Electronic Supplementary Information

Mechanochemical synthesis of pyrrolo[1,2-*a*]indoles *via* consecutive C-C and C-N bond formation in presence of ionic liquid: Antimicrobial and photophysical studies

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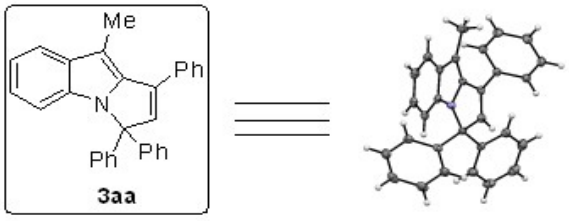
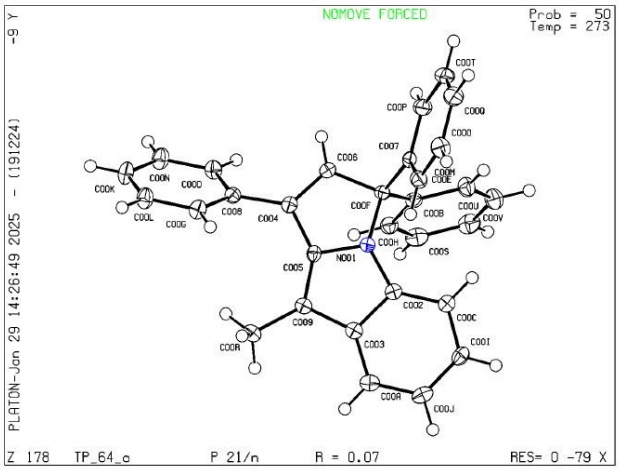
1. General Information:

No purification of the chemicals has been carried out after purchasing from commercial sources. Solvents, reagents, and chemicals were purchased from Aldrich, Fluka, Merck, SRL, Spectrochem, and Process Chemicals. ^{1}H NMR spectra were determined as solutions in $CDCl_3$ on a 400 MHz spectrometer. $^{13}C\{1H\}$ NMR and ^{19}F NMR spectra were recorded at 100 MHz and 376 MHz in $CDCl_3$ solution, respectively. Chemical shifts are in parts per million (δ) and reported as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (double doublet), and J (coupling constants) in Hz. Slide (made of glass) coated with silica gel has been used for thin-layer chromatography. Silica gel (100−200 mesh) as the stationary phase and ethyl acetate/petroleum ether was used for column chromatography. Melting points were determined on a glass disk with an electric hot plate and are uncorrected. A Borosilicate glass tube was used as a reaction tube.

2. Structure Determination (X-ray crystallographic data of 3aa):

The colorless crystals of **3aa** were obtained by crystallization from a solution in dichloromethane/ hexane. Chemical Formula: $\mathbf{C_{30}H_{23}N}$.





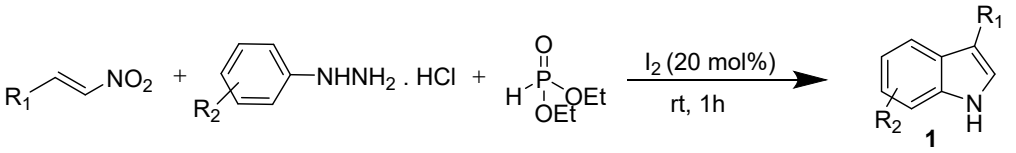
ORTEP (with 50% probability) diagram for the structure ***9-methyl-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole*** (**3aa**)

Wavelength	0.71073 Å	
Formula	$C_{30}H_{23}N$	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 11.3687(4) Å	α = 90 °
	b= 17.6290 (7) Å	β = 108.254 °
	c = 11.5663 (5) Å	γ = 90 °
Volume	2201.45 (19) $Å^3$	
Z	4	
R-factor (%)	7	

The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication with a CCDC reference number CCDC 2457288.

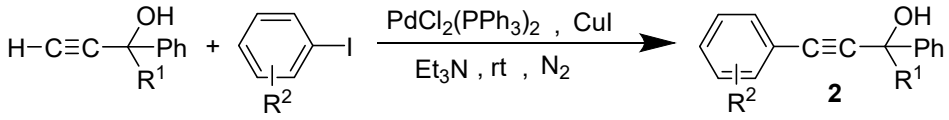
3. Experimental Procedures:

3.1. Typical procedure for the synthesis of 3-substituted indoles 1:



The synthesis of **1** was carried out according to the described method.[1] In a round bottom flask, 10 mmol of nitro styrene, 10 mmol of phenyl hydrazine hydrochloride, 20 mmol of diethyl phosphite and 20 mol% of iodine were stirred at room temperature for 1h. The mixture was then poured into 40 mL of a saturated sodium thiosulfate solution and extracted with dichloromethane. The extract was dried over anhydrous Na_2SO_4. Dichloromethane was removed in a vacuum and evaporated into a crude product. The crude product was passed through a silica gel column using petroleum ether as eluent. The eluent was removed in a vacuum, and the corresponding indole was obtained.

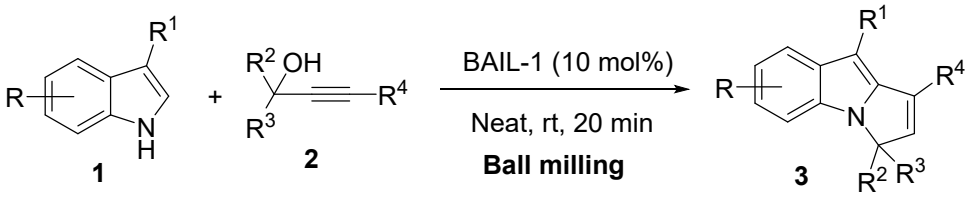
3.2. General procedure for the synthesis of substituted propargyl alcohols (2):



The starting propargyl alcohols were prepared according to the previously reported method.[2] To a mixture of bis(triphenylphosphine)palladium dichloride (0.1 mmol) and tri-ethylamine solution (60 mL) of iodoarene (10 mmol) under a nitrogen atmosphere in a flask equipped with a magnetic stirrer. Then, add alkyne moiety and the reaction mixture was allowed to stir for 6 h at room temperature. After completion of the reaction (monitored by TLC), the mixture was diluted with saturated saline water (3 × 15 mL), and extracted with ethyl acetate. The combined organic layer was collected and dried over anhydrous Na_2SO_4. The residue was purified by column chromatography on silica gel to get the desired products.

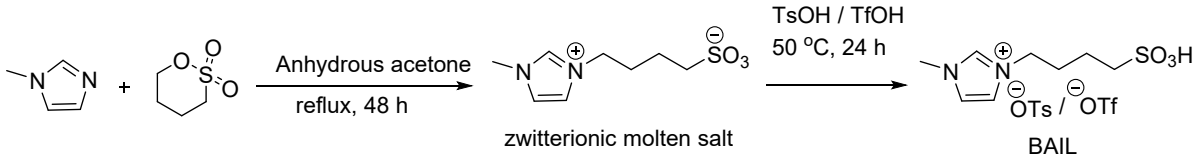
The propargylic alcohol **2a** (R^1 = Ph , R^2 = H) was purchased commercially from TCI Chemicals. **2b**,[3] **2c**,[3] **2d**,[4] **2e**[5] are known compounds, and their spectral data showed good agreement with the literature data.

3.3. General procedure for the synthesis of 3:



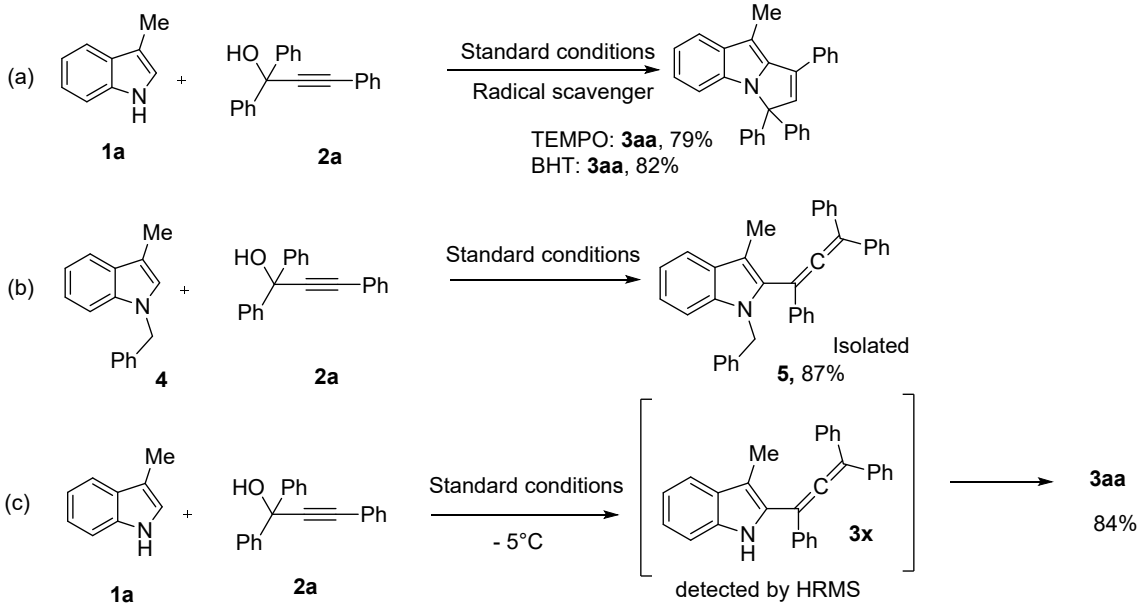
A grinding beaker (50 mL) and milling balls (4 × 10 mm) were set as a reaction chamber. For each reaction, a mixture of propargyl alcohol (1 mmol), 3-substituted indole (1 mmol), with 10 mol% of Brønsted acidic ionic liquid were milled for 20 min at 500 rpm at room temperature. After completion of reaction (monitored by TLC), the mixture was diluted with saturated saline water (3 × 15 mL), and extracted with ethyl acetate. The combined organic layer was collected and dried over anhydrous Na_2SO_4. The residue was purified by column chromatography on silica gel to get the desired products.

3.4. General procedure for the synthesis of Brønsted acidic ionic liquids (BAILs):



Brønsted acidic ionic liquids (BAILS) were prepared according to the previously reported method.[6] A mixture of an equivalent amount of 1-methylimidazole and corresponding butane sultone was refluxed in anhydrous acetone for 48 h to get the zwitterionic molten salt in about 99% yield. After washing the salt with diethyl ether and toluene to remove any unreacted starting materials, the solid was dried in vacuo. Then, a stoichiometric amount of corresponding sulfonic acid was added and the mixture was stirred for 240 h at 50 °C, during which time the solid zwitterion dissolved/liquefied and resulted in the formation of $–SO_3H$ acidic ionic liquids (BAILs) with yield of ~98%. The IL phase was then washed repeatedly with toluene and ether to remove non-ionic residues and dried in vacuo.

4. Mechanistic investigation:



5. Antimicrobial assay for the compounds 3am & 3ak

5.1 Antimicrobial activity using Agar well diffusion method

The agar well diffusion method was used to evaluate the antibacterial activity of test compounds **3am** and **3ak**.[7] To begin the assay, microbial inocula were evenly spread on sterile nutrient agar plates. Uniform wells were then made using a sterile cork borer. Five bacterial strains were tested: Gram-positive *Bacillus cereus* (ATCC 13061), *Listeria monocytogenes* (MTCC 657), *Staphylococcus aureus* (MTCC 96), Gram-negative *Salmonella typhimurium* (MTCC 98) and *Escherichia coli* (MTCC 1667). All strains were cultured in nutrient broth to the logarithmic phase and standardized to an optical density (OD) of 0.5 at 600 nm. Test compounds, dissolved in DMSO, were added to the wells at concentrations of 50, 25, and 10 mg/ml (25 µl per well). The plates were then incubated at 37°C for 12–16 hours. Following incubation, the zones of inhibition were measured to assess antimicrobial activity.[8]

5.2 Minimum Inhibitory Concentration (MIC) value determination

The lowest concentration of an antimicrobial agent that inhibits bacterial growth is known as the minimum inhibitory concentration or MIC.[9] A modified resazurin-based assay determined the MIC value of **3am** and **3ak**.[10] Resazurin is a blue dye that is reduced to pink resorufin by metabolically active cells, serving as an indicator of cell viability. In this assay, test compounds were prepared at concentrations of 1000, 500, 250, and 125 µg/mL in a 96-well microtiter plate. Each well was filled using a micropipette with the test compound, bacterial suspension, and 0.01% resazurin solution. The negative control consisted of bacterial cultures in DMSO without any test compound, while ciprofloxacin served as the positive control. After 10 hours of incubation at 37°C, the minimum inhibitory concentration (MIC) was determined as the lowest concentration that retained the blue colour of resazurin, indicating the absence of bacterial growth.[11]

5.3 SEM analysis of bacterial strains

To evaluate the effectiveness of compound 3am, which was found to be more effective than the others, morphological changes in bacterial cells were examined using scanning electron microscopy (SEM). The analysis provided insights into structural alterations caused by the

treatment. Two bacterial strains, *Bacillus cereus* and *Staphylococcus aureus*, were cultured in fresh nutrient broth and treated with compound 3am at its minimum inhibitory concentration (MIC). After overnight incubation, the bacterial cells were fixed with 2.5% glutaraldehyde, centrifuged, and dehydrated through a graded ethanol series (10% to 90%). Following critical point drying, the samples were mounted on metal stubs, coated with gold using an ion sputter, and imaged using a high-resolution SEM (Carl Zeiss Gemini 450).[12]

5.4 Results

5.4.1. Antimicrobial activity using the Agar well diffusion method

Significant variations in the antibacterial activity were found for the compounds **3am**, **3ak**, **3ap**, **3ar**, **3ax**, but two of them showed the best activity against five bacterial strains found using the agar well diffusion experiment. The compound **3am** (25 mg/ml) demonstrated greater activity with inhibitory zones that ranged from 8±0.5 mm for *Bacillus cereus* to 6±1.5 mm for *Listeria monocytogenes*. On the other hand, smaller zones were produced by the compound **3ak** (25 mg/ml), with zones measuring 3.5±1.0 mm for *Listeria monocytogenes* and for *Escherichia coli* inhibition zones measuring 5.5±1.0 mm (Table S1). In the antibacterial assay, the compound **3am** exhibited a greater inhibitory zone than **3ak**, as shown in Figure S1.

Table S1 Inhibition zone of antimicrobial activity for the **3ak** and **3am** using the agar well diffusion method

Test materials (25 mg/mL)	Zone of Inhibition (mm) (Mean± SD)				
	Escherichia coli	*Staphylococcus aureus*	*Salmonella typhimurium*	*Bacillus cereus*	*Listeria monocytogenes*
3ak	5.5±1.0	4.5±1.5	4.5±1.5	4±1.0	3.5±1.0
3am	7.0±1.5	7.5±0.5	7 ±1.5	8±0.5	6±1.5

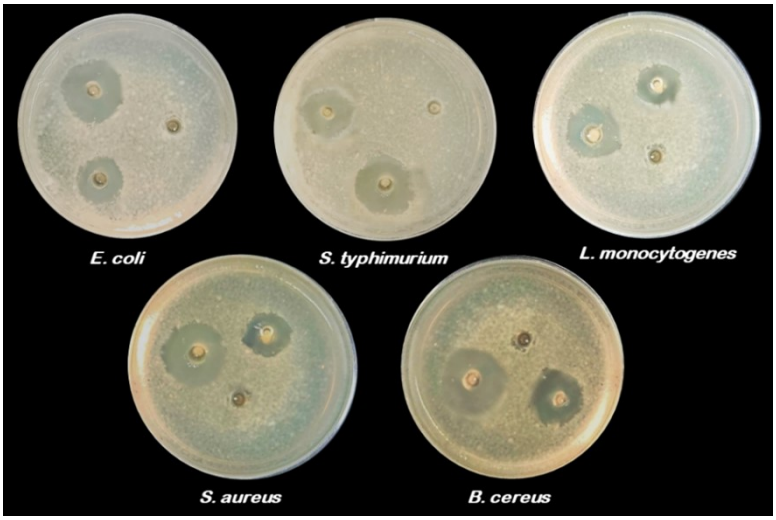


Figure S1 Antibacterial screening of **3am** and **3ak** against five bacterial strains (agar-well diffusion method). A larger inhibition zone indicates for **3am**, whereas a smaller one indicates **3ak.**

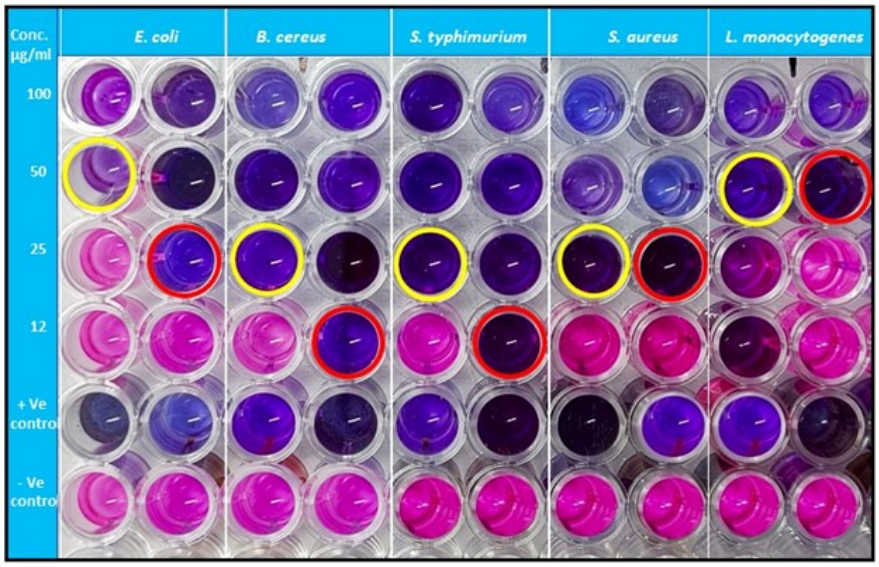


Figure S2 The microtiter plate, after a 14-hour incubation period, showed the antibacterial activity of the test compounds against the five bacterial strains. Blue wells signify the inhibition of bacterial growth, while pink wells show the growth of bacteria. Red circles represent the value of **3am**, while yellow circles represent the value of **3ak**. Positive and negative controls are below

Table S2 MIC values of the compounds **3ak** and **3am** against different bacterial strains

List of Bacterial strains	Gram-positive/Gram-negative	MIC values of 3ak (µg/mL)	MIC values of 3am(µg/mL)	MIC values of ciprofloxacin (µg/mL)
Bacillus cereus	*Gm +ve*	25	12	03
Salmonella typhimurium	*Gm -ve*	25	12	03
Escherichia coli	*Gm -ve*	50	25	02
Staphylococcus aureus	*Gm +ve*	25	25	01
Listeria monocytogenes	*Gm +ve*	50	50	02

5.4.2 Evaluation of Minimum Inhibitory Concentration (MIC):

The minimum concentration of an antimicrobial agent needed to inhibit bacterial growth can be determined by the Minimum Inhibitory Concentration (MIC). A redox indicator called resazurin detects the metabolic activities of bacteria. Positive responses were indicated by a continuous blue coloring, whereas responses that were negative were indicated by changing the color to pink or colorless. Although the compounds **3am**, **3ak**, **3ap**, **3ar**, and **3ax** exhibited good antibacterial activity, MIC values were determined only for **3am** and **3ak**, as these two compounds demonstrated the best bioactivity. MIC values for compound **3ak** ranged from 25 to 50 µg/ml against each tested bacterial strain. Meanwhile, MIC values for **3am** ranged from 12 to 25 µg/ml against test bacteria and exhibited stronger antibacterial activity (Table S2). The higher antibacterial potency of compound **3am** is demonstrated by these MIC values over **3ak**, which were also confirmed by triple replicates (Figure S2).

Similarly, scanning electron microscopy (SEM) provides a direct and effective method for evaluating the mechanism of antibacterial action by revealing structural damage in bacterial cells. The images clearly differentiate between live and dead cells, demonstrating the impact of the treatment. A comparison between untreated cells and those treated with compound **3am** allows for a more precise assessment of cell integrity. This visual evidence

underscores the compound's antibacterial potential by highlighting its ability to disrupt and destroy the bacterial cell wall (Figure S3).

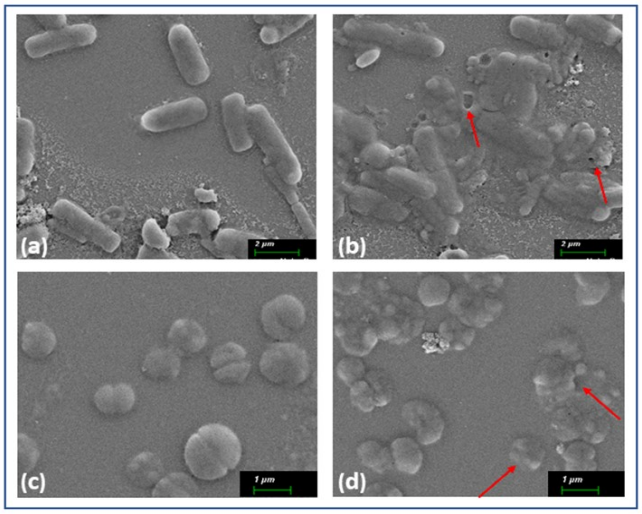


Figure S3 FE-SEM images of a Gram-negative and a Gram-positive bacterium: (a) *E. coli* before treatment; (b) *E. coli* after treatment with **3am**; (c) *S. aureus* before treatment; (d) *S. aureus* after treatment with **3am**. Red arrows indicate dead bacterial cells.

6. Photophysical Studies:

We studied the photophysical behavior of these 3*H*-pyrrolo[1,2-*a*]indole derivatives. The spectroscopic results are shown for **3ae** (Figure S4). The principal absorption band falls between 325 and 346 nm in the experiment. All of the examined compounds were found to be fluorescent in the blue region (λ_{em}= 422-463 nm, Figure S5).[13] The electron donating group present in **3ad** and **3ae** have relatively high emission wavelengths while the electron withdrawing group present in 3an showed the low emission wavelength. The fluorescence quantum yield (Φ) of the synthesized compounds are in the range of 0.02-0.43 in acetonitrile. Here tryptophan is used as a reference at λ_{ex} = 280 nm (Φ_R= 0.14 at 298 K).[14] The thiomethyl group on the arene moiety of 3*H*-pyrrolo[1,2-*a*]indole in compound 3ae shows higher Φ (0.43) value and higher stokes shift value (123 nm). These values indicate the distortion of the π conjugated system in excited state.[15] Compound 3an showed the lower Stokes shift value (97 nm) and relatively lower quantum yield value (0.16). Remarkable differences between alkyl and aryl substituted 3*H*-pyrrolo[1,2-*a*]indole derivatives were also found in fluorescence quantum yield. Compound **3ae** exhibited ~21-fold higher quantum yield value and longer emission wavelength than compound **3aa**. Additionally, the molar absorptivity (ε_{max}) for **3ab** (-OMe) is higher (25000 $M^{-1}cm^{-1}$) and lower (7000 $M^{-1}cm^{-1)}$ for **3an** (-CF_3),

which indicates the probability of transition from ground state(S_0) to first excited electronic state (S_1) is higher for those derivatives with strong electron donating group comparative to strong electron withdrawing group.[16] These photophysical properties with high quantum yield and Stokes shift value establish the compounds as unique material for potential bioimaging[17] and further utilized them as fluoroprobes.

In addition, we examine the solvatofluorochromic properties of selected five synthesized compounds by changing the solvent polarity from non-polar to polar solvents. Figure S4(c) shows the emission spectra of **3ae** in *n*-hexane, THF, methanol, acetonitrile and DMSO. The results of solvent effect with **3ai**, **3at**, **3an** and **3aw** are shown here. With increase in the polarity of solvents, the compounds show a moderate bathochromic shift. The emission maxima of **3ae** locates at 448 nm in *n*-hexane, while the emission spectra shift to 464 nm in DMSO. In general, the compounds have high dipole moments in excited state as compared to their corresponding ground state due to electronic excitations.[18] The high dipole moment of compounds interacts with the environment of the polarity of solvents and results the slight shifts of emission maxima to longer wavelengths.[19] The observed trend in photoluminescence characteristics is evidently showed that 3*H*-pyrrolo[1,2-*a*]indole derivatives have good tendency to photoluminescence properties.

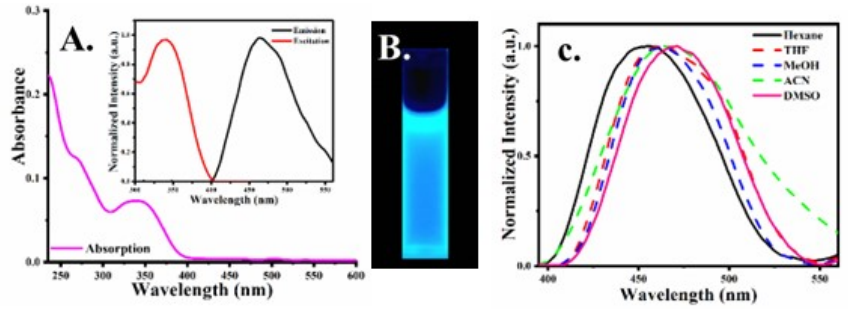


Figure S4 Photophysical behavior of compound **3ae**: (a) The UV-Vis absorption characteristic of compound **3ae** in acetonitrile (ACN) solvent medium, inset indicates the normalized excitation and emission spectra of the same, (b) the high emissive image of compound **3ae** in ACN solution under fluorescence light and (c) the solvent dependent normalized emission spectra of compound **3ae.**

6.1. Steady state UV-Vis absorbance and fluorescence spectroscopic measurements:

UV-Vis absorption spectra of the selected thirteen compounds were recorded in acetonitrile solution with the help of a UV-Vis-NIR spectrophotometer (Shimadzu UV 1800 pc) within

the wavelength range of 200-600 nm. The fluorescence emission and corresponding excitation spectra of the same compounds in acetonitrile solution were obtained using a Perkin Elmer LS55 fluorescence spectrophotometer at the excitation wavelength (λ_{ex}) 290 nm to get the maximum fluorescence intensity. The slit width was fixed at 7/2.5 nm for both the excitation and emission beams. The spectroscopic studies were carried out at 25^{o} C and no change was observed in the spectra of all experimental solutions for a long time period. During experimental studies, this nullifies any possibility of degradation of the sample solutions. Molar extinction coefficient (ε) of the thirteen compounds in acetonitrile solution for the maximum absorption band was determined with the help of Beer-Lambert's law (A= εcl) where concentration (c) of the compounds in micro molar range and path length (l) was kept as 1 cm and 'A' represent the absorbance. For calculation of the Stokes shifts, considered the lowest energetic absorption band of compounds.

6.2. Fluorescence Quantum Yield (Φ) calculations of compounds:

The relative fluorescence quantum yields (Φ) of the selected thirteen compounds were calculated in acetonitrile solution by using the following equation:

$$\Phi = \Phi_R \times \frac{I}{I_R} \times \frac{OD_R}{OD} \times \frac{\eta_R^2}{\eta^2} \quad \ldots(1)$$

Where Φ_R represents the quantum yield of reference, here tryptophan in a water medium is used as reference; I and I_R denote the area under the fluorescence peak of samples and reference respectively; OD and OD_R indicate the absorbance for samples and reference respectively; η and η_R are the refractive index of respective solvent. Here, refractive indexes of the medium (η= 1.333, water) and (η = 1.344, acetonitrile). The absorbance value of sample compounds and reference was kept between 0.01 to 0.1 to avoid self-quenching and self-aggregation. Quantum yield value (Φ_R= 0.14 at 298 K) of tryptophan in water medium at λ_{ex} = 280 nm used as reference.[14]

UV-Vis absorbance and steady-state fluorescence spectra were measured to understand the photo-physical behaviour of 3*H*-pyrrolo[1,2-*a*]indole derivatives. Here we selected thirteen 3*H*-pyrrolo[1,2-*a*]indole derivatives (**3ae, 3au, 3ab, 3af, 3at, 3ai, 3ah, 3ad, 3an, 3aw, 3ax, 3aj and 3aa**) in acetonitrile medium for UV-Vis absorbance measurement and the concentration of all measured solutions is fixed at 5μM. Similarly, the excitation and emission spectra of the same solutions were recorded in the same medium. Selected

compounds manifest captivating photo-physical behaviours; the detailed spectral results are summarized in **Table S3**. **Table S3** contains the values of λ_{abs} (wavelengths related to several absorption bands), the excitation wavelength (λ_{ex}), maxima of emission wavelength (λ_{max}), molar extinction coefficients, ε (at the wavelength having the highest absorbance), Stokes shifts and fluorescence quantum yields. **Figure S5** indicates the absorption and normalized excitation and emission spectra of compounds (**3au-3aa**). From all the figures, it is evidently noticed that the excitation and absorption spectra nearly resemble, signifying the purity of the compounds. The UV-Vis spectral patterns show mainly one absorption band (λ_{abs}) at ~325-346 nm. No remarkable changes are observed in the absorption spectra upon the substitution of 3-position of the indole ring. Electron donating groups as substituents show the red shift as compared to the electron withdrawing group as substituents. The fluorescence emission studies show an intense emission band in visible region at ~ 422-463 nm (λ_{em}) (**Table S3**). The emission studies of compound (**3ae** and **3ad**) show a red shift in the emission maximum upon increase the conjugation compared to other compounds.

Table S3 Summarized photo-physical parameters of the selected thirteen indole derivatives

Compounds	Absorption (λ_{abs}) (nm)	Excitation (λ_{ex}) (nm)	Emission λ_{max} (nm)	Molar Extinction Coefficient (ε) ($10^4 M^{-1}cm^{-1}$)	Stokes Shift (nm)	Quantum Yield (Φ)
3ae	340	290	463	1.0	123	0.43
3au	346	290	457	1.5	111	0.41
3ab	335	290	452	2.5	117	0.38
3af	335	290	456	1.8	121	0.37
3at	330	290	450	2.2	120	0.31
3ai	331	290	451	1.2	120	0.29
3ah	330	290	448	1.3	118	0.24
3ad	337	290	463	1.2	126	0.19
3an	325	290	422	0.7	97	0.16
3aw	333	290	451	1.8	118	0.14
3ax	330	290	453	1.0	123	0.11
3aj	333	290	450	1.3	117	0.09
3aa	330	290	430	1.2	100	0.02

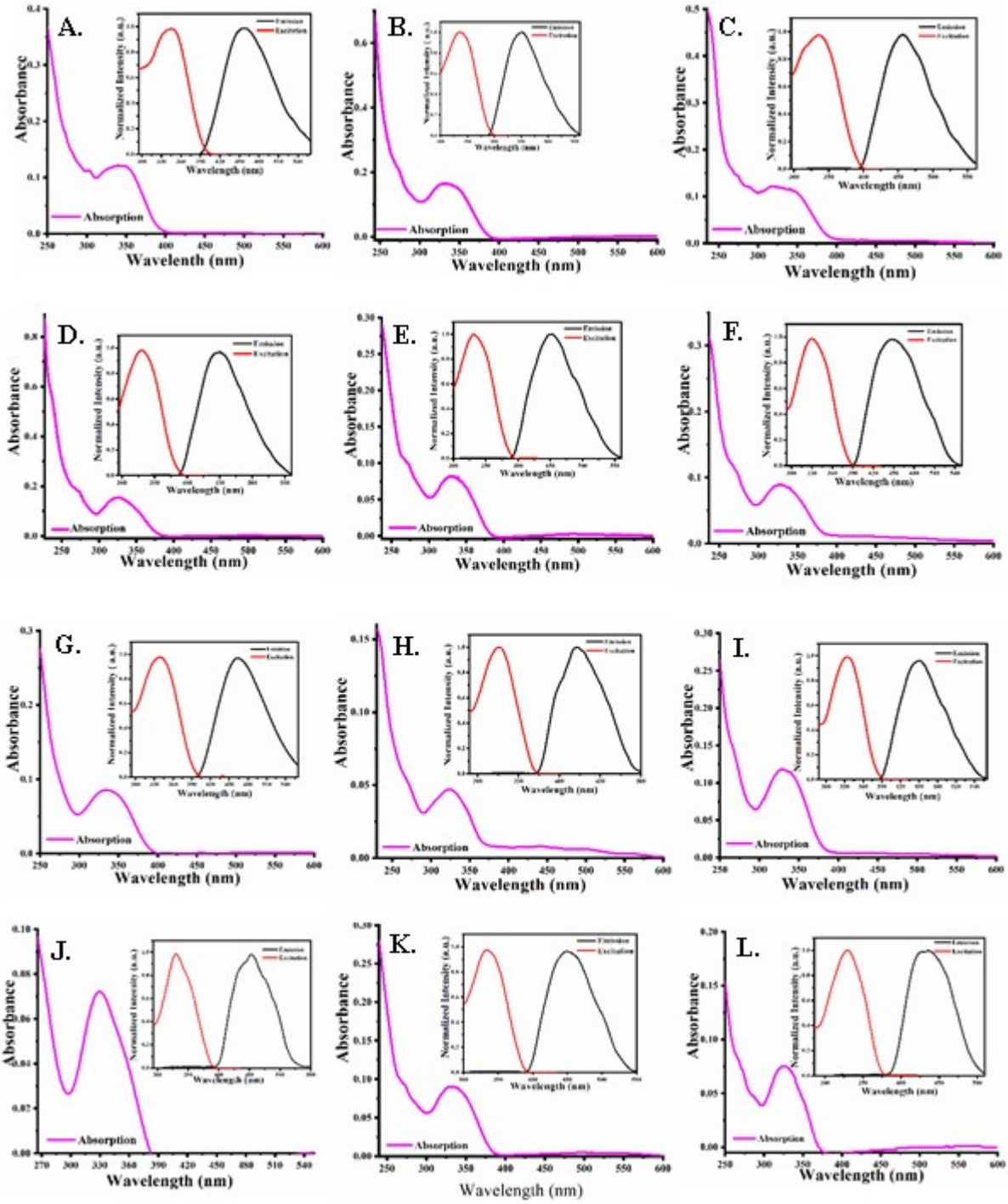


Figure S5 (**A-L**) UV-Vis absorption spectra of compounds (**3au-3aa**) in acetonitrile medium respectively (compound final concentration: 5μM), inset shows the normalized excitation and emission spectra of the same.

Furthermore, the solvatofluorochromic properties of selected five compounds are examined in various solvents as the polar substituents of aromatic ring are sensitive to the variation of solvents. **Figure S6** shows the emission spectra of selected compounds are in n-hexane, THF, methanol, acetonitrile and DMSO. With increase in the polarity of solvents, the compounds show a moderate bathochromic shift. Here all the five compounds exhibited same observations with the effect of solvents. The emission maxima of **3ai**, **3at** and **3aw** locate at 439 nm, and for **3an** at 410 nm in *n*-hexane, while the emission spectra shift to 453 nm for first three compounds and 425 nm for **3an** in DMSO. In general, the compounds have high dipole moments in excited state as compared to their corresponding ground state due to electronic excitations.[20] The high dipole moment of the compounds interacts with the environment of the polarity of solvents and results the slight shifts of emission maxima to longer wavelengths.[21] The observed trend in photoluminescence characteristics are evidently showed that 3*H*-pyrrolo[1,2-*a*]indole derivatives have good tendency to photoluminescence properties.

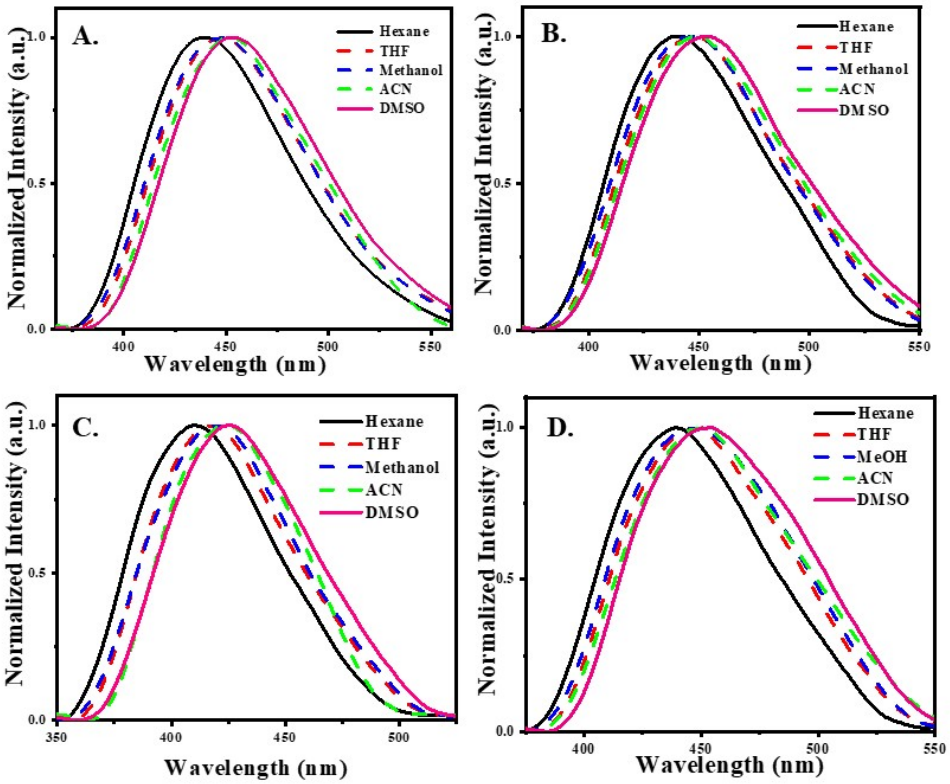
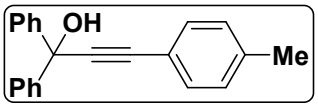
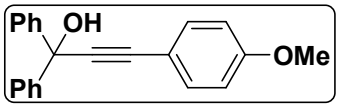


Figure S6 Normalized fluorescence emission spectra of compounds; **A. 3ai, B. 3at, C. 3an** and **D. 3aw** in different solvent medium.

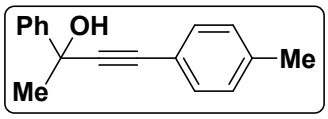
7. Spectroscopic data of synthesized compounds:



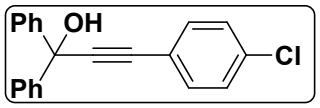
1,1-Diphenyl-3-(p-tolyl)prop-2-yn-1-ol **(2b)[3]:** Yield: 72%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.72 (t, J = 7.2 Hz, 4H), 7.44 (d, J = 8 Hz, 2H), 7.40-7.36(m, 4H), 7.33-7.29 (m, 2H), 7.18 (d, J = 8.0 Hz, 2H), 2.93 (s, 1H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ *145.2*, 139.0, 131.8, 129.2, 128.4, 127.8, 126.2, 119.4, 91.0, 87.5, 74.9, 21.7.



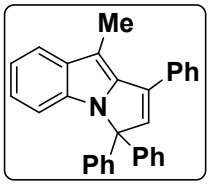
3-(4-Methoxyphenyl)-1,1-diphenylprop-2-yn-1-ol **(2c)[3]:** Yield: 74%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60 (d, J = 8.0 Hz, 4H), 7.37 (t, J = 6.8 Hz, 2H), 7.27 (t, J = 7.6 Hz, 4H), 7.21-7.17 (m, 2H), 6.78 (d, J = 8.8 Hz, 2H), 3.73 (s, 3H), 2.85 (s, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ *160.0*, 145.3, 133.4, 128.4, 127.8, 126.2, 114.5, 114.0, 90.4, 87.3, 75.0, 55.4.



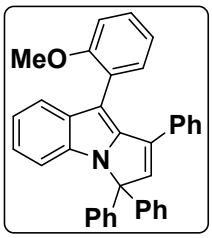
2-Phenyl-4-(p-tolyl)but-3-yn-2-ol **(2d)[4]:** Yield: 76%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.75-7.73 (m, 2H), 7.41-7.37 (m, 4H), 7.32 (t, J = 7.6 Hz, 1H), 7.14 (d, J = 8.0 Hz, 2H), 2.52 (s, 1H), 2.36 (s, 3H), 1.87 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ *145.9*, 138.8, 131.7, 129.2, 128.4, 127.8, 125.1, 119.5, 91.8, 85.2, 70.5, 33.5, 21.6.



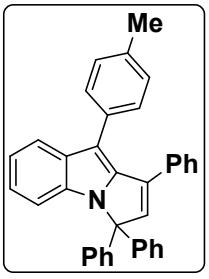
1,1-Diphenyl-3-(p-tolyl)prop-2-yn-1-ol **(2e)[5]:** Yield: 71%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.67 (t, J = 7.2 Hz, 4H), 7.44 (d, J = 8.4 Hz, 2H), 7.38-7.34 (m, 4H), 7.32-7.28 (m, 4H), 2.92 (s, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ *144.9*, 134.9, 133.1, 128.8, 128.5, 128.0, 126.1, 121.0, 92.7, 86.2, 74.9.



9-Methyl-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3aa)[22]:** Yield: 84%; 333 mg; white solid; mp 120-122 ºC; R_f = 0.60 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68 (t, J = 6.8 Hz, 2H), 7.61 (d, J = 8 Hz, 1H), 7.48-7.42 (m, 3H), 7.35-7.26 (m, 10H), 7.06-6.94 (m, 3H), 6.67 (s, 1H), 2.37 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ *140.5*, 140.2, 139.6, 136.4, 134.4, 134.1, 133.8, 128.6, 128.4, 128.3, 127.4, 121.9, 119.7, 118.8, 110.5, 103.0, 75.5, 9.7.

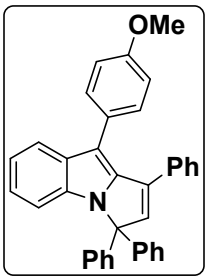


9-(2-Methoxyphenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ab):** Yield: 77%; 377 mg; white solid; mp 180-182 °C; R_f = 0.50 (petroleum ether/EtOAc = 90/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.70-7.68 (m, 1H), 7.55-7.53 (m, 1H), 7.39-7.21 (m, 14H), 7.16-7.01 (m, 6H), 6.87 (s, 1H), 6.67 (d, J = 8 Hz, 1H), 3.16 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 157.1, 141.1, 140.0, 139.9, 139.6, 136.9, 134.4, 133.6, 132.8, 131.9, 128.7, 128.7, 128.3, 128.0, 127.8(3C), 127.4, 123.5, 121.9, 120.8, 120.1, 119.5, 110.6, 110.5, 104.7, 75.7, 54.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{28}NO]^+$: 490.2165; Found : 490.2169.

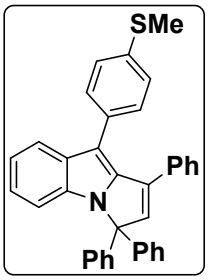


1,3,3-Triphenyl-9-(p-tolyl)-3H-pyrrolo[1,2-a]indole **(3ac):** Yield: 83%; 393 mg; white solid; mp 134-136 ºC; R_f = 0.6 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.96-7.94 (m, 1H), 7.53-7.49 (m, 9H), 7.48-7.44 (m, 3H), 7.41-7.36 (m, 3H), 7.33-7.29 (m, 2H), 7.26-7.20 (m, 5H), 7.00 (s, 1H), 2.54 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ

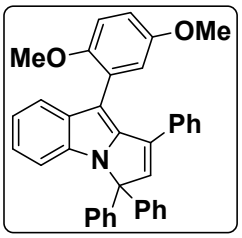
140.7, 139.7, 139.7, 136.2, 135.7, 134.3, 132.7, 132.5, 131.2, 130.7, 128.7, 128.6, 128.4, 128.3, 128.2, 127.9, 122.3, 120.7, 119.6, 110.7, 110.3, 75.6, 21.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{28}N]^+$: 474.2222; Found : 474.2209.



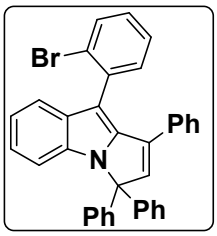
9-(4-Methoxyphenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ad):** Yield: 85%; 416 mg; off white solid; mp 182-184 ºC; R_f = 0.50 (petroleum ether/EtOAc = 90/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.65-7.63 (m, 1H), 7.24-7.7.20 (m, 9H), 7.19-7.16 (m, 3H), 7.12-7.10 (m, 3H), 7.03 (t, J = δ Hz, 2H), 6.97-6.94 (m, 3H), 6.70 (s, 1H), 6.68-6.66 (m, 2H), 3.70 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 158.2, 140.6, 139.7, 139.6, 136.1, 134.2, 132.7, 132.5, 131.8, 128.7, 128.4, 128.3, 128.2, 127.9(2C), 126.6, 122.3, 120.6, 119.5, 113.4, 110.6, 109.9, 75.6, 55.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{28}NO]^+$: 490.2165; Found : 490.2160.



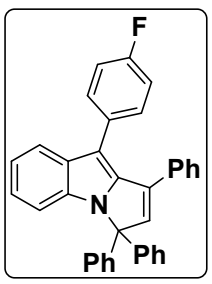
9-(4-(Methylthio)phenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ae):** Yield: 80%; 405 mg; off white solid; mp 184-186 ºC; R_f = 0.65 (petroleum ether/EtOAc = 90/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81-7.79 (m, 1H), 7.40-7.35 (m, 9H), 7.34-7.24 (m, 6H), 7.21-7.15 (m, 4H), 7.13-7.09 (m, 3H), 6.87 (s, 1H), 2.53 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.0, 139.9, 139.5, 136.0, 135.8, 134.3, 132.6, 132.2, 131.2, 131.2, 130.2, 128.7, 128.4, 128.3, 128.0, 127.9, 126.4, 122.4, 120.5, 119.7, 110.7, 109.6, 75.8, 16.38; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{28}NS]^+$: 506.1973; Found : 506.1967.



9-(2,5-Dimethoxyphenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3af):** Yield: 80%; 416 mg; white solid; mp 214-216 °C; R_f = 0.3 (petroleum ether/EtOAc = 90/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.74-7.72 (m, 1H), 7.68-7.65 (m, 2H), 7.39-7.31 (m, 13H), 7.26-7.22 (m, 1H), 7.18-7.15 (m, 2H), 7.09-7.07 (m, 3H), 6.88 (s, 1H), 6.85-6.82 (m, 1H), 6.63(d, J = 8 Hz, 1H), 3.74 (s, 3H), 3.17 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 153.1, 151.4, 141.1, 140.2, 139.8, 139.6, 136.8, 134.3, 133.5, 132.6, 128.7(2C), 128.3, 127.9, 127.8(2C), 127.5, 124.1, 122.0, 120.9, 119.5, 117.4, 113.2, 111.5, 110.6, 104.8, 75.7, 55.8, 55.0; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{37}H_{30}NO_2]^+$: 520.2271; Found : 520.2303.

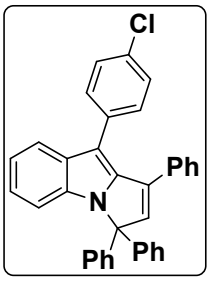


9-(2-Bromophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ag):** Yield: 77%; 415 mg; off white solid; mp 150-152 ºC; R_f = 0.50 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49-7.47 (m, 1H), 7.42-7.340 (m, 1H), 7.38-7.36 (m, 1H), 7.33 (d, J = 4.4 Hz, 4H), 7.30-7.260 (m, 6H), 7.21-7.18 (m, 3H), 7.15-7.08 (m, 2H), 7.04-7.00 (m, 5H) 6.83 (s, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.1, 140.4, 139.6, 139.4, 136.1, 135.8, 133.9, 133.1, 132.6(2C), 128.8, 128.7, 128.6, 128.4, 128.2, 128.1, 127.9(2C), 127.8, 127.7, 126.9, 126.4, 122.2, 120.7, 119.6, 110.7, 108.7, 75.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{25}BrN]^+$: 538.1165; Found : 538.1167.

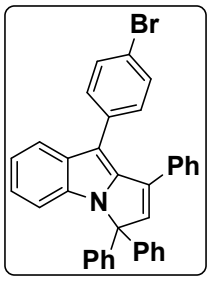


9-*(4-Fluorophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole* **(3ah):** Yield: 76%; 363 mg; off white solid; mp 198-200 ºC; R_f = 0.4 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.76-7.74 (m, 1H), 7.44-7.34 (m, 10H), 7.31-7.26 (m, 5H), 7.20 (t, J =

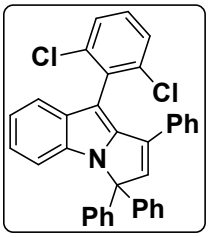
7.6 Hz, 2H), 7.15-7.08 (m, 3H), 6.95 (t, J = 8.8 Hz, 2H), 6.87 (s, 1H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz): δ 161.6 (d, J = 243 Hz), 141.0, 140.0, 139.5, 135.9, 134.2, 132.5, 132.2 (d, J = 9 Hz), 130.2, 128.8, 128.3(2C), 128.0(2C), 122.4, 120.0 (d, J = 56 Hz), 114.7 (d, J = 22 Hz), 109.9 (d, J = 171 Hz), 75.8; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{25}FN]^+$: 478.1971; Found : 478.1954.



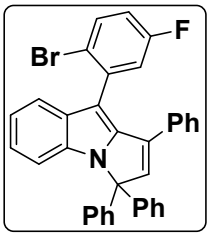
9-(4-Chlorophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ai):** Yield: 80%, 395 mg; off white solid; mp 208-210 ºC; R_f = 0.50 (petroleum ether/EtOAc = 95/05); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.77-7.75 (m, 1H), 7.42-7.35 (m, 10H), 7.30-7.28 (m, 3H), 7.24-7.20 (m, 6H), 7.13 (t, J = 3.6 Hz, 1H), 7.12-7.09 (m, 2H), 6.87 (s, 1H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz): δ 141.3, 140.1, 139.4, 135.9, 134.2, 132.7, 132.5, 132.0(2C), 131.9, 128.8, 128.4(2C), 128.3, 128.1, 128.0, 122.5, 120.3, 119.9, 110.8, 108.9, 75.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{25}ClN]^+$: 494.1670; Found : 494.1638.



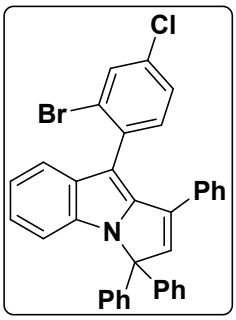
9-(4-Bromophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3aj):** Yield: 62%; 334 mg; radish solid; mp 216-218 ºC; R_f = 0.60 (petroleum ether/EtOAc = 95/05); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.72-7.70 (m, 1H), 7.37-7.32 (m, 6H), 7.31-7.29 (m, 5H), 7.27-7.24 (m, 4H), 7.18-7.12 (m, 4H), 7.09-7.04 (m, 3H), 6.83 (s, 1H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz): δ 141.4, 140.1, 139.4, 135.9, 134.3, 133.2, 132.5, 132.3, 132.0, 131.0, 128.8, 128.5, 128.4, 128.3, 128.1, 128.0, 122.5, 120.3, 120.1, 119.9, 110.9, 108.9, 75.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{25}BrN]^+$: 338.1165; Found : 338.1156.



9-(2,6-Dichlorophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ak):** Yield: 77%; 407 mg; off white solid; mp 128-130 °C; R_f = 0.45 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.33-7.28 (m, 10H), 7.24-7.21 (m, 5H), 7.14-7.10 (m, 2H), 7.06-7.00 (m, 5H), 6.84 (s, 1H); $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 140.4, 139.4, 137.3, 136.0, 134.3, 133.1, 132.5, 132.0, 129.0, 128.8, 128.3, 128.2, 128.0, 127.8, 127.7, 127.4, 122.1, 120.8, 119.7, 110.9, 103.9, 76.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{24}Cl_2N]^+$: 528.1280; Found : 528.1254.

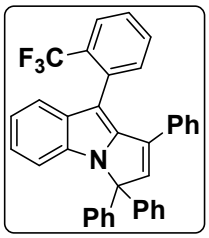


9-(2-Bromo-5-fluorophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3al):** Yield: 80%; 445 mg; off white solid; mp 152-154 °C; R_f = 0.35 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.51-7.47 (m, 2H), 7.42-7.32 (m, 10H), 7.29 (d, J = 7.2 Hz, 2 H), 7.24-7.19 (m, 2H), 7.16-7.09 (m, 5H), 6.94-6.90 (m, 2H); $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 161.6 (d, J = 245 Hz), 141.1 (d, J = 53 Hz), 139.4, 139.1, 137.8(d, J = 9 Hz), 135.9, 133.9, 133.7(2C), 132.4 (d, J = 36 Hz), 128.8(2C), 128.6, 128.3, 128.2, 128.0 (2C), 127.9, 127.6, 122.4, 120.7(2C), 120.5, 119.9(2C), 119.7, 115.7 (d, J = 22 Hz), 110.8, 107.6, 76.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{24}BrFN]^+$: 556.1071; Found : 556.1054.

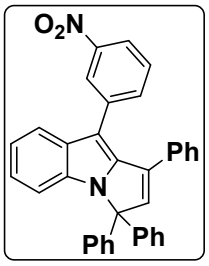


9-(2-Bromo-4-chlorophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3am):** Yield: 71%; 406.7 mg; light yellow solid; mp 110-112 ºC; R_f = 0.50 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.56 (d, J = 2 Hz, 1H), 7.43-7.41 (m, 1H), 7.39-7.36 (m, 5H),

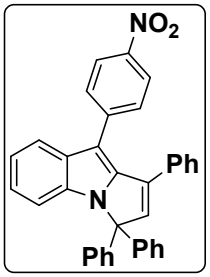
7.35-7.33 (m, 3H), 7.31-7.29 (m, 2H), 7.27 (s, 1H), 7.25-7.21 (m, 4H), 7.14-7.06 (m, 5H), 6.88 (s, 1H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz): δ 141.4, 140.7, 139.5, 139.3, 135.9, 134.6, 134.0, 133.7, 133.4, 132.5, 132.4, 132.3, 128.8(2C), 128.3, 128.2, 128.0(3C), 127.7, 127.2, 126.7, 122.3, 120.5, 119.8, 110.9, 107.4, 76.1; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{24}BrClN]^+$: 572.0775; Found : 572.0775.



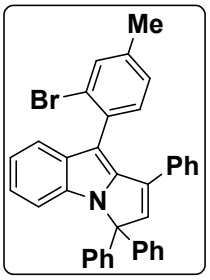
1,3,3-Triphenyl-9-(2-(trifluoromethyl)phenyl)-3H-pyrrolo[1,2-a]indole **(3an):** Yield: 76%; 401 mg; off white solid; mp 174-176 ºC; R_f = 0.20 (petroleum ether/EtOAc = 90/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.75 (d, J = 8 Hz, 1H), 7.67-7.62 (m, 2H), 7.56-7.38 (m, 12H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.17-7.12 (m, 5H), 7.98 (t, *J* = 1.6 Hz, 1H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz): δ 140.3 (q, *J* = 239 Hz), 135.9, 134.1, 134.0, 133.9, 133.7, 132.5, 131.3, 131.2, 131.0, 130.7, 128.8, 128.7, 128.4, 127.9 (q, *J* = 14 Hz), 127.6, 127.5, 126.1(q, *J* = 15 Hz), 125.4, 123.0, 122.7, 122.2, 120.6, 119.9, 119.6, 110.6, 106.0, 75.8; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{25}F_3N]^+$: 528.1934; Found : 528.1938.



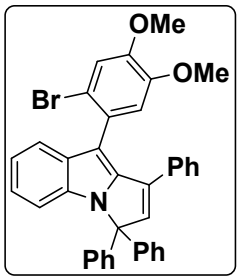
9-(3-Nitrophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ao):** Yield: 79%; 399 mg; yellow solid; mp 246-248 °C; R_f = 0.40 (petroleum ether/EtOAc = 85/15); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.80 (d, J = 8 Hz, 1H), 7.65 (d, J = 7.6 Hz, 1H), 7.42-7.34 (m, 11H), 7.27-7.25 (m, 3H), 7.19-7.13 (m, 5H), 6.91 (s, 1H); $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100 MHz): δ 147.8, 142.1, 141.0, 139.0, 136.3, 135.9, 135.5, 134.3, 132.3, 131.4, 128.8, 128.6, 128.4, 128.2(2C), 128.1, 125.4, 122.9, 120.7, 120.4, 119.8, 111.1, 107.5, 76.2; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{25}N_2O_2]^+$: 505.1911; Found : 505.1939.



9-(4-Nitrophenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ap):** Yield: 80%; 404 mg; yellow solid; mp 247-249 °C; R_f = 0.40 (petroleum ether/EtOAc = 85/15); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.06 (d, J = 8 Hz, 2H), 7.80 (d, J = 8 Hz, 1H), 7.43-7.34 (m, 12H), 7.31-7.26 (m, 3H), 7.21-7.12 (m, 5H), 6.93 (d, J = 1.6 Hz, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 145.7, 142.7, 141.5, 141.3, 138.8, 135.5, 134.3, 132.4, 131.3, 130.9, 128.9, 128.8, 128.3(2C), 128.2(2C), 123.1, 123.0, 120.5, 120.0, 111.2, 108.0, 76.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{35}H_{25}N_2O_2]^+$: 505.1911; Found : 505.1933.

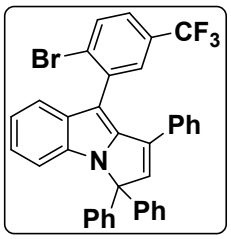


9-(2-Bromo-4-methylphenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3aq):** Yield: 72%; 398 mg; off white solid; mp 88-90 °C; R_f = 0.50 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47-7.45 (m, 1H), 7.40-7.38 (m, 5H), 7.36-7.31 (m, 6H), 7.29-7.26 (m, 3H), 7.22-7.18 (m, 1H), 7.11-7.06 (m, 6H), 6.88 (d, J = 1.2 Hz, 1H), 2.38 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.1, 140.3, 139.8, 139.5, 138.7, 136.2, 134.0, 133.1, 132.8, 132.7, 128.8, 128.7, 128.4, 128.3, 128.1, 127.9, 127.8, 127.7, 126.1, 122.1, 120.8, 119.5, 110.7, 108.6, 75.9, 20.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{27}BrN]^+$: 552.1321; Found : 552.1299.

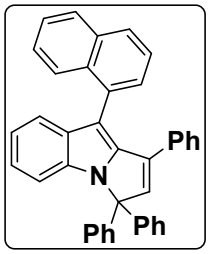


9-(2-Bromo-4,5-dimethoxyphenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3ar):** Yield: 78%; 500 mg; brown solid; mp 241-243 °C; R_f = 0.60 (petroleum ether/EtOAc = 85/15); ^{1}H

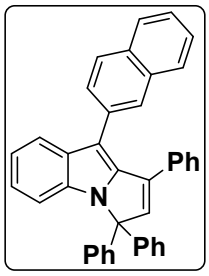
NMR ($CDCl_3$, 400 MHz): δ 7.57-7.53 (m, 1H), 7.40-7.28 (m, 12H), 7.26-7.22 (m, 1H), 7.15-7.07 (m, 6H), 7.92-6.85 (m, 2H), 3.93 (s, 3H), 3.67 (s, 3H); $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 148.7, 147.9, 141.0, 140.4, 139.6, 139.4, 136.1, 133.9, 132.7, 132.4, 128.8, 128.7, 128.4, 128.2, 127.9(2C), 127.8, 127.7, 122.2, 121.0, 119.6, 116.1, 115.7, 115.4, 110.8, 108.7, 75.9, 56.3, 56.0; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{37}H_{29}BrNO_2]^+$: 598.1376; Found : 598.1386.



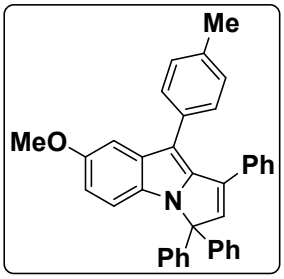
9-(2-Bromo-5-(trifluoromethyl)phenyl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3as):** Yield: 80%; 485 mg; grey solid; mp 102-104 °C; R_f = 0.60 (petroleum ether/EtOAc = 85/15); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.68 (d, J = 8.4 Hz, 1H), 7.61 (s, 1H), 7.46 (t, J = 5.2 Hz, 1H), 7.40-7.34 (m, 11H), 7.20 (d, J = 7.6 Hz, 3H), 7.12-7.07 (m, 5H), 6.91 (s, 1H); $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 141.7, 141.0, 139.3, 139.1, 136.9, 135.8, 132.9 (q, J = 202 Hz), 130.0 (q, J = 13 Hz), 129.6, 129.2, 128.8, 128.3(2C), 128.3 (q, J = 28 Hz), 127.7, 125.2, 125.0 , 124.9, 122.5, 120.6, 119.9, 111.0, 107.2, 76.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{24}BrF_3N]^+$: 606.1039; Found: 606.1021.



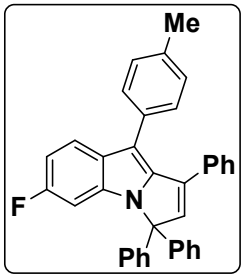
9-(Naphthalen-1-yl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3at):** Yield: 73%; 372 mg; radish solid; mp 182-184 ºC R_f = 0.80 (petroleum ether/EtOAc = 95/05); ^1H NMR ($CDCl_3$, 400 MHz): δ 7.89 (d, J = 8 Hz, 1H), 7.85 (d, J = 8 Hz, 1H), 7.80 (d, J = 8 Hz, 1H), 7.42-7.40 (m, 5H), 7.38-7.30 (m, 9H), 7.29-7.25 (m, 1H), 7.13-6.97 (m, 6H), 6.87 (s, 1H), 6.82 (t, J = 7.6 Hz, 2H); $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 141.4, 140.3, 139.8, 139.7, 136.1, 134.2, 133.8, 133.6, 133.3, 132.2, 129.6, 128.8(2C), 128.4, 128.3, 128.0(2C), 127.9, 127.5, 127.3, 126.9, 125.6(2C), 125.2, 122.2, 121.3, 119.5, 110.8, 107.8, 75.9; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{39}H_{28}N]^+$: 510.2216; Found: 510.2221.



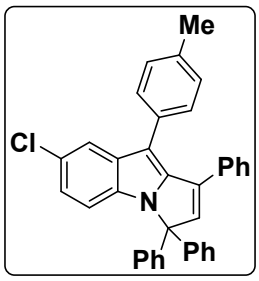
9-(Naphthalen-2-yl)-1,3,3-triphenyl-3H-pyrrolo[1,2-a]indole **(3au):** Yield: 60%; 306 mg; off white solid; mp 224-226 °C; R_f = 0.80 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87-7.85 (m, 1H), 7.81-7.79 (m, 1H), 7.73 (s, 1H), 7.65 (d, J = 8 Hz, 1H), 7.59-7.57 (m, 1H), 7.44-7.41 (m, 3H), 7.37-7.33 (m, 9H), 7.27-7.25 (m, 3H), 7.14-7.07 (m, 4H), 7.02-6.98 (m, 2H), 6.85 (s, 1H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.2, 140.2, 139.5, 136.2, 134.4, 133.4, 132.7, 132.3, 132.0, 131.7, 129.5, 129.3, 128.8, 128.4, 128.4, 128.3, 128.1, 127.9, 127.6, 127.1, 125.8, 125.4, 122.5, 120.7, 119.8, 110.8, 110.2, 104.8, 75.8; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{39}H_{28}N]^+$: 510.2216; Found: 510.2211.



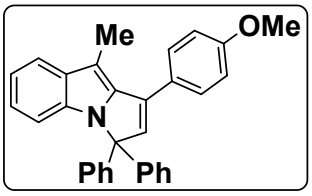
7-Methoxy-1,3,3-triphenyl-9-(p-tolyl)-3H-pyrrolo[1,2-a]indole **(3av):** Yield: 76%; 383 mg; yellow solid; mp 138-140 °C; R_f = 0.50 (petroleum ether/EtOAc = 90/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.28-7.19 (m, 10H), 7.17-7.12 (m, 4H), 7.08 (d, J = 8 Hz, 2H), 7.03 (t, J = 7.6, 2H), 6.95 (d, J = 7.6 Hz, 2H), 6.84 (d , J = 8.8 Hz, 1H), 6.71 (s, 1H), 6.65-6.62 (m, 1H), 3.69(s, 3H), 2.27 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 154.2, 140.6, 140.3, 139.7, 136.2, 135.6, 132.8, 132.7, 131.3, 130.6, 129.5, 128.7, 128.6, 128.4, 128.3, 128.1, 127.9, 112.3, 111.3, 109.9, 102.5, 75.6, 55.9, 21.4; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{37}H_{30}NO]^+$: 504.2322; Found: 504.2353.



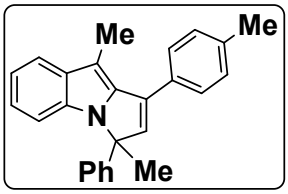
6-Fluoro-1,3,3-triphenyl-9-(p-tolyl)-3H-pyrrolo[1,2-a]indole **(3aw):** Yield: 79%; 388 mg; off white solid; mp 138-140 °C; R_f = 0.40 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.75-7.72 (m, 1H), 7.44-7.39 (m, 9H), 7.35-7.29 (m, 3H), 7.27-7.18 (m, 5H), 7.11(d, 2H), 6.93-6.91 (m, 1H), 6.87 (s, 1H), 6.84-6.81 (m, 1H), 2.43 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 160.0 (d, J = 237 Hz), 141.2, 140.4, 140.0, 139.3, 139.2, 136.0 (d, J = 13 Hz), 134.2, 132.5, 131.3, 130.8, 130.6, 129.0, 128.8(2C), 128.6, 128.4, 128.2(2C), 128.0, 127.9, 127.8, 121.4 (d, J = 10 Hz), 110.4, 108.1 (d, J = 24 Hz), 97.1 (d, J = 27 Hz), 97.0, 75.7, 21.3;; ^{19}F NMR ($CDCl_3$, 376 MHz): δ -119.7; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{27}FN]^+$: 492.2122; Found : 492.2145.



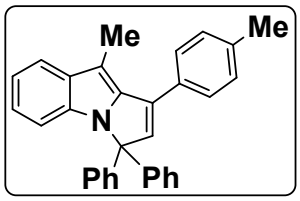
7-Chloro-1,3,3-triphenyl-9-(p-tolyl)-3H-pyrrolo[1,2-a]indole **(3ax):** Yield: 73%; 371 mg; white solid; mp 220-222 °C; R_f = 0.50 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.69 (t, J = 9.2 Hz, 13H), 7.34-7.22 (m, 13H), 7.11 (d, J = 6 Hz, 4H), 7.02-7.6.96 (m, 3H), 6.94-6.89 (m, 3H), 6.84 (s, 1H), 2.34 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.2, 141.0, 139.4, 136.1, 133.6, 132.6, 132.4, 130.6, 130.5, 128.4, 128.7, 128.4, 128.3, 128.2, 128.1, 128.0, 125.6, 122.6, 120.2, 111.5, 110.0, 75.9, 21.3; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{36}H_{27}ClN]^+$: 508.1827; Found : 508.1853.



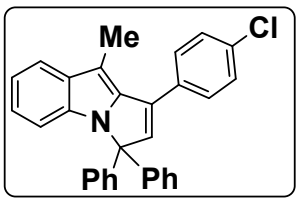
1-(4-Methoxyphenyl)-9-methyl-3,3-diphenyl-3H-pyrrolo[1,2-a]indole **(3ay):** Yield: 76%; 325 mg; off white solid; mp 184-186 °C; R_f = 0.50 (petroleum ether/EtOAc = 90/10); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60 (d, J = 8.8 Hz, 3H), 7.33-7.24 (m, 10H), 7.05-6.93 (m, 5H), 6.59 (s, 1H), 3.87 (s, 3H), 2.37 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 159.9, 140.8, 140.3, 138.6, 135.9, 134.4, 134.1, 129.6, 128.6, 128.2, 127.7, 126.1, 121.8, 119.6, 118.7, 113.9, 110.5, 102.8, 75.4, 55.5, 9.8; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{31}H_{26}NO]^+$: 428.2009; Found : 428.2036.



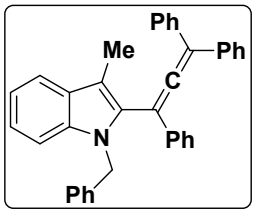
3,9-Dimethyl-3-phenyl-1-(p-tolyl)-3H-pyrrolo[1,2-a]indole **(3az):** Yield: 74%; 259 mg; off white solid; mp 122-124 °C; R_f = 0.70 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.68-7.66 (m, 1H), 7.53 (d, J = 8 Hz, 1H), 7.34-7.26 (m, 5H), 7.20 (d, J = 7.6 Hz, 2H), 7.13-7.08 (m, 2H), 7.02-7.00 (m, 1H), 6.38 (s, 1H), 2.44 (s, 3H), 2.39 (s, 3H), 2.01 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.7, 141.1, 140.1, 138.2, 135.6, 134.0, 133.4, 131.0, 129.2, 128.8, 128.2, 127.4, 126.0, 121.6, 119.7, 118.6, 109.9, 101.9, 68.5, 24.0, 21.4, 9.7; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{26}H_{24}N]^+$: 350.1903; Found : 350.1906.



9-Methyl-3,3-diphenyl-1-(p-tolyl)-3H-pyrrolo[1,2-a]indole **(3ba):** Yield: 68%; 280 mg; off white solid; mp 141-143 °C; R_f = 0.55 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.63-7.57 (m, 3H), 7.36-7.27 (m, 12H), 7.09-7.00 (m, 2H), 6.96 (d, J = 7.6 Hz, 1H), 6.65 (s, 1H), 2.43 (s, 3H), 2.39 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 140.6, 140.2, 139.1, 138.4, 136.2, 134.3, 134.1, 130.8, 129.2, 128.6, 128.2, 127.7, 121.8, 119.6, 118.7, 110.4, 102.9, 75.4, 21.5, 9.8; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{31}H_{26}N]^+$: 412.2060; Found : 412.2073.



1-(4-Chlorophenyl)-9-methyl-3,3-diphenyl-3H-pyrrolo[1,2-a]indole **(3bb):** Yield: 76%; 328 mg; white solid; mp 177-179 °C; R_f = 0.6 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58 (d, J = 8.4 Hz, 3H), 7.41 (d, J = 8.4 Hz, 2H), 7.32-7.27 (m, 6H), 7.23 (t, J = 6.4 Hz, 4H), 7.04-6.98 (m, 2H), 6.92 (d, J = 7.6 Hz, 1H), 6.64 (s, 1H), 2.33 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 140.0, 139.9, 139.8, 135.2, 134.4, 134.0, 132.2, 129.7, 128.8, 128.7, 128.2, 127.8, 122.1, 119.8, 118.9, 110.5, 103.1, 75.5, 9.73; HRMS (ESI-TOF) m/z: $[M+H]^+$ Calculated for $[C_{30}H_{23}ClN]^+$: 432.1514; Found: 432.1505.



1-Benzyl-3-methyl-2-(1,3,3-triphenylpropa-1,2-dien-1-yl)-1H-indole **(5):** Yield: 87%; 424 mg; off white gummy; R_f = 0.70 (petroleum ether/EtOAc = 95/05); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60 (t, J = 5.2 Hz, 1H), 7.27-7.25 (m, 4H), 7.22-7.18 (m, 11H), 7.14-7.10 (m, 3H), 7.07-7.02 (m, 3H), 6.73 (d, J = 6.4 Hz, 1H), 5.10 (s, 2H), 2.13 (s, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 209.6, 138.1, 137.2, 135.8, 135.7, 130.9, 128.9, 128.8, 128.7, 128.5, 128.4, 127.8, 127.7, 126.9, 126.7, 126.1, 122.1, 119.3, 119.0, 112.8, 111.2, 110.3, 102.7, 47.6, 9.7.

7. Calculation of Green Chemistry Metrics (EcoScale and E-factor):

(a) Calculation of EcoScale indexes under ball milling

The penalty points for synthesis of coumarin derivatives for the synthesis of pyrrolo[1,2-*a*]indoles (**3**) under ball milling

Parameter	**Penalty**
1. Yields 60-85%	20-7.5
2. Price of reaction components	
Indoles	0
Propargyl alcohols	0
BAIL-1	0
3. Safety	
non-dangerous for environment, non-toxic, non-flammable	0
4. Technical setup	
Unconventional activation technique	2
5. Temperature/time	
Room temperature < 1 h	0
6. Workup and purification	
Classical chromatography	10
Penalty points total:	32-19.5

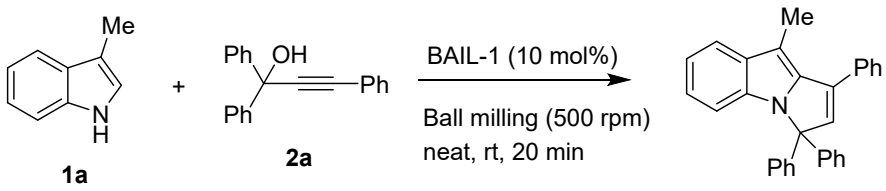
EcoScale Score = 100 - Total penalty points = 68-80.5

EcoScale Score for the synthesis of 9-methyl-1,3,3-triphenyl-3*H*-pyrrolo[1,2-*a*]indole (3aa) under the ball-milling conditions:

Parameter	**Penalty**
1. Yields 84%	8
2. Price of reaction components	
3-Methyl-1*H*-indole (**1a**)	0
Propargyl alcohol (**2a**)	0
BAIL-1	0
3. Safety	
non-dangerous for environment, non-toxic, non-flammable	0
4. Technical setup	
Unconventional activation technique	2
5. Temperature/time	
Room temperature < 1 h	0
6. Workup and purification	
Classical chromatography	10
Penalty points total:	20

EcoScale Score = 100 - Total penalty points
= 80

(c) Calculation of E-factor for the synthesis of 9-methyl-1,3,3-triphenyl-3*H*-pyrrolo[1,2-*a*]indole (3aa) under the ball-milling conditions:



E-factor calculation for the synthesis of 3aa under the ball-milling conditions:

Reactant 1 (**1a**):	3-Methyl-1*H*-indole	0.131 g	1 mmol	FW 131.18
Reactant 2 (**2a**):	1,1,3-Triphenylprop-2-yn-1-ol	0.284 g	1 mmol	FW 284.36
Reagent:	BAIL-1	0.039 g	0.1 mmol	FW 390
Solvent:	—	—	—	—
Auxiliary (grinding):	—	—	—	—
Product (**3aa**):	9-methyl-1,3,3-triphenyl-3*H*-pyrrolo[1,2-*a*]indole	0.333 g	0.84 mmol	FW 397.52

Product yield = 84%

$$\text{E-factor} = \frac{0.131 + 0.284 + (0.039-0.036) - (0.333)}{0.333}$$ **= 0.25 Kg waste/1 Kg product**

Note: (i) Calculations were donw on 1 mmol scale. (ii) When the authors have not reported the amount of solvent used in the work-up and purification procedure, we have nnot accounted for solvent and considered that soovent can be recovered. The catalyst was recovered in 94% amount.

8. References:

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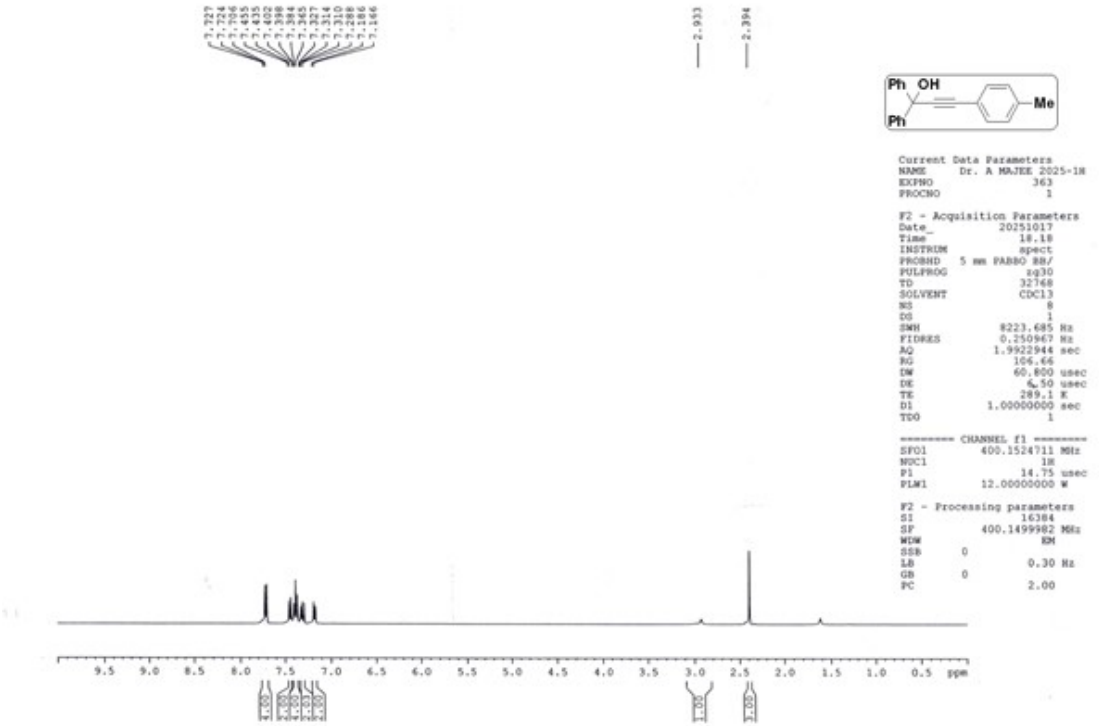
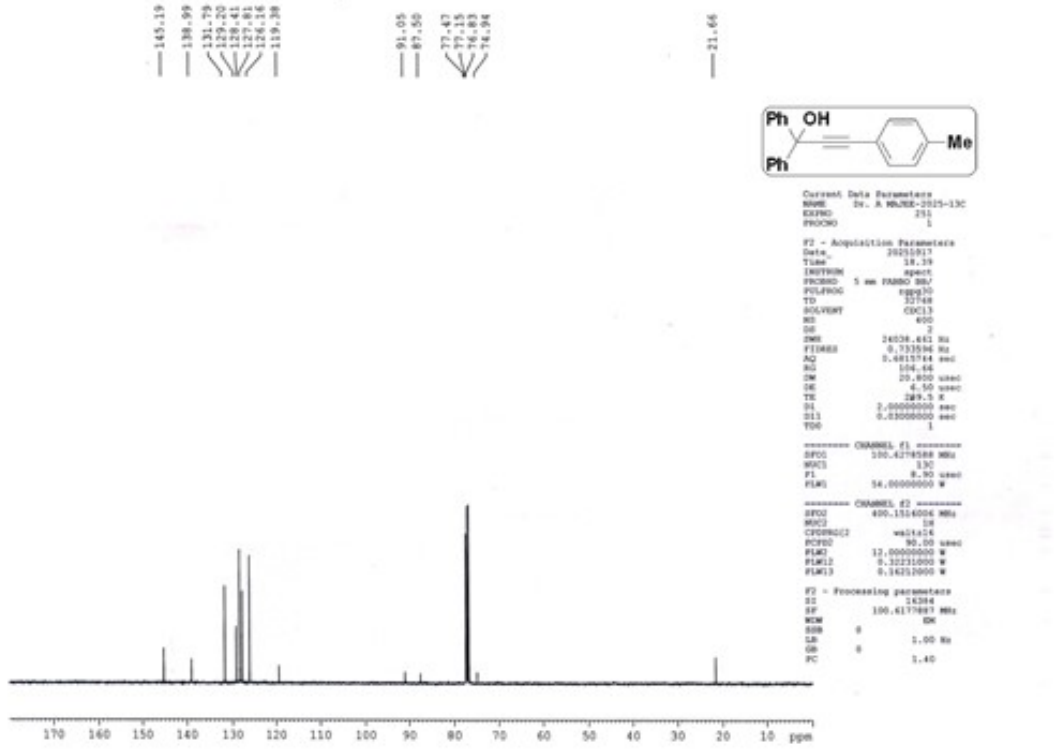
9. ^{1}H, and ^{13}C NMR spectra of synthesized compounds:

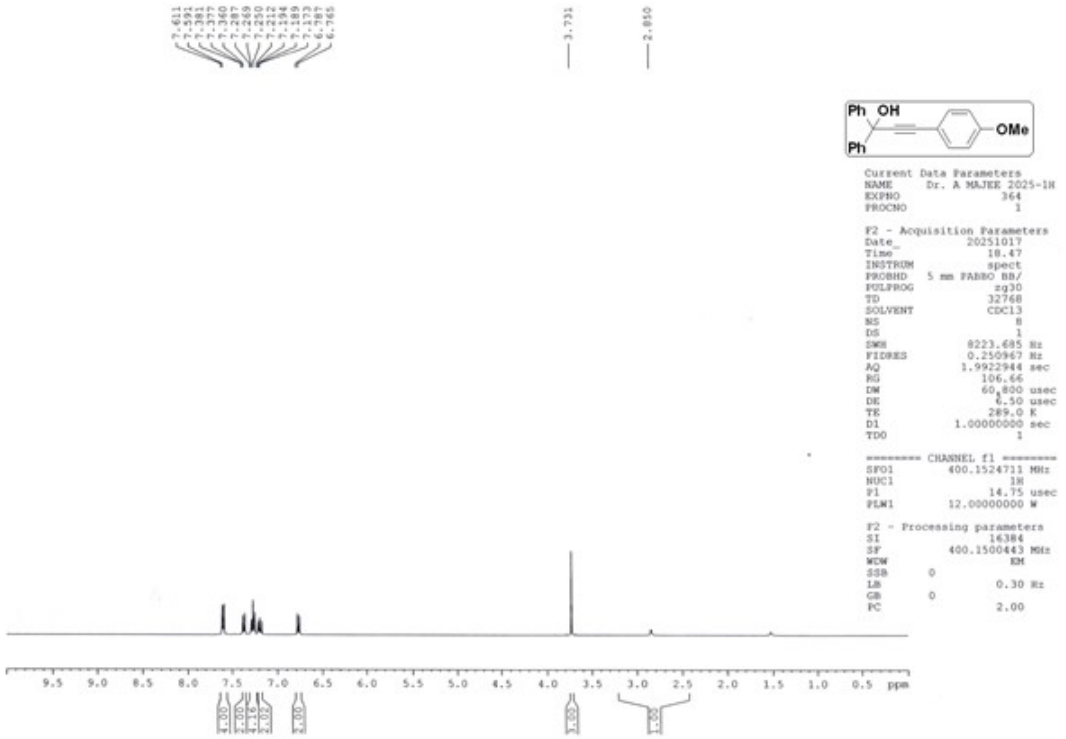
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



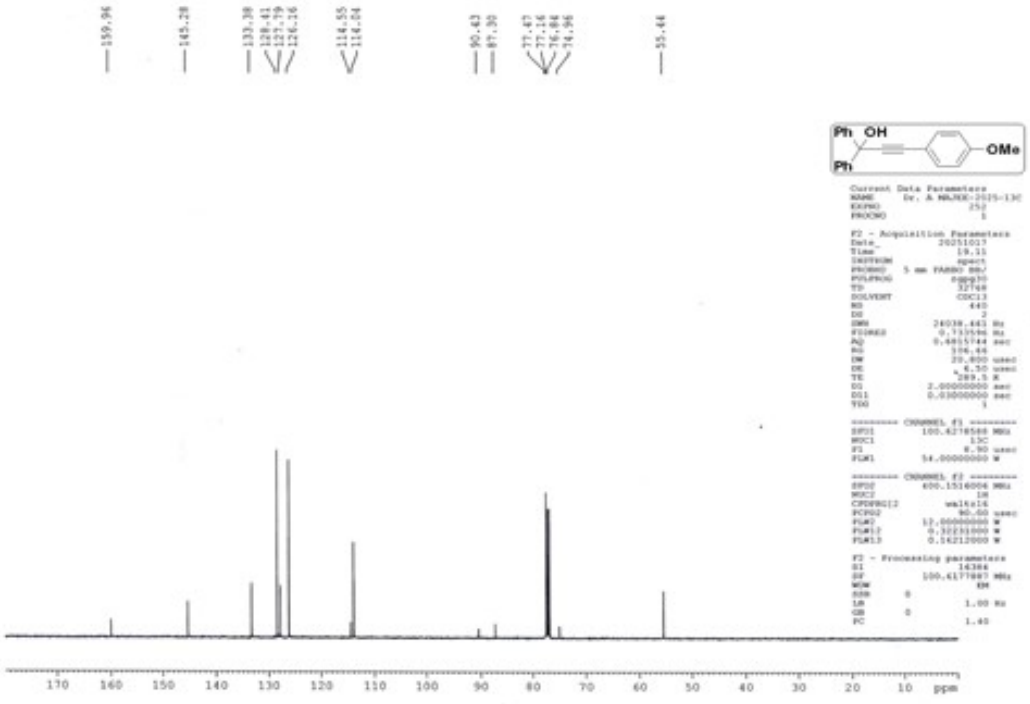
^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



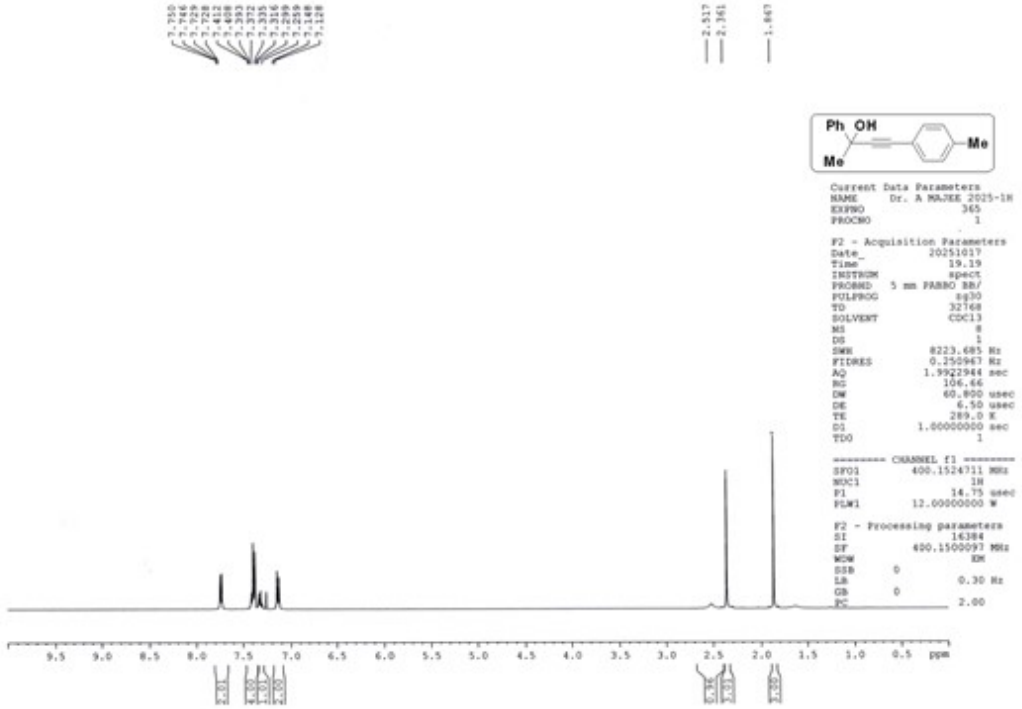
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



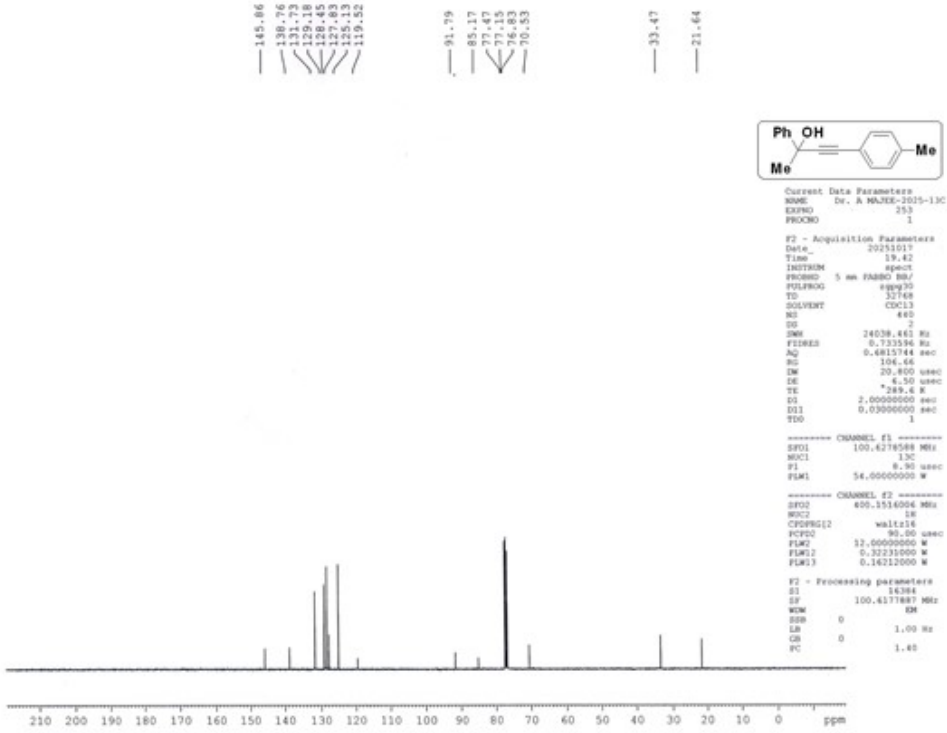
^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



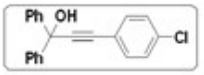
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

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PROCNO                   1

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PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                   8
DS                   1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG              106.66
DW               60.800 usec
DE                6.50 usec
TE              291.8 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1              1H
P1               14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
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WDW                EM
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LB                0.30 Hz
GB       0
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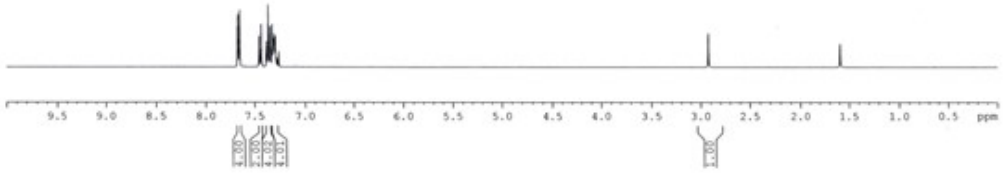
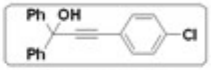


^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$

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PROCNO                   1

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Time              17.30
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PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                 440
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG              106.66
DW               20.800 usec
DE                6.50 usec
TE              292.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         100.6278580 MHz
NUC1              13C
P1                8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2              1H
CPDPRG[2          waltz16
PCPD2            90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
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WDW                EM
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LB                1.00 Hz
GB       0
PC                1.40
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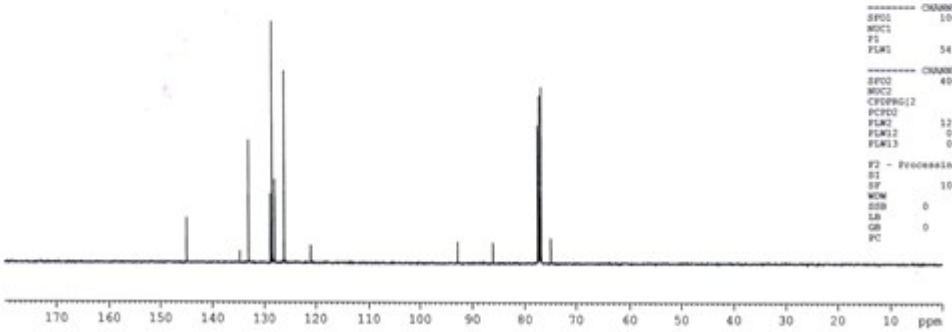
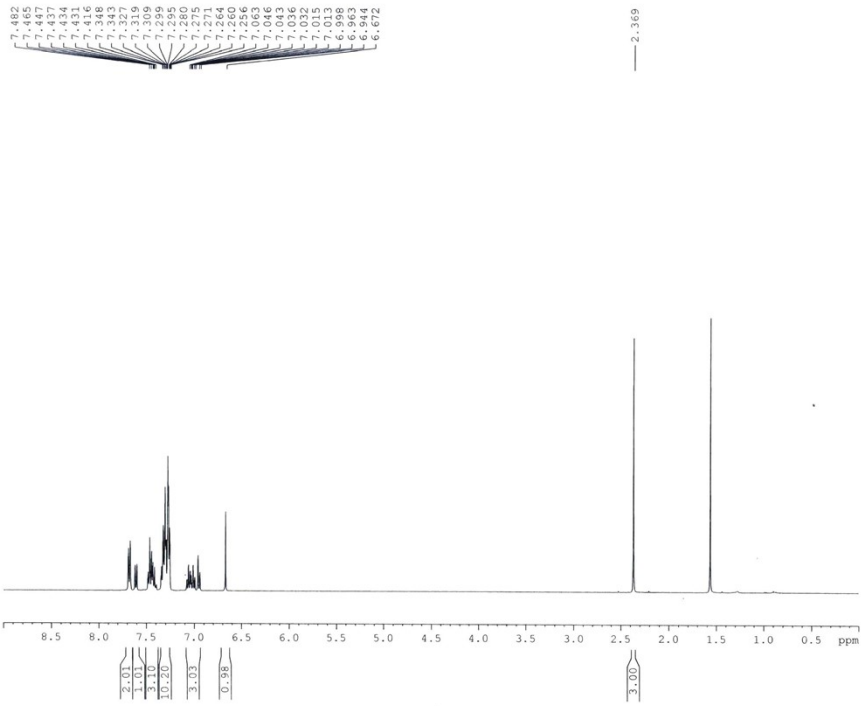
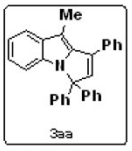


^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



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PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
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DS                      1
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                1.9922944 sec
RG                   186.42
DW                   60.800 usec
DE                    6.50 usec
TE                   295.7 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
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NUC1                     1H
P1                   14.75 usec
PLW1           12.00000000 W

F2 - Processing parameters
SI                    16384
SF              400.1500046 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    2.00
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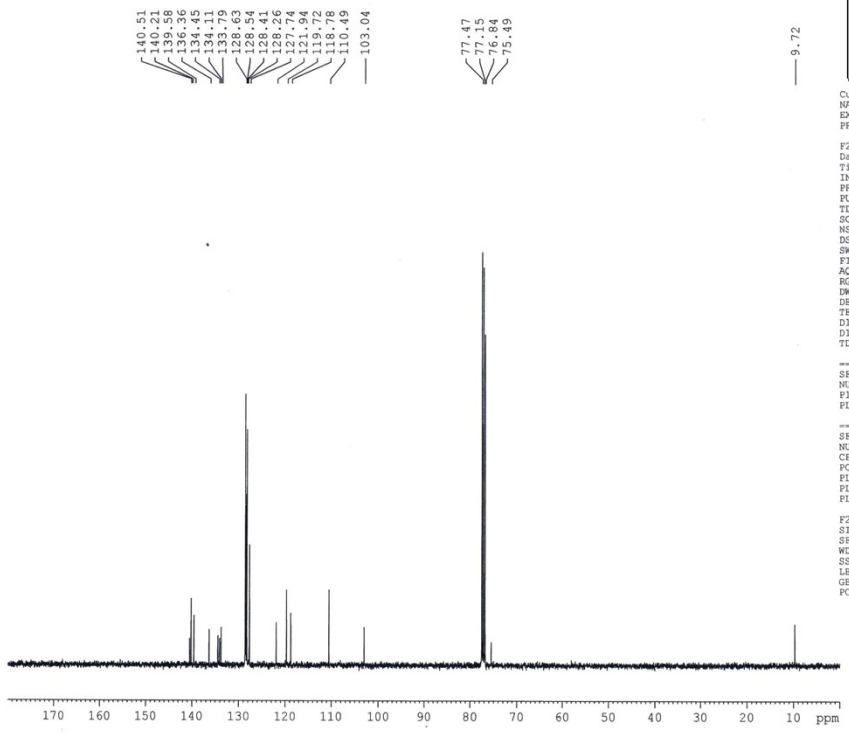
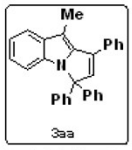
$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$



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PROCNO                    1

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PULPROG           zgpg30
TD                  32768
SOLVENT             CDCl3
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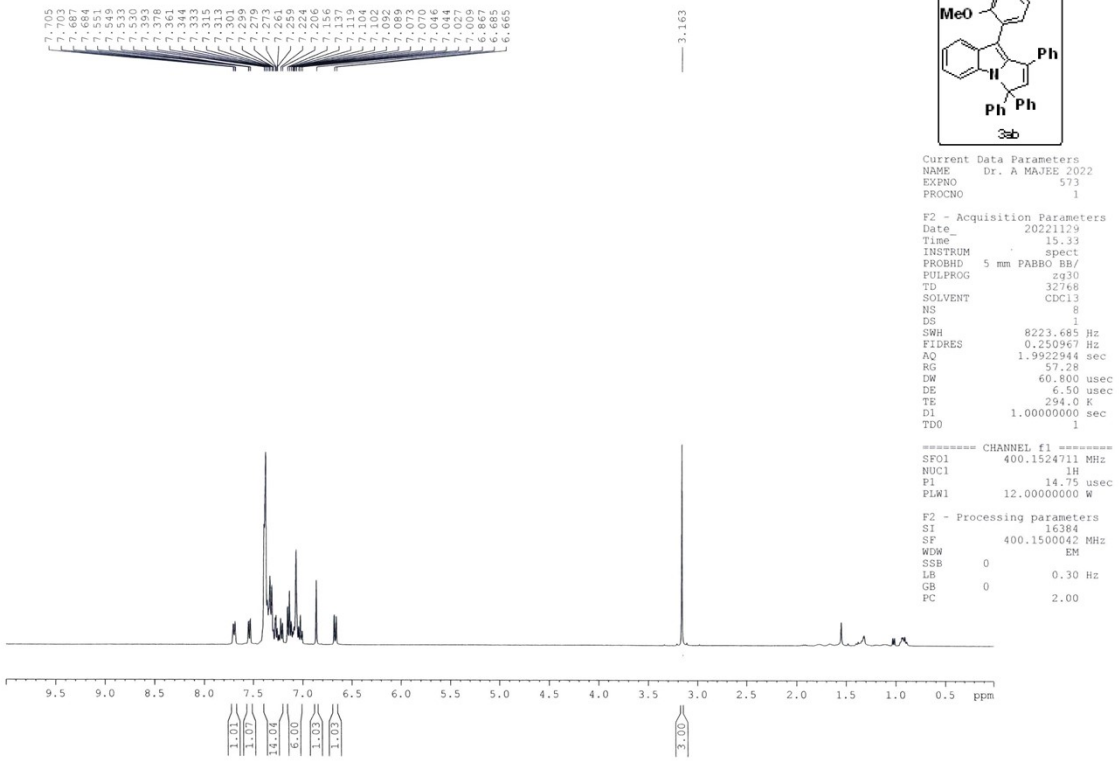
DS                      2
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                   186.42
DW                   20.800 usec
DE                    6.50 usec
TE                   300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            100.6278588 MHz
NUC1                    13C
P1                    8.90 usec
PLW1           54.00000000 W

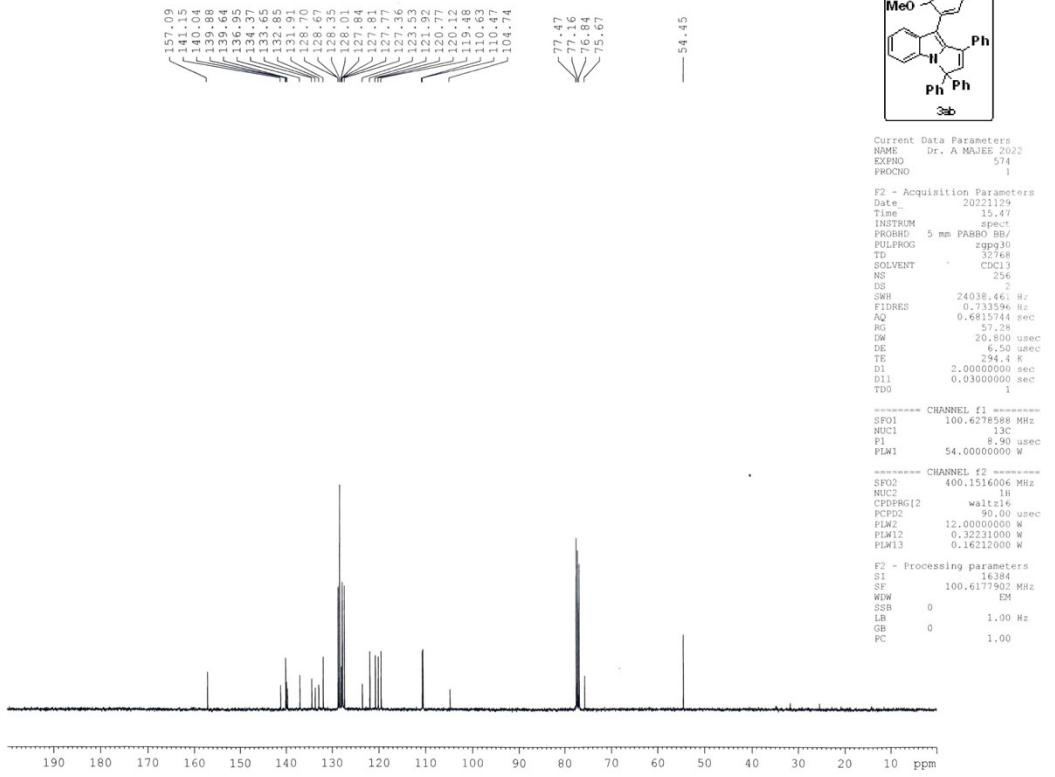
======== CHANNEL f2 ========
SFO2            400.1516006 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2           12.00000000 W
PLW12           0.32231000 W
PLW13           0.16212000 W

F2 - Processing parameters
SI                    16384
SF              100.6177844 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

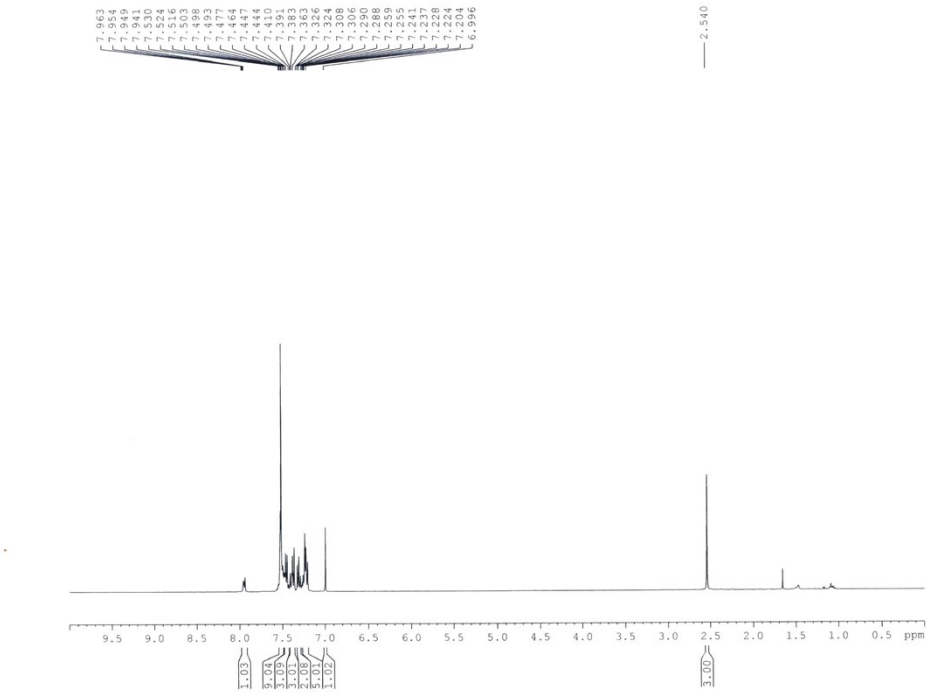
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

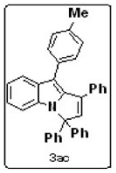


^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



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PROCNO                   1

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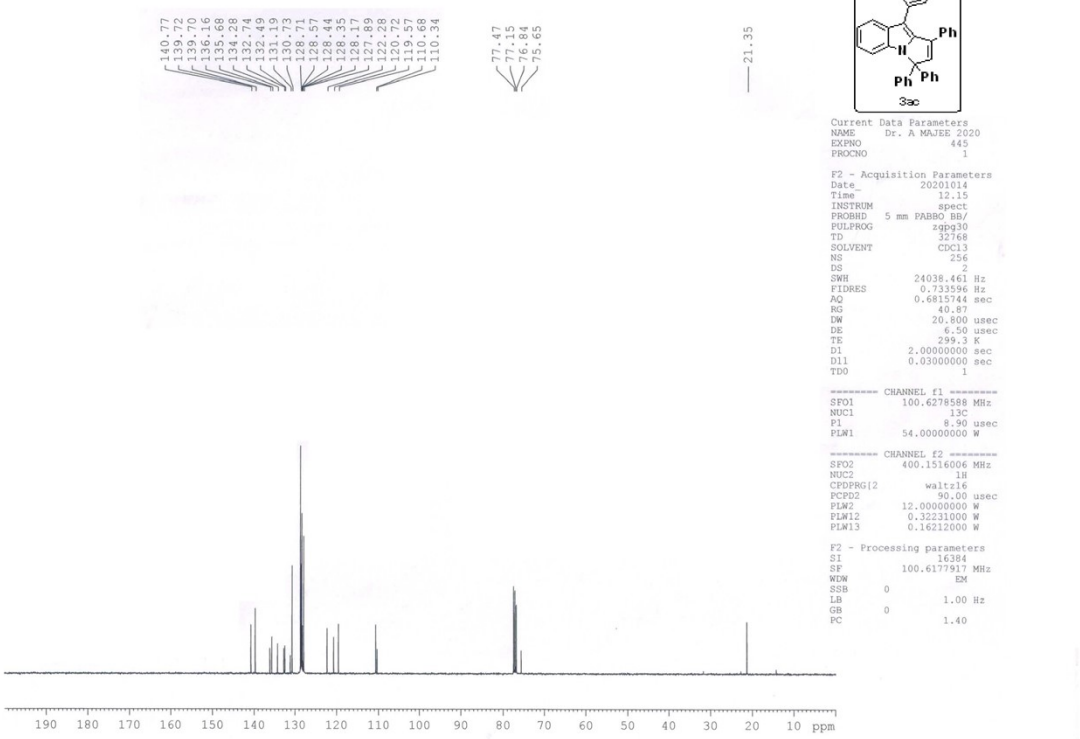
TD               32768
SOLVENT           CDCl3
NS                   8
DS                   1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                40.87
DW              60.800 usec
DE               6.50 usec
TE              298.6 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1524711 MHz
NUC1                   1H
P1                 14.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                 16384
SF          400.1499555 MHz
WDW                   EM
SSB          0
LB                 0.30 Hz
GB           0
PC                 2.00
```

^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$

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PROCNO                   1

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PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
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SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                40.87
DW              20.800 usec
DE               6.50 usec
TE              299.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1                   13C
P1                 8.90 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
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SSB          0
LB                 1.00 Hz
GB           0
PC                 1.40
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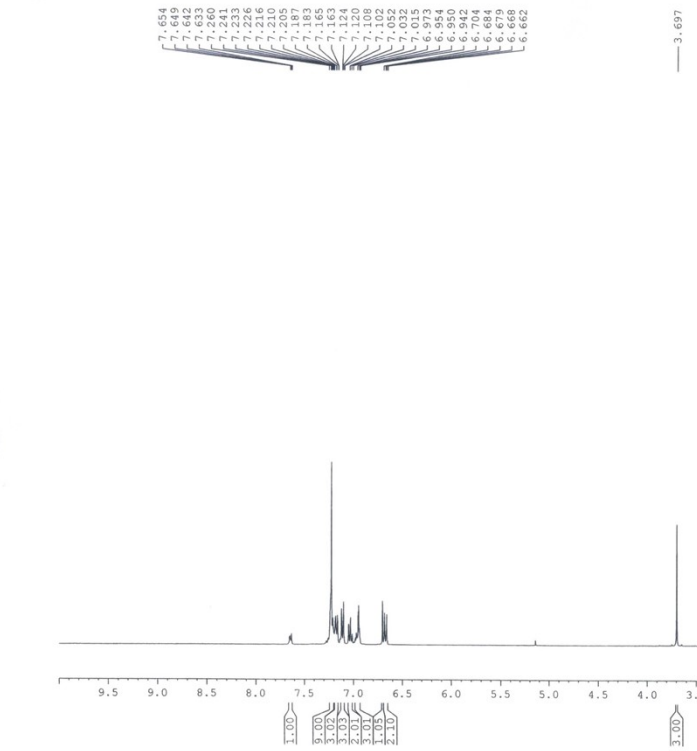
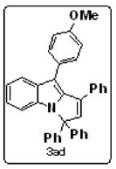
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



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PROCNO                  1

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PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                32.25
DW               60.800 usec
DE                6.50 usec
TE               293.9 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
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NUC1                  1H
P1                14.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                16384
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WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
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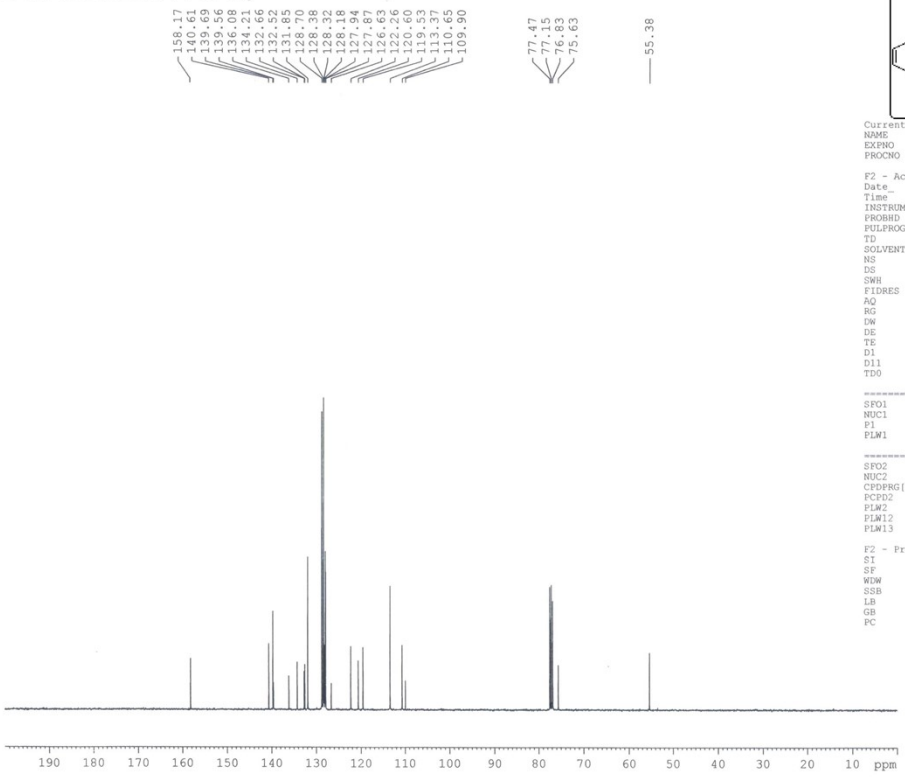
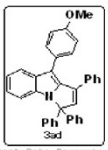
IR : 100 MHz, Solvent : $CDCl_3$



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PROCNO                  1

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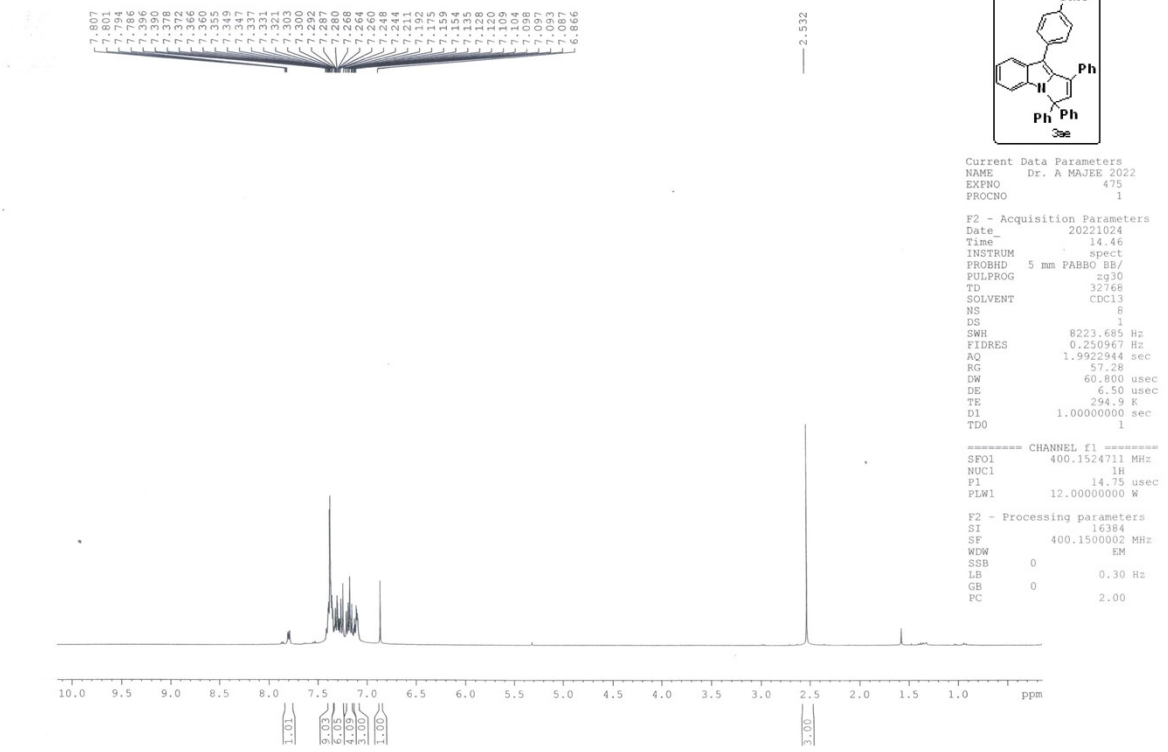
PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
NS                  440
DS                    2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                32.25
DW               20.800 usec
DE                6.50 usec
TE               294.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1                  13C
P1                 8.90 usec
PLW1        54.00000000 W

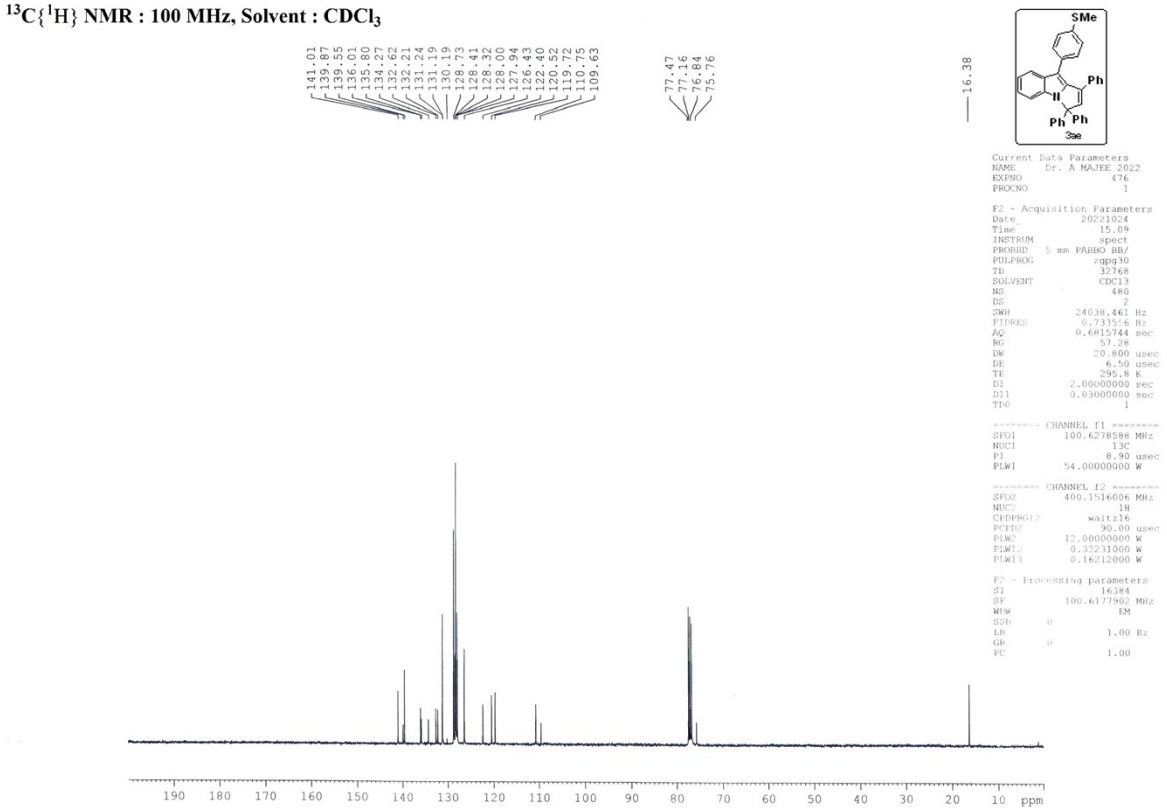
======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177946 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

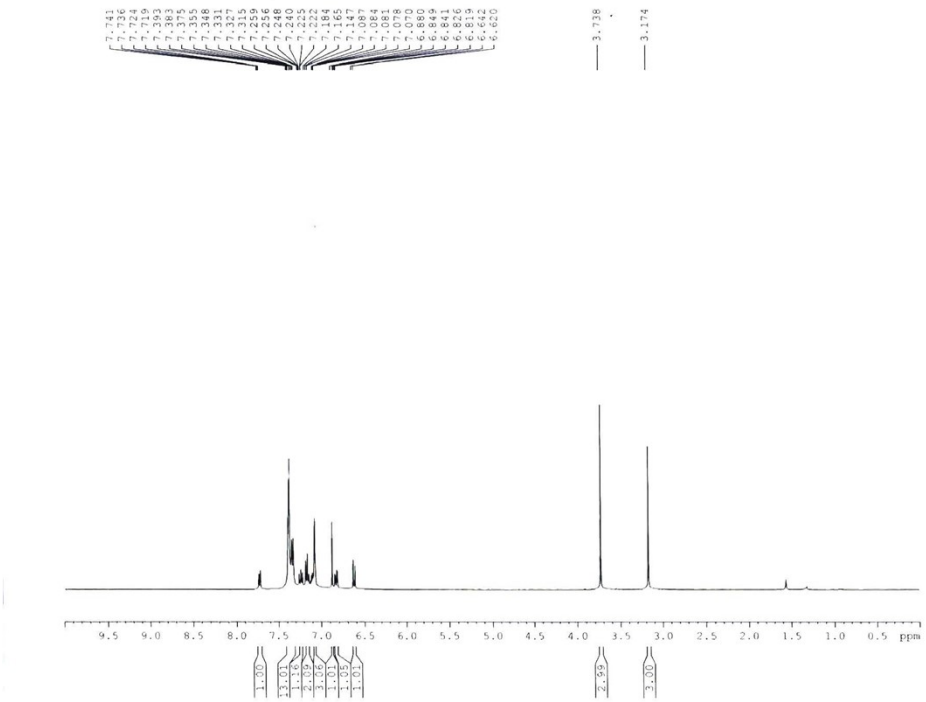
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

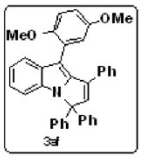


^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



^{1}H NMR : 400 MHz, Solvent : $CDCl_3$





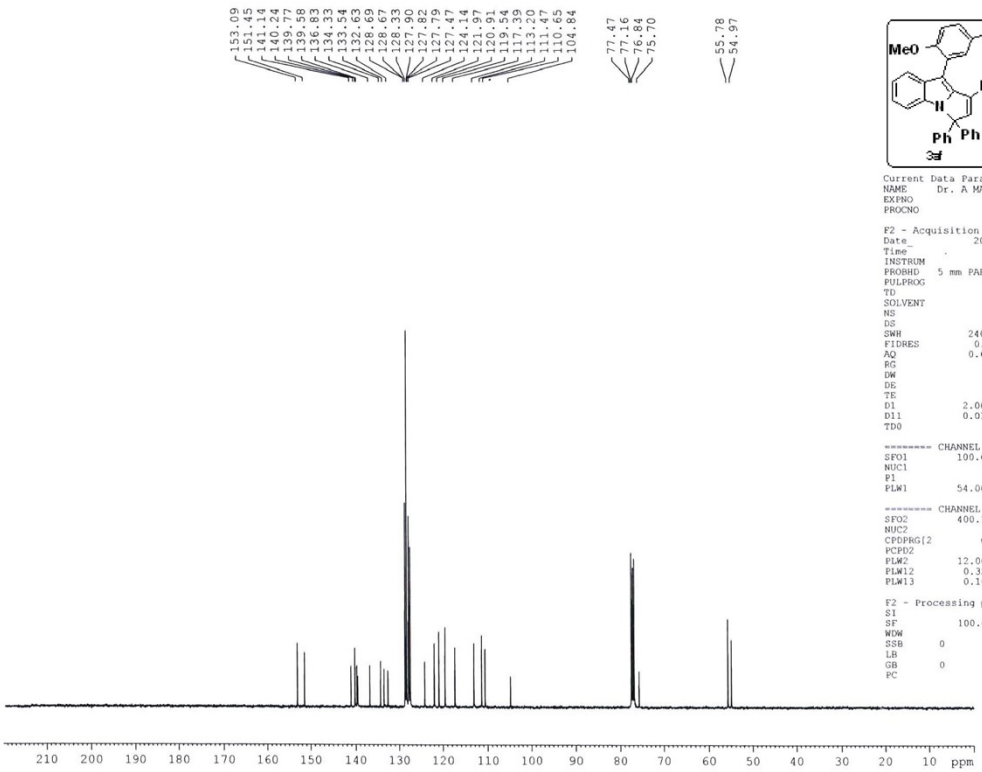

```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                506
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221107
Time                13.09
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             CDCl3
NS                     8
DS                     1
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9922944 sec
RG                 62.69
DW                60.800 usec
DE                 6.50 usec
TE                294.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1524711 MHz
NUC1                  1H
P1                 14.75 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                  16384
SF            400.1500083 MHz
WDW                    EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  2.00
```

^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$




```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                507
PROCNO                 1

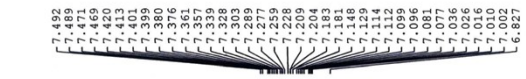
F2 - Acquisition Parameters
Date_           20221107
Time                13.35
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT             CDCl3
NS                   512
DS                     2
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 62.69
DW                20.800 usec
DE                 6.50 usec
TE                294.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

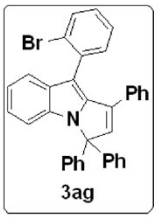
======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                  13C
P1                  8.90 usec
PLW1          54.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2          12.00000000 W
PLW12          0.32231000 W
PLW13          0.16212000 W

F2 - Processing parameters
SI                  16384
SF            100.6177932 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



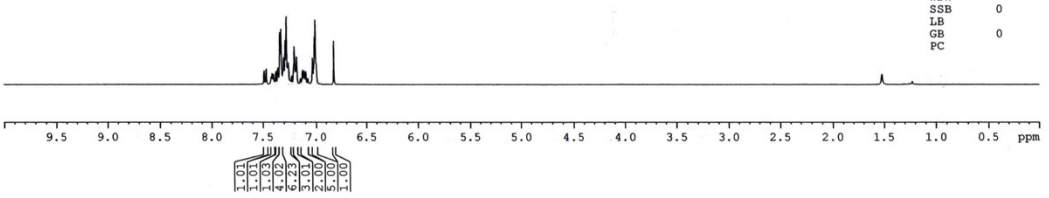



```
Current Data Parameters
NAME      Dr. A MAJEE 2025-1H
EXPNO                  361
PROCNO                   1

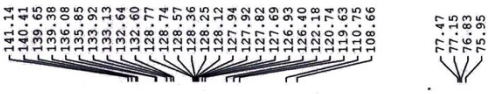
F2 - Acquisition Parameters
Date_              20251017
Time                 11.34
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT              CDCl3
NS                       8
DS                       1
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                1.9922944 sec
RG                   77.59
DW                  60.800 usec
DE                   6.50 usec
TE                  290.6 K
D1                1.00000000 sec
TD0                      1

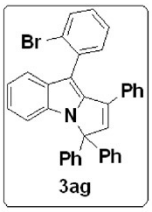
======== CHANNEL f1 ========
SFO1          400.1524711 MHz
NUC1                    1H
P1                   14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                   16384
SF            400.1500318 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    2.00
```



^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$





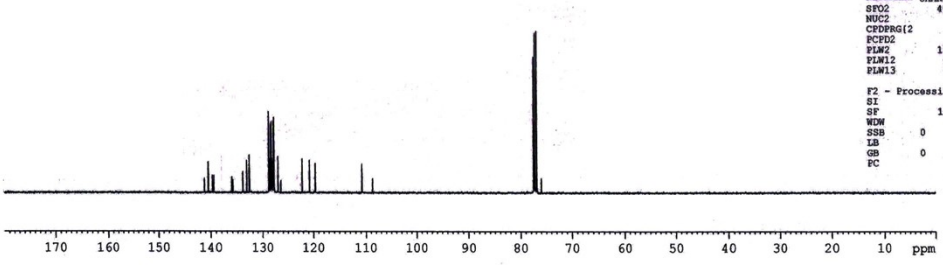

```
Current Data Parameters
NAME      Dr. A MAJEE-2025-13C
EXPNO                  248
PROCNO                   1

F2 - Acquisition Parameters
Date_              20251017
Time                 12.03
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  32768
SOLVENT              CDCl3
NS                     600
DS                       2
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                   77.59
DW                  20.800 usec
DE                   6.50 usec
TE                  290.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

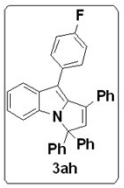
======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                   13C
P1                    8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                   16384
SF            100.6177902 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

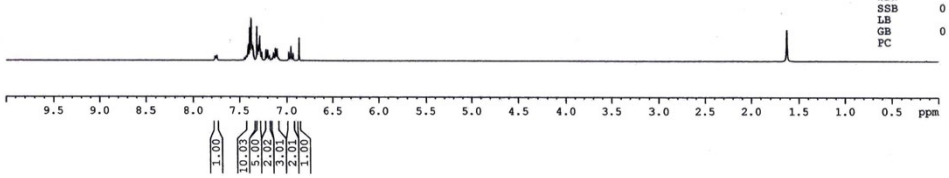



```
Current Data Parameters
NAME      Dr. A MAJEE 2025-1H
EXPNO                  372
PROCNO                   1

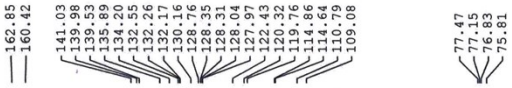
F2 - Acquisition Parameters
Date_           20251022
Time_              17.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG               186.42
DW              60.800 usec
DE               6.50 usec
TE              293.8 K
D1            1.00000000 sec
TD0                   1

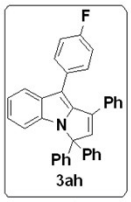
======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1                 1H
P1                14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                16384
SF           400.1499881 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```



^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$





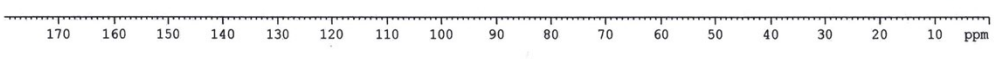

```
Current Data Parameters
NAME      Dr. A MAJEE-2025-13C
EXPNO                  260
PROCNO                   1

F2 - Acquisition Parameters
Date_           20251022
Time              18.02
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                 1200
DS                    2
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               186.42
DW              20.800 usec
DE               6.50 usec
TE              293.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

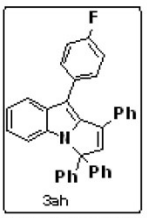
======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1                13C
P1                8.90 usec
PLW1         54.00000000 W

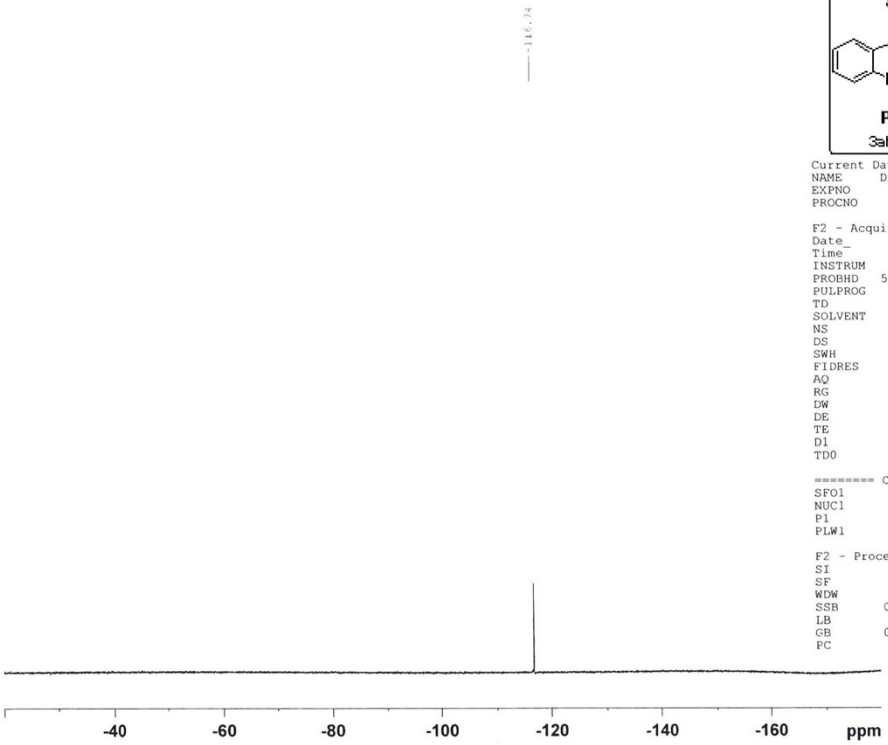
======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF           100.6177858 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



^{19}F NMR : 376 MHz, Solvent : $CDCl_3$



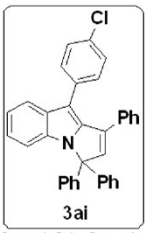



```
Current Data Parameters
NAME      Dr. A MAJEE 2024
EXPNO                  488
PROCNO                   1

F2 - Acquisition Parameters
Date_              20241217
Time                  17.50
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgflqn
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              89285.711 Hz
FIDRES            2.724784 Hz
AQ                0.1835008 sec
RG                   186.42
DW                  5.600 usec
DE                  6.50 usec
TE                  289.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          376.4795333 MHz
NUC1                    19F
P1                   12.50 usec
PLW1          20.00000000 W

F2 - Processing parameters
SI                   16384
SF            376.5171850 MHz
WDW                     EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00
```

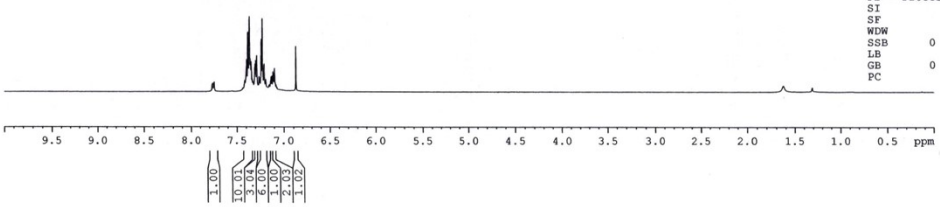


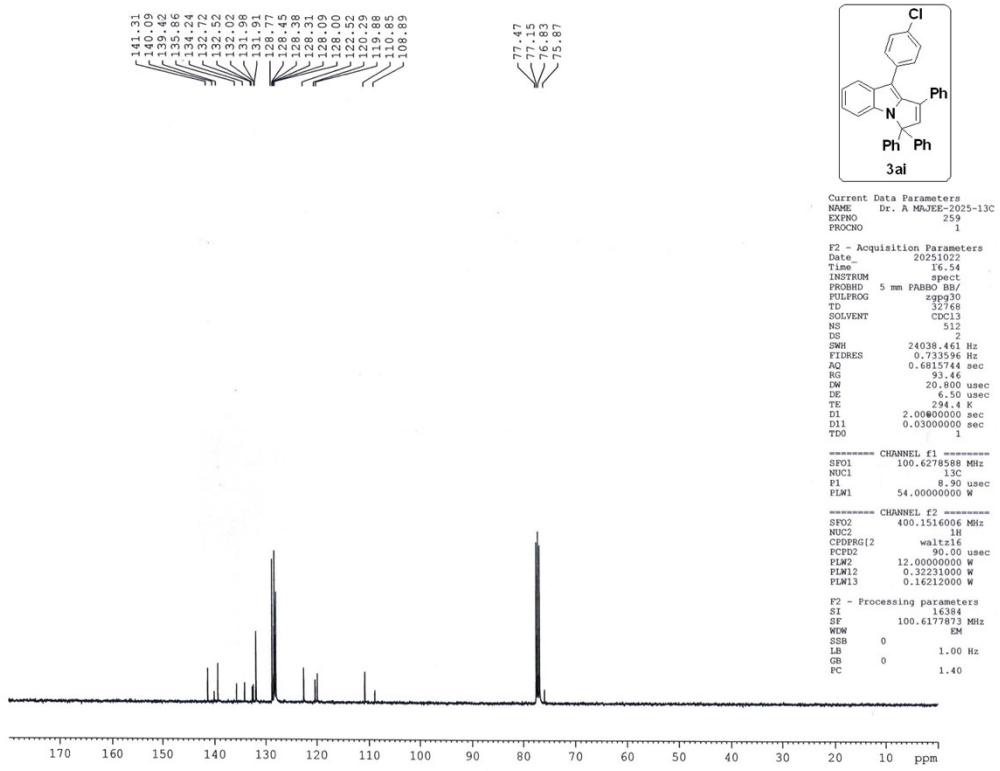

```
Current Data Parameters
NAME      Dr. A MAJEE 2025-1H
EXPNO                  371
PROCNO                   1

F2 - Acquisition Parameters
Date_              20251022
Time                  16.26
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       1
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                1.9922944 sec
RG                   93.46
DW                  60.800 usec
DE                   6.50 usec
TE                  294.1 K
D1              1.00000000 sec
TD0                      1

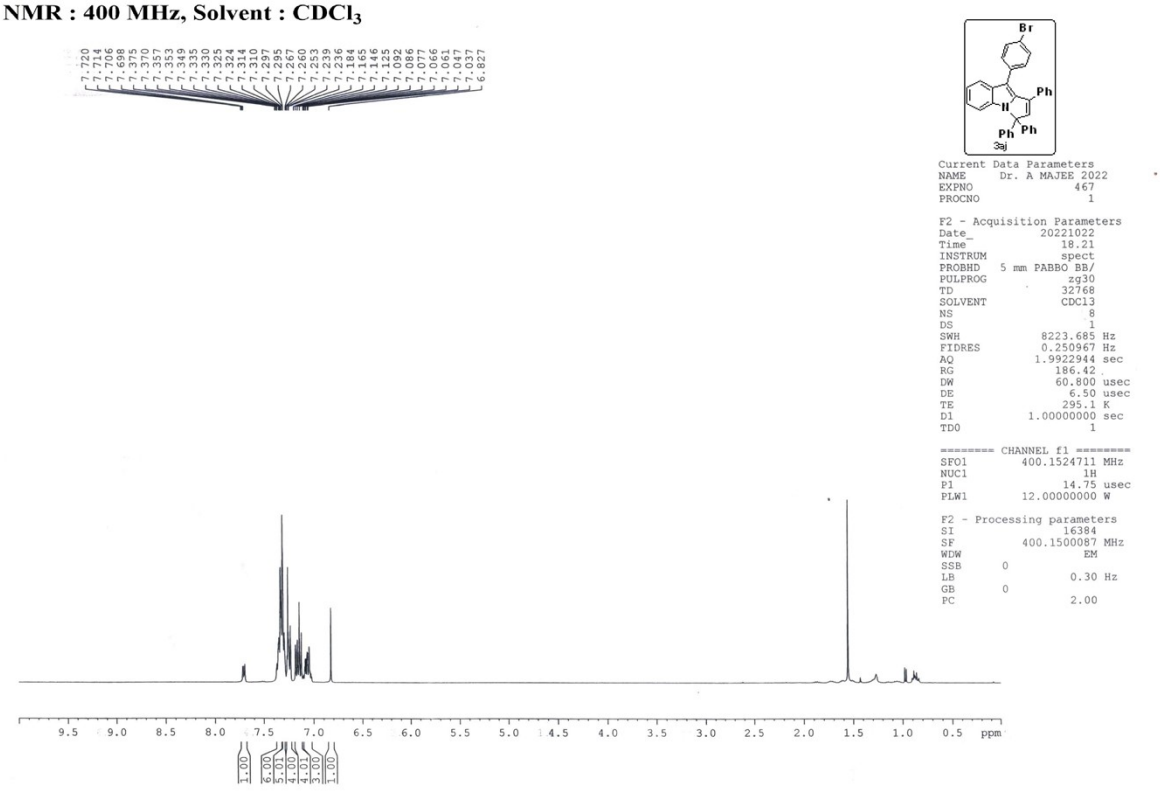
======== CHANNEL f1 ========
SFO1          400.1524711 MHz
NUC1                    1H
P1                   14.75 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                   16384
SF            400.1499952 MHz
WDW                     EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   2.00
```

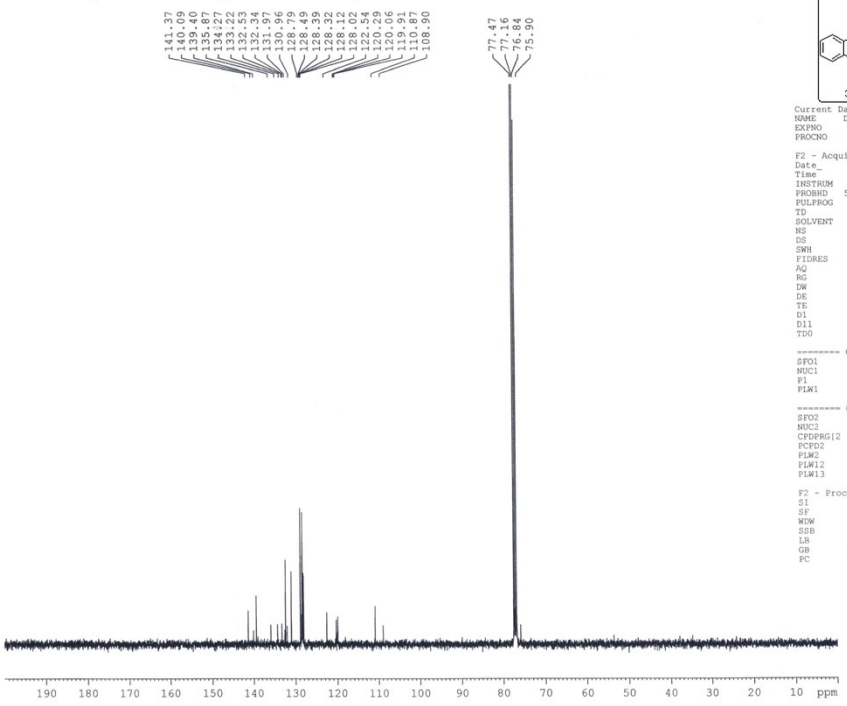


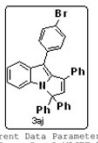


^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$






```
Current Data Parameters
NAME        Dr. A MAJEE 2022
EXPNO                   468
PROCNO                    1

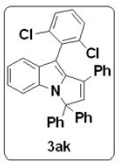
F2 - Acquisition Parameters
Date_               20221022
Time                   18.46
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     512
DS                       2
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                   186.42
DW                  20.800 usec
DE                   6.50 usec
TE                  295.6 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6278588 MHz
NUC1                     13C
P1                      8.90 usec
PLW1           54.00000000 W

======== CHANNEL f2 ========
SFO2           400.1516006 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2           12.00000000 W
PLW12           0.32231000 W
PLW13           0.16212000 W

F2 - Processing parameters
SI                       16384
SF             100.6177843 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.00
```

^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

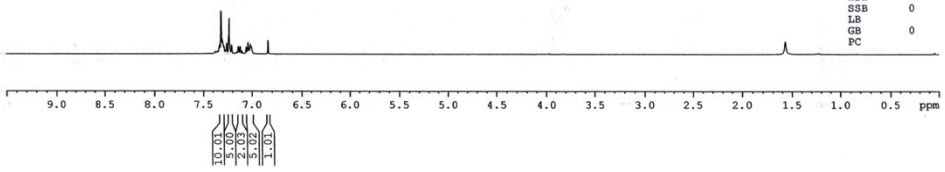



```
Current Data Parameters
NAME        Dr. A MAJEE 2025-1H
EXPNO                   358
PROCNO                    1

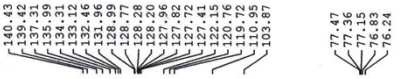
F2 - Acquisition Parameters
Date_               20251016
Time                   16.41
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                   32768
SOLVENT              CDCl3
NS                       8
DS                       1
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                1.9922944 sec
RG                   186.42
DW                  60.800 usec
DE                   6.50 usec
TE                  290.0 K
D1              1.00000000 sec
TD0                      1

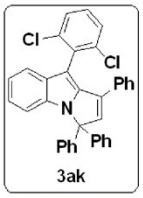
======== CHANNEL f1 ========
SFO1           400.1524711 MHz
NUC1                      1H
P1                    14.75 usec
PLW1           12.00000000 W

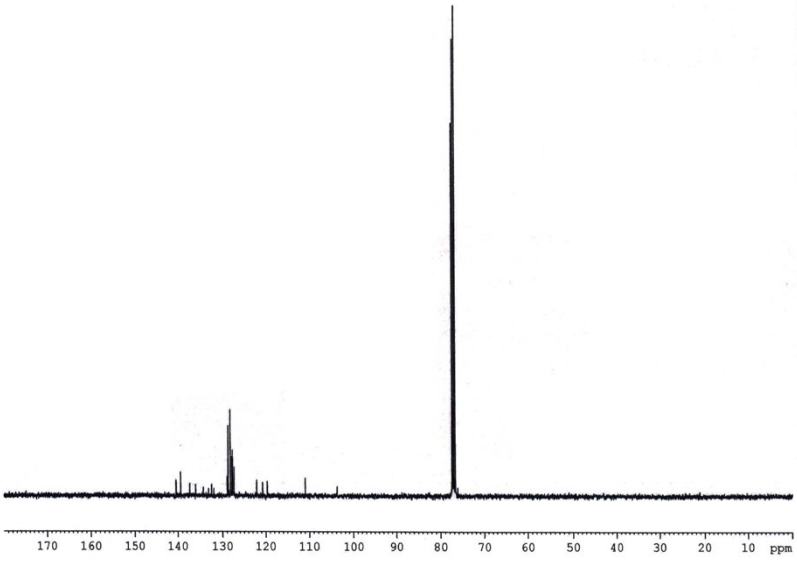
F2 - Processing parameters
SI                       16384
SF             400.1500202 MHz
WDW                         EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      2.00
```



$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$








```
Current Data Parameters
NAME      Dr. A MAJEE-2025-13C
EXPNO              247
PROCNO               1

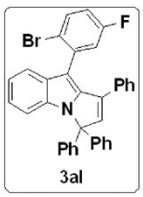
F2 - Acquisition Parameters
Date_          20251016
Time               17.17
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  720
DS                    2
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                186.42
DW              20.800 usec
DE               6.50 usec
TE              290.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

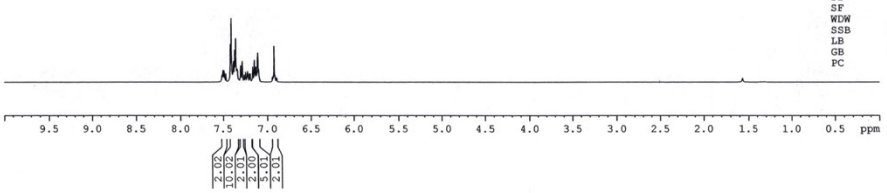
======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2               1H
CPDPRG[2          waltz16
PCPD2            90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF           100.6177873 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{1}H NMR : 400 MHz, Solvent : $CDCl_3$





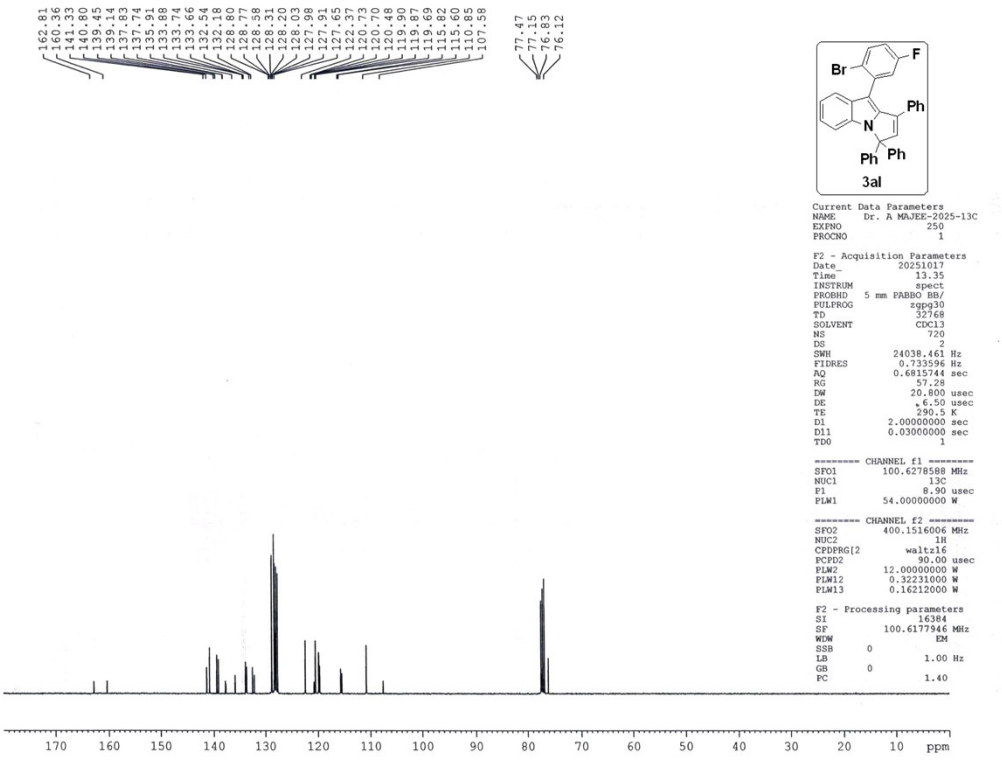

```
Current Data Parameters
NAME      Dr. A MAJEE 2025-1H
EXPNO              362
PROCNO               1

F2 - Acquisition Parameters
Date_          20251017
Time               12.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                57.28
DW              60.800 usec
DE               6.50 usec
TE              290.0 K
D1            1.00000000 sec
TD0                  1

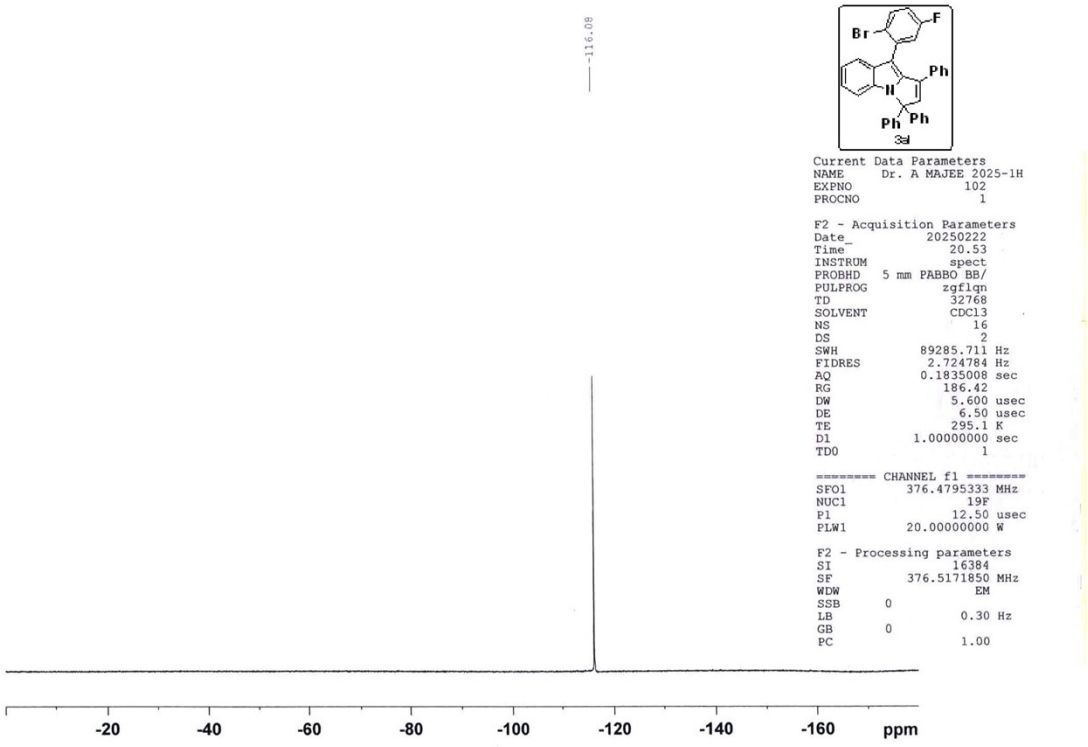
======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1               1H
P1               14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                16384
SF           400.1500097 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

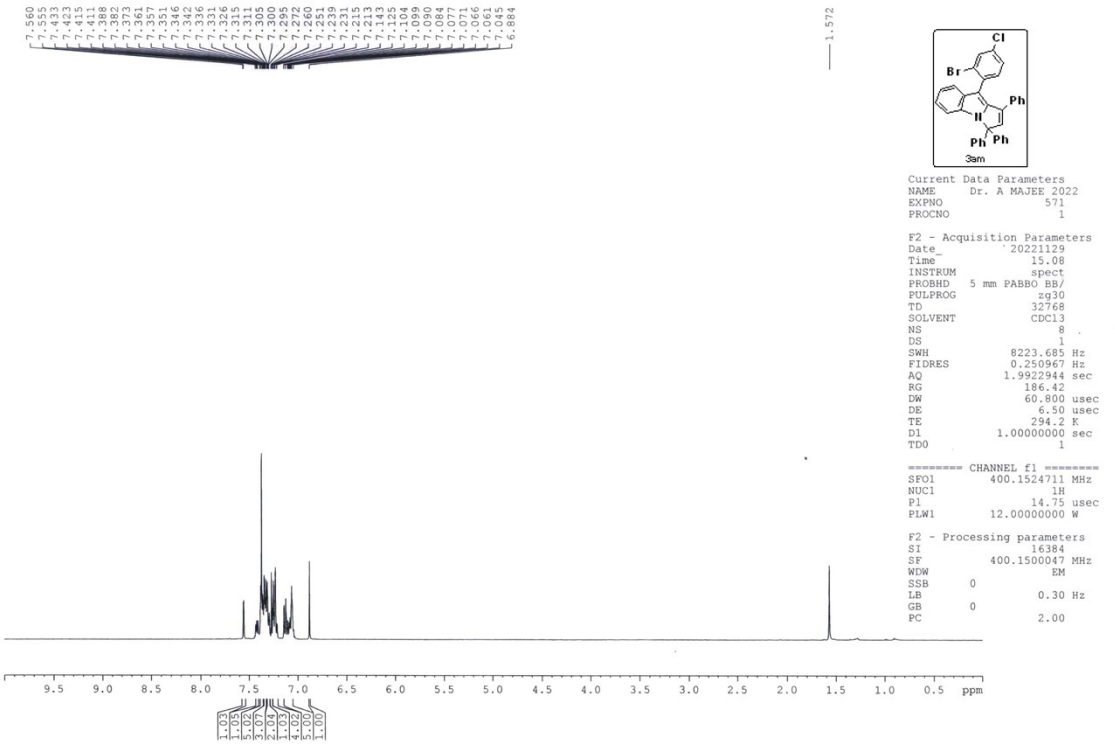
$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$



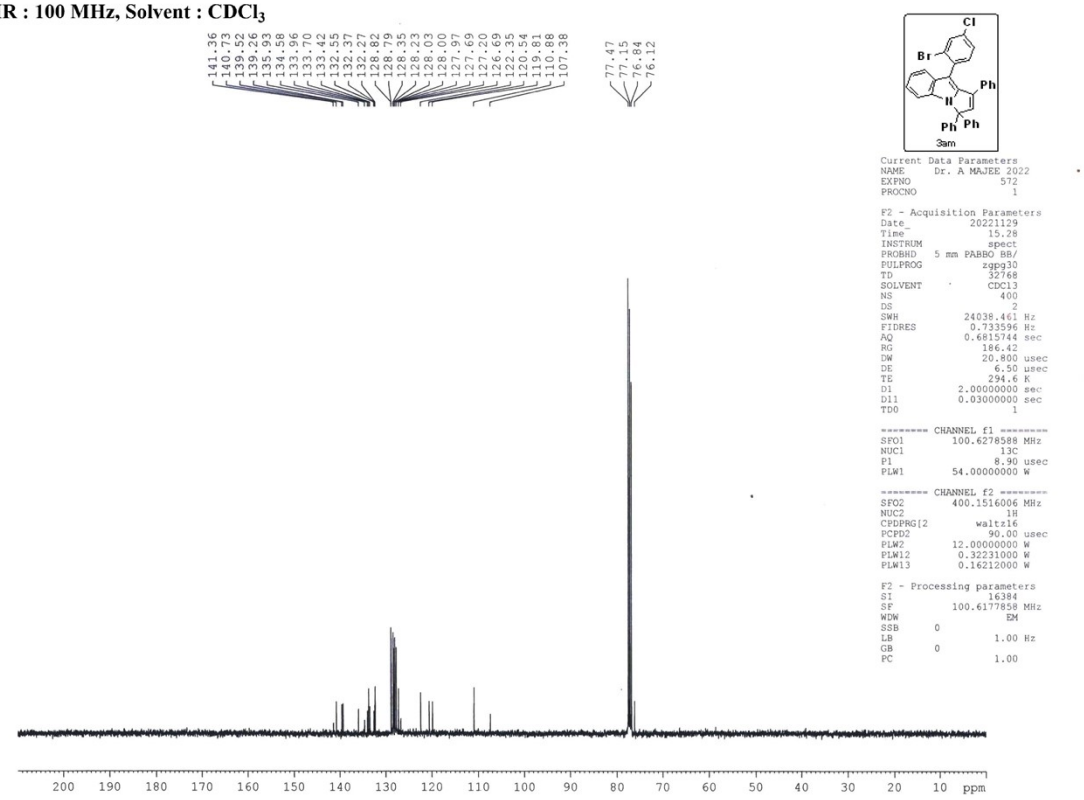
^{19}F NMR : 376 MHz, Solvent : $CDCl_3$



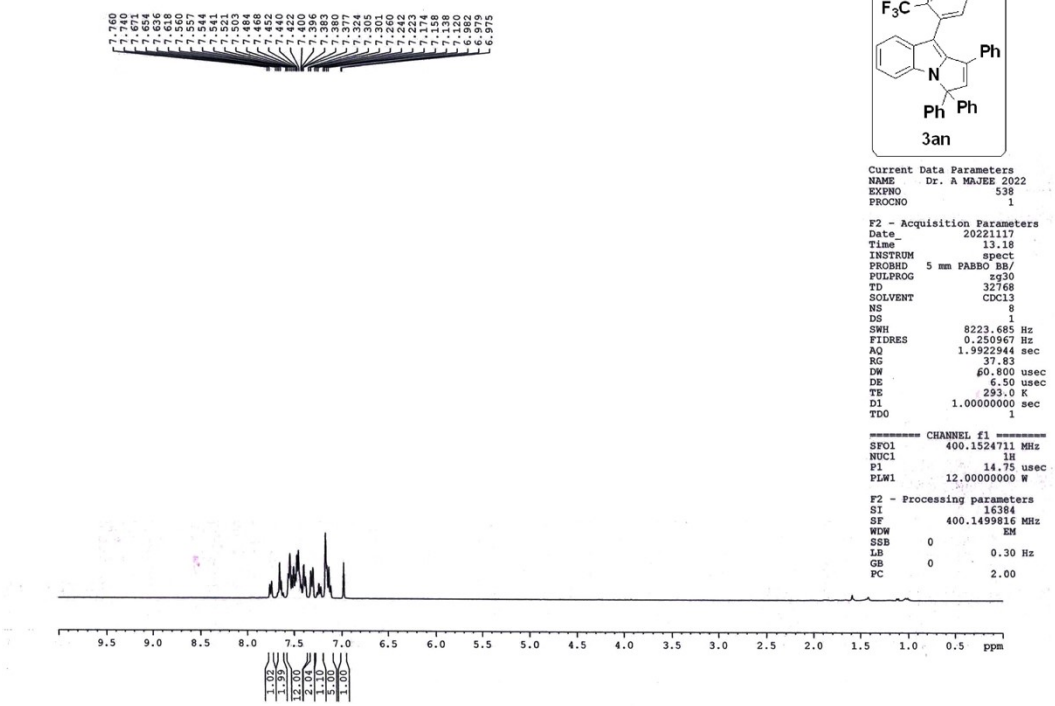
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



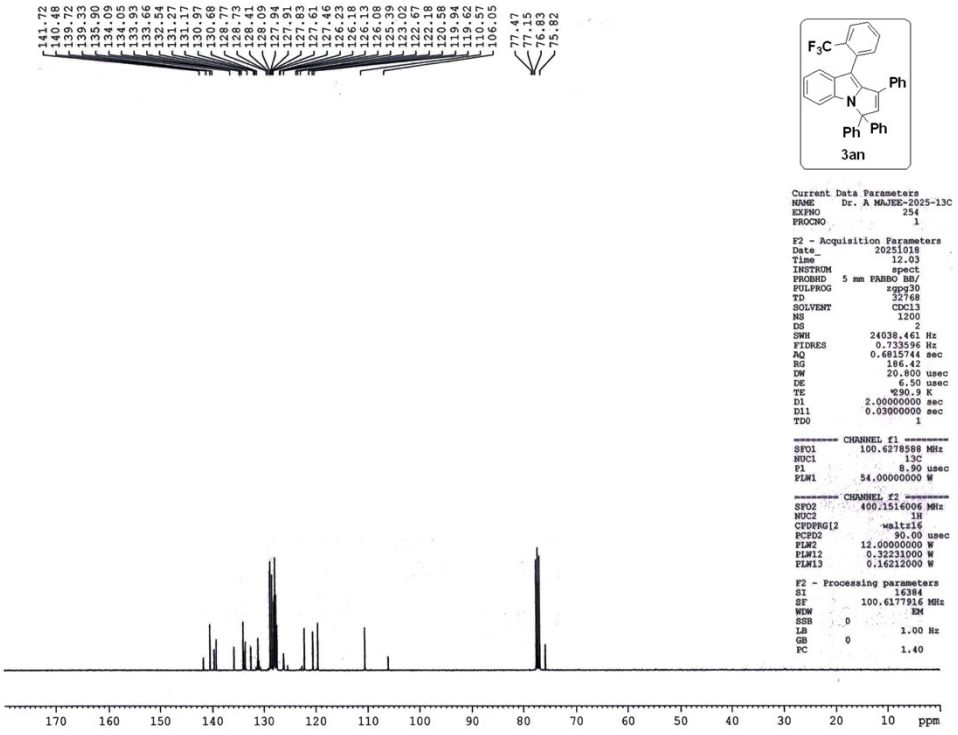
^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



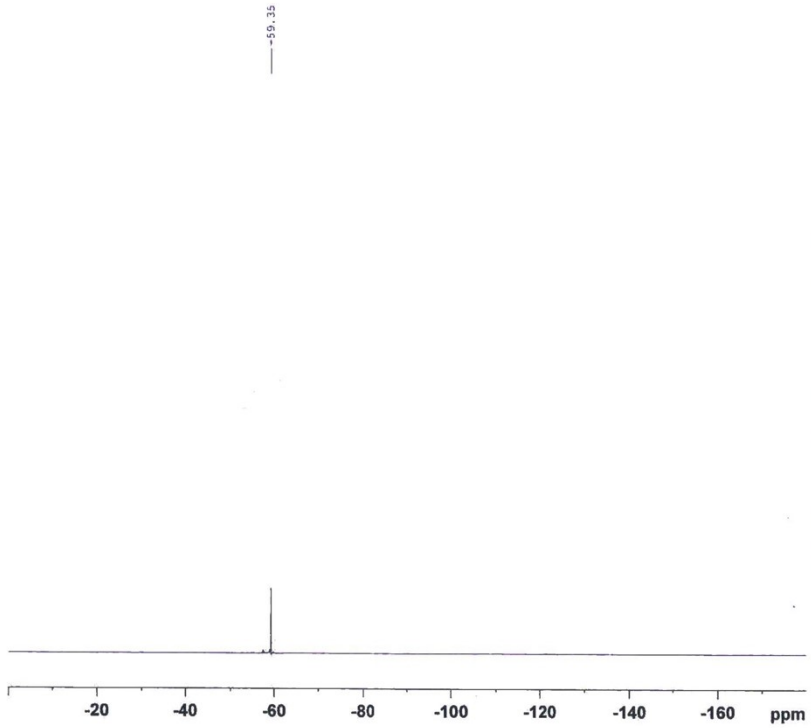
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

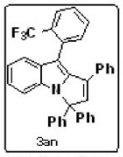


^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



^{19}F NMR : 376 MHz, Solvent : $CDCl_3$





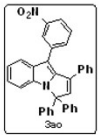

```
Current Data Parameters
NAME      Dr. A MAJEE 2024
EXPNO                489
PROCNO                 1

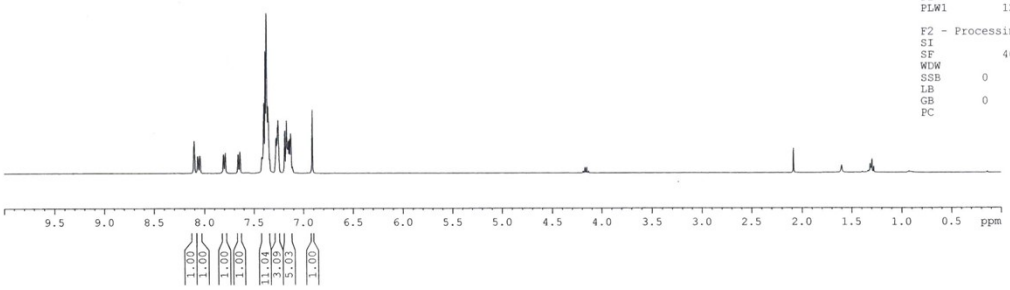
F2 - Acquisition Parameters
Date_           20241217
Time              18.01
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgflqn
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           89285.711 Hz
FIDRES         2.724784 Hz
AQ             0.1835008 sec
RG                186.42
DW                 5.600 usec
DE                 6.50 usec
TE                289.2 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        376.4795333 MHz
NUC1               19F
P1                12.50 usec
PLW1        20.00000000 W

F2 - Processing parameters
SI                16384
SF          376.5171850 MHz
WDW                EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H NMR : 400 MHz, Solvent : $CDCl_3$





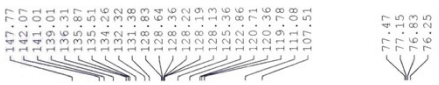

```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                581
PROCNO                 1

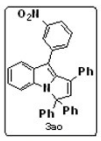
F2 - Acquisition Parameters
Date_           20221203
Time              22.29
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES         0.250967 Hz
AQ             1.9922944 sec
RG                 47.25
DW                60.800 usec
DE                 6.50 usec
TE                292.4 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1524711 MHz
NUC1               1H
P1                14.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                16384
SF          400.1500092 MHz
WDW                EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 2.00
```

$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$





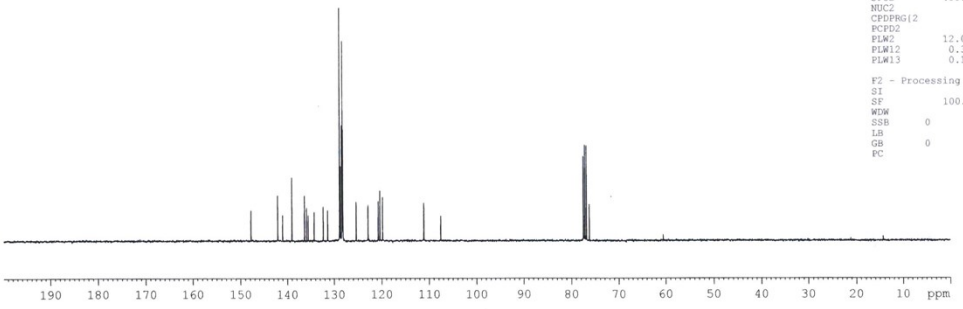
Current Data Parameters
NAME Dr. A MAJEE 2022
EXPNO 582
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221203
Time 22.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 180
DS 2
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 47.25
DW 20.800 usec
DE 6.50 usec
TE 292.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

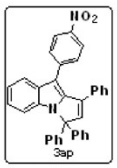
======== CHANNEL f1 ========
SFO1 100.6278588 MHz
NUC1 13C
P1 8.90 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.1516006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.32231000 W
PLW13 0.16212000 W

F2 - Processing parameters
SI 16384
SF 100.6177946 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

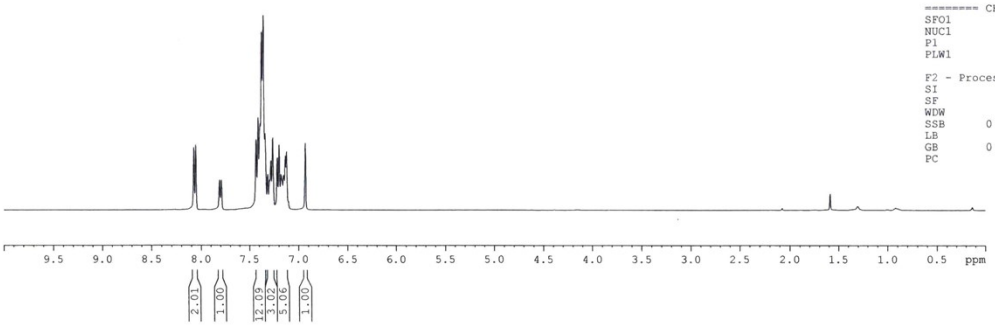


Current Data Parameters
NAME Dr. A MAJEE 2022
EXPNO 579
PROCNO 1

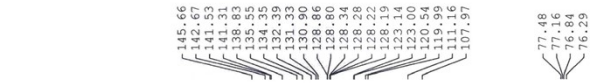
F2 - Acquisition Parameters
Date_ 20221203
Time 22.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 1
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9922944 sec
RG 47.25
DW 60.800 usec
DE 6.50 usec
TE 292.3 K
D1 1.00000000 sec
TD0 1

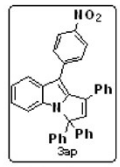
======== CHANNEL f1 ========
SFO1 400.1524711 MHz
NUC1 1H
P1 14.75 usec
PLW1 12.00000000 W

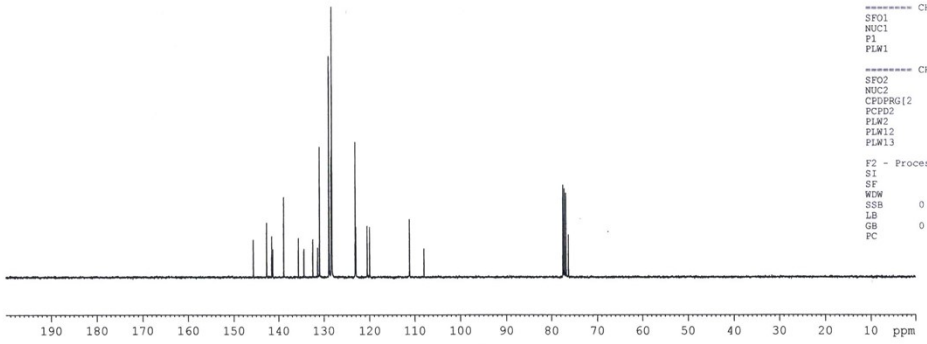
F2 - Processing parameters
SI 16384
SF 400.1500123 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$








```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO              580
PROCNO               1

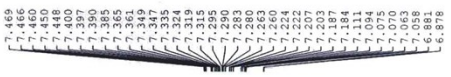
F2 - Acquisition Parameters
Date_          20221203
Time             22.22
INSTRUM          spect
PROBHD  5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                 256
DS                   2
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                47.25
DW               20.800 usec
DE                6.50 usec
TE              292.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

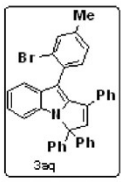
======== CHANNEL f1 ========
SFO1        100.6278588 MHz
NUC1              13C
P1                8.90 usec
PLW1         54.00000000 W

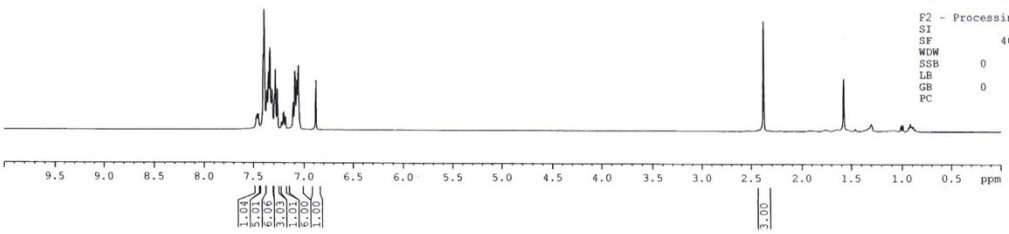
======== CHANNEL f2 ========
SFO2        400.1516006 MHz
NUC2              1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF          100.6177946 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```

^{1}H NMR : 400 MHz, Solvent : $CDCl_3$







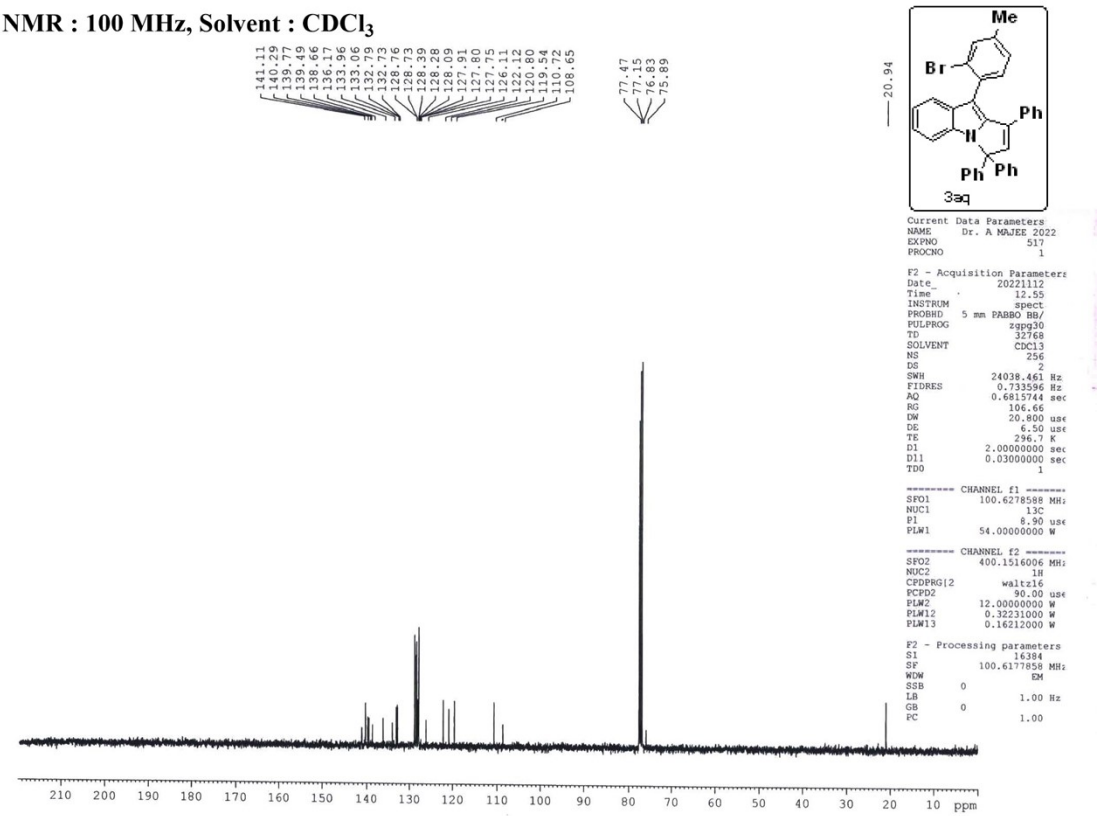

```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO              516
PROCNO               1

F2 - Acquisition Parameters
Date_          20221112
Time             12.42
INSTRUM          spect
PROBHD  5 mm PABBO BB/
PULPROG           zg30
TD              32768
SOLVENT          CDCl3
NS                  16
DS                   1
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                106.66
DW               60.800 usec
DE                6.50 usec
TE              296.3 K
D1           1.00000000 sec
TD0                  1

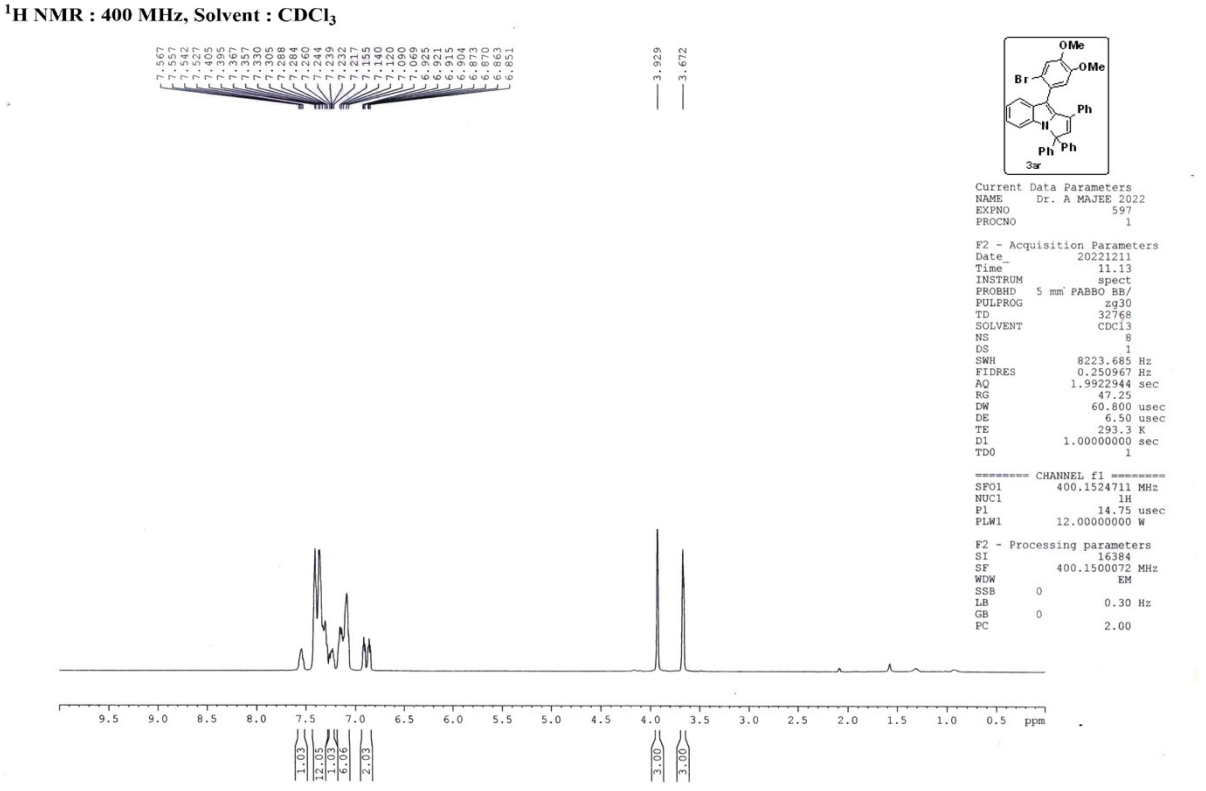
======== CHANNEL f1 ========
SFO1        400.1527111 MHz
NUC1              1H
P1               14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                16384
SF          400.1499992 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                2.00
```

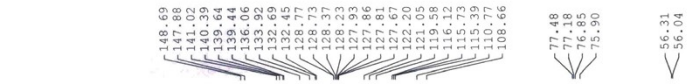
$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$

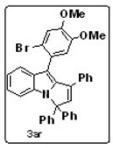


^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$





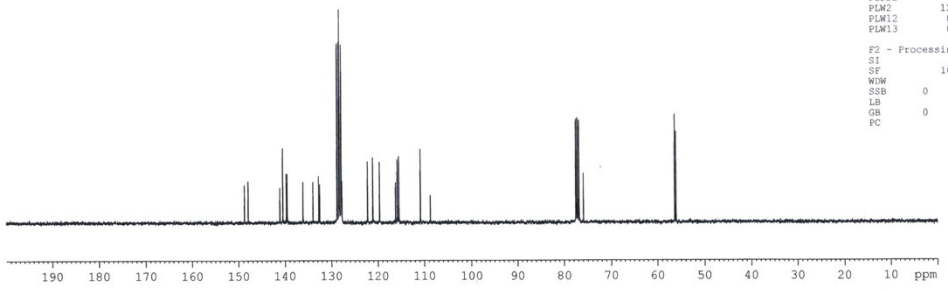

```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                  598
PROCNO                   1

F2 - Acquisition Parameters
Date_            20221211
Time                11.34
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  400
DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                47.25
DW               20.800 usec
DE                6.50 usec
TE               293.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

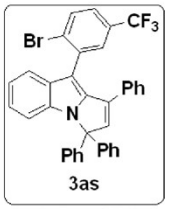
======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1                  13C
P1                 8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                 16384
SF           100.6177932 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.00
```



^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

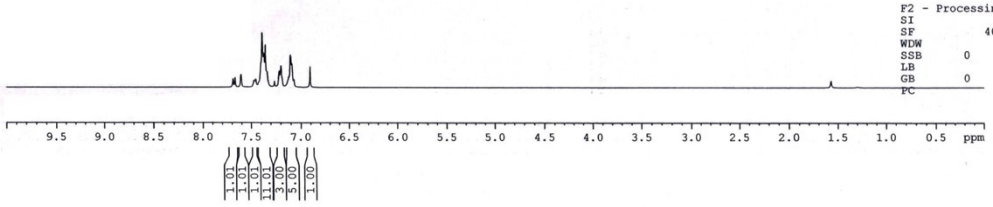



```
Current Data Parameters
NAME      Dr. A MAJEE 2025-1H
EXPNO                  360
PROCNO                   1

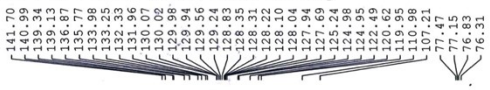
F2 - Acquisition Parameters
Date_            20251017
Time                12.13
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES         0.250967 Hz
AQ             1.9922944 sec
RG                *67.81
DW               60.800 usec
DE                6.50 usec
TE               290.2 K
D1            1.00000000 sec
TD0                   1

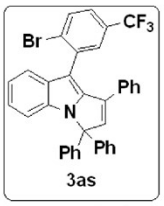
======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1                  1H
P1                14.75 usec
PLW1         12.00000000 W

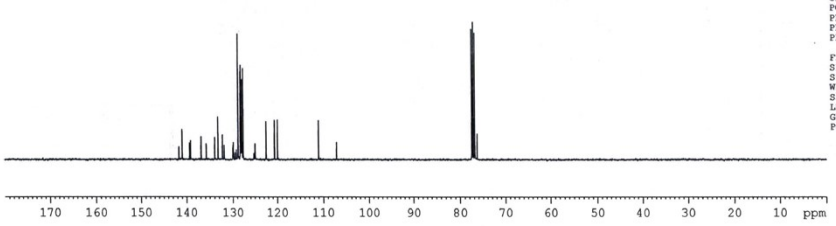
F2 - Processing parameters
SI                 16384
SF           400.1500092 MHz
WDW                   EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 2.00
```



$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$








```
Current Data Parameters
NAME        Dr. A MAJEE-2025-13C
EXPNO                        249
PROCNO                         1

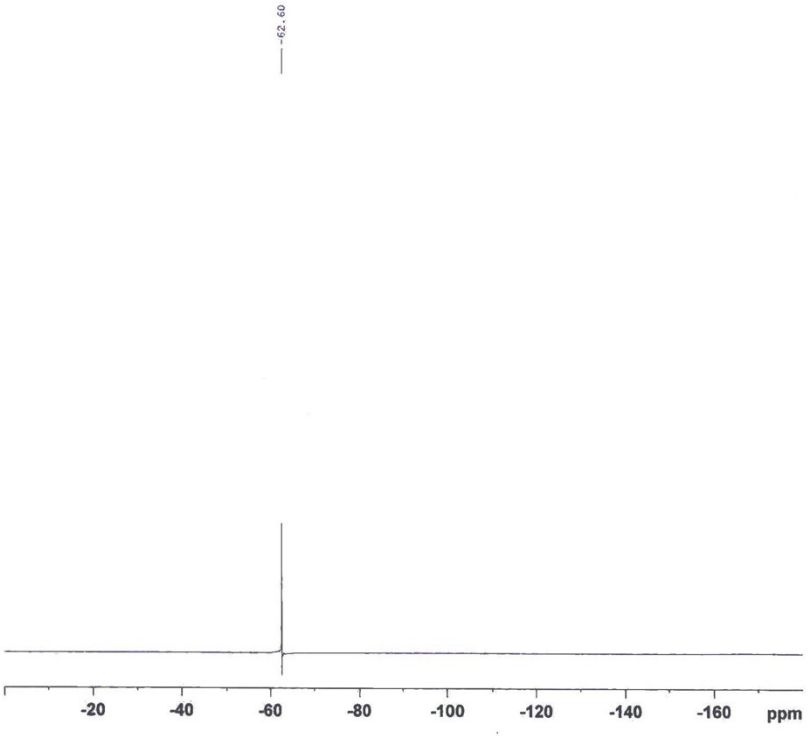
F2 - Acquisition Parameters
Date_                   20251017
Time                       12.46
INSTRUM                    spect
PROBHD   5 mm PABBO BB/
PULPROG                 zgpg30
TD                         32768
SOLVENT                    CDCl3
NS                           600
DS                             2
SWH                  24038.461 Hz
FIDRES                0.733596 Hz
AQ                    0.6815744 sec
RG                         62.69
DW                        20.800 usec
DE                         6.50 usec
TE                        290.6 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                            1

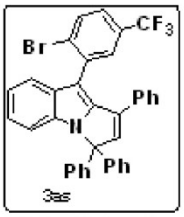
======== CHANNEL f1 ========
SFO1                100.6278588 MHz
NUC1                        13C
P1                        8.90 usec
PLW1                54.00000000 W

======== CHANNEL f2 ========
SFO2                400.1516006 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                12.00000000 W
PLW12                0.32231000 W
PLW13                0.16212000 W

F2 - Processing parameters
SI                         16384
SF                  100.6177902 MHz
WDW                           EM
SSB          0
LB                         1.00 Hz
GB           0
PC                         1.40
```

^{19}F NMR : 376 MHz, Solvent : $CDCl_3$





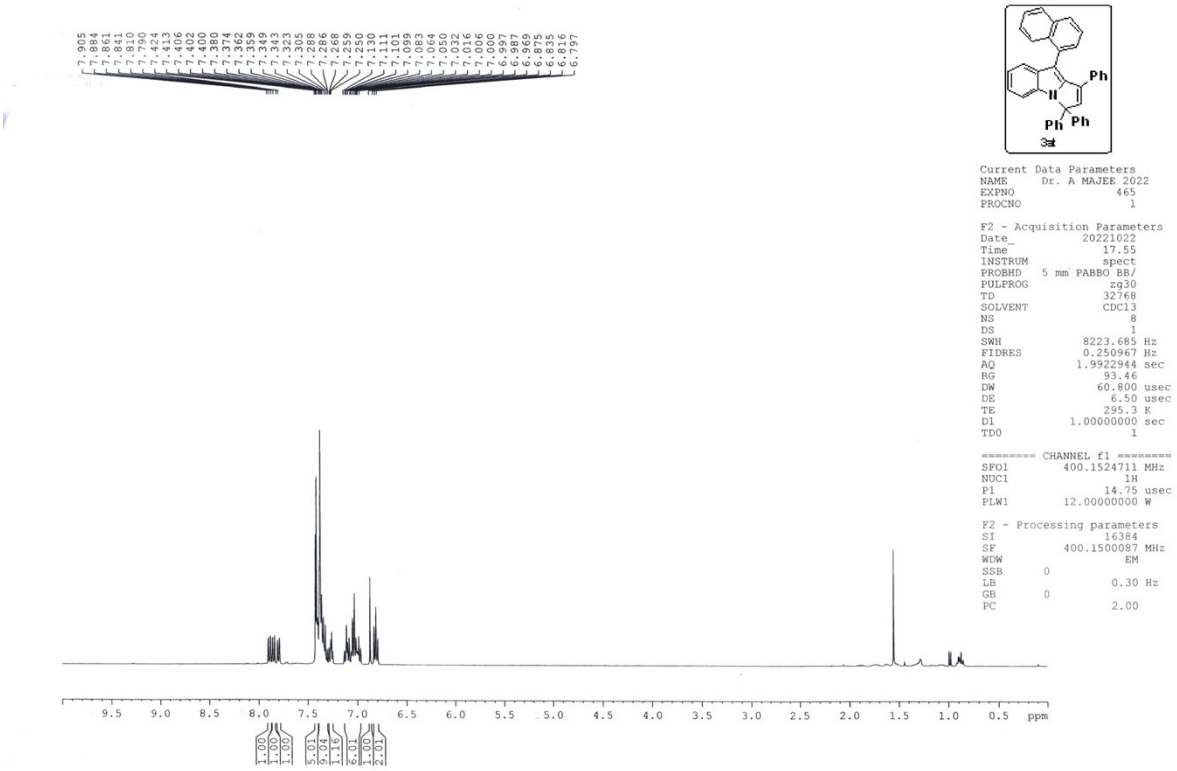

```
Current Data Parameters
NAME        Dr. A MAJEE 2024
EXPNO                        491
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20241217
Time                       18.13
INSTRUM                    spect
PROBHD   5 mm PABBO BB/
PULPROG                 zgflqn
TD                         32768
SOLVENT                    CDCl3
NS                            16
DS                             2
SWH                  89285.711 Hz
FIDRES                2.724784 Hz
AQ                    0.1835008 sec
RG                        186.42
DW                        5.600 usec
DE                         6.50 usec
TE                        289.1 K
D1                    1.00000000 sec
TD0                            1

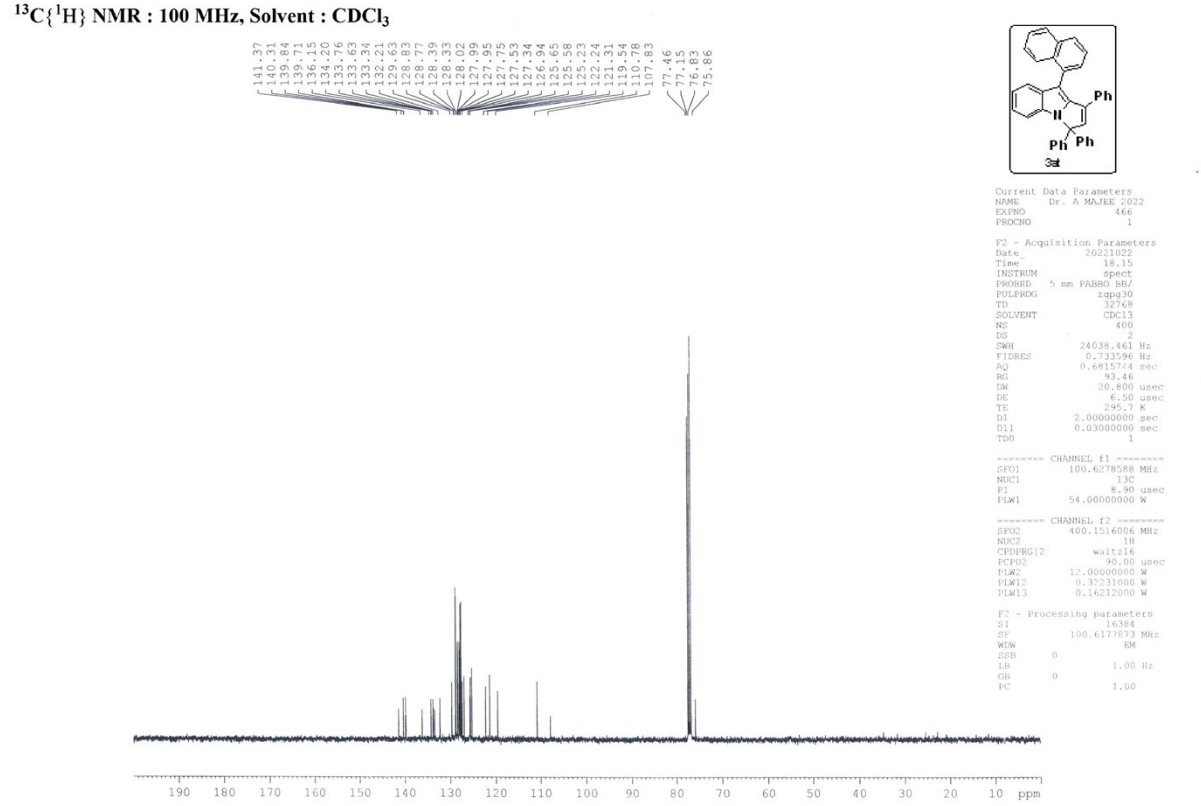
======== CHANNEL f1 ========
SFO1                376.4795333 MHz
NUC1                        19F
P1                       12.50 usec
PLW1                20.00000000 W

F2 - Processing parameters
SI                         16384
SF                  376.5171850 MHz
WDW                           EM
SSB          0
LB                         0.30 Hz
GB           0
PC                         1.00
```

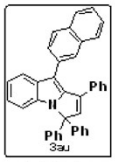
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

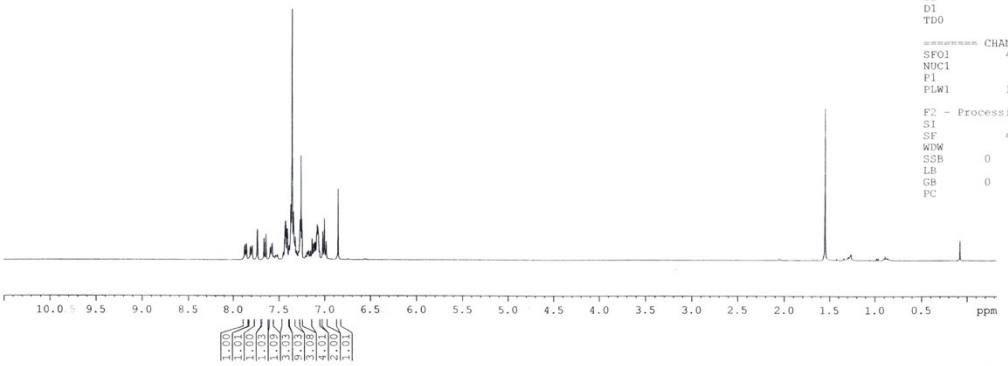



```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                 490
PROCNO                  1

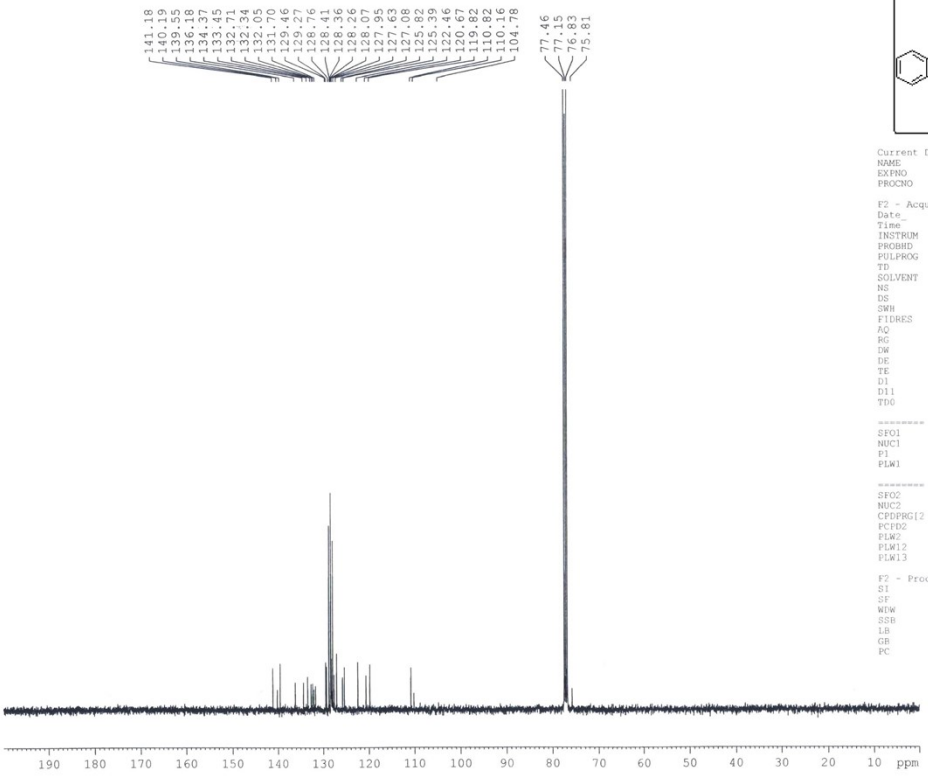
F2 - Acquisition Parameters
Date_           20221030
Time              13.03
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES         0.250967 Hz
AQ             1.9922944 sec
RG               168.31
DW               60.800 usec
DE                6.50 usec
TE               295.9 K
D1             1.00000000 sec
TD0                   1

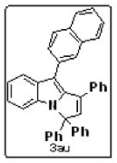
======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1               1H
P1               14.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                16384
SF           400.1500087 MHz
WDW                EM
SSB       0
LB               0.30 Hz
GB        0
PC               2.00
```



^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$






```
Current Data Parameters
NAME      Dr. A MAJEE 2022
EXPNO                 491
PROCNO                  1

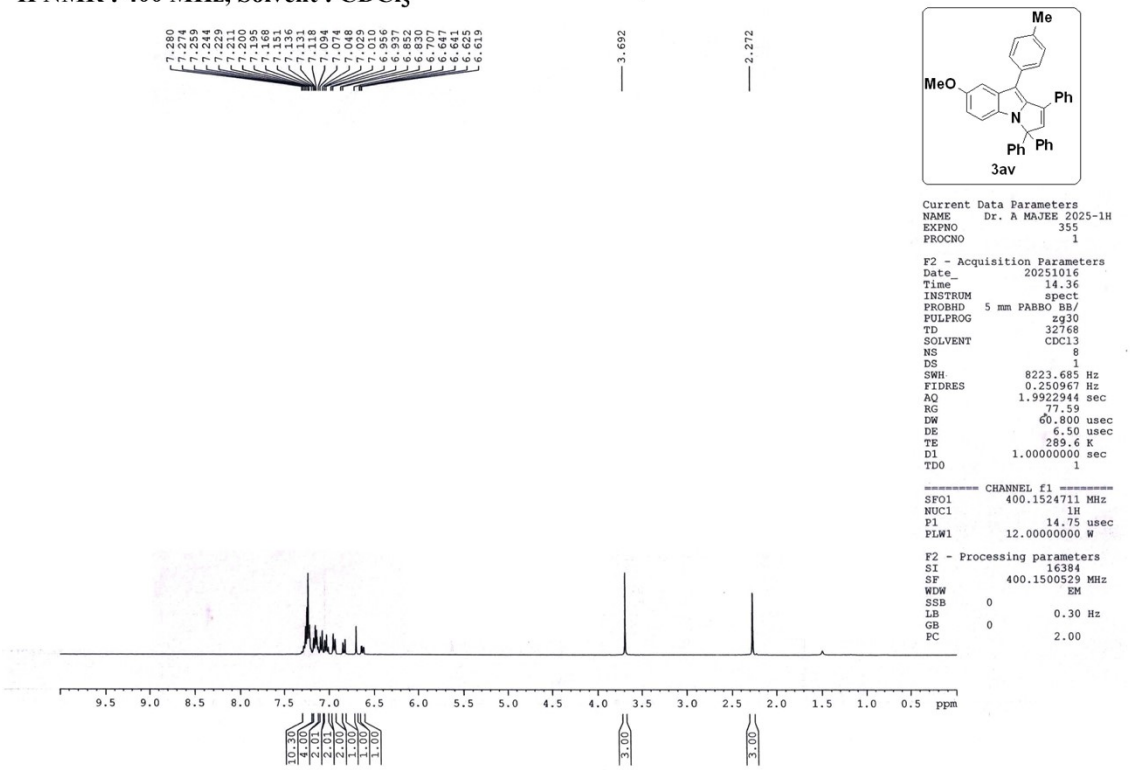
F2 - Acquisition Parameters
Date_           20221030
Time              13.36
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT           CDCl3
NS                  680
DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG               168.31
DW               20.800 usec
DE                6.50 usec
TE               295.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1               13C
P1                8.90 usec
PLW1         54.00000000 W

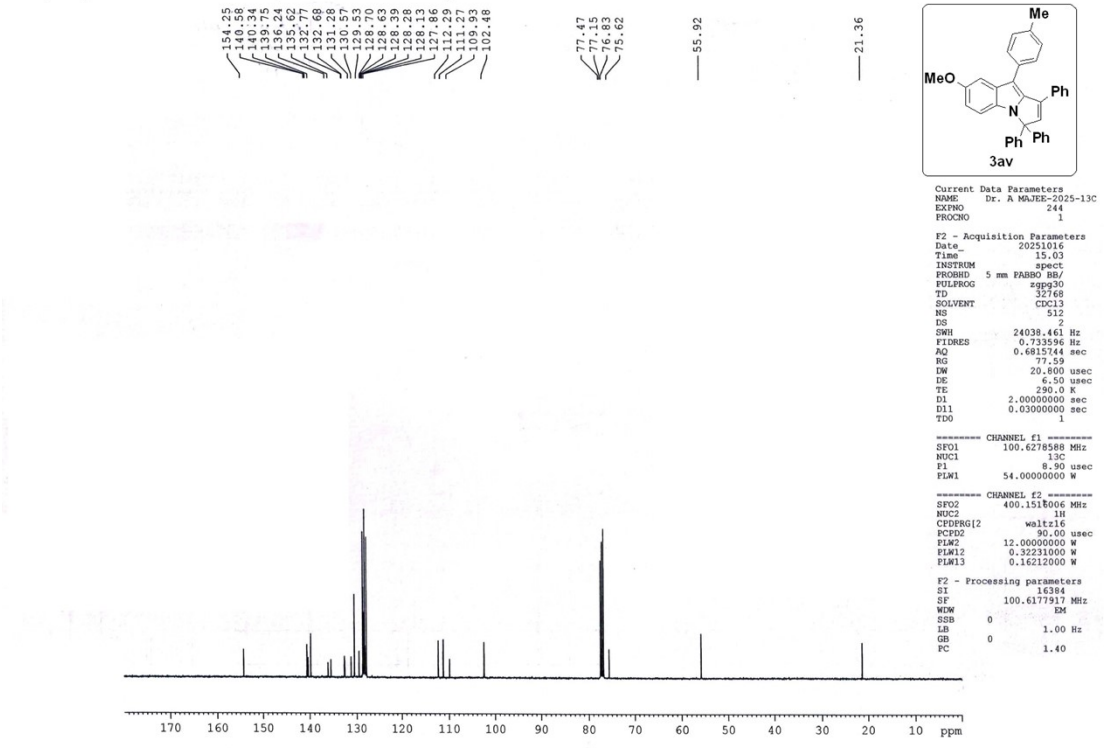
======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.32231000 W
PLW13         0.16212000 W

F2 - Processing parameters
SI                16384
SF           100.6177858 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.00
```

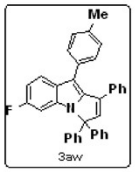
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$



^{1}H NMR : 400 MHz, Solvent : $CDCl_3$

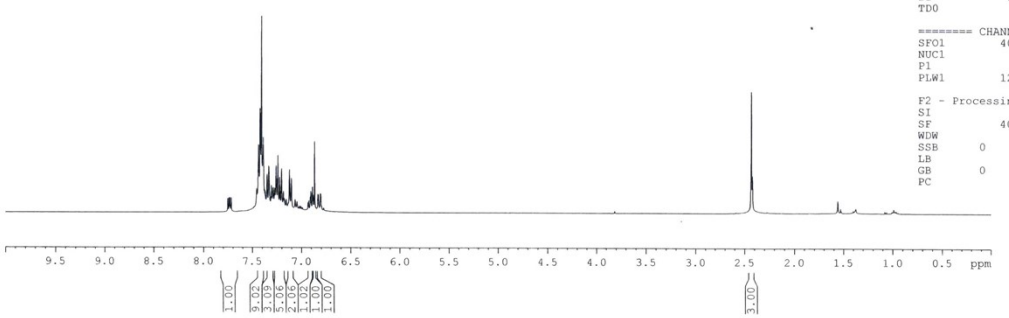



```
Current Data Parameters
NAME       Dr. A MAJEE 2023
EXPNO                 474
PROCNO                  1

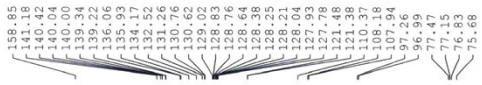
F2 - Acquisition Parameters
Date_          20230708
Time               20.50
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES         0.250967 Hz
AQ             1.9922944 sec
RG                32.25
DW               60.800 usec
DE                6.50 usec
TE                297.7 K
D1             1.00000000 sec
TD0                   1

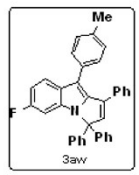
======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1                   1H
P1                 14.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                 16384
SF           400.1500036 MHz
WDW                   EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 2.00
```



^{13}C{^{1}H} NMR : 100 MHz, Solvent : $CDCl_3$





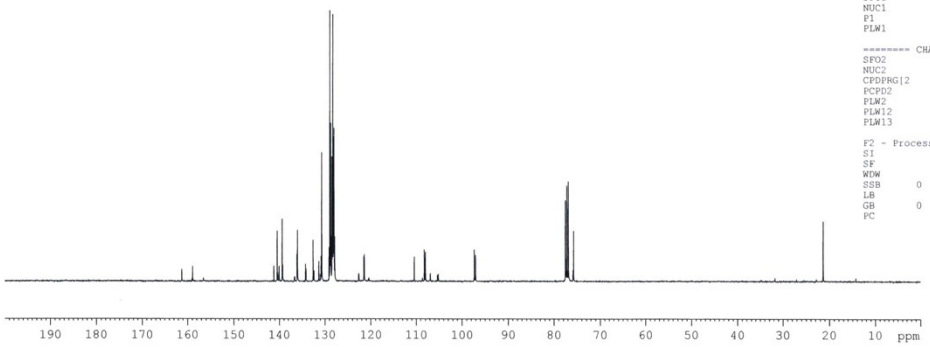

```
Current Data Parameters
NAME       Dr. A MAJEE 2023
EXPNO                 476
PROCNO                  1

F2 - Acquisition Parameters
Date_          20230708
Time               21.31
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  800
DS                    2
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             0.6815744 sec
RG                32.25
DW               20.800 usec
DE                6.50 usec
TE                298.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                   1

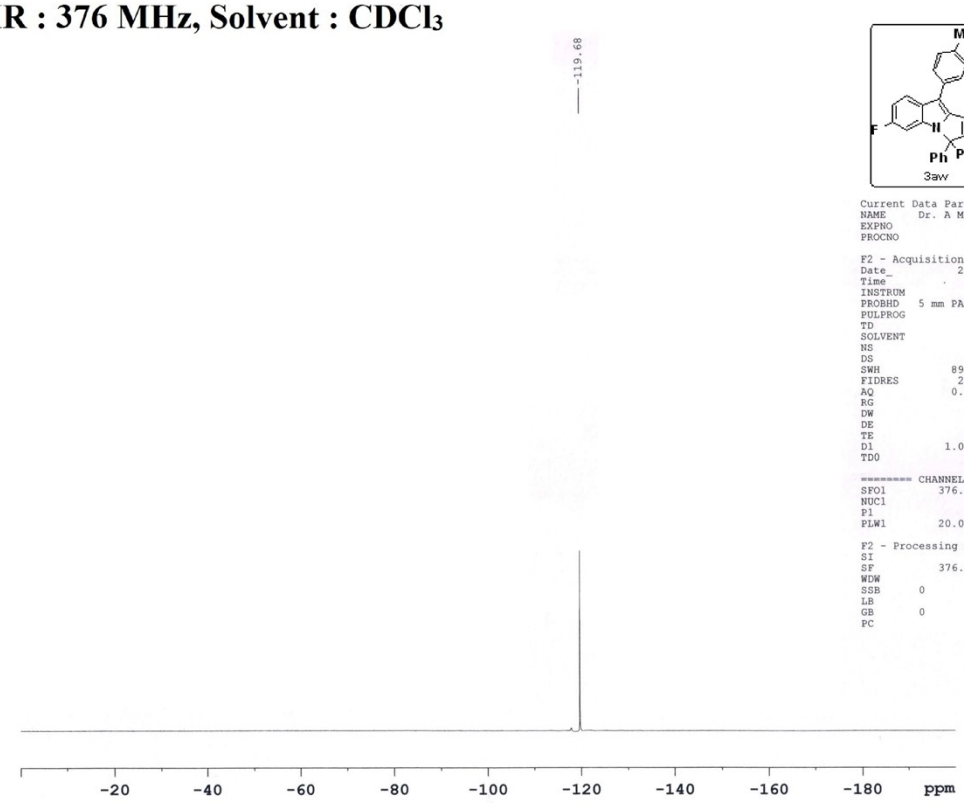
======== CHANNEL f1 ========
SFO1         100.6278588 MHz
NUC1                  13C
P1                 8.90 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2         400.1516006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2        12.00000000 W
PLW12        0.32231000 W
PLW13        0.16212000 W

F2 - Processing parameters
SI                 16384
SF           100.6177961 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.00
```



^{19}F NMR : 376 MHz, Solvent : $CDCl_3$



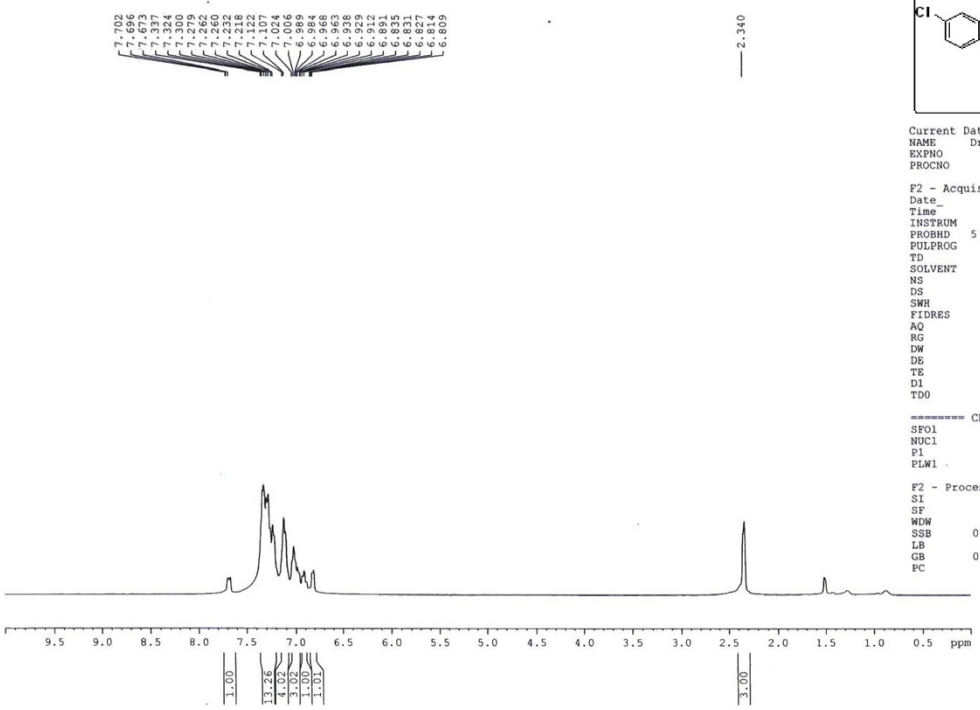

```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO                 475
PROCNO                  1

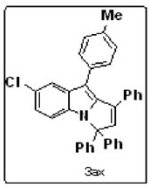
F2 - Acquisition Parameters
Date_           20230708
Time              20.52
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgflqn
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           89285.711 Hz
FIDRES        2.724784 Hz
AQ            0.1835008 sec
RG                32.25
DW               5.600 usec
DE               6.50 usec
TE               297.6 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         376.4795333 MHz
NUC1                 19F
P1                12.50 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                16384
SF          376.5171850 MHz
WDW                  EM
SSB       0
LB               0.30 Hz
GB        0
PC               1.00
```

^{1}H NMR : 400 MHz, Solvent : $CDCl_3$





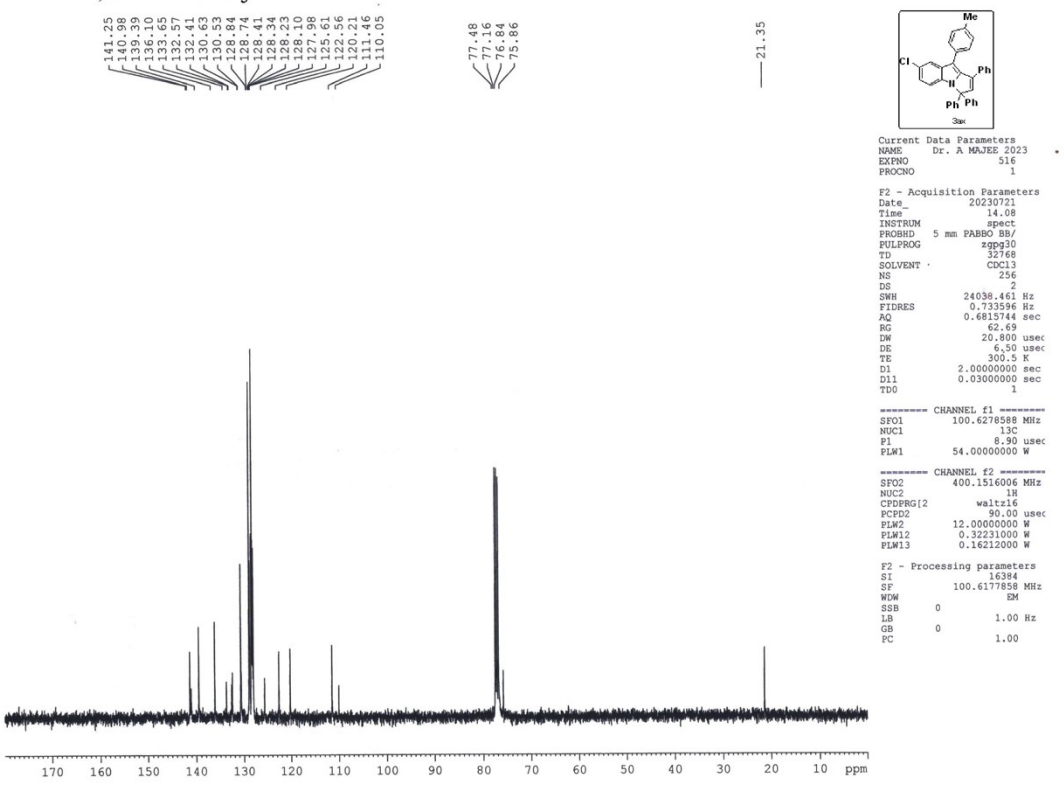

```
Current Data Parameters
NAME      Dr. A MAJEE 2023
EXPNO                 515
PROCNO                  1

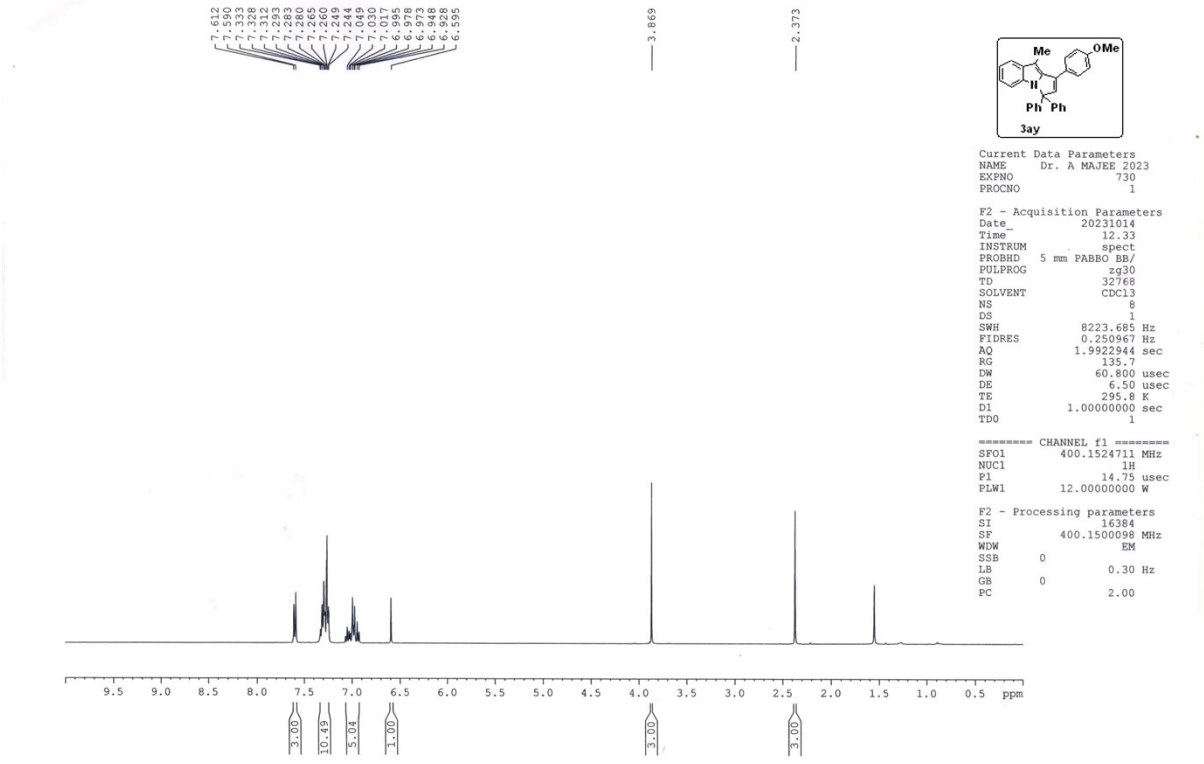
F2 - Acquisition Parameters
Date_           20230721
Time              13.47
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                32768
SOLVENT           CDCl3
NS                    8
DS                    1
SWH            8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9922944 sec
RG                62.69
DW               60.800 usec
DE               6.50 usec
TE               299.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1524711 MHz
NUC1                  1H
P1               14.75 usec
PLW1         12.00000000 W

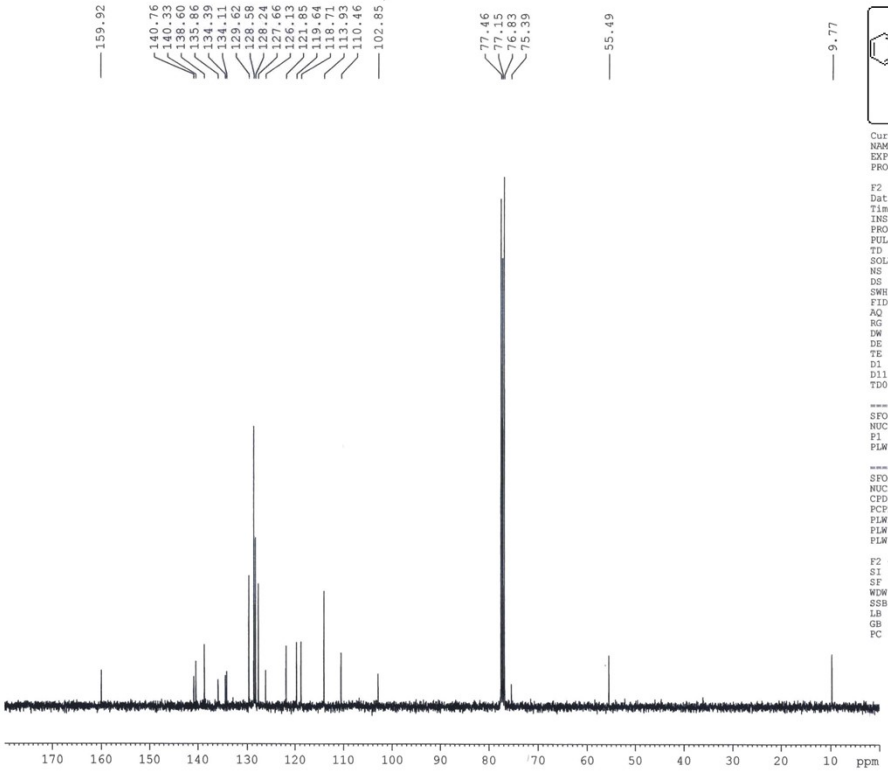
F2 - Processing parameters
SI                16384
SF          400.1500218 MHz
WDW                  EM
SSB       0
LB               0.30 Hz
GB        0
PC               2.00
```

$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$





$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$




```
Current Data Parameters
NAME        Dr. A MAJEE 2023
EXPNO                   731
PROCNO                    1

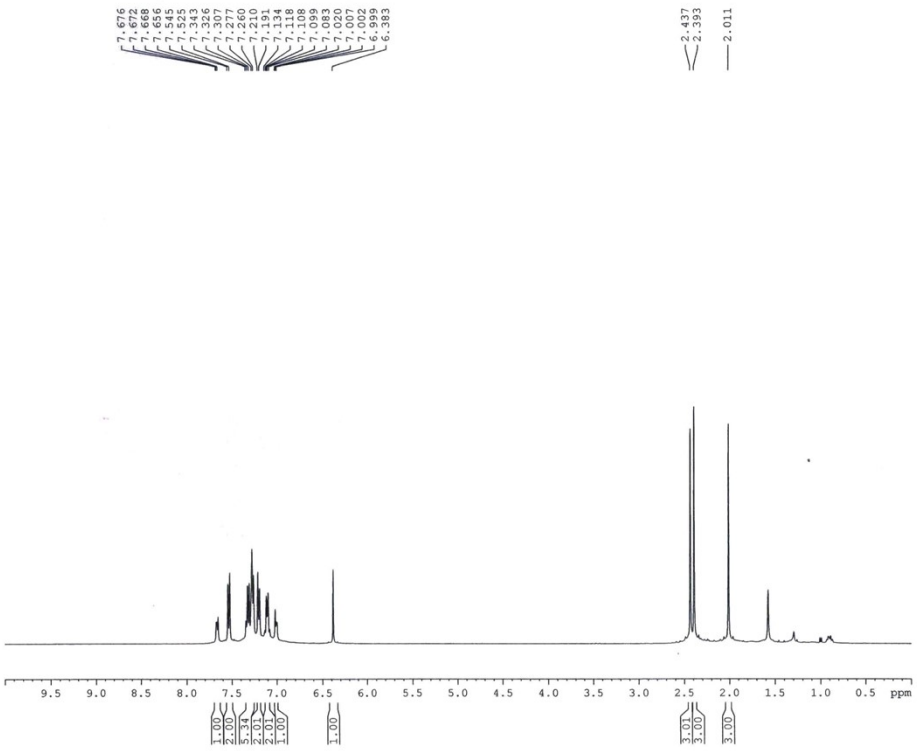
F2 - Acquisition Parameters
Date_               20231014
Time                   12.58
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG             zgpg30
TD                     32768
SOLVENT                CDCl3
NS                       400
DS                         2
SWH                24038.461 Hz
FIDRES              0.733596 Hz
AQ                  0.6815744 sec
RG                     186.42
DW                   20.800 usec
DE                    6.50 usec
TE                    296.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             100.6278588 MHz
NUC1                      13C
P1                       8.90 usec
PLW1            54.00000000 W

======== CHANNEL f2 ========
SFO2             400.1516006 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2            12.00000000 W
PLW12            0.32231000 W
PLW13            0.16212000 W

F2 - Processing parameters
SI                       16384
SF               100.6177857 MHz
WDW                         EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.00
```

^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



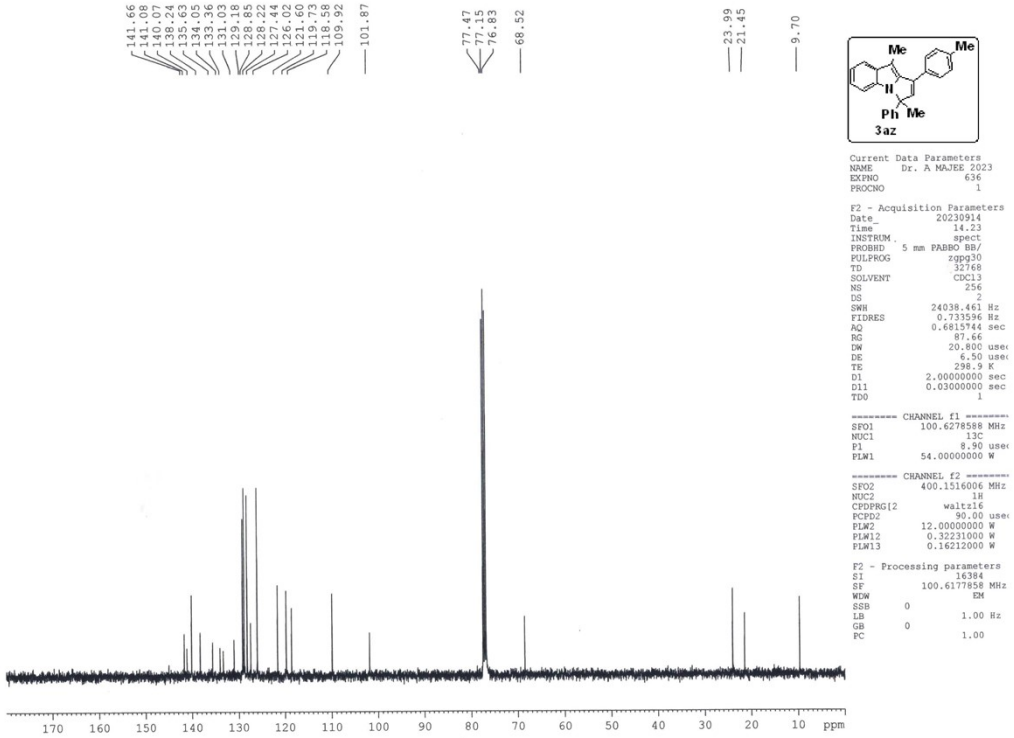

```
Current Data Parameters
NAME        Dr. A MAJEE 2023
EXPNO                   635
PROCNO                    1

F2 - Acquisition Parameters
Date_               20230914
Time                   14.09
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG                zg30
TD                     32768
SOLVENT                CDCl3
NS                         8
DS                         1
SWH                 8223.685 Hz
FIDRES              0.250967 Hz
AQ                  1.9922944 sec
RG                     87.66
DW                   60.800 usec
DE                    6.50 usec
TE                    298.4 K
D1                 1.00000000 sec
TD0                        1

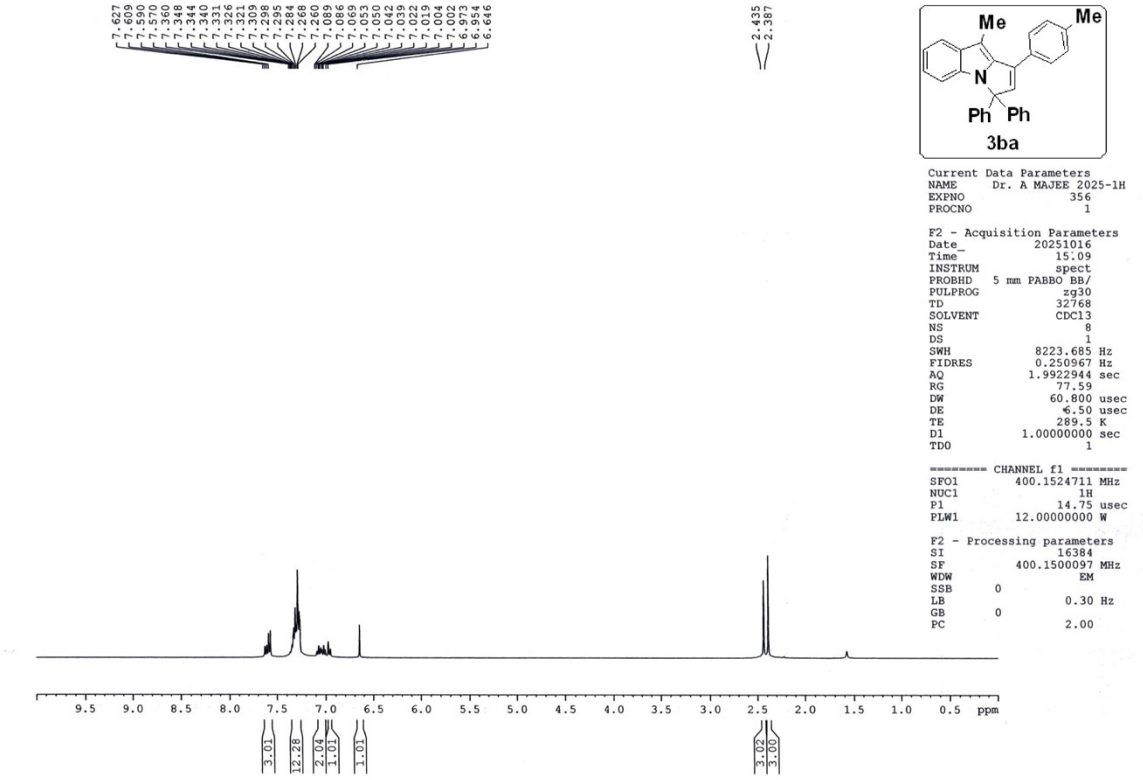
======== CHANNEL f1 ========
SFO1             400.1524711 MHz
NUC1                      1H
P1                   14.75 usec
PLW1            12.00000000 W

F2 - Processing parameters
SI                       16384
SF               400.1500037 MHz
WDW                         EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    2.00
```

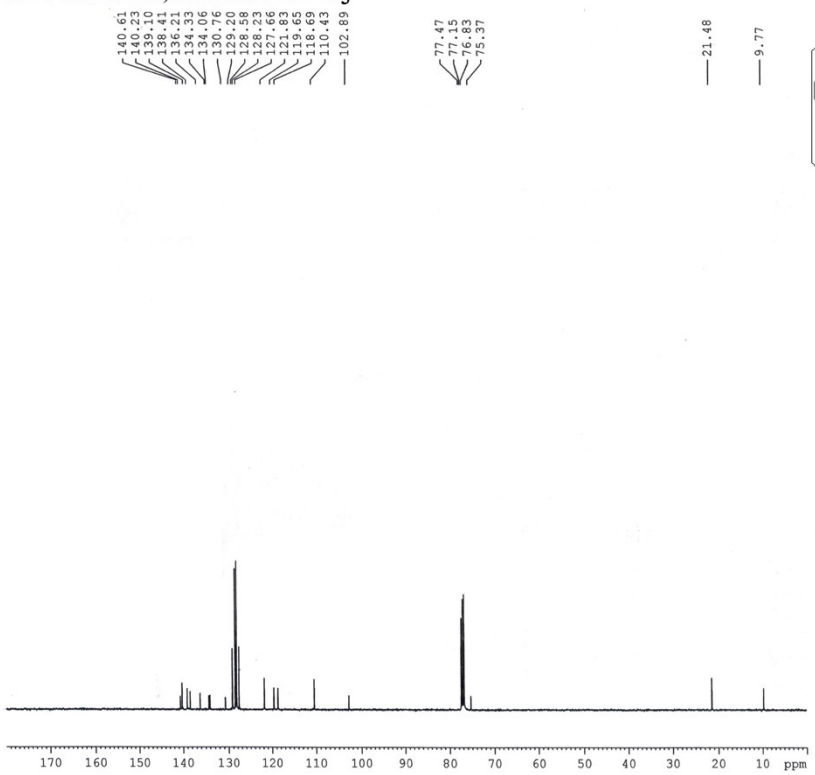
$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$



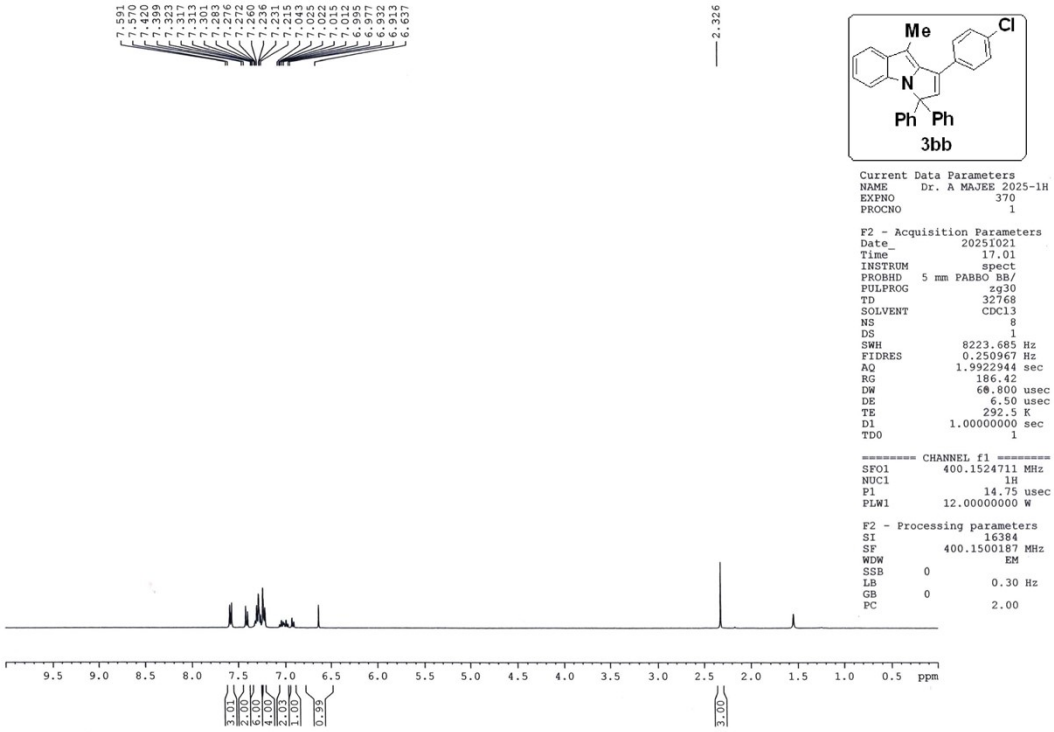
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



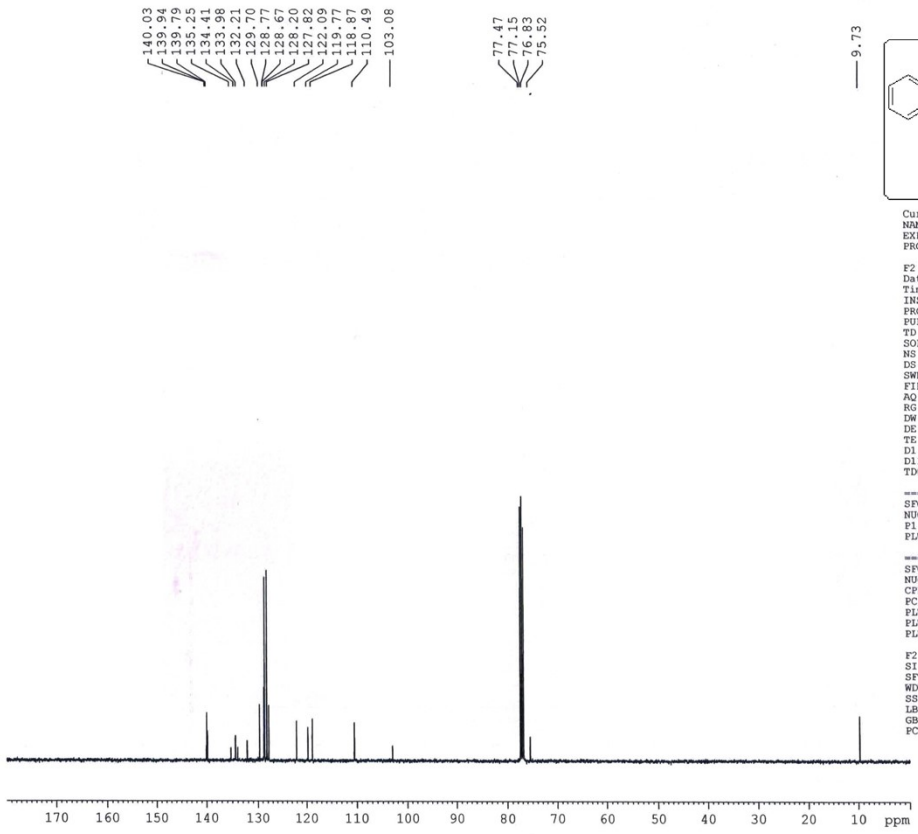
$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$



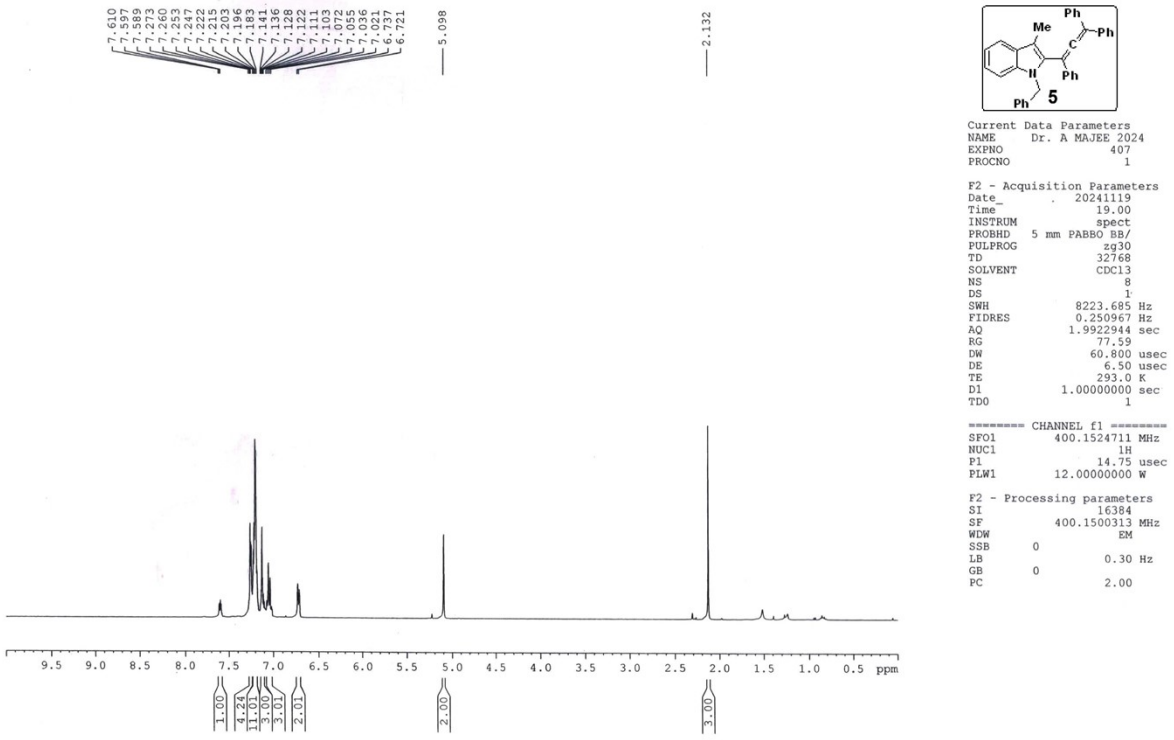
^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



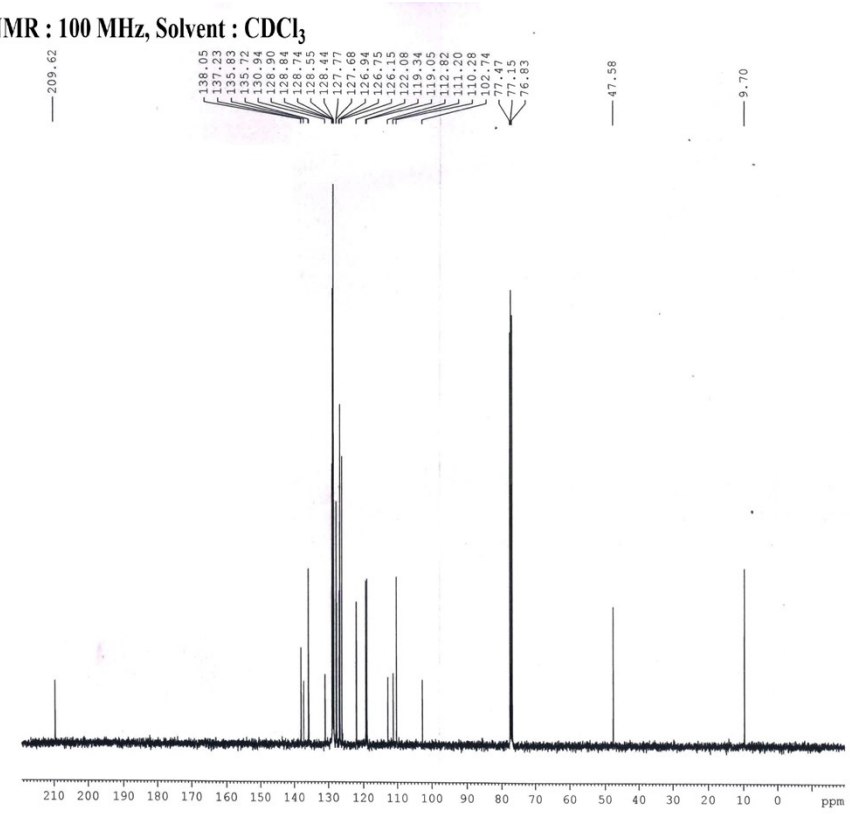
$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$

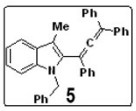


^{1}H NMR : 400 MHz, Solvent : $CDCl_3$



$^{13}C\{^{1}H\}$ NMR : 100 MHz, Solvent : $CDCl_3$






```
Current Data Parameters
NAME        Dr. A MAJEE 2024
EXPNO                  408
PROCNO                   1

F2 - Acquisition Parameters
Date_              20241119
Time                 19.31
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   512
DS                     2
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 77.59
DW                20.800 usec
DE                 6.50 usec
TE                293.5 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6278588 MHz
NUC1                  13C
P1                   8.90 usec
PLW1         54.00000000 W

======== CHANNEL f2 ========
SFO2          400.1516006 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.00000000 W
PLW12          0.32231000 W
PLW13          0.16212000 W

F2 - Processing parameters
SI                   16384
SF            100.6177887 MHz
WDW                    EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.00
```