecules	**λ_{abs} (nm)**	**ε ($10^4 mol^{-1}Lcm^{-1}$)**	**λ_{emi} (nm)**	**Quantum Yield(ϕ)**
3a	230, 305	3.2, 0.85	395	0.38
3b	319	1.3	390	0.29
3c	230, 310	3.0, 1.0	398	0.31
3d	237, 313	3.9, 0.81	409	0.29
3da	237, 315	3.9,0.81	401	0.19
3db	262, 315	3.3,0.76	401	0.18
3dc	253, 330	2.3,0.42	408	0.45
3e	234, 305	3.4, 0.95	390	0.37
3f	233, 308	3.4, 1.2	372	0.28
3g	236, 314	3.7, 1.0	409	0.17
3h	238, 313	2.1, 1.1	404	0.37
3i	235, 325	1.7, 0.38	449	0.68
3j	226, 263, 314	3.1, 4.2, 0.93	410	0.23
3k	230, 305	3.0, 0.86	443	0.39
3l	230, 305	1.7, 0.82	394	0.38
3m	230, 314	3.1, 0.26	397	0.32
3n	230, 314	4.6, 0.63	401	0.48
3o	225, 305	2.1, 0.84	417	0.19
3p	230, 320	5.5, 0.26	398	0.36
3q	240, 305	1.0, 1.1	390	0.05
3r	244, 305	2.1, 0.98	393	0.33
3s	225, 305	4.5, 0.98	395	0.38
3t	227, 305	5.5, 1.4	396	0.22
3u	233, 310	1.7, 0.31	396	0.46
3v	231, 308	3.8, 0.94	393	0.41
3w	230, 308	3.3, 0.84	393	0.39
3x	230, 308	3.2, 0.82	394	0.41

3y	230, 308	3.9, 1.1	401	0.24

Photophysical study

Absorbance Study

The UV-vis absorption spectra were obtained by scanning a freshly prepared solution in a cuvette of 1 cm path length in methanol with a Shimadzu UV-2600 absorption spectrophotometer equipped with a TCC-260 thermoelectrically temperature-controlled cell holder in the wavelength range of 200-800 nm. The molar absorption coefficient (ε)was calculated using Lambert Beer-law (A= εcl);[5,6] the path length was kept at 1cm, and the sample concentration (c) was around 10^{-6} M. The absorbance (A) values of the solutions were kept between 0.1 to 1 for determination.

Fluorescence Study

A Jobin Yvon-Spex Fluorolog-3 spectrophotometer with a temperature-controlled water-cooled cuvette holder was used to measure the steady-state fluorescence spectra. The slit for the fluorescence study was 2/1 or 1/1. To minimize error due to self-aggregation or self-quenching, all measurements were performed while keeping the concentration of the samples and reference at a low value of 5μM. The solutions absorbance (A) values were kept below 0.1. Fluorescence quantum yields were measured using a secondary standard quinine sulphate (λ_{abs}= 350 nm) in 0.1N H_2SO_4 (ϕ = 0.55 at 298 K).[5-7] The quantum yield was calculated using the equations below.

$$\frac{\Phi_s}{\Phi_r} = \frac{I_s}{I_r} \times \frac{A_r}{A_s} \times \frac{n_s^2}{n_r^2}$$

Where the subscripts ‘r’ and ‘s’ stand for reference and sample, respectively, I stand for the integrated area under the emission curve and A stand for the absorbance at a particular excitation wavelength, n represents the refractive index of the medium.

Results and discussion

Absorbance Study

Because all of these compounds are soluble in methanol, we use methanol as a solvent and prepare the required concentration for this experiment. All compounds have two absorbance bands, one near about 230 nm and one above 230 nm. Because all of the compounds are

aromatic, different types of electronic transitions occur. At 230 nm, π -π* electronic transition occurs, and above 230 nm, n-π* transition occurs. The absorbance maxima of all compounds due to the π-π* electronic transition remain nearly constant with the change of different substitutes at different positions, but above the 230 nm transition, the absorbance maxima change with the change of different substitutes, and these changes occur between 300 nm and 330 nm (**Fig.1**, Table S1). In terms of electronic transition, **3a** to **3t** compounds can be divided into four groups: (i) 305 nm (**3a, 3e, 3k, 3o, 3l, 3s, 3q, 3r, 3t**), (ii) 308-310 nm (3c, 3f), (iii) 313-315 nm (**3d, 3da, 3db, 3g, 3h, 3n, 3p, 3j, 3m**), and (iv) 319-330 nm (**3b, 3dc, 3p, 3i**). Redshift or bathochromic shift occurs from group one to group four absorbance maxima (**Fig.2**). As the electron-donating group shifted its absorbance maxima towards red, the electron-drawing group shifted its absorbance maxima towards blue. Because the **3p** compound contains two electron-donating groups (methyl and methoxy), it exhibits a nearly 15 nm redshift when compared to the **3a** compound (from 305 nm to 320 nm). The **3j** compound exhibits a bathochromic shift compared to the **3a** compound. Because **3h** (from 305 to 310 nm) and **3n** (from 305 nm to 314 nm) contain phenyl and methyl groups, respectively, they exhibit more redshift than **3a**. For the **3u to 3y** compounds, no significant change was observed in absorbance maxima.

Solvatochromism Study:

Absorption studies:

The absorbance study of the **3i** compound was measured in the different organic solvents to study the solvatochromism effect. Among all the compounds, this compound shows the highest redshift and high quantum yield, hence we chose this compound for further study. Absorbance maxima and absorbance coefficient are listed here. We previously discussed that this compound showed two absorption bands. In this case, we only show above 230 nm absorption band which is obtained due to n-π* transition (**Fig. S6**). The absorption band of compound **3i** was observed when the solvent polarity increased from cyclohexane to DMSO. The absorption maxima were shown at 310 nm in non-polar solvents like dioxane, THF. In polar aprotic solvent and polar protic solvent, absorption maxima remain unchanged at 325 nm. In cyclohexane and ether, it showed absorption maxima at 319 nm and 315 nm. Non-polar solvents (Cyclohexane < 1,4-dioxane < THF < DCM) showed higher molar extinction coefficient values than polar aprotic solvent (DMF, DMSO) and polar protic solvent (MeOH).

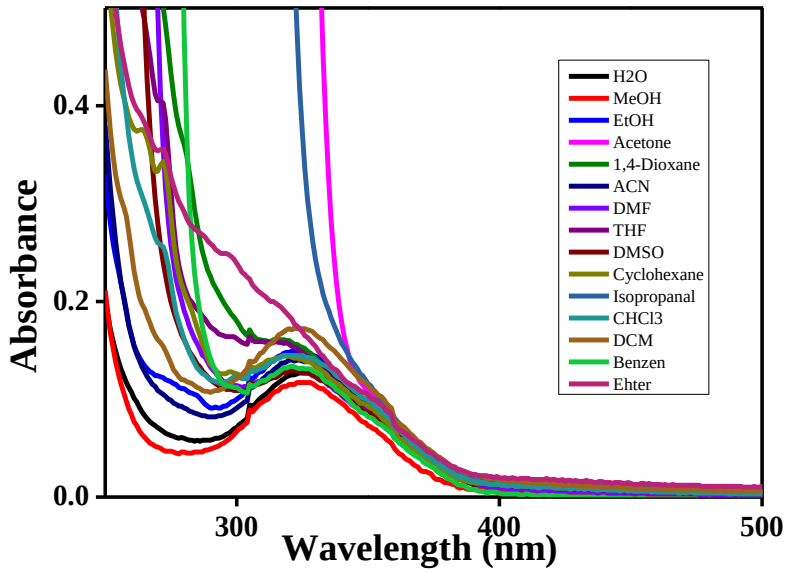


Figure S6. Absorbance spectra of **3i** compound in different solvents

Fluorescence Study of 3i:

The fluorescence study of the **3i** compound in selected solvents which were also used in the absorption study was carried out. The emission maxima in different solvents are tabulated (**Table S4**). The emission maxima increases (redshift) with the increases in the solvent polarity of the selected solvent. Solvent polarity was more affected in the case of the emission study than the absorption study. The emission maxima shift from 418 nm to 454 nm as follows: cyclohexane (418 nm), ether (427 nm), Benzene (430 nm), $CHCl_3$(433 nm), dioxane (439 nm), MeOH (445 nm), DMSO (454 nm). In the same solvent, the quantum yield was also calculated to evaluate the solvatochromism effect. The calculated quantum yield was also tabulated (**Table S4**). The fluorescence quantum yield of the **3i** compound from 0.95 in nonpolar solvent ($CHCl_3$, Benzene) to 0.27 in highly polar solvent DMSO was observed. The **3i** compound exhibited slight fluorescent color variation under UV irradiation with 365 nm by changing the solvent from cyclohexane to DMSO. The results in absorption and emission spectra can be explained by the stabilization of the charge-separated excited states of the **3i** compound. In the excited state due to intramolecular charge transfer and the charged-separated excited state can be stabilized more effectively than the ground state in polar solvent, which is the cause of the red shift in absorption and emission maxima. For optical properties solvents have a vital role because it stimulates major changes in the position, intensity, and shape of the absorption and emission bands. The emission spectra of the **3i** compound were affected by solvents shown in

Fig.S7, a solvatochromic shift from less brightness to more brightness was clearly visible upon UV irradiation (**Fig.S9**). The **3i** compound shows a positive solvatochromism effect confirmed by the red-shift (35 nm) with increasing the polarity of the solvents. Stokes shift of **3i** compound was calculated in different solvents and the values are obtained in the range of 6245-8742 cm^{-1} (**Table S4**). The Stokes shift values significantly increase with the increases of the solvent polarity of the solvents which indicates the different charge distribution in the excited state as compared to the ground state. Plotting the stokes shifts (Δν) against the solvent polarity parameter Δf (ϵ, n) (calculate using equation 1, where ϵ and n are the dielectric constant and reflective index of different solvents.), shows almost a linear relationship according to the Lippert-Mataga plot for compound **3i** (**Fig.S10**). The change of the solvent polarity indicated the enhancement or diminished electron density in the structure, as well as the intermolecular charge transfer due to the strong interaction with the solvent.

$$\Delta f(\epsilon, n) = \frac{\epsilon - 1}{2\epsilon + 1} - \frac{n^2 - 1}{2n^2 + 1} \quad \text{.....1}$$

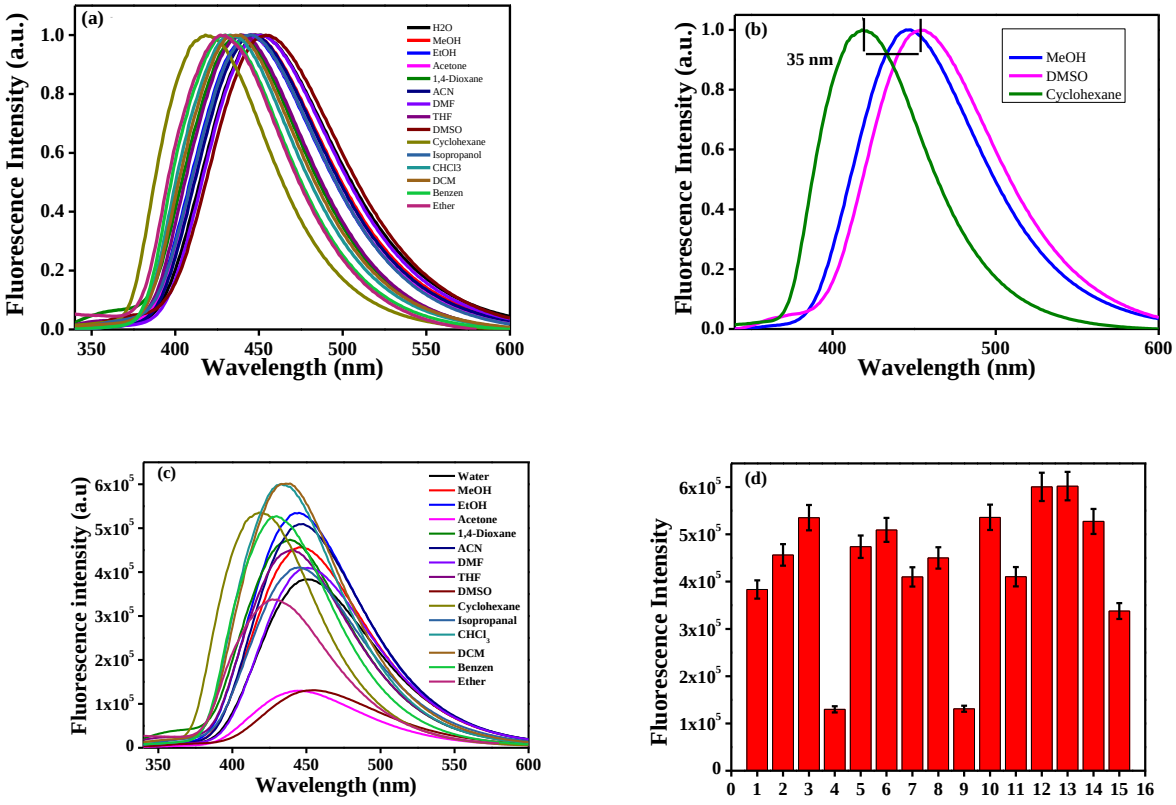


Figure S7. (a) Normalize emission spectra of **3i** compound in different solvents, (b) Emission maxima shift in different solvents, (c) Fluorescence spectra of **3i** compound, (d) Bar plot of fluorescence intensity change in different solvents (1 to 15 are water to ether in table 2)

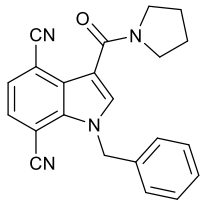
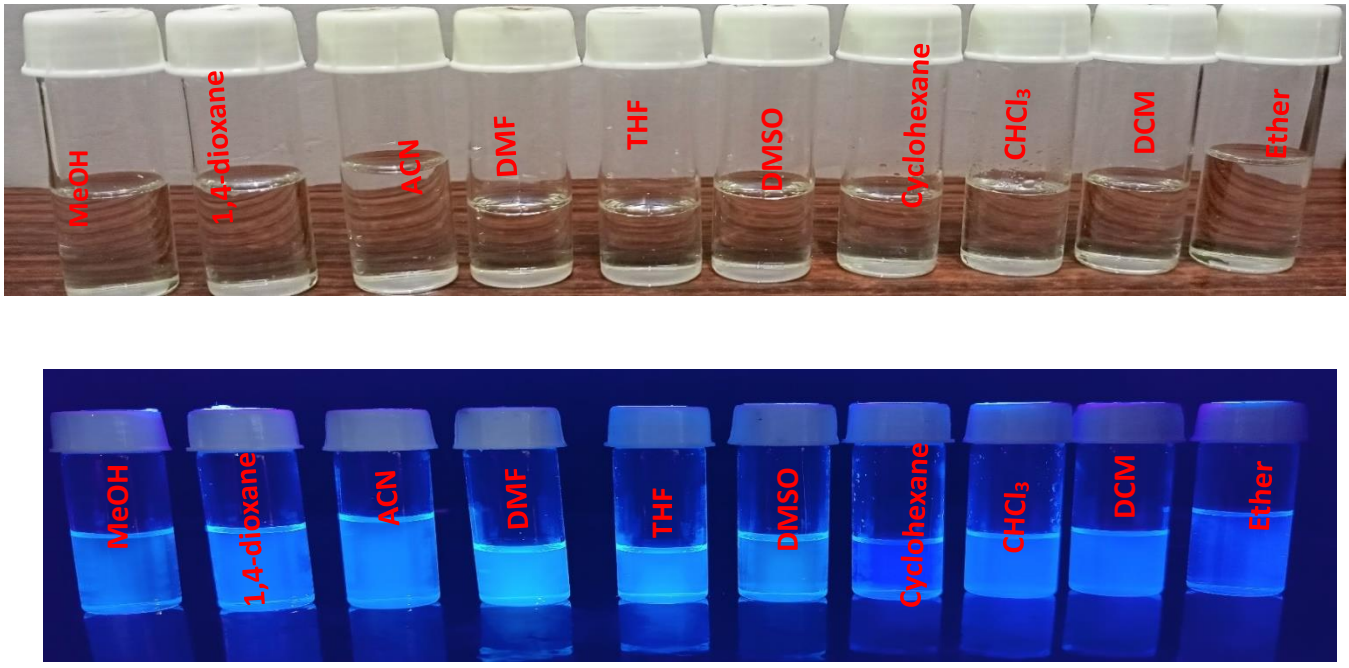


Figure S8. Structure of **3i** compound



FigureS9. Photograph of **3i** compound in the naked eye (above) and under UV irradiation (below) (excitation 365 nm) in different organic solvents

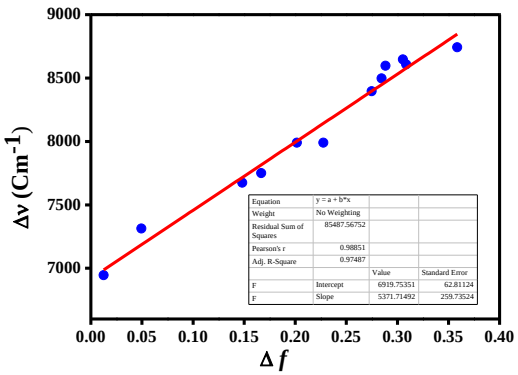


Figure S10. The relationship between stokes shift (cm^{-1}) and the solvent polarity parameter (Δf) for the compound **3i** in different solvents

Table S4: Photophysical parameters of **3i** compound in different solvents

Sl No	Solvent	Dielectric constant	λ_{abs}(nm)	ε/(10^4mol^{-1}Lcm^{-1})	λ_{emi}(nm)	Stokes shift (cm^{-1})	QY
1	**Water**	78.6	325	0.50	451	8596	0.64
2	**MeOH**	32.7	325	0.38	445	8297	0.68
3	**EtOH**	24.55	325	0.59	445	8297	0.76
4	**Acetone**	20.7	325	0.87	447	8397	0.21
5	**1,4-Dioxane**	2.25	310	0.64	439	7990	0.67
6	**ACN**	37.5	325	0.56	448	8448	0.75
7	**DMF**	36.7	325	0.51	451	8596	0.75
8	**THF**	7.58	310	0.64	439	7990	0.61
9	**DMSO**	46.7	324	0.51	454	8742	0.28
10	**Cyclohexane**	2.02	319	0.56	418	6245	0.72
11	**Isopropanol**	17.9	325	0.17	445	8297	0.21
12	**$CHCl_3$**	4.81	325	0.58	433	7675	0.92
13	**DCM**	8.93	325	0.69	439	7990	0.77
14	**Benzene**	2.27	325	0.52	430	7513	0.98
15	**Ether**	4.33	315	0.64	427	7350	0.42

Fluorescence Lifetime Studies:

We have measured the fluorescence lifetime of the **3i** compound in different organic solvents. From fluorescence lifetime measurements we get a clear idea about the excited state phenomena of **3i** compound in different solvents. In all solvents, the fluorescence decays of the **3i** compound were fitted by using the triexponential function. In all these solvents **3i** compound showed three decay components, in between them one is fast, one is the slow component and the other is an intermediate component. The average lifetime of the **3i** compound in different solvents was tabulated. (Table 3) The average lifetime in a polar aprotic solvent (DMSO) is 5.76 ns and in non-polar solvent cyclohexane is 9.44 ns. These compounds have almost the same average lifetime in some polar protic, aprotic and nonpolar solvents (**Fig. S11**).

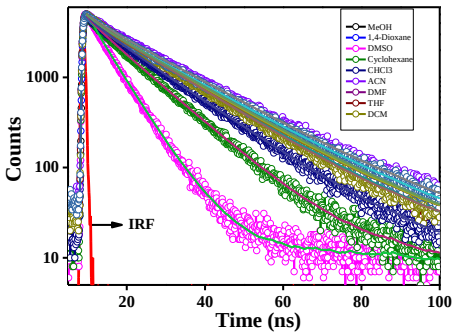


Figure S11. Fluorescence lifetime of **3i** compound in different organic solvents

Table S5. Fluorescence lifetime parameter of **3i** compound in different solvents

Name	τ_1	τ_2	τ_3	α_1	α_2	α_3	$<\tau>^a$	χ^2
MeOH	0.018	5.06	16.75	16.2	10.58	73.22	12.79	1.06
Dioxane	0.696	3.57	17.38	15.79	14.52	69.69	12.74	1.08
DMSO	2.245	6.19	18.89	13.18	86.06	0.76	5.76	1.00
Cyclohexane	0.952	5.04	11.69	15.49	8.89	75.62	9.44	1.01
$CHCl_3$	1.018	6.28	14.94	20.04	9.75	70.20	11.30	1.03
Ether	0.695	3.85	18.29	16.42	14.78	68.79	13.27	1.00
DMF	0.111	3.93	17.29	17.51	12.33	70.17	12.64	1.04
ACN	0.031	4.05	18.48	15.90	9.45	74.64	14.18	1.06
DCM	0.032	3.45	16.33	15.91	9.32	74.77	12.54	1.04
THF	0.055	3.24	17.62	14.13	14.05	71.82	13.12	1.02

a Experimental errors in the determination of lifetime ±5%

3. X-ray crystallographic data: The crystal structures have been deposited at the Cambridge Crystallographic Data Centre. CCDC No of **3d** is 2267151. The structure solution and refinement were processed by SHELXTL.

3.1 Method of crystallization: Compound **3d** was dissolved in a minimum volume of chloroform and kept at room temperature for slow evaporation. Cuboid -shaped yellow colour crystal was formed and was subjected to x-ray analysis.

3.2 Single crystal x-ray data of compound 3d (CCDC No: 2267151)

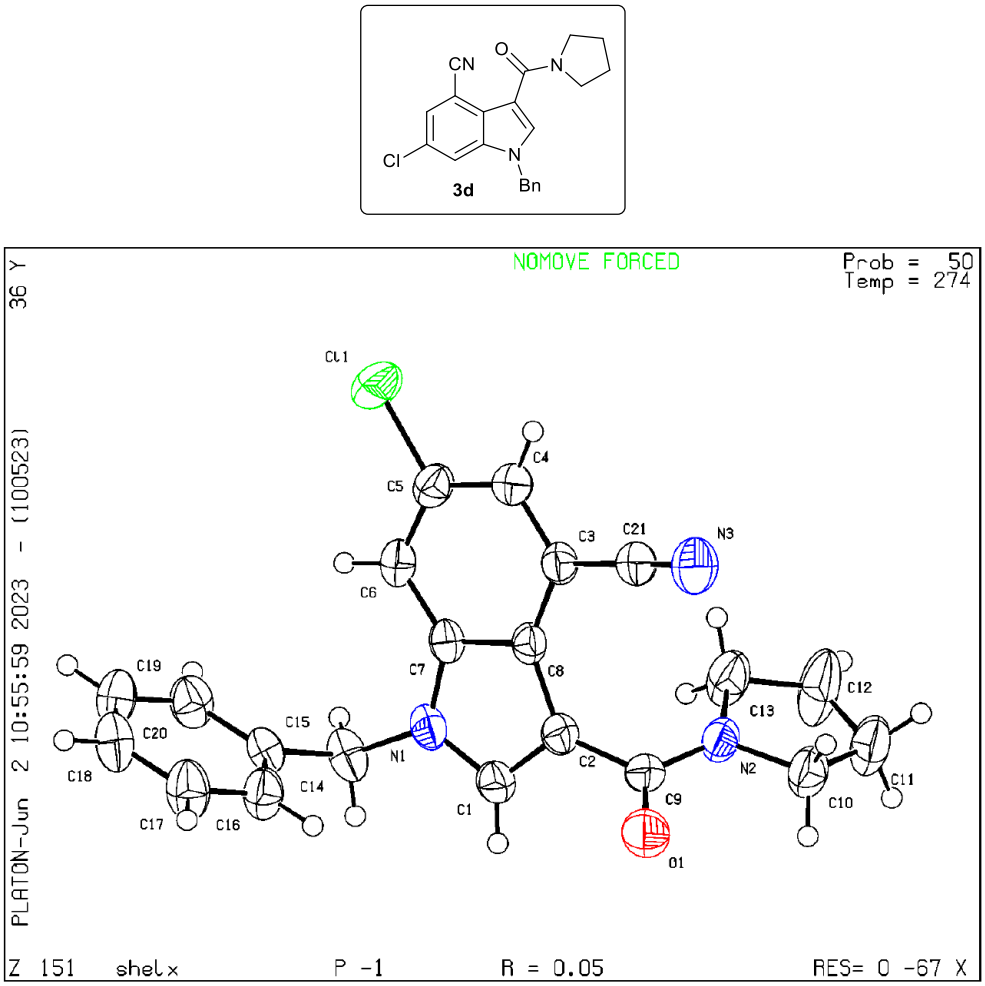


Figure: S6 ORTEP view of the molecular structure of **3d** with thermal ellipsoids drawn at the 50% probability level.

3.3 Crystal data and structure refinement for compound 3d (CCDC no: 2267151)

Bond precision:	C-C = 0.0031 A		Wavelength=0.71073
Cell:	a=8.059(9)	b=8.883(10)	c=12.824(18)
	alpha=99.80(4)	beta=90.05(5)	gamma=94.96(3)
Temperature: 274 K			

	Calculated	Reported
Volume	901.2(19)	901.1(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H17 Cl N3 O	?
Sum formula	C21 H17 Cl N3 O	C21 H17 Cl N3 O
Mr	362.83	362.83
Dx,g cm-3	1.337	1.337
Z	2	2
Mu (mm-1)	0.227	0.227
F000	378.0	378.0
F000'	378.43	
h,k,lmax	11,12,18	11,12,17
Nref	5299	5203
Tmin,Tmax	0.958,0.971	0.724,0.746
Tmin'	0.958	

Correction method= # Reported T Limits: Tmin=0.724 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max)= 30.050

R(reflections)= 0.0494(4080) wR2(reflections)= 0.1430(5203)

S = 1.037 Npar= 235

References:

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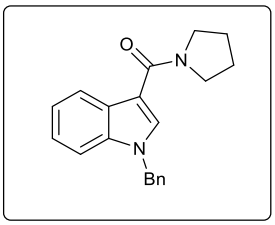
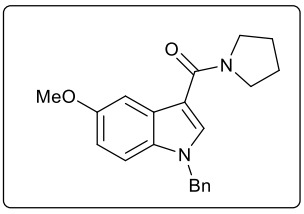
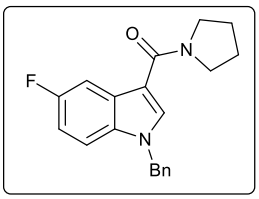
Analytical Data



(1-Benzyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1a)[4]: Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 94%, 1.43 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (m, 1H), 7.44 (s, 1H), 7.31-7.26 (m, 4H), 7.22 (d, *J* = 3.0 Hz, 2H), 7.12 (d, *J* = 6.8 Hz, 2H), 5.33 (s, 2H), 3.68 (s, 4H), 1.93 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.1, 136.5, 136.0, 129.9, 128.8, 127.8, 127.7, 126.7, 122.7, 122.2, 121.2, 121.0, 111.6, 109.7, 50.2, 48.6, 46.6, 26.2, 24.4.

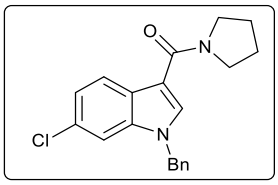


(1-Benzyl-5-methoxy-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1b); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 91%, 1.52 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 2.4 Hz, 1H), 7.41 (s, 1H), 7.30 – 7.24 (m, 3H), 7.11 (d, *J* = 8.9 Hz, 1H), 7.09 – 7.05 (m, 2H), 6.84 (dd, *J* = 8.9, 2.5 Hz, 1H), 5.27 (d, *J* = 4.1 Hz, 2H), 3.85 (s, 3H), 3.67 (t, *J* = 6.6 Hz, 4H), 1.92 (t, *J* = 6.7 Hz, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.4, 155.5, 136.7, 131.3, 130.4, 129.0, 128.8, 128.0, 127.0, 126.9, 113.9, 111.1, 110.7, 103.7, 55.9, 55.9, 50.7, 47.8, 25.5. FT-IR: $\tilde{\nu}$ 2951, 2872, 1592, 1525, 1423, 1288, 1221 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{23}N_2O_2$; 335.1754, found 335.1754.

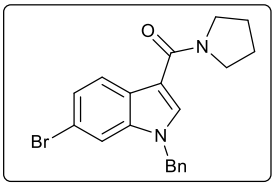


(1-Benzyl-5-fluoro-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1c); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 92%, 1.49 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 9.9 Hz, 1H), 7.49 (s, 1H), 7.25 (d, *J* = 5.1 Hz, 3H), 7.17 – 7.00 (m, 3H), 6.90 (dd, *J* = 12.1, 5.5 Hz, 1H), 5.24 (s, 2H), 3.64 (brs, 4H), 1.89 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.0, 164.8, 159.6, 157.8, 136.1, 132.5, 131.6, 128.8, 128.5, 128.4, 127.9, 126.6, 111.3, 111.1, 111.0,

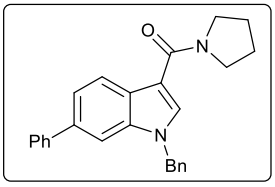
110.0, 110.6, 107.5, 107.3, 50.5, 48.8, 46.6, 26.4, 24.0. FT-IR: $\tilde{\nu}$ 2974, 2874, 1592, 1527, 1423, 1285, 1187 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{20}FN_2O$; 323.1554, found 323.1556.



(1-Benzyl-6-chloro-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1d); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 90%, 1.521 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.6 Hz, 1H), 7.40 (s, 1H), 7.25 – 7.31 (m, 4H), 7.18 (dd, *J* = 8.6, 1.1 Hz, 1H), 7.08 (d, *J* = 6.4 Hz, 2H), 5.27 (s, 2H), 3.65 (brs, 4H), 1.93 (brs, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 136.5, 136.0, 130.5, 129.1, 128.9, 128.2, 126.8, 126.5, 123.5, 122.0, 111.9, 109.8, 50.5, 49.0, 46.7, 26.6, 24.3. FT-IR: $\tilde{\nu}$ 2925, 2872, 1594, 1529, 1432, 1378, 1321, 1185 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{20}ClN_2O$; 339.1259, found 339.1262.

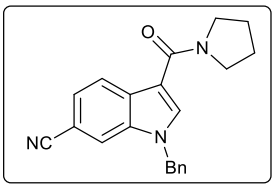


(1-Benzyl-6-bromo-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1da): Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 89%, 1.7 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.6 Hz, 1H), 7.42 (s, 1H), 7.38 (s, 1H), 7.31 (d, *J* = 7.3 Hz, 4H), 7.09 (d, *J* = 6.4 Hz, 2H), 5.27 (s, 2H), 3.65 (brs, 4H), 1.93 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.7, 137.0, 136.1, 130.3, 129.2, 128.3, 126.9, 126.9, 124.7, 123.9, 116.7, 112.8, 112.2, 50.5, 48.8, 46.7, 26.6, 24.4. FT-IR: $\tilde{\nu}$ = 2972, 2872, 1592, 1527, 1429, 137, 1320, 1185 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{20}BrN_2O$; 383.0754, found 383.0763.

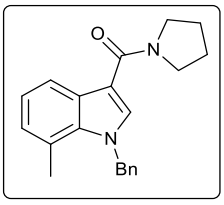


(1-Benzyl-6-phenyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1db): Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 88%, 1.67 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.3 Hz, 1H), 7.49 (d, *J* = 7.3 Hz, 2H), 7.38 (m, 1H), 7.35 (d, *J* = 6.9 Hz, 2H), 7.33 – 7.25 (m,

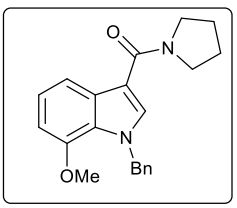
3H), 7.25 – 7.13 (m, 5H), 7.04 (d, *J* = 6.9 Hz, 2H), 5.25 (s, 2H), 3.58 (brs, 4H), 1.84-1.81 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.3, 142.1, 136.8, 136.6, 136.5, 130.5, 129.1, 128.8, 128.8, 127.5, 127.1, 127.0, 126.9, 122.7, 121.2, 112.0, 108.3, 50.4, 47.4, 46.2, 26.0, 24.0. FT-IR: $\tilde{\nu}$ = 2969, 2928, 1598, 1532, 1434, 1379, 1185 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{26}H_{25}N_2O$; 381.1961, found 381.1967.



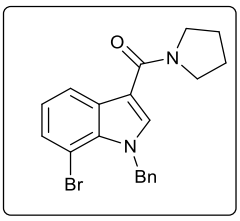
1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-6-carbonitrile (1dc): Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 78%, 1.28 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.3 Hz, 1H), 7.61-7.57 (m, 2H), 7.40 (d, *J* = 8.3 Hz, 1H), 7.28 (m, 3H), 7.09 (d, *J* = 4.7 Hz, 2H), 5.34 (s, 2H), 3.64 (brs, 4H), 1.94 (brs, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 135.4, 135.0, 133.0, 131.1, 129.2, 128.5, 126.8, 124.0, 123.4, 120.3, 114.9, 112.5, 105.6, 50.8, 48.9, 46.7, 26.6, 24.3. FT-IR: $\tilde{\nu}$ = 2973, 2874, 221, 1594, 1530, 1434, 1384, 1326, 1187 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{20}N_3O$; 330.1601, found 330.1608.



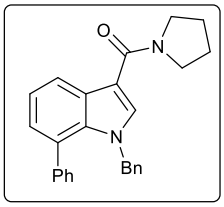
(1-Benzyl-7-methyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1e); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 93%, 1.48 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.0 Hz, 1H), 7.36 (s, 1H), 7.27 – 7.19 (m, 3H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.89 (t, *J* = 7.9 Hz, 3H), 5.50 (s, 2H), 3.64 (brs, 4H), 2.46 (s, 3H), 1.84 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.2, 138.6, 134.7, 131.8, 128.7, 128.5, 127.4, 125.5, 125.3, 121.2, 120.9, 120.1, 111.3, 52.3, 48.8, 46.4, 26.3, 24.2, 19.2. FT-IR: $\tilde{\nu}$ 2977, 2848, 1593, 1533, 1493, 1448, 1382, 1318, 1201 cm^{-1}. HRMS: Calculated for $[M+Na]^+$ $C_{21}H_{22}N_2NaO$; 341.1624, found 341.1613.



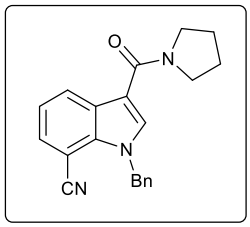
(1-Benzyl-7-methoxy-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1f); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 95%, 1.54 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 8.1, 0.7 Hz, 1H), 7.31 (s, 1H), 7.24 (ddd, *J* = 18.7, 12.2, 4.3 Hz, 3H), 7.07 (t, *J* = 7.9 Hz, 3H), 6.63 (d, *J* = 7.7 Hz, 1H), 5.60 (s, 2H), 3.78 (s, 3H), 3.62 (brs, 4H), 1.88 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.4, 147.5, 138.8, 130.8, 129.9, 128.6, 127.4, 126.7, 126.0, 121.6, 114.9, 112.1, 103.8, 55.4, 53.0, 46.6, 25.8. FT-IR: $\tilde{\nu}$ 2972, 1595, 1495, 1445, 1382, 1318, 1265, 1205 cm-1. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{23}N_2O_2$; 335.1754, found 335.1761.



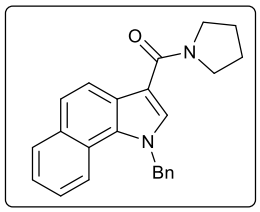
(1-Benzyl-7-bromo-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1g); Eluent: 60% ethyl acetate in hexane. Brown solid. Yield 89%, 1.7 g, ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 7.3 Hz, 2H), 7.27 (dt, *J* = 6.7, 4.5 Hz, 3H), 7.04 (t, *J* = 7.8 Hz, 1H), 7.00 (d, *J* = 7.2 Hz, 2H), 5.83 (s, 2H), 3.64 (brs, 4H), 1.92 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.6, 138.2, 132.7, 132.6, 130.9, 128.9, 128.4, 127.8, 126.4, 122.4, 121.9, 112.2, 103.8, 51.9, 49.0, 46.6, 26.5, 24.6. FT-IR: $\tilde{\nu}$ 2975, 2925, 2869, 1599, 1532, 1416, 1308, 1263, 1183 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{20}BrN_2O$; 383.0754, found 383.0757.



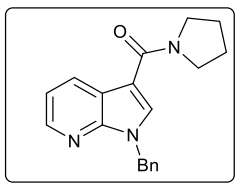
(1-Benzyl-7-phenyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1h); Eluent: 60% ethyl acetate in hexane. Brown solid. Yield 91%, 1.73 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 6.7 Hz, 1H), 7.40 (d, *J* = 3.9 Hz, 1H), 7.38 – 7.23 (m, 5H), 7.22 – 7.09 (m, 5H), 7.07 – 6.99 (m, 1H), 6.53 (s, 2H), 4.95 (d, *J* = 3.2 Hz, 2H), 3.71 (brs, 4H), 1.96 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.4, 139.9, 137.6, 133.4, 132.1, 129.9, 128.9, 128.5, 127.8, 127.41, 127.37, 127.2, 126.2, 125.8, 121.5, 121.0, 112.1, 52.4, 47.5, 44.2, 29.8, 25.7. FT-IR: $\tilde{\nu}$ 3098, 3028, 2923, 2874, 1591, 1537, 1447, 1327, 1178 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{26}H_{25}N_2O$; 381.1961, found 381.1943.



1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-7-carbonitrile (1i); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 90%, 1.48 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.57 (dd, *J* = 7.4, 0.8 Hz, 1H), 7.47 (s, 1H), 7.26 – 7.35 (m, 4H), 7.15 – 7.07 (m, 2H), 5.74 (s, 2H), 3.64 (brs, 4H), 1.95 – 1.99 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.1, 136.4, 134.3, 131.9, 130.0, 129.7, 129.2, 128.3, 128.2, 127.0, 121.1, 118.1, 112.8, 94.4, 51.2, 48.9, 46.7, 26.6, 24.8. FT-IR: $\tilde{\nu}$ = 2973, 2222, 1598, 1537, 1434, 1323, 1178 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{20}N_3O$; 330.1601, found 330.1609.

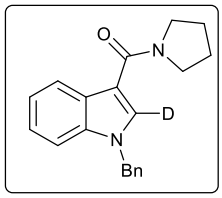


(1-Benzyl-1*H*-benzo[*g*]indol-3-yl)(pyrrolidin-1-yl)methanone (1j); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 88%, 1.56 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.7 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.93 (d, *J* = 7.5 Hz, 1H), 7.64 (d, *J* = 8.7 Hz, 1H), 7.47 – 7.22 (m, 7H), 7.08 (d, *J* = 6.8 Hz, 2H), 5.80 (s, 2H), 3.72 (brs, 4H), 1.95 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.4, 137.0, 131.9, 130.2, 129.9, 129.3, 129.2, 128.0, 126.2, 125.7, 125.5, 124.0, 122.9, 122.4, 121.5, 121.0, 113.0, 54.1, 47.9, 43.6, 29.8, 25.6. FT-IR: $\tilde{\nu}$ = 2924, 2870, 1600, 1536, 1437, 1370, 1264, 1184 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{24}H_{23}N_2O$; 355.1805, found 355.1800.



(1-Benzyl-1*H*-pyrrolo[2,3-b]pyridin-3-yl)(pyrrolidin-1-yl)methanone (1k); Eluent: 80% ethyl acetate in hexane. Brown solid. Yield 85%, 1.25 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (dd, *J* = 7.9, 1.4 Hz, 1H), 8.34 (dd, *J* = 4.7, 1.4 Hz, 1H), 7.45 (s, 1H), 7.21-7.26 (m, 3H), 7.15 (dd, *J* = 7.8, 4.8 Hz, 3H), 5.46 (s, 2H), 3.59 (brs, 4H), 1.86 (brs, 4H). ^{13}C NMR (125 MHz,

$CDCl_3$) δ 174.0, 164.4, 147.2, 144.1, 136.9, 131.1, 129.5, 128.8, 127.9, 127.5, 120.3, 117.6, 110.2, 48.7, 48.1, 46.7, 26.6, 24.2. FT-IR: $\tilde{\nu}$ = 2923, 2869, 1591, 1527, 1450, 1341, 1175, 1114 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{20}N_3O$; 306.1601, found 306.1596.



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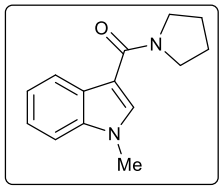
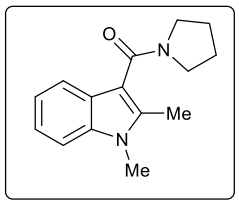
(1-Benzyl-1*H*-indol-3-yl-2-d)(pyrrolidin-1-yl)methanone (1l); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 94%, 1.43 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (m, 1H), 7.25 (m, 1H), 7.23 – 7.19 (m, 3H), 7.18 – 7.14 (m, 2H), 7.08 – 7.03 (m, 2H), 5.26 (s, 2H), 3.61 (t, *J* = 6.5 Hz, 4H), 1.91 – 1.82 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.3, 136.5, 136.1, 128.9, 127.9, 127.7, 126.9, 122.8, 122.3, 121.2, 111.7, 109.8, 50.4, 47.6, 25.5. FT-IR: $\tilde{\nu}$ = 2968, 2858, 1586, 1497, 1429, 1385, 1340, 1192 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{20}DN_2O$; 306.1711, found 306.1709.

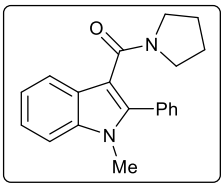


(1-Methyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1m)[4]; Eluent: 80% ethyl acetate in hexane. Brown solid. Yield 94%, 1.07 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (t, *J* = 7.9 Hz, 1H), 7.38 (s, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.28 (d, *J* = 7.0 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 3.81 (s, 3H), 3.69 (brs, 4H), 1.95 (brs, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 136.5, 130.8, 127.4, 122.7, 122.2, 121.1, 111.1, 109.4, 47.8, 33.3, 25.6.

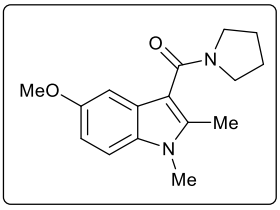


(1,2-Dimethyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1n); Eluent: 90% ethyl acetate in hexane. Brown solid. Yield 91%, 1.10 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.7 Hz, 1H), 7.27 (d, *J* = 9.1 Hz, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.4 Hz, 1H), 3.69 (m, 5H), 3.39 (brs, 2H), 2.51 (s, 3H), 1.95 (brs, 2H), 1.86 (brs, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ

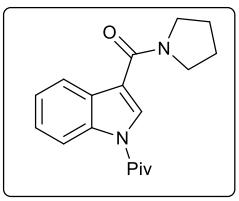
167.4, 137.6, 136.4, 125.4, 121.3, 120.3, 119.7, 110.5, 109.2, 48.7, 46.0, 29.6, 26.2, 24.9, 11.7. FT-IR: $\tilde{\nu}$ = 2975, 2875, 1649, 1598, 1428, 1340, 1044 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{15}H_{19}N_2O$; 243.1492, found 243.1514.



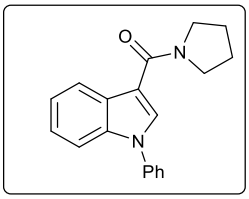
(1-Methyl-2-phenyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1o); Eluent: 80% ethyl acetate in hexane. Brown solid. Yield 90%, 1.37 g. ^1H NMR (400 MHz, $CDCl_3$) δ 8.46 (m, 1H), 7.49 (d, *J* = 4.7 Hz, 3H), 7.40 (d, *J* = 4.5 Hz, 2H), 7.38 – 7.33 (m, 3H), 3.50 (s, 3H), 3.25 (t, *J* = 6.6 Hz, 2H), 2.80 (t, *J* = 6.9 Hz, 2H), 1.79 – 1.65 (m, 2H), 1.65 – 1.57 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 188.0, 165.7, 148.8, 137.1, 130.7, 129.9, 129.5, 128.1, 126.7, 124.0, 123.5, 122.6, 111.5, 109.9, 46.3, 44.5, 31.0, 25.6, 23.8. FT-IR: $\tilde{\nu}$ = 3053, 2951, 2878, 1612, 1466, 1389, 1262, 1087 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{21}N_2O$; 305.1648, found 305.1649.



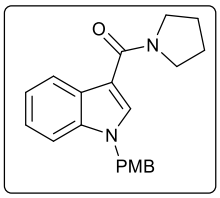
(5-Methoxy-1,2-dimethyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1p); Eluent: 80% ethyl acetate in hexane. Brown solid. Yield 78%, 1.06 g. ^1H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 8.8 Hz, 1H), 6.93 (s, 1H), 6.82 (dd, *J* = 8.8, 2.3 Hz, 1H), 3.83 (s, 3H), 3.61 (s, 5H), 3.40 (s, 2H), 2.46 (s, 3H), 1.93 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.5, 154.8, 138.0, 131.7, 125.9, 111.0, 109.8, 102.2, 56.1, 48.7, 29.7, 24.8, 11.8. FT-IR: $\tilde{\nu}$ = 2966, 1600, 1490, 1432, 1363, 1230, 1158 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{21}N_2O_2$; 273.1598, found 273.1595.



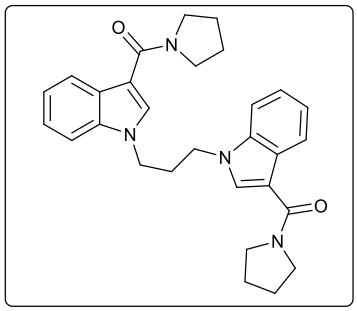
2,2-Dimethyl-1-(3-(pyrrolidine-1-carbonyl)-1*H*-indol-1-yl)propan-1-one (1q); Eluent: 60% ethyl acetate in hexane. Brown solid. Yield 87%, 1.29 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.3 Hz, 1H), 7.98 (s, 1H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.38 (m, 1H), 7.33 (dd, *J* = 11.1, 3.9 Hz, 1H), 3.65 (brs, 4H), 1.97 (t, *J* = 6.6 Hz, 4H), 1.52 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.2, 164.4, 136.7, 127.4, 126.1, 126.0, 124.3, 121.2, 117.9, 117.3, 47.8, 41.5, 28.9, 25.5. FT-IR: $\tilde{\nu}$ = 2923, 2875, 1695, 1610, 1566, 1438, 1310, 1181 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{23}N_2O_2$; 299.1754, found 299.1752.



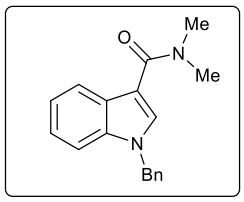
(1-Phenyl-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1r); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 74%, 430 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (m, 1H), 7.49 (s, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.35 (d, *J* = 8.2 Hz, 3H), 7.27 (t, *J* = 7.2 Hz, 1H), 7.13 (m, 2H), 3.60 (brs, 4H), 1.82 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.3, 139.0, 136.0, 129.9, 129.4, 128.0, 127.5, 124.9, 123.4, 122.4, 121.8, 113.7, 110.6, 49.0, 46.5, 26.5, 24.4. FT-IR: $\tilde{\nu}$ = 2970, 2872, 1595, 1501, 1455, 1366, 1317, 1226, 1015 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{19}N_2O$; 291.1492, found 291.1481.



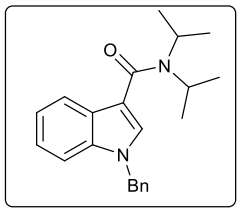
(1-(4-Methoxybenzyl)-1*H*-indol-3-yl)(pyrrolidin-1-yl)methanone (1s)[4]; Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 93%, 1.55 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 5.9, 2.8 Hz, 1H), 7.41 (s, 1H), 7.29 (m, 1H), 7.21 (dd, *J* = 5.9, 2.8 Hz, 2H), 7.06 (d, *J* = 8.3 Hz, 2H), 5.24 (s, 2H), 3.76 (s, 3H), 3.66 (brs, 4H), 1.92 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.5, 159.4, 136.1, 129.9, 128.5, 128.4, 127.7, 122.8, 122.3, 121.2, 114.2, 111.7, 109.9, 55.4, 50.0, 48.8, 46.6, 26.3, 24.6.



(Propane-1,3-diylbis(1*H*-indole-1,3-diyl))bis(pyrrolidin-1-ylmethanone) (1t); Eluent: 100% ethyl acetate in hexane. Brown solid. Yield 78%, 1.82 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (m, 1H), 7.28 (s, 1H), 7.24 (dd, *J* = 6.4, 3.3 Hz, 3H), 4.13 (t, *J* = 6.6 Hz, 2H), 3.68 (brs, 2H), 3.55 (s, 2H), 2.47 (m, 1H), 1.93 (brs, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 135.5, 129.3, 127.8, 122.8, 122.5, 121.3, 111.7, 109.4, 48.8, 46.9, 45.1, 43.5, 29.5, 25.8, 26.6, 24.1. FT-IR: $\tilde{\nu}$ = 2973, 2874, 1590, 1530, 1443, 1341, 1215 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{29}H_{33}N_4O_2$; 469.2598, found 469.2592.

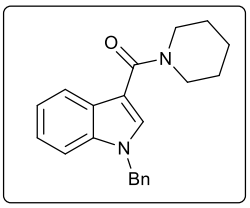


1-Benzyl-*N*,*N*-dimethyl-1*H*-indole-3-carboxamide (1u); Eluent: 90% ethyl acetate in hexane. Brown solid. Yield 85%, 1.18 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 – 7.76 (m, 1H), 7.39 (s, 1H), 7.29 – 7.21 (m, 4H), 7.17 (m, 2H), 7.10 (d, *J* = 6.6 Hz, 2H), 5.27 (s, 2H), 3.11 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.6, 136.6, 136.2, 130.4, 129.0, 128.0, 127.1, 127.0, 122.7, 121.5, 121.1, 111.3, 110.2, 50.5, 37.7. FT-IR: $\tilde{\nu}$ = 1615, 1539, 1467, 1393, 1337, 1258, 1176 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{19}N_2O$; 279.1492, found 279.1484.

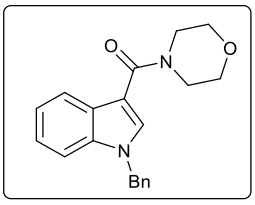


1-Benzyl-*N*,*N*-diisopropyl-1*H*-indole-3-carboxamide (1v); Eluent: 60% ethyl acetate in hexane. Brown solid. Yield 81%, 1.35 g. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (m, 1H), 7.31 – 7.20 (m, 5H), 7.16 (dd, *J* = 13.6, 6.3 Hz, 2H), 7.11 (d, *J* = 7.1 Hz, 2H), 5.25 (s, 2H), 3.95 (brs, 2H), 1.38 (brs, 6H), 1.36 (brs, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.7, 136.7, 136.0, 128.9,

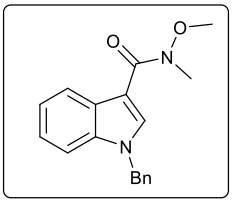
127.9, 127.5, 127.1, 122.5, 120.8, 120.6, 113.6, 110.0, 50.3, 48.3, 21.3. FT-IR: $\tilde{\nu}$ = 2966, 1607, 1532, 1438, 1367, 1296, 1205, 1153 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{27}N_2O$; 335.2118, found 335.2112.



(1-Benzyl-1*H*-indol-3-yl)(piperidin-1-yl)methanone (1w); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 92%, 1.46 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (dd, *J* = 6.3, 2.7 Hz, 1H), 7.46 (s, 1H), 7.34 – 7.27 (m, 4H), 7.24 – 7.19 (m, 2H), 7.16 (d, *J* = 7.8 Hz, 2H), 5.31 (s, 2H), 3.66 (s, 4H), 1.76 – 1.66 (m, 2H), 1.62 (d, *J* = 3.9 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 136.5, 136.1, 130.6, 129.0, 128.0, 127.1, 126.6, 122.5, 121.0, 120.9, 111.6, 110.3, 50.5, 46.3, 26.4, 24.8. FT-IR: $\tilde{\nu}$ = 2924, 2853, 1603, 1532, 1441, 1225, 1198 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{23}N_2O$; 319.1805, found 319.1812.

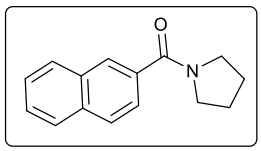


(1-Benzyl-1*H*-indol-3-yl)(morpholino)methanone (1x); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 89%, 1.42 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.67 (m, 1H), 7.50 (s, 1H), 7.31 (d, *J* = 6.2 Hz, 4H), 7.23 (dd, *J* = 6.4, 2.8 Hz, 2H), 7.16 (d, *J* = 7.1 Hz, 2H), 5.33 (s, 2H), 3.74 (brs, 8H).^{13}C NMR (125 MHz, $CDCl_3$) δ 166.8, 136.3, 136.3, 131.3, 129.1, 128.2, 127.2, 126.3, 122.8, 121.4, 120.8, 110.7, 110.5, 67.3, 50.7, 45.9. FT-IR: $\tilde{\nu}$ = 2848, 1593, 1525, 1437, 1243, 1198, 1110 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{21}N_2O_2$; 321.1598, found 321.1597.

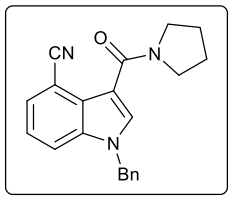


1-Benzyl-*N*-methoxy-*N*-methyl-1*H*-indole-3-carboxamide (1y); Eluent: 80% ethyl acetate in hexane. Brown solid. Yield 81%, 1.19 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.6 Hz,

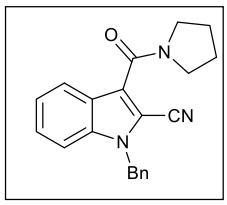
1H), 7.93 (s, 1H), 7.36 – 7.23 (m, 6H), 7.17 – 7. 12 (m, 2H), 5.34 (s, 2H), 3.68 (s, 3H), 3.41 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 136.4, 136.0, 133.2, 128.9, 128.7, 128.0, 126.9, 122.9, 122.7, 121.7, 109.8, 107.7, 60.6, 50.5, 33.2. FT-IR: $\tilde{\nu}$ = 3098, 2923, 1591, 1537, 1447, 1327, 1178 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{18}H_{19}N_2O_2$; 295.1441, found 295.1439.



Naphthalen-2-yl(pyrrolidin-1-yl)methanone (1z); Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 92%, 1.03 g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.86 (brs, 3H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.56 – 7.45 (m, 2H), 3.71 (brs, 2H), 3.49 (s, 2H), 1.97 (s, 2H), 1.88 (s, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.9, 134.7, 134.0, 132.8, 128.6, 128.2, 127.9, 127.2, 127.1, 126.7, 124.6, 49.8, 46.4, 26.6, 24.6. FT-IR: $\tilde{\nu}$ = 2971, 2875, 1611, 1416, 1340, 1191 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{15}H_{16}NO$; 226.1226, found 226.1232.

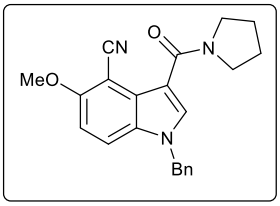


1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3a): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 83%, 54.6 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53-7.50 (m, 3H), 7.30 (dd, *J* = 6.0, 3.8 Hz, 3H), 7.23 (m, 1H), 7.12 (d, *J* = 6.0 Hz, 2H), 5.34 (s, 2H), 3.70 (brs, 2H), 3.35 (brs, 2H), 1.94 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.2, 136.0, 135.7, 130.5, 129.1, 128.4, 127.4, 127.1, 125.4, 122.2, 117.8, 115.3, 112.8, 103.4, 50.8, 48.9, 46.0, 25.9, 24.8. FT-IR: $\tilde{\nu}$ = 2972, 2877, 2221, 1604, 1536, 1455, 1345, 1302, 1188 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{20}N_3O$; 330.1601, found 330.1594.

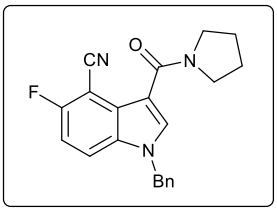


1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-2-carbonitrile (4a); Eluent: 30% ethyl acetate in hexane. Viscous gel. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 1H), 7.30 – 7.13 (m, 6H), 7.07 (d, *J* = 6.7 Hz, 2H), 5.38 (s, 2H), 3.64 (brs, 2H), 3.44 (brs, 2H), 1.89 (brs,

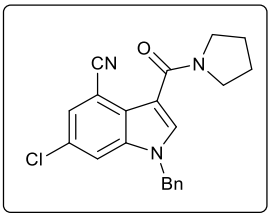
2H), 1.82 (brs, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8, 137.2, 135.5, 129.2, 128.4, 127.0, 126.8, 124.9, 123.1, 122.7, 122.4, 112.8, 111.0, 108.9, 49.4, 48.7, 46.3, 26.3, 24.6. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{20}N_3O$; 330.1601, found 330.1604.



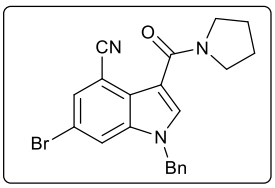
1-Benzyl-5-methoxy-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3b): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 78%, 56 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (s, 1H), 7.41 (d, *J* = 9.0 Hz, 1H), 7.33 - 7.32 (m, 3H), 7.12 (d, *J* = 6.5 Hz, 2H), 6.87 (d, *J* = 9.1 Hz, 1H), 5.29 (s, 2H), 3.94 (s, 3H), 3.73 (brs, 2H), 3.35 (brs, 2H), 1.98 (m, 2H), 1.92 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.5, 158.9, 135.8, 131.4, 131.1, 129.2, 128.4, 127.2, 126.1, 116.1, 115.3, 112.4, 107.4, 91.2, 57.1, 50.9, 48.8, 46.0, 25.9, 24.8. FT-IR: $\tilde{\nu}$ = 2970, 2876, 2216, 1608, 1539, 1427, 1340, 1302, 1254, 1181, 1105 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{22}N_3O_2$; 360.1707, found 360.1704.



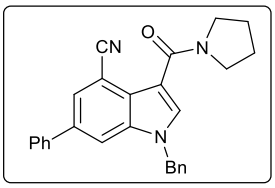
1-Benzyl-5-fluoro-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3c): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 64%, 44.4 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.45 (m, 1H), 7.35 – 7.29 (m, 3H), 7.16 – 7.09 (m, 2H), 7.01 (m, 1H), 5.32 (s, 2H), 3.71 (s, 2H), 3.37 (s, 2H), 1.97 (brs, 2H), 1.94 (brs, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.7, 161.0 (d, *J* = 251.6 Hz), 160.0, 135.3, 132.2 (d, *J* = 40.2 Hz), 129.2, 128.5, 127.1, 125.3 (d, *J* = 2.5 Hz), 116.6 (d, *J* = 9.9 Hz), 113.0 (d, *J* = 16.0 Hz), 110.7 (d, *J* = 24.6 Hz), 91.2 (d, *J* = 18.4 Hz), 51.0, 48.9, 46.0, 26.0, 24.7. FT-IR: $\tilde{\nu}$ = 2972, 2877, 2226, 1609, 1536, 1426, 1343, 1239, 1187 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{19}FN_3O$; 348.1507, found 348.1500.



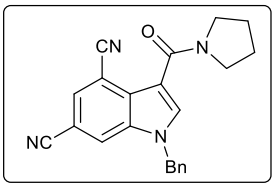
1-Benzyl-6-chloro-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3d): Eluent: 80% ethyl acetate in hexane. Brown solid. Yield 81%, 58.8 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.46 (m, 3H), 7.37 – 7.29 (m, 3H), 7.16 – 7.10 (m, 2H), 5.30 (s, 2H), 3.69 (brs, 2H), 3.34 (brs, 2H), 1.93 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.6, 136.6, 135.1, 131.3, 129.3, 128.7, 128.2, 127.3, 127.2, 124.2, 116.5, 115.3, 113.0, 104.4, 51.0, 49.0, 46.2, 26.0, 24.7. FT-IR: $\tilde{\nu}$ = 2974, 2879, 2225, 1606, 153, 1455, 1381, 1304, 1181 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{19}ClN_3O$; 364.1211, found 364.1210.



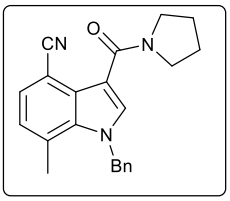
1-Benzyl-6-bromo-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3da): Eluent: 70% ethyl acetate in hexane. Viscous gel. Yield 77%, 62.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (s, 1H), 7.61 (s, 1H), 7.45 (s, 1H), 7.34-7.33 (m, 3H), 7.15 – 7.07 (m, 2H), 5.30 (s, 2H), 3.72-3.69 (m, 2H), 3.34-3.31 (m, 2H), 2.02 – 1.85 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.4, 136.8, 135.1, 130.9, 129.7, 129.3, 128.7, 127.1, 124.5, 118.1, 116.5, 114.9, 113.7, 104.9, 50.8, 48.8, 46.0, 26.0, 24.7. FT-IR: $\tilde{\nu}$ = 2971, 2877, 2225, 1614, 1534, 1440, 1380, 1304 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{19}BrN_3O$; 408.0706 found 408.0714.



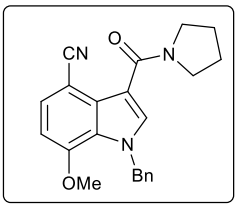
1-Benzyl-6-phenyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3db): Eluent: 70% ethyl acetate in hexane. Viscous gel. Yield 62%, 56.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.69 (s, 1H), 7.56 – 7.49 (m, 3H), 7.47-7.44 (m, 2H), 7.39-7.33 (m, 4H), 7.17-7.16 (m, 2H), 5.39 (s, 2H), 3.76 (brs, 2H), 3.41 (brs, 2H), 2.01-1.94 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 139.9, 136.8, 136.3, 135.6, 130.9, 129.3, 129.2, 128.6, 127.9, 127.4, 127.2, 127.1, 124.6, 117.9, 113.5, 113.4, 103.9, 50.8, 48.9, 46.0, 26.1, 24.8. FT-IR: $\tilde{\nu}$ = 2926, 2855, 2222, 1614, 1541, 1455, 1379, 1308 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{27}H_{24}N_3O$; 406.1914 found 406.1925.



1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4,6-dicarbonitrile (3dc); Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 54 %, 38.2 mg. ^{1}H NMR (400 MHz, DMSO) δ 8.63 (s, 1H), 8.41 (s, 1H), 8.12 (s, 1H), 7.37 – 7.25 (m, 5H), 5.60 (s, 2H), 3.35 (brs, 4H), 1.86 (brs, 4H). ^{13}C NMR (100 MHz, DMSO) δ 161.8, 136.7, 135.5, 134.8, 129.9, 128.9, 128.0, 127.4, 127.2, 120.7, 118.5, 116.1, 112.9, 104.1, 103.5, 49.7, 48.2, 45.6, 25.7, 24.2. FT-IR: $\tilde{\nu}$ = 2925, 2876, 2228, 1613, 1536, 1441, 1310, 1190 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{19}N_4O$; 355.1553 found 355.1557.

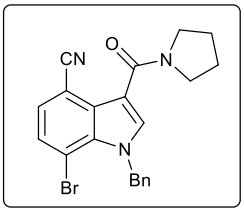


1-Benzyl-7-methyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3e): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 82%, 56.3 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.0 Hz, 2H), 7.29 (t, *J* = 7.6 Hz, 3H), 6.95 (d, *J* = 7.5 Hz, 1H), 6.91 (d, *J* = 6.9 Hz, 2H), 5.59 (s, 2H), 3.72 (s, 2H), 3.34 (s, 2H), 2.56 (s, 3H), 1.95 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.3, 137.9, 134.8, 132.0, 129.3, 128.1, 127.8, 127.7, 126.2, 125.7, 125.4, 118.0, 113.3, 101.4, 52.9, 48.8, 46.0, 26.0, 24.8, 20.0. FT-IR: $\tilde{\nu}$ = 2971, 2876, 2220, 1631, 1544, 1451, 1385, 1303, 1180 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{22}N_3O$; 344.1757, found 344.1752.

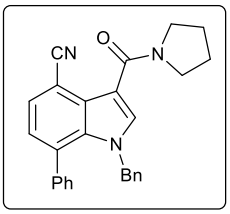


1-Benzyl-7-methoxy-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3f): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 89%, 63.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.2 Hz, 1H), 7.36 (s, 1H), 7.30 (dd, *J* = 9.5, 6.5 Hz, 3H), 7.11 (d, *J* = 6.9 Hz, 2H), 6.68 (d, *J* = 8.2 Hz, 1H), 5.62 (s, 2H), 3.92 (s, 3H), 3.73 (brs, 2H), 3.34 (brs, 2H), 1.96 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.2, 151.4, 138.0, 130.6, 129.5, 128.9, 127.9, 127.3, 127.0, 125.5, 118.3, 113.9, 103.7, 96.0, 55.9, 53.2, 48.5, 45.9, 25.6. FT-IR: $\tilde{\nu}$ = 2934, 2213,

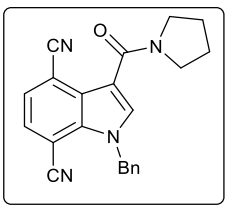
1605, 1540, 1387, 1304, 1186 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{22}N_3O_2$; 360.1707, found 360.1708.



1-Benzyl-7-bromo-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3g): Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 70%, 57 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 2H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.30 – 7.22 (m, 3H), 6.99 (d, *J* = 7.0 Hz, 2H), 5.80 (s, 2H), 3.68 (s, 2H), 3.27 (s, 2H), 1.91 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.2, 137.2, 132.8, 132.7, 129.1, 128.1, 127.91, 127.86, 127.8, 126.5, 117.1, 113.9, 110.1, 103.0, 52.2, 48.7, 45.9, 25.9, 24.8. FT-IR: $\tilde{\nu}$ = 2924, 2874, 2222, 1617, 1544, 1454, 1380, 1331, 1289, 1181 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{19}BrN_3O$; 408.0706, found 408.0711.

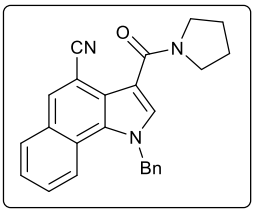


1-Benzyl-7-phenyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3h): Eluent: 70% ethyl acetate in hexane. Brown solid. Yield 67%, 54.2 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.41 (s, 1H), 7.37 (m, 1H), 7.29 (dd, *J* = 10.4, 4.7 Hz, 2H), 7.19 – 7.08 (m, 5H), 7.25 (m, 1H), 6.50 (d, *J* = 7.1 Hz, 2H), 4.92 (s, 2H), 3.73 (s, 2H), 3.40 (s, 2H), 1.97 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.2, 138.1, 136.7, 133.2, 132.7, 132.3, 129.3, 128.6, 128.3, 128.2, 127.7, 127.0, 126.6, 126.2, 125.3, 117.8, 113.2, 102.4, 52.5, 48.9, 46.0, 25.9, 24.8. FT-IR: $\tilde{\nu}$ = 2924, 2875, 2220, 1616, 1537, 1454, 1384, 1336, 1268, 1179 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{27}H_{24}N_3O$; 406.1914, found 406.1916.

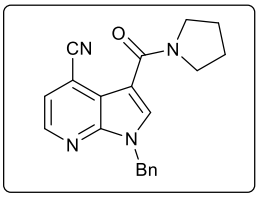


1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4,7-dicarbonitrile (3i): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 58%, 41 mg. ^{1}H NMR (500 MHz, DMSO-D_6) δ 8.24 (s, 1H),

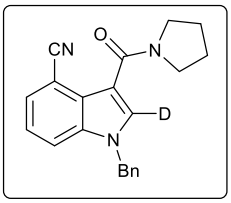
7.86 (d, *J* = 7.8 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.29 (d, *J* = 7.2 Hz, 1H), 7.07 (d, *J* = 7.5 Hz, 2H), 5.83 (s, 2H), 3.51 (brs, 2H), 3.39 (brs, 2H), 1.88 (brs, 4H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 161.6, 136.9, 134.2, 133.4, 128.8, 128.6, 127.7, 126.6, 126.1, 116.3, 116.2, 113.0, 107.2, 98.6, 50.2, 48.0, 45.4, 25.5, 24.0. FT-IR: $\tilde{\nu}$ = 2925, 2222, 1599, 1541, 1458, 1337, 1178 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{19}N_4O$ 355.1553, found 355.1550.



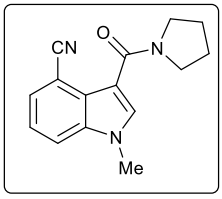
1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-benzo[*g*]indole-4-carbonitrile (3j): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 68%, 51.5 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.86 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.46 – 7.34 (m, 3H), 7.26 –7.19 (m, 3H), 7.01 (d, *J* = 7.1 Hz, 2H), 5.74 (s, 2H), 3.71 – 3.68 (m, 2H), 3.31 – 3.28 (m, 2H), 1.96 – 1.90 (m, 2H), 1.88 – 1.84 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.4, 137.0, 131.9, 130.2, 129.9, 129.3, 129.2, 128.0, 126.2, 125.7, 125.5, 124.0, 122.9, 122.4, 121.5, 121.0, 120.7, 113.0, 54.1, 47.9, 43.6, 29.8, 25.6. FT-IR: $\tilde{\nu}$ = 2969, 2222, 1618, 1545, 1440, 1357, 1185 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{25}H_{22}N_3O$; 380.1757, found 380.1751.



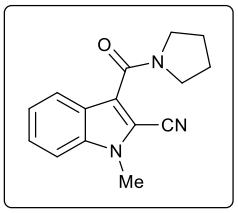
1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-pyrrolo[2,3-*b*]pyridine-4-carbonitrile (3k): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 62%, 40.9 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (m, 1H), 7.60 (s, 1H), 7.46 (m, 1H), 7.32 (s, 3H), 7.26 (d, *J* = 2.2 Hz, 2H), 5.52 (s, 2H), 3.72 (s, 2H), 3.40 (s, 2H), 1.95 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.2, 147.6, 143.6, 136.1, 130.7, 129.2, 128.5, 128.1, 121.0, 117.1, 116.2, 111.9, 111.8, 49.0, 48.7, 46.2, 26.2, 24.7. FT-IR: $\tilde{\nu}$ = 2970, 2847, 2231, 1595, 1525, 1452, 1344, 1186 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{19}N_4O$; 331.1553, found 331.1543.



1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile-2-d (3l): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 84%, 55.4 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.49 (m, 2H), 7.31 (d, *J* = 6.8 Hz, 3H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 6.2 Hz, 2H), 5.34 (s, 2H), 3.71 (s, 2H), 3.37 (s, 2H), 1.95 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.1, 136.0, 135.7, 130.4, 129.2, 128.4, 127.4, 127.1, 125.4, 122.2, 117.8, 115.2, 113.2, 103.5, 50.8, 48.9, 46.0, 26.0, 24.7. FT-IR: $\tilde{\nu}$ = 2969, 2876, 2221, 1604, 1534, 1424, 13441302, 1189 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{19}DN_3O$; 331.1664, found 331.1642.

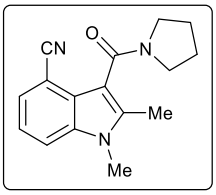


1-Methyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3m): Eluent: 100% ethyl acetate. Viscous gel. Yield 51%, 25.8 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.3 Hz, 1H), 7.52 (d, *J* = 7.4 Hz, 1H), 7.43 (s, 1H), 7.28 (t, *J* = 7.9 Hz, 1H), 3.83 (s, 3H), 3.72 (brs, 2H), 3.34 (brs, 2H), 1.97 (brs, 2H), 1.92 (brs, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.3, 136.5, 131.1, 127.3, 125.1, 122.0, 117.9, 114.7, 112.7, 103.3, 48.9, 46.0, 33.4, 25.9, 24.7. FT-IR: $\tilde{\nu}$ = 2922, 2853, 2221, 1604, 1537, 1458, 1345, 1301, 1153 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{15}H_{16}N_3O$; 254.1288, found 254.1290.

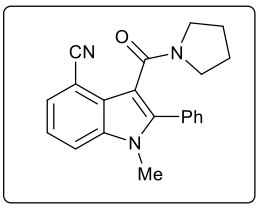


1-Methyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-2-carbonitrile (4m): Eluent: 40% ethyl acetate in hexane. Viscous gel. Yield 29%, 14.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.2 Hz, 1H), 7.43(m, 1H), 7.36 (d, *J* = 8.4 Hz, 1H), 7.26 (dd, *J* = 8.2, 6.9 Hz, 1H), 3.91 (s, 3H), 3.74 (brs, 2H), 3.53 (brs, 2H), 1.99 (brs, 2H), 1.91 (brs, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9, 137.6, 126.6, 124.5, 122.5, 122.3, 112.7, 110.4, 109.3, 48.7, 46.2, 31.8, 26.2, 24.7.

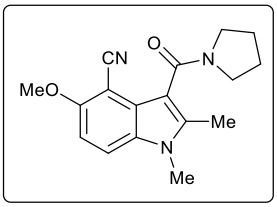
FT-IR: $\tilde{\nu}$ = 2873, 2226, 1609, 1537, 1423, 1326, 1226, 1164 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{15}H_{16}N_3O$; 254.1288, found 254.1284.



1,2-Dimethyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3n): Eluent: 100% ethyl acetate. Viscous gel. Yield 48%, 25.6 mg. ^{1}HNMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.2 Hz, 1H), 7.45 (d, *J* = 7.3 Hz, 1H), 7.20 (t, *J* = 7.8 Hz, 1H), 3.77 (s, 2H), 3.71 (s, 3H), 3.41 (s, 1H), 3.09 (d, *J* = 4.9 Hz, 1H), 2.51 (s, 3H), 2.04 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.1, 139.2, 136.5, 126.6, 125.0, 121.0, 118.1, 113.9, 101.7, 48.5, 45.9, 30.0, 25.9, 24.9, 11.6. FT-IR: $\tilde{\nu}$ = 2971, 2877, 2219, 1605, 1443, 1352, 1296, 1166 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{18}N_3O$; 268.1444, found 268.1449.

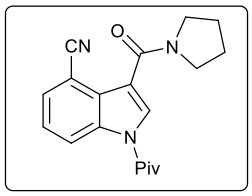


1-Methyl-2-phenyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3o): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 42%, 27.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.4 Hz, 1H), 7.63 (d, *J* = 8.1 Hz, 1H), 7.52 (d, *J* = 7.1 Hz, 3H), 7.47 – 7.36 (m, 3H), 3.59 (s, 3H), 3.43 (t, *J* = 6.4 Hz, 2H), 2.93 (t, *J* = 6.7 Hz, 2H), 1.80 – 1.71 (m, 2H), 1.70 – 1.61 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 186.5, 164.5, 149.6, 137.7, 130.8, 130.7, 130.3, 129.2, 128.4, 125.8, 123.4, 118.7, 114.8, 113.0, 105.4, 47.0, 45.4, 31.3, 25.9, 23.8. FT-IR: $\tilde{\nu}$ = 2923, 2222, 1634, 1431, 1352, 1133 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{20}N_3O$; 330.1601, found 330.1589.

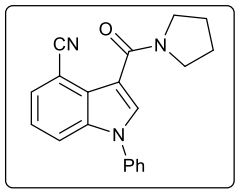


5-Methoxy-1,2-dimethyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3p); Eluent: 100% ethyl acetate. Viscous gel. Yield 43%, 25.5 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ

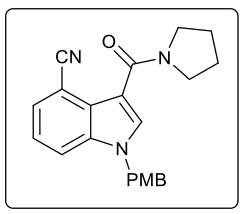
7.38 (d, *J* = 8.8 Hz, 1H), 6.82 (d, *J* = 8.9 Hz, 1H), 3.93 (s, 3H), 3.81 – 3.69 (m, 2H), 3.66 (s, 3H), 3.40 (m, 1H), 3.05 (m, 1H), 2.47 (s, 3H), 2.08 – 1.91 (m, 3H), 1.81 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 140.1, 131.6, 126.9, 125.6, 115.6, 114.6, 105.7, 57.0, 48.4, 45.9, 30.0, 25.9, 24.9, 11.5. FT-IR: $\tilde{\nu}$ = 2954, 2231, 1721, 1642, 1482, 1438, 1285 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{20}N_3O_2$; 298.1550, found 298.1554.



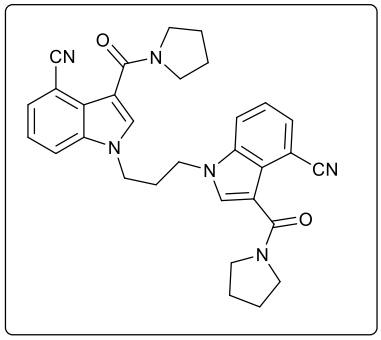
1-Pivaloyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3q): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 75%, 48.4 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (d, *J* = 8.5 Hz, 1H), 8.03 (s, 1H), 7.63 (d, *J* = 7.5 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 3.74 (brs, 2H), 3.31 (brs, 2H), 1.98 (brs, 4H), 1.51 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 177., 162.6, 136.7, 129.7, 126.7, 126.4, 125.7, 122.3, 118.3, 116.8, 103.4, 48.6, 46.0, 41.7, 28.7, 26.0, 24.7. FT-IR: $\tilde{\nu}$ = 2924, 2223, 1712, 1592, 1442, 1332, 1289, 1178 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{22}N_3O_2$; 324.1707, found 324.1703.



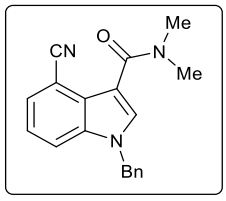
1-Phenyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3r): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 63%, 39.7 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.66 (m, 2H), 7.60 – 7.52 (m, 3H), 7.46 (d, *J* = 4.3 Hz, 3H), 7.29 (m, 1H), 3.76 (brs, 2H), 3.43 (brs, 2H), 1.97 (brs, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 137.9, 135.9, 130.1, 129.8, 128.2, 127.9, 125.6, 125.0, 122.9, 117.7, 116.0, 114.5, 103.4, 48.9, 46.0, 26.0, 24.7. FT-IR: $\tilde{\nu}$ = 2923, 2874, 2220, 1616, 1545, 1499, 1445, 1371, 1294, 1168 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{20}H_{18}N_3O$; 316.1444, found 316.1450.



1-(4-Methoxybenzyl)-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3s): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 83%, 59.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.3 Hz, 1H), 7.54 (d, *J* = 7.9 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.14 (d, *J* = 8.3 Hz, 2H), 6.89 (d, *J* = 8.3 Hz, 2H), 5.31 (s, 2H), 3.81 (brs, 3H), 3.72 (brs, 2H), 3.39 (brs, 2H), 1.98 (brs, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 159.7, 135.9, 130.7, 128.8, 127.5, 127.4, 125.3, 122.2, 117.9, 115.4, 114.5, 111.9, 103.2, 55.4, 50.4, 49.1, 46.2, 25.9, 24.6. FT-IR: $\tilde{\nu}$ = 2970, 2878, 2222, 1609, 1514, 1441, 1346, 1303, 1249, 1177 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{22}N_3O_2$; 360.1707, found 360.1691.

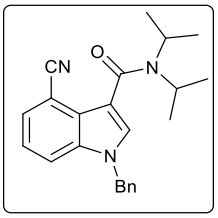


1,1'-(Propane-1,3-diyl)bis(3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile) (3t): Eluent: 10% methanol in ethyl acetate. Viscous gel. Yield 71%, 73.5 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.3 Hz, 2H), 7.44 (s, 2H), 7.37 (d, *J* = 8.2 Hz, 2H), 7.20 (t, *J* = 7.8 Hz, 2H), 4.16 (brs, 4H), 3.71 (brs, 4H), 3.30 (brs, 4H), 2.40 (brs, 2H), 1.97 (brs, 4H), 1.90 (brs, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.9, 135.6, 129.4, 127.5, 125.2, 122.4, 117.7, 114.6, 113.8, 103.6, 48.8, 46.0, 43.7, 30.1, 26.0, 24.7. FT-IR: $\tilde{\nu}$ = 2925, 2875, 2221, 1603, 1535, 1447, 1346, 1301, 1192 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{31}H_{31}N_6O_2$; 519.2503, found 519.2518.

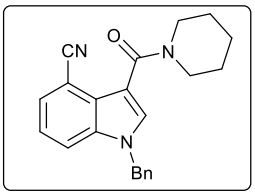


1-Benzyl-4-cyano-*N*,*N*-dimethyl-1*H*-indole-3-carboxamide (3u): Eluent: 100% ethyl acetate. Viscous gel. Yield 86%, 52.1 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (m, 2H), 7.50 (s, 1H), 7.33 (m, 3H), 7.25 (m, 1H), 7.14 (d, *J* = 6.9 Hz, 2H), 5.35 (s, 2H), 3.17 (s, 3H), 3.04 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 166.2, 136.0, 135.6, 131.2, 130.0, 128.4, 127.5, 127.2, 125.7, 122.3, 117.8, 115.4, 111.8, 111.7, 103.3, 50.8, 39.3, 35.1. FT-IR: $\tilde{\nu}$ = 2926, 2222,

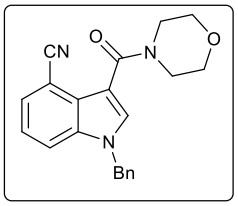
1621, 1540, 1455, 1394, 1262, 1143 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{18}N_3O$; 304.1444, found 304.1442.



1-Benzyl-4-cyano-*N*,*N*-diisopropyl-1*H*-indole-3-carboxamide (3v): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 58%, 41.6 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 – 7.47 (m, 2H), 7.36 – 7.20 (m, 5H), 7.12 (d, *J* = 6.6 Hz, 2H), 5.34 (s, 2H), 3.83 (brs, 2H), 1.40 (brs, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.0, 136.1, 136.0, 129.2, 128.4, 128.1, 127.11, 127.09, 126.0, 122.3, 117.8, 114.9, 114.0, 103.5, 50.7, 47.0, 20.9. FT-IR: $\tilde{\nu}$ = 2971, 2222, 1618, 1537, 1434, 1618, 1288, 1209, 1157 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{23}H_{26}N_3O$; 360.2070, found 360.2056.

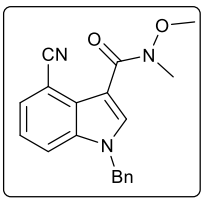


1-Benzyl-3-(piperidine-1-carbonyl)-1*H*-indole-4-carbonitrile (3w): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 66%, 45.3 mg. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 – 7.50 (m, 2H), 7.46 (s, 1H), 7.32 (p, *J* = 6.0 Hz, 3H), 7.24 (t, *J* = 7.9 Hz, 1H), 7.15 (d, *J* = 7.2 Hz, 2H), 5.34 (s, 2H), 3.63 (brs, 4H), 1.67 (brs, 2H), 1.60 (s, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.4, 136.1, 135.7, 130.7, 129.2, 128.5, 127.5, 127.2, 127.7, 125.8, 122.3, 118.0, 115.2, 112.1, 103.4, 50.9, 26.0, 24.7. FT-IR: $\tilde{\nu}$ = 2936, 2856, 2222, 1615, 1537, 1433, 1345, 1257, 1212 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{22}H_{22}N_3O$; 344.1757, found 344.1742.

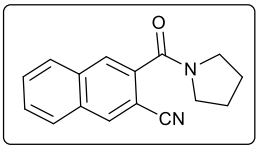


1-Benzyl-3-(morpholine-4-carbonyl)-1*H*-indole-4-carbonitrile (3x): Eluent: 80% ethyl acetate in hexane. Viscous gel. Yield 71%, 49 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.7, 4.6 Hz, 2H), 7.51 (s, 1H), 7.35 (d, *J* = 5.8 Hz, 3H), 7.29 (d, *J* = 6.1 Hz, 1H), 7.17 (d, *J* =

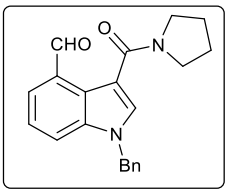
7.4 Hz, 2H), 5.37 (s, 2H), 3.75 (brs, 8H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.7, 136.1, 135.5, 131.0, 129.2, 128.5, 127.6, 127.2, 125.6, 122.5, 118.0, 115.4, 111.0, 103.2, 66.7, 53.5, 50.9. FT-IR: $\tilde{\nu}$ = 2909, 2854, 2224, 1618, 1537, 1430, 1343, 1250, 1109 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{20}N_3O_2$; 346.1550, found 346.1550.



1-Benzyl-4-cyano-*N*-methoxy-*N*-methyl-1*H*-indole-3-carboxamide (3y): Eluent: 70% ethyl acetate in hexane. Viscous gel. Yield 78%, 49.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (s, 1H), 7.57 (d, *J* = 7.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.31 (d, *J* = 6.5 Hz, 3H), 7.23 (t, *J* = 7.9 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 2H), 5.37 (s, 2H), 3.55 (s, 3H), 3.42 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.3, 136.2, 135.6, 133.3, 129.2, 128.5, 128.4, 127.0, 126.4, 122.3, 118.7, 115.0, 109.7, 104.7, 61.1, 50.8, 33.5. FT-IR: $\tilde{\nu}$ = 2924, 2220, 1616, 1537, 1454, 1384, 1336, 1268, 1179 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{19}H_{18}N_3O_2$; 320.1394, found 320.1394.

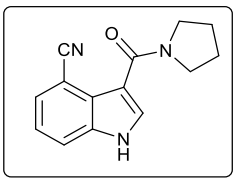


3-(Pyrrolidine-1-carbonyl)-2-naphthonitrile (**3z,** major isomer); Eluent: 60% ethyl acetate in hexane. Viscous gel. Yield 82%, 41.2 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 7.95 (s, 1H), 7.93 – 7.85 (m, 2H), 7.68-7.63 (m, 2H), 3.76-3.72 (m, 2H), 3.39 – 3.32 (m, 2H), 2.05 – 1.98 (m, 2H), 1.95 – 1.90 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 135.6, 134.2, 133.8, 132.1, 129.9, 128.6, 128.5, 128.4, 127.4, 117.6, 107.2, 48.9, 46.2, 26.2, 24.5. FT-IR: $\tilde{\nu}$ = 2972, 2879, 2225, 1630, 1474, 1420, 1341, 1192 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{16}H_{15}N_2O$; 251.1179, found 251.1184.

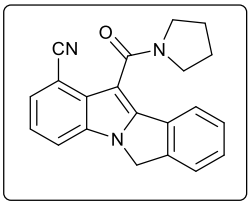


1-Benzyl-3-(pyrrolidine-1-carbonyl)-1*H*-indole-4-carbaldehyde (5): Eluent: 100% ethyl acetate. Viscous gel. Yield 87%, 57.8 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.36 (s, 1H), 7.76

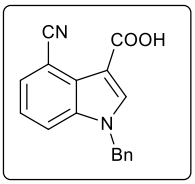
(d, *J* = 7.1 Hz, 1H), 7.56 (d, *J* = 8.2 Hz, 1H), 7.47 (s, 1H), 7.32 (d, *J* = 7.2 Hz, 4H), 7.14 (d, *J* = 5.7 Hz, 2H), 5.37 (s, 2H), 3.73 (brs, 2H), 3.23 (brs, 2H), 1.95 (brs, 2H), 1.85 (brs, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.0, 166.9, 137.1, 136.1, 131.0, 129.6, 129.2, 128.4, 127.1, 125.7, 123.6, 122.3, 116.3, 113.5, 50.8, 29.8, 25.3. FT-IR: $\tilde{\nu}$ = 2925, 1676, 1605, 1534, 1455, 1345, 1247 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{21}N_2O_2$; 333.1598, found 333.1601.



3-(Pyrrolidine-1-carbonyl)-1*H*-indole-4-carbonitrile (6): Eluent: 5% methanol in ethyl. Brown solid. Yield 92%, 44 mg. ^{1}H NMR (400 MHz, DMSO- D_6) δ 12.03 (s, 1H), 7.88 (t, *J* = 2.6 Hz, 1H), 7.80 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.58 (dd, *J* = 7.0, 2.0 Hz, 1H), 7.30 (m, 1H), 3.50 (brs, 2H), 3.37 (brs, 2H), 1.85 (brs, 4H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 163.3, 135.8, 128.4, 127.0, 124.2, 121.7, 118.1, 117.4, 112.2, 101.7, 48.0, 45.4, 25.6, 24.1. FT-IR: $\tilde{\nu}$ = 3415, 2981, 2254, 1660, 1542, 1456, 1436, 1248 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{14}N_{14}N_3O$; 240.1131, found 240.1128.

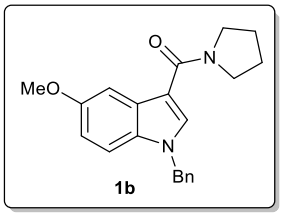


11-(Pyrrolidine-1-carbonyl)-6*H*-isoindolo[2,1-a]indole-1-carbonitrile (7); Eluent: 60% ethyl acetate in hexane. Viscous gel. Yield 72%, 47 mg. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 6.0, 2.0 Hz, 1H), 7.50 (d, *J* = 8.2 Hz, 1H), 7.36 (d, *J* = 6.8 Hz, 1H), 7.31 (d, *J* = 7.4 Hz, 1H), 7.27 – 7.22 (m, 2H), 7.11 (t, *J* = 7.8 Hz, 1H), 5.23 (d, *J* = 16.9 Hz, 1H), 4.94 (d, *J* = 16.8 Hz, 1H), 3.89 – 3.75 (m, 2H), 3.45 (m, 1H), 3.09 (m, 1H), 2.06 (m, 1H), 2.0-1.91 (m, 2H), 1.76 (m, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.2, 145.0, 142.1, 133.1, 130.7, 129.0, 128.9, 128.5, 126.9, 123.6, 122.9, 121.6, 118.1, 114.7, 103.3, 103.0, 49.1, 48.5, 45.9, 26.0, 24.8. FT-IR: $\tilde{\nu}$ = 2924, 2870, 2218, 1605, 1436, 1348, 1208, 1168 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{21}H_{18}N_3O$; 328.1444, found 328.1445.



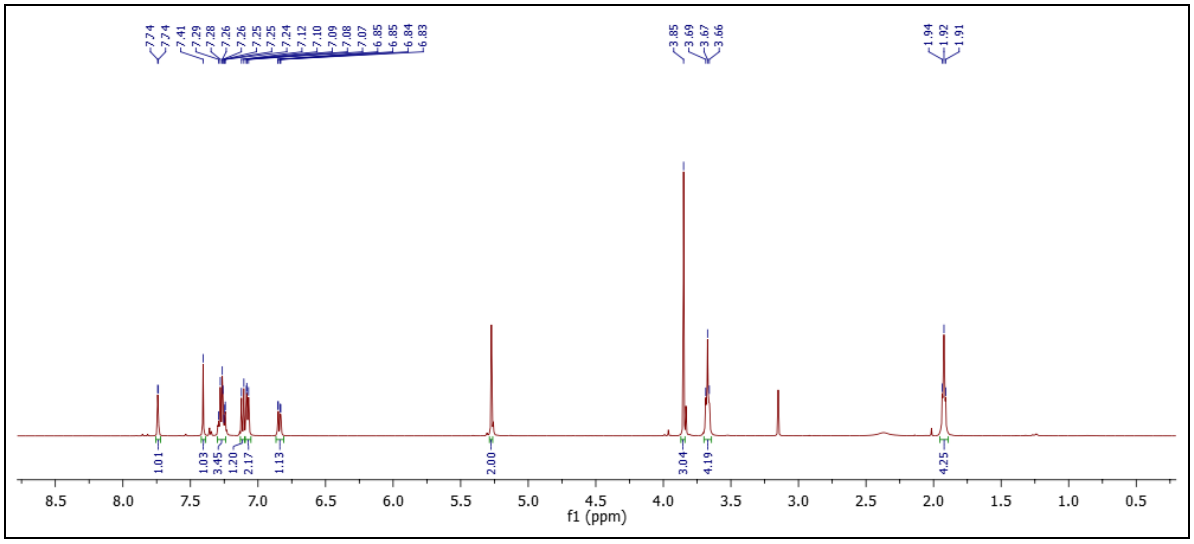
1-Benzyl-4-cyano-1*H*-indole-3-carboxylic acid (8): Eluent: 60% ethyl acetate in hexane. White solid. Yield 89%, 49.2 mg. ^{1}H NMR (400 MHz, DMSO-D_6) δ 12.42 (s, 1H), 8.47 (s, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 7.4 Hz, 1H), 7.37 – 7.30 (m, 3H), 7.27 (d, *J* = 7.3 Hz, 3H), 5.58 (s, 2H). ^{13}C NMR (125 MHz, DMSO-D_6) δ 164.1, 138.2, 137.0, 136.5, 130.0, 128.7, 127.8, 127.2, 124.6, 122.4, 118.6, 116.5, 107.2, 103.3, 49.6. FT-IR: $\tilde{\nu}$ = 3396, 2224, 1697, 1530, 1456, 1402, 1338, 1192 cm^{-1}. HRMS: Calculated for $[M+H]^+$ $C_{17}H_{13}N_2O_2$; 277.0972, found 277.0970.

Spectra:

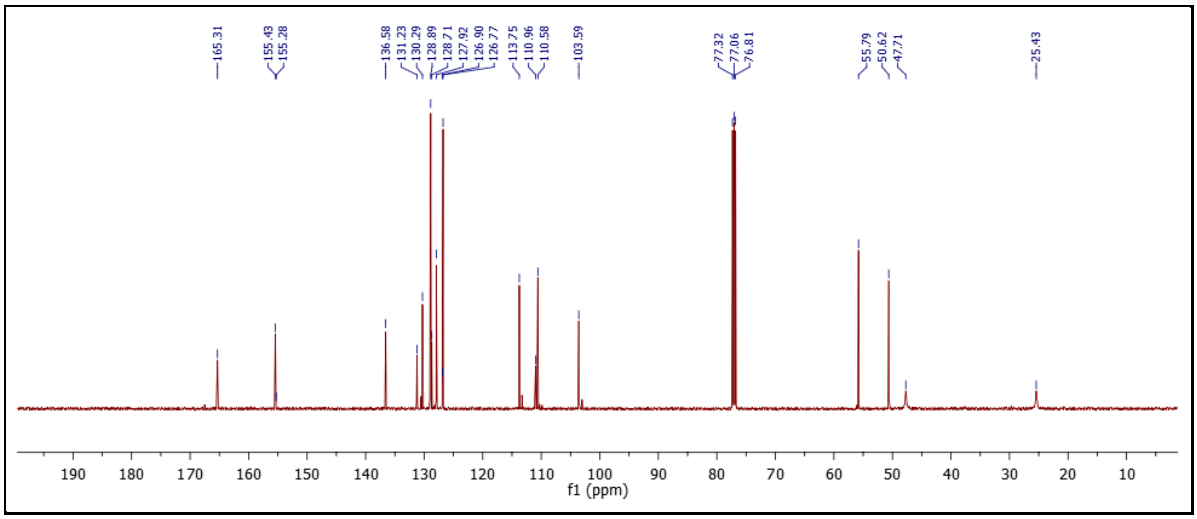


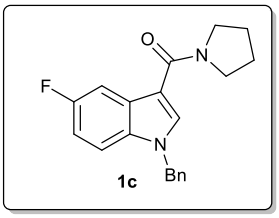
1b

^{1}H NMR (500 MHz, $CDCl_3$)

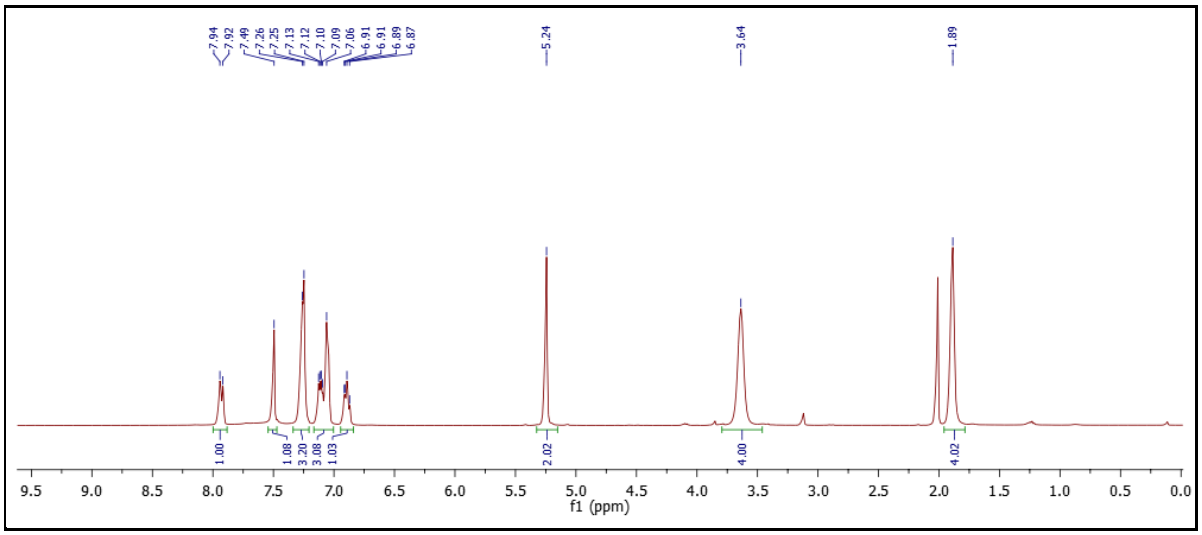


^{13}C NMR (125 MHz, $CDCl_3$)

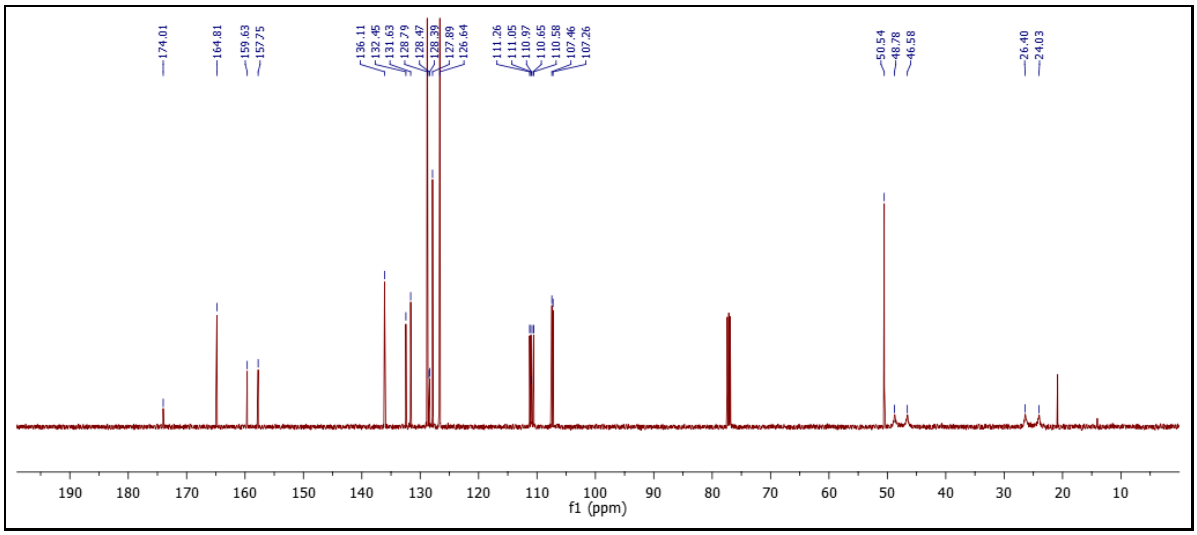


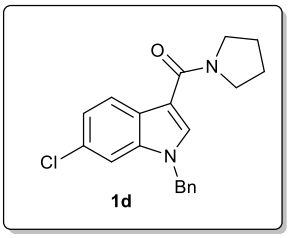


^{1}H NMR (400 MHz, $CDCl_3$)



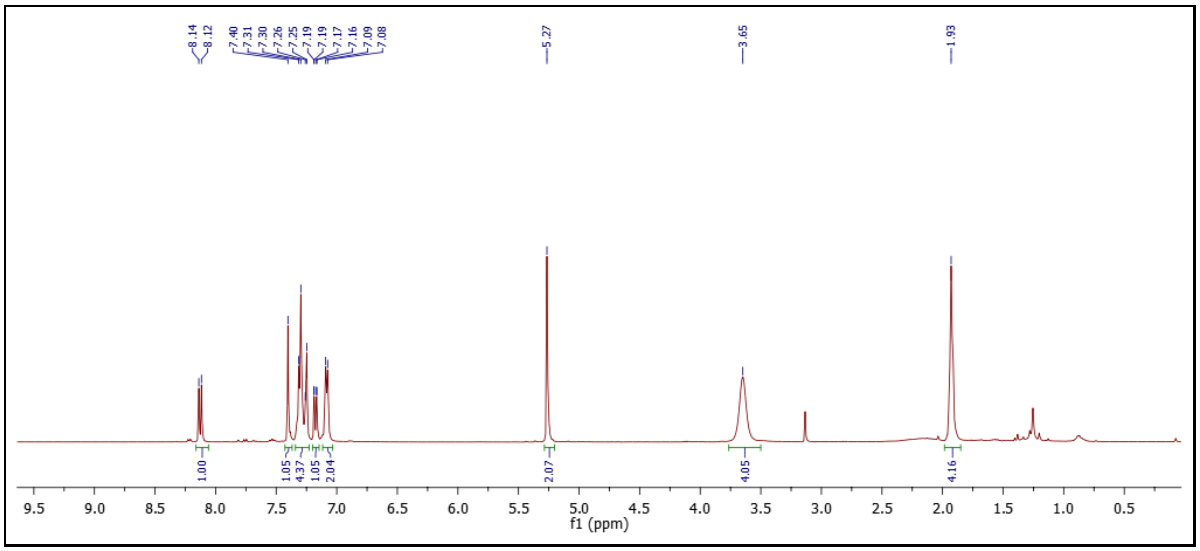
^{13}C NMR (126 MHz, $CDCl_3$)



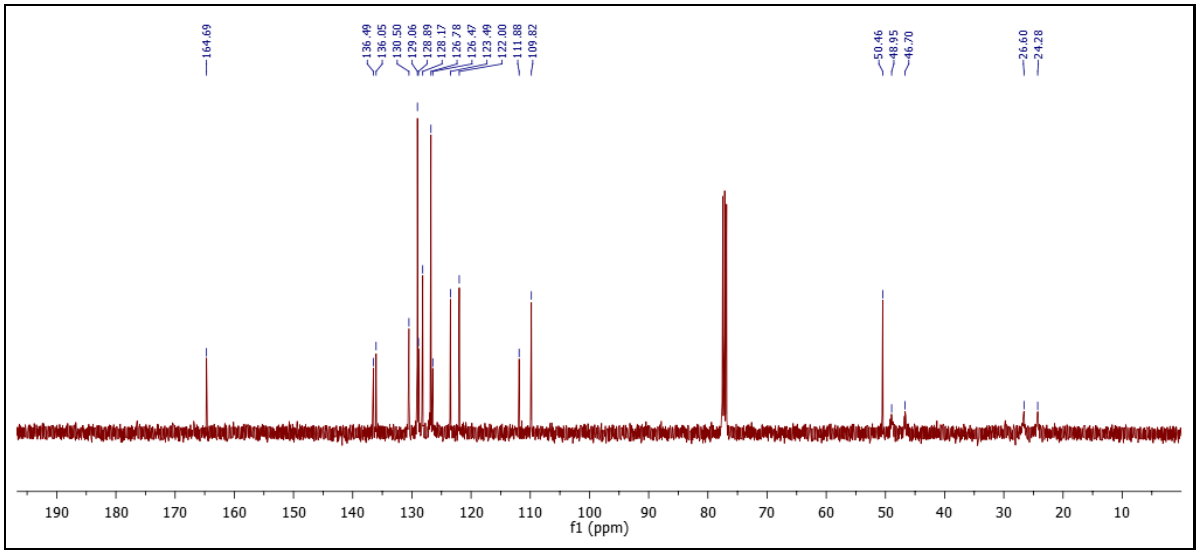


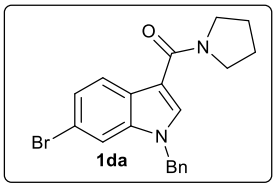
1d

^{1}H NMR (400 MHz, $CDCl_3$)



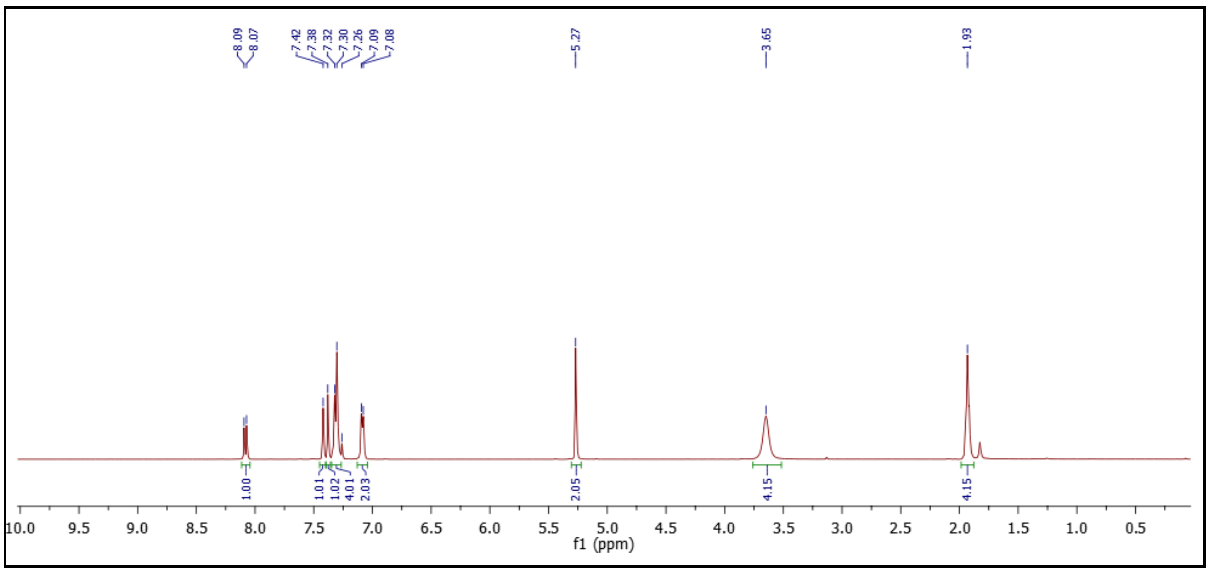
^{13}C NMR (100 MHz, $CDCl_3$)



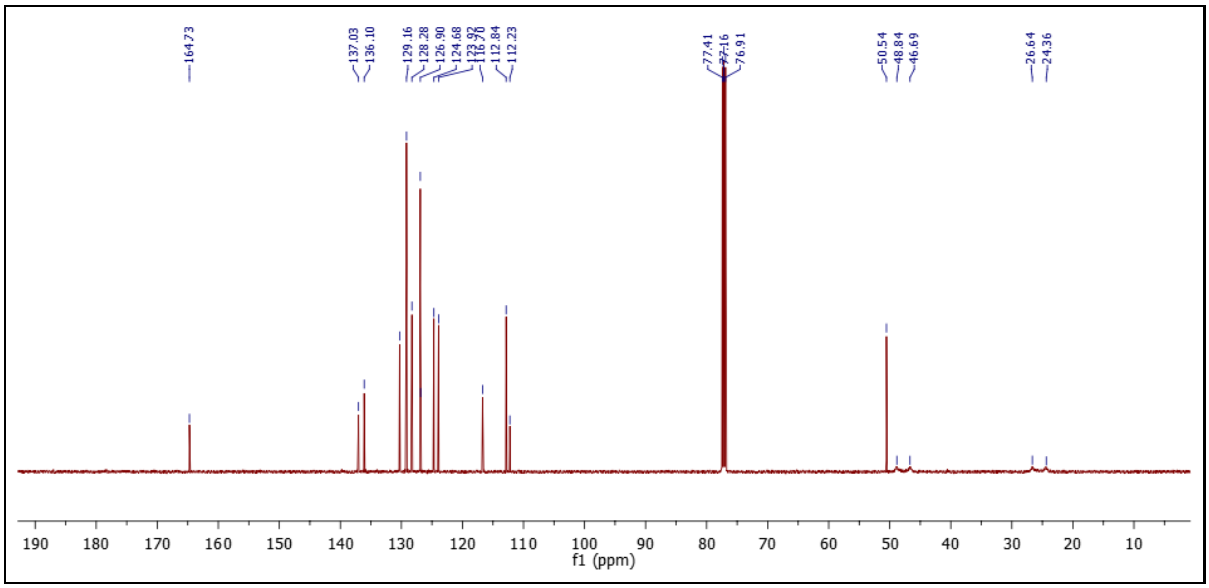


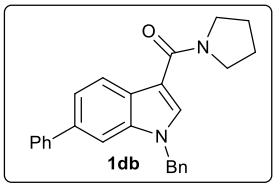
1da

^{1}H NMR (400 MHz, $CDCl_3$)

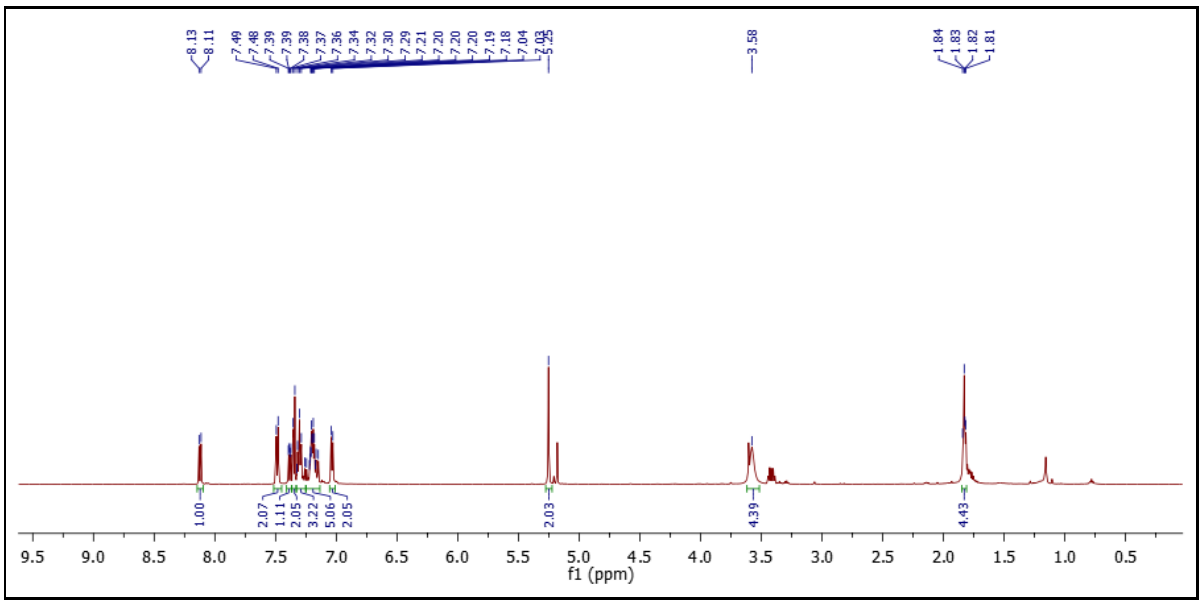


^{13}C NMR (125 MHz, $CDCl_3$)

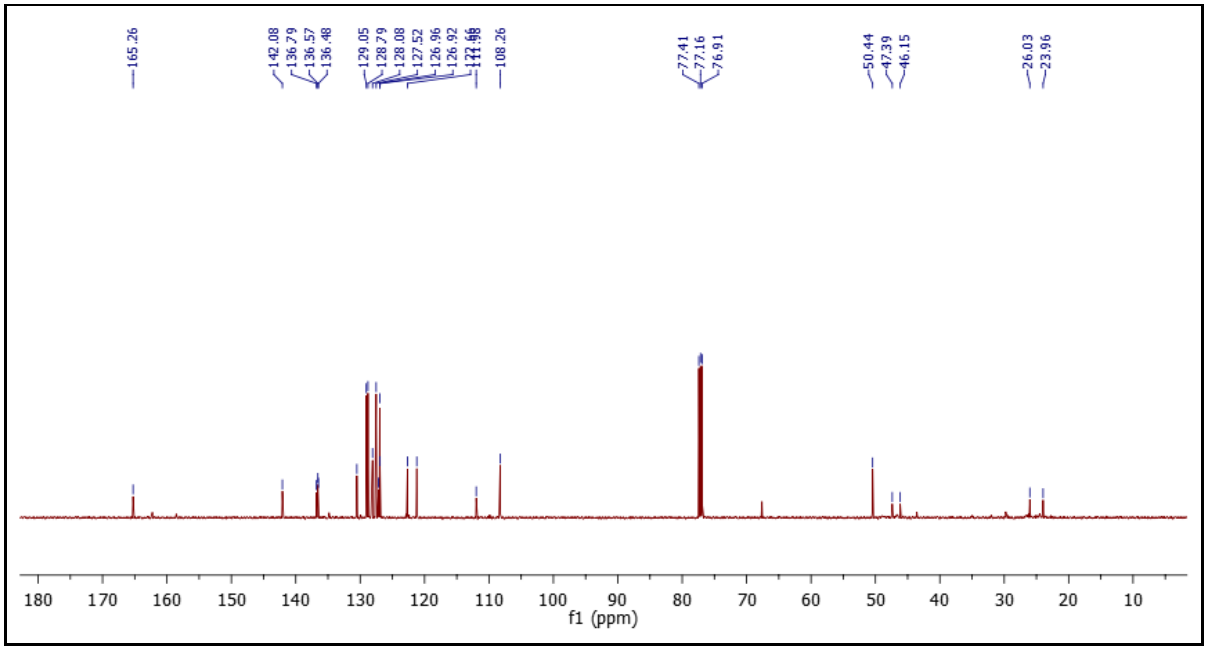


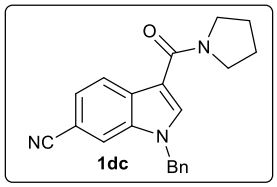


^{1}H NMR (500 MHz, $CDCl_3$)



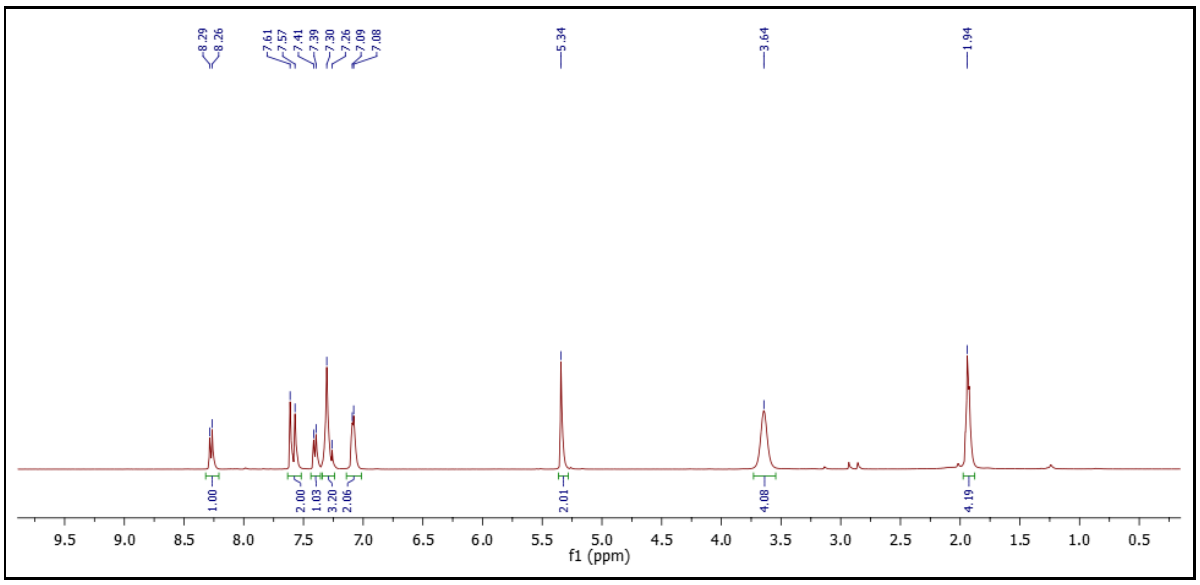
^{13}C NMR (125 MHz, $CDCl_3$)



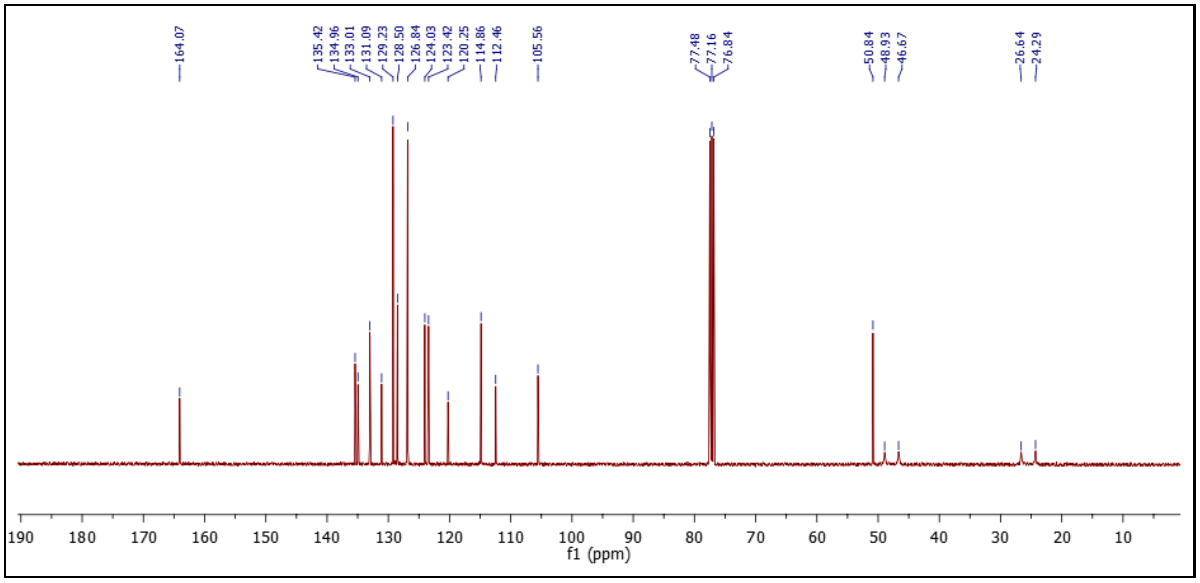


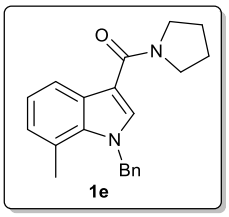
1dc

^{1}H NMR (400 MHz, $CDCl_3$)



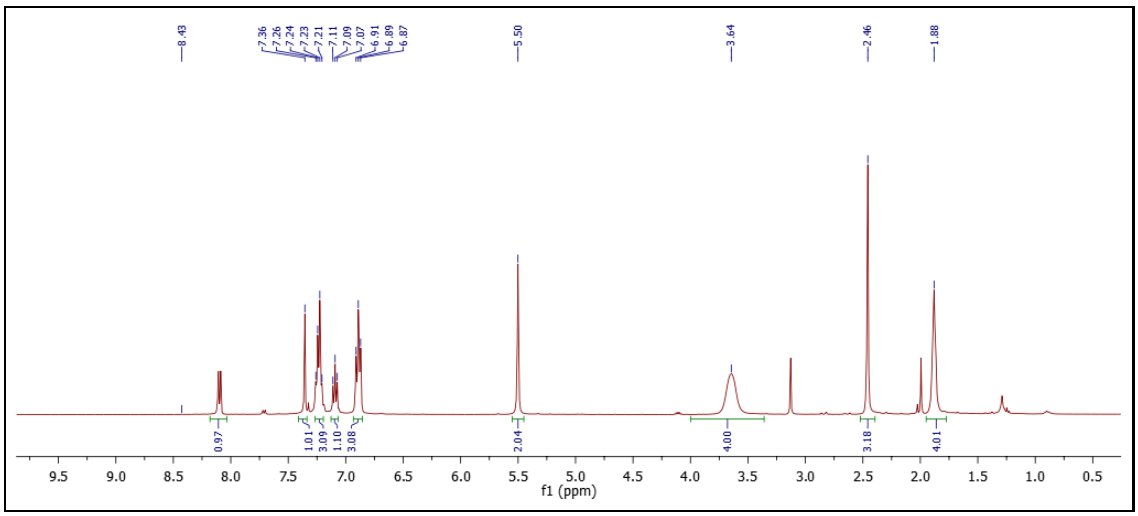
^{13}C NMR (100 MHz, $CDCl_3$)



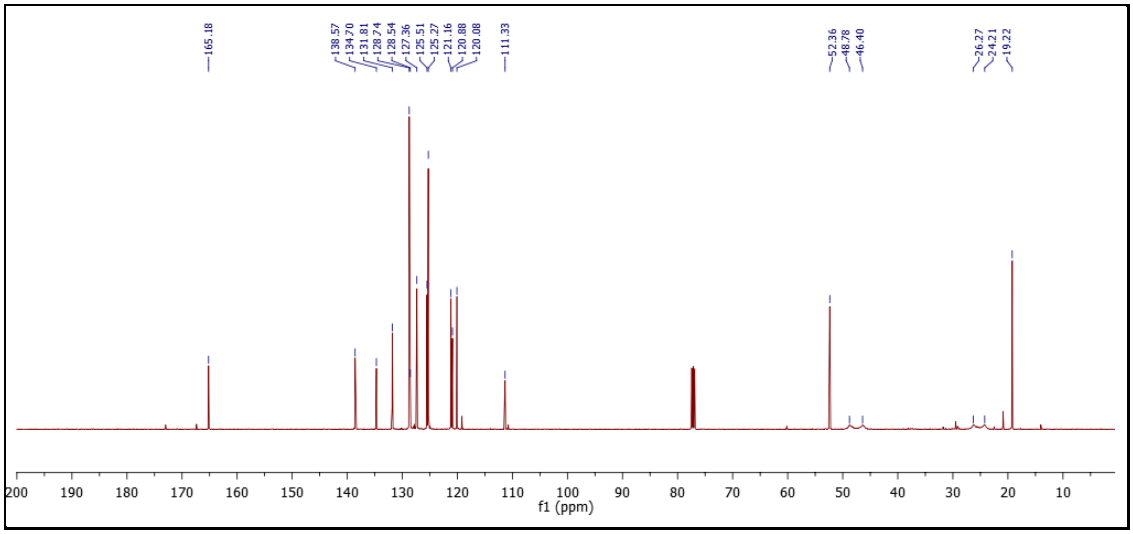


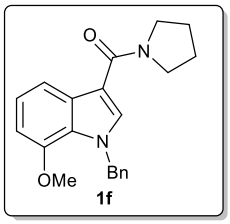
1e

^{1}H NMR (400 MHz, $CDCl_3$)



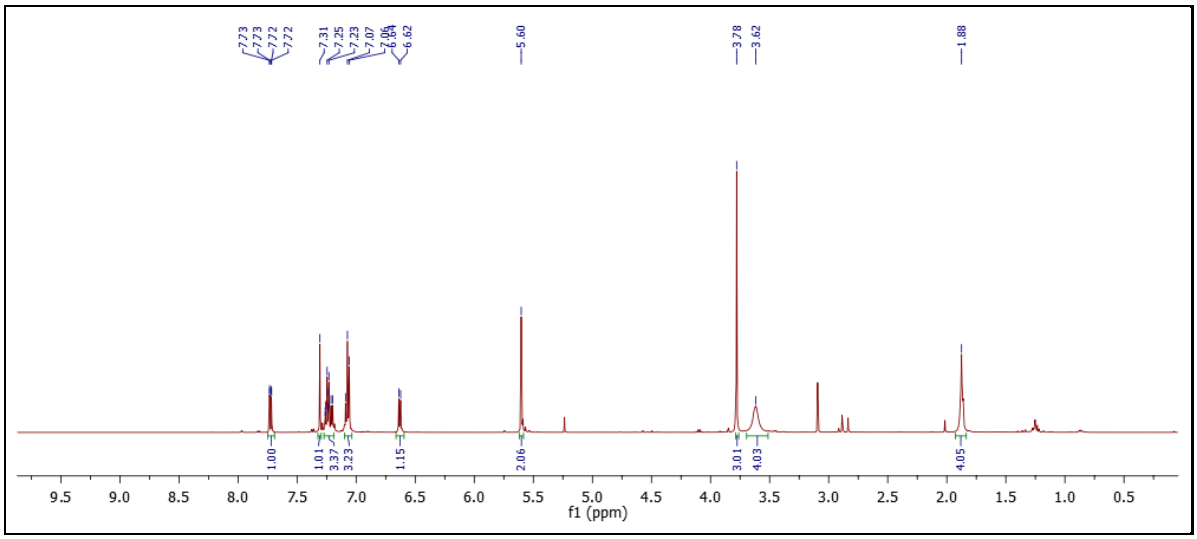
^{13}C NMR (125 MHz, $CDCl_3$)



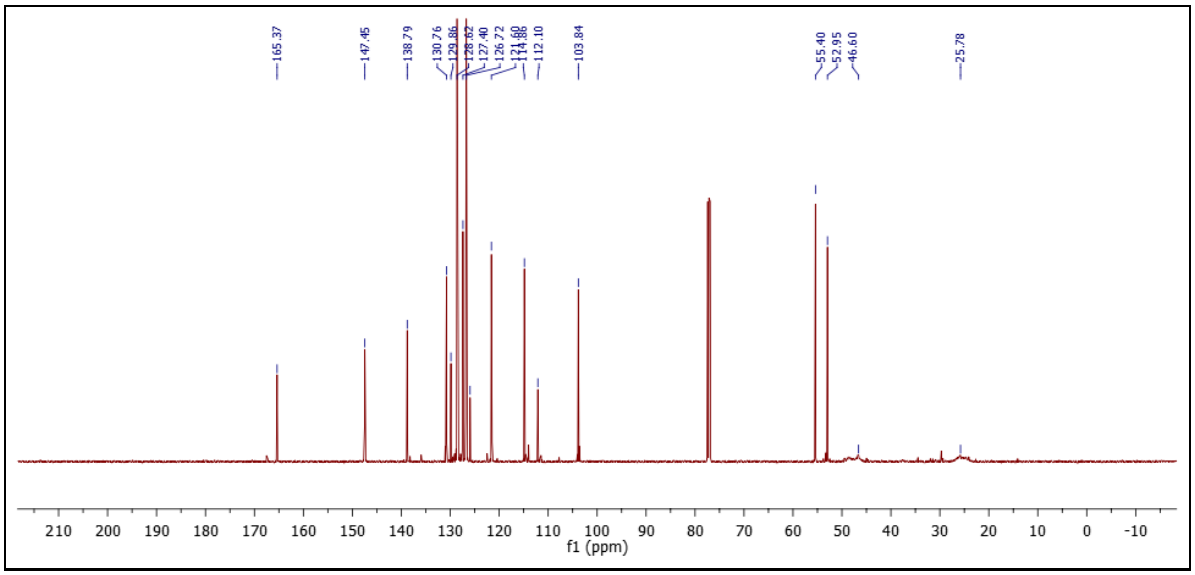


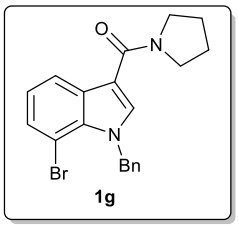
1f

^{1}H NMR (500 MHz, $CDCl_3$)



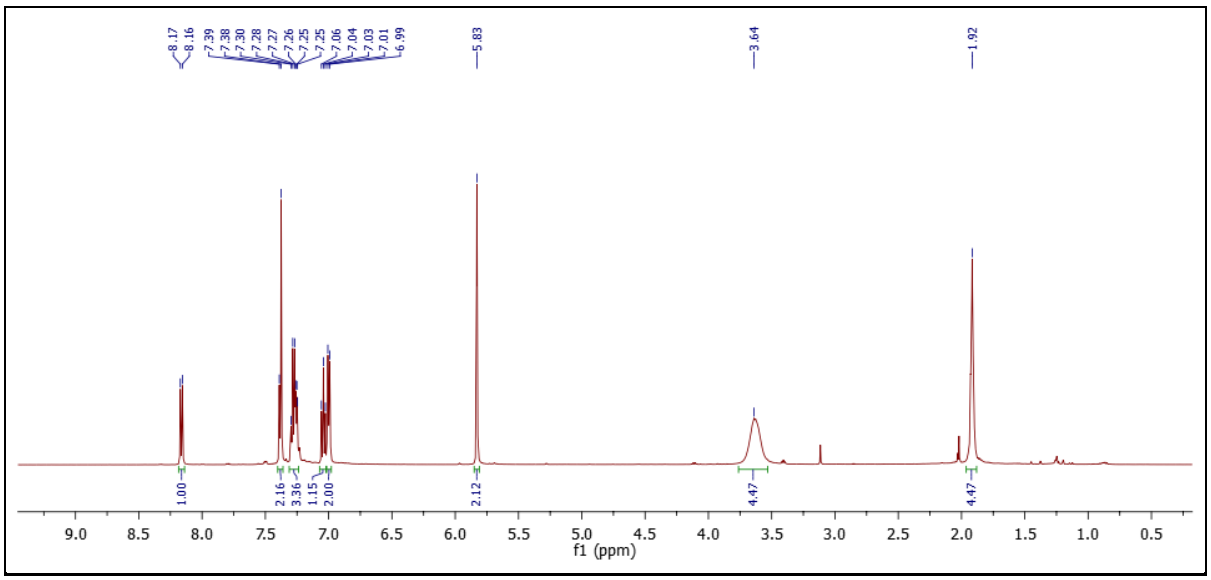
^{13}C NMR (125 MHz, $CDCl_3$)



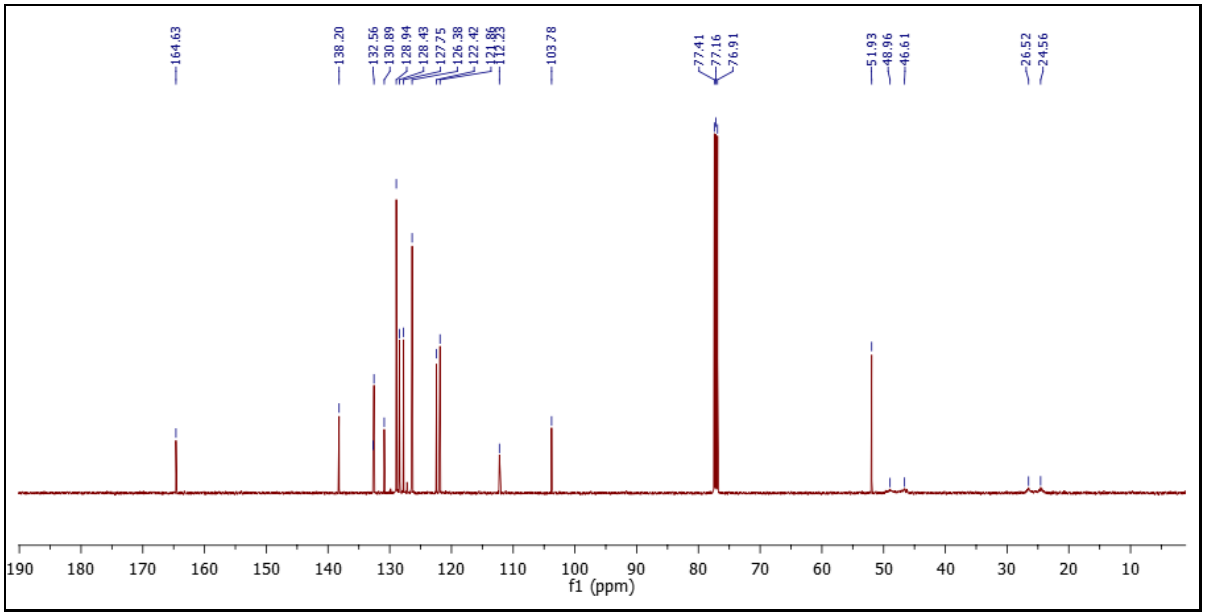


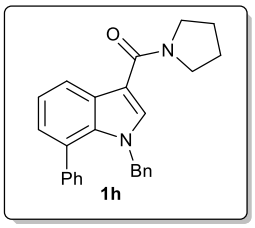
1g

^{1}H NMR (500 MHz, $CDCl_3$)



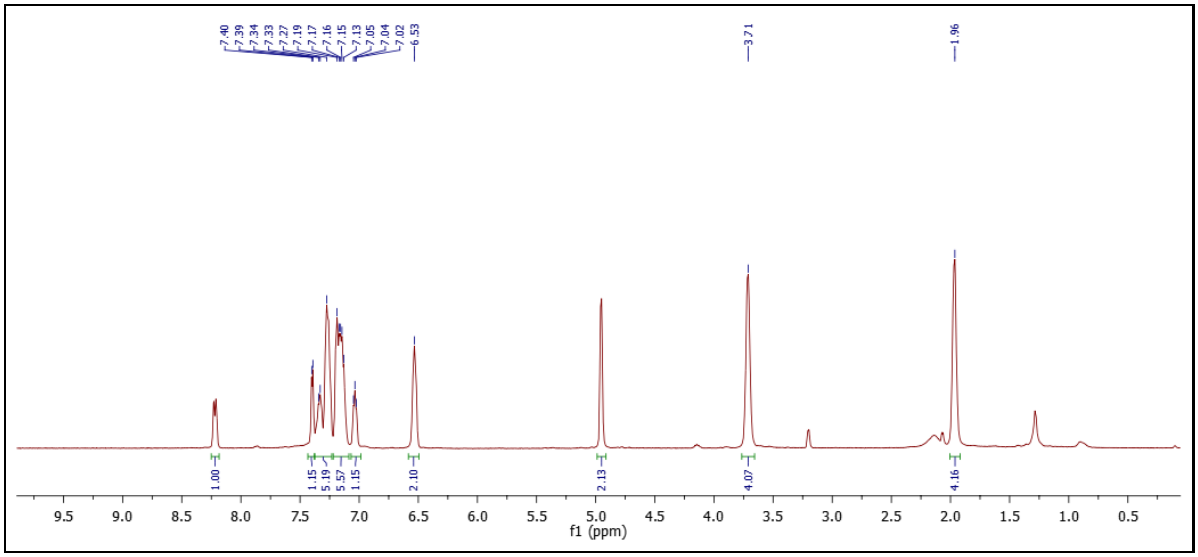
^{13}C NMR (125 MHz, $CDCl_3$)



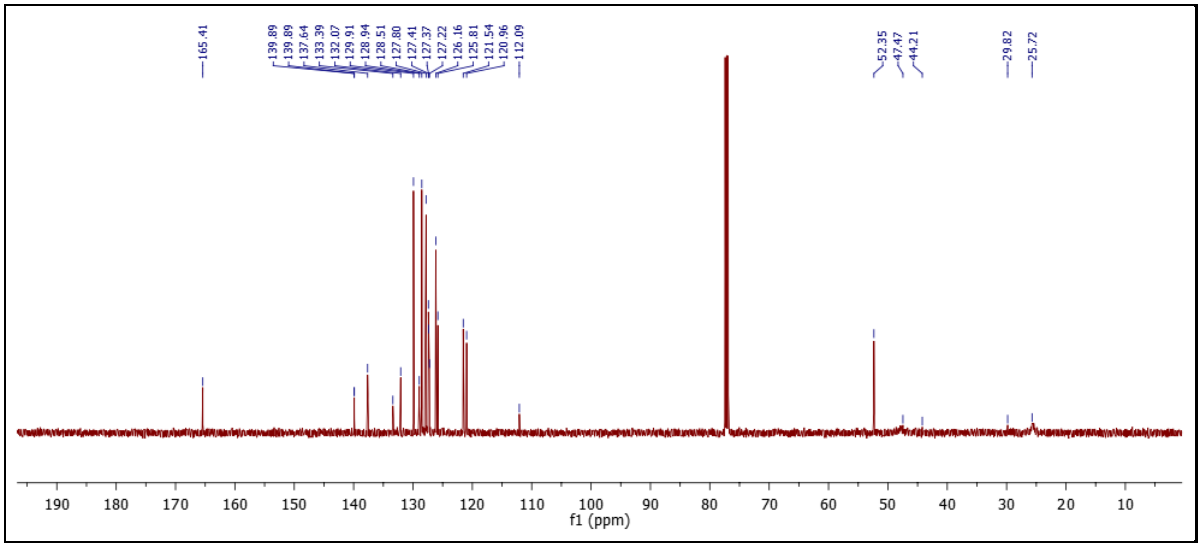


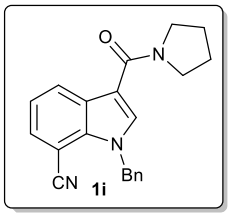
1h

^{1}H NMR (400 MHz, $CDCl_3$)

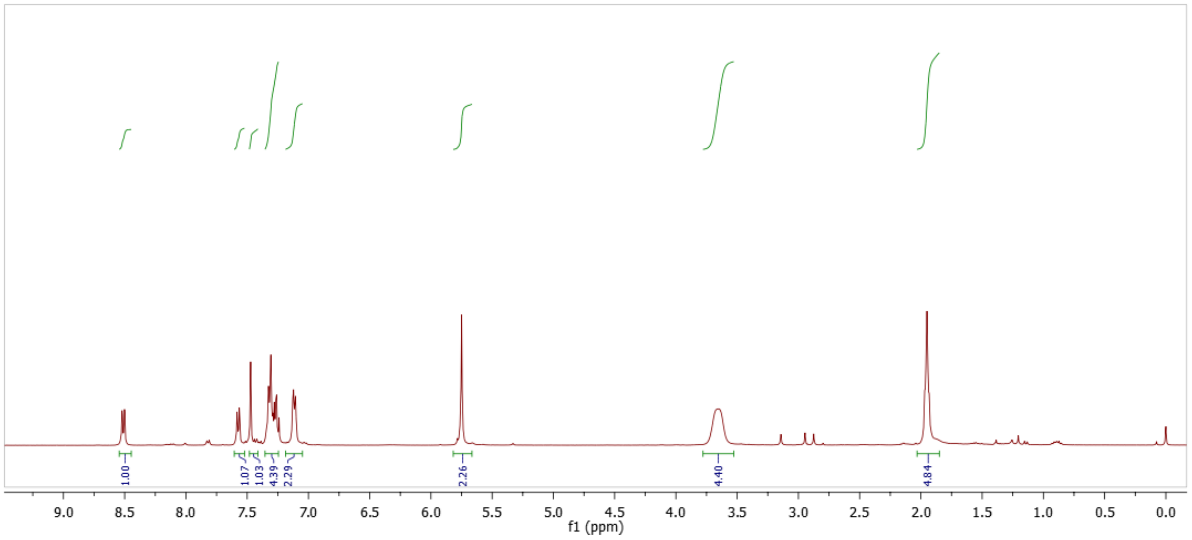


^{13}C NMR (125 MHz, $CDCl_3$)

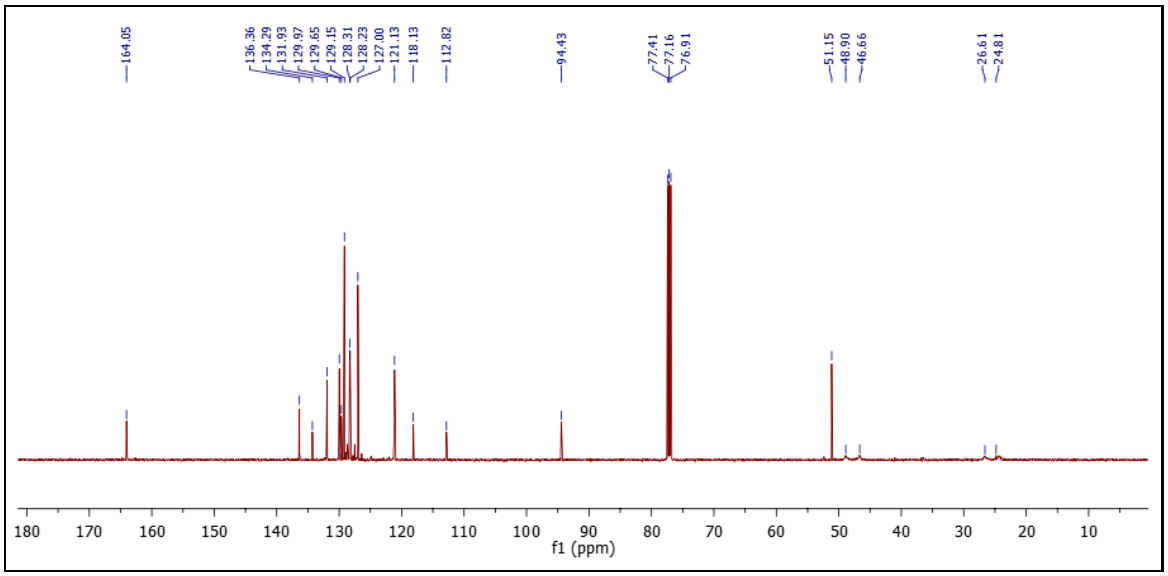


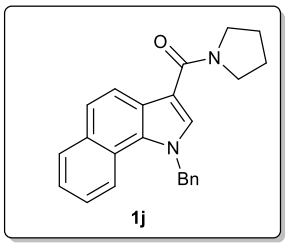


^{1}H NMR (400 MHz, $CDCl_3$)



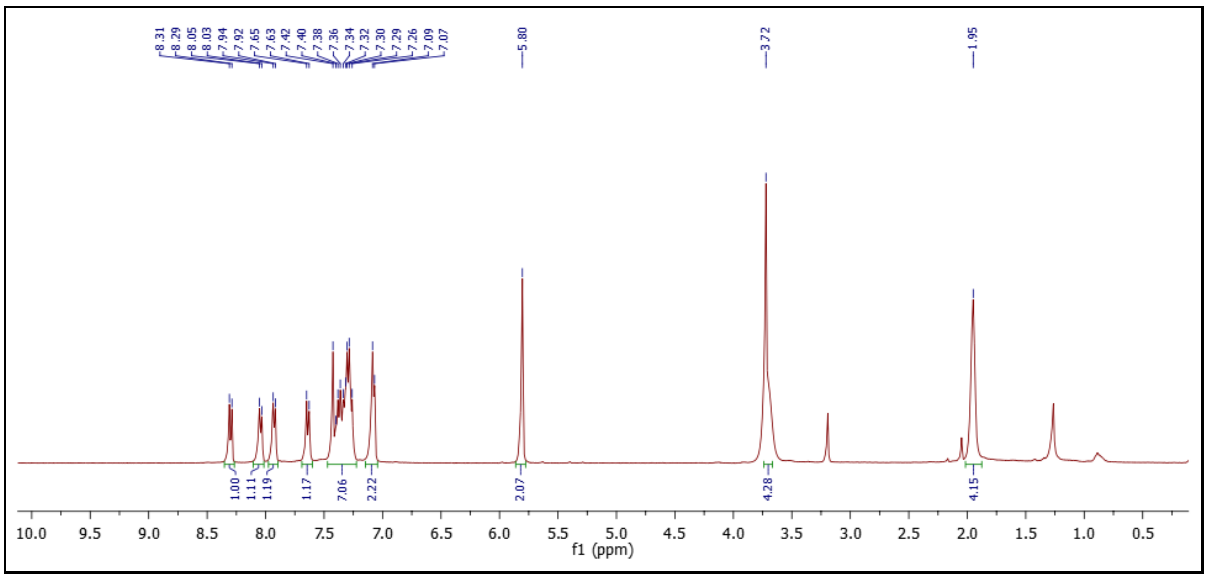
^{13}C NMR (125 MHz, $CDCl_3$)



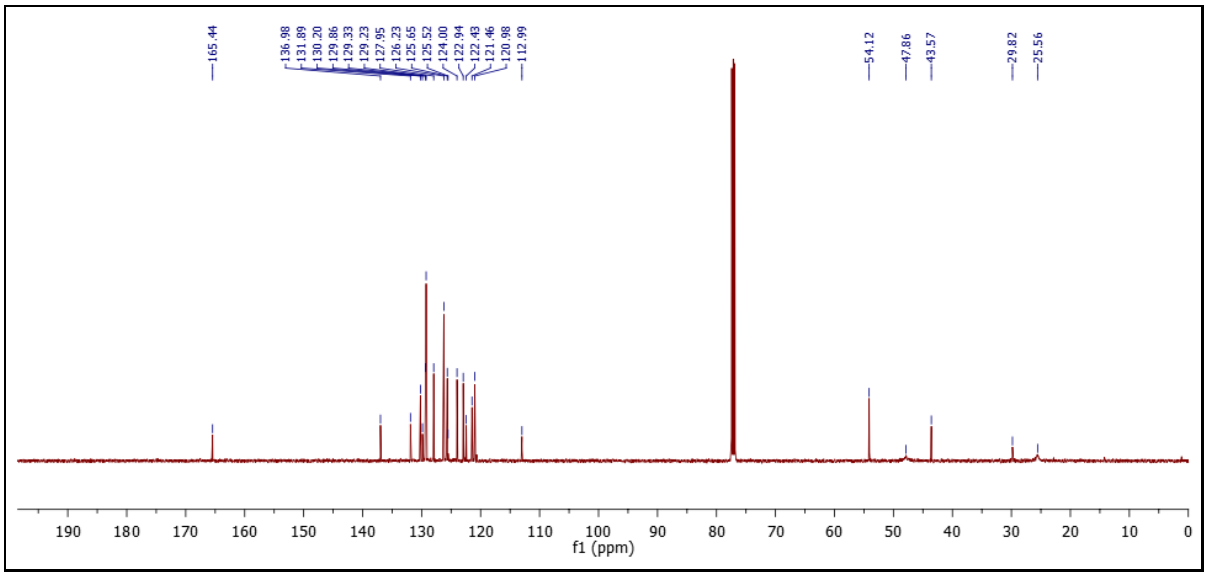


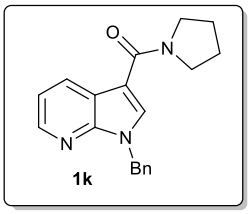
1j

^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)





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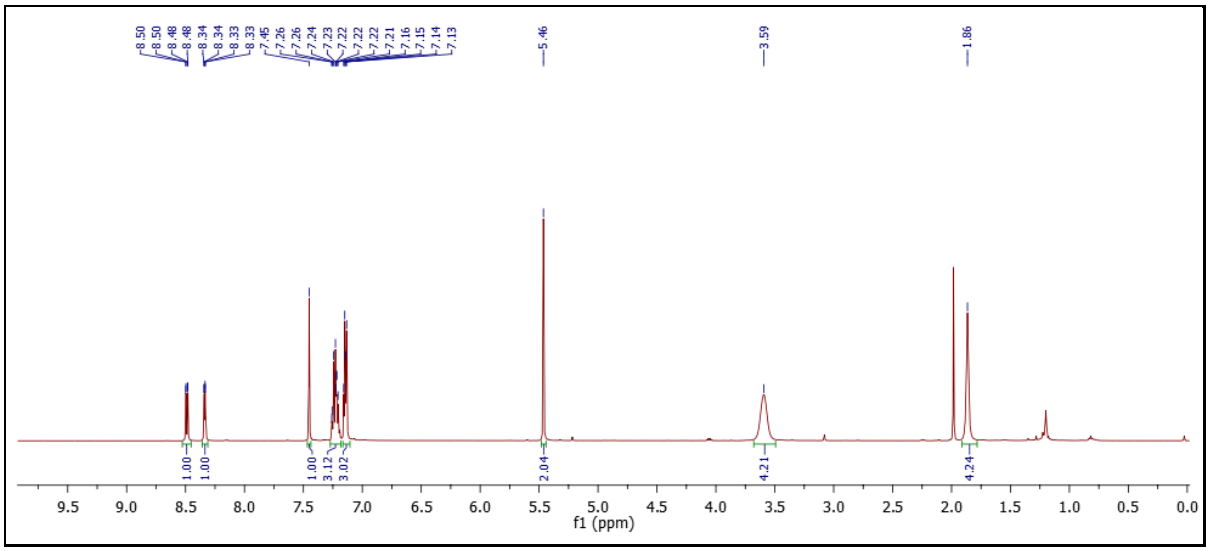
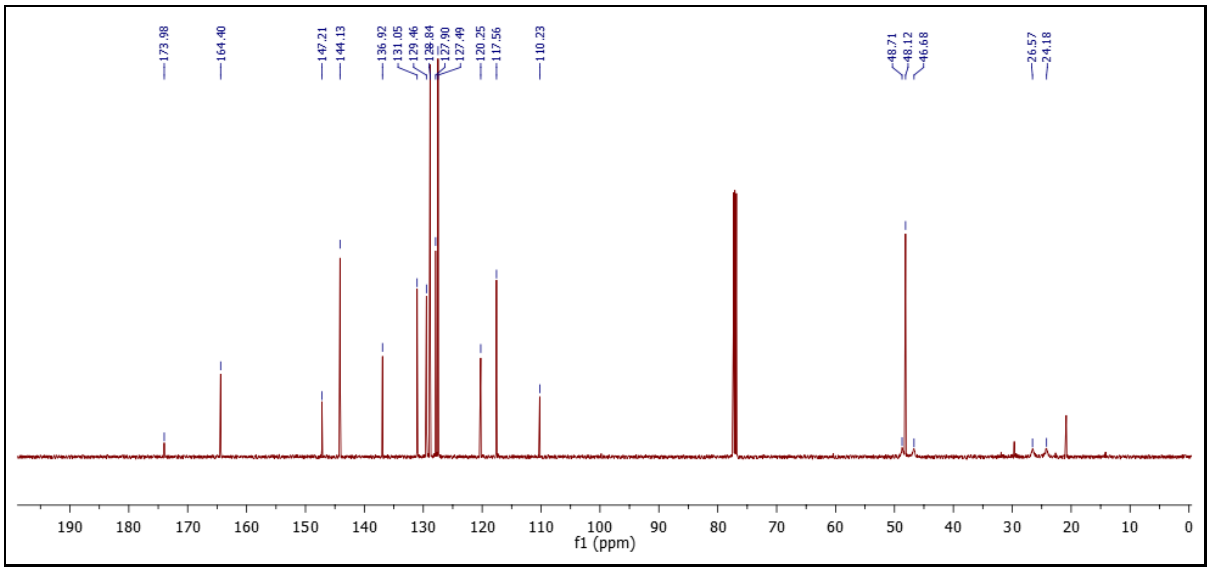
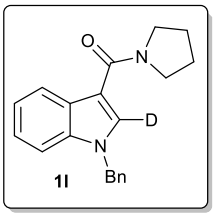
^{1}H NMR (500 MHz, $CDCl_3$)



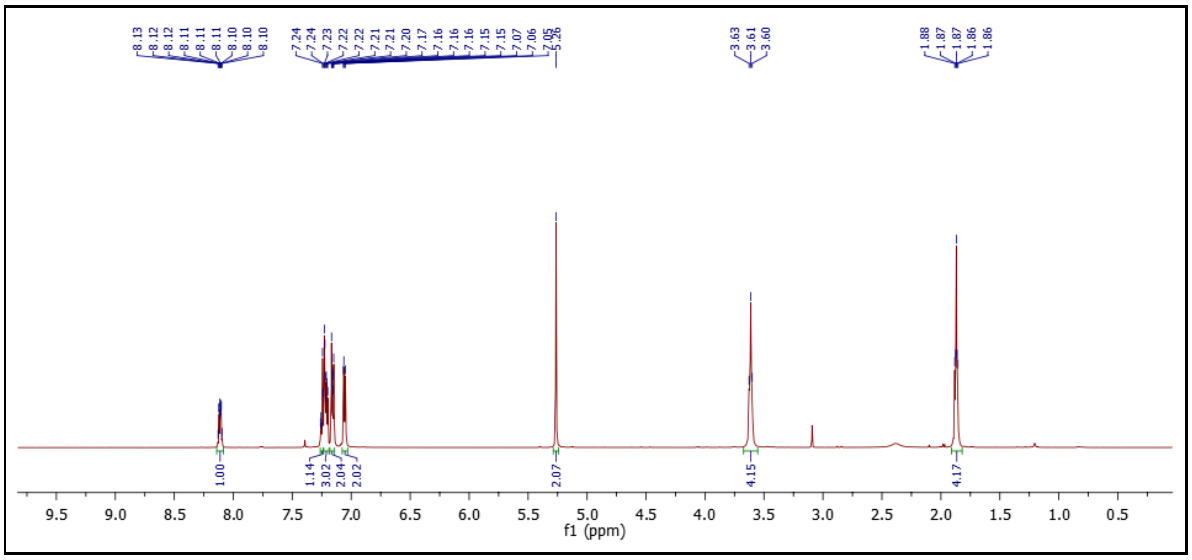
^{13}C NMR (125 MHz, $CDCl_3$)



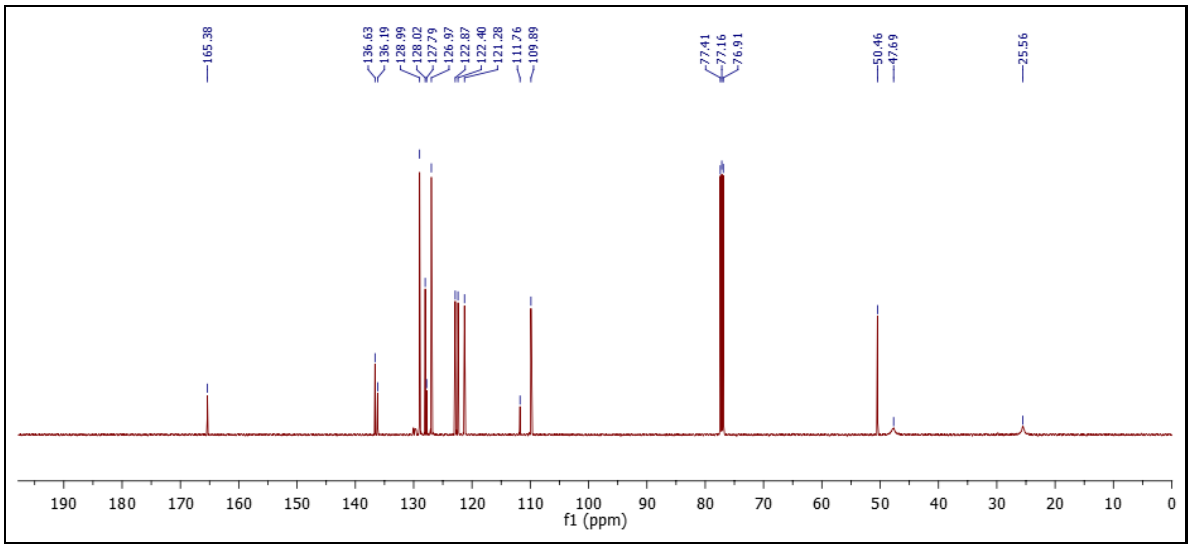


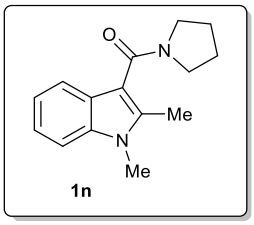
1l

^{1}H NMR (500 MHz, $CDCl_3$)



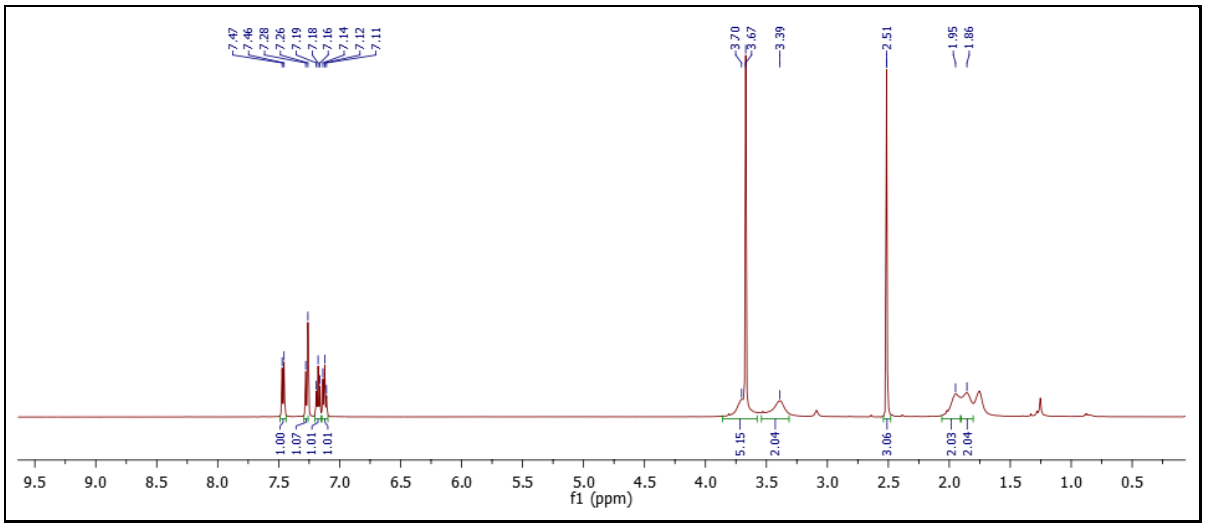
^{13}C NMR (125 MHz, $CDCl_3$)



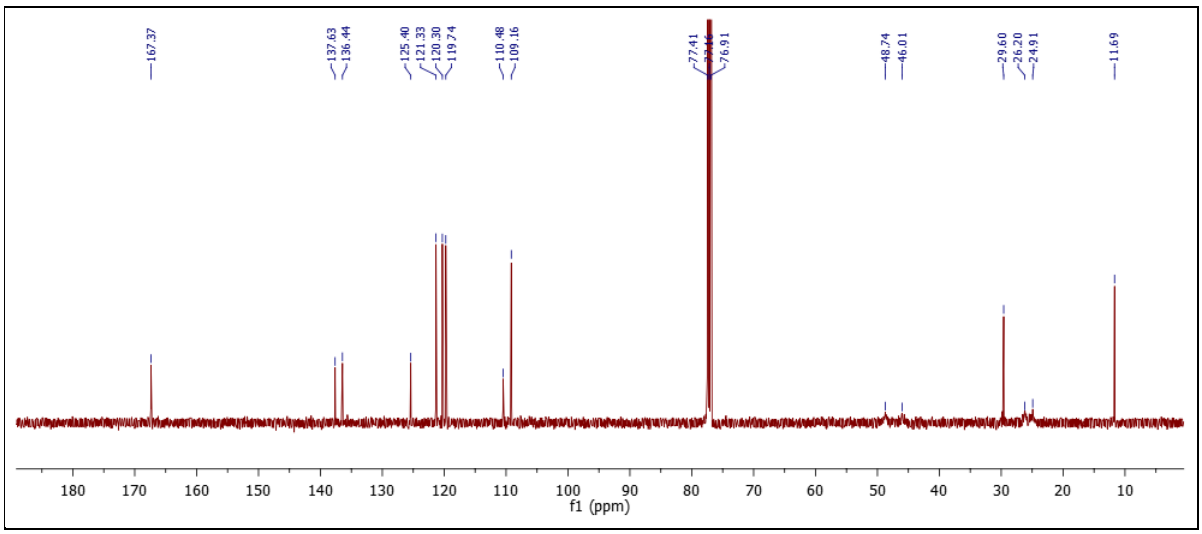


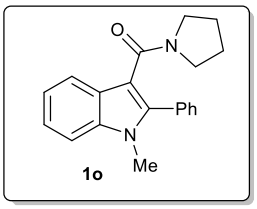
1n

^{1}H NMR (500 MHz, $CDCl_3$)

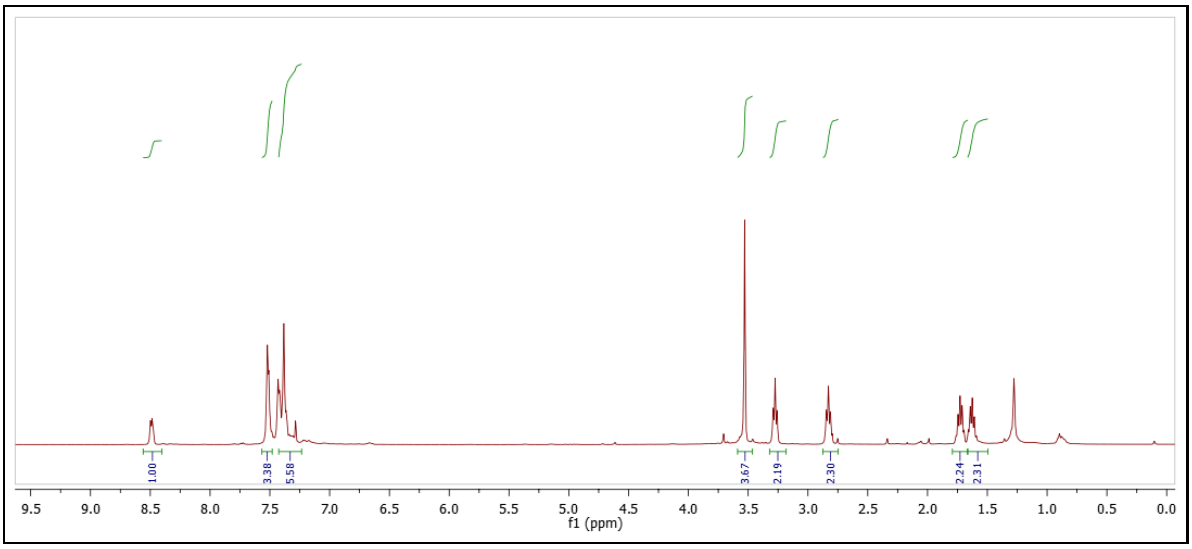


^{13}C NMR (125 MHz, $CDCl_3$)

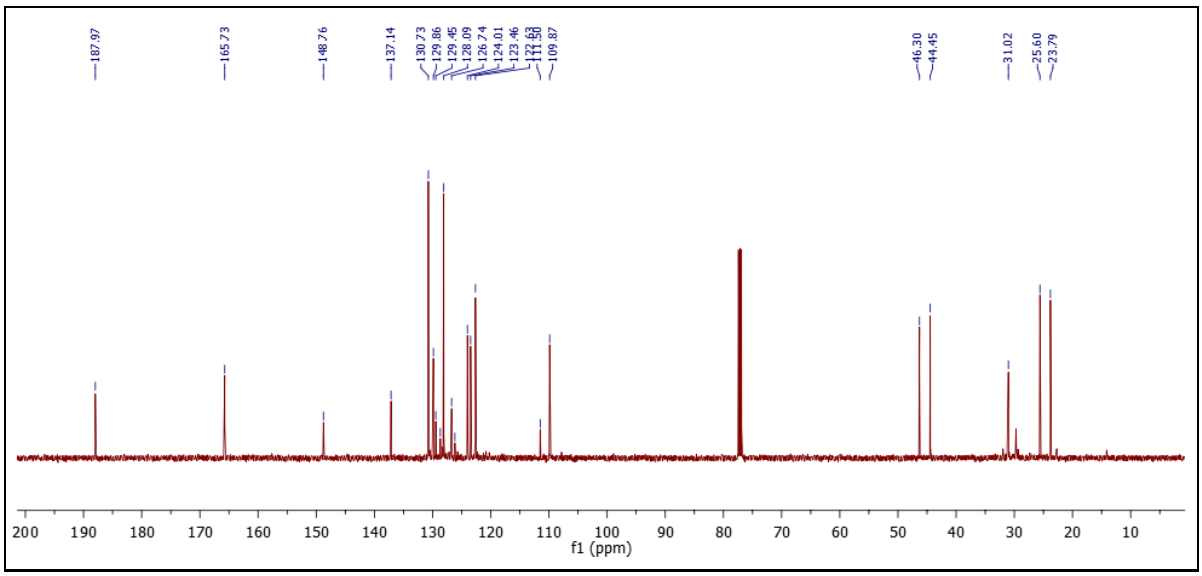


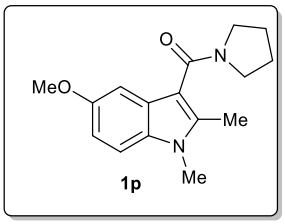


^{1}H NMR (400 MHz, $CDCl_3$)

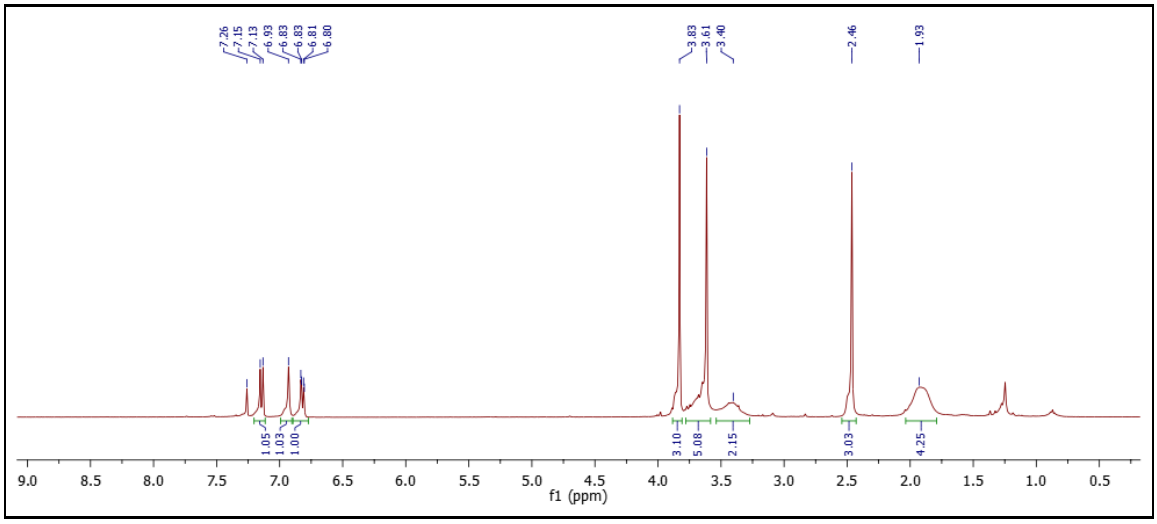


^{13}C NMR (125 MHz, $CDCl_3$)

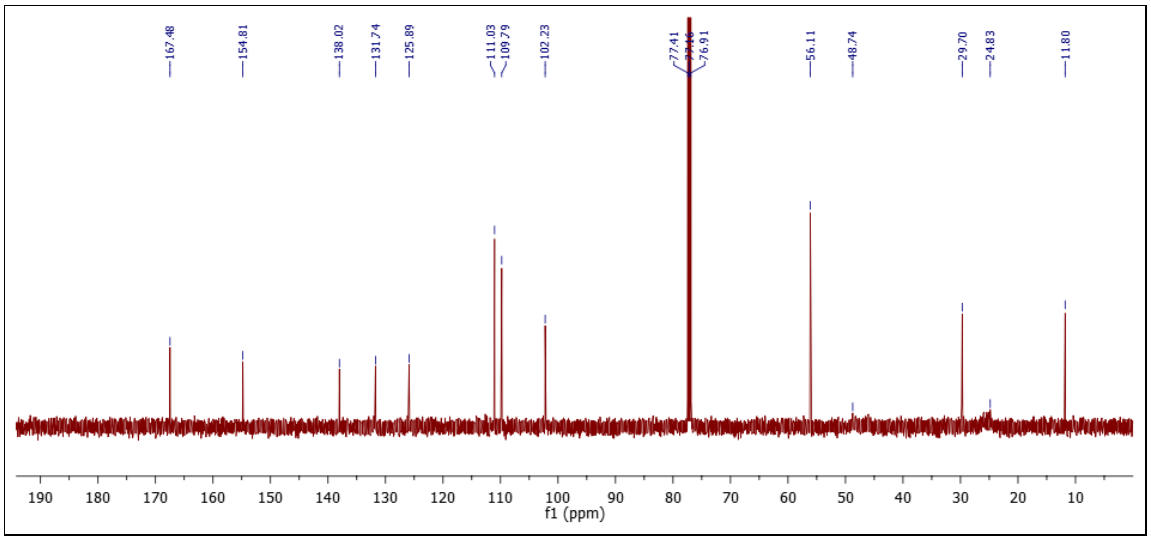


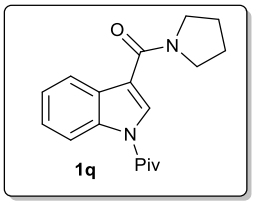


^{1}H NMR (400 MHz, $CDCl_3$)

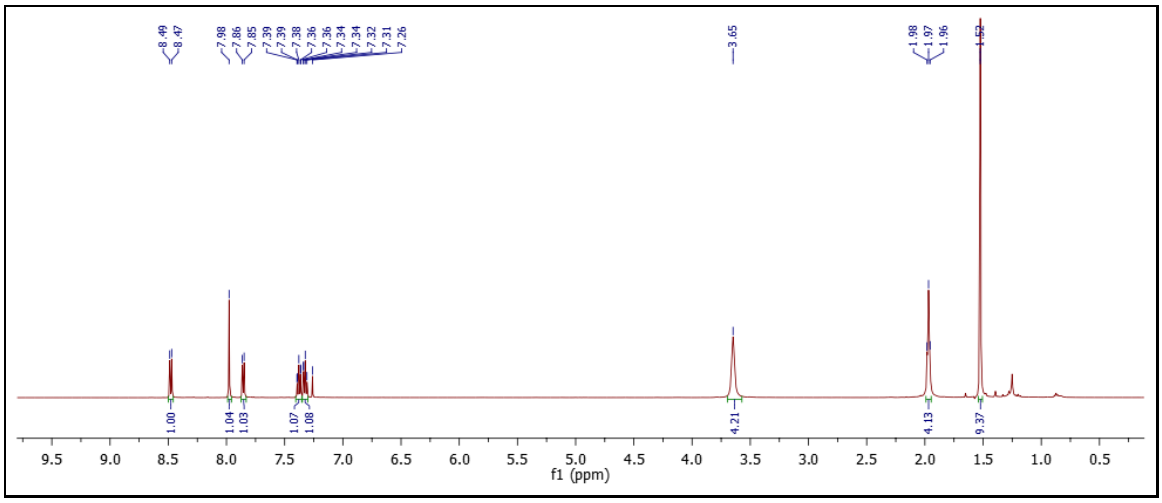


^{13}C NMR (125 MHz, $CDCl_3$)

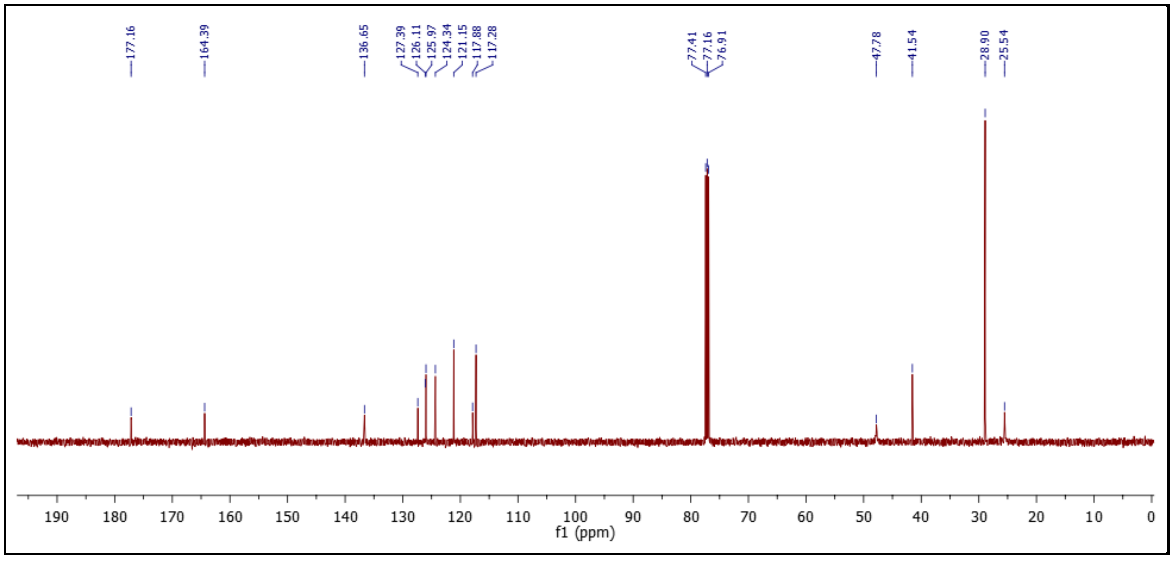


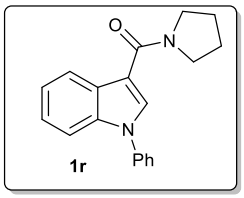


^{1}H NMR (500 MHz, $CDCl_3$)

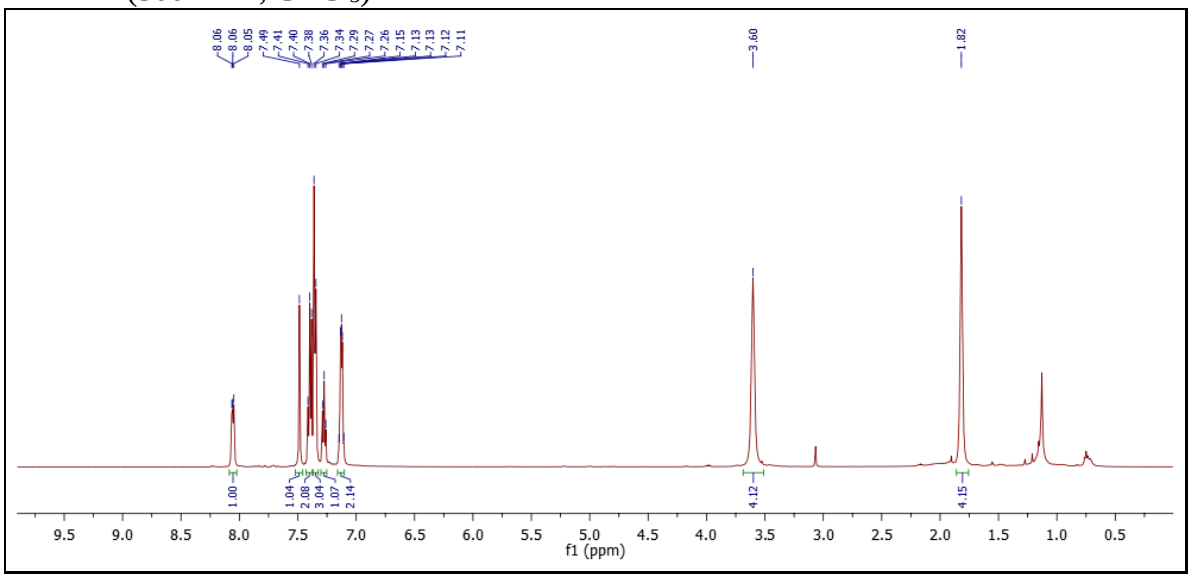


^{13}C NMR (125 MHz, $CDCl_3$)

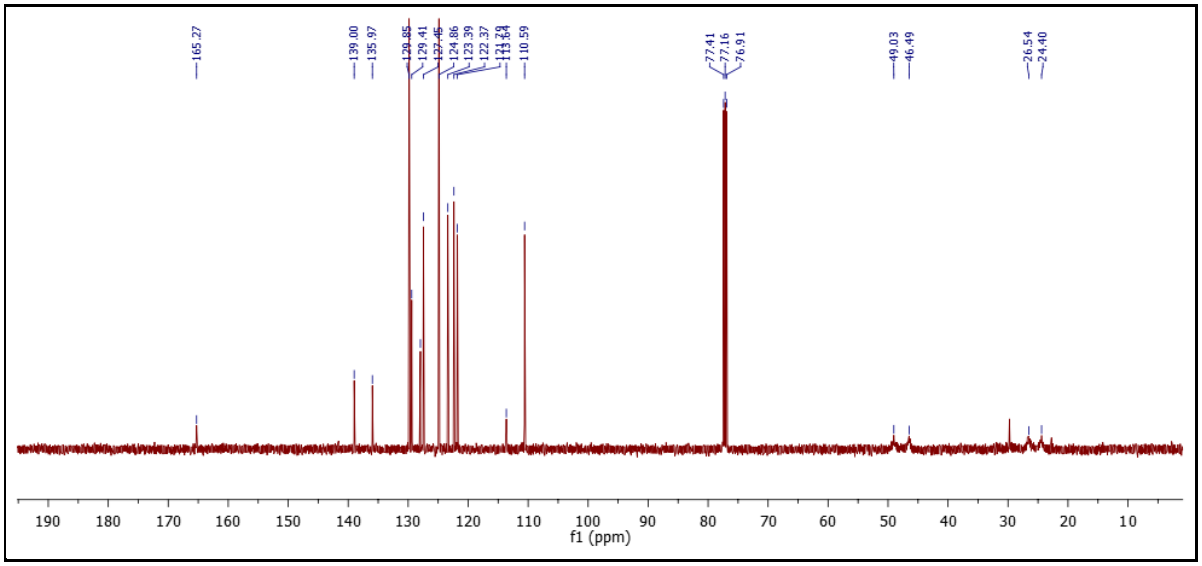


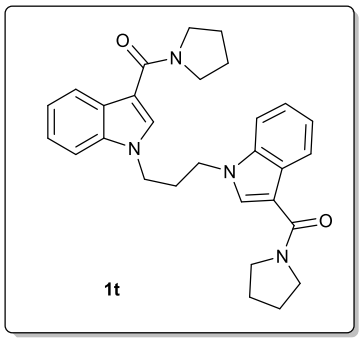


^{1}H NMR (500 MHz, $CDCl_3$)

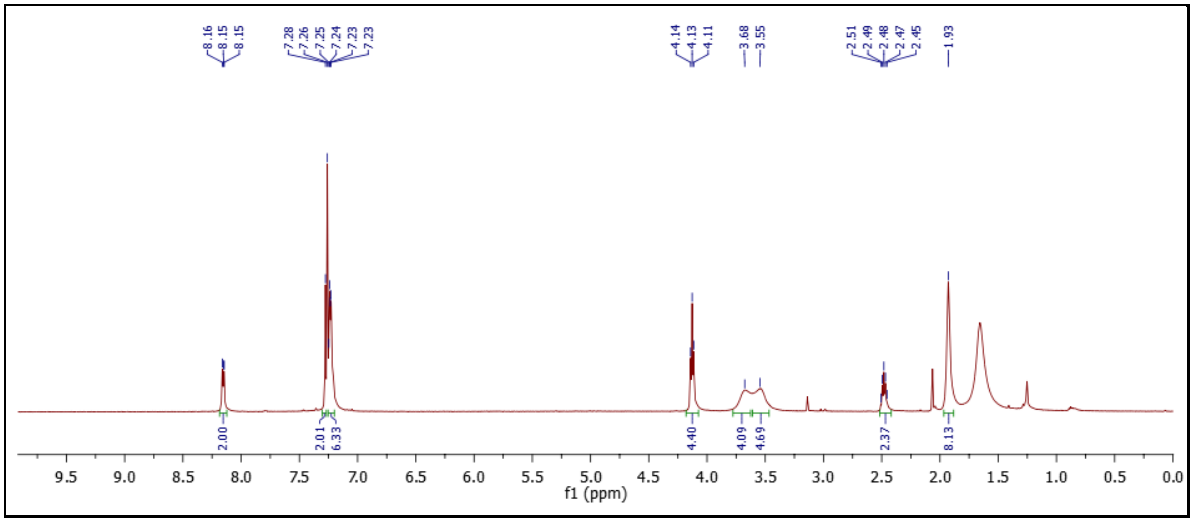


^{13}C NMR (125 MHz, $CDCl_3$)

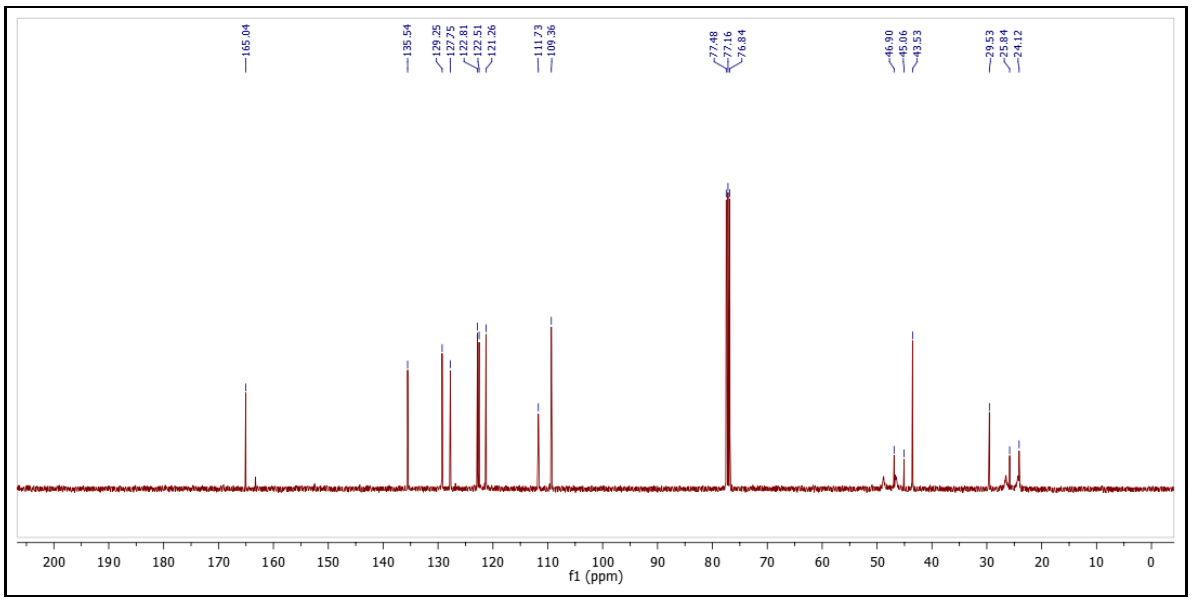


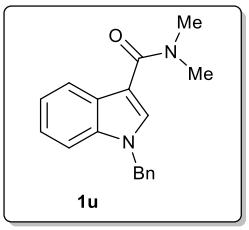


^{1}H NMR (500 MHz, $CDCl_3$)



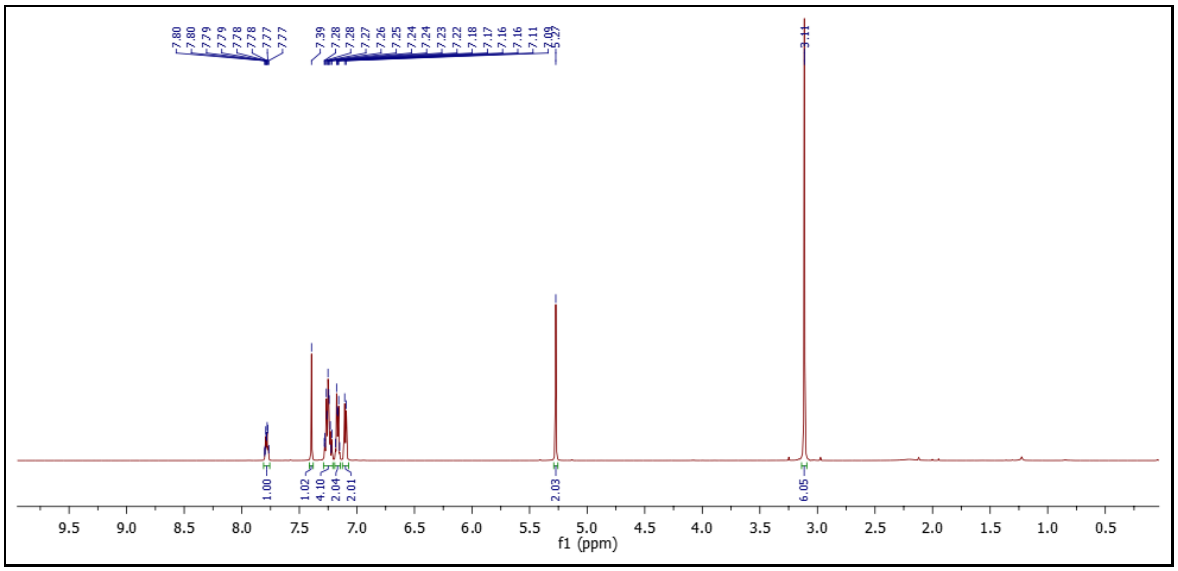
^{13}C NMR (100 MHz, $CDCl_3$)



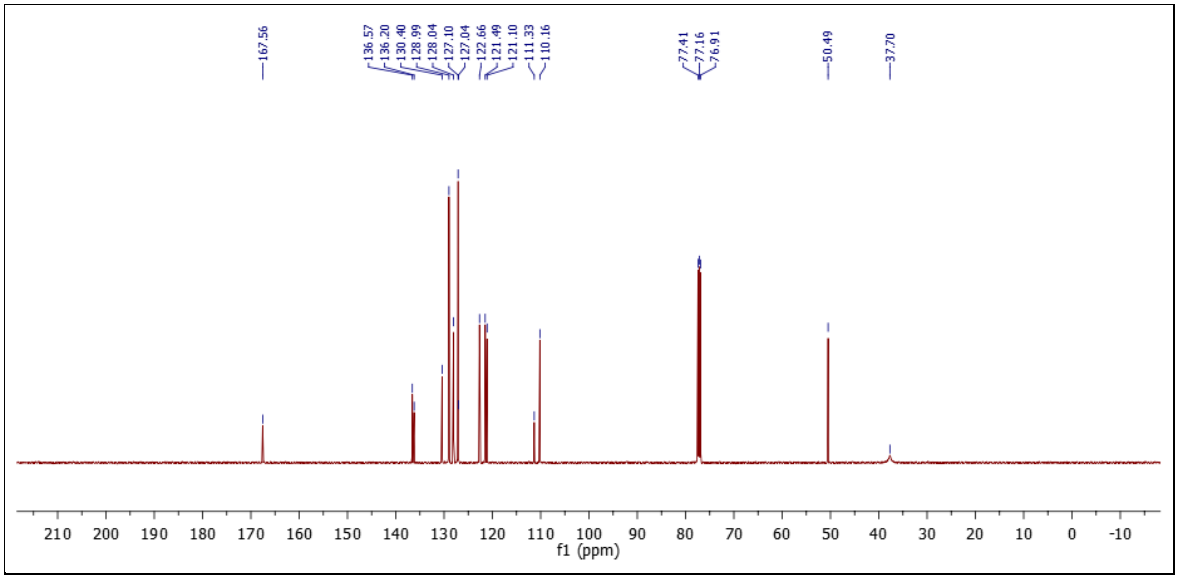


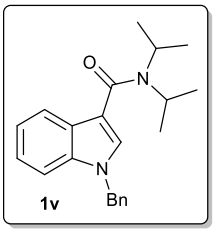
1u

^{1}H NMR (500 MHz, $CDCl_3$)

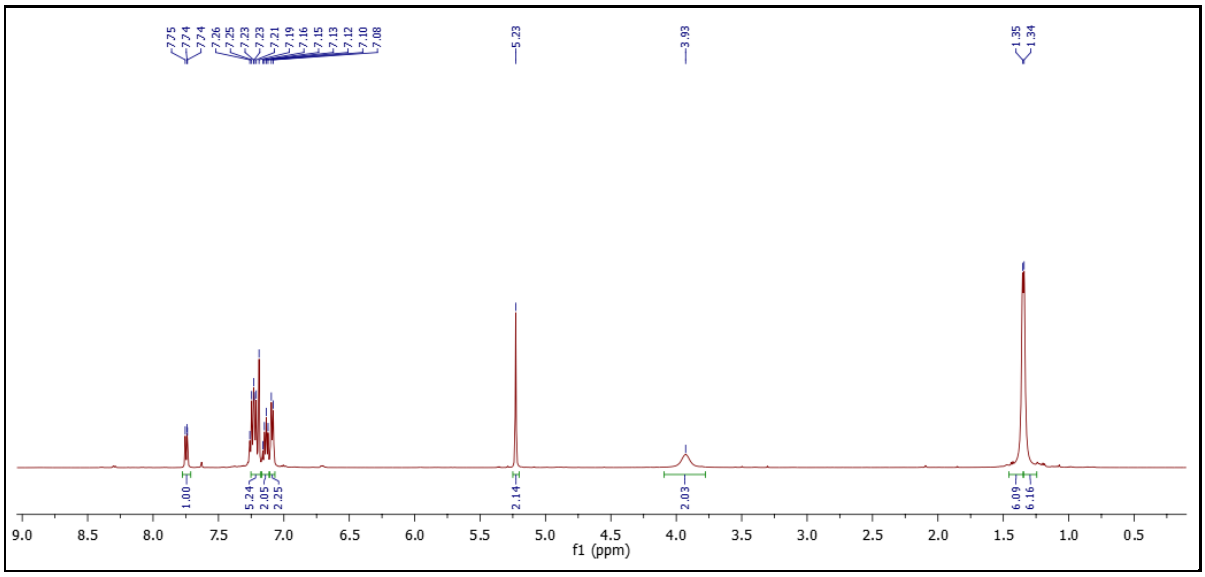


^{13}C NMR (125 MHz, $CDCl_3$)

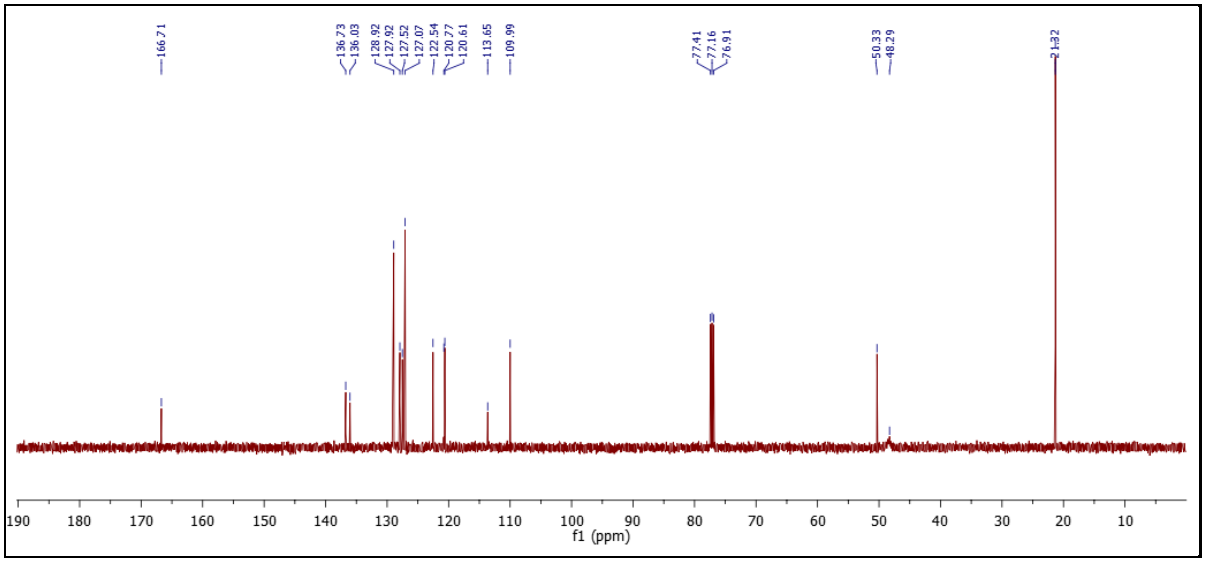


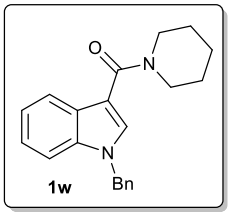


^{1}H NMR (500 MHz, $CDCl_3$)

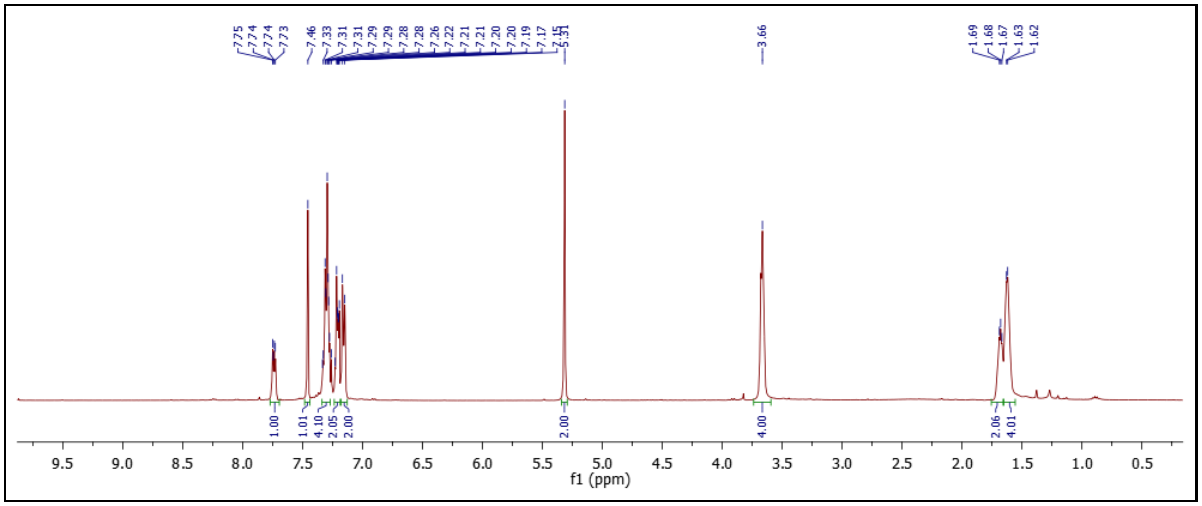


^{13}C NMR (125 MHz, $CDCl_3$)

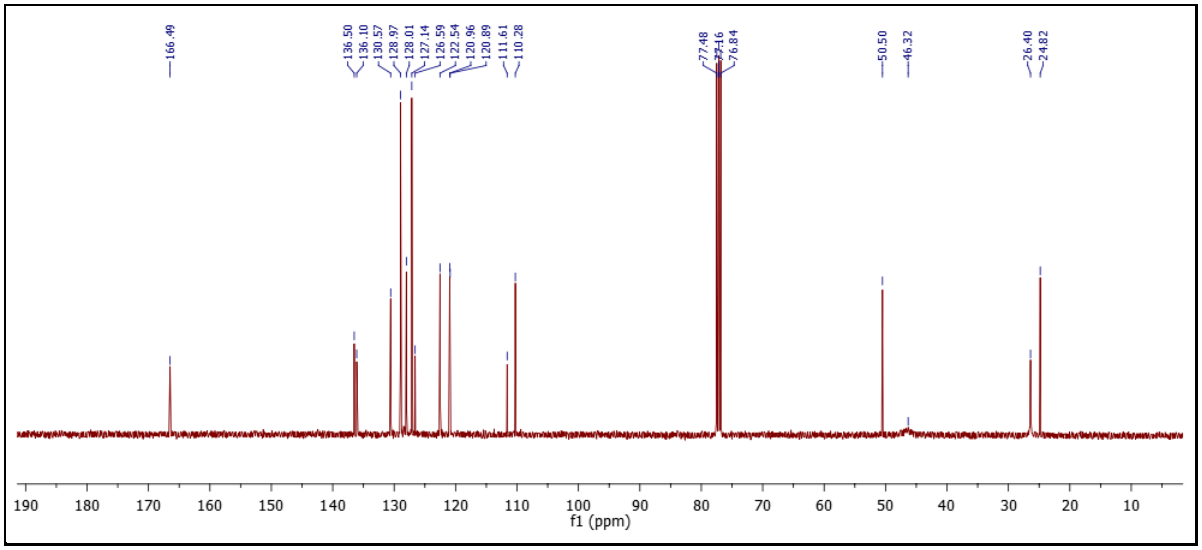


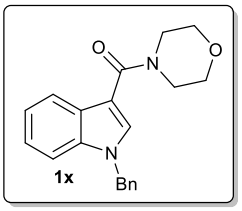


^{1}H NMR (400 MHz, $CDCl_3$)

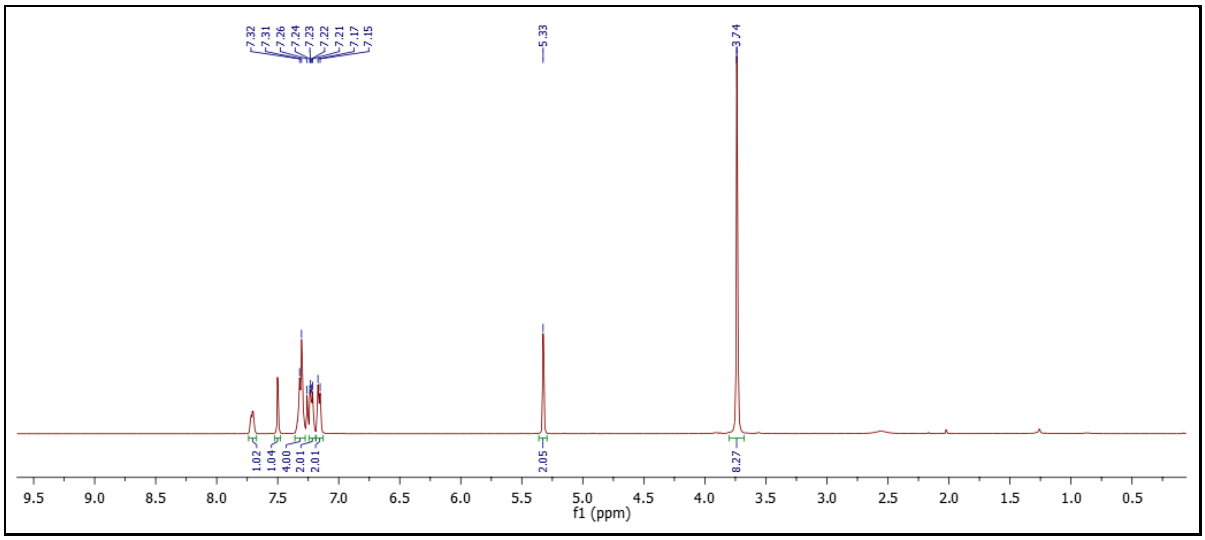


^{13}C NMR (100 MHz, $CDCl_3$)

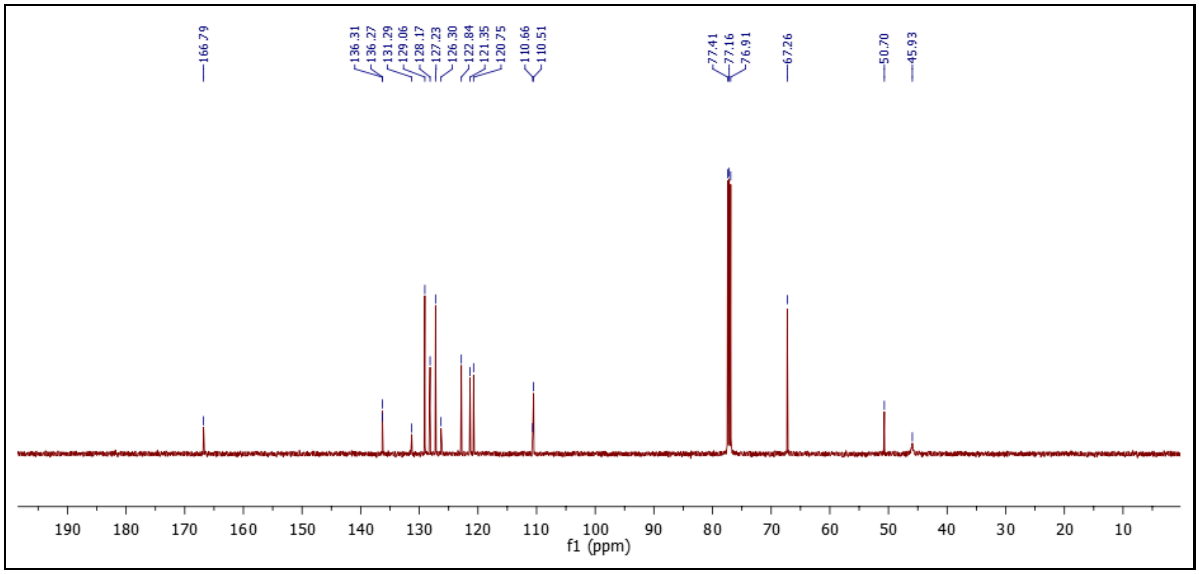


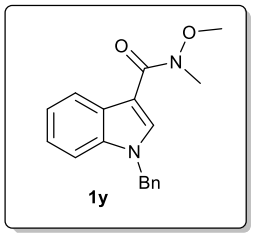


^{1}H NMR (400 MHz, $CDCl_3$)



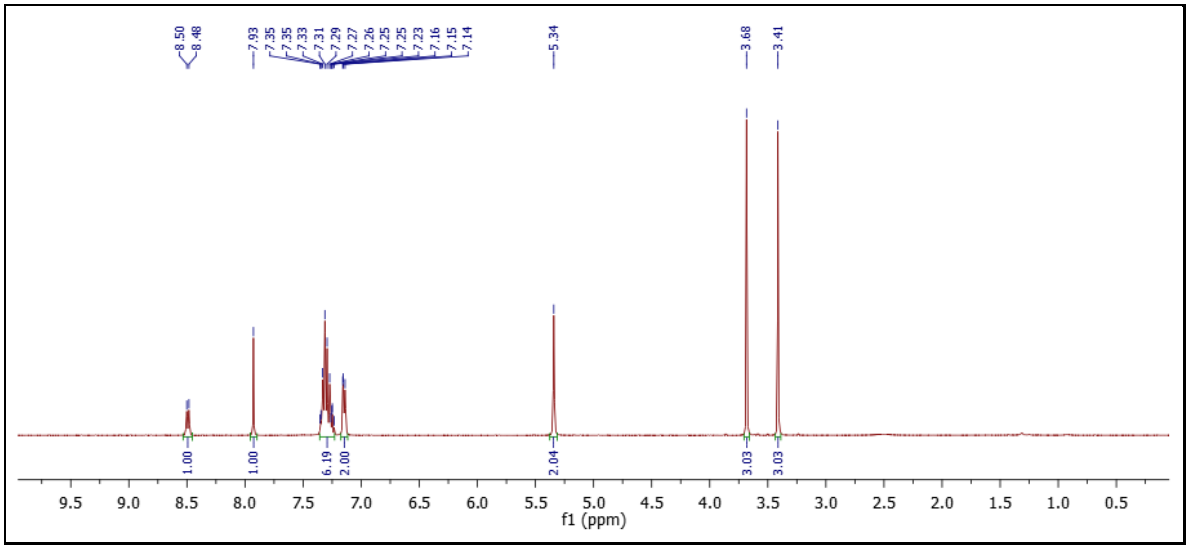
^{13}C NMR (125 MHz, $CDCl_3$)



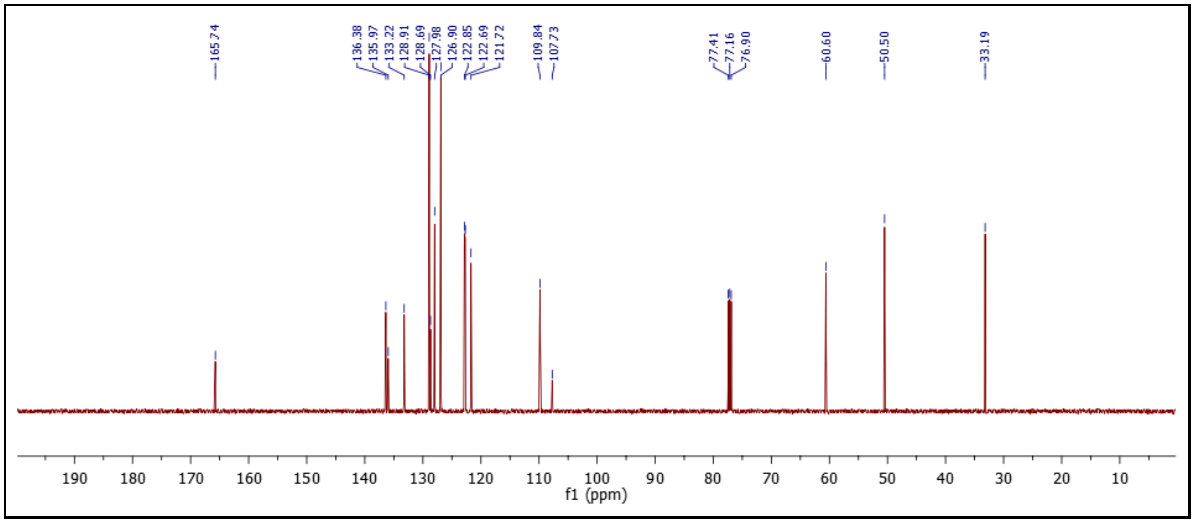


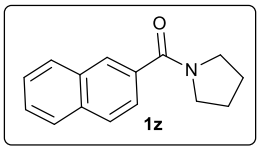
1y

^{1}H NMR (400 MHz, $CDCl_3$)

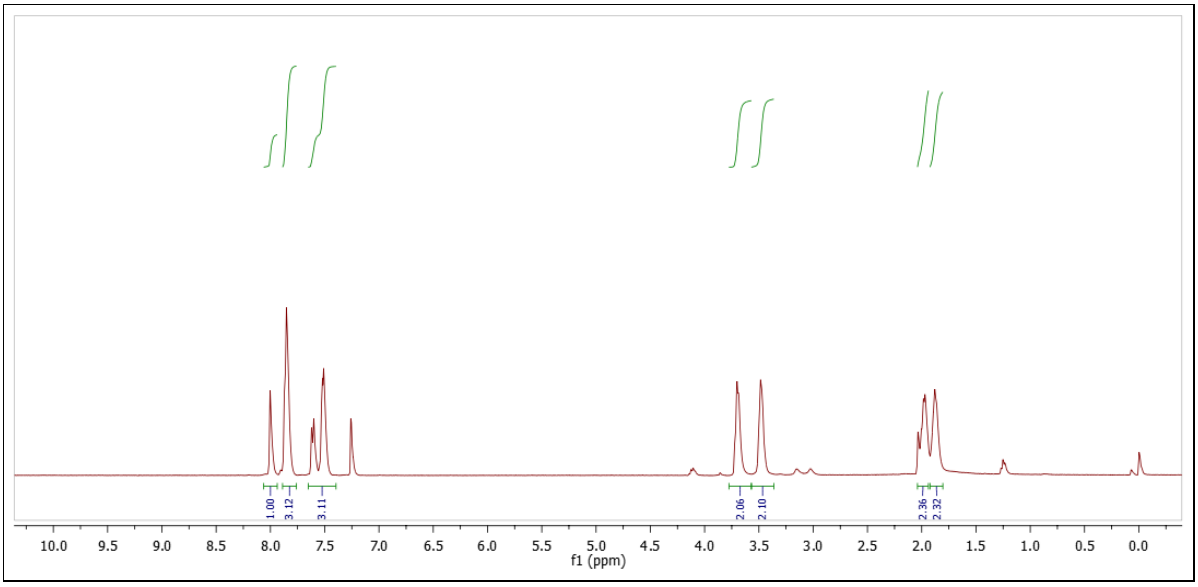


^{13}C NMR (125 MHz, $CDCl_3$)

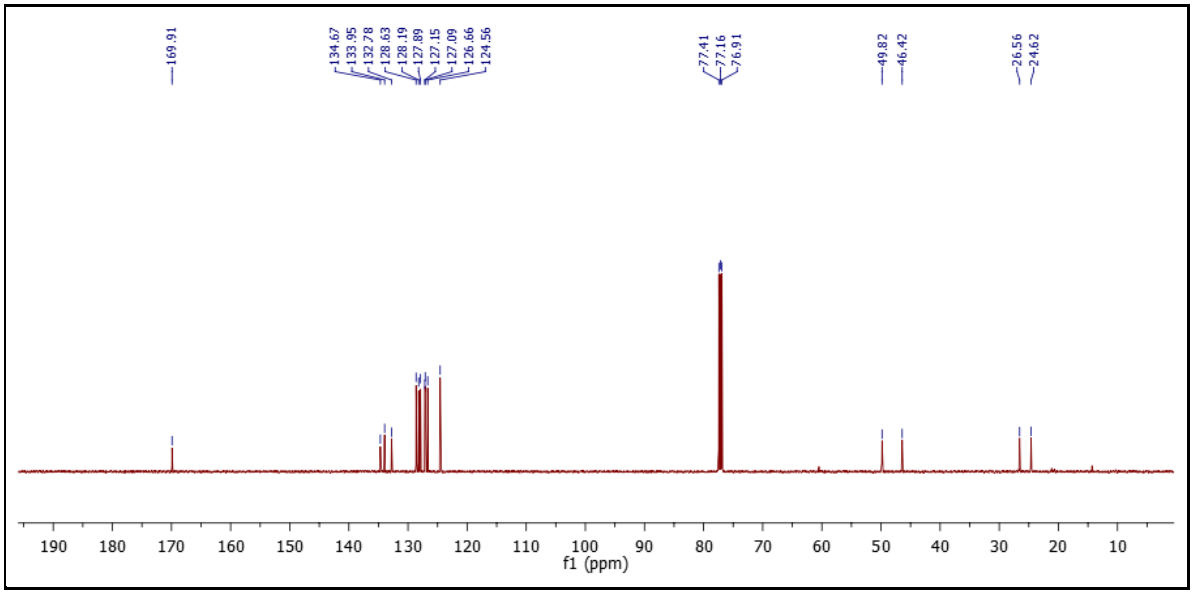


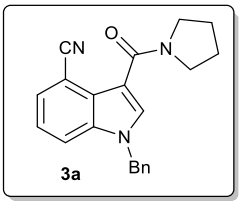


^{1}H NMR (400 MHz, $CDCl_3$)

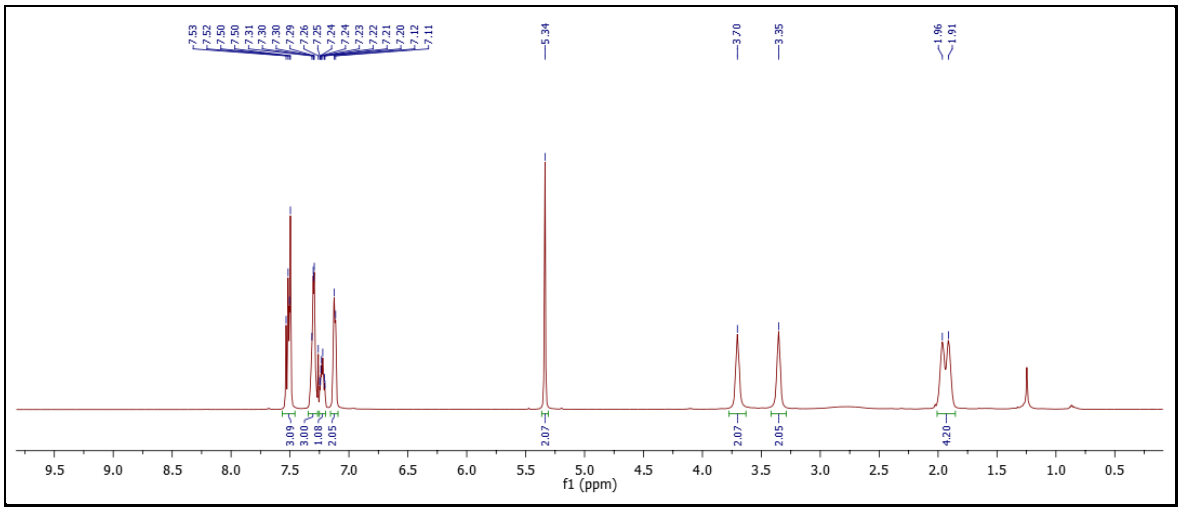


^{13}C NMR (125 MHz, $CDCl_3$)

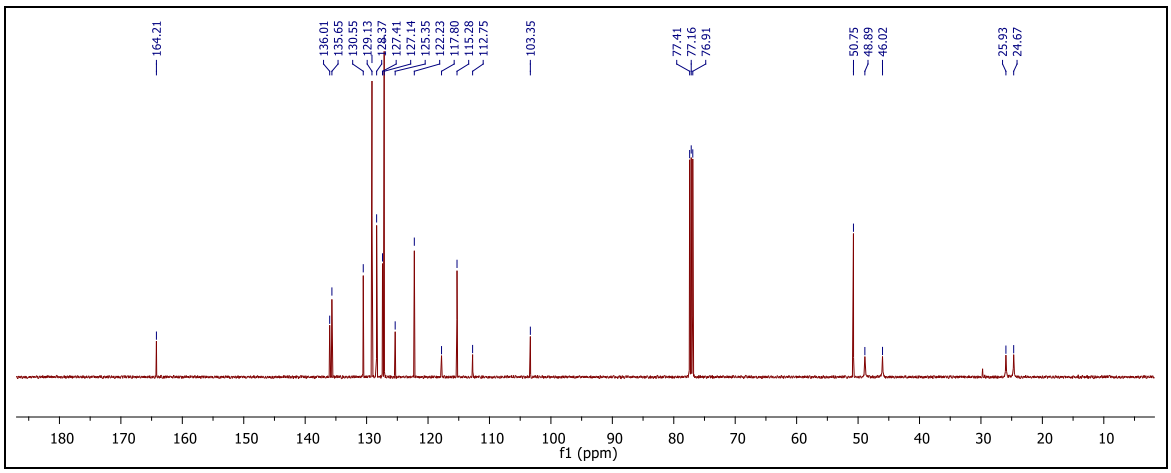


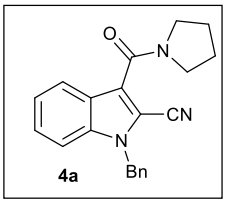


^{1}H NMR (500 MHz, $CDCl_3$)



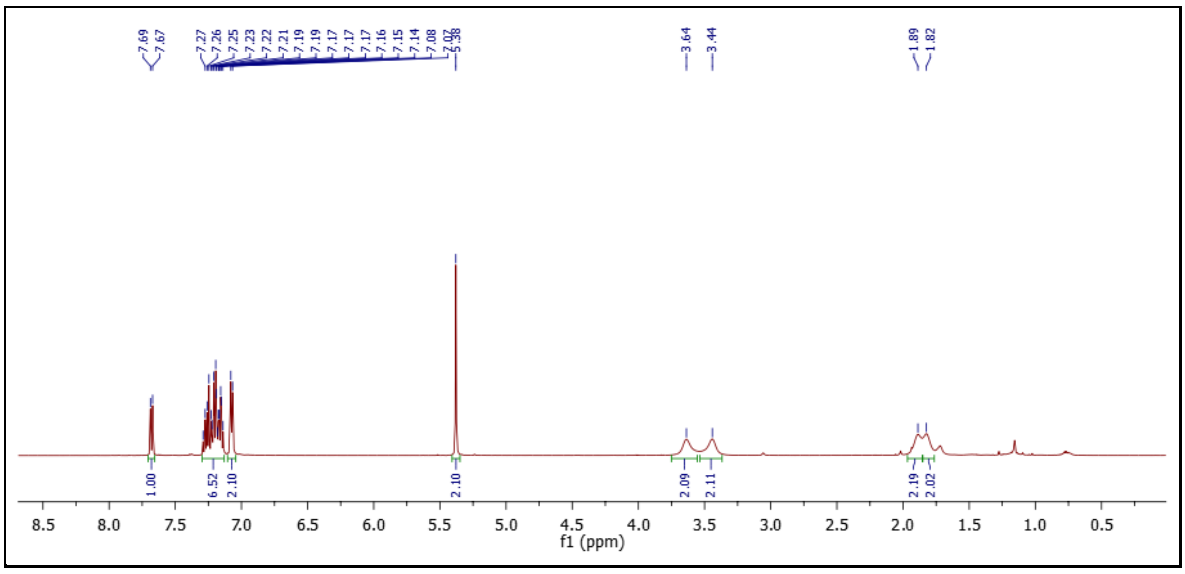
^{13}C NMR (125 MHz, $CDCl_3$)



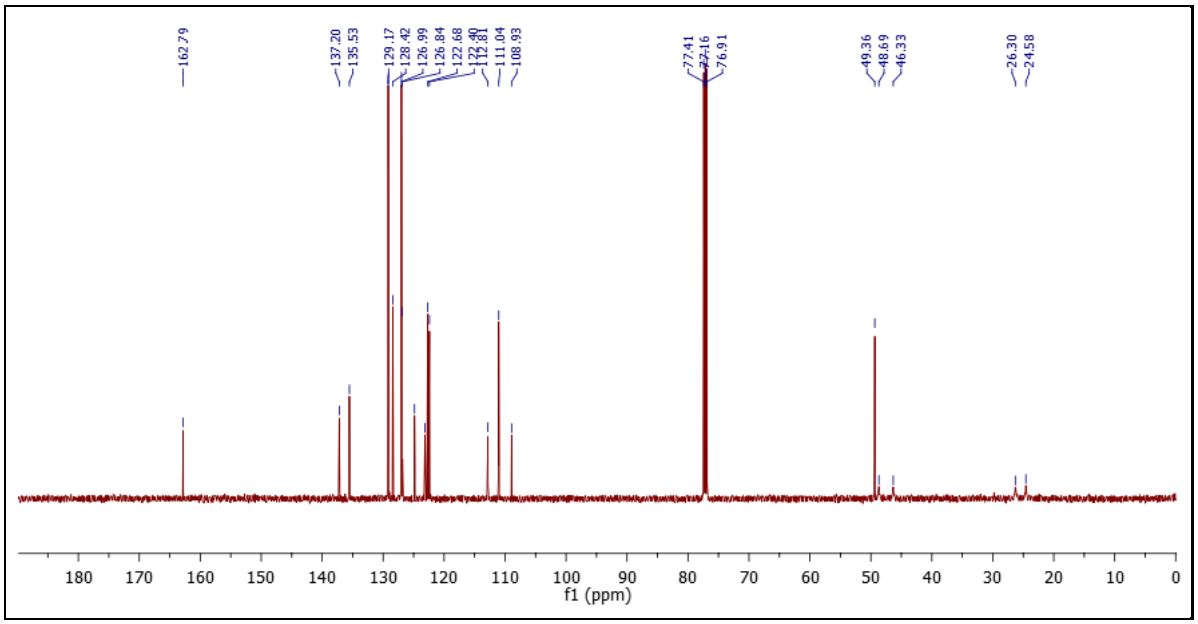


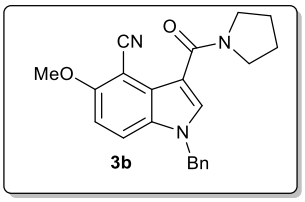
4a

^{1}H NMR (500 MHz, $CDCl_3$)

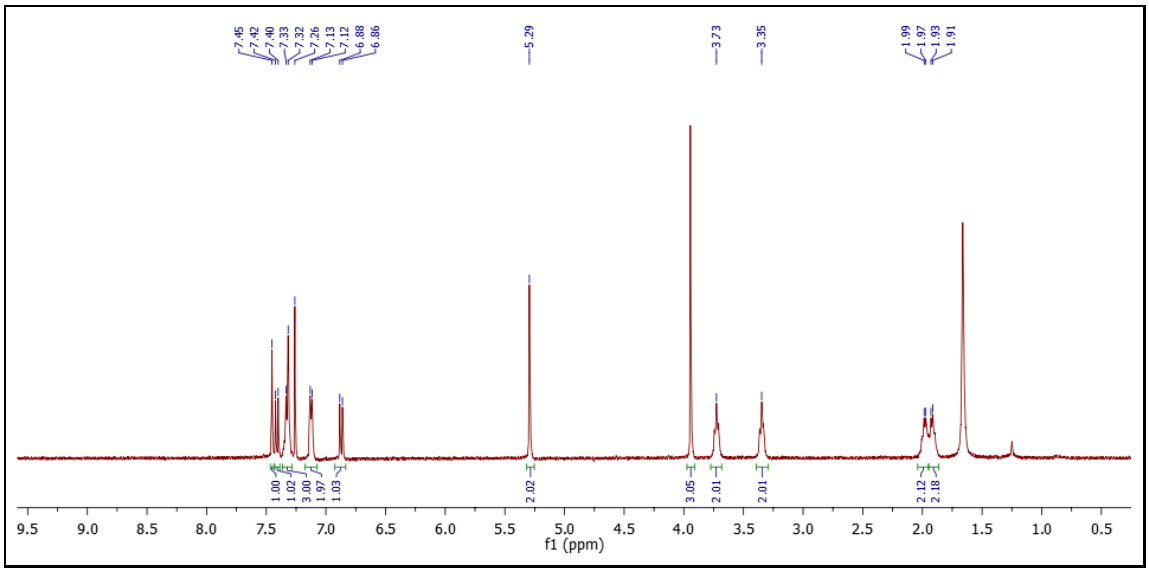


^{13}C NMR (125 MHz, $CDCl_3$)

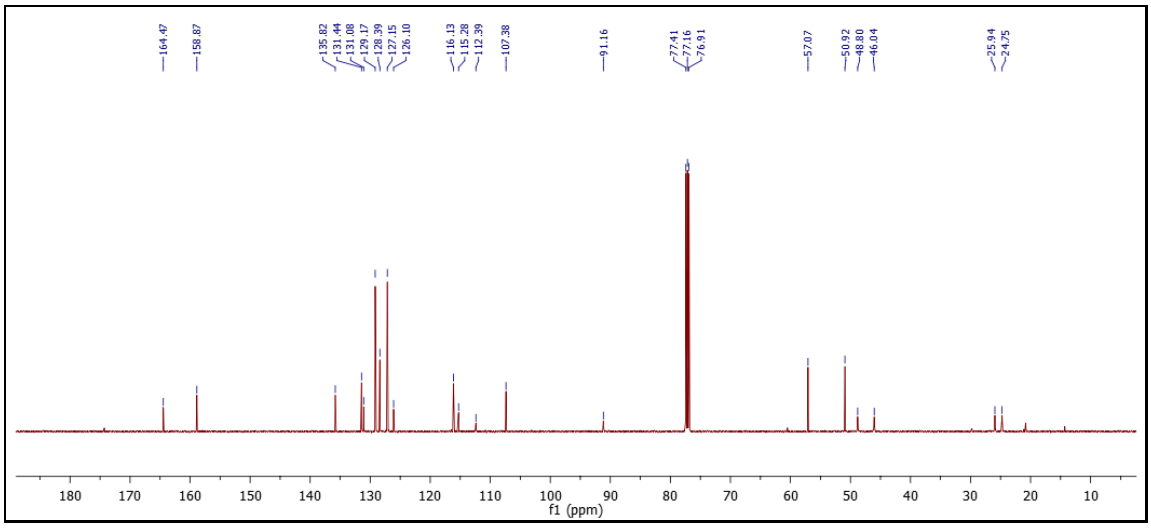


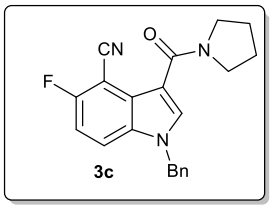


^{1}H NMR (400 MHz, $CDCl_3$)

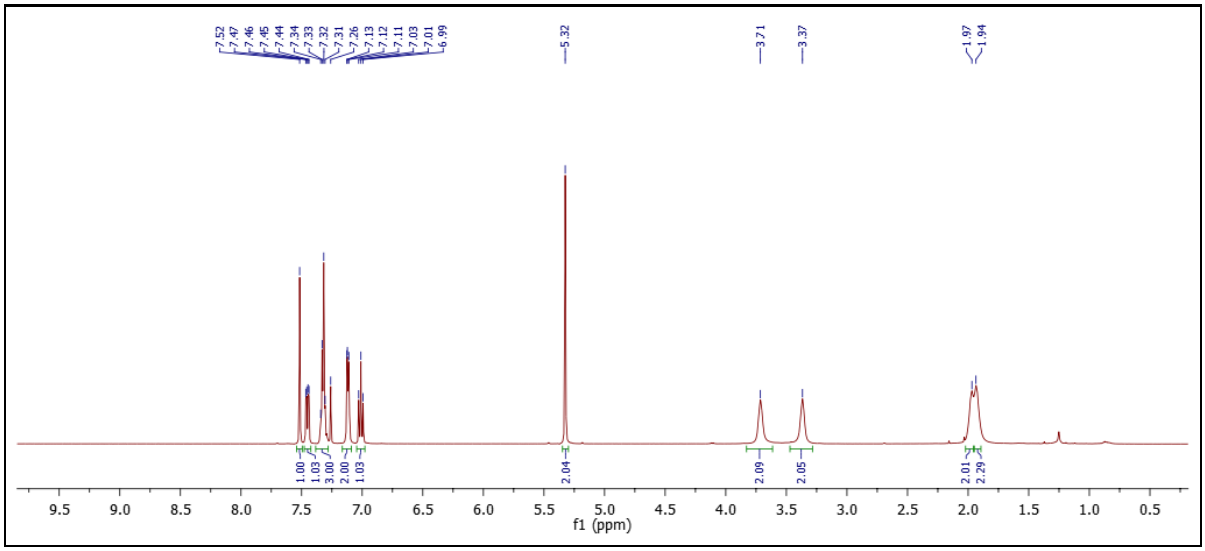


^{13}C NMR (125 MHz, $CDCl_3$)

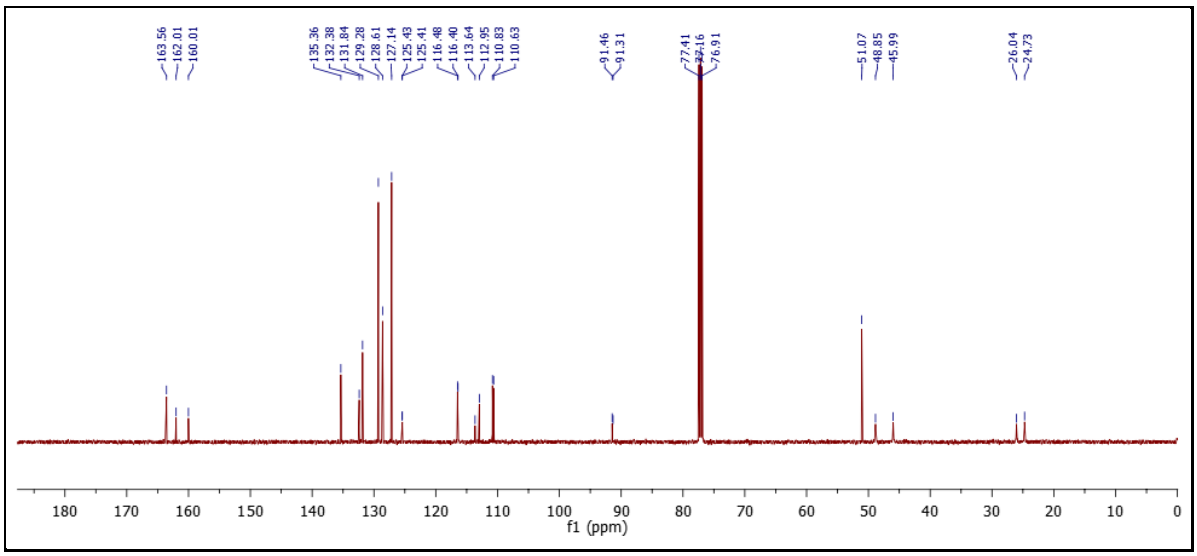


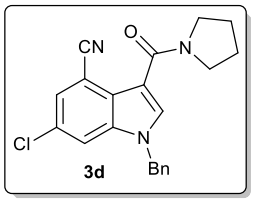


^{1}H NMR (400 MHz, $CDCl_3$)

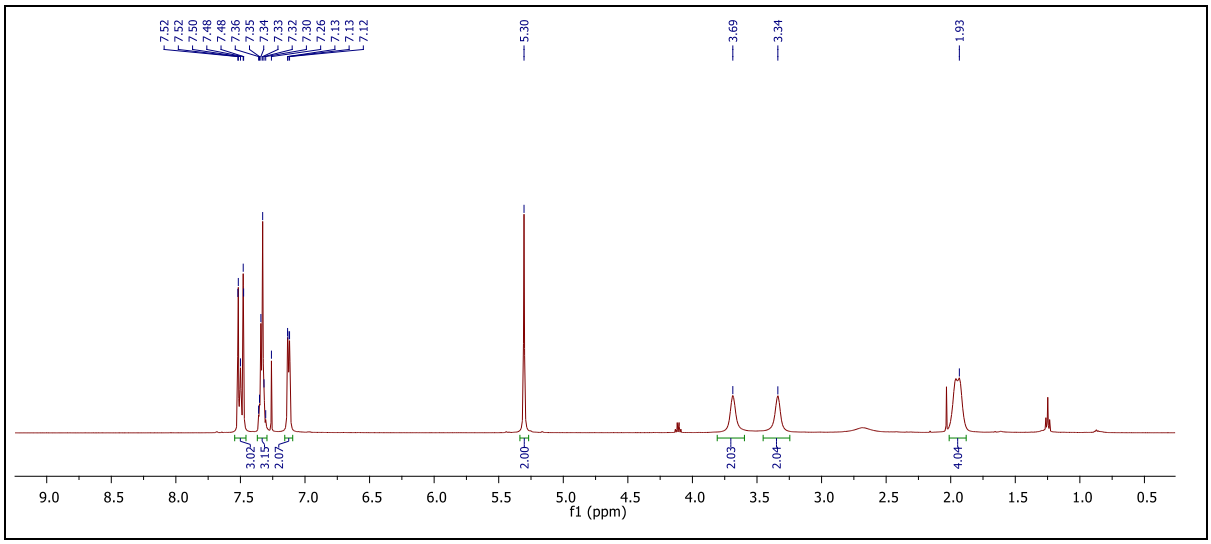


^{13}C NMR (125 MHz, $CDCl_3$)

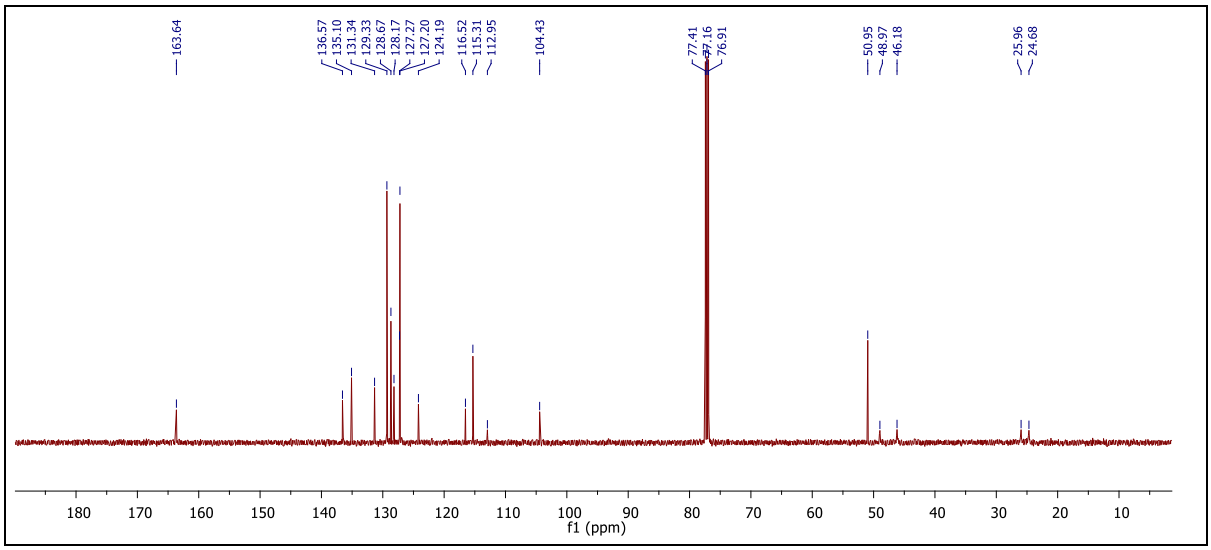


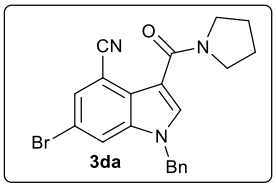


^{1}H NMR (500 MHz, $CDCl_3$)

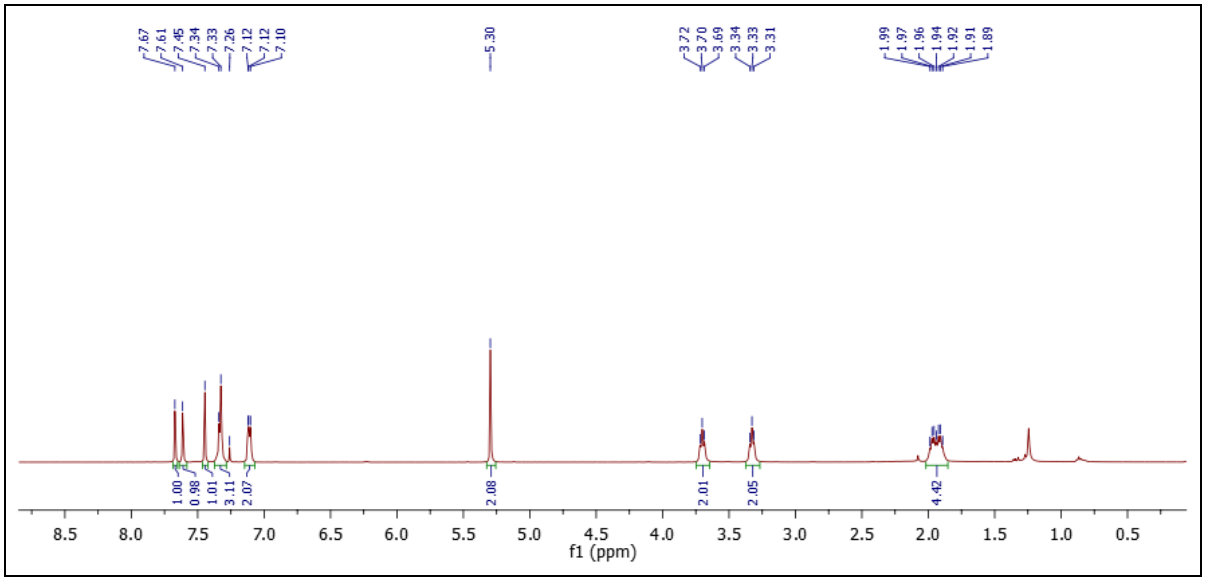


^{13}C NMR (125 MHz, $CDCl_3$)

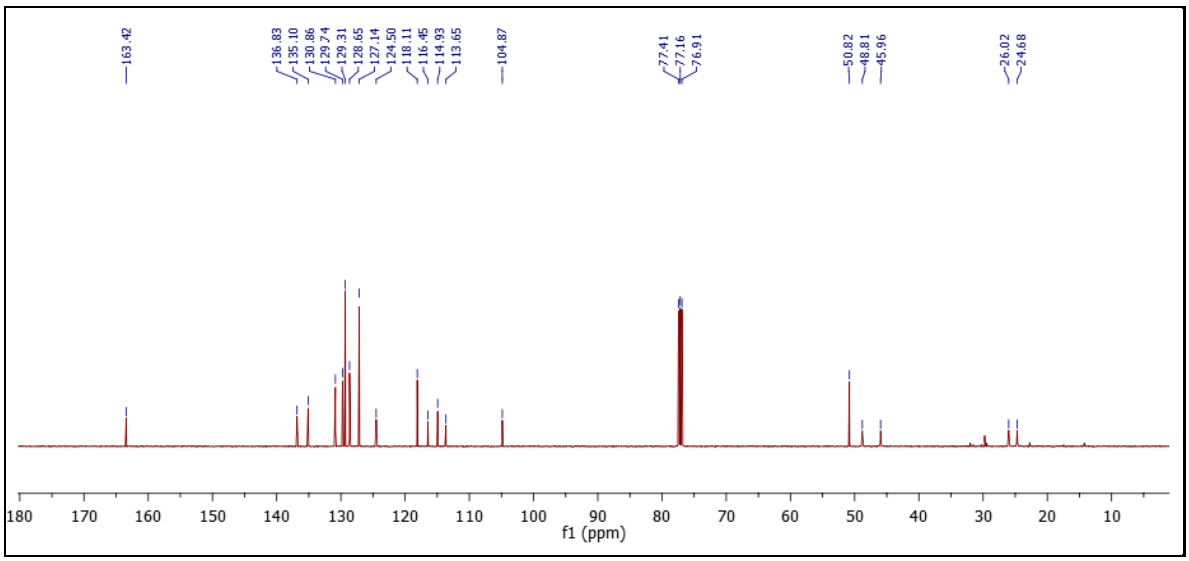


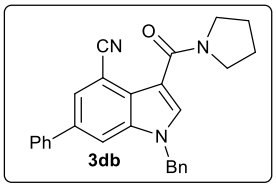


^{1}H NMR (400 MHz, $CDCl_3$)

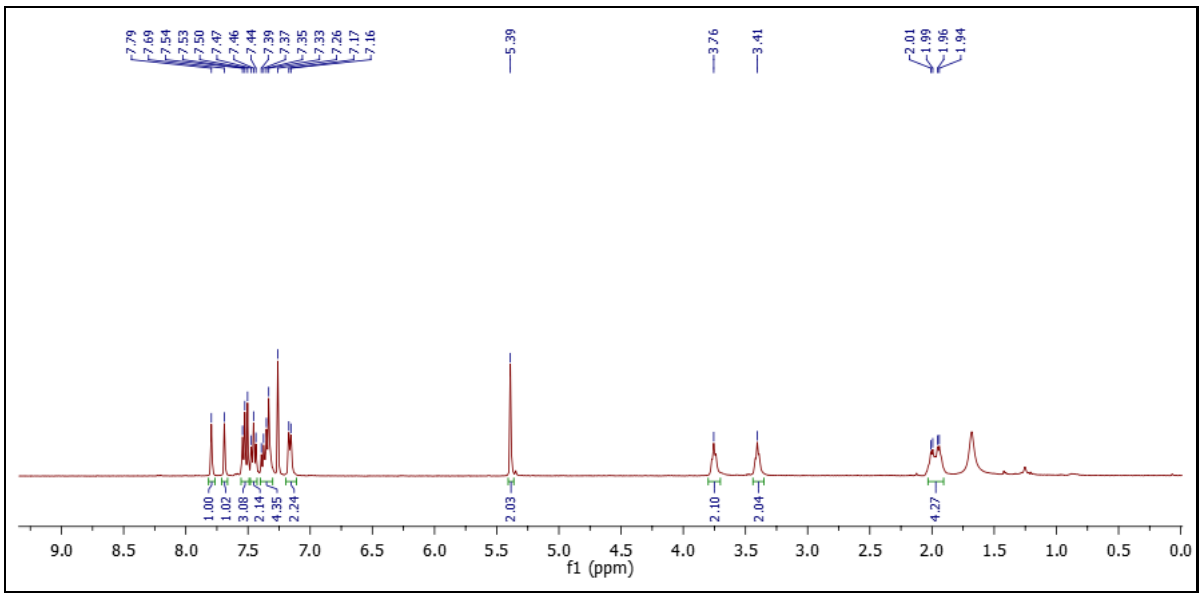


^{13}C NMR (125 MHz, $CDCl_3$)

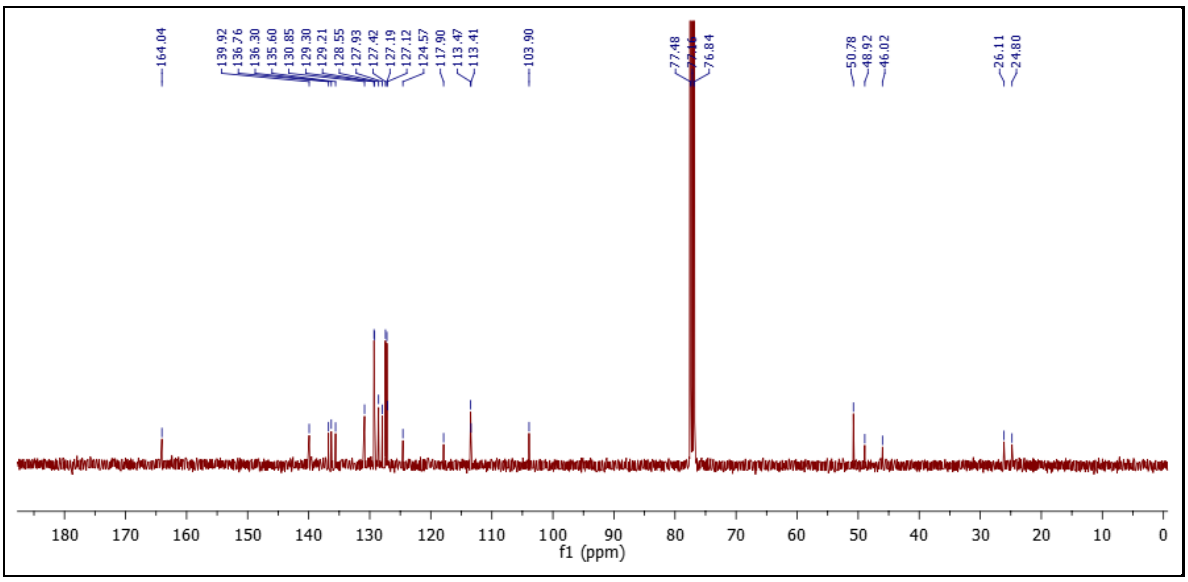


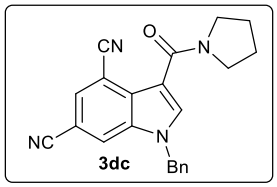


^{1}H NMR (400 MHz, $CDCl_3$)



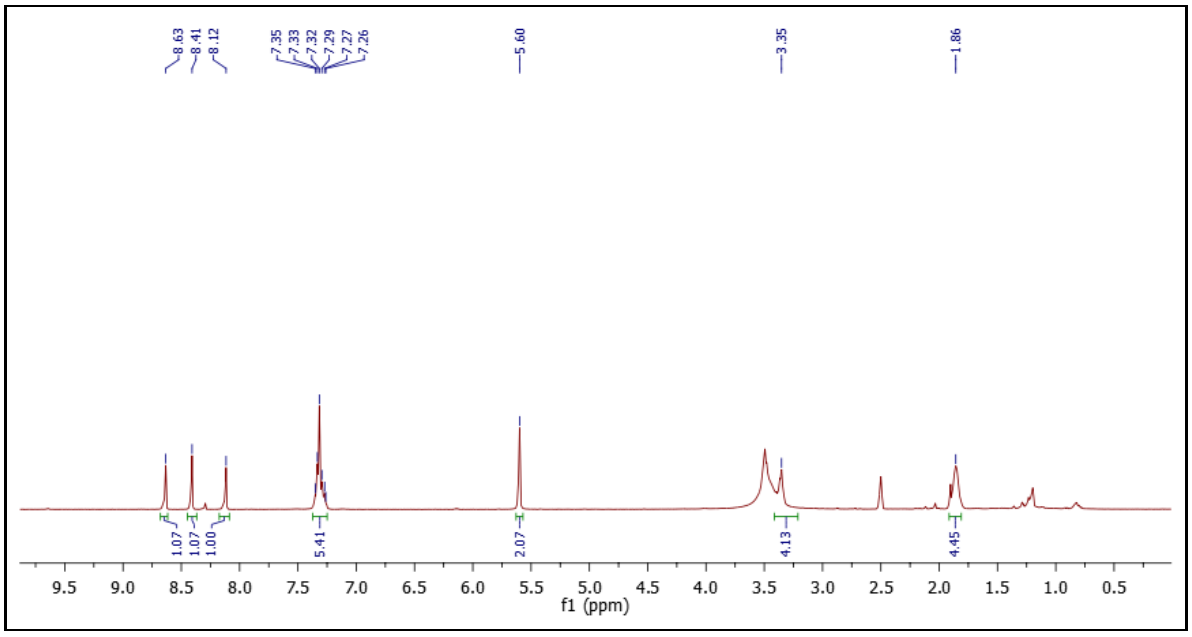
^{13}C NMR (125 MHz, $CDCl_3$)



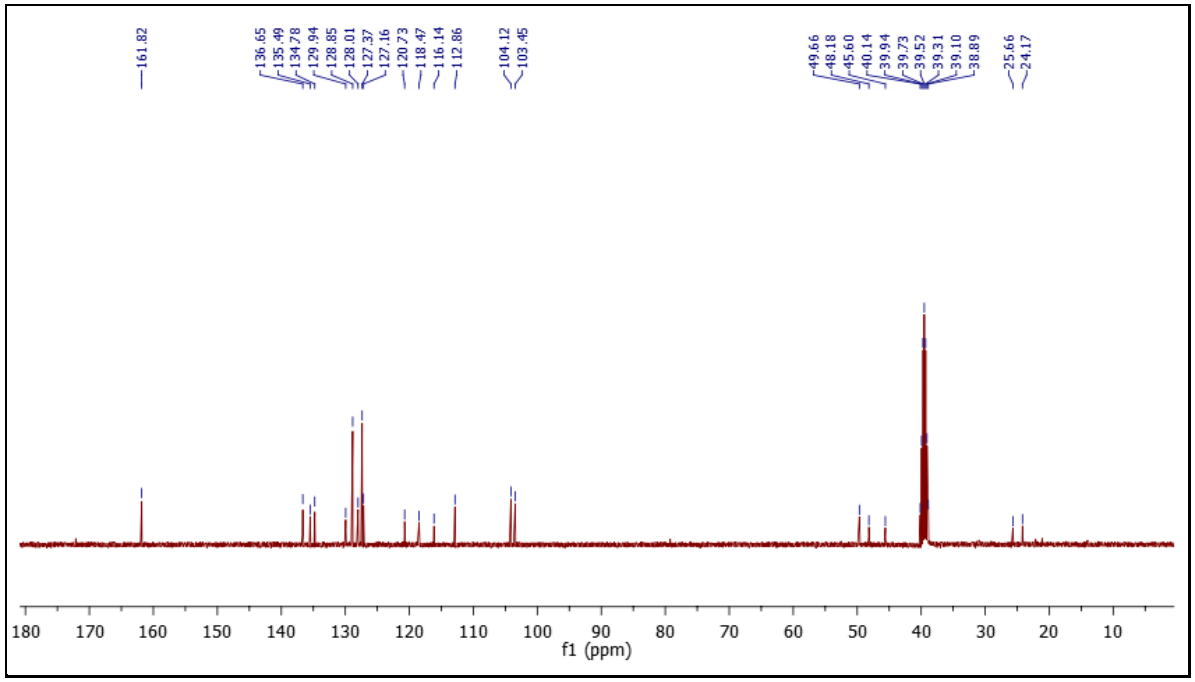


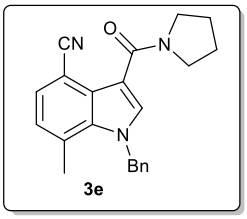
3dc

^{1}H NMR (400 MHz, DMSO-D_6)



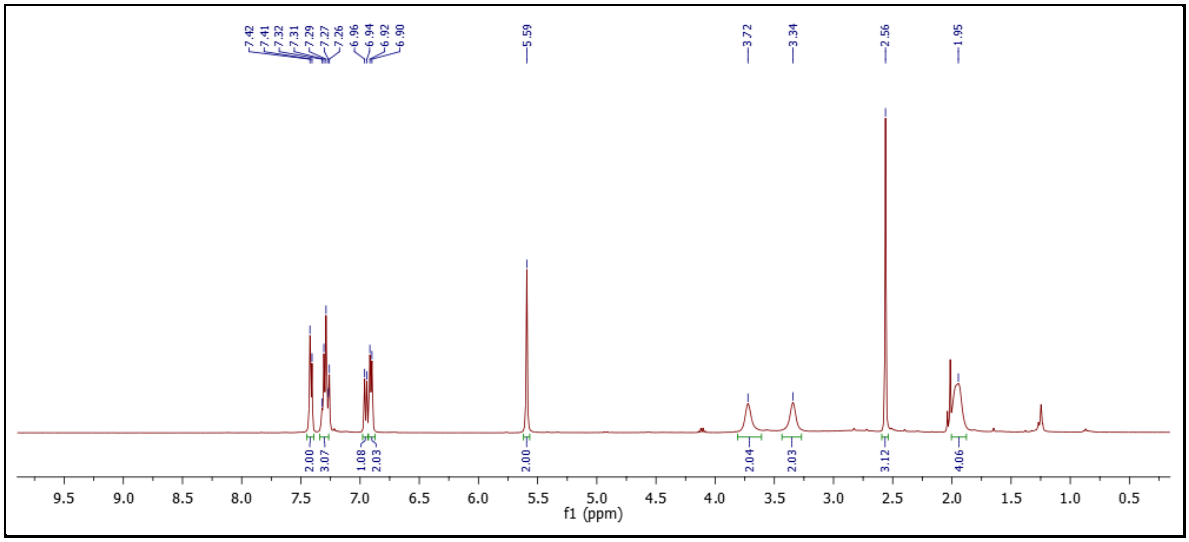
^{13}C NMR (100 MHz, DMSO-D_6)



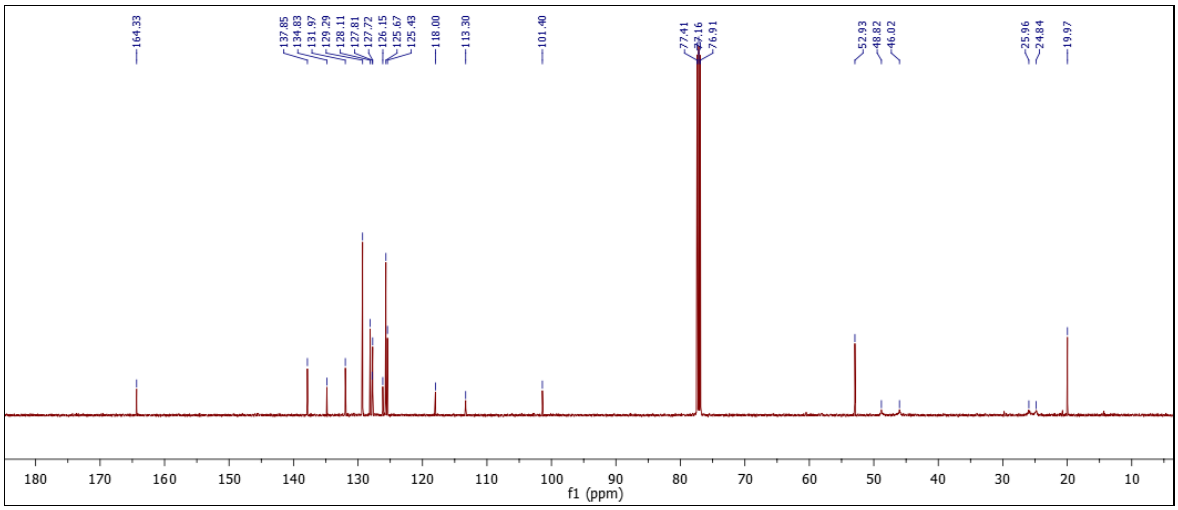


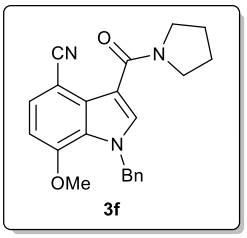
3e

^{1}H NMR (400 MHz, $CDCl_3$)



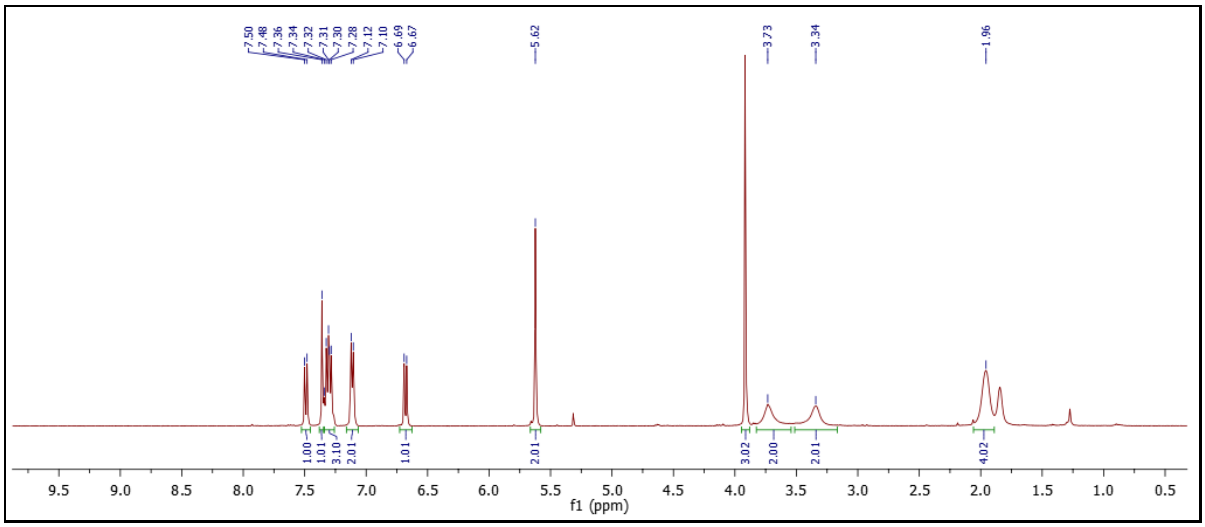
^{13}C NMR (125 MHz, $CDCl_3$)



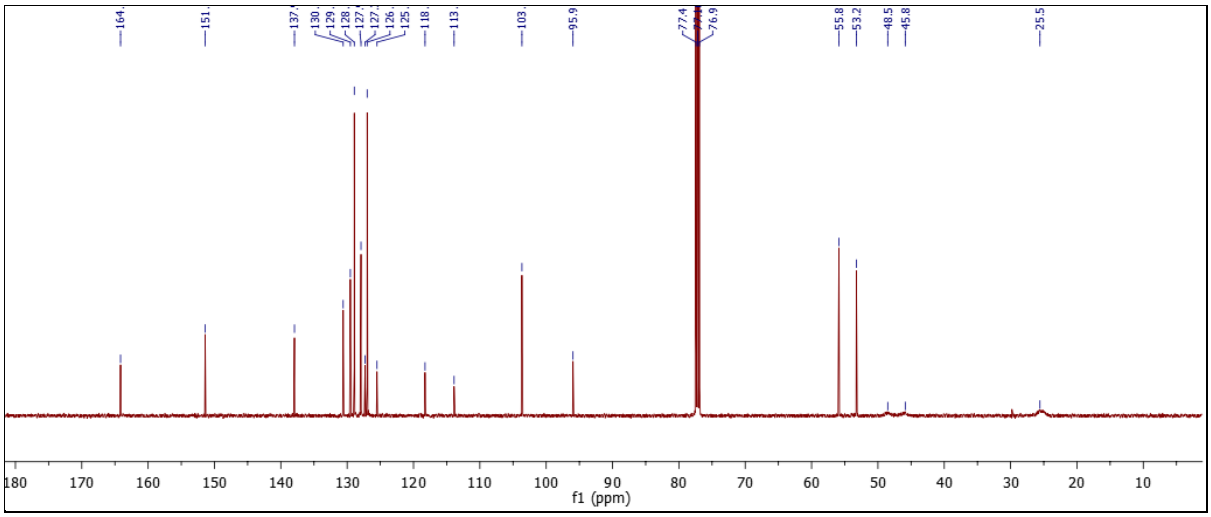


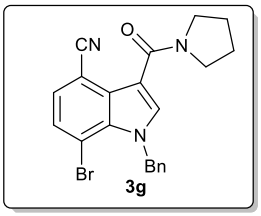
3f

^{1}H NMR (400 MHz, $CDCl_3$)

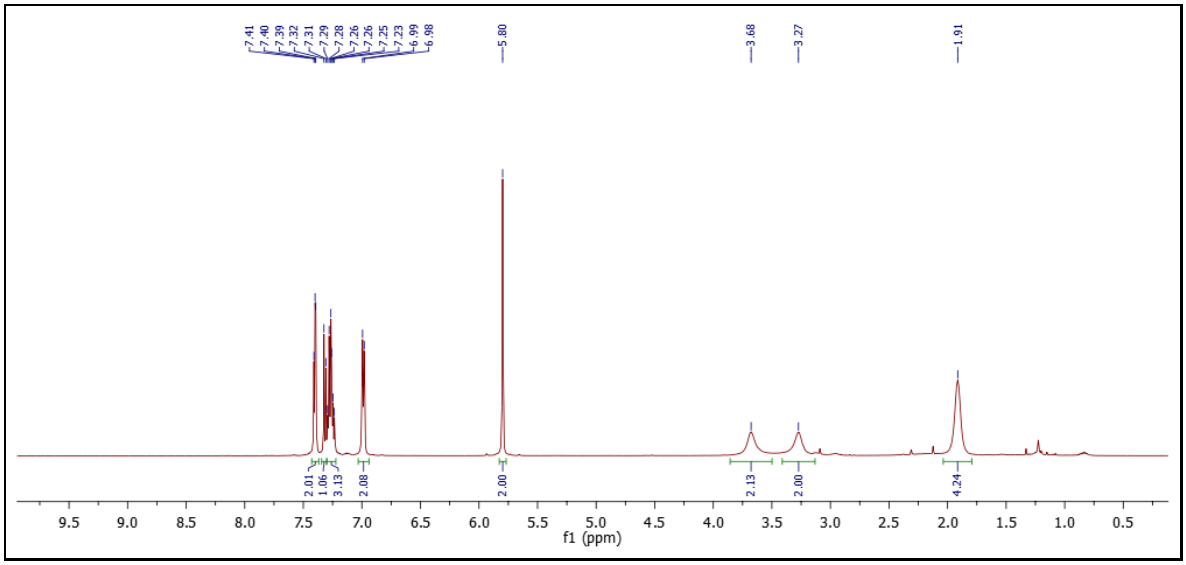


^{13}C NMR (125 MHz, $CDCl_3$)

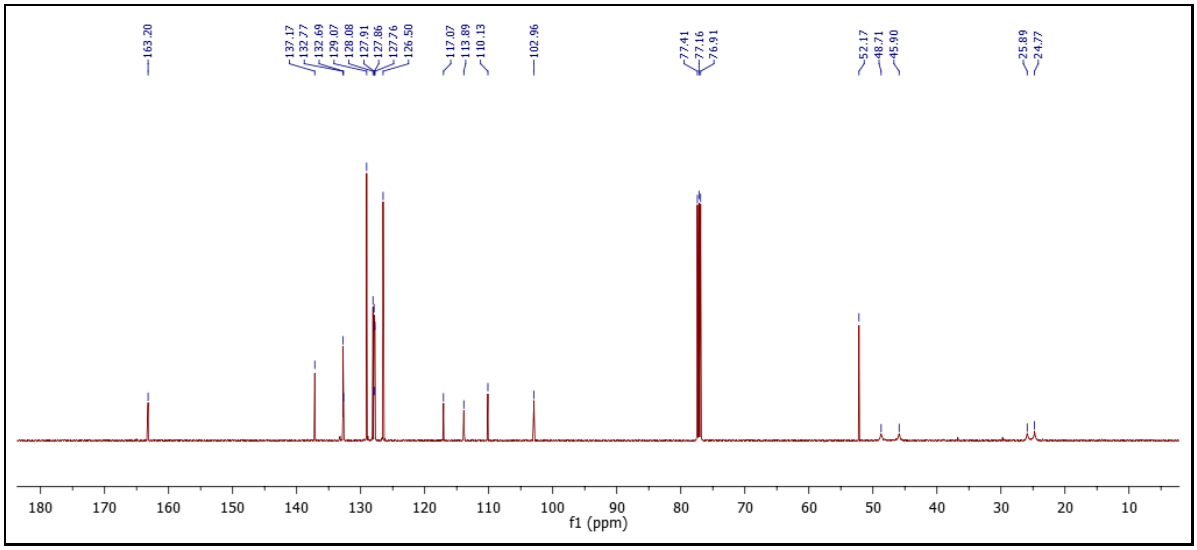


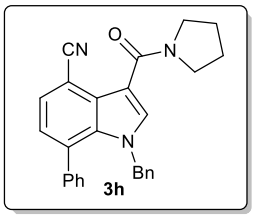


^{1}H NMR (500 MHz, $CDCl_3$)

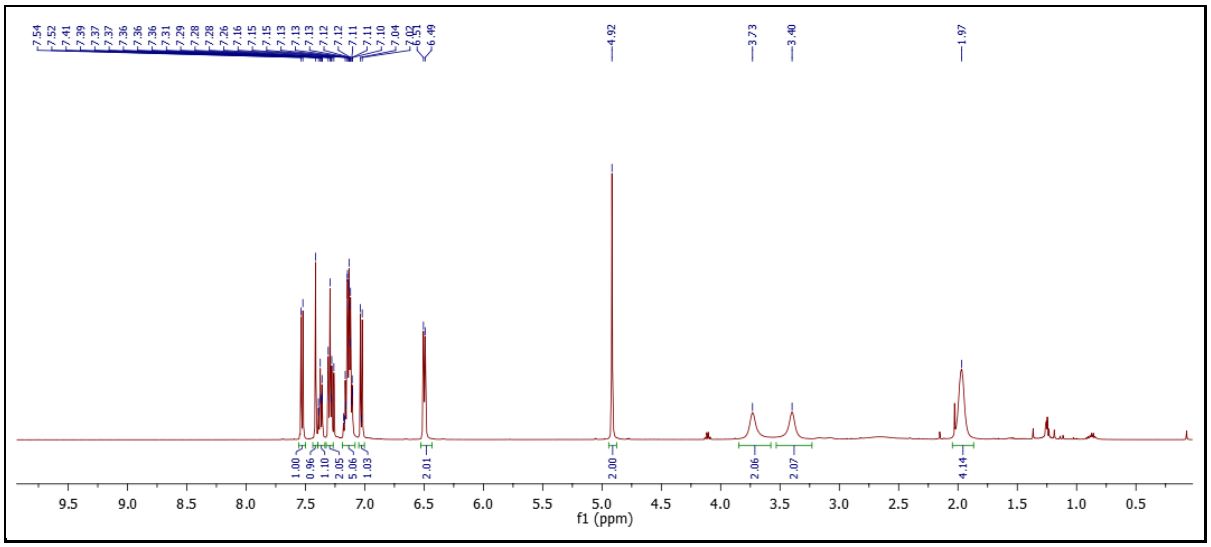


^{13}C NMR (125 MHz, $CDCl_3$)

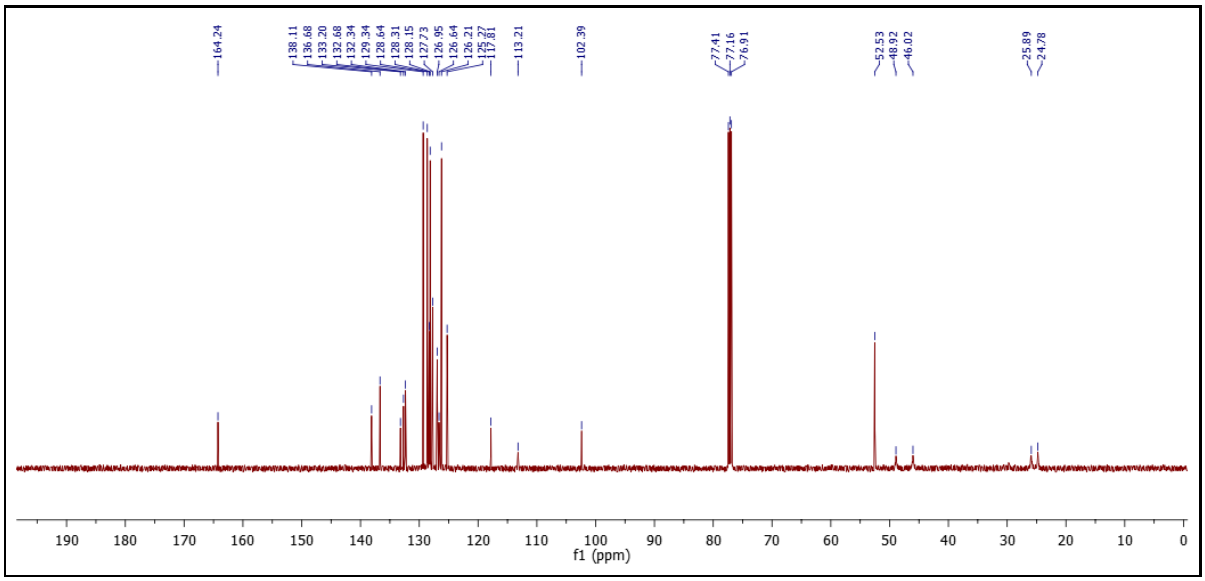


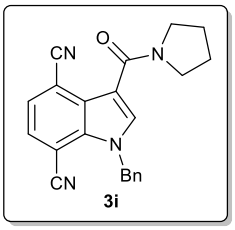


^{1}H NMR (500 MHz, $CDCl_3$)



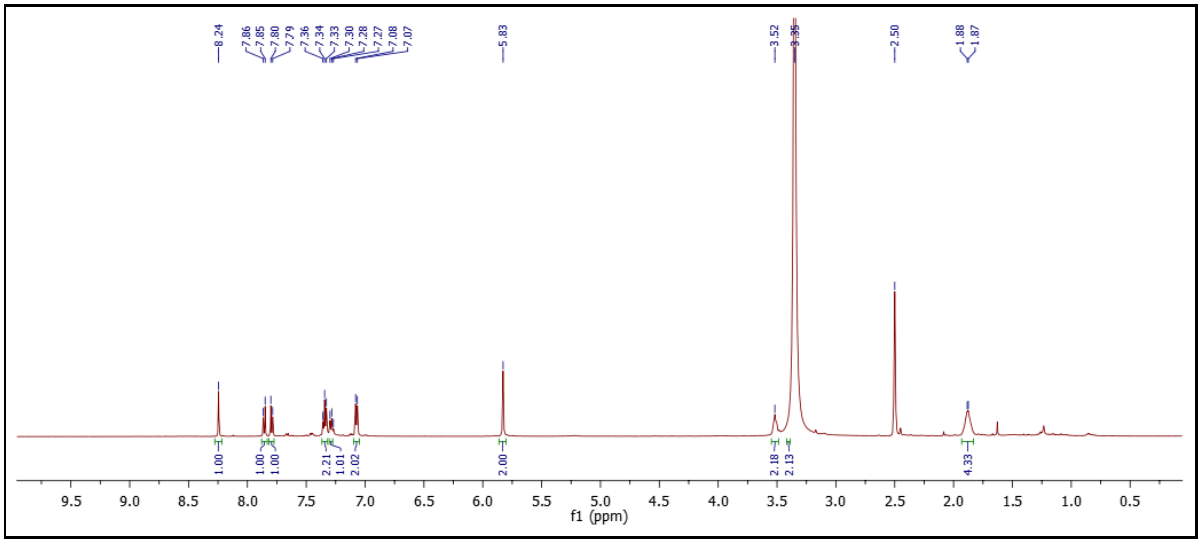
^{13}C NMR (125 MHz, $CDCl_3$)



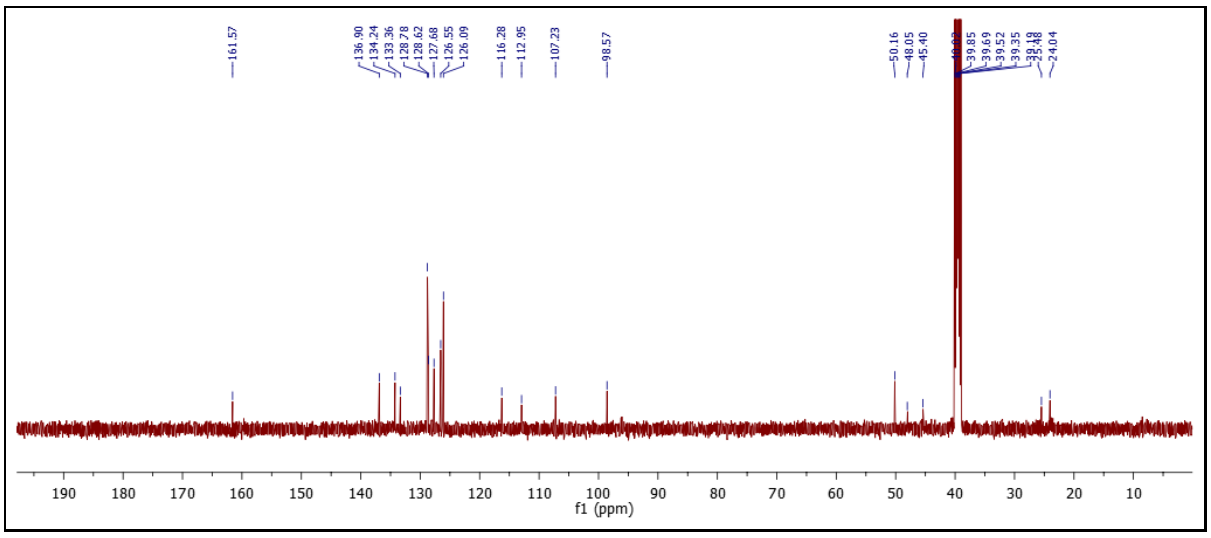


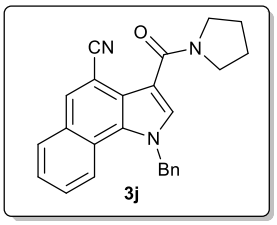
3i

^{1}H NMR (500 MHz, DMSO-D$_6$)



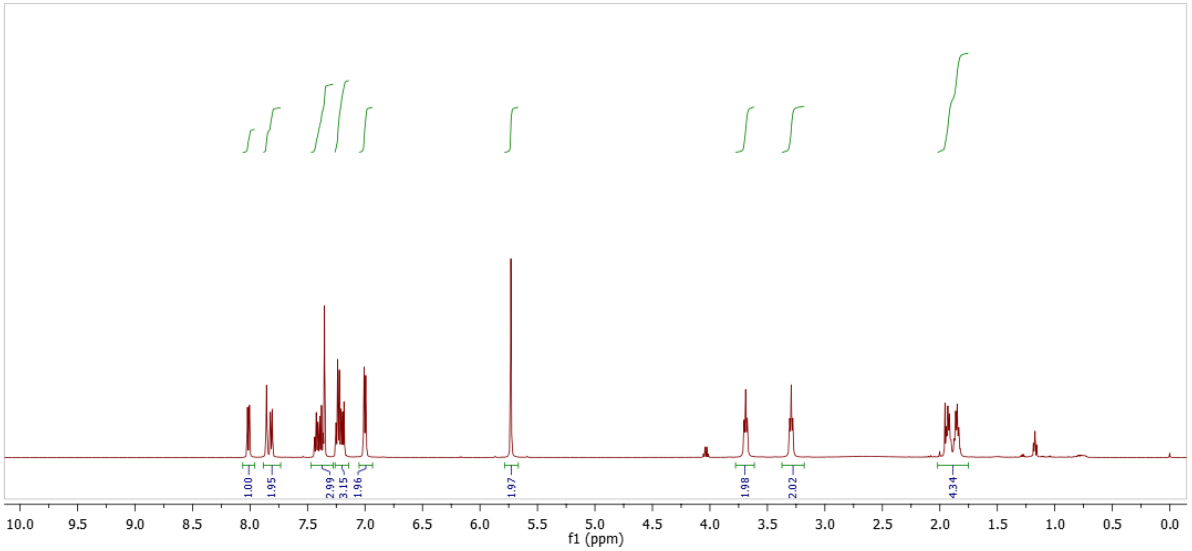
^{13}C NMR (125 MHz, DMSO-D$_6$)



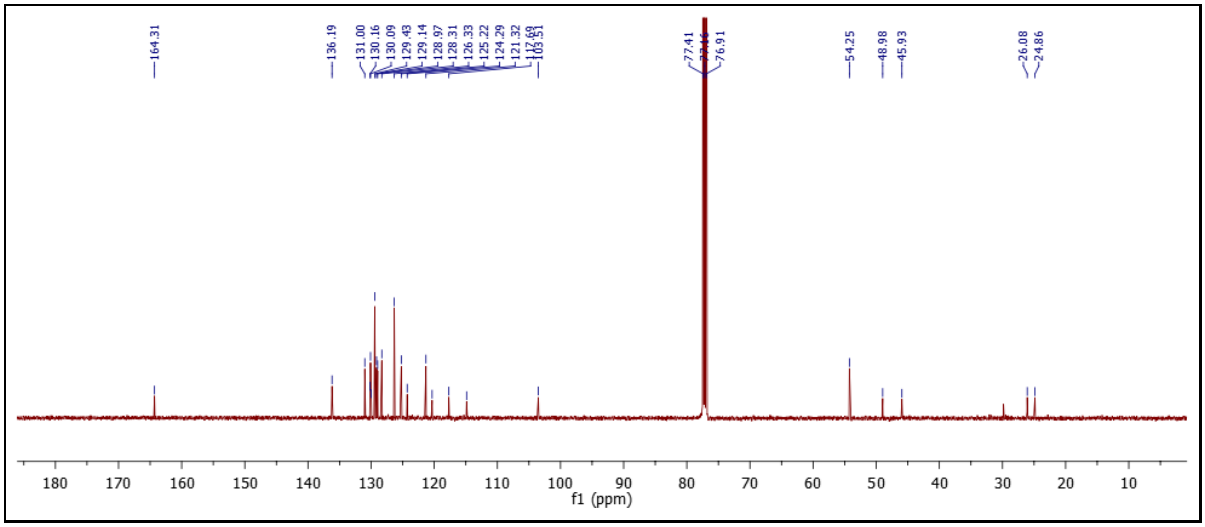


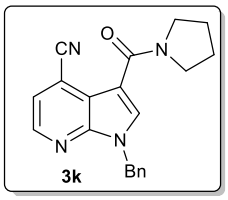
3j

^{1}H NMR (500 MHz, $CDCl_3$)

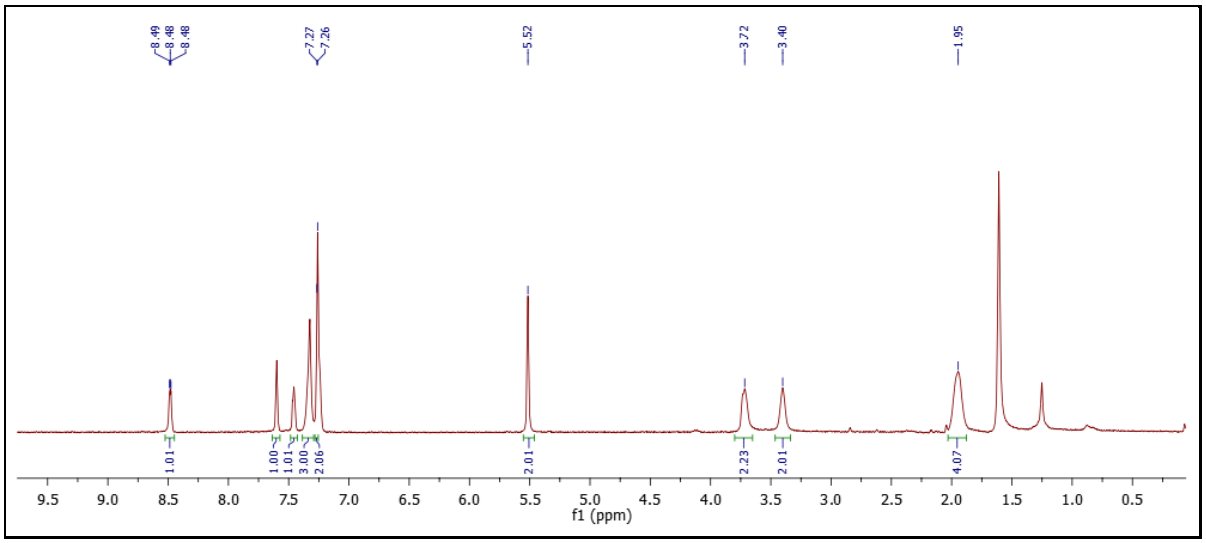


^{13}C NMR (125 MHz, $CDCl_3$)

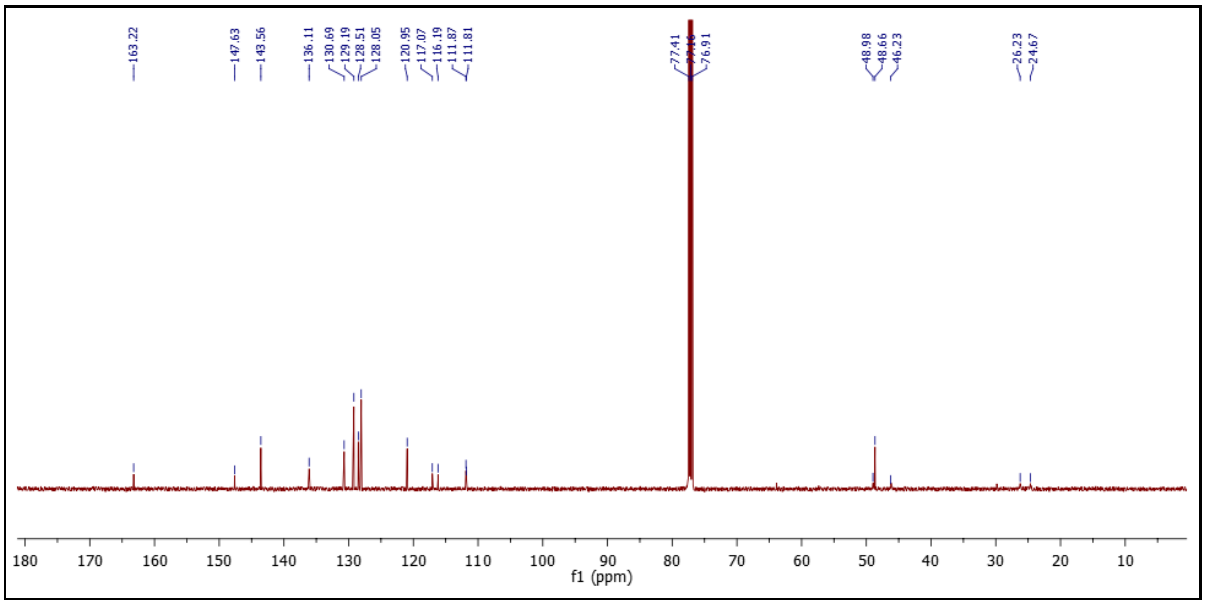


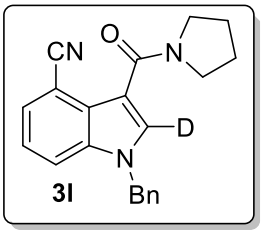


^{1}HNMR (400 MHz, $CDCl_3$)

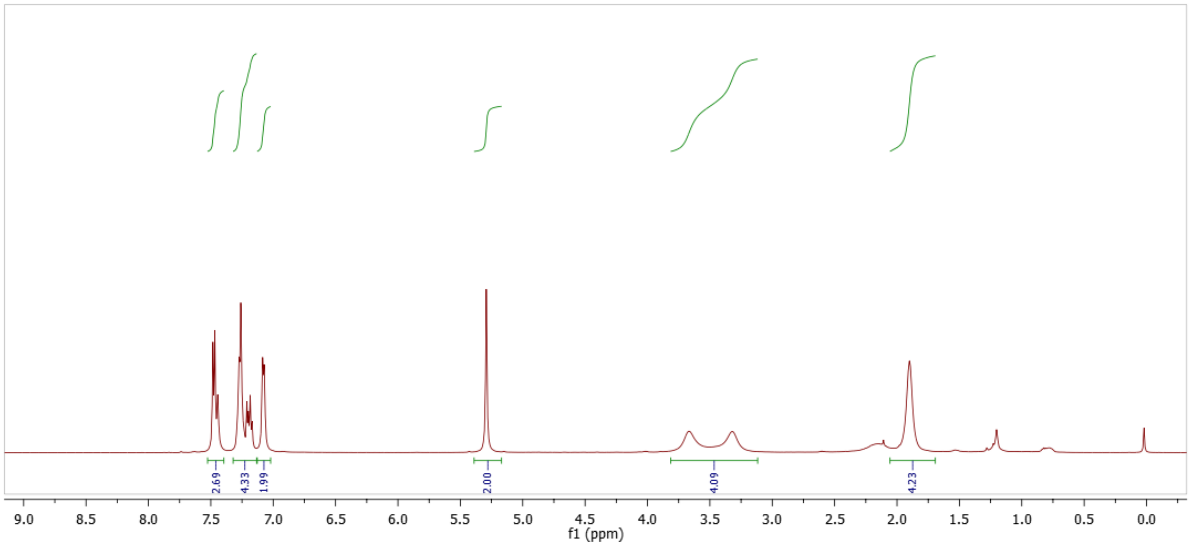


^{13}C NMR (125 MHz, $CDCl_3$)

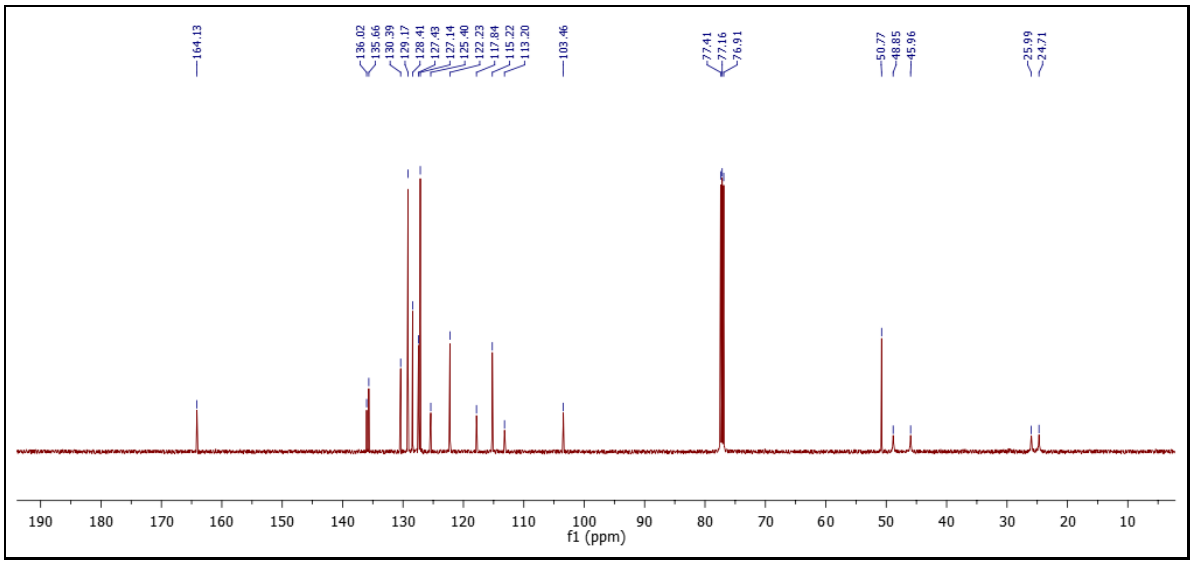


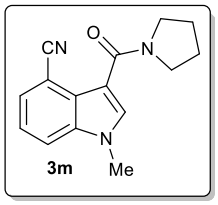


^{1}H NMR (500 MHz, $CDCl_3$)

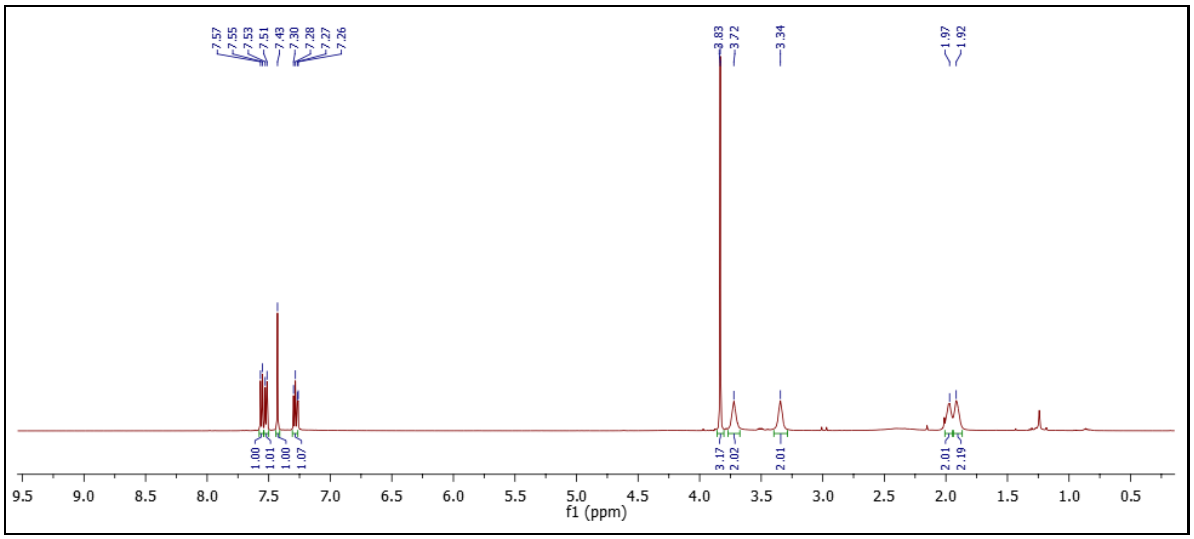


^{13}C NMR (125 MHz, $CDCl_3$)

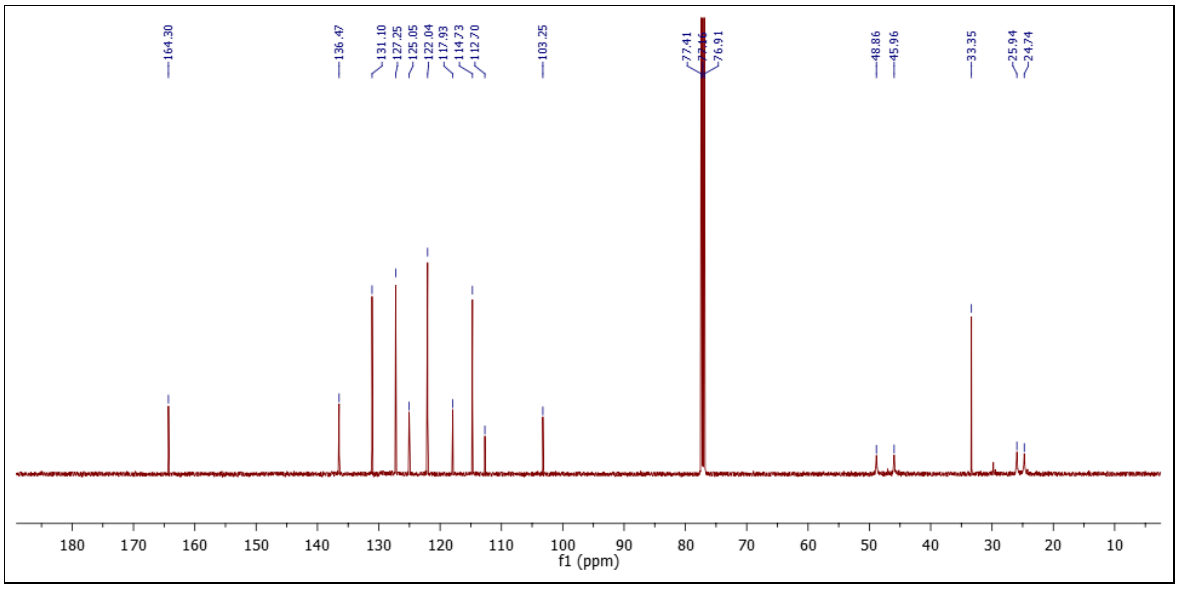


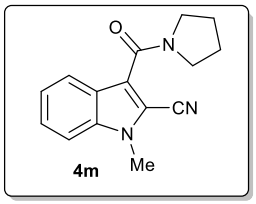


^{1}H NMR (500 MHz, $CDCl_3$)

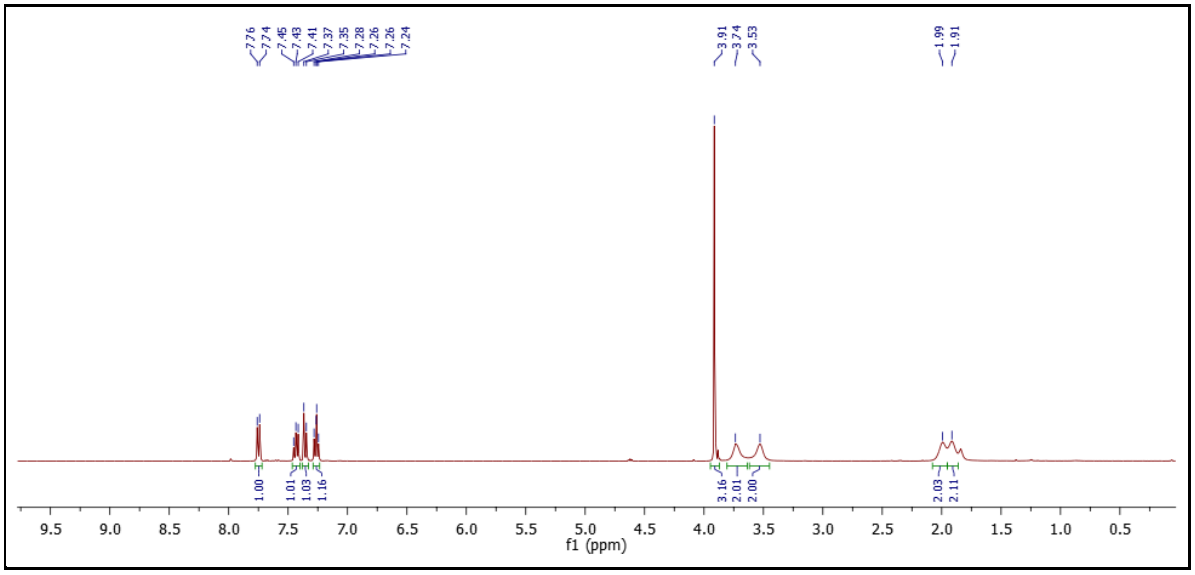


^{13}C NMR (125 MHz, $CDCl_3$)

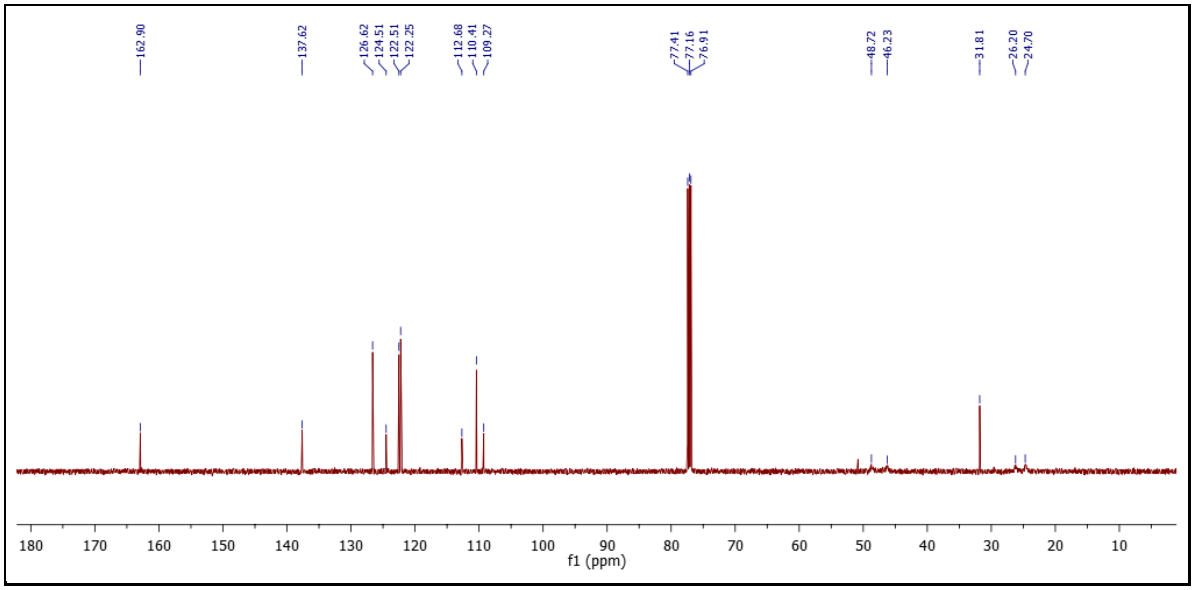


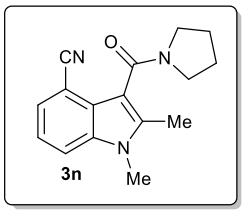


^{1}H NMR (400 MHz, $CDCl_3$)

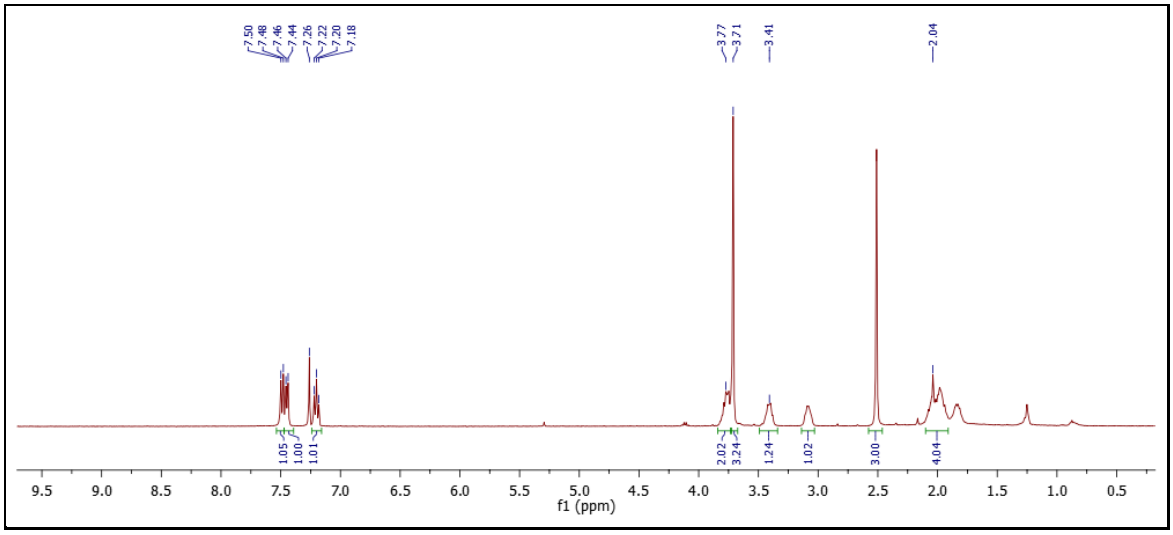


^{13}C NMR (100 MHz, $CDCl_3$)

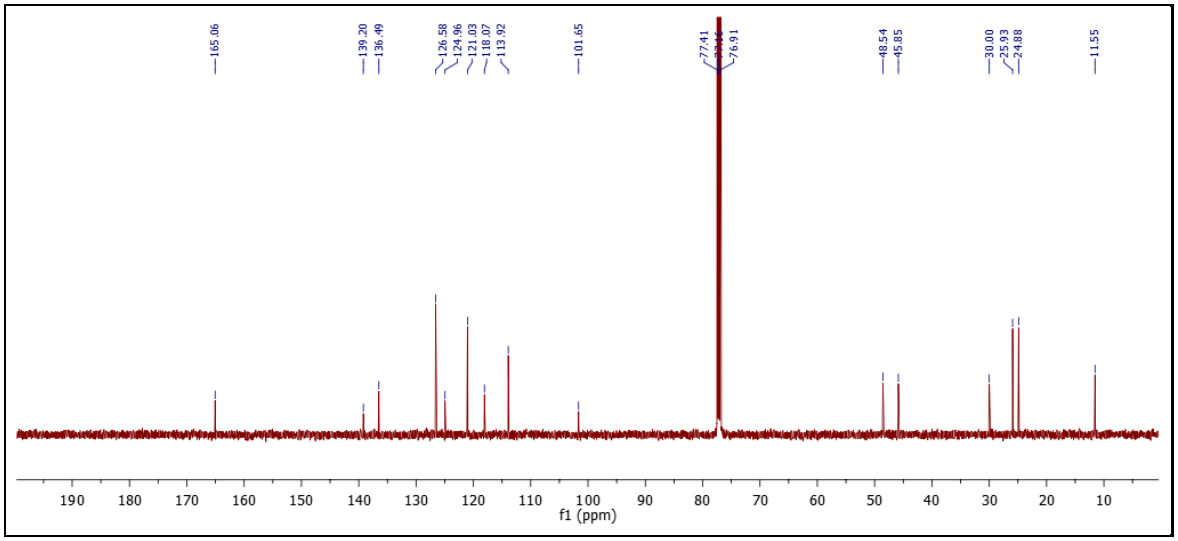


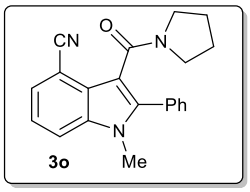


^{1}HNMR (400 MHz, $CDCl_3$)

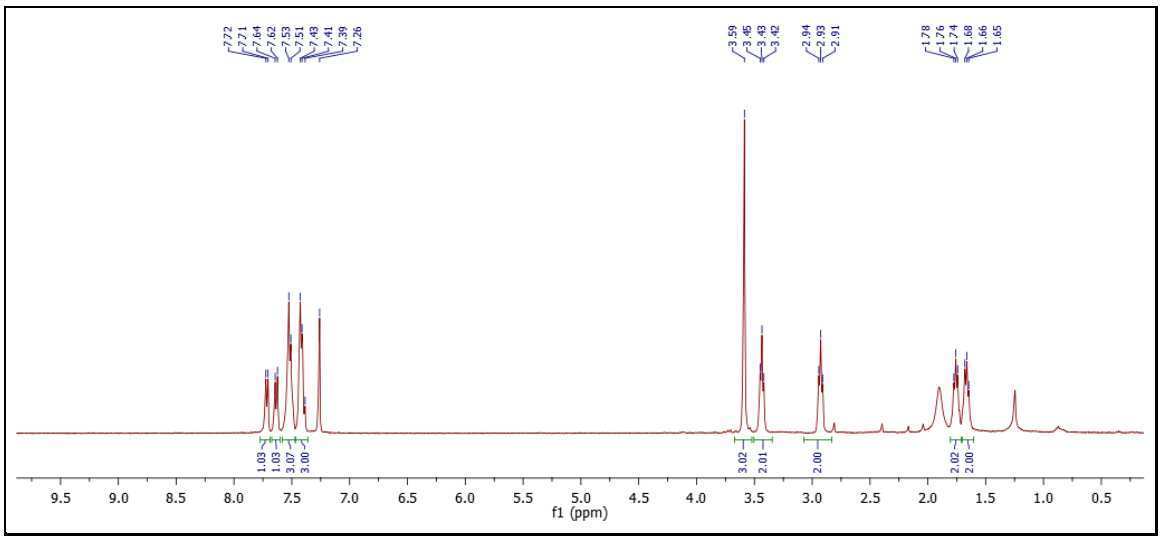


^{13}C NMR (125 MHz, $CDCl_3$)

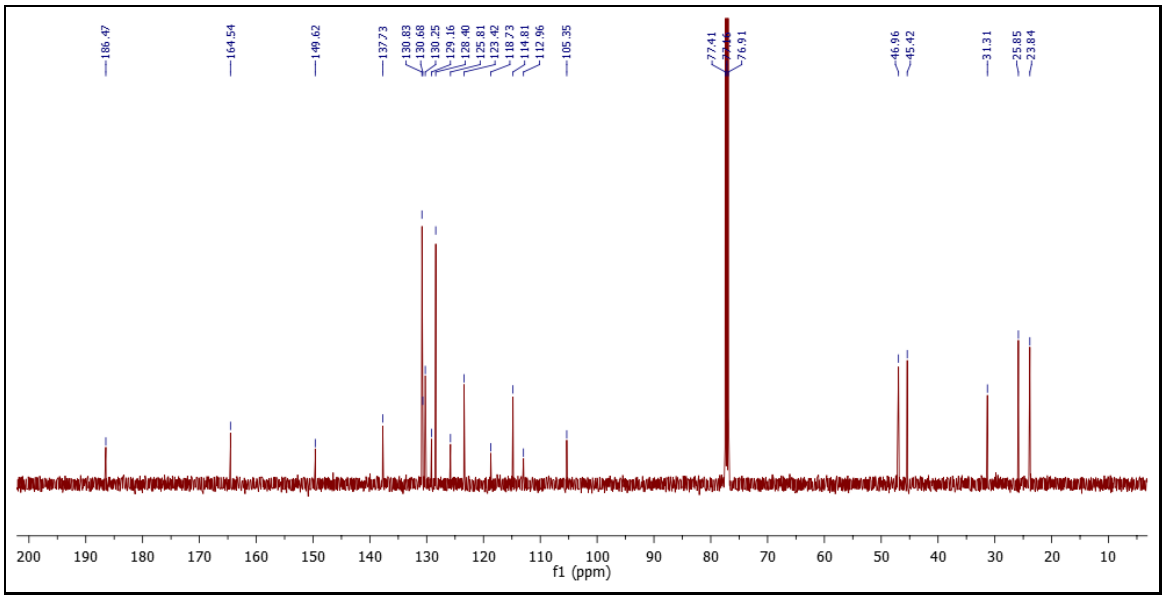


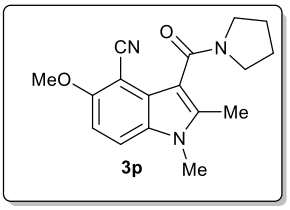


^{1}H NMR (400 MHz, $CDCl_3$)

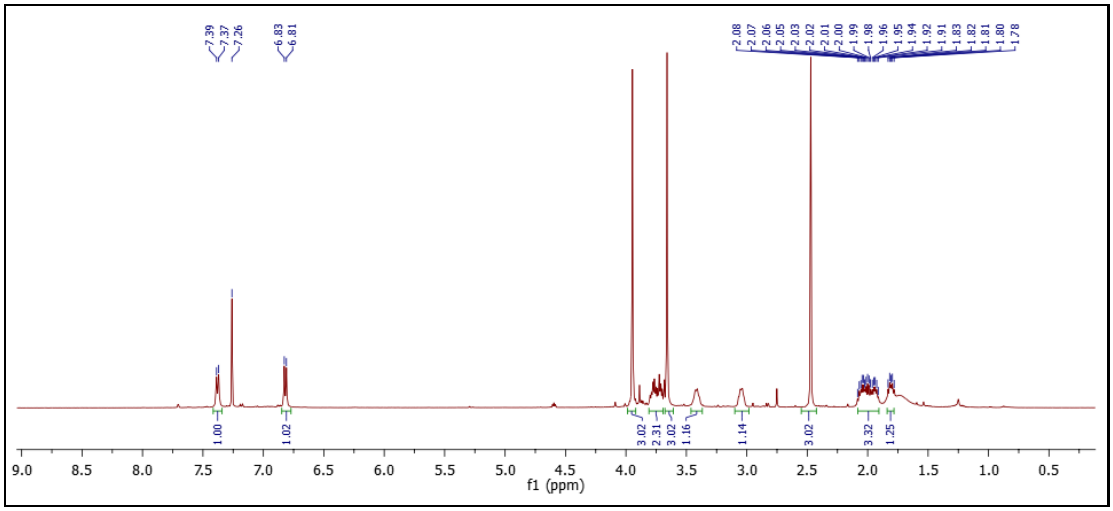


^{13}C NMR (125 MHz, $CDCl_3$)

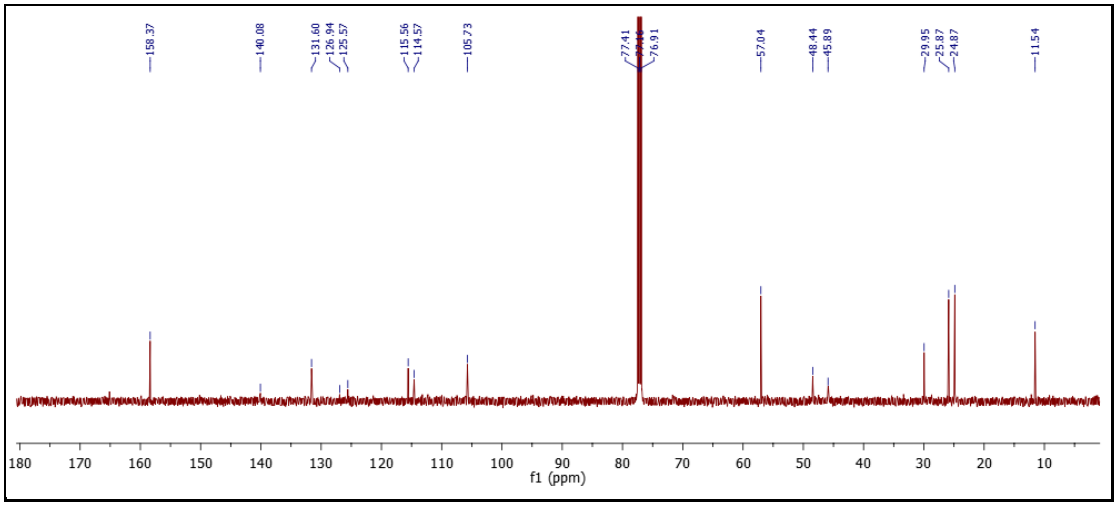


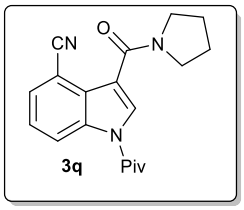


^{1}H NMR (500 MHz, $CDCl_3$)



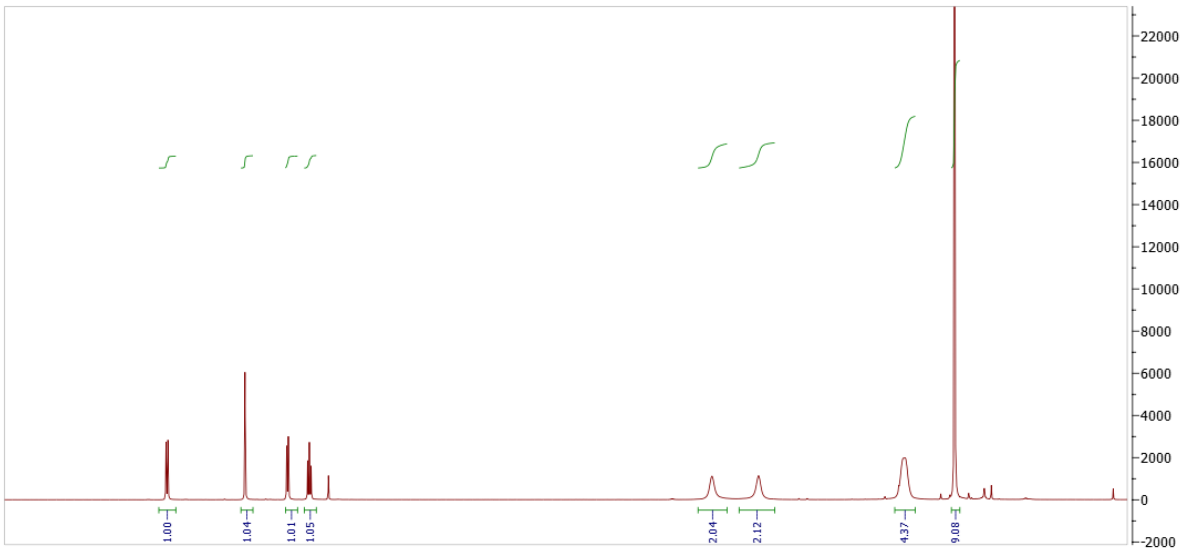
^{13}C NMR (125 MHz, $CDCl_3$)



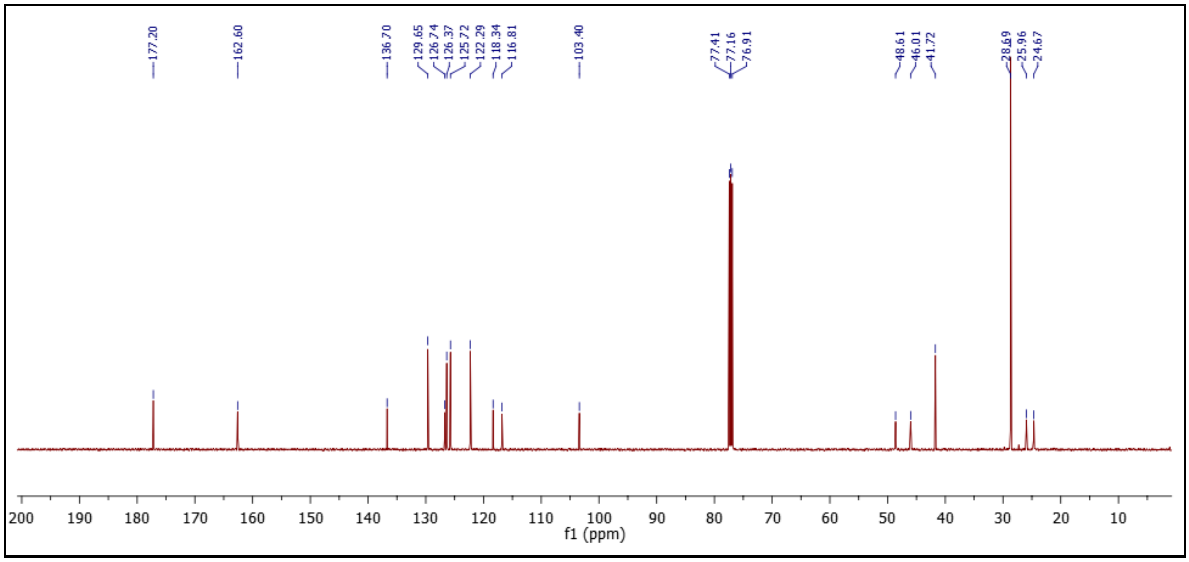


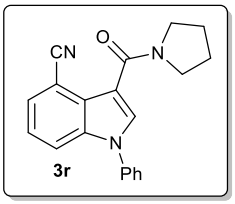
3q

^{1}H NMR (500 MHz, $CDCl_3$)

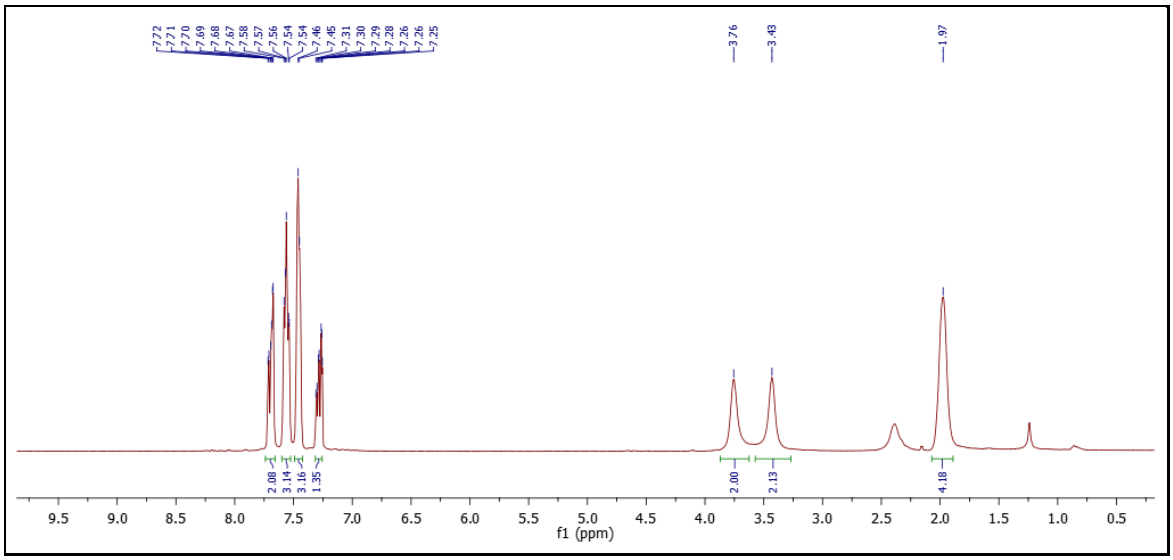


^{13}C NMR (125 MHz, $CDCl_3$)

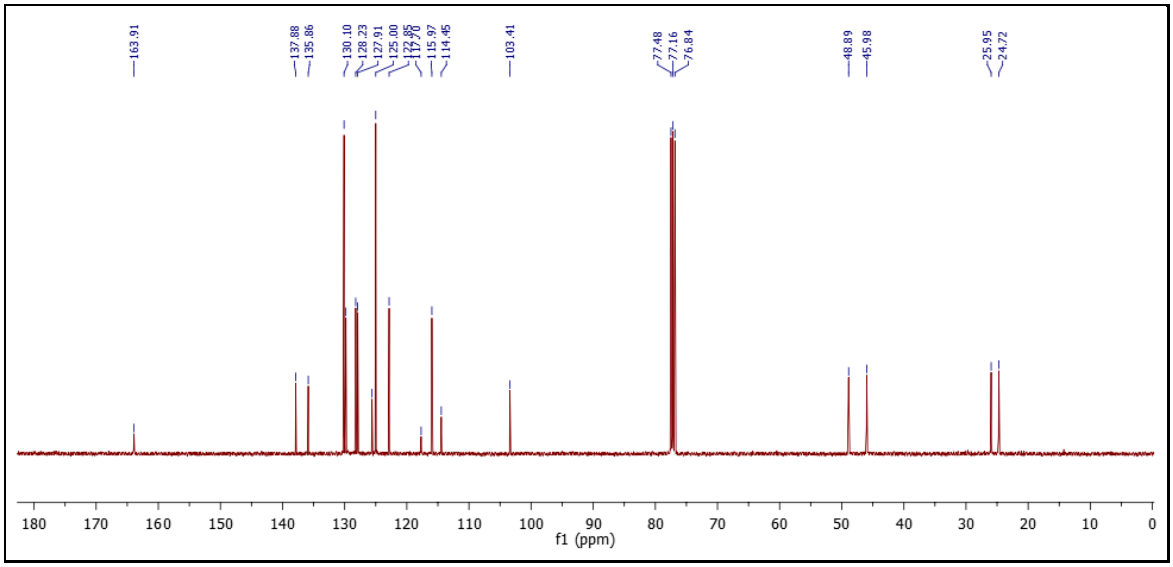


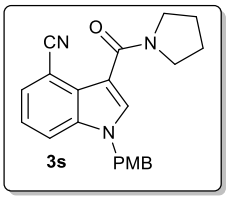


^{1}H NMR (400 MHz, $CDCl_3$)

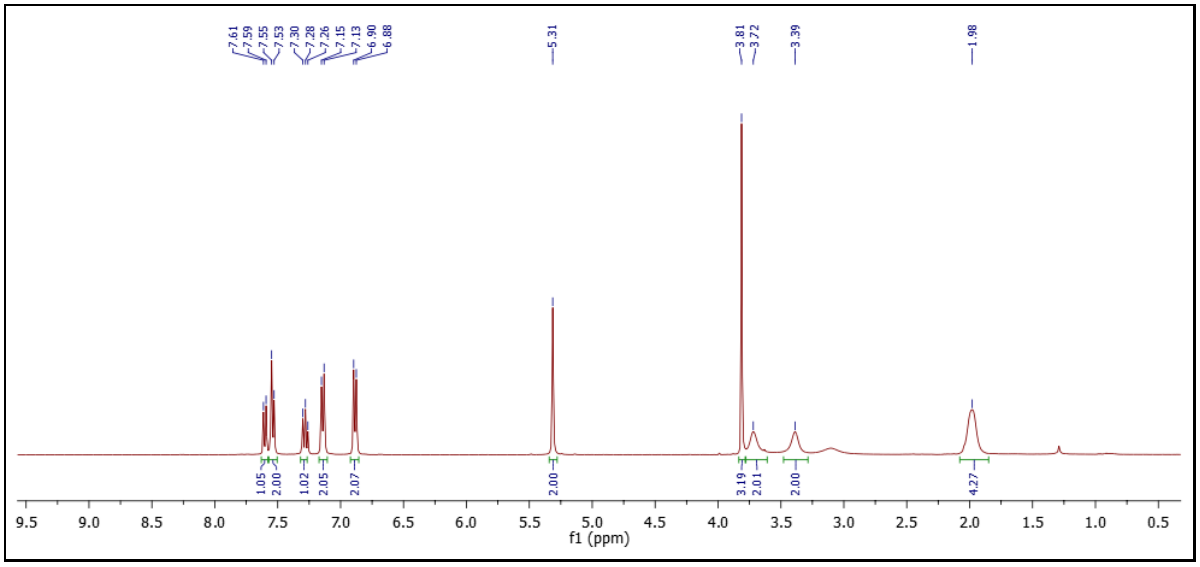


^{13}C NMR (100 MHz, $CDCl_3$)

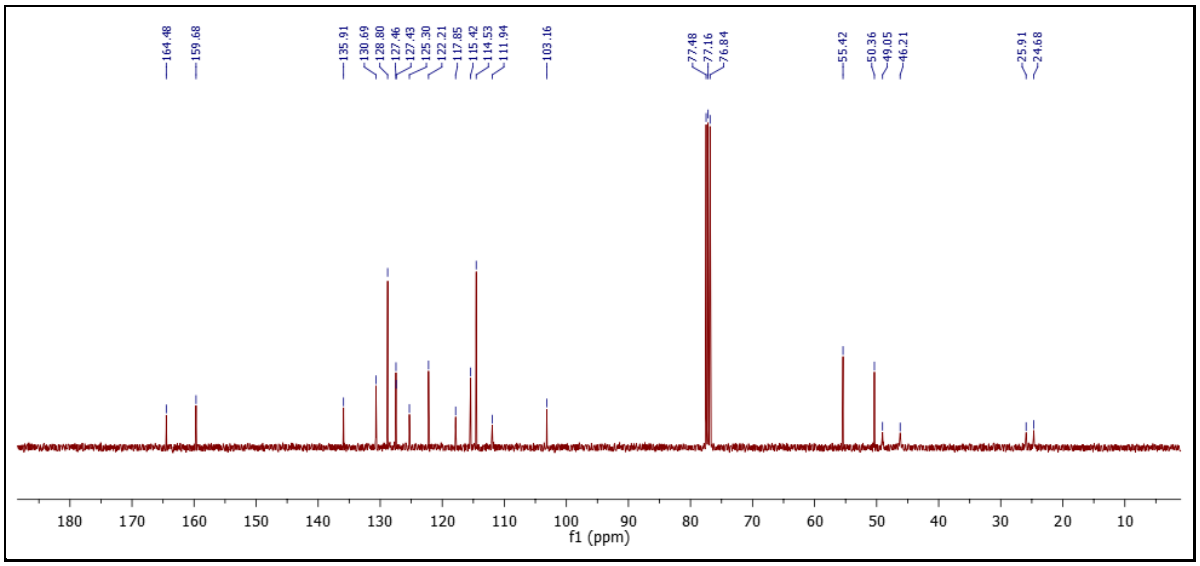


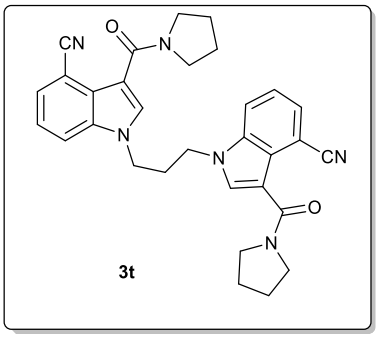


^{1}H NMR (400 MHz, $CDCl_3$)



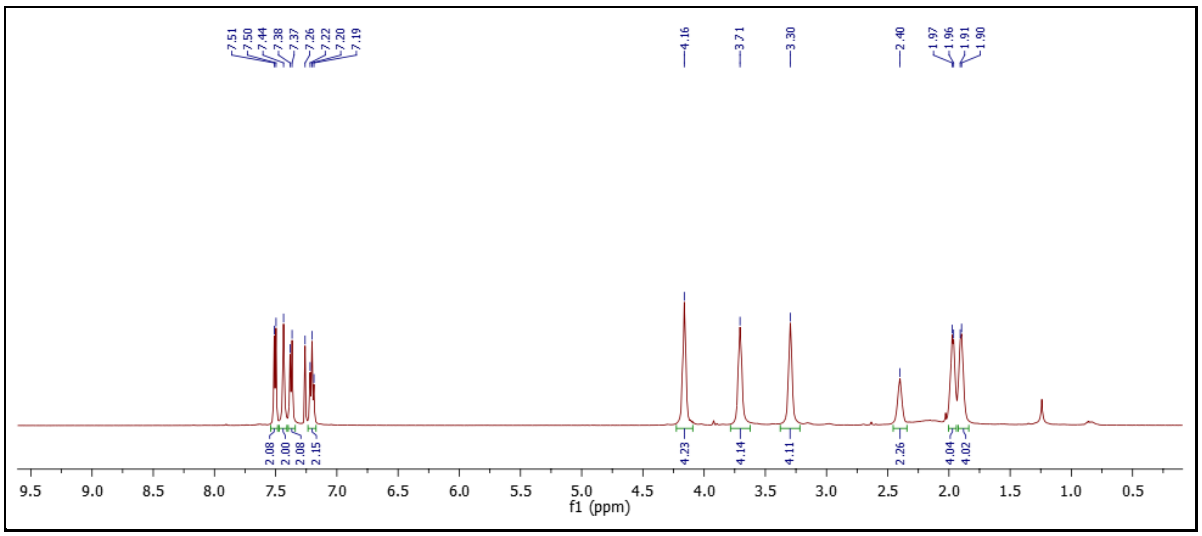
^{13}C NMR (100 MHz, $CDCl_3$)



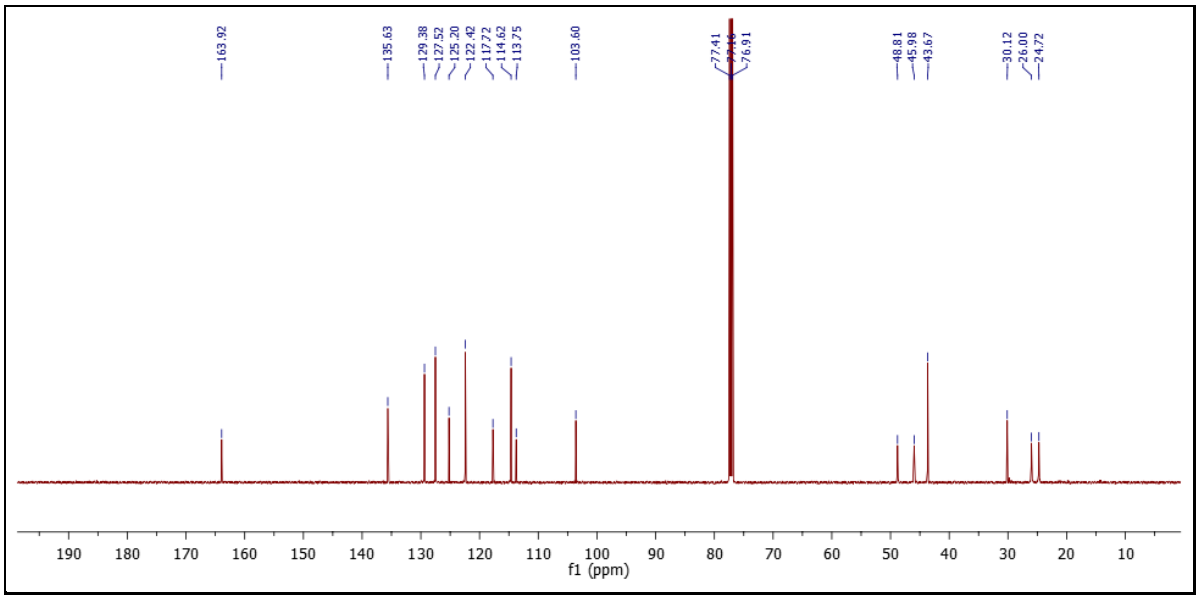


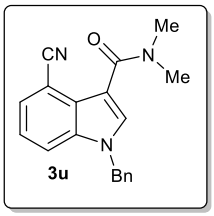
3t

^{1}H NMR (500 MHz, $CDCl_3$)

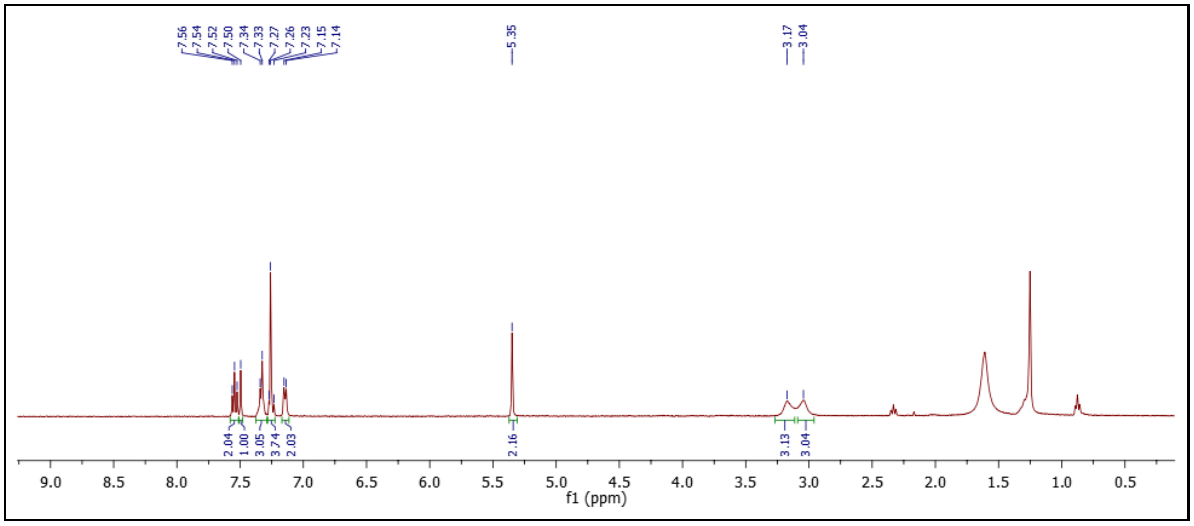


^{13}C NMR (125 MHz, $CDCl_3$)

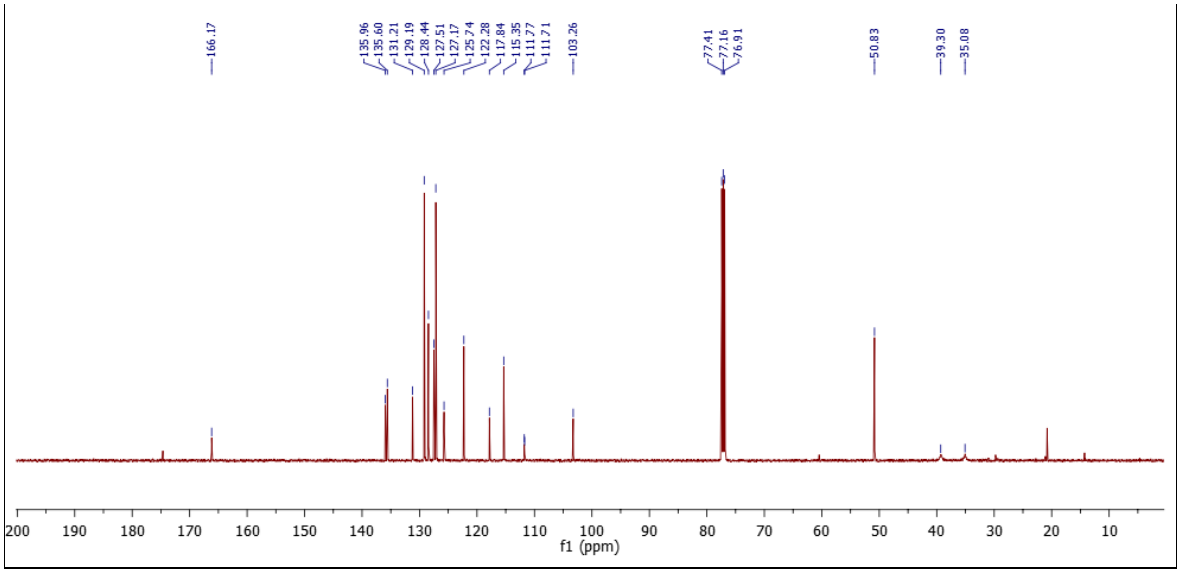


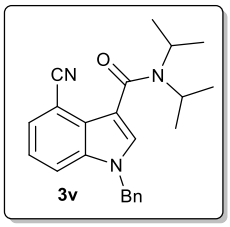


^{1}H NMR (400 MHz, $CDCl_3$)

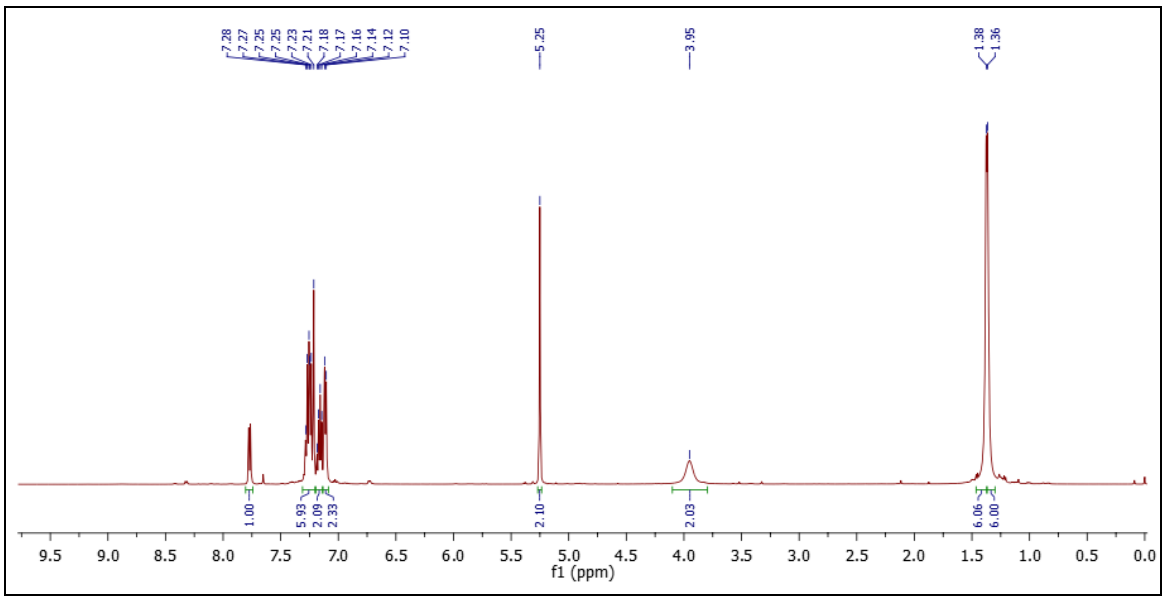


^{13}C NMR (125 MHz, $CDCl_3$)

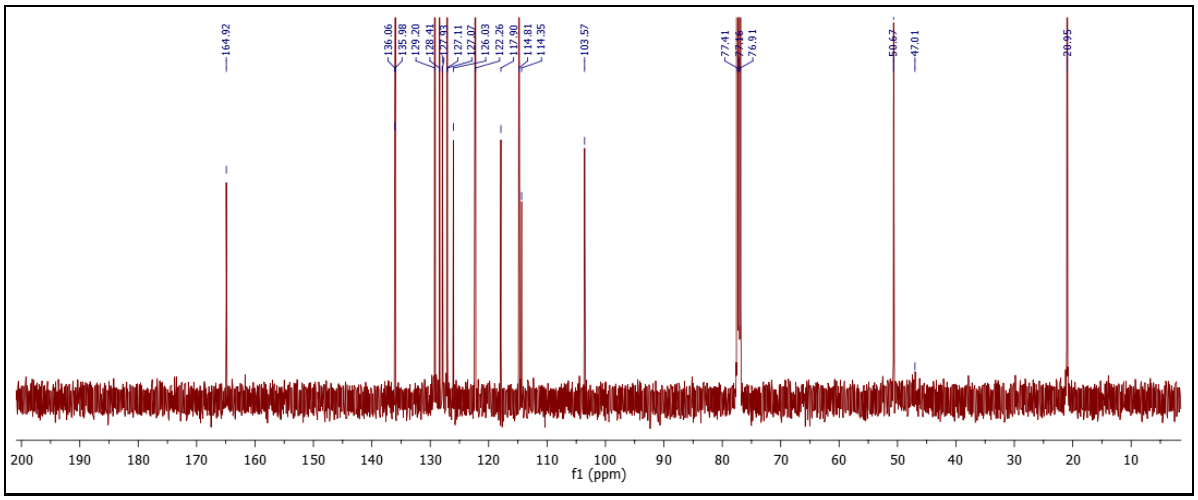


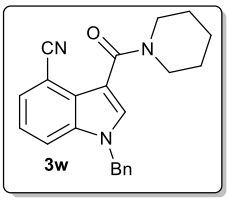


^{1}H NMR (500 MHz, $CDCl_3$)

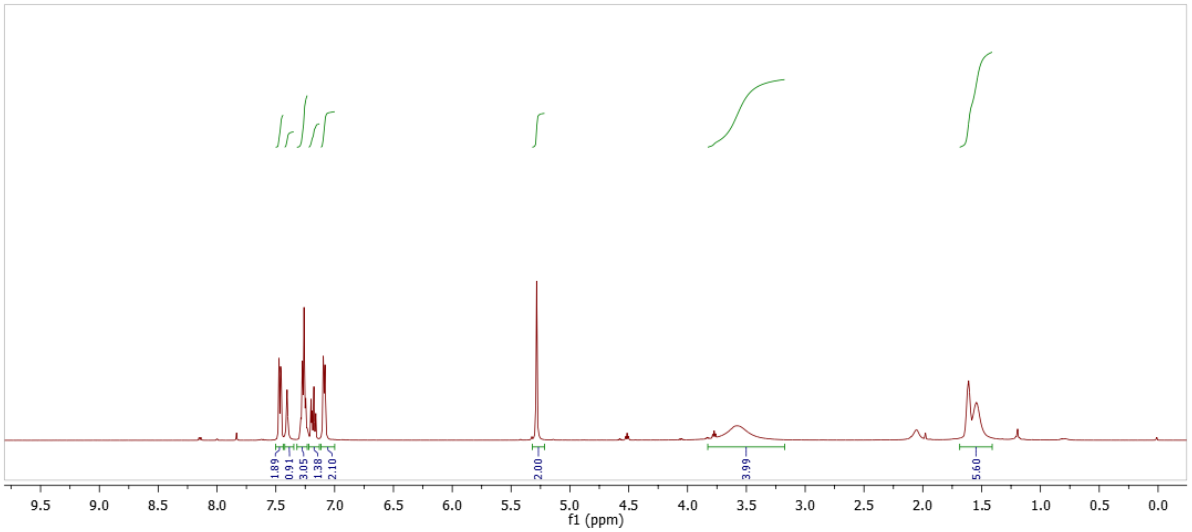


^{13}C NMR (125 MHz, $CDCl_3$)

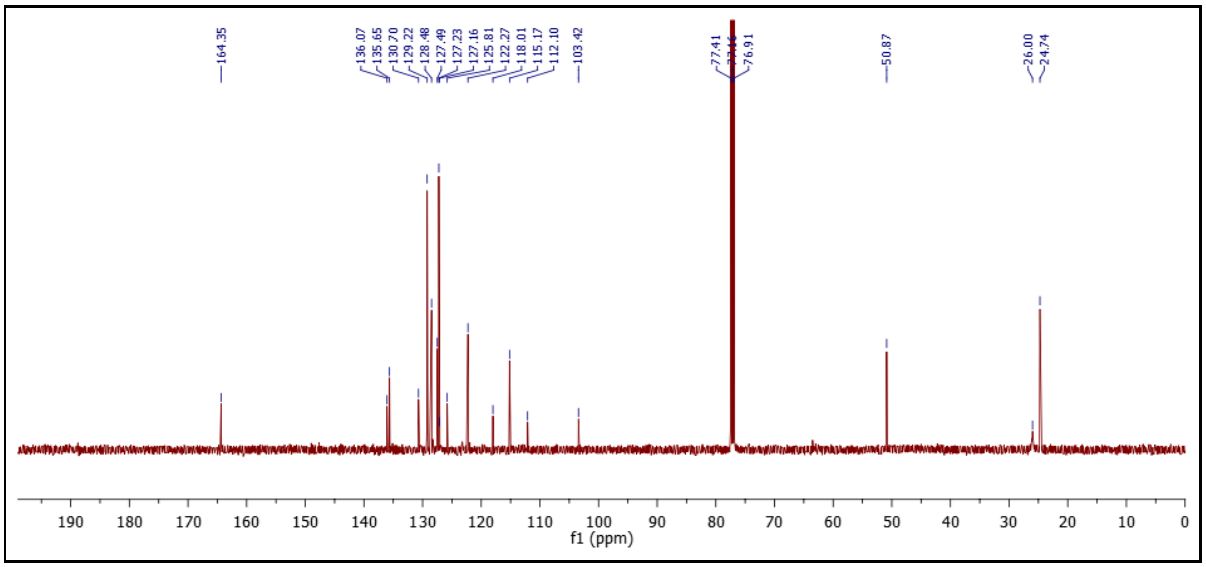


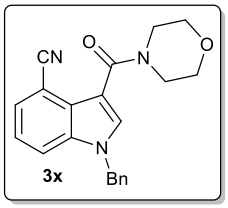


^{1}H NMR (500 MHz, $CDCl_3$)

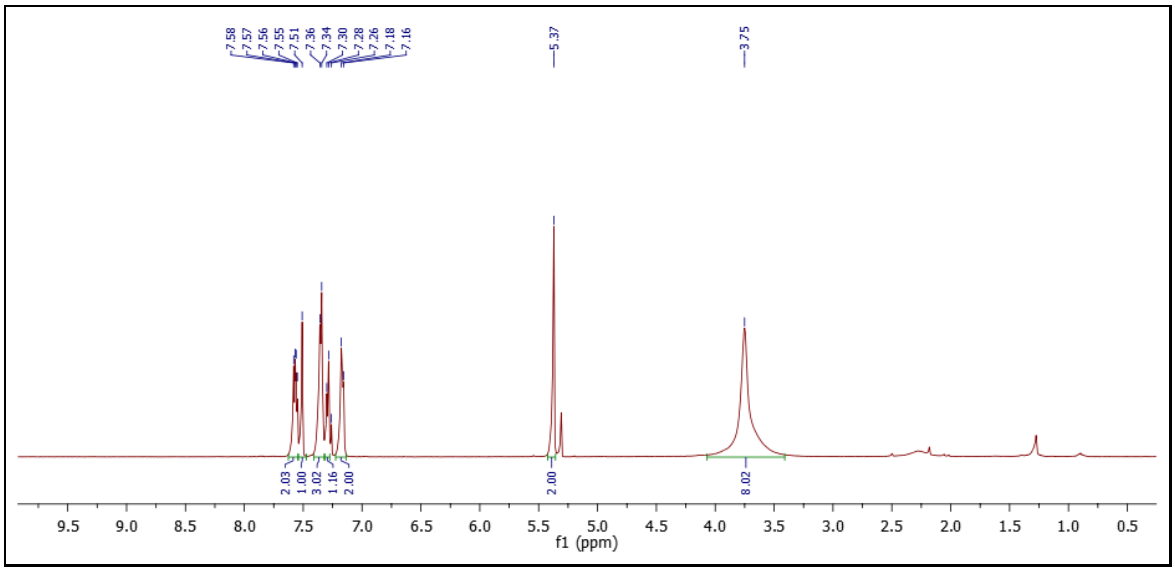


^{13}C NMR (125 MHz, $CDCl_3$)

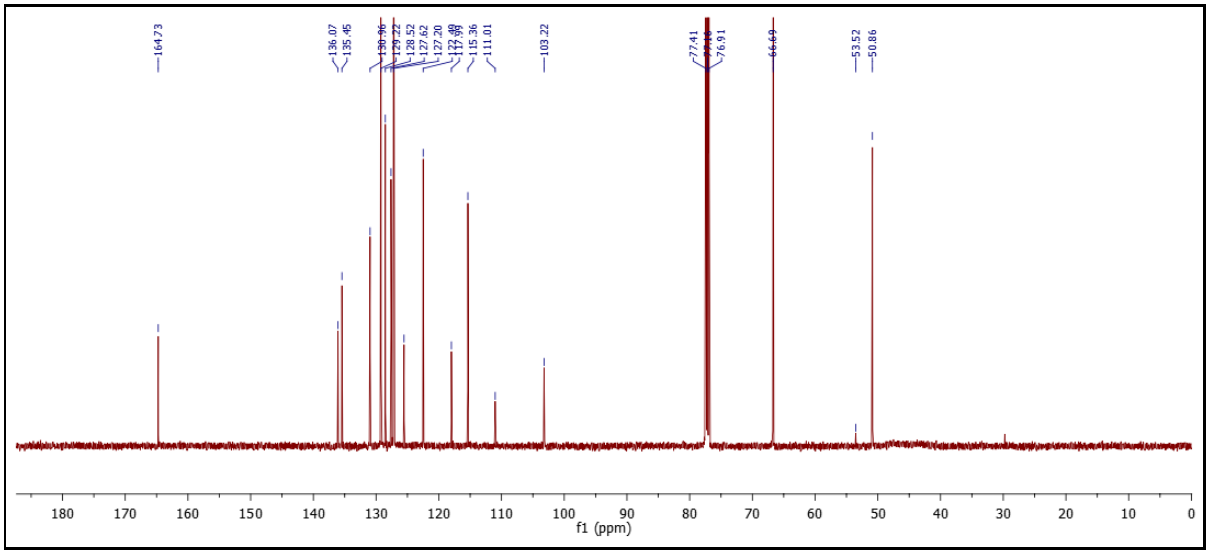


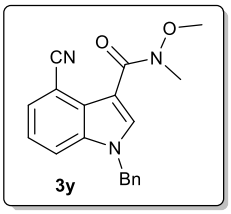


^{1}H NMR (400 MHz, $CDCl_3$)

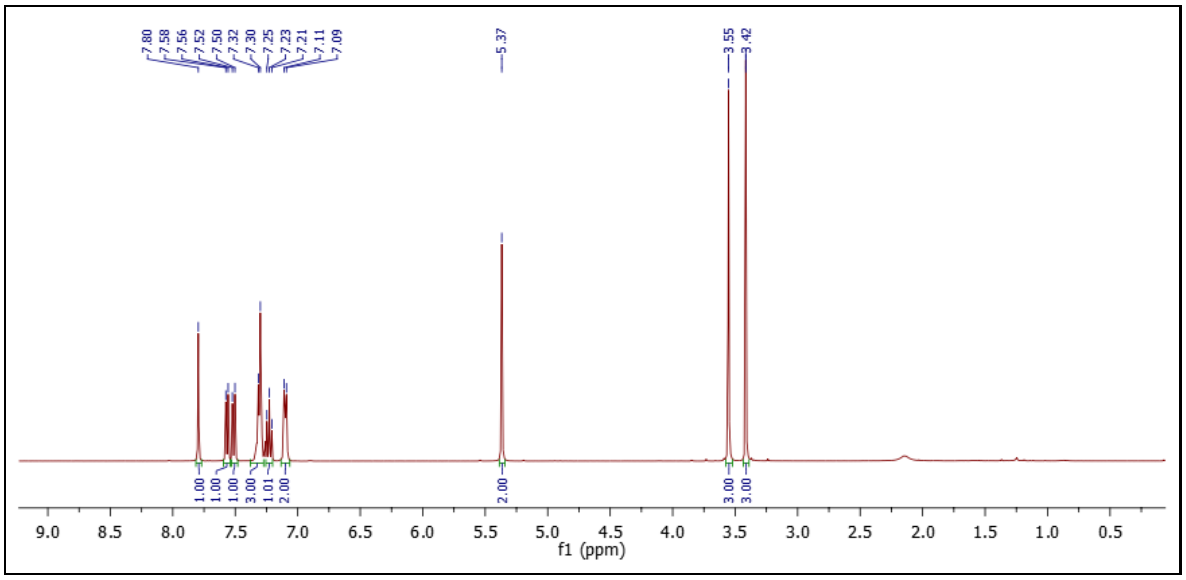


^{13}C NMR (125 MHz, $CDCl_3$)

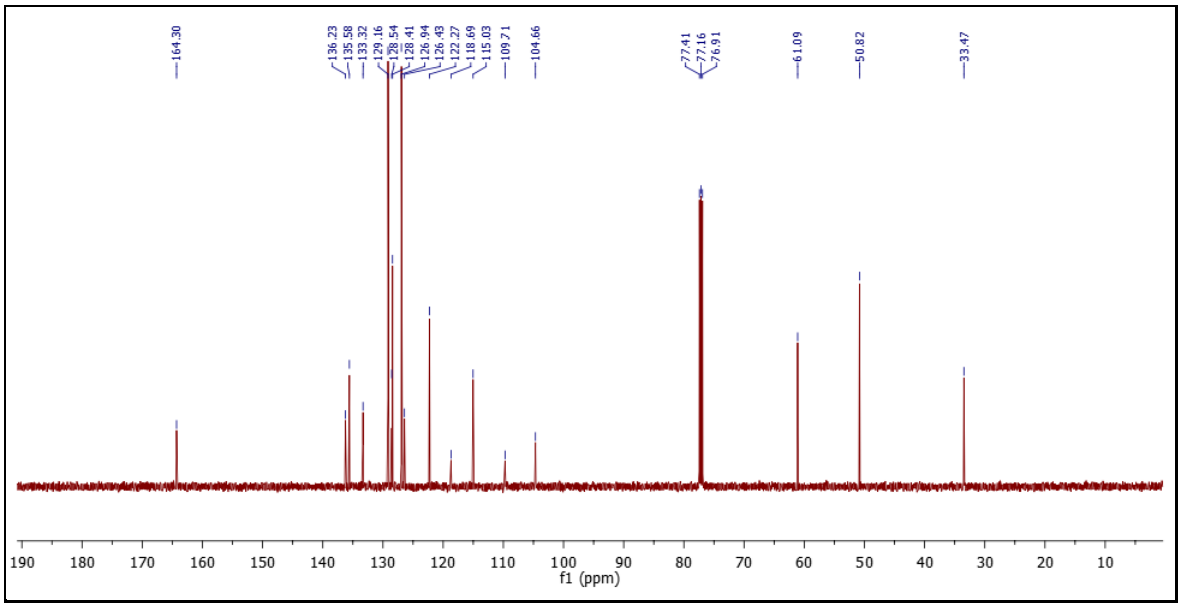


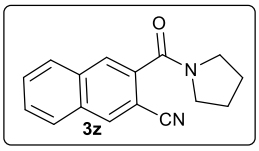


^{1}H NMR (400 MHz, $CDCl_3$)



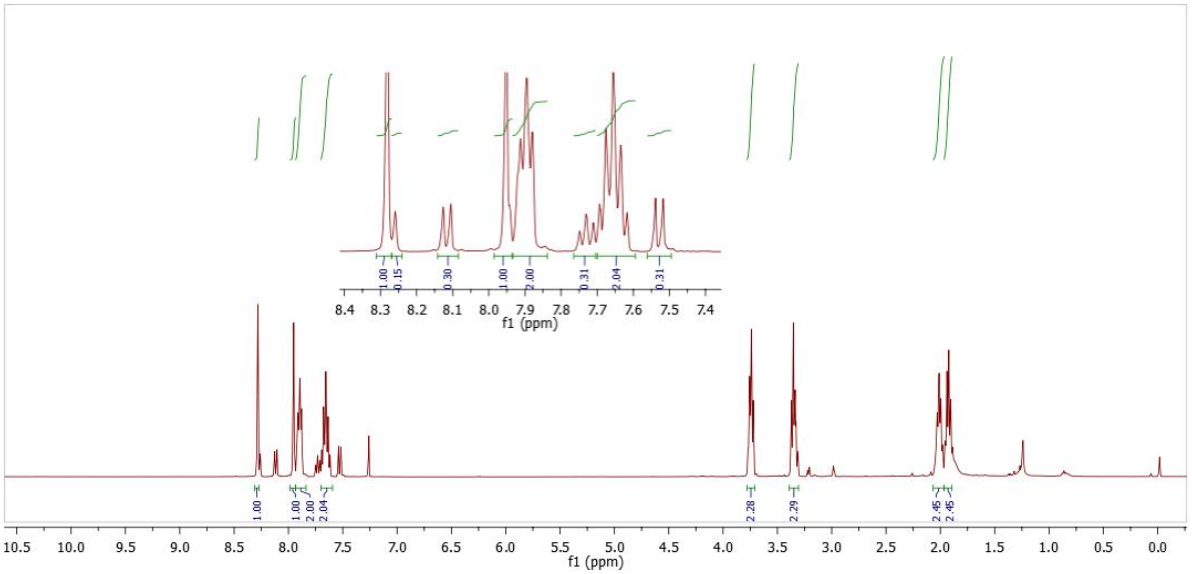
^{13}C NMR (125 MHz, $CDCl_3$)



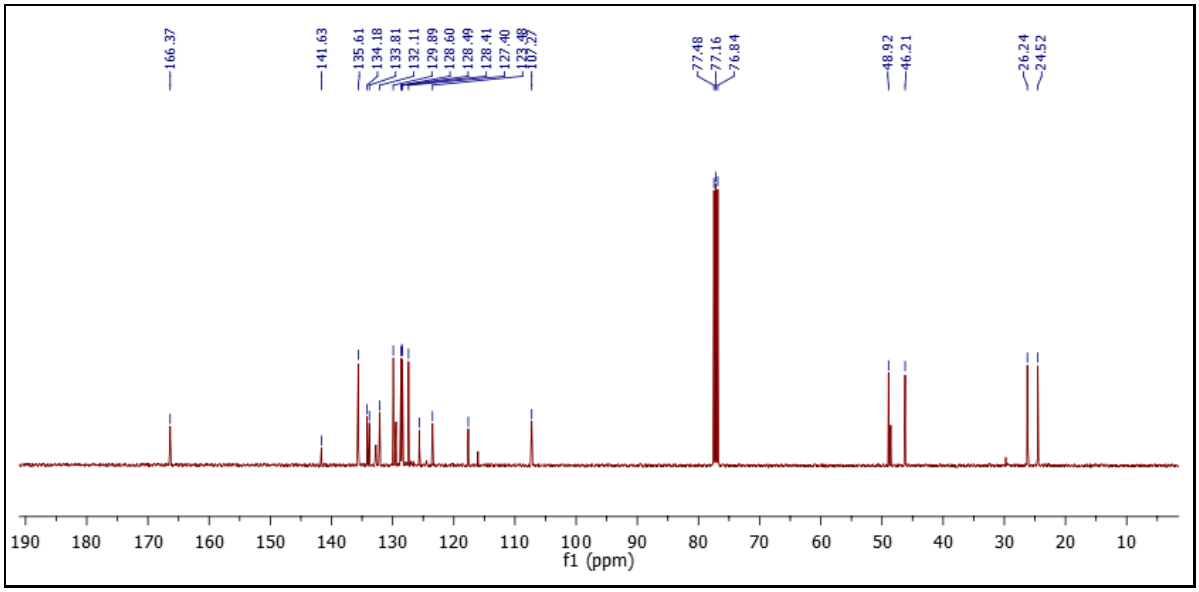


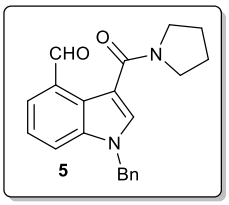
(major isomer)

^{1}H NMR (400 MHz, $CDCl_3$)



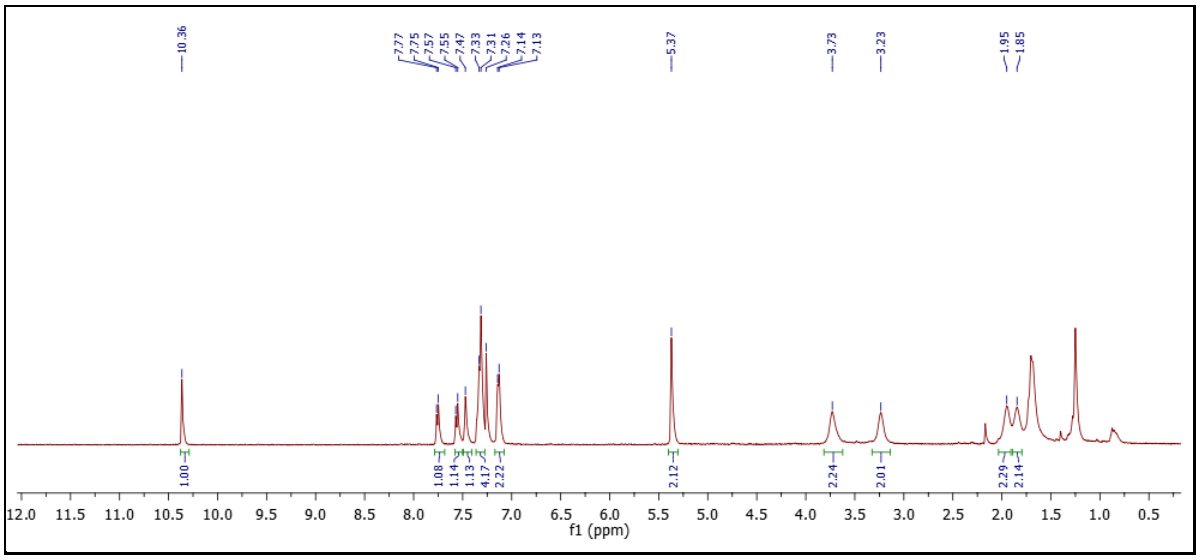
^{13}C NMR (100 MHz, $CDCl_3$)



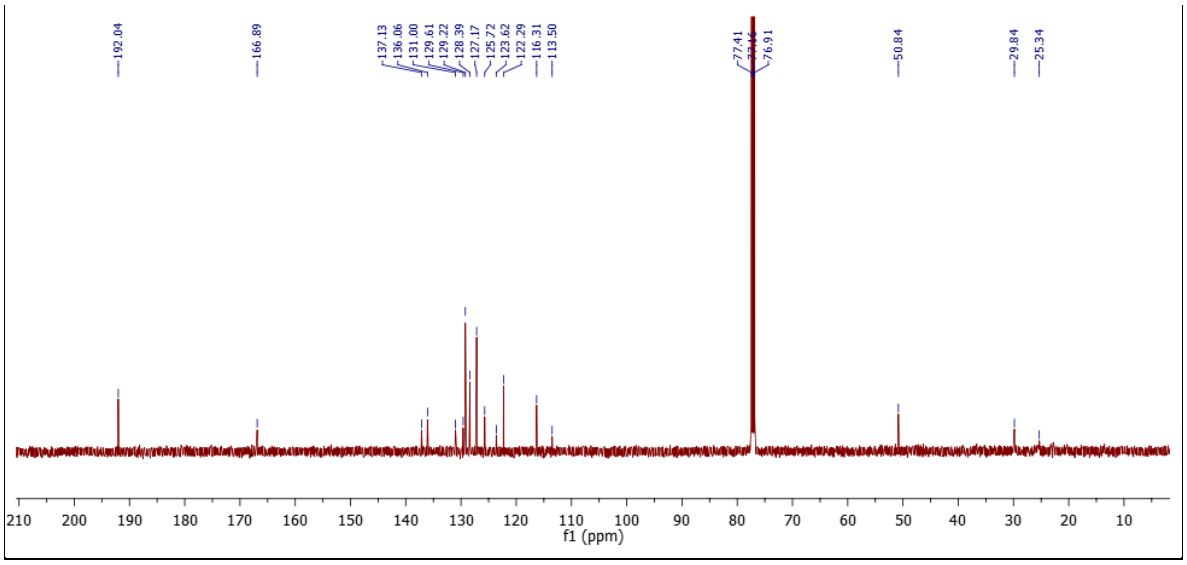


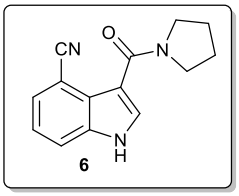
5

^{1}H NMR (400 MHz, $CDCl_3$)

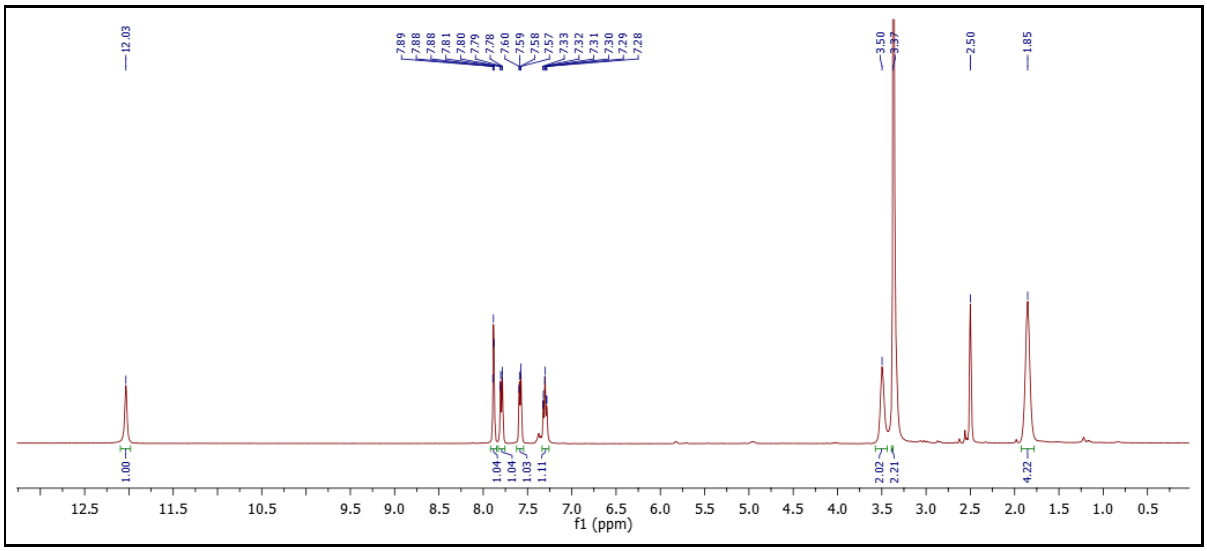


^{13}C NMR (125 MHz, $CDCl_3$)

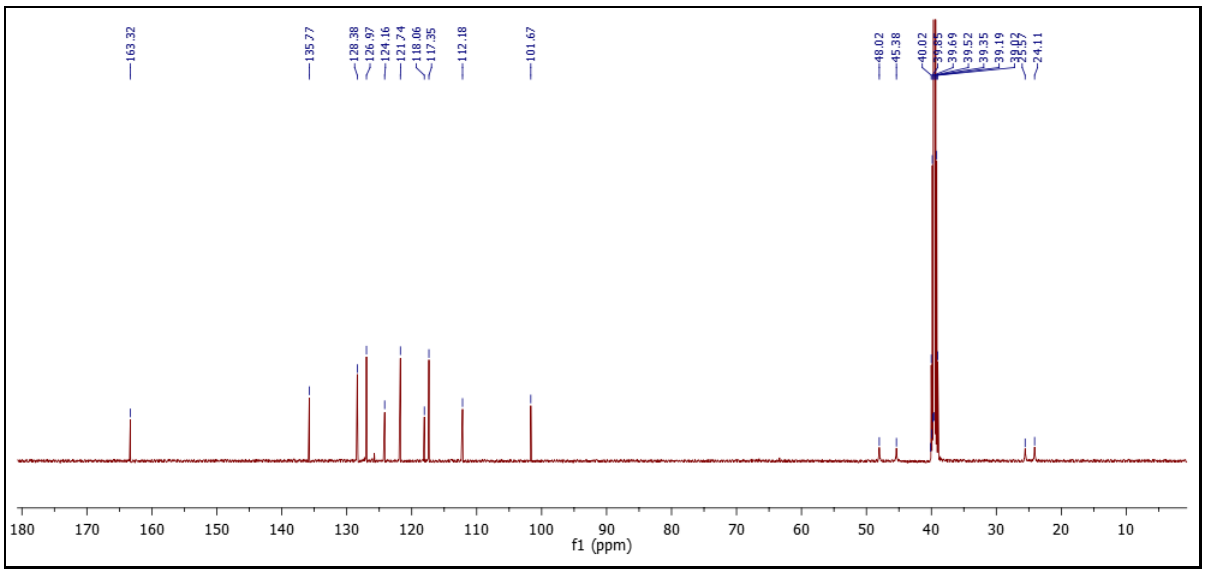


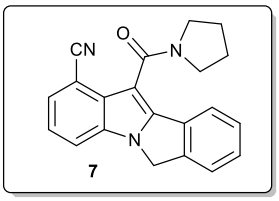


^{1}H NMR (400 MHz, DMSO-D$_6$)



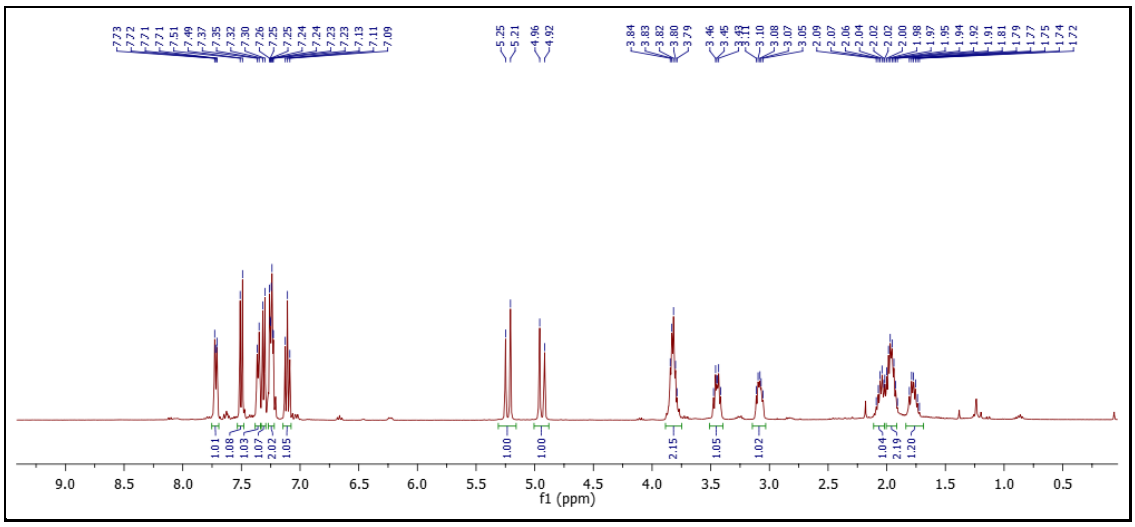
^{13}C NMR (125 MHz, DMSO-D$_6$)



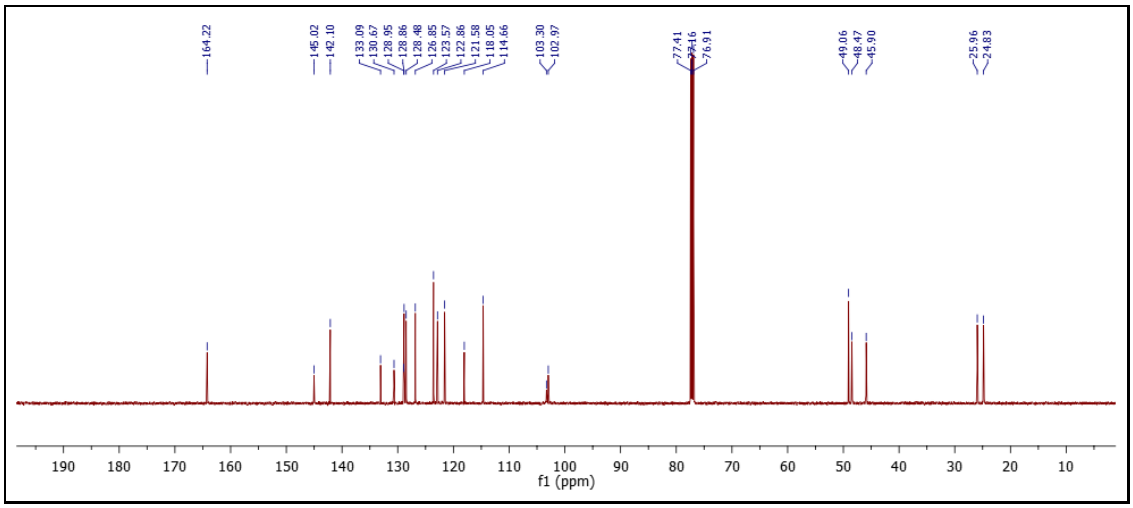


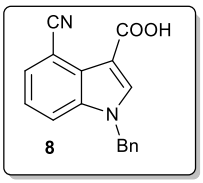
7

^{1}H NMR (400 MHz, $CDCl_3$)

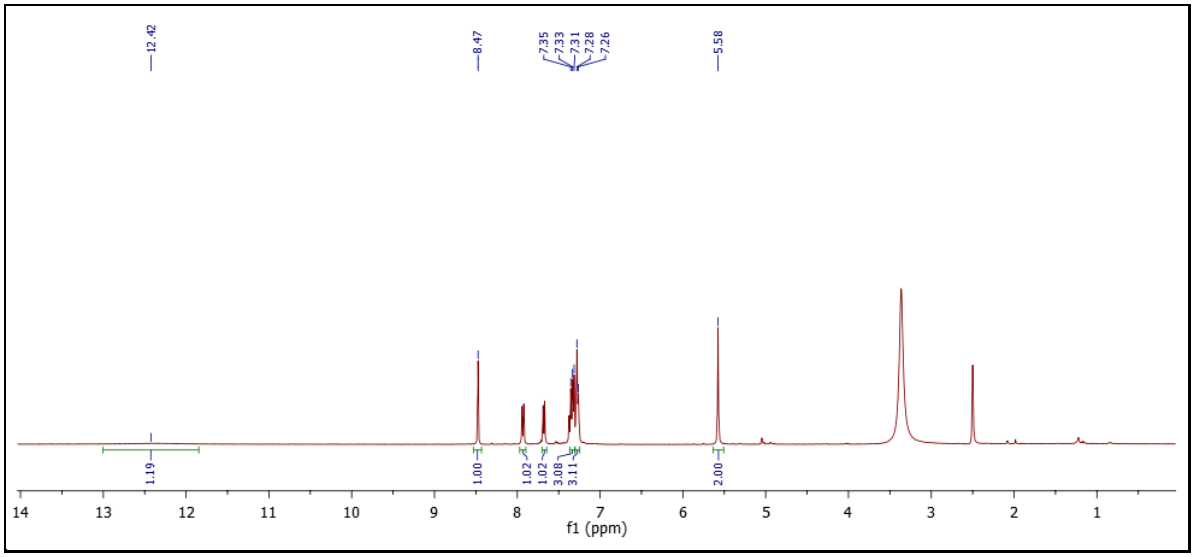


^{13}C NMR (125 MHz, $CDCl_3$)





^{1}H NMR (400 MHz, DMSO-D$_6$)



^{13}C NMR (125 MHz, DMSO-D$_6$)