Supporting Information

Visible light-driven direct access to imine-containing azaarene-substituted highly functionalized pyrroles

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1. General information

General procedures and methods

Experiments involving moisture and/or air sensitive components were performed under a positive pressure of argon in oven-dried glassware equipped with a rubber septum inlet. Dried solvents and liquid reagents were transferred by oven-dried syringes or hypodermic syringe cooled to ambient temperature in a desiccator. Reactions mixtures were stirred in 25 mL Schlenk tube with Teflon-coated magnetic stirring bars unless otherwise stated. Moisture in non-volatile reagents/compounds was removed in high *vacuo* by means of an oil pump and subsequent purging with nitrogen. Solvents were removed *in vacuo* under ~30 mmHg and heated with a water bath at 30–35 ºC using rotary evaporator with aspirator. The condenser was cooled with running water at 0 ºC.

All experiments were monitored by analytical thin layer chromatography (TLC). TLC was performed on pre-coated plates, 60 F_{254}. After elution, plate was visualized under UV illumination at 254 nm for UV active material. Further visualization was achieved by staining $Ce(SO_4)_2$ solution. For those using the aqueous stains, the TLC plates were heated on a hot plate.

Columns for flash chromatography (FC) contained *silica gel* 200–300 mesh. Columns were packed as slurry of *silica gel* in petroleum ether and equilibrated solution using the appropriate solvent system. The elution was assisted by applying pressure of about 2 atm with an air pump.

Instrumentations

Proton nuclear magnetic resonance (^{1}H NMR) and carbon NMR (^{13}C NMR) were recorded in $CDCl_3$ otherwise stated. Chemical shifts are reported in parts per million (ppm), using the residual solvent signal as an internal standard: $CDCl_3$ (^{1}H NMR: δ 7.26, singlet; ^{13}C NMR: δ 77.0, triplet). Multiplicities were given as: *s* (singlet), *d* (doublet), *t* (triplet), *q* (quartet), *quintet*, *m* (multiplets), *dd* (doublet of doublets), *dt* (doublet of triplets), and *br* (broad). Coupling constants (*J*) were recorded in hertz (Hz). The number of proton atoms (*n*) for a given resonance was indicated by *n*H. The number of carbon atoms (*n*) for a given resonance was indicated by *n*C. HRMS (Analyzer: TOF) was reported in units of mass of charge ratio (m/z). Mass samples were dissolved in CH_3CN (HPLC Grade) unless otherwise stated. Melting points were determined on a melting point apparatus.

Materials

All commercial reagents were purchased with the highest purity grade. They were used without further purification unless specified. All solvents used, mainly petroleum ether (PE) and ethyl acetate (EtOAc) were distilled. Anhydrous dichloromethane (DCM), DCE, CH_3COCH_3, CH_3CN, DMSO were freshly distilled from CaH_2 and stored under N_2 atmosphere. THF, $CHCl_3$ and toluene were freshly distilled from sodium/benzophenone

before use. All compounds synthesized were stored in a −20 ºC freezer and light-sensitive compounds were protected with aluminium foil.

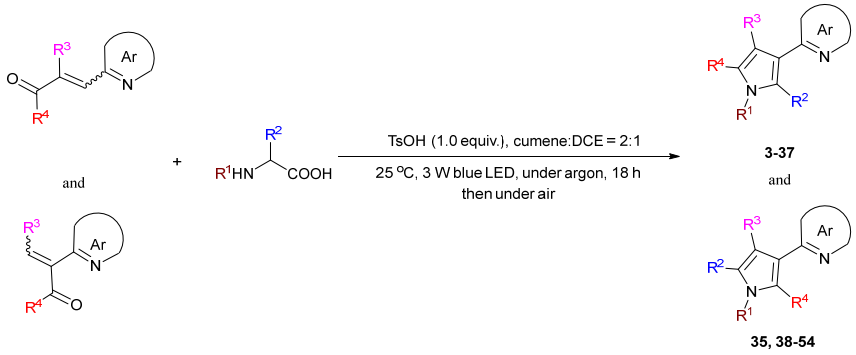
2. General procedures

2.1 Preparation of staring materials

1,2-Diphenyl-3-(pyridin-2-yl)prop-2-en-1-one and other corresponding *α,β*-unsaturated ketone derivatives were prepared based on the reported procedures.[1]

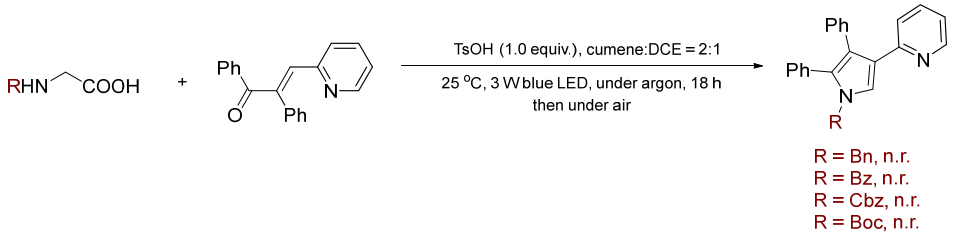
Representative procedure: A solution of 1,2-diphenylethan-1-one (1.96 g, 10 mmol), picolinaldehyde (1.06 g, 10 mmol), AcOH (0.5 mL) and piperidine (0.2 mL) in 25 mL toluene was refluxed overnight using a Dean-stark apparatus. After cooling to room temperature, the reaction was quenched by the addition of saturated aqueous $NaHCO_3$ solution (10 mL). The aqueous layer was extracted with ethyl acetate (3 × 30 mL) and the combined organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated under reduced pressure. The solvent was removed under vacuum and the resultant residue was purified by flash chromatography on *silica gel* (ethyl acetate/petroleum ether, 1:10 v/v) to afford the (*Z/E*)-1,2-Diphenyl-3-(pyridin-2-yl)prop- 2-en-1-one in 80% yield.

2.2 General procedures for the synthesis of azaarene-substituted pyrroles

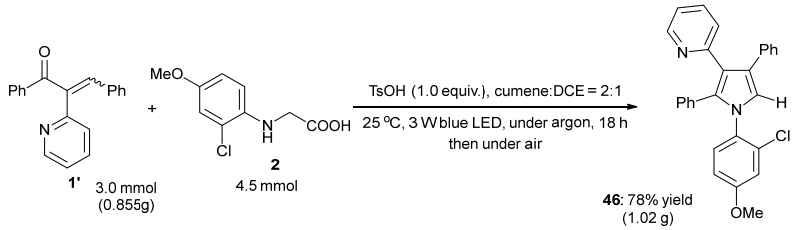


β-Azaarene-substituted enones or *α*-azaarene-substituted enones (0.1 mmol, 1.0 equiv.) and *N*-aryl amino acids (0.15 mmol, 1.5 equiv.) with TsOH (0.1 mmol, 1.0 equiv.) in cumene/DCE (v/v = 2:1, 4.5 mL) was added into a 10 mL Schlenk tube, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere at 25 °C (the temperature was maintained in an incubator) and irradiated by a 3 W blue LED (λ_{max} = 452 nm) for 18 h. After completion, the reaction mixture was removing the solvent and purification by a short *silica gel* column, followed by gradient elution with petroleum ether/ethyl acetate (100/1–10/1 ratio). Removing the solvent *in vacuo*, afforded products **3-54**.

2.3 Unsuccessful substrates

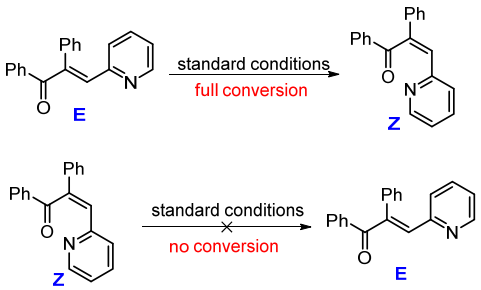


3. Gram-scale synthesis

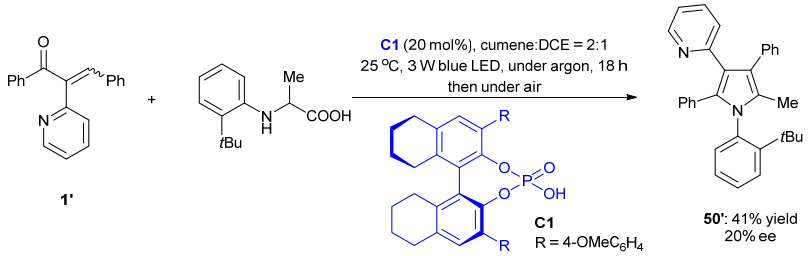


1' (3 mmol, 1.0 equiv.) and **2** (4.5 mmol, 1.5 equiv.) with TsOH (3 mmol, 1.0 equiv.) in cumene/DCE (v/v = 2: 1, 120 mL) was added into a 300 mL Schlenk tube, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere at 25 °C (the temperature was maintained in an incubator) and irradiated by a 3 W blue LED (λ_{max} = 452 nm) for 18 h. After completion of the reaction, the reaction mixture was removing the solvent and purification by a short *silica gel* column, followed by gradient elution with petroleum ether/ethyl acetate (100/1–10/1 ratio). Removing the solvent *in vacuo*, afforded product **46** as a gray solid in 78% yield (1.02 g).

4. *E*/*Z* Isomerization experiments.

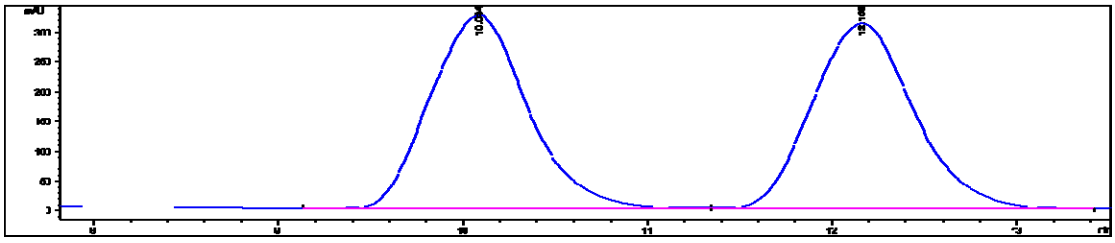


5. Asymmetric experiments

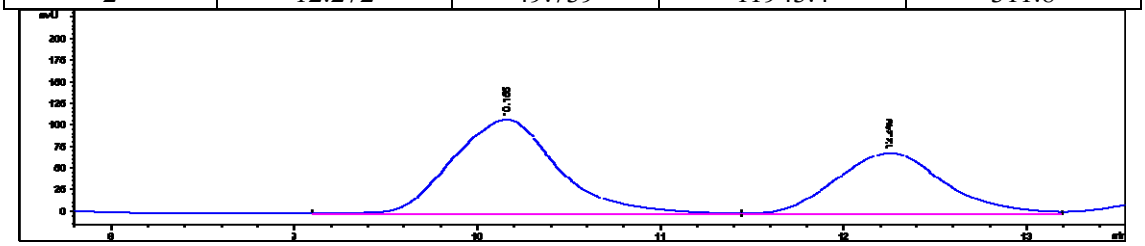


1' (0.1 mmol, 1.0 equiv.) and (2-(*tert*-butyl)phenyl)alanine (0.15 mmol, 1.5 equiv.) with **C1** (0.02 mmol, 0.2 equiv.) in cumene/DCE (v/v = 2:1, 4.5 mL) was added into a 10 mL Schlenk tube, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere at 25 °C (the temperature was maintained in an incubator) and irradiated by a 3 W blue LED (λ_{max} = 452 nm) for 18 h. After completion of the reaction, the reaction mixture was removing the solvent and purification by a short *silica gel* column, followed by gradient elution with petroleum ether/ethyl acetate (100/1–10/1 ratio). Removing the solvent *in vacuo*, afforded products **50'** as a gray solid in 41% yield (18.1 mg) and 20% ee.

The ee was determined by HPLC analysis: CHIRALPAK IG (4.6 mm i.d. x 250 mm); hexane/2-propanol = 90/10; flow rate 1.0 mL/min; 25 °C; 254 nm; retention time: 10.2 min (major) and 12.2 min (minor).



Entry	Retention Time	%Area	Area	Height
1	10.048	50.261	12068.6	325.6
2	12.272	49.739	11943.4	311.8



Entry	Retention Time	%Area	Area	Height
1	10.155	60.104	4517.6	109.7
2	12.249	39.896	2998.7	71.5

6. UV/Vis absorption and NMR studies

6.1 UV-vis absorption spectra

UV-vis absorption spectroscopy was performed using a spectrophotometer, equipped with a temperature control unit at 25 °C. The samples were measured in a 1.5 mL quartz cuvettes fitted with a PTFE stopper. **1'**, **2** and TsOH were prepared as a 0.1 mM solution with fresh DCE as the solvent for measurement.

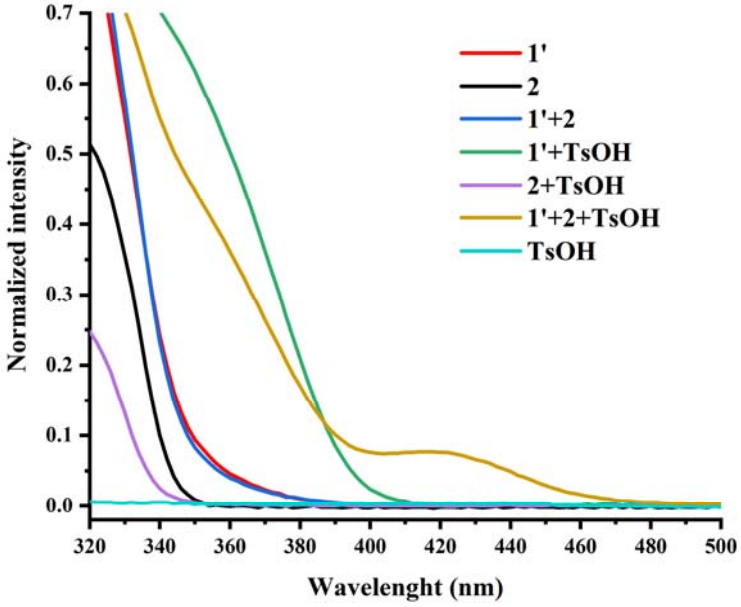


Fig. S1. UV-vis absorption spectra of **1'**, **2** and TsOH.

Comments: The results indicate that EDA complex of **1'** and TsOH is generated in the reaction system.

6.2 Emission spectrum of the LED light

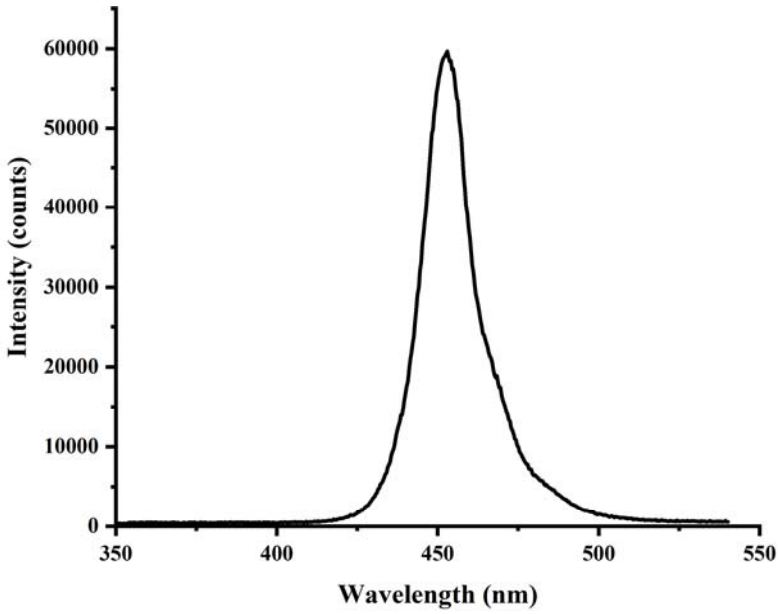


Fig. S2. Emission spectrum of the 3 W Blue LED light.

6.3 Stoichiometry of the EDA Complex in Solution

The Job's plot was constructed to evaluate the stoichiometry of the EDA complex[2] between unsaturated ketone derivative **1'** and TsOH. We measured the absorption of DCE solutions at 400 nm with different donor/acceptor ratios with constant concentration (0.05 M) of the two components. All the absorption spectra were recorded in 1 cm path quartz cuvettes using a UV/Vis spectrometer. The absorbance values were plotted against the molar fraction (%) of **1'**. The maximal absorbance at 50% molar fraction of **1'** indicated the 1:1 stoichiometry of the EDA complex in solution.

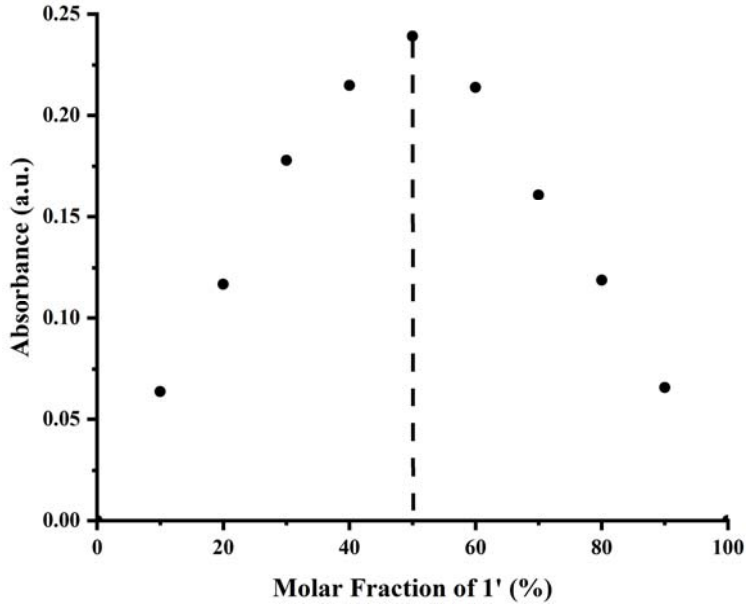


Fig. S3. Job's plots of the EDA complexes between **1'** and TsOH.

6.4 Determination of the Association Constant (K_{EDA})

The association constant of the EDA complex formed between TsOH and **1** was determined spectrophotometrically in DCE, employing the Benesi-Hildebrand methodology[3]. We measured the absorption of solutions with constant concentration of TsOH and **1** (0.03 M) at 400 nm, and added an excess of TsOH to increase the donor/acceptor ratios. All the absorption spectra were recorded in 1 cm path quartz cuvettes using a UV/Vis spectrometer. According to the methodology, a straight line was obtained when the reciprocal of the absorbance (A) was plotted against the reciprocal of the concentration of the partner in excess. Data obtained were displayed in Table S1. The association constants (K_{EDA}) were calculated by dividing the intercept by the slope: 15.9 M^{-1} for the **1**/TsOH complex; 18.3 M^{-1} for the **1'**/TsOH complex;

Table S1: Data obtained by UV/vis absorption spectra for EDA in DCE, with [**1**] = 0.03 M

[TsOH]	1/ [TsOH] (M^{-1})	Abs_{EDA}	1/ (Abs_{EDA}-A_0)
0.03	33.3	0.555	1.802
0.04	25	0.632	1.581

0.05	20	0.713	1.403
0.06	16.7	0.840	1.190
0.07	14.3	0.910	1.099
0.08	12.5	0.943	1.061

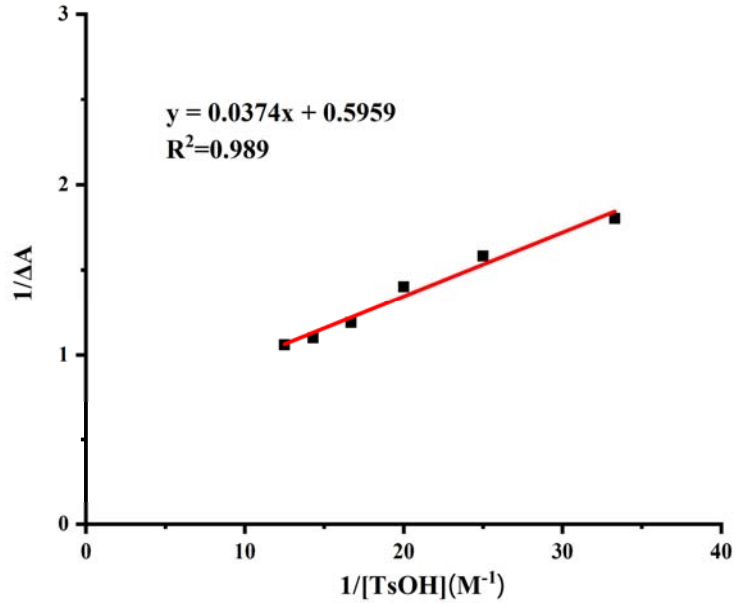


Fig. S4. Hildebrand-Benesi plots for the EDA complexes generated in DCE upon association of the **1** and TsOH.

Table S2: Data obtained by UV/vis absorption spectra for EDA in DCE, with [**1'**] = 0.03 M

[TsOH]	1/ [TsOH] (M^{-1})	Abs_{EDA}	1/ (Abs_{EDA}-A_0)
0.03	33.3	0.196	5.102
0.04	25	0.216	4.632
0.05	20	0.245	4.081
0.06	16.7	0.284	3.522
0.07	14.3	0.300	3.333
0.08	12.5	0.333	3.001

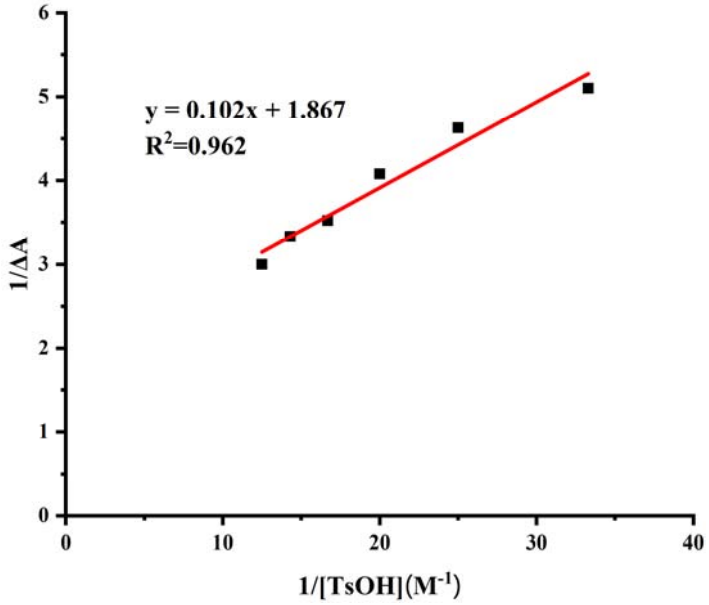


Fig. S5. Hildebrand-Benesi plots for the EDA complexes generated in DCE upon association of the **1'** and TsOH.

6.5 NMR Titration Experiments

Solutions containing equal molar concentrations of the donor (TsOH, 0.2 M in acetone-D6) and the acceptor (**1**, 0.2 M in Acetone-D6) were prepared and mixed to cover acceptor/donor ratio from 0%, 10%, 20% to 100% donor (from 1 to 11 in Figure S6).

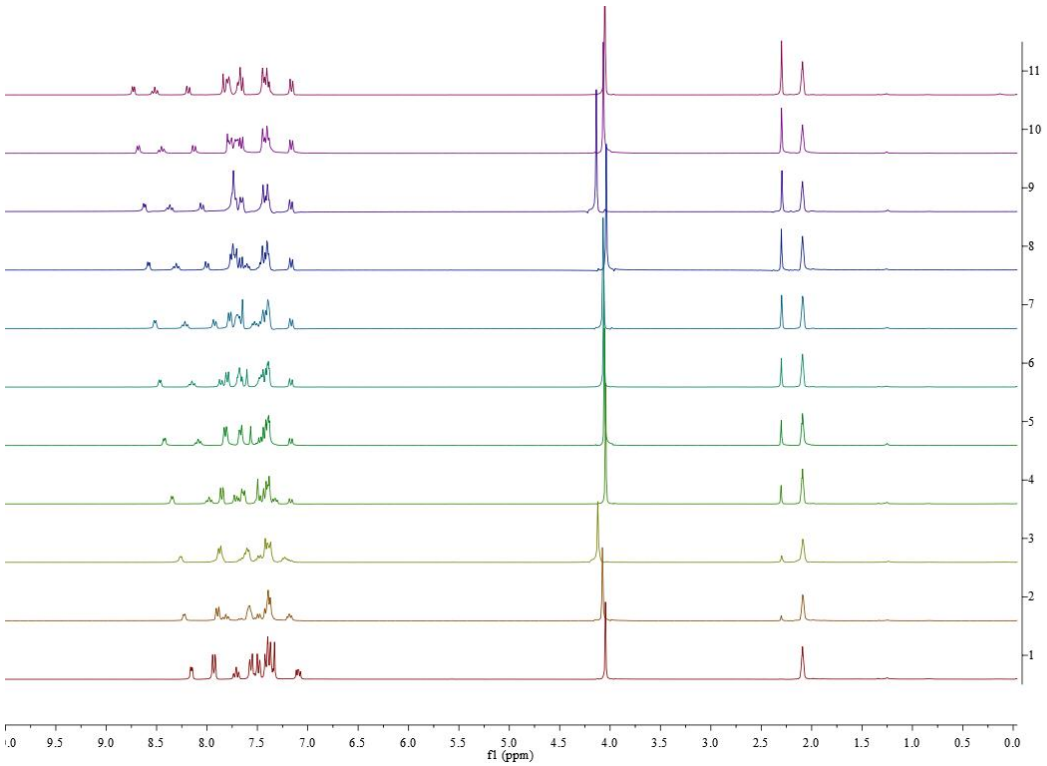


Fig. S6. ^{1}H NMR titration between TsOH and **1**.

In NMR titration experiments, we observed ^{1}H NMR signal of **1** shifted downfield with the addition of TsOH.

Solutions containing equal molar concentrations of the donor (TsOH, 0.2 M in acetone-D6) and the acceptor (**1'**, 0.2 M in Acetone-D6) were prepared and mixed to cover acceptor/donor ratio from 0%, 10%, 20% to 100% donor (from 1 to 11 in Figure S7).

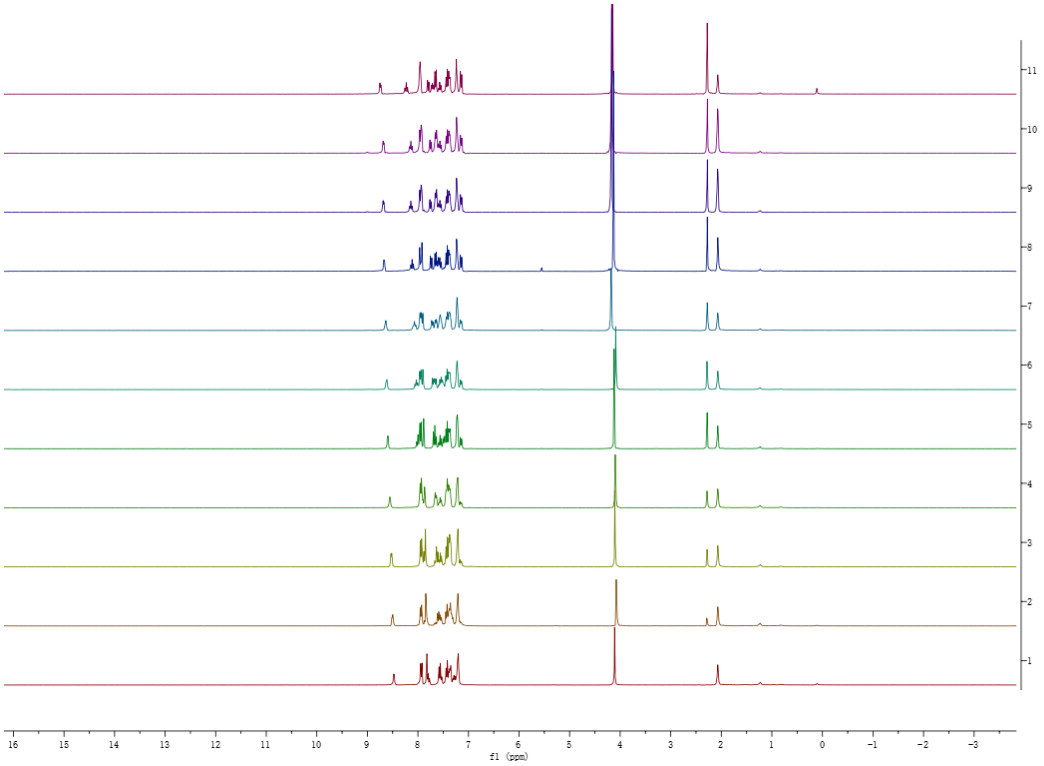


Fig. S7. ^{1}H NMR titration between TsOH and **1'**.

In NMR titration experiments, we observed ^{1}H NMR signal of **1'** shifted downfield with the addition of TsOH.

7. Emission quenching experiment

Emission intensities were recorded on a spectrofluorometer. EDA complex of **1** and TsOH solution was excited at 400 nm and the emission intensity at 460 nm was observed. A solution of EDA complexes (5.0×10^{-5} M) in mixed cumene: DCE (V/V = 2: 1) was added to the appropriate amount of quencher in 3.0 mL volumetric flask under N_2. The solution was transferred to a 3.0 mL quartz cell and the emission spectrum of the sample was collected.

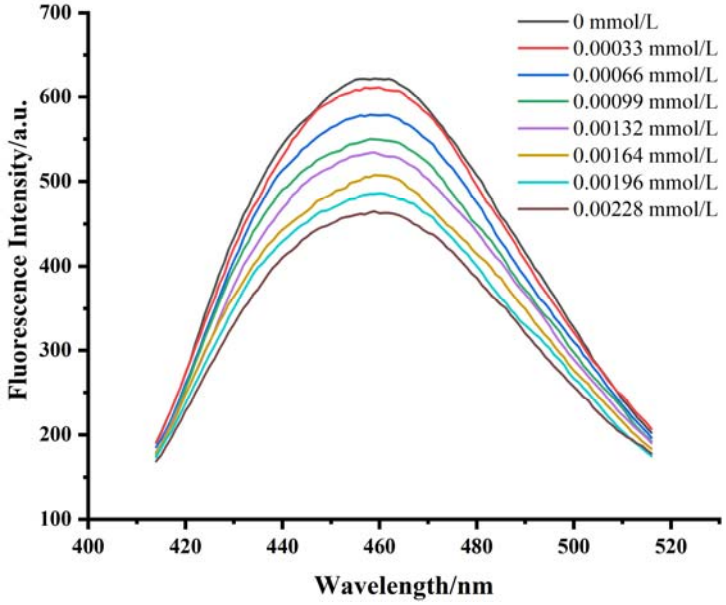


Fig. S8. Different concentrations of **2**.

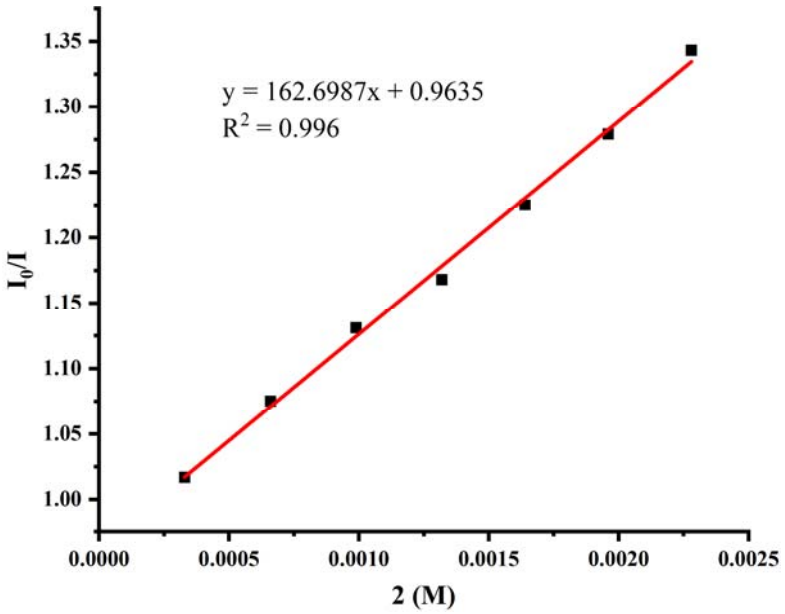


Fig. S9. Stern–Volmer quenching experiment of EDA complexe and **2** in DCE.

8. Cyclic voltammetry measurement

Electrochemical potentials were obtained with a standard set of conditions to main internal consistency. Cyclic voltammograms were collected with a potentiostat. Samples were prepared with 0.01 mmol of **1**, in 10 mL of 0.1 M tetrabutylammonium hexafluorophosphate in anhydrous acetonitrile. Measurements employed a radium glassy carbon working electrode, platinum wire counter electrode, saturated KCl silver-silver chloride reference electrode. The obtained value was referenced to Ag/AgCl. The obtained value was referenced to Ag/AgCl and converted to SCE by adding 0.03 V.

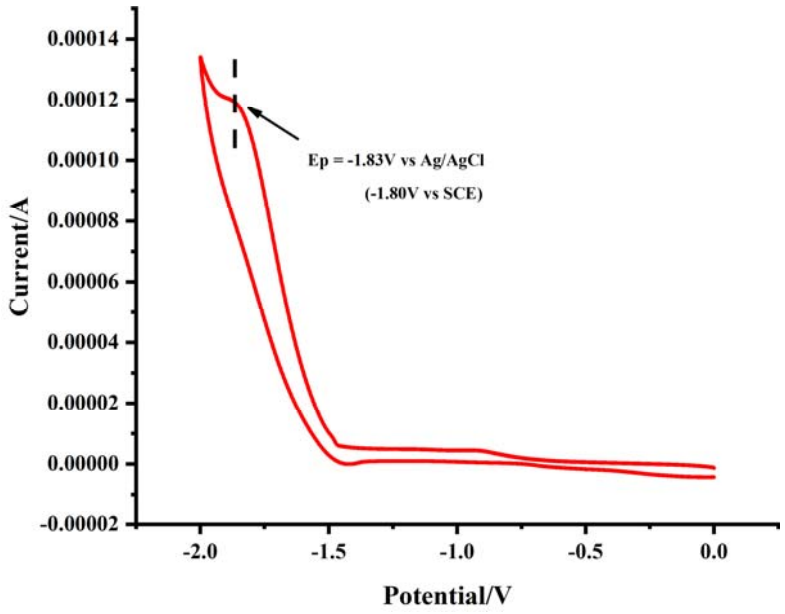


Fig. S10. Cyclic voltammogram of **1** in MeCN.

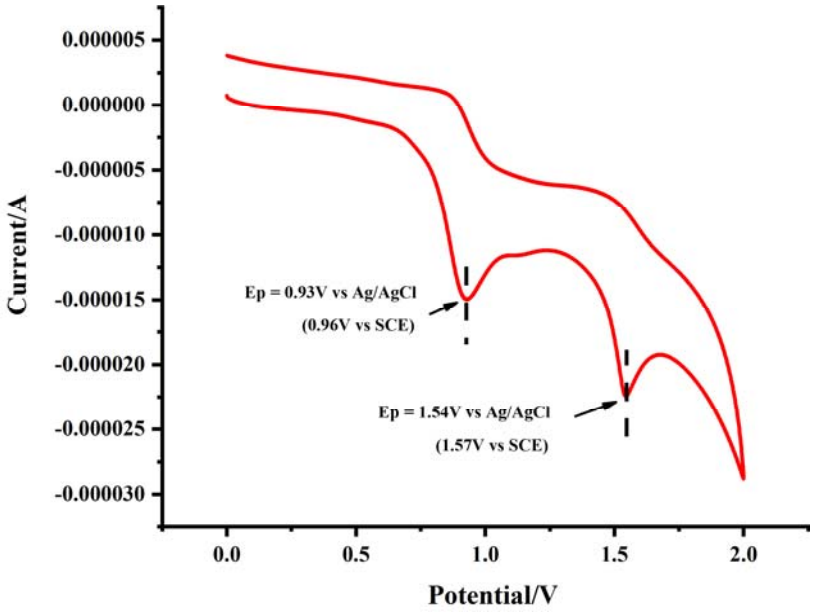


Fig. S11. Cyclic voltammogram of **2** in MeCN.

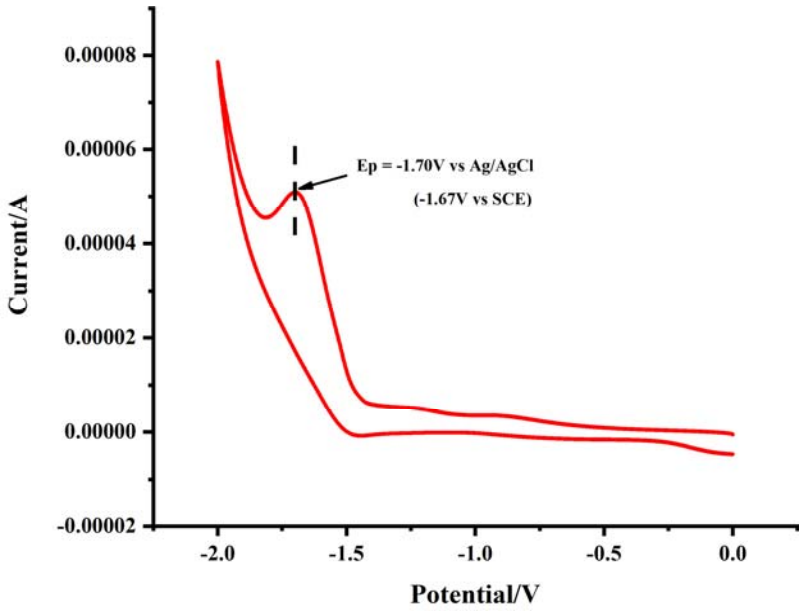


Fig. S12. Cyclic voltammogram of **1'** in MeCN.

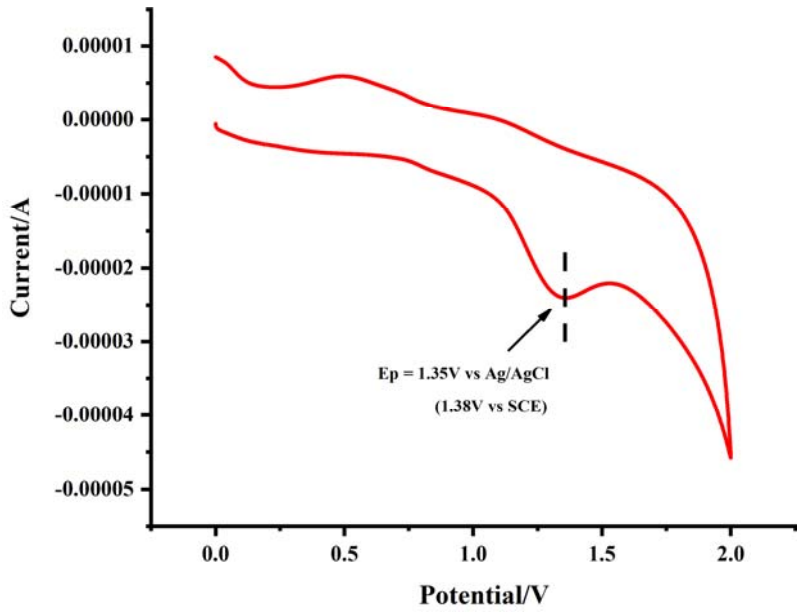
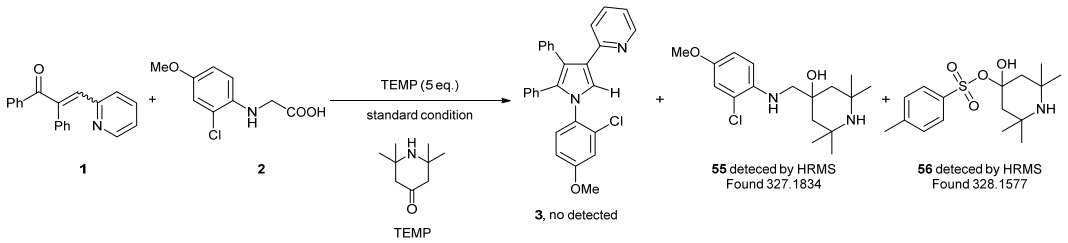


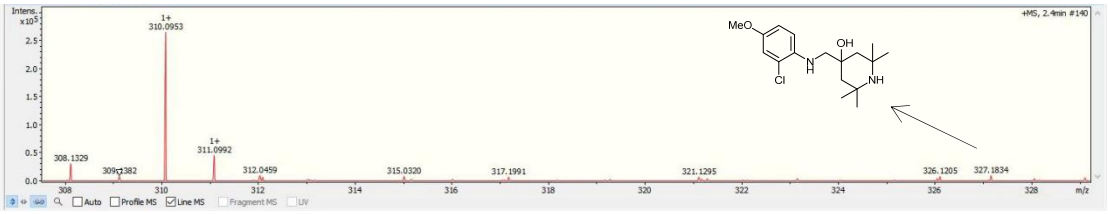
Fig. S13. Cyclic voltammogram of TsOH in MeCN.

9. Other experiments for exploring mechanism

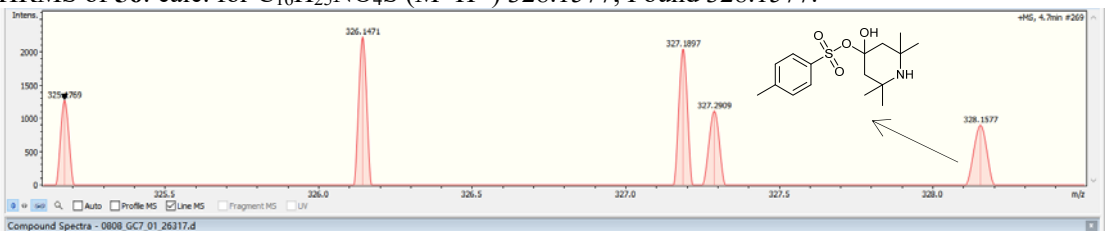


1 (0.1 mmol, 1.0 equiv.), **2** (0.15 mmol, 1.5 equiv.), TsOH (0.1 mmol, 1.0 equiv.) and TEMP (0.5mmol, 5 equiv.) in cumene/DCE (v/v = 2:1, 4.5 mL) was added into a 10 mL Schlenk tube, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere at 25 °C (the temperature was maintained in an incubator) and irradiated by a 3 W blue LED (λmax = 452 nm) for 18 h. (The reaction solution was detected by HRMS analysis and the **3** was not found, **55** and **56** were detected by HRMS)

HRMS of **55**: calc. for $C_{17}H_{27}ClN_2O_2$ ($M+H^+$) 327.1834; Found 327.1834.



HRMS of **56**: calc. for $C_{16}H_{25}NO_4S$ ($M+H+$) 328.1577; Found 328.1577.



10. X-Ray crystallographic data

The structure of products was confirmed by X-ray crystallographic analysis of a single crystal of compound **28** (CCDC**2256338)**.

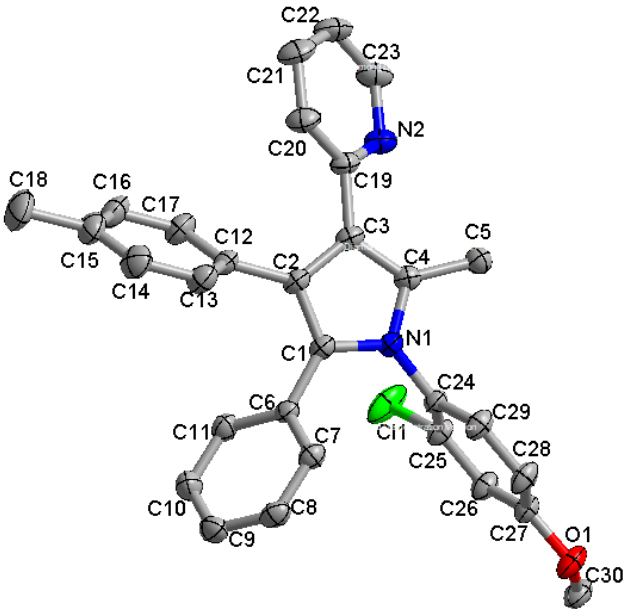


Fig. S14. Relative configuration of product **28**

Displacement ellipsoids are drawn at the 30% probability level.

(Solvents: ethyl acetate/petroleum ether = 1:10)

Table S3 Crystal data and structure refinement for **28** (CCDC **2256338)**.

Identification code	
Empirical formula	$C_{30}H_{25}ClN_2O$
Formula weight	464.97
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	6.72673(14)
b/Å	18.4617(4)
c/Å	19.8732(5)
α/°	90
β/°	93.1900(19)
γ/°	90
Volume/Å^3	2464.16(10)
Z	4
ρ_{calc}g/cm^3	1.253
μ/mm^{-1}	1.559
F(000)	976.0
Crystal size/mm^3	0.16 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.914 to 141.588

Index ranges	$-8 \le h \le 6$, $-22 \le k \le 22$, $-24 \le l \le 21$
Reflections collected	9959
Independent reflections	4654 [R_{int} = 0.0330, R_{sigma} = 0.0464]
Data/restraints/parameters	4654/0/310
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0582, wR_2 = 0.1552
Final R indexes [all data]	R_1 = 0.0719, wR_2 = 0.1722
Largest diff. peak/hole / e Å^{-3}	0.34/-0.45

Table S4 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters (Å$^2 \times 10^3$) for **28**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cl1	-148.0(12)	4450.3(5)	3971.9(4)	86.4(3)
O1	5688(3)	4011.2(11)	5675.4(9)	63.2(5)
N1	1881(3)	3312.8(10)	3195.6(9)	40.6(4)
N2	-3645(3)	2296.2(12)	2642.7(11)	53.7(5)
C1	2092(3)	3645.2(12)	2574.7(10)	40.6(5)
C2	691(3)	3343.1(12)	2124.1(11)	42.9(5)
C3	-448(3)	2834.6(12)	2487.2(11)	42.7(5)
C4	321(3)	2827.1(12)	3144.8(11)	42.5(5)
C5	-199(4)	2385.6(14)	3739.3(13)	52.8(6)
C6	3528(3)	4230.4(12)	2467.3(10)	41.2(5)
C7	5551(3)	4162.7(13)	2639.3(12)	46.9(5)
C8	6866(4)	4712.2(16)	2501.9(13)	54.5(6)
C9	6194(4)	5342.0(15)	2193.0(13)	59.3(6)
C10	4186(4)	5417.5(15)	2025.6(14)	62.4(7)
C11	2866(4)	4871.8(15)	2161.0(13)	53.5(6)
C12	514(4)	3527.6(13)	1394.0(11)	48.2(5)
C13	2156(4)	3469.3(16)	1006.6(13)	60.4(7)
C14	2028(5)	3638.3(19)	324.0(14)	72.5(8)
C15	274(6)	3873.2(18)	10.9(14)	72.6(8)
C16	-1373(5)	3936.4(19)	395.8(15)	75.6(9)
C17	-1261(4)	3770.4(17)	1079.6(14)	61.9(7)
C18	138(8)	4066(3)	-734.1(16)	107.4(14)
C19	-2185(3)	2406.7(12)	2219.6(12)	45.5(5)
C20	-2335(4)	2153.2(16)	1561.4(14)	61.0(7)
C21	-4081(5)	1808.7(18)	1328.9(17)	74.9(9)
C22	-5568(4)	1704.8(18)	1761.6(18)	75.2(9)
C23	-5280(4)	1947.8(16)	2410.0(16)	65.5(7)
C24	2854(3)	3513.8(12)	3827.3(10)	40.0(4)
C25	2044(3)	4016.4(13)	4239.6(11)	46.4(5)
C26	2916(4)	4203.0(14)	4863.7(11)	49.9(5)
C27	4669(4)	3864.6(13)	5079.4(11)	47.1(5)
C28	5488(4)	3345.8(16)	4680.3(13)	56.7(6)
C29	4597(4)	3171.3(14)	4059.8(12)	51.0(6)
C30	4843(5)	4516.5(16)	6119.0(13)	62.8(7)

Table S5 Anisotropic Displacement Parameters ($Å^2×10^3$) for **28**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	69.7(5)	111.7(6)	74.2(5)	-31.1(4)	-27.6(4)	49.1(4)
O1	66.5(11)	79.5(12)	41.4(9)	-11.2(8)	-17.0(8)	17.2(9)
N1	38.6(9)	47.0(9)	35.7(9)	-2.4(7)	-1.7(7)	-0.2(7)
N2	44.8(10)	55.4(11)	60.9(12)	-10.8(9)	1.6(9)	-6.3(9)
C1	37.4(10)	48.1(11)	35.8(10)	-3.1(8)	-2.0(8)	0.6(9)
C2	38.9(10)	51.1(12)	38.0(11)	-5.6(9)	-3.2(8)	1.3(9)
C3	37.3(10)	47.6(11)	42.9(11)	-8.9(9)	-0.6(8)	0.7(9)
C4	40.3(10)	43.2(10)	44.0(11)	-3.7(9)	1.1(8)	-0.7(9)
C5	51.4(13)	57.3(14)	49.6(13)	4.4(11)	0.9(10)	-5.8(11)
C6	39.7(11)	50.2(11)	33.2(10)	-3.5(8)	-1.3(8)	-3.4(9)
C7	42.2(11)	52.6(12)	45.7(12)	-3.7(9)	-0.1(9)	4.0(10)
C8	37.5(11)	72.6(16)	53.2(14)	-6.3(12)	-0.2(9)	-5.0(11)
C9	60.0(15)	65.3(15)	52.8(14)	1.9(12)	4.8(11)	-18.7(12)
C10	65.5(16)	58.8(15)	62.2(16)	14.6(12)	-2.9(12)	-5.1(12)
C11	45.0(12)	61.6(14)	52.9(13)	8.3(11)	-7.2(10)	0.3(10)
C12	51.1(12)	55.6(13)	36.7(11)	-5.1(9)	-7.4(9)	-3.6(10)
C13	54.8(14)	80.9(18)	45.2(13)	-3.9(12)	-0.8(10)	-0.9(13)
C14	81(2)	93(2)	44.8(14)	-6.7(14)	11.3(13)	-6.6(17)
C15	101(2)	76.3(19)	39.7(13)	-1.4(13)	-4.0(14)	-4.3(17)
C16	82(2)	88(2)	53.4(16)	-2.9(15)	-25.1(15)	8.8(17)
C17	57.7(15)	77.7(17)	48.8(14)	-4.4(12)	-10.0(11)	4.9(13)
C18	156(4)	122(3)	42.3(17)	9.9(18)	-12(2)	-3(3)
C19	43.0(11)	41.5(10)	51.5(12)	-9.4(9)	-2.7(9)	-0.6(9)
C20	61.4(15)	64.4(15)	57.0(15)	-19.7(12)	2.1(12)	-5.6(12)
C21	77(2)	78.2(19)	68.1(18)	-29.9(15)	-11.6(15)	-7.9(15)
C22	54.9(16)	73.3(18)	95(2)	-19.6(17)	-15.6(15)	-15.0(14)
C23	46.8(13)	67.1(16)	82.2(19)	-11.3(14)	0.2(12)	-10.9(12)
C24	38.9(10)	46.5(11)	34.2(10)	-0.3(8)	-1.4(8)	-1.5(8)
C25	40.9(11)	54.9(12)	42.4(11)	-1.6(9)	-5.6(9)	7.9(9)
C26	53.5(13)	56.1(13)	39.8(11)	-9.0(10)	-1.5(9)	10.2(11)
C27	50.1(12)	55.6(13)	34.7(11)	0.4(9)	-5.8(9)	2.8(10)
C28	48.6(13)	72.8(16)	47.2(13)	-3.7(11)	-10.2(10)	21.8(12)
C29	49.0(12)	59.8(14)	43.7(12)	-7.6(10)	-3.4(9)	14.9(10)
C30	78.4(18)	67.6(16)	41.0(13)	-10.2(11)	-11.4(12)	2.9(14)

Table S6 Bond Lengths for **28**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C25	1.735(2)	C9	C10	1.380(4)
O1	C27	1.362(3)	C10	C11	1.379(4)
O1	C30	1.424(3)	C12	C13	1.385(4)
N1	C1	1.392(3)	C12	C17	1.391(4)
N1	C4	1.380(3)	C13	C14	1.390(4)
N1	C24	1.432(3)	C14	C15	1.374(5)
N2	C19	1.344(3)	C15	C16	1.386(5)
N2	C23	1.334(3)	C15	C18	1.520(4)

C1	C2	1.381(3)	C16	C17	1.391(4)
C1	C6	1.472(3)	C19	C20	1.388(3)
C2	C3	1.432(3)	C20	C21	1.392(4)
C2	C12	1.489(3)	C21	C22	1.369(5)
C3	C4	1.378(3)	C22	C23	1.368(4)
C3	C19	1.484(3)	C24	C25	1.371(3)
C4	C5	1.493(3)	C24	C29	1.389(3)
C6	C7	1.390(3)	C25	C26	1.386(3)
C6	C11	1.393(3)	C26	C27	1.382(3)
C7	C8	1.383(4)	C27	C28	1.378(3)
C8	C9	1.379(4)	C28	C29	1.379(3)

Table S7 Bond Angles for **28**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C27	O1	C30	118.0(2)	C17	C12	C2	122.1(2)
C1	N1	C24	126.78(18)	C12	C13	C14	121.1(3)
C4	N1	C1	109.64(17)	C15	C14	C13	121.2(3)
C4	N1	C24	122.75(18)	C14	C15	C16	118.0(3)
C23	N2	C19	118.3(2)	C14	C15	C18	121.2(3)
N1	C1	C6	123.49(18)	C16	C15	C18	120.7(3)
C2	C1	N1	107.28(19)	C15	C16	C17	121.3(3)
C2	C1	C6	129.2(2)	C12	C17	C16	120.6(3)
C1	C2	C3	107.64(19)	N2	C19	C3	116.4(2)
C1	C2	C12	123.7(2)	N2	C19	C20	121.4(2)
C3	C2	C12	128.69(19)	C20	C19	C3	122.1(2)
C2	C3	C19	126.9(2)	C19	C20	C21	118.9(3)
C4	C3	C2	107.54(18)	C22	C21	C20	119.2(3)
C4	C3	C19	125.5(2)	C23	C22	C21	118.4(3)
N1	C4	C5	120.5(2)	N2	C23	C22	123.7(3)
C3	C4	N1	107.84(19)	C25	C24	N1	121.49(19)
C3	C4	C5	131.6(2)	C25	C24	C29	117.8(2)
C7	C6	C1	122.6(2)	C29	C24	N1	120.65(19)
C7	C6	C11	117.9(2)	C24	C25	Cl1	119.23(17)
C11	C6	C1	119.4(2)	C24	C25	C26	122.7(2)
C8	C7	C6	120.9(2)	C26	C25	Cl1	118.03(18)
C9	C8	C7	120.6(2)	C27	C26	C25	118.5(2)
C8	C9	C10	119.0(2)	O1	C27	C26	124.0(2)
C11	C10	C9	120.7(3)	O1	C27	C28	116.2(2)
C10	C11	C6	120.9(2)	C28	C27	C26	119.8(2)
C13	C12	C2	120.1(2)	C27	C28	C29	120.6(2)
C13	C12	C17	117.8(2)	C28	C29	C24	120.5(2)

Table S8 Torsion Angles for **28**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cl1	C25	C26	C27	-179.5(2)	C6	C7	C8	C9	0.3(4)
O1	C27	C28	C29	-178.4(3)	C7	C6	C11	C10	0.8(4)
N1	C1	C2	C3	2.2(2)	C7	C8	C9	C10	0.3(4)
N1	C1	C2	C12	-176.5(2)	C8	C9	C10	C11	-0.3(4)
N1	C1	C6	C7	54.4(3)	C9	C10	C11	C6	-0.3(4)

N1	C1	C6	C11	-127.8(2)	C11	C6	C7	C8	-0.8(3)
N1	C24	C25	Cl1	-3.1(3)	C12	C2	C3	C4	177.2(2)
N1	C24	C25	C26	177.7(2)	C12	C2	C3	C19	-4.6(4)
N1	C24	C29	C28	-177.4(2)	C12	C13	C14	C15	0.4(5)
N2	C19	C20	C21	3.2(4)	C13	C12	C17	C16	1.0(4)
C1	N1	C4	C3	1.3(2)	C13	C14	C15	C16	-0.1(5)
C1	N1	C4	C5	178.8(2)	C13	C14	C15	C18	179.4(3)
C1	N1	C24	C25	88.5(3)	C14	C15	C16	C17	0.2(5)
C1	N1	C24	C29	-95.4(3)	C15	C16	C17	C12	-0.7(5)
C1	C2	C3	C4	-1.5(2)	C17	C12	C13	C14	-0.9(4)
C1	C2	C3	C19	176.7(2)	C18	C15	C16	C17	-179.2(3)
C1	C2	C12	C13	54.1(3)	C19	N2	C23	C22	-0.9(4)
C1	C2	C12	C17	-125.0(3)	C19	C3	C4	N1	-178.1(2)
C1	C6	C7	C8	177.0(2)	C19	C3	C4	C5	4.8(4)
C1	C6	C11	C10	-177.1(2)	C19	C20	C21	C22	-2.5(5)
C2	C1	C6	C7	-128.4(3)	C20	C21	C22	C23	0.2(5)
C2	C1	C6	C11	49.3(3)	C21	C22	C23	N2	1.6(5)
C2	C3	C4	N1	0.1(2)	C23	N2	C19	C3	176.4(2)
C2	C3	C4	C5	-177.0(2)	C23	N2	C19	C20	-1.5(4)
C2	C3	C19	N2	-143.8(2)	C24	N1	C1	C2	-171.9(2)
C2	C3	C19	C20	34.1(4)	C24	N1	C1	C6	5.7(3)
C2	C12	C13	C14	180.0(3)	C24	N1	C4	C3	171.50(19)
C2	C12	C17	C16	-179.9(3)	C24	N1	C4	C5	-11.0(3)
C3	C2	C12	C13	-124.4(3)	C24	C25	C26	C27	-0.3(4)
C3	C2	C12	C17	56.5(4)	C25	C24	C29	C28	-1.2(4)
C3	C19	C20	C21	-174.6(3)	C25	C26	C27	O1	178.7(2)
C4	N1	C1	C2	-2.2(2)	C25	C26	C27	C28	-1.1(4)
C4	N1	C1	C6	175.5(2)	C26	C27	C28	C29	1.4(4)
C4	N1	C24	C25	-80.0(3)	C27	C28	C29	C24	-0.3(4)
C4	N1	C24	C29	96.2(3)	C29	C24	C25	Cl1	-179.34(19)
C4	C3	C19	N2	34.0(3)	C29	C24	C25	C26	1.5(4)
C4	C3	C19	C20	-148.1(3)	C30	O1	C27	C26	3.4(4)
C6	C1	C2	C3	-175.3(2)	C30	O1	C27	C28	-176.8(3)
C6	C1	C2	C12	6.0(4)					

Table S9 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **28**.

Atom	*x*	*y*	*z*	U(eq)
H5A	962	2132	3916	79
H5B	-1216	2042	3604	79
H5C	-678	2698	4081	79
H7	6027	3742	2850	56
H8	8216	4657	2619	65
H9	7080	5710	2099	71
H10	3717	5841	1819	75
H11	1517	4933	2046	64
H13	3365	3314	1207	73
H14	3151	3591	75	87
H16	-2576	4093	193	91

H17	-2383	3822	1329	74
H18A	1338	4306	-849	161
H18B	-979	4381	-827	161
H18C	-33	3632	-997	161
H20	-1287	2213	1280	73
H21	-4235	1651	885	90
H22	-6747	1475	1618	90
H23	-6280	1865	2705	79
H26	2334	4548	5131	60
H28	6652	3111	4831	68
H29	5169	2821	3795	61
H30A	5741	4591	6505	94
H30B	3602	4331	6262	94
H30C	4615	4969	5889	94

11. References

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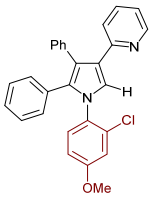
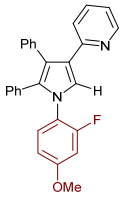
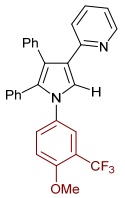
12. Characterization data



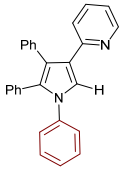
2-(1-(2-Chloro-4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (3): brown solid; Mp: 174.3-175.6 °C; 40.6 mg, 93% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.0 Hz, 1H), 7.45 (s, 1H), 7.39 – 7.34 (m, 1H), 7.20 (m, 5H), 7.12 (d, *J* = 8.7 Hz, 1H), 7.05 (dt, *J* = 5.4, 3.0 Hz, 3H), 7.02 – 6.98 (m, 1H), 6.98 – 6.92 (m, 3H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.69 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.77 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 154.3, 149.2, 135.6, 133.2, 132.8, 131.6, 131.0, 130.6, 130.5, 127.9, 127.5, 126.6, 126.1, 124.2, 123.9, 122.3, 121.9, 120.3, 114.8, 112.9, 55.6; HRMS (ESI) m/z 437.1412 ($M+H^+$), calc. for $C_{28}H_{21}ClN_2O$ 437.1415.



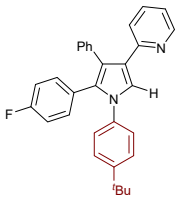
2-(1-(2-Fluoro-4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (4): white solid; Mp: 166.1-167.3 °C; 34.5 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.8 Hz, 1H), 7.50 (s, 1H), 7.41 – 7.33 (m, 1H), 7.18 (dd, *J* = 7.2, 3.6 Hz, 5H), 7.13 – 7.05 (m, 4H), 7.04 – 6.99 (m, 1H), 6.98 – 6.92 (m, 2H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.66 – 6.56 (m, 2H), 3.78 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ160.0 (d, *J* = 10.1 Hz), 157.7 (d, *J* = 250.5 Hz), 154.2, 149.1, 135.7 (d, *J* = 17.4 Hz), 133.2, 131.6, 131.0, 130.5, 129.7 (d, *J* = 2.0 Hz), 128.0, 127.6, 126.8, 126.2, 124.3, 124.0, 122.4, 122.2, 120.8, 120.7, 120.4, 109.7 (d, *J* = 3.3 Hz), 102.2 (d, *J* = 23.6 Hz), 55.7; ^{19}F NMR (471 MHz, $CDCl_3$) δ -119.0; HRMS (ESI) m/z 421.1705 ($M+H^+$), calc. for $C_{28}H_{21}FN_2O$ 421.1711.



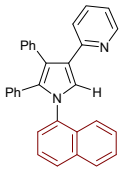
2-(1-(4-Methoxy-3-(trifluoromethyl)phenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (5): brown solid; Mp: 134.8-135.7 °C; 37.6 mg, 80% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.56 (d, *J* = 4.8 Hz, 1H), 7.60 (s, 1H), 7.49 (d, *J* = 2.5 Hz, 1H), 7.41 – 7.36 (m, 1H), 7.21 (td, *J* = 5.7, 2.4 Hz, 6H), 7.12 (dd, *J* = 5.0, 1.8 Hz, 3H), 7.06 – 7.01 (m, 1H), 6.96 (dd, *J* = 6.5, 3.1 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.9 (q, *J* = 1.6 Hz), 154.0, 149.2, 135.7, 135.3, 132.3 (q, *J* = 23.8 Hz), 131.3, 131.0, 130.5, 128.0, 127.8, 127.0, 126.3, 124.5 (q, *J* = 5.2 Hz), 123.2, 122.2, 120.6, 119.1, 118.7, 114.0, 112.1, 56.1; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.8; HRMS (ESI) m/z 471.1674 ($M+H^+$), calc. for $C_{29}H_{21}F_3N_2O$ 471.1679.



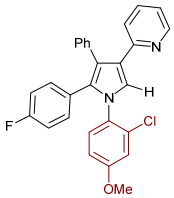
2-(1,4,5-Triphenyl-1*H*-pyrrol-3-yl)pyridine (6): yellow oil; 32.8 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.7 Hz, 1H), 7.47 (d, *J* = 9.9 Hz, 1H), 7.34 (d, *J* = 8.3 Hz, 1H), 7.30 (s, 1H), 7.27 (s, 1H), 7.22 (d, *J* = 4.1 Hz, 4H), 7.20 – 7.13 (m, 4H), 7.13 – 7.08 (m, 3H), 7.04 (t, *J* = 8.7 Hz, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.1, 149.2, 136.9, 133.4, 132.0, 130.3, 128.5, 127.9, 126.9, 126.5, 125.8, 123.7, 122.6, 121.1; HRMS (ESI) m/z 373.1695 ($M+H^+$), calc. for $C_{27}H_{20}N_2$ 373.1699.



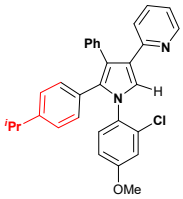
2-(1-(4-(Tert-butyl)phenyl)-5-(4-fluorophenyl)-4-phenyl-1*H*-pyrrol-3-yl) pyridine (7): yellow oil; 31.7 mg, 71% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.9 Hz, 1H), 7.60 (s, 1H), 7.43 – 7.33 (m, 2H), 7.32 – 7.26 (m, 3H), 7.22 (td, *J* = 4.2, 2.5 Hz, 3H), 7.17 (m, 2H), 7.08 (d, *J* = 4.5 Hz, 1H), 7.05 – 6.99 (m, 1H), 6.93 (dd, *J* = 8.8, 2.6 Hz, 2H), 6.88 – 6.81 (m, 1H), 6.81 – 6.75 (m, 1H), 1.31 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.2, 149.9, 149.2, 137.1, 135.8, 135.5, 132.6 (d, *J* = 8.1 Hz), 131.1, 128.0, 126.3, 125.7, 125.3, 123.5, 123.0, 122.1, 120.4, 114.7 (d, *J* = 21.4 Hz), 34.5, 31.3.; ^{19}F NMR (471 MHz, $CDCl_3$) δ -115.8; HRMS (ESI) m/z 447.2226 ($M+H^+$), calc. for $C_{31}H_{27}FN_2$ 447.2231.



2-(1-(Naphthalen-1-yl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (8): yellow solid; Mp: 159.7-160.4 °C; 32.1 mg, 76% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.3 Hz, 1H), 7.90 – 7.76 (m, 3H), 7.62 (s, 1H), 7.48 (q, *J* = 5.6, 4.0 Hz, 2H), 7.43 – 7.30 (m, 3H), 7.26 (s, 1H), 7.24 (s, 4H), 7.07 – 7.01 (m, 1H), 6.91 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.4, 149.2, 136.6, 135.8, 135.7, 134.0, 133.9, 131.7, 131.1, 130.8, 130.3, 128.3, 128.0, 127.9, 127.4, 127.0, 126.5, 126.4, 126.1, 125.9, 125.2, 124.9, 123.5, 122.4, 120.4; HRMS (ESI) m/z 423.1851 ($M+H^+$), calc. for $C_{31}H_{22}N_2$ 423.1856.

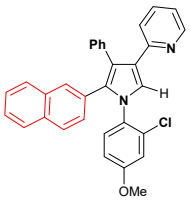


2-(1-(2-Chloro-4-methoxyphenyl)-5-(4-fluorophenyl)-4-phenyl-1*H*-pyrrol -3-yl)pyridine (9): yellow oil; 35.5 mg, 78% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.54 (d, *J* = 5.7 Hz, 1H), 7.43 (s, 1H), 7.38 (td, *J* = 7.8, 1.9 Hz, 1H), 7.25 – 7.10 (m, 6H), 7.04 – 7.00 (m, 1H), 6.95 – 6.84 (m, 4H), 6.80 – 6.69 (m, 3H), 3.79 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.6 (d, *J* = 246.6 Hz), 159.9, 159.5, 154.2, 149.2, 135.7, 135.4, 132.9, 132.2 (d, *J* = 8.1 Hz), 132.2, 131.0, 130.6, 130.3, 128.0, 127.7 (d, *J* = 3.4 Hz), 126.2, 124.1, 123.9, 122.3, 122.0, 120.4, 114.9, 114.9 (d, *J* = 7.9 Hz), 113.0, 55.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -114.9； HRMS (ESI) m/z 455.1317 ($M+H^+$), calc. for $C_{28}H_{20}ClFN_2O$ 455.1321.

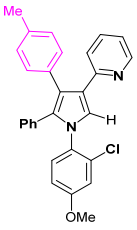


2-(1-(2-Chloro-4-methoxyphenyl)-5-(4-isopropylphenyl)-4-phenyl-1*H*-p yrrol-3-yl)pyridine (10): brown solid; Mp: 178.9-179.6 °C; 42.6 mg, 89% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.8 Hz, 1H), 7.42 (s, 1H), 7.36 (td, *J* = 7.8, 1.8 Hz, 1H), 7.24 – 7.16 (m, 5H), 7.09 (d, *J* = 8.8 Hz, 1H), 7.03 – 6.98 (m, 1H), 6.95 (d, *J* = 2.8 Hz, 1H), 6.87 (q, *J* = 8.1 Hz, 5H), 6.69 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.79 (s, 3H), 2.76 (m, 1H), 1.14 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 154.4, 149.2, 147.0, 135.7, 135.6, 133.3, 132.8, 130.7, 130.3, 128.8, 127.9, 126.0,

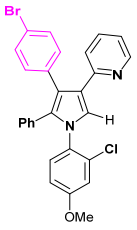
125.6, 124.1, 123.8, 122.4, 121.6, 120.3, 114.8, 112.9, 55.6, 33.5, 23.7; HRMS (ESI) m/z 479.1880 ($M+H^+$), calc. for $C_{31}H_{27}ClN_2O$ 479.1885.



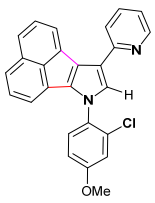
2-(1-(2-Chloro-4-methoxyphenyl)-5-(naphthalen-2-yl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (11): brown solid; Mp: 158.3-159.7 °C; 38.5 mg, 79% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.1 Hz, 1H), 7.72 – 7.65 (m, 1H), 7.51 (d, *J* = 10.1 Hz, 3H), 7.46 – 7.31 (m, 4H), 7.27 – 7.12 (m, 6H), 7.10 – 7.00 (m, 2H), 6.97 – 6.82 (m, 2H), 6.66 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 154.3, 149.3, 135.6, 135.5, 133.1, 132.8, 132.8, 131.9, 131.1, 130.6, 130.6, 129.6, 129.2, 128.4, 128.0, 128.0, 127.4, 127.0, 126.2, 125.7, 125.6, 124.5, 124.1, 122.4, 120.4, 114.9, 113.0, 55.6; HRMS (ESI) m/z 487.1570 ($M+H^+$), calc. for $C_{32}H_{23}ClN_2O$ 487.1572.



2-(1-(2-Chloro-4-methoxyphenyl)-5-phenyl-4-(p-tolyl)-1*H*-pyrrol-3-yl)pyridine (12): brown solid; Mp: 179.8-180.6 °C; 39.7 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.1 Hz, 1H), 7.43 (s, 1H), 7.37 (td, *J* = 7.8, 1.8 Hz, 1H), 7.14 – 7.00 (m, 9H), 6.99 – 6.93 (m, 3H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.69 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.77 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 154.5, 149.2, 135.5, 135.5, 133.1, 132.7, 132.4, 131.8, 130.8, 130.6, 130.6, 128.7, 127.5, 126.5, 124.1, 124.0, 122.3, 121.8, 120.3, 114.8, 112.9, 55.6, 21.2; HRMS (ESI) m/z 451.1568 ($M+H^+$), calc. for $C_{29}H_{23}ClN_2O$ 451.1572.

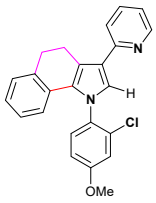


2-(4-(4-Bromophenyl)-1-(2-chloro-4-methoxyphenyl)-5-phenyl-1*H*-pyrrol-3-yl)pyridine (13): brown solid; Mp: 152.2-153.2 °C; 43.8 mg, 85% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.6 Hz, 1H), 7.47 – 7.39 (m, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.13 – 7.01 (m, 7H), 7.00 – 6.81 (m, 4H), 6.69 (dd, *J* = 8.8, 2.7 Hz, 1H), 3.78 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.4, 154.1, 149.4, 135.7, 134.5, 133.3, 132.8, 132.6, 131.3, 131.1, 130.6, 130.6, 130.3, 127.7, 126.9, 124.3, 123.9, 122.4, 120.5, 120.1, 114.9, 112.9, 55.6; HRMS (ESI) m/z 515.0519 ($M+H^+$), calc. for $C_{28}H_{20}BrClN_2O$ 515.0521.

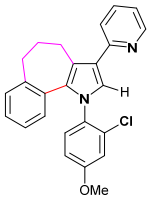


7-(2-Chloro-4-methoxyphenyl)-9-(pyridin-2-yl)-7*H*-acenaphtho[1,2-b]pyrrole (14): yellow oil; 30.6 mg, 75% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.75 (d, *J* = 5.1 Hz, 1H), 8.30 (d, *J* = 6.8 Hz, 1H), 7.82 – 7.74 (m, 2H), 7.65 (dd, *J* = 8.2, 4.5 Hz, 2H), 7.59 – 7.51 (m, 2H), 7.38 (s, 1H), 7.35 – 7.30 (m, 1H), 7.17 (t, *J* = 4.1 Hz, 2H), 7.04 – 6.93 (m, 2H), 3.92 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.0, 154.2, 149.4, 139.8, 136.5, 133.5, 132.8, 131.7, 130.2, 129.4, 129.1, 128.9, 127.9, 126.7, 125.9,

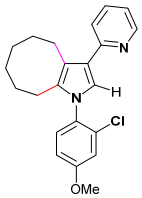
125.4, 123.0, 120.7, 120.2, 118.1, 115.7, 113.6, 55.9; HRMS (ESI) m/z 409.1097 ($M+H^+$), calc. for $C_{26}H_{17}ClN_2O$ 409.1102.



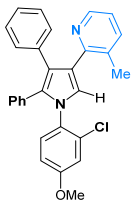
1-(2-Chloro-4-methoxyphenyl)-3-(pyridin-2-yl)-4,5-dihydro-1*H*-benzo[g]indole (15): yellow oil; 29.0 mg, 75% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.7 Hz, 1H), 7.68 (t, *J* = 7.7 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.7 Hz, 1H), 7.28 (s, 1H), 7.22 (d, *J* = 7.3 Hz, 1H), 7.16 – 7.07 (m, 2H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.90 (t, *J* = 7.7 Hz, 2H), 6.41 (d, *J* = 7.7 Hz, 1H), 3.89 (s, 3H), 3.11 (dd, *J* = 7.9, 5.6 Hz, 2H), 2.99 (t, *J* = 7.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.8, 154.5, 149.1, 136.5, 135.9, 132.8, 131.3, 130.3, 130.0, 129.3, 128.0, 126.2, 125.1, 124.8, 121.1, 120.6, 120.3, 120.0, 115.4, 113.5, 55.8, 30.7, 21.9; HRMS (ESI) m/z 387.1253 ($M+H^+$), calc. for $C_{24}H_{19}ClN_2O$ 387.1259.



1-(2-Chloro-4-methoxyphenyl)-3-(pyridin-2-yl)-1,4,5,6-tetrahydrobenzo[6,7]cyclohepta[1,2-b]pyrrole (16): yellow oil; 32.9 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.5 Hz, 1H), 7.71 (t, *J* = 7.7 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.37 – 7.27 (m, 3H), 7.17 – 7.07 (m, 2H), 6.97 (t, *J* = 7.5 Hz, 1H), 6.92 (d, *J* = 2.5 Hz, 1H), 6.83 (dd, *J* = 8.7, 2.4 Hz, 1H), 6.63 (d, *J* = 7.6 Hz, 1H), 3.81 (s, 3H), 2.80 (m, 3H), 2.60 (dd, *J* = 13.3, 6.8 Hz, 1H), 2.36 (m, 2H); 13C NMR (75 MHz, CDCl3) δ 159.3, 154.4, 149.1, 141.2, 136.8, 132.8, 132.4, 130.6, 130.0, 129.4, 127.1, 126.1, 125.5, 123.3, 121.9, 121.3, 120.3, 115.2, 113.3, 55.7, 34.4, 32.8, 21.6; HRMS (ESI) m/z 401.1412 ($M+H^+$), calc. for $C_{25}H_{21}ClN_2O$ 401.1415.

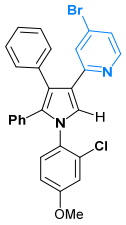


1-(2-Chloro-4-methoxyphenyl)-3-(pyridin-2-yl)-4,5,6,7,8,9-hexahydro-1*H*-cycloocta[b]pyrrole (17): yellow oil; 31.6 mg, 86% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.7 Hz, 1H), 7.65 (t, *J* = 7.4 Hz, 1H), 7.51 (s, 1H), 7.25 (d, *J* = 6.6 Hz, 1H), 7.21 – 7.11 (m, 1H), 7.05 (m, 2H), 6.86 (dd, *J* = 8.6, 2.3 Hz, 1H), 3.85 (s, 3H), 2.96 (p, *J* = 6.5 Hz, 2H), 2.60 – 2.32 (m, 2H), 1.91 – 1.61 (m, 3H), 1.55 – 1.32 (m, 5H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.7, 155.2, 148.6, 136.6, 133.6, 133.1, 130.5, 130.3, 121.6, 121.1, 119.8, 118.3, 115.1, 113.0, 55.8, 30.5, 29.7, 26.1, 25.8, 23.4; HRMS (ESI) m/z 367.1569 ($M+H^+$), calc. for $C_{22}H_{23}ClN_2O$ 367.1572.

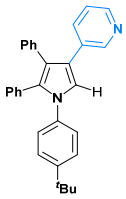


2-(1-(2-Chloro-4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-3-methylpyridine (18): brown oil; 39.7 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.5 Hz, 1H), 7.41 (d, *J* = 7.0 Hz, 1H), 7.11 (s, 4H), 7.02 (m, 7H), 6.97 (d, *J* = 2.4 Hz, 1H), 6.95 – 6.88 (m, 2H), 6.66 (dd, *J* = 8.8, 2.6 Hz, 1H), 3.79 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.3, 156.1, 149.1, 137.8, 136.8, 132.0, 130.5,

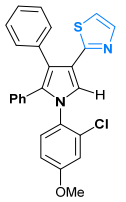
130.3, 129.0, 128.5, 128.2, 126.9, 126.5, 125.3, 123.7, 123.6, 122.8, 122.6, 121.0, 117.1, 113.0, 55.3, 21.4; HRMS (ESI) m/z 451.1568 ($M+H^+$), calc. for $C_{29}H_{23}ClN_2O$ 451.1572.



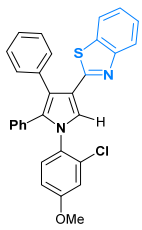
4-Bromo-2-(1-(2-chloro-4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (19): brown oil; 44.4 mg, 86% yield; ^1H NMR (300 MHz, $CDCl_3$) δ 8.34 (d, J = 5.2 Hz, 1H), 7.49 (s, 1H), 7.24 (s, 2H), 7.21 – 7.16 (m, 3H), 7.10 (m, 5H), 7.02 (s, 1H), 6.97 – 6.91 (m, 3H), 6.71 (d, J = 8.8 Hz, 1H), 3.79 (d, J = 1.3 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.5, 155.6, 149.6, 134.9, 133.5, 132.8, 131.4, 130.9, 130.6, 130.5, 130.4, 128.1, 127.6, 126.8, 126.5, 125.4, 124.8, 123.5, 122.0, 114.9, 113.0, 55.7; HRMS (ESI) m/z 515.0516 ($M+H^+$), calc. for $C_{28}H_{20}BrClN_2O$ 515.0521.



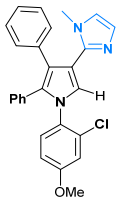
3-(1-(4-(Tert-butyl)phenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (20): yellow oil; 33.0 mg, 77% yield; ^1H NMR (300 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.40 (d, J = 4.7 Hz, 1H), 7.40 (d, J = 7.9 Hz, 1H), 7.31 (d, J = 8.3 Hz, 2H), 7.17 (d, J = 3.2 Hz, 4H), 7.14 – 7.04 (m, 8H), 6.97 (d, J = 7.6 Hz, 2H), 1.31 (d, J = 1.1 Hz, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.0, 148.5, 146.2, 137.2, 135.8, 134.9, 132.0, 131.6, 131.0, 130.9, 128.1, 127.7, 126.8, 126.1, 125.8, 125.3, 123.1, 122.9, 121.5, 120.7, 34.6, 31.3; HRMS (ESI) m/z 429.2322 ($M+H^+$), calc. for $C_{31}H_{28}N_2$ 429.2325.



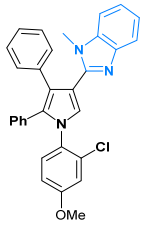
2-(1-(2-Chloro-4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)thiazole (21): yellow solid; Mp: 173.6-174.5 °C; 35.9 mg, 81% yield; ^1H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, J = 3.3 Hz, 1H), 7.53 (s, 1H), 7.29 (d, J = 8.5 Hz, 5H), 7.17 (d, J = 8.8 Hz, 1H), 7.08 – 7.01 (m, 4H), 6.95 (dd, J = 6.8, 2.3 Hz, 3H), 6.73 (dd, J = 8.8, 2.8 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.0, 159.5, 141.7, 134.4, 133.4, 132.7, 131.7, 131.1, 130.4, 130.3, 130.2, 128.1, 127.6, 127.0, 126.8, 123.2, 122.4, 118.8, 117.2, 115.0, 113.1, 55.7; HRMS (ESI) m/z 443.0976 ($M+H^+$), calc. for $C_{26}H_{19}ClN_2OS$ 443.0980.



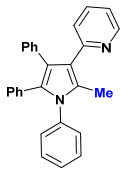
2-(1-(2-Chloro-4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)benzo[d]thiazole (22): yellow oil; 38.9 mg, 79% yield; ^1H NMR (300 MHz, $CDCl_3$) δ 7.95 (d, J = 10.2 Hz, 1H), 7.69 (d, J = 7.9 Hz, 2H), 7.44 – 7.29 (m, 6H), 7.20 (d, J = 8.9 Hz, 2H), 7.05 (dd, J = 8.9, 5.1 Hz, 3H), 7.00 – 6.89 (m, 3H), 6.75 (dd, J = 8.8, 2.4 Hz, 1H), 3.81 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.4, 159.7, 152.8, 134.1, 133.8, 133.4, 132.8, 131.9, 130.9, 130.4, 130.3, 130.1, 128.7, 127.6, 127.3, 126.9, 126.3, 125.7, 124.5, 123.9, 122.9, 122.5, 122.0, 121.2, 115.1, 113.1, 55.7; HRMS (ESI) m/z 493.1133 ($M+H^+$), calc. for $C_{30}H_{21}ClN_2OS$ 493.1136.



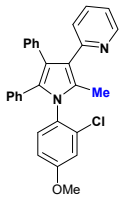
2-(1-(2-Chloro-4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-imidazole (23): yellow oil; 36.1 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (dd, *J* = 9.0, 5.5 Hz, 2H), 7.18 – 7.09 (m, 6H), 7.07 – 6.98 (m, 3H), 6.96 (dd, *J* = 6.8, 3.1 Hz, 3H), 6.85 (s, 1H), 6.66 (dd, *J* = 8.4, 2.2 Hz, 1H), 3.79 (s, 3H), 3.02 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.4, 143.7, 135.2, 132.9, 131.7, 131.5, 130.8, 130.7, 130.2, 129.4, 128.0, 127.9, 127.8, 127.0, 125.7, 125.0, 122.8, 120.7, 114.9, 113.3, 112.9, 55.6, 33.1; HRMS (ESI) m/z 440.1519 ($M+H^+$), calc. for $C_{27}H_{22}ClN_3O$ 440.1524.



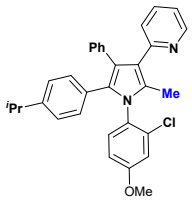
2-(1-(2-Chloro-4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)-1-methyl-1*H*-benzo[d]imidazole (24): yellow oil; 37.7 mg, 77% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 6.7, 1.7 Hz, 1H), 7.30 (s, 1H), 7.29 – 7.23 (m, 2H), 7.21 (t, *J* = 3.0 Hz, 1H), 7.13 (dd, *J* = 5.1, 1.9 Hz, 3H), 7.11 – 7.05 (m, 5H), 7.01 (m,3H), 6.96 (d, *J* = 2.8 Hz, 1H), 6.69 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.78 (s, 3H), 3.14 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 150.3, 143.1, 136.0, 135.0, 132.9, 132.2, 131.3, 130.8, 130.7, 130.0, 129.5, 128.2, 127.9, 127.1, 125.9, 125.8, 122.7, 121.9, 121.8, 119.3, 114.9, 113.2, 112.9, 109.3, 55.6, 30.5; HRMS (ESI) m/z 490.1675 ($M+H^+$), calc. for $C_{31}H_{24}ClN_3O$ 490.1681.



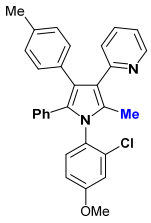
2-(2-Methyl-1,4,5-triphenyl-1*H*-pyrrol-3-yl)pyridine (25): yellow oil; 33.6 mg, 87% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 – 8.49 (m, 1H), 7.51 – 7.44 (m, 1H), 7.33 (s, 1H), 7.25 – 7.18 (m, 4H), 7.18 – 6.96 (m, 12H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.2, 149.2, 136.9, 133.4, 132.0, 130.3, 128.5, 127.9, 126.9, 126.5, 125.8, 123.7, 122.6, 121.1, 116.2, 108.5, 105.9, 12.9; HRMS (ESI) m/z 387.1851 ($M+H^+$), calc. for $C_{28}H_{22}N_2$ 387.1856.



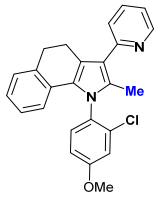
2-(1-(2-Chloro-4-methoxyphenyl)-2-methyl-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (26): gray solid; Mp: 189.4-190.6 °C; 39.2 mg, 87% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.5 Hz, 1H), 7.48 – 7.38 (m, 1H), 7.10 (d, *J* = 3.0 Hz, 2H), 7.08 (s, 3H), 7.04 (dd, *J* = 6.7, 3.4 Hz, 4H), 7.02 – 6.98 (m, 3H), 6.97 (d, *J* = 2.4 Hz, 1H), 6.90 (d, *J* = 7.9 Hz, 1H), 6.71 (dd, *J* = 8.7, 2.3 Hz, 1H), 3.79 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.3, 156.1, 149.1, 136.9, 132.0, 130.5, 130.2, 128.5, 127.5, 126.8, 126.5, 123.7, 123.7, 122.8, 122.6, 121.1, 117.1, 116.1, 113.0, 108.4, 105.8, 55.3, 12.8.; HRMS (ESI) m/z 451.1566 ($M+H^+$), calc. for $C_{29}H_{23}ClN_2O$ 451.1572.



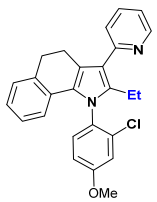
2-(1-(2-Chloro-4-methoxyphenyl)-5-(4-isopropylphenyl)-2-methyl-4-phenyl-1*H*-pyrrol-3-yl)pyridine (27): gray solid; Mp: 179.4-180.3 °C; 42.4 mg, 86% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.2 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.19 (m, 2H), 7.07 (s, 2H), 7.03 (d, *J* = 3.8 Hz, 2H), 6.97 (dd, *J* = 6.8, 2.9 Hz, 2H), 6.89 (d, *J* = 5.3 Hz, 5H), 6.72 (dd, *J* = 8.7, 2.8 Hz, 1H), 3.79 (s, 3H), 2.83 – 2.69 (m, 1H), 2.22 (s, 3H), 1.14 (d, *J* = 6.9 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.4, 156.2, 149.1, 148.8, 136.8, 131.1, 130.5, 128.3, 127.3, 126.4, 125.8, 125.7, 124.9, 124.6, 123.7, 123.6, 122.8, 121.1, 117.2, 116.2, 113.0, 108.4, 105.8, 55.3, 34.1, 23.9, 12.8; HRMS (ESI) m/z 493.2037 ($M+H^+$), calc. for $C_{32}H_{29}ClN_2O$ 493.2041.



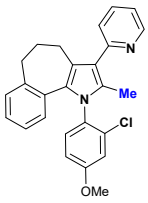
2-(1-(2-Chloro-4-methoxyphenyl)-2-methyl-5-phenyl-4-(p-tolyl)-1*H*-pyrrol-3-yl)pyridine (28): brown solid; Mp: 169.4-170.2 °C; 40.5 mg, 87% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.5 Hz, 1H), 7.44 (t, *J* = 7.1 Hz, 1H), 7.11 – 7.02 (m, 6H), 6.96 (dd, *J* = 10.3, 7.9 Hz, 3H), 6.89 (s, 4H), 6.71 (dd, *J* = 8.7, 2.4 Hz, 1H), 3.78 (s, 3H), 2.28 – 2.21 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.3, 156.1, 149.1, 137.8, 136.8, 132.0, 130.5, 130.3, 129.0, 128.5, 128.2, 127.5, 126.9, 126.5, 125.3, 123.7, 123.6, 122.8, 122.6, 121.0, 117.1, 116.1, 113.0, 108.4, 105.8, 55.3, 21.4, 12.8; HRMS (ESI) m/z 465.1723 ($M+H^+$), calc. for $C_{30}H_{25}ClN_2O$ 465.1728.



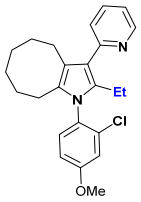
1-(2-Chloro-4-methoxyphenyl)-2-methyl-3-(pyridin-2-yl)-4,5-dihydro-1*H*-benzo[g]indole (29): yellow oil; 32.5 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.5 Hz, 1H), 7.71 (t, *J* = 7.0 Hz, 1H), 7.34 (d, *J* = 7.9 Hz, 1H), 7.29 (s, 1H), 7.15 (dd, *J* = 9.8, 5.2 Hz, 3H), 6.98 – 6.83 (m, 3H), 6.32 (d, *J* = 7.6 Hz, 1H), 3.90 (s, 3H), 2.91 (t, *J* = 4.7 Hz, 4H), 2.23 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.1, 156.2, 149.1, 135.9, 134.4, 131.2, 130.3, 129.7, 128.8, 128.0, 126.2, 124.4, 124.0, 120.8, 120.0, 119.4, 115.4, 114.6, 114.3, 113.7, 55.8, 30.8, 21.4, 11.2; HRMS (ESI) m/z 401.1411 ($M+H^+$), calc. for $C_{25}H_{21}ClN_2O$ 401.1415.



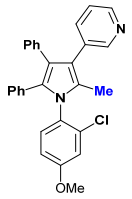
1-(2-Chloro-4-methoxyphenyl)-2-ethyl-3-(pyridin-2-yl)-4,5-dihydro-1*H*-benzo[g]indole (30): yellow oil; 35.7 mg, 86% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.4 Hz, 1H), 7.71 (t, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 8.8 Hz, 2H), 7.14 (m, 3H), 6.93 (dd, *J* = 7.5, 4.3 Hz, 2H), 6.85 (t, *J* = 7.4 Hz, 1H), 6.27 (d, *J* = 7.8 Hz, 1H), 3.91 (s, 3H), 2.88 (m, 4H), 2.67 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.1, 156.6, 149.2, 137.0, 136.0, 134.8, 131.5, 130.1, 129.7, 128.0, 126.2, 124.4, 123.8, 120.8, 120.1, 119.4, 115.4, 113.5, 55.8, 30.8, 21.4, 18.4, 14.6; HRMS (ESI) m/z 415.1565 ($M+H^+$), calc. for $C_{26}H_{23}ClN_2O$ 415.1572.



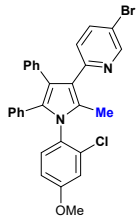
1-(2-Chloro-4-methoxyphenyl)-2-methyl-3-(pyridin-2-yl)-1,4,5,6-tetrahydrobenzo[6,7]cyclohepta[1,2-b]pyrrole (31): yellow oil; 34.9 mg, 84% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.2 Hz, 1H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 5.2 Hz, 1H), 7.21 – 7.08 (m, 2H), 7.06 – 6.91 (m, 3H), 6.86 – 6.77 (m, 1H), 6.68 (d, *J* = 7.5 Hz, 1H), 3.82 (s, 3H), 2.75 (m, 2H), 2.50 (t, *J* = 7.1 Hz, 2H), 2.32 (dt, *J* = 10.4, 4.9 Hz, 2H), 2.21 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 155.9, 149.4, 141.3, 135.7, 134.2, 133.3, 131.4, 130.2, 129.7, 129.6, 129.3, 126.9, 125.5, 124.3, 121.6, 121.3, 120.0, 115.2, 113.3, 55.7, 34.8, 33.0, 21.4, 11.4; HRMS (ESI) m/z 415.1566 ($M+H^+$), calc. for $C_{26}H_{23}ClN_2O$ 415.1572.



1-(2-Chloro-4-methoxyphenyl)-2-ethyl-3-(pyridin-2-yl)-4,5,6,7,8,9-hexahydro-1*H*-cycloocta[b]pyrrole (32): yellow oil; 30.8 mg, 78% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.8 Hz, 1H), 7.65 (td, *J* = 7.7, 1.8 Hz, 1H), 7.35 (d, *J* = 7.9 Hz, 1H), 7.23 (d, *J* = 8.7 Hz, 1H), 7.09 (dd, *J* = 6.6, 1.6 Hz, 1H), 7.06 (d, *J* = 2.7 Hz, 1H), 6.89 (dd, *J* = 8.7, 2.8 Hz, 1H), 3.86 (s, 3H), 2.83 – 2.56 (m, 2H), 2.61 – 2.32 (m, 4H), 1.62 (t, *J* = 8.8 Hz, 2H), 1.51 – 1.34 (m, 6H), 0.84 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.7, 156.6, 149.2, 135.6, 134.8, 132.8, 131.7, 129.8, 129.3, 124.1, 120.0, 119.7, 118.1, 115.0, 113.0, 55.7, 31.0, 29.4, 26.1, 25.8, 23.5, 23.3, 18.5, 14.9; HRMS (ESI) m/z 395.1879 ($M+H^+$), calc. for $C_{24}H_{27}ClN_2O$ 395.1885.

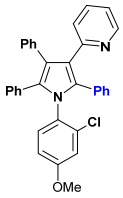


3-(1-(2-Chloro-4-methoxyphenyl)-2-methyl-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (33): yellow oil; 36.9 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.43 (d, *J* = 4.4 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.22 (dd, *J* = 7.8, 5.1 Hz, 1H), 7.16 (d, *J* = 8.8 Hz, 1H), 7.13 – 7.04 (m, 6H), 7.02 (d, *J* = 5.3 Hz, 2H), 6.96 (dd, *J* = 8.0, 3.4 Hz, 3H), 6.75 (dd, *J* = 8.5, 2.4 Hz, 1H), 3.80 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.8, 149.4, 145.0, 139.1, 134.8, 134.5, 132.9, 131.9, 131.5, 130.8, 129.2, 128.8, 127.8, 127.6, 126.7, 125.6, 123.2, 122.1, 117.2, 115.0, 113.1, 55.7, 11.1; HRMS (ESI) m/z 451.1567 ($M+H^+$), calc. for $C_{29}H_{23}ClN_2O$ 451.1572.

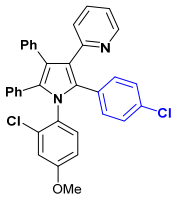


5-Bromo-2-(1-(2-chloro-4-methoxyphenyl)-2-methyl-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (34): white solid; Mp: 141.2-142.3 ºC; 46.6 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.69 (d, *J* = 2.0 Hz, 1H), 7.52 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 2.1 Hz, 1H), 7.11 (d, *J* = 5.6 Hz, 3H), 7.05 (dd, *J* = 7.8, 4.1 Hz, 5H), 7.00 – 6.99 (m, 1H), 6.97 (d, *J* = 3.0 Hz, 1H), 6.79 – 6.69 (m, 2H), 3.79 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.7, 158.0, 150.1, 138.9, 138.6, 136.5, 135.3, 134.4, 132.8, 132.0, 131.6, 130.8, 129.2, 129.0, 128.8,

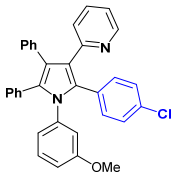
128.4, 128.2, 127.8, 127.6, 127.2, 126.6, 125.6, 125.3, 122.1, 117.0, 114.9, 113.1, 55.6, 11.2; HRMS (ESI) m/z 529.0673 ($M+H^+$), calc. for $C_{29}H_{22}BrClN_2O$ 529.0677.



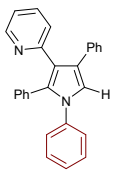
2-(1-(2-Chloro-4-methoxyphenyl)-2,4,5-triphenyl-1*H*-pyrrol-3-yl)pyridine (35): yellow oil; 41.0 mg, 85 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.41 (d, *J* = 3.7 Hz, 1H), 7.40 (td, *J* = 7.7, 1.8 Hz, 1H), 7.07 (m, 10H), 6.99 (m, 8H), 6.75 (d, *J* = 2.7 Hz, 1H), 6.62 (dd, *J* = 8.7, 2.8 Hz, 1H), 3.71 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 155.4, 149.0, 135.2, 135.1, 134.4, 133.5, 132.4, 132.2, 132.1, 131.9, 131.1, 130.8, 130.7, 129.4, 127.5, 127.4, 127.4, 126.6, 125.9, 125.3, 122.9, 122.8, 120.4, 114.4, 112.7, 55.5; HRMS (ESI) m/z 513.1724 ($M+H^+$), calc. for $C_{34}H_{25}ClN_2O$ 513.1728.



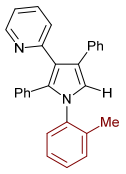
2-(1-(2-Chloro-4-methoxyphenyl)-2-(4-chlorophenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (36): brown oil; 44.3 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.48 (d, *J* = 3.7 Hz, 1H), 7.72 – 7.38 (m, 2H), 7.11 (m, 9H), 7.04 (s, 2H), 7.01 – 6.92 (m, 5H), 6.76 (d, *J* = 2.4 Hz, 1H), 6.63 (dd, *J* = 8.7, 2.6 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.5, 156.2, 149.2, 136.9, 132.1, 130.6, 130.4, 129.8, 128.7, 128.6, 127.0, 126.6, 126.5, 123.8, 123.7, 122.9, 122.7, 121.1, 117.3, 113.1, 55.4; HRMS (ESI) m/z 547.1334 ($M+H^+$), calc. for $C_{34}H_{24}Cl_2N_2O$ 547.1339.



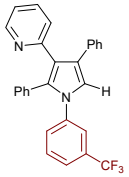
2-(2-(4-Chlorophenyl)-1-(3-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (37): yellow oil; 42.6 mg, 83% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.45 (d, *J* = 4.5 Hz, 1H), 7.55 – 7.40 (m, 1H), 7.06 (m, 11H), 6.94 (d, *J* = 6.1 Hz, 4H), 6.87 (d, *J* = 8.3 Hz, 2H), 6.75 – 6.69 (m, 1H), 6.51 (d, *J* = 7.9 Hz, 1H), 6.44 (s, 1H), 3.52 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.3, 156.1, 149.1, 136.8, 134.2, 133.4, 132.0, 130.5, 130.3, 129.6, 128.5, 128.5, 127.8, 126.9, 126.5, 126.4, 125.8, 123.7, 123.6, 122.8, 122.6, 121.0, 117.1, 113.0, 55.3; HRMS (ESI) m/z 513.1724 ($M+H^+$), calc. for $C_{34}H_{25}ClN_2O$ 513.1728.



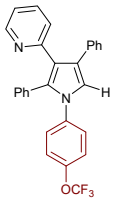
2-(1,2,4-Triphenyl-1*H*-pyrrol-3-yl)pyridine (38): yellow oil; 32.9 mg, 88 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.6 Hz, 1H), 7.45 (t, *J* = 7.4 Hz, 1H), 7.29 (d, *J* = 7.7 Hz, 2H), 7.22 (d, *J* = 4.1 Hz, 4H), 7.19 – 7.13 (m, 4H), 7.13 – 7.07 (m, 4H), 7.03 (d, *J* = 7.6 Hz, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.3, 149.0, 140.0, 135.0, 132.7, 131.6, 130.9, 128.9, 128.2, 128.1, 127.7, 126.8, 126.7, 126.1, 125.9, 125.8, 125.3, 121.5, 120.9; HRMS (ESI) m/z 373.1694 ($M+H^+$), calc. for $C_{27}H_{20}N_2$ 373.1699.



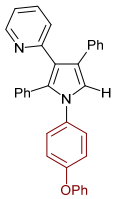
2-(2,4-Diphenyl-1-(o-tolyl)-1*H*-pyrrol-3-yl)pyridine (39): yellow oil; 31.3 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 5.0 Hz, 1H), 7.50 (s, 1H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.29 (s, 1H), 7.26 (s, 2H), 7.21 (q, *J* = 3.7, 3.0 Hz, 5H), 7.15 (t, *J* = 6.9 Hz, 2H), 7.02 (p, *J* = 5.8 Hz, 4H), 6.88 (d, *J* = 8.2 Hz, 2H), 2.00 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.2, 149.2, 137.8, 136.9, 132.0, 130.3, 129.0, 128.5, 128.2, 126.9, 126.5, 125.3, 123.7, 122.6, 121.1, 21.4; HRMS (ESI) m/z 387.1851 ($M+H^+$), calc. for $C_{28}H_{22}N_2$ 387.1856.



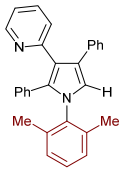
2-(2,4-Diphenyl-1-(3-(trifluoromethyl)phenyl)-1*H*-pyrrol-3-yl)pyridine (40): green solid; Mp: 164.2-164.9 °C; 34.8 mg, 79 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.7 Hz, 1H), 7.72 (s, 1H), 7.49 (d, *J* = 7.1 Hz, 2H), 7.43 – 7.30 (m, 3H), 7.24 – 7.18 (m, 4H), 7.10 (m, 5H), 7.00 – 6.93 (m, 2H), 6.86 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.6, 148.9, 140.4, 136.2, 135.1, 132.1, 131.7, 131.2, 131.2, 131.0 (q, *J* = 3.1 Hz), 130.6, 129.4, 128.8, 128.1, 127.9, 127.2, 126.5, 123.9, 123.4, 123.4, 123.3, 123.3, 122.4 (q, *J* = 3.8 Hz), 121.6, 120.7; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.9; HRMS (ESI) m/z 441.1569 ($M+H^+$), calc. for $C_{28}H_{19}F_3N_2$ 441.1573.



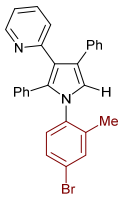
(4,5-Diphenyl-1-(4-(trifluoromethoxy)phenyl)-1*H*-pyrrol-3-yl)pyridine (41): brown solid; Mp: 140.2-141.1 °C; 34.2 mg, 90 % yield; ^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.56 (d, *J* = 4.8 Hz, 1H), 7.61 (s, 1H), 7.42 – 7.34 (m, 1H), 7.26 – 7.23 (m, 1H), 7.22 (d, *J* = 2.3 Hz, 2H), 7.20 (d, *J* = 3.1 Hz, 2H), 7.18 (d, *J* = 2.3 Hz, 2H), 7.14 (s, 2H), 7.12 (dd, *J* = 4.8, 2.4 Hz, 3H), 7.03 (td, *J* = 7.5, 4.9, 1.0 Hz, 1H), 6.98 – 6.93 (m, 2H), 6.85 (d, *J* = 8.0 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.9, 149.3, 147.5 (q, *J* = 1.9 Hz),138.4, 135.7, 135.3, 131.9, 131.3, 131.0, 130.9, 128.0, 127.8, 126.9, 126.4, 124.7, 123.5, 123.3, 122.1, 121.2, 120.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -57.9; HRMS (ESI) m/z 457.1514 ($M+H^+$), calc. for $C_{28}H_{19}F_3N_2O$ 457.1522.



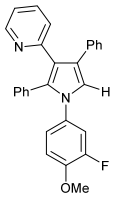
2-(1-(4-Phenoxyphenyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (42): brown solid; Mp: 167.3-168.4 °C; 39.0 mg, 84 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.6 Hz, 1H), 7.47 (d, *J* = 5.9 Hz, 1H), 7.39 – 7.32 (m, 2H), 7.22 (d, *J* = 3.4 Hz, 4H), 7.11 (d, *J* = 8.0 Hz, 8H), 7.06 – 6.98 (m, 5H), 6.91 (d, *J* = 8.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.7, 156.0, 155.3, 149.0, 135.7, 135.1, 135.0, 132.9, 131.5, 130.9, 129.8, 128.2, 128.1, 127.7, 127.3, 126.8, 126.1, 125.8, 125.2, 123.7, 121.5, 120.9, 119.1, 118.8; HRMS (ESI) m/z 465.1958 ($M+H^+$), calc. for $C_{33}H_{24}N_2O$ 465.1962.



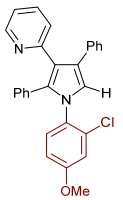
2-(1-(2,6-Dimethylphenyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (43): yellow oil; 32.8 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.53 (d, *J* = 4.1 Hz, 1H), 7.51 – 7.46 (m, 1H), 7.40 – 7.32 (m, 1H), 7.22 (d, *J* = 4.2 Hz, 3H), 7.16 (m, 3H), 7.05 (m, 6H), 6.89 (d, *J* = 7.5 Hz, 2H), 6.85 (s, 1H), 2.08 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.2, 149.1, 137.7, 136.8, 132.0, 130.3, 129.9, 128.5, 128.1, 126.9, 126.5, 126.0, 123.6, 122.6, 121.1, 21.3; HRMS (ESI) m/z 401.2007 ($M+H^+$), calc. for $C_{29}H_{24}N_2$ 401.2012.



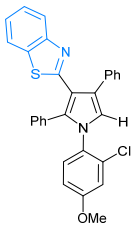
2-(1-(4-Bromo-2-methylphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (44): white solid; Mp: 174.2-175.3 °C; 36.3 mg, 78 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.7 Hz, 1H), 7.40 (d, *J* = 6.5 Hz, 2H), 7.31 (d, *J* = 5.8 Hz, 2H), 7.22 (d, *J* = 5.2 Hz, 3H), 7.20 – 7.12 (m, 3H), 7.09 – 6.99 (m, 4H), 6.85 (t, *J* = 7.5 Hz, 3H), 1.98 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.1, 149.1, 138.3, 137.7, 135.9, 135.5, 133.5, 133.0, 131.5, 131.0, 130.4, 129.9, 129.4, 128.1, 127.7, 126.7, 126.3, 123.7, 122.3, 122.2, 121.7, 120.5, 17.7; HRMS (ESI) m/z 465.0956 ($M+H^+$), calc. for $C_{28}H_{21}BrN_2$ 465.0961.



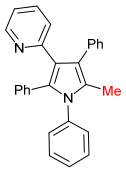
2-(1-(3-Fluoro-4-methoxyphenyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (45): yellow oil; 33.6 mg, 80 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.7 Hz, 1H), 7.61 (s, 1H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.25 – 7.14 (m, 5H), 7.14 – 7.07 (m, 3H), 7.04 (dd, *J* = 7.3, 5.2 Hz, 1H), 6.95 (t, *J* = 5.9 Hz, 3H), 6.91 – 6.80 (m, 3H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.9, 151.6 (d, *J* = 247.7 Hz), 148.8, 146.6, 146.5, 136.1, 135.4, 133.00 (d, *J* = 8.6 Hz), 132.2, 131.4, 131.0 (d, *J* = 8.3 Hz), 128.0, 127.8, 126.9, 126.3, 123.7, 123.6, 123.1, 122.3, 121.7 (d, *J* = 3.6 Hz), 120.5, 114.3 (d, *J* = 20.7 Hz), 121.6 (d, *J* = 3.6 Hz), 56.3; ^{19}F NMR (471 MHz, $CDCl_3$) δ -133.1; HRMS (ESI) m/z 421.1706 ($M+H^+$), calc. for $C_{28}H_{21}FN_2O$ 421.1711.



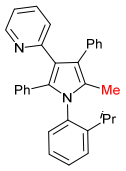
2-(1-(2-Chloro-4-methoxyphenyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (46): gray solid; Mp: 178.5-179.6 °C; 38.4 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.59 – 8.45 (m, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.30 – 7.13 (m, 6H), 7.12 – 6.98 (m, 8H), 6.95 (s, 1H), 6.70 (d, *J* = 8.8 Hz, 1H), 3.79 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.4, 155.5, 149.1, 135.5, 135.2, 134.0, 132.9, 131.6, 130.7, 130.6, 130.5, 128.3, 128.0, 127.6, 126.7, 126.0, 125.7, 125.0, 122.2, 122.0, 120.8, 115.0, 113.0, 55.7; HRMS (ESI) m/z 437.1411 ($M+H^+$), calc. for $C_{28}H_{21}ClN_2O$ 437.1415.



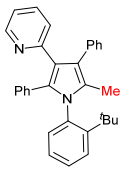
2-(1-(2-Chloro-4-methoxyphenyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)benzo[d]thiazole (47): brown solid; Mp: 196.2-197.3 °C; 43.4 mg, 88 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.4 Hz, 1H), 7.70 (d, *J* = 9.0 Hz, 1H), 7.39 – 7.32 (m, 1H), 7.26 (s, 2H), 7.14 (t, *J* = 10.0 Hz, 11H), 6.74 (s, 1H), 6.63 (d, *J* = 6.9 Hz, 1H), 3.71 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 153.3, 136.1, 135.5, 134.3, 134.2, 133.2, 132.1, 131.5, 131.1, 131.0, 130.9, 128.9, 127.7, 127.6, 127.6, 127.0, 126.0, 125.3, 124.2, 123.4, 122.9, 121.1, 116.2, 114.5, 112.8, 55.5; HRMS (ESI) m/z 493.1132 ($M+H^+$), calc. for $C_{30}H_{21}ClN_2OS$ 493.1136.



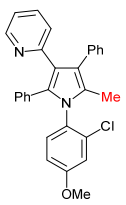
2-(5-Methyl-1,2,4-triphenyl-1*H*-pyrrol-3-yl)pyridine (48): yellow oil; 35.2 mg, 91 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.54 (d, *J* = 3.7 Hz, 1H), 7.47 (m, 1H), 7.43 – 7.30 (m, 1H), 7.22 (m, 5H), 7.18 – 7.15 (m, 1H), 7.14 – 7.07 (m, 6H), 7.04 (d, *J* = 7.2 Hz, 4H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.1, 149.1, 136.9, 131.1, 127.5, 127.3, 125.8, 124.9, 124.6, 123.7, 121.1, 116.2, 108.4, 105.8, 12.8; HRMS (ESI) m/z 387.1851 ($M+H^+$), calc. for $C_{28}H_{22}N_2$ 387.1856.



2-(1-(2-Isopropylphenyl)-5-methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (49): yellow oil; 32.1 mg, 75 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.54 – 8.36 (m, 1H), 7.48 (d, *J* = 6.4 Hz, 2H), 7.40 – 7.28 (m, 3H), 7.26 (s, 2H), 7.22 (d, *J* = 8.3 Hz, 4H), 7.00 (s, 6H), 2.61 – 2.34 (m, 1H), 2.07 (s, 3H), 1.03 (d, *J* = 5.6 Hz, 3H), 0.54 (d, *J* = 5.9 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.1, 149.1, 136.9, 132.0, 130.3, 128.5, 128.3, 126.9, 126.5, 126.4, 125.7, 123.7, 122.6, 121.1, 116.2, 108.4, 105.8, 34.1, 23.9, 12.8; HRMS (ESI) m/z 429.2320 ($M+H^+$), calc. for $C_{31}H_{28}N_2$ 429.2325.

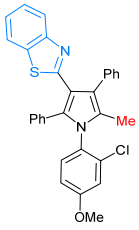


2-(1-(2-(Tert-butyl)phenyl)-5-methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (50): yellow oil; 34.5 mg, 78 % yield; 20% ee;^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 (d, *J* = 4.1 Hz, 1H), 7.47 – 7.42 (m, 1H), 7.35 (dt, *J* = 7.4, 2.3 Hz, 3H), 7.29 (s, 1H), 7.23 (d, *J* = 6.1 Hz, 2H), 7.19 – 7.14 (m, 3H), 7.02 – 6.86 (m, 7H), 0.98 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.9, 147.5, 136.0, 135.3, 135.2, 133.0, 132.5, 131.0, 130.4, 130.1, 128.7, 128.6, 127.7, 127.3, 126.1, 126.0, 125.9, 125.3, 121.9, 120.2, 36.0, 31.4, 12.1; HRMS (ESI) m/z 443.2478 ($M+H^+$), calc. for $C_{32}H_{30}N_2$ 443.2482.

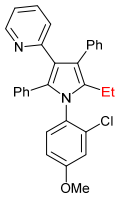


2-(1-(2-Chloro-4-methoxyphenyl)-5-methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (51): yellow solid; Mp: 191.2-192.3 °C; 40.1 mg, 89 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.39 – 7.32 (m, 1H), 7.26 – 7.11 (m, 6H), 7.06 (s, 5H), 6.95 (m, 3H), 6.75 (d, *J* = 8.6 Hz, 1H), 3.79 (s, 3H), 2.10 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 155.6, 148.9, 136.0, 135.1, 134.5, 132.5, 132.2, 131.7, 130.6,

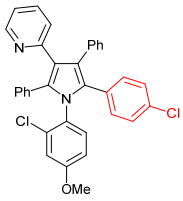
130.4, 129.6, 128.3, 127.7, 127.5, 126.4, 125.7, 125.4, 122.4, 121.7, 120.2, 114.9, 113.1, 55.6, 11.1; HRMS (ESI) m/z 451.1568 ($M+H^+$), calc. for $C_{29}H_{23}ClN_2O$ 451.1572.



2-(1-(2-Chloro-4-methoxyphenyl)-5-methyl-2,4-diphenyl-1*H*-pyrrol-3-yl)benzo[d]thiazole (52): brown solid; Mp: 124.4-125.3 °C; 41.1 mg, 81 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.39 – 7.35 (m, 2H), 7.31 (d, *J* = 7.7 Hz, 2H), 7.28 – 7.20 (m, 5H), 7.18 – 7.12 (m, 4H), 6.96 (d, *J* = 2.7 Hz, 1H), 6.75 (dd, *J* = 8.7, 2.8 Hz, 1H), 3.79 (s, 3H), 2.06 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.4, 159.8, 153.3, 136.0, 135.0, 134.6, 134.4, 131.5, 131.2, 131.1, 130.8, 128.9, 128.8, 127.8, 127.7, 127.5, 126.1, 125.2, 124.0, 122.8, 122.1, 121.0, 115.7, 115.0, 113.2, 55.6, 11.0; HRMS (ESI) m/z 507.1288 ($M+H^+$), calc. for $C_{31}H_{23}ClN_2OS$ 507.1293.

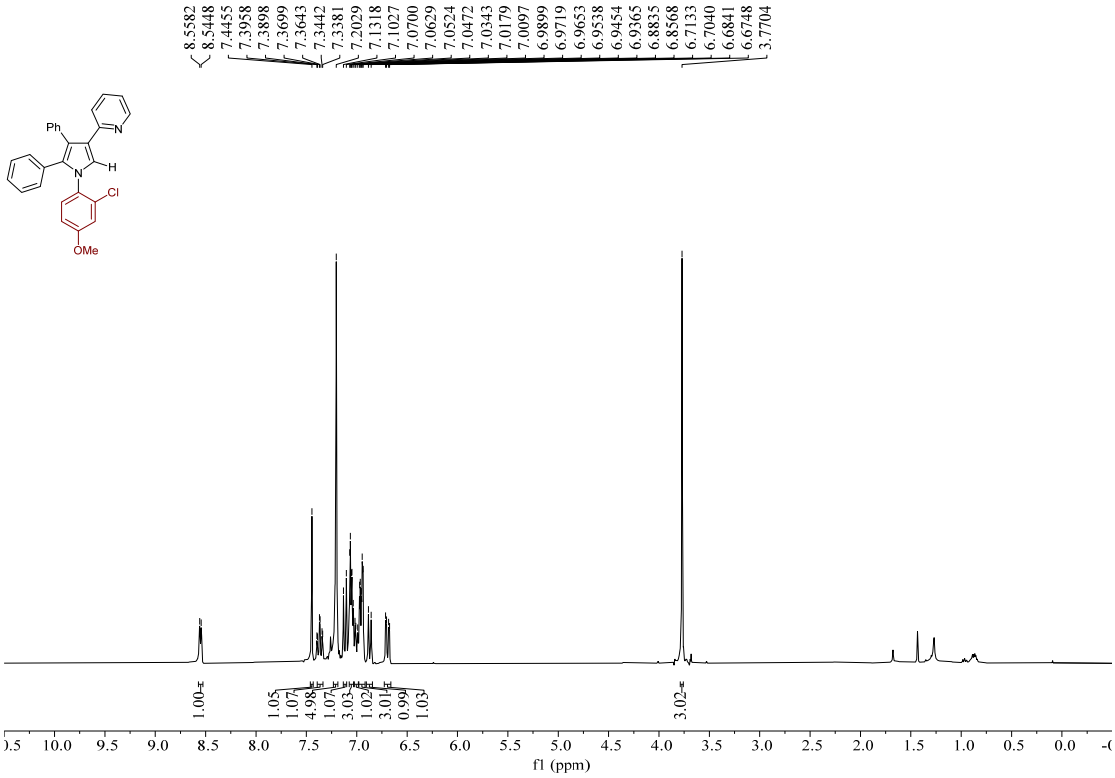


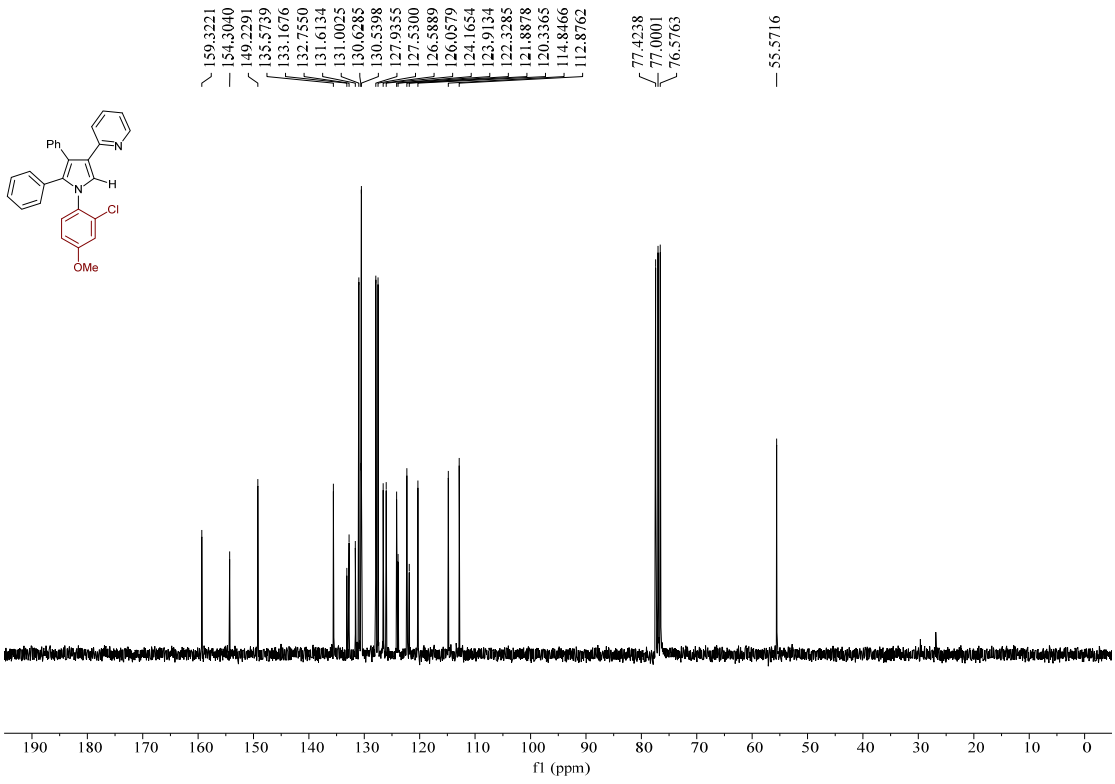
2-(1-(2-Chloro-4-methoxyphenyl)-5-ethyl-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (53): brown solid; Mp: 116.8-117.4 °C; 39.5 mg, 85 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.43 – 8.29 (m, 1H), 7.33 (d, *J* = 6.9 Hz, 1H), 7.24 (m, 6H), 7.04 (s, 5H), 6.93 (s, 3H), 6.78 (d, *J* = 8.0 Hz, 1H), 3.80 (s, 3H), 2.69 – 2.51 (m, 1H), 2.50 – 2.36 (m, 1H), 0.97 – 0.84 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.6, 155.6, 148.9, 136.1, 135.1, 134.7, 133.8, 132.5, 132.2, 132.0, 130.8, 130.3, 129.4, 127.7, 127.4, 126.4, 125.6, 125.5, 121.7, 120.1, 114.8, 112.9, 55.6, 18.4, 14.9; HRMS (ESI) m/z 465.1724 ($M+H^+$), calc. for $C_{30}H_{25}ClN_2O$ 465.1728.

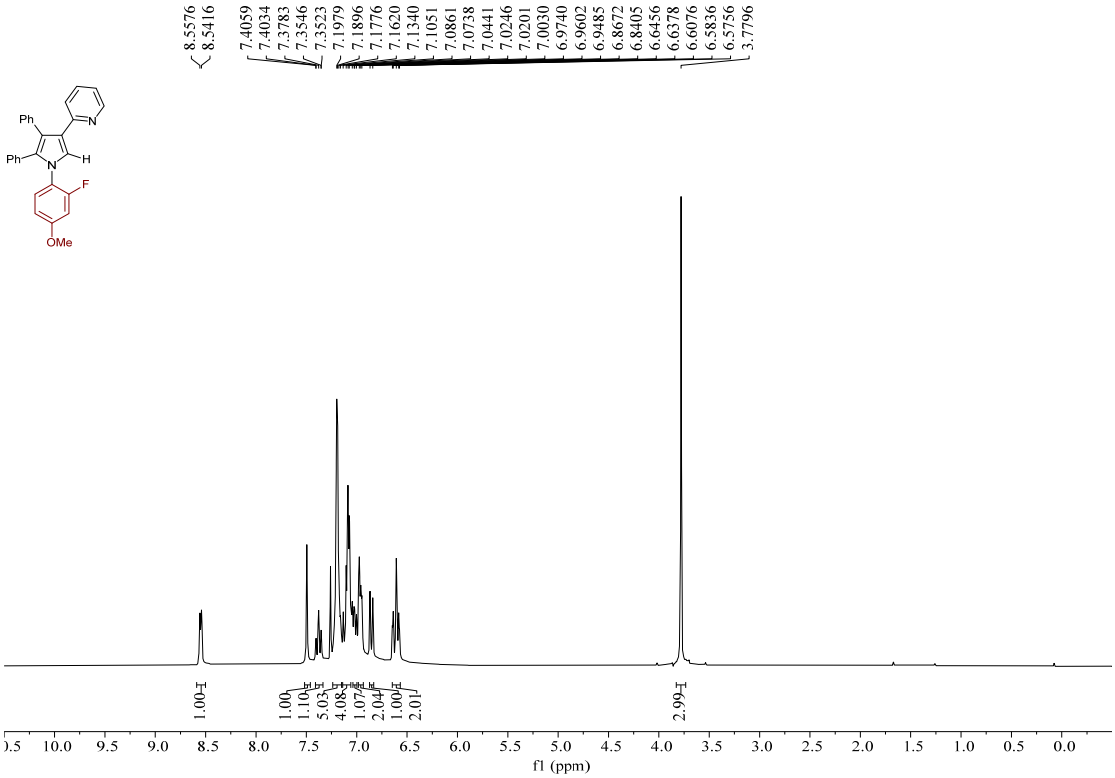


2-(1-(2-Chloro-4-methoxyphenyl)-5-(4-chlorophenyl)-2,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (54): yellow oil; 44.9 mg, 82 % yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.47 – 8.33 (m, 1H), 7.38 (d, *J* = 7.5 Hz, 1H), 7.05 (m, 10H), 6.98 (s, 5H), 6.90 (d, *J* = 7.7 Hz, 2H), 6.76 (s, 1H), 6.63 (d, *J* = 8.8 Hz, 1H), 3.74 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.5, 155.1, 149.1, 135.2, 134.8, 134.4, 133.9, 132.7, 132.3, 132.1, 131.7, 131.1, 130.8, 130.7, 129.1, 127.9, 127.6, 127.5, 126.8, 125.8, 125.5, 123.3, 123.0, 120.5, 114.6, 112.9, 55.5; HRMS (ESI) m/z 547.1334 ($M+H^+$), calc. for $C_{34}H_{24}Cl_2N_2O$ 547.1339.

13. Copies of NMR spectra



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7.1051
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H
F
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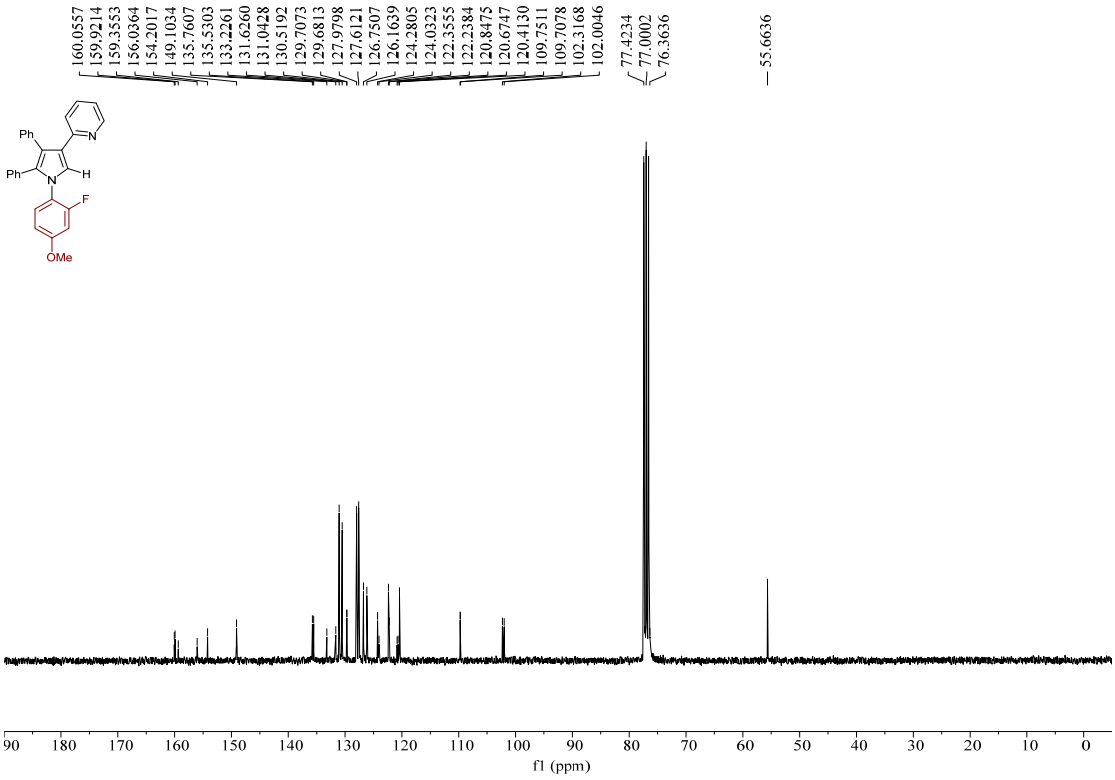
f1 (ppm)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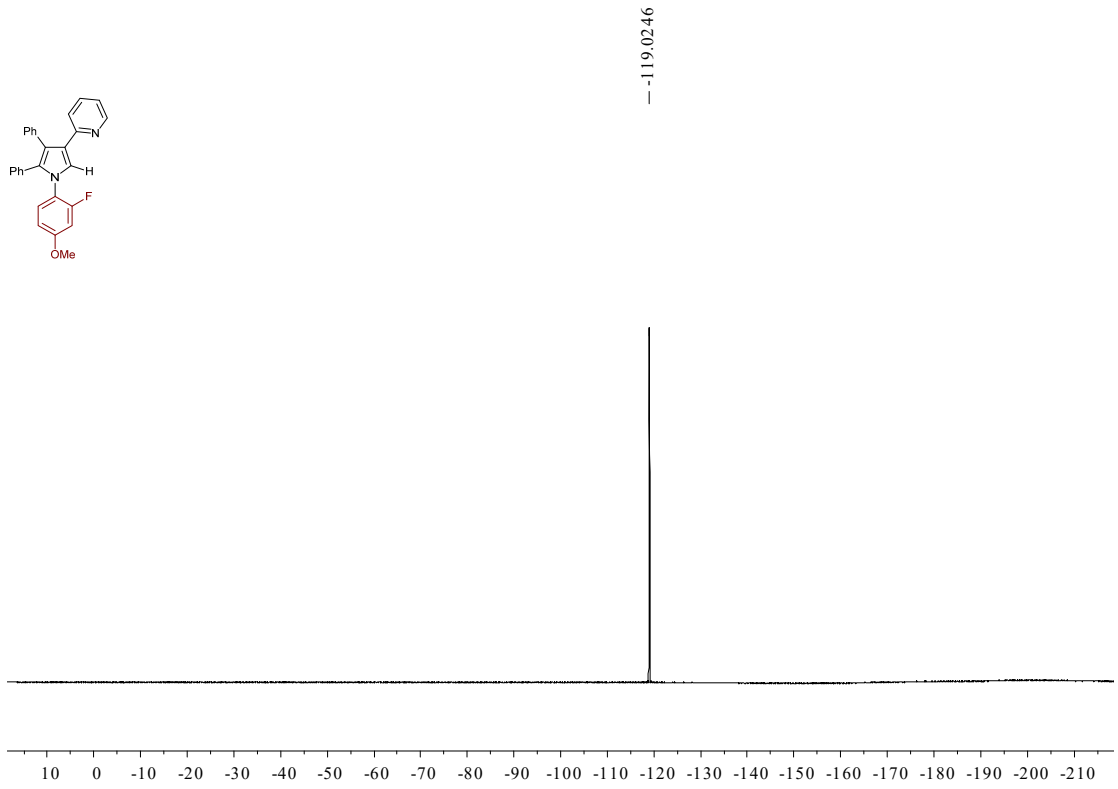
f1 (ppm)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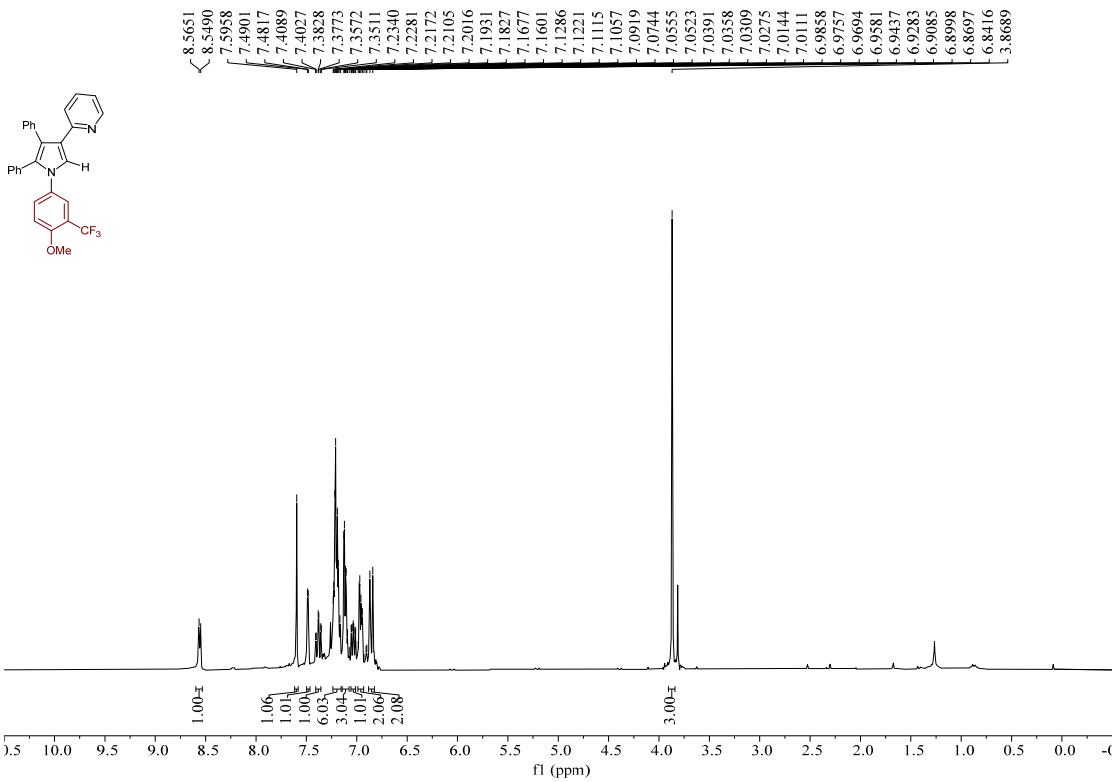
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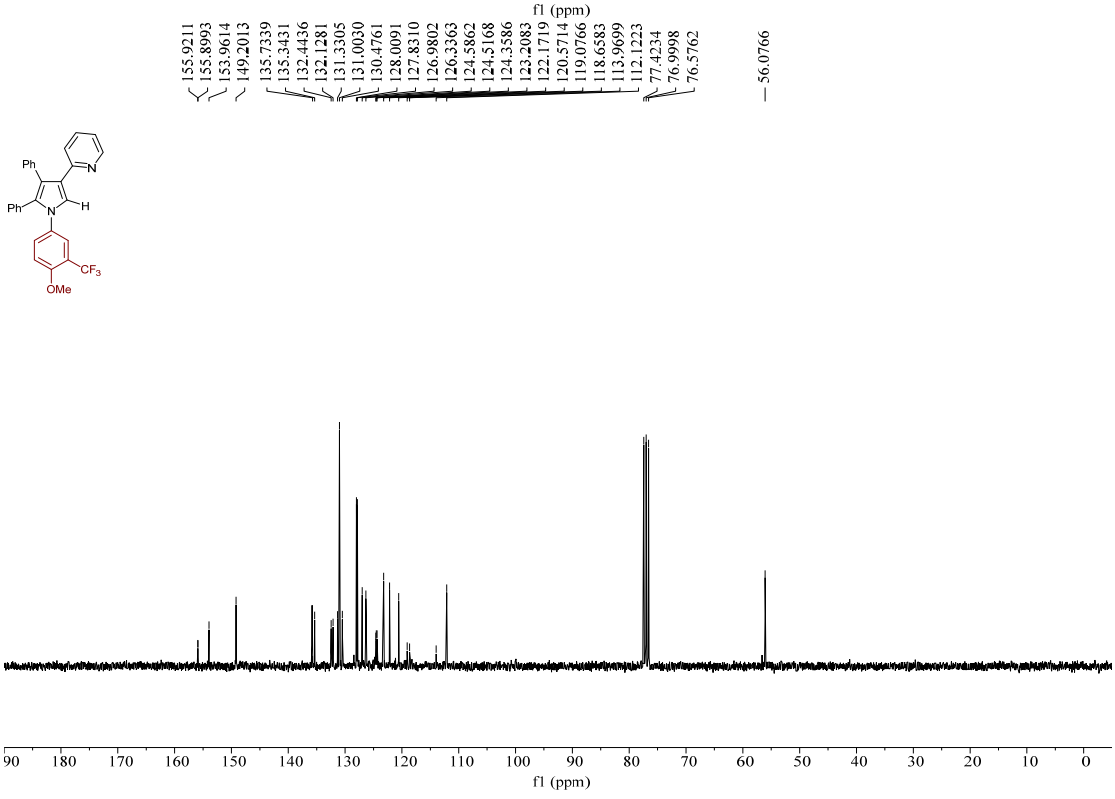
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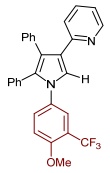
OMe
f1 (ppm)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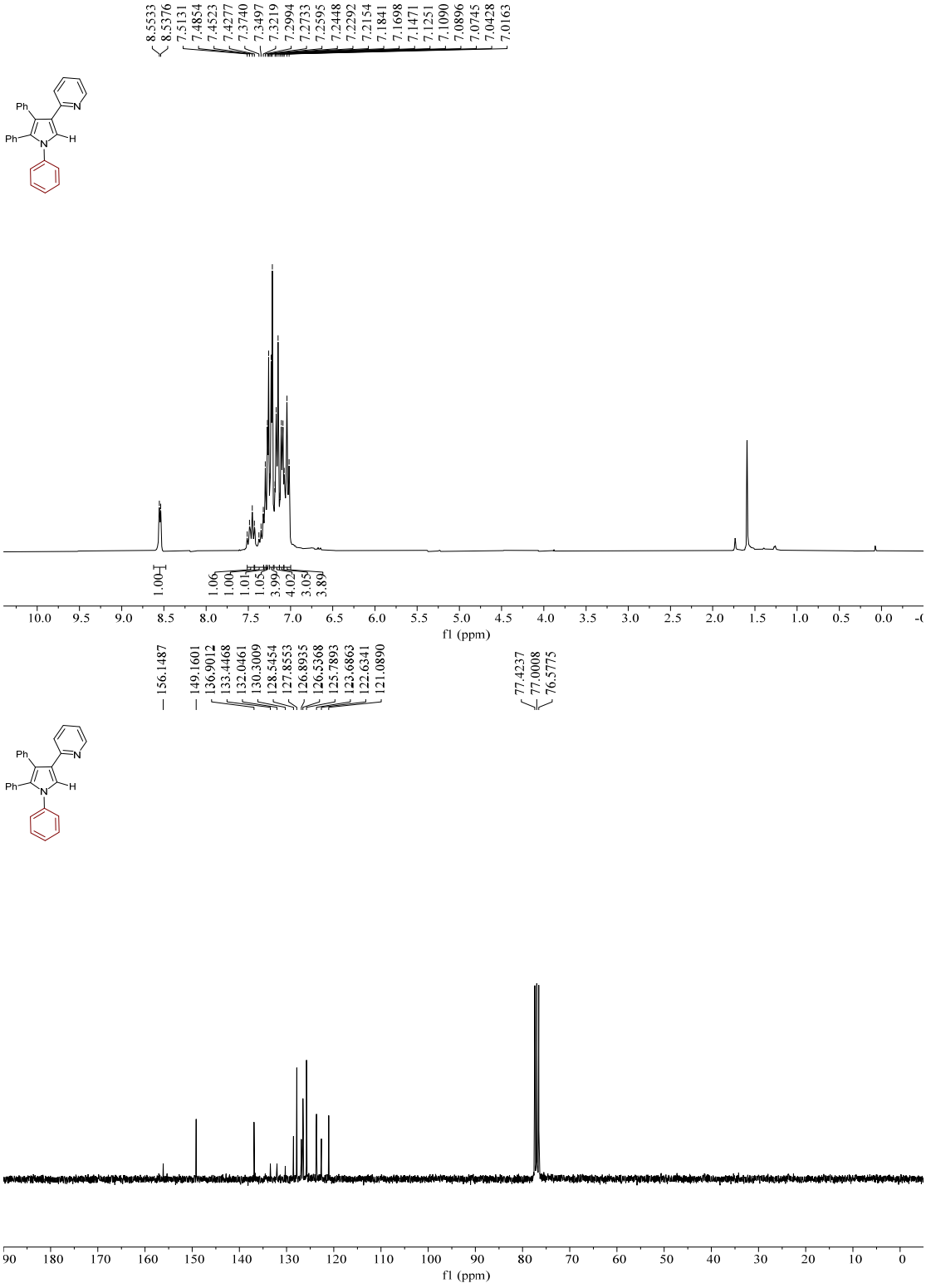
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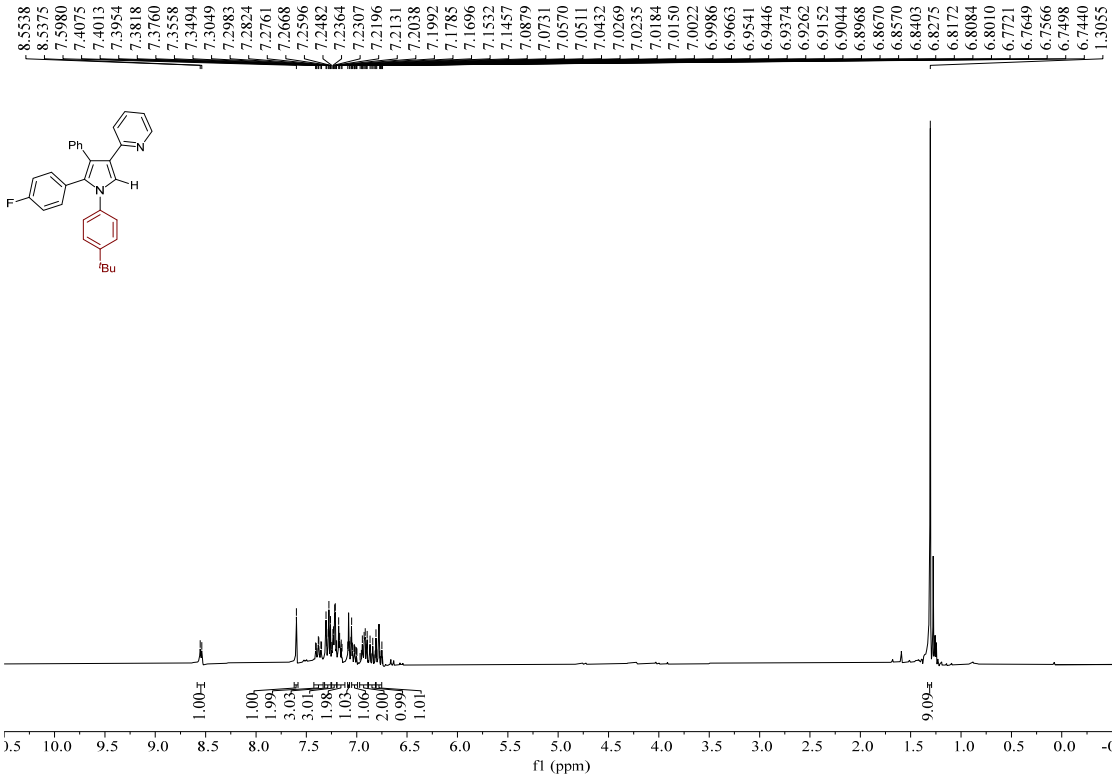
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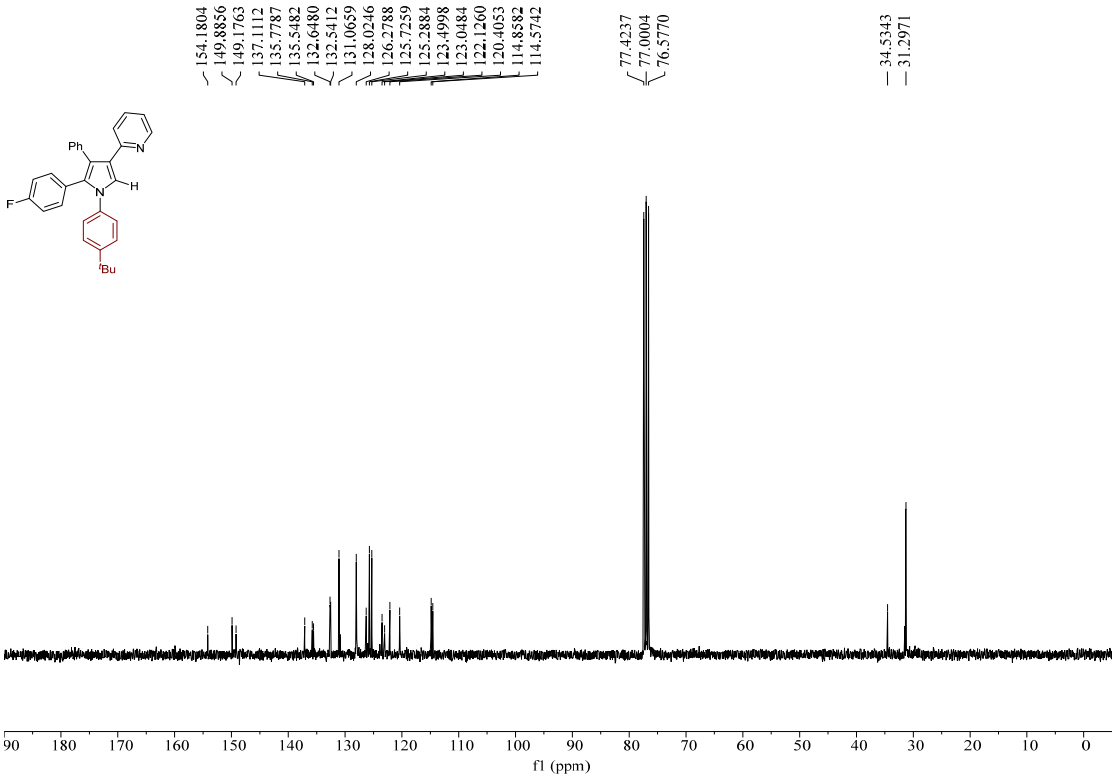
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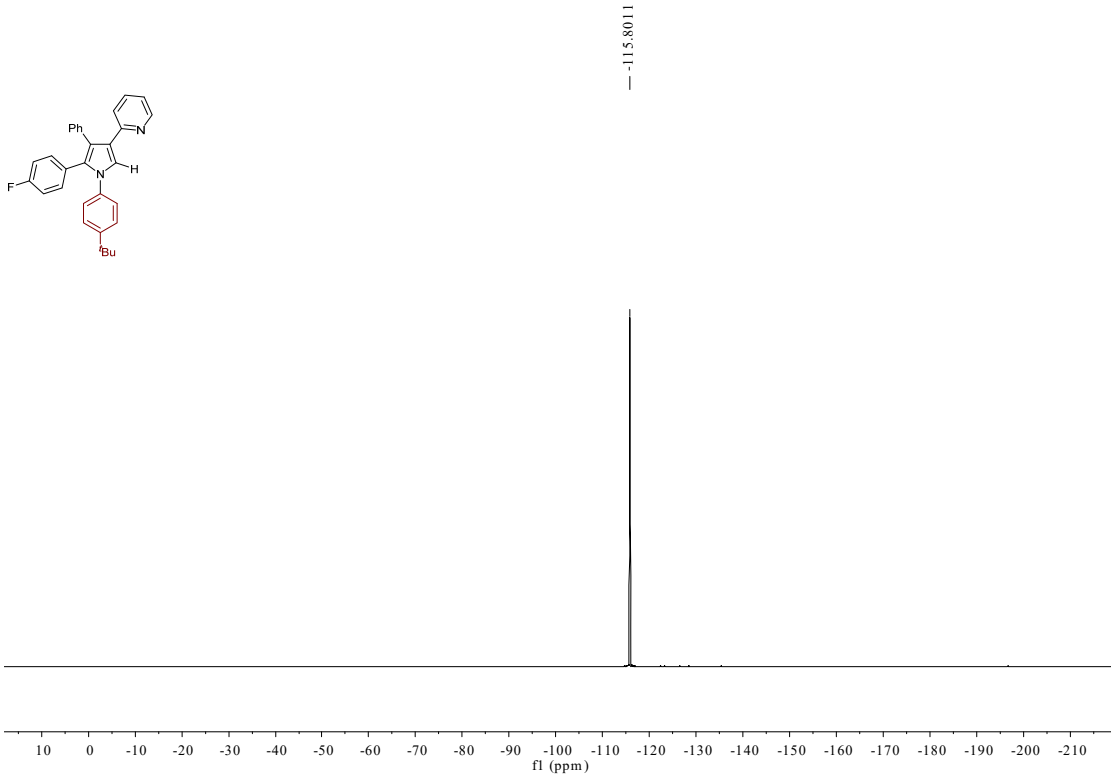
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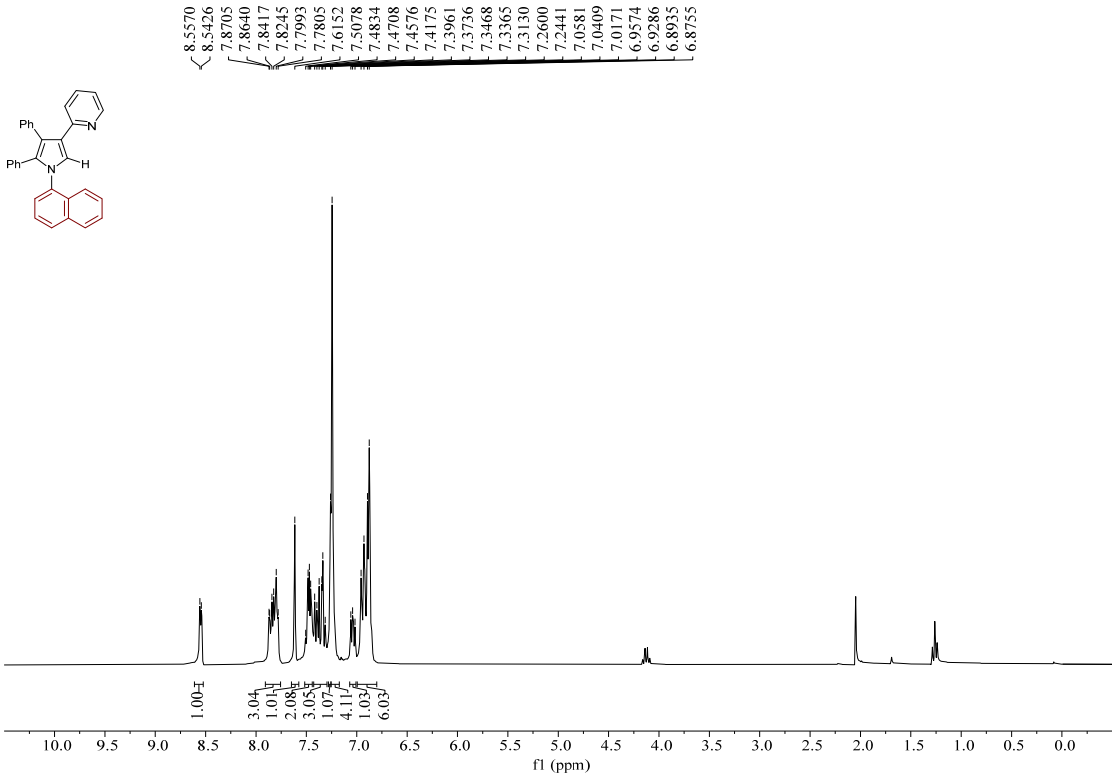
f1 (ppm)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1.07
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1.03
6.03
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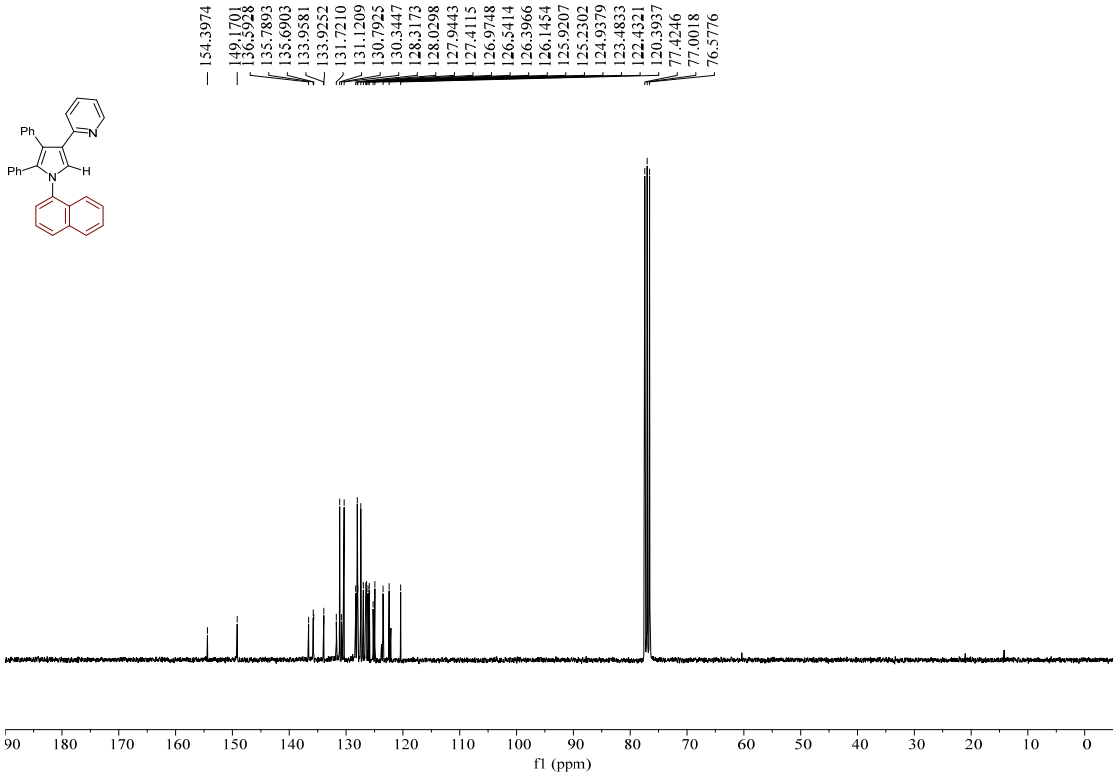
f1 (ppm)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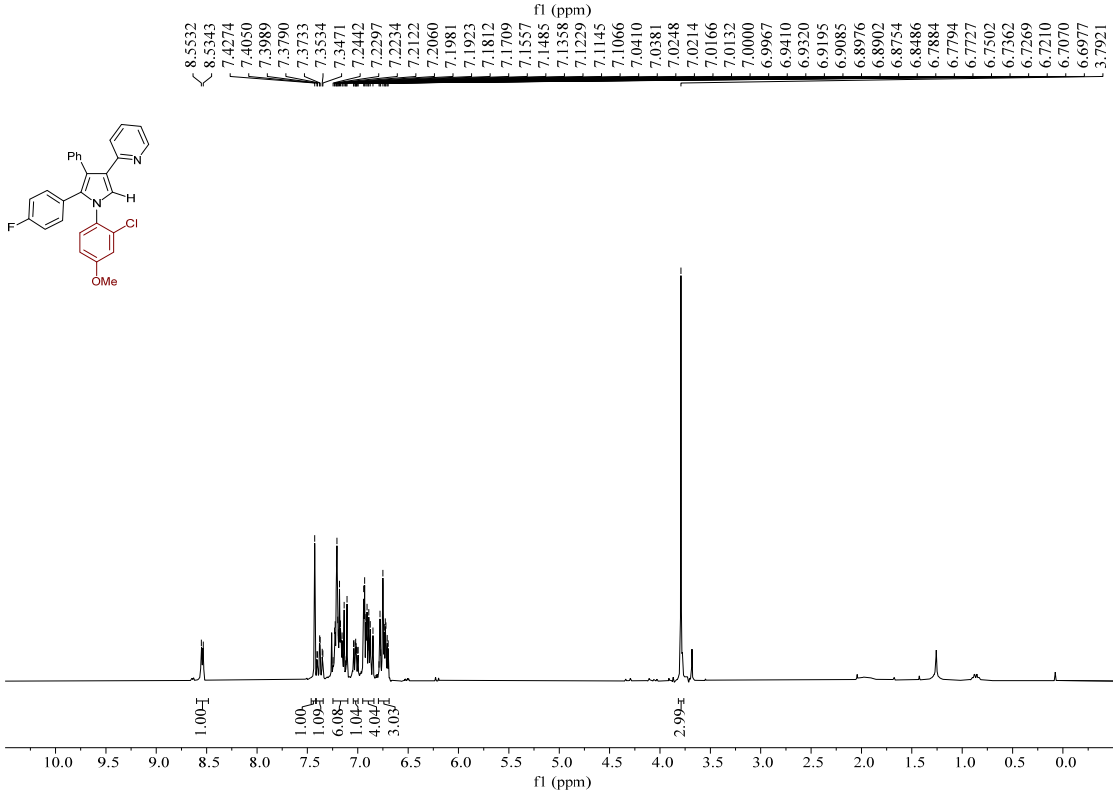
f1 (ppm)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4.04
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2.99
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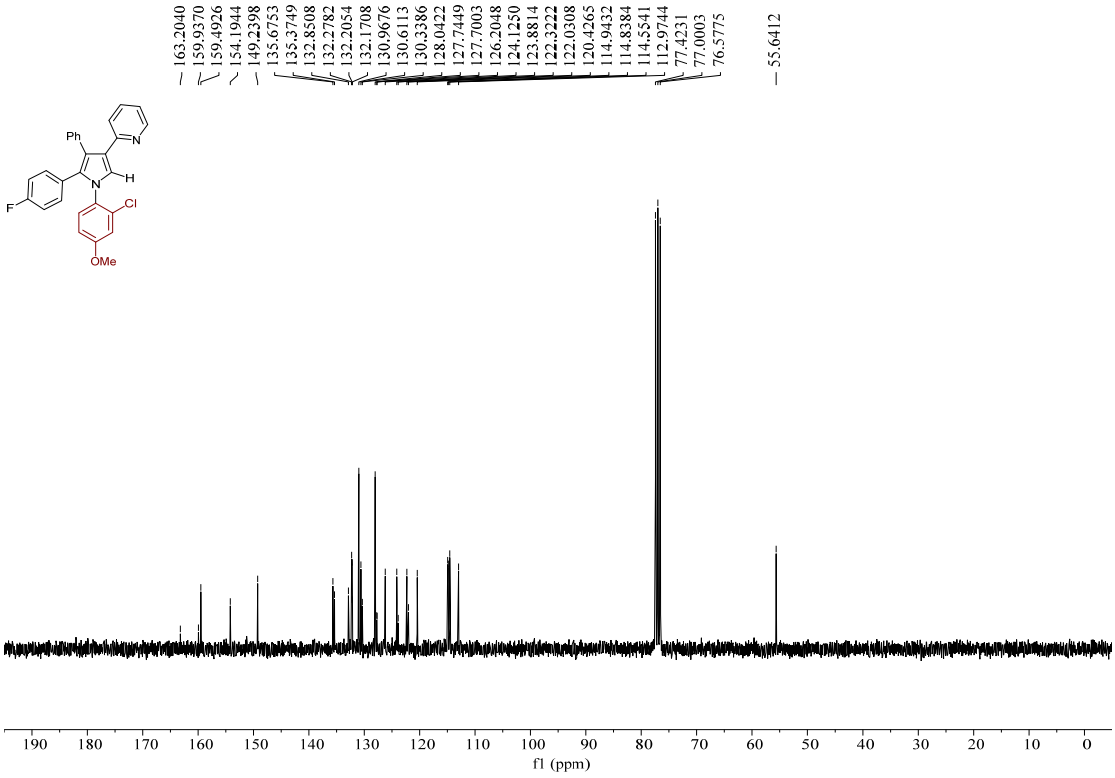
f1 (ppm)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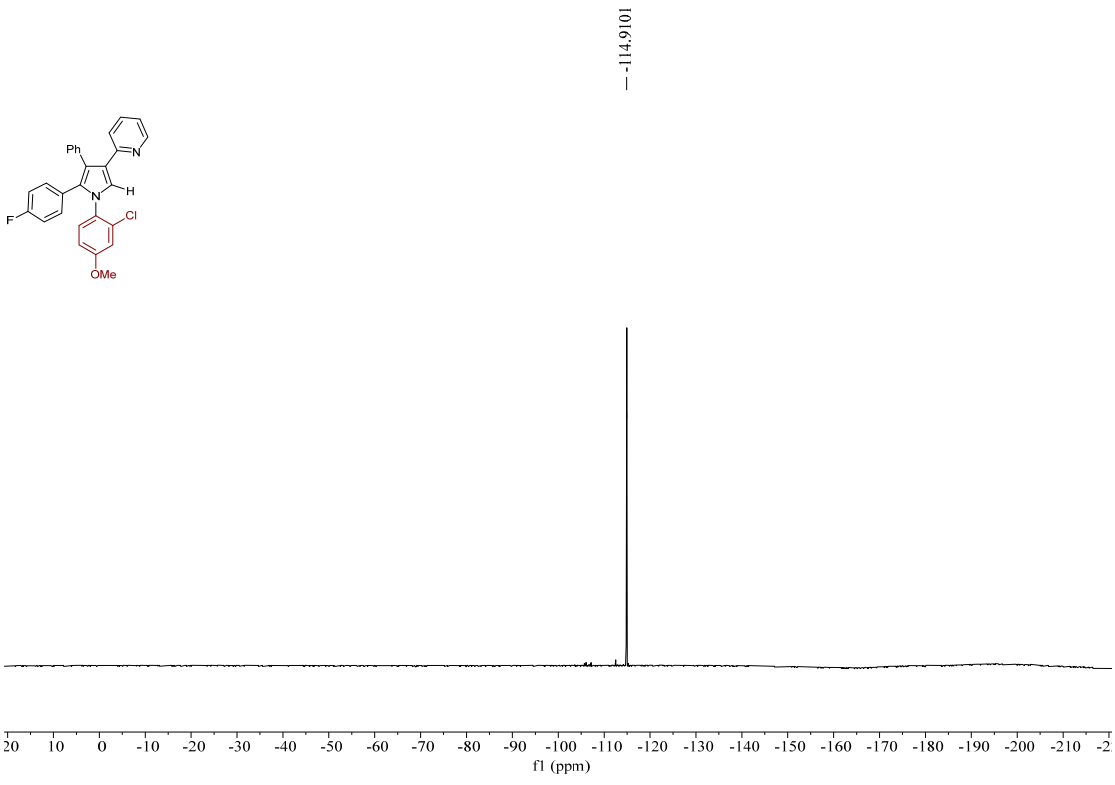
f1 (ppm)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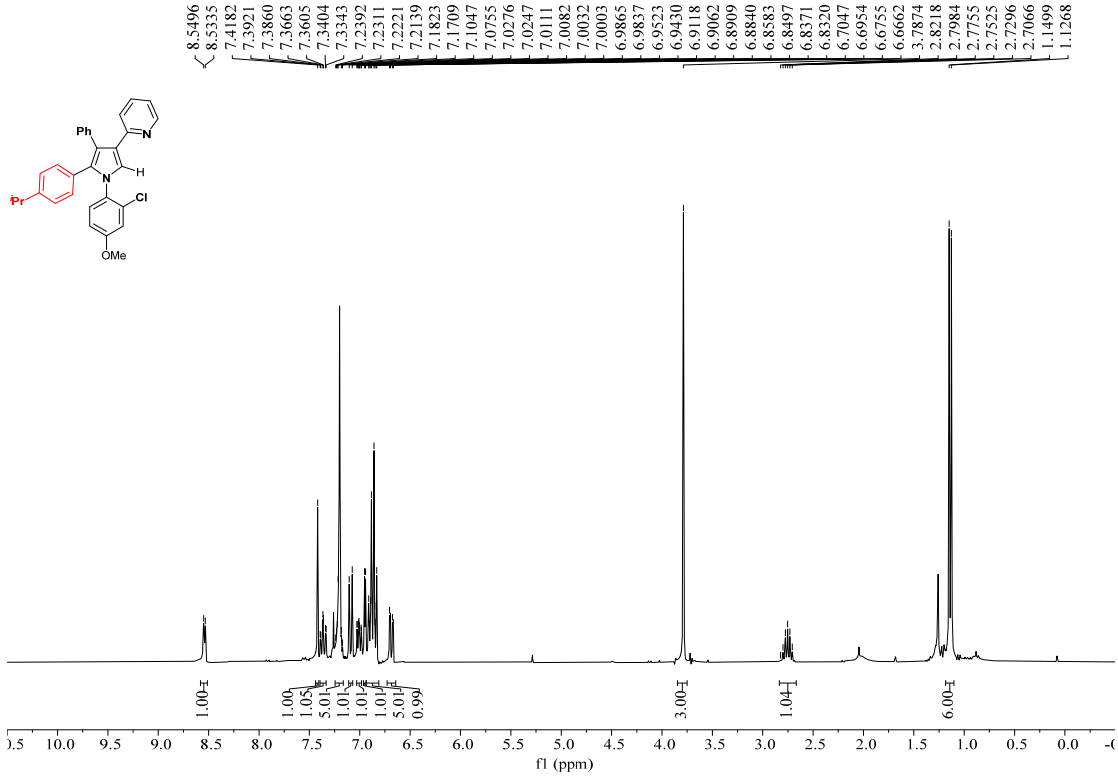
f1 (ppm)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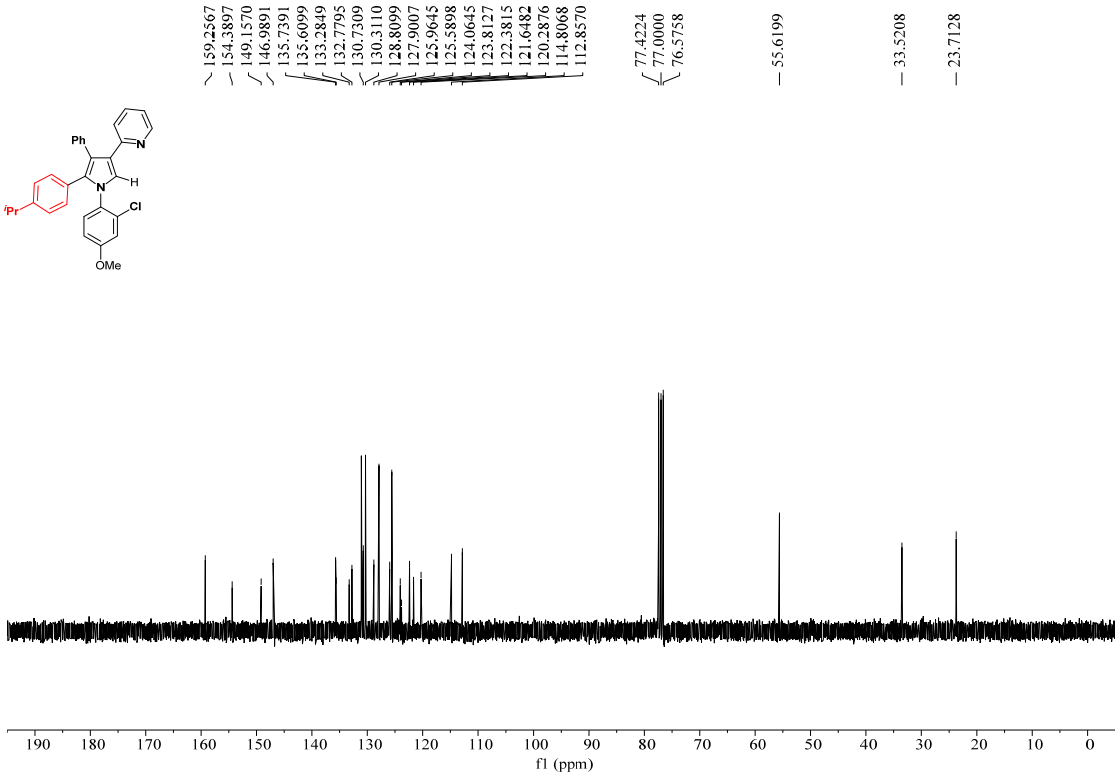
1.01
1.01
5.01
0.99
3.00
1.04
6.00
f1 (ppm)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127.9007
125.9645
125.5898
124.0645
123.8127
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114.8068
112.8570
77.4224
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H
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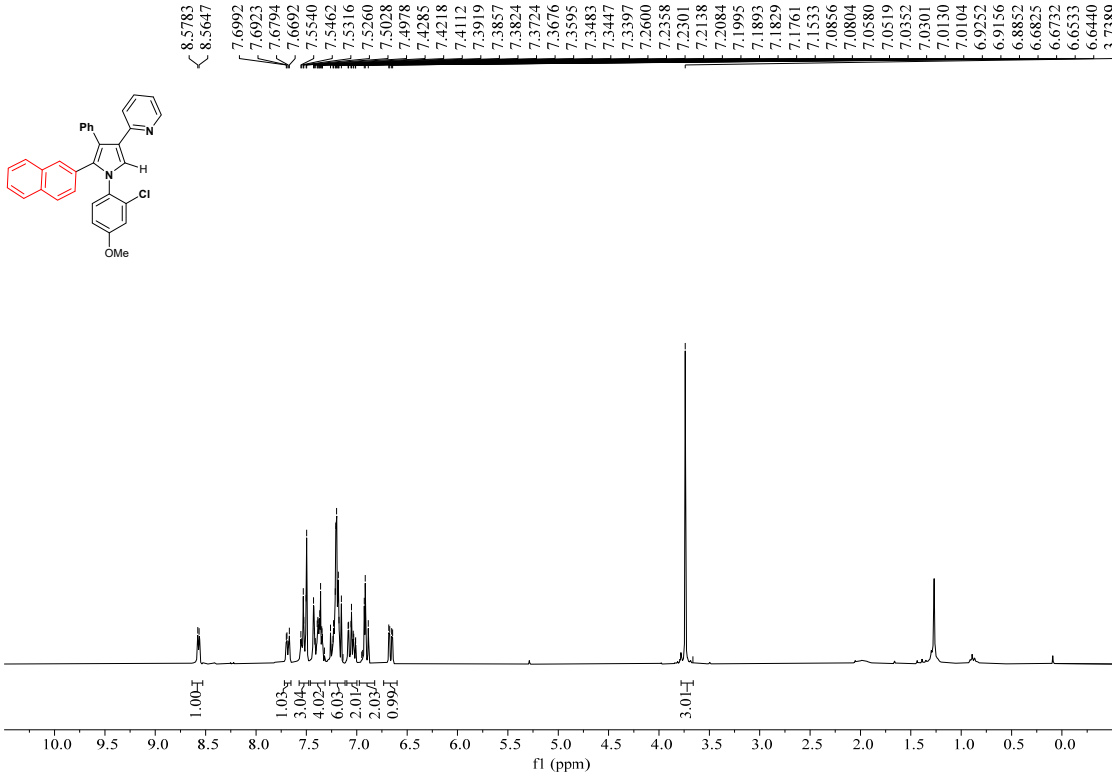
Cl
iPr
OMe
f1 (ppm)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7.3724
7.3676
7.3595
7.3483
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7.2301
7.2138
7.2084
7.1995
7.1893
7.1829
7.1761
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7.0804
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7.0519
7.0352
7.0301
7.0130
7.0104
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6.9156
6.8852
6.6825
6.6732
6.6533
6.6440
Ph
N
H
N
Cl
OMe
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1.03
3.04
4.02
6.03
2.01
2.03
0.99
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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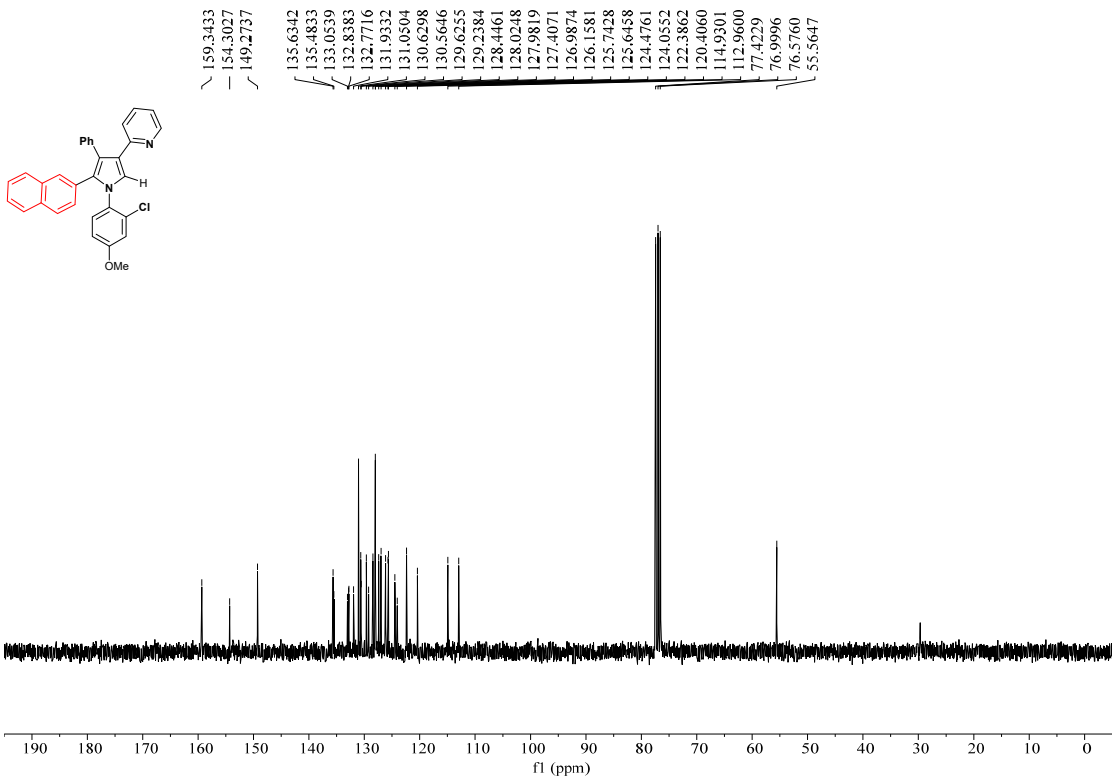
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122.3862
120.4060
114.9301
112.9600
77.4229
76.9996
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Ph
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H
N
Cl
OMe
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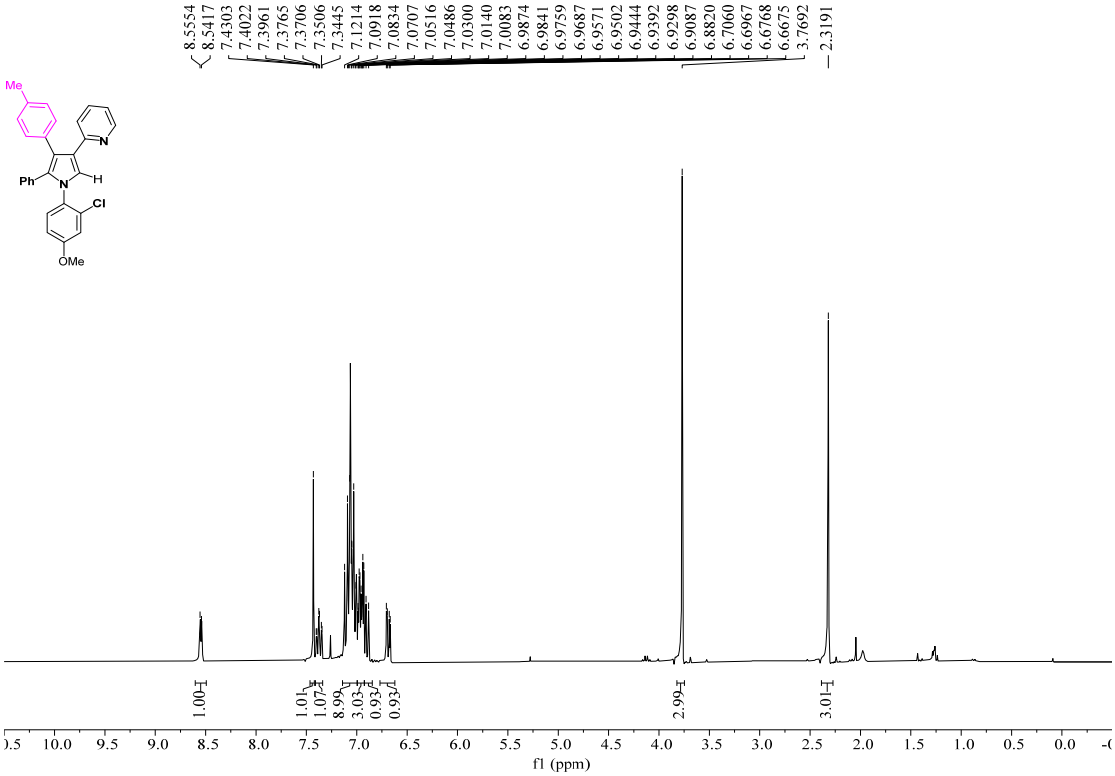
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7.0707
7.0516
7.0486
7.0300
7.0140
7.0083
6.9874
6.9841
6.9759
6.9687
6.9571
6.9502
6.9444
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6.7060
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6.6768
6.6675
3.7692
2.3191
Me
Ph
N
H
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OMe
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1.07
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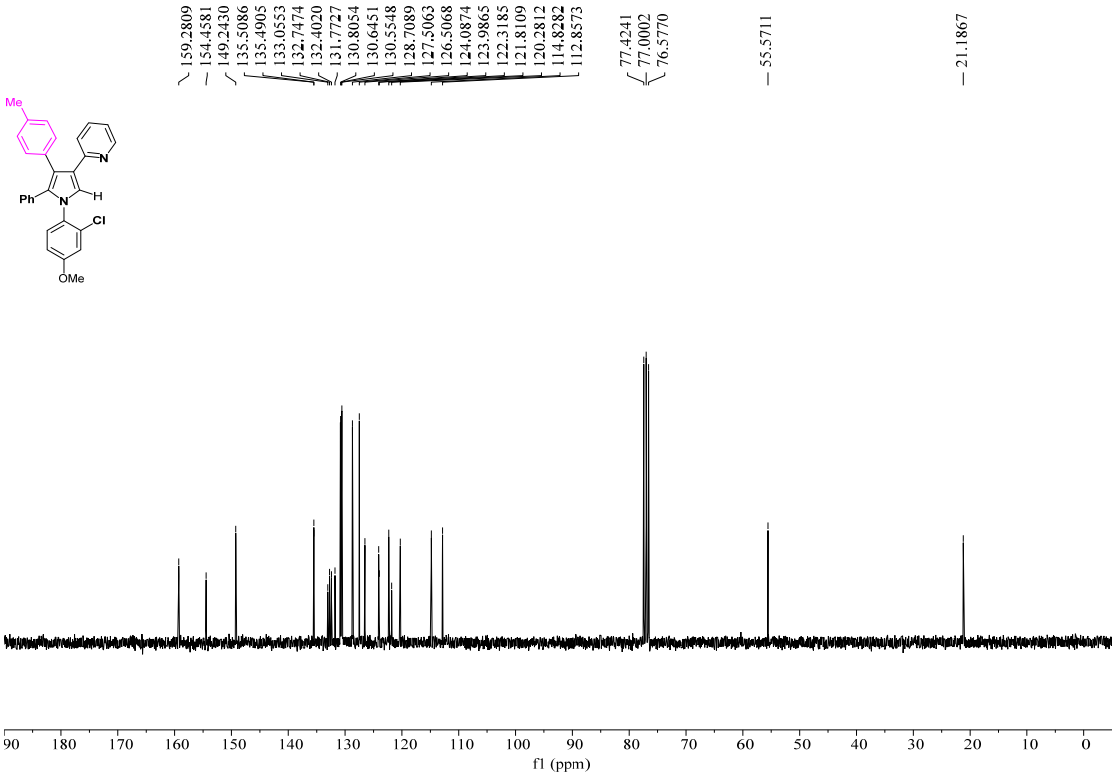
3.01
f1 (ppm)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Ph
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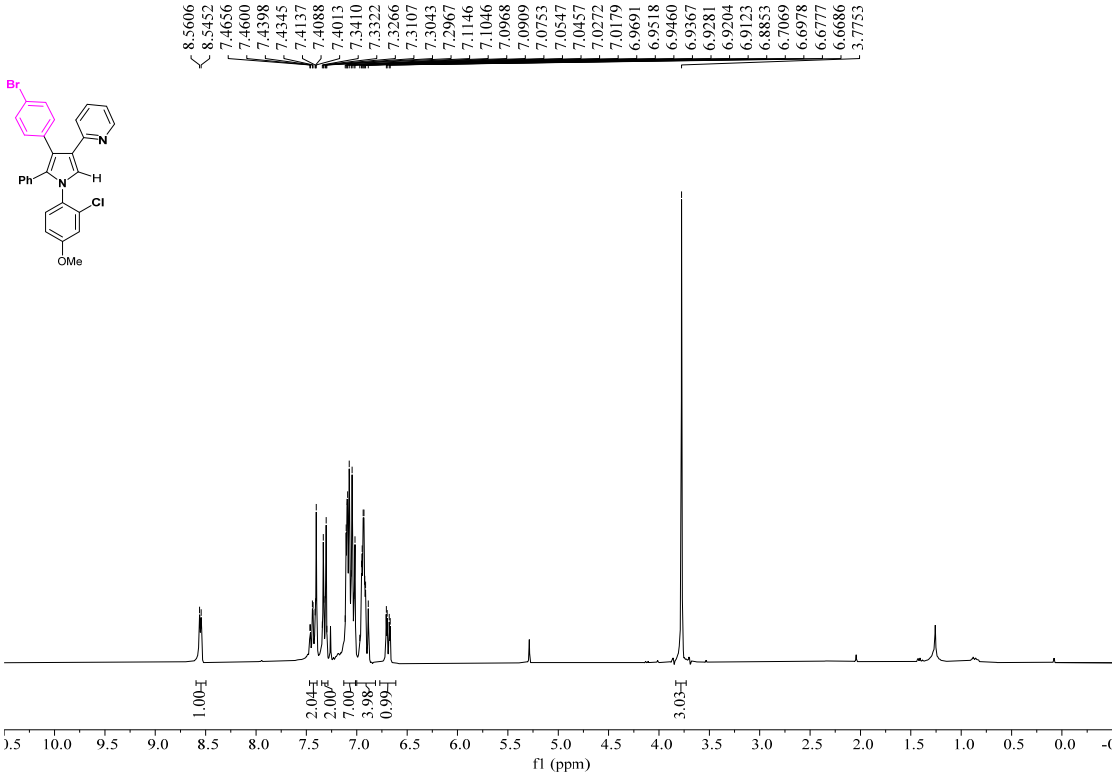
Cl
OMe
f1 (ppm)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7.3266
7.3107
7.3043
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7.1146
7.1046
7.0968
7.0909
7.0753
7.0547
7.0457
7.0272
7.0179
6.9691
6.9518
6.9460
6.9367
6.9281
6.9204
6.9123
6.8853
6.7069
6.6978
6.6777
6.6686
3.7753
Br
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Ph
N
H
Cl
OMe
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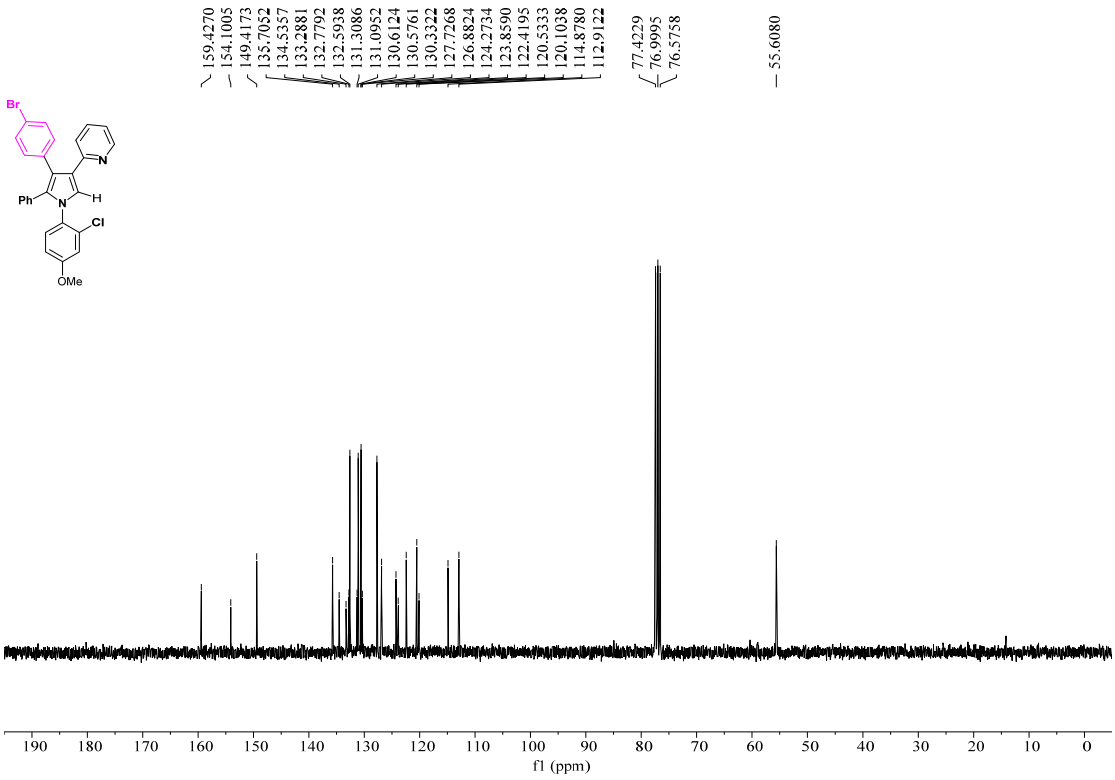
2.00
7.00
3.98
0.99
3.03
f1 (ppm)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124.2734
123.8590
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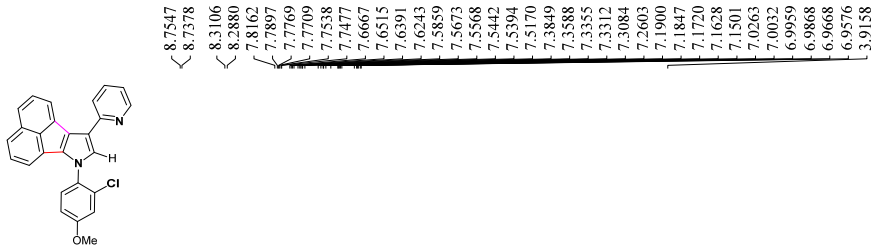
55.6080
Br
N
Ph
N
H
Cl
OMe
f1 (ppm)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7.3355
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7.2603
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7.1847
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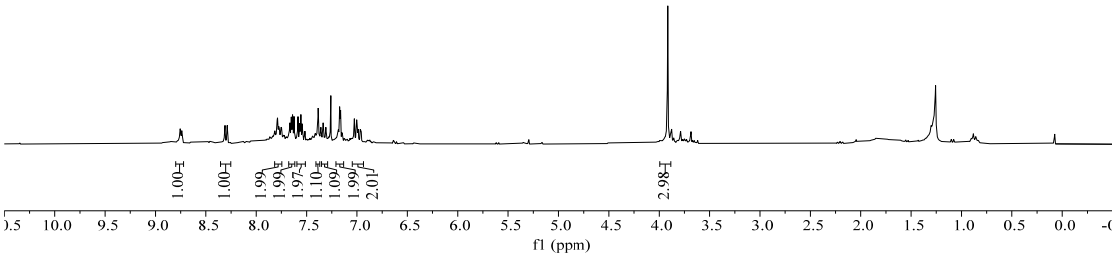
H
N
Cl
OMe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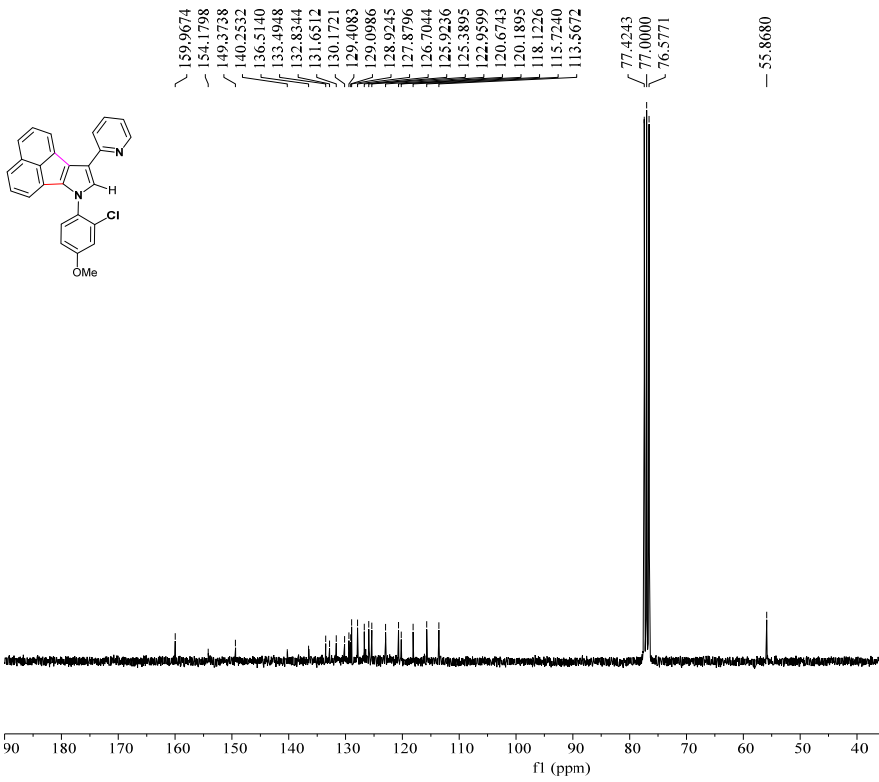
1.10
1.09
1.99
2.01
2.98
f1 (ppm)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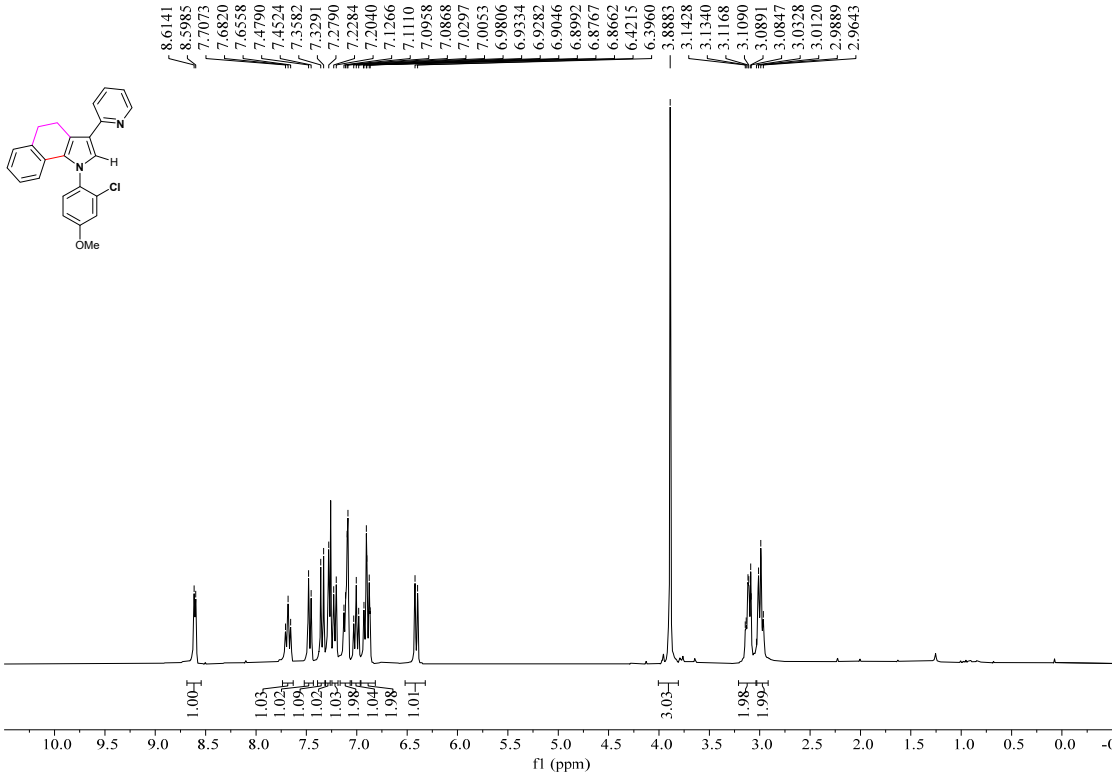
N
Cl
OMe
f1 (ppm)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7.2284
7.2040
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7.0958
7.0868
7.0297
7.0053
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6.9334
6.9282
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3.1340
3.1168
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3.0120
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H
N
Cl
OMe
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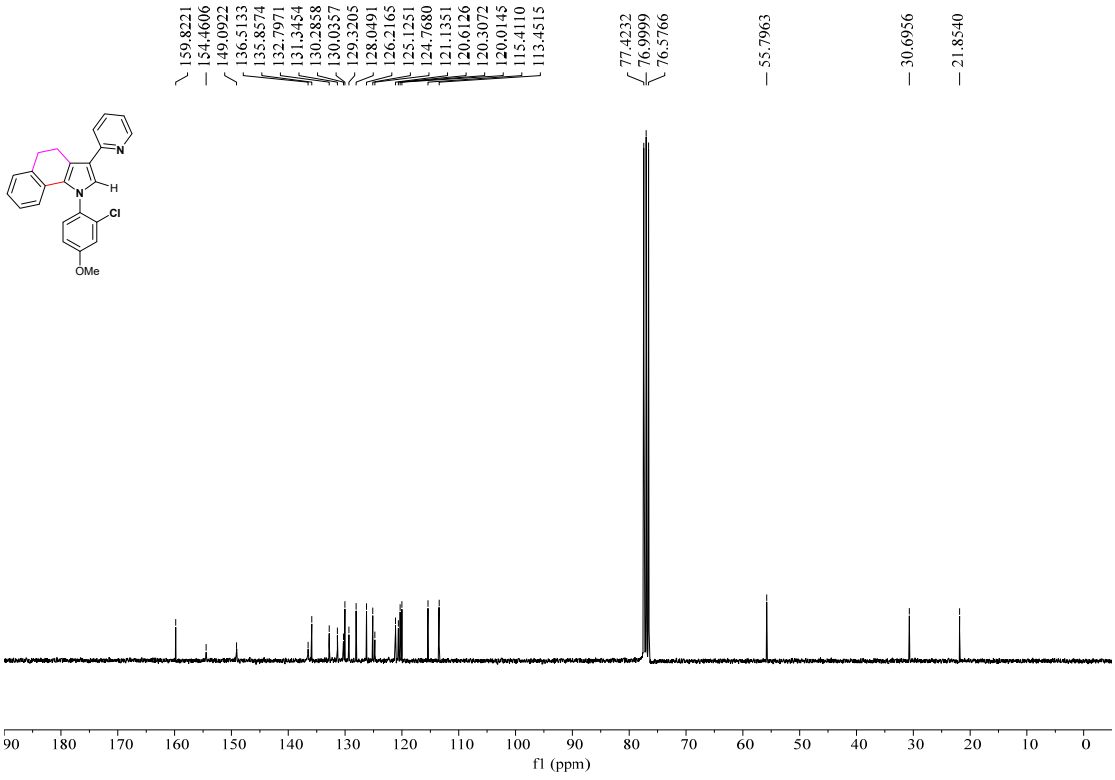
1.03
1.02
1.09
1.02
1.03
1.98
1.04
1.98
1.01
3.03
1.98
1.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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H
N
Cl
OMe
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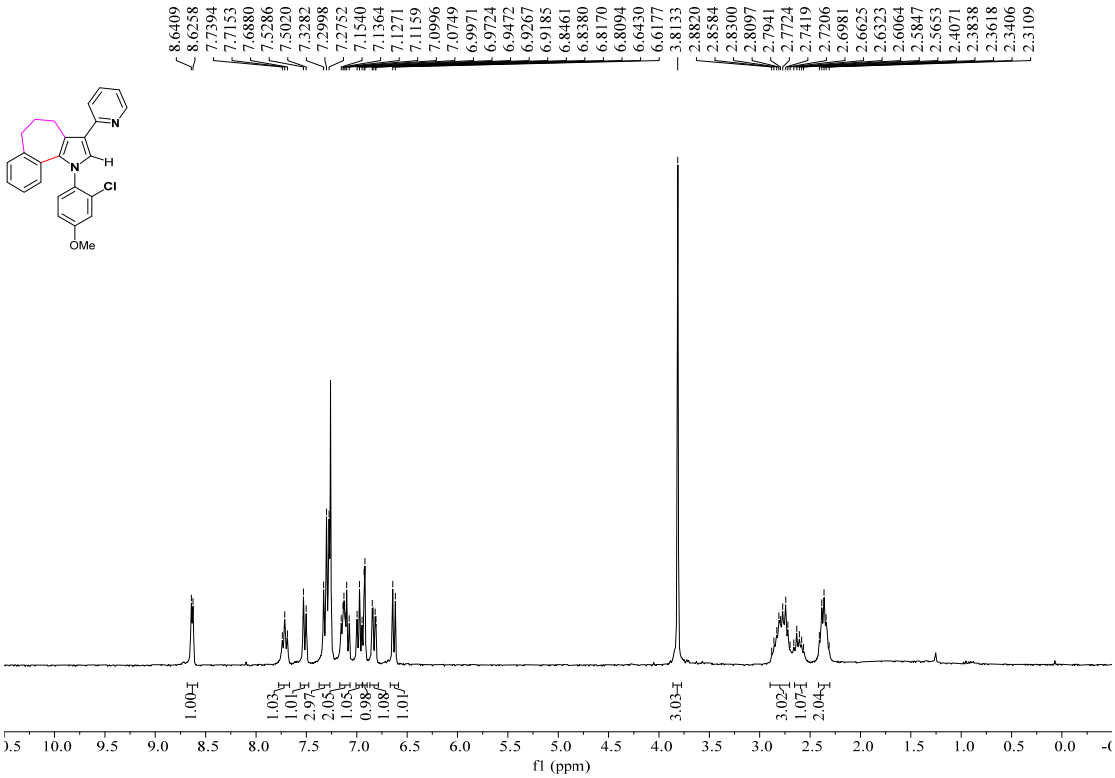
f1 (ppm)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2.7724
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N
Cl
OMe
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1.03
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1.08
1.01
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3.02
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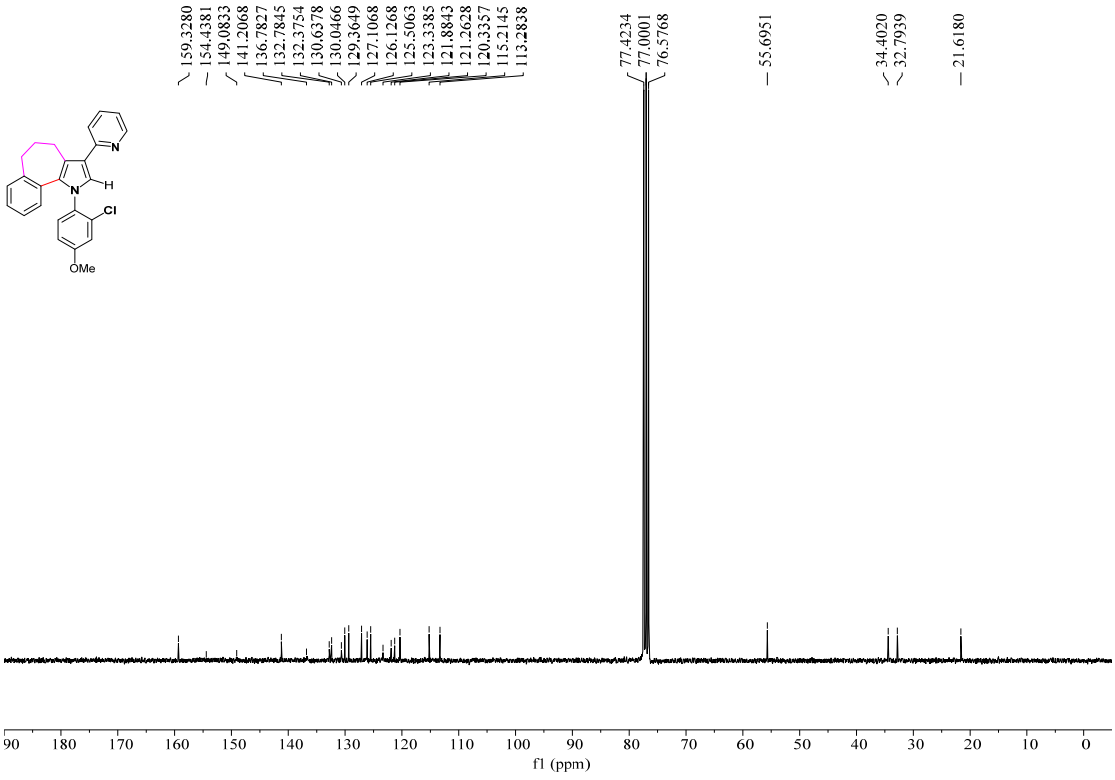
2.04
f1 (ppm)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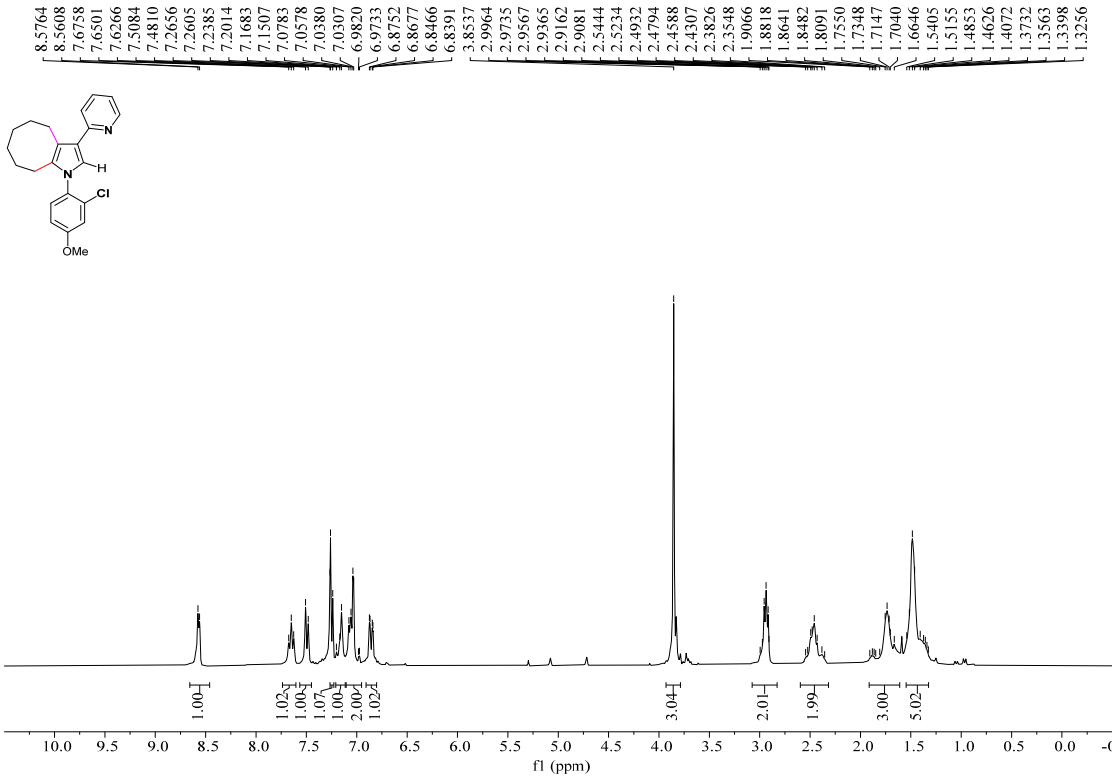
OMe
f1 (ppm)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H
N
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OMe
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1.02
1.00
1.07
1.00
2.00
1.02
3.04
2.01
1.99
3.00
5.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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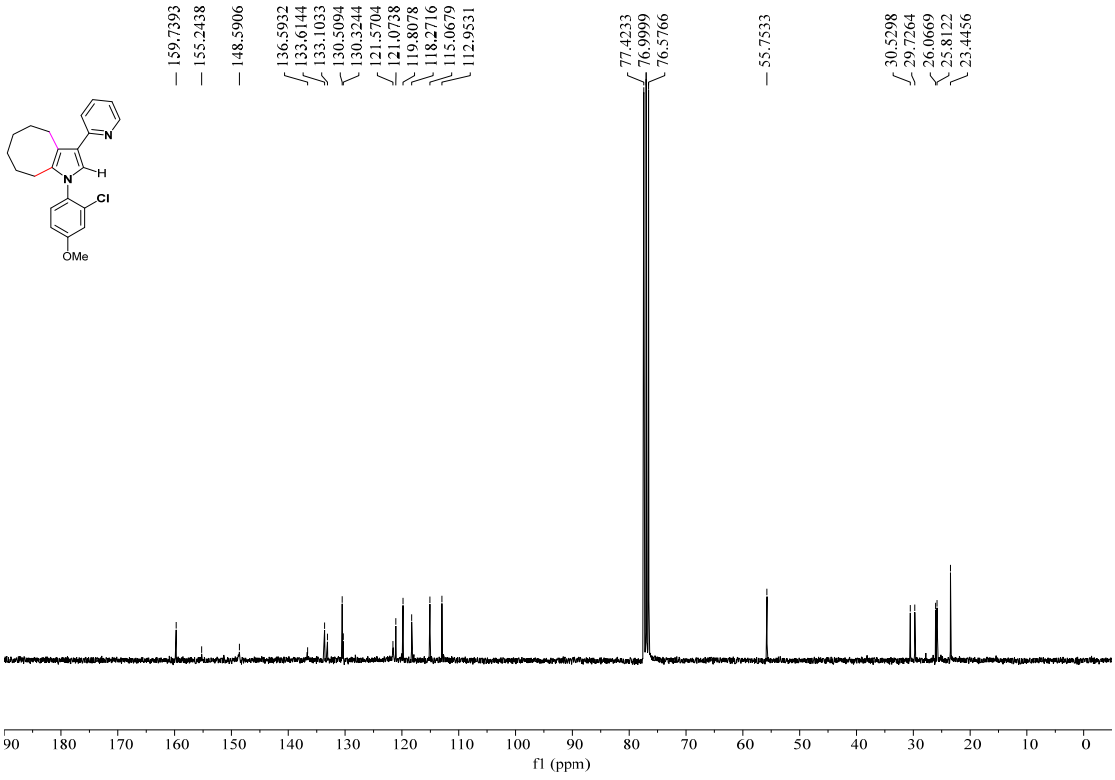
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76.5766
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H
N
Cl
OMe
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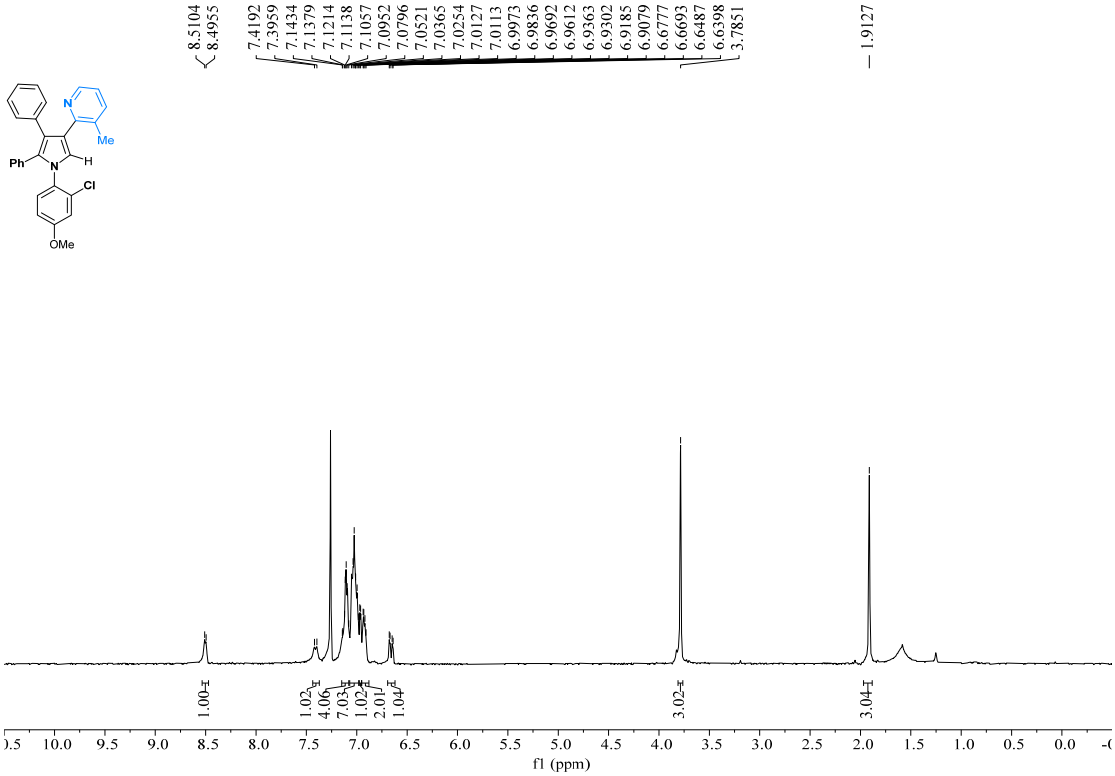
f1 (ppm)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6.9302
6.9185
6.9079
6.6777
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6.6487
6.6398
3.7851
1.9127
N
Me
Ph
N
H
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OMe
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4.06
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1.02
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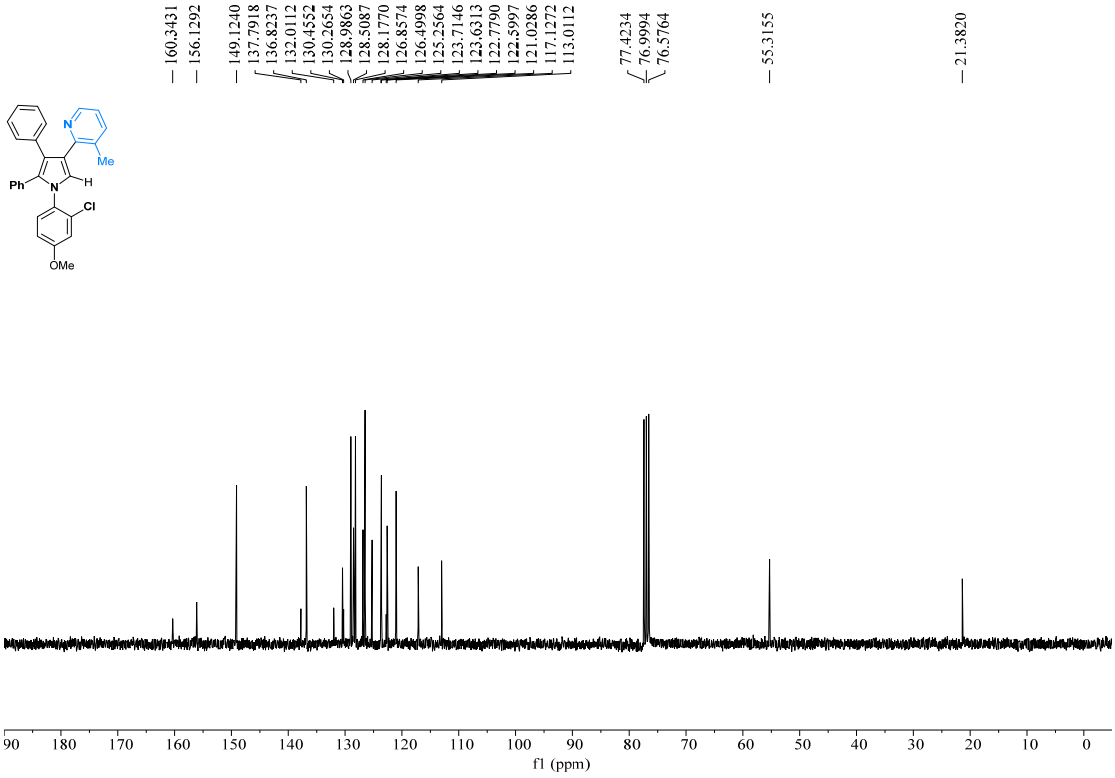
1.04
3.02
3.04
f1 (ppm)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121.0286
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113.0112
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21.3820
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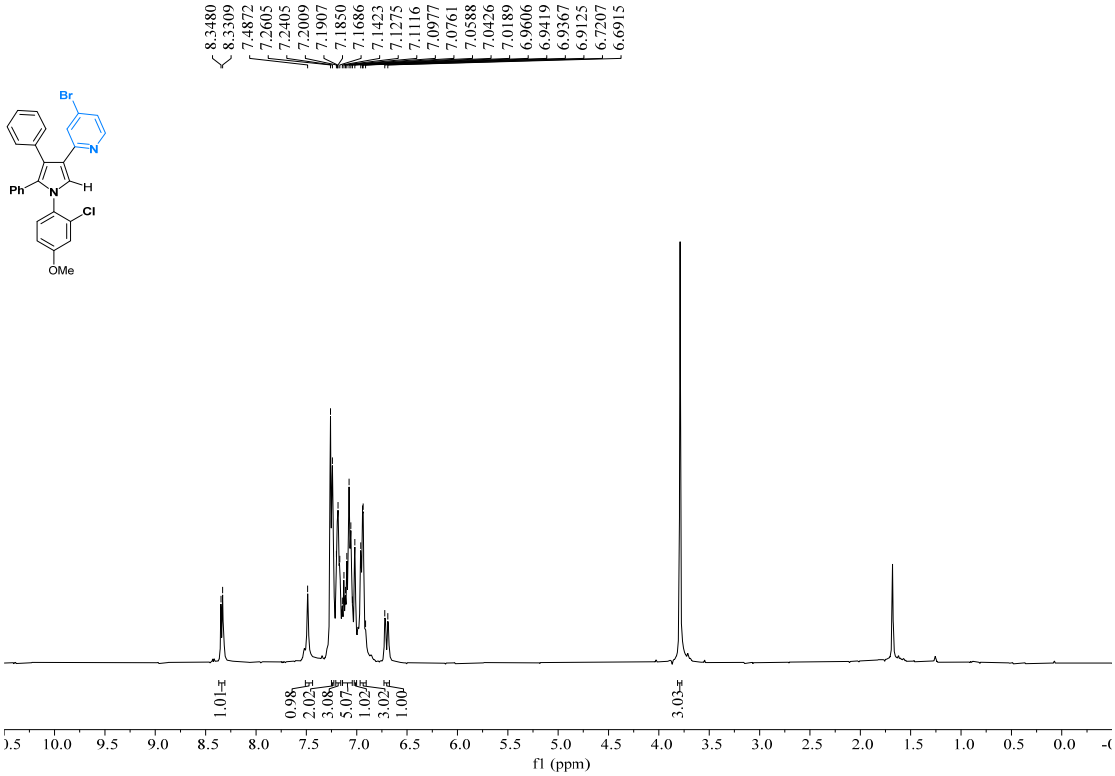
Me
Ph
N
H
Cl
OMe
f1 (ppm)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7.0977
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7.0588
7.0426
7.0189
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6.9419
6.9367
6.9125
6.7207
6.6915
Br
N
Ph
N
H
Cl
OMe
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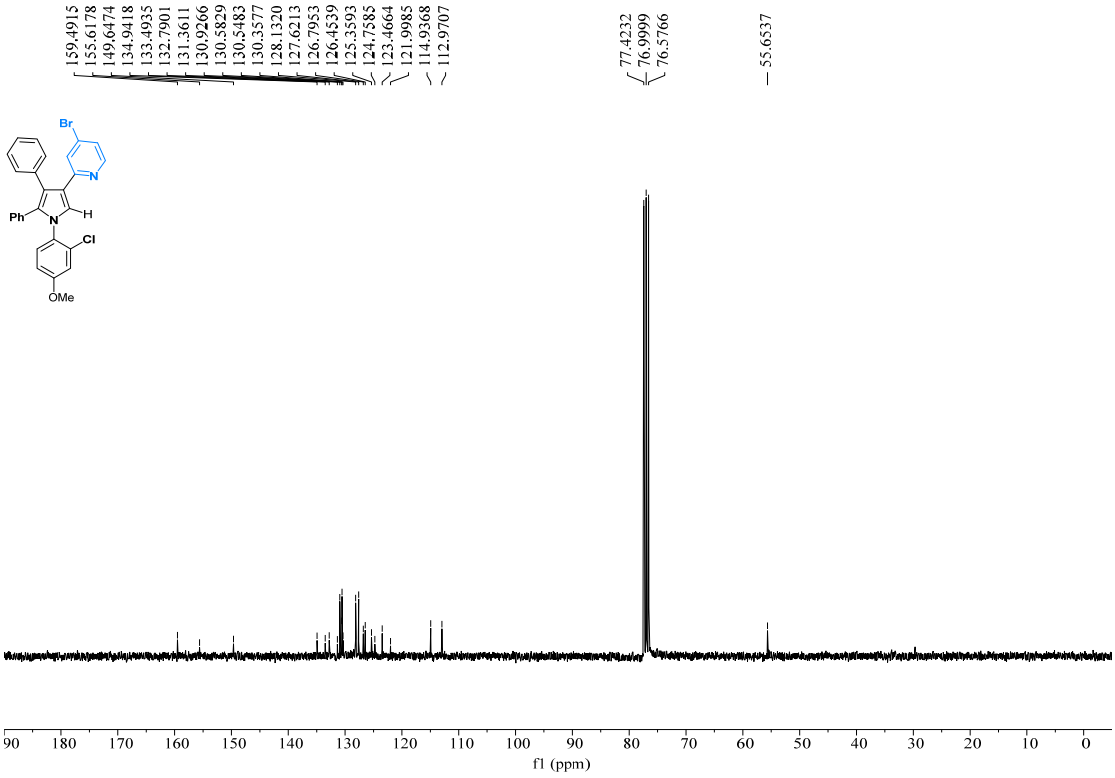
3.08
5.07
1.02
3.02
1.00
3.03
f1 (ppm)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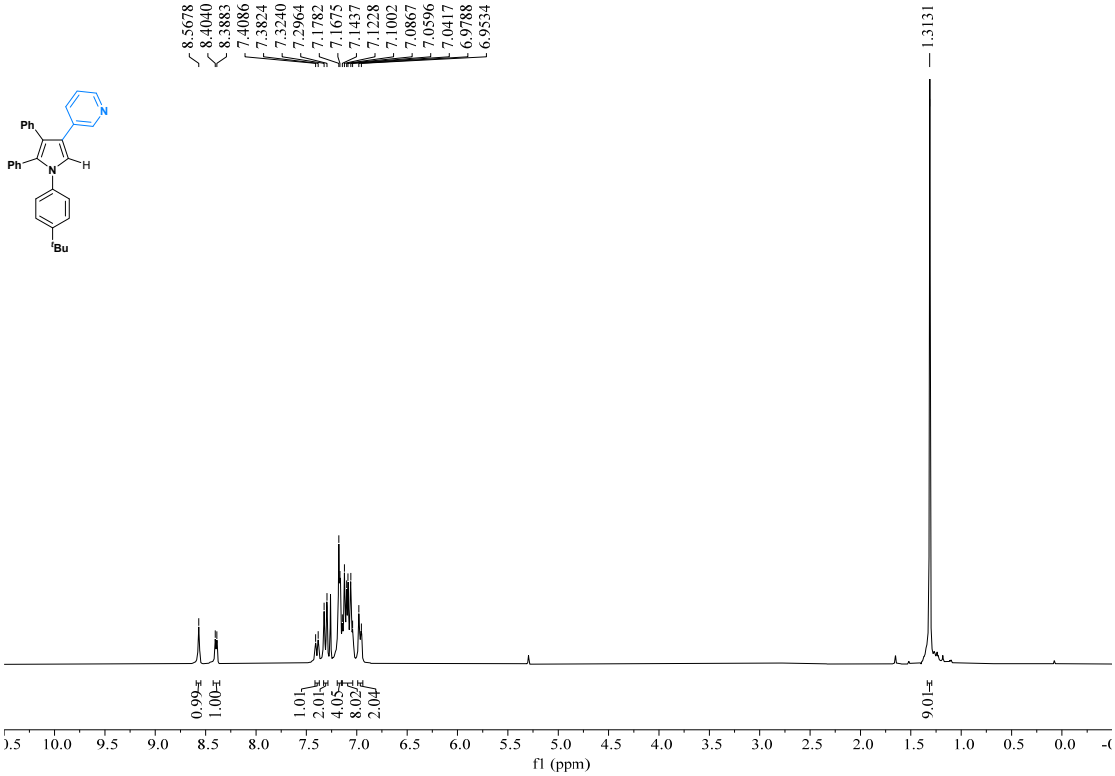
Cl
OMe
f1 (ppm)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7.0417
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8.02
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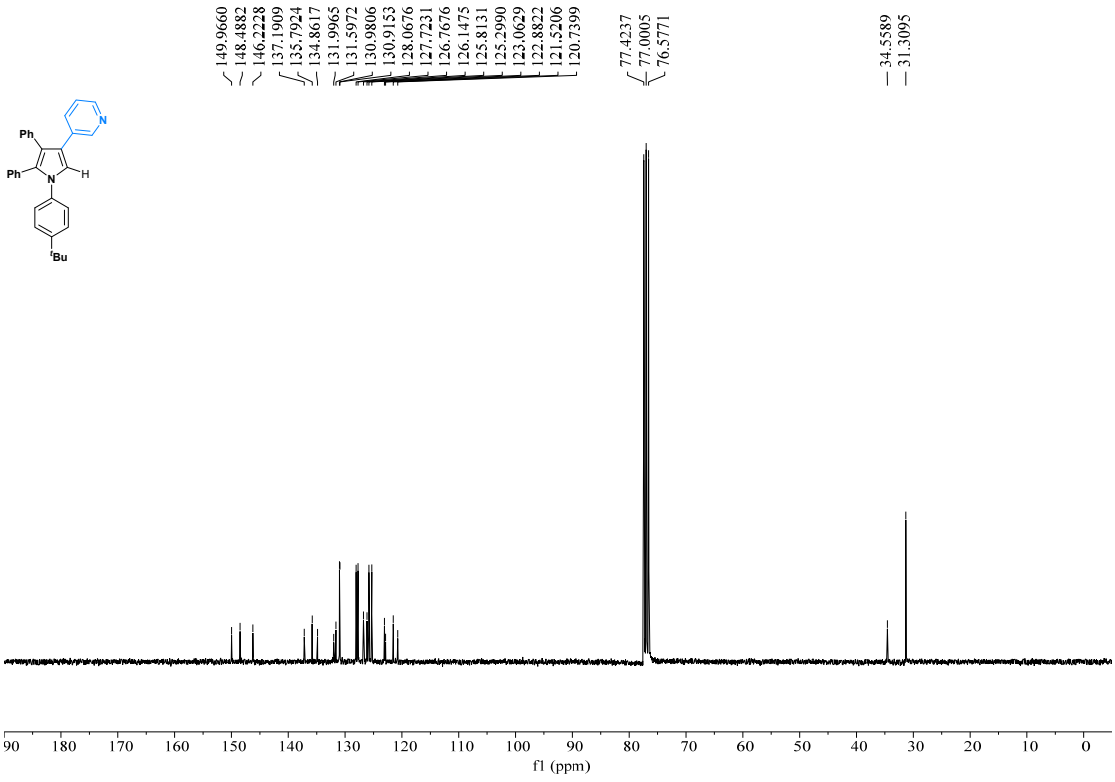
9.01
f1 (ppm)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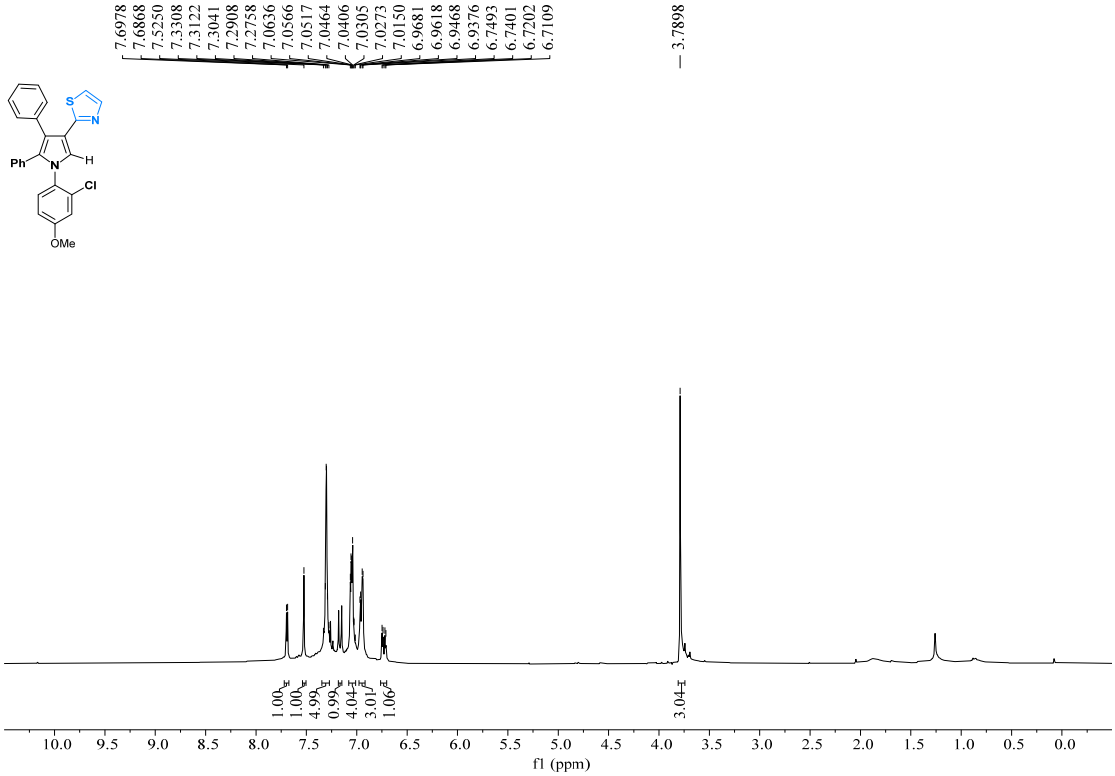
31.3095
Ph
Ph
N
H
tBu
f1 (ppm)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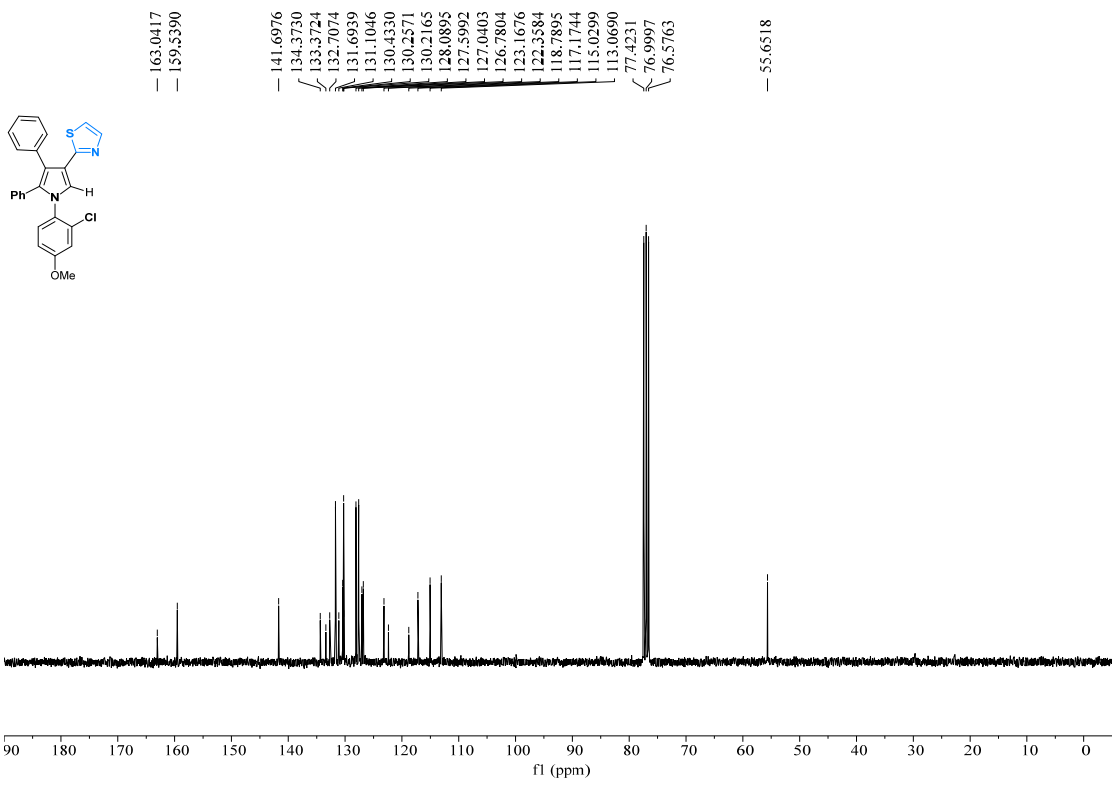
7.0517
7.0464
7.0406
7.0305
7.0273
7.0150
6.9681
6.9618
6.9468
6.9376
6.7493
6.7401
6.7202
6.7109
3.7898
Ph
N
H
S
N
Cl
OMe
1.00
1.00
4.99
0.99
4.04
3.01
1.06
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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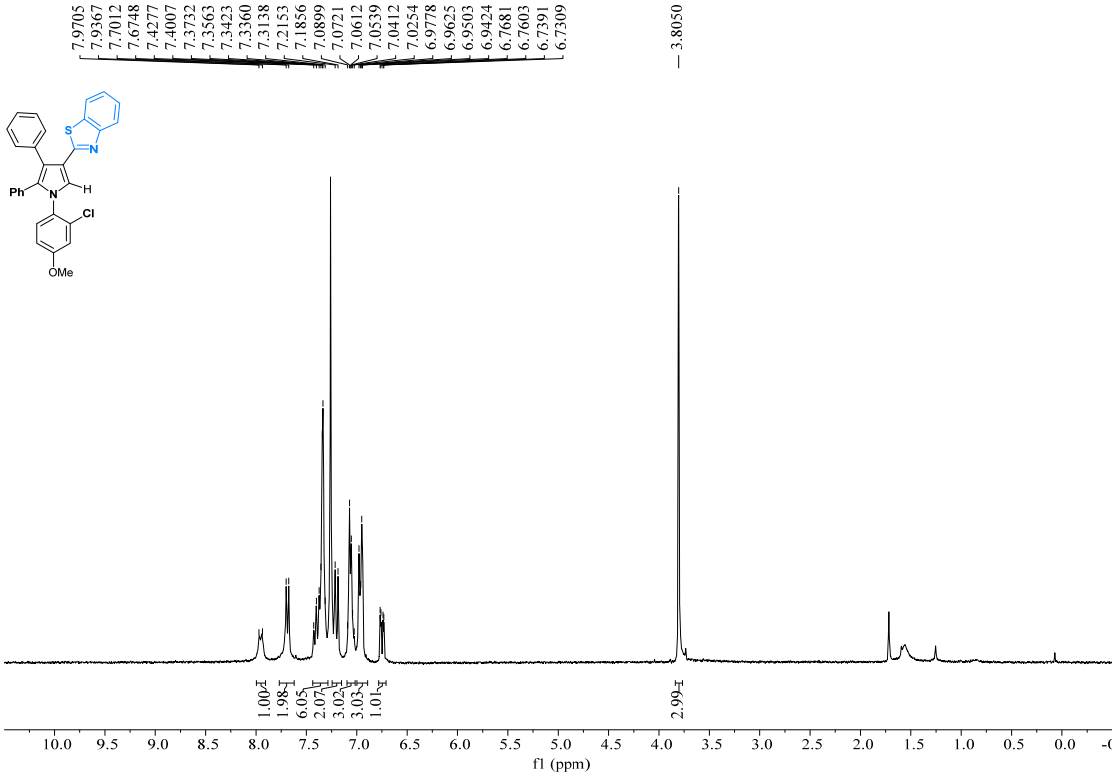
130.2165
128.0895
127.5992
127.0403
126.7804
123.1676
122.3584
118.7895
117.1744
115.0299
113.0690
77.4231
76.9997
76.5763
55.6518
Ph
N
H
S
N
Cl
OMe
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.0539
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6.9503
6.9424
6.7681
6.7603
6.7391
6.7309
3.8050
Ph
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H
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3.03
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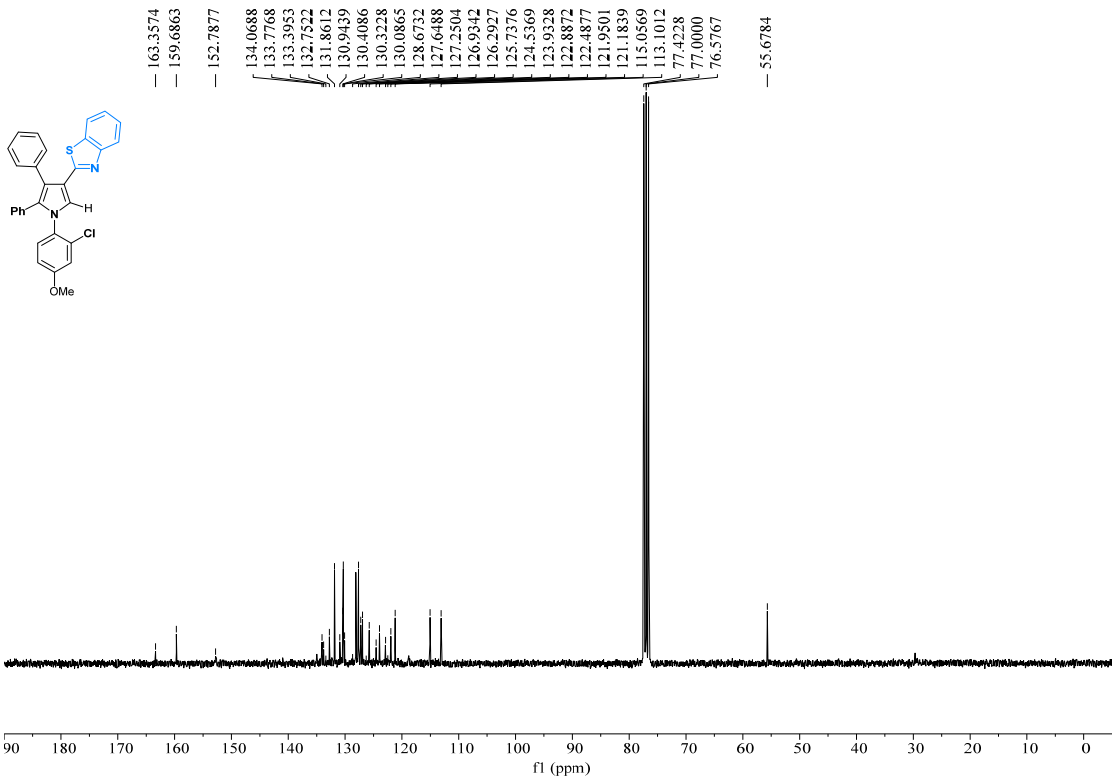
f1 (ppm)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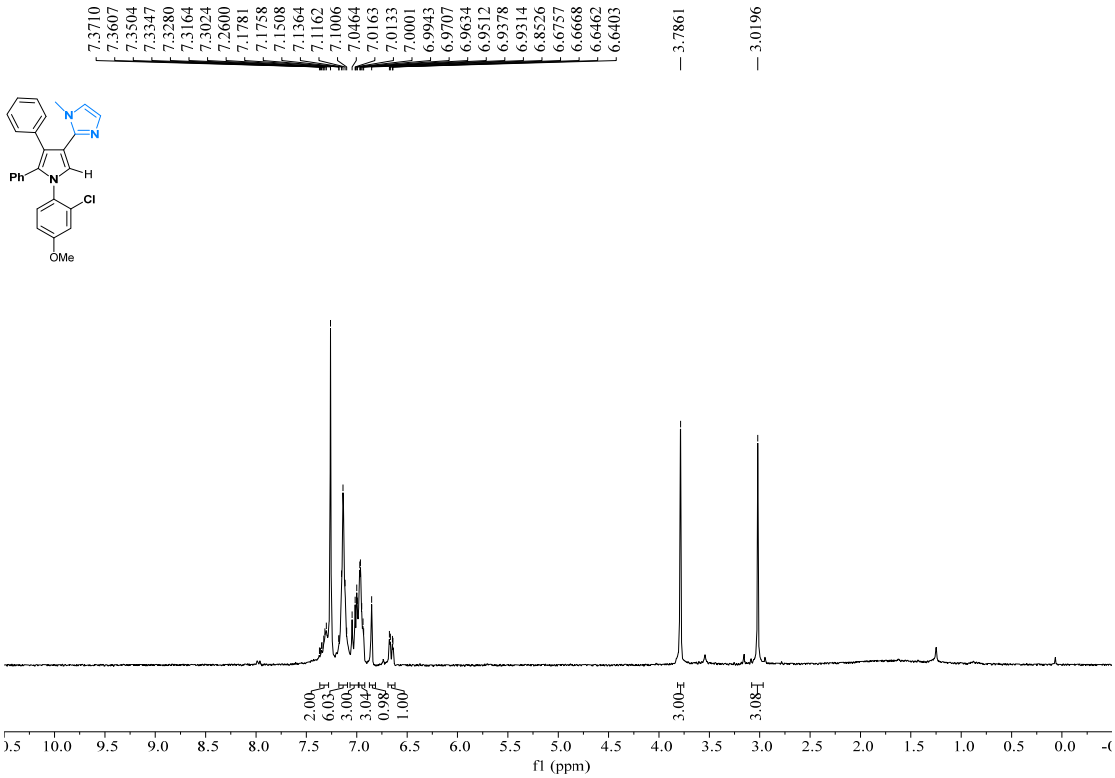
Cl
OMe
f1 (ppm)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7.1508
7.1364
7.1162
7.1006
7.0464
7.0163
7.0133
7.0001
6.9943
6.9707
6.9634
6.9512
6.9378
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6.6462
6.6403
3.7861
3.0196
Ph
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H
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3.00
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0.98
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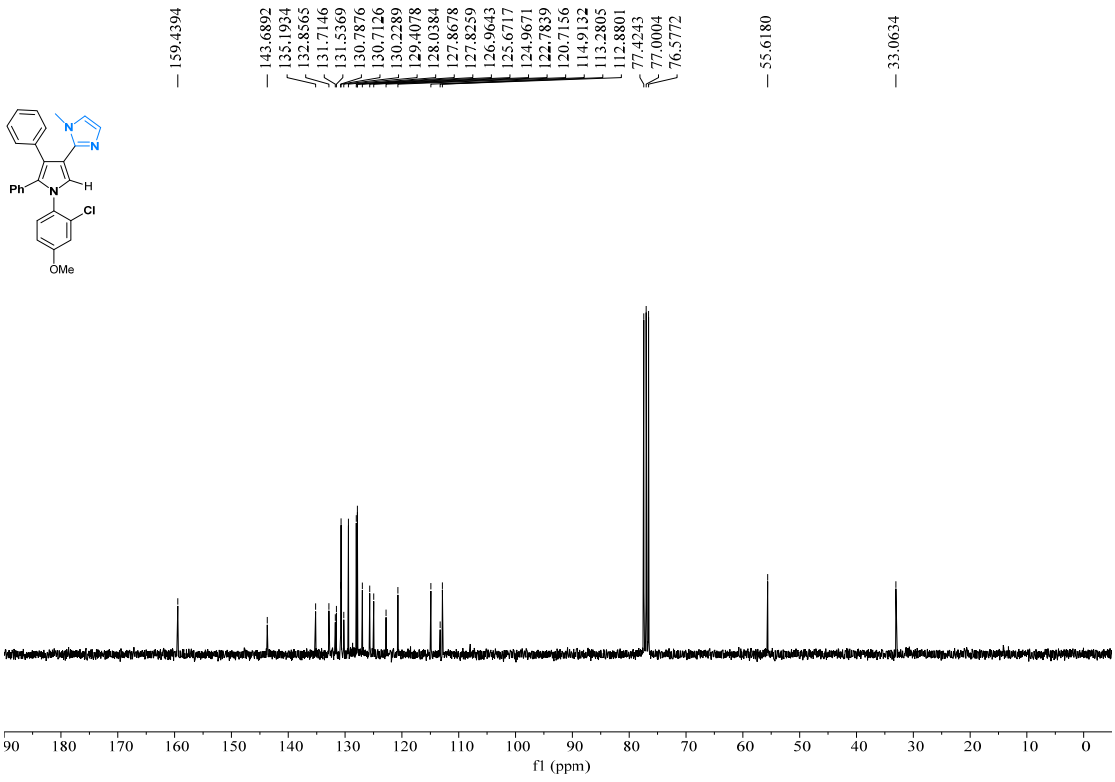
3.00
3.08
f1 (ppm)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122.7839
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113.2805
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Ph
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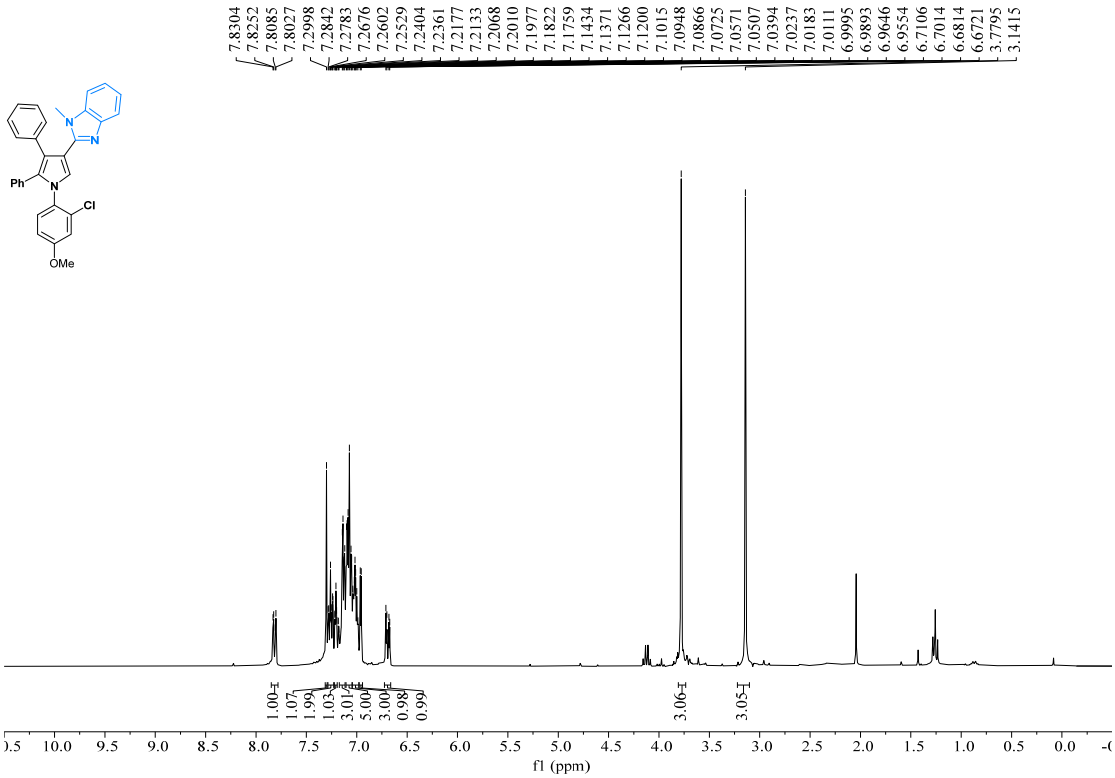
H
Cl
OMe
f1 (ppm)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7.2602
7.2529
7.2404
7.2361
7.2177
7.2133
7.2068
7.2010
7.1977
7.1822
7.1759
7.1434
7.1371
7.1266
7.1200
7.1015
7.0948
7.0866
7.0725
7.0571
7.0507
7.0394
7.0237
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7.0111
6.9995
6.9893
6.9646
6.9554
6.7106
6.7014
6.6814
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3.7795
3.1415
Ph
N
Cl
OMe
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1.03
3.01
5.00
3.00
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0.99
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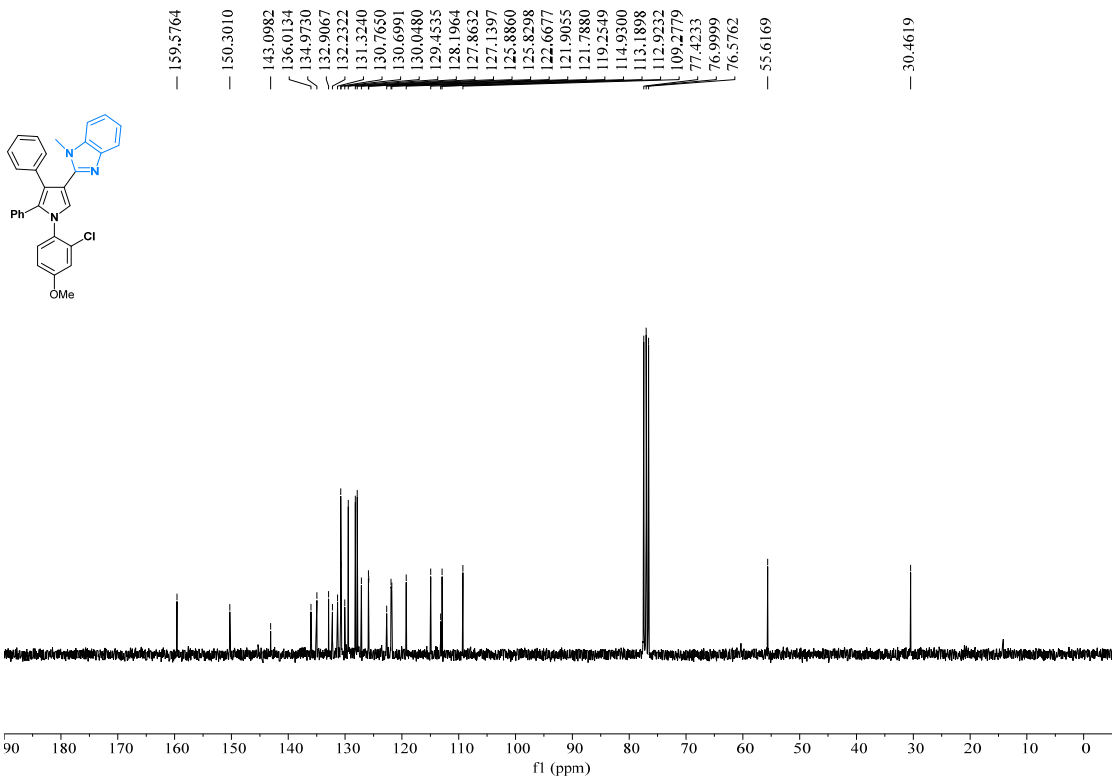
3.05
f1 (ppm)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121.7880
119.2549
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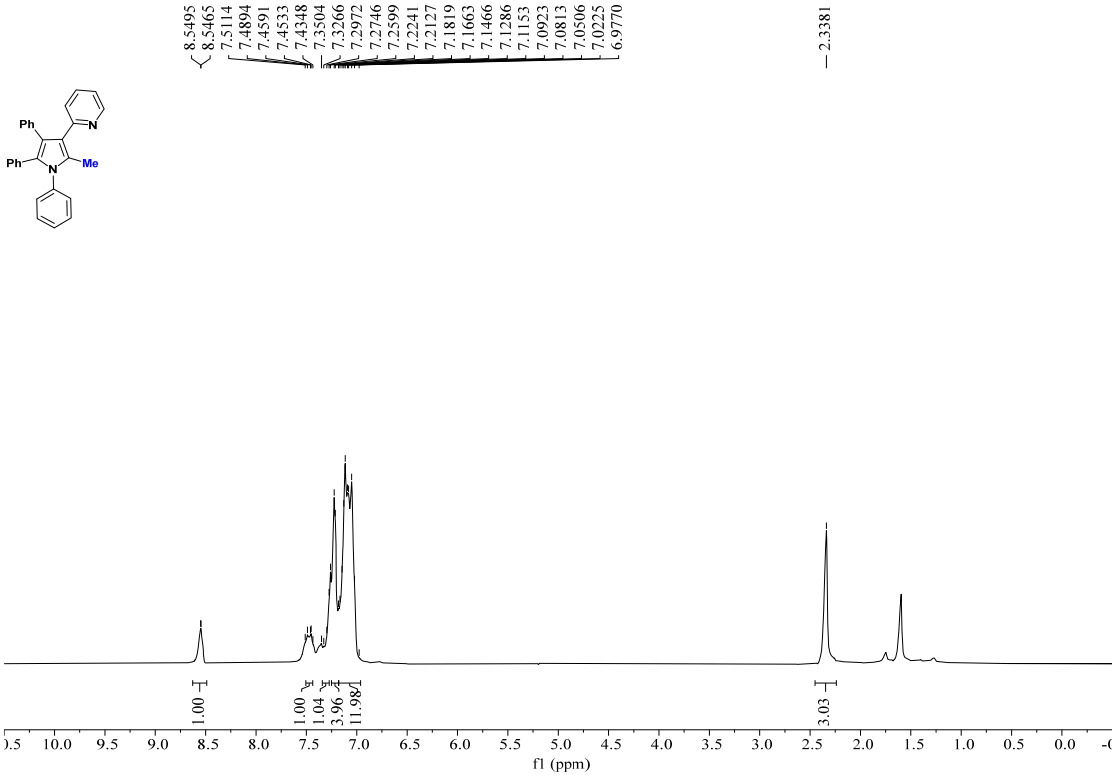
Cl
OMe
f1 (ppm)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7.2127
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7.1466
7.1286
7.1153
7.0923
7.0813
7.0506
7.0225
6.9770
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Me
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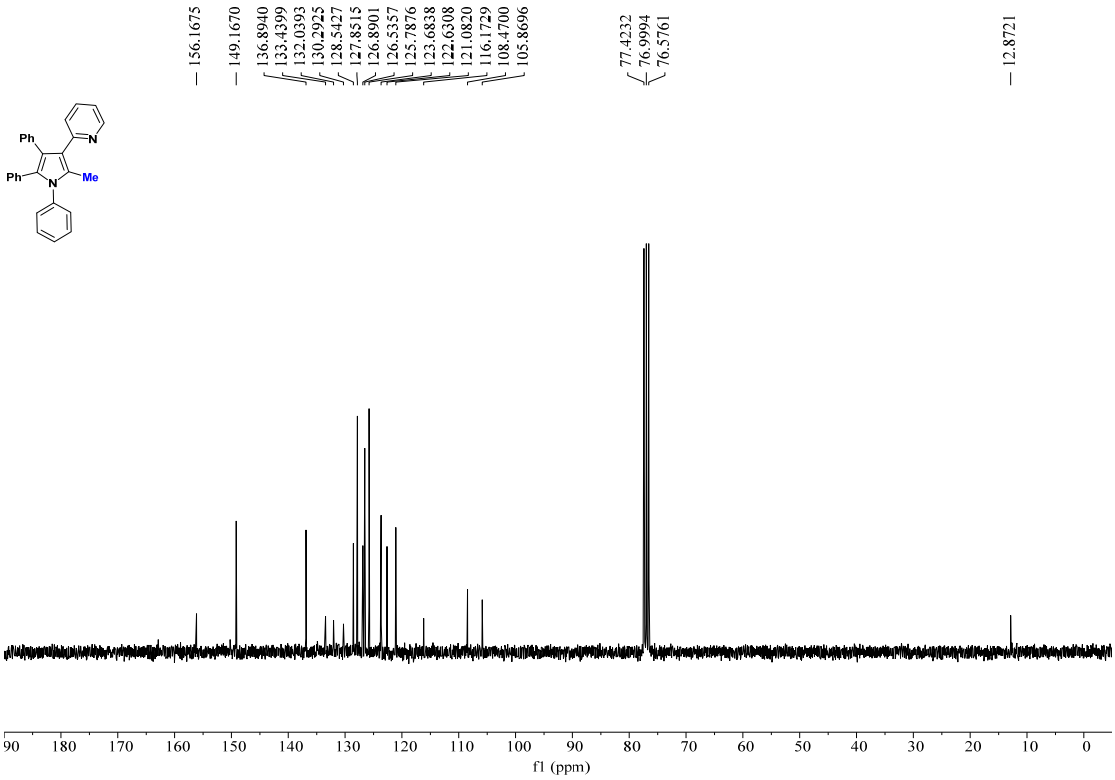
3.03
f1 (ppm)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121.0820
116.1729
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76.5761
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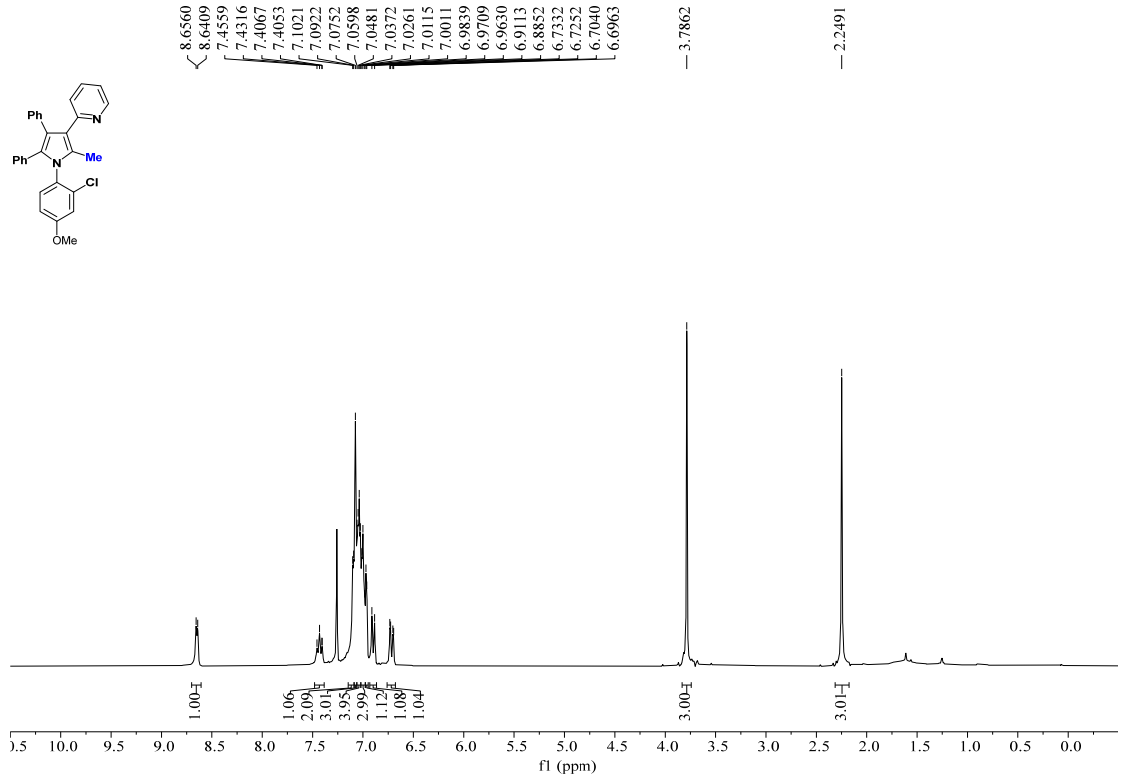
Ph
Ph
N
Me
N
f1 (ppm)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6.8852
6.7332
6.7252
6.7040
6.6963
3.7862
2.2491
Ph
Ph
N
Me
Cl
OMe
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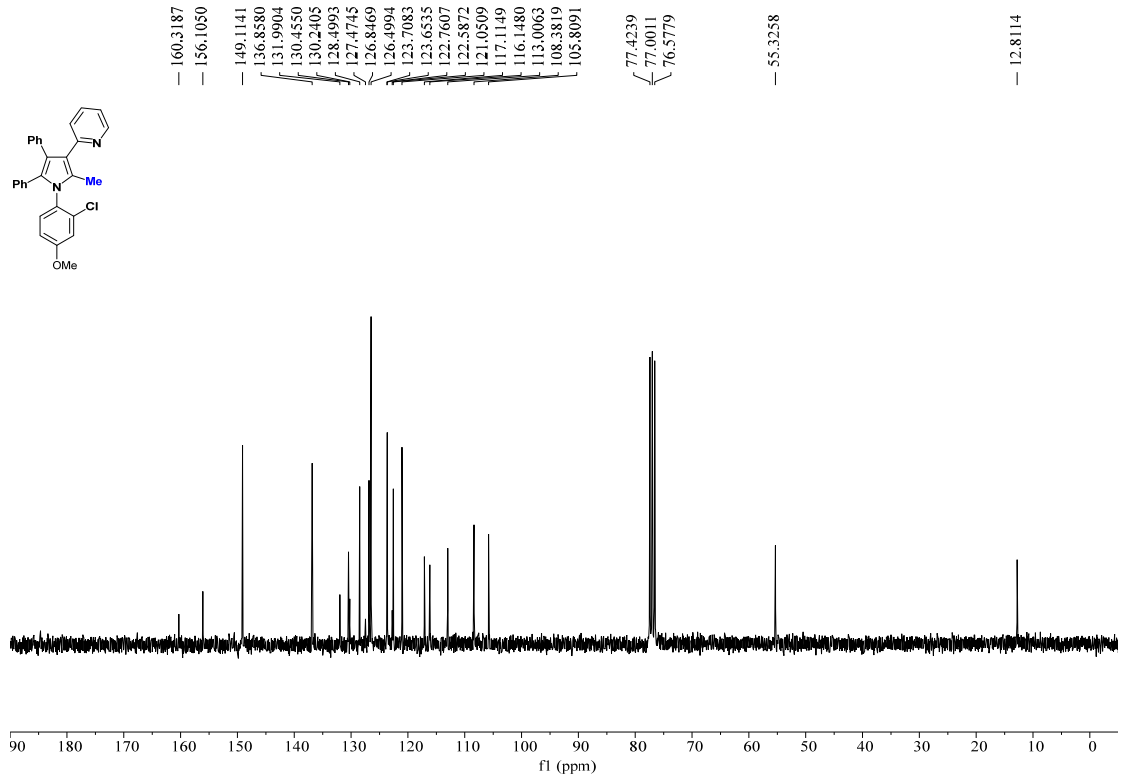
3.95
2.99
1.12
1.08
1.04
3.00
3.01
f1 (ppm)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116.1480
113.0063
108.3819
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Ph
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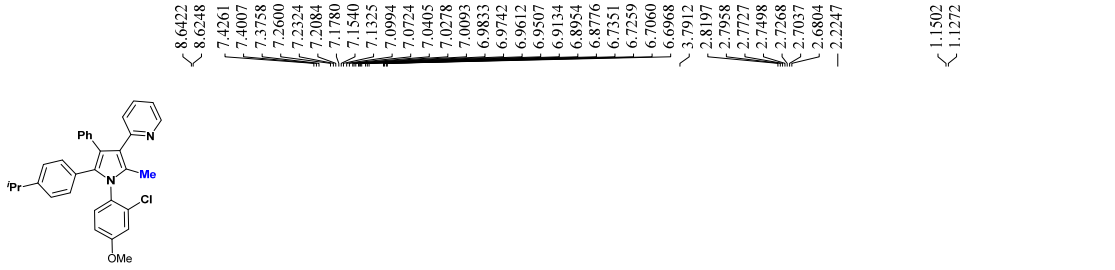
Me
Cl
OMe
f1 (ppm)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Ph
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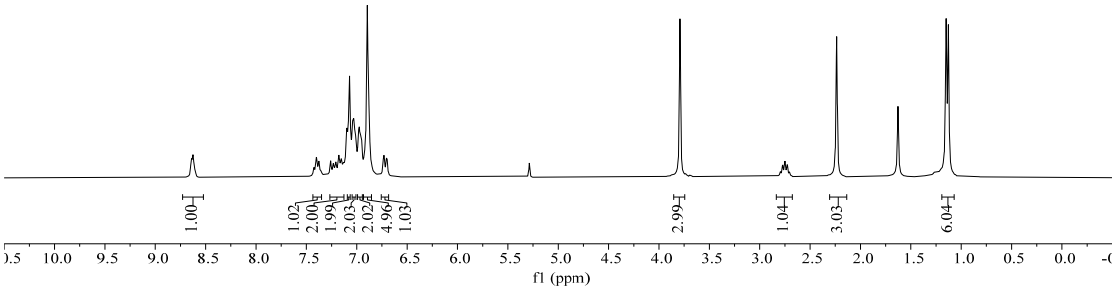
Me
iPr
N
Cl
OMe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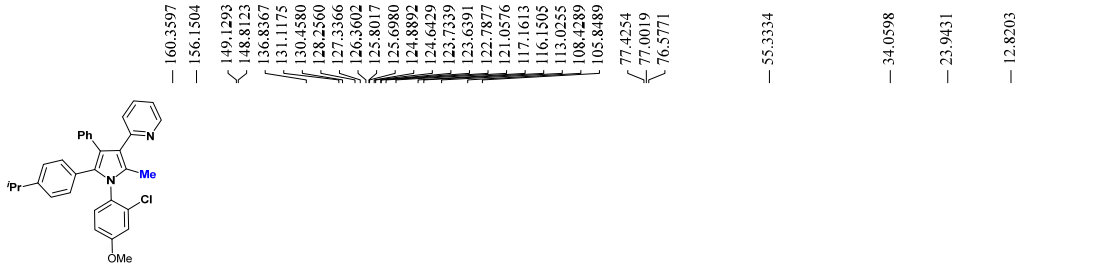
1.03
2.99
1.04
3.03
6.04
f1 (ppm)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Ph
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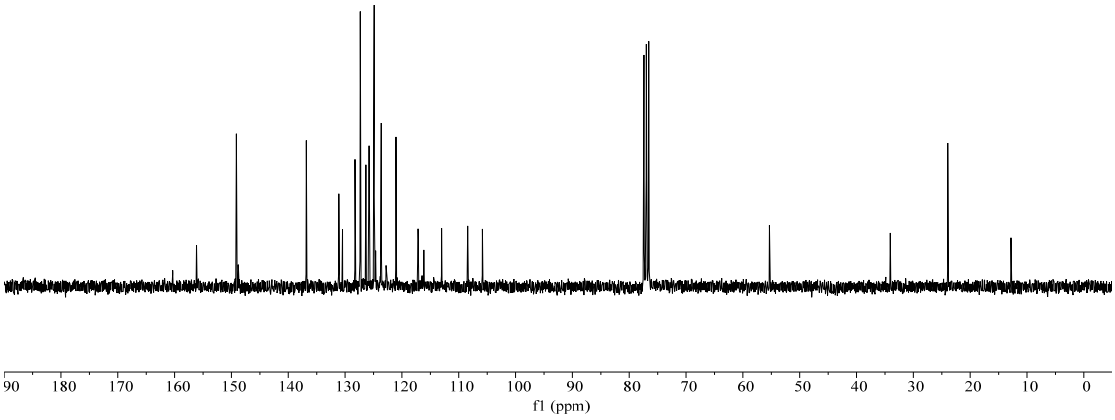
N
Cl
OMe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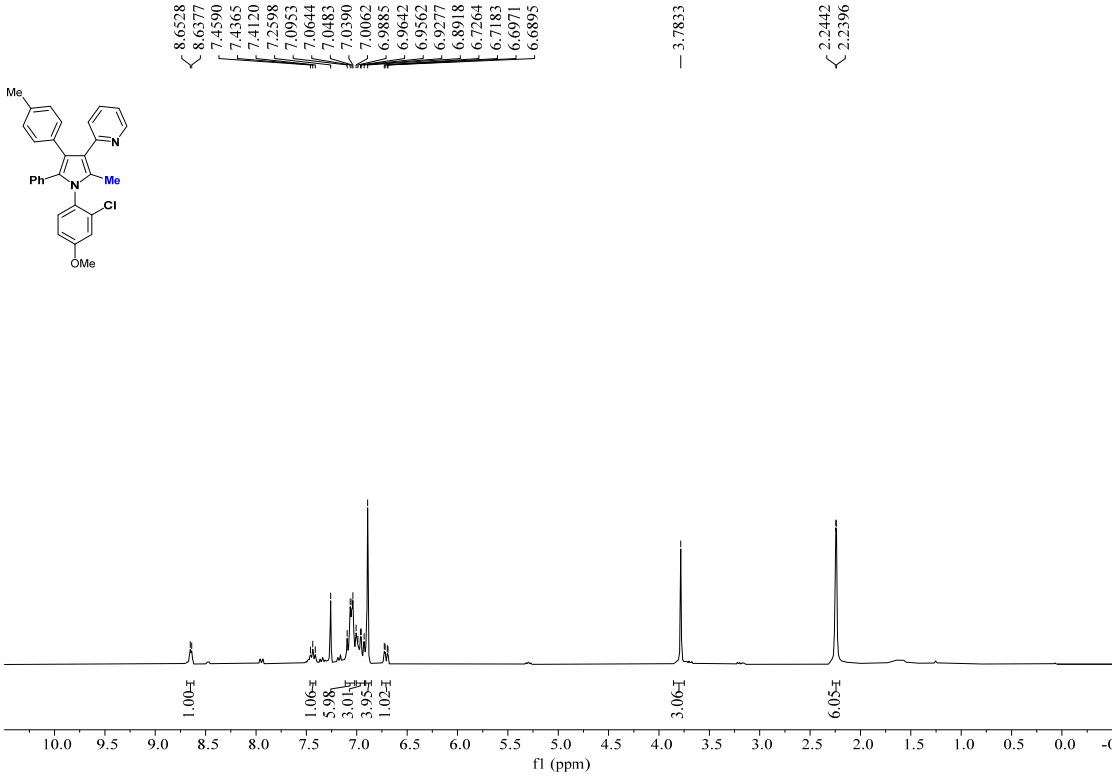
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6.7183
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2.2442
2.2396
Me
Ph
N
Me
Cl
OMe
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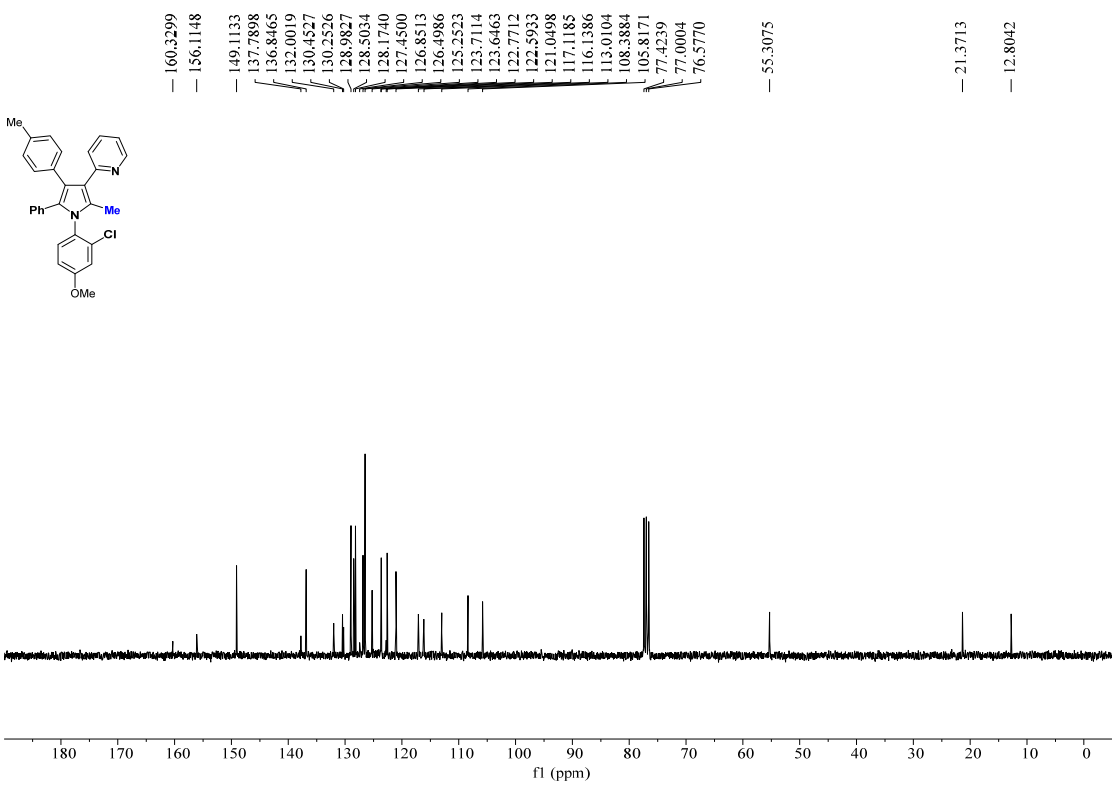
1.06
5.98
3.01
3.95
1.02
3.06
6.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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108.3884
105.8171
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Ph
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Me
Cl
OMe
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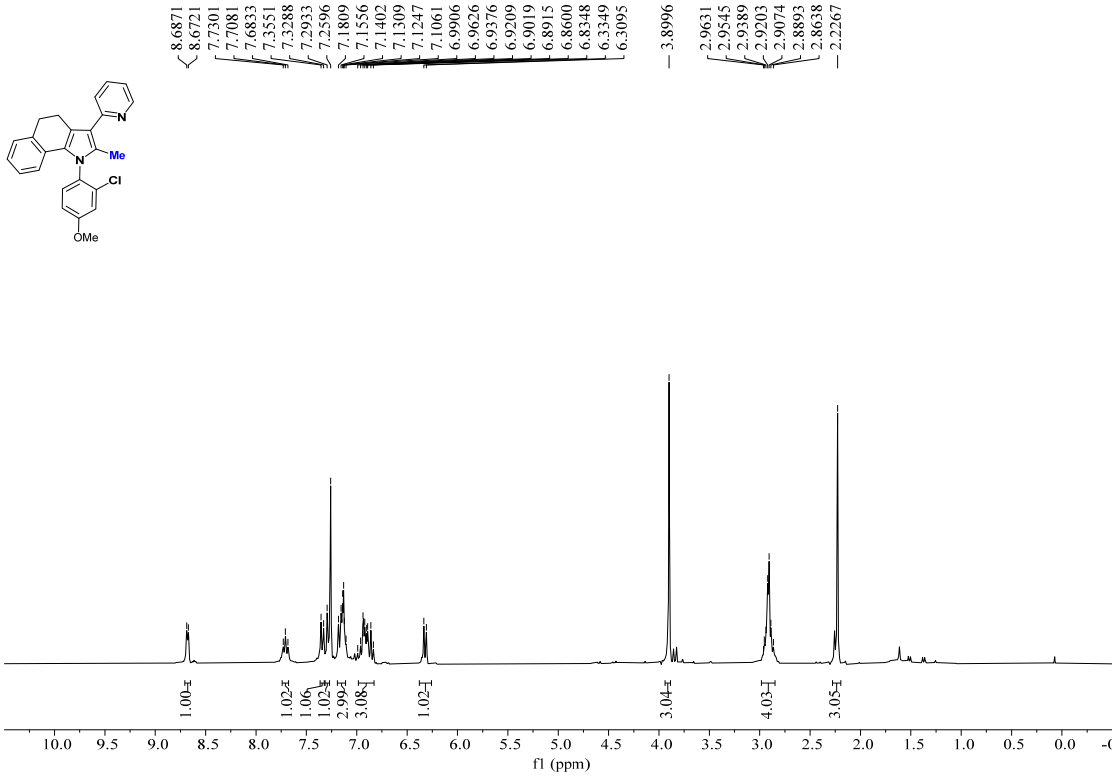
f1 (ppm)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1.02
2.99
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1.02
3.04
4.03
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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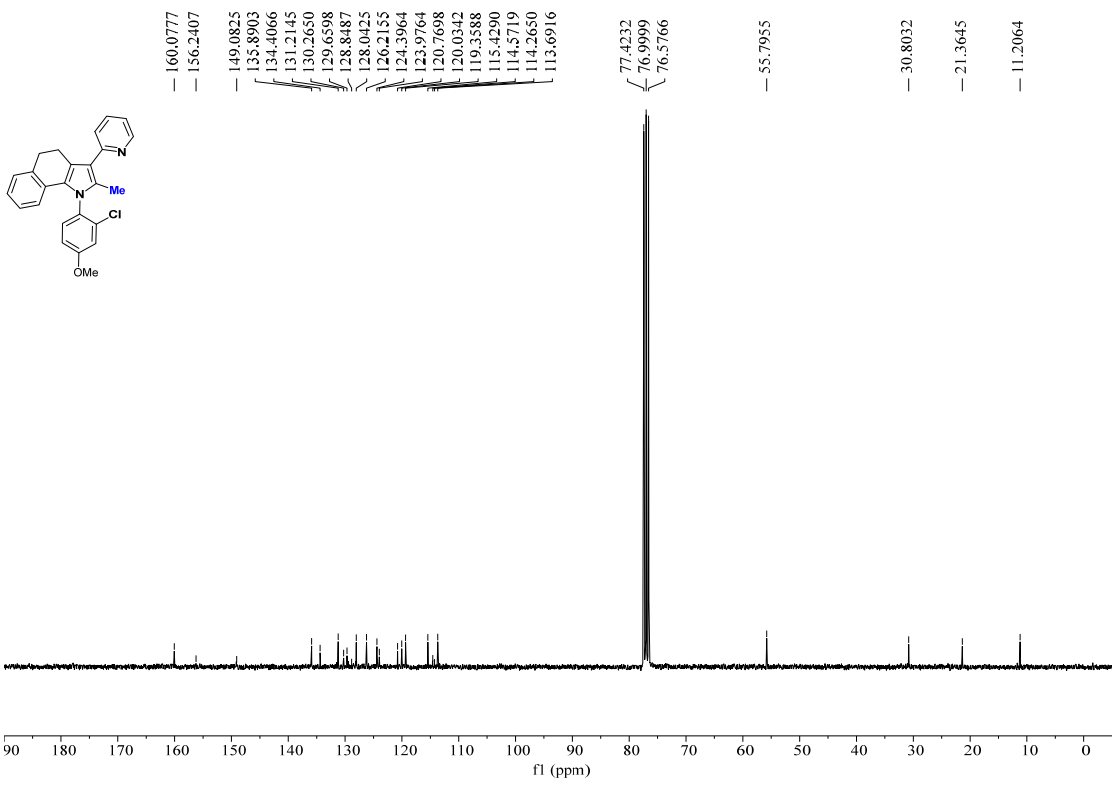
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76.5766
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Me
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Cl
OMe
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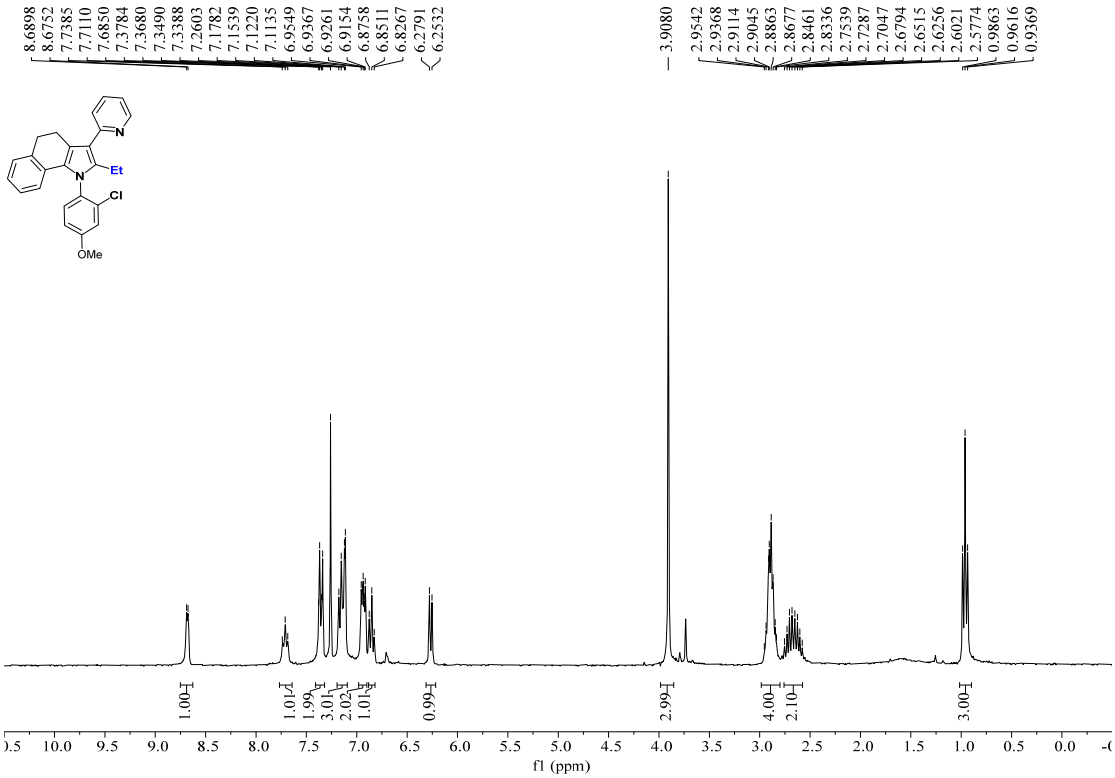
f1 (ppm)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2.6021
2.5774
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0.9369
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Et
N
Cl
OMe
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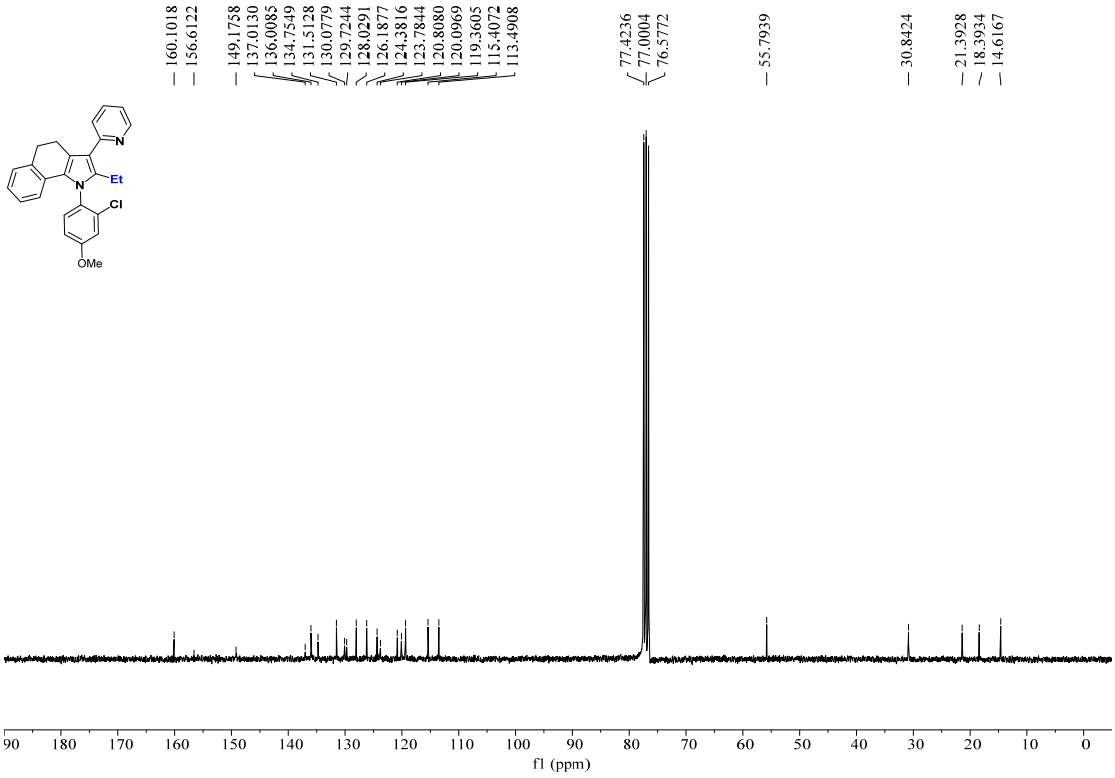
3.00
f1 (ppm)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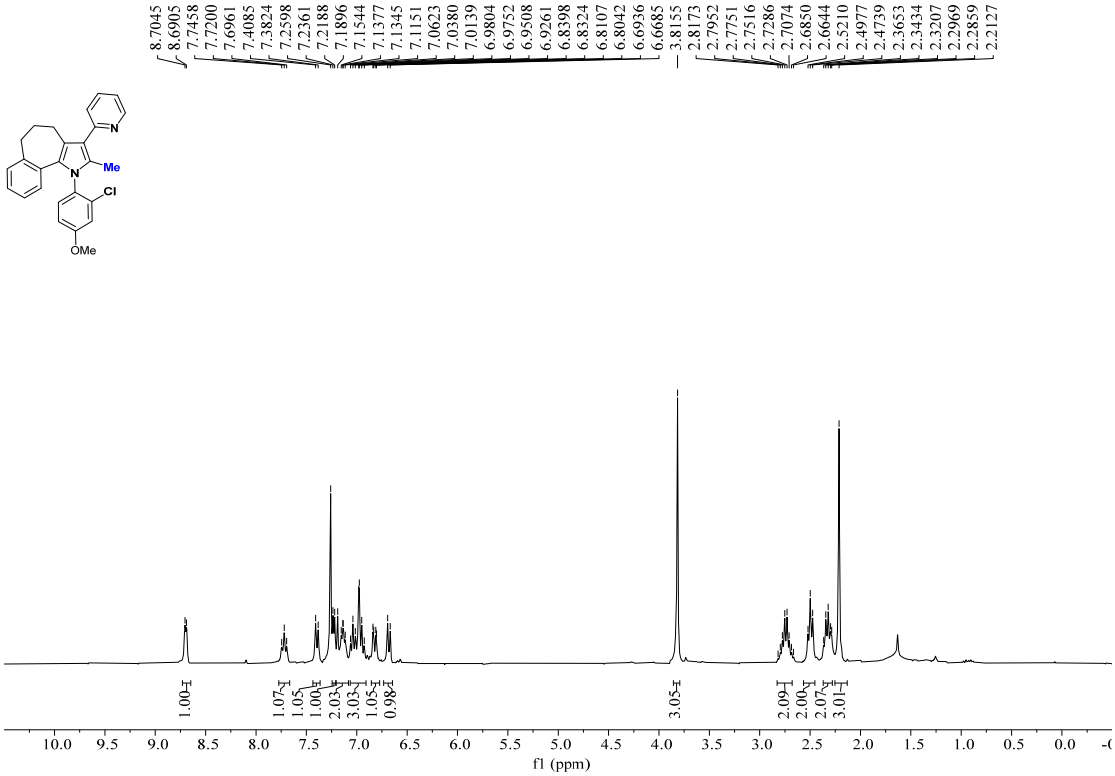
Cl
OMe
f1 (ppm)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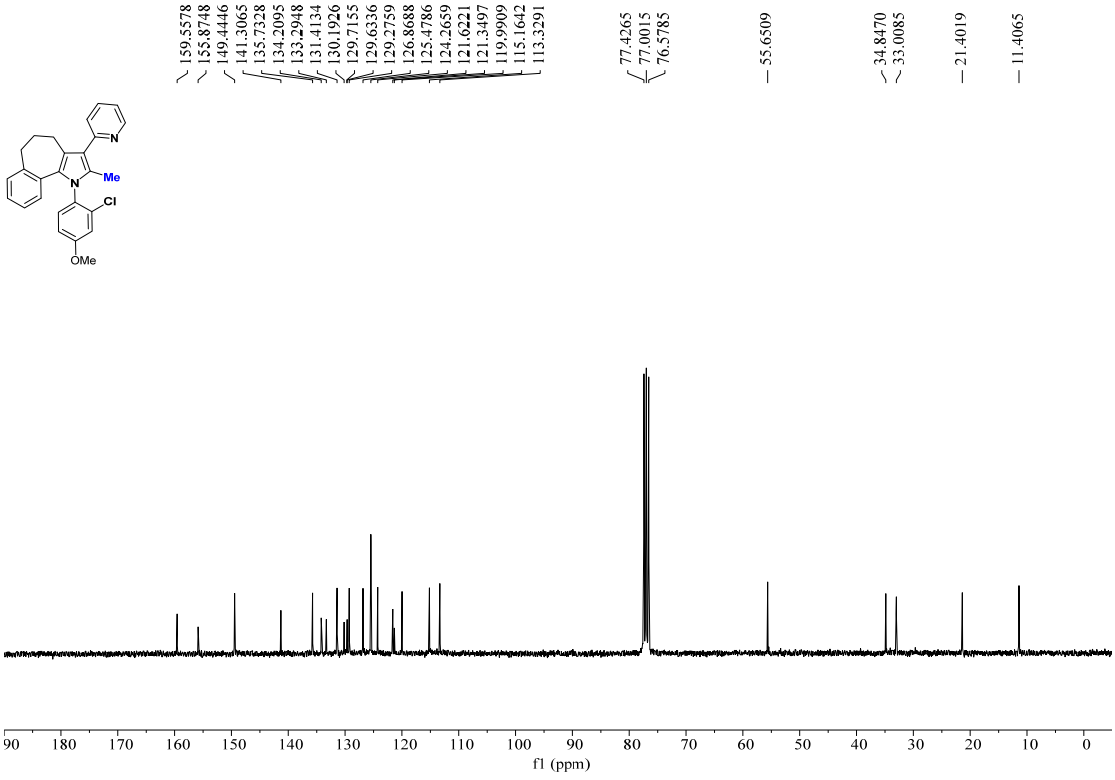
1.07
1.05
1.00
2.03
3.03
1.05
0.98
3.05
2.09
2.00
2.07
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.2759
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125.4786
124.2659
121.6221
121.3497
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113.3291
77.4265
77.0015
76.5785
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34.8470
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Me
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Cl
OMe
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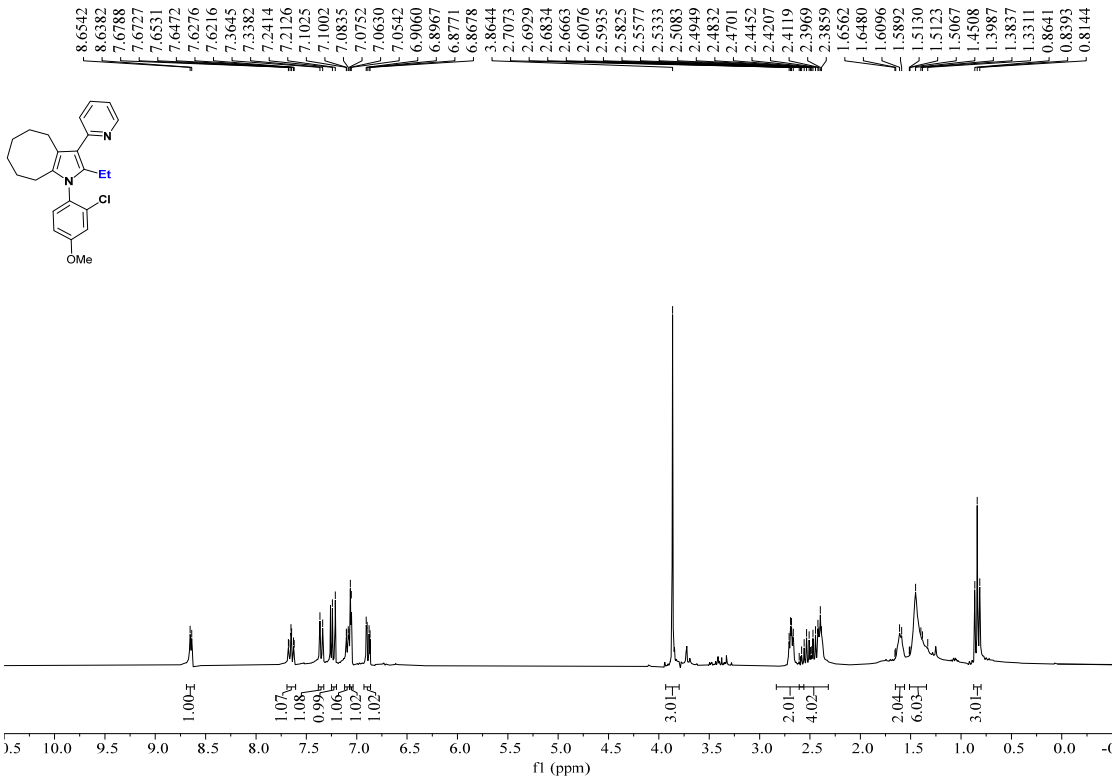
f1 (ppm)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6.8771
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2.4832
2.4701
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2.4207
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1.07
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1.02
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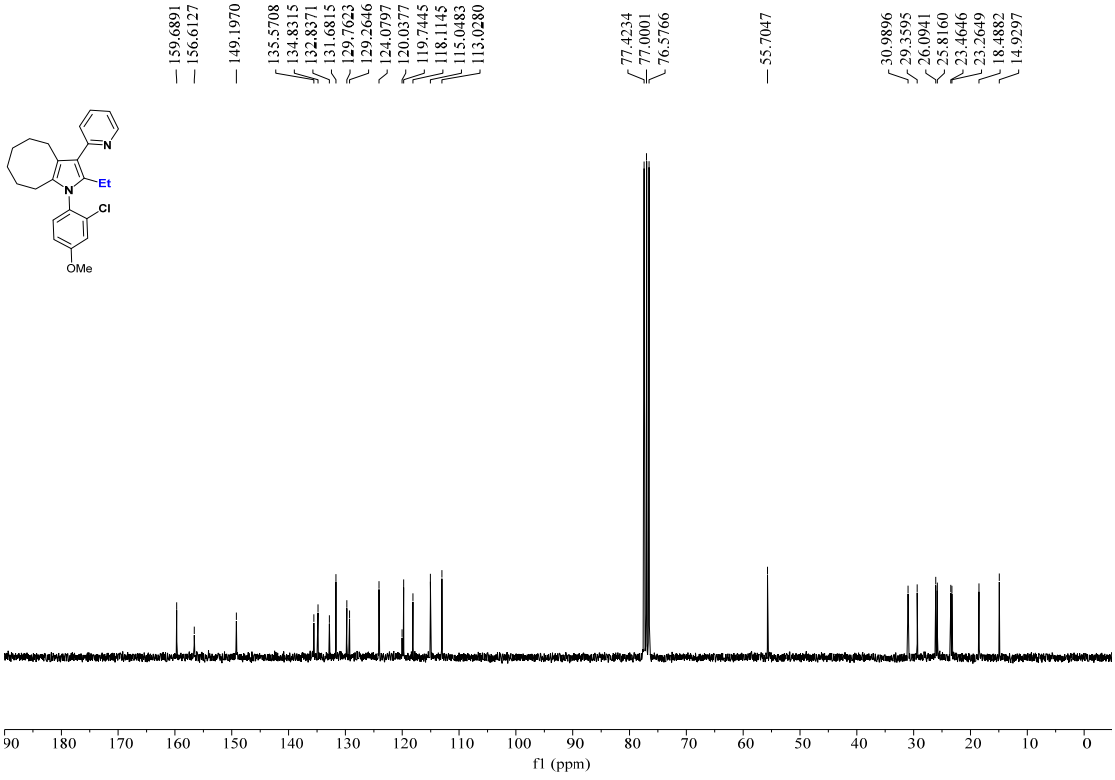
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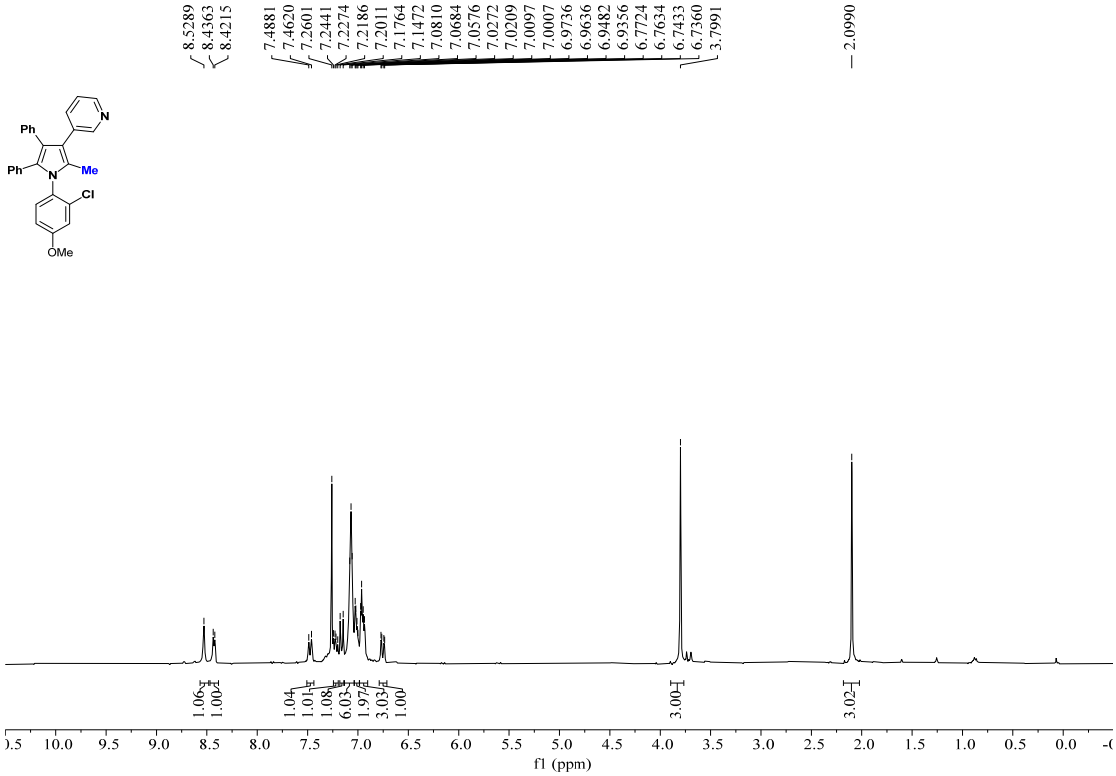
Cl
OMe
f1 (ppm)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7.0810
7.0684
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6.9482
6.9356
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6.7433
6.7360
3.7991
2.0990
Ph
Ph
N
Me
Cl
OMe
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1.01
1.08
6.03
1.97
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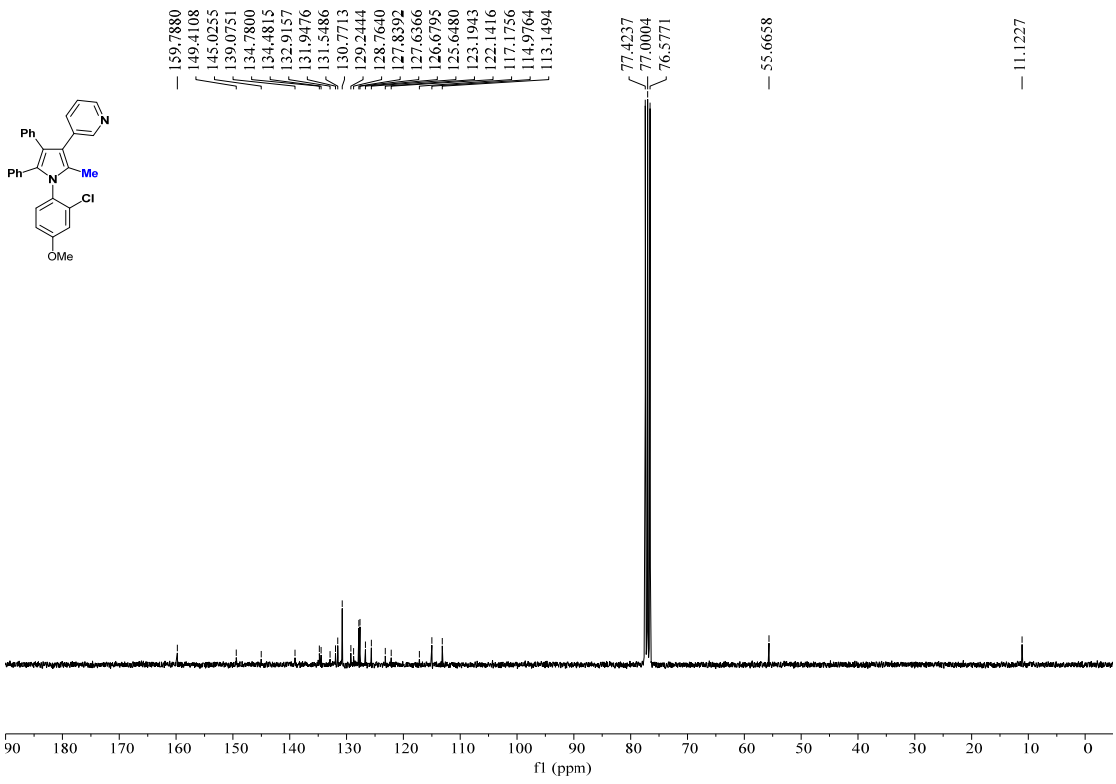
3.02
f1 (ppm)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Ph
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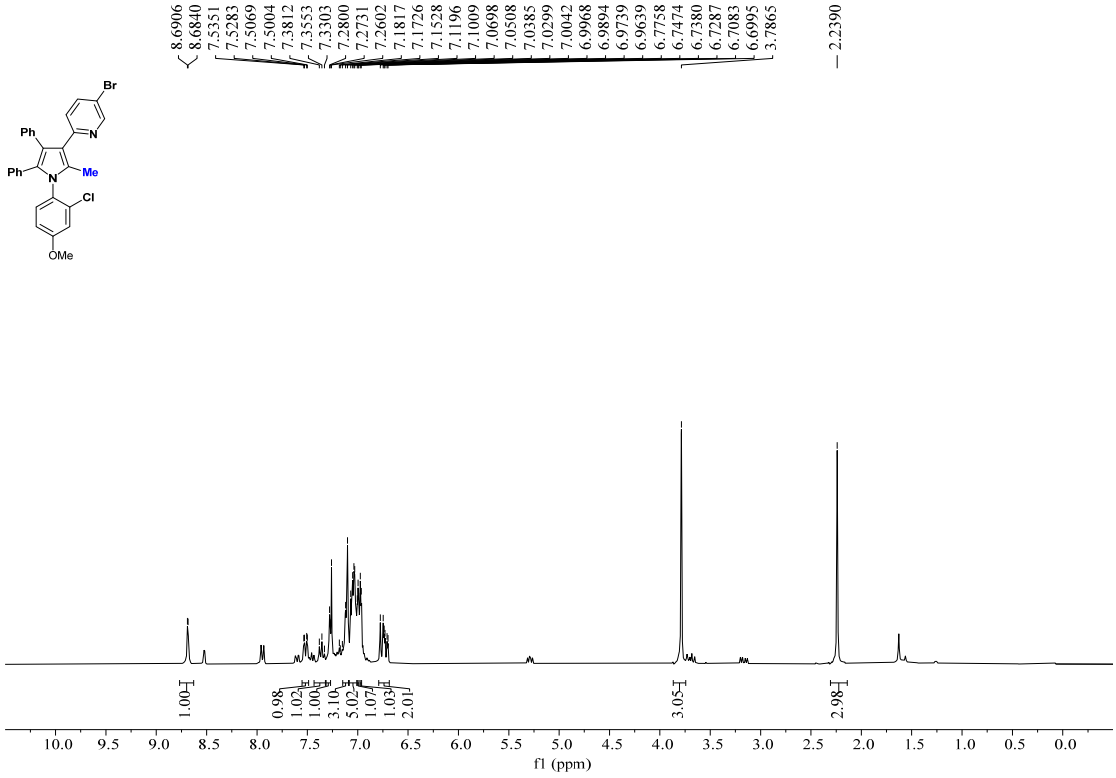
Me
Cl
OMe
f1 (ppm)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7.1817
7.1726
7.1528
7.1196
7.1009
7.0698
7.0508
7.0385
7.0299
7.0042
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6.9739
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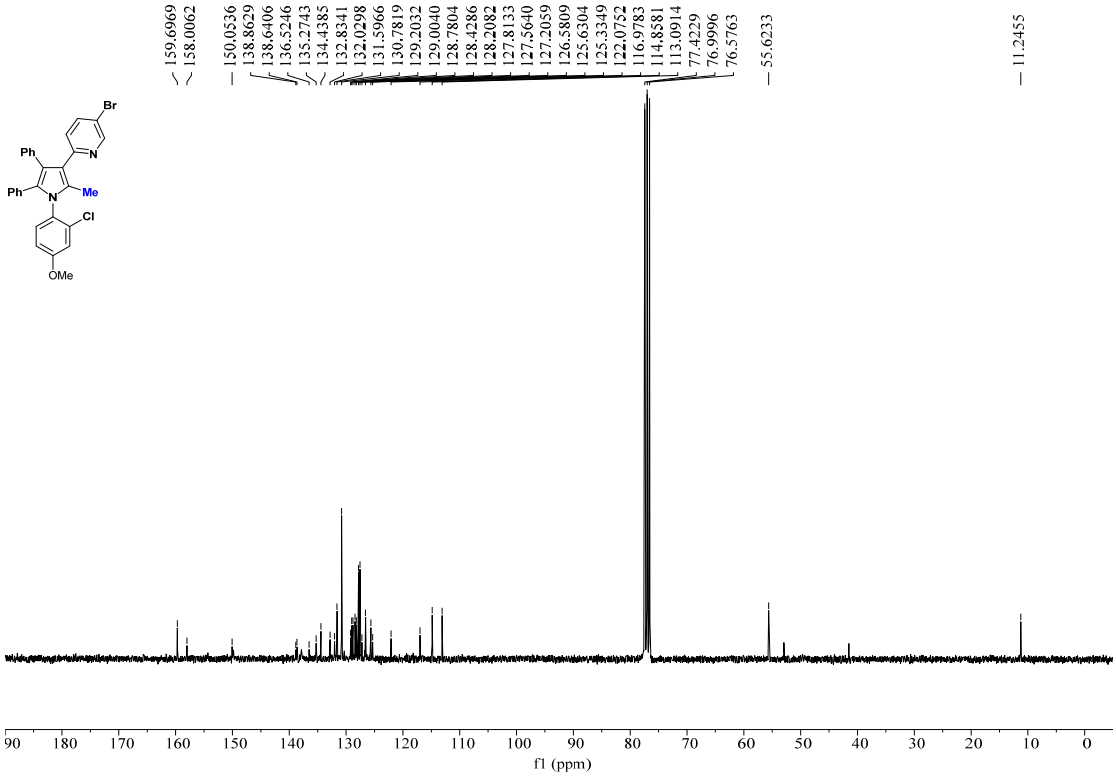
6.7758
6.7474
6.7380
6.7287
6.7083
6.6995
3.7865
2.2390
Br
Ph
Ph
N
Me
N
Cl
OMe
1.00
0.98
1.02
1.00
3.10
5.02
1.07
1.03
2.01
3.05
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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128.4286
128.2082
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113.0914
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55.6233
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Me
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Cl
OMe
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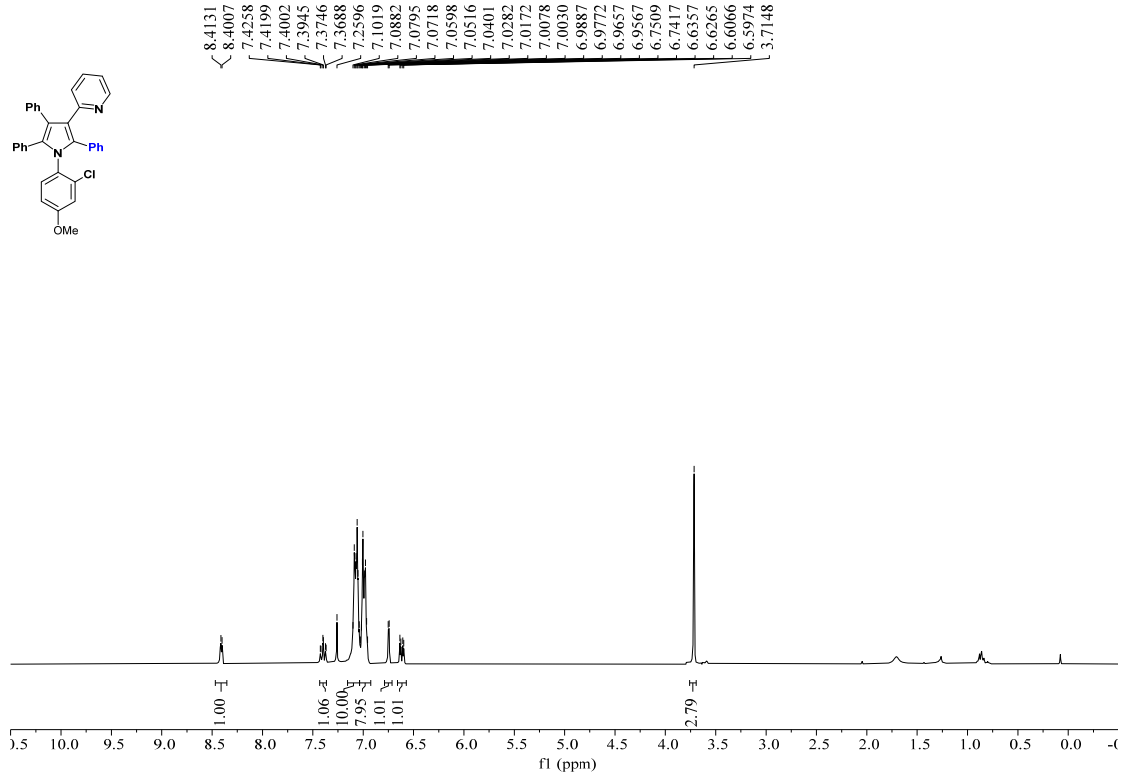
f1 (ppm)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7.0795
7.0718
7.0598
7.0516
7.0401
7.0282
7.0172
7.0078
7.0030
6.9887
6.9772
6.9657
6.9567
6.7509
6.7417
6.6357
6.6265
6.6066
6.5974
3.7148
Ph
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Ph
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Cl
OMe
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10.00
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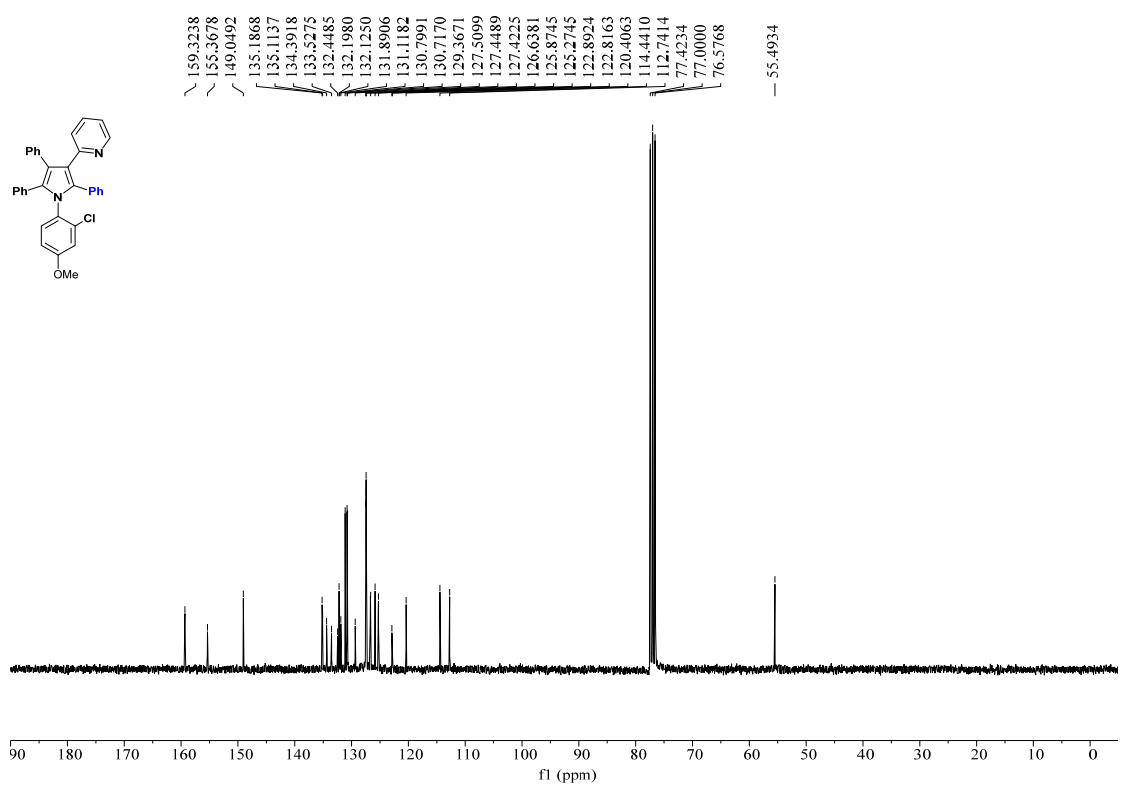
1.01
1.01
2.79
f1 (ppm)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Ph
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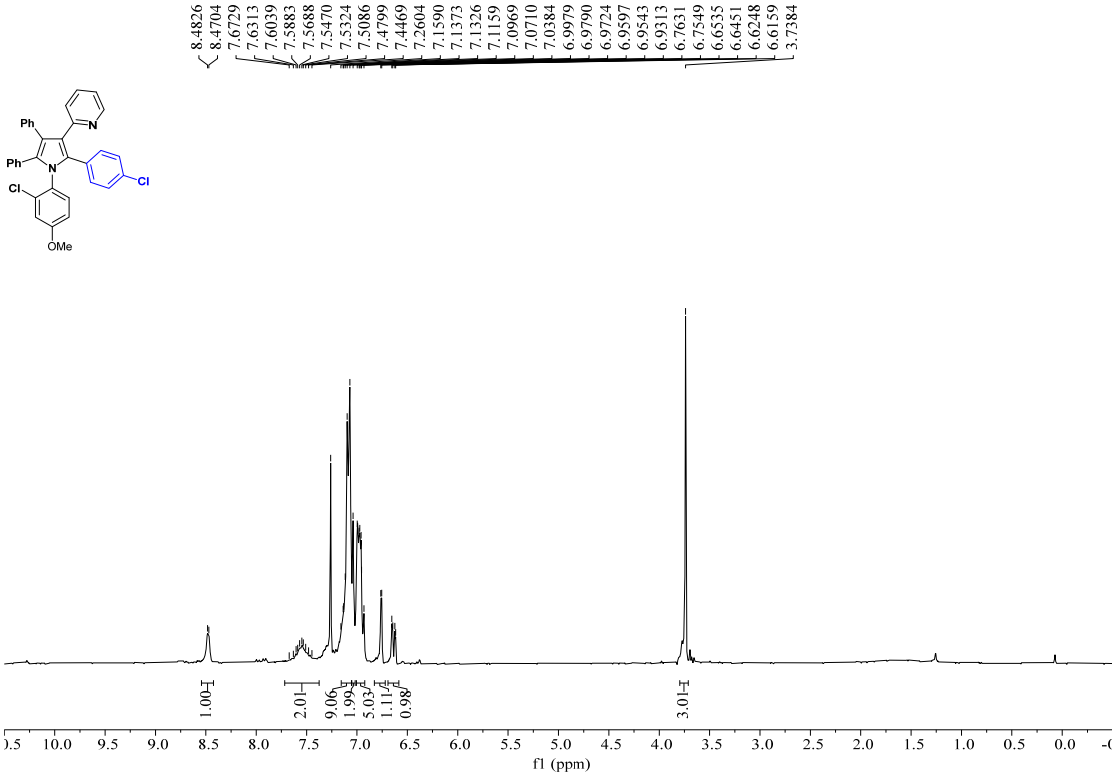
Ph
N
Cl
OMe
f1 (ppm)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7.0710
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6.9790
6.9724
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6.9543
6.9313
6.7631
6.7549
6.6535
6.6451
6.6248
6.6159
3.7384
Ph
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Cl
Cl
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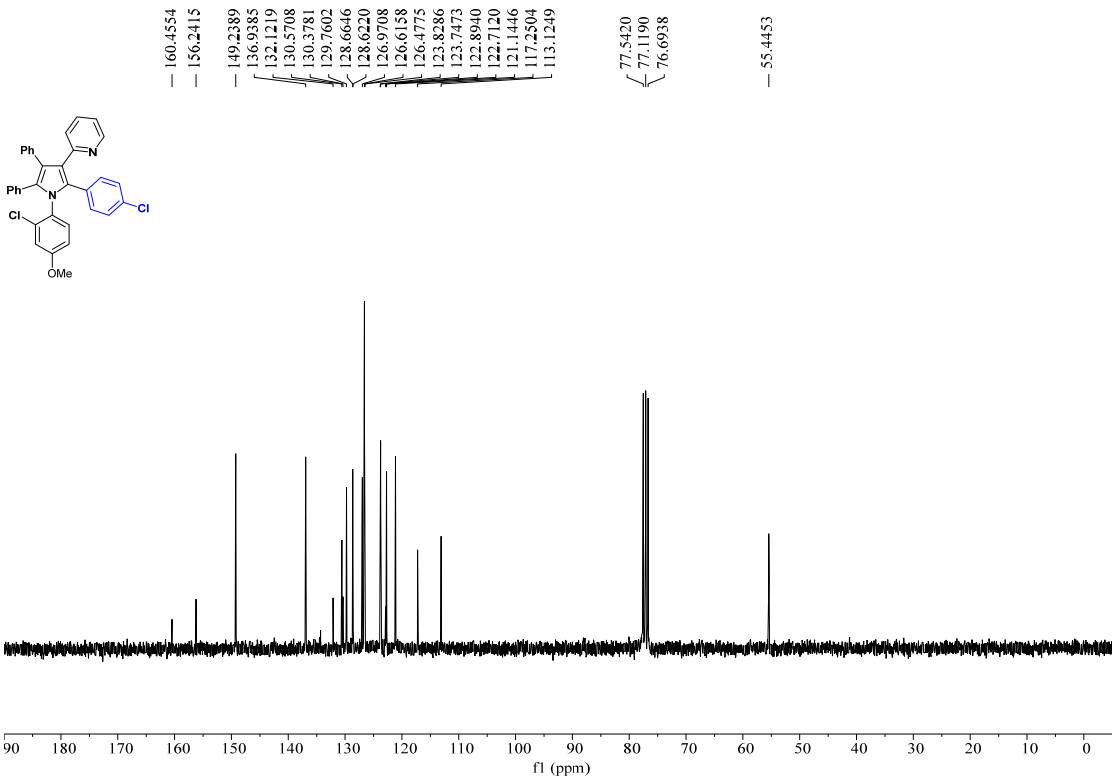
3.01
f1 (ppm)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122.7120
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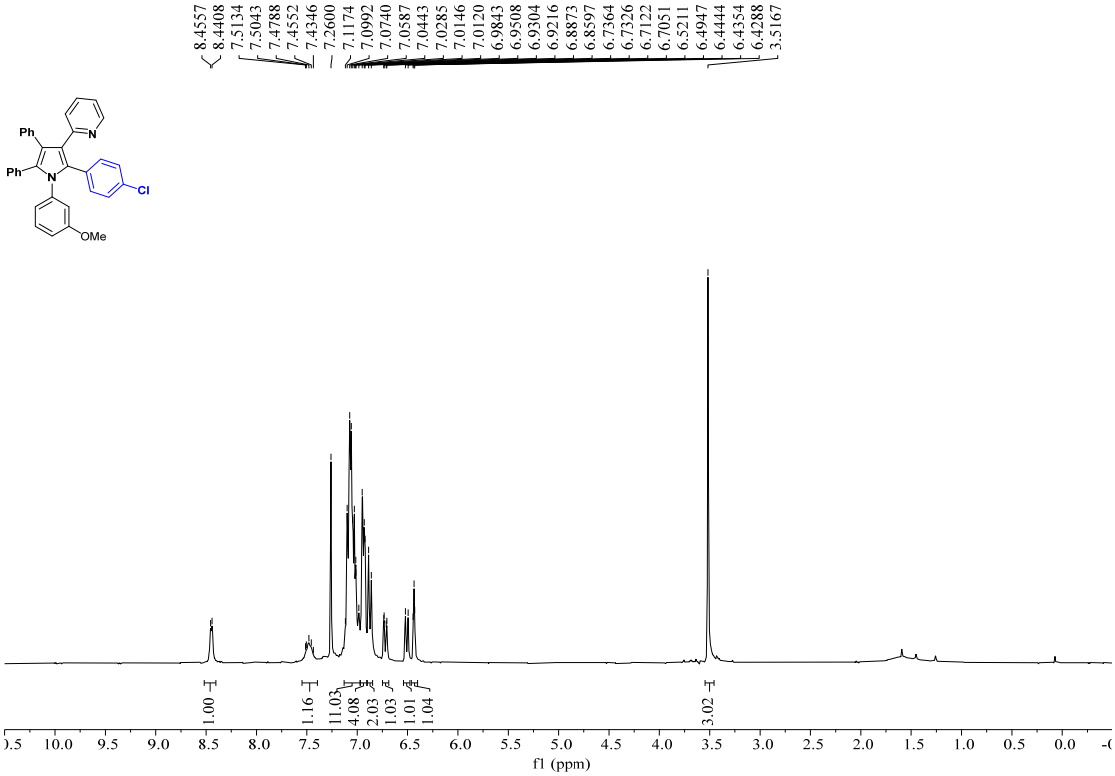
Ph
Ph
N
Cl
Cl
OMe
f1 (ppm)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7.0443
7.0285
7.0146
7.0120
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6.8597
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6.7051
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6.4947
6.4444
6.4354
6.4288
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Ph
Ph
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OMe
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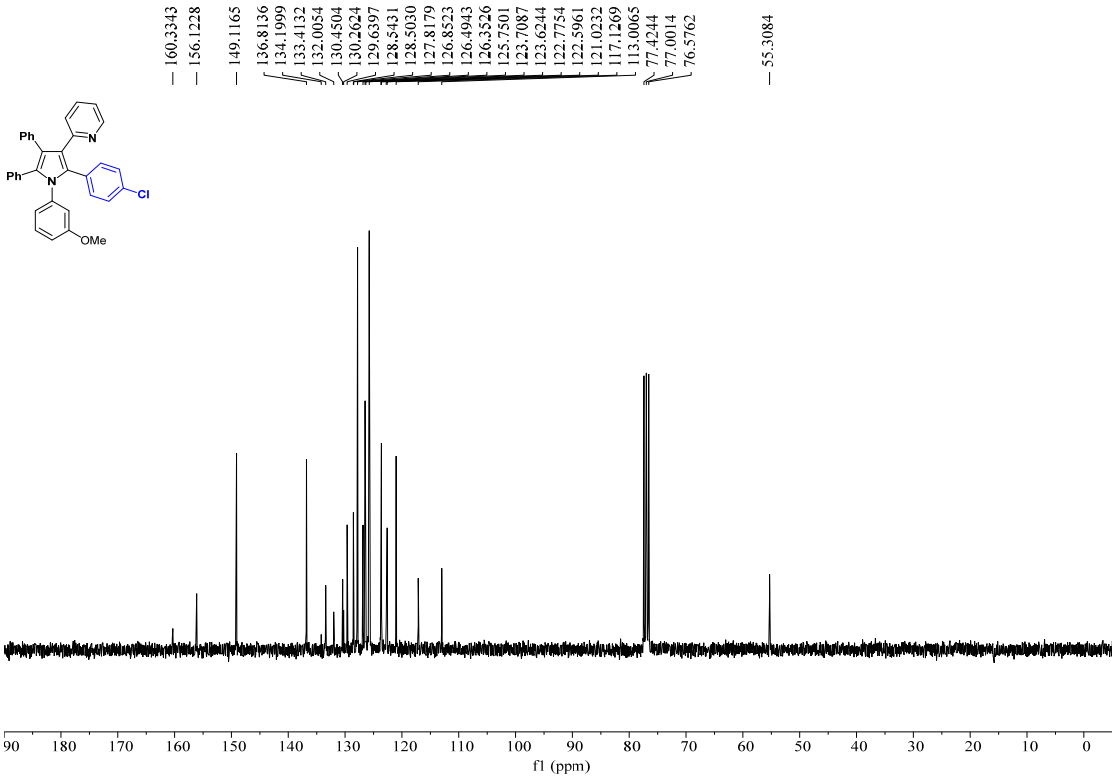
1.01
1.04
3.02
f1 (ppm)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Ph
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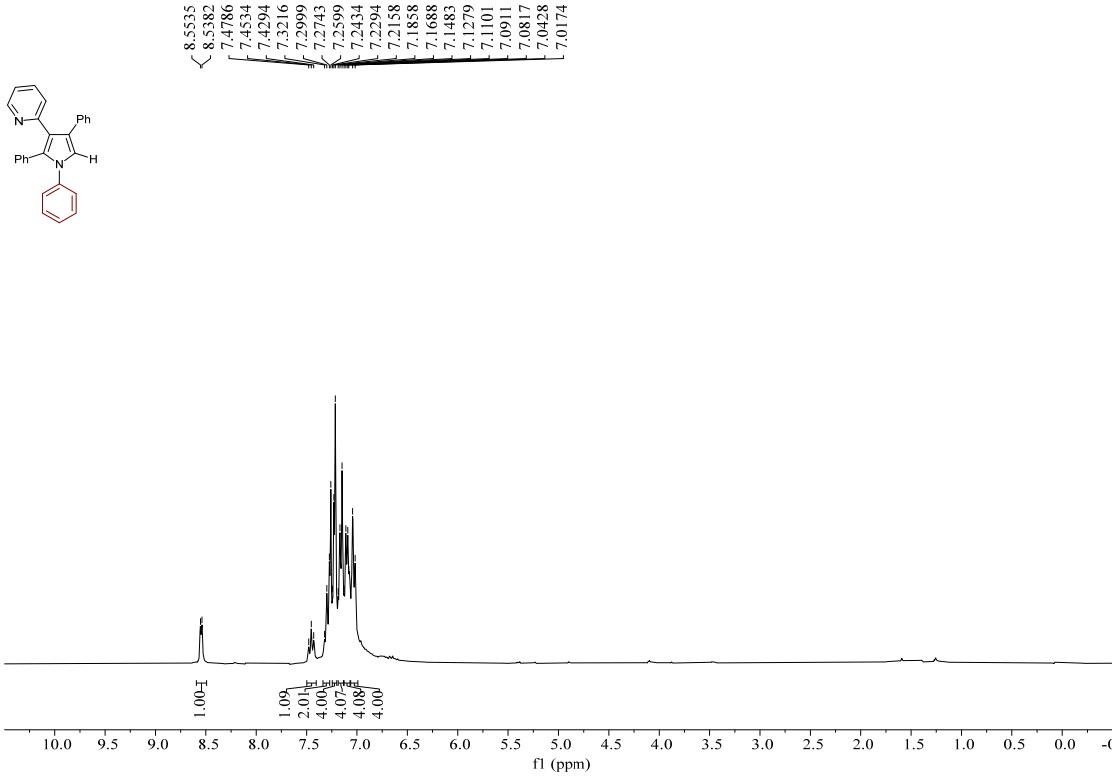
Cl
OMe
f1 (ppm)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7.1483
7.1279
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7.0817
7.0428
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4.00
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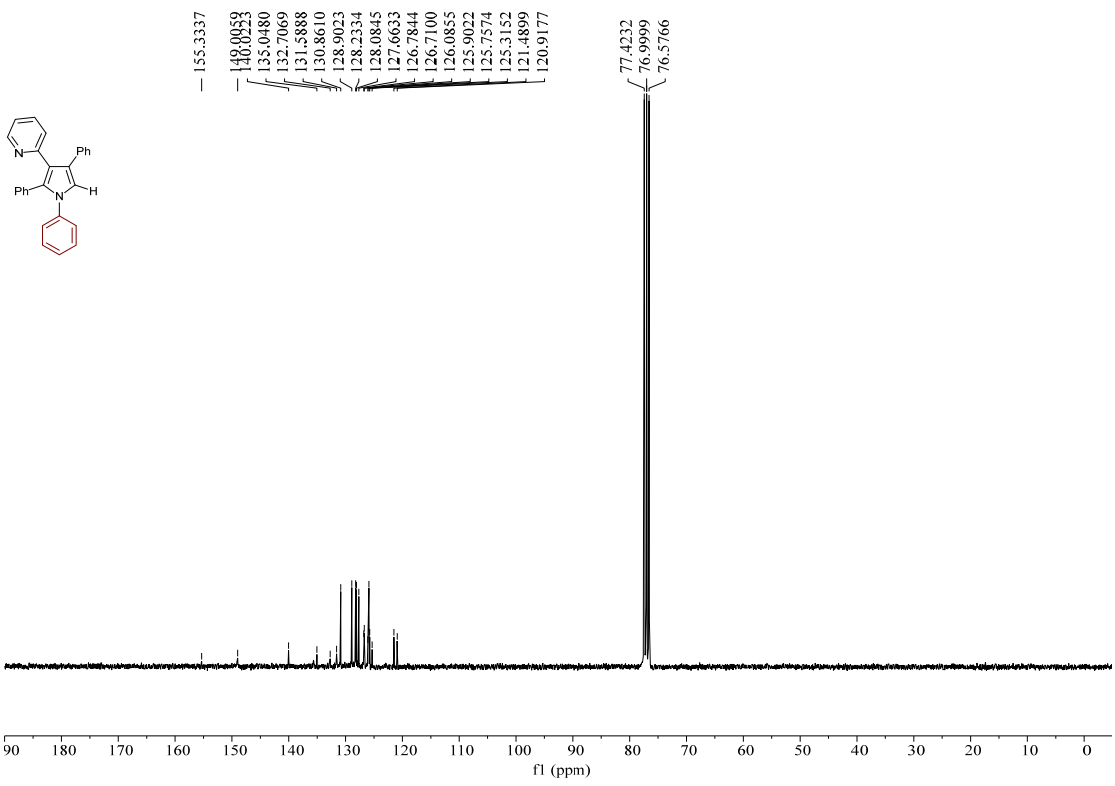
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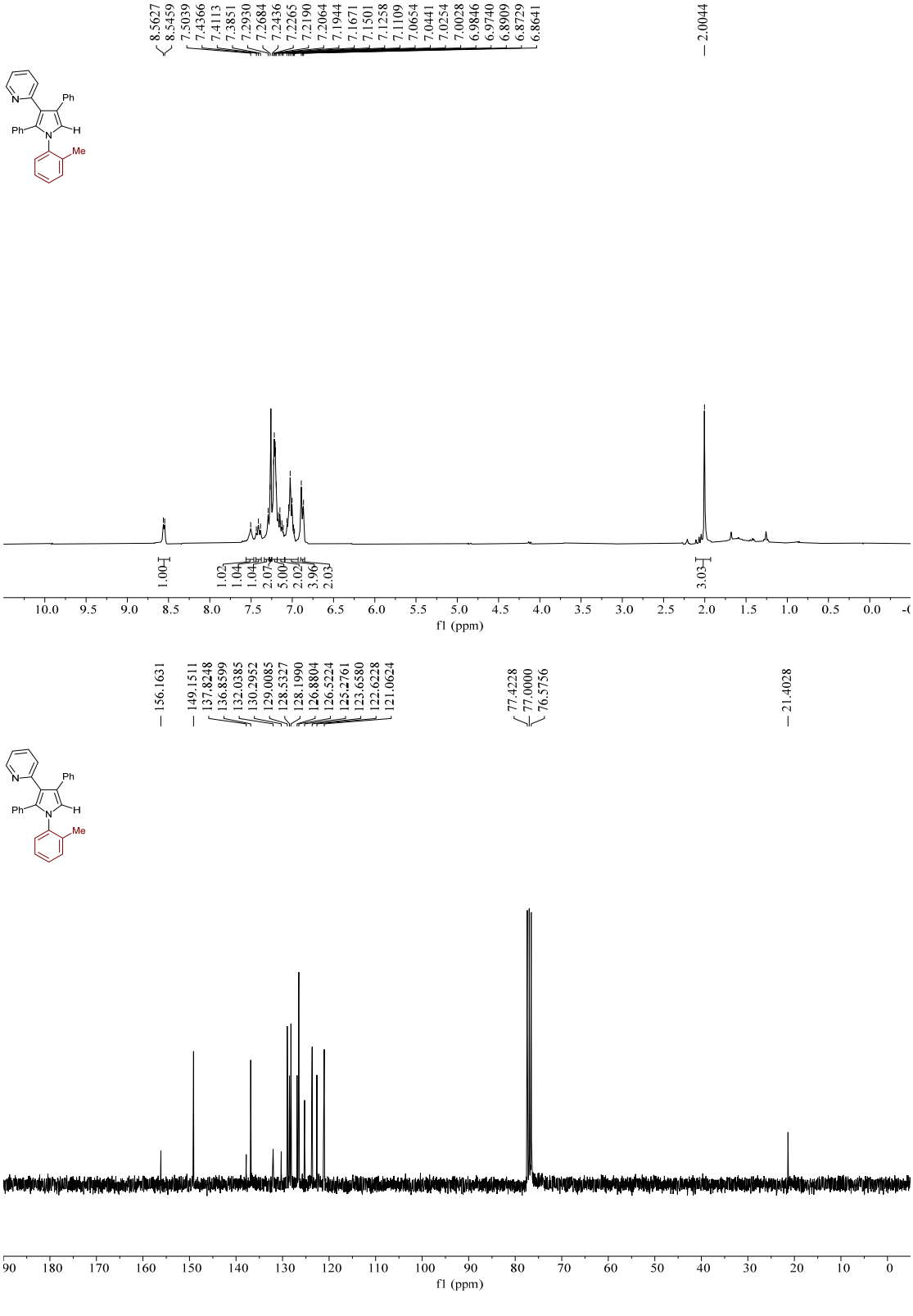
H
f1 (ppm)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Ph
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N
N
Me
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1.02
1.04
1.04
2.07
5.00
2.02
3.96
2.03
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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Me
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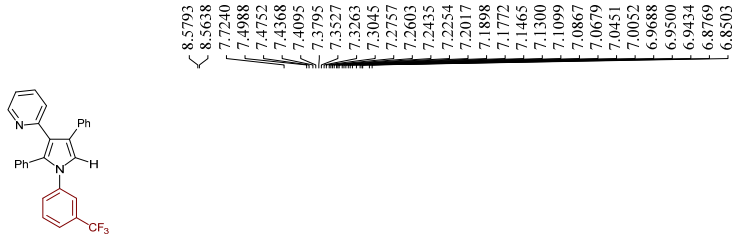
f1 (ppm)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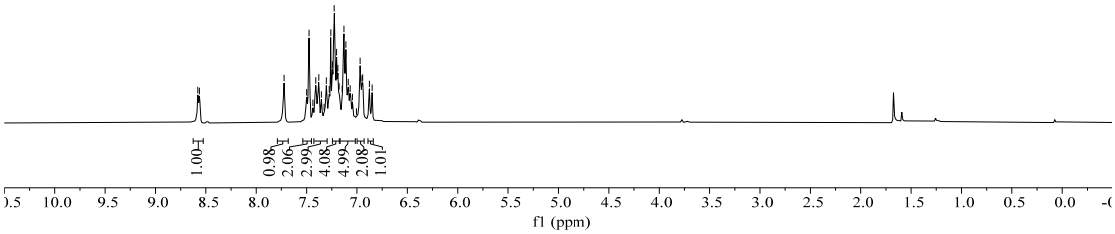
Ph
H
N
CF3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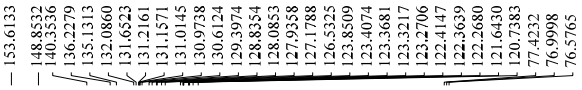
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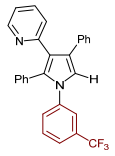
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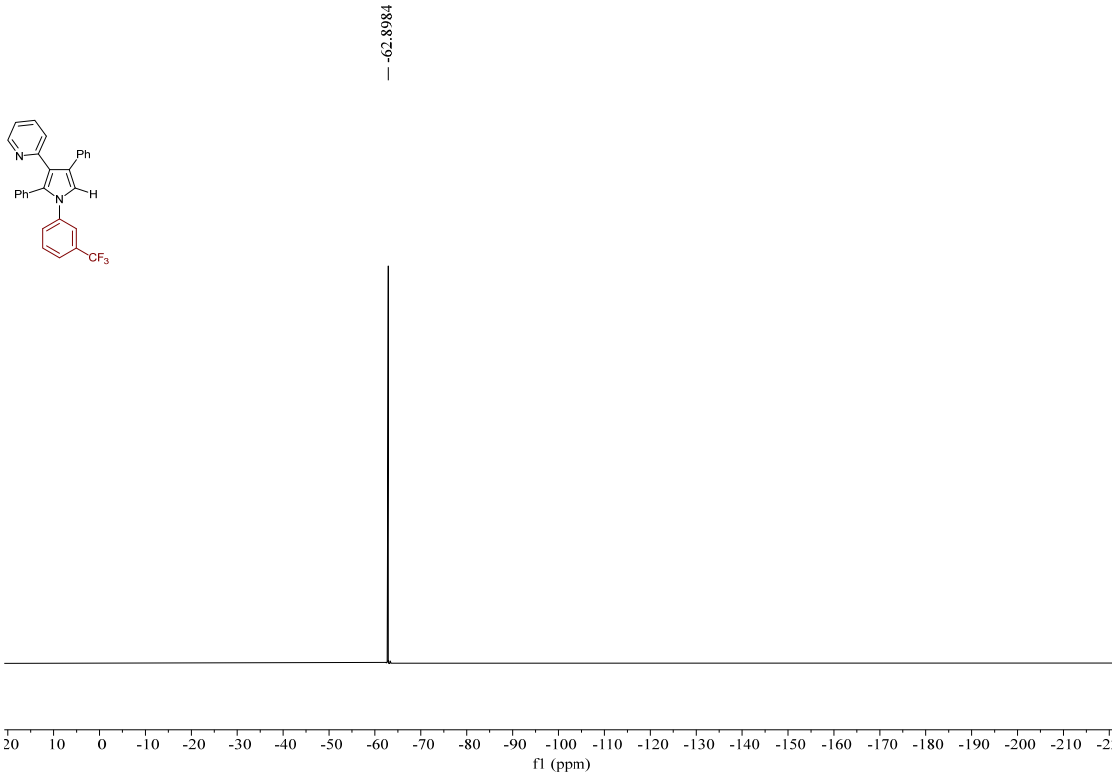
Ph
Ph
H
N
CF3

f1 (ppm)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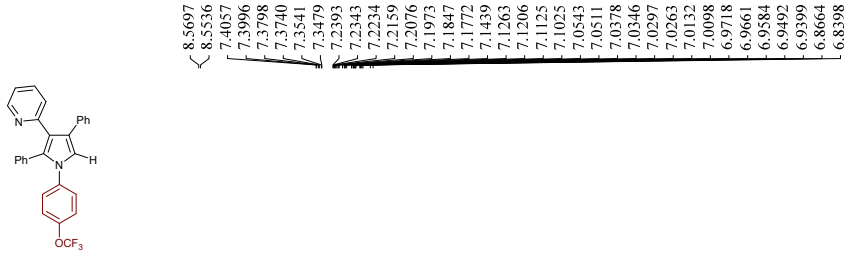
f1 (ppm)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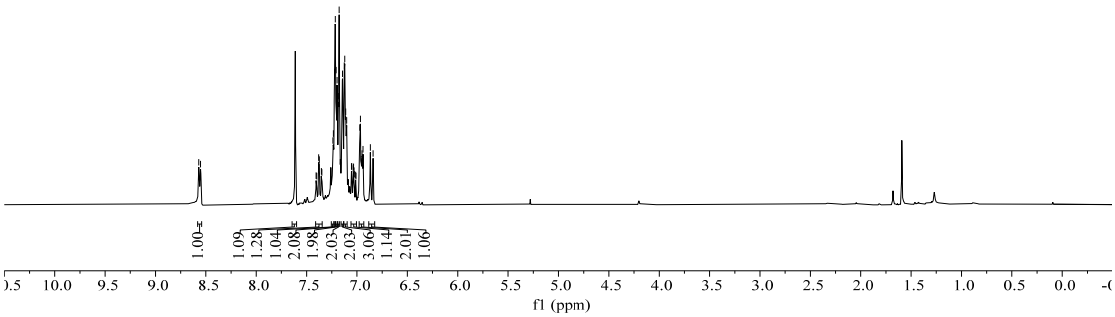
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1.06
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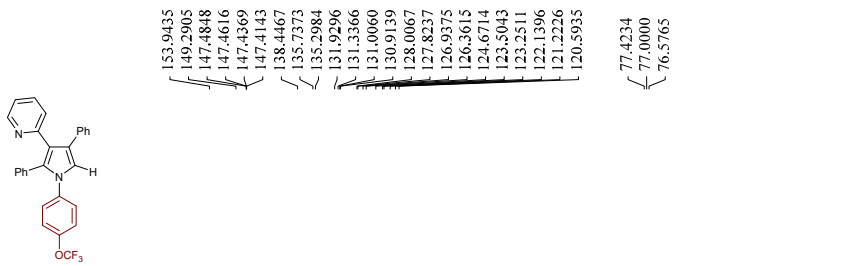
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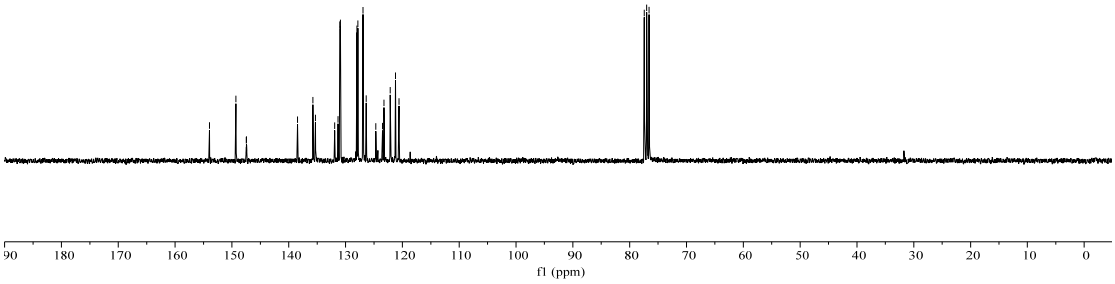
Ph
H
N
OCF3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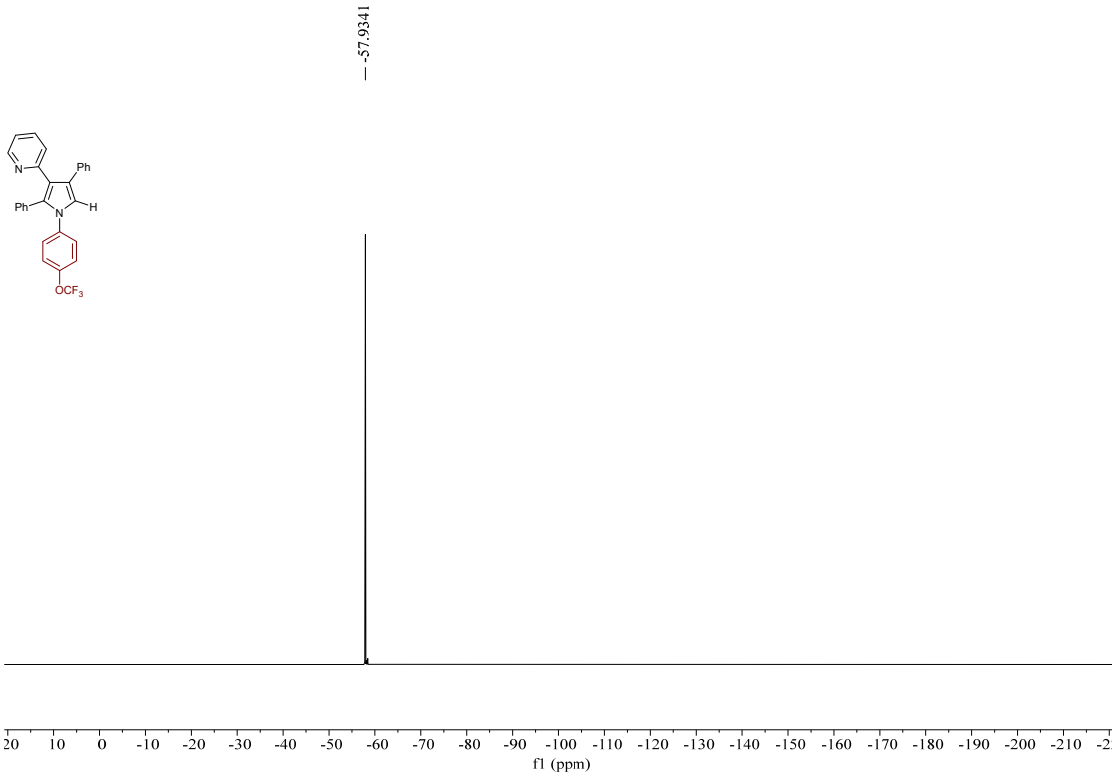
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Ph
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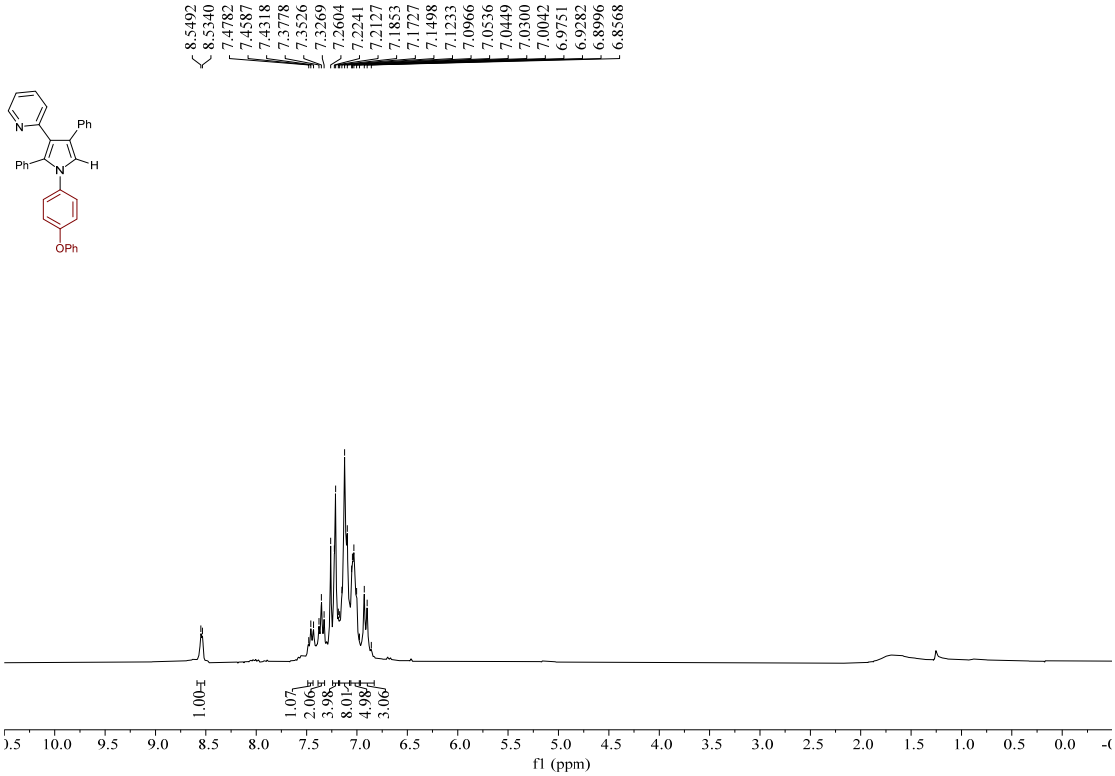
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7.2127
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7.1498
7.1233
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7.0536
7.0449
7.0300
7.0042
6.9751
6.9282
6.8996
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Ph
H
OPh
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1.07
2.06
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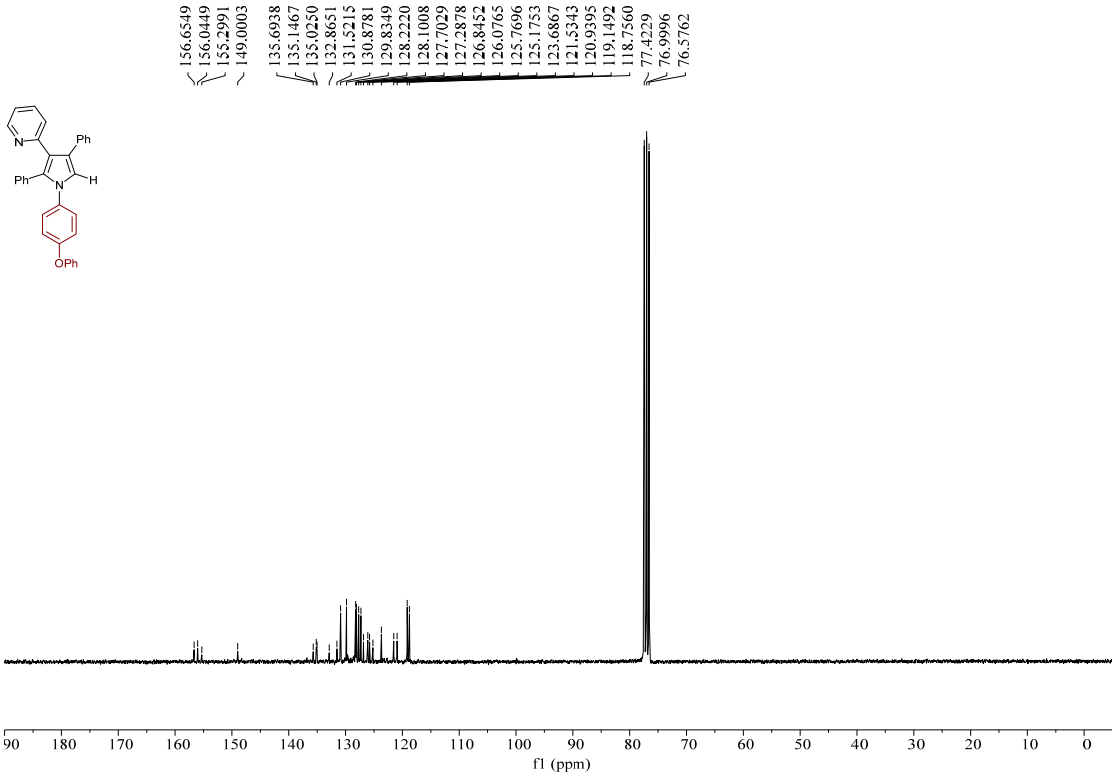
8.01
4.98
3.06
f1 (ppm)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125.1753
123.6867
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118.7560
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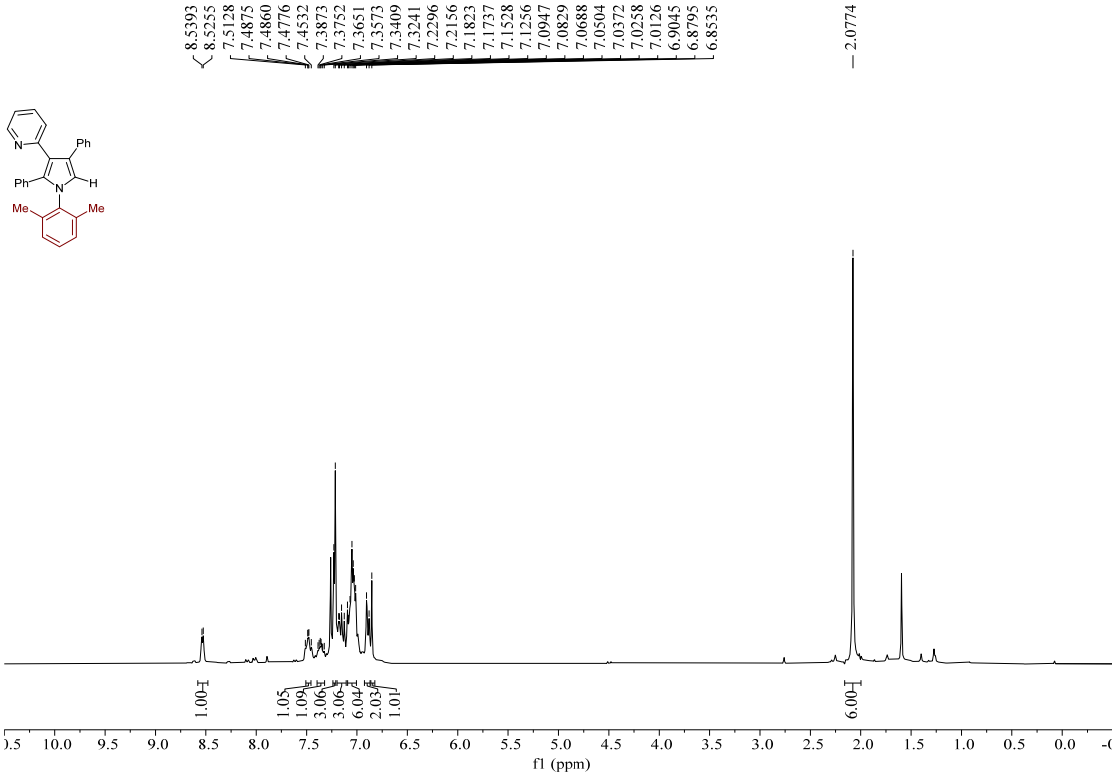
76.9996
76.5762
Ph
Ph
H
OPh
f1 (ppm)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7.2156
7.1823
7.1737
7.1528
7.1256
7.0947
7.0829
7.0688
7.0504
7.0372
7.0258
7.0126
6.9045
6.8795
6.8535
2.0774
Ph
Ph
N
H
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Me
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1.05
1.09
3.06
3.06
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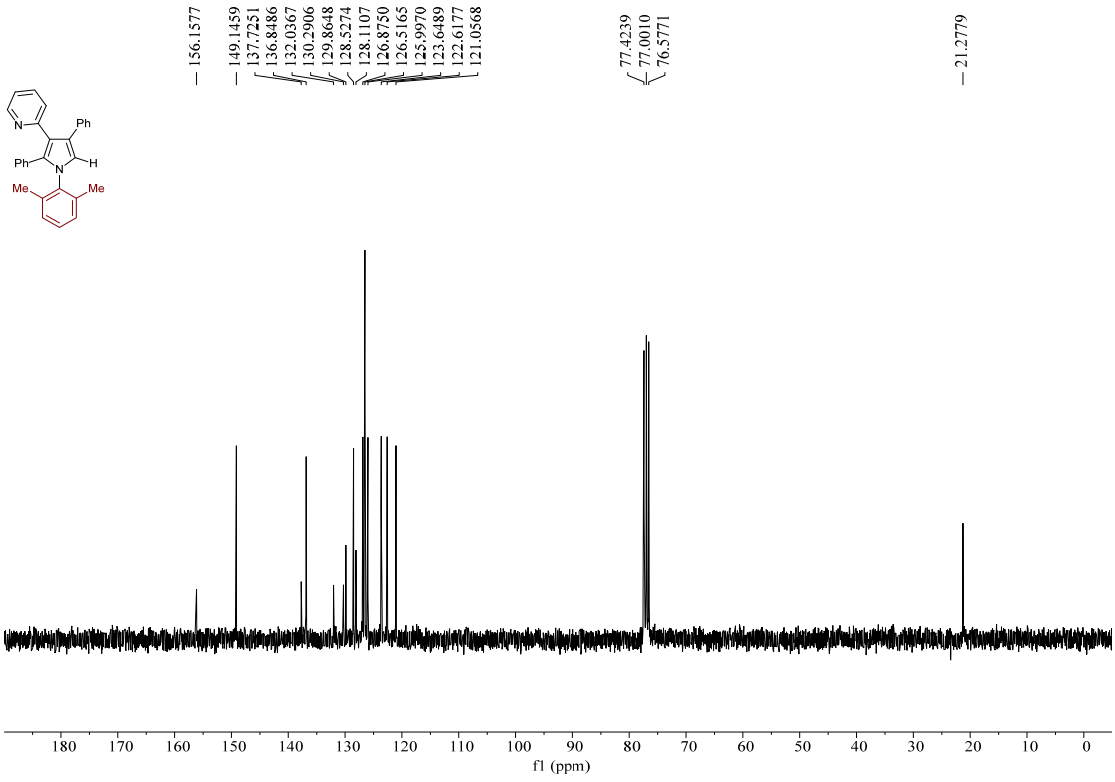
2.03
1.01
6.00
f1 (ppm)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123.6489
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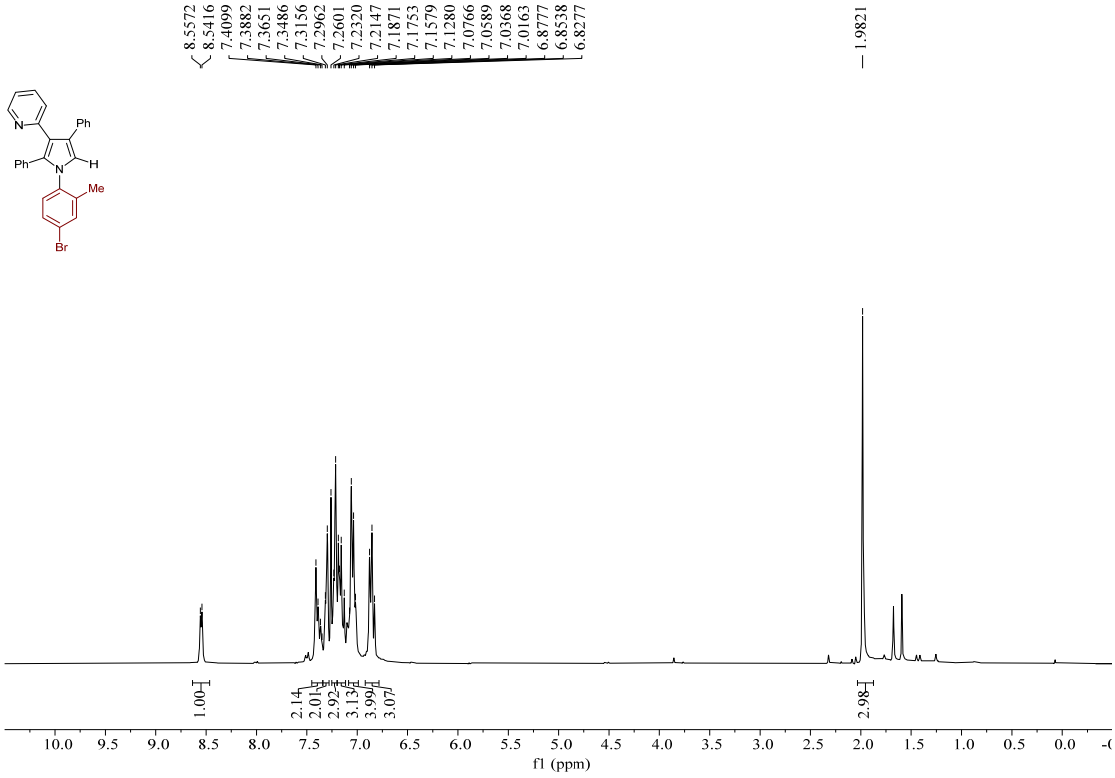
Ph
Ph
N
H
Me
Me
f1 (ppm)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7.1871
7.1753
7.1579
7.1280
7.0766
7.0589
7.0368
7.0163
6.8777
6.8538
6.8277
1.9821
Ph
Ph
H
Me
Br
1.00
2.14
2.01
2.92
3.13
3.99
3.07
2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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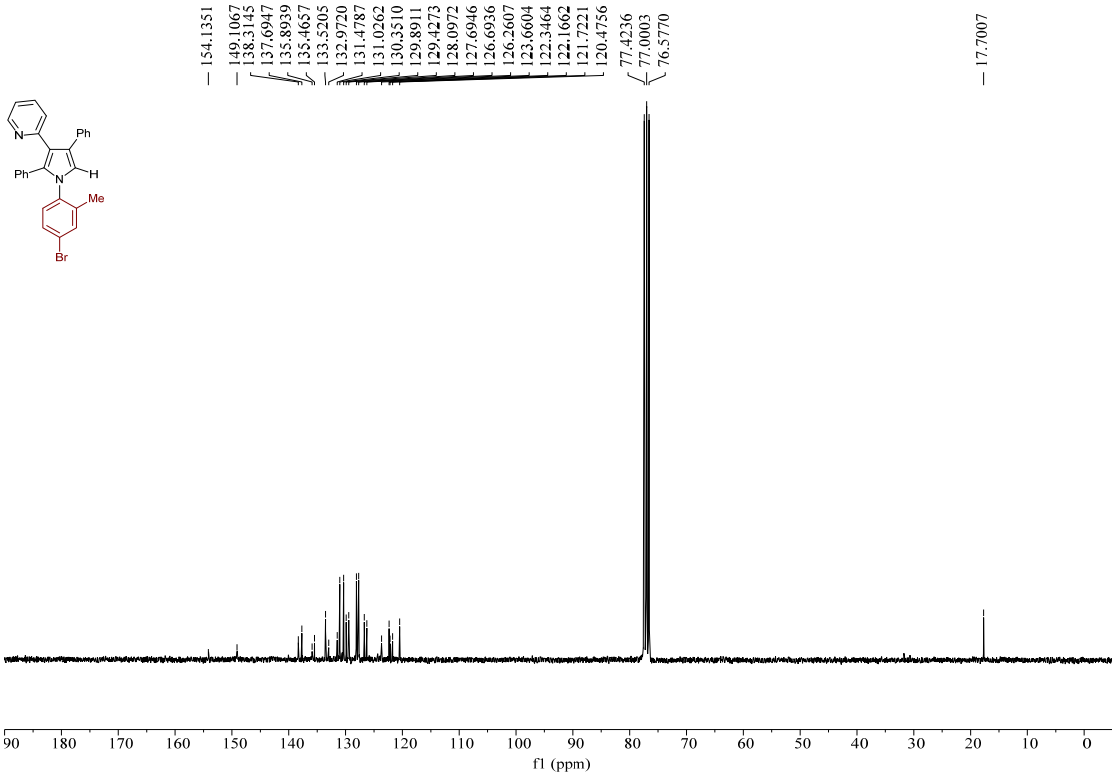
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135.8939
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133.5205
132.9720
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129.8911
129.4273
128.0972
127.6946
126.6936
126.2607
123.6604
122.3464
122.1662
121.7221
120.4756
77.4236
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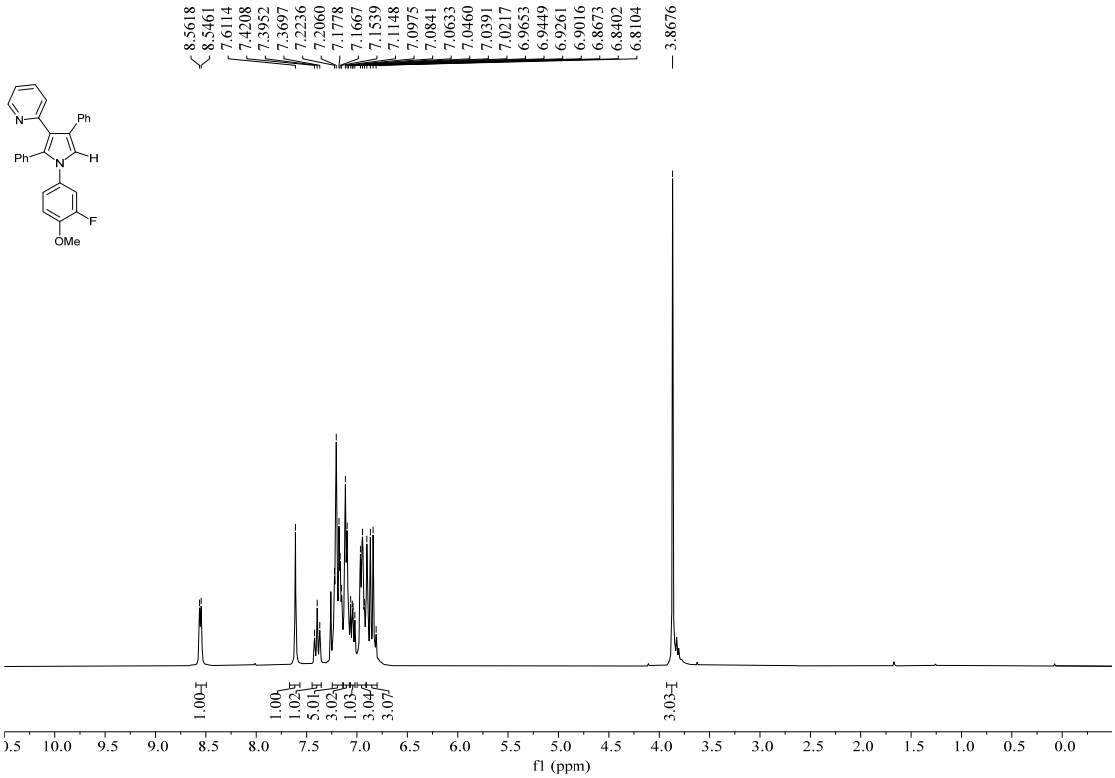
17.7007
Ph
Ph
H
Me
Br
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.3697
7.2236
7.2060
7.1778
7.1667
7.1539
7.1148
7.0975
7.0841
7.0633
7.0460
7.0391
7.0217
6.9653
6.9449
6.9261
6.9016
6.8673
6.8402
6.8104
3.8676
Ph
Ph
H
N
F
OMe
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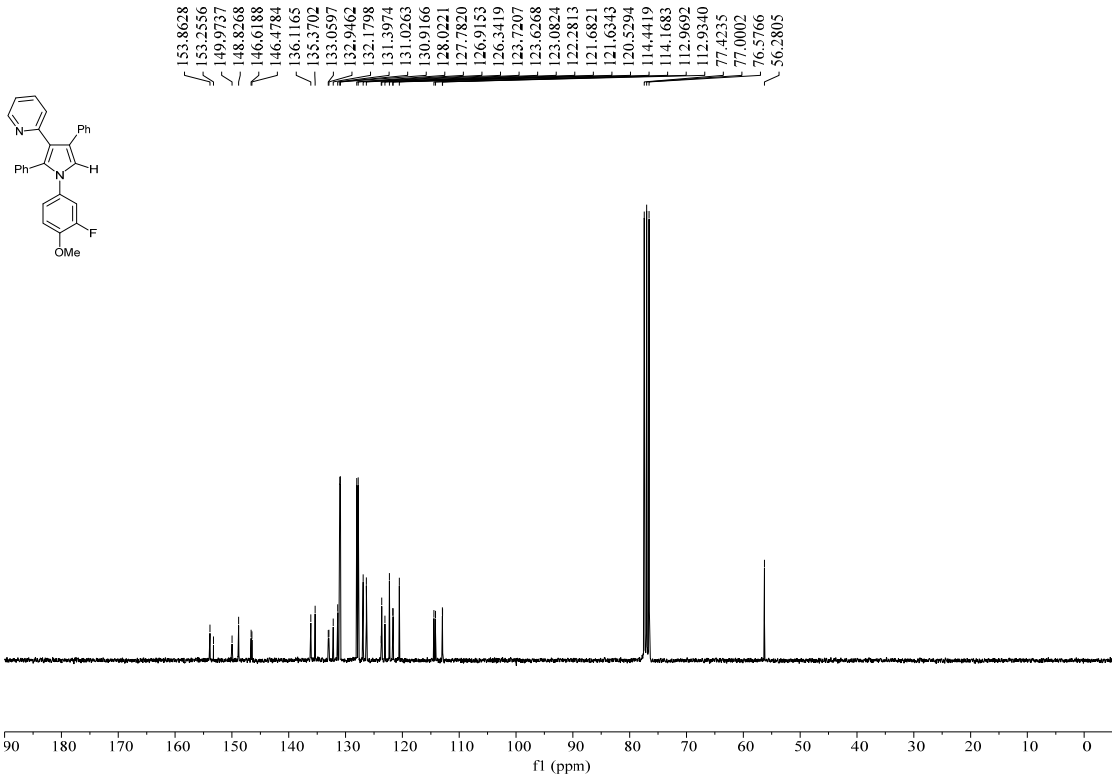
1.00
1.02
5.01
3.02
1.03
3.04
3.07
3.03
f1 (ppm)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131.3974
131.0263
130.9166
128.0221
127.7820
126.9153
126.3419
123.7207
123.6268
123.0824
122.2813
121.6821
121.6343
120.5294
114.4419
114.1683
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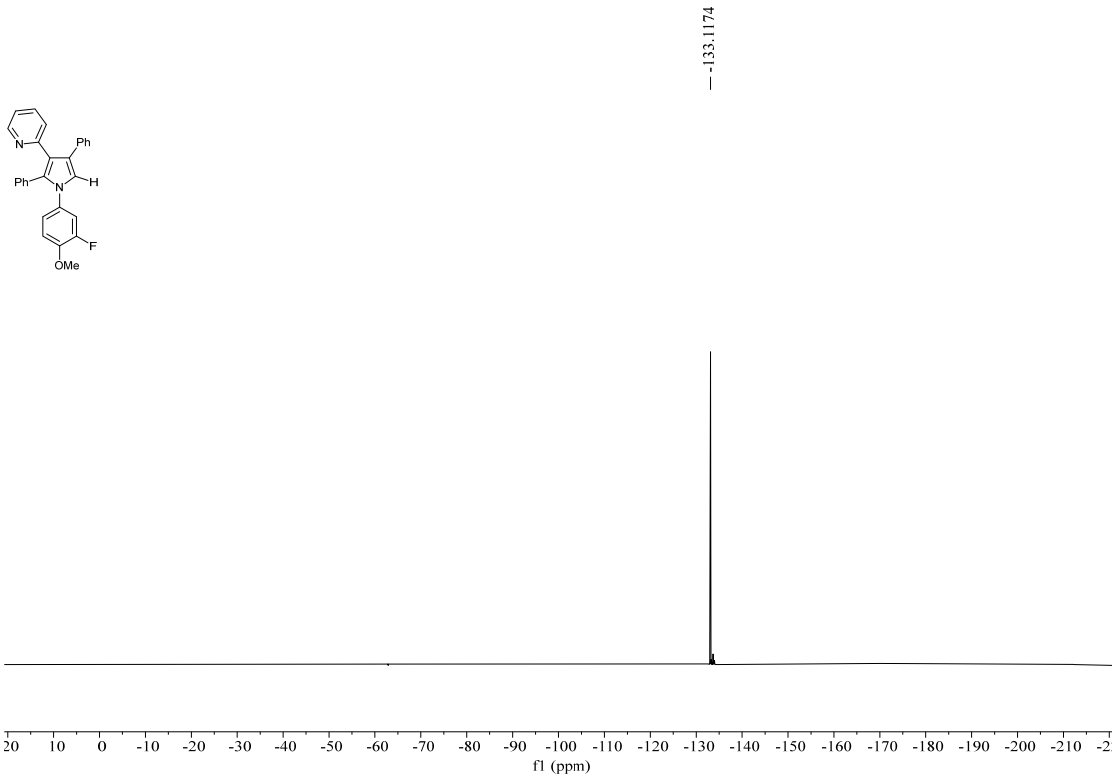
112.9340
77.4235
77.0002
76.5766
56.2805
Ph
Ph
H
N
F
OMe
f1 (ppm)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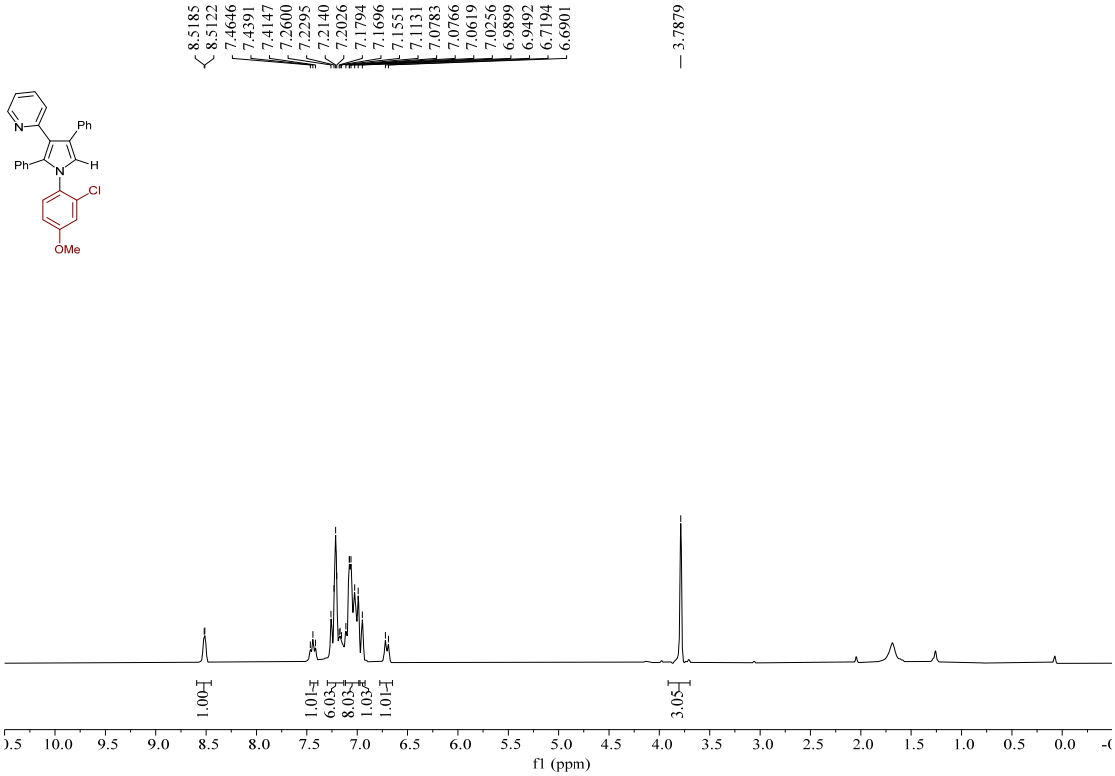
Ph
Ph
N
H
F
OMe
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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7.2295
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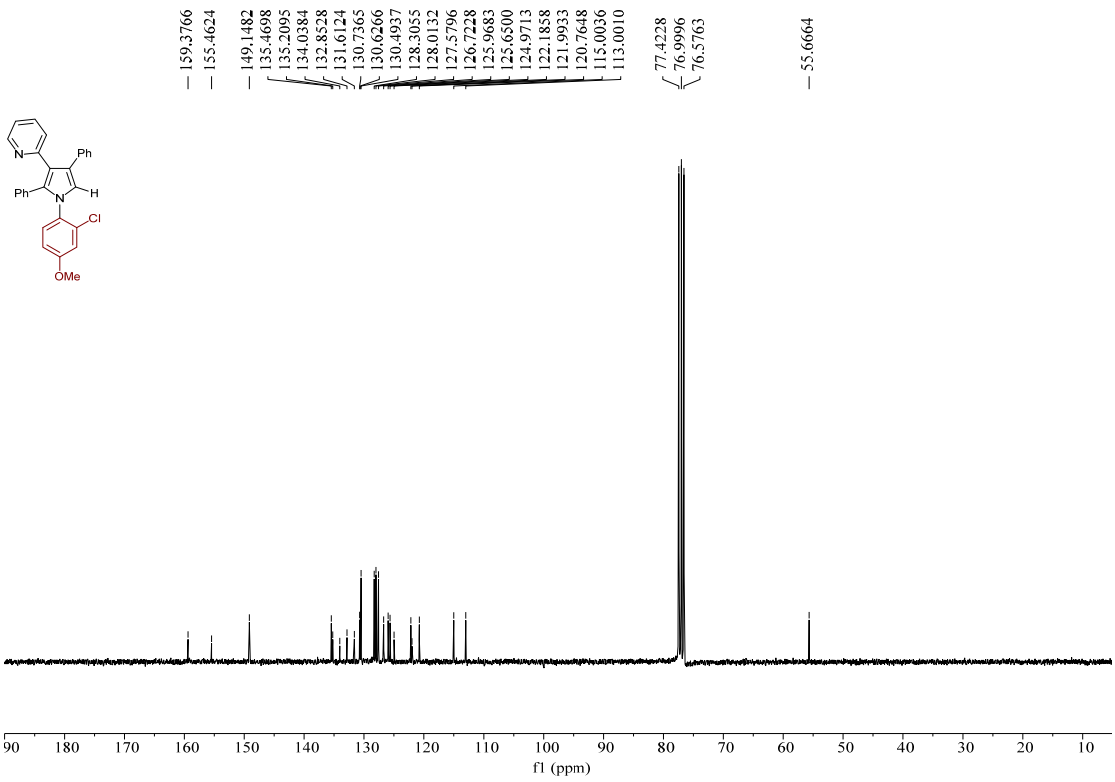
7.1696
7.1551
7.1131
7.0783
7.0766
7.0619
7.0256
6.9899
6.9492
6.7194
6.6901
3.7879
Ph
Ph
H
Cl
OMe
1.00
1.01
6.03
8.03
1.03
1.01
3.05
f1 (ppm)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130.4937
128.3055
128.0132
127.5796
126.7228
125.9683
125.6500
124.9713
122.1858
121.9933
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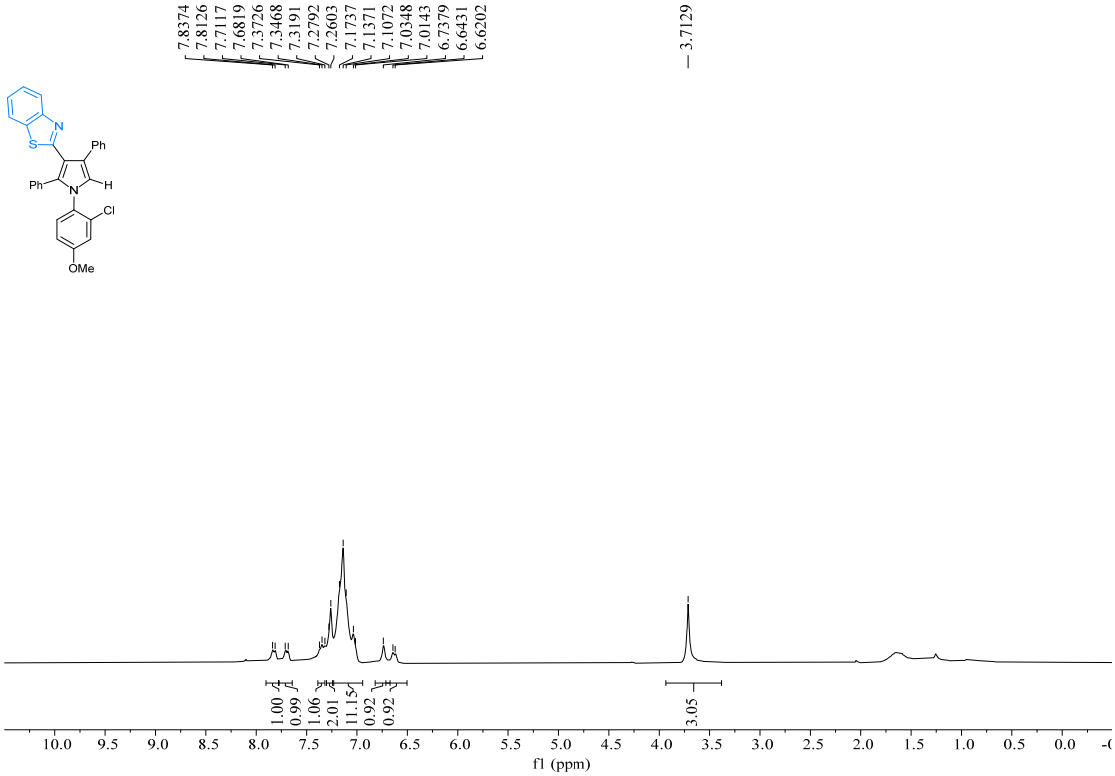
Ph
Ph
H
Cl
OMe
f1 (ppm)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7.3191
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7.2603
7.1737
7.1371
7.1072
7.0348
7.0143
6.7379
6.6431
6.6202
3.7129
Ph
Ph
H
Cl
OMe
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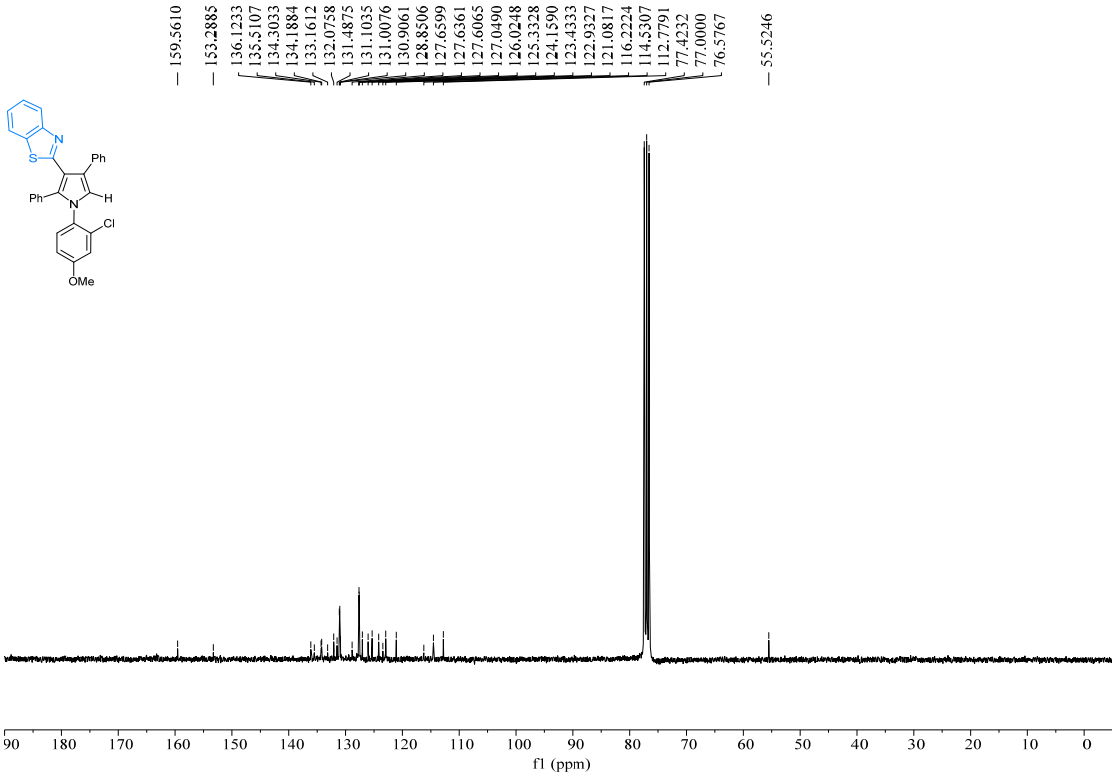
0.99
1.06
2.01
11.15
0.92
0.92
3.05
f1 (ppm)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127.6361
127.6065
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126.0248
125.3328
124.1590
123.4333
122.9327
121.0817
116.2224
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77.0000
76.5767
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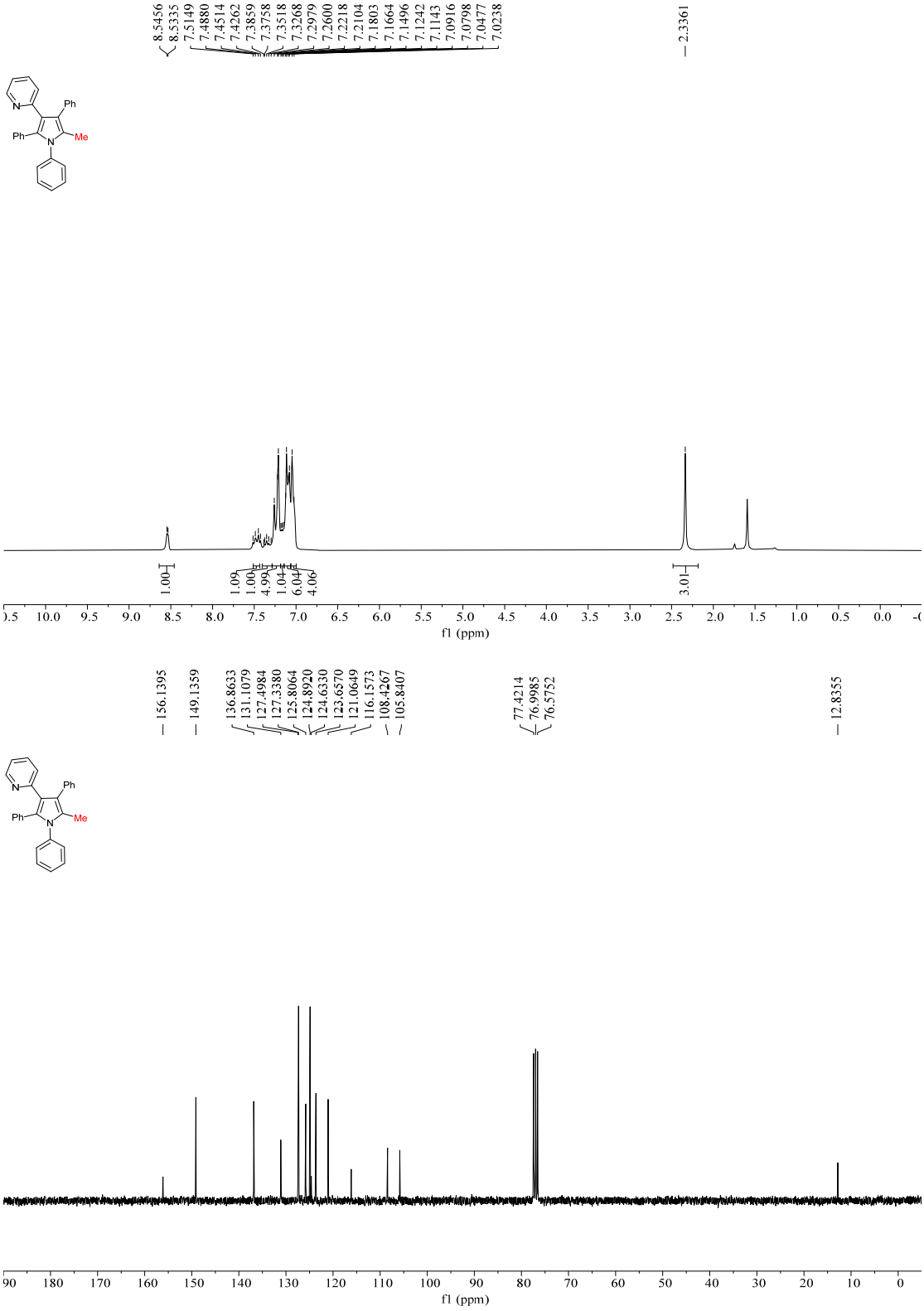
Ph
Ph
H
Cl
OMe
f1 (ppm)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7.2600
7.2218
7.2104
7.1803
7.1664
7.1496
7.1242
7.1143
7.0916
7.0798
7.0477
7.0238
2.3361
Ph
Ph
Me
N
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1.09
1.00
4.99
1.04
6.04
4.06
3.01
f1 (ppm)
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127.3380
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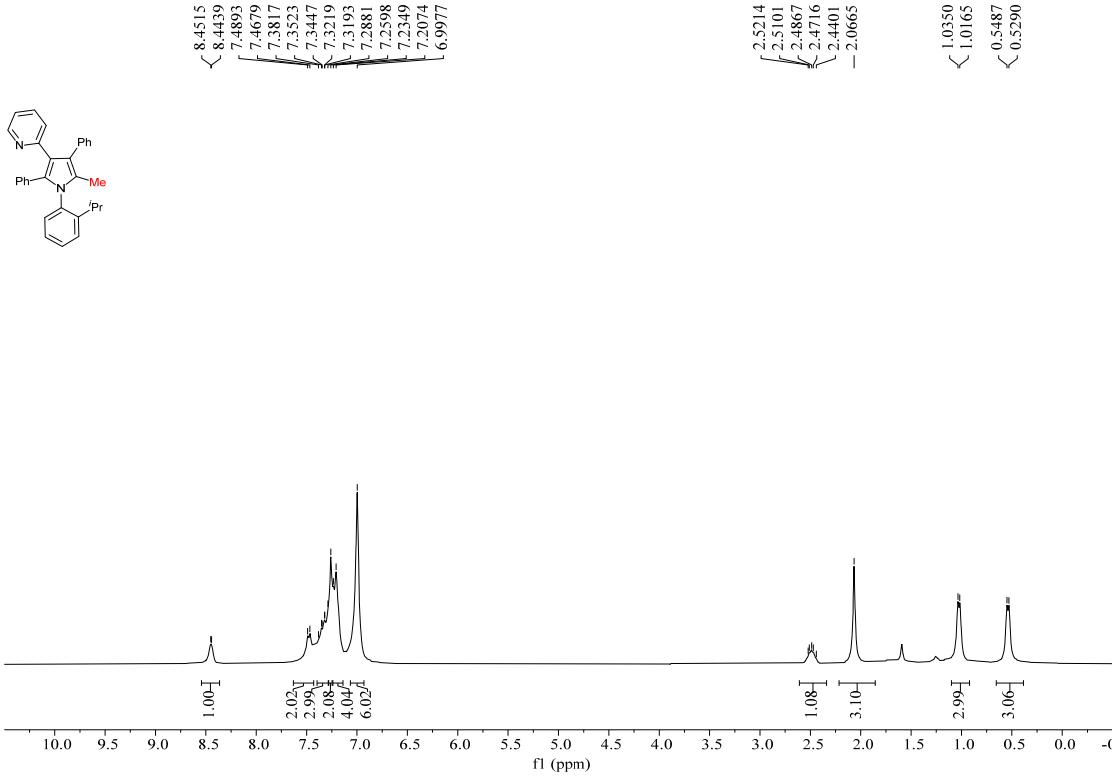
f1 (ppm)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7.2881
7.2598
7.2349
7.2074
6.9977
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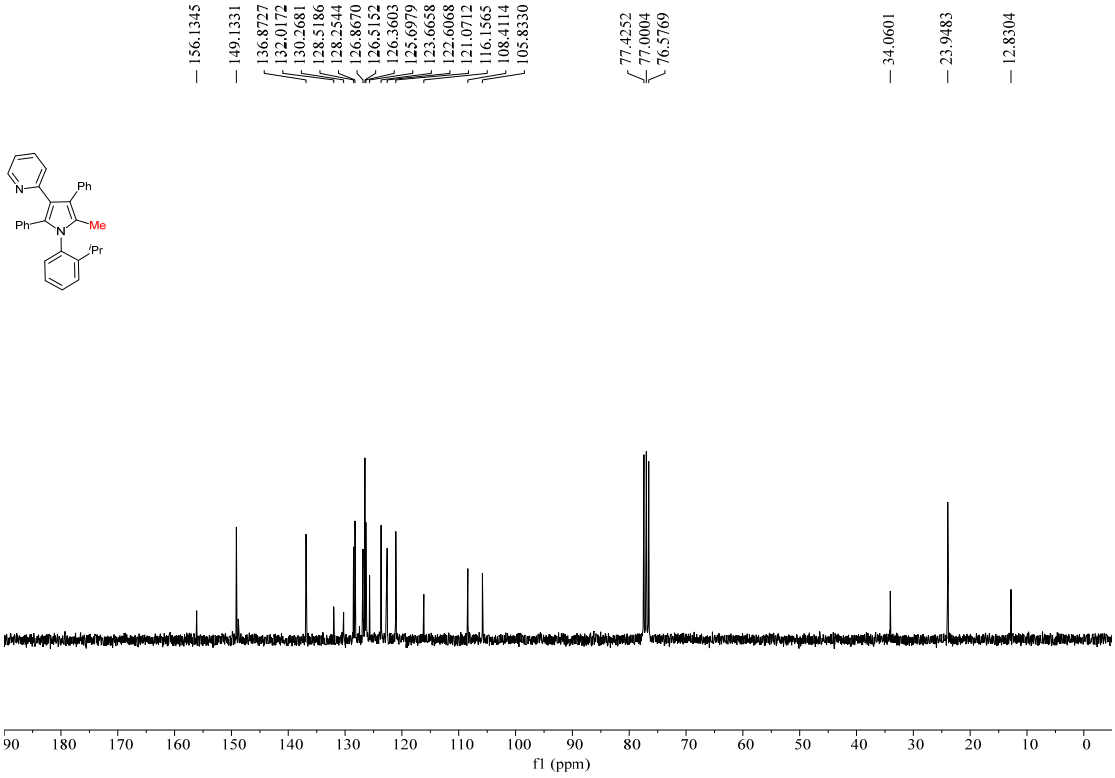
2.5101
2.4867
2.4716
2.4401
2.0665
1.0350
1.0165
0.5487
0.5290
Ph
Ph
N
Me
iPr
1.00
2.02
2.99
2.08
4.04
6.02
1.08
3.10
2.99
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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116.1565
108.4114
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77.0004
76.5769
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Ph
N
Me
iPr
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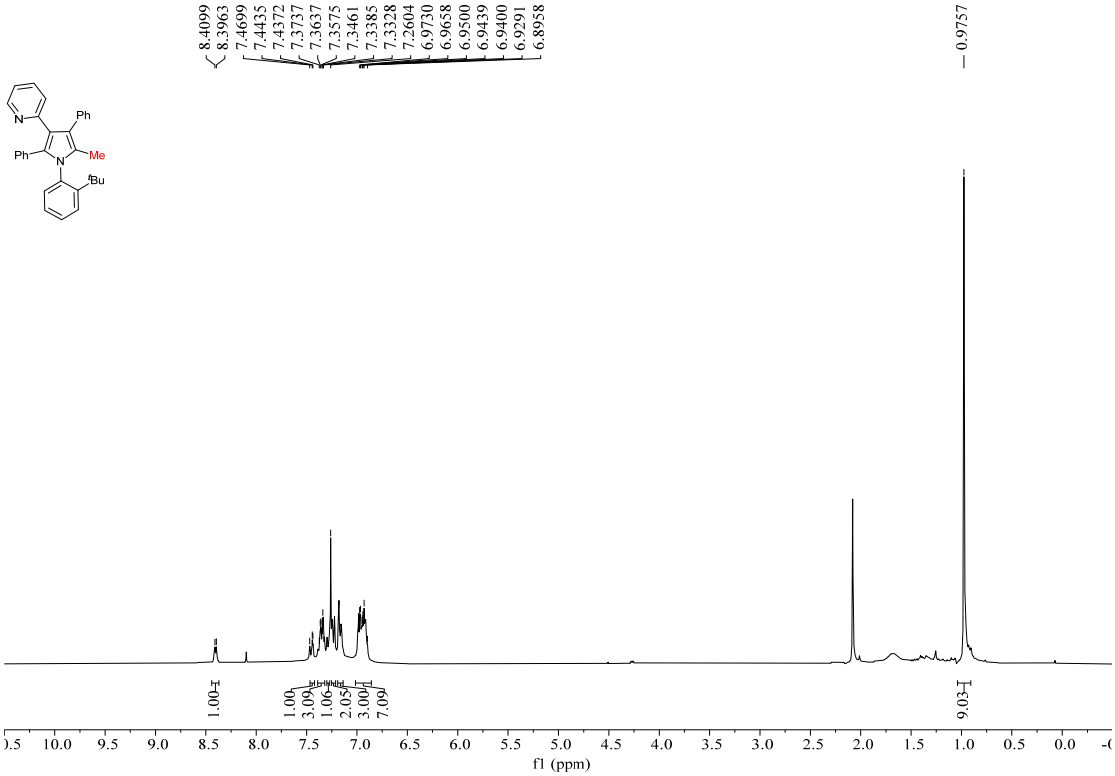
f1 (ppm)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7.2604
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6.9658
6.9500
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6.8958
0.9757
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N
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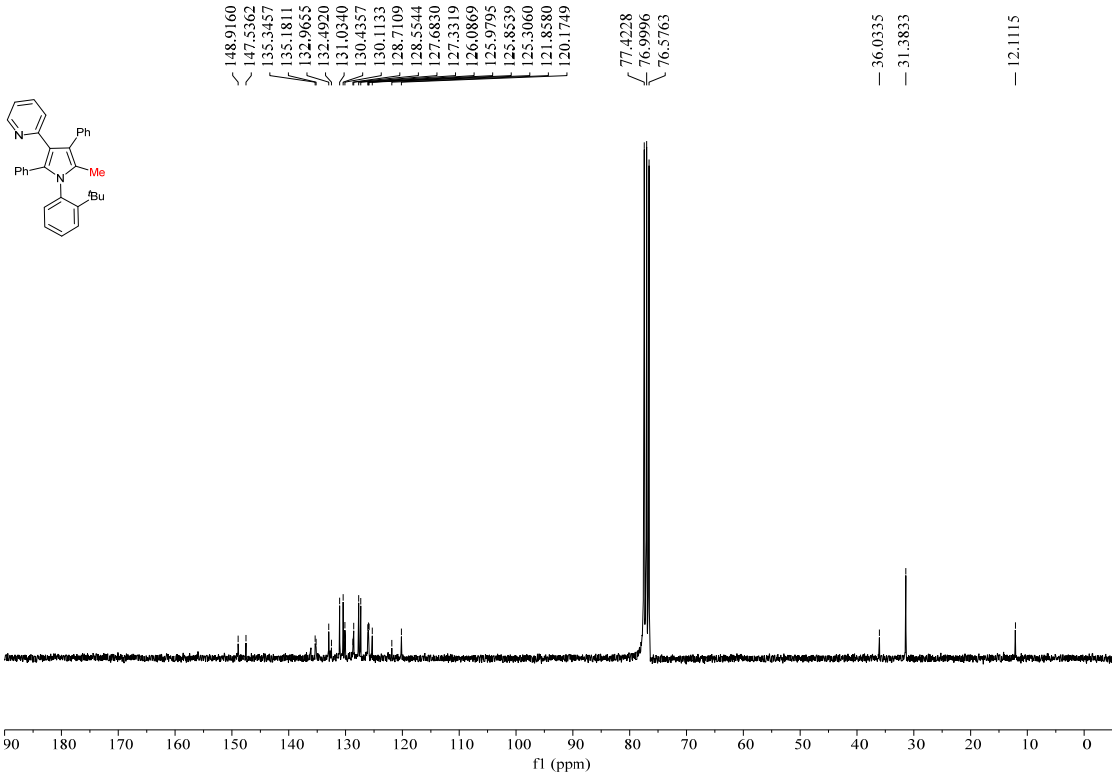
1.00
3.09
1.06
2.05
3.00
7.09
9.03
f1 (ppm)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126.0869
125.9795
125.8539
125.3060
121.8580
120.1749
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Ph
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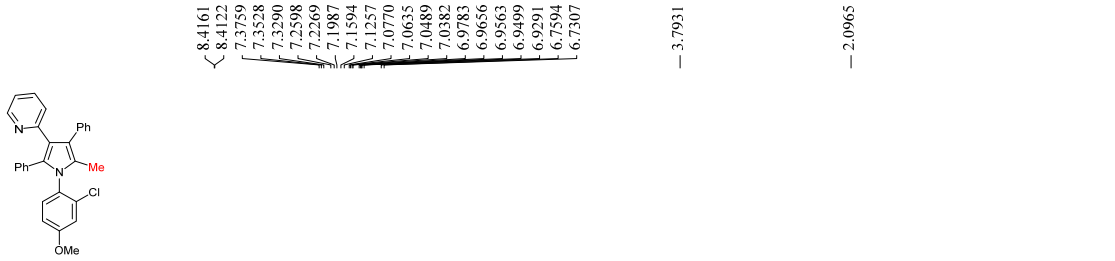
tBu
N
f1 (ppm)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7.0489
7.0382
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6.9563
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3.7931
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Ph
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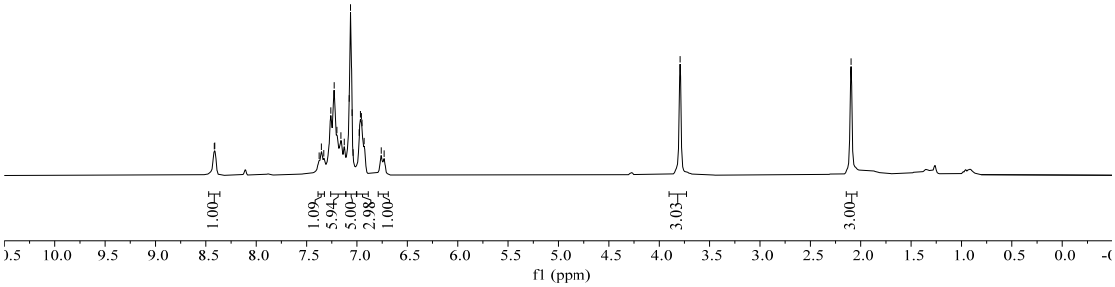
Ph
Me
N
Cl
OMe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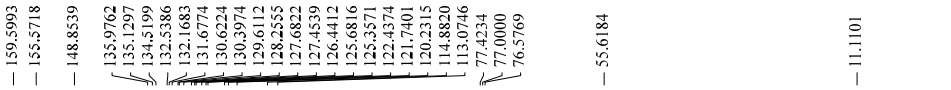
3.00
f1 (ppm)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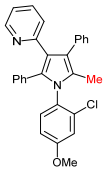
Ph
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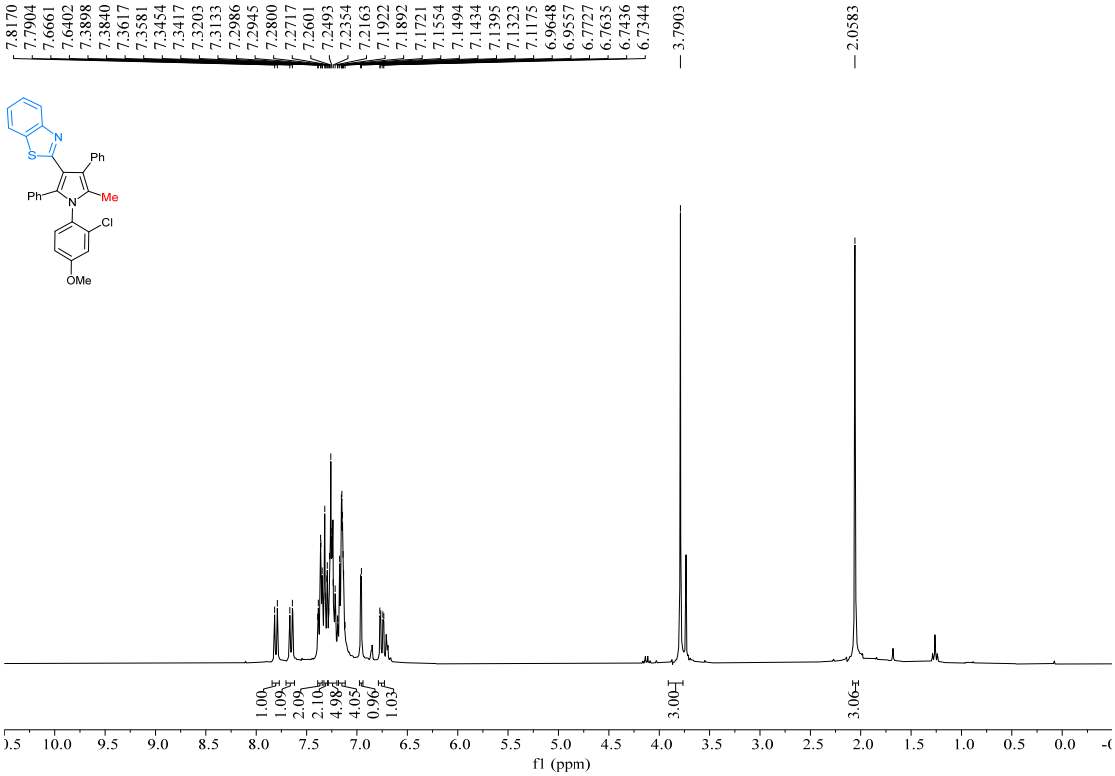
Ph
Me
N
Cl
OMe

f1 (ppm)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6.7344
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Ph
N
Me
Cl
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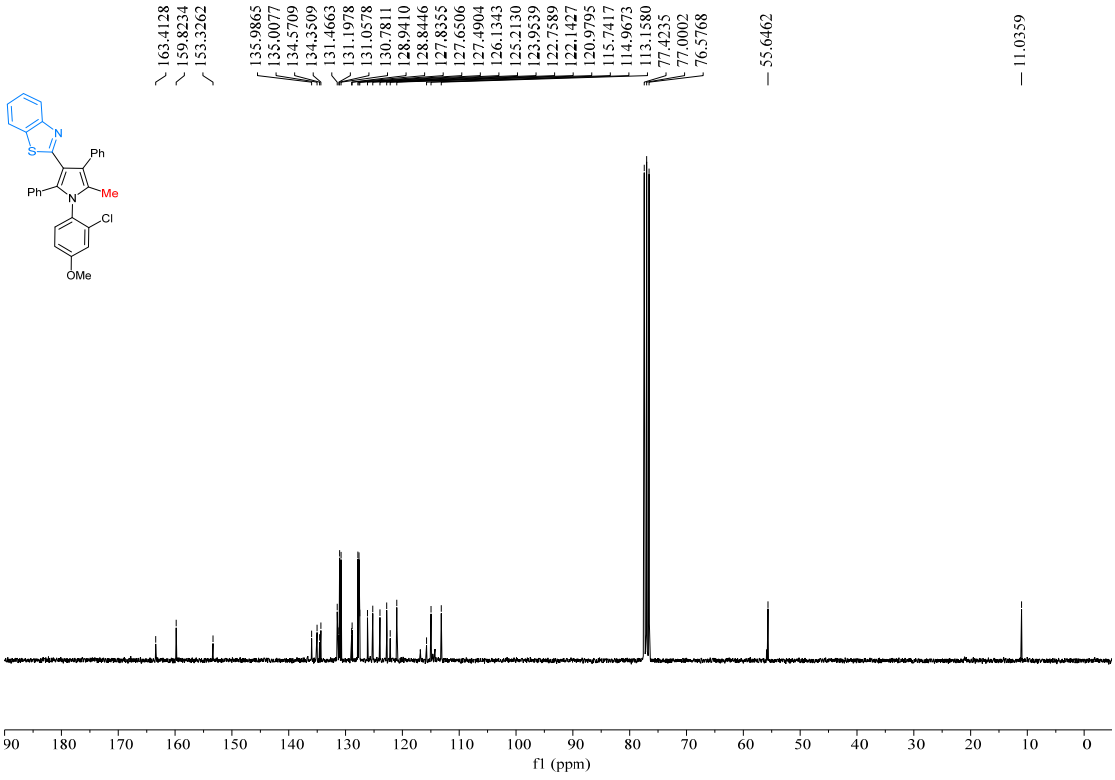
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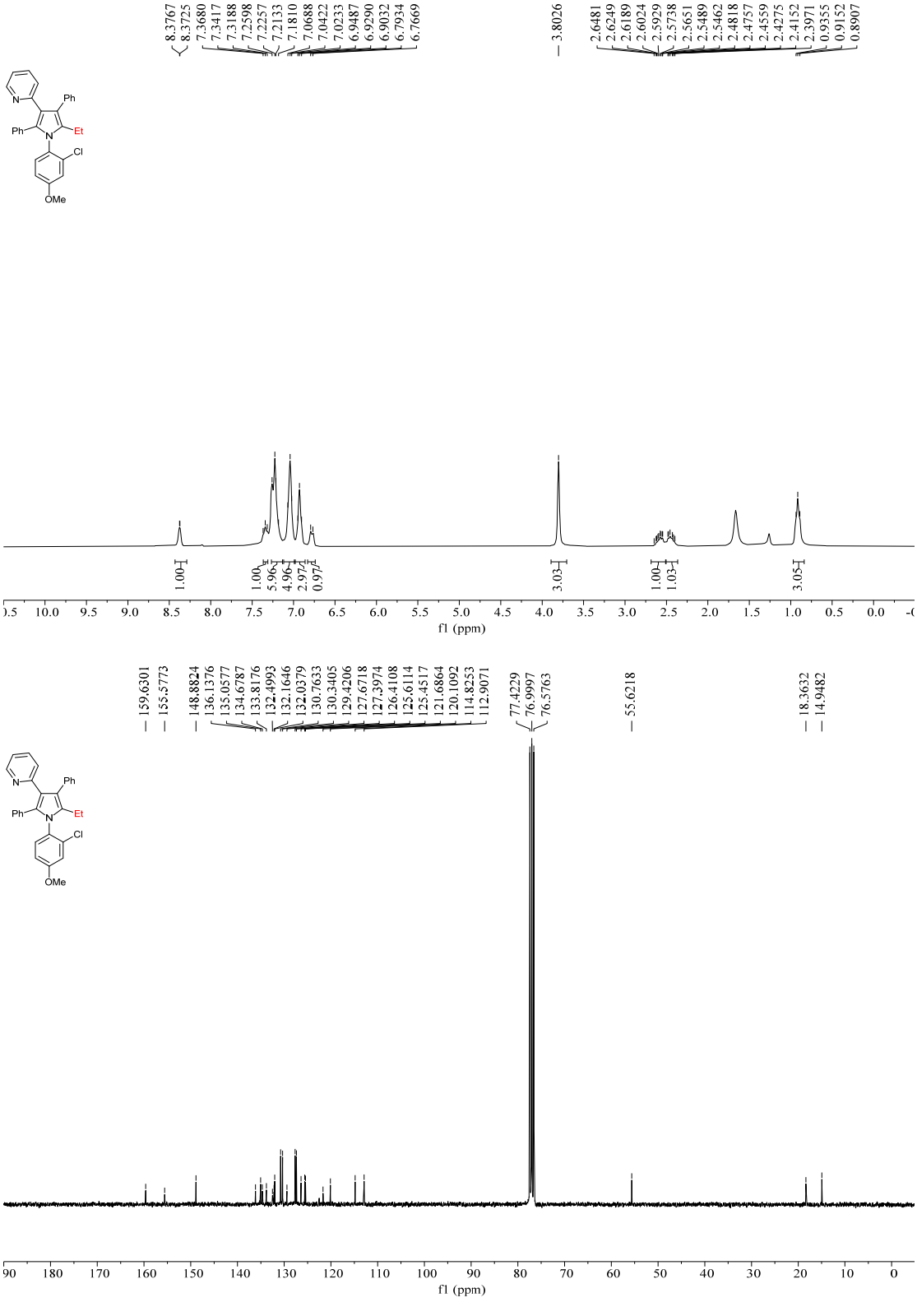
114.9673
113.1580
77.4235
77.0002
76.5768
55.6462
11.0359
Ph
Ph
N
Me
Cl
OMe
f1 (ppm)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7.3188
7.2598
7.2257
7.2133
7.1810
7.0688
7.0422
7.0233
6.9487
6.9290
6.9032
6.7934
6.7669
3.8026
2.6481
2.6249
2.6189
2.6024
2.5929
2.5738
2.5651
2.5489
2.5462
2.4818
2.4757
2.4559
2.4275
2.4152
2.3971
0.9355
0.9152
0.8907
Ph
Ph
Et
N
N
Cl
OMe
1.00
1.00
5.96
4.96
2.97
0.97
3.03
1.00
1.03
3.05
f1 (ppm)
159.6301
155.5773
148.8824
136.1376
135.0577
134.6787
133.8176
132.4993
132.1646
132.0379
130.7633
130.3405
129.4206
127.6718
127.3974
126.4108
125.6114
125.4517
121.6864
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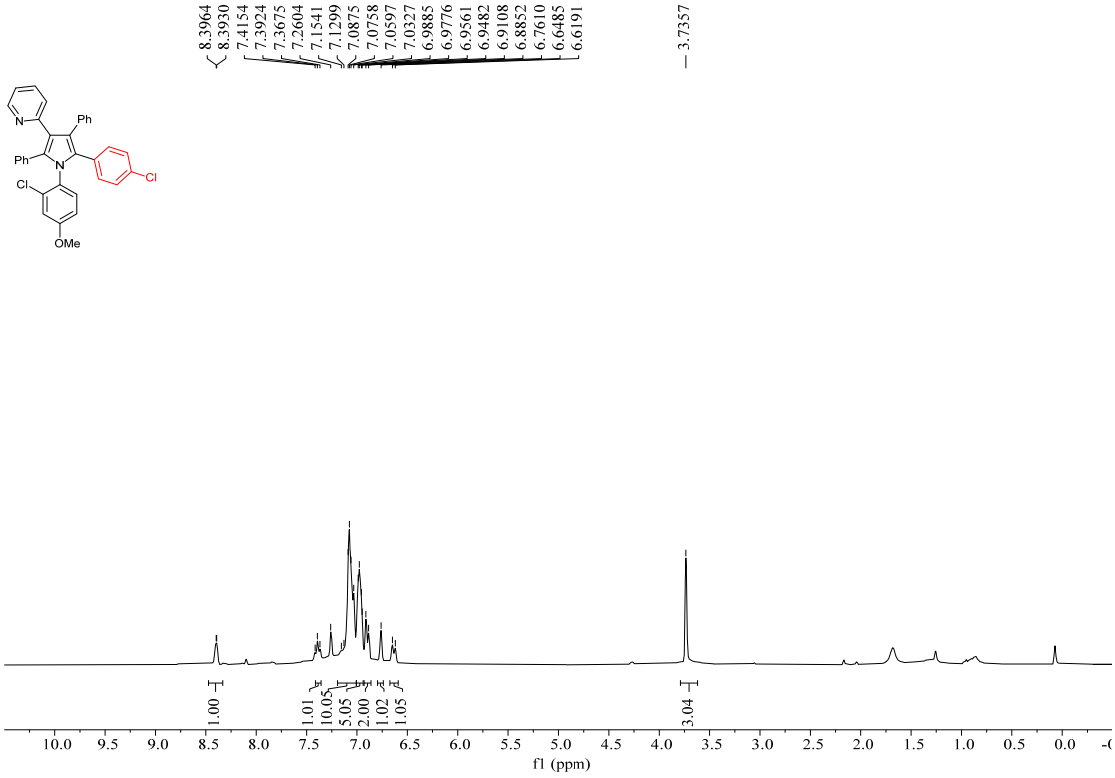
112.9071
77.4229
76.9997
76.5763
55.6218
18.3632
14.9482
f1 (ppm)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8.3930
7.4154
7.3924
7.3675
7.2604
7.1541
7.1299
7.0875
7.0758
7.0597
7.0327
6.9885
6.9776
6.9561
6.9482
6.9108
6.8852
6.7610
6.6485
6.6191
3.7357
Ph
Ph
N
Cl
Cl
OMe
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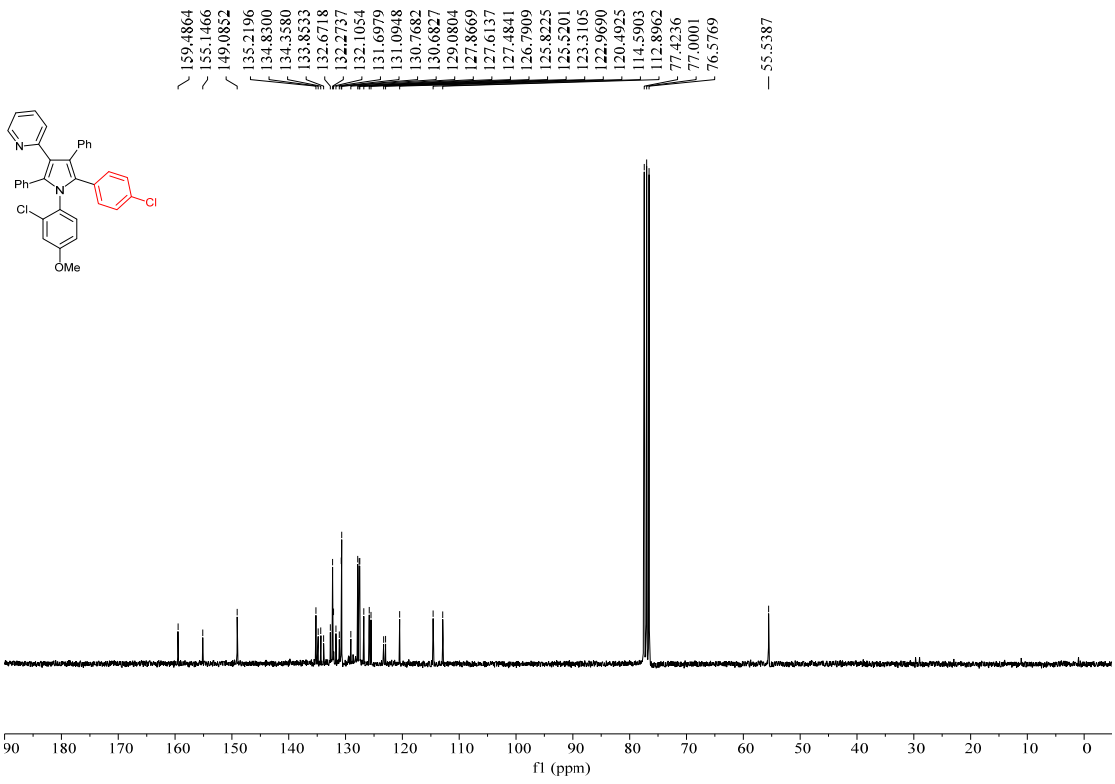
1.01
10.05
5.05
2.00
1.02
1.05
3.04
f1 (ppm)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131.6979
131.0948
130.7682
130.6827
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127.8669
127.6137
127.4841
126.7909
125.8225
125.5201
123.3105
122.9690
120.4925
114.5903
112.8962
77.4236
77.0001
76.5769
55.5387
Ph
Ph
N
Cl
Cl
OMe
f1 (ppm)