SUPPORTING INFORMATION

$FeCl_3$ Mediated Reaction of 9-Fluorine Propargylic Alcohol with 2-(7-azaindole-3-methelene) aniline: Synthesis, Photophysical and anti-Alzheimer Properties of 1H-Pyrrolo[2,3-b]pyridin-3-yl)methyl)phenyl)-2-(9H-fluoren-9-ylidene)-1-phenylethan-1-imines

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Content

1. General remarks

All the reactions were carried out in oven-dried glassware. The progress of reactions was monitored by Thin Layer Chromatography (TLC), and purification of crude compounds was performed by column chromatography using silica gel (100-200 mesh). The NMR spectra were recorded on a Bruker-400 MHz NMR spectrometer (400 MHz for ^{1}H NMR and 100.6 MHz for ^{13}C NMR) with $CDCl_3$ as the solvent and TMS as the internal standard. Integrals are per assignments; Coupling constants (J) were reported in Hertz (Hz). All ^{13}C NMR spectra reported are proton decoupled. Multiplicity is indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), dt (doublet triplet), td (triplet of doublet), br s (broad singlet). HRMS analyses were recorded using a Q-TOF Micro mass spectrometer (with different mass analyses depending on instrument availability). Yields refer to quantities obtained after column chromatography.

Reagents, including ABTS (2,2′-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid)), ascorbic acid, potassium persulfate, DPPH (2,2-diphenyl-1-picrylhydrazyl), MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide), and DMSO (Dimethyl sulfoxide) were obtained from Sigma-Aldrich, India. Additionally, Acetylthiocholine iodide (ATCI), Acetylcholinesterase (AChE) (Sigma), 5,5′-dithiobis [2-nitrobenzoic acid] (DTNB), DCFH-DA (2′, 7′-dichlorofluorescein diacetate), and $A\beta_{1\text{-}42}$, SDS, and TBA were also purchased from Sigma. Neuro-2a cells were purchased from ATCC. DMEM and Fetal bovine serum (FBS) from Gibco.

2. Experimental procedure

2.1 General procedure for the synthesis of compounds 2a and 2b

In a sealed tube, a mixture of 5-substituted-N-methyl-7-azaindole (1g), 2-aminobenzyl alcohol (1.2 equiv), and *p*-TSA (1 equiv) as a catalyst was heated in an ethanol: water (3mL, 1:1) solvent system to 120 °C for 6 hours. After the reaction was complete (monitored by TLC every two hours), the mixture was diluted with ethyl acetate and washed with distilled water. The combined organic layer was dried over anhyd. Na_2SO_4, and the solvent was removed under reduced pressure. The resulting crude mixture was purified by alumina column. (Gradient eluent: hexane: EtOAc), affording compounds **2a** and **2b** in good yields.

2.2 General procedure for the synthesis of compounds 3a-3k

In a 50 mL RBF, propargylic alcohol derivative **1a-o** of 9-fluorenone (50mg) and C-3 alkylated 7-azaindonyl aniline **2a** (1 equiv.) in 1,2-dichloroethane (3 mL), $FeCl_3$ (1 equiv.) was added. The resulting reaction mixture was stirred at room temperature. After the completion of the reaction (monitored by TLC), the reaction mixture was diluted with DCM and washed with saturated brine and distilled water. The combined organic layer was dried over anhyd. Na_2SO_4, and the solvent was removed *in vacuo*. The crude mixture was purified through a silica gel column (Gradient eluent: Hexane: Ethyl acetate), affording the corresponding compounds **3a-k** in good yields (See table 2 in the main text).

2.3 DPPH method

The synthesized compounds were tested for their antioxidant properties using the 1,1-diphenyl-2-picrylhydrazyl (DPPH) method. In this procedure[1], all compounds were diluted to final concentrations of 5, 10, 20, 30, 40, and 50 µg/mL. Methanolic DPPH solution (1 mL, 0.3 mmol) was added to 300 µL of compound solutions of different concentrations. The tube was kept at ambient temperature in the dark for 30 min, and the absorbance was measured at 517 nm using a UV-Vis 1800 spectrophotometer (Epoch™ 2 Microplate Spectrophotometer). The scavenging activity was calculated by following the formula:

$$\%\text{Inhibition} = \left[\frac{A_{control} - A_{sample}}{A_{control}}\right] x100$$

Where A-control is the blank, and A-sample is the absorbance of different samples. The methanolic DPPH solution (1 mL, 0.3 mM) was used as a control. The inhibitory concentration (IC_{50}) is the concentration required to exhibit 50% antiradical activity. The IC_{50} values were calculated % inhibition and concentration. The experiments were run in triplicate.

2.4 ABTS method

ABTS radical scavenging activity was measured following the method described by *Burgart et al*., with minor modifications[2]. The ABTS stock solution was prepared by combining equal

volumes of 7 mM ABTS and 2.45 mM potassium persulfate, then incubating the mixture for 12–16 hours at room temperature in the dark. Next, 1 ml of ABTS solution was mixed with 1 mg/ml ascorbic acid at concentrations ranging from 0.02 to 0.10 mg/ml. The mixture was incubated in the dark at room temperature for 10 minutes. For the control, 1 ml of ABTS solution was combined with 0.50 ml of double-distilled water. Absorbance was measured at 734 nm, with the control solution showing a value of 0.25 ± 0.03. Scavenging activity was calculated as a percent inhibition using the following equation.

$$\%\text{Inhibition} = \left[\frac{A_{control} - A_{sample}}{A_{control}}\right] x100$$

Sample concentrations of 5, 10, 20, 30, 40, and 50 µg/mL were used to plot calibration curves and determine IC_{50} values, with concentration or log concentration on the x-axis and percentage inhibition on the y-axis. The IC_{50} is defined as the concentration of a compound that produces 50% of the maximal response. IC_{50} values indicate the antioxidant capacity of the tested materials. Ascorbic acid served as the standard, and all experiments were performed in triplicate.

2.5 Biocompatibility Assay (MTT assay)

Neuro-2a (N2a) mouse neuroblastoma cell line from ATCC was cultured in DMEM with 10% FBS for the study[3]. The cells were trypsinized, added to 96-well culture plates (5 × 10^4 cells/100 µL/well), and incubated at 37 °C for 24 h. The cells were treated with all compounds at concentrations of 5µg to 60 µg, along with 2% DMSO as a positive control, for 12 hours at 37°C. Post-treatment, 5 mg/mL of MTT in the complete medium was added to each well and incubated at 37°C for 4 h. Cell viability was assessed by measuring absorbance at 570 nm using the Epoch™ 2 Microplate Spectrophotometer (Agilent Technologies, USA).

2.6 Measurement of Cellular Antioxidant Activity (CAA)

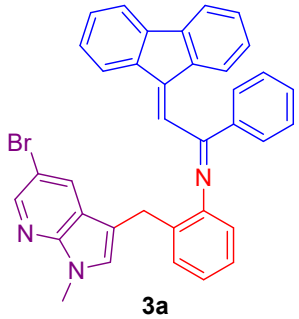
Cellular antioxidant activity (CAA) was assessed according to the method of Yanmei Feng and Pratap *et al.*, with modifications[4]. Neuro 2A cells were seeded at a density of 1 × 10^5 cells per well in 96-well plates. After 16 hours, cells were exposed to 10µg concentrations of the test compounds for 24 hours. Subsequently, cells were incubated with DCF-DA for 30 minutes at 37 °C in a CO_2 incubator. $A\beta_{1-42}$ (10µM) was then added, and fluorescence was measured (emission at 538 nm, excitation at 485 nm) every 5 minutes for 1 hour at 37 °C. The percentage of CAA was determined by comparing the increase in fluorescence between control and $A\beta_{1-42}$ treated cells.

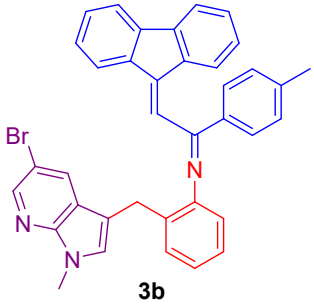
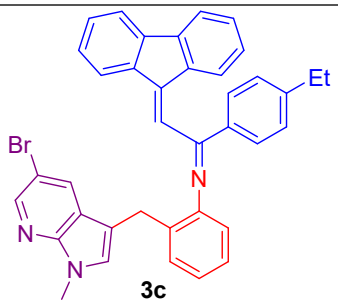
2.7 Assessment of Acetylcholinesterase Activity in Neuro-2a Neuronal Cell Cultures

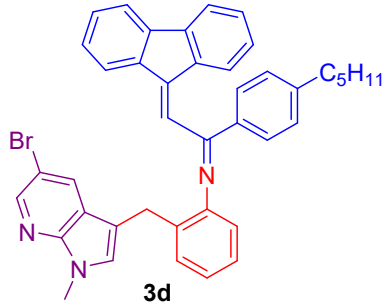
A biochemical assay was performed to measure acetylcholinesterase (AChE) activity in Neuro-2a cells, with minor modifications to established protocols[5]. Crude cell lysates were analyzed. Neuro-2a cells were seeded at 1.0 × 10^4 cells per well in 96-well plates (Eppendorf, Germany) and exposed to various concentrations of test compounds (5–30 µg) diluted in DMEM medium without fetal bovine serum (FBS), with a final volume of 0.10 mL per well. Plates were

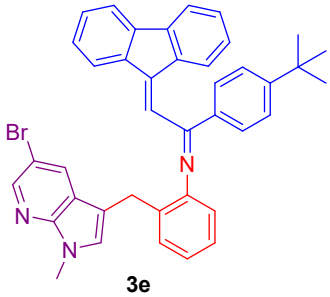
incubated for 24 hours at 37 °C in a 5% CO_2 atmosphere. For crude protein lysate preparation, cells were washed once with 200 µL of phosphate-buffered saline (PBS; 137 mM NaCl, 27 mM KCl, 10 mM Na_2HPO_4, 1.8 mM KH_2PO_4, pH=7.4) and lysed in a buffer containing 150 mM NaCl, 1% Triton X-100, and 50 mM Tris, pH 8.0. Aliquots of crude protein lysates (10 µL) were subjected to the AChE enzymatic assay using a modified spectrophotometric method as described by Ellman *et al.* AChE activity was quantified as the amount of acetylthiocholine iodine substrate hydrolyzed in nmol per minute or as a percentage of substrate hydrolyzed relative to the control. $A\beta_{1\text{-}40}$ (10 µM) was used as a positive control.

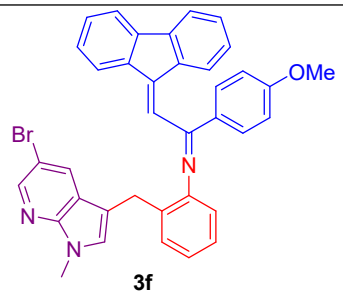
Spectroscopic data of new compounds

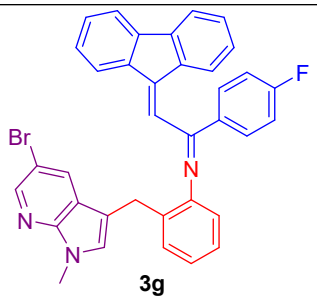
Compound	Physical and Spectroscopic data
 **3a**	N-(2-((5-Bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl) methyl)phenyl)-2-(9H-fluoren-9-ylidene)-1-phenylethan-1-imine **(3a)** **Nature**: Yellowish solid **Yield:** 81% (83mg) **R_f (20% EtOAc-Hexane)**: 0.54 **Melting point:** 155-158°C **FTIR (ATR) ν_{max}**: 2920, 1592, 1478, 1441, 1402, 1348, 1270, 1210, 1143, 1080, 1021, 878, 844, 763, 723, 691, 664, 622, 593, 563 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS)**: δ 8.27 (d, *J* = 2.1 Hz, 1H), 8.02 – 7.93 (m, 2H), 7.84 (d, *J* = 2.2 Hz, 1H), 7.58 (ddt, *J* = 17.3, 7.6, 1.0 Hz, 2H), 7.48 – 7.41 (m, 1H), 7.41 – 7.30 (m, 3H), 7.25 (d, *J* = 1.8 Hz, 1H), 7.19 (qd, *J* = 7.6, 1.1 Hz, 2H), 7.11 (ddt, *J* = 7.8, 5.9, 1.0 Hz, 2H), 7.05 – 6.97 (m, 2H), 6.85 (td, *J* = 7.6, 1.1 Hz, 1H), 6.71 – 6.65 (m, 2H), 6.31 (s, 1H), 4.00 (s, 2H), 3.52 (s, 3H). **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 146.2, 143.0, 141.2, 140.7, 139.6, 137.7, 137.2, 135.5, 131.1, 130.2, 129.7, 129.4, 129.1, 129.0, 128.7, 128.6, 128.3, 127.2, 127.1, 126.9, 125.8, 124.4, 121.6, 120.6, 120.0, 119.6, 119.2, 112.3, 110.9, 30.8, 28.0 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ 131.1, 129.7, 129.4, 129.1, 129.0, 128.7, 128.6, 128.3, 127.2, 127.1, 126.9, 125.8, 124.4, 120.6, 120.0, 119.6, 119.2, 30.8, 28.0 ppm.

	HRMS (ESI): Calcd. for $C_{36}H_{26}BrN_3$ $[M+H]^+$ *m/z*: 580.1388; Found *m/z*=580.1389
 **3b**	N-(2-((5-bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-2-(9H-fluoren-9-ylidene)-1-(p-tolyl)ethan-1-imine **(3b)** **Nature**: Yellowish solid **Yield:** 77% (81mg) **R_f (20% EtOAc-Hexane)**: 0.52 **Melting point:** 159-162℃ **FTIR (ATR) ν_{max}**: 1586, 1561, 1480, 1442, 1406, 1346, 1272, 1207, 1178, 1146, 1104, 1014, 827, 767, 727, 621, 595, 566, 535, 462 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS):** δ 8.18 (d, *J* = 2.1 Hz, 1H), 7.85 – 7.68 (m, 3H), 7.59 – 7.40 (m, 2H), 7.21 (td, *J* = 7.4, 1.1 Hz, 1H), 7.15 (dt, *J* = 6.5, 1.4 Hz, 1H), 7.10 – 7.06 (m, 5H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.89 (tt, *J* = 7.4, 5.6 Hz, 2H), 6.77 (td, *J* = 7.6, 1.1 Hz, 1H), 6.57 (d, *J* = 4.1 Hz, 2H), 6.22 (s, 1H), 3.89 (s, 2H), 3.43 (s, 3H). **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 149.7, 146.1, 143.0, 141.4, 141.1, 140.4, 139.6, 137.7, 135.6, 134.5, 130.2, 129.6, 129.4, 129.0, 128.9, 128.6, 128.2, 127.1, 127.0, 126.9, 125.8, 124.2, 121.6, 120.5, 120.3, 120.5, 119.6, 119.6, 119.2, 112.3, 110.9, 30.8, 27.9, 21.5 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ 143.0, 129.6, 129.4, 129.0, 128.9, 128.6, 128.2,127.1, 127.0, 126.9, 125.8, 124.2, 120.5, 120.3, 119.6, 119.6, 119.2 ppm. **HRMS (ESI):** Calcd. for $C_{37}H_{28}BrN_3$ $[M+H]^+$ *m/z*: 594.1545; Found *m/z:* 594.1550
 **3c**	N-(2-((5-bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-1-(4-ethylphenyl)-2-(9H-fluoren-9-ylidene)ethan-1-imine **(3c)** **Nature**: Yellowish solid **Yield:** 79% (84 mg) **Melting point:** 159-161℃ **R_f (20% EtOAc-Hexane)**: 0.56

	FTIR (ATR) ν_{max}: 3054, 2963, 2923, 1587, 1480, 1443, 1408, 1344, 1273, 1208, 1146, 1076, 1014, 878, 838, 767, 726, 621, 594, 426 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS)** δ 8.19 (d, *J* = 2.1 Hz, 1H), 7.83 – 7.79 (m, 2H), 7.76 (d, *J* = 2.2 Hz, 1H), 7.50 (ddt, *J* = 16.4, 7.5, 0.9 Hz, 2H), 7.23 (td, *J* = 7.5, 1.2 Hz, 1H), 7.15 – 7.00 (m, 7H), 6.96 – 6.85 (m, 2H), 6.78 (td, *J* = 7.6, 1.1 Hz, 1H), 6.63 – 6.49 (m, 2H), 6.25 (s, 1H), 3.91 (s, 2H), 3.44 (s, 3H) ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 146.1, 142.9, 141.1, 140.4, 139.6, 137.7, 135.6, 134.6, 130.2, 129.7, 129.4, 129.0, 128.9, 128.6, 128.4, 128.2, 127.0, 126.9, 125.8, 124.2, 121.6, 120.6, 120.4, 119.6, 119.6, 119.3, 112.3, 110.9, 30.8, 28.8, 27.9, 15.2 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ 129.7, 129.4, 129.0, 128.9, 128.6,128.4, 128.2, 127.1, 127.0, 126.9, 125.8, 124.2, 120.6, 120.4, 119.6, 19.6, 119.3, 30.8, 28.8, 27.9, 15.2 ppm. **HRMS (ESI):** Calcd. for $C_{38}H_{30}BrN_3$ M^+ *m/z*: 607.1623; Found *m/z:* 607.1627
 **3d**	N-(2-((5-bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-2-(9H-fluoren-9-ylidene)-1-(4-pentylphenyl)ethan-1-imine **(3d)** **Nature**: Pale yellowish powder **Yield:** 76% (87mg) **Melting point:** 164-166℃ **R_f (20% EtOAc-Hexane)**: 0.54 **FTIR (ATR) ν_{max}**: 2923, 2854, 1590, 1478, 1443, 1407, 1348, 1267, 1210, 1178, 1142, 1082, 1011, 879, 842, 771, 728, 668, 622, 594 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS):** δ 8.19 (d, *J* = 2.2 Hz, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.77 (d, *J* = 2.1 Hz, 1H), 7.51 (ddt, *J* = 17.4, 7.5, 1.0 Hz, 2H), 7.25 (td, *J* = 7.4, 1.1 Hz, 1H), 7.14 – 7.09 (m, 5H), 7.05 (d, *J* = 7.9 Hz, 2H), 6.93 (tt, *J* = 7.5, 5.6 Hz, 2H), 6.78 (td, *J* = 7.6, 1.1

	Hz, 1H), 6.64 – 6.59 (m, 2H), 6.25 (s, 1H), 3.93 (s, 2H), 3.45 (s, 3H), 2.61 – 2.52 (m, 2H), 1.56 – 1.51 (m, 4H), 1.23 (dd, *J* = 7.4, 3.1 Hz, 2H), 0.84 – 0.79 (m, 3H) ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 146.1, 143.0, 141.2, 139.6, 137.7, 135.6, 129.7, 129.5, 129.1, 129.0, 128.8, 128.7, 128.4, 127.2, 128.4, 127.2, 127.1, 126.9, 125.9, 124.3, 121.7, 120.6, 119.6, 119.6, 112.3, 110.9, 35.8, 31.4, 30.8, 28.0, 22.5, 14.0 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ 143.0, 129.8, 129.5, 129.1, 129.0, 128.9, 128.7, 128.4, 127.2, 127.1, 126.9, 125.9, 120.6, 119.7, 119.6, 5.9, 31.5, 30.9, 28.0, 22.5, 14.0 ppm. **HRMS (ESI):** Calcd. for $C_{41}H_{36}BrN_3$ $[M+H]^+$ *m/z*: 650.2171; Found *m/z:* 650.2175.
 **3e**	N-(2-((5-bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-1-(4-(tert-butyl)phenyl)-2-(9H-fluoren-9-ylidene)ethan-1-imine **(3e)** **Nature**: Yellowish solid **Yield:** 82% (92mg) **R_f (20% EtOAc-Hexane)**: 0.52 **Melting point:** 163-165℃ **FTIR (ATR) ν_{max}**: 2957, 1586, 1476, 1445, 1405, 1361, 1269, 1202, 1145, 1113, 1082, 1013, 845, 768, 724, 699, 619, 598, 568 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS)** δ δ 8.19 (t, *J* = 1.6 Hz, 1H), 7.86 – 7.80 (m, 2H), 7.77 (dd, *J* = 2.0, 1.2 Hz, 1H), 7.50 (dd, *J* = 15.9, 7.5 Hz, 2H), 7.31 (d, *J* = 8.3 Hz, 2H), 7.24 (td, *J* = 7.4, 1.3 Hz, 1H), 7.15 – 7.03 (m, 5H), 6.90 (td, *J* = 6.6, 1.8 Hz, 2H), 6.79 (t, *J* = 7.6 Hz, 1H), 6.60 (d, *J* = 5.1 Hz, 2H), 6.29 (d, *J* = 1.1 Hz, 1H), 3.91 (s, 2H), 3.44 (s, 3H), 1.24 (s, 9H) ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 149.6, 146.1, 143.0, 141.1, 140.4, 139.6, 137.7, 135.6, 134.3, 130.3, 129.7, 129.4, 129.0, 128.9, 128.6, 128.1, 127.2, 127.0, 126.9, 125.8, 125.6, 124.2, 121.7, 120.6, 120.4, 119.6, 119.6, 119.3, 112.3, 110.9, 34.9, 30.8, 27.9 ppm.

	DEPT-135 (101.6 MHz, $CDCl_3$/TMS): δ 129.7, 129.4, 129.0, 128.9, 128.6, 128.1, 127.2, 127.0, 126.9, 125.8, 125.6, 124.2, 120.6, 120.4, 119.6, 119.6, 119.3, 31.1, 30.8, 27.9 ppm. **HRMS (ESI):** Calcd. for $C_{40}H_{34}BrN_3$ $[M+H]^+$ *m/z*: 636.2014; Found *m/z:* 636.2012
 **3f**	N-(2-((5-Bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-2-(9H-fluoren-9-ylidene)-1-(4-methoxyphenyl)ethan-1-imine **(3f)** **Nature**: Dirty white powder **Yield:** 79% (85mg) **R_f (20% EtOAc-Hexane)**: 0. 51 **Melting point:** 158-161°C **^{1}H NMR (400 MHz, $CDCl_3$/TMS)** δ 8.19 (d, *J* = 2.2 Hz, 1H), 7.88 – 7.82 (m, 2H), 7.76 (d, *J* = 2.2 Hz, 1H), 7.52 (ddt, *J* = 16.1, 7.5, 1.0 Hz, 2H), 7.25 (td, *J* = 7.4, 1.1 Hz, 1H), 7.20 – 7.10 (m, 4H), 7.05 (dt, *J* = 7.7, 0.9 Hz, 1H), 6.96 – 6.87 (m, 2H), 6.84 – 6.77 (m, 3H), 6.62 – 6.56 (m, 2H), 6.23 (s, 1H), 3.91 (s, 2H), 3.75 (s, 3H), 3.47 (s, 3H) ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 149.7, 146.1, 143.0, 141.2, 140.4, 139.6, 137.7, 135.6, 130.3, 130.0, 129.8, 129.6, 129.5, 129.0, 128.9, 128.6, 127.2, 127.1, 127.0, 125.9, 124.1, 121.7, 120.5, 120.4, 119.6, 119.6, 119.4, 114.0, 112.4, 110.9, 55.4, 30.9, 27.9 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ 130.0, 129.6, 129.5. 129.0, 128.9, 128.6, 127.2, 127.1, 127.0, 125.9, 124.1, 120.5, 120.4, 119.6, 119.4, 114.0, 55.4, 30.9, 27.9 ppm. **HRMS (ESI):** Calcd. for $C_{37}H_{28}BrN_3O$ $[M+H]^+$ *m/z*: 612.1474; Found *m/z:* 612.1467.



3g

N-(2-((5-bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-2-(9H-fluoren-9-ylidene)-1-(4-fluorophenyl)ethan-1-imine **(3g)**

Nature: Yellow powder

Yield: 85% (90mg)

R_f (20% EtOAc-Hexane): 0. 45

Melting point: 155-158℃

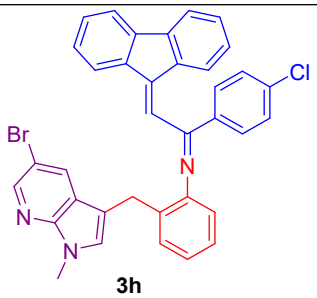
FTIR (ATR) ν_{max}: 1597, 1570, 1480, 1442, 1406, 1348, 1273, 1216, 1148, 1086, 1011, 884, 842, 767, 730, 696, 671, 622, 594, 569 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$/TMS): δ 8.19 (d, *J* = 2.2 Hz, 1H), 7.92 – 7.84 (m, 2H), 7.74 (d, *J* = 2.2 Hz, 1H), 7.51 (ddt, *J* = 14.8, 7.6, 1.0 Hz, 2H), 7.25 (td, *J* = 7.4, 1.1 Hz, 1H), 7.21 – 7.18 (m, 1H), 7.12 (tt, *J* = 7.5, 1.2 Hz, 2H), 7.05 (dt, *J* = 7.7, 0.9 Hz, 1H), 7.02 – 6.91 (m, 5H), 6.80 (td, *J* = 7.6, 1.1 Hz, 1H), 6.58 (d, *J* = 9.1 Hz, 2H), 6.21 (s, 1H), 3.91 (s, 2H), 3.47 (s, 3H) ppm.

^{13}C NMR (101.6 MHz, $CDCl_3$/TMS): δ 146.1, 143.1, 141.3, 141.0, 139.6, 137.5, 135.3, 133.3, 130.5, 130.4, 129.8, 129.4, 129.2, 128.5, 127.2, 127.1, 127.0, 125.7, 124.5, 121.6, 120.6, 119.7, 119.7, 119.5, 119.2, 115.9, 115.7, 112.3, 110.9, 30.9, 27.9 ppm.

DEPT-135 (101.6 MHz, $CDCl_3$/TMS): δ 130.4, 129.8, 129.4, 129.2, 129.2, 128.5, 127.2, 127.1, 127.0, 125.7, 124.5, 120.6, 119.7, 119.7, 119.5, 119.2, 115.9, 115.7, 30.9, 27.9 ppm.

HRMS (ESI): Calcd. for $C_{36}H_{25}BrFN_3$ $[M+H]^+$ *m/z*: 598.1294; Found *m/z:* 598.1294



3h

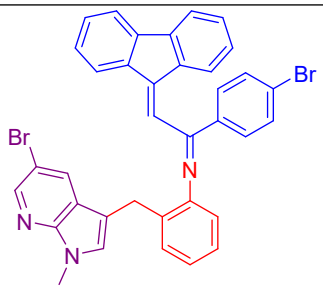
N-(2-((5-Bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-1-(4-chlorophenyl)-2-(9H-fluoren-9-ylidene)ethan-1-imine **(3h)**

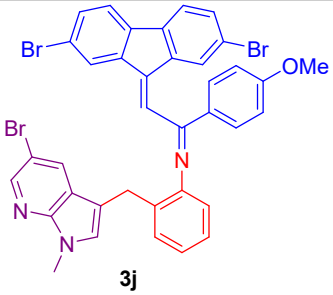
Nature: Yellowish solid

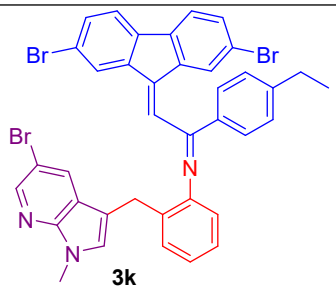
Yield: 77% (83mg)

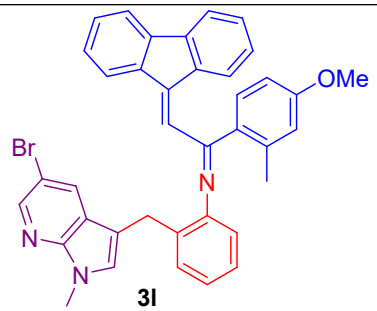
R_f (20% EtOAc-Hexane): 0. 44

Melting point: 161-163℃

	^{1}H NMR (400 MHz, $CDCl_3$/TMS): δ 8.18 (d, *J* = 2.1 Hz, 1H), 7.84 – 7.78 (m, 2H), 7.73 (d, *J* = 2.2 Hz, 1H), 7.50 (ddt, *J* = 14.2, 7.6, 0.9 Hz, 2H), 7.29 – 7.20 (m, 3H), 7.20 – 7.17 (m, 1H), 7.12 (ddd, *J* = 8.2, 7.4, 0.9 Hz, 2H), 7.05 (dt, *J* = 7.6, 1.0 Hz, 1H), 6.99 (dt, *J* = 7.7, 0.9 Hz, 1H), 6.96 – 6.90 (m, 2H), 6.80 (td, *J* = 7.6, 1.1 Hz, 1H), 6.64 – 6.52 (m, 2H), 6.18 (s, 1H), 3.91 (s, 2H), 3.46 (s, 3H) ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 146.1, 143.1, 141.3, 141.1, 139.6, 137.5, 137.3, 135.6, 135.3, 130.4, 129.7, 129.6, 129.4, 129.2, 129.2, 129.0, 128.5, 127.2, 127.1, 127.0, 125.7, 124.6, 121.6, 120.6, 119.8, 119.7, 119.3, 119.1, 112.3, 110.9, 30.8, 28.0 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ 129.7, 129.6, 129.4, 129.2, 129.2, 129.0, 128.5, 127.2, 127.1, 127.0, 125.7, 124.6, 120.6, 119.8, 119.7, 119.3, 119.1, 30.8, 28.0 ppm. **HRMS (ESI):** Calcd. for $C_{36}H_{25}BrClN_3$ $[M+H]^+$ *m/z*: 614.0999; Found *m/z:* 614.0999
 **3i**	N-(2-((5-Bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-1-(4-bromophenyl)-2-(9H-fluoren-9-ylidene)ethan-1-imine **(3i)** **Nature**: Brownish solid **Yield:** 75% (87mg) **R_f (20% EtOAc-Hexane)**: 0. 46 **Melting point:** 160-162℃ **FTIR (ATR) ν_{max}**: 1589, 1476, 1436, 1403, 1354, 1270, 1224, 1146, 1065, 1021, 943, 910, 878, 836, 775, 726, 676, 651, 622, 592 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS):** δ 8.71 (d, *J* = 7.8 Hz, 1H), 8.16 (dd, *J* = 10.7, 2.1 Hz, 2H), 7.81 (dd, *J* = 18.3, 2.1 Hz, 2H), 7.64 – 7.57 (m, 3H), 7.55 – 7.51 (m, 2H), 7.49 – 7.41 (m, 3H), 7.29 (tdd, *J* = 7.5, 2.9, 1.1 Hz, 2H), 7.25 (dt, *J* = 7.5, 1.9 Hz, 2H), 7.23 – 7.18 (m, 1H), 7.16 – 7.14 (m, 1H), 7.14 – 7.06 (m, 3H), 7.04 (dd, *J* = 2.3, 1.7 Hz, 4H), 6.97 (td, *J* = 7.6, 1.2 Hz, 1H), 6.94 – 6.82 (m, 5H), 6.80 – 6.72 (m, 2H), 6.66 (d, *J* = 1.1 Hz, 1H), 6.60 – 6.47 (m, 2H), 6.32 (dd, *J* =

	7.6, 1.7 Hz, 1H), 4.04 (s, 2H), 3.96 (s, 2H), 3.56 (s, 3H), 3.47 (s, 3H).ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 143.0, 143.0, 134.3, 132.8, 131.8, 130.9, 130.3, 130.1, 129.9, 129.5, 129.4, 129.3, 129.2, 129.2, 128.8, 128.5, 128.0, 127.6, 127.3, 127.3, 127.2, 127.2, 126.7, 125.6, 125.0, 121.0, 120.7, 120.1, 119.7, 119.6, 119.5, 119.4, 31.0, 30.9, 28.0, 27.9 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ129.3, 129.2, 129.2, 128.8, 128.5, 128.0, 127.6, 127.4, 127.3, 127.2, 127.2, 126.7, 125.6, 125.0, 124.9, 124.5, 121.0, 120.7, 120.1, 119.7, 119.6, 119.6, 119.5, 119.4, 31.0, 30.9, 21.0, 27.9 ppm. **HRMS (ESI):** Calcd. for $C_{36}H_{25}Br_2N_3$ $[M+H]^+$ *m/z*: 660.0473; Found *m/z:* 660.0477.
 **3j**	N-(2-((5-Bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-2-(2,7-dibromo-9H-fluoren-9-ylidene)-1-(4-methoxyphenyl) ethan-1-imine **(3j)** **Nature**: Yellowish solid **Yield:** 73% (99mg) **R_f (20% EtOAc-Hexane)**: 0. 49 **Melting point:** 168-170℃ **FTIR (ATR) ν_{max}**: 2919, 1569, 1448, 1402, 1314, 1254, 1209, 1163, 1065, 1025, 954, 880, 838, 803, 751, 661, 623, 587, 514, 433 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS):** δ 8.20 (d, *J* = 2.2 Hz, 1H), 7.82 – 7.69 (m, 3H), 7.39 – 7.31 (m, 2H), 7.30 – 7.25 (m, 1H), 7.24 – 7.19 (m, 3H), 7.14 (d, *J* = 1.6 Hz, 1H), 6.96 (pd, *J* = 7.4, 1.7 Hz, 2H), 6.87 – 6.78 (m, 2H), 6.62 – 6.53 (m, 2H), 6.27 (s, 1H), 3.92 (s, 2H), 3.77 (s, 3H), 3.48 (s, 3H) ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 146.0, 143.2, 139.1, 138.9, 138.3, 137.4, 136.9, 132.1, 131.9, 130.4, 129.9, 129.9, 129.6, 129.5, 128.5, 127.1, 124.5, 123.8, 123.3, 121.5, 121.4, 121.1, 121.0, 120.8, 119.2, 114.2, 112.4, 111.0, 55.4, 30.9, 27.9 ppm.

	DEPT-135 (101.6 MHz, $CDCl_3$/TMS): δ 143.2, 132.1, 131.9, 129.9, 129.9, 129.6, 128.8, 128.5, 127.1, 124.5, 123.8, 123.3, 121.0, 120.8, 119.2, 114.2, 55.4, 30.9, 27.9 ppm. **HRMS (ESI):** Calcd. for $C_{37}H_{26}Br_3N_3O$ $[M+H]^+$ *m/z*: 767.9684; Found *m/z:* 767.9701.
 **3k**	N-(2-((5-Bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-2-(2,7-dibromo-9H-fluoren-9-ylidene)-1-(4-ethylphenyl) ethan-1-imine **(3k)** **Nature**: Yellowish solid **Yield:** 75% (100mg) **R_f (20% EtOAc-Hexane)**: 0. 51 **Melting point:** 167-170°C **FTIR (ATR) ν_{max}**: 1589, 1563, 1475, 1449, 1401, 1300, 1263, 1205, 1176, 1140, 1062, 1008, 942, 880,839, 809, 747, 661, 622, 587 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS):** δ 8.18 (d, *J* = 2.1 Hz, 1H), 7.73 (dd, *J* = 7.8, 1.6 Hz, 3H), 7.39 – 7.31 (m, 2H), 7.26 (dd, *J* = 8.1, 2.2 Hz, 1H), 7.21 (d, *J* = 1.8 Hz, 1H), 7.18 – 7.14 (m, 4H), 7.13 (d, *J* = 1.8 Hz, 1H), 6.96 (pd, *J* = 7.4, 1.7 Hz, 2H), 6.58 (d, *J* = 6.8 Hz, 2H), 6.32 (s, 1H), 3.92 (s, 2H), 3.47 (s, 3H), 2.62 (q, *J* = 7.6 Hz, 2H), 1.18 (t, *J* = 7.5 Hz, 3H) ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 148.2, 146.1, 143.2, 139.2, 138.9, 138.4, 137.5, 136.9, 134.5, 132.1, 131.9, 130.4, 130.0, 129.5, 128.4, 128.2, 127.1, 124.6, 123.8, 123.2, 121.5, 121.4, 121.1, 121.0, 120.8, 119.1, 1123, 111.0, 30.9, 28.8, 27.9, 15.3 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ 143.2, 132.1, 131.9, 130.0, 129.5, 128.9, 128.5, 128.4, 128.2, 127.1, 124.6, 123.8, 123.2, 121.0, 120.8, 119.1, 30.9, 28.8, 27.9, 15.3 ppm. **HRMS (ESI):** Calcd. for $C_{38}H_{28}Br_3N_3$ $[M+Na]^+$ *m/z*: 785.9731. Found *m/z:* 785.9797



3l

N-(2-((5-Bromo-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl) phenyl)-2-(9H-fluoren-9-ylidene)-1-(4-methoxy-2-methylphenyl) ethan-1-imine **(3l)**

Nature: Brownish solid

Yield: 71% (78 mg)

R_f (20% EtOAc-Hexane): 0. 54

Melting point: 157-160℃

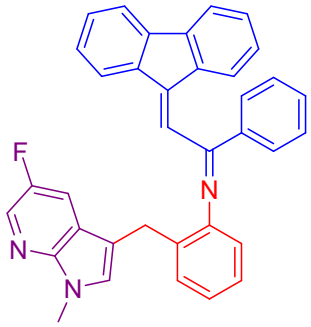
FTIR (ATR) ν_{max}: 2920, 1597, 1558, 1477, 1442, 1406, 1314, 1243, 1205, 1163, 1128, 1034, 875, 845, 811, 772, 727, 667, 622, 593 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$/TMS): δ 8.24 (d, *J* = 2.1 Hz, 1H), 7.81 (d, *J* = 2.2 Hz, 1H), 7.55 (dd, *J* = 16.1, 7.5 Hz, 2H), 7.44 (d, *J* = 8.7 Hz, 1H), 7.40 – 7.27 (m, 3H), 7.26 – 7.10 (m, 3H), 7.09 – 6.96 (m, 3H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.86 (td, *J* = 7.6, 1.1 Hz, 1H), 6.80 (d, *J* = 2.7 Hz, 1H), 6.73 – 6.66 (m, 2H), 6.62 (dd, *J* = 8.6, 2.7 Hz, 1H), 6.44 (s, 1H), 3.98 (s, 2H), 3.80 (s, 3H), 3.56 (s, 3H), 2.57 (s, 3H).ppm.

^{13}C NMR (101.6 MHz, $CDCl_3$/TMS): δ 146.2, 143.0, 141.2, 140.1, 139.8, 139.5, 138.3, 135.3, 132.3, 132.0, 130.7, 130.0, 129.4, 129.0, 128.9, 128.6, 127.1, 127.1, 126.9, 125.7, 124.1, 122.1, 121..6, 120.4, 122.1, 121.7, 120.5, 119.6, 119.5, 119.5, 117.5, 112.3, 110.9, 55.2, 30.9, 28.1, 22.8 ppm.

DEPT-135 (101.6 MHz, $CDCl_3$/TMS): δ 132.3, 129.8, 129.4, 129.0, 128.9, 128.6, 127.1, 127.1, 126.9, 125.7, 124.1, 122.1, 120.5, 119.6, 119.5, 117.5, 110.9, 55.2, 30.9, 28.1, 22.8 ppm.

HRMS (ESI): Calcd. for $C_{38}H_{30}BrN_3O$ $[M+H]^+$ *m/z*: 626.1630; Found *m/z:* 626.1329.



3p

2-(9H-fluoren-9-ylidene)-N-(2-((5-fluoro-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl)phenyl)-1-phenylethan-1-imine **(3p)**

Nature: Yellow solid

Yield: 71% (51 mg)

R_f (20% EtOAc-Hexane): 0. 41

Melting point: 135-137°C

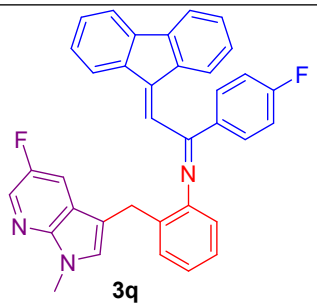
FTIR (ATR) $_{max}$: 2915, 1569, 1536, 1485, 1444, 1405, 1345, 1273, 1227, 1126, 918, 873, 834, 762, 731, 687, 609, 465 cm^{-1}.

^{1}H NMR (400 MHz, $CDCl_3$/TMS): δ 8.05 (dd, *J* = 2.7, 1.8 Hz, 1H), 7.93 – 7.82 (m, 2H), 7.51 (ddt, *J* = 14.1, 7.6, 0.9 Hz, 2H), 7.39 – 7.32 (m, 2H), 7.32 – 7.27 (m, 2H), 7.24 (td, *J* = 7.5, 1.1 Hz, 1H), 7.20 – 7.17 (m, 1H), 7.10 (tdd, *J* = 7.5, 1.8, 1.1 Hz, 2H), 7.05 (dt, *J* = 7.8, 0.9 Hz, 1H), 7.01 (dt, *J* = 7.6, 0.9 Hz, 1H), 6.96 – 6.87 (m, 2H), 6.78 (td, *J* = 7.6, 1.1 Hz, 1H), 6.66 (s, 1H), 6.61 – 6.57 (m, 1H), 6.22 (s, 1H), 3.93 (s, 2H), 3.49 (s, 3H).ppm.

^{13}C NMR (101.6 MHz, $CDCl_3$/TMS): δ 149.6, 144.7, 141.2, 14.7, 139.6, 137.6, 137.2, 135.5, 131.1, 130.8, 130.3, 129.7, 129.3, 129.0, 129.0, 128.7, 128.3, 127.1, 127.0, 126.9, 125.8, 124.3, 120.5, 120.0, 120.0, 119.9, 119.9, 119.6, 119.1, 119.1, 113.1, 112.9,112.3, 30.9, 28.1 ppm.

DEPT-135 (101.6 MHz, $CDCl_3$/TMS): δ 130.8, 129.7, 129.3, 129.0, 129.0, 128.7, 128.3, 127.1, 127.0, 126.9, 125.8, 124.3, 120.5, 120.0, 119.6, 119.1, 113.1, 112.9, 30.9, 28.1 ppm.

HRMS (ESI): Calcd. for $C_{36}H_{26}FN_3$ $[M+H]^+$ *m/z*: 520.2189; Found *m/z:* 520.2186.



3q

2-(9H-fluoren-9-ylidene)-N-(2-((5-fluoro-1-methyl-1H-pyrrolo[2,3-b]pyridin-3-yl)methyl)phenyl)-1-(4-fluorophenyl)ethan-1-imine **(3q)**

Nature: Pale Yellow powder

Yield: 65% (28 mg)

R_f (20% EtOAc-Hexane): 0. 43

Melting point: 131-132°C

	FTIR (ATR) $_{max}$: 2918, 1577, 1494, 1444, 1405, 1345, 1270, 1231, 1150, 921, 874, 832, 761, 733, 688, 605, 462 cm^{-1}. **^{1}H NMR (400 MHz, $CDCl_3$/TMS):** δ 8.06 (dd, *J* = 2.7, 1.8 Hz, 1H), 7.95 – 7.84 (m, 2H), 7.52 (ddt, *J* = 12.3, 7.6, 1.0 Hz, 2H), 7.31 (dd, *J* = 9.0, 2.7 Hz, 1H), 7.25 (td, *J* = 7.5, 1.1 Hz, 1H), 7.21 – 7.19 (m, 0H), 7.12 (qd, *J* = 7.4, 1.1 Hz, 2H), 7.02 (dt, *J* = 7.7, 1.0 Hz, 2H), 7.00 – 6.95 (m, 2H), 6.94 – 6.89 (m, 2H), 6.81 (td, *J* = 7.6, 1.1 Hz, 1H), 6.67 (s, 1H), 6.61 – 6.56 (m, 1H), 6.20 (s, 1H), 3.93 (s, 2H), 3.51 (s, 3H).ppm. **^{13}C NMR (101.6 MHz, $CDCl_3$/TMS):** δ 163.9, 149.4, 144.7, 141.3, 140.9, 139.6, 137.5, 135.4, 133.4, 131.1, 130.9, 130.5, 130.4, 129.7, 129.2, 129.1, 127.2, 127.1, 127.0, 125.7, 124.5, 120.5, 119.9, 119.7, 119.7, 119.7, 119.6, 119.1, 115.8, 115.6, 113.1, 112.9, 112.4, 112.4, 31.6, 28.1 ppm. **DEPT-135 (101.6 MHz, $CDCl_3$/TMS):** δ 13127.1, 127.0, 125.7, 130.4, 129.7, 129.2, 129.1, 127.2, 127.1, 127.0, 125.7, 124.5,120.5, 119.7, 119.7, 119.6, 119.1, 115.8, 115.6, 113.1, 112.9 31.6, 28.1 ppm. **HRMS (ESI):** Calcd. for $C_{36}H_{25}F_2N_3$ $[M+H]^+$ *m/z*: 538.2095; Found *m/z:* 538.1915.

Scanned copies of ^{1}H, ^{13}C, DEPT-135, FT-IR and HRMS spectra

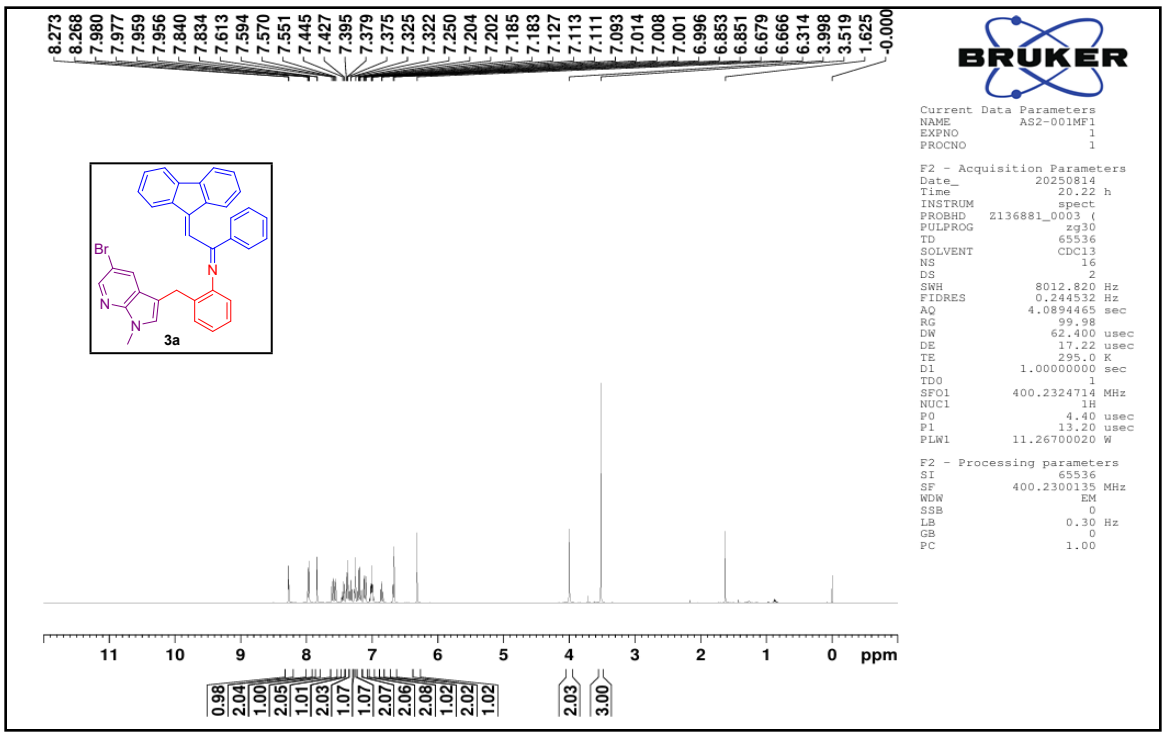


Fig 1 ^{1}H NMR spectrum of compound **3a**

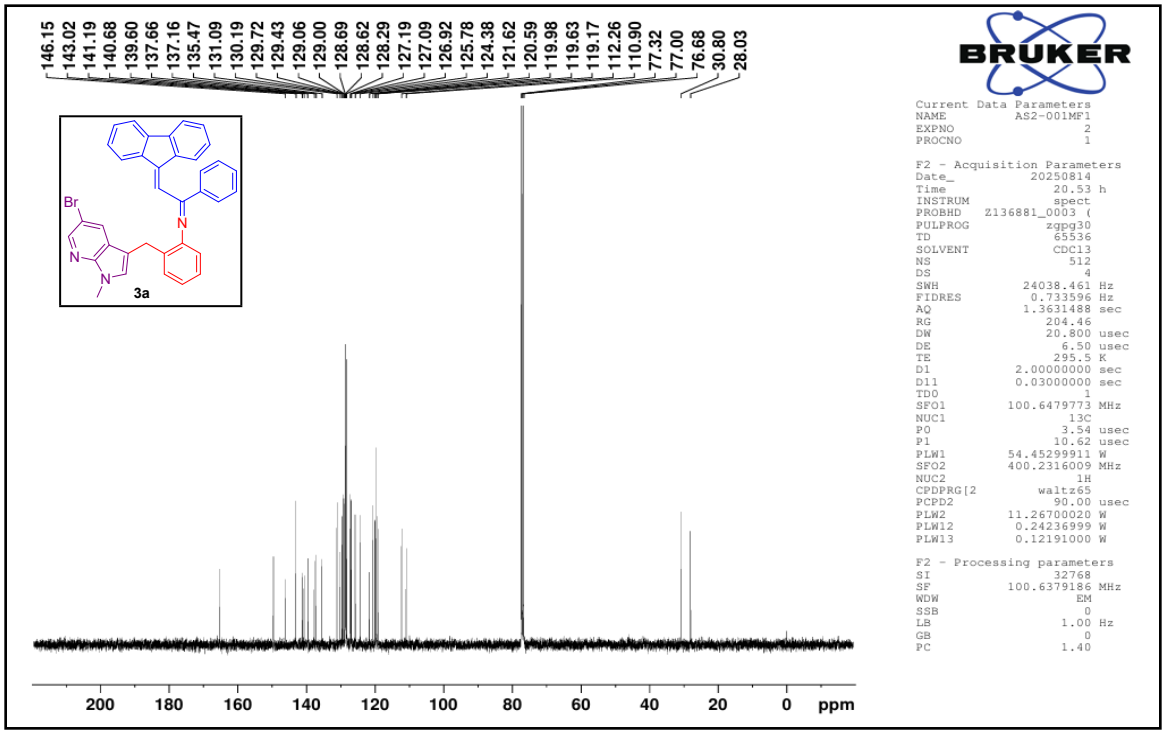


Fig 2 ^{13}C NMR spectrum of compound **3a**

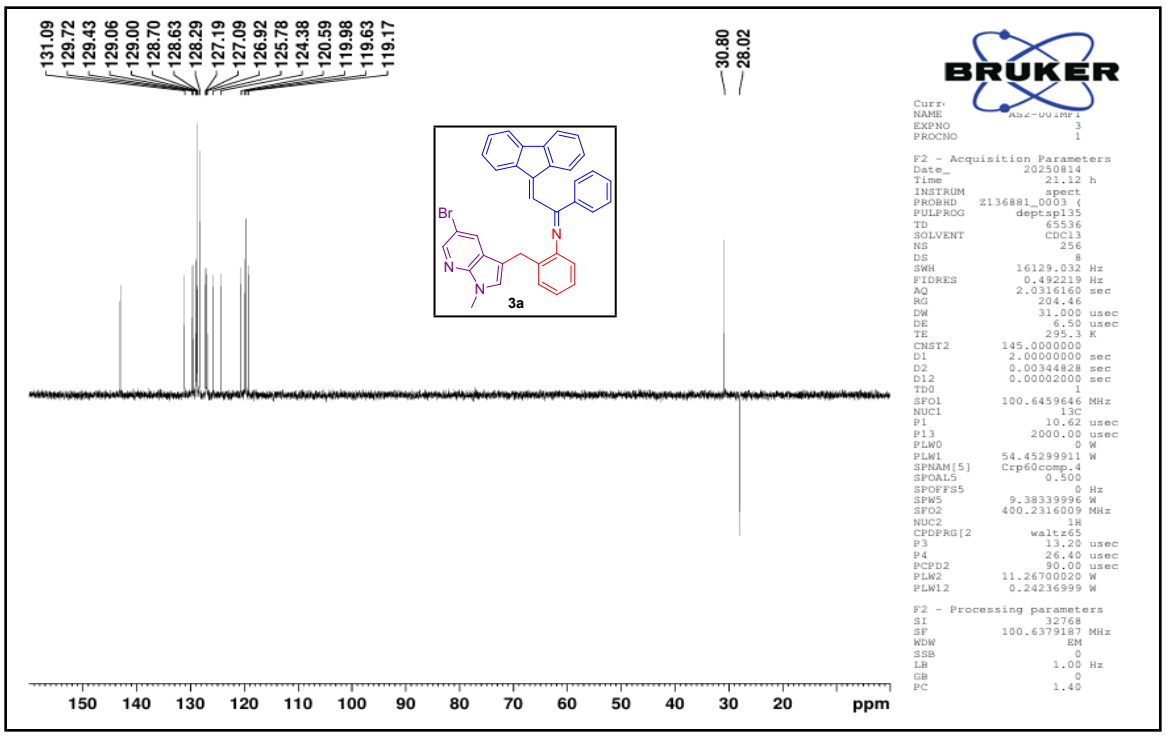


Fig 3 DEPT-135 NMR spectrum of compound **3a**

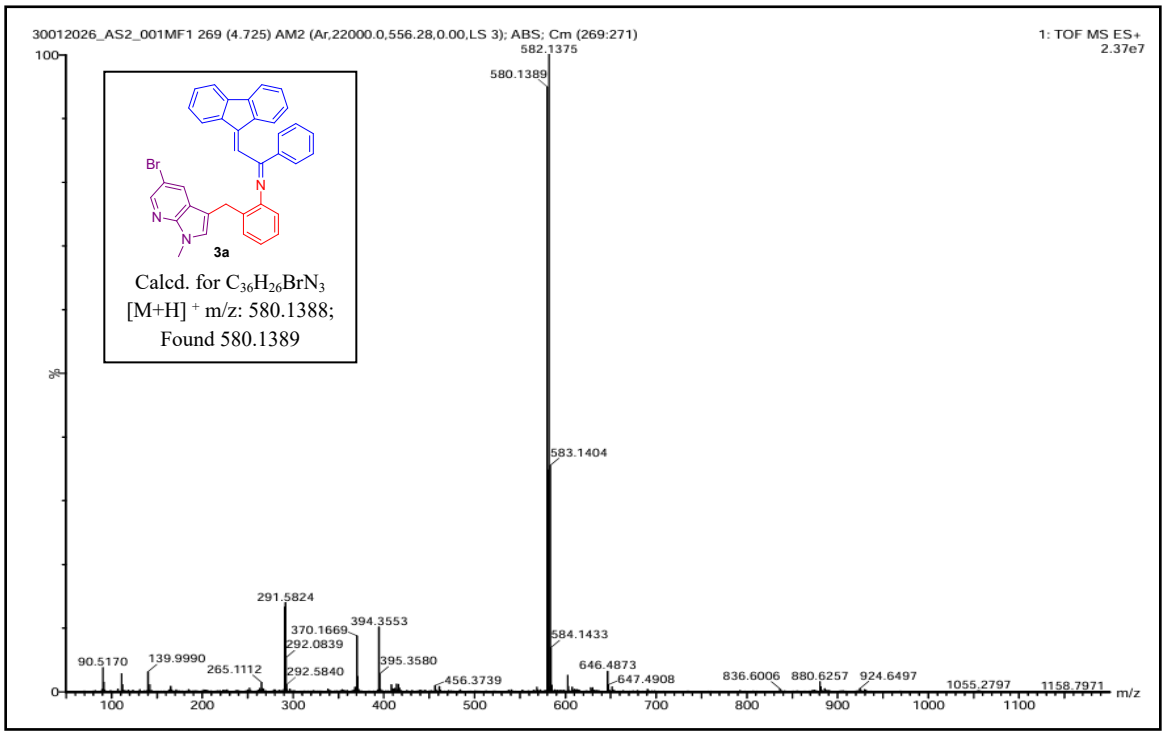


Fig 4 HRMS spectrum of compound **3a**

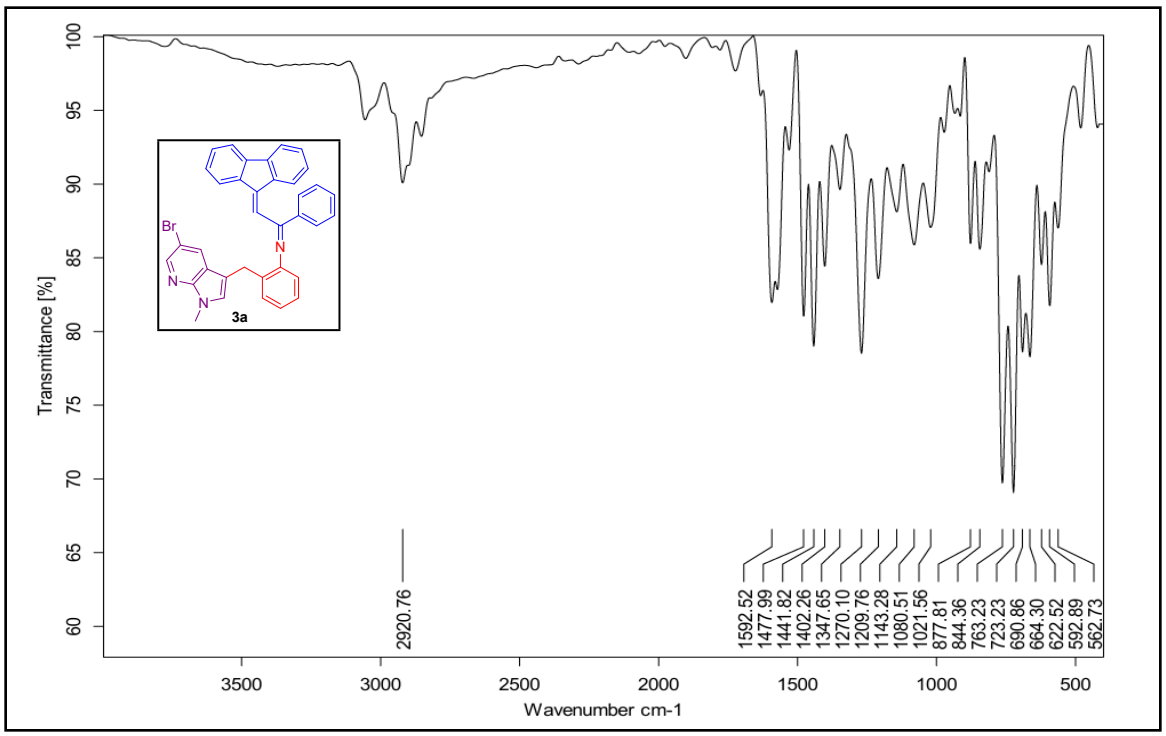


Fig 5 FT-IR spectrum of compound **3a**

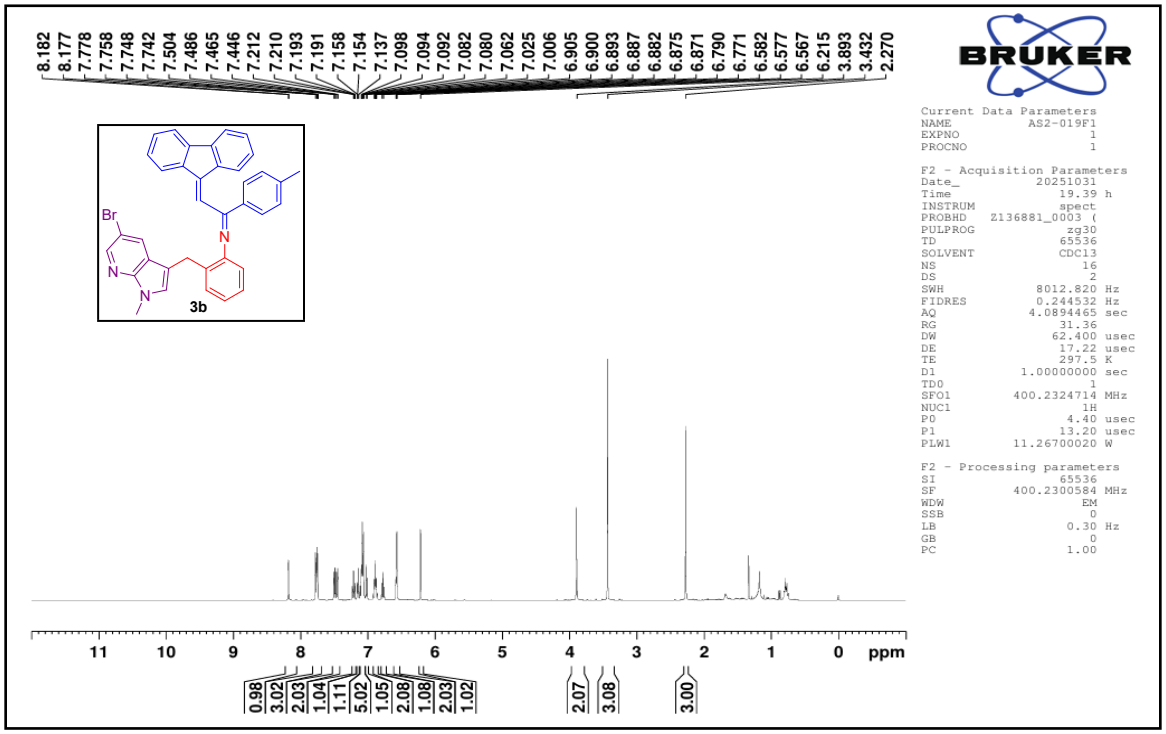


Fig 6 ^{1}H NMR spectrum of **3b**

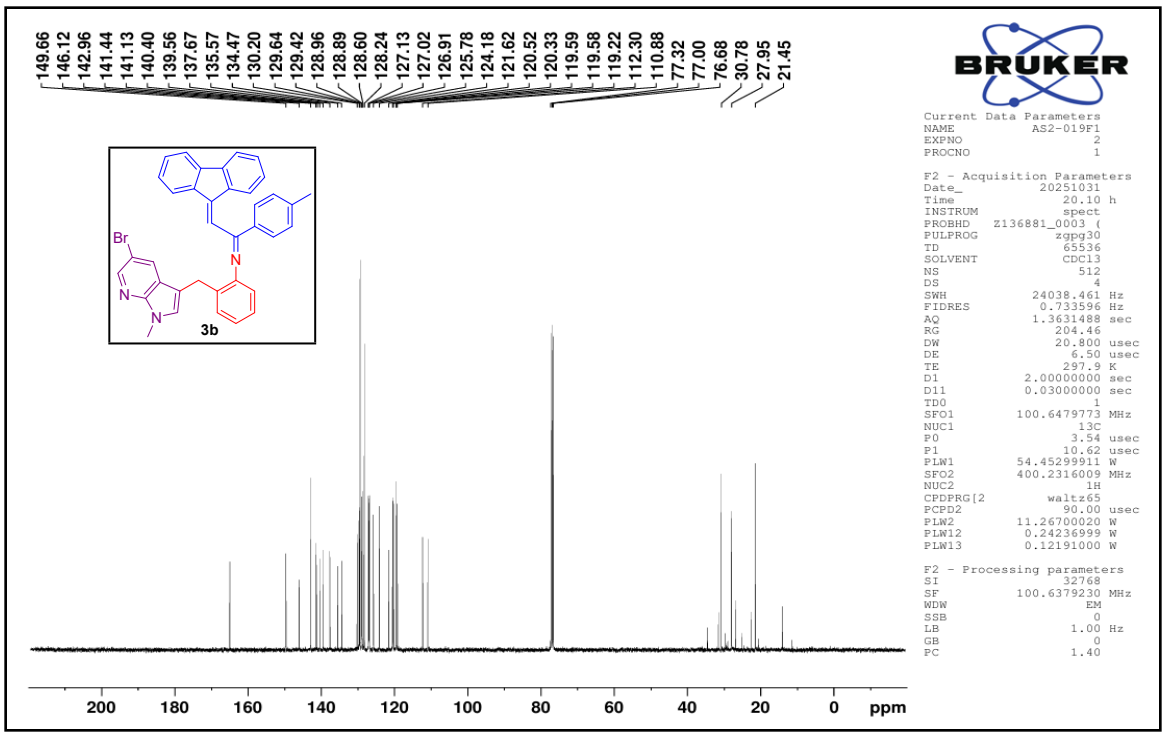


Fig 7 ^{13}C NMR spectrum of compound **3b**

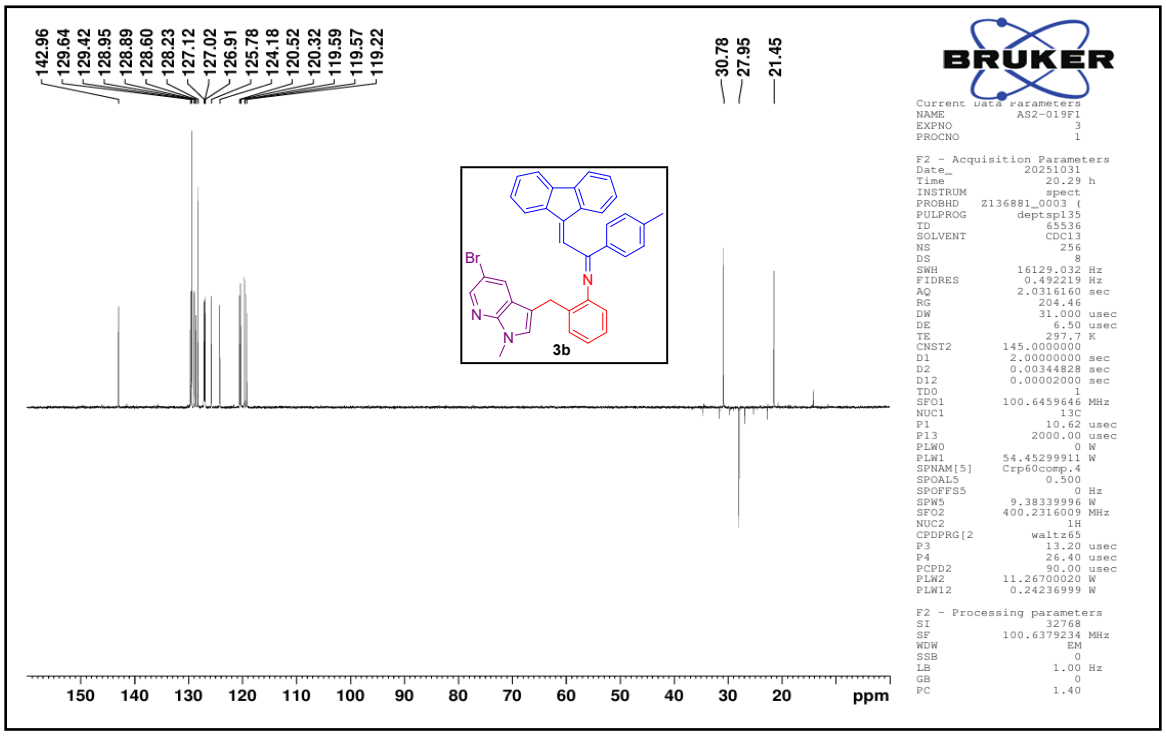


Fig 8 DEPT-135 NMR spectrum of compound **3b**

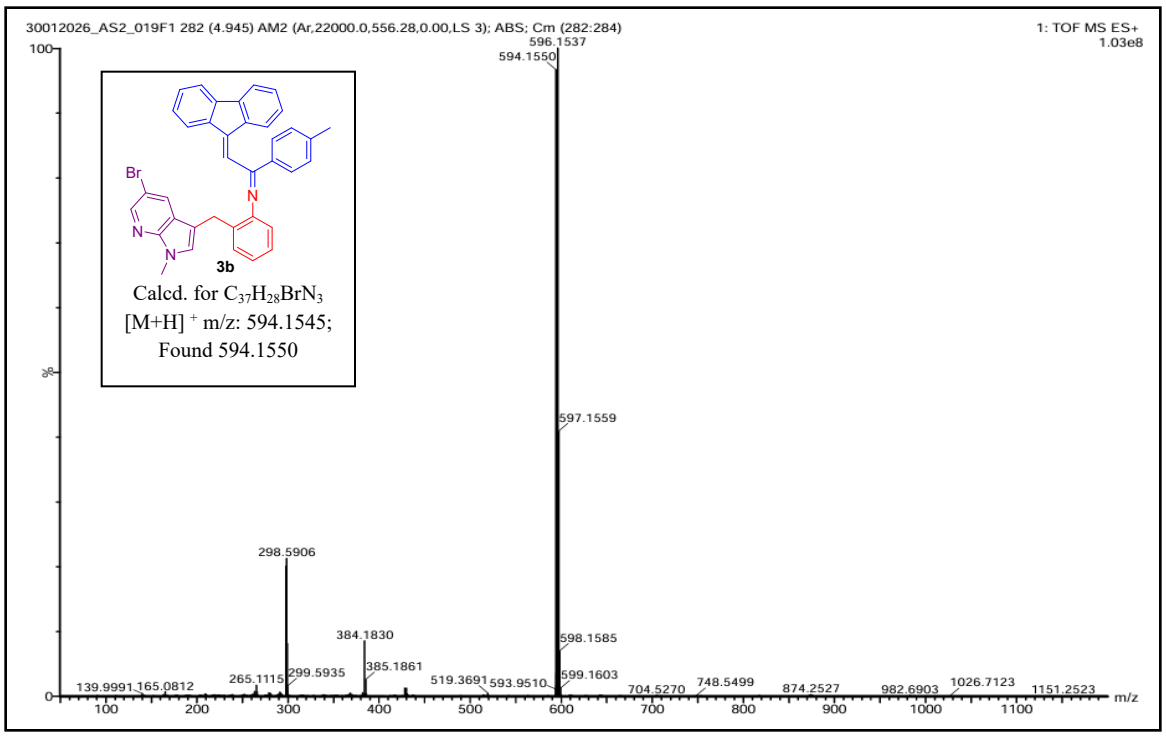


Fig 9 HRMS spectrum of compound **3b**

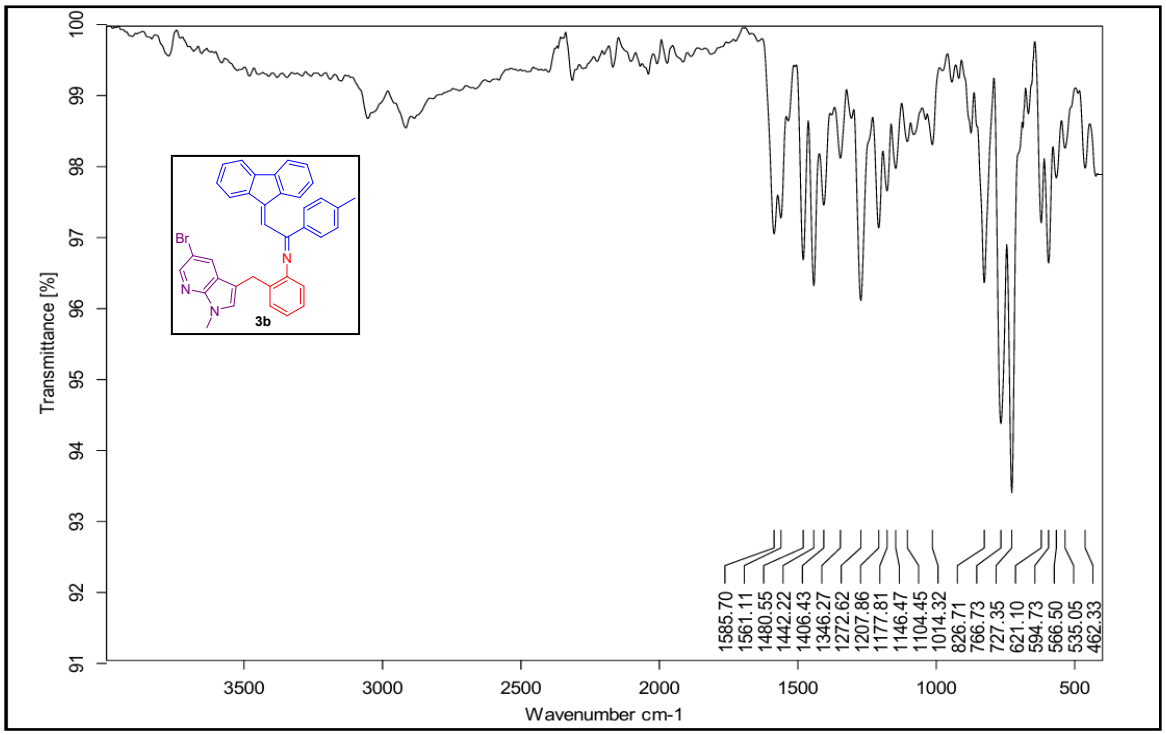


Fig 10 FT-IR spectrum of compound **3b**

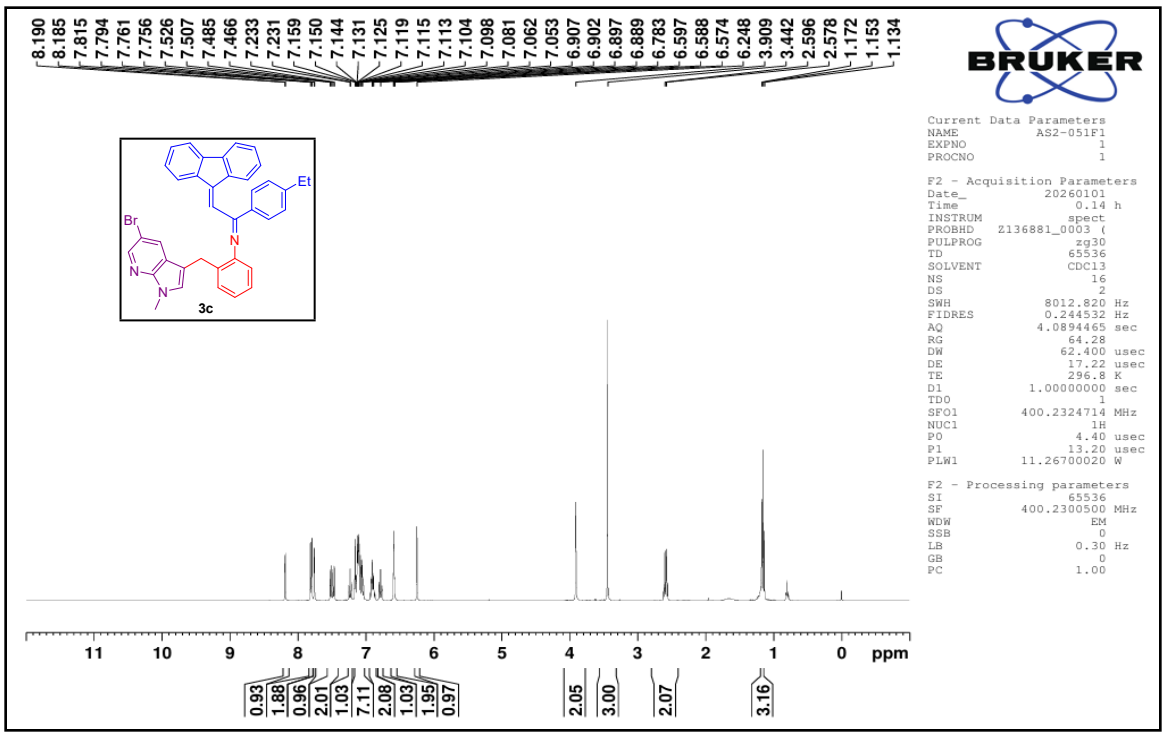


Fig 11 ^{1}H NMR spectrum of **3c**

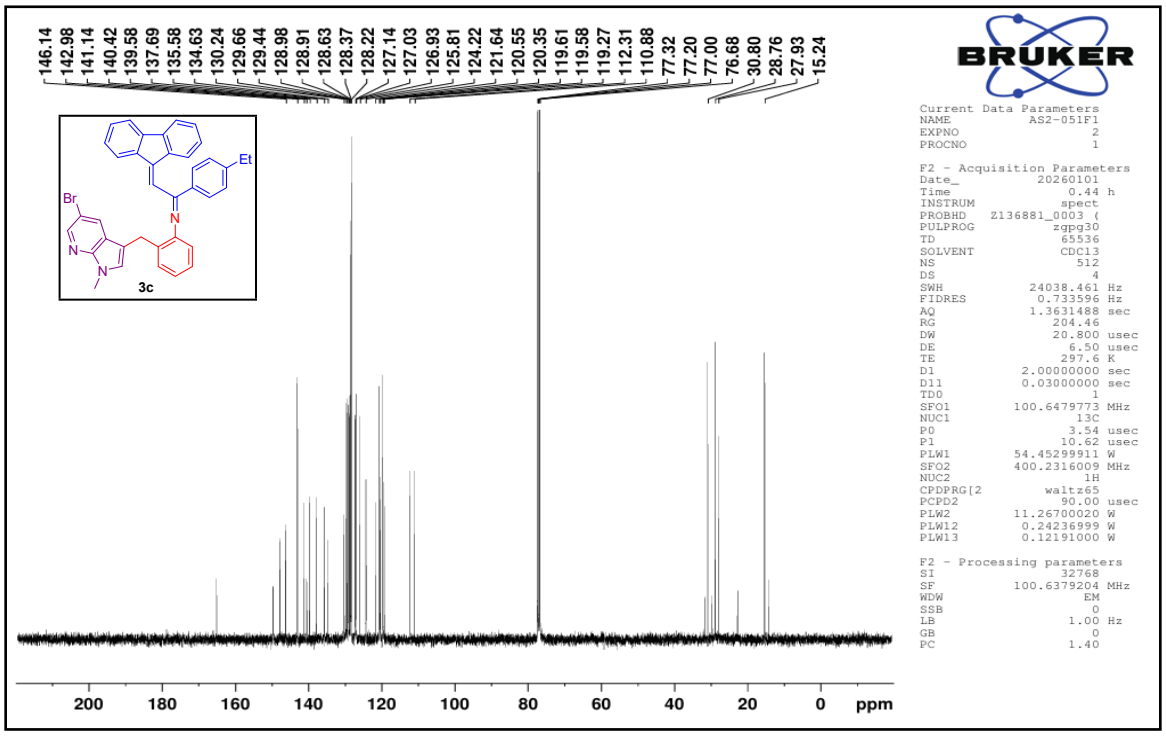


Fig 12 ^{13}C NMR spectrum of compound **3c**

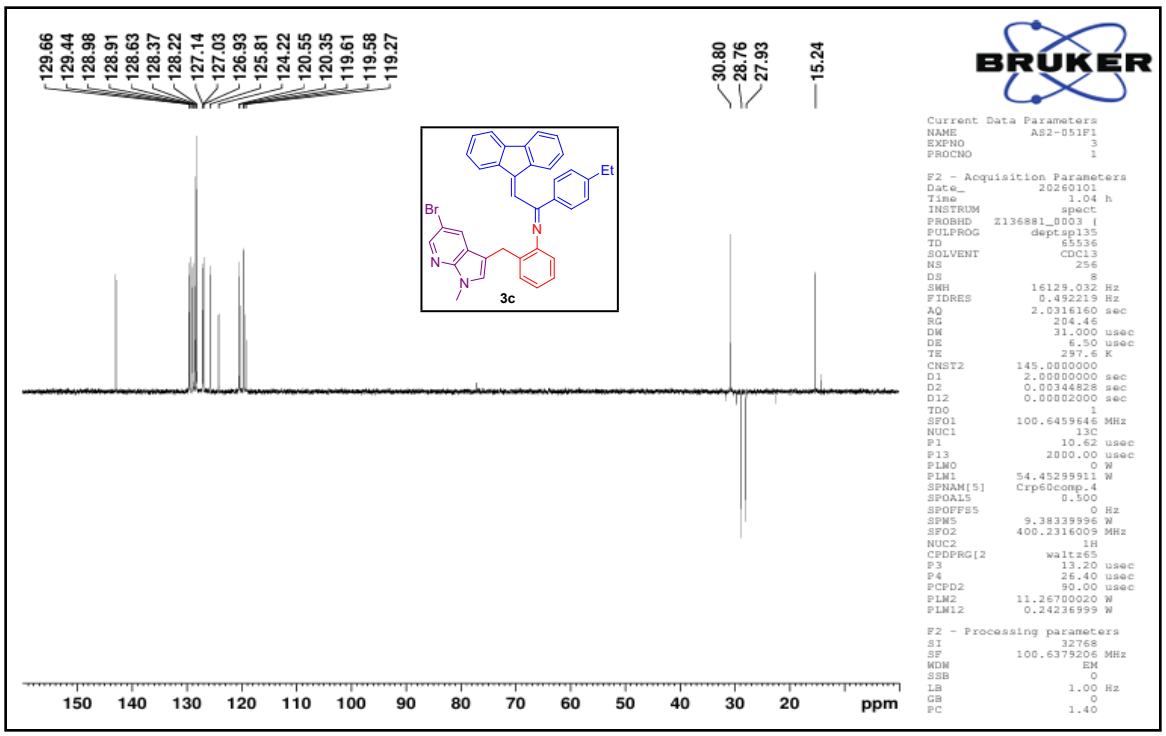


Fig 13 DEPT-135 NMR spectrum of compound **3c**

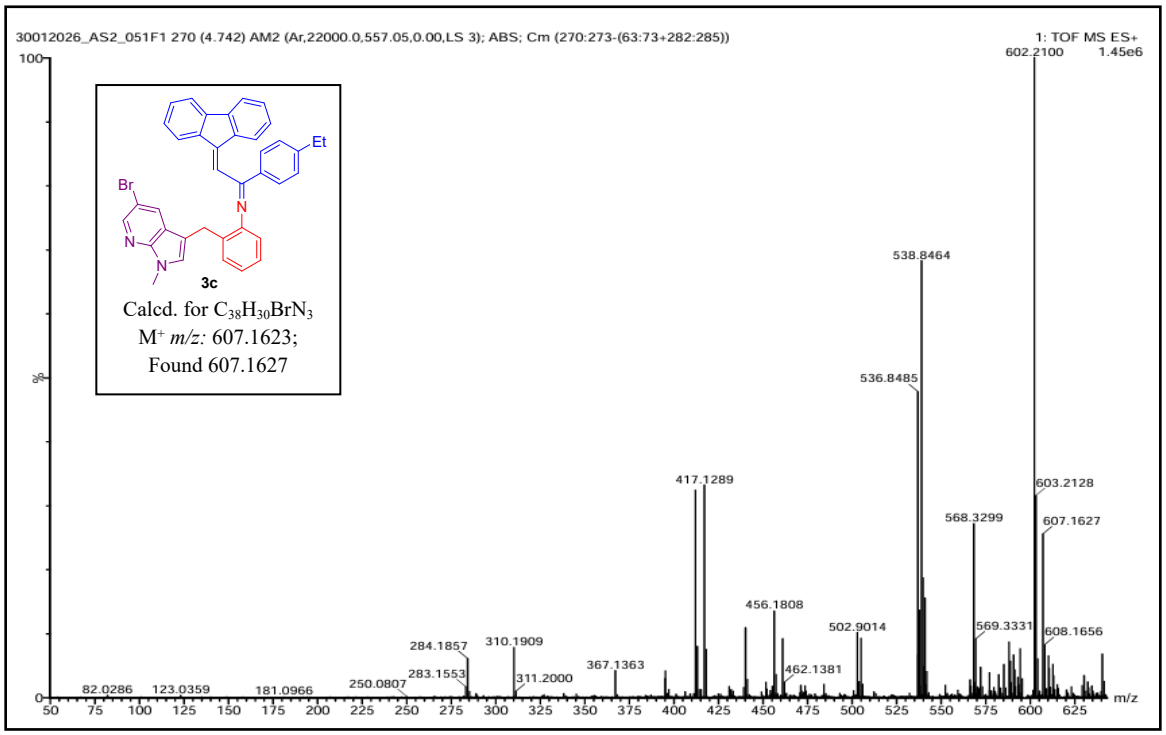


Fig 14 HRMS spectrum of compound **3c**

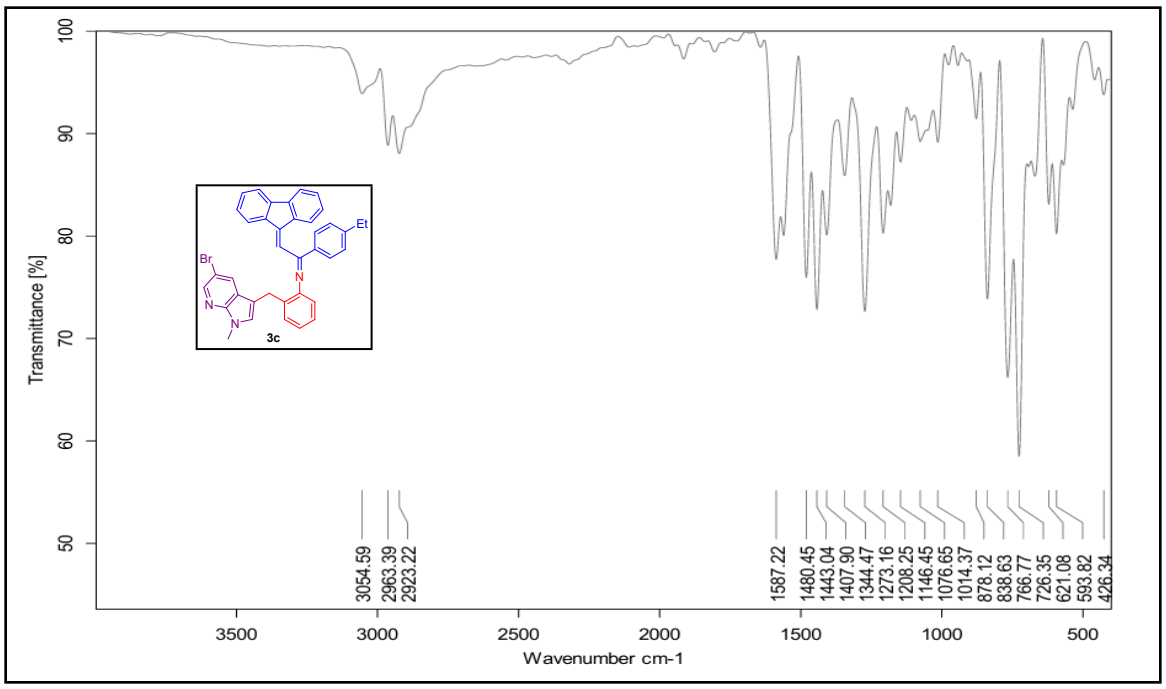


Fig 15 FT-IR spectrum of compound **3c**

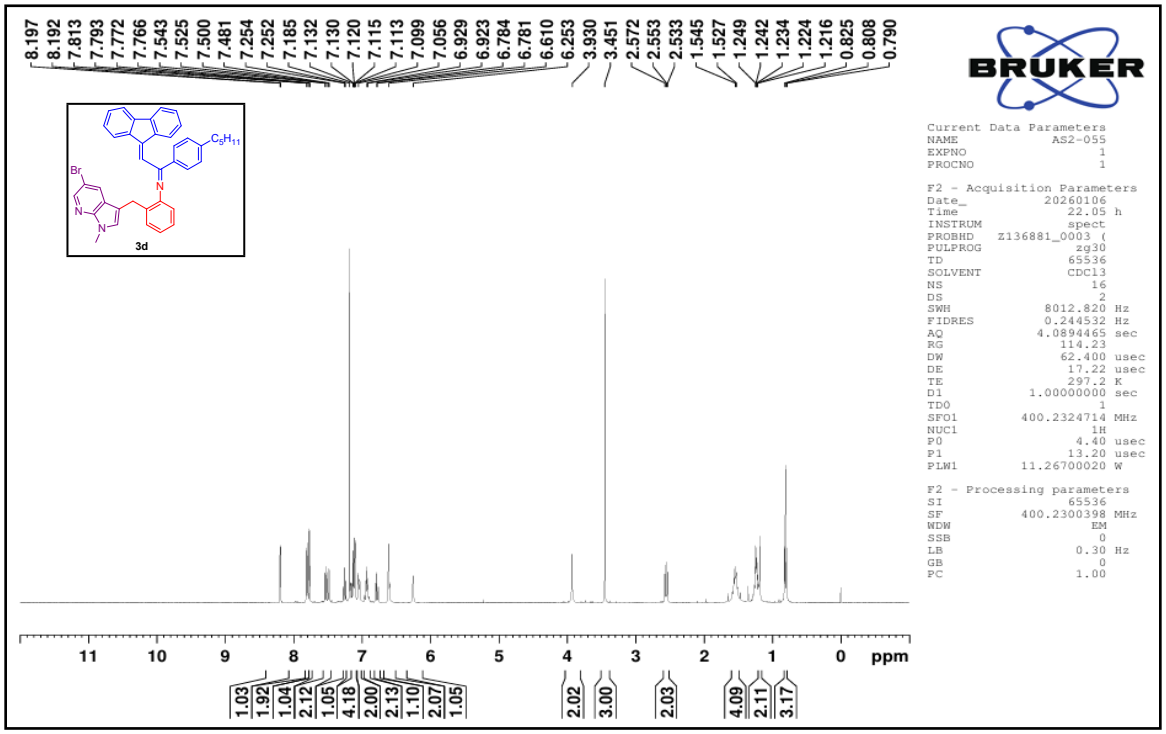


Fig 16 ^{1}H NMR spectrum of **3d**

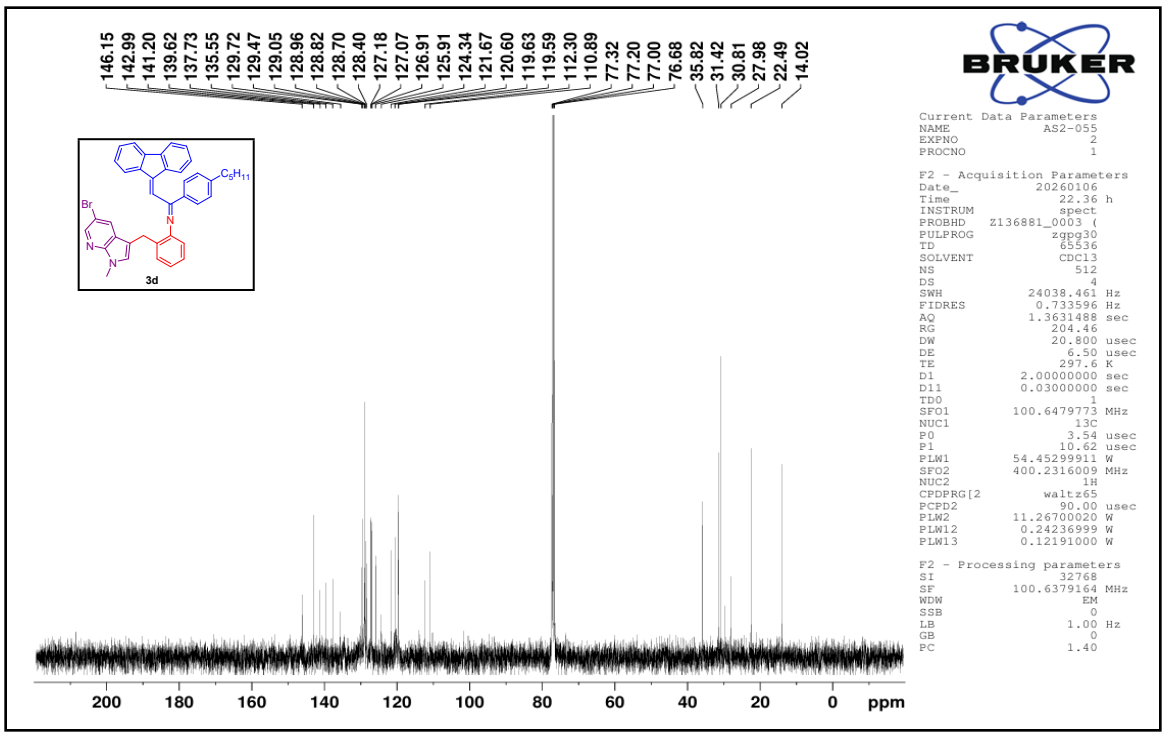


Fig 17 ^{13}C NMR spectrum of compound **3d**

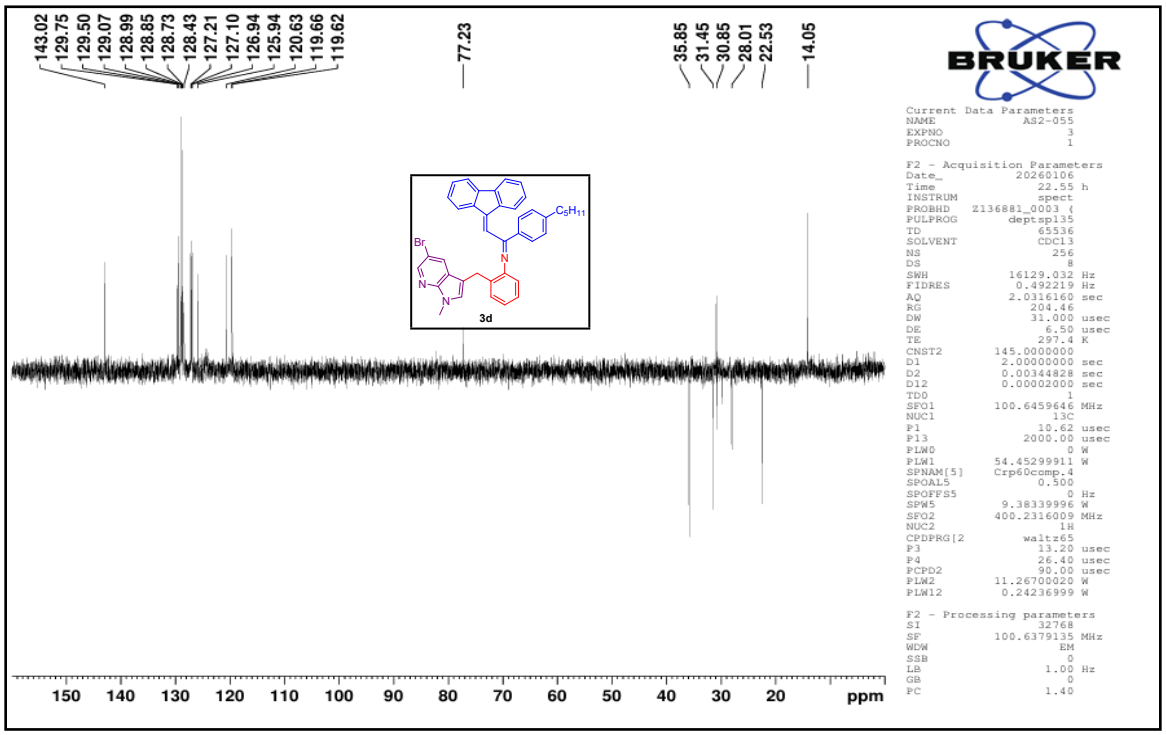


Fig 18 DEPT-135 NMR spectrum of compound **3d**

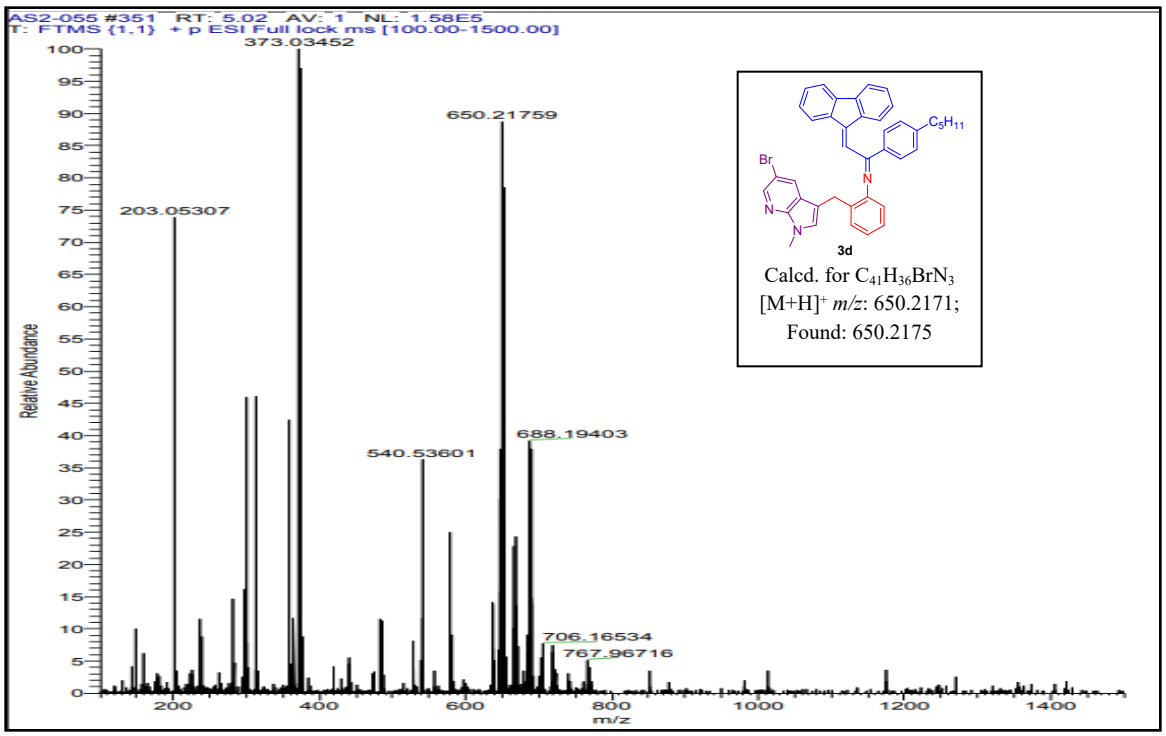


Fig 19 HRMS spectrum of compound **3d**

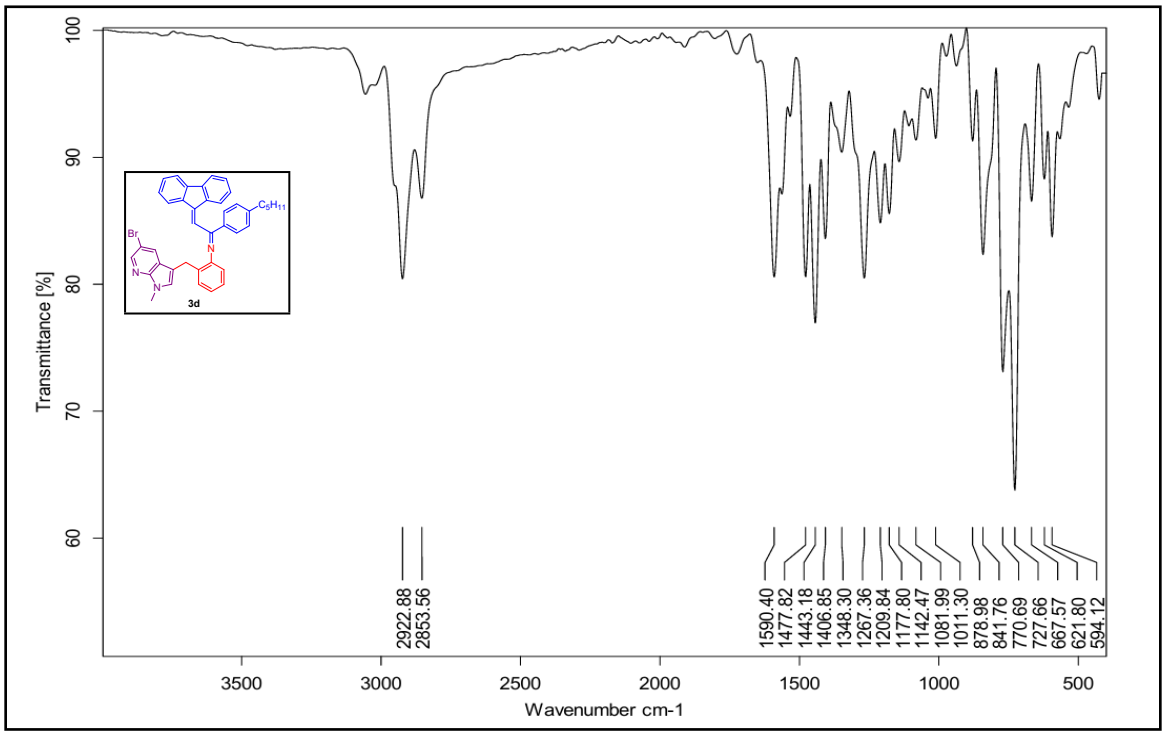


Fig 20 FT-IR spectrum of compound **3d**

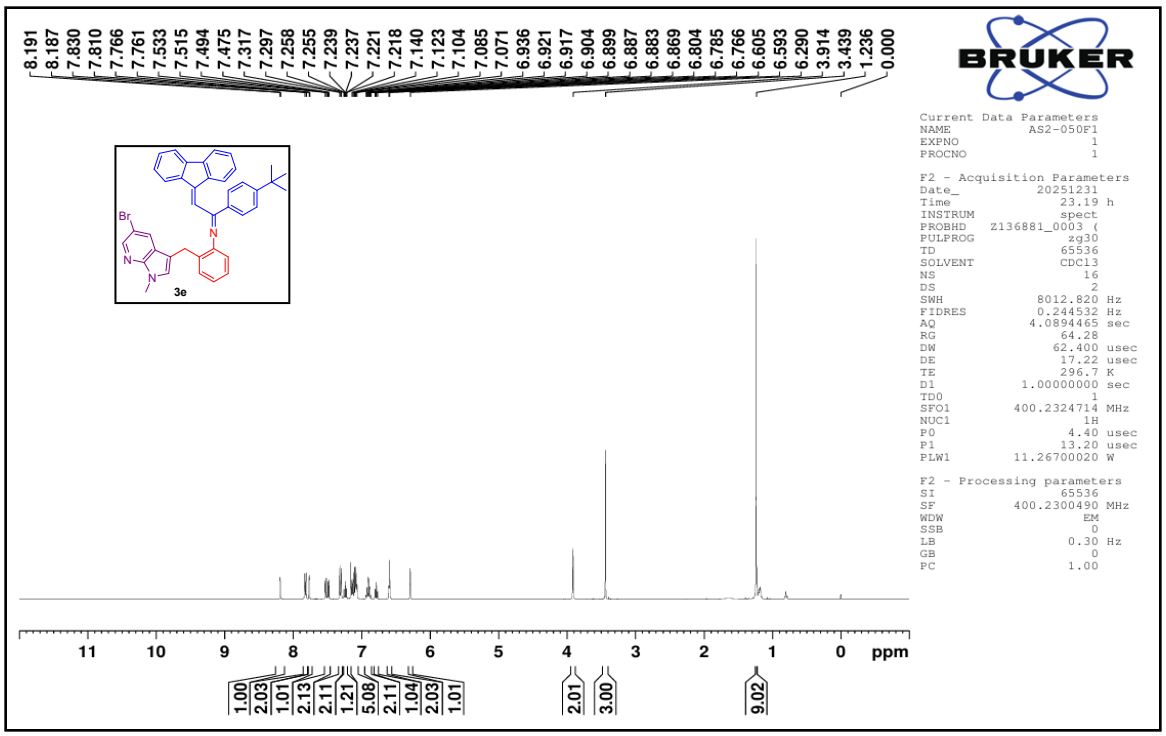


Fig 21 ^{1}H NMR spectrum of **3e**

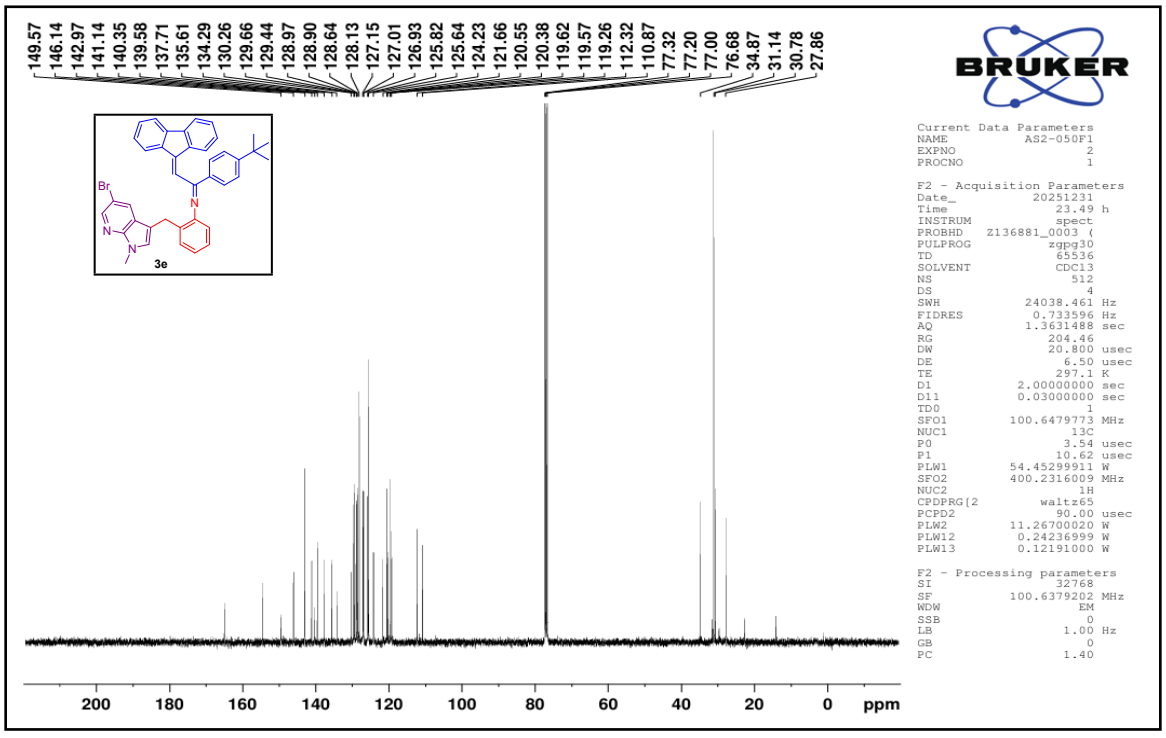


Fig 22 ^{13}C NMR spectrum of compound **3e**

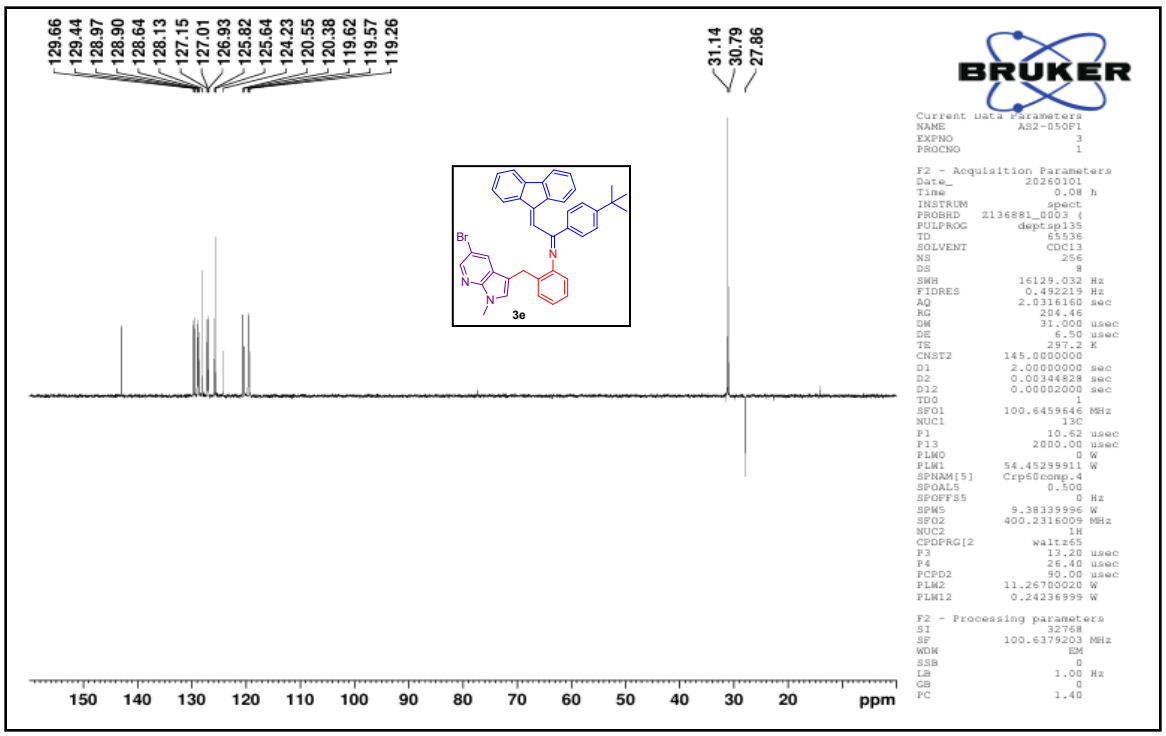


Fig 23 DEPT-135 NMR spectrum of compound **3e**

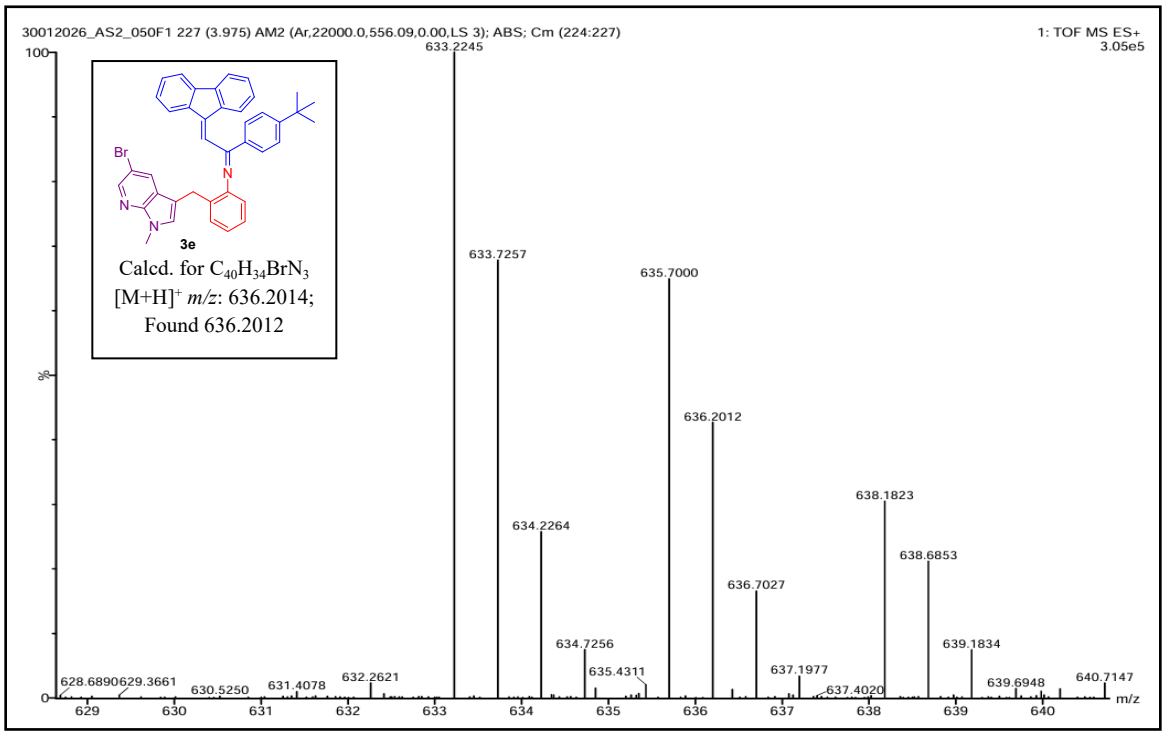


Fig 24 HRMS spectrum of compound **3e**

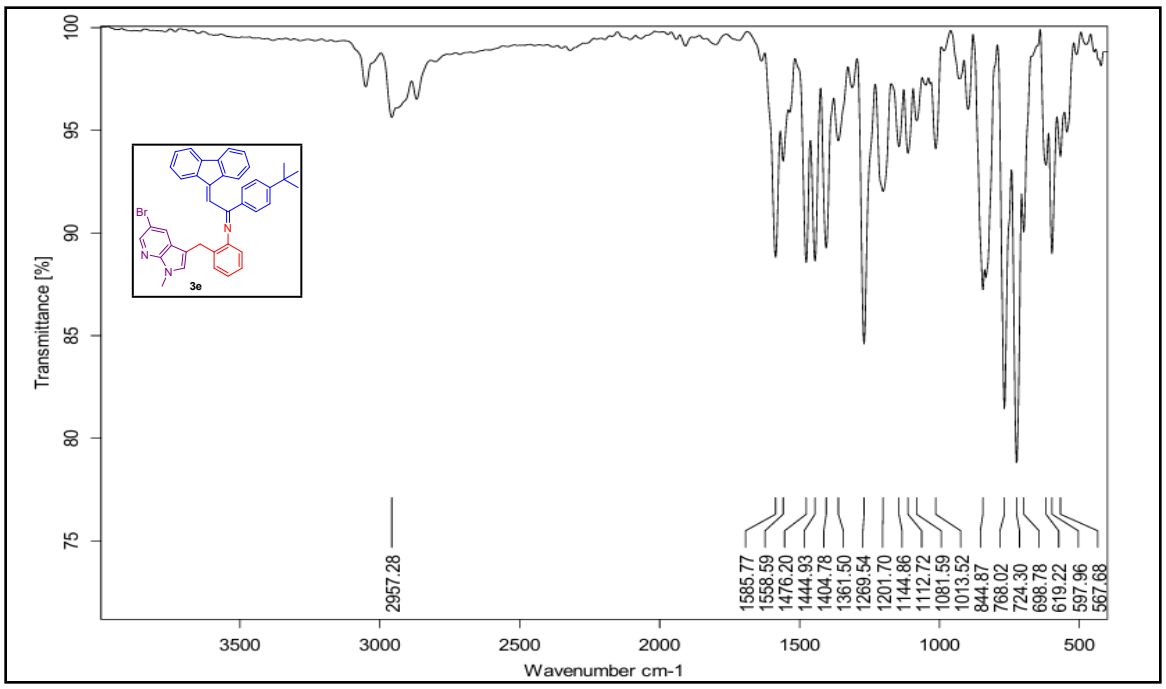


Fig 25 FT-IR spectrum of compound **3e**

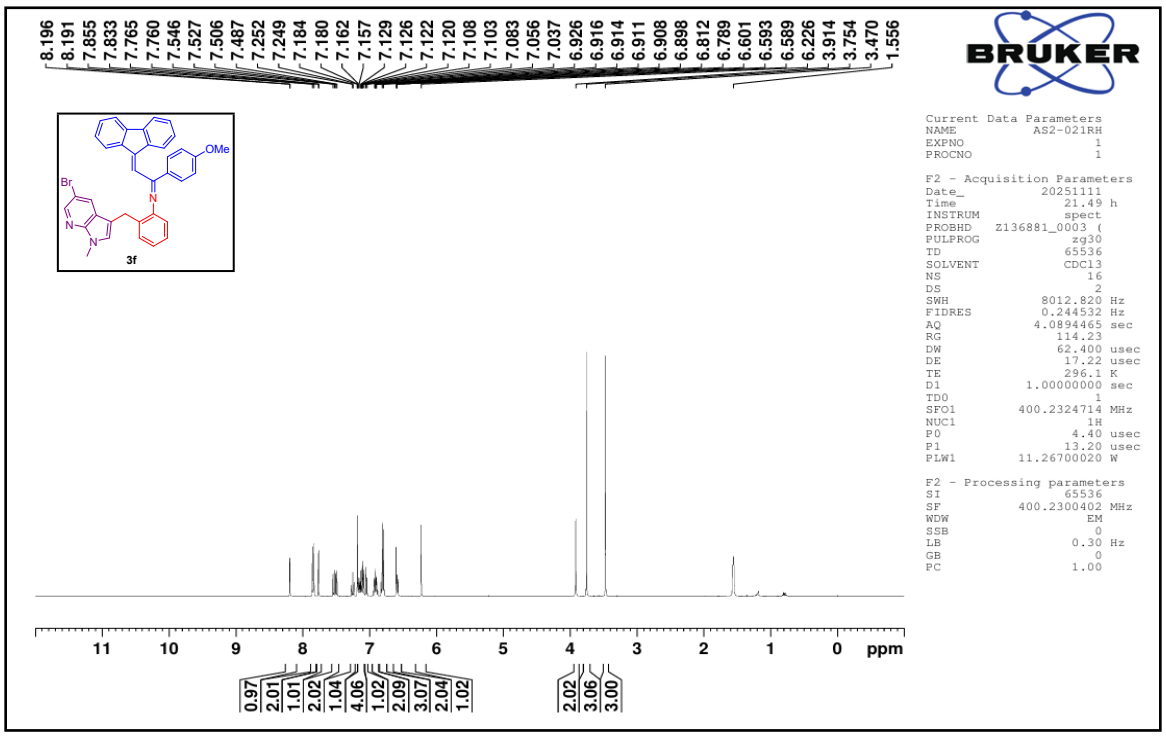


Fig 26 ^{1}H NMR spectrum of **3f**

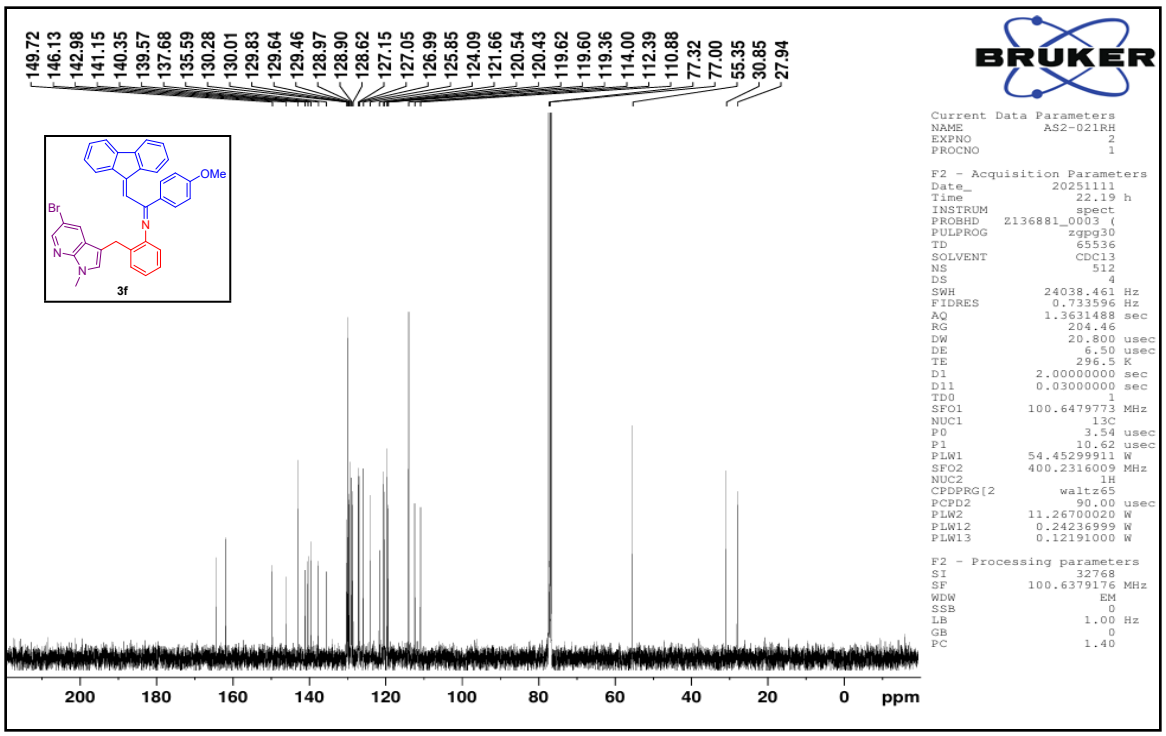


Fig 27 ^{13}C NMR spectrum of compound **3f**

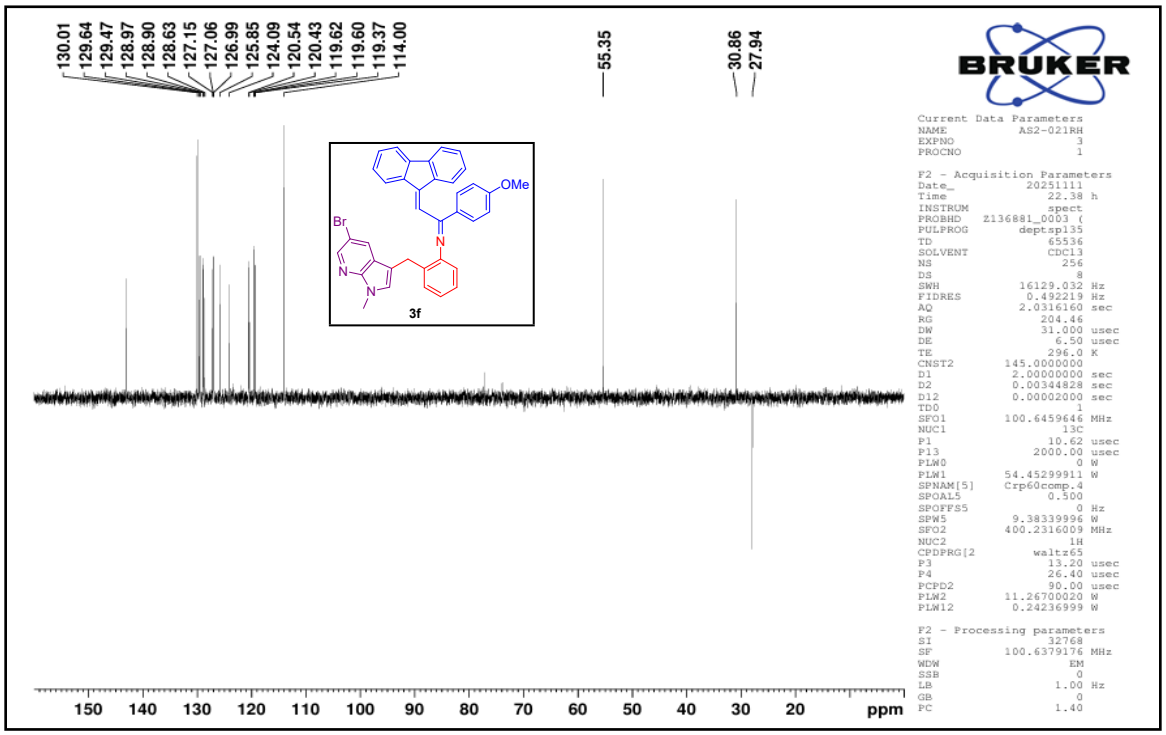


Fig 28 DEPT-135 NMR spectrum of compound **3f**

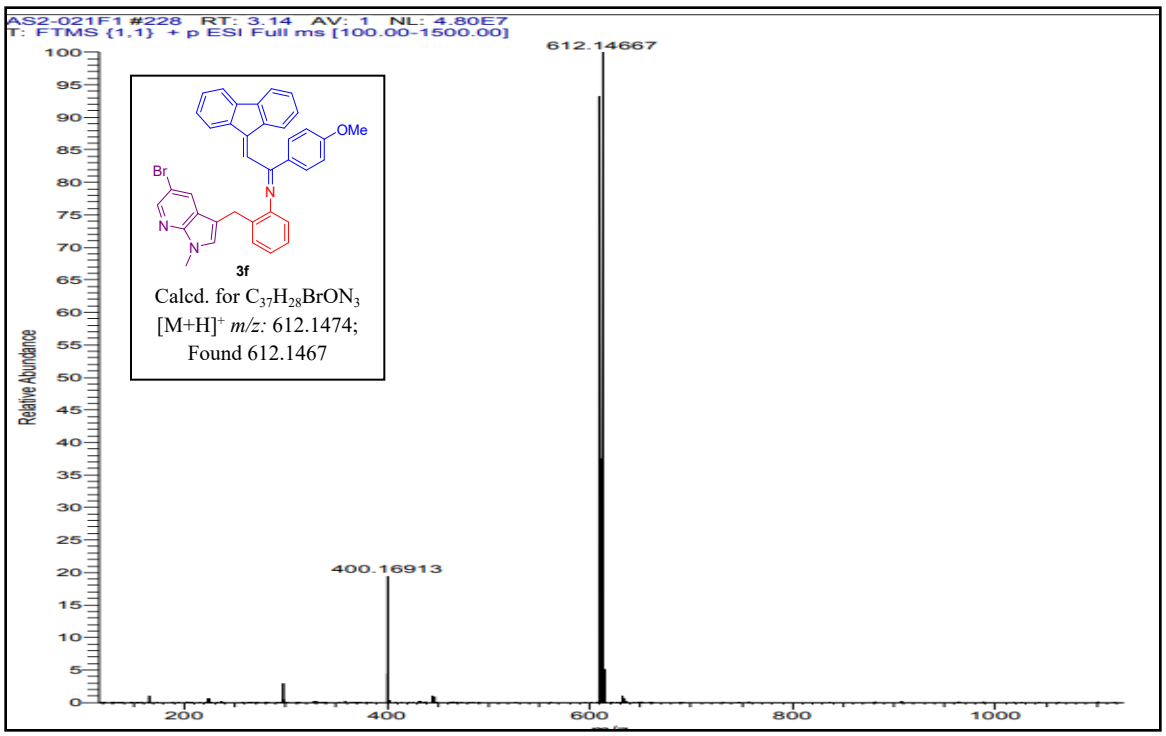


Fig 29 HRMS spectrum of compound **3f**

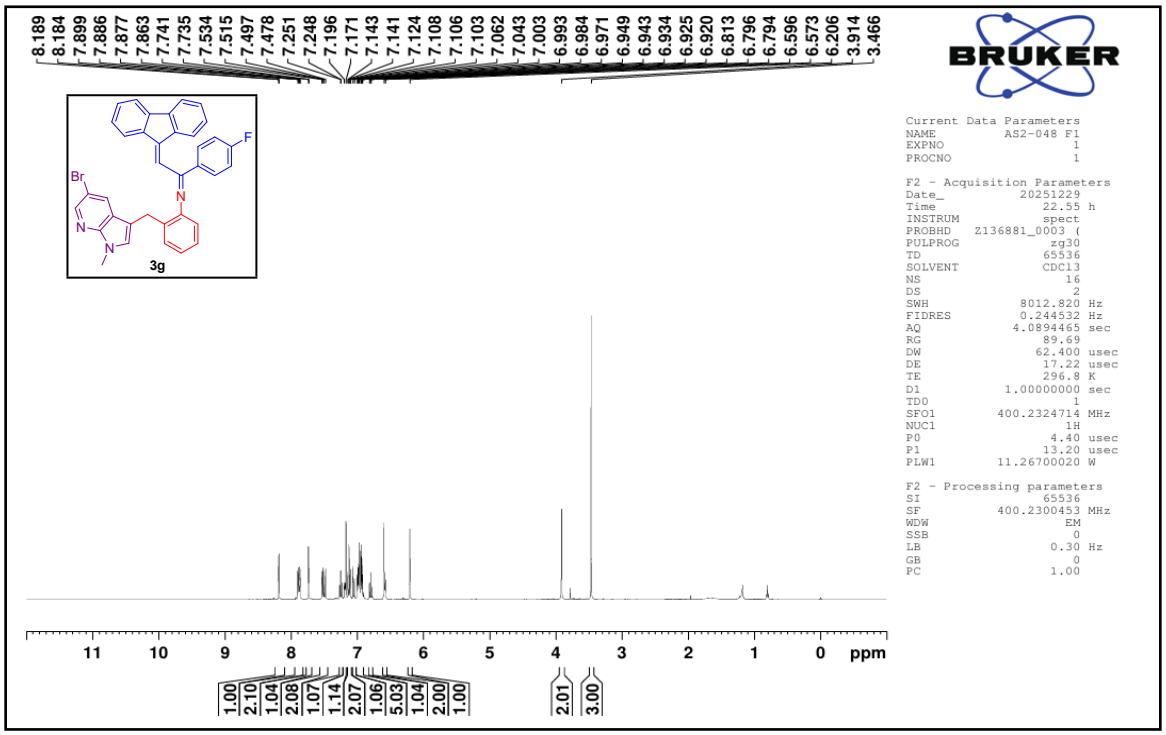


Fig 30 ^{1}H NMR spectrum of **3g**

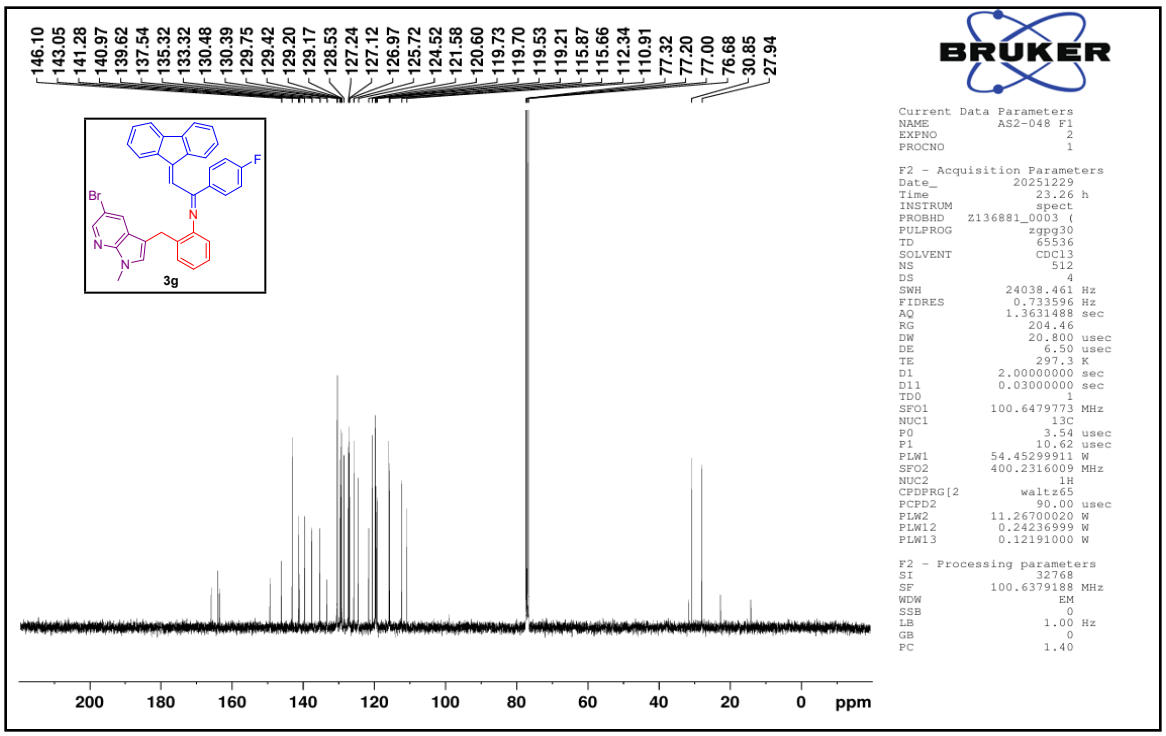


Fig 31 ^{13}C NMR spectrum of compound **3g**

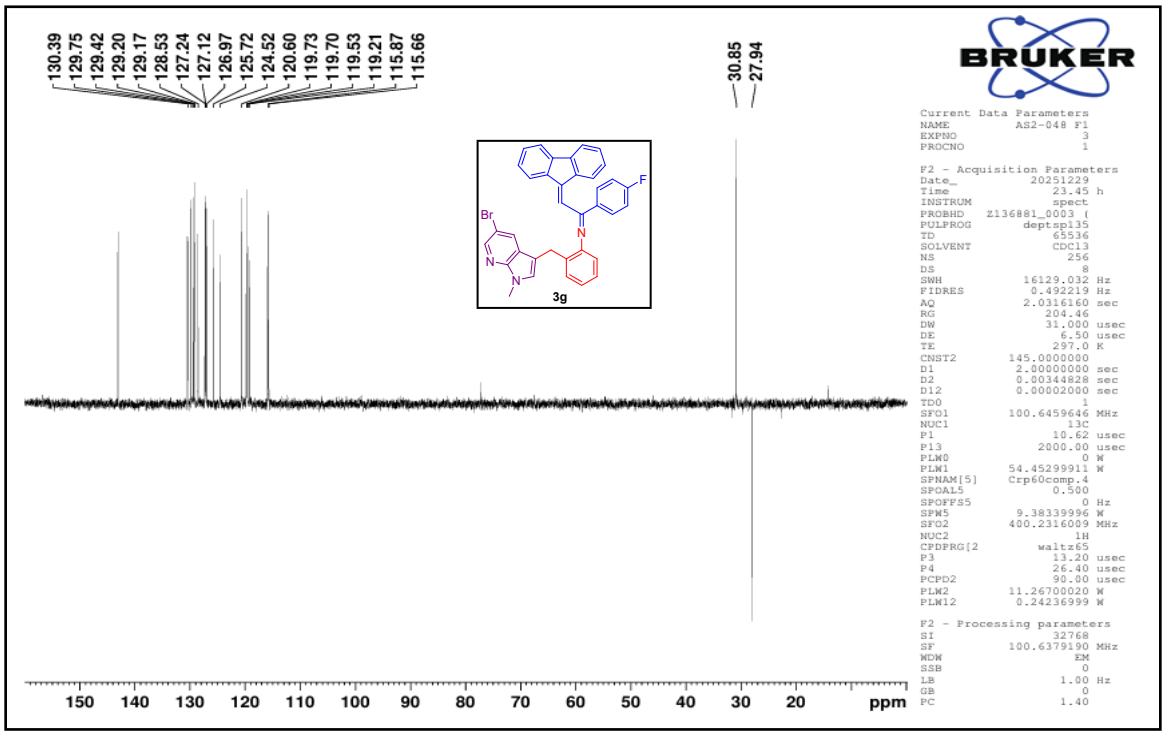


Fig 32 DEPT-135 NMR spectrum of compound **3g**

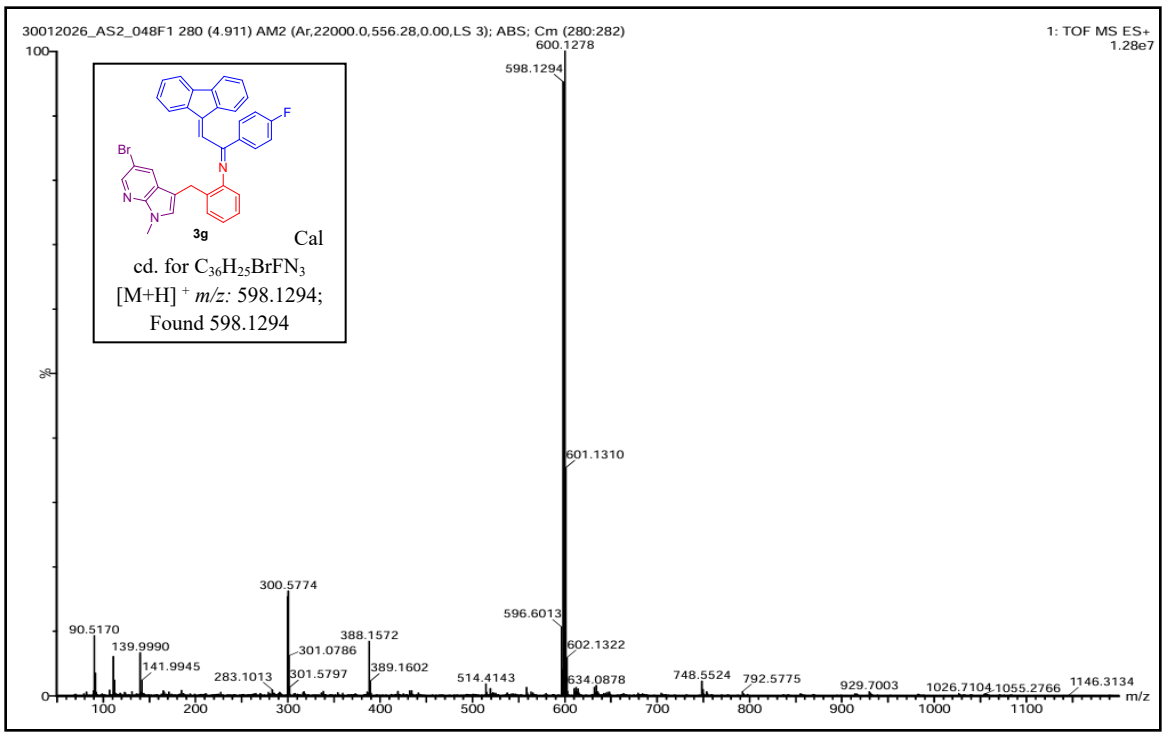


Fig 33 HRMS spectrum of compound **3g**

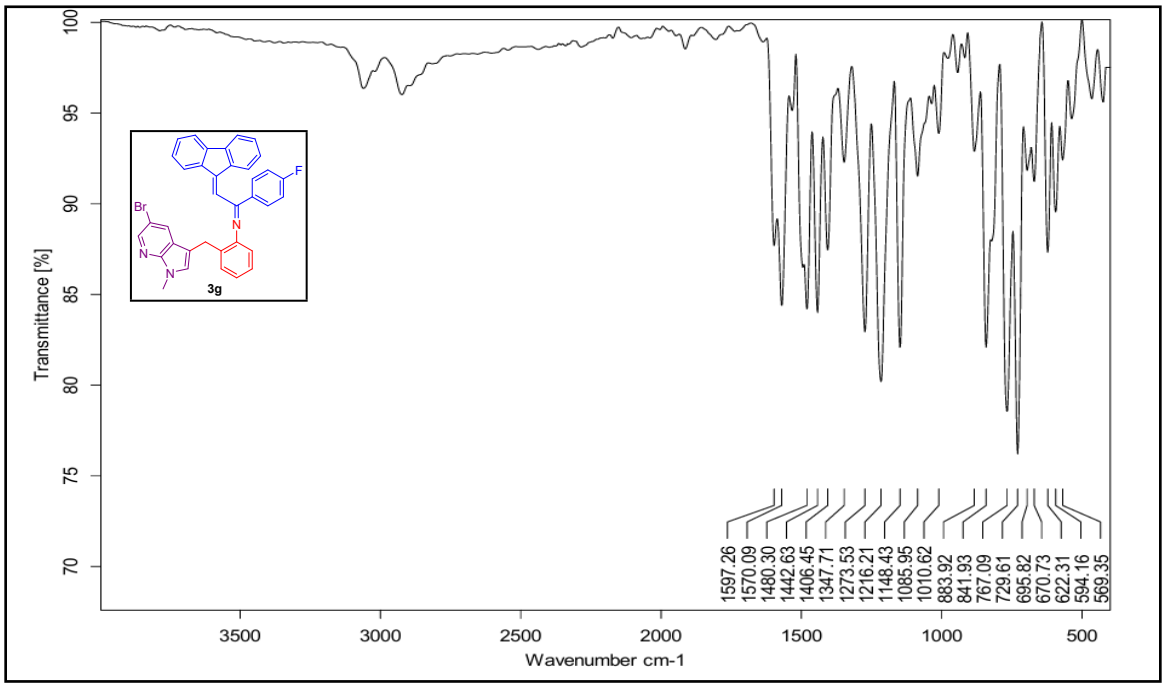


Fig 34 FT-IR spectrum of compound **3g**

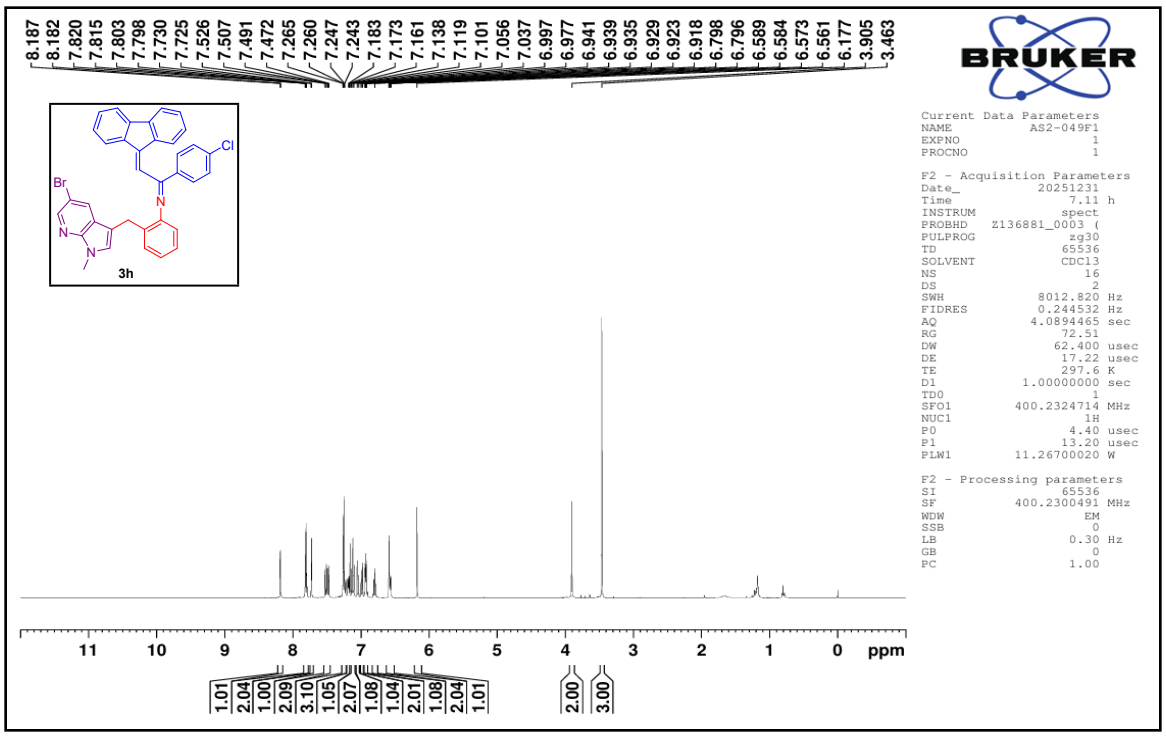


Fig 35 ^{1}H NMR spectrum of compound **3h**

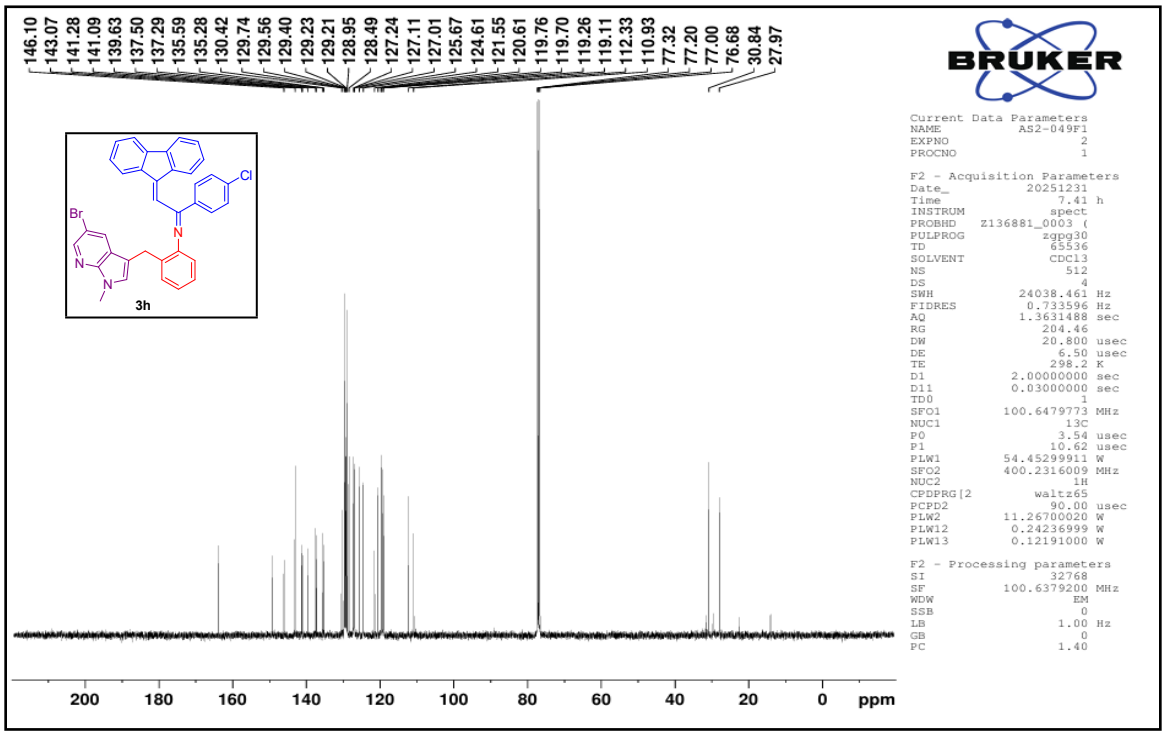


Fig 36 ^{13}C NMR spectrum of compound **3h**

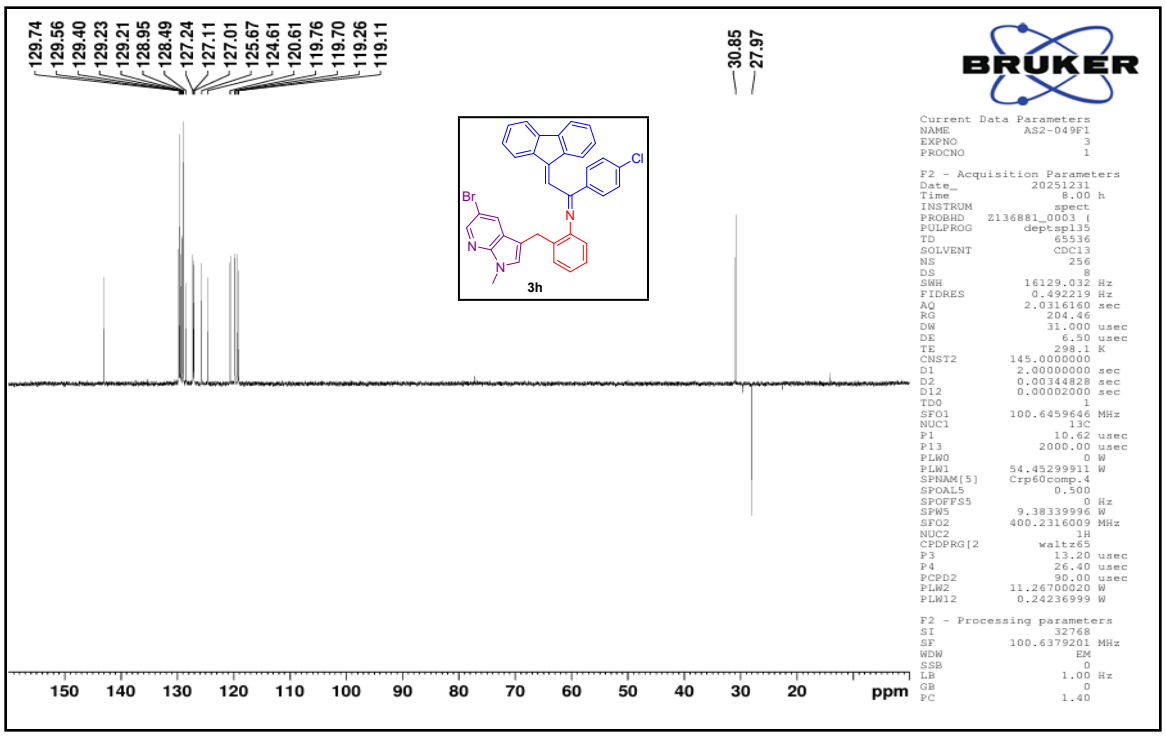


Fig 37 DEPT-135 NMR spectrum of compound **3h**

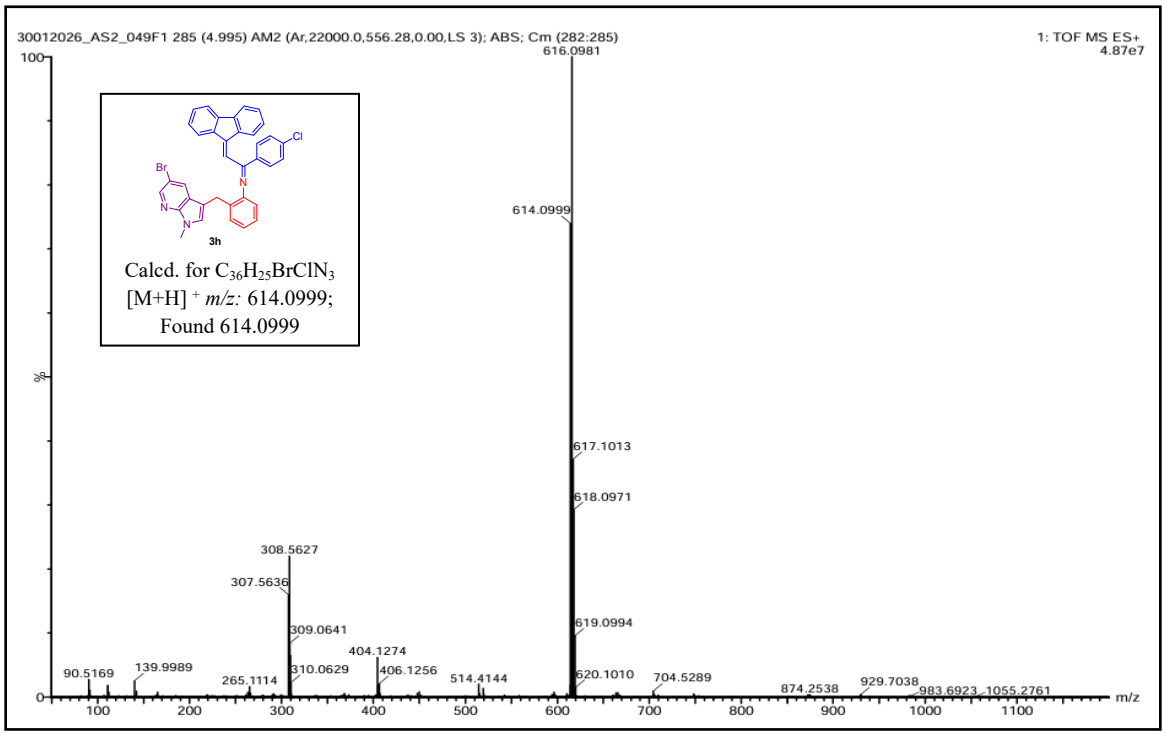


Fig 38 HRMS spectrum of compound **3h**

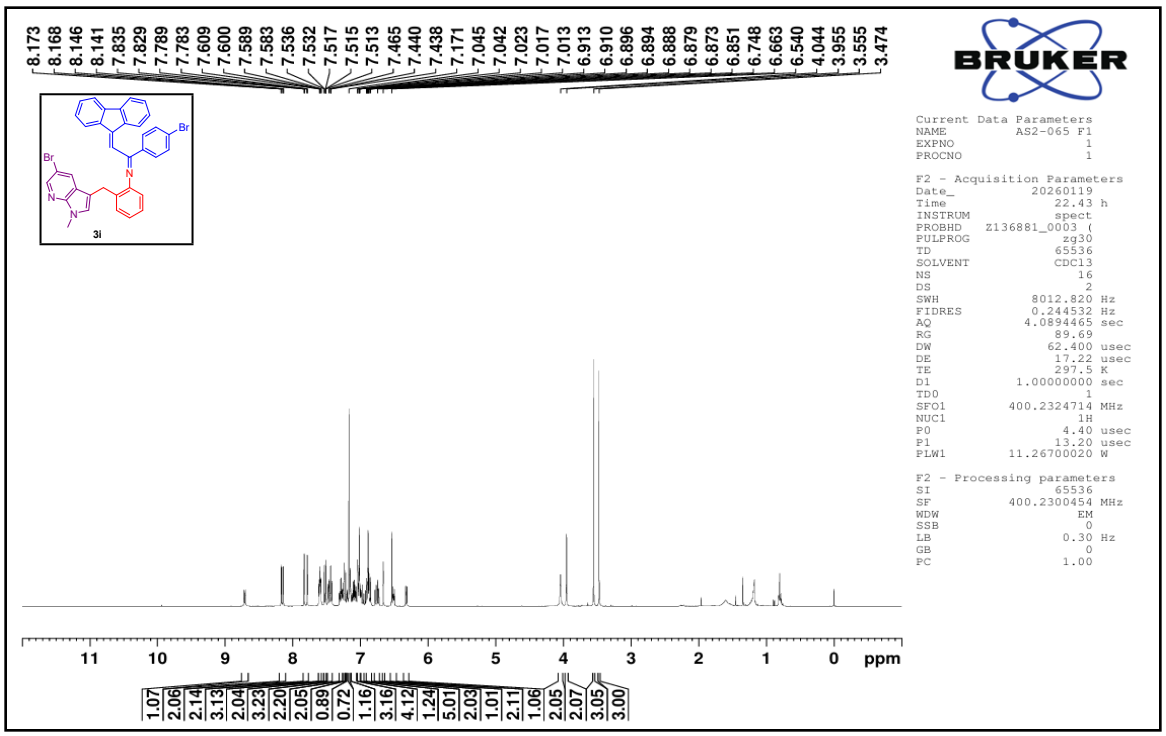


Fig 39 ^{1}H NMR spectrum of **3i**

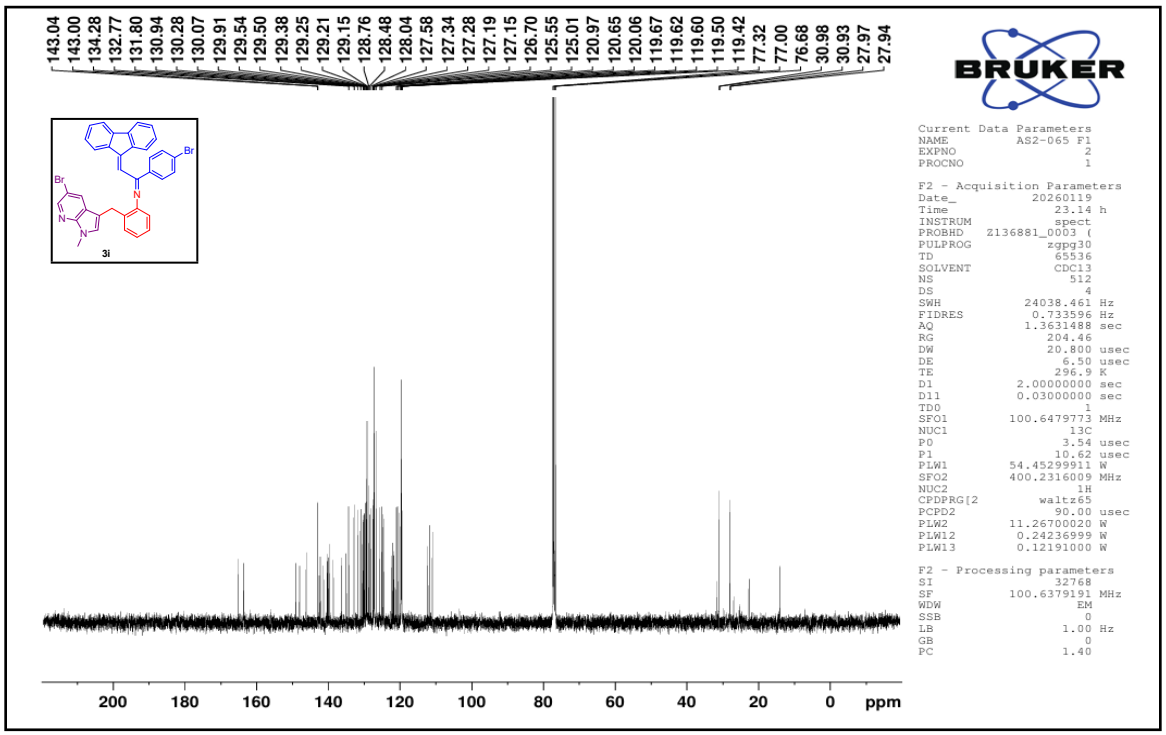


Fig 40 ^{13}C NMR spectrum of compound **3i**

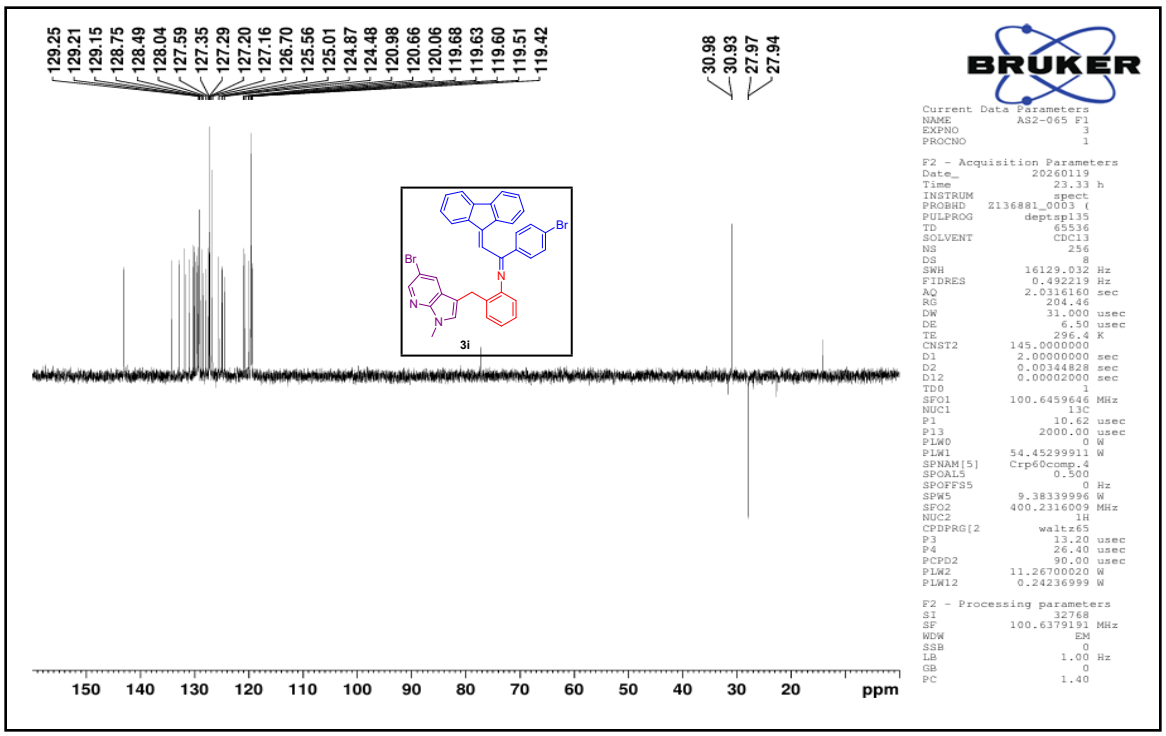


Fig 41 DEPT-135 NMR spectrum of compound **3i**

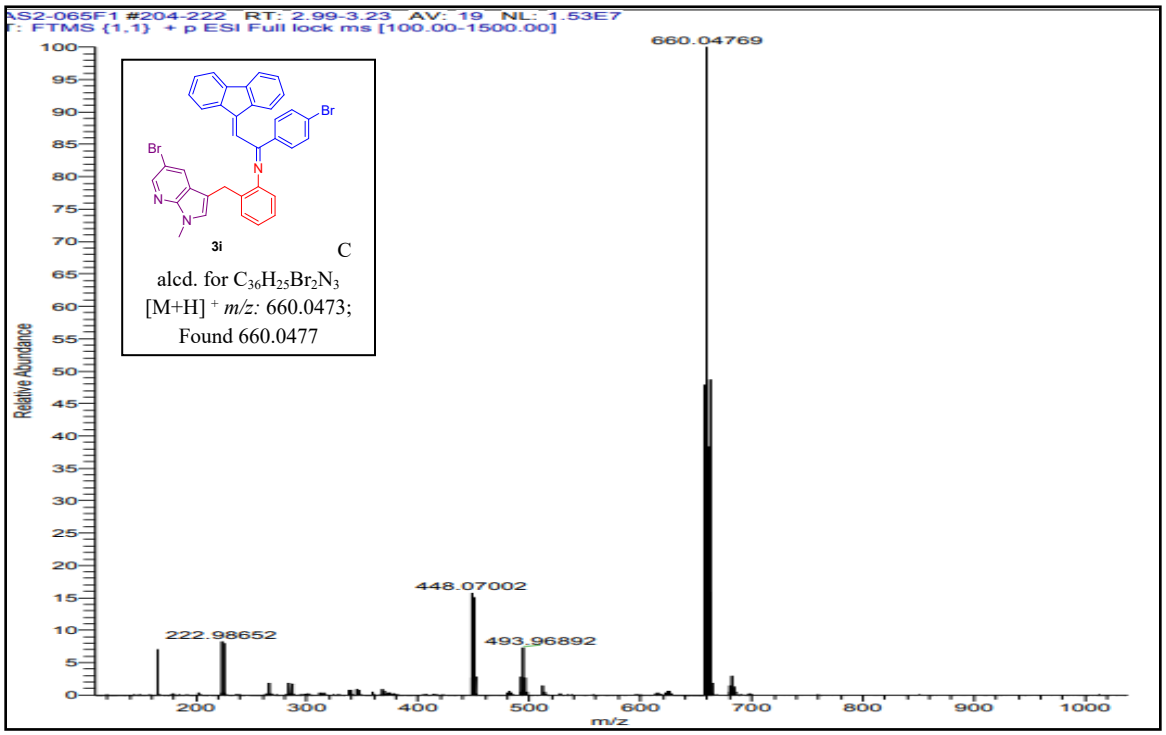


Fig 42 HRMS spectrum of compound **3i**

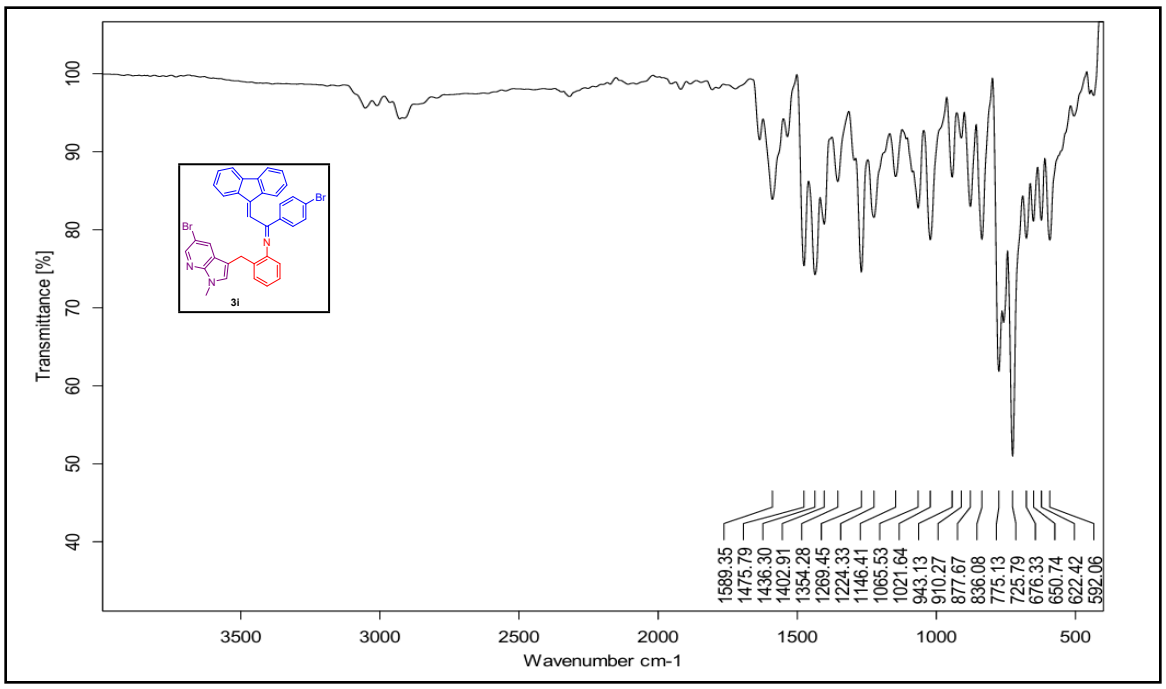


Fig 43 FT-IR spectrum of compound **3i**

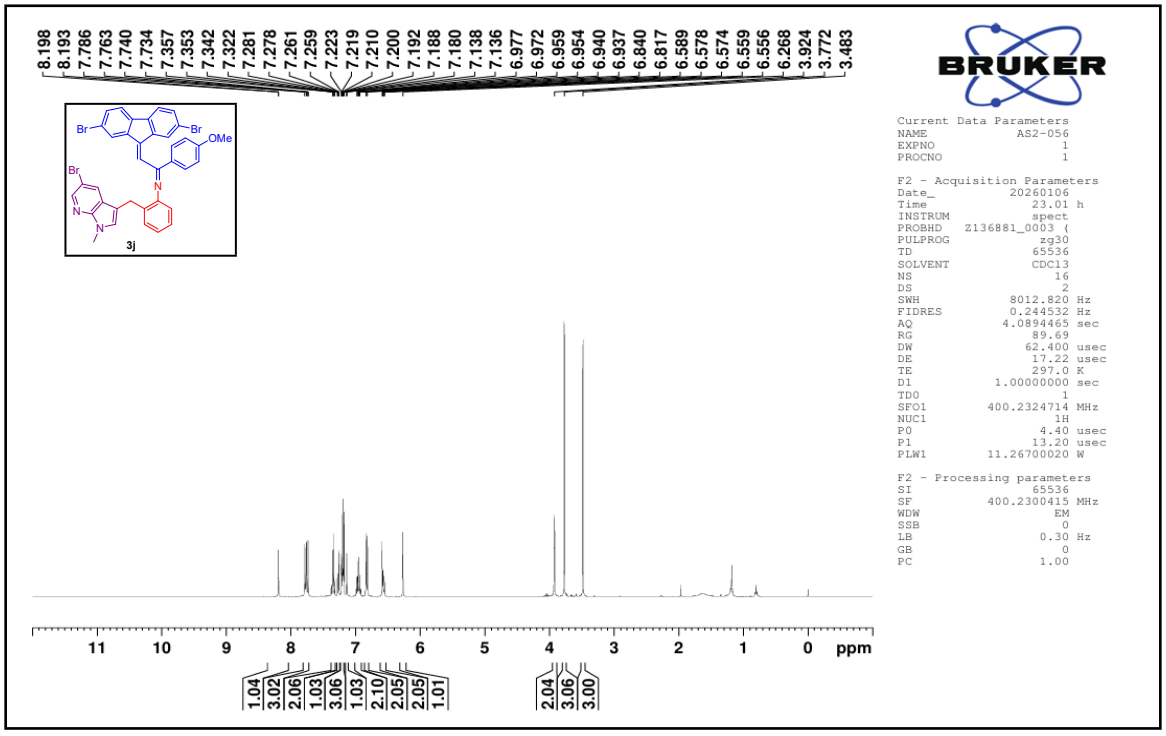


Fig 44 ^{1}H NMR spectrum of **3j**

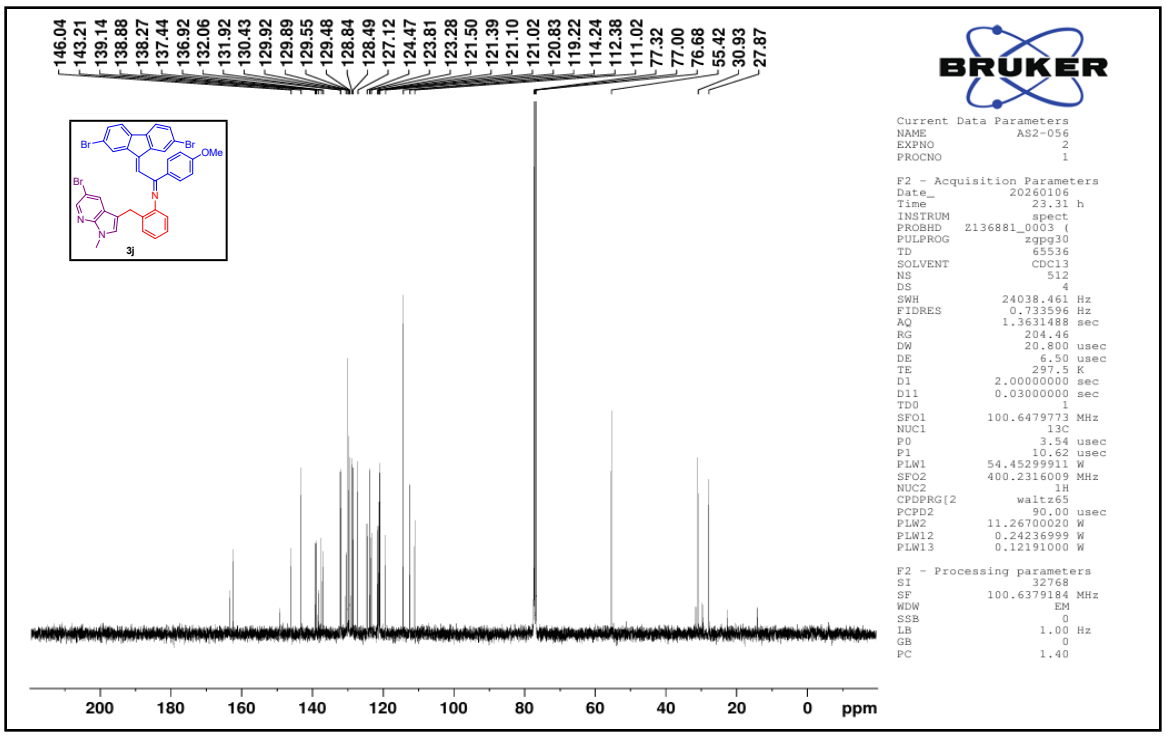


Fig 45 ^{13}C NMR spectrum of compound **3j**

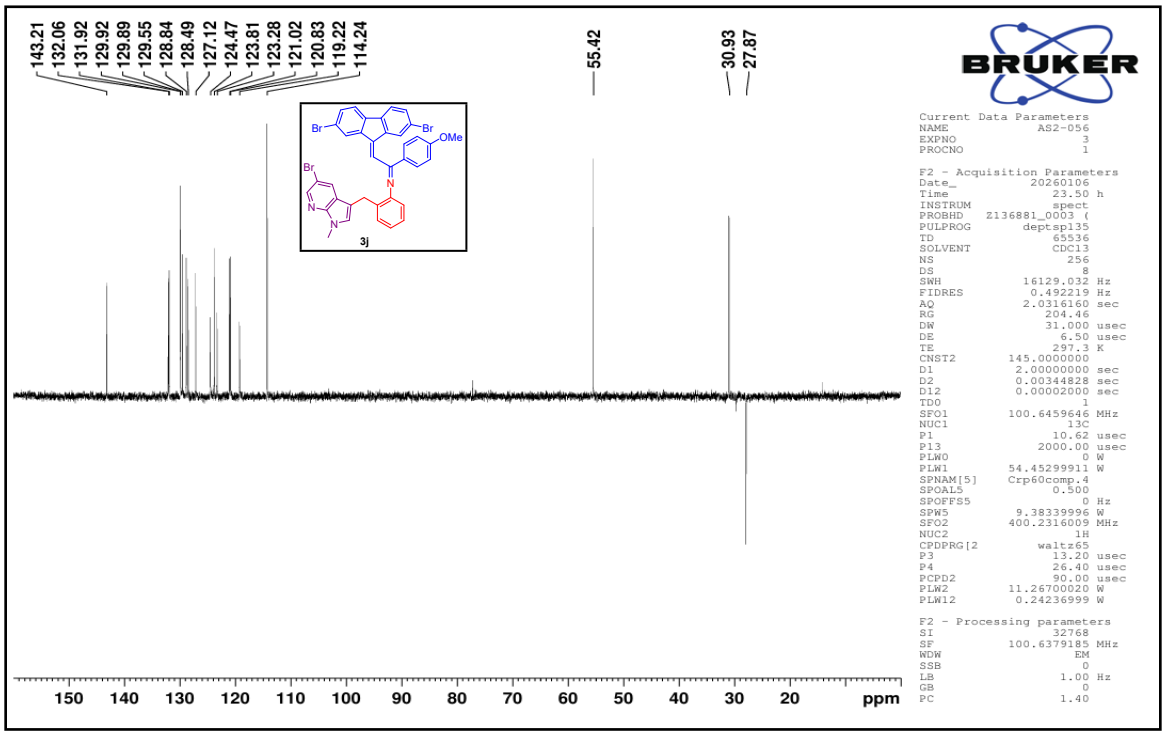


Fig 46 DEPT-135 NMR spectrum of compound **3j**

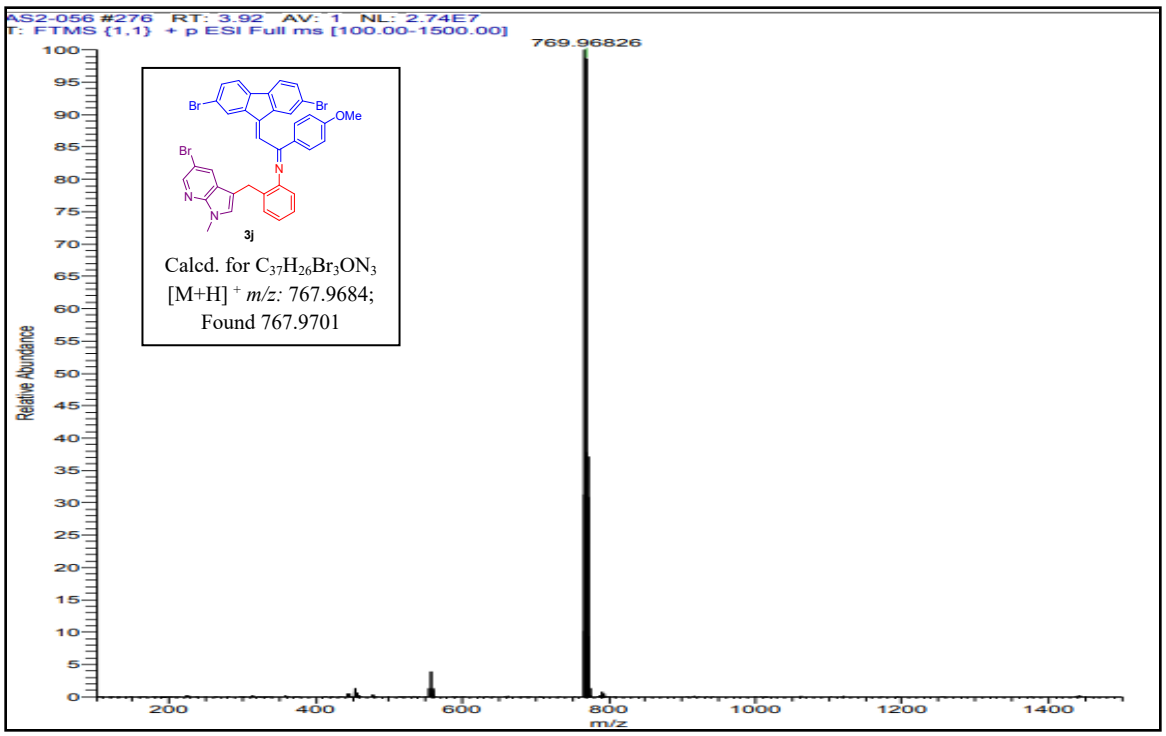


Fig 47 HRMS spectrum of compound **3j**

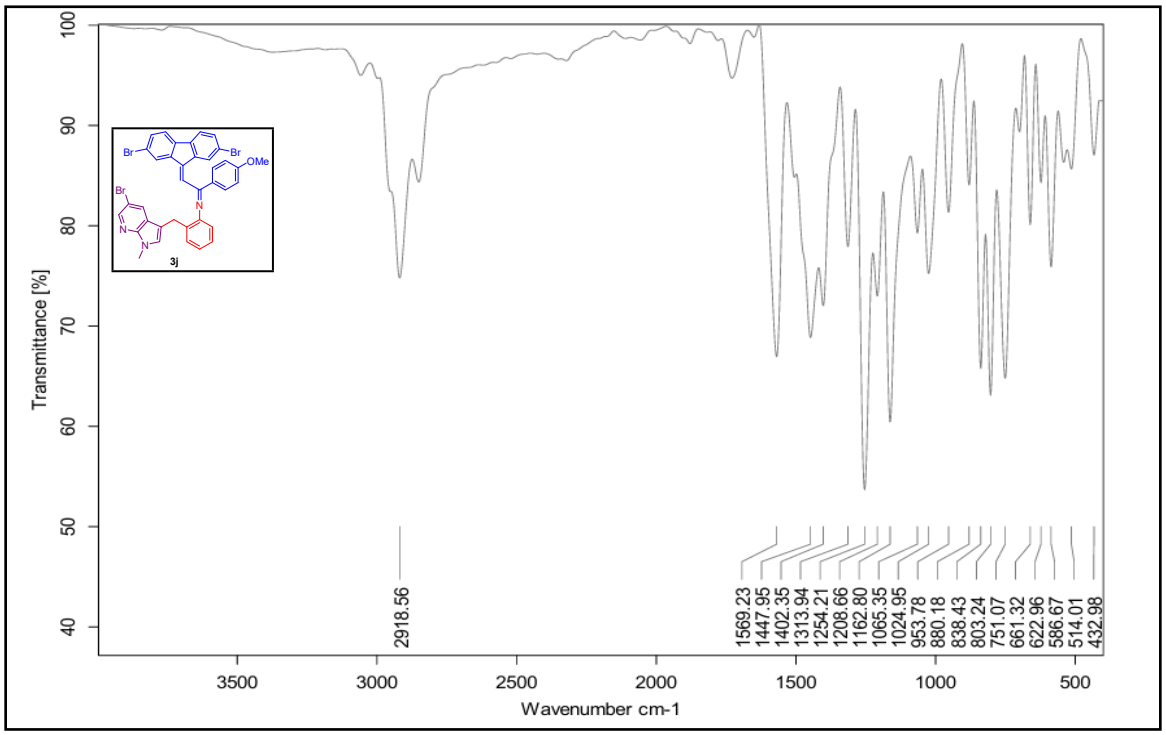


Fig 48 FT-IR spectrum of compound **3j**

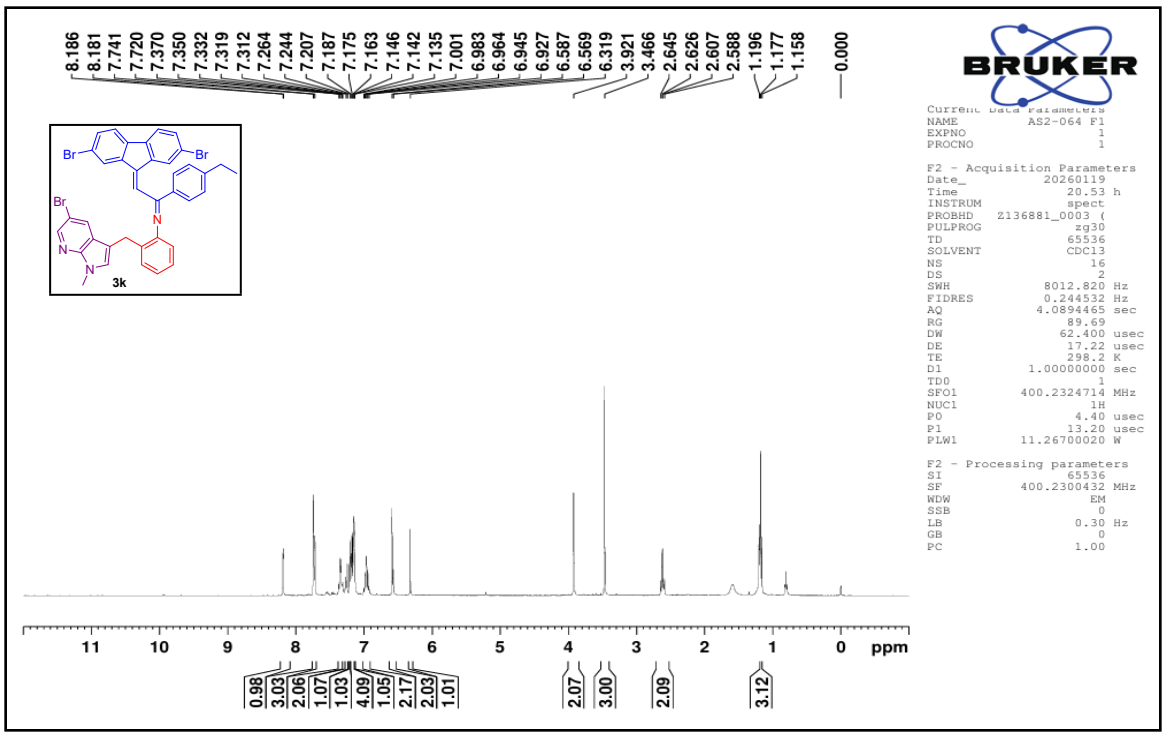


Fig 49 ^{1}H NMR spectrum of compound **3k**

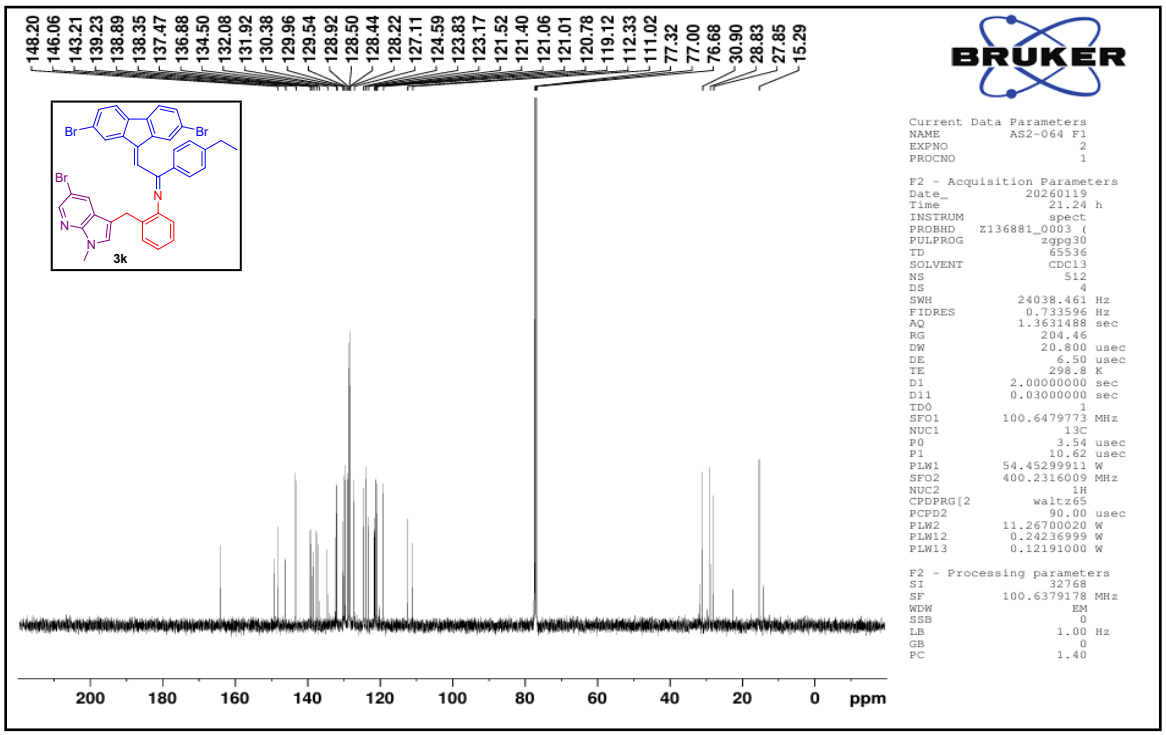


Fig 50 ^{13}C NMR spectrum of compound **3k**

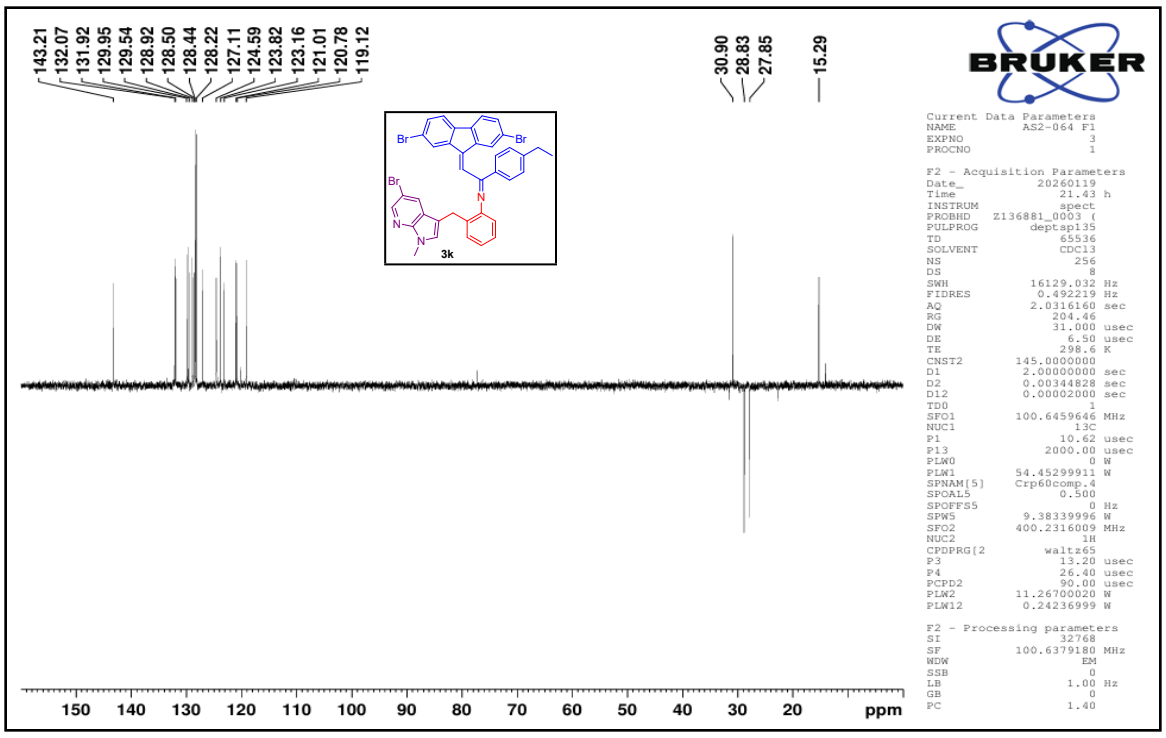


Fig 51 DEPT-135 NMR spectrum of compound **3k**

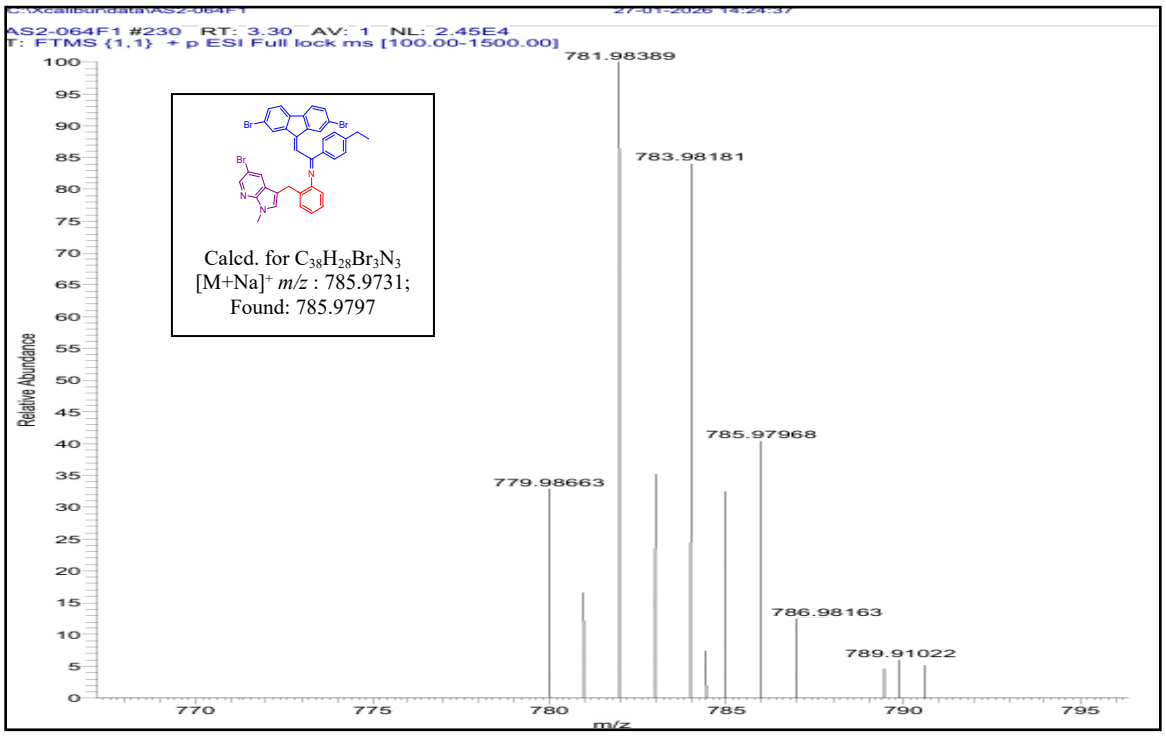


Fig 52 HRMS Spectrum of compound **3k**

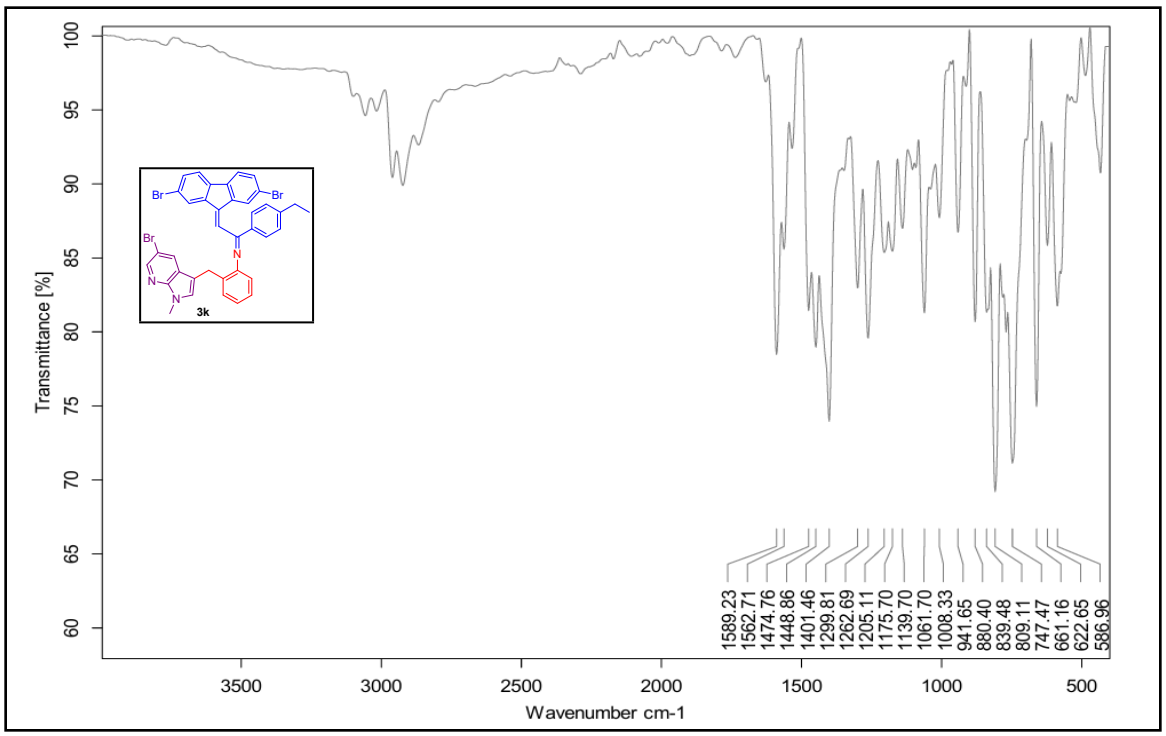


Fig 53 FT-IR Spectrum of compound **3k**

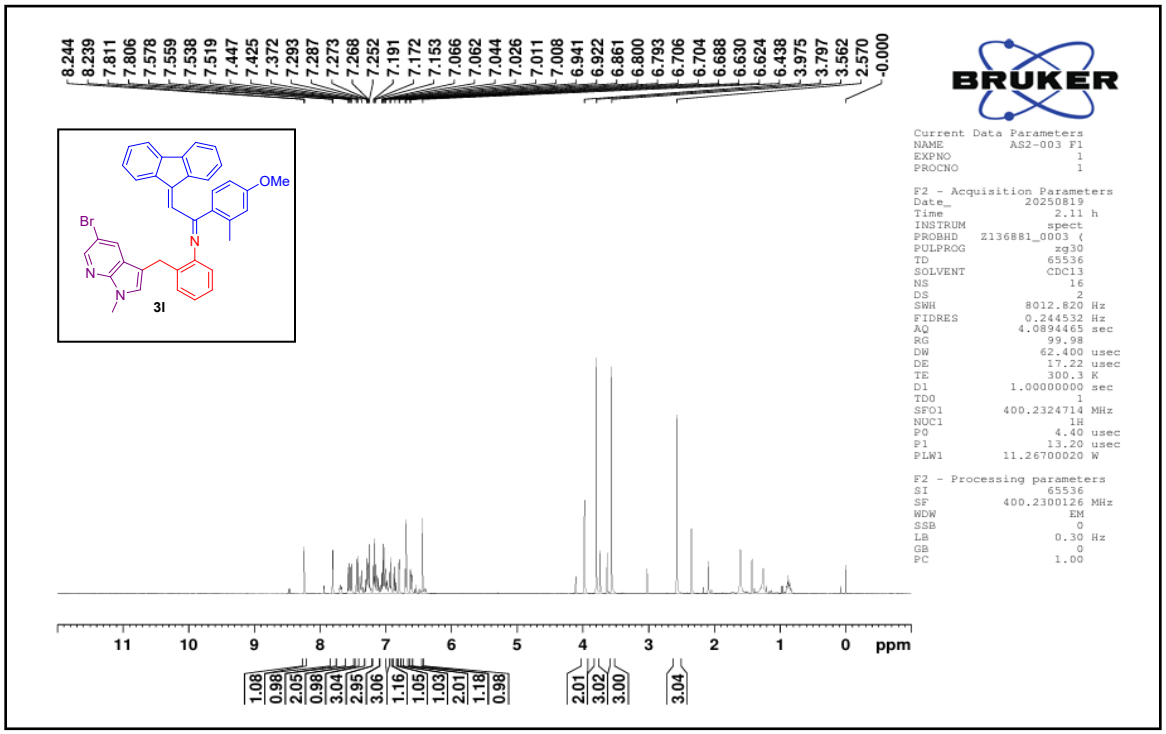


Fig 54 ^{1}H NMR spectrum of compound **3l**

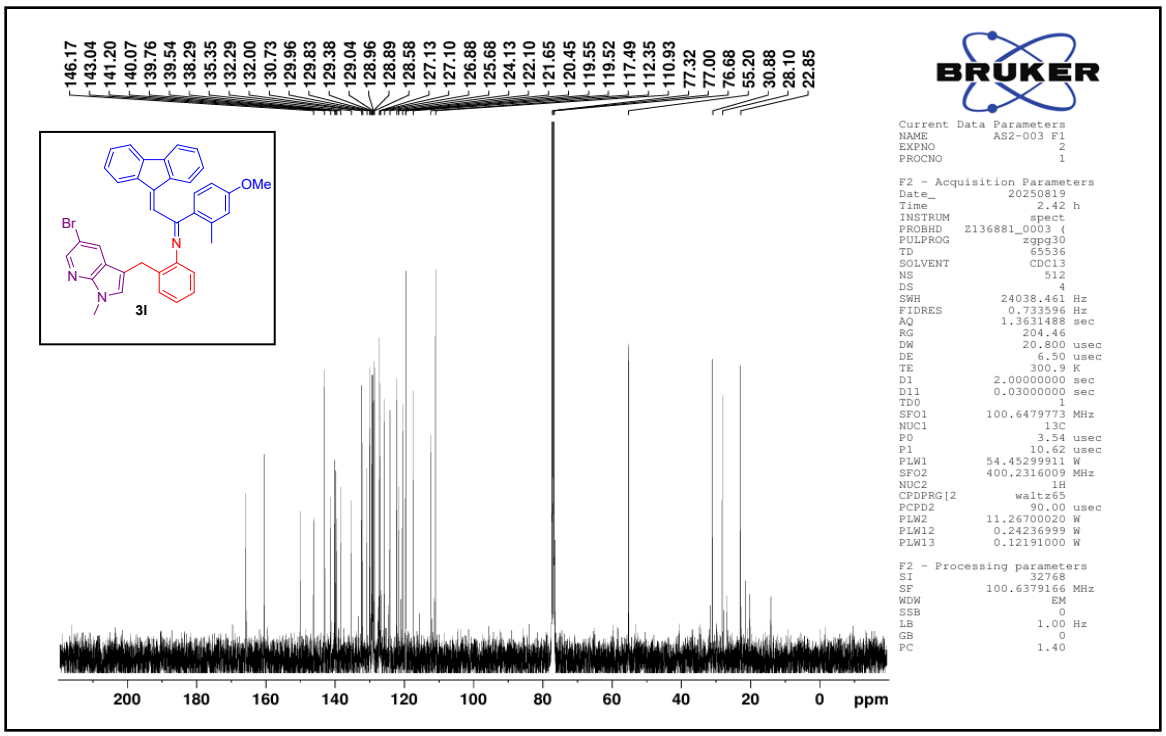


Fig 55 ^{13}C NMR spectrum of compound **3l**

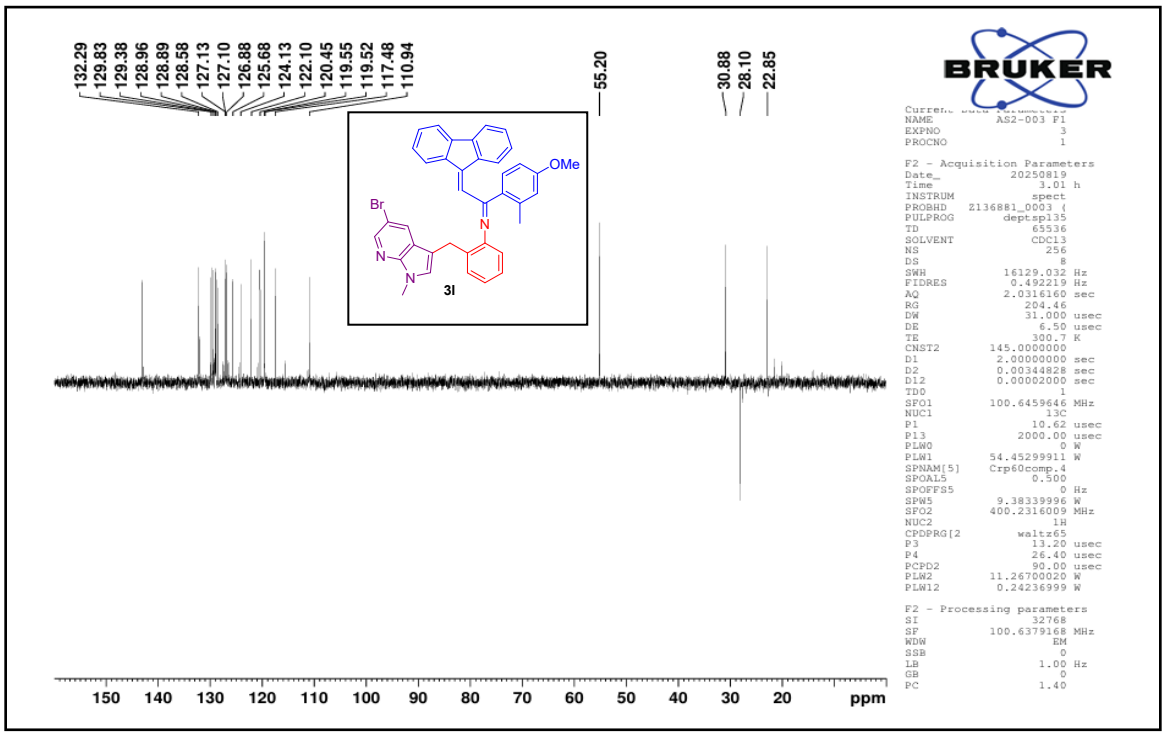


Fig 56 DEPT-135 NMR spectrum of compound **3l**

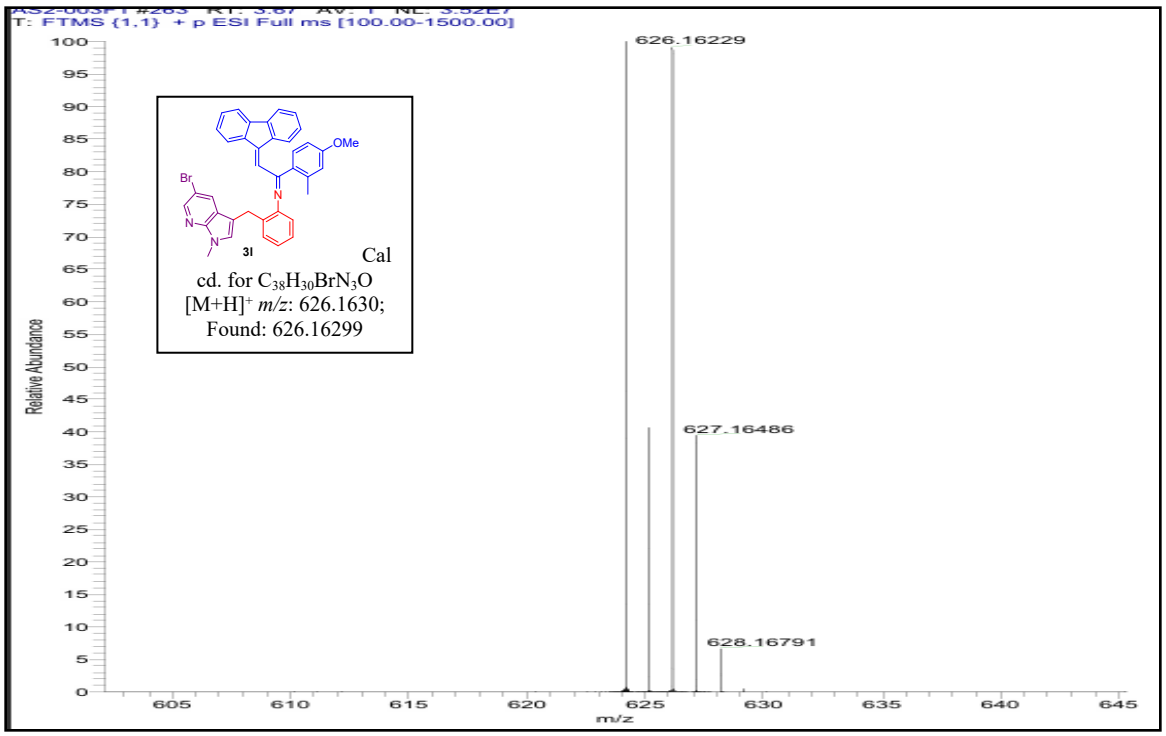


Fig 57 HRMS Spectrum of compound **3l**

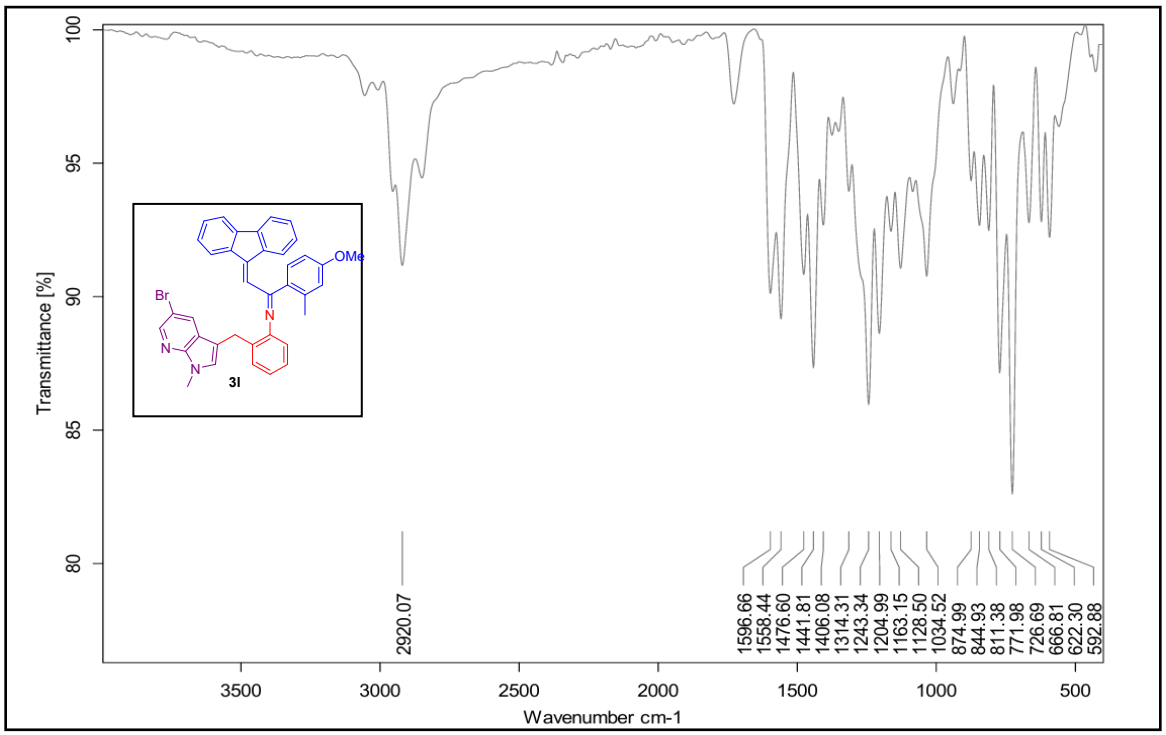


Fig 58 FT-IR spectrum of compound **3l**

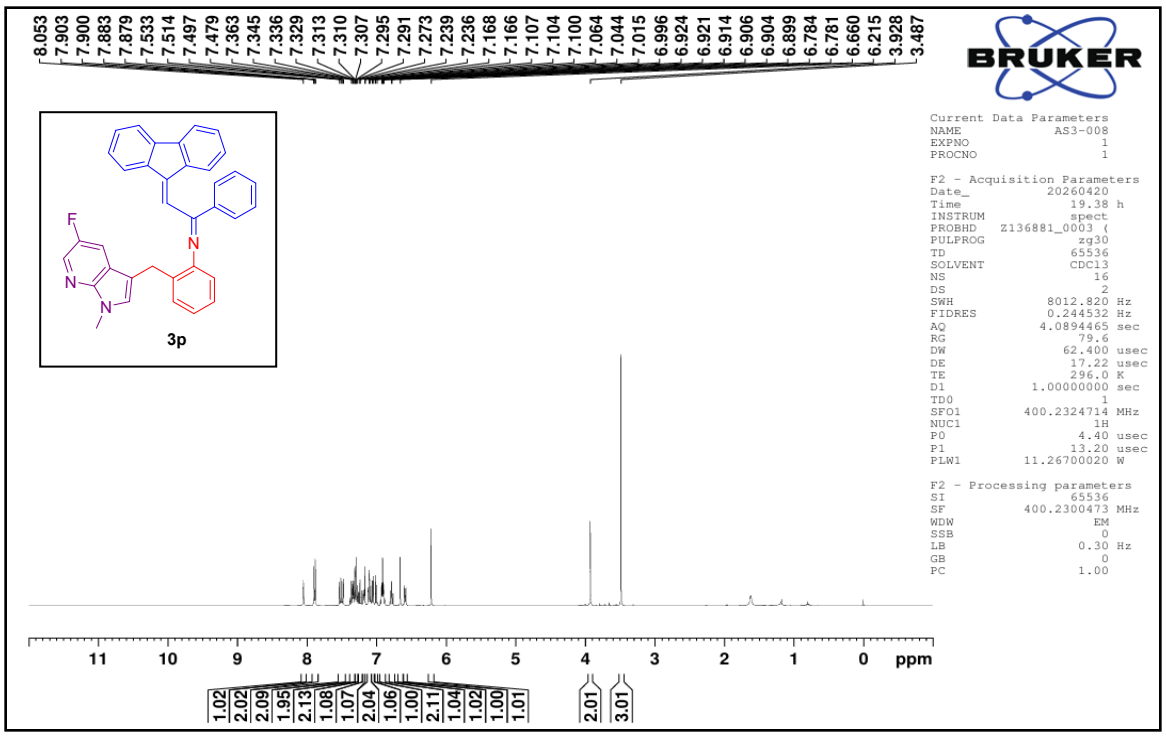


Fig 59 ^{1}H NMR spectrum of compound **3p**

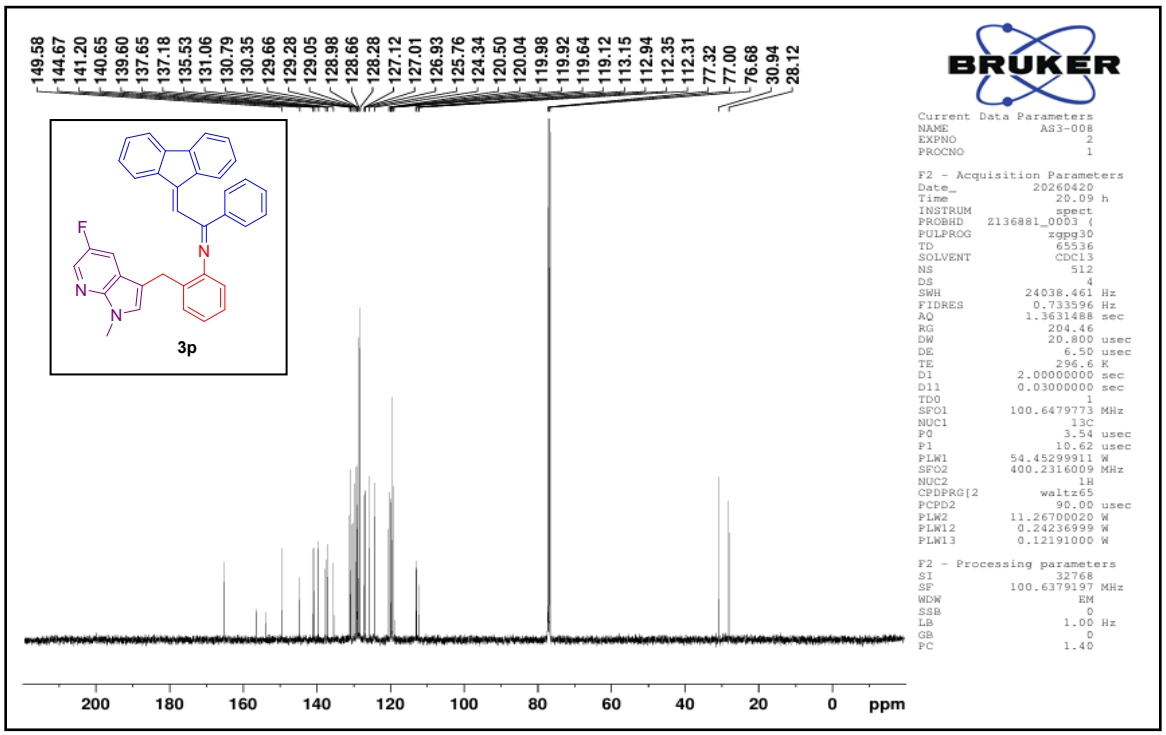


Fig 60 ^{13}C NMR spectrum of compound **3p**

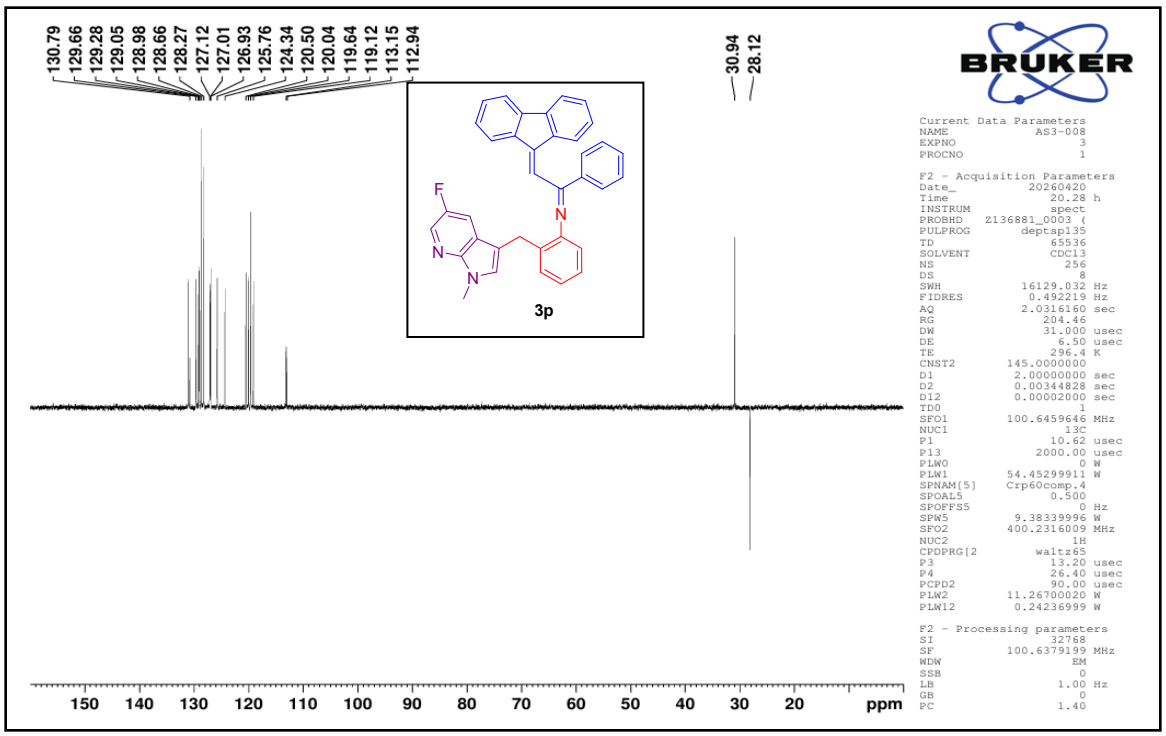


Fig 61 DEPT-135 NMR spectrum of compound **3p**

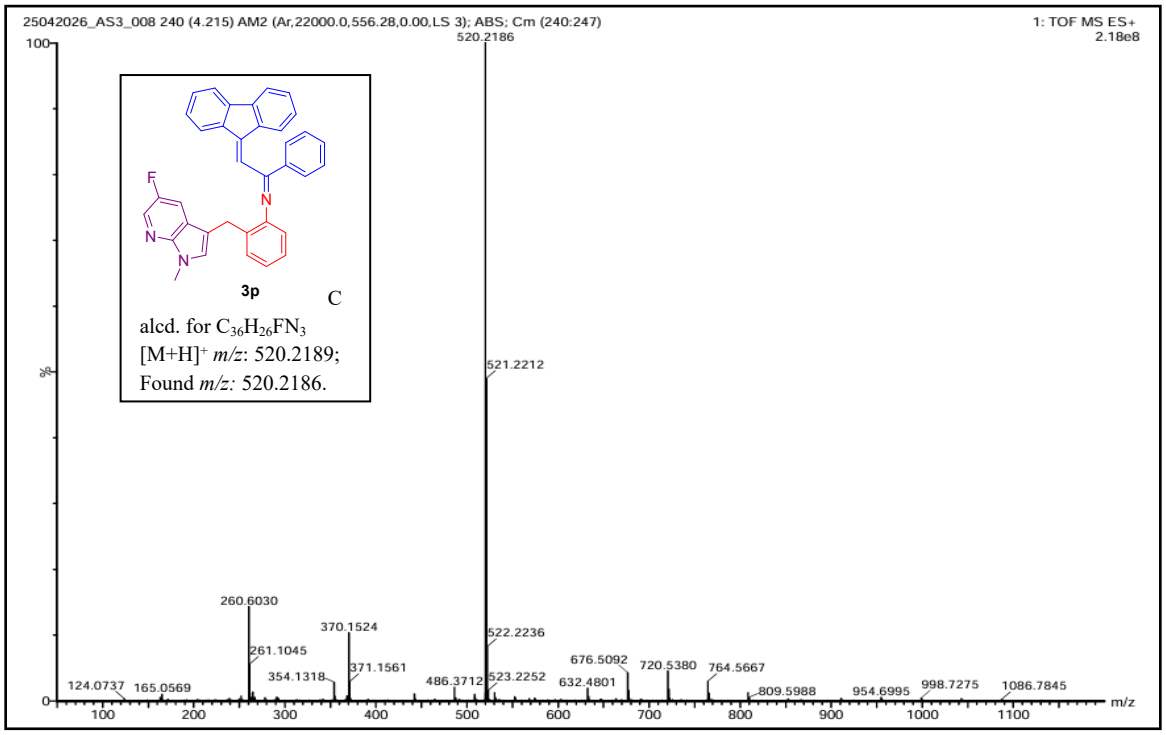


Fig 62 HRMS Spectrum of compound **3p**

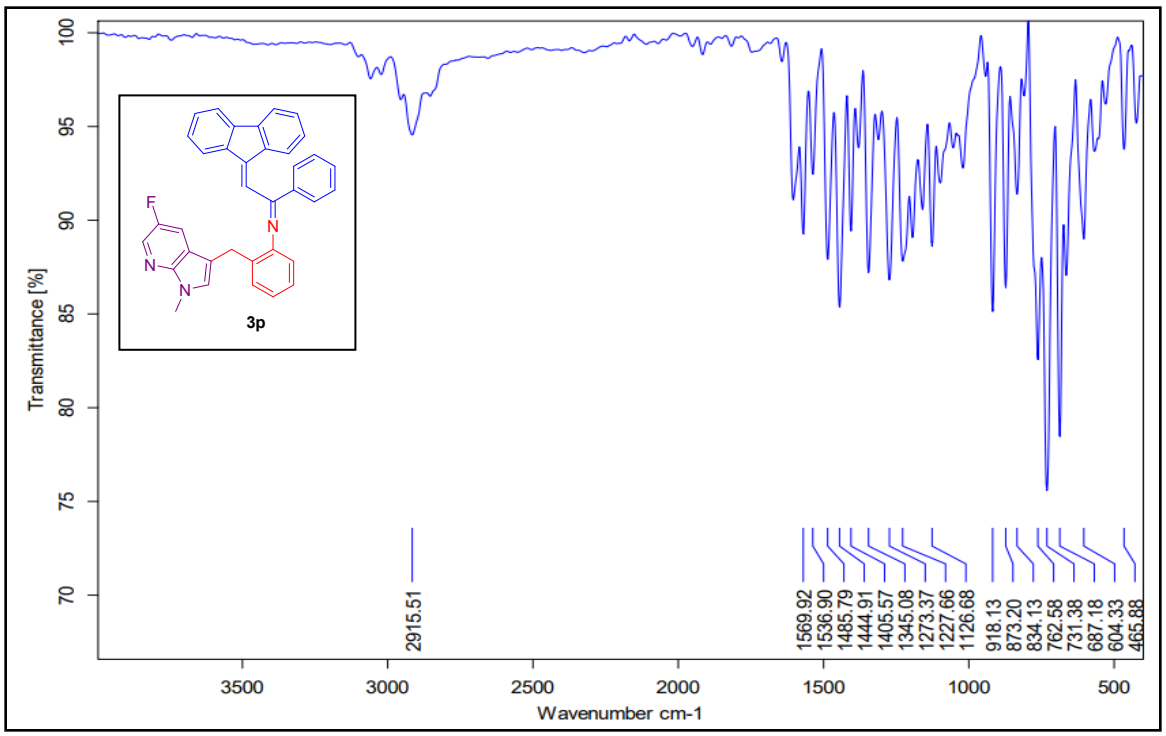


Fig 63 FT-IR spectrum of compound **3p**

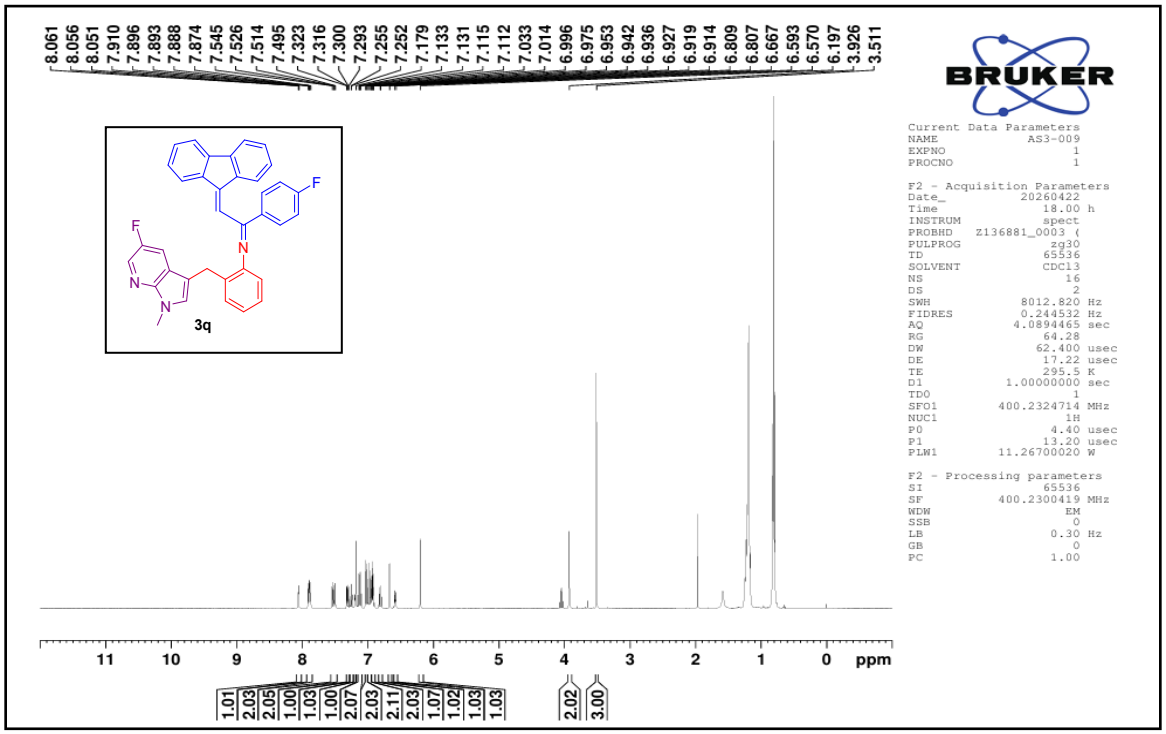


Fig 64 ^{1}H NMR spectrum of compound **3q**

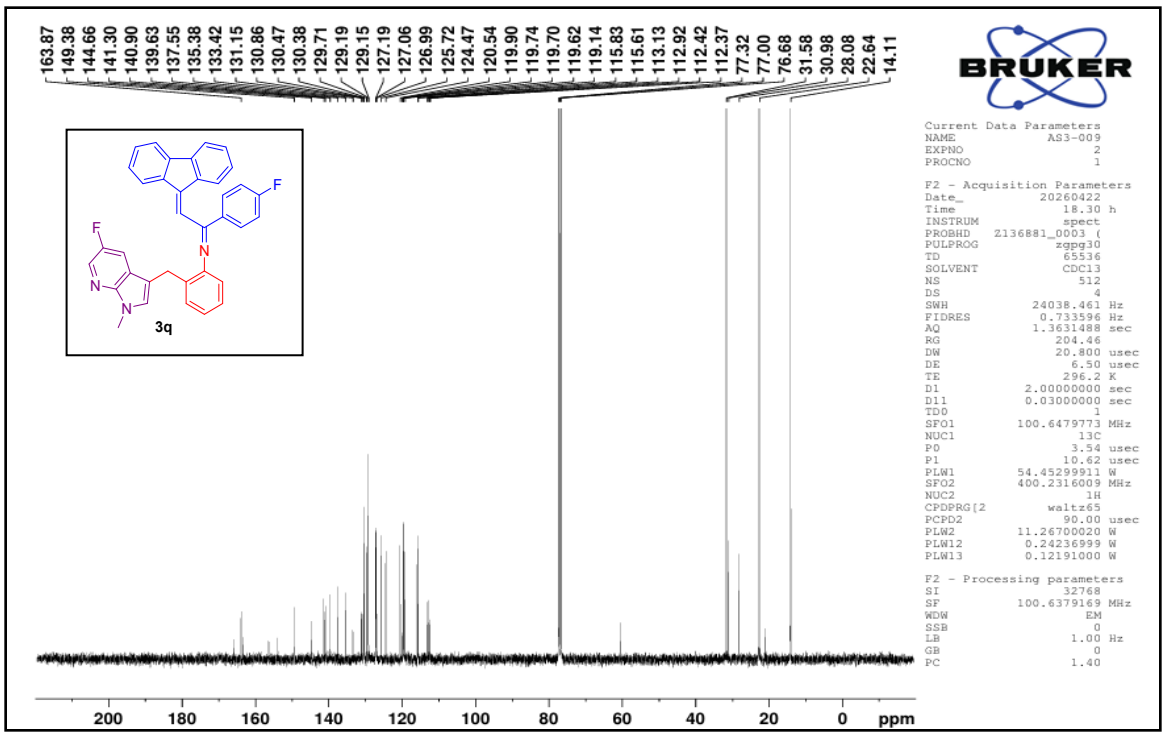


Fig 65 ^{13}C NMR spectrum of compound **3q**

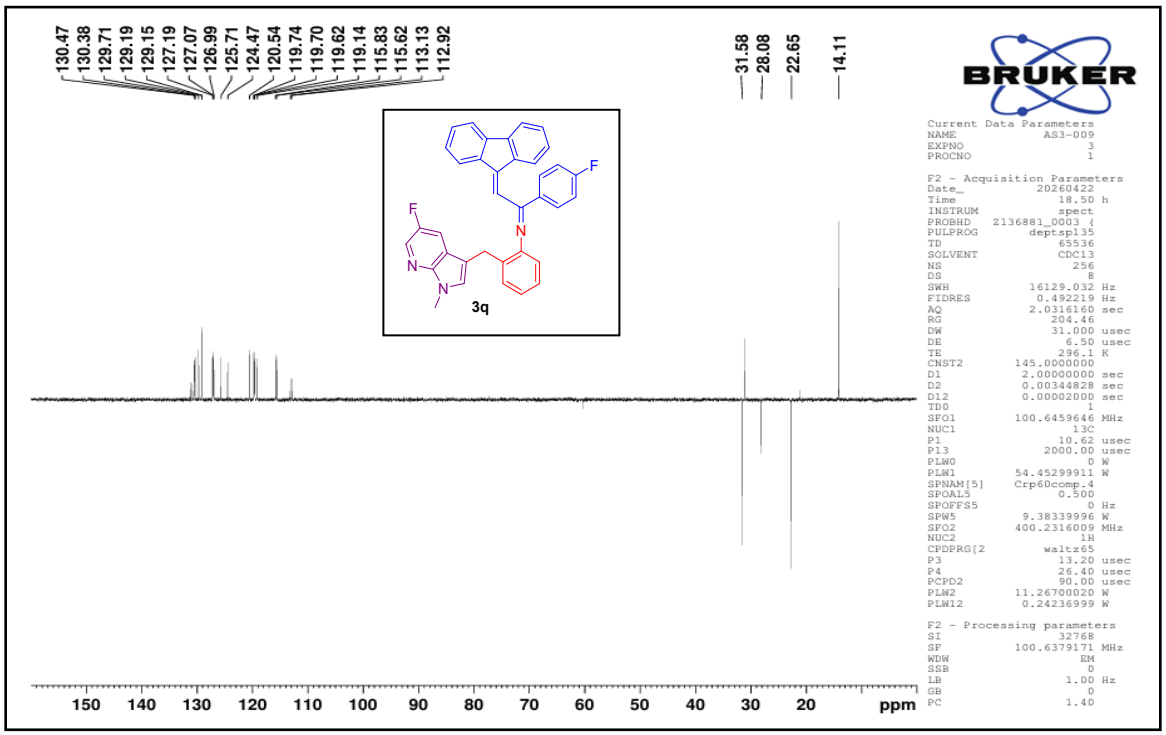


Fig 66 DEPT-135 NMR spectrum of compound **3q**

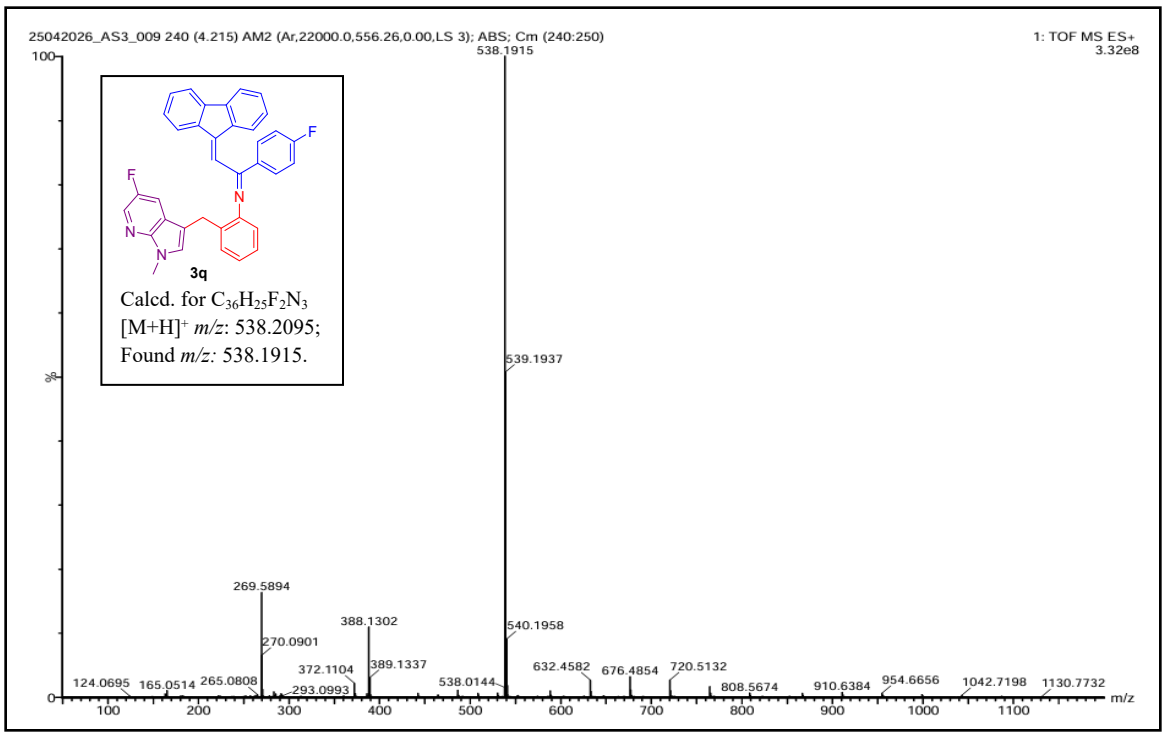


Fig 67 HRMS Spectrum of compound **3q**

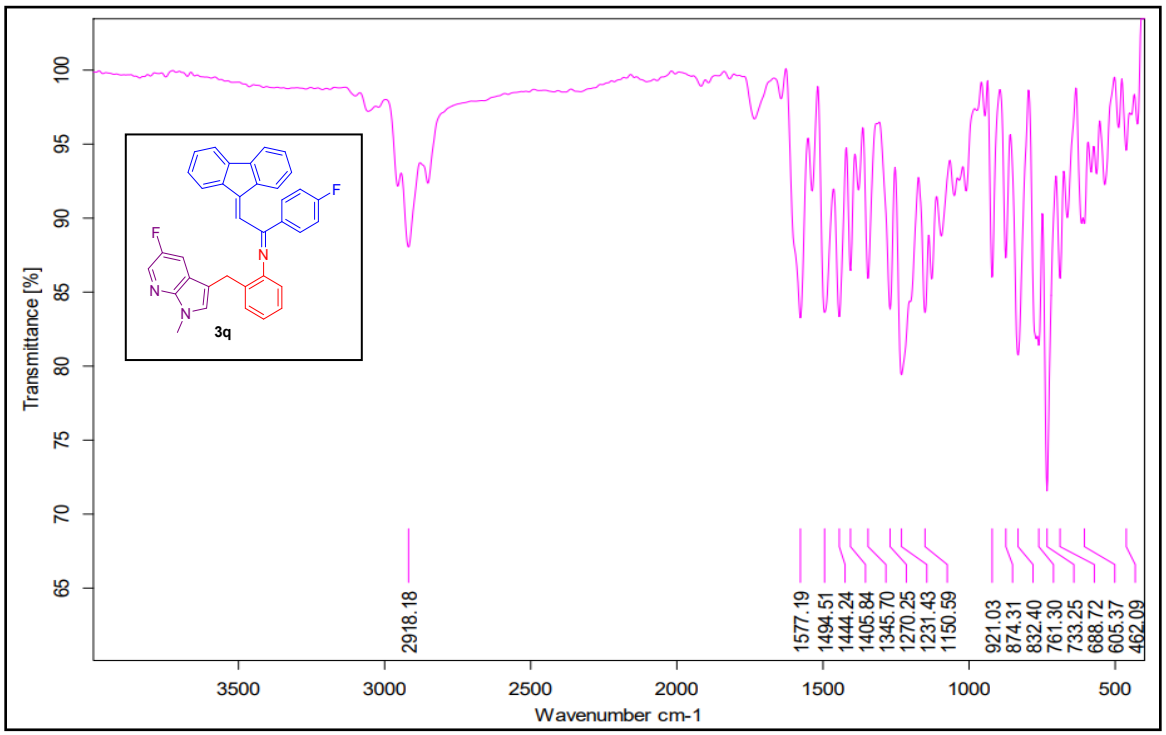


Fig 68 FT-IR spectrum of compound **3q**

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PS_019_100226_0m_a

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: PS_019_100226_0m_a

Bond precision: C-C = 0.0084 A Wavelength=0.71073

Cell: a=13.8227(6) b=52.886(2) c=8.2911(3)
alpha=90 beta=96.478(2) gamma=90

Temperature: 294 K

	Calculated	Reported
Volume	6022.3(4)	6022.3(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C37 H28 Br N3	C37 H28 Br N3
Sum formula	C37 H28 Br N3	C37 H28 Br N3
Mr	594.52	594.53
Dx,g cm-3	1.311	1.311
Z	8	8
Mu (mm-1)	1.395	1.395
F000	2448.0	2448.0
F000’	2446.45	
h,k,lmax	16,62,9	16,62,9
Nref	10595	10590
Tmin,Tmax	0.818,0.894	0.636,0.746
Tmin’	0.778	

Correction method= # Reported T Limits: Tmin=0.636 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.000

wR2(reflections)=

R(reflections)= 0.0653(5401)

0.2477(10590)

S = 1.119 Npar= 754

References

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