Supporting Information

Radical-based functionalization-oriented construction: rapid assembly of 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 °C using rotary evaporator with aspirator. The condenser was cooled with running water at 0 °C.

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.

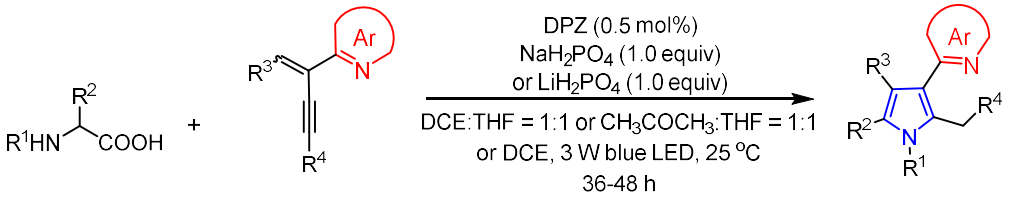
2. General procedures

2.1 Preparation of staring materials

2-(2-Enynyl)pyridines and other corresponding 1,3-enyne derivatives were prepared based on the reported procedures.[1-5]

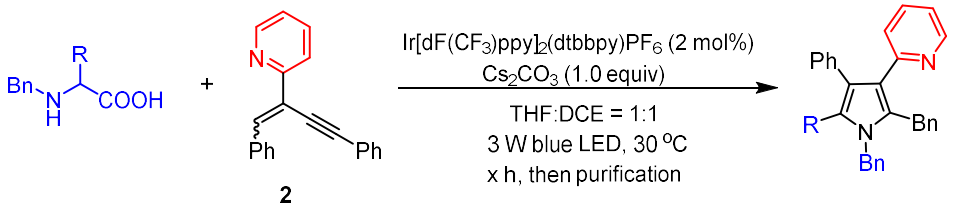
Representative procedure: To a solution of the benzyl triphenylphosphonium bromide (1.2 equiv.) in anhydrous THF at 0 °C, *n*-butyllithium (1.6 M in Hexane, 1.2 equiv.) was added dropwise by syringe over 5 minutes. After 30 minutes, 2-pyridyl-substituted alkynyl ketone (1.0 equiv.) was added to the orange reaction mixture. After completion of the reaction (monitored by TLC), The reaction was quenched with water and the mixture was extracted with ethyl acetate (3 x 20 mL). The combined organic phase was washed with brine, dried over Na_2SO_4, and filtered. 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 (*E*/*Z*)-2-(2-enynyl)pyridine in 78% yield.

2.2 General procedures for the synthesis of *N*-aryl substituted pyrroles



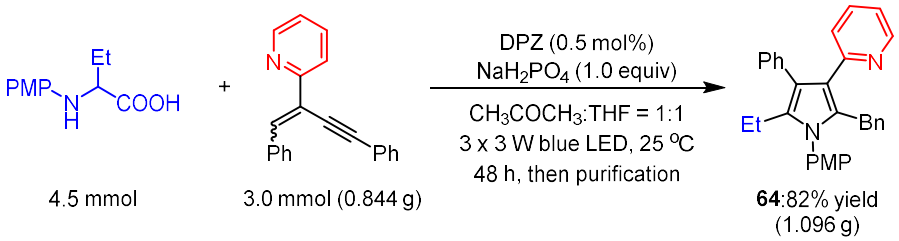
35.5 μL (0.0005 mmol, 0.005 equiv.) of DPZ solution (1.0 mg of DPZ in 200 μL of toluene) was added into a 10 mL Schlenk tube, and then solvent was removed *in vacuo*. Subsequently, *N*-aryl amino acids (0.15 mmol, 1.5 equiv.) and 1,3-enynes (0.1 mmol, 1.0 equiv.) with NaH_2PO_4 (0.1 mmol, 1.0 equiv.) for **1-16, 18-65, 67-68, 70-76, 78, 80-84, 86-89**; trifluoroacetic acid (0.1 mmol, 1.0 equiv.) for **66**; LiH_2PO_4 (0.1 mmol, 1.0 equiv.) for **69** and **85** in THF: DCE = 1:1 (4.0 mL) for **1-36, 38-62, 73**; DCE (4.0 mL) for **37, 71**; THF: CH_3COCH_3 = 1:1 (4.0 mL) for **63-70, 72, 74-76, 78, 80-89** were sequentially added, 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 = 450−455 nm) from a 1.0 cm distance for 36-48 h for **1-16, 18-36, 38-70, 72-76, 78, 80-89**; for 60 h for **37, 71**. 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 **1-16, 18-76, 78, 80-89**.

2.3 General procedures for the synthesis of *N*-benzyl substituted pyrroles



In a 10 mL of Schlenk tube, $Ir[dF(CF_3)ppy]_2(dtbbpy)PF_6$ (0.002 mmol, 0.02 equiv.), ***N***-benzyl amino acid (0.15 mmol, 1.5 equiv.), 2-(2-enynyl)pyridine **2** (0.1 mmol, 1.0 equiv.), Cs_2CO_3 (0.1 mol, 1.0 equiv.) and THF:DCE = 1:1 (4.0 mL) for **17** and **77**; $THF:CH_3COCH_3$ = 1:1 (4.0 mL) for **79** were sequentially added, degassed three times by freeze-pump-thaw method. The reaction mixture was stirred under an argon atmosphere at 30 °C (the temperature was maintained in an incubator) for **17** and **77**; 25 °C (the temperature was maintained in an incubator) for **79**, then irradiated by a 3 W blue LED (λ = 450−455 nm) for **17** for 60 h; 3 x 3 W blue LED (λ = 450−455 nm) for **77** and **79** for 48 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 (30/1–5/1 ratio). Removing the solvent *in vacuo*, afforded products **17**, **77** and **79**.

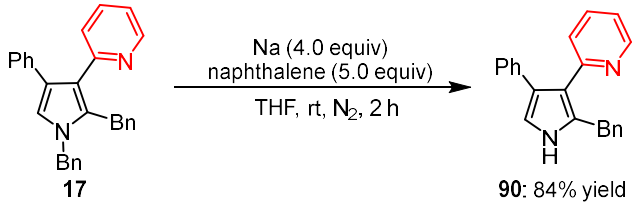
3. Gram-scale synthesis



4.5 mmol | 3.0 mmol (0.844 g) | **64**:82% yield (1.096 g)

In a 100 mL of Schlenk tube, DPZ (0.015 mmol, 0.005 equiv.), 2-((4-methoxyphenyl)amino)butanoic acid (4.5 mmol, 1.5 equiv.), 1,3-enynes (3.0 mmol, 1.0 equiv), NaH_2PO_4 (3.0 mmol, 1.0 equiv.) and THF: DCE = 1:1 (60 mL) were sequentially added, 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 3 x 3 W blue LED (λ = 450−455 nm) for 48 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 (10/1–5/1 ratio). Removing the solvent *in vacuo*, afforded product **64** as a light yellow solid in 82% yield (1.096 g).

4. Transformation of product 17



To a solution of Na (0.4 mmol, 4.0 equiv.) in dry THF (5.0 mL) was added naphthalene (0.5 mmol, 5.0 equiv.) under N_2 atmosphere. After being stirred at room temperature for 1 h, and then the compound **17** (0.1 mmol, 1.0 equiv.) in THF was added at 0 °C. After that, the reaction mixture was stirred at the temperature for another 2 h. The reaction was carefully quenched by dropping saturated ammonium chloride solution and the residue was extracted with DCM (3 × 20 mL). The combined organic layers were dried over Na_2SO_4, filtered, the reaction mixture was removing the solvent and purification by column chromatography on *silica gel*, followed by gradient elution with petroleum ether/ethyl acetate (20/1–10/1 ratio). Removing the solvent *in vacuo*, afforded product **90** in 84% yield.

5. Emission quenching experiments

Emission intensities were recorded on a spectrofluorometer. DPZ solution was excited at 448 nm and the emission intensity at 525 nm was observed. A solution of DPZ (5.0×10^{-5} M) in mixed THF: DCE (V/V = 1:1) 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.

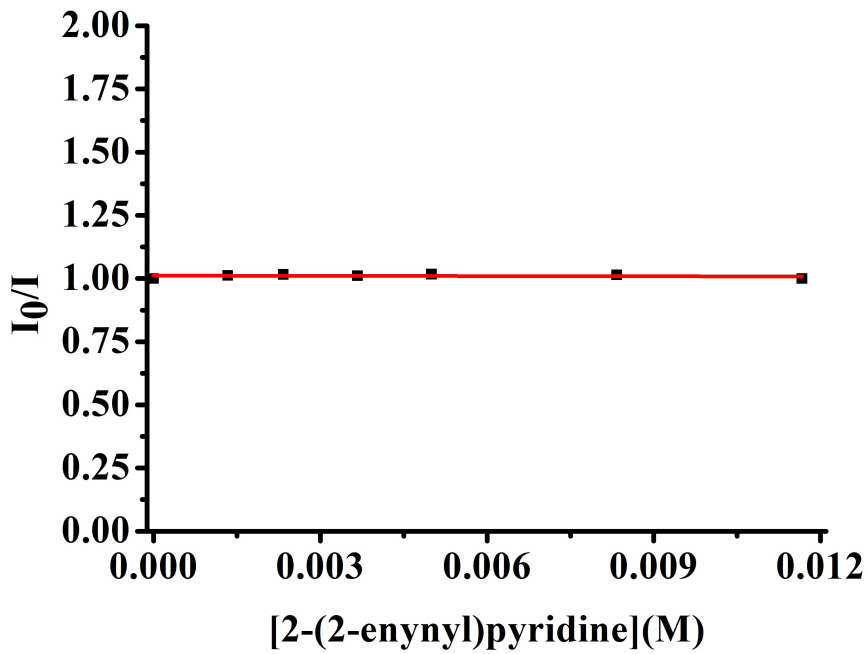


Fig. S1. Stern–Volmer quenching experiment of DPZ and **2.**

（No quenching observed）

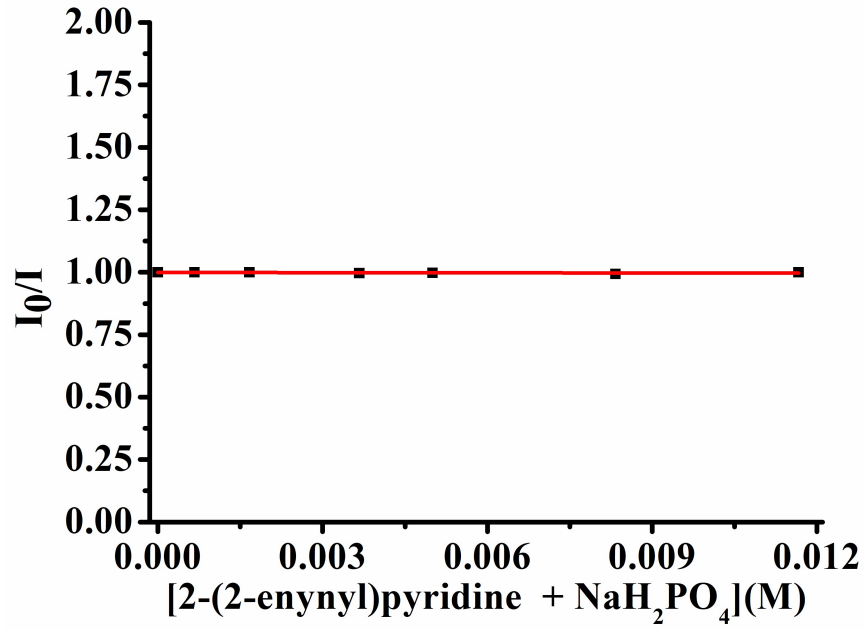


Fig. S2. Stern–Volmer quenching experiment of DPZ and **2** + NaH_2PO_4**.**

（No quenching observed）

6. 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 **2**, 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.

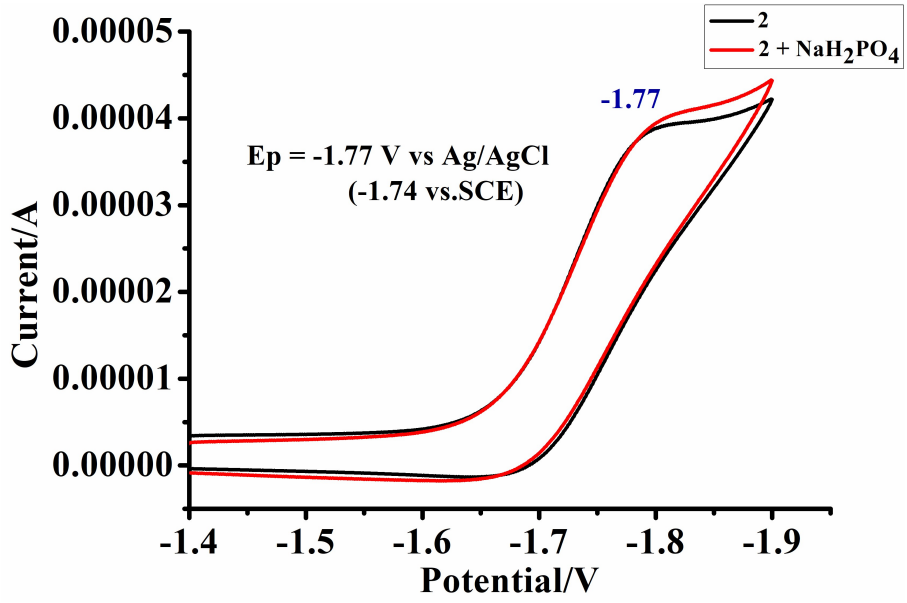


Fig. S3. Cyclic voltammogram of **2** in MeCN.

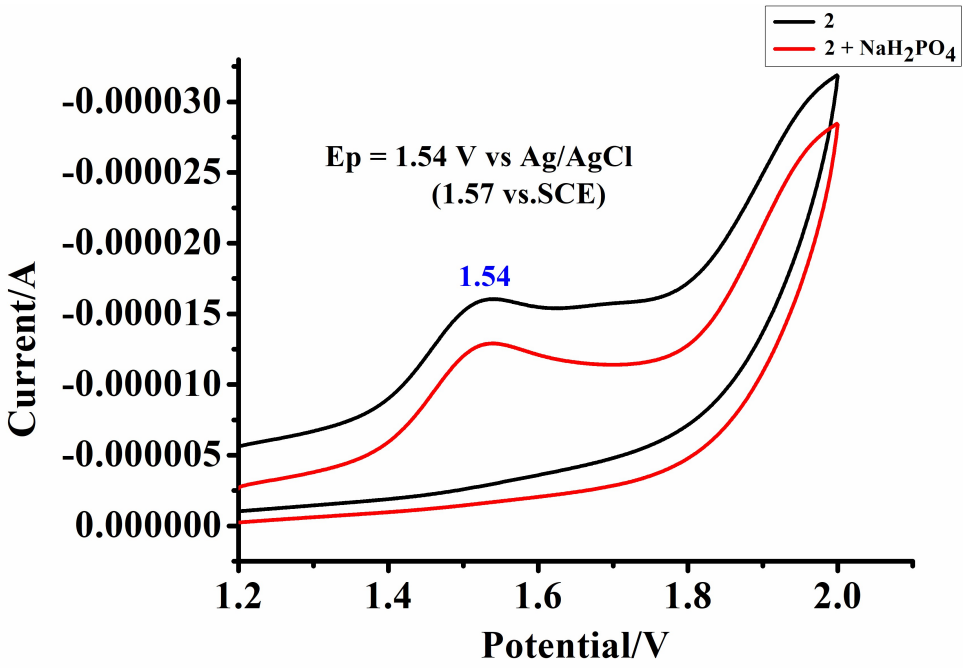


Fig. S4. Cyclic voltammogram of **2** in MeCN.

7. X-Ray crystallographic data

The structure of products was confirmed by *X*-ray crystallographic analysis of a single crystal of compound **18** (CCDC 2049838).

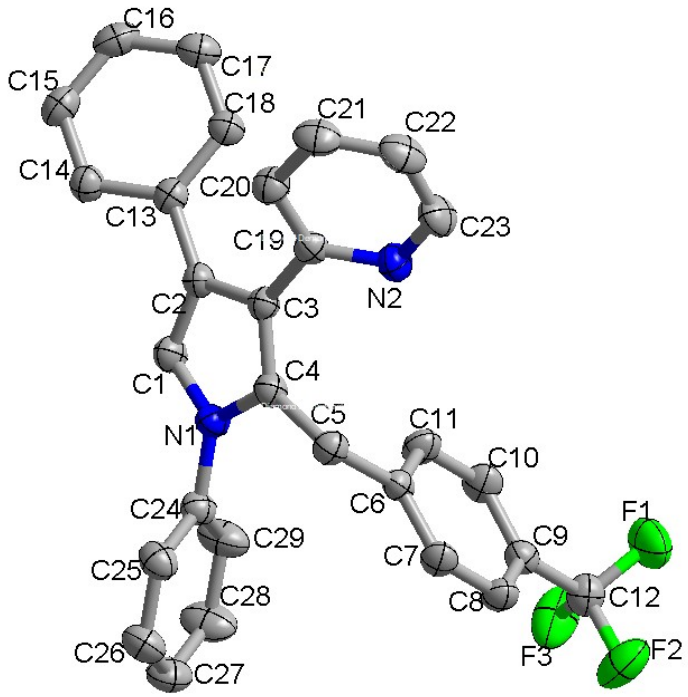


Fig. S5. Absolute configuration of product generated from the reduction of **18**
Displacement ellipsoids are drawn at the 30% probability level.
(Solvents: ethyl acetate/petroleum ether = 1:10)

Table S1 Crystal data and structure refinement for 20200518.

Identification code	20200518
Empirical formula	$C_{29}H_{21}F_3N_2$
Formula weight	454.48
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.4838(4)
b/Å	10.8493(5)
c/Å	22.4754(10)
α/°	90
β/°	94.262(4)
γ/°	90
Volume/Å^3	2306.18(17)
Z	4
ρ_{calc}g/cm^3	1.309
μ/mm^{-1}	0.774

F(000)	944.0
Crystal size/mm^3	0.18 × 0.14 × 0.09
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.89 to 134.154
Index ranges	-11 ≤ h ≤ 9, -12 ≤ k ≤ 8, -26 ≤ l ≤ 22
Reflections collected	8519
Independent reflections	4112 [R_{int} = 0.0378, R_{sigma} = 0.0527]
Data/restraints/parameters	4112/31/318
Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0574, wR_2 = 0.1373
Final R indexes [all data]	R_1 = 0.0892, wR_2 = 0.1615
Largest diff. peak/hole / e Å^{-3}	0.23/-0.19

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 20200518. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N1	3542(2)	7183(2)	7203.7(10)	54.4(6)
N2	1444(3)	7158(2)	8831.0(11)	64.6(7)
C1	4738(3)	6623(3)	7458.6(13)	56.0(7)
C2	4682(3)	6589(2)	8065.0(12)	49.0(6)
C3	3357(3)	7151(2)	8186.0(11)	48.2(6)
C4	2685(3)	7502(2)	7648.9(12)	51.3(6)
C5	1252(3)	8046(3)	7503.3(13)	54.0(6)
C6	187(3)	7147(2)	7212.4(11)	48.0(6)
C7	-987(3)	7575(3)	6874.6(13)	57.5(7)
C8	-1958(3)	6779(3)	6599.2(13)	59.9(7)
C9	-1777(3)	5518(2)	6657.8(12)	53.8(6)
C10	-620(3)	5073(3)	6999.4(14)	65.5(8)
C11	350(3)	5882(3)	7276.9(14)	63.1(8)
C12	-2783(3)	4644(3)	6359.0(15)	66.1(8)
C13	5753(3)	5990(2)	8476.5(12)	48.8(6)
C14	7175(3)	6001(3)	8349.4(13)	58.2(7)
C15	8185(3)	5384(3)	8710.5(15)	68.1(8)
C16	7806(3)	4753(3)	9204.4(14)	69.3(8)
C17	6414(3)	4738(3)	9337.2(13)	65.6(8)
C18	5388(3)	5345(3)	8975.6(12)	55.9(7)
C19	2815(3)	7410(2)	8773.2(12)	49.7(6)
C20	3671(3)	7920(3)	9233.9(13)	62.7(7)
C21	3100(4)	8197(3)	9764.3(14)	76.5(9)
C22	1693(4)	7970(3)	9816.9(15)	78.6(10)
C23	930(4)	7459(3)	9346.7(15)	76.1(9)
C24	3250(3)	7372(3)	6571.6(12)	55.0(7)
C25	3311(4)	8538(3)	6337.8(14)	66.1(8)
C26	3047(4)	8712(3)	5730.3(14)	74.2(9)

C27	2726(4)	7741(3)	5362.0(14)	74.8(9)
C28	2677(5)	6580(4)	5598.8(16)	94.8(13)
C29	2940(5)	6393(3)	6205.9(15)	83.8(11)
F1	-3344(4)	3875(3)	6736.2(13)	113.4(11)
F2	-3910(3)	5184(2)	6074.4(16)	112.6(11)
F3	-2232(3)	3935(3)	5961.9(16)	121.5(13)
F1A	-4040(20)	4570(30)	6581(14)	113.4(11)
F2A	-3060(30)	4910(30)	5782(7)	112.6(11)
F3A	-2300(30)	3506(16)	6396(14)	121.5(13)

Table S3 Anisotropic Displacement Parameters ($Å^2×10^3$) for 20200518. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
N1	52.4(13)	65.1(15)	46.4(12)	2.2(10)	7.3(9)	6.3(11)
N2	55.8(14)	79.3(17)	59.8(15)	-2.6(12)	13.1(11)	-0.8(12)
C1	50.6(15)	60.8(17)	57.4(17)	1.1(13)	10.2(12)	7.2(13)
C2	47.6(14)	48.5(14)	51.2(15)	-1.0(11)	5.6(11)	-0.5(11)
C3	46.7(13)	48.9(14)	49.2(14)	-0.7(11)	4.5(11)	0.5(11)
C4	51.5(14)	51.5(14)	51.2(15)	-1.9(12)	5.5(11)	1.2(12)
C5	55.0(15)	51.2(15)	56.0(16)	0.7(12)	4.8(12)	5.1(12)
C6	49.1(14)	49.5(14)	46.2(14)	7.0(11)	8.9(10)	6.3(11)
C7	59.0(16)	45.3(14)	67.5(18)	10.3(13)	0.7(13)	5.8(13)
C8	56.9(16)	58.3(17)	63.1(18)	11.3(14)	-5.3(13)	4.3(14)
C9	54.8(15)	53.4(15)	54.0(16)	3.0(12)	10.1(12)	0.6(12)
C10	66.9(18)	46.4(15)	83(2)	6.2(14)	2.2(15)	6.9(14)
C11	56.7(16)	55.6(17)	75(2)	9.3(14)	-6.9(14)	10.3(14)
C12	62.6(18)	59.2(18)	77(2)	-5.6(15)	9.8(15)	0.9(15)
C13	50.8(14)	42.7(13)	52.8(15)	-7.1(11)	3.2(11)	0.9(11)
C14	53.4(16)	58.6(16)	62.8(17)	0.7(13)	6.0(12)	0.7(13)
C15	50.2(16)	75(2)	78(2)	-6.0(17)	-3.1(14)	4.3(15)
C16	71(2)	69.0(19)	65.0(19)	-6.4(15)	-15.5(15)	15.7(16)
C17	83(2)	61.7(18)	52.0(17)	1.9(13)	2.8(15)	7.8(16)
C18	59.0(16)	54.8(16)	54.2(16)	-0.6(12)	5.1(12)	1.7(13)
C19	50.5(14)	46.7(13)	52.4(15)	3.5(11)	6.4(11)	7.1(12)
C20	63.1(17)	63.5(18)	61.4(18)	-7.8(14)	3.6(13)	-2.0(14)
C21	103(3)	74(2)	52.3(18)	-11.7(15)	-0.5(17)	4.0(19)
C22	100(3)	82(2)	57.0(19)	-3.0(16)	25.6(18)	21(2)
C23	72(2)	95(2)	64(2)	0.1(17)	24.4(16)	7.4(18)
C24	56.1(15)	60.4(16)	49.3(15)	0.8(12)	9.0(11)	5.9(13)
C25	78(2)	63.8(18)	57.5(18)	-4.3(14)	11.4(14)	-8.3(16)
C26	93(2)	70(2)	60.6(19)	12.7(16)	12.9(17)	0.2(18)
C27	90(2)	84(2)	50.6(18)	0.2(16)	4.8(15)	9.0(19)
C28	151(4)	75(2)	57(2)	-14.2(17)	-3(2)	-8(2)
C29	132(3)	62(2)	57(2)	0.8(15)	2.6(19)	-1(2)

F1	125(2)	103(2)	112(2)	14.7(16)	7.3(17)	-54.6(19)
F2	87.1(19)	80.9(16)	161(3)	-5.1(17)	-48.8(18)	-3.0(14)
F3	93.6(18)	147(3)	126(3)	-82(2)	21.2(17)	-15.5(17)
F1A	125(2)	103(2)	112(2)	14.7(16)	7.3(17)	-54.6(19)
F2A	87.1(19)	80.9(16)	161(3)	-5.1(17)	-48.8(18)	-3.0(14)
F3A	93.6(18)	147(3)	126(3)	-82(2)	21.2(17)	-15.5(17)

Table S4 Bond Lengths for 20200518.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.374(3)	C12	F3	1.316(4)
N1	C4	1.379(3)	C12	F1A	1.332(14)
N1	C24	1.442(3)	C12	F2A	1.335(14)
N2	C19	1.344(3)	C12	F3A	1.316(14)
N2	C23	1.331(4)	C13	C14	1.399(4)
C1	C2	1.368(4)	C13	C18	1.388(4)
C2	C3	1.440(4)	C14	C15	1.381(4)
C2	C13	1.473(4)	C15	C16	1.375(5)
C3	C4	1.376(4)	C16	C17	1.375(4)
C3	C19	1.479(4)	C17	C18	1.387(4)
C4	C5	1.495(4)	C19	C20	1.383(4)
C5	C6	1.517(4)	C20	C21	1.379(4)
C6	C7	1.380(4)	C21	C22	1.370(5)
C6	C11	1.388(4)	C22	C23	1.354(5)
C7	C8	1.376(4)	C24	C25	1.373(4)
C8	C9	1.384(4)	C24	C29	1.361(4)
C9	C10	1.379(4)	C25	C26	1.383(4)
C9	C12	1.471(4)	C26	C27	1.360(5)
C10	C11	1.386(4)	C27	C28	1.369(5)
C12	F1	1.329(4)	C28	C29	1.384(5)
C12	F2	1.339(4)			

Table S5 Bond Angles for 20200518.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	C4	108.7(2)	F3	C12	F2	106.0(3)
C1	N1	C24	124.4(2)	F1A	C12	C9	115.9(13)
C4	N1	C24	126.8(2)	F1A	C12	F2A	105.0(15)
C23	N2	C19	117.0(3)	F2A	C12	C9	112.5(12)
C2	C1	N1	109.6(2)	F3A	C12	C9	111.6(13)
C1	C2	C3	106.0(2)	F3A	C12	F1A	104(2)
C1	C2	C13	124.1(2)	F3A	C12	F2A	107.6(15)
C3	C2	C13	129.7(2)	C14	C13	C2	119.9(2)
C2	C3	C19	128.0(2)	C18	C13	C2	121.9(2)
C4	C3	C2	107.8(2)	C18	C13	C14	118.1(3)
C4	C3	C19	124.1(2)	C15	C14	C13	120.9(3)

N1	C4	C5	121.0(2)	C16	C15	C14	120.3(3)
C3	C4	N1	107.9(2)	C17	C16	C15	119.6(3)
C3	C4	C5	130.9(2)	C16	C17	C18	120.7(3)
C4	C5	C6	114.0(2)	C17	C18	C13	120.4(3)
C7	C6	C5	120.3(2)	N2	C19	C3	116.8(2)
C7	C6	C11	118.0(3)	N2	C19	C20	121.8(3)
C11	C6	C5	121.7(2)	C20	C19	C3	121.4(3)
C8	C7	C6	121.5(3)	C21	C20	C19	119.2(3)
C7	C8	C9	120.2(3)	C22	C21	C20	118.9(3)
C8	C9	C12	121.5(3)	C23	C22	C21	118.3(3)
C10	C9	C8	119.2(3)	N2	C23	C22	124.8(3)
C10	C9	C12	119.4(3)	C25	C24	N1	119.9(3)
C9	C10	C11	120.2(3)	C29	C24	N1	120.1(3)
C10	C11	C6	120.9(3)	C29	C24	C25	120.1(3)
F1	C12	C9	113.0(3)	C24	C25	C26	119.6(3)
F1	C12	F2	103.7(3)	C27	C26	C25	120.8(3)
F2	C12	C9	113.8(3)	C26	C27	C28	119.2(3)
F3	C12	C9	114.2(3)	C27	C28	C29	120.6(3)
F3	C12	F1	105.2(3)	C24	C29	C28	119.7(3)

Table S6 Torsion Angles for 20200518.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C1	C2	C3	0.8(3)	C8	C9	C12	F2	-4.9(5)
N1	C1	C2	C13	176.4(2)	C8	C9	C12	F3	116.9(4)
N1	C4	C5	C6	69.5(3)	C8	C9	C12	F1A	-71.6(19)
N1	C24	C25	C26	179.2(3)	C8	C9	C12	F2A	49.2(16)
N1	C24	C29	C28	-179.3(4)	C8	C9	C12	F3A	170.1(16)
N2	C19	C20	C21	-1.1(5)	C9	C10	C11	C6	-0.7(5)
C1	N1	C4	C3	0.6(3)	C10	C9	C12	F1	57.8(4)
C1	N1	C4	C5	-175.4(2)	C10	C9	C12	F2	175.7(3)
C1	N1	C24	C25	-108.6(3)	C10	C9	C12	F3	-62.4(4)
C1	N1	C24	C29	70.3(4)	C10	C9	C12	F1A	109.0(18)
C1	C2	C3	C4	-0.4(3)	C10	C9	C12	F2A	-130.2(16)
C1	C2	C3	C19	-176.1(3)	C10	C9	C12	F3A	-9.2(17)
C1	C2	C13	C14	34.3(4)	C11	C6	C7	C8	-1.2(4)
C1	C2	C13	C18	-141.8(3)	C12	C9	C10	C11	179.0(3)
C2	C3	C4	N1	-0.1(3)	C13	C2	C3	C4	-175.7(3)
C2	C3	C4	C5	175.4(3)	C13	C2	C3	C19	8.6(5)
C2	C3	C19	N2	-137.5(3)	C13	C14	C15	C16	-0.3(5)
C2	C3	C19	C20	44.2(4)	C14	C13	C18	C17	0.5(4)
C2	C13	C14	C15	-176.2(3)	C14	C15	C16	C17	0.0(5)
C2	C13	C18	C17	176.7(3)	C15	C16	C17	C18	0.5(5)
C3	C2	C13	C14	-151.2(3)	C16	C17	C18	C13	-0.8(5)
C3	C2	C13	C18	32.7(4)	C18	C13	C14	C15	0.1(4)

C3	C4	C5	C6	-105.4(3)	C19	N2	C23	C22	-1.6(5)
C3	C19	C20	C21	177.1(3)	C19	C3	C4	N1	175.8(2)
C4	N1	C1	C2	-0.9(3)	C19	C3	C4	C5	-8.7(5)
C4	N1	C24	C25	72.5(4)	C19	C20	C21	C22	-0.7(5)
C4	N1	C24	C29	-108.6(4)	C20	C21	C22	C23	1.3(5)
C4	C3	C19	N2	47.5(4)	C21	C22	C23	N2	-0.1(6)
C4	C3	C19	C20	-130.8(3)	C23	N2	C19	C3	-176.1(3)
C4	C5	C6	C7	-157.9(3)	C23	N2	C19	C20	2.2(4)
C4	C5	C6	C11	22.4(4)	C24	N1	C1	C2	-179.9(3)
C5	C6	C7	C8	179.1(3)	C24	N1	C4	C3	179.6(3)
C5	C6	C11	C10	-178.8(3)	C24	N1	C4	C5	3.6(4)
C6	C7	C8	C9	0.2(5)	C24	C25	C26	C27	0.1(5)
C7	C6	C11	C10	1.4(5)	C25	C24	C29	C28	-0.4(6)
C7	C8	C9	C10	0.6(4)	C25	C26	C27	C28	-0.5(6)
C7	C8	C9	C12	-178.8(3)	C26	C27	C28	C29	0.4(7)
C8	C9	C10	C11	-0.3(5)	C27	C28	C29	C24	0.0(7)
C8	C9	C12	F1	-122.8(3)	C29	C24	C25	C26	0.3(5)

Table S7 Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 20200518.

Atom	x	y	z	U(eq)
H1	5473	6314	7251	67
H5A	1342	8742	7238	65
H5B	893	8354	7868	65
H7	-1124	8420	6832	69
H8	-2739	7089	6373	72
H10	-491	4227	7044	79
H11	1121	5572	7510	76
H14	7443	6428	8017	70
H15	9125	5396	8619	82
H16	8487	4339	9447	83
H17	6158	4317	9673	79
H18	4449	5319	9068	67
H20	4621	8074	9187	75
H21	3660	8532	10081	92
H22	1274	8162	10166	94
H23	-23	7307	9387	91
H25	3528	9208	6587	79
H26	3089	9502	5572	89
H27	2543	7864	4954	90
H28	2464	5911	5349	114
H29	2904	5602	6363	101

Table S8 Atomic Occupancy for 20200518.

Atom ***Occupancy*** **Atom** ***Occupancy*** **Atom** ***Occupancy***

F1	0.912(4)	F2	0.912(4)	F3	0.912(4)
F1A	0.088(4)	F2A	0.088(4)	F3A	0.088(4)

8. DFT calculation

I. Computation Details

All the calculations in this work were performed on the basis of density functional theory (DFT) in the Gaussian G16 package (Revision B.01).[6] Geometry optimizations and frequencies were calculated with the B3LYP,[7] dispersion-corrected with the D3 version of Grimme's dispersion with Becke-Johnson damping (B3LYP-D3(BJ))[8] and a basis set of 6-31G(d, p).[9] All of the optimized geometries had been characterized as minima (zero imaginary frequencies) or transition state structures (a single imaginary frequency) at the same level of theory. Intrinsic reaction coordinate (IRC)[10] calculations were also carried out to inspect whether each of the transition structures actually connected the proposed reactant and product. The mixed solvent THF/DCE (Ɛ= 8.78, R_{solv} = 2.03 Å) was evaluated by single-point energy calculation with SMD solvation model[11] using M06-2X functional method[12] on the basis sets of 6-311+G(d, p). Atomic charges were computed using natural population analysis (NPA).[13] The key 3D structures were prepared using the CYL view visualization program.[14]

II. Cartesian coordination and energies for the all the calculated species were performed at the SMD/M06/6-311++G** level in solvent phase.

1

Sum of electronic and thermal Free Energies=-515.316811

C	1.94005400	1.51236300	-0.27116900
C	0.75391200	0.83686900	-0.56049900
C	0.65627100	-0.54509100	-0.33693500
C	1.76927300	-1.22115400	0.19217200
C	2.94221200	-0.53636600	0.48362600
C	3.04090300	0.83814300	0.25130200
H	1.99312200	2.58213400	-0.45115200
H	-0.08917100	1.39575000	-0.95025600
H	1.70360800	-2.29182200	0.36763300
H	3.78685200	-1.08120200	0.89498100
H	3.95793000	1.37131200	0.47877500
N	-0.48896800	-1.28681100	-0.66433600
H	-0.59976800	-2.10001000	-0.07283300
C	-1.73525600	-0.61019400	-0.91001300
H	-2.47841100	-1.34253900	-1.24587300
H	-1.63333500	0.11207500	-1.72351400
C	-2.31436200	0.08438100	0.32129800
O	-2.06825000	-0.21593200	1.46552400
O	-3.18188900	1.06394800	-0.02464800
H	-3.53498100	1.42414500	0.80690000

2

Sum of electronic and thermal Free Energies=-863.594483

C	-0.15110800	-0.41475700	0.00117300
C	-1.36186000	-0.53509600	0.00910500
C	-2.78506900	-0.61451700	0.03112100
C	-3.51284200	-0.04828500	1.09649400

C	-3.48299500	-1.25284400	-1.01242800
C	-4.90254400	-0.12130700	1.11231000
H	-2.97438700	0.44227000	1.90072500
C	-4.87275000	-1.31869600	-0.98920100
H	-2.92263500	-1.68446500	-1.83571500
C	-5.58654500	-0.75753700	0.07213600
H	-5.45420800	0.31571100	1.93990200
H	-5.40107300	-1.81047000	-1.80134500
H	-6.67104600	-0.81135700	0.08622500
C	1.27058900	-0.35032500	0.00354400
C	1.98299400	0.81135100	-0.00536400
H	3.05886800	0.66521100	0.03419100
C	1.55189100	2.20066400	-0.05764100
C	2.55010600	3.18893500	0.08429000
C	0.22263700	2.63157700	-0.25534500
C	2.23997100	4.54331400	0.04561200
H	3.58100900	2.87560500	0.22624800
C	-0.08260900	3.98721300	-0.30142900
H	-0.56417500	1.90160800	-0.37992500
C	0.91775200	4.95008400	-0.14725800
H	3.02746700	5.28178300	0.16113500
H	-1.11233600	4.29495200	-0.45700100
H	0.67169300	6.00670000	-0.18316500
C	1.99806500	-1.65421900	0.03304100
C	1.30374500	-2.87190400	-0.00831000
C	2.02428800	-4.06157900	0.01000000
H	0.22278200	-2.87228300	-0.05960800
C	4.01676600	-2.75694800	0.11525300
C	3.41417100	-4.01297500	0.07292200
H	1.50472400	-5.01375900	-0.02653100
H	5.10057300	-2.67023100	0.16976100
H	4.01598300	-4.91479000	0.08634600
N	3.34126500	-1.60848100	0.09694200

3

Sum of electronic and thermal Free Energies=-326.111122

C	-1.35847800	1.33286700	-0.01590900
C	0.01293600	1.09392500	-0.04560800
C	0.49392000	-0.22836500	-0.02612900
C	-0.43143900	-1.28940400	0.00615800
C	-1.79603300	-1.03317000	0.02895100
C	-2.27430000	0.28076600	0.02351900
H	-1.71373700	2.35915200	-0.03360900
H	0.70574700	1.92413500	-0.10948600
H	-0.06745400	-2.31409500	0.02109500
H	-2.49225800	-1.86621400	0.05460900
H	-3.34067300	0.47856900	0.04435300
N	1.85121400	-0.51685700	-0.03084600
H	2.08547300	-1.48873500	-0.16996500
C	2.89676300	0.37952000	0.01417400
H	3.88968300	-0.04518600	0.05236300
H	2.71451300	1.35353700	0.44562900

TS1

Sum of electronic and thermal Free Energies=-1189.688841

C	-1.76646200	0.60034400	0.56263000
C	-2.84868400	0.24715300	0.12867000
C	-4.05569700	-0.23845100	-0.44646000
C	-4.02449100	-1.37590300	-1.27942700
C	-5.28686600	0.41200200	-0.22428700
C	-5.19113200	-1.83814900	-1.87837200
H	-3.07699900	-1.86798200	-1.45844800
C	-6.44931400	-0.06239800	-0.82423200
H	-5.31891800	1.29743200	0.41491600
C	-6.40641000	-1.18604900	-1.65366700
H	-5.15289900	-2.70106700	-2.52944600
H	-7.39319900	0.44789700	-0.64551700
H	-7.31534600	-1.54411200	-2.12676300
C	-0.47105200	1.03871200	0.93817100
C	0.53801100	0.18141200	1.28831000
H	1.50382200	0.66105800	1.40847400
C	0.52106900	-1.24464000	1.57411200
C	1.76975800	-1.88844800	1.69916200
C	-0.64288300	-2.02174500	1.74814400
C	1.85635500	-3.25438900	1.94679000
H	2.67417300	-1.30089600	1.57749900
C	-0.55180200	-3.38530400	2.00756100
H	-1.61658800	-1.54834900	1.69294500
C	0.69354400	-4.01262200	2.09926600
H	2.82959900	-3.72449800	2.03248900
H	-1.46157200	-3.96303900	2.14700400
H	0.75576000	-5.07730200	2.30053500
C	-0.17495800	2.48510800	0.78188900
C	-1.20314800	3.41886100	0.56650800
C	-0.88031900	4.76413600	0.43583500
H	-2.22938000	3.07970000	0.50650800
C	1.41126100	4.15598800	0.72182900
C	0.45638300	5.15277400	0.51596100
H	-1.66211200	5.49985000	0.27322300
H	2.46862600	4.41160900	0.78228900
H	0.75459300	6.19089500	0.41859300
N	1.11826600	2.86173000	0.85154700
C	4.75243700	1.02437200	-1.11766300
C	3.47007400	0.47920600	-1.11549300
C	3.30253200	-0.89880400	-1.34578100
C	4.43605800	-1.70982200	-1.53775300
C	5.70747100	-1.14921900	-1.52704000
C	5.87703000	0.22520400	-1.32885000
H	4.86911900	2.08924700	-0.93849100
H	2.61467800	1.10783400	-0.89576200
H	4.30663900	-2.77530900	-1.71191000
H	6.57243100	-1.78751700	-1.68389200
H	6.87120200	0.66215200	-1.33177800
N	2.03590500	-1.47628500	-1.40022500
H	1.98929700	-2.46477800	-1.21327000
C	0.85392900	-0.79491400	-1.41904100
H	-0.05762500	-1.35417200	-1.28696500
H	0.83934400	0.21673100	-1.79212300

4

Sum of electronic and thermal Free Energies=-1189.723465

C	0.78485900	1.02641700	0.06394500
C	-0.11907700	1.84094800	0.25692000
C	-1.19610600	2.72435000	0.48194900
C	-2.52547800	2.23985000	0.49748200
C	-0.96605400	4.10457500	0.68661500
C	-3.58494700	3.11812600	0.68708300
H	-2.70930700	1.18218900	0.33083400
C	-2.03577500	4.97171500	0.88300400
H	0.05248800	4.47839100	0.68511600
C	-3.34761100	4.48451200	0.87224200
H	-4.60461200	2.73817400	0.67465000
H	-1.84728200	6.03070700	1.03128300
H	-4.17965600	5.16706200	1.02137800
C	1.80023900	0.11880200	-0.16213800
C	1.50293600	-1.34822800	-0.39218400
H	2.48203400	-1.82262500	-0.48580300
C	0.77597600	-2.05622700	0.74227200
C	1.28516200	-3.28640700	1.17575200
C	-0.39402100	-1.57558800	1.34361400
C	0.64488500	-4.02313100	2.17184700
H	2.19577200	-3.67124900	0.72416700
C	-1.03620100	-2.30753000	2.34041000
H	-0.81274800	-0.63032000	1.02704900
C	-0.52045400	-3.53294300	2.76070700
H	1.05702300	-4.97771300	2.48695400
H	-1.94733200	-1.91735100	2.78480200
H	-1.02237200	-4.10305800	3.53716100
C	3.17568900	0.59159500	-0.24203600
C	3.50193400	1.94774200	-0.01213400
C	4.82391800	2.35274200	-0.10270600
H	2.71407400	2.64900500	0.23520000
C	5.39452400	0.09187500	-0.63765500
C	5.80393500	1.40967000	-0.42316800
H	5.09149400	3.38979100	0.07476300
H	6.12690500	-0.67292500	-0.88996700
H	6.85086600	1.68239100	-0.50435700
N	4.13031300	-0.31849700	-0.55278800
C	-3.29060300	-2.85652400	-0.90137800
C	-1.97813200	-2.53137900	-1.23957300
C	-1.66466300	-1.24056500	-1.69803900
C	-2.71211900	-0.30468700	-1.81986800
C	-4.01582600	-0.64136100	-1.47265600
C	-4.32112700	-1.92142700	-1.00732100
H	-3.50057800	-3.85880500	-0.53469900
H	-1.19710100	-3.26935400	-1.10253400
H	-2.48442200	0.69165500	-2.18360400
H	-4.79960800	0.10576800	-1.56914100
H	-5.33775900	-2.18470800	-0.73447700
N	-0.38667300	-0.85316900	-2.06999100
H	-0.27203500	0.14503300	-2.16196400
C	0.83248600	-1.56934000	-1.79010500
H	1.56965900	-1.27562500	-2.54441600
H	0.65893000	-2.64026900	-1.92023200

5

Sum of electronic and thermal Free Energies=-1189.852241

C	0.98595700	0.93059600	0.02859700
C	0.25453000	1.92150800	0.14815100
C	-0.58831500	3.03043000	0.31112600
C	-1.98853200	2.87806300	0.51596300
C	-0.08078800	4.35828600	0.28643300
C	-2.81474300	3.98344900	0.66737600
H	-2.40266700	1.87648100	0.55193900
C	-0.92108200	5.45201600	0.44704800
H	0.98457000	4.50291300	0.13591700
C	-2.29777900	5.28387000	0.63507200
H	-3.88081900	3.82827800	0.81958700
H	-0.49726500	6.45375200	0.42204100
H	-2.95029700	6.14379900	0.75514900
C	1.80819200	-0.17438700	-0.10234700
C	1.23892200	-1.56435900	-0.33878600
H	2.11371300	-2.22048900	-0.38945800
C	0.30840600	-2.13966400	0.71870500
C	0.25703800	-3.53329400	0.87250000
C	-0.55769600	-1.36290000	1.49776300
C	-0.64680300	-4.13790500	1.74532100
H	0.93537500	-4.14829100	0.28418400
C	-1.46512800	-1.96372600	2.37210500
H	-0.52812400	-0.28382300	1.40254000
C	-1.52185700	-3.35016300	2.49445600
H	-0.66687600	-5.22114900	1.84115400
H	-2.13909100	-1.33702800	2.94928300
H	-2.23504500	-3.81340200	3.17246600
C	3.23243600	-0.00196600	-0.13693000
C	3.84236400	1.27939000	0.04894400
C	5.21305100	1.40400100	0.00984000
H	3.20445900	2.13815800	0.22426200
C	5.34707500	-0.94045100	-0.38531600
C	6.01415600	0.26771300	-0.21439800
H	5.67100500	2.38166400	0.15259700
H	5.92300300	-1.85228700	-0.56220600
H	7.09730500	0.32445000	-0.24963600
N	4.02373200	-1.09766000	-0.35726700
C	-3.65130400	-2.52391700	-0.90957900
C	-2.32527700	-2.33067600	-1.28455600
C	-1.84289500	-1.03797200	-1.56883000
C	-2.75367200	0.03688800	-1.47959500
C	-4.07423500	-0.17107700	-1.10266500
C	-4.54424200	-1.45496300	-0.81285600
H	-3.98413000	-3.53120300	-0.67189600
H	-1.65246900	-3.17806700	-1.30189500
H	-2.39930400	1.04185800	-1.68917300
H	-4.73435000	0.68685300	-1.02973900
H	-5.57616300	-1.61784700	-0.50951100
N	-0.54492500	-0.77290000	-1.97753300
H	-0.28501200	0.19650800	-1.83209400
C	0.57854800	-1.66684000	-1.74675700
H	1.34997200	-1.41417500	-2.48065000
H	0.26260900	-2.69472700	-1.95198200

I

Sum of electronic and thermal Free Energies=-1995.748692

C	-0.01306900	1.09853300	1.22407800
C	-0.84469100	0.36822100	1.78775200
C	-1.86471900	-0.41657000	2.34034600
C	-1.61772900	-1.72396600	2.85075100
C	-3.21943400	0.03293100	2.33849300
C	-2.65980600	-2.53040700	3.29156600
H	-0.59342100	-2.08305300	2.89323100
C	-4.24462400	-0.78630100	2.79224300
H	-3.43092000	1.03213500	1.96925800
C	-3.98395100	-2.07911400	3.26536300
H	-2.43510100	-3.52736200	3.66330400
H	-5.26824500	-0.41479900	2.77034200
H	-4.79411800	-2.71812500	3.60216200
C	0.86242200	1.92260600	0.56460500
C	2.25747900	1.49867300	0.12749800
H	2.85012800	2.41899800	0.10129100
C	3.02127700	0.51211900	0.98758000
C	4.38461400	0.74742600	1.21303500
C	2.48515400	-0.68480400	1.48472300
C	5.18591400	-0.17219300	1.88912600
H	4.82224500	1.67303100	0.84545900
C	3.27825600	-1.60777600	2.16348200
H	1.43381500	-0.88863000	1.34910300
C	4.63583400	-1.36268400	2.36294300
H	6.24068500	0.04356400	2.04549000
H	2.83346800	-2.52955700	2.52368000
H	5.25608900	-2.08537100	2.88584100
C	0.40923900	3.22139600	0.13139400
C	-0.89260700	3.71535300	0.44035700
C	-1.26095500	4.97977900	0.03699100
H	-1.57643800	3.08370800	0.99442600
C	0.88623700	5.21173500	-0.96947900
C	-0.35435700	5.77330500	-0.68855700
H	-2.25243100	5.35711900	0.27778400
H	1.61948300	5.78002000	-1.54608100
H	-0.60807200	6.77502900	-1.02739300
N	1.27618100	3.99052500	-0.59047800
C	3.11376100	-3.27109100	-1.56900200
C	2.89315400	-1.90258200	-1.47830500
C	1.64497000	-1.35266900	-1.85812000
C	0.66412400	-2.23696500	-2.37655000
C	0.89937200	-3.60505800	-2.43914200
C	2.12499600	-4.14428600	-2.03062200
H	4.07460200	-3.65752600	-1.25364200
H	3.66582200	-1.26561900	-1.06597600
H	-0.27960800	-1.82313400	-2.72144600
H	0.11093600	-4.24933100	-2.81985700
H	2.30283900	-5.21388600	-2.07458500
N	1.31604700	-0.02502600	-1.70034300
H	0.37736800	0.24642900	-1.97485900
C	2.23584100	1.04981500	-1.37021200
H	1.93343400	1.93934700	-1.93608900
H	3.24407300	0.78486700	-1.70014100
P	-2.94825400	-0.58726500	-1.76712500
O	-4.06083800	0.30107500	-0.95730500
H	-4.07427500	-0.03427500	-0.04710100

O	-3.66607900	-0.71137600	-3.23966900
H	-3.15492800	-0.13558000	-3.82572500
O	-1.63912500	0.17023200	-1.95707900
O	-2.82174200	-1.92576500	-1.08115700
Na	-0.80701400	-1.24212700	-0.23438300

TS2

Sum of electronic and thermal Free Energies= -1995.749810

C	-1.46307600	0.50407300	-0.47392700
C	-1.82755800	-0.67067900	-0.85700000
C	-2.79004300	-1.51519300	-0.12673400
C	-3.93638300	-0.99258200	0.49741200
C	-2.52545700	-2.89216300	-0.01260100
C	-4.78484300	-1.81575900	1.23572400
H	-4.14753600	0.06885300	0.39850900
C	-3.37090200	-3.70702600	0.73907000
H	-1.63099200	-3.28870300	-0.48757000
C	-4.50226800	-3.17781600	1.36560700
H	-5.66599400	-1.39376600	1.71327300
H	-3.14537300	-4.76635300	0.83325100
H	-5.16099400	-3.82029000	1.94419800
C	-1.07678000	1.71202900	-0.04340400
C	0.00874500	1.89552200	1.02026400
H	-0.27024100	2.81906600	1.54360400
C	0.05527700	0.76973400	2.05106600
C	1.25581500	0.36699000	2.66572600
C	-1.11526600	0.08077600	2.41236900
C	1.28631400	-0.70869900	3.56033300
H	2.18843600	0.86453200	2.43040500
C	-1.08813700	-0.99562200	3.29831400
H	-2.05728900	0.36459300	1.96297400
C	0.11721700	-1.40572700	3.87052300
H	2.23373000	-1.00343900	4.00347700
H	-2.01145700	-1.52459200	3.51385900
H	0.14640500	-2.25535400	4.54639900
C	-1.72012000	2.92214300	-0.56142600
C	-2.70746700	2.85778700	-1.57554200
C	-3.30031300	4.02256700	-2.02379200
H	-2.97465000	1.89080900	-1.98662600
C	-1.92190600	5.22628900	-0.49483400
C	-2.90743000	5.25153200	-1.47401200
H	-4.05959800	3.98260100	-2.80058000
H	-1.57507200	6.15657100	-0.04410400
H	-3.34330300	6.18990500	-1.80136000
N	-1.33610200	4.11143100	-0.04245200
C	5.60412200	1.22034000	1.03999600
C	4.25304700	1.54217900	0.89264900
C	3.44449900	0.85056000	-0.03262600
C	4.05556000	-0.15667400	-0.81926300
C	5.40020300	-0.46067700	-0.65636600
C	6.19422700	0.21763300	0.27624400
H	6.19711300	1.77454800	1.76378700
H	3.84619300	2.34382600	1.49751300
H	3.43534900	-0.68539900	-1.53965900
H	5.83623300	-1.24088300	-1.27525400
H	7.24554600	-0.02651800	0.39581800

N	2.07147100	1.05858800	-0.16801100
H	1.67379400	0.64784000	-1.02033500
C	1.38577500	2.21617500	0.38913100
H	1.22413000	2.99284400	-0.36755600
H	2.01811600	2.66492900	1.15564100
P	0.64298400	-2.25770400	-2.28836700
O	-0.79767300	-1.99457300	-2.84632700
H	-1.30010800	-1.29122200	-1.95996300
O	1.44090600	-3.11010400	-3.45943700
H	1.43807100	-4.02135000	-3.13662800
O	1.40355400	-0.94374000	-2.04019700
O	0.63154800	-3.15398200	-1.02786500
Na	1.04575900	-1.37224600	0.22989800

II

Sum of electronic and thermal Free Energies=-1995.760355

C	-1.58705200	0.47690900	-0.48023800
C	-1.90524700	-0.72748600	-0.87240200
C	-2.80700300	-1.63249500	-0.13587900
C	-3.76497400	-1.16946400	0.78091800
C	-2.65492200	-3.01542700	-0.33626900
C	-4.53994000	-2.06941000	1.50890500
H	-3.90085800	-0.09833800	0.90868600
C	-3.43432900	-3.90849700	0.39770700
H	-1.91045600	-3.34916800	-1.05748600
C	-4.37281800	-3.44436000	1.32284600
H	-5.27847800	-1.69950400	2.21569900
H	-3.30328800	-4.97657500	0.24743600
H	-4.97598500	-4.14784100	1.89101400
C	-1.27440600	1.68326000	-0.04242600
C	-0.10262600	1.96476100	0.90155500
H	-0.41541800	2.84311800	1.47972300
C	0.21594000	0.85102300	1.89014300
C	1.51242000	0.69842300	2.41701500
C	-0.76972800	-0.04832800	2.32903700
C	1.81584400	-0.33750000	3.30728400
H	2.31251600	1.36114700	2.11228600
C	-0.47016000	-1.08956500	3.21032300
H	-1.78070700	0.03980800	1.95728800
C	0.82919700	-1.24854200	3.69875400
H	2.83159400	-0.43547400	3.68014100
H	-1.25581400	-1.78296300	3.49432200
H	1.06955700	-2.06568100	4.37246500
C	-2.05182900	2.85806200	-0.50758900
C	-3.08221400	2.72077900	-1.46172200
C	-3.79446900	3.83982800	-1.85698600
H	-3.29405600	1.73931200	-1.87027000
C	-2.43836800	5.13043000	-0.37777200
C	-3.47276600	5.08533100	-1.30498700
H	-4.59025400	3.74873700	-2.59108400
H	-2.14706900	6.07755800	0.07501000
H	-4.00253700	5.98864600	-1.58946700
N	-1.74086600	4.05862900	0.01799000
C	5.45229700	1.83018100	0.51840300
C	4.10064700	2.12140300	0.32173200
C	3.25665800	1.21103700	-0.35518500

C	3.84755900	0.02536800	-0.87015100
C	5.19315500	-0.24011400	-0.66241600
C	6.01612000	0.64938300	0.04263200
H	6.06998200	2.55289100	1.04755300
H	3.71657900	3.07055900	0.67874000
H	3.20780500	-0.66029700	-1.42128800
H	5.60742700	-1.16094100	-1.06569000
H	7.06824200	0.43158000	0.20024800
N	1.90419300	1.40103200	-0.53020600
H	1.41638000	0.63502700	-1.02220600
C	1.14062100	2.45086800	0.09901100
H	0.78134800	3.19099200	-0.62709500
H	1.78680100	2.99992200	0.78702000
P	0.77190000	-2.50618500	-1.92476600
O	-0.54869500	-2.65048500	-2.68506400
H	-1.38838300	-1.18126000	-1.73773300
O	1.97685500	-2.92728800	-3.01126200
H	1.54576600	-2.87947500	-3.87428700
O	1.07520900	-1.02769100	-1.49997700
O	0.97812300	-3.41337900	-0.68821000
Na	1.37363100	-1.70100300	0.57715000

TS2'

Sum of electronic and thermal Free Energies=-1995.746450

C	-0.55233600	-0.06268800	0.64905800
C	0.34114200	-0.34190200	1.43886700
C	1.38266200	-0.79163600	2.28127400
C	2.71591800	-0.34005900	2.10534100
C	1.13582900	-1.76890000	3.28107000
C	3.74343000	-0.83925500	2.90138800
H	2.93225600	0.38317600	1.31415500
C	2.18047100	-2.26976000	4.05588600
H	0.13480700	-2.12700200	3.39798700
C	3.48863200	-1.80635600	3.87859600
H	4.77229600	-0.47645000	2.73295700
H	1.97198900	-3.02781100	4.79710400
H	4.30510600	-2.19625900	4.48447400
C	-1.58556400	0.26740100	-0.26760600
C	-1.32834100	1.54336100	-1.10097900
H	-2.29035500	1.77384500	-1.56958500
C	-0.96650900	2.75382900	-0.25750700
C	-1.93446900	3.73521200	-0.00480900
C	0.30628100	2.92550400	0.30581400
C	-1.63822700	4.86018700	0.76313300
H	-2.93620600	3.58380900	-0.39191900
C	0.60861000	4.05383700	1.06682900
H	1.06668000	2.17532100	0.14577300
C	-0.36041800	5.02941700	1.29807000
H	-2.40946100	5.60430400	0.94702800
H	1.60706200	4.16598200	1.48106000
H	-0.12572300	5.90816200	1.89428500
C	-2.95474100	0.08693900	0.30113500
C	-3.29192100	-1.16280900	0.86935400
C	-4.56791400	-1.34542800	1.37365800
H	-2.56556200	-1.97323100	0.83771300
C	-5.08243100	0.87984700	0.68284700

C	-5.49291800	-0.29808100	1.29539300
H	-4.85235800	-2.30156000	1.80358200
H	-5.77574500	1.71676700	0.57994800
H	-6.50407800	-0.39878600	1.67925000
N	-3.85106200	1.08330600	0.19321700
C	3.90412800	2.41888800	-1.77153000
C	2.54948000	2.12519100	-1.92213800
C	2.09522300	0.78611800	-1.88871000
C	3.07290700	-0.23243000	-1.71727400
C	4.41576400	0.08477300	-1.56868700
C	4.85534300	1.41424900	-1.58801200
H	4.21572000	3.46057100	-1.79658100
H	1.84031900	2.93394800	-2.03864800
H	2.73539000	-1.26362500	-1.74687700
H	5.13601400	-0.72291600	-1.44690000
H	5.90783200	1.65636700	-1.47186900
N	0.78812800	0.41096700	-2.00675000
H	0.62630300	-0.60122300	-2.01847300
C	-0.35810900	1.24778600	-2.28710600
H	-0.95214700	0.71661000	-3.03712700
H	-0.03412800	2.19369500	-2.73335600
P	-0.75884100	-2.85997500	-1.64026700
O	-1.69816600	-1.67236600	-2.03839400
H	-1.59529000	-0.75209700	-1.15566900
O	-1.12878600	-4.06790300	-2.70961000
H	-0.98353300	-3.71652700	-3.59748600
O	0.72991000	-2.46302500	-1.84244500
O	-0.99078000	-3.42145100	-0.23431400
Na	1.01881900	-2.63607400	0.34235500

II'

Sum of electronic and thermal Free Energies=-1995.753628

C	-0.39838500	0.09794700	0.71629300
C	0.56229000	0.00647400	1.45737200
C	1.78069000	-0.11731300	2.19162800
C	3.00341900	0.22916100	1.57794800
C	1.79835200	-0.62957000	3.50522200
C	4.20175100	0.06560900	2.26502500
H	3.00138500	0.60280600	0.56163000
C	3.00579600	-0.78959900	4.18209600
H	0.85813900	-0.89415100	3.97909400
C	4.21097900	-0.44349800	3.56633600
H	5.13072800	0.32702600	1.76756100
H	3.00480600	-1.18565400	5.19363400
H	5.15016900	-0.57340900	4.09622100
C	-1.55033500	0.21039900	-0.16672800
C	-1.36134900	1.24862400	-1.30632300
H	-2.36584500	1.37824500	-1.72062000
C	-0.90482100	2.63363700	-0.88734200
C	-1.76007600	3.72483400	-1.09391200
C	0.35278200	2.89108600	-0.32462500
C	-1.37663400	5.02386800	-0.76612900
H	-2.75056300	3.54078900	-1.49791700
C	0.74140700	4.18845200	0.00951600
H	1.03828200	2.07483100	-0.15250700
C	-0.11883900	5.26348000	-0.21125400

H	-2.06369100	5.84849000	-0.93829800
H	1.72468200	4.35402900	0.44185100
H	0.18525700	6.27435200	0.04730300
C	-2.82908300	0.34987400	0.64810100
C	-3.33299500	-0.80888100	1.26356400
C	-4.50110400	-0.69633800	2.00715400
H	-2.81216700	-1.75825200	1.11881100
C	-4.55844800	1.62702900	1.44067100
C	-5.13038900	0.54822100	2.10724900
H	-4.92528600	-1.57173300	2.49183500
H	-5.02480500	2.61109200	1.47973400
H	-6.04675700	0.67713400	2.67614500
N	-3.42923700	1.54248300	0.72280100
C	3.80999200	1.39789700	-1.95692100
C	2.43909700	1.21559600	-2.13638300
C	1.85646200	-0.06482800	-1.98862300
C	2.72916500	-1.15233100	-1.70122000
C	4.08959800	-0.94619600	-1.52812900
C	4.65386000	0.33214100	-1.63906100
H	4.21988800	2.39974100	-2.06480800
H	1.81572400	2.06880300	-2.37198000
H	2.29116000	-2.14494900	-1.65007400
H	4.72503800	-1.80031700	-1.30432100
H	5.71916700	0.48733400	-1.49758700
N	0.52379200	-0.32487800	-2.10638900
H	0.25945500	-1.31693600	-1.97873400
C	-0.53417700	0.58963200	-2.46976700
H	-1.25249500	-0.01327700	-3.03047200
H	-0.15579000	1.37757200	-3.13136200
P	-1.28062100	-3.21755100	-1.05041900
O	-2.17849600	-2.21884600	-1.78427400
H	-1.68161100	-0.75856500	-0.69695700
O	-1.72975500	-4.73233700	-1.58615000
H	-2.26266300	-4.55688900	-2.37255100
O	0.23823000	-3.03083000	-1.40053300
O	-1.41491500	-3.24237600	0.49744000
Na	0.65188200	-2.53503800	0.69212200

III

Sum of electronic and thermal Free Energies=-1996.248010

C	-1.47893400	0.44561900	-0.54923600
C	-1.56847800	-0.79610700	-0.96661600
C	-2.59273000	-1.76359600	-0.53299800
C	-3.79363600	-1.36104600	0.07302300
C	-2.33857100	-3.13320500	-0.70216900
C	-4.70665300	-2.30745200	0.52704300
H	-4.00938800	-0.30093300	0.16929100
C	-3.25548800	-4.07803100	-0.24370000
H	-1.41817000	-3.44455200	-1.18779100
C	-4.43738300	-3.67074900	0.37611300
H	-5.63352900	-1.98399900	0.99135900
H	-3.04662400	-5.13570100	-0.37308900
H	-5.15046700	-4.40880600	0.73023900
C	-1.38983300	1.67099900	-0.07386200
C	-0.55906800	1.98646300	1.17648600
H	-1.04955100	2.84415600	1.65031700

C	-0.50520000	0.83367100	2.17550100
C	0.67157300	0.49038700	2.86493600
C	-1.65142000	0.06543500	2.42953800
C	0.70642800	-0.60248500	3.73903400
H	1.58319200	1.05770300	2.71488500
C	-1.62057100	-1.02612600	3.29514500
H	-2.57577200	0.30599000	1.92026200
C	-0.43680600	-1.37407100	3.94758100
H	1.63396900	-0.84948900	4.24656300
H	-2.52161900	-1.61288200	3.44234500
H	-0.40541300	-2.23251600	4.61052200
C	-2.03885600	2.81652000	-0.76753000
C	-2.78823000	2.63129200	-1.94225200
C	-3.38105100	3.73288100	-2.54173400
H	-2.89113900	1.63668400	-2.36166000
C	-2.44963200	5.08240900	-0.80295900
C	-3.21268500	4.99354900	-1.96322200
H	-3.96572000	3.61351100	-3.44871300
H	-2.28866900	6.04411000	-0.32034500
H	-3.65698400	5.88125600	-2.39997700
N	-1.87354800	4.02856400	-0.21203800
C	5.18030700	2.18664600	0.90057000
C	3.78583500	2.27064300	0.92083800
C	3.02114100	1.49813800	0.03434000
C	3.68570200	0.65920300	-0.88057700
C	5.07368500	0.58489800	-0.88629000
C	5.83522900	1.34596800	0.00463700
H	5.75301800	2.79534600	1.59417800
H	3.31475500	2.94951300	1.62123500
H	3.09520600	0.04530400	-1.55434200
H	5.56103700	-0.08271600	-1.59029200
H	6.91842300	1.28447300	-0.00229400
N	1.60395500	1.44935300	0.07067300
H	1.21789300	1.22023500	-0.84116800
C	0.83247200	2.49251900	0.74787500
H	0.70434600	3.38634600	0.12693500
H	1.37098000	2.80616600	1.64148800
P	1.80787000	-2.69239200	-1.48401500
O	0.79817600	-3.76551100	-2.21821200
H	-0.77468300	-1.16304300	-1.62361600
O	3.25565000	-2.97226100	-2.19198300
H	3.25240000	-2.58258900	-3.07771000
O	1.30842400	-1.30554000	-1.84679400
O	1.92733800	-3.01698800	-0.01198300
Na	1.17813500	-0.99573300	0.58247600
H	0.95255800	-4.64389400	-1.84140700

TS3

Sum of electronic and thermal Free Energies=-1996.222860

C	0.89644300	0.68393700	-0.26885800
C	0.75607200	1.47176800	0.81252800
C	1.17730000	1.12839100	2.17293000
C	1.82540800	-0.08131300	2.49810600
C	0.91904200	2.03816500	3.21796300
C	2.18008800	-0.36747000	3.81260900
H	2.05399600	-0.79189900	1.71283700

C	1.28376100	1.75024800	4.52848700
H	0.41866800	2.97486200	2.98719000
C	1.91531800	0.54334300	4.83682700
H	2.67533000	-1.30785900	4.03674000
H	1.07030500	2.46911800	5.31431900
H	2.19922600	0.31779500	5.85986300
C	1.54026600	-0.28435800	-0.95451000
C	0.69950500	-1.05457500	-1.94065800
H	1.36107600	-1.48653800	-2.69667800
C	-0.11944900	-2.20646600	-1.36600100
C	-0.22316200	-2.45106200	0.00847400
C	-0.78099800	-3.07849500	-2.24759200
C	-0.95266100	-3.54008900	0.49452800
H	0.25912500	-1.78124200	0.70765000
C	-1.50983200	-4.17405600	-1.77334000
H	-0.69941200	-2.91431400	-3.31923800
C	-1.59539800	-4.41181800	-0.39235600
H	-1.03210400	-3.69293300	1.56539300
H	-1.98172500	-4.85632500	-2.47536200
H	-2.14051100	-5.27300500	-0.01661800
C	2.98951700	-0.48170200	-0.91503500
C	3.83792600	0.32015500	-0.12015600
C	5.20155100	0.07195000	-0.12749900
H	3.41912500	1.11792900	0.47983700
C	4.79608900	-1.70783400	-1.66547100
C	5.70542200	-0.96847200	-0.91314600
H	5.86724700	0.68141900	0.47671000
H	5.14281600	-2.52650000	-2.29447900
H	6.76450500	-1.20074000	-0.93988300
N	3.47864700	-1.48623000	-1.67648600
C	-0.11265000	4.43930500	-2.73607400
C	0.07751500	3.06977100	-2.57868300
C	-0.82573100	2.32631100	-1.80614000
C	-1.90024800	2.97026600	-1.17603800
C	-2.07241200	4.34437200	-1.33514000
C	-1.18674000	5.08456400	-2.11802200
H	0.59064800	5.00849000	-3.33632600
H	0.93782200	2.58727100	-3.02893500
H	-2.59353600	2.38640300	-0.57998400
H	-2.90881200	4.83415800	-0.84599700
H	-1.32661800	6.15344700	-2.24304700
N	-0.62678500	0.94767400	-1.54804900
H	-1.43025000	0.54883500	-1.02087200
C	-0.19174600	0.03435200	-2.60043300
H	0.39768100	0.57911800	-3.33766200
H	-1.06130200	-0.39837100	-3.10610400
P	-3.02517900	-0.28821600	1.20642300
O	-1.64537400	-0.24064300	2.04728600
H	0.32875100	2.46323500	0.67174600
O	-3.84026300	1.05292800	1.65635200
H	-4.16372600	0.95584700	2.56335500
O	-2.76313100	-0.12513100	-0.29567600
O	-3.76200900	-1.55977800	1.55998600
Na	-3.42154700	-2.27050300	-0.56086500
H	-0.99161500	0.38633100	1.68307800

IV

Sum of electronic and thermal Free Energies= -1996.241697

C	0.46486900	0.70361700	-0.65637600
C	0.70851800	1.63228600	0.35158900
C	1.76473700	1.63083200	1.35093500
C	2.45464200	0.47058600	1.76907200
C	2.08188500	2.84012500	2.01195400
C	3.40788400	0.52545200	2.78206000
H	2.22716900	-0.48107800	1.30749000
C	3.03646900	2.89020600	3.01920600
H	1.56011200	3.74720700	1.71715500
C	3.71383200	1.73135800	3.41200000
H	3.91680300	-0.38739800	3.07867000
H	3.25708600	3.83885700	3.50108000
H	4.46279900	1.76986300	4.19680700
C	1.07107700	-0.40387100	-1.24166200
C	0.05465600	-1.27131500	-1.94671400
H	0.49133500	-1.71986800	-2.84473700
C	-0.52023400	-2.42394900	-1.12172400
C	-0.12273500	-2.65182600	0.20125100
C	-1.45377800	-3.29994300	-1.69909400
C	-0.63192900	-3.73159700	0.92893700
H	0.57945400	-1.96833900	0.66178600
C	-1.97156400	-4.38319300	-0.97960600
H	-1.76060600	-3.14858500	-2.73147100
C	-1.55751100	-4.60518400	0.34298300
H	-0.31289000	-3.88429300	1.95480200
H	-2.67107000	-5.06593100	-1.45431700
H	-1.93636700	-5.45723200	0.89997200
C	2.46387400	-0.76365800	-1.28865300
C	3.51071700	0.14058200	-0.98675000
C	4.82516400	-0.28895800	-1.07981400
H	3.27917400	1.15918400	-0.70746300
C	4.00565500	-2.41700400	-1.78516100
C	5.09435300	-1.60117300	-1.47747100
H	5.63521000	0.39625100	-0.84666900
H	4.16921400	-3.44154400	-2.11859800
H	6.10870300	-1.97719700	-1.55592900
N	2.73122100	-2.03417400	-1.69931700
C	-1.01591200	4.12355700	-2.92966900
C	-0.59479400	2.85434900	-2.54505600
C	-1.37595200	2.12606800	-1.64856300
C	-2.55453000	2.64195700	-1.11898700
C	-2.96407600	3.91887300	-1.51083300
C	-2.20205900	4.65611700	-2.41513900
H	-0.41424100	4.70192200	-3.62323000
H	0.33820900	2.43693400	-2.90898600
H	-3.12507100	2.05706700	-0.40582500
H	-3.87850000	4.33467700	-1.10046600
H	-2.52408500	5.64831300	-2.71481100
N	-0.94679400	0.78830500	-1.24295500
H	-1.62293400	0.44067500	-0.47898000
C	-1.00187200	-0.23148100	-2.34644200
H	-0.72639800	0.26079300	-3.27896400
H	-2.02808600	-0.59794000	-2.41498300
P	-2.41159800	-0.08605900	2.00867000
O	-0.85938000	0.09396300	2.36257000

H	0.11997600	2.54504800	0.30974800
O	-3.13606000	1.30399600	2.45970800
H	-3.11830300	1.39487500	3.42316200
O	-2.62710900	-0.15471500	0.47844200
O	-2.96277900	-1.29590300	2.72501600
Na	-3.22199500	-2.33894900	0.75544700
H	-0.36746200	0.68251400	1.73117700

TS4-1

Sum of electronic and thermal Free Energies=-1996.228124

C	-0.04937000	1.14881000	-0.15522700
C	-0.27064800	1.03286900	1.27194400
C	0.65639600	0.32266800	2.15853600
C	1.71179000	-0.51831500	1.72148500
C	0.41331900	0.33709700	3.55149800
C	2.43186100	-1.32054600	2.61217900
H	2.01013800	-0.50111900	0.67955400
C	1.13329300	-0.45786000	4.43348700
H	-0.38717900	0.96648400	3.93082800
C	2.14590900	-1.30793100	3.97554400
H	3.24791000	-1.93197000	2.23199500
H	0.89934500	-0.41903400	5.49372200
H	2.70887200	-1.92455500	4.66826000
C	1.09076600	1.16798200	-0.92258300
C	0.75727500	0.71838500	-2.34516300
H	1.38027100	1.23469600	-3.08050300
C	0.96331800	-0.79686000	-2.49541300
C	2.17085700	-1.37105800	-2.04865400
C	-0.01317000	-1.65873900	-3.00787600
C	2.36714500	-2.75391600	-2.07118500
H	2.95921200	-0.71268900	-1.70273700
C	0.17563200	-3.04448000	-3.02921800
H	-0.95715000	-1.26706100	-3.36595100
C	1.35904500	-3.60407100	-2.54861600
H	3.31322500	-3.16676200	-1.73115200
H	-0.61373200	-3.68393400	-3.41158700
H	1.50800000	-4.67949100	-2.56792400
C	2.41730900	1.63646300	-0.55450600
C	2.68351300	2.29541900	0.66669700
C	3.96222100	2.76511300	0.92098300
H	1.88799900	2.43661100	1.38509900
C	4.61761900	1.93404300	-1.21641000
C	4.96509400	2.58289100	-0.03492800
H	4.17638000	3.27192100	1.85730600
H	5.36149700	1.77395200	-1.99526800
H	5.97878800	2.93227300	0.12809400
N	3.39257400	1.47046100	-1.48116900
C	-3.46849100	3.77282700	-0.01377600
C	-2.30628100	3.05151500	-0.27978500
C	-2.39547900	1.73114600	-0.72852900
C	-3.64408900	1.14067100	-0.92503700
C	-4.80387900	1.86981500	-0.66802300
C	-4.71921500	3.18467000	-0.20952700
H	-3.39694100	4.79537300	0.34388100
H	-1.32807900	3.49888800	-0.13515400
H	-3.70312000	0.10986900	-1.25764000

H	-5.77301400	1.40312900	-0.81190900
H	-5.62348300	3.74724800	0.00007500
N	-1.20705600	0.97059100	-1.03701900
H	-1.54312000	-0.58559800	-0.74523000
C	-0.70126300	1.18411400	-2.42167400
H	-0.72734100	2.25492500	-2.65645900
H	-1.33795600	0.66176600	-3.13617800
P	-2.22727300	-1.90506000	0.96503100
O	-2.39425600	-0.54044800	1.68588500
H	-0.84519000	1.82980900	1.74652900
O	-3.73317800	-2.44086100	0.71838900
H	-3.77263500	-3.37658500	0.96108000
O	-1.61164100	-1.58028200	-0.49436600
O	-1.35261500	-2.97962200	1.55699200
Na	0.45660000	-2.47549900	0.29863500
H	-1.50417200	0.12426500	1.48558700

TS4-2

Sum of electronic and thermal Free Energies=-1996.227274

C	-0.73727600	-0.33285100	-0.73078800
C	-1.90024100	-0.54681500	-0.03615700
C	-2.75106000	0.32658800	0.76092000
C	-2.46217300	1.66024800	1.13408900
C	-3.94716100	-0.23470500	1.27543600
C	-3.32600000	2.37891400	1.95754400
H	-1.55163200	2.13201100	0.80259000
C	-4.80595300	0.48868700	2.09214000
H	-4.19187400	-1.26119100	1.01481900
C	-4.50368300	1.80874500	2.43808800
H	-3.06690800	3.39896600	2.22560600
H	-5.71409900	0.02142200	2.46210800
H	-5.17140900	2.37753300	3.07744500
C	0.07922800	0.81344700	-1.06095900
C	1.37287200	0.32158700	-1.75863700
H	1.51176300	0.90666900	-2.67503400
C	2.68566700	0.47678200	-0.98504100
C	2.89682000	1.62984900	-0.20968200
C	3.73751900	-0.44923700	-1.07698300
C	4.09259500	1.82881800	0.48213300
H	2.11422700	2.37776600	-0.17858200
C	4.94488900	-0.25497100	-0.39019700
H	3.63669200	-1.33388400	-1.69580700
C	5.12613500	0.88509400	0.40445300
H	4.22172500	2.72689100	1.07816400
H	5.74915100	-0.97786000	-0.50081600
H	6.06660600	1.05202800	0.92199500
C	-0.45385900	2.08614800	-1.53815100
C	-1.82987000	2.32973600	-1.75158100
C	-2.24117000	3.57349700	-2.20640700
H	-2.54686100	1.53789400	-1.58119800
C	0.04799600	4.23270500	-2.25702800
C	-1.28938700	4.56401600	-2.46078000
H	-3.29751600	3.76591800	-2.37241700
H	0.83011100	4.96313700	-2.46168600
H	-1.56995900	5.55027900	-2.81403200
N	0.46773100	3.04595500	-1.81188500
C	-2.04730300	-4.23949400	-2.49547800

C	-1.43359600	-3.00127900	-2.32520100
C	-0.58941200	-2.78661300	-1.23084100
C	-0.37569400	-3.80547900	-0.30232700
C	-0.99661400	-5.04396700	-0.47448400
C	-1.82817400	-5.26437400	-1.57142400
H	-2.70296600	-4.40350500	-3.34499100
H	-1.62053100	-2.19214700	-3.02341300
H	0.26218000	-3.61707800	0.55454600
H	-0.83176500	-5.83302000	0.25247800
H	-2.31033400	-6.22774900	-1.70441300
N	0.06981900	-1.51817200	-1.04438600
H	0.84023800	-1.45959200	0.34790300
C	0.99685600	-1.12112100	-2.12549600
H	0.48278300	-1.13496800	-3.09421500
H	1.81777300	-1.83783600	-2.17010800
P	0.80349900	-0.28620200	2.35617500
O	0.53605700	1.07679700	1.62367800
H	-2.22720800	-1.58109400	-0.01429500
O	-0.58393000	-0.81176100	2.95178800
H	-1.34759300	-0.48229800	2.44058400
O	1.32664200	-1.35686000	1.25501000
O	1.89361800	-0.24015700	3.38625900
Na	3.47800900	-0.83530200	1.95001000
H	0.39316100	1.03069600	0.57709000

V

Sum of electronic and thermal Free Energies=-1996.268932

C	0.64637600	0.81925500	-0.51454800
C	1.62726300	1.56034300	0.02739700
C	2.82555100	1.03905500	0.69880300
C	2.76783500	-0.06080200	1.57224300
C	4.07012000	1.64287400	0.45455300
C	3.93716900	-0.57236700	2.13084600
H	1.80376300	-0.48679400	1.82955500
C	5.23509200	1.13083200	1.01982300
H	4.12000900	2.50645700	-0.20392000
C	5.17416800	0.01091000	1.85159600
H	3.87750000	-1.42787000	2.79717600
H	6.19064800	1.60292200	0.80960200
H	6.08192700	-0.39317800	2.28994300
C	0.52675200	-0.68471100	-0.66190800
C	-0.57275300	-0.90075700	-1.76558500
H	-0.10265600	-1.38130200	-2.63077700
C	-1.71717700	-1.81687900	-1.34144600
C	-1.50807400	-2.83145400	-0.39176600
C	-2.98347900	-1.72694900	-1.94155500
C	-2.54087500	-3.70107000	-0.03177800
H	-0.52912700	-2.95036800	0.05993800
C	-4.02146900	-2.59661600	-1.58654700
H	-3.17315400	-0.97950600	-2.70474700
C	-3.80677300	-3.58824900	-0.62033100
H	-2.35330600	-4.46849200	0.71254000
H	-4.98642700	-2.51192900	-2.07863000
H	-4.60304400	-4.27650700	-0.35182400
C	1.79246200	-1.44977900	-0.97492500
C	2.82462700	-0.91994500	-1.75621100
C	3.95534200	-1.69299700	-1.99270700

H	2.75126400	0.09575600	-2.12577100
C	2.92569800	-3.43484500	-0.72222700
C	4.01585400	-2.98016800	-1.46003900
H	4.78097900	-1.29402300	-2.57396000
H	2.92578300	-4.43670500	-0.29769600
H	4.88228000	-3.61534800	-1.61036900
N	1.83616900	-2.69686900	-0.48162100
C	-1.14878700	4.85440800	-2.22379300
C	-0.87078700	3.48624700	-2.24868100
C	-0.80995500	2.76449500	-1.05349700
C	-1.03002100	3.41857500	0.16757300
C	-1.29168600	4.78474600	0.18226600
C	-1.35334200	5.50910300	-1.01143400
H	-1.19924500	5.40625900	-3.15751100
H	-0.70159000	2.98868000	-3.19693300
H	-1.01766600	2.85199500	1.09261400
H	-1.46551800	5.28181300	1.13140800
H	-1.56742300	6.57300200	-0.99455900
N	-0.56609100	1.35776400	-1.03609800
H	-1.68604300	0.77216600	0.27525000
C	-0.97564200	0.53446800	-2.17838400
H	-0.43543400	0.81881300	-3.09173900
H	-2.04224500	0.67575900	-2.35975600
P	-1.74542500	-0.03917000	2.39210800
O	-0.35684100	-0.59571200	2.28385500
H	1.54135400	2.64099500	-0.04964900
O	-1.66808000	1.43712200	3.11685100
H	-0.79556800	1.50409200	3.52897100
O	-2.35031900	0.39410100	0.89756600
O	-2.90324100	-0.84998700	2.94184800
Na	-3.91754300	-1.19603900	1.05973100
H	0.15367200	-1.04950500	0.29882300

TS5

Sum of electronic and thermal Free Energies=-1996.244359

C	-0.57168300	0.05294500	-1.05209700
C	-1.24069200	1.29895400	-0.75772500
C	-0.41177800	2.55938100	-0.80524600
C	0.19194100	3.05320400	0.35746700
C	-0.23260300	3.24555900	-2.01189100
C	0.99160400	4.19418600	0.29832300
H	0.04295500	2.52450600	1.29314800
C	0.55801100	4.39257500	-2.06741200
H	-0.70971300	2.87054100	-2.91421100
C	1.17955300	4.86524600	-0.91075700
H	1.47121400	4.55784400	1.20214000
H	0.69163200	4.91390000	-3.01101200
H	1.80242500	5.75400900	-0.95136600
C	0.78368600	-0.38050000	-0.58447800
C	1.04099600	-1.70550400	-1.34291100
H	1.42459500	-1.47854800	-2.34563700
C	2.00399100	-2.63261000	-0.63968100
C	3.12493400	-3.11944900	-1.31685600
C	1.79338900	-3.00306500	0.69759700
C	4.02839300	-3.97040200	-0.67880300
H	3.29397300	-2.82745300	-2.35044400

C	2.69804700	-3.85240900	1.33124100
H	0.93379000	-2.61678400	1.24314300
C	3.81509400	-4.33923900	0.64837300
H	4.89600000	-4.34008800	-1.21726700
H	2.53017000	-4.12991500	2.36736900
H	4.51671600	-4.99900200	1.15009600
C	1.93374600	0.57258300	-0.47767300
C	2.49819800	1.21783100	-1.57992900
C	3.57299300	2.07629200	-1.37876300
H	2.07644100	1.07216100	-2.56842200
C	3.45169400	1.55078600	0.95217300
C	4.06711700	2.24509100	-0.08582800
H	4.01397700	2.61017500	-2.21442900
H	3.79696700	1.65705600	1.97729400
H	4.90312200	2.90565100	0.11650200
N	2.40862600	0.73401900	0.76866200
C	-4.65297600	-1.23525500	-2.91718100
C	-3.26485100	-1.10505900	-2.86575000
C	-2.63384300	-1.10705300	-1.62413000
C	-3.34679900	-1.24583600	-0.43113300
C	-4.73244100	-1.37965500	-0.50031000
C	-5.38429000	-1.37265100	-1.73599900
H	-5.16032800	-1.23019600	-3.87651900
H	-2.67585300	-0.99527000	-3.77070800
H	-2.79480100	-1.24626700	0.50727500
H	-5.30428500	-1.49565800	0.41529400
H	-6.46403300	-1.47712100	-1.78003600
N	-1.20220100	-1.00482100	-1.53940900
H	-1.57871700	1.13841900	0.38517900
C	-0.39188200	-2.24295700	-1.46640900
H	-0.57098800	-2.85986400	-2.34902900
H	-0.69103200	-2.78285500	-0.56356600
P	-1.06449200	-0.11419600	2.58087200
O	-0.84701000	-1.29175700	1.62557100
H	-2.16927900	1.38412500	-1.32772800
O	0.39876600	0.55454400	2.93161200
H	1.07870100	0.39884800	2.24679300
O	-1.89634800	1.04325100	1.85048300
O	-1.75868000	-0.36047600	3.92628500
Na	-3.15651800	1.23817700	3.59807500
H	0.49935100	-0.68202500	0.44258300

VI

Sum of electronic and thermal Free Energies=-1996.275562

C	-0.39655000	-0.15172000	-1.03170500
C	-1.18202800	1.13351600	-1.11061400
C	-0.38590000	2.35120600	-1.52789000
C	-0.51907600	3.55021700	-0.82211700
C	0.47790200	2.30510600	-2.62684600
C	0.20888500	4.67829400	-1.19884700
H	-1.16084700	3.57948100	0.05238300
C	1.21325900	3.42821000	-3.00007700
H	0.59045100	1.37566100	-3.17830100
C	1.08233100	4.61995900	-2.28490500
H	0.10357800	5.59971800	-0.63355700
H	1.88946700	3.37361800	-3.84823600
H	1.65769100	5.49486300	-2.57245900

C	0.90560000	-0.37533700	-0.64428300
C	1.29702600	-1.78691300	-1.08136300
H	1.74190500	-1.72534900	-2.08808100
C	2.25142100	-2.56382600	-0.20112400
C	3.19734000	-3.40952000	-0.79135200
C	2.20078700	-2.48062300	1.19622500
C	4.07224400	-4.16365200	-0.00977100
H	3.24850400	-3.47437100	-1.87572900
C	3.07621800	-3.23228200	1.97860800
H	1.48777900	-1.82325800	1.68108100
C	4.01341800	-4.07623200	1.38084700
H	4.79997500	-4.81364300	-0.48655800
H	3.02707100	-3.15160300	3.06020800
H	4.69567700	-4.65713200	1.99405400
C	1.90762200	0.59229500	-0.21880200
C	3.25030400	0.46100200	-0.62421500
C	4.17982800	1.41772700	-0.24420800
H	3.54801300	-0.38067100	-1.23630300
C	2.43924300	2.53845000	0.93690600
C	3.77122900	2.49471100	0.54447900
H	5.21349400	1.32808200	-0.56427900
H	2.06423600	3.33409500	1.57492200
H	4.46470100	3.26506000	0.86150200
N	1.53899100	1.61526500	0.58327000
C	-4.17944200	-2.55425600	-2.90150000
C	-2.82679500	-2.24950100	-2.77279200
C	-2.36639300	-1.55972400	-1.64461600
C	-3.26293500	-1.17646300	-0.63993100
C	-4.61884800	-1.46674100	-0.79302200
C	-5.08246500	-2.15713300	-1.91304800
H	-4.53009500	-3.08859000	-3.77917300
H	-2.11840800	-2.52908800	-3.54634900
H	-2.91694900	-0.65477900	0.24982200
H	-5.31493800	-1.15548700	-0.01920100
H	-6.13892300	-2.38444800	-2.01796800
N	-0.96863800	-1.31249900	-1.53613300
H	-1.68724100	1.32131800	-0.15834300
C	-0.08606800	-2.44749100	-1.21479600
H	-0.13153900	-3.21932000	-1.98470900
H	-0.39154500	-2.88881200	-0.25421300
P	-1.37486300	0.74495100	2.62413900
O	-0.40503100	-0.51296000	2.23575700
H	-1.98695800	0.96645200	-1.83517300
O	-0.58182800	2.03988300	2.10926100
H	0.18631300	1.82734300	1.48496300
O	-2.71314000	0.62445000	1.86735000
O	-1.57919900	0.74758000	4.12973700
Na	-3.73756700	0.56397100	3.81571800
H	-0.19306000	-0.52374800	1.28246500

VII

Sum of electronic and thermal Free Energies=-1190.357968

C	0.54922000	-0.30732000	-0.92233000
C	1.09203000	-1.64392000	-0.53746000
C	0.07794000	-2.76315000	-0.61033000
C	-0.56526000	-3.21720000	0.54554000

C	-0.24409000	-3.33596000	-1.84531000
C	-1.53281000	-4.21753000	0.45726000
H	-0.32482000	-2.75406000	1.49795000
C	-1.20989000	-4.33748000	-1.93216000
H	0.26173000	-2.98994000	-2.74379000
C	-1.86056000	-4.77706000	-0.77848000
H	-2.03712000	-4.55534000	1.35745000
H	-1.45320000	-4.77436000	-2.89632000
H	-2.61580000	-5.55479000	-0.84243000
C	-0.68918000	0.29981000	-0.48963000
C	-0.85364000	1.53158000	-1.41523000
H	-1.25682000	1.18623000	-2.37830000
C	-1.74717000	2.64020000	-0.91100000
C	-2.74163000	3.14821000	-1.75366000
C	-1.60830000	3.17296000	0.37896000
C	-3.58416000	4.17554000	-1.32911000
H	-2.85921000	2.73177000	-2.75131000
C	-2.45337000	4.19818000	0.80099000
H	-0.85314000	2.77538000	1.05136000
C	-3.44026000	4.70423000	-0.04716000
H	-4.35153000	4.55687000	-1.99637000
H	-2.34055000	4.59963000	1.80363000
H	-4.09552000	5.50167000	0.29079000
C	-1.93614000	-0.46675000	-0.18060000
C	-2.70373000	-1.05820000	-1.19012000
C	-3.87577000	-1.72364000	-0.85349000
H	-2.36142000	-1.02045000	-2.21802000
C	-3.45397000	-1.13515000	1.42380000
C	-4.26698000	-1.76137000	0.48434000
H	-4.47097000	-2.21033000	-1.61962000
H	-3.71391000	-1.14334000	2.47932000
H	-5.17423000	-2.26830000	0.79443000
N	-2.31877000	-0.50094000	1.10718000
C	4.61144000	0.62559000	-3.22437000
C	3.23127000	0.64697000	-3.03493000
C	2.71679000	0.51781000	-1.74359000
C	3.55193000	0.37971000	-0.63212000
C	4.93090000	0.35123000	-0.84250000
C	5.46213000	0.47595000	-2.12701000
H	5.02053000	0.72065000	-4.22509000
H	2.55338000	0.75221000	-3.87623000
H	3.12522000	0.27899000	0.36858000
H	5.59389000	0.23480000	0.00962000
H	6.53741000	0.45697000	-2.27572000
N	1.29685000	0.58894000	-1.55770000
H	1.48646000	-1.51720000	0.48727000
C	0.61790000	1.90973000	-1.62650000
H	0.83179000	2.39857000	-2.57808000
H	0.99469000	2.51612000	-0.79659000
H	1.95666000	-1.86247000	-1.17081000

9. References

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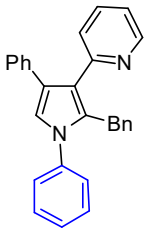
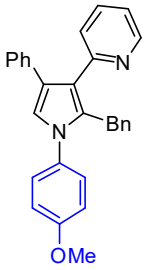
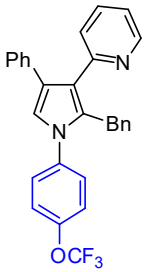
10. Characterization data for products



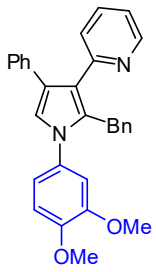
2-(2-Benzyl-1,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (9): yellow oil; 34.2 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.0 Hz, 1H), 7.48 (t, *J* = 6.9 Hz, 1H), 7.35 – 7.29 (m, 3H), 7.23 (d, *J* = 4.2 Hz, 4H), 7.18 (s, 3H), 7.12 – 7.06 (m, 2H), 7.02 (d, *J* = 6.2 Hz, 3H), 6.90 (s, 1H), 6.78 – 6.67 (m, 2H), 4.24 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.6, 149.2, 140.1, 139.7, 135.7, 135.4, 132.1, 128.9, 128.2, 128.1, 128.1, 127.9, 127.6, 126.7, 125.7, 125.6, 125.5, 124.3, 121.8, 120.8, 120.6, 30.6; HRMS (ESI) m/z 387.1854 ($M+H^+$), calc. for $C_{28}H_{22}N_2$ 387.1856.



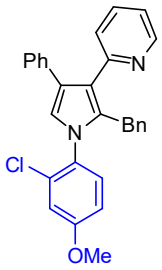
2-(2-Benzyl-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (10): yellow oil; 38.5 mg, 92% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (dd, *J* = 5.3, 1.8 Hz, 1H), 7.49 (td, *J* = 7.7, 1.8 Hz, 1H), 7.23 (d, *J* = 3.9 Hz, 4H), 7.18 (dd, *J* = 5.1, 3.5 Hz, 1H), 7.11 – 7.07 (m, 4H), 7.05 (d, *J* = 7.2 Hz, 3H), 6.85 (dd, *J* = 7.1, 1.6 Hz, 3H), 6.77 – 6.73 (m, 2H), 4.22 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 155.6, 149.1, 140.2, 135.8, 135.5, 132.6, 132.4, 128.2, 128.1, 128.0, 127.9, 125.7, 125.6, 125.5, 123.9, 121.0, 120.6, 114.0, 55.5, 30.5; HRMS (ESI) m/z 417.1959 ($M+H^+$), calc. for $C_{29}H_{24}N_2O$ 417.1961.



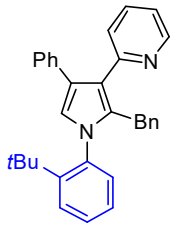
2-(2-Benzyl-4-phenyl-1-(4-(trifluoromethoxy)phenyl)-1*H*-pyrrol-3-yl)pyridine (11): yellow oil; 39.9 mg, 85% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (dd, *J* = 5.1, 1.8 Hz, 1H), 7.50 (td, *J* = 7.7, 1.8 Hz, 1H), 7.25 – 7.21 (m, 4H), 7.20 – 7.16 (m, 5H), 7.12 – 7.08 (m, 2H), 7.03 (dd, *J* = 5.8, 4.2 Hz, 3H), 6.87 (s, 1H), 6.72 (dd, *J* = 7.1, 2.2 Hz, 2H), 4.22 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.3, 149.3, 148.2, 139.7, 138.3, 135.8, 135.1, 132.2, 128.3, 128.2,128.1, 128.1, 128.0, 125.8, 125.7, 124.7, 121.4, 120.8, 120.6, 30.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ –57.97; HRMS (ESI) m/z 471.1676 ($M+H^+$), calc. for $C_{29}H_{21}F_3N_2O$ 471.1679.



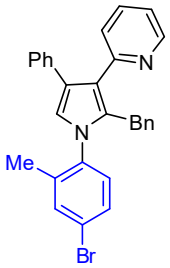
2-(2-Benzyl-1-(3,4-dimethoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (12): yellow oil; 42.9 mg, 96% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.66 – 8.61 (m, 1H), 7.49 (td, *J* = 7.8, 1.9 Hz, 1H), 7.25 – 7.21 (m, 4H), 7.20 – 7.15 (m, 1H), 7.14 – 7.04 (m, 5H), 6.93 (s, 1H), 6.89 – 6.82 (m, 2H), 6.43 (t, *J* = 2.3 Hz, 1H), 6.34 (d, *J* = 2.3 Hz, 2H), 4.26 (s, 2H), 3.63 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.7, 155.5, 149.3, 141.3, 140.5, 135.7, 135.3, 131.6, 128.2, 128.1, 128.0, 125.6, 125.6, 125.5, 124.2, 120.6, 104.8, 100.5, 55.3, 30.7; HRMS (ESI) m/z 447.2062 ($M+H^+$), calc. for $C_{30}H_{26}N_2O_2$ 447.2067.



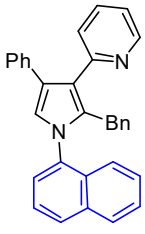
2-(2-Benzyl-1-(2-chloro-4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (13): yellow oil; 37.3 mg, 83% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.66 (dd, *J* = 5.4, 1.6 Hz, 1H), 7.52 (td, *J* = 7.7, 1.6 Hz, 1H), 7.23 (d, *J* = 4.1 Hz, 4H), 7.20 – 7.16 (m, 1H), 7.15 – 7.10 (m, 2H), 7.06 – 6.99 (m, 4H), 6.96 (d, *J* = 2.8 Hz, 1H), 6.77 (s, 1H), 6.76 – 6.70 (m, 3H), 4.25 (d, *J* = 16.1 Hz, 1H), 4.04 (d, *J* = 15.8 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.7, 155.6, 149.3, 139.6, 135.6, 135.4, 133.4, 133.00, 130.6, 129.9, 128.3, 128.1, 127.8, 125.7, 125.6, 125.5, 124.0, 120.9, 120.5, 114.9, 112.8, 55.7, 30.7; HRMS (ESI) m/z 451.1571 ($M+H^+$), calc. for $C_{29}H_{23}ClN_2O$ 451.1572.



2-(2-Benzyl-1-(2-(*tert*-butyl)phenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (14): yellow oil; 38.1 mg, 86% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.1 Hz, 1H), 7.58 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.48 (td, *J* = 7.7, 1.8 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.23 (t, *J* = 6.6 Hz, 4H), 7.20 – 7.15 (m, 1H), 7.09 (dd, *J* = 11.3, 5.1 Hz, 2H), 7.03 (dd, *J* = 7.1, 3.3 Hz, 4H), 6.85 (s, 1H), 6.80 – 6.70 (m, 3H), 4.43 (d, *J* = 15.7 Hz, 1H), 3.71 (d, *J* = 15.8 Hz, 1H), 1.22 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.3, 139.7, 138.9, 136.8, 135.6, 132.00, 128.7, 128.7, 128.5, 128.3, 128.1, 127.8, 125.9, 125.8, 125.5, 123.4, 122.2, 120.4, 36.0, 31.7, 31.3; HRMS (ESI) m/z 443.2479 ($M+H^+$), calc. for $C_{32}H_{30}N_2$ 443.2482.

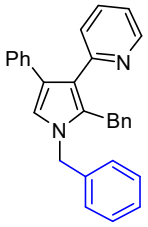


2-(2-Benzyl-1-(4-bromo-2-methylphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (15): Brown solid; Mp: 82-83 °C; 40.7 mg, 85% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.2 Hz, 1H), 7.53 (td, *J* = 7.8, 1.8 Hz, 1H), 7.34 (s, 1H), 7.31 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.26 – 7.21 (m, 4H), 7.19 (dd, *J* = 6.1, 2.4 Hz, 1H), 7.15 (d, *J* = 3.2 Hz, 1H), 7.13 (s, 1H), 7.06 – 7.00 (m, 3H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.73 – 6.63 (m, 3H), 4.08 (s, 2H), 1.79 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.3, 149.1, 139.4, 138.8, 137.5, 135.9, 135.3, 133.5, 132.7, 130.0, 129.5, 129.3, 128.4, 128.3, 128.2, 127.9, 125.8, 125.7, 125.7, 124.3, 122.2, 120.7, 120.2, 116.3, 30.7, 17.1; HRMS (ESI) m/z 479.1115 ($M+H^+$), calc. for $C_{29}H_{23}BrN_2$ 479.1117.

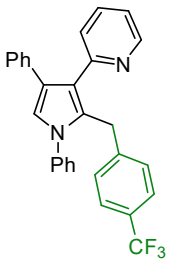


2-(2-Benzyl-1-(naphthalen-1-yl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (16): yellow oil; 34.4 mg, 79% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.8 Hz, 1H), 7.87 (d, *J* = 7.8 Hz, 2H), 7.55 (td, *J* = 8.0, 1.3 Hz, 1H), 7.48 (dd, *J* = 7.7, 5.7 Hz, 2H), 7.42 (d, *J* = 4.7 Hz, 1H), 7.37 (d, *J* = 8.1 Hz, 1H), 7.26 – 7.23 (m, 4H), 7.22 (s, 1H), 7.18 (d, *J* = 7.7 Hz, 2H), 7.13 (d, *J* = 7.6 Hz, 1H), 6.94 (s, 1H), 6.88 – 6.83 (m, 3H), 6.53 (dd, *J* = 6.1, 2.5 Hz, 2H), 4.30 (d, *J* = 16.0 Hz, 1H), 3.85 (d, *J* = 15.9 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.63, 149.18, 139.81, 135.99, 135.43, 133.85,

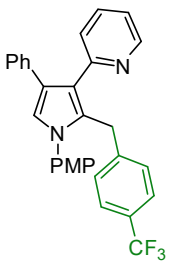
131.05, 128.72, 128.29, 128.18, 128.12, 127.73, 127.61, 127.09, 126.45, 125.84, 125.62, 125.33, 124.87, 124.04, 123.44, 121.79, 120.63, 77.42, 77.00, 76.58, 30.82; HRMS (ESI) m/z 437.2011 ($M+H^+$), calc. for $C_{32}H_{24}N_2$ 437.2012.



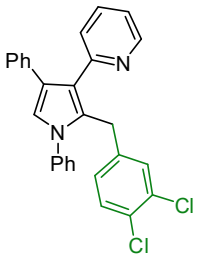
2-(1,2-Dibenzyl-4-phenyl-1*H*-pyrrol-3-yl)pyridine (17): yellow oil; 36.2 mg, 90% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.5 Hz, 1H), 7.49 (t, *J* = 7.2 Hz, 1H), 7.28 (d, *J* = 7.4 Hz, 3H), 7.25 (s, 1H), 7.20 (d, *J* = 6.9 Hz, 5H), 7.17 – 7.13 (m, 2H), 7.11 (s, 1H), 7.06 (dd, *J* = 11.7, 5.6 Hz, 5H), 6.76 (s, 1H), 4.88 (s, 2H), 4.24 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.3, 148.6, 139.7, 137.2, 135.5, 131.4, 128.7, 128.4, 128.2, 128.1, 128.1, 127.5, 126.9, 126.0, 125.8, 125.5, 123.6, 120.6, 120.2, 50.7, 30.3; HRMS (ESI) m/z 401.2011 ($M+H^+$), calc. for $C_{29}H_{24}N_2$ 401.2012.



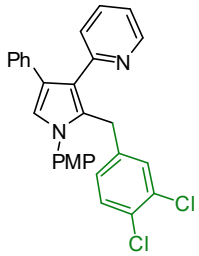
2-(1,4-Diphenyl-2-(4-(trifluoromethyl)benzyl)-1*H*-pyrrol-3-yl)pyridine (18): yellow solid; Mp: 162.4-163.3 °C; 35.4 mg, 78% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (ddd, *J* = 4.9, 1.7, 0.8 Hz, 1H), 7.52 – 7.46 (m, 1H), 7.36 (dd, *J* = 5.0, 1.7 Hz, 3H), 7.29 (s, 1H), 7.27 (s, 1H), 7.25 – 7.22 (m, 4H), 7.18 (dt, *J* = 6.2, 2.5 Hz, 3H), 7.12 – 7.08 (m, 1H), 7.06 (d, *J* = 7.8 Hz, 1H), 6.90 (s, 1H), 6.83 (d, *J* = 8.0 Hz, 2H), 4.31 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.3, 149.3, 144.2, 139.5, 135.8, 135.2, 131.1, 129.1, 128.4, 128.3, 128.2, 127.8, 126.7, 125.8, 125.7, 124.9, 124.8, 124.7, 124.4, 122.4, 121.9, 121.1, 120.8, 30.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ –62.35; HRMS (ESI) m/z 455.1727 ($M+H^+$), calc. for $C_{29}H_{21}F_3N_2$ 455.1730.



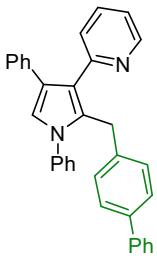
2-(1-(4-Methoxyphenyl)-4-phenyl-2-(4-(trifluoromethyl)benzyl)-1*H*-pyrrol-3-yl)pyridine (19): yellow oil; 36.4 mg, 75% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.1 Hz, 1H), 7.49 (td, *J* = 7.7, 1.8 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.25 – 7.22 (m, 3H), 7.21 – 7.17 (m, 1H), 7.12 – 7.04 (m, 4H), 6.86 (dd, *J* = 5.8, 3.0 Hz, 5H), 4.27 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 155.4, 149.3, 144.4, 135.7, 135.3, 132.4, 131.4, 128.5, 128.3, 128.2, 128.0, 125.7, 125.6, 124.9, 124.8, 124.7, 124.1, 121.5, 121.3, 120.7, 114.1, 55.5, 30.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ –62.30; HRMS (ESI) m/z 485.1837 ($M+H^+$), calc. for $C_{30}H_{23}F_3N_2O$ 485.1835.



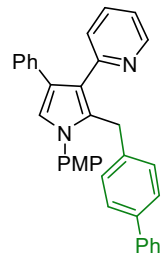
2-(2-(3,4-Dichlorobenzyl)-1,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (20): yellow oil; 32.7 mg, 72% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.1 Hz, 1H), 7.44 – 7.38 (m, 1H), 7.31 (dd, *J* = 5.2, 1.8 Hz, 3H), 7.15 (d, *J* = 4.2 Hz, 4H), 7.11 (dd, *J* = 6.5, 3.1 Hz, 3H), 7.05 – 7.00 (m, 1H), 6.96 (d, *J* = 7.9 Hz, 1H), 6.91 (t, *J* = 1.8 Hz, 1H), 6.81 (s, 1H), 6.51 (d, *J* = 1.7 Hz, 2H), 4.12 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.00, 149.1, 143.4, 139.3, 135.9, 135.1, 134.2, 130.6, 129.2, 128.4, 128.2, 128.1, 126.8, 126.8, 125.9, 125.8, 125.7, 124.4, 121.1, 120.8, 30.3; HRMS (ESI) m/z 455.1076 ($M+H^+$), calc. for $C_{28}H_{20}Cl_2N_2$ 455.1076.



2-(2-(3,4-Dichlorobenzyl)-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (21): yellow oil; 35.3 mg, 73% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.1 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.26 – 7.22 (m, 4H), 7.12 – 7.08 (m, 2H), 7.06 (d, *J* = 2.8 Hz, 2H), 7.02 (dd, *J* = 4.8, 3.0 Hz, 2H), 6.90 (d, *J* = 8.9 Hz, 2H), 6.85 (s, 1H), 6.60 (d, *J* = 1.8 Hz, 2H), 4.15 (s, 2H), 3.85 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 155.2, 149.4, 143.5, 135.7, 135.2, 134.1, 132.2, 130.9, 128.3, 128.2, 128.1, 126.9, 125.8, 125.6, 124.0, 121.3, 120.7, 114.2, 55.6, 30.3; HRMS (ESI) m/z 485.1175 ($M+H^+$), calc. for $C_{29}H_{22}Cl_2N_2O$ 485.1182.

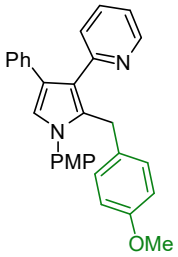


2-(2-([1,1'-Biphenyl]-4-ylmethyl)-1,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (22): yellow oil; 40.4 mg, 87% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.7 Hz, 1H), 7.50 – 7.45 (m, 3H), 7.38 – 7.31 (m, 5H), 7.29 – 7.25 (m, 3H), 7.22 (dd, *J* = 6.1, 3.1 Hz, 6H), 7.18 – 7.14 (m, 1H), 7.11 – 7.05 (m, 2H), 6.91 (s, 1H), 6.78 (d, *J* = 8.1 Hz, 2H), 4.28 (s, 2H);^{13}C NMR (75 MHz, $CDCl_3$) δ 155.5, 149.2, 140.9, 139.7, 139.2, 138.3, 135.7, 135.4, 132.00, 129.00, 128.6, 128.5, 128.3, 128.2, 127.6, 126.9, 126.8, 126.7, 126.6, 125.7, 125.6, 124.3, 120.8, 120.6, 30.3; HRMS (ESI) m/z 463.2164 ($M+H^+$), calc. for $C_{34}H_{26}N_2$ 463.2169.

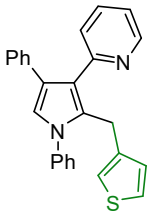


2-(2-([1,1'-Biphenyl]-4-ylmethyl)-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (23): yellow oil; 43.8 mg, 89% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.3 Hz, 1H), 7.52 – 7.47 (m, 3H), 7.36 (d, *J* = 7.8 Hz, 2H), 7.31 – 7.27 (m, 3H), 7.23 (d, *J* = 4.6 Hz, 4H), 7.19 – 7.15 (m, 1H), 7.14 – 7.08 (m, 4H), 6.87 (s, 2H), 6.83 (d, *J* = 5.1 Hz, 2H), 6.79 (s, 1H), 4.24 (s, 2H), 3.81 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 155.6, 149.2, 140.9,

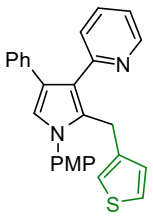
139.4, 138.3, 135.8, 135.4, 132.6, 132.3, 128.6, 128.5, 128.2, 128.1, 128.0, 126.9, 126.8, 126.6, 125.7, 125.6, 123.9, 121.1, 120.6, 116.4, 114.7, 114.0, 55.5, 30.2; HRMS (ESI) m/z 493.2271 ($M+H^+$), calc. for$C_{35}H_{28}N_2O$ 493.2274.



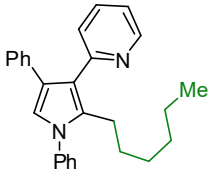
2-(2-(4-Methoxybenzyl)-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (24): yellow oil; 28.5 mg, 64% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.2 Hz, 1H), 7.51 (dd, *J* = 7.7, 6.0 Hz, 1H), 7.23 (d, *J* = 1.1 Hz, 1H), 7.22 – 7.20 (m, 3H), 7.18 (d, *J* = 1.8 Hz, 1H), 7.12 – 7.07 (m, 4H), 6.86 (d, *J* = 9.4 Hz, 3H), 6.65 (d, *J* = 8.7 Hz, 2H), 6.59 (d, *J* = 8.8 Hz, 2H), 4.14 (s, 2H), 3.83 (s, 3H), 3.70 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 157.5, 135.4, 133.0, 132.6, 132.3, 129.1, 128.2, 128.2, 128.0, 125.8, 125.6, 124.0, 121.1, 120.6, 114.0, 113.4, 55.5, 55.1, 29.7; HRMS (ESI) m/z 447.2064 ($M+H^+$), calc. for $C_{30}H_{26}N_2O_2$ 447.2067.



2-(1,4-Diphenyl-2-(thiophen-3-ylmethyl)-1*H*-pyrrol-3-yl)pyridine (25): yellow oil; 31.2 mg, 79% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.2 Hz, 1H), 7.50 (td, *J* = 7.7, 1.7 Hz, 1H), 7.38 (t, *J* = 5.9 Hz, 3H), 7.25 (s, 2H), 7.24 – 7.21 (m, 4H), 7.19 – 7.15 (m, 1H), 7.12 (d, *J* = 5.0 Hz, 1H), 7.08 (d, *J* = 7.8 Hz, 1H), 7.01 (dd, *J* = 4.9, 3.0 Hz, 1H), 6.89 (s, 1H), 6.49 (dd, *J* = 4.9, 0.8 Hz, 1H), 6.42 (d, *J* = 1.8 Hz, 1H), 4.21 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.5, 149.1, 140.3, 139.7, 135.8, 135.3, 132.0, 129.00, 128.3, 128.2, 128.00, 127.7, 126.7, 125.7, 124.7, 124.3, 120.7, 120.7, 120.6, 25.6; HRMS (ESI) m/z 393.1414 ($M+H^+$), calc. for $C_{26}H_{20}N_2S$ 393.1420.

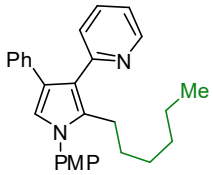


2-(1-(4-Methoxyphenyl)-4-phenyl-2-(thiophen-3-ylmethyl)-1*H*-pyrrol-3-yl)pyridine (26): yellow oil; 35.0 mg, 83% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.1 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.23 (s, 1H), 7.21 (d, *J* = 2.6 Hz, 3H), 7.19 – 7.17 (m, 1H), 7.15 (s, 1H), 7.12 (s, 1H), 7.08 (dd, *J* = 6.3, 2.6 Hz, 2H), 7.02 (dd, *J* = 4.9, 3.0 Hz, 1H), 6.89 (d, *J* = 8.9 Hz, 2H), 6.83 (s, 1H), 6.51 (dd, *J* = 4.9, 1.0 Hz, 1H), 6.45 (d, *J* = 1.8 Hz, 1H), 4.16 (s, 2H), 3.85 (s, 3H);^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 155.8, 149.4, 140.5, 135.6, 135.5, 132.6, 132.2, 128.2, 128.1, 128.1, 128.0, 125.6, 125.5, 124.7, 123.9, 120.9, 120.7, 120.5, 114.8, 114.0, 55.5, 26.0; HRMS (ESI) m/z 423.1523 ($M+H^+$), calc. for $C_{27}H_{22}N_2OS$ 423.1526.

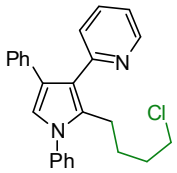


2-(2-Hexyl-1,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (27): yellow oil; 34.3 mg, 90% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.2 Hz, 1H),

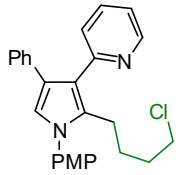
7.54 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.48 (s, 1H), 7.46 (s, 1H), 7.44 (s, 1H), 7.41 (d, *J* = 3.0 Hz, 1H), 7.22 (s, 1H), 7.20 (s, 3H), 7.18 (d, *J* = 0.8 Hz, 1H), 7.13 (d, *J* = 6.0 Hz, 1H), 7.08 (d, *J* = 7.9 Hz, 2H), 6.86 (s, 1H), 2.90 – 2.79 (m, 2H), 1.20 – 1.14 (m, 2H), 1.09 – 1.02 (m, 2H), 0.96 (d, *J* = 3.1 Hz, 4H), 0.72 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.8, 148.9, 140.1, 135.5, 134.5, 129.1, 128.3, 128.1, 127.5, 126.5, 125.8, 125.5, 124.2, 120.4, 120.2, 31.0, 29.5, 28.6, 24.4, 22.3, 13.9; HRMS (ESI) m/z 381.2329 ($M+H^+$), calc. for $C_{27}H_{28}N_2$ 381.2325.



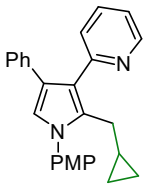
2-(2-Hexyl-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (28): yellow oil; 37.9 mg, 92% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.1 Hz, 1H), 7.50 (td, *J* = 7.7, 1.8 Hz, 1H), 7.34 (d, *J* = 8.8 Hz, 2H), 7.22 – 7.18 (m, 4H), 7.17 – 7.13 (m, 1H), 7.10 (dd, *J* = 5.0, 3.5 Hz, 1H), 7.06 (d, *J* = 7.7 Hz, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.81 (s, 1H), 3.87 (s, 3H), 2.82 – 2.74 (m, 2H), 1.23 – 1.16 (m, 2H), 1.12 – 1.03 (m, 2H), 1.02 – 0.95 (m, 4H), 0.74 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.8, 156.1, 149.2, 135.6, 135.4, 134.6, 133.0, 128.2, 128.0, 127.7, 125.6, 125.4, 123.8, 120.3, 120.3, 120.3, 114.1, 55.5, 31.0, 29.6, 28.6, 24.3, 22.3, 13.9; HRMS (ESI) m/z 411.2427 ($M+H^+$), calc. for $C_{28}H_{30}N_2O$ 411.2431.



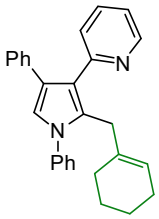
2-(2-(4-Chlorobutyl)-1,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (29): yellow oil; 34.2 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.3 Hz, 1H), 7.55 – 7.46 (m, 3H), 7.43 (d, *J* = 7.3 Hz, 2H), 7.23 – 7.18 (m, 4H), 7.15 (d, *J* = 4.0 Hz, 1H), 7.11 (d, *J* = 6.9 Hz, 1H), 7.06 (d, *J* = 7.9 Hz, 1H), 6.87 (s, 1H), 3.22 (t, *J* = 6.6 Hz, 2H), 2.90 (t, *J* = 7.4 Hz, 2H), 1.47 (dt, *J* = 13.4, 6.7 Hz, 2H), 1.40 – 1.29 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.6, 149.1, 139.9, 135.7, 135.3, 133.3, 129.3, 128.3, 128.1, 127.7, 126.4, 125.7, 125.6, 124.3, 120.9, 120.5, 120.5, 44.4, 31.7, 26.7, 23.6; HRMS (ESI) m/z 387.1619 ($M+H^+$), calc. for $C_{25}H_{23}ClN_2$ 387.1623.



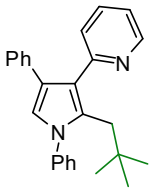
2-(2-(4-Chlorobutyl)-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (30): yellow oil; 35.8 mg, 86% yield;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.1 Hz, 1H), 7.49 (td, *J* = 7.7, 1.7 Hz, 1H), 7.33 (d, *J* = 8.8 Hz, 2H), 7.17 (ddd, *J* = 8.4, 7.6, 4.6 Hz, 5H), 7.11 – 7.08 (m, 1H), 7.04 (d, *J* = 7.9 Hz, 1H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.81 (s, 1H), 3.86 (s, 3H), 3.23 (t, *J* = 6.7 Hz, 2H), 2.82 (dd, *J* = 19.5, 12.0 Hz, 2H), 1.48 (dt, *J* = 13.7, 6.8 Hz, 2H), 1.35 (dt, *J* = 13.5, 6.6 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.00, 155.8, 149.2, 135.5, 133.6, 132.8, 128.9, 128.6, 128.2, 128.1, 127.7, 125.6, 125.5, 123.9, 120.6, 120.4, 114.3, 55.5, 44.4, 31.8, 26.8, 23.6; HRMS (ESI) m/z 417.1724 ($M+H^+$), calc. for $C_{26}H_{25}ClN_2O$ 417.1728.



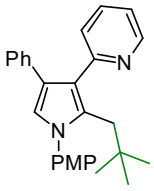
2-(2-(Cyclopropylmethyl)-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (31): yellow oil; 30.9 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.1 Hz, 1H), 7.53 (td, *J* = 7.7, 1.7 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.21 (s, 1H), 7.19 (d, *J* = 1.4 Hz, 3H), 7.16 (d, *J* = 2.8 Hz, 1H), 7.11 (t, *J* = 5.6 Hz, 2H), 7.01 – 6.96 (m, 2H), 6.83 (s, 1H), 3.87 (s, 3H), 2.75 (d, *J* = 6.7 Hz, 2H), 0.56 – 0.48 (m, 1H), 0.14 – 0.07 (m, 2H), -0.38 (q, *J* = 4.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 156.2, 149.2, 135.6, 135.4, 134.2, 133.7, 133.2, 128.2, 128.1, 128.0, 125.9, 125.4, 123.9, 120.6, 120.4, 114.2, 55.5, 28.8, 11.2, 4.5; HRMS (ESI) m/z 381.1964 ($M+H^+$), calc. for $C_{26}H_{24}N_2O$ 381.1961.



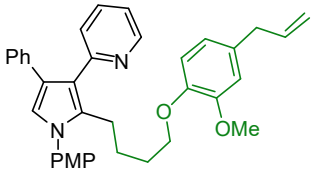
2-(2-(Cyclohex-1-en-1-ylmethyl)-1,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (32): yellow oil; 33.1 mg, 85% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.8 Hz, 1H), 7.52 (td, *J* = 7.7, 1.8 Hz, 1H), 7.47 – 7.43 (m, 1H), 7.42 – 7.35 (m, 4H), 7.22 (d, *J* = 4.2 Hz, 4H), 7.17 – 7.08 (m, 3H), 6.92 (s, 1H), 4.90 (s, 1H), 3.45 (s, 2H), 1.68 (s, 2H), 1.52 (s, 2H), 1.40 – 1.29 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.9, 149.1, 140.1, 135.5, 135.5, 135.1, 131.3, 128.8, 128.1, 128.0, 127.3, 126.4, 125.5, 125.4, 124.0, 122.6, 122.00, 120.4, 120.3, 32.9, 27.9, 25.1, 22.7, 22.2; HRMS (ESI) m/z 391.2164 ($M+H^+$), calc. for $C_{28}H_{26}N_2$ 391.2169.



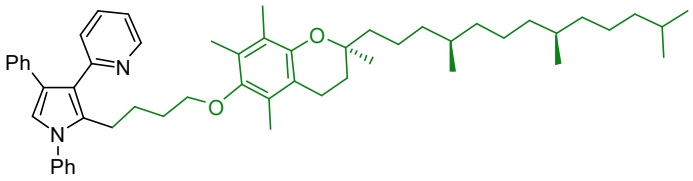
2-(2-Neopentyl-1,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (33): brown solid; Mp: 157.3-158.6 °C; 31.7 mg, 86% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.3 Hz, 1H), 7.38 (d, *J* = 7.9 Hz, 2H), 7.34 (d, *J* = 5.4 Hz, 3H), 7.31 – 7.27 (m, 1H), 7.12 (d, *J* = 1.4 Hz, 1H), 7.09 (d, *J* = 4.3 Hz, 2H), 7.08 – 7.03 (m, 2H), 7.02 (d, *J* = 4.8 Hz, 1H), 6.93 (d, *J* = 7.9 Hz, 1H), 6.76 (s, 1H), 2.98 (s, 2H), 0.30 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.7, 148.9, 140.8, 135.5, 131.5, 129.1, 128.4, 128.0, 127.1, 126.9, 126.7, 125.5, 124.4, 121.4, 120.5, 36.2, 34.2, 29.4; HRMS (ESI) m/z 367.2164 ($M+H^+$), calc. for $C_{26}H_{26}N_2$ 367.2169.



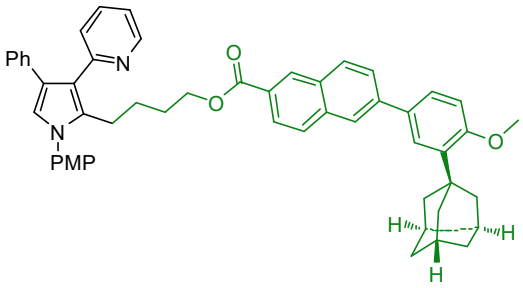
2-(1-(4-Methoxyphenyl)-2-neopentyl-4-phenyl-1*H*-pyrrol-3-yl)pyridine (34): yellow solid; Mp: 148.2-149.8 °C; 27.3 mg, 69% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.9 Hz, 1H), 7.51 (dd, *J* = 10.9, 4.5 Hz, 1H), 7.34 – 7.30 (m, 2H), 7.21 (d, *J* = 1.8 Hz, 1H), 7.19 (s, 1H), 7.16 (s, 2H), 7.14 (d, *J* = 1.8 Hz, 1H), 7.12 – 7.09 (m, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.99 – 6.95 (m, 2H), 6.81 (s, 1H), 3.87 (d, *J* = 4.6 Hz, 3H), 3.03 (s, 2H), 0.42 (d, *J* = 6.5 Hz, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.5, 156.7, 148.6, 135.9, 135.6, 133.8, 131.9, 128.4, 128.1, 128.0, 126.7, 125.5, 124.1, 121.6, 120.5, 114.1, 55.5, 36.2, 34.1, 29.5; HRMS (ESI) m/z 397.2269 ($M+H^+$), calc. for $C_{27}H_{28}N_2O$ 397.2274.



2-(2-(4-(4-Allyl-2-methoxyphenoxy)butyl)-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (35): yellow oil; 47.8 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.1 Hz, 1H), 7.46 (td, *J* = 7.7, 1.8 Hz, 1H), 7.33 (d, *J* = 8.8 Hz, 2H), 7.20 (dd, *J* = 10.1, 4.4 Hz, 5H), 7.06 (dd, *J* = 8.1, 5.2 Hz, 2H), 6.97 – 6.92 (m, 2H), 6.81 (s, 1H), 6.68 – 6.64 (m, 2H), 6.60 (d, *J* = 8.3 Hz, 1H), 5.95 (ddd, *J* = 16.9, 6.7, 3.4 Hz, 1H), 5.11 – 5.07 (m, 1H), 5.04 (s, 1H), 3.84 (s, 3H), 3.79 (s, 3H), 3.66 (t, *J* = 6.7 Hz, 2H), 3.32 (d, *J* = 6.6 Hz, 2H), 2.95 – 2.85 (m, 2H), 1.56 (dd, *J* = 14.0, 7.1 Hz, 2H), 1.38 (dd, *J* = 14.8, 7.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 155.9, 149.2, 146.7, 137.7, 135.6, 135.5, 133.9, 132.9, 132.5, 128.2, 128.1, 127.7, 125.6, 125.5, 123.9, 120.5, 120.3, 120.3, 115.5, 114.2, 112.9, 112.2, 68.3, 55.8, 55.4, 39.7, 28.3, 25.9, 24.0; HRMS (ESI) m/z 545.2800 ($M+H^+$), calc. for $C_{36}H_{36}N_2O_3$ 545.2799.

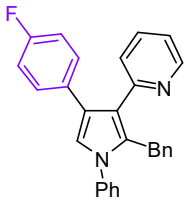


2-(1,4-Diphenyl-2-(4-(((S)-2,5,7,8-tetramethyl-2-((4R,8R)-4,8,12-trimethyltridecyl)chroman-6-yl)oxy)butyl)-1H-pyrrol-3-yl)pyridine (36): yellow oil; 43.9 mg, 56% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.66 (d, *J* = 4.0 Hz, 1H), 7.53 – 7.40 (m, 6H), 7.21 (s, 4H), 7.16 – 7.06 (m, 3H), 6.88 (s, 1H), 3.36 (t, *J* = 6.1 Hz, 2H), 2.94 (t, *J* = 7.1 Hz, 2H), 2.54 (t, *J* = 6.4 Hz, 2H), 2.07 – 1.97 (m, 9H), 1.77 (dd, *J* = 14.8, 6.8 Hz, 3H), 1.53 (dd, *J* = 13.3, 6.5 Hz, 6H), 1.39 (s, 3H), 1.29 (d, *J* = 6.4 Hz, 10H), 1.19 – 1.07 (m, 8H), 0.88 (d, *J* = 6.7 Hz, 12 H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.9, 149.2, 148.4, 147.5, 140.1, 135.5, 133.8, 129.2, 128.3, 128.1, 127.7, 127.6, 126.5, 125.7, 125.7, 125.6, 124.3, 122.6, 121.1, 120.5, 120.3, 117.3, 74.7, 72.6, 40.1, 40.1, 39.4, 37.6, 37.4, 37.4, 37.3, 37.3, 32.8, 32.7, 31.3, 31.2, 29.7, 28.0, 26.3, 24.8, 24.6, 24.4, 23.8, 22.7, 22.6, 21.0, 20.6, 19.7, 19.7, 19.6, 12.7, 11.9, 11.7; HRMS (ESI) m/z 781.5659 ($M+H^+$), calc. for $C_{54}H_{72}N_2O_2$ 781.5667.

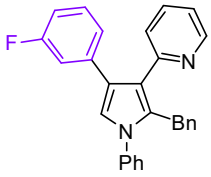


4-(1-(4-Methoxyphenyl)-4-phenyl-3-(pyridin-2-yl)-1H-pyrrol-2-yl)butyl6-(3-((3r,5r,7r)-adamantan-1-yl)-4-methoxyphenyl)-2-naphthoate (37): yellow oil; 57.1 mg, 72% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.2 Hz, 1H), 8.50 (s, 1H), 8.02 (s, 1H), 7.99 – 7.94 (m, 2H), 7.90 (d, *J* = 8.7 Hz, 1H), 7.80 (dd, *J* = 8.6, 1.5 Hz, 1H), 7.62 (d, *J* = 2.2 Hz, 1H), 7.55 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.44 (td, *J* = 7.7, 1.7 Hz, 1H), 7.34 (d, *J* = 8.8 Hz, 2H), 7.23 – 7.20 (m, 3H), 7.20 – 7.14 (m, 2H), 7.10 – 7.04 (m, 2H), 7.00 (d, *J* = 8.5 Hz, 1H), 6.92 (d, *J* = 8.8

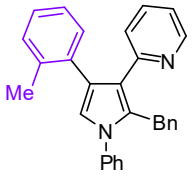
Hz, 2H), 6.83 (s, 1H), 4.13 (t, J = 6.1 Hz, 2H), 3.91 (s, 3H), 3.78 (s, 3H), 2.94 (t, J = 7.4 Hz, 2H), 2.20 (s, 6H), 2.12 (s, 3H), 1.82 (s, 6H), 1.59 – 1.52 (m, 2H), 1.49 – 1.41 (m, 2H); ^{13}C NMR (75 MHz, CD_2Cl_2) δ 166.6, 159.0, 158.9, 141.3, 139.0, 135.9, 135.4, 134.1, 132.7, 132.5, 131.2, 130.6, 129.6, 129.0, 128.3, 128.1, 128.1, 127.7, 127.2, 126.4, 126.2, 125.9, 125.8, 125.7, 125.6, 125.5, 125.2, 124.7, 124.0, 120.8, 120.5, 114.3, 112.1, 64.5, 55.4, 55.1, 40.6, 37.2, 37.1, 29.1, 28.1, 26.2, 24.2; HRMS (ESI) m/z 793.3992 (M+H$^+$), calc. for $C_{54}H_{52}N_2O_4$ 793.4000.



2-(2-Benzyl-4-(4-fluorophenyl)-1-phenyl-1*H*-pyrrol-3-yl)pyridine (38): yellow oil; 33.3 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (ddd, J = 4.8, 1.6, 0.9 Hz, 1H), 7.51 (td, J = 7.7, 1.8 Hz, 1H), 7.37 – 7.31 (m, 3H), 7.22 – 7.16 (m, 4H), 7.13 – 7.02 (m, 5H), 6.97 – 6.91 (m, 2H), 6.88 (s, 1H), 6.73 (dd, J = 7.3, 2.0 Hz, 2H), 4.24 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.3 (d, J = 242.7 Hz), 155.4, 149.3, 140.00, 139.6, 135.8, 132.0, 131.4 (d, J = 3.2 Hz), 129.6 (d, J = 7.7 Hz), 128.9, 128.1, 127.9, 127.6, 126.7, 125.5, 125.5, 123.3, 121.8, 120.7, 120.6, 115.0 (d, J = 21.1 Hz), 30.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ –117.59, –117.60; HRMS (ESI) m/z 405.1758 (M+H$^+$), calc. for $C_{28}H_{21}FN_2$ 405.1762.

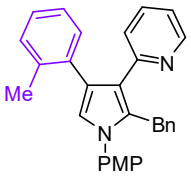


2-(2-Benzyl-4-(3-fluorophenyl)-1-phenyl-1*H*-pyrrol-3-yl)pyridine (39): yellow oil; 30.2 mg, 75% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.66 (dd, J = 5.2, 1.9 Hz, 1H), 7.53 (td, J = 7.7, 1.8 Hz, 1H), 7.36 – 7.33 (m, 3H), 7.21 – 7.16 (m, 3H), 7.14 – 7.11 (m, 2H), 7.03 (dd, J = 5.9, 4.5 Hz, 3H), 6.99 (d, J = 7.8 Hz, 1H), 6.95 – 6.90 (m, 2H), 6.85 (dd, J = 8.4, 6.1 Hz, 1H), 6.72 (dd, J = 7.2, 2.0 Hz, 2H), 4.21 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.7 (d, J = 242.7 Hz), 155.2, 149.4, 139.9, 139.5, 137.7, 137.6, 135.9, 132.2, 129.5 (d, J = 8.6 Hz), 129.0, 128.1, 127.9, 127.7, 126.7, 125.6, 123.8 (d, J = 2.7 Hz), 123.2, 121.0, 120.9, 114.7 (d, J = 21.6 Hz), 112.5, 112.2, 30.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ –113.93, –113.94; HRMS (ESI) m/z 405.1756 (M+H$^+$), calc. for $C_{28}H_{21}FN_2$ 405.1762.

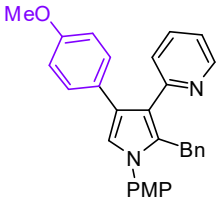


2-(2-Benzyl-1-phenyl-4-(*o*-tolyl)-1*H*-pyrrol-3-yl)pyridine (40): white solid; Mp: 103.3-104.7 °C; 31.7 mg, 79% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (dd, J = 4.9, 0.9 Hz, 1H), 7.38 (d, J = 1.7 Hz, 1H), 7.36 (d, J = 1.8 Hz, 1H), 7.34 (d, J = 1.5 Hz, 2H), 7.31 (d, J = 2.9 Hz, 1H), 7.23 (d, J = 2.6 Hz, 2H), 7.21 (d, J = 1.9 Hz, 1H), 7.19 – 7.15 (m, 3H), 7.06 (s, 1H), 7.04 (s, 2H), 7.01 – 6.98 (m, 1H), 6.86 (d, J = 8.0 Hz, 1H), 6.78 (d, J = 2.1 Hz, 1H), 6.75 (s, 1H), 4.44 (s, 2H), 2.08 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.6, 148.8, 140.4, 139.8, 136.9, 135.9, 135.4, 131.7,

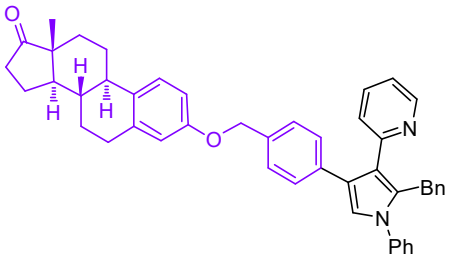
131.3, 131.0, 130.0, 128.9, 128.1, 127.9, 127.5, 126.7, 126.6, 125.4, 125.4, 124.1, 123.6, 121.2, 120.1, 30.7, 20.4; HRMS (ESI) m/z 401.2006 ($M+H^+$), calc. for $C_{29}H_{24}N_2$ 401.2012.



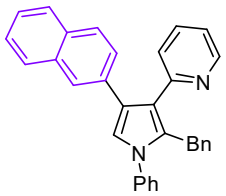
2-(2-Benzyl-1-(4-methoxyphenyl)-4-(*o*-tolyl)-1*H*-pyrrol-3-yl)pyridine (41): yellow oil; 24.8 mg, 58% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.0 Hz, 1H), 7.47 – 7.39 (m, 2H), 7.39 – 7.35 (m, 1H), 7.24 – 7.22 (m, 2H), 7.19 (s, 1H), 7.17 – 7.11 (m, 4H), 7.07 (dd, *J* = 11.7, 6.6 Hz, 2H), 6.94 – 6.92 (m, 1H), 6.90 (d, *J* = 2.8 Hz, 1H), 6.87 – 6.82 (m, 2H), 6.76 (s, 1H), 4.45 (s, 2H), 3.90 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 140.6, 136.9, 135.6, 132.8, 131.8, 131.6, 131.0, 130.00, 128.2, 128.0, 127.9, 126.5, 125.4, 124.1, 123.3, 121.5, 120.0, 114.00, 55.5, 30.7, 20.5; HRMS (ESI) m/z 431.2121 ($M+H^+$), calc. for $C_{30}H_{26}N_2O$ 431.2118.



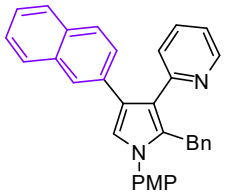
2-(2-Benzyl-1,4-bis(4-methoxyphenyl)-1*H*-pyrrol-3-yl)pyridine (42): white solid; Mp: 133.4-134.7 °C; 19.3 mg, 43% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.62 (dt, *J* = 7.6, 4.0 Hz, 1H), 7.52 – 7.46 (m, 1H), 7.17 – 7.11 (m, 3H), 7.11 – 7.06 (m, 4H), 7.03 (s, 2H), 6.86 – 6.78 (m, 5H), 6.73 (d, *J* = 5.6 Hz, 2H), 4.21 (s, 2H), 3.82 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.8, 157.7, 140.3, 135.7, 132.7, 132.2, 129.3, 128.1, 128.00, 127.9, 125.6, 125.5, 123.5, 120.5, 120.5, 113.9, 113.6, 55.5, 55.2, 30.5; HRMS (ESI) m/z 447.2060 ($M+H^+$), calc. for $C_{30}H_{26}N_2O_2$ 447.2067.



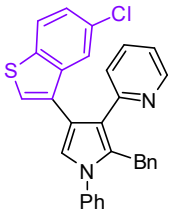
(8S,9R,13R,14R)-3-((4-(5-Benzyl-1-phenyl-4-(pyridin-2-yl)-1*H*-pyrrol-3-yl)benzyl)oxy)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one (43): yellow oil; 46.8 mg, 70% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.2 Hz, 1H), 7.54 (td, *J* = 7.8, 1.7 Hz, 1H), 7.33 (dd, *J* = 5.8, 3.7 Hz, 3H), 7.29 (s, 1H), 7.24 (s, 1H), 7.22 (d, *J* = 1.8 Hz, 1H), 7.17 (dd, *J* = 7.0, 2.8 Hz, 3H), 7.12 (dd, *J* = 5.4, 2.3 Hz, 3H), 7.03 – 7.00 (m, 2H), 6.91 (s, 1H), 6.80 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.74 (s, 1H), 6.72 – 6.68 (m, 2H), 6.64 (dd, *J* = 8.4, 2.6 Hz, 1H), 4.99 (s, 2H), 4.23 (s, 2H), 2.92 – 2.87 (m, 2H), 2.84 – 2.79 (m, 1H), 2.51 (ddd, *J* = 11.5, 8.4, 3.8 Hz, 2H), 2.16 (dd, *J* = 8.8, 3.9 Hz, 1H), 2.09 (d, *J* = 4.6 Hz, 1H), 1.97 (d, *J* = 8.6 Hz, 2H), 1.55 – 1.48 (m, 5H), 0.92 (s, 2H), 0.90 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 221.0, 156.9, 155.1, 154.3, 148.6, 139.8, 139.6, 137.7, 136.5, 134.9, 134.4, 132.5, 132.2, 128.9, 128.3, 128.1, 127.9, 127.7, 127.5, 126.7, 126.3, 126.1, 125.5, 123.9, 120.9, 120.9, 115.5, 114.9, 113.1, 112.4, 70.0, 50.4, 48.0, 44.0, 38.4, 38.3, 35.8, 31.5, 30.6, 29.6, 29.4, 26.5, 25.9, 21.5, 13.8; HRMS (ESI) m/z 669.3477 ($M+H^+$), calc. for $C_{47}H_{44}N_2O_2$ 669.3476.



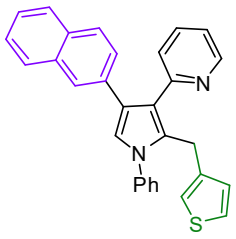
2-(2-Benzyl-4-(naphthalen-2-yl)-1-phenyl-1*H*-pyrrol-3-yl)pyridine (44): brown solid; Mp: 73.4-74.7 °C; 33.2 mg, 76% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.2 Hz, 1H), 7.81 – 7.77 (m, 1H), 7.74 – 7.69 (m, 3H), 7.46 – 7.40 (m, 3H), 7.38 – 7.33 (m, 4H), 7.26 – 7.23 (m, 2H), 7.14 – 7.10 (m, 2H), 7.08 (d, *J* = 6.0 Hz, 2H), 7.04 (d, *J* = 3.7 Hz, 2H), 6.77 (dd, *J* = 7.3, 1.8 Hz, 2H), 4.31 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.5, 149.2, 140.0, 139.7, 135.8, 133.6, 133.00, 132.2, 131.8, 128.9, 128.1, 127.9, 127.7, 127.6, 127.5, 127.5, 127.4, 126.7, 126.1, 125.8, 125.7, 125.5, 125.1, 124.2, 121.1, 120.7, 30.6; HRMS (ESI) m/z 437.2010 ($M+H^+$), calc. for $C_{32}H_{24}N_2$ 437.2012.



2-(2-Benzyl-1-(4-methoxyphenyl)-4-(naphthalen-2-yl)-1*H*-pyrrol-3-yl)pyridine (45): yellow oil; 34.5 mg, 74% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.66 (dd, *J* = 5.5, 1.5 Hz, 1H), 7.80 – 7.76 (m, 1H), 7.71 (d, *J* = 1.8 Hz, 2H), 7.68 (s, 1H), 7.47 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.43 – 7.39 (m, 2H), 7.33 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.14 (s, 1H), 7.12 (d, *J* = 2.7 Hz, 2H), 7.09 (d, *J* = 5.5 Hz, 2H), 7.05 (s, 2H), 6.98 (s, 1H), 6.90 – 6.85 (m, 2H), 6.80 – 6.76 (m, 2H), 4.26 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 155.5, 149.1, 140.2, 135.9, 133.6, 133.1, 132.6, 132.6, 131.8, 128.1, 128.0, 127.9, 127.7, 127.5, 127.5, 126.0, 125.8, 125.7, 125.5, 125.0, 123.9, 121.4, 120.6, 116.4, 114.7, 114.0, 55.5, 30.6; HRMS (ESI) m/z 467.2120 ($M+H^+$), calc. for $C_{33}H_{26}N_2O$ 467.2118.

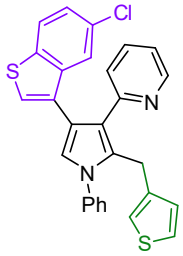


2-(2-Benzyl-4-(5-chlorobenzo[*b*]thiophen-3-yl)-1-phenyl-1*H*-pyrrol-3-yl) pyridine (46): yellow oil; 35.4 mg, 74% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.4 Hz, 1H), 7.72 (t, *J* = 5.3 Hz, 2H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.39 (d, *J* = 1.7 Hz, 1H), 7.37 (d, *J* = 1.6 Hz, 2H), 7.27 (dd, *J* = 4.0, 2.1 Hz, 2H), 7.25 – 7.23 (m, 1H), 7.16 (s, 1H), 7.09 (d, *J* = 6.7 Hz, 1H), 7.05 (d, *J* = 7.1 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.80 – 6.75 (m, 2H), 4.38 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.9, 148.8, 140.0, 139.9, 139.5, 138.2, 136.3, 132.3, 130.6, 130.4, 129.0, 128.1, 128.0, 127.9, 126.8, 125.6, 125.0, 124.9, 124.5, 123.5, 123.1, 121.6, 120.8, 117.0, 30.7; HRMS (ESI) m/z 477.1174($M+H^+$), calc. for $C_{30}H_{21}ClN_2S$ 477.1187.

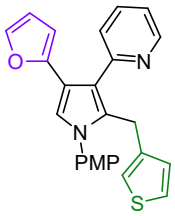


2-(4-(Naphthalen-2-yl)-1-phenyl-2-(thiophen-3-ylmethyl)-1*H*-pyrrol-3-yl)pyridine (47): yellow oil; 35.6 mg, 80% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.2 Hz, 1H), 7.80 – 7.76 (m, 1H), 7.69 (d, *J* = 6.8 Hz, 3H), 7.53 – 7.47 (m, 1H), 7.44 – 7.37 (m, 5H), 7.34 – 7.27 (m, 3H), 7.17 – 7.13 (m, 1H), 7.10 (d, *J* = 7.9 Hz, 1H), 7.04 – 6.99 (m, 2H), 6.53 (dd, *J* = 4.9, 0.9 Hz, 1H), 6.50 (d, *J* = 1.8 Hz, 1H), 4.30 (s, 2H); ^{13}C NMR (75 MHz,

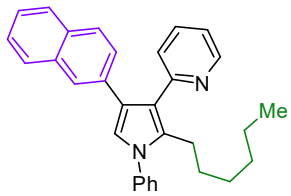
$CDCl_3$) δ 155.3, 149.0, 140.2, 139.6, 136.0, 133.7, 132.9, 132.3, 131.9, 129.0, 128.0, 127.8, 127.7, 127.5, 127.4, 126.7, 126.1, 125.8, 125.8, 125.1, 124.8, 124.3, 121.1, 120.8, 120.7, 25.7; HRMS (ESI) m/z 443.1570 ($M+H^+$), calc. for $C_{30}H_{22}N_2S$ 443.1576.



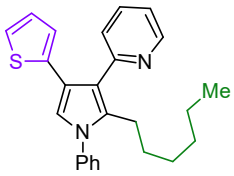
2-(4-(5-Chlorobenzo[*b*]thiophen-3-yl)-1-phenyl-2-(thiophen-3-ylmethyl)-1*H*-pyrrol-3-yl)pyridine (48): yellow oil; 40.1 mg, 83% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.1 Hz, 1H), 7.71 (dd, *J* = 9.0, 5.2 Hz, 2H), 7.42 (d, *J* = 6.8 Hz, 4H), 7.30 (d, *J* = 2.3 Hz, 1H), 7.28 – 7.22 (m, 2H), 7.16 (s, 1H), 7.07 – 7.02 (m, 2H), 6.97 (t, *J* = 3.9 Hz, 2H), 6.55 (d, *J* = 4.9 Hz, 1H), 6.49 (d, *J* = 1.8 Hz, 1H), 4.31 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.9, 148.9, 140.1, 139.9, 139.4, 138.2, 136.2, 132.1, 130.6, 130.4, 129.1, 128.0, 127.9, 126.8, 124.9, 124.5, 123.5, 123.0, 121.4, 120.9, 120.7, 116.9, 25.8; HRMS (ESI) m/z 483.0740 ($M+H^+$), calc. for $C_{28}H_{19}ClN_2S_2$ 483.0751.



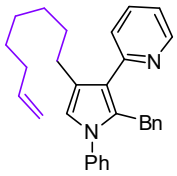
2-(4-(Furan-2-yl)-1-(4-methoxyphenyl)-2-(thiophen-3-ylmethyl)-1*H*-pyrrol-3-yl)pyridine (49): black solid; Mp: 127.4-129.0 °C; 28.0 mg, 68% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (d, *J* = 5.0 Hz, 1H), 7.66 (td, *J* = 7.7, 1.6 Hz, 1H), 7.35 (d, *J* = 7.9 Hz, 1H), 7.28 (d, *J* = 1.1 Hz, 1H), 7.19 (s, 1H), 7.11 (d, *J* = 8.8 Hz, 2H), 7.04 (s, 1H), 7.04 – 7.01 (m, 1H), 6.88 (t, *J* = 5.9 Hz, 2H), 6.54 (d, *J* = 4.8 Hz, 1H), 6.49 (s, 1H), 6.28 (dd, *J* = 3.2, 1.9 Hz, 1H), 5.90 (d, *J* = 3.2 Hz, 1H), 4.04 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 150.0, 140.1, 132.3, 128.0, 127.9, 125.4, 124.9, 121.2, 120.9, 120.4, 114.3, 114.1, 110.8, 104.6, 55.5, 25.6; HRMS (ESI) m/z 413.1315 ($M+H^+$), calc. for $C_{25}H_{20}N_2O_2S$ 413.1318.



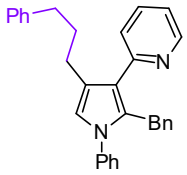
2-(2-Hexyl-4-(naphthalen-2-yl)-1-phenyl-1*H*-pyrrol-3-yl)pyridine (50): yellow oil; 35.2 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.72 – 8.67 (m, 1H), 7.81 – 7.73 (m, 2H), 7.68 (d, *J* = 8.5 Hz, 3H), 7.51 (d, *J* = 1.9 Hz, 1H), 7.48 (d, *J* = 2.2 Hz, 3H), 7.44 (dd, *J* = 5.1, 2.6 Hz, 2H), 7.42 – 7.37 (m, 3H), 7.31 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.13 (dd, *J* = 4.4, 3.1 Hz, 1H), 7.10 (d, *J* = 7.8 Hz, 1H), 6.98 (s, 1H), 2.92 – 2.84 (m, 2H), 1.25 – 1.19 (m, 2H), 1.07 (d, *J* = 6.8 Hz, 2H), 1.03 – 0.97 (m, 4H), 0.74 (t, *J* = 7.0 Hz, 3H);^{13}C NMR (75 MHz, $CDCl_3$) δ 155.8, 148.9, 140.1, 135.8, 134.7, 133.7, 133.1, 131.8, 129.2, 127.7, 127.6, 127.5, 127.5, 127.4, 126.5, 126.0, 125.8, 125.7, 125.0, 124.2, 120.6, 120.5, 31.0, 29.5, 28.6, 24.5, 22.3, 13.9; HRMS (ESI) m/z 431.2473 ($M+H^+$), calc. for $C_{31}H_{30}N_2$ 431.2482.



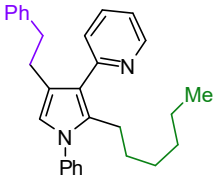
2-(2-Hexyl-1-phenyl-4-(thiophen-2-yl)-1*H*-pyrrol-3-yl)pyridine (51): yellow oil; 31.3 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.1 Hz, 1H), 7.61 (td, *J* = 7.7, 1.8 Hz, 1H), 7.49 (dd, *J* = 7.3, 1.5 Hz, 1H), 7.45 (s, 1H), 7.43 – 7.37 (m, 3H), 7.28 – 7.24 (m, 1H), 7.20 – 7.15 (m, 1H), 7.06 (dd, *J* = 5.1, 1.0 Hz, 1H), 6.92 (s, 1H), 6.88 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.67 (dd, *J* = 3.5, 0.9 Hz, 1H), 2.79 – 2.71 (m, 2H), 1.19 – 1.12 (m, 2H), 1.05 (dd, *J* = 13.3, 6.6 Hz, 2H), 0.99 – 0.92 (m, 4H), 0.72 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.3, 148.9, 139.8, 137.6, 135.9, 134.4, 129.2, 127.7, 127.1, 126.5, 125.8, 123.9, 122.8, 120.9, 120.3, 117.2, 31.0, 29.4, 28.6, 24.4, 22.3, 13.9; HRMS (ESI) m/z 387.1883 ($M+H^+$), calc. for $C_{25}H_{26}N_2S$ 387.1889.



2-(2-Benzyl-4-(oct-7-en-1-yl)-1-phenyl-1*H*-pyrrol-3-yl)pyridine (52): yellow oil; 25.6 mg, 61% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.0 Hz, 1H), 7.64 (td, *J* = 7.7, 1.7 Hz, 1H), 7.35 – 7.32 (m, 1H), 7.31 – 7.26 (m, 3H), 7.16 – 7.10 (m, 3H), 7.07 (dd, *J* = 11.6, 4.3 Hz, 3H), 6.79 – 6.73 (m, 2H), 6.63 (s, 1H), 5.79 (ddt, *J* = 16.9, 10.1, 6.7 Hz, 1H), 5.09 – 4.78 (m, 2H), 4.14 (s, 2H), 2.69 – 2.58 (m, 2H), 2.05 – 1.96 (m, 2H), 1.56 – 1.47 (m, 2H), 1.32 (dd, *J* = 9.7, 4.5 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.3, 149.1, 140.4, 140.1, 139.2, 128.8, 128.00, 127.1, 126.5, 125.5, 124.1, 123.4, 120.4, 119.9, 114.0, 33.8, 30.7, 30.1, 29.4, 28.9, 28.8, 25.8; HRMS (ESI) m/z 421.2640 ($M+H^+$), calc. for $C_{30}H_{32}N_2$ 421.2638.

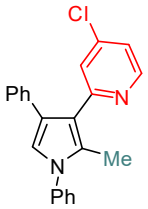


2-(2-Benzyl-1-phenyl-4-(3-phenylpropyl)-1*H*-pyrrol-3-yl)pyridine (53): yellow oil; 26.2 mg, 61% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.1 Hz, 1H), 7.61 (td, *J* = 7.7, 1.8 Hz, 1H), 7.29 (d, *J* = 7.4 Hz, 4H), 7.24 (d, *J* = 7.4 Hz, 2H), 7.16 – 7.12 (m, 5H), 7.11 – 7.09 (m, 1H), 7.08 – 7.02 (m, 3H), 6.77 (d, *J* = 6.8 Hz, 2H), 6.65 (s, 1H), 4.15 (s, 2H), 2.76 – 2.69 (m, 2H), 2.67 – 2.62 (m, 2H), 1.86 (dt, *J* = 15.4, 7.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.8, 149.1, 142.7, 140.4, 140.1, 136.1, 130.3, 128.8, 128.4, 128.1, 128.00, 127.1, 126.5, 125.5, 124.1, 122.9, 120.4, 120.1, 35.7, 31.9, 30.7, 25.5; HRMS (ESI) m/z 429.2318 ($M+H^+$), calc. for $C_{31}H_{48}N_2$ 429.2325.

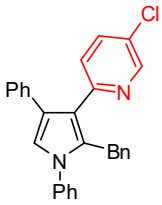


2-(2-Hexyl-4-phenethyl-1-phenyl-1*H*-pyrrol-3-yl)pyridine (54): yellow oil; 27.8 mg, 68% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.1 Hz, 1H), 7.70 (td, *J* = 7.7, 1.6 Hz, 1H), 7.43 (d, *J* = 7.4 Hz, 2H), 7.35 (ddd, *J* = 6.7, 4.3, 1.5 Hz, 4H), 7.23 (dd, *J* = 6.3, 4.7 Hz, 3H), 7.14 (t, *J* = 7.3 Hz, 5H), 6.59 (s, 1H), 2.93 – 2.86 (m, 2H), 2.83 – 2.77 (m, 2H), 2.77 – 2.72 (m, 2H), 1.18 – 1.13 (m, 2H), 1.06 – 0.94 (m, 6H), 0.72 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$)

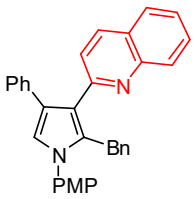
δ 155.9, 148.9, 142.7, 140.4, 136.2, 133.1, 129.0, 128.4, 128.2, 127.2, 126.4, 125.6, 124.3, 122.4, 120.3, 119.5, 36.7, 31.0, 29.6, 28.6, 28.2, 24.5, 22.3, 13.9; HRMS (ESI) m/z 409.2630 ($M+H^+$), calc. for $C_{29}H_{32}N_2$ 409.2638.



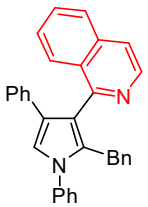
2-(2-Methyl-1,4-diphenyl-1*H*-pyrrol-3-yl)pyridine (55): yellow solid; 171-173 °C; 22.0 mg, 64% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.54 (d, *J* = 5.4 Hz, 1H), 7.47 (d, *J* = 6.4 Hz, 2H), 7.40 (d, *J* = 6.4 Hz, 3H), 7.26 (dd, *J* = 5.0, 2.3 Hz, 2H), 7.22 (s, 2H), 7.20 (d, *J* = 2.6 Hz, 1H), 7.11 (dd, *J* = 5.4, 2.0 Hz, 1H), 7.08 (d, *J* = 1.4 Hz, 1H), 6.89 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.1, 149.7, 143.5, 139.6, 135.0, 130.1, 129.2, 128.3, 128.3, 127.5, 126.1, 126.0, 125.4, 124.5, 120.6, 120.1, 119.7, 12.0; HRMS (ESI) m/z 345.1158 ($M+H^+$), calc. for $C_{22}H_{17}ClN_2$ 345.1153.



2-(2-Benzyl-1,4-diphenyl-1*H*-pyrrol-3-yl)-5-chloropyridine (56): yellow oil; 36.1 mg, 86% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, *J* = 2.2 Hz, 1H), 7.43 (dd, *J* = 8.5, 2.6 Hz, 2H), 7.34 (d, *J* = 0.9 Hz, 1H), 7.33 (d, *J* = 2.4 Hz, 2H), 7.23 (d, *J* = 2.2 Hz, 3H), 7.20 (d, *J* = 2.2 Hz, 1H), 7.18 (dd, *J* = 4.4, 1.7 Hz, 2H), 7.03 (dd, *J* = 6.9, 5.9 Hz, 4H), 6.89 (s, 1H), 6.74 (dd, *J* = 7.3, 1.9 Hz, 2H), 4.22 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.7, 147.9, 139.9, 139.6, 135.6, 135.2, 132.3, 129.0, 128.9, 128.3, 128.3, 128.1, 128.0, 127.7, 126.7, 126.2, 125.8, 125.6, 124.3, 121.0, 120.5, 30.6; HRMS (ESI) m/z 421.1465 ($M+H^+$), calc. for $C_{28}H_{21}ClN_2$ 421.1466.

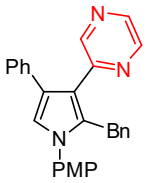


2-(2-Benzyl-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)quinoline (57): yellow oil; 32.6 mg, 70% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.6 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.47 (t, *J* = 7.0 Hz, 1H), 7.25 (dd, *J* = 10.0, 7.0 Hz, 4H), 7.19 (d, *J* = 2.6 Hz, 1H), 7.17 (s, 1H), 7.14 – 7.10 (m, 2H), 6.99 (dd, *J* = 5.8, 4.4 Hz, 3H), 6.91 – 6.87 (m, 2H), 6.85 (t, *J* = 2.6 Hz, 1H), 6.76 – 6.70 (m, 2H), 4.34 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 156.4, 148.3, 140.2, 135.5, 135.1, 133.3, 132.6, 129.2, 129.0, 128.4, 128.2, 128.1, 127.8, 127.4, 126.3, 125.7, 125.7, 125.4, 124.3, 124.2, 121.2, 114.0, 55.5, 30.6; HRMS (ESI) m/z 467.2108 ($M+H^+$), calc. for $C_{33}H_{26}N_2O$ 467.2118.

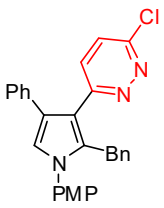


1-(2-Benzyl-1,4-diphenyl-1*H*-pyrrol-3-yl)isoquinoline (58): yellow solid; Mp: 85.2-86.5 °C; 30.1 mg, 69% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (d, *J* = 5.7 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.59 (d, *J* = 5.7 Hz, 1H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.37 (t, *J* = 6.0 Hz, 3H), 7.33 – 7.27 (m, 3H), 7.09 (s, 1H), 7.04 (s, 2H), 7.03 – 6.96 (m, 3H), 6.89 – 6.84 (m, 3H), 6.61 (dd, *J*

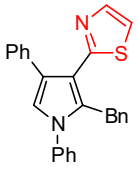
= 6.4, 2.8 Hz, 2H), 4.17 (d, *J* = 16.4 Hz, 1H), 3.85 (d, *J* = 16.2 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.2, 139.8, 139.4, 136.3, 135.3, 132.7, 129.9, 129.0, 128.6, 128.2, 128.1, 128.1, 127.7, 127.6, 127.1, 126.7, 126.4, 125.4, 125.4, 125.3, 120.0, 119.6, 31.0; HRMS (ESI) m/z 437.2014 ($M+H^+$), calc. for $C_{32}H_{24}N_2$ 437.2012.



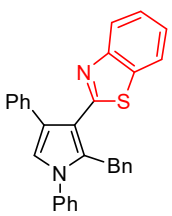
2-(2-Benzyl-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyrazine (59): yellow solid; Mp: 123.6-125.0 °C; 34.6 mg, 83% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 – 8.49 (m, 1H), 8.30 – 8.25 (m, 2H), 7.25 – 7.22 (m, 1H), 7.19 (d, *J* = 7.3 Hz, 2H), 7.07 (s, 1H), 7.06 – 7.03 (m, 2H), 6.84 (d, *J* = 5.9 Hz, 1H), 6.82 (s, 1H), 6.77 (d, *J* = 6.8 Hz, 1H), 4.16 (s, 2H), 3.80 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 151.7, 146.3, 143.8, 140.6, 139.7, 135.00, 133.5, 132.3, 128.5, 128.3, 128.1, 128.0, 128.00, 126.1, 125.8, 124.2, 121.6, 117.9, 114.1, 55.5, 30.6; HRMS (ESI) m/z 440.1725 ($M+Na^+$), calc. for $C_{28}H_{23}N_3O$ 440.1733.



3-(2-Benzyl-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)-6-chloropyridazine (60): brown solid; Mp: 119.6-121.0 °C; 37.0 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (d, *J* = 7.5 Hz, 2H), 7.23 – 7.16 (m, 4H), 7.13 – 7.09 (m, 2H), 7.04 (dd, *J* = 7.9, 6.7 Hz, 4H), 6.87 (dd, *J* = 5.8, 3.1 Hz, 3H), 6.79 (d, *J* = 2.2 Hz, 1H), 6.77 (s, 1H), 4.25 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 157.6, 153.9, 139.7, 134.7, 133.9, 132.1, 130.7, 128.6, 128.5, 128.2, 128.00, 127.00, 126.3, 125.7, 124.1, 121.7, 116.7, 114.2, 55.5, 30.7; HRMS (ESI) m/z 452.1517 ($M+H^+$), calc. for $C_{28}H_{22}ClN_3O$ 452.1524.

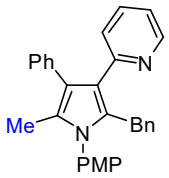


2-(2-Benzyl-1,4-diphenyl-1*H*-pyrrol-3-yl)thiazole (61): brown solid; Mp: 98.7-100.0 °C; 28.6 mg, 73% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, *J* = 3.4 Hz, 1H), 7.37 (s, 1H), 7.35 (d, *J* = 3.0 Hz, 2H), 7.32 (d, *J* = 2.0 Hz, 2H), 7.31 (s, 1H), 7.27 (d, *J* = 2.6 Hz, 1H), 7.20 (dd, *J* = 5.2, 2.4 Hz, 3H), 7.08 (d, *J* = 7.2 Hz, 3H), 6.87 (s, 1H), 6.85 – 6.80 (m, 2H), 4.30 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.4, 142.0, 139.5, 139.3, 134.4, 133.0, 129.0, 128.2, 128.0, 127.9, 126.7, 126.4, 125.7, 124.9, 121.1, 119.0, 115.2, 30.9; HRMS (ESI) m/z 393.1418 ($M+H^+$), calc. for $C_{26}H_{20}N_2S$ 393.1420.

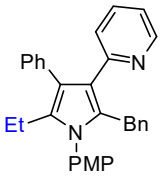


2-(2-Benzyl-1,4-diphenyl-1*H*-pyrrol-3-yl)benzo[*d*]thiazole (62): yellow solid; Mp: 144.1-145.0 °C; 34.1 mg, 77% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.43 – 7.38 (m, 3H), 7.37 – 7.33 (m, 3H), 7.33 – 7.26 (m, 4H), 7.17 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.05 (d, *J*

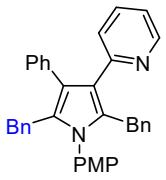
= 6.6 Hz, 3H), 6.86 (s, 1H), 6.85 – 6.77 (m, 2H), 4.41 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.9, 153.4, 139.4, 139.2, 135.9, 134.4, 133.9, 129.4, 129.1, 128.3, 128.2, 128.1, 128.0, 126.8, 126.6, 125.7, 125.5, 125.2, 124.2, 122.7, 121.5, 121.2, 115.7, 31.0; HRMS (ESI) m/z 443.1575 ($M+H^+$), calc. for $C_{30}H_{22}N_2S$ 443.1576.



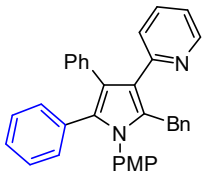
2-(2-Benzyl-1-(4-methoxyphenyl)-5-methyl-4-phenyl-1*H*-pyrrol-3-yl)pyridine (63): yellow oil; 32.7 mg, 76% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 4.9 Hz, 1H), 7.40 – 7.34 (m, 1H), 7.24 – 7.20 (m, 2H), 7.16 (d, *J* = 2.9 Hz, 2H), 7.14 (s, 1H), 6.99 (dd, *J* = 4.9, 2.1 Hz, 4H), 6.96 (s, 1H), 6.93 (d, *J* = 2.1 Hz, 1H), 6.89 (d, *J* = 7.9 Hz, 1H), 6.84 – 6.80 (m, 2H), 6.68 – 6.63 (m, 2H), 4.15 (s, 2H), 3.80 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 155.7, 148.6, 140.5, 136.2, 135.7, 131.2, 131.0, 130.3, 129.8, 128.3, 127.9, 127.7, 127.1, 125.4, 125.3, 125.3, 120.4, 120.1, 114.0, 55.4, 30.9, 11.5; HRMS (ESI) m/z 431.2110 ($M+H^+$), calc. for $C_{30}H_{26}N_2O$ 431.2118.



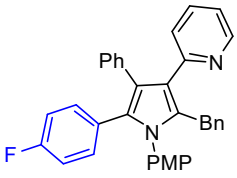
2-(2-Benzyl-5-ethyl-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (64): yellow oil; 36.0 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.9 Hz, 1H), 7.42 (dd, *J* = 7.7, 6.0 Hz, 1H), 7.36 (dd, *J* = 7.2, 4.6 Hz, 1H), 7.32 – 7.30 (m, 1H), 7.29 (s, 1H), 7.28 – 7.22 (m, 3H), 7.08 (s, 1H), 7.05 (dd, *J* = 4.8, 2.0 Hz, 3H), 7.02 (s, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 6.91 – 6.85 (m, 2H), 6.73 (dd, *J* = 7.1, 2.2 Hz, 2H), 4.21 (s, 2H), 3.89 (s, 3H), 2.47 (q, *J* = 7.4 Hz, 2H), 0.84 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 156.0, 148.9, 140.6, 136.5, 135.4, 133.2, 131.7, 131.1, 130.9, 130.4, 130.2, 128.3, 127.9, 127.7, 125.4, 125.3, 125.2, 120.3, 119.9, 113.8, 55.4, 30.8, 18.1, 15.1; HRMS (ESI) m/z 445.2267 ($M+H^+$), calc. for $C_{31}H_{28}N_2O$ 445.2274.



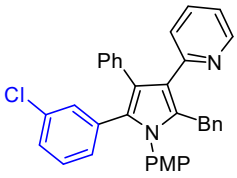
2-(2,5-Dibenzyl-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (65): yellow oil; 41.5 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.1 Hz, 1H), 7.41 (dd, *J* = 7.6, 6.4 Hz, 1H), 7.24 (d, *J* = 4.3 Hz, 4H), 7.19 (dd, *J* = 8.8, 4.9 Hz, 2H), 7.02 (dd, *J* = 4.5, 2.8 Hz, 6H), 6.99 (d, *J* = 1.7 Hz, 2H), 6.92 (d, *J* = 8.0 Hz, 1H), 6.71 – 6.67 (m, 2H), 6.64 (d, *J* = 3.3 Hz, 4H), 4.18 (s, 2H), 3.81 (s, 2H), 3.76 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 140.4, 140.2, 136.0, 130.5, 130.4, 130.0, 129.6, 128.2, 128.1, 128.1, 127.8, 127.7, 125.7, 125.5, 125.4, 125.3, 122.3, 120.1, 113.5, 55.4, 30.9; HRMS (ESI) m/z 507.2424 ($M+H^+$), calc. for $C_{36}H_{30}N_2O$ 507.2431.



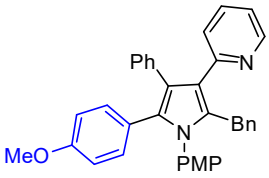
2-(2-Benzyl-1-(4-methoxyphenyl)-4,5-diphenyl-1*H*-pyrrol-3-yl)pyridine (66): yellow oil; 38.4 mg, 78% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.9 Hz, 1H), 7.42 (td, *J* = 7.7, 1.8 Hz, 1H), 7.10 (d, *J* = 1.4 Hz, 2H), 7.08 (s, 4H), 7.04 (d, *J* = 4.3 Hz, 3H), 7.01 (d, *J* = 3.8 Hz, 3H), 6.98 (s, 1H), 6.95 (s, 1H), 6.92 (d, *J* = 3.7 Hz, 1H), 6.88 – 6.82 (m, 4H), 6.68 – 6.65 (m, 2H), 4.21 (s, 2H), 3.74 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.7, 155.8, 149.1, 140.5, 135.6, 135.5, 132.3, 131.9, 131.2, 130.8, 130.3, 128.3, 127.9, 127.6, 127.4, 126.2, 125.7, 125.5, 125.3, 122.1, 120.4, 116.4, 114.8, 113.4, 55.3, 30.8; HRMS (ESI) m/z 493.2261 ($M+H^+$), calc. for $C_{35}H_{28}N_2O$ 493.2274.



2-(2-Benzyl-5-(4-fluorophenyl)-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (67): yellow oil; 40.3 mg, 79% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.4 Hz, 1H), 7.44 (t, *J* = 7.0 Hz, 1H), 7.09 (d, *J* = 1.6 Hz, 4H), 7.08 (s, 3H), 7.01 (dd, *J* = 6.8, 2.6 Hz, 2H), 6.96 (d, *J* = 7.9 Hz, 1H), 6.92 (s, 1H), 6.89 (d, *J* = 2.9 Hz, 1H), 6.86 (d, *J* = 6.1 Hz, 2H), 6.82 (d, *J* = 2.8 Hz, 2H), 6.75 – 6.66 (m, 4H), 4.21 (s, 2H), 3.76 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4 (d, *J* = 244.6 Hz), 158.8, 155.4, 148.8, 140.3, 135.8, 135.3, 132.8 (d, *J* = 8.0 Hz), 130.9 (d, *J* = 3.4 Hz), 130.7, 130.3, 128.3, 127.9, 127.7, 125.8, 125.5, 122.2, 120.5, 114.6 (d, *J* = 21.2 Hz), 113.5, 55.3, 30.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ –115.56; HRMS (ESI) m/z 511.2172 ($M+H^+$), calc. for $C_{35}H_{27}FN_2O$ 511.2180.

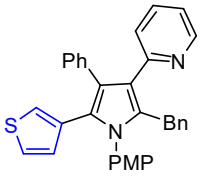


2-(2-Benzyl-5-(3-chlorophenyl)-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (68): yellow oil; 43.1 mg, 82% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.61 (dd, *J* = 4.9, 0.8 Hz, 1H), 7.44 (td, *J* = 7.8, 1.6 Hz, 1H), 7.11 (dd, *J* = 5.1, 3.1 Hz, 4H), 7.07 (s, 2H), 7.05 – 7.00 (m, 3H), 7.00 – 6.97 (m, 1H), 6.95 (s, 1H), 6.93 – 6.90 (m, 2H), 6.85 (dd, *J* = 5.4, 3.4 Hz, 4H), 6.79 (dd, *J* = 7.5, 1.4 Hz, 1H), 6.70 (d, *J* = 8.9 Hz, 2H), 4.22 (s, 2H), 3.76 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.9, 140.2, 135.0, 134.1, 133.2, 131.0, 130.7, 130.7, 130.4, 130.2, 129.3, 128.7, 128.3, 127.9, 127.8, 126.5, 125.8, 125.8, 125.6, 122.8, 120.6, 113.6, 55.4, 30.8; HRMS (ESI) m/z 527.1876 ($M+H^+$), calc. for $C_{35}H_{27}ClN_2O$ 527.1885.

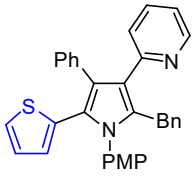


2-(2-Benzyl-1,5-bis(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (69): yellow oil; 45.9 mg, 88% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.9 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.11 – 7.06 (m, 6H), 7.05 – 7.02 (m, 3H), 6.96 (d, *J* = 7.9 Hz, 1H), 6.85 (dd, *J* = 8.7, 3.7 Hz, 6H), 6.67 (d, *J* = 8.9 Hz, 2H), 6.56 (d, *J* = 8.8 Hz, 2H), 4.21 (s, 2H), 3.75 (s, 3H), 3.67 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.6, 157.9, 155.8, 148.9, 140.5, 135.7, 135.6,

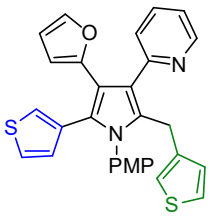
132.3, 132.0, 131.7, 131.2, 130.8, 130.3, 128.3, 127.9, 127.6, 125.7, 125.4, 125.2, 124.7, 121.6, 120.3, 113.4, 112.9, 55.3, 54.9, 30.8; HRMS (ESI) m/z 523.2366 ($M+H^+$), calc. for $C_{36}H_{30}N_2O_2$ 523.2380.



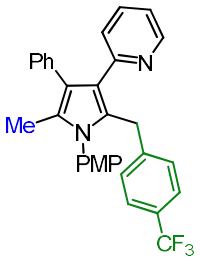
2-(2-Benzyl-1-(4-methoxyphenyl)-4-phenyl-5-(thiophen-3-yl)-1*H*-pyrrol-3-yl)pyridine (70): yellow solid; Mp: 134.3-135.6 ºC; 40.3 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.60 (d, J = 4.1 Hz, 1H), 7.42 (td, J = 7.8, 1.7 Hz, 1H), 7.17 – 7.13 (m, 3H), 7.09 (dd, J = 5.0, 2.5 Hz, 3H), 7.06 (s, 2H), 7.03 (d, J = 6.9 Hz, 1H), 6.95 (d, J = 3.3 Hz, 1H), 6.94 – 6.91 (m, 2H), 6.88 (s, 1H), 6.86 – 6.81 (m, 2H), 6.73 (d, J = 8.9 Hz, 2H), 6.60 (dd, J = 2.9, 1.1 Hz, 1H), 6.50 (dd, J = 5.0, 1.1 Hz, 1H), 4.20 (s, 2H), 3.79 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 155.5, 148.7, 140.4, 135.7, 132.6, 132.6, 132.3, 131.3, 130.8, 130.2, 129.4, 128.3, 127.9, 127.8, 127.1, 125.7, 125.5, 124.0, 123.6, 122.4, 120.4, 113.6, 55.4, 30.9; HRMS (ESI) m/z 499.1837 ($M+H^+$), calc. for $C_{33}H_{26}N_2OS$ 499.1839.



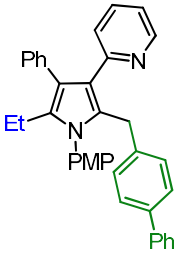
2-(2-Benzyl-1-(4-methoxyphenyl)-4-phenyl-5-(thiophen-2-yl)-1*H*-pyrrol-3-yl)pyridine (71): yellow oil; 35.9 mg, 72% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.60 (d, J = 4.8 Hz, 1H), 7.45 (t, J = 7.4 Hz, 1H), 7.18 – 7.13 (m, 5H), 7.10 – 7.04 (m, 4H), 7.03 – 7.01 (m, 1H), 6.95 (dd, J = 8.2, 5.3 Hz, 3H), 6.82 – 6.78 (m, 2H), 6.75 (s, 1H), 6.73 (d, J = 2.3 Hz, 1H), 6.69 (dd, J = 5.1, 3.6 Hz, 1H), 6.49 (dd, J = 3.5, 0.9 Hz, 1H), 4.23 (s, 2H), 3.78 (d, J = 6.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 140.0, 135.1, 133.4, 130.9, 130.6, 130.5, 128.6, 128.3, 127.9, 127.8, 126.1, 126.0, 125.8, 125.6, 123.9, 120.6, 116.4, 114.8, 114.3, 113.6, 55.4, 31.0; HRMS (ESI) m/z 499.1839 ($M+H^+$), calc. for $C_{33}H_{26}N_2OS$ 499.1839.



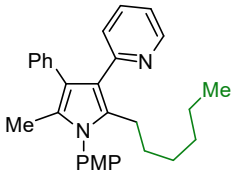
2-(4-(Furan-2-yl)-1-(4-methoxyphenyl)-5-(thiophen-3-yl)-2-(thiophen-3-ylmethyl)-1*H*-pyrrol-3-yl)pyridine (72): yellow solid; Mp: 145.0-146.6 ºC; 30.6 mg, 62% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.63 (d, J = 4.1 Hz, 1H), 7.56 (td, J = 7.8, 1.8 Hz, 1H), 7.31 (d, J = 1.0 Hz, 1H), 7.15 (d, J = 7.9 Hz, 1H), 7.12 – 7.08 (m, 1H), 7.02 (ddd, J = 6.6, 5.0, 3.0 Hz, 2H), 6.93 (d, J = 8.9 Hz, 2H), 6.81 – 6.76 (m, 3H), 6.62 (dd, J = 5.0, 1.0 Hz, 1H), 6.57 (d, J = 4.9 Hz, 1H), 6.48 (d, J = 1.8 Hz, 1H), 6.29 (dd, J = 3.2, 1.9 Hz, 1H), 5.97 (d, J = 3.2 Hz, 1H), 4.13 (s, 2H), 3.80 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.0, 155.1, 149.4, 148.8, 141.0, 140.2, 135.8, 132.5, 131.8, 130.9, 129.9, 128.9, 128.6, 128.2, 124.6, 124.0, 123.7, 120.9, 120.7, 116.4, 114.7, 113.7, 112.1, 110.7, 108.5, 55.3, 25.9; HRMS (ESI) m/z 495.1194 ($M+H^+$), calc. for $C_{29}H_{22}N_2O_2S_2$ 495.1195.



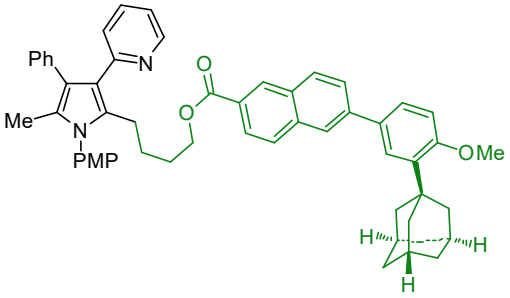
2-(1-(4-Methoxyphenyl)-5-methyl-4-phenyl-2-(4-(trifluoromethyl)benzyl)-1*H*-pyrrol-3-yl)pyridine (73): yellow oil; 39.8 mg, 80% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (d, *J* = 4.2 Hz, 1H), 7.33 (dd, *J* = 7.6, 6.1 Hz, 1H), 7.19 (dd, *J* = 6.9, 5.0 Hz, 4H), 7.11 (t, *J* = 6.1 Hz, 3H), 6.95 (dd, *J* = 6.6, 5.3 Hz, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 9.5 Hz, 2H), 6.75 (d, *J* = 8.4 Hz, 3H), 4.17 (s, 2H), 3.76 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3, 155.4, 148.6, 144.7, 136.0, 135.8, 130.8, 130.3, 129.7, 128.6, 128.0, 127.5, 125.5, 125.4, 124.7, 124.7, 124.6, 124.6, 120.6, 120.2, 114.2, 55.5, 31.0, 11.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ –62.25; HRMS (ESI) m/z 499.1990 ($M+H^+$), calc. for $C_{31}H_{25}F_3N_2O$ 499.1992.



2-(2-([1,1'-Biphenyl]-4-ylmethyl)-5-ethyl-1-(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyridine (74): yellow oil; 43.7 mg, 84% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.76 (d, *J* = 4.9 Hz, 1H), 7.71 (d, *J* = 9.1 Hz, 2H), 7.58 (d, *J* = 7.3 Hz, 2H), 7.51 (t, *J* = 7.4 Hz, 3H), 7.44 (s, 1H), 7.42 (d, *J* = 1.8 Hz, 1H), 7.39 (s, 2H), 7.38 (s, 1H), 7.35 (d, *J* = 1.5 Hz, 2H), 7.32 (s, 1H), 7.29 (s, 1H), 7.04 (t, *J* = 8.9 Hz, 3H), 6.93 (d, *J* = 8.0 Hz, 2H), 4.48 (s, 2H), 3.98 (s, 3H), 2.58 (q, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 141.0, 139.7, 138.2, 136.3, 133.4, 130.8, 130.4, 130.2, 128.7, 128.6, 127.9, 126.9, 126.8, 126.4, 125.5, 125.5, 120.4, 120.1, 116.4, 114.8, 113.9, 55.5, 30.6, 18.2, 15.1; HRMS (ESI) m/z 521.2587 ($M+H^+$), calc. for $C_{37}H_{32}N_2O$ 521.2587.

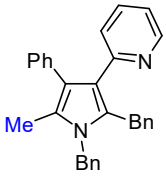


2-(2-Hexyl-1-(4-methoxyphenyl)-5-methyl-4-phenyl-1*H*-pyrrol-3-yl)pyridine (75): yellow oil; 34.3 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.3 Hz, 1H), 7.41 (td, *J* = 8.0, 1.0 Hz, 1H), 7.28 (d, *J* = 2.2 Hz, 1H), 7.26 – 7.24 (m, 2H), 7.22 (s, 1H), 7.15 (t, *J* = 6.2 Hz, 3H), 7.00 (d, *J* = 8.8 Hz, 3H), 7.00 (d, *J* = 8.8 Hz, 3H), 6.87 (d, *J* = 7.9 Hz, 1H), 3.88 (s, 3H), 2.73 (dd, *J* = 9.9, 5.5 Hz, 2H), 2.00 (s, 3H), 1.21 – 1.14 (m, 2H), 1.07 – 1.00 (m, 2H), 0.98 – 0.91 (m, 4H), 0.72 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1, 156.1, 148.6, 136.3, 133.6, 131.4, 130.3, 129.7, 127.8, 126.3, 125.3, 125.2, 122.3, 120.3, 119.8, 114.2, 55.5, 31.0, 29.8, 28.7, 24.7, 22.3, 14.0, 11.6; HRMS (ESI) m/z 425.2585 ($M+H^+$), calc. for $C_{29}H_{32}N_2O$ 521.2587.

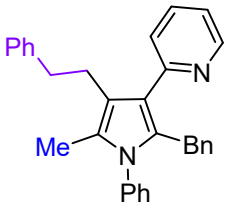


4-(1-(4-Methoxyphenyl)-5-methyl-4-phenyl-3-(pyridin-2-yl)-1*H*-pyrrol-2-yl)butyl 6-(3-((3r,5r,7r)-adamantan-1-yl)-4-methoxyphenyl)-2-naphthoate (76) : yellow oil; 49.2 mg,

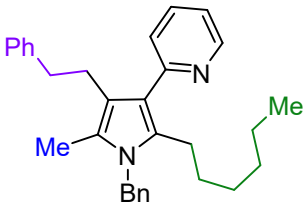
61% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.4 Hz, 1H), 8.47 (s, 1H), 8.00 (d, *J* = 7.9 Hz, 2H), 7.96 (s, 1H), 7.93 – 7.89 (m, 2H), 7.80 (dd, *J* = 8.6, 1.0 Hz, 1H), 7.60 (d, *J* = 1.8 Hz, 1H), 7.55 (dd, *J* = 8.3, 1.8 Hz, 2H), 7.30 (s, 1H), 7.27 (s, 1H), 7.23 (d, *J* = 8.4 Hz, 2H), 7.18 (d, *J* = 3.6 Hz, 1H), 7.12 (d, *J* = 7.0 Hz, 2H), 7.00 (d, *J* = 8.5 Hz, 2H), 6.96 (s, 1H), 6.93 (s, 1H), 4.09 (t, *J* = 6.1 Hz, 2H), 3.91 (s, 3H), 3.81 (s, 3H), 3.02 (s, 2H), 2.19 (s, 6H), 2.11 (s, 3H), 1.98 (s, 3H), 1.81 (s, 6H), 1.49 (dd, *J* = 8.0, 6.4 Hz, 2H), 1.34 (d, *J* = 7.2 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.6, 159.2, 158.9, 157.7, 156.8, 141.3, 139.0, 135.9, 132.5, 131.2, 131.0, 130.6, 130.3, 129.6, 129.5, 128.1, 127.9, 127.2, 126.9, 126.4, 125.9, 125.7, 125.5, 125.4, 124.7, 120.5, 120.1, 114.4, 112.1, 64.6, 55.4, 55.1, 49.1, 40.6, 37.2, 37.1, 33.9, 29.1, 24.9, 11.5; HRMS (ESI) m/z 807.4148 ($M+H^+$), calc. for $C_{55}H_{54}N_2O_4$ 807.4156.



2-(1,2-Dibenzyl-5-methyl-4-phenyl-1*H*-pyrrol-3-yl)pyridine (77): yellow oil; 31.1 mg, 75% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.56 (d, *J* = 4.3 Hz, 1H), 7.44 – 7.38 (m, 1H), 7.29 (s, 1H), 7.27 – 7.24 (m, 3H), 7.22 (d, *J* = 2.9 Hz, 1H), 7.18 (d, *J* = 5.9 Hz, 5H), 7.13 (d, *J* = 7.0 Hz, 1H), 7.06 (d, *J* = 7.1 Hz, 2H), 7.02 (d, *J* = 6.1 Hz, 1H), 6.96 (d, *J* = 7.2 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 1H), 4.97 (s, 2H), 4.30 (s, 2H), 2.15 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.1, 137.7, 136.2, 130.5, 128.7, 128.4, 128.1, 127.9, 127.1, 126.2, 125.9, 125.7, 125.5, 125.4, 120.9, 120.1, 47.3, 30.5, 10.7; HRMS (ESI) m/z 415.2171 ($M+H^+$), calc. for $C_{30}H_{26}N_2$ 415.2169.

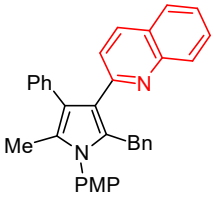


2-(2-Benzyl-5-methyl-4-phenethyl-1-phenyl-1*H*-pyrrol-3-yl)pyridine (78): yellow oil; 30.4 mg, 71% yield; ^{1}H NMR (300 MHz, CD_2Cl_2) δ 8.66 (d, *J* = 3.8 Hz, 1H), 7.63 (t, *J* = 6.9 Hz, 1H), 7.31 (d, *J* = 6.3 Hz, 4H), 7.22 (t, *J* = 7.1 Hz, 2H), 7.16 – 7.03 (m, 7H), 6.98 (d, *J* = 3.5 Hz, 2H), 6.73 (d, *J* = 5.9 Hz, 2H), 3.96 (s, 2H), 2.95 – 2.87 (m, 2H), 2.72 – 2.64 (m, 2H), 1.79 (s, 3H); ^{13}C NMR (75 MHz, CD_2Cl_2) δ 157.0, 150.0, 143.4, 141.3, 139.2, 136.4, 129.4, 129.3, 129.1, 128.6, 128.5, 128.4, 128.3, 126.9, 126.0, 126.0, 124.3, 122.7, 120.7, 118.2, 38.1, 31.4, 27.9, 10.7; HRMS (ESI) m/z 429.2323 ($M+H^+$), calc. for $C_{31}H_{28}N_2$ 429.2325.

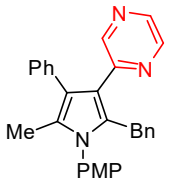


2-(1-Benzyl-2-hexyl-5-methyl-4-phenethyl-1*H*-pyrrol-3-yl)pyridine (79): yellow oil; 27.5 mg, 63% yield; ^{1}H NMR (300 MHz, CD_2Cl_2) δ 8.65 (d, *J* = 4.7 Hz, 1H), 7.67 (td, *J* = 7.7, 1.9 Hz, 1H), 7.32 – 7.28 (m, 2H), 7.26 (d, *J* = 3.2 Hz, 1H), 7.22 (d, *J* = 7.3 Hz, 1H), 7.18 (d, *J* = 7.4 Hz, 2H), 7.14 – 7.09 (m, 2H), 7.07 – 7.03 (m, 2H), 6.89 (d, *J* = 7.1 Hz, 2H), 5.06 (s, 2H), 2.83 (dd, *J* = 9.1, 6.5 Hz, 2H), 2.59 (dd, *J* = 12.3, 5.1 Hz, 4H), 1.90 (s, 3H), 1.43 – 1.32 (m, 3H), 1.15 (td, *J* = 13.5, 8.1 Hz, 7H), 0.80 (t, *J* = 6.8

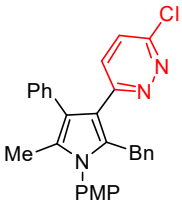
Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.6, 149.8, 143.4, 139.6, 136.1, 131.2, 129.1, 129.1, 128.5, 127.4, 126.2, 125.9, 125.0, 124.4, 121.2, 120.3, 118.1, 47.3, 38.2, 31.9, 31.4, 29.5, 27.8, 25.2, 23.1, 14.3, 10.0; HRMS (ESI) m/z 437.2948 ($M+H^+$), calc. for $C_{31}H_{36}N_2$ 437.2951.



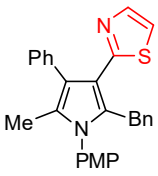
2-(2-Benzyl-1-(4-methoxyphenyl)-5-methyl-4-phenyl-1*H*-pyrrol-3-yl) quinoline (80): yellow oil; 37.0 mg, 77% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 (d, J = 7.7 Hz, 1H), 7.83 (d, J = 8.6 Hz, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.65 (t, J = 7.7 Hz, 1H), 7.44 (t, J = 7.3 Hz, 1H), 7.27 (d, J = 0.9 Hz, 1H), 7.24 (d, J = 2.0 Hz, 2H), 7.20 (dd, J = 6.5, 2.5 Hz, 1H), 7.04 – 6.97 (m, 6H), 6.87 (d, J = 8.9 Hz, 2H), 6.68 (dd, J = 6.5, 2.8 Hz, 2H), 4.32 (s, 2H), 3.85 (s, 3H), 2.02 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 156.6, 148.3, 140.6, 136.4, 134.9, 131.1, 130.4, 129.9, 129.2, 129.0, 128.4, 128.1, 127.8, 127.4, 127.3, 126.2, 125.5, 125.4, 124.2, 120.7, 114.1, 105.3, 55.6, 31.1, 11.6; HRMS (ESI) m/z 481.2273 ($M+H^+$), calc. for $C_{34}H_{28}N_2O$ 481.2274.



2-(2-Benzyl-1-(4-methoxyphenyl)-5-methyl-4-phenyl-1*H*-pyrrol-3-yl)pyr azine (81): brown solid; Mp: 100.2-101.5 ºC; 16.8 mg, 39% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.48 (dd, J = 2.3, 1.6 Hz, 1H), 8.22 (d, J = 2.5 Hz, 1H), 8.15 (d, J = 1.2 Hz, 1H), 7.29 (d, J = 7.4 Hz, 2H), 7.25 – 7.22 (m, 1H), 7.20 (d, J = 1.5 Hz, 1H), 7.18 (s, 1H), 7.05 (dd, J = 5.8, 4.2 Hz, 3H), 6.99 – 6.94 (m, 2H), 6.87 – 6.83 (m, 2H), 6.78 – 6.73 (m, 2H), 4.14 (s, 2H), 3.84 (s, 3H), 2.00 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 152.0, 146.1, 143.6, 140.1, 140.0, 135.8, 132.2, 130.7, 130.2, 129.7, 128.3, 128.2, 127.9, 127.6, 125.9, 125.6, 120.4, 117.6, 114.1, 55.4, 30.9, 11.4; HRMS (ESI) m/z 432.2073 ($M+H^+$), calc. for $C_{29}H_{25}N_3O$ 432.2070.

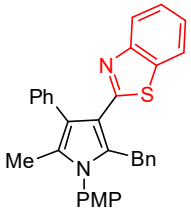


3-(2-Benzyl-1-(4-methoxyphenyl)-5-methyl-4-phenyl-1*H*-pyrrol-3-yl)-6-chloropyridazine (82): yellow oil; 39.1 mg, 84% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30 (d, J = 7.5 Hz, 2H), 7.24 (d, J = 7.2 Hz, 1H), 7.20 – 7.16 (m, 2H), 7.11 (d, J = 9.0 Hz, 1H), 7.06 – 6.99 (m, 4H), 6.97 (s, 1H), 6.87 (d, J = 8.9 Hz, 3H), 6.78 – 6.73 (m, 2H), 4.20 (s, 2H), 3.84 (s, 3H), 1.98 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.4, 157.6, 153.4, 139.9, 135.4, 133.0, 130.5, 130.3, 129.7, 128.4, 128.3, 128.0, 127.8, 127.0, 126.1, 125.6, 120.3, 116.2, 114.2, 55.5, 31.1, 11.4; HRMS (ESI) m/z 466.1682 ($M+H^+$), calc. for $C_{29}H_{24}ClN_3O$ 466.1681.

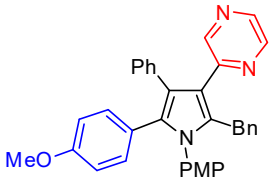


2-(2-Benzyl-1-(4-methoxyphenyl)-5-methyl-4-phenyl-1*H*-pyrrol-3-yl)thiaz ole (83): yellow oil; 35.3 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70 (d, J = 3.3 Hz, 1H), 7.40 – 7.28 (m, 6H), 7.09 (d, J = 3.5 Hz, 4H), 6.95 (d, J = 8.9 Hz, 2H), 6.87 (s, 1H), 6.85 – 6.81 (m, 2H), 4.26 (s, 2H), 3.84 (s, 3H), 1.93

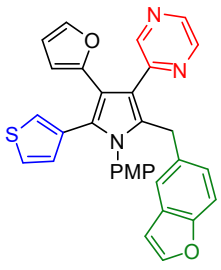
(s, 3H);^{13}C NMR (75 MHz, $CDCl_3$) δ 164.1, 159.3, 141.9, 140.1, 135.5, 131.8, 131.1, 130.6, 129.7, 128.4, 128.0, 127.9, 127.5, 126.3, 125.5, 120.9, 117.8, 114.9, 114.1, 55.5, 31.3, 11.3; HRMS (ESI) m/z 437.1682 ($M+H^+$), calc. for $C_{28}H_{24}N_2OS$ 437.1682.



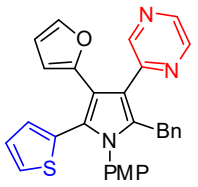
2-(2-Benzyl-1-(4-methoxyphenyl)-5-methyl-4-phenyl-1*H*-pyrrol-3-yl)benzo[*d*]thiazole (84): yellow solid; Mp: 176.3-177.6 ºC; 30.6 mg, 63% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.35 (dd, *J* = 8.9, 3.1 Hz, 5H), 7.25 – 7.18 (m, 2H), 7.08 – 7.03 (m, 3H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.88 – 6.80 (m, 4H), 4.40 (s, 2H), 3.84 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.5, 159.4, 153.4, 140.0, 135.6,135.2, 133.2, 131.2, 130.5, 129.7, 128.5, 128.1, 128.0, 127.9, 126.5, 125.6, 125.3, 123.7, 122.3, 121.2, 121.0, 115.0, 114.1, 55.5, 31.4, 11.2; HRMS (ESI) m/z 487.1844 ($M+H^+$), calc. for $C_{32}H_{26}N_2OS$ 487.1839.



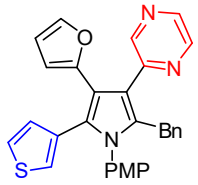
2-(2-Benzyl-1,5-bis(4-methoxyphenyl)-4-phenyl-1*H*-pyrrol-3-yl)pyrazine (85): brown solid; Mp 143.5-145.0 ºC; 43.9 mg, 84% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.53 – 8.49 (m, 1H), 8.25 (d, *J* = 2.5 Hz, 1H), 8.18 (s, 1H), 7.14 (s, 1H), 7.11 (d, *J* = 3.1 Hz, 3H), 7.08 (s, 2H), 7.04 (dd, *J* = 5.7, 1.9 Hz, 2H), 6.89 – 6.83 (m, 6H), 6.68 (d, *J* = 8.8 Hz, 2H), 6.57 (d, *J* = 8.7 Hz, 2H), 4.20 (s, 2H), 3.75 (s, 3H), 3.67 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.8, 158.1, 151.9, 146.4, 143.6, 140.4, 139.9, 135.2, 133.1, 132.3, 132.2, 130.9, 130.7, 130.2, 128.2, 128.0, 125.8, 125.7, 124.3, 121.7, 118.1, 113.6, 113.0, 55.3, 54.9, 30.9; HRMS (ESI) m/z 524.2333 ($M+H^+$), calc. for $C_{35}H_{29}N_3O_2$ 524.2333.



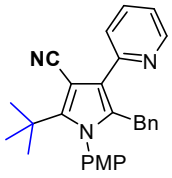
2-(2-(Benzofuran-5-ylmethyl)-4-(furan-2-yl)-1-(4-methoxyphenyl)-5-(thiophen-3-yl)-1*H*-pyrrol-3-yl)pyrazine (86): yellow oil; 42.8 mg, 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.41 (s, 1H), 8.32 (d, *J* = 2.4 Hz, 1H), 7.53 (d, *J* = 2.1 Hz, 1H), 7.34 (d, *J* = 1.0 Hz, 1H), 7.21 (d, *J* = 8.5 Hz, 1H), 7.02 (dd, *J* = 4.9, 2.7 Hz, 2H), 6.85 (s, 1H), 6.81 (d, *J* = 3.1 Hz, 2H), 6.76 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.69 (d, *J* = 8.8 Hz, 2H), 6.63 (d, *J* = 5.0 Hz, 1H), 6.59 (d, *J* = 2.0 Hz, 1H), 6.32 (dd, *J* = 3.1, 1.9 Hz, 1H), 6.03 (d, *J* = 3.2 Hz, 1H), 4.22 (s, 2H), 3.76 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 153.4, 151.3, 148.8, 145.6, 144.9, 143.6, 141.4, 141.0, 134.2, 133.90, 131.4, 130.6, 129.9, 129.3, 128.8, 127.1, 124.7, 124.4, 124.0, 120.5, 118.7, 113.8, 112.0, 110.9, 110.6, 108.8, 106.4, 55.4, 30.7; HRMS (ESI) m/z 530.1533 ($M+H^+$), calc. for $C_{32}H_{23}N_3O_3S$ 530.1533.



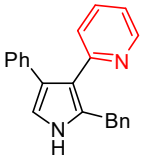
2-(2-Benzyl-4-(furan-2-yl)-1-(4-methoxyphenyl)-5-(thiophen-2-yl)-1*H*-pyrrol-3-yl)pyrazine (87): brown solid; Mp: 142.3-143.7 °C;; 37.7 mg, 75% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.37 (d, *J* = 16.5 Hz, 2H), 7.34 (d, *J* = 1.1 Hz, 1H), 7.12 (dd, *J* = 5.2, 1.0 Hz, 1H), 7.09 (s, 1H), 7.07 (d, *J* = 1.5 Hz, 1H), 6.92 – 6.88 (m, 2H), 6.80 (dd, *J* = 6.1, 2.3 Hz, 3H), 6.75 – 6.71 (m, 2H), 6.66 (dd, *J* = 3.6, 1.0 Hz, 1H), 6.32 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.08 (d, *J* = 2.9 Hz, 1H), 4.14 (s, 2H), 3.78 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.4, 151.2, 148.3, 145.7, 143.7, 141.6, 141.0, 139.3, 134.5, 132.4, 130.2, 130.1, 128.5, 128.2, 128.0, 126.9, 126.3, 126.3, 125.8, 118.9, 116.6, 114.7, 113.8, 113.3, 111.0, 109.1, 55.4, 31.0; HRMS (ESI) m/z 490.1588 ($M+H^+$), calc. for $C_{30}H_{23}N_3O_2S$ 490.1584.



2-(2-Benzyl-4-(furan-2-yl)-1-(4-methoxyphenyl)-5-(thiophen-3-yl)-1*H*-pyrrol-3-yl)pyrazine (88): yellow oil; 40.6 mg, 83% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.40 (s, 1H), 8.35 (s, 1H), 7.34 (d, *J* = 1.1 Hz, 1H), 7.12 (dd, *J* = 5.2, 1.0 Hz, 1H), 7.09 (s, 1H), 7.07 (d, *J* = 1.5 Hz, 1H), 6.92 – 6.88 (m, 2H), 6.80 (dd, *J* = 6.1, 2.3 Hz, 3H), 6.75 – 6.71 (m, 2H), 6.66 (dd, *J* = 3.6, 1.0 Hz, 1H), 6.32 (dd, *J* = 3.2, 1.9 Hz, 1H), 6.08 (d, *J* = 2.9 Hz, 1H), 4.14 (s, 2H), 3.78 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.2, 151.4, 148.8, 145.7, 143.6, 141.4, 141.0, 139.5, 133.7, 131.5, 130.6, 129.9, 129.3, 128.9, 128.2, 128.0, 125.8, 124.4, 124.0, 118.9, 113.8, 112.0, 110.9, 108.8, 55.4, 30.9; HRMS (ESI) m/z 490.1588 ($M+H^+$), calc. for $C_{30}H_{23}N_3O_2S$ 490.1584.

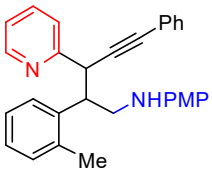


5-Benzyl-2-(*tert*-butyl)-1-(4-methoxyphenyl)-4-(pyridin-2-yl)-1*H*-pyrrole-3-carbonitrile (89): yellow oil; 18.1 mg, 43% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.4 Hz, 1H), 7.81 (t, *J* = 7.4 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.06 – 7.02 (m, 3H), 6.85 (d, *J* = 8.7 Hz, 2H), 6.75 (d, *J* = 9.0 Hz, 2H), 6.65 (dd, *J* = 6.4, 2.9 Hz, 2H), 3.94 (s, 2H), 3.82 (s, 3H), 1.29 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.9, 149.7, 148.5, 138.9, 131.4, 131.1, 130.7, 128.1, 128.0, 125.9, 124.5, 122.0, 118.3, 116.0, 114.7, 114.3, 113.5, 90.3, 55.5, 34.9, 31.5, 30.9; HRMS (ESI) m/z 422.2220 ($M+H^+$), calc. for $C_{28}H_{27}N_3O$ 422.2227.



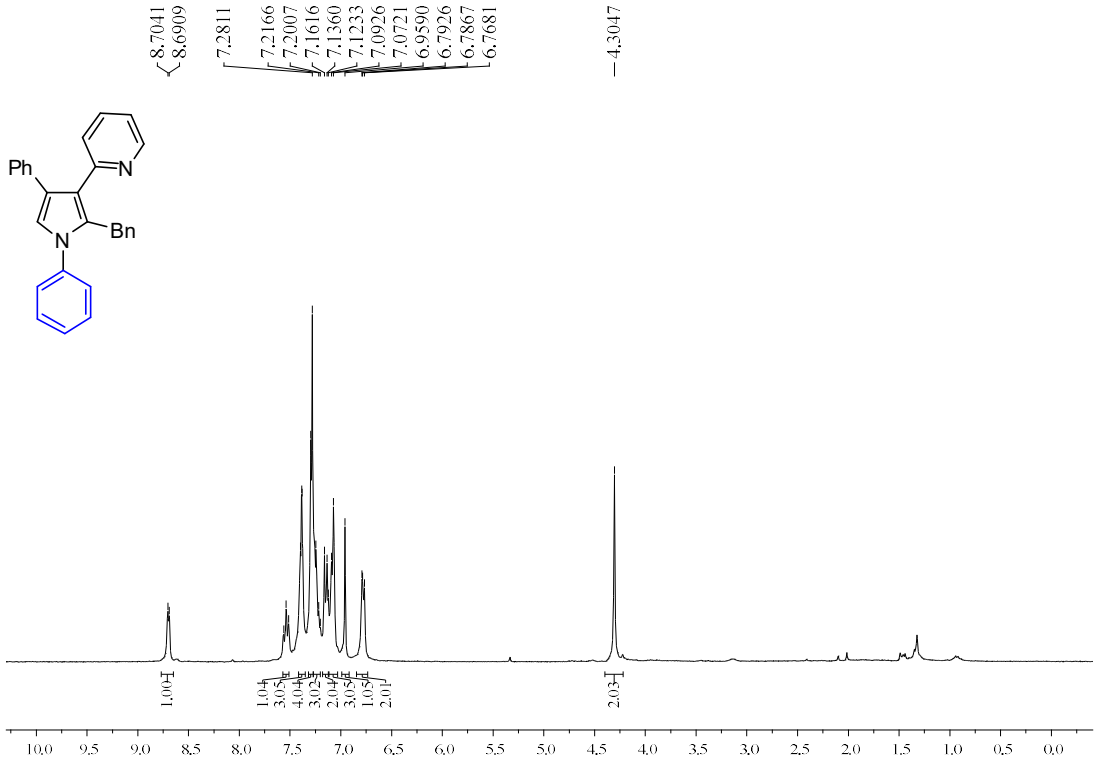
2-(2-Benzyl-4-phenyl-1*H*-pyrrol-3-yl)pyridine (90): yellow oil; 22.3 mg, 72% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.4 Hz, 1H), 8.25 (s, 1H), 7.50 (td, *J* = 7.8, 1.7 Hz, 1H), 7.30 (d, *J* = 7.3 Hz, 2H), 7.21 (dd, *J* = 8.4, 3.4 Hz, 7H), 7.18 – 7.15 (m, 1H), 7.13 – 7.08 (m, 1H), 7.06 (d, *J* = 7.9 Hz, 1H), 6.73 (d,

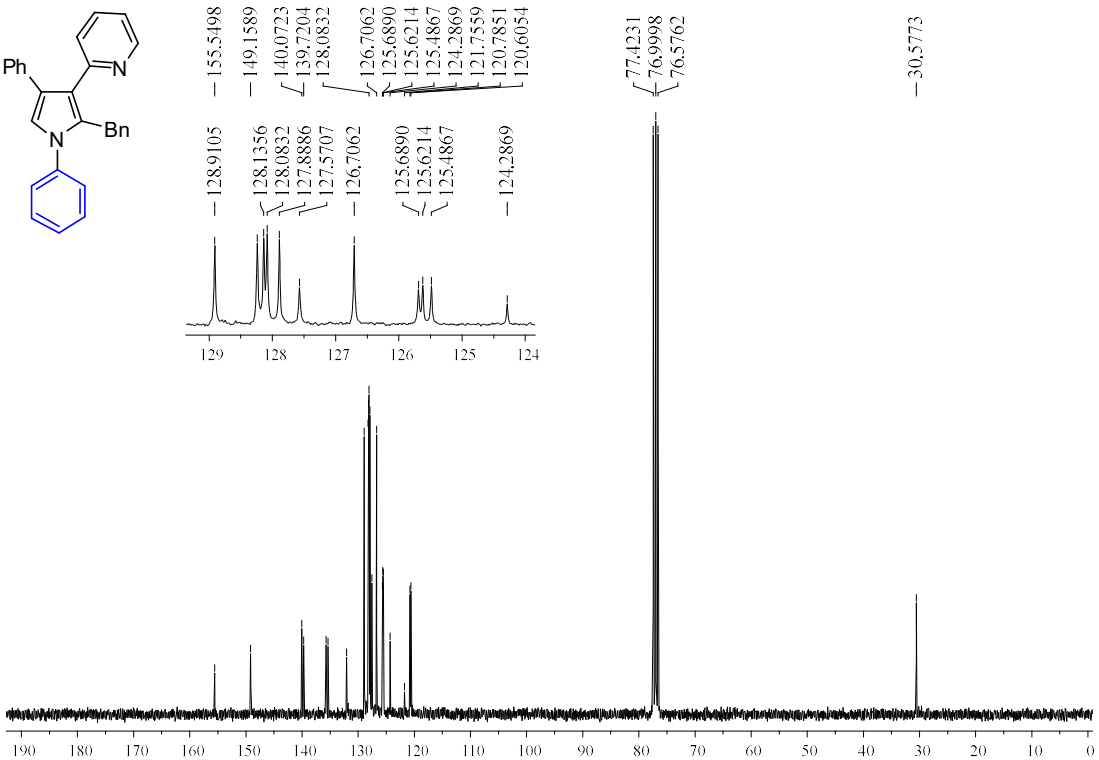
J = 2.6 Hz, 1H), 4.25 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.3, 148.8, 139.2, 135.8, 135.8, 131.1, 128.9, 128.6, 128.4, 128.1, 126.4, 125.6, 125.4, 124.5, 120.4, 119.0, 118.5, 115.5, 32.6; HRMS (ESI) m/z 311.1542 ($M+H^+$), calc. for $C_{22}H_{18}N_2$ 311.1543.

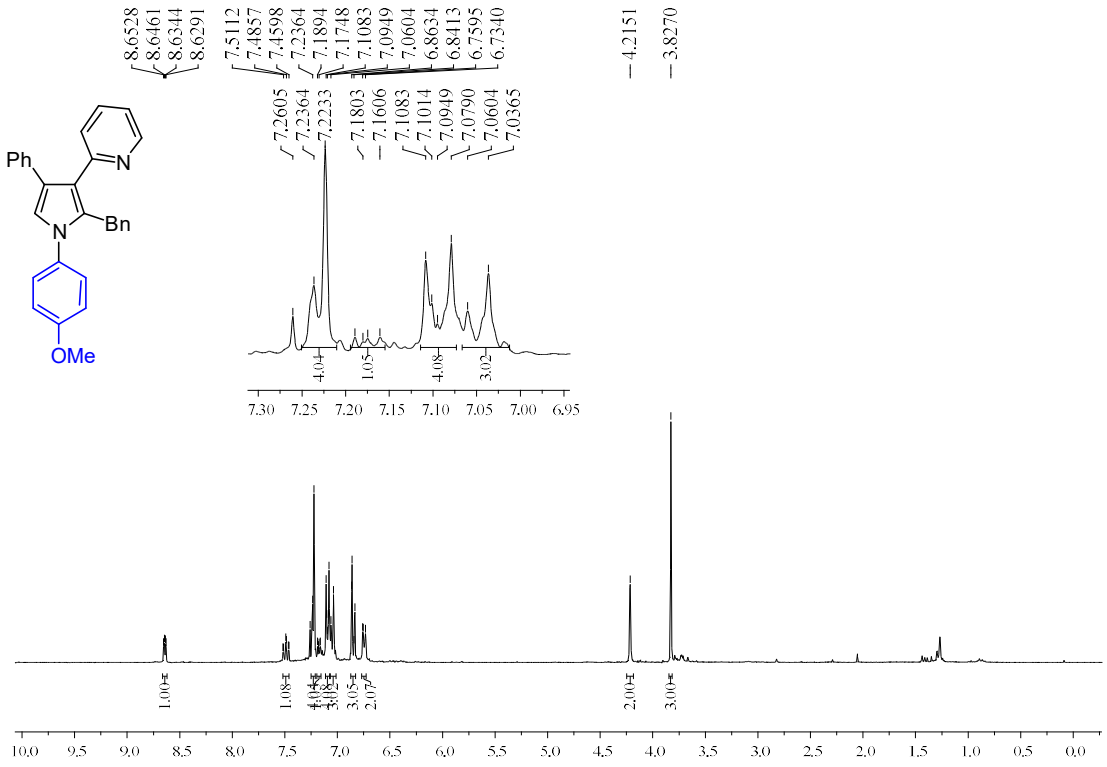


4-Methoxy-*N*-(5-phenyl-3-(pyridin-2-yl)-2-(*o*-tolyl)pent-4-yn-1-yl)anil ine (91): yellow oil; 7.3 mg, 17% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.60 (d, J = 4.1 Hz, 1H), 7.70 (d, J = 7.7 Hz, 1H), 7.56 (td, J = 7.7, 1.7 Hz, 1H), 7.41 (dd, J = 6.7, 3.1 Hz, 2H), 7.35 – 7.33 (m, 2H), 7.28 (d, J = 7.5 Hz, 1H), 7.24 – 7.14 (m, 4H), 7.06 (d, J = 7.5 Hz, 1H), 6.80 – 6.76 (m, 2H), 6.54 (t, J = 6.2 Hz, 2H), 4.61 (d, J = 6.4 Hz, 1H), 3.96 (dd, J = 14.5, 6.5 Hz, 1H), 3.78 (s, 3H), 3.74 – 3.70 (m, 1H), 3.60 – 3.54 (m, 1H), 1.83 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.7, 152.1, 148.9, 142.1, 138.1, 137.5, 136.5, 131.5, 130.0, 128.2, 128.0, 127.2, 126.7, 125.9, 123.3, 122.9, 122.1, 114.8, 114.5, 88.5, 85.6, 55.7, 48.5, 45.3, 44.2, 19.4; HRMS (ESI) m/z 433.2272 ($M+H^+$), calc. for $C_{30}H_{28}N_2O$ 433.2274.

11. Copies of NMR spectra



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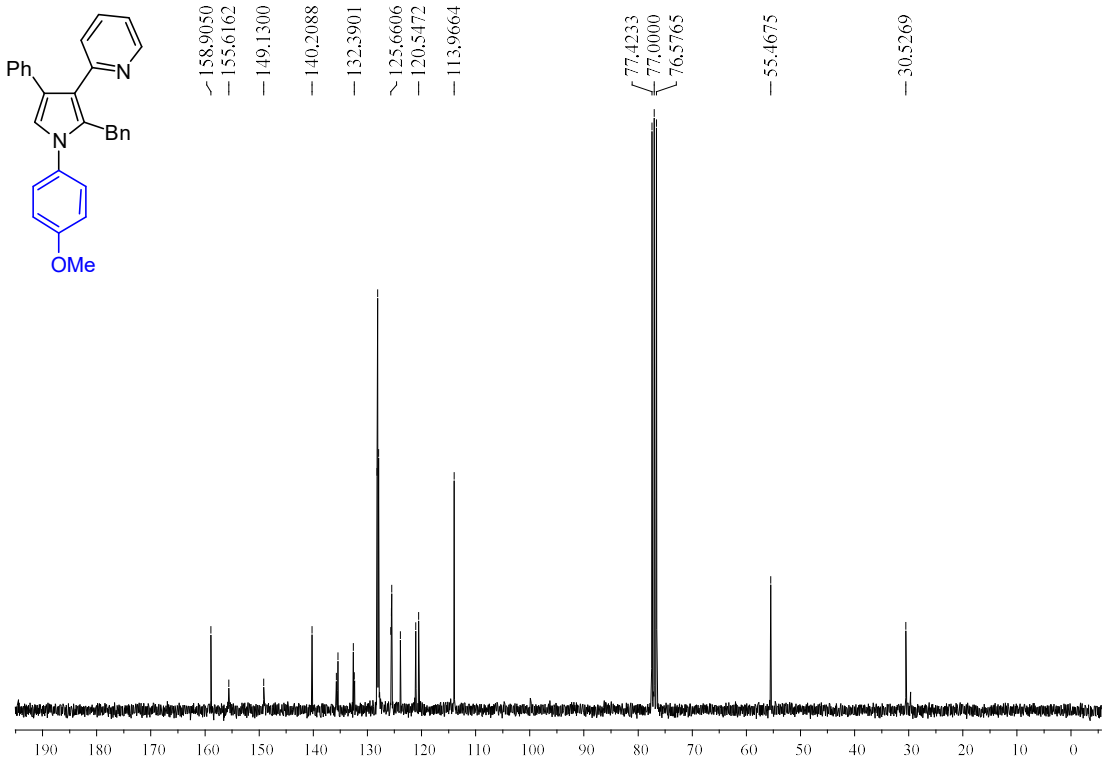
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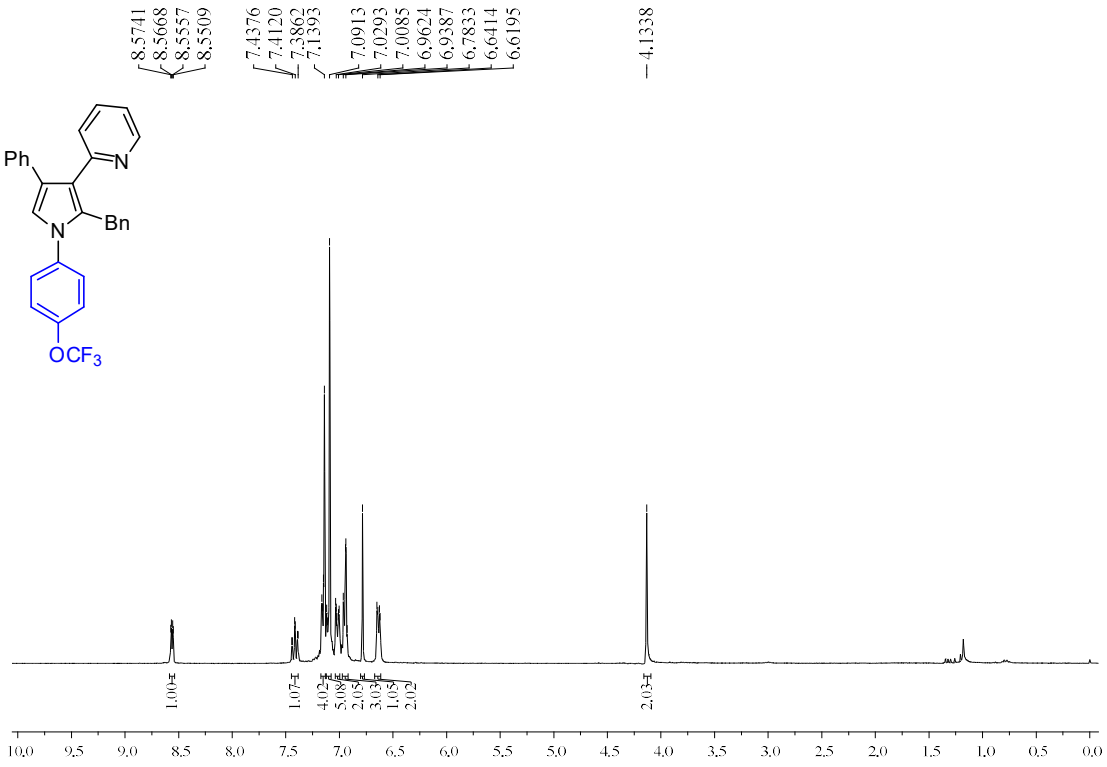
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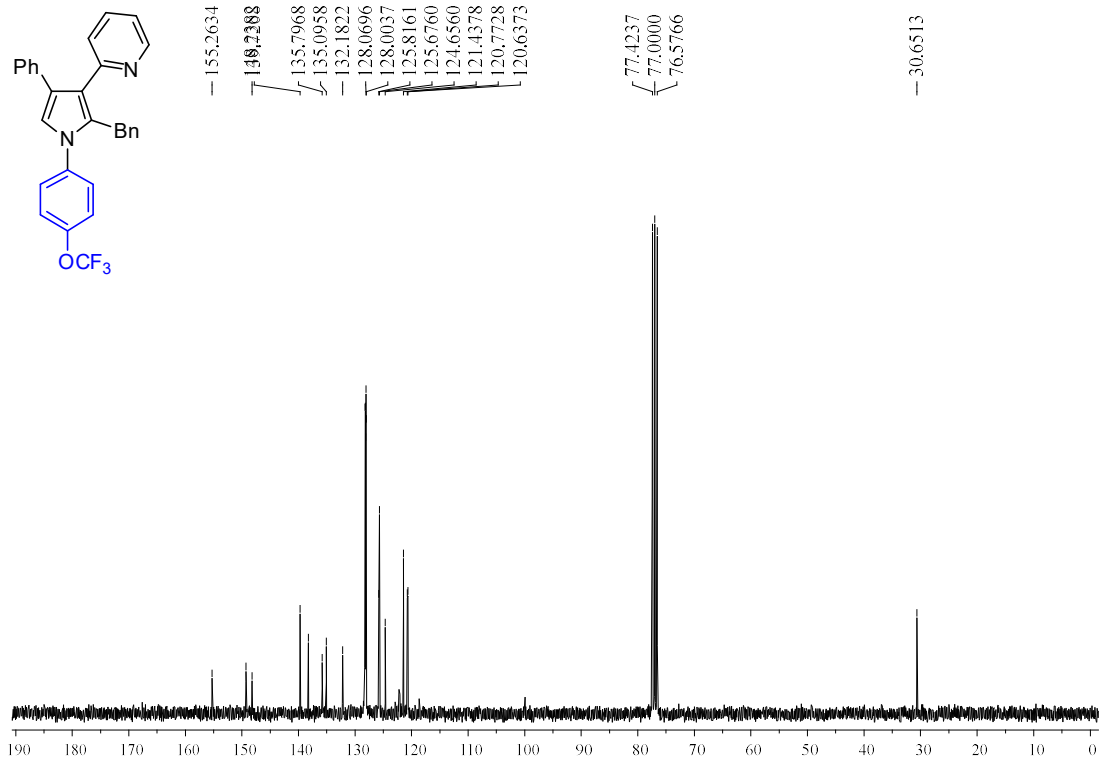
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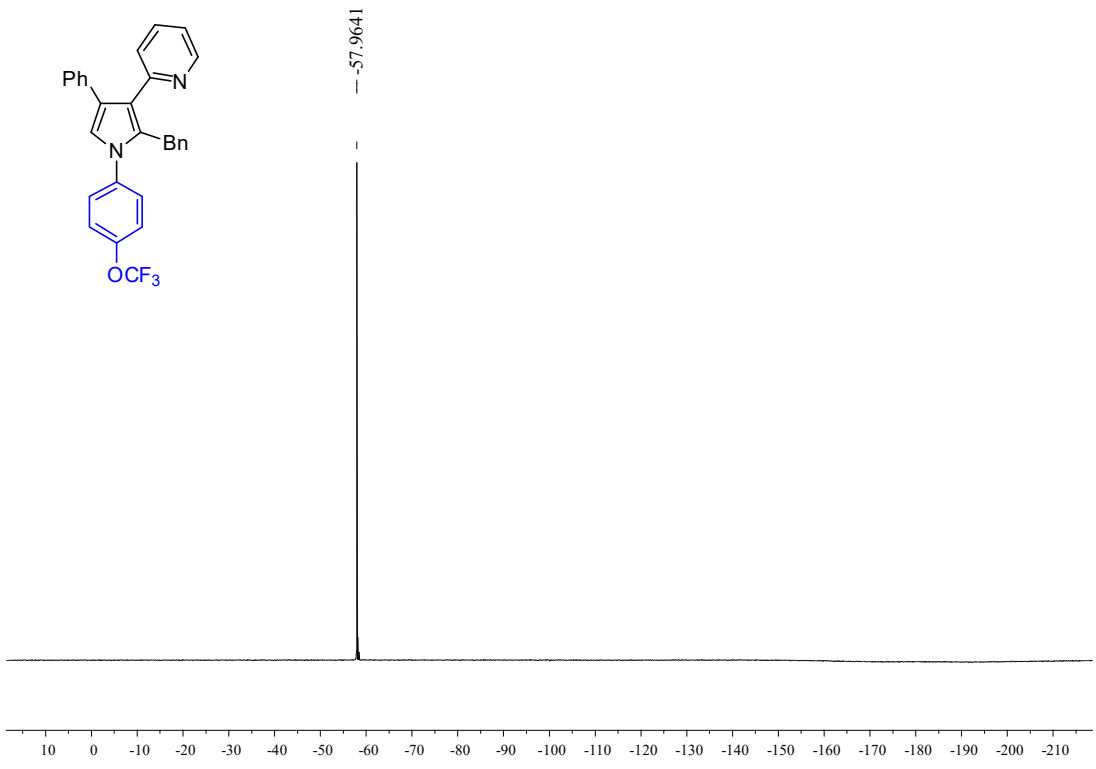
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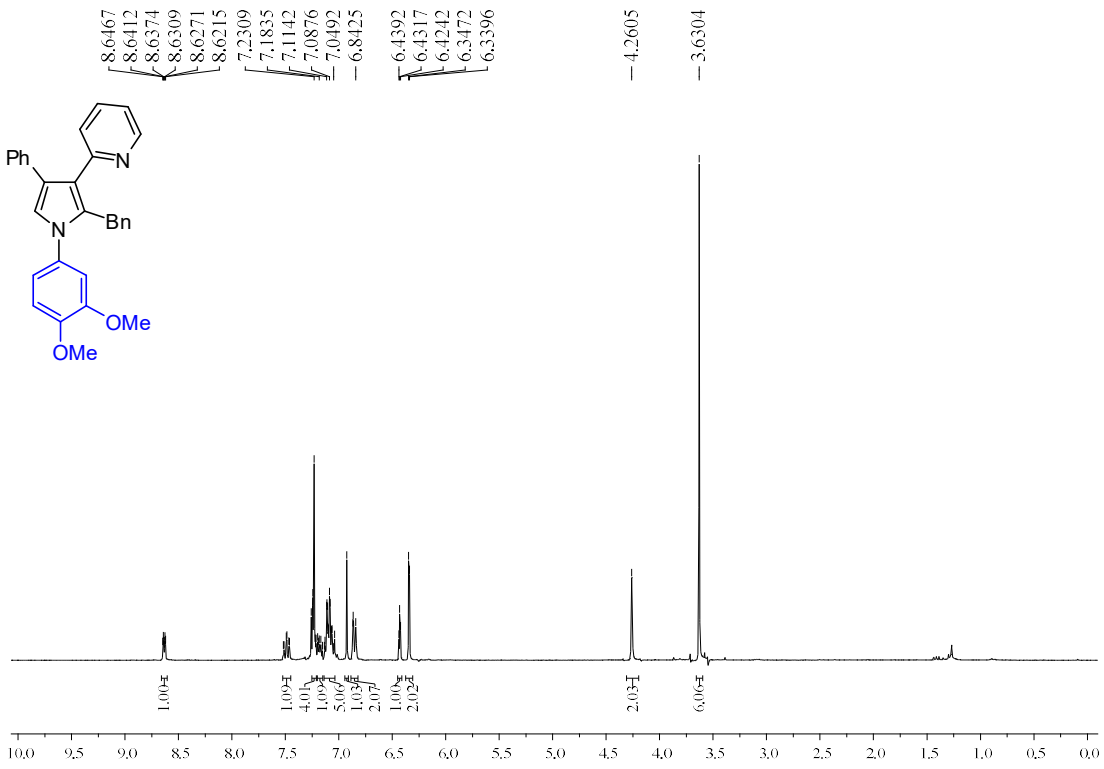
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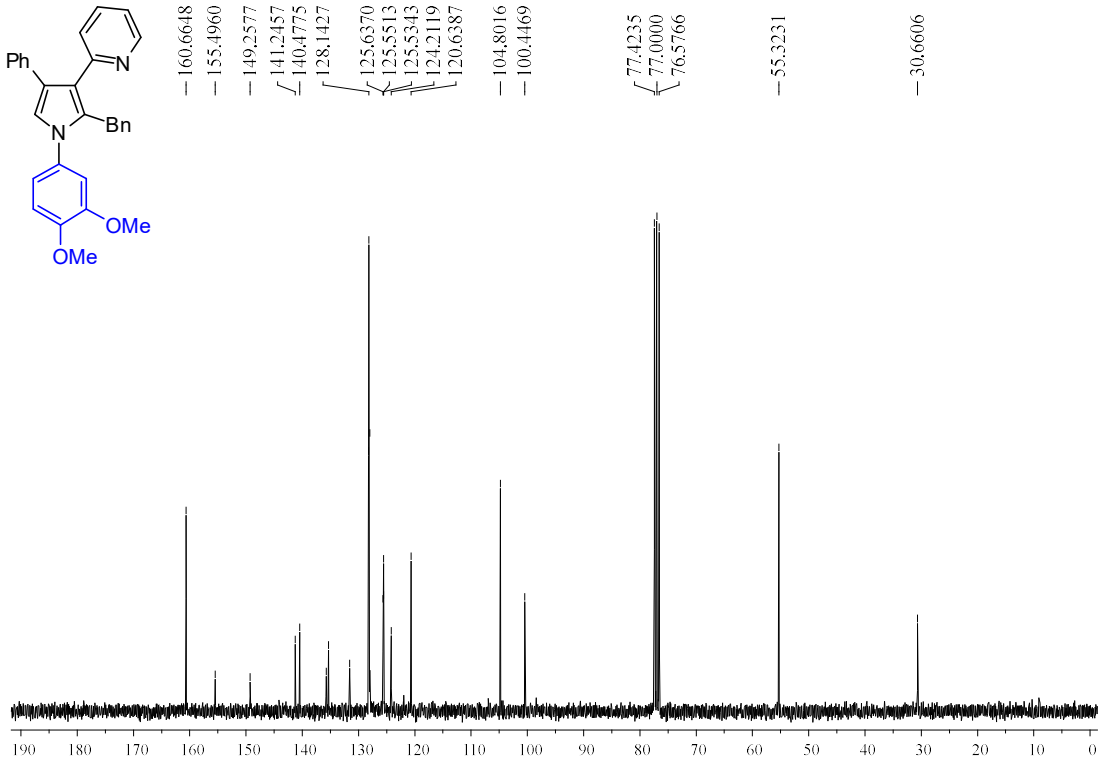
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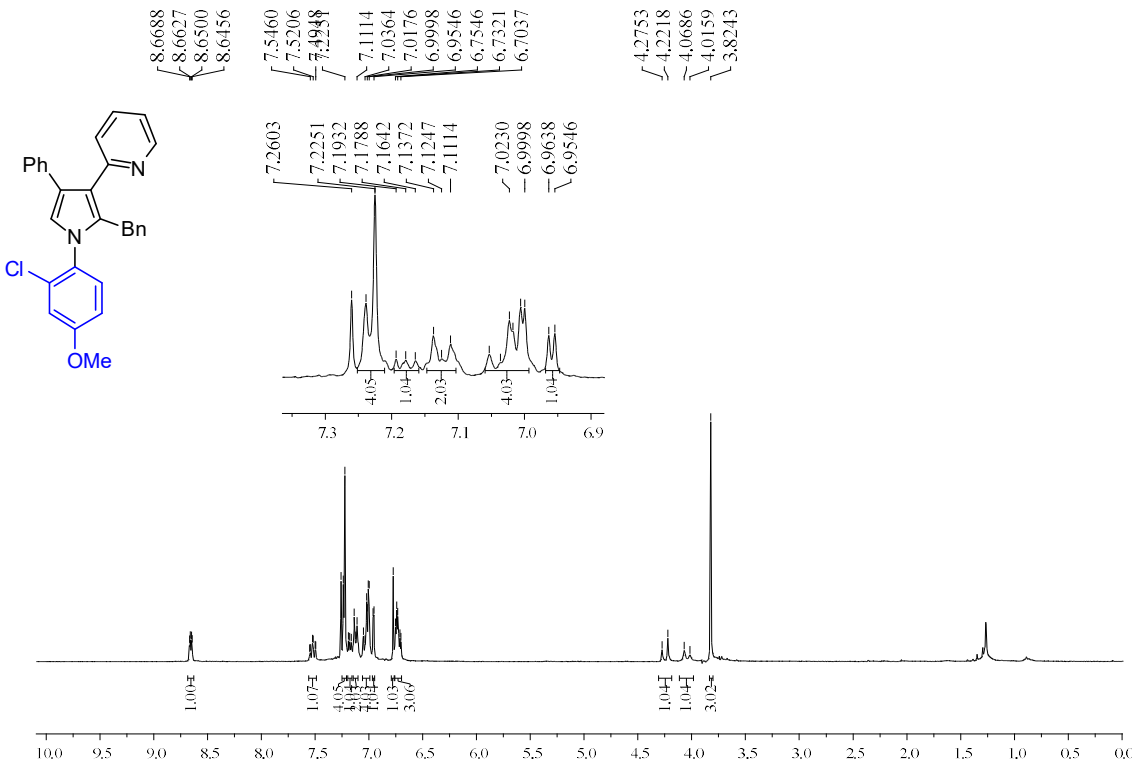
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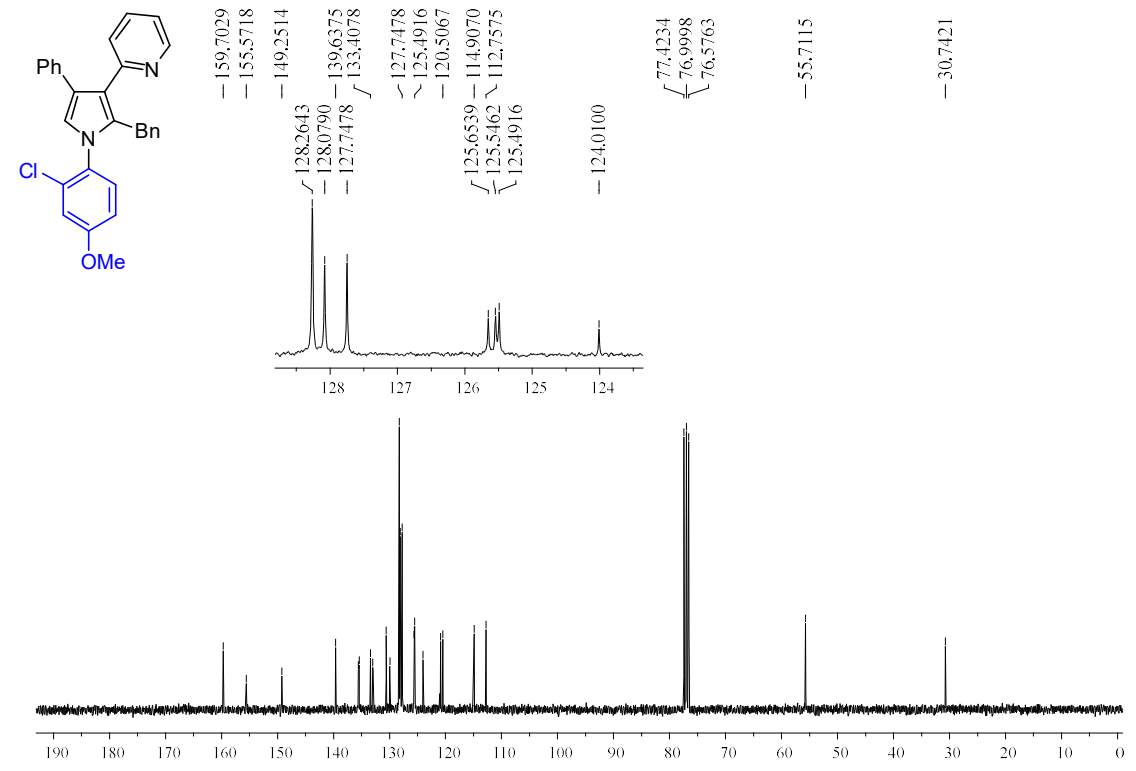
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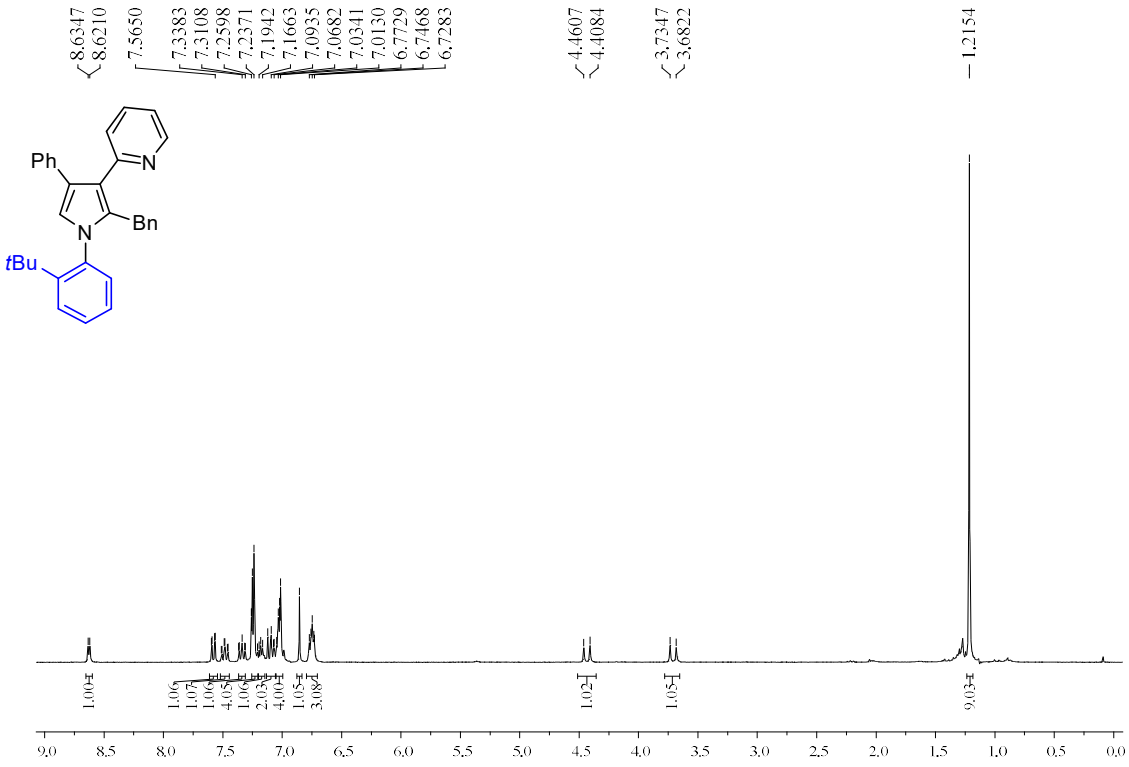
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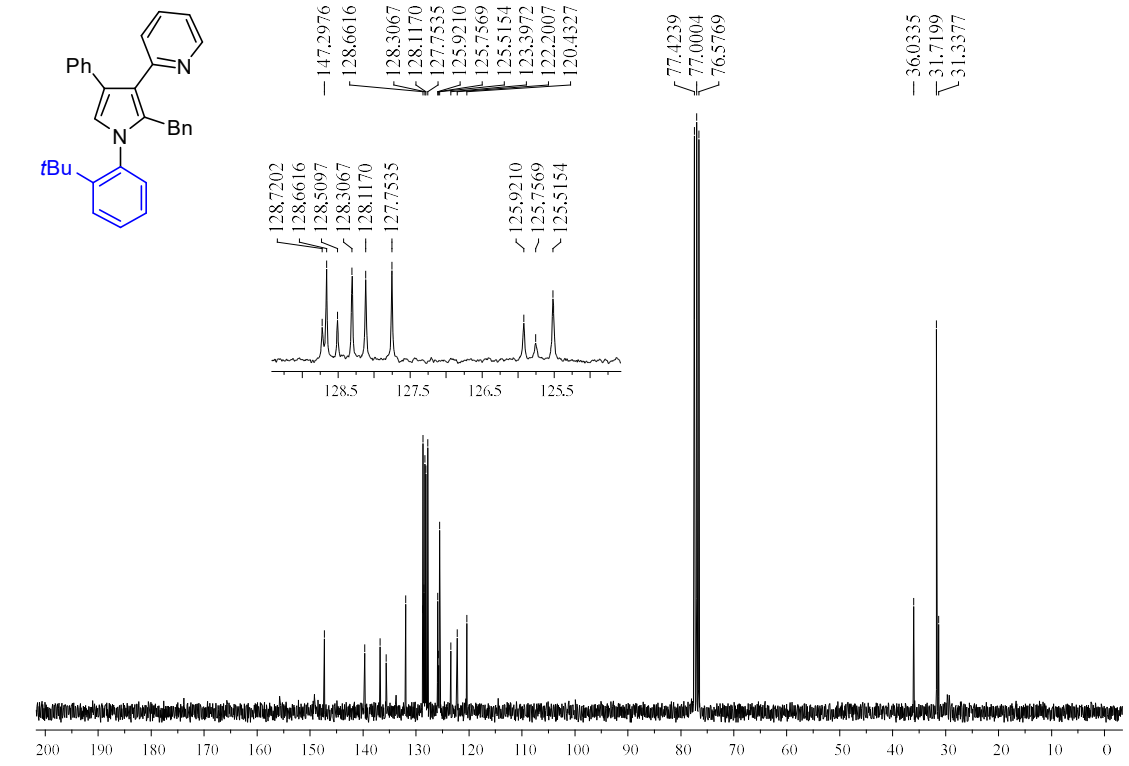
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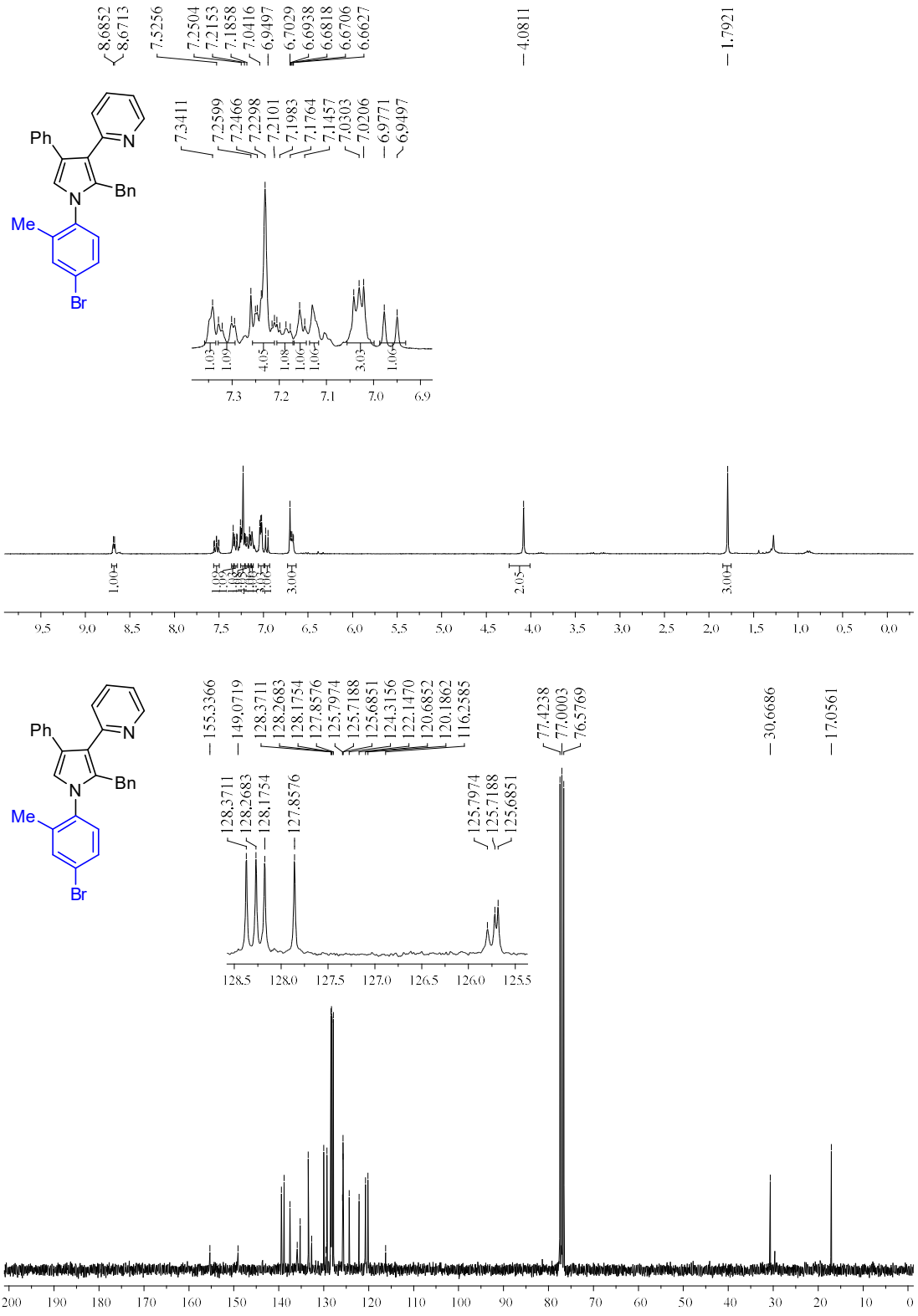
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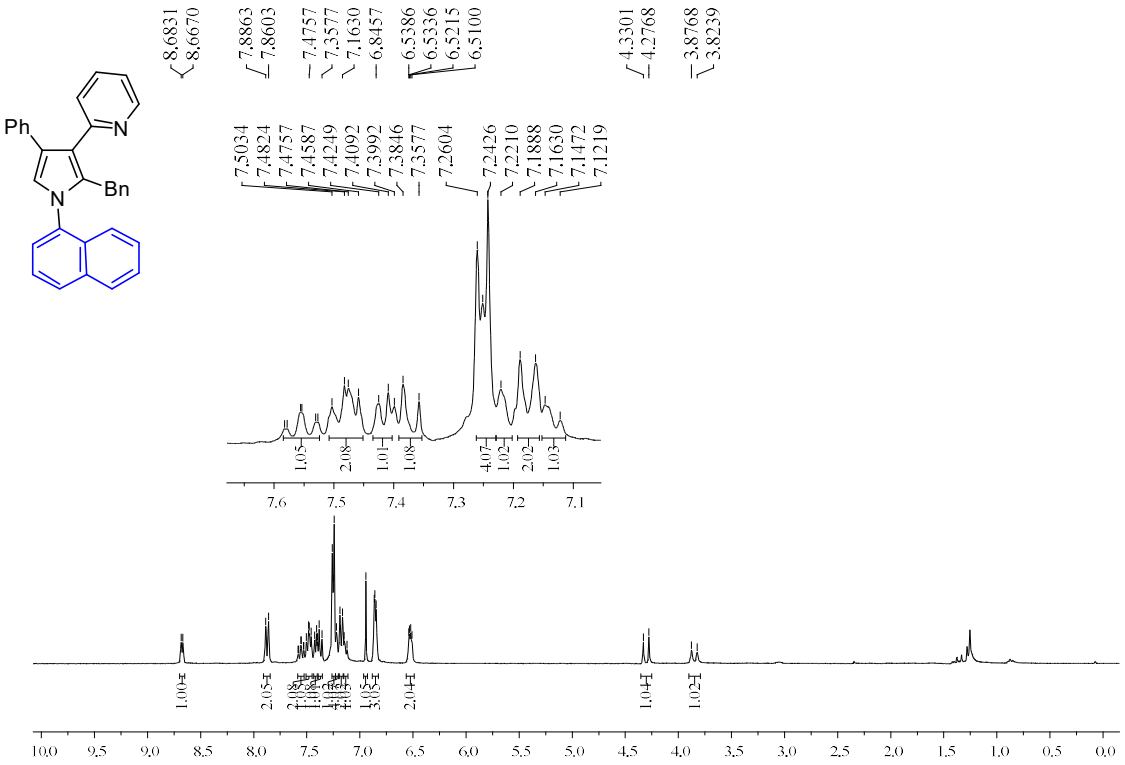
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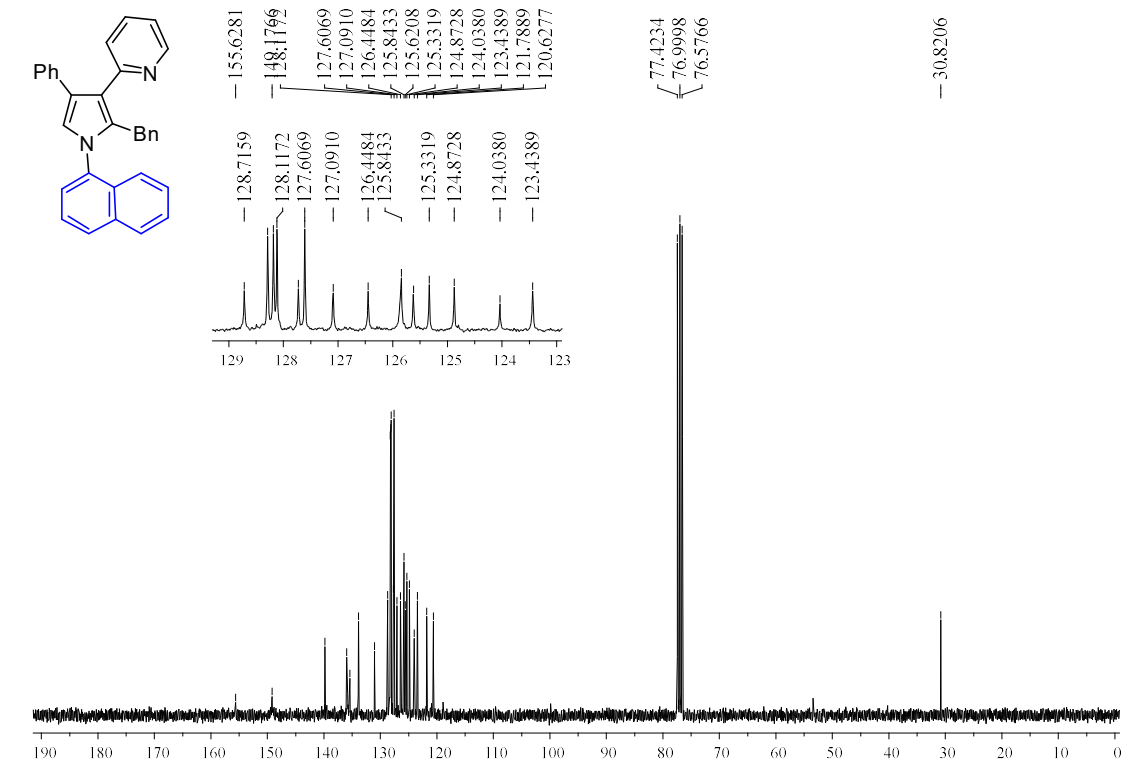
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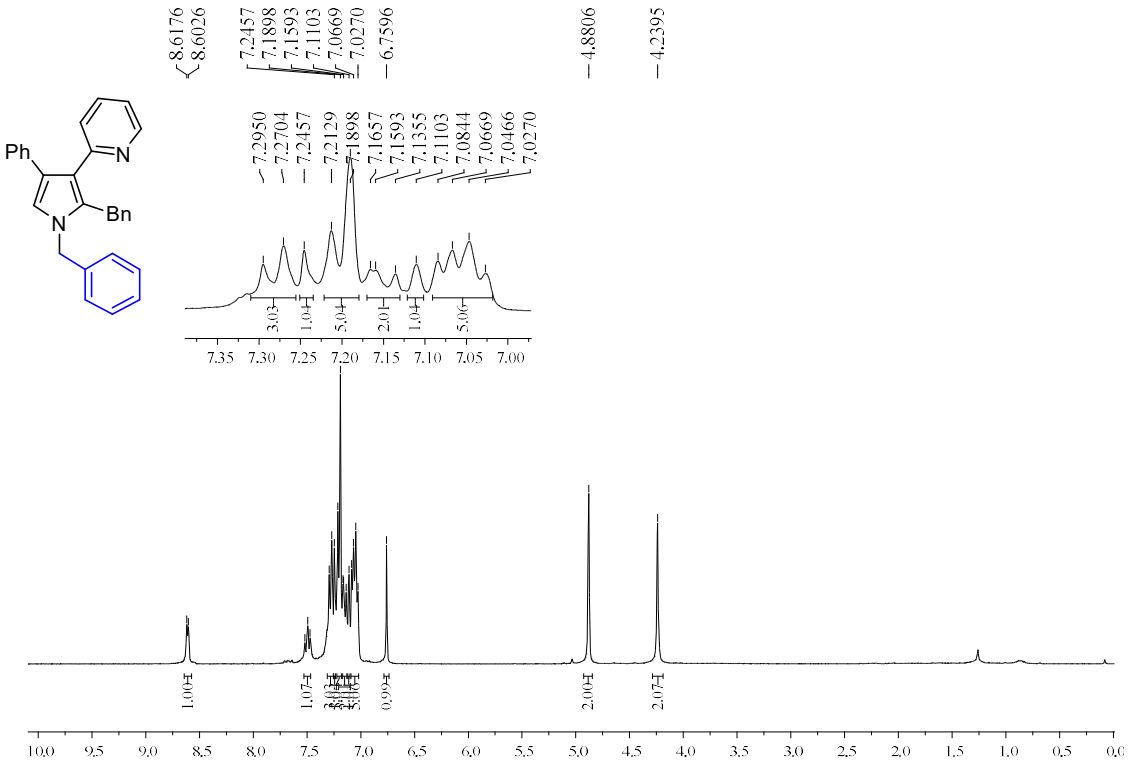
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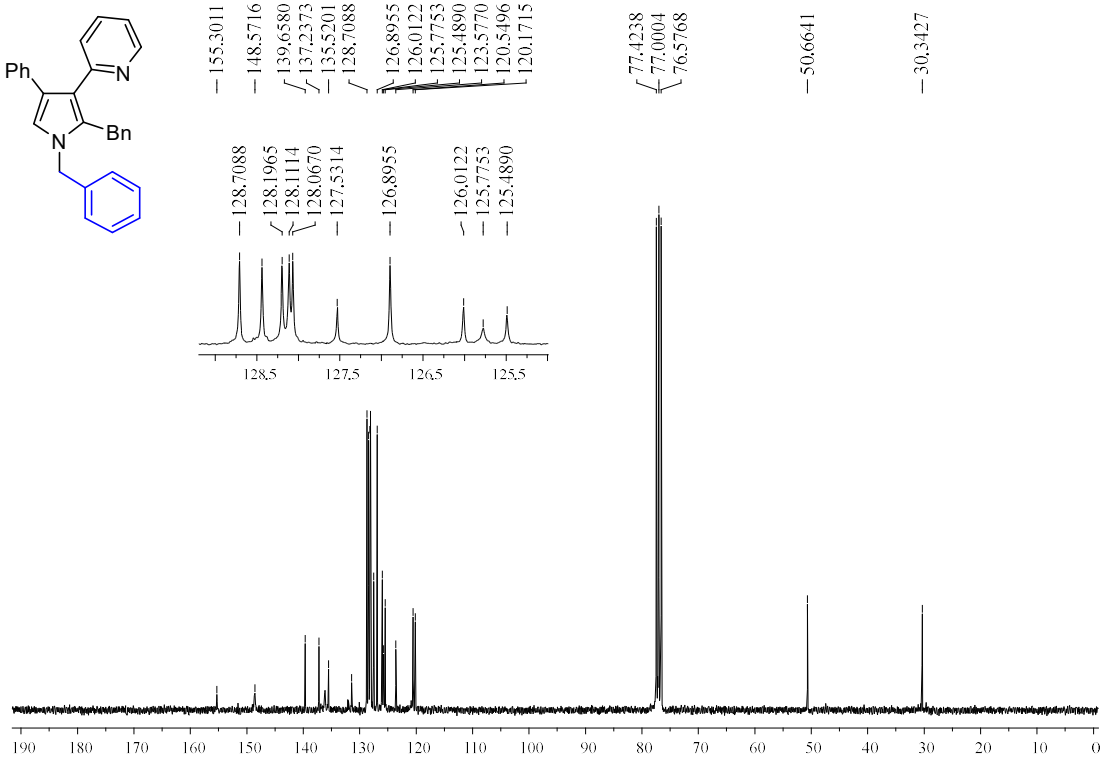
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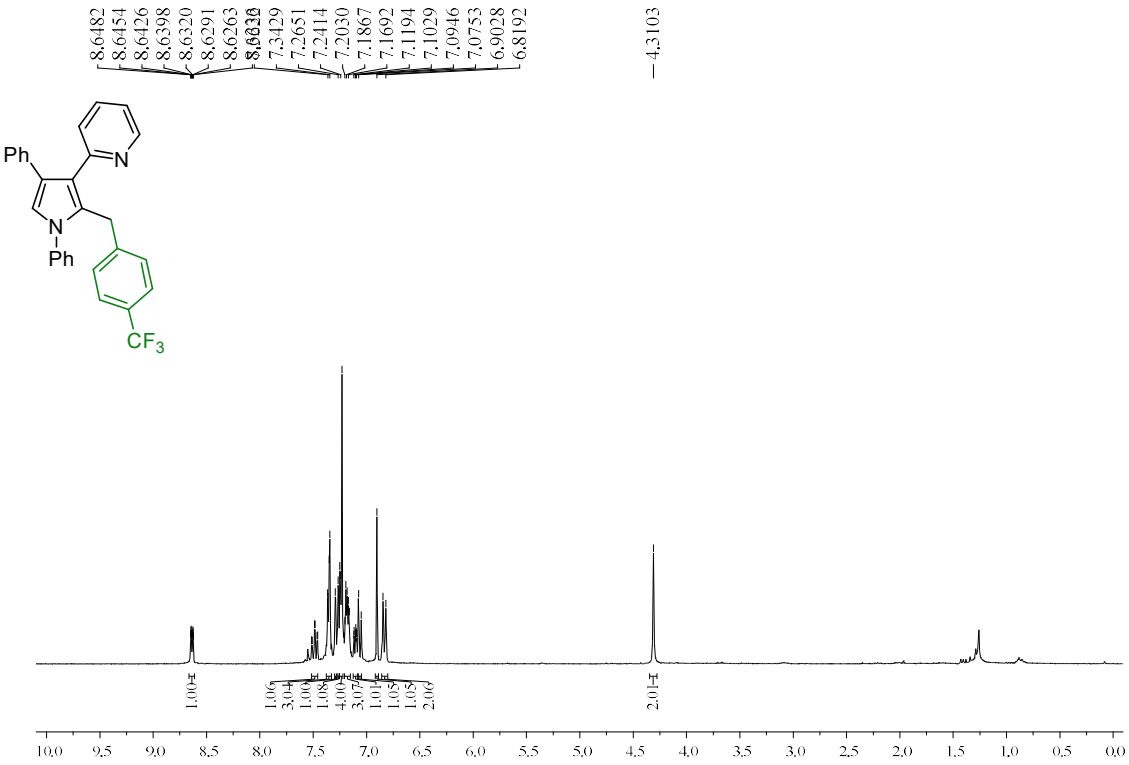
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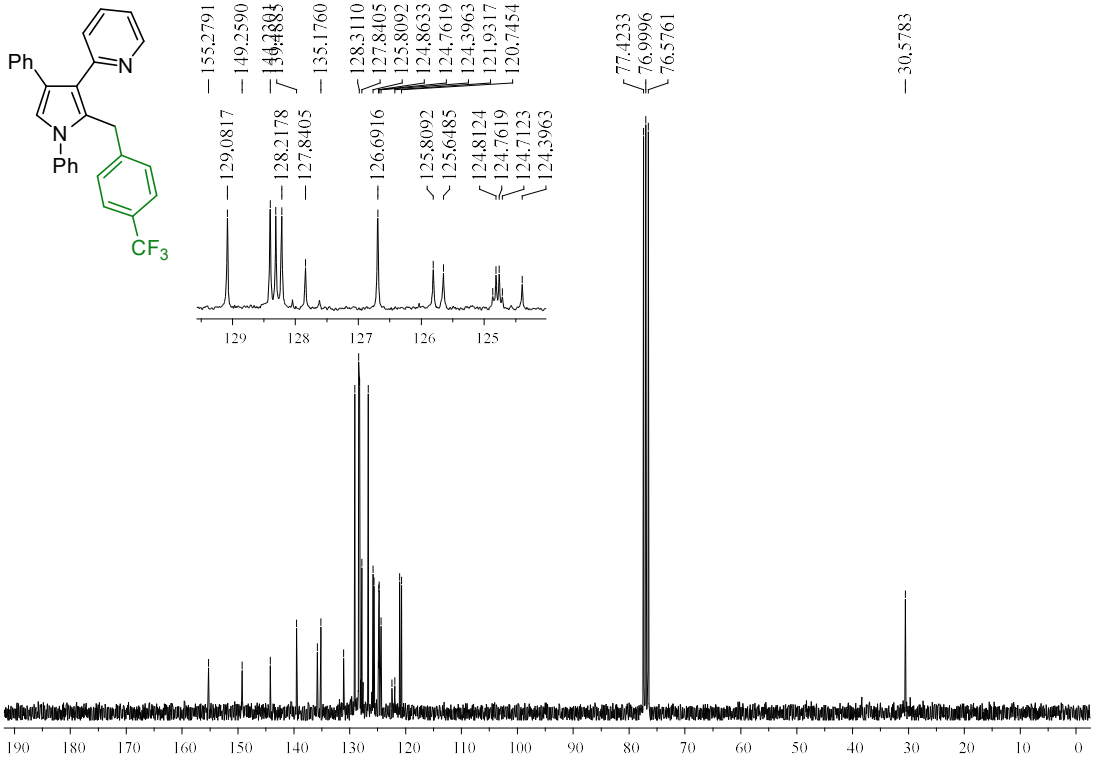
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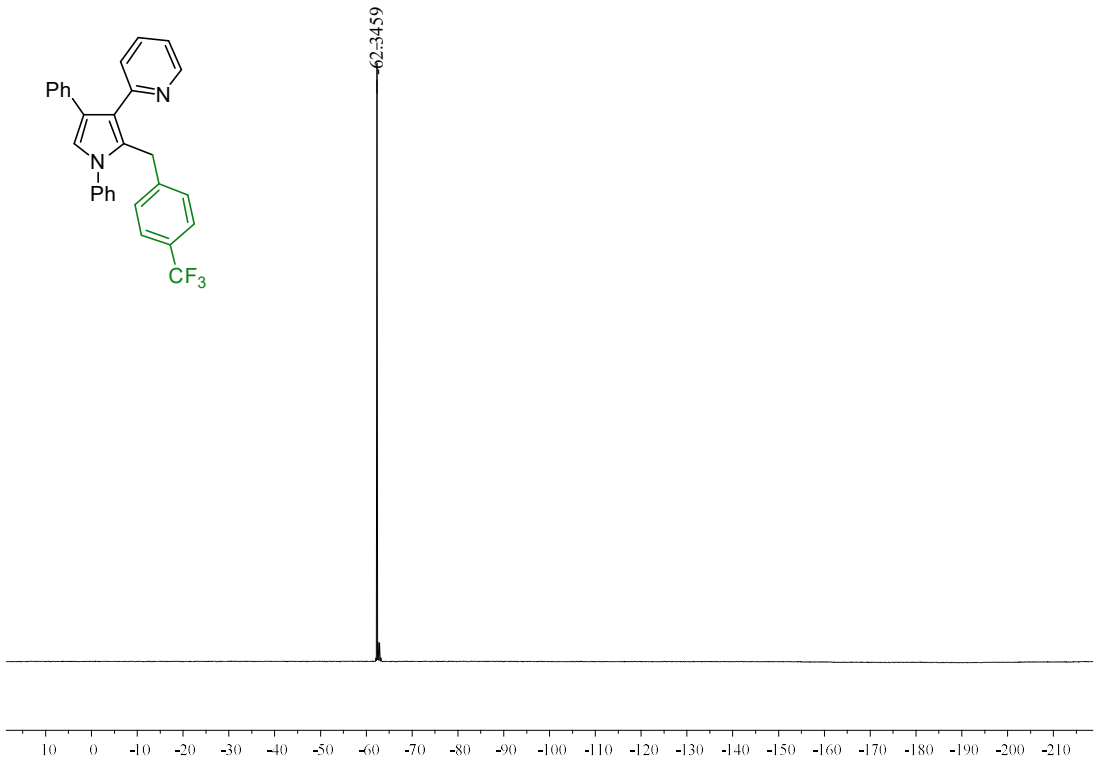
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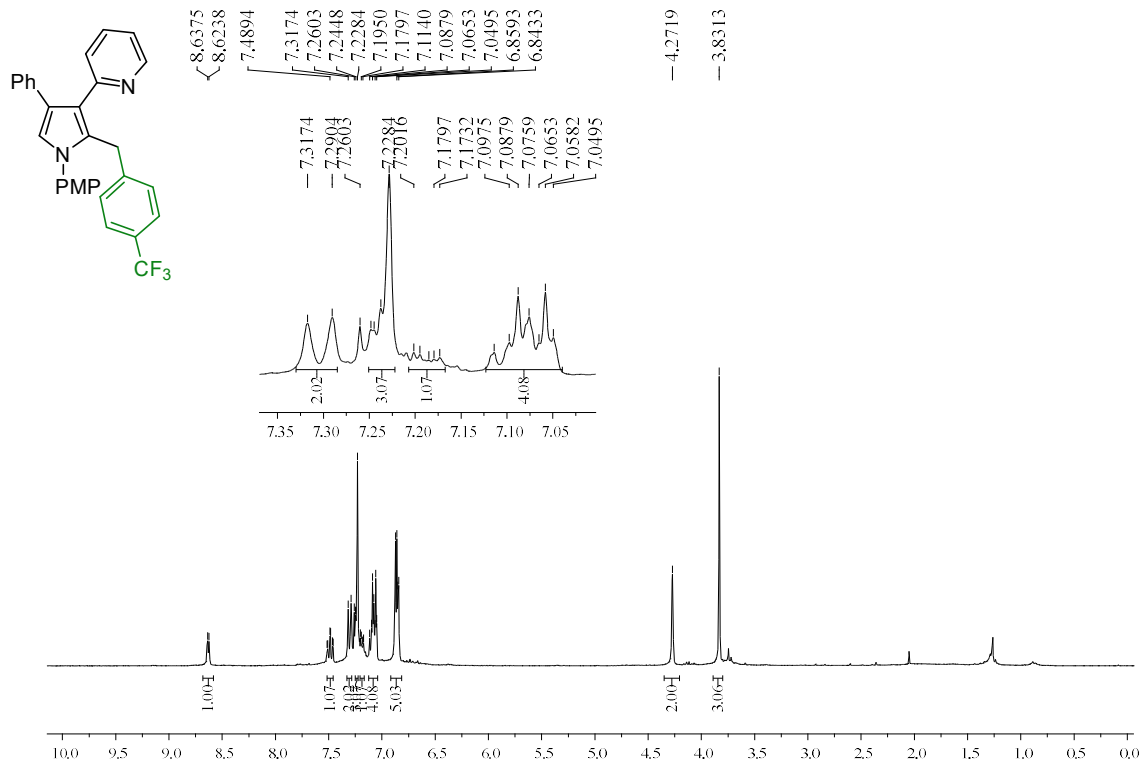
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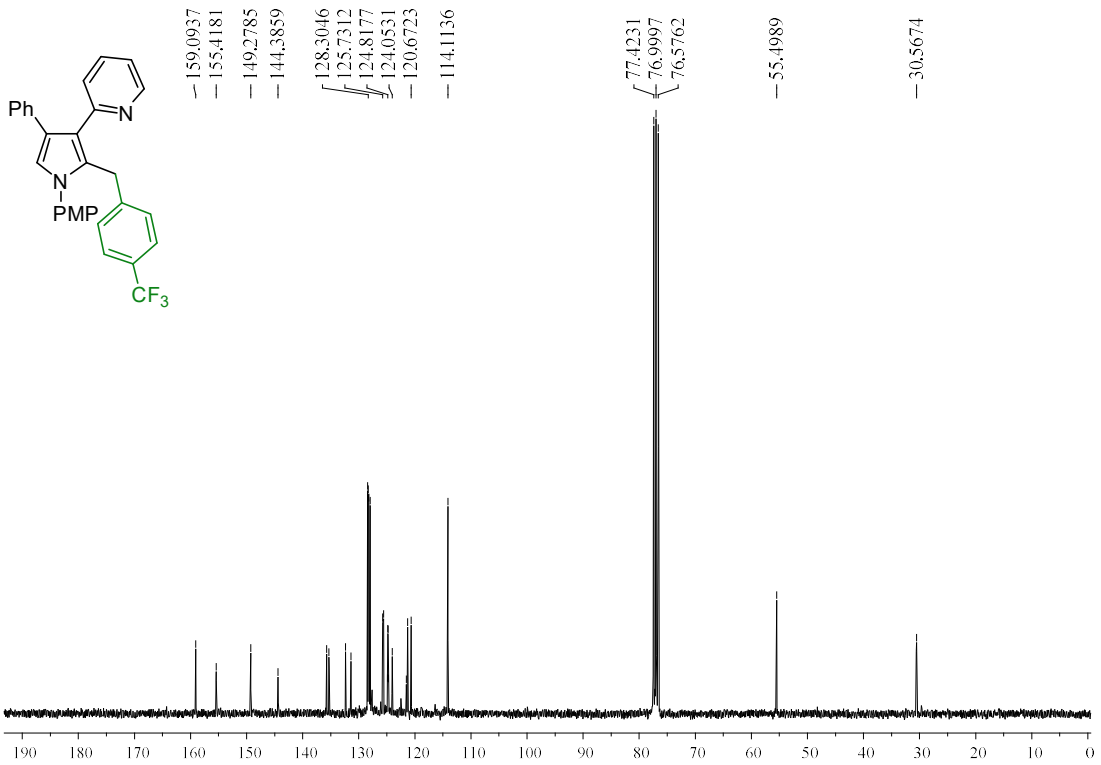
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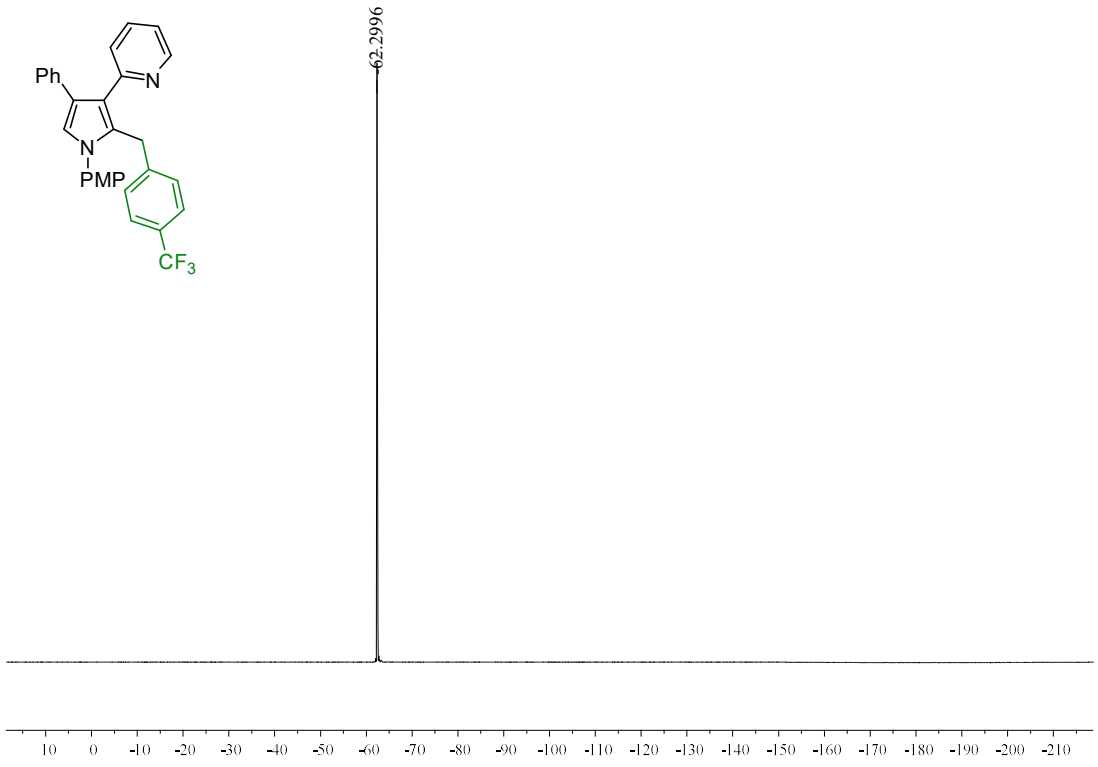
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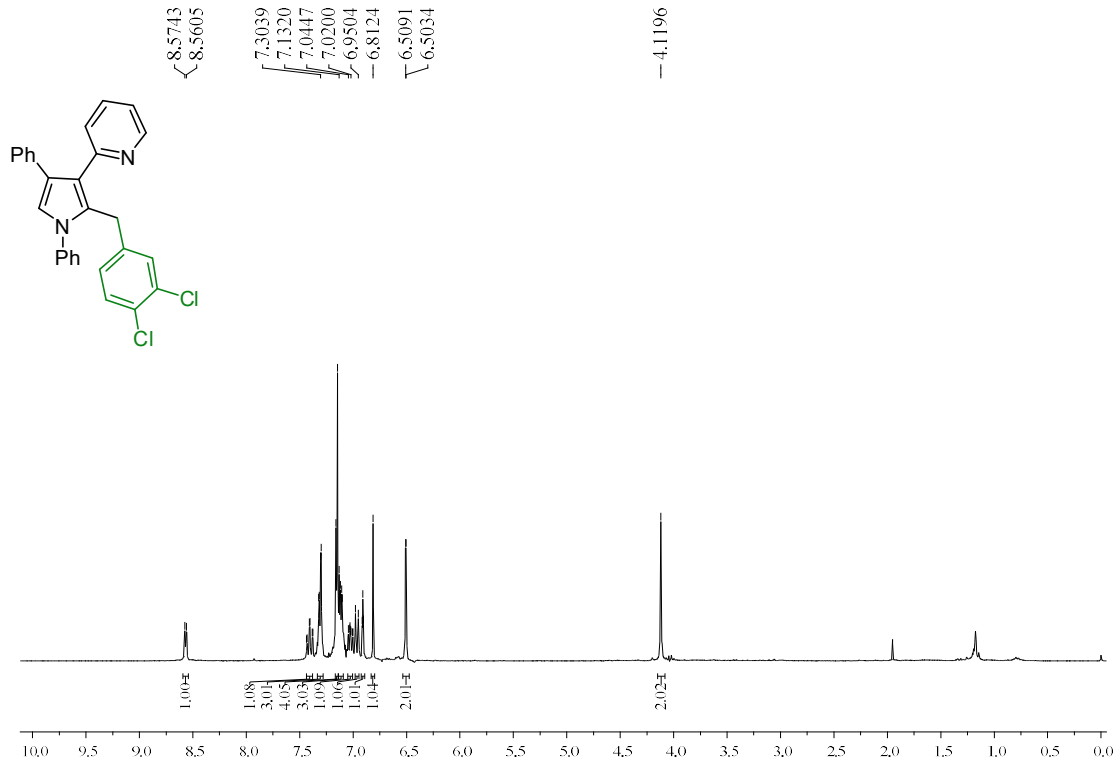
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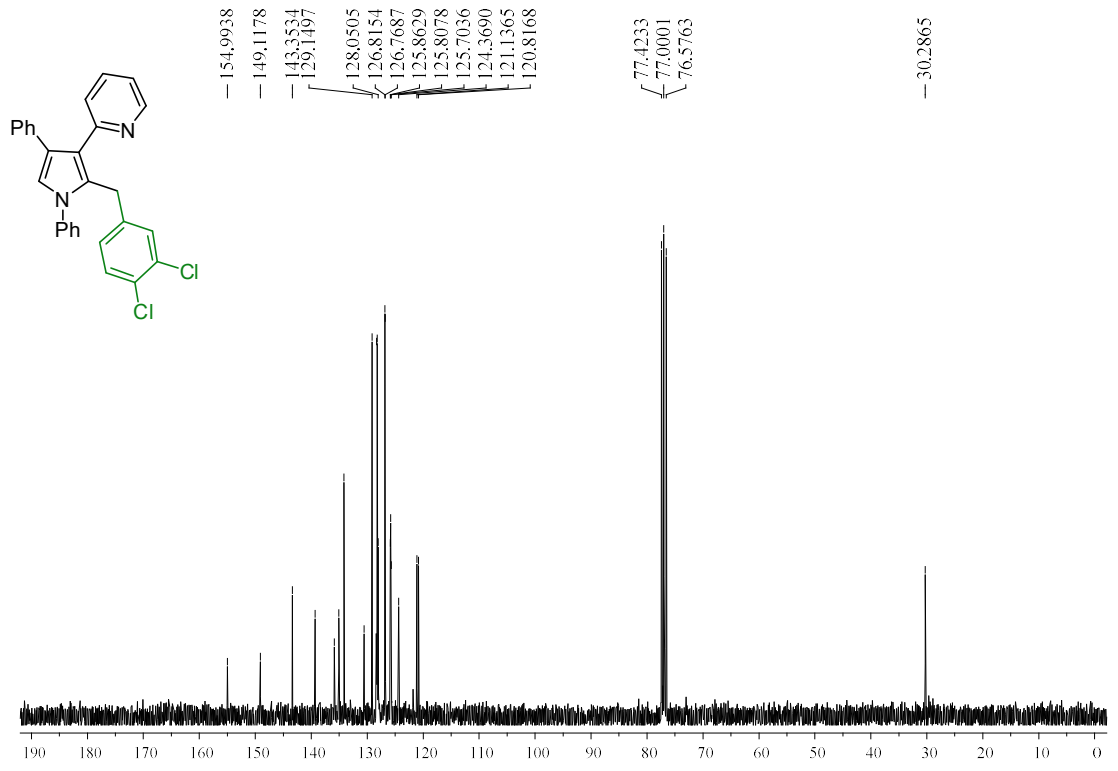
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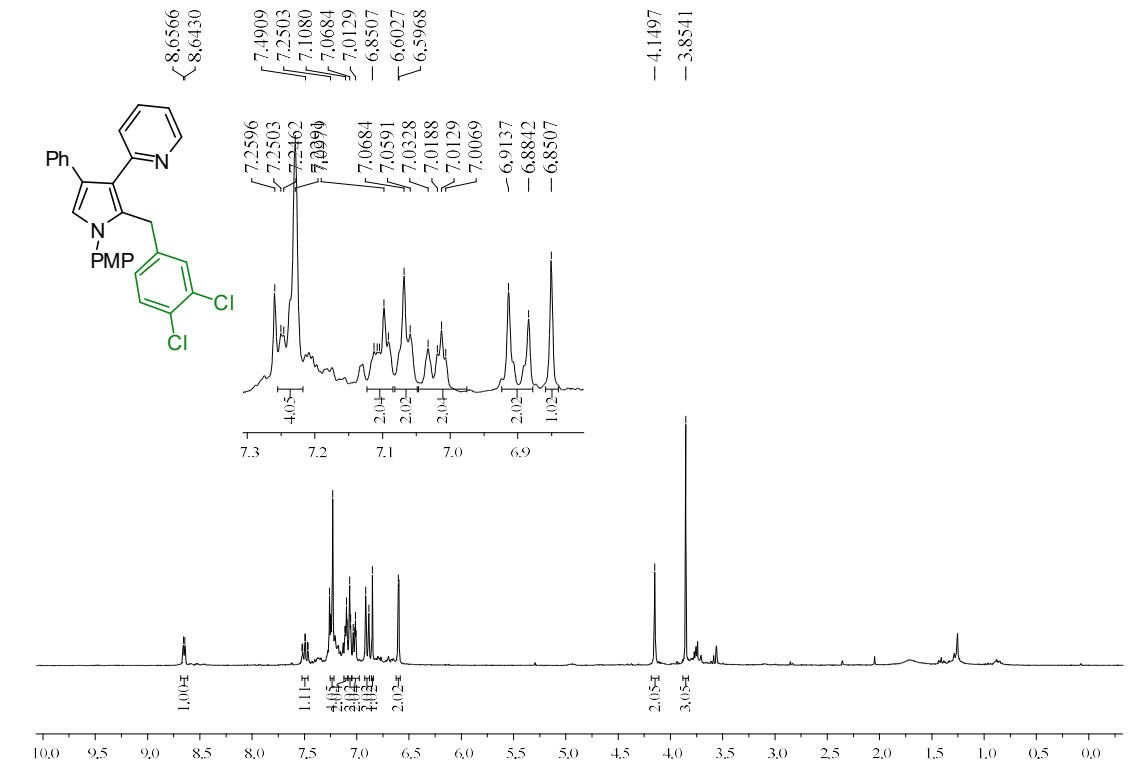
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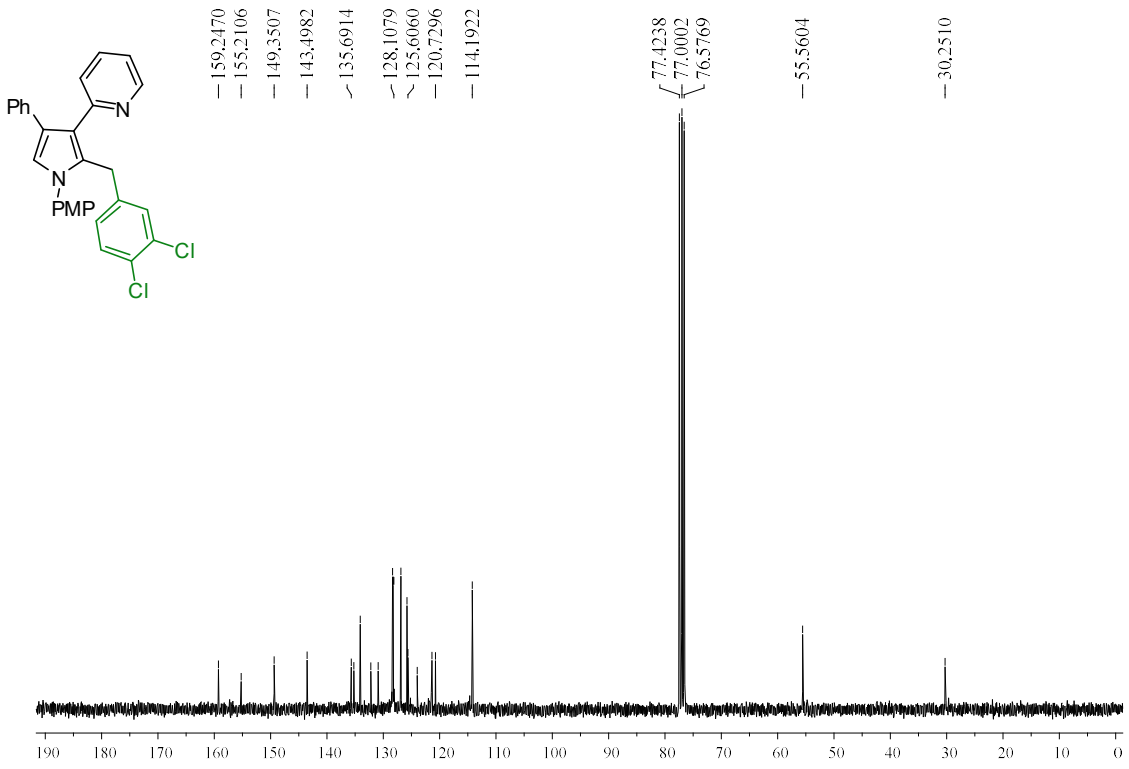
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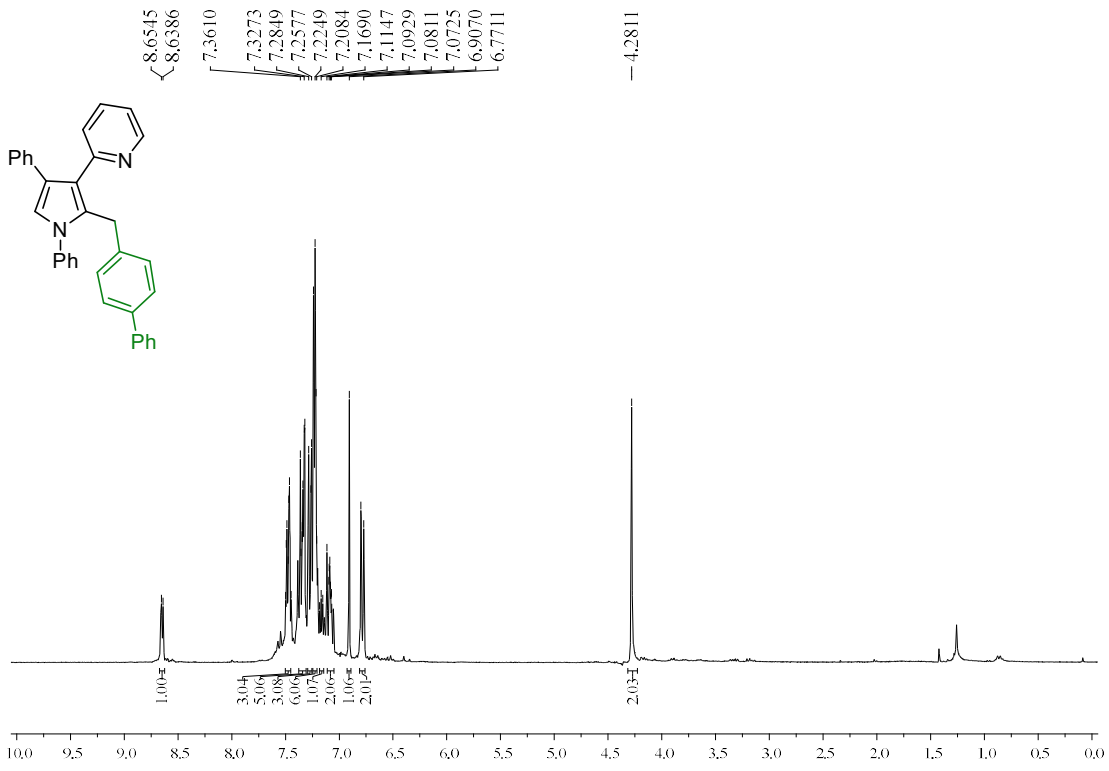
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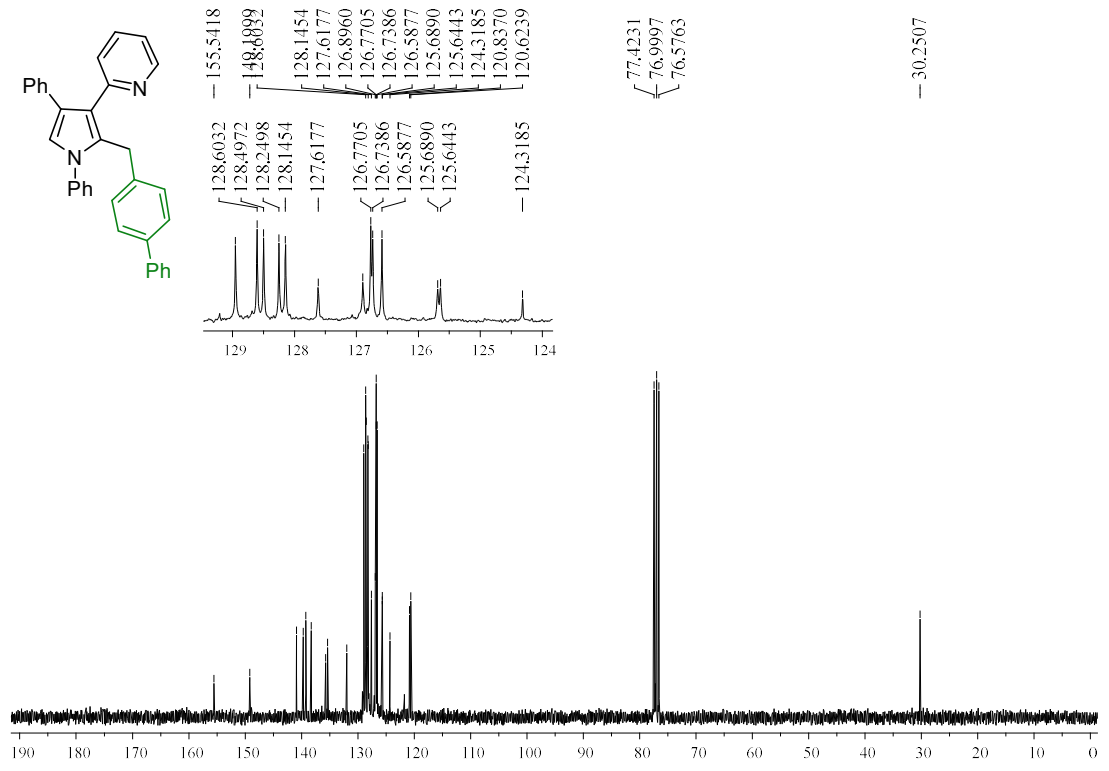
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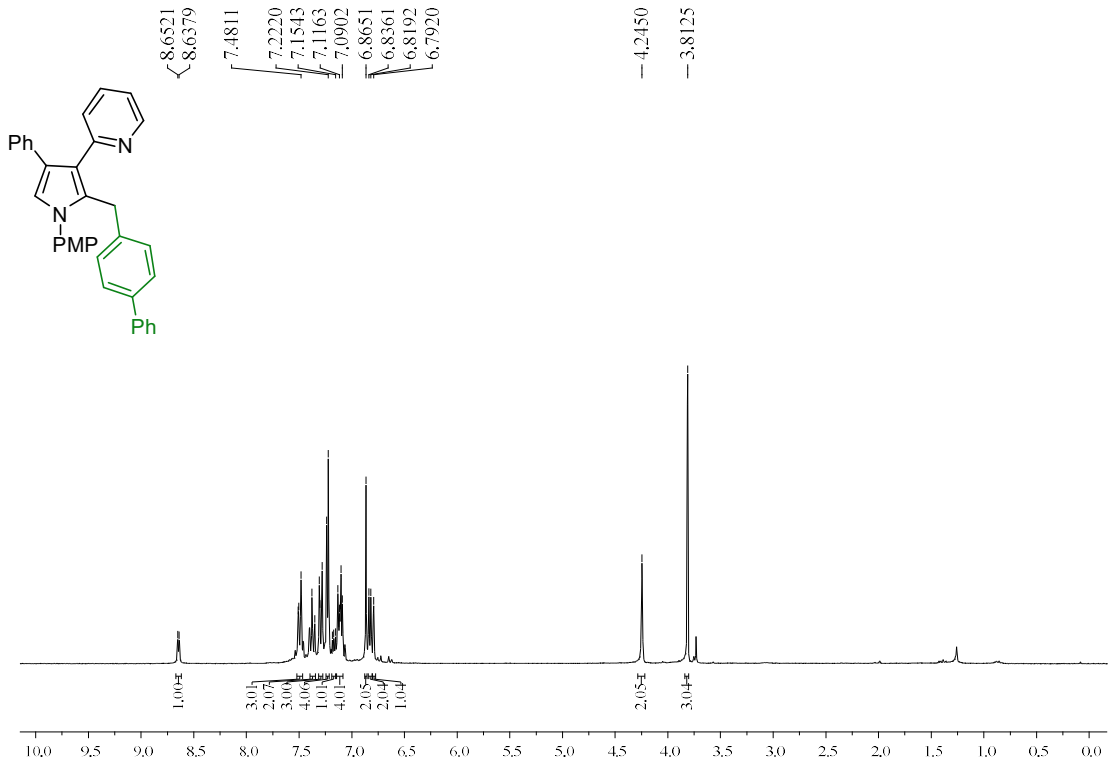
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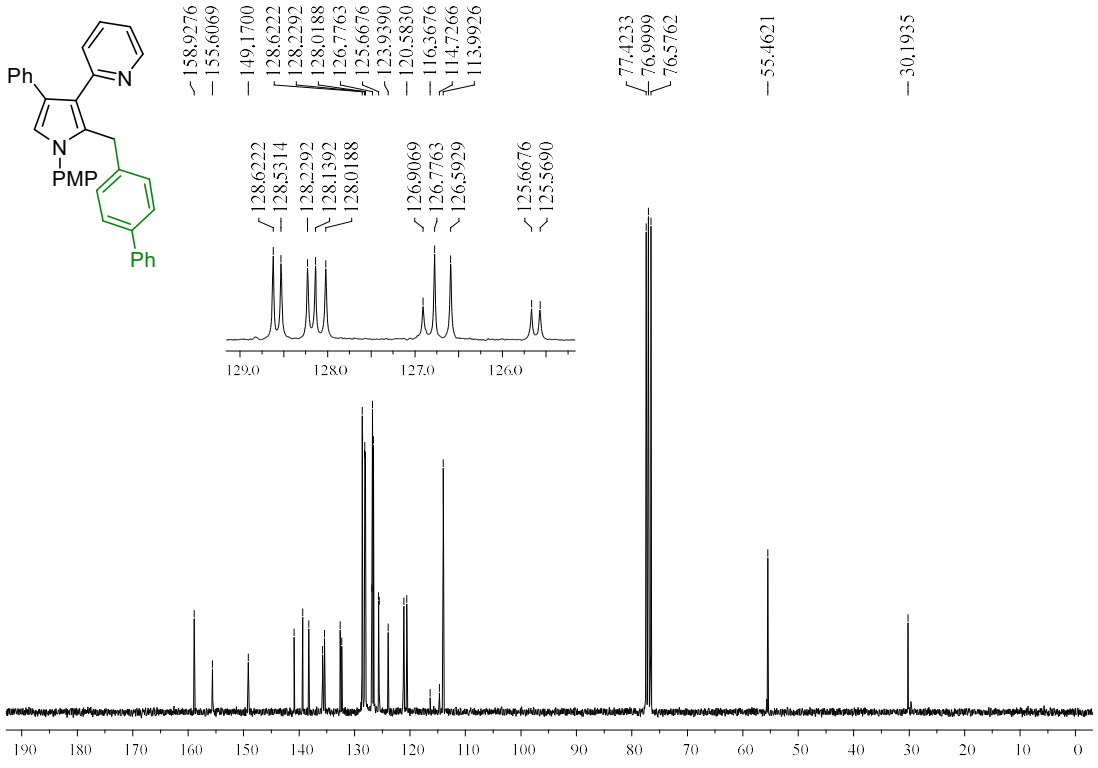
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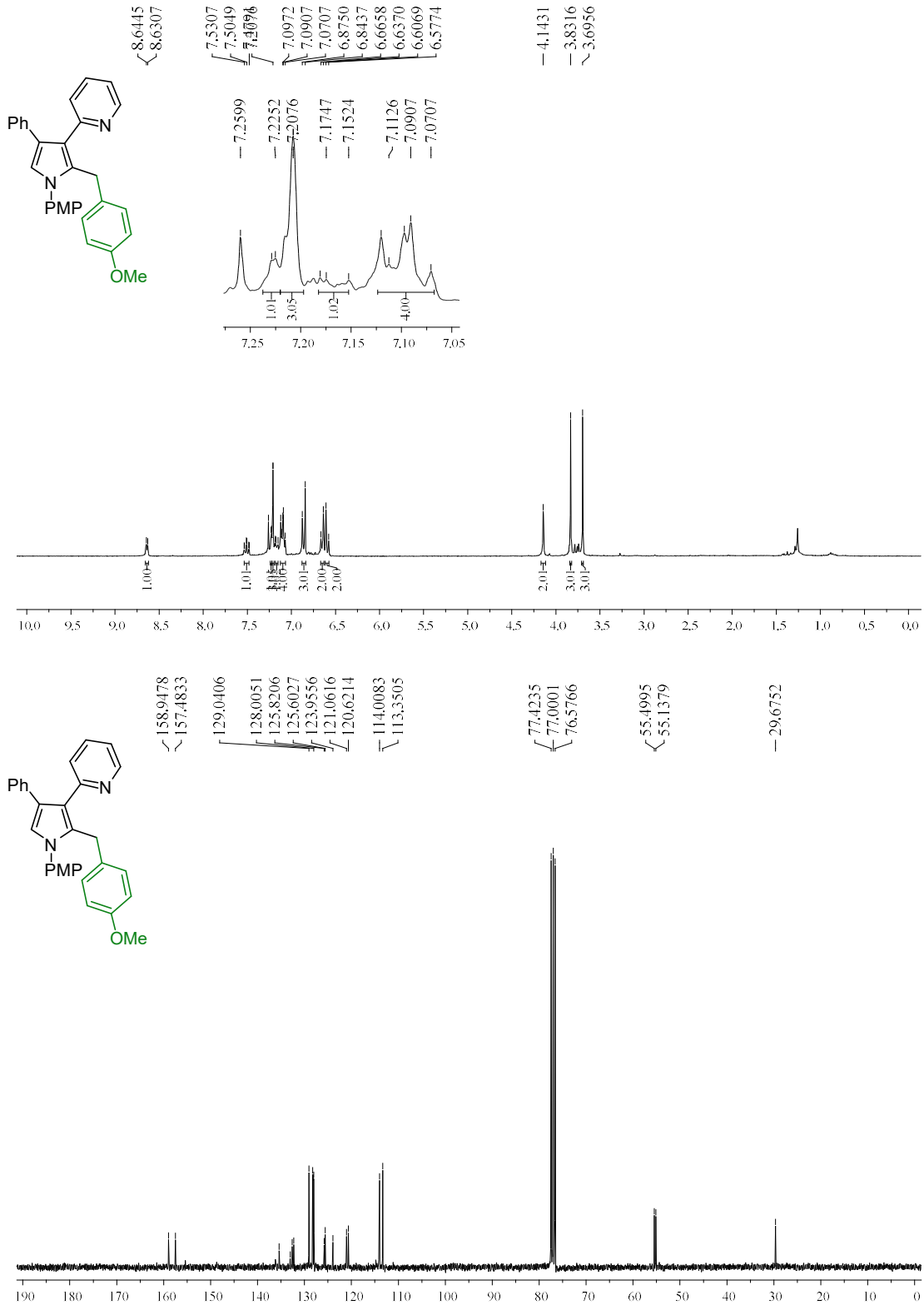
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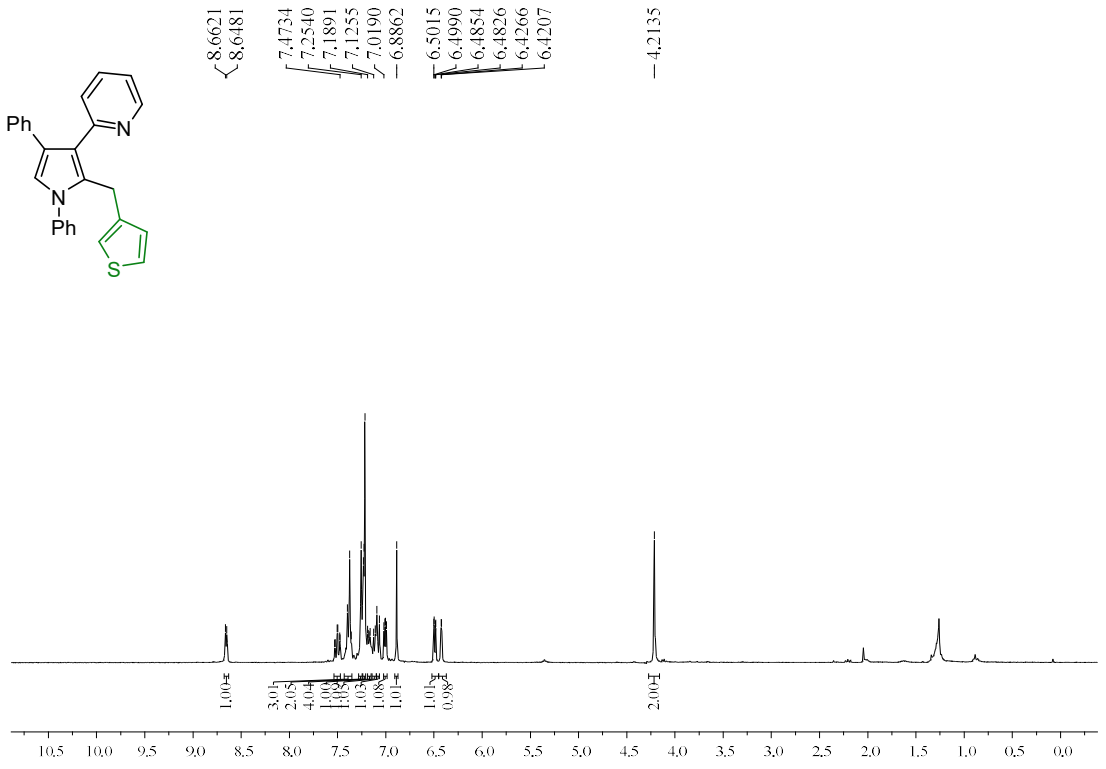
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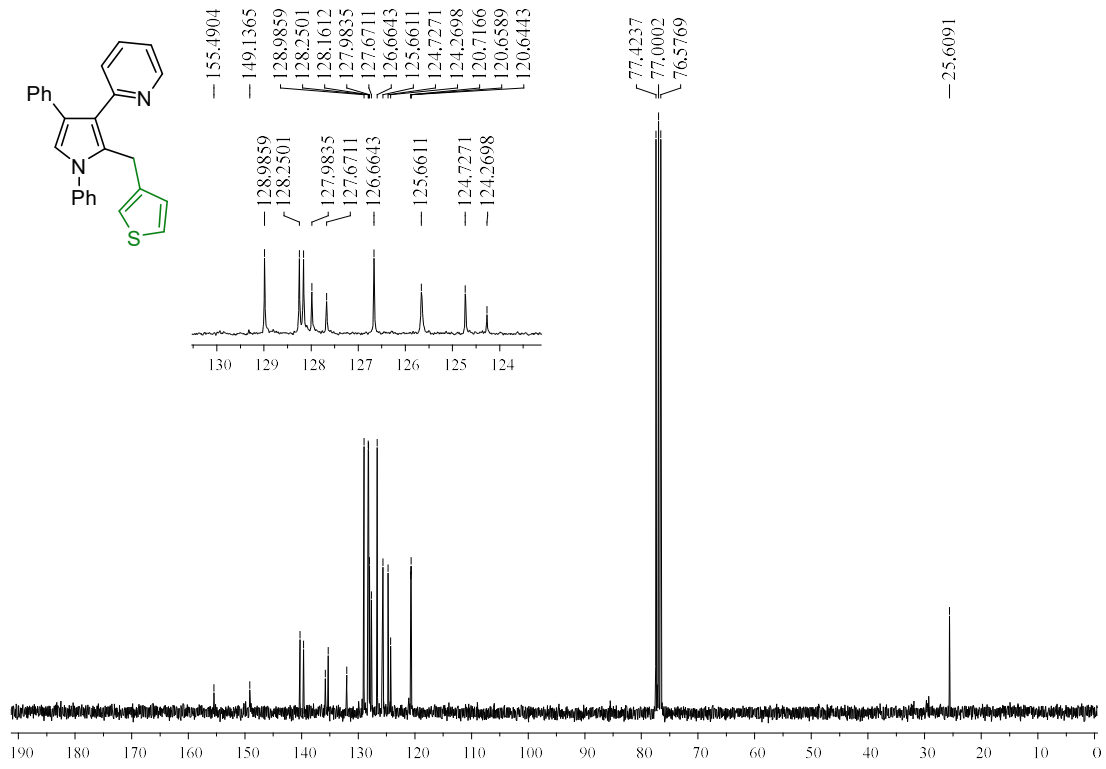
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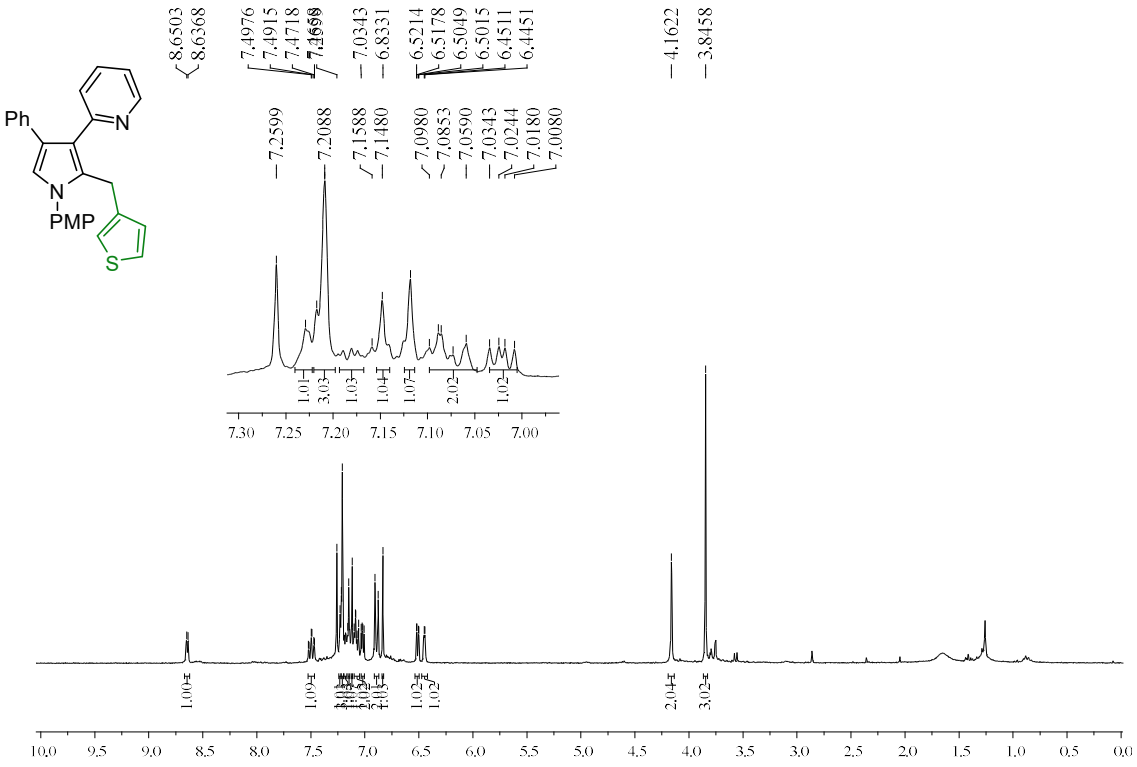
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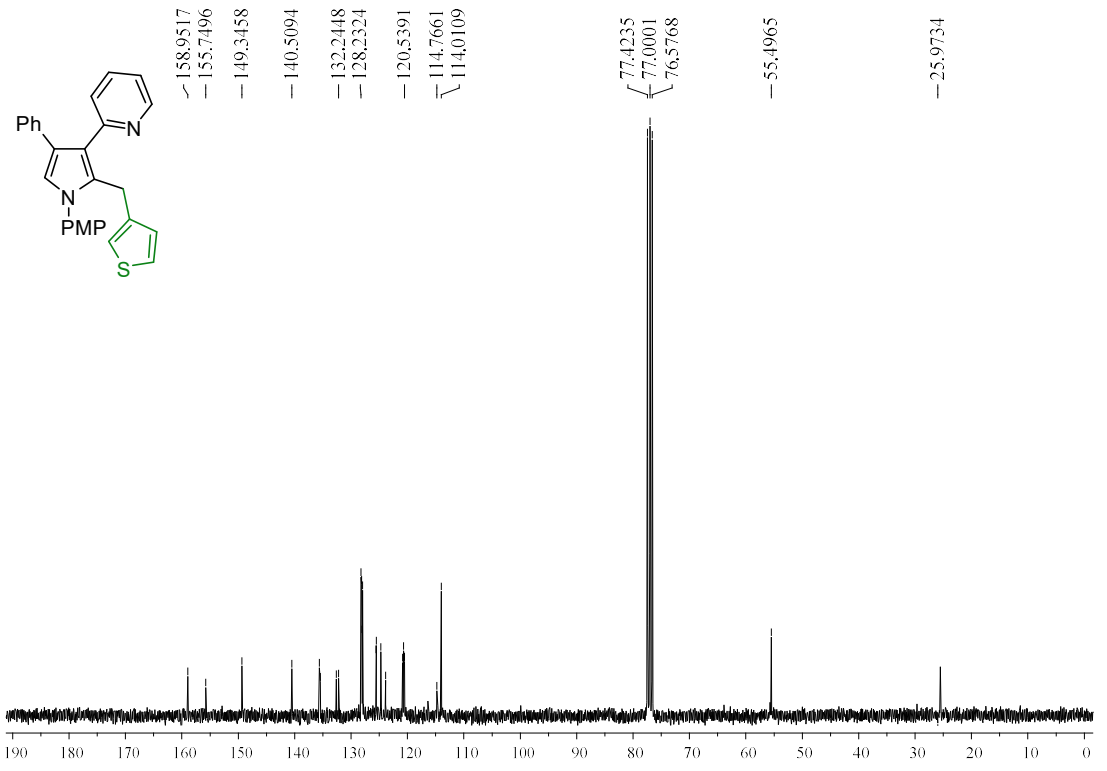
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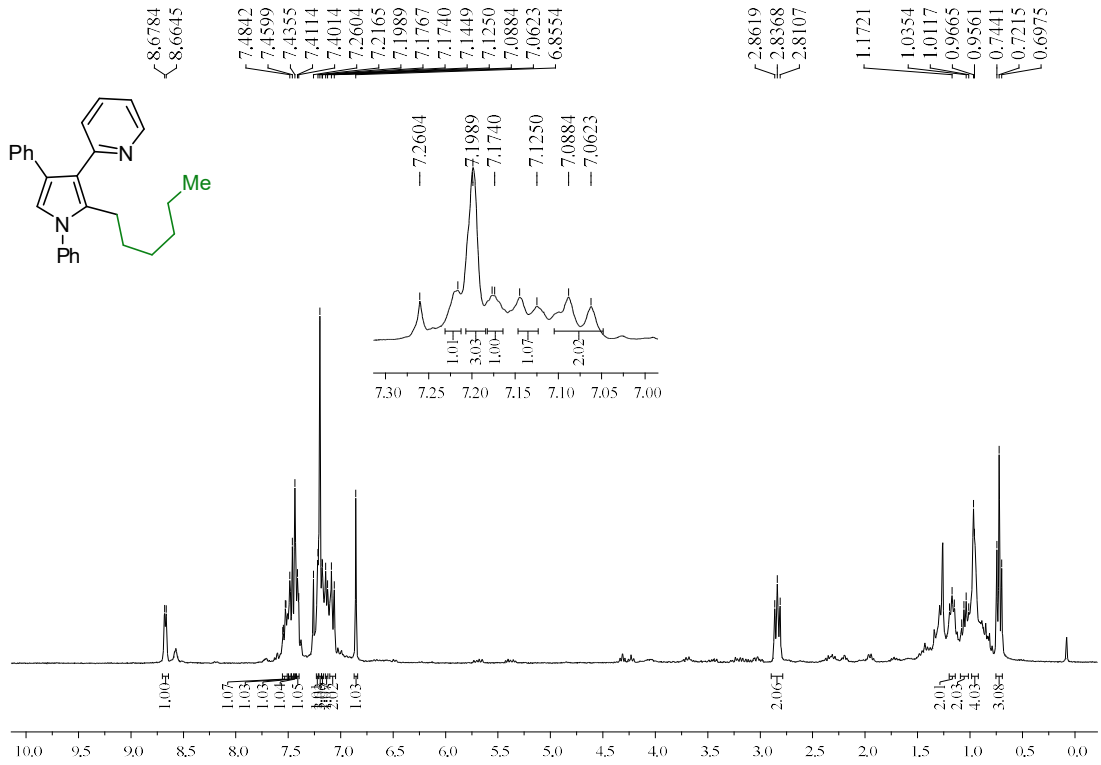
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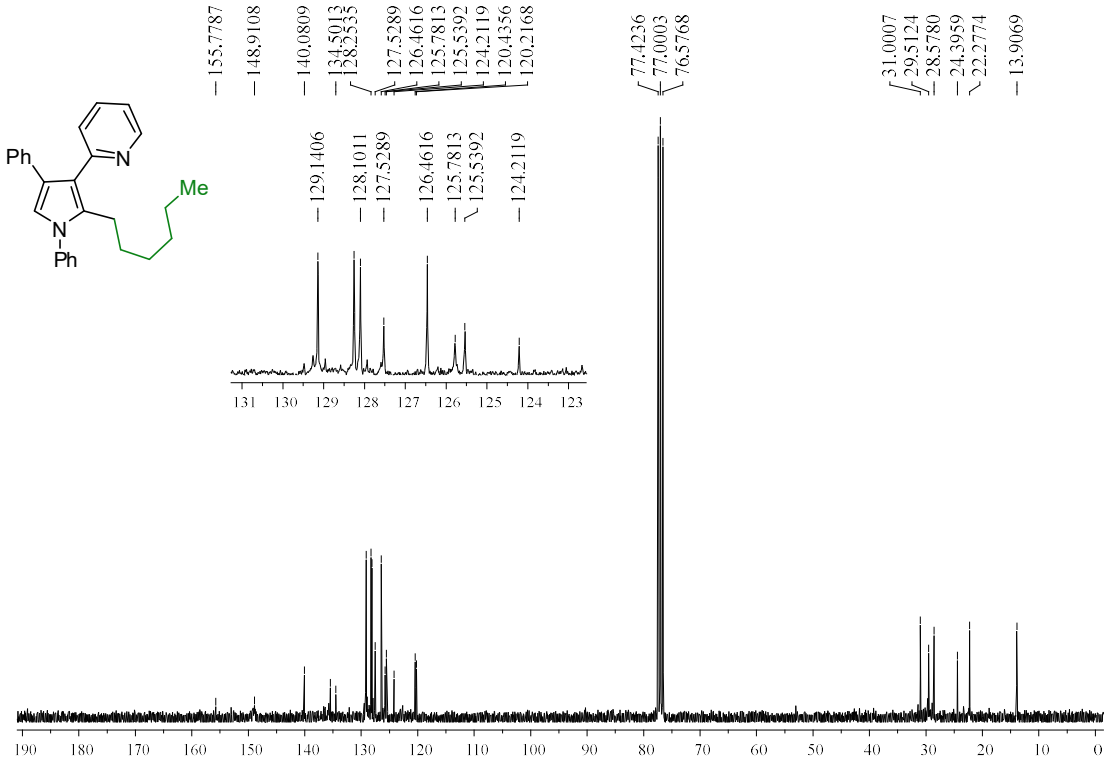
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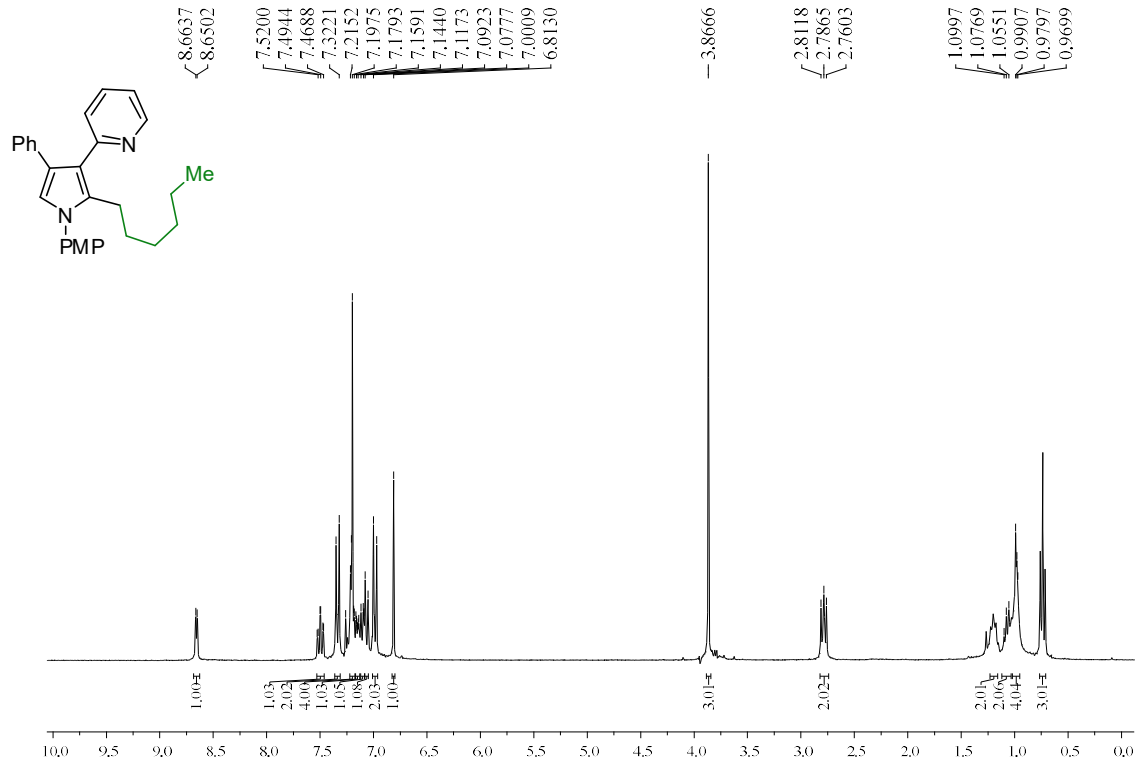
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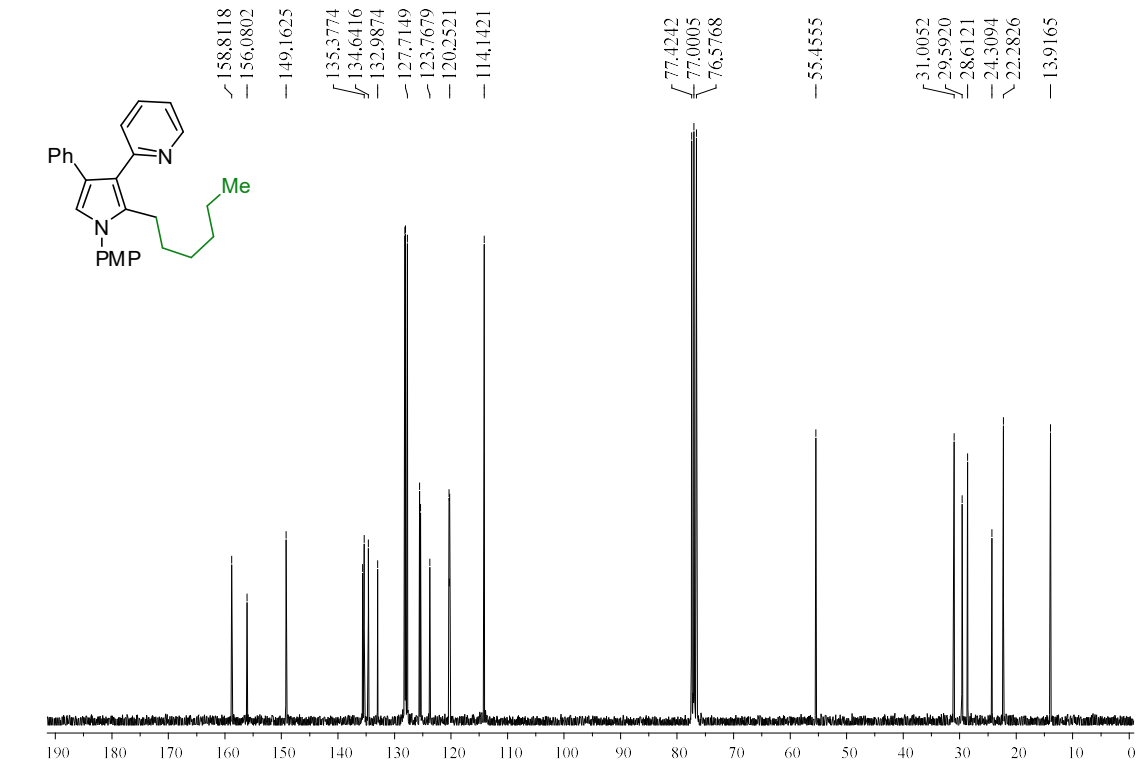
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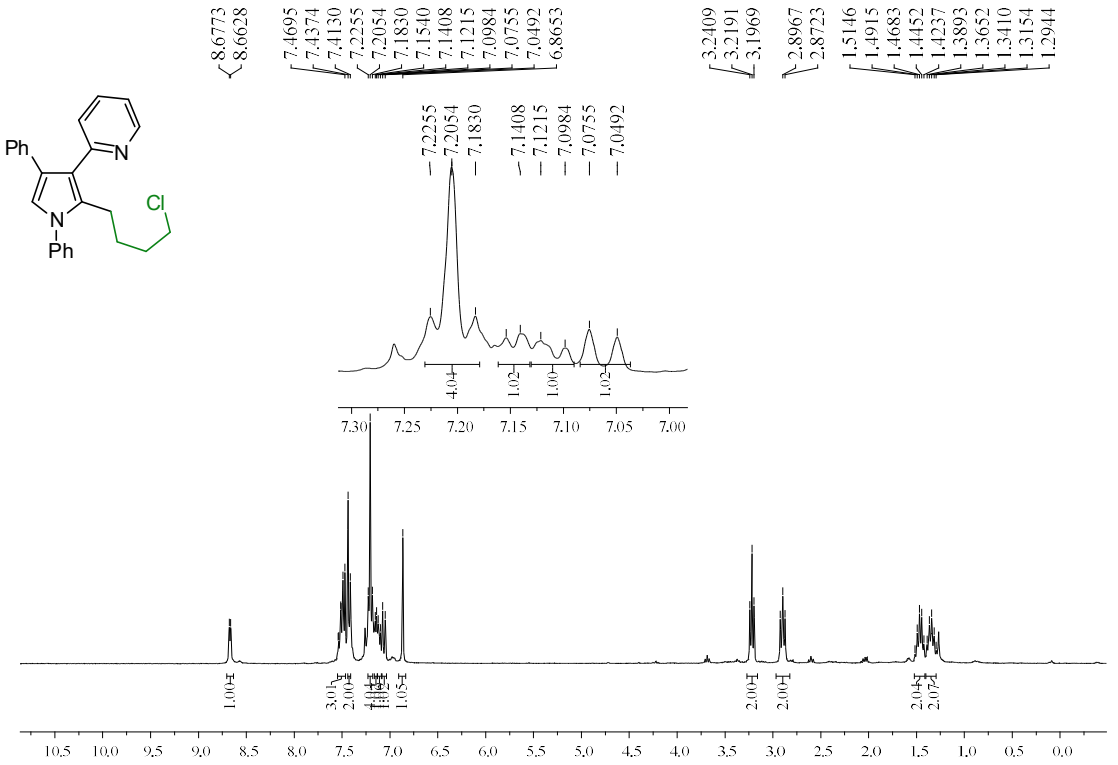
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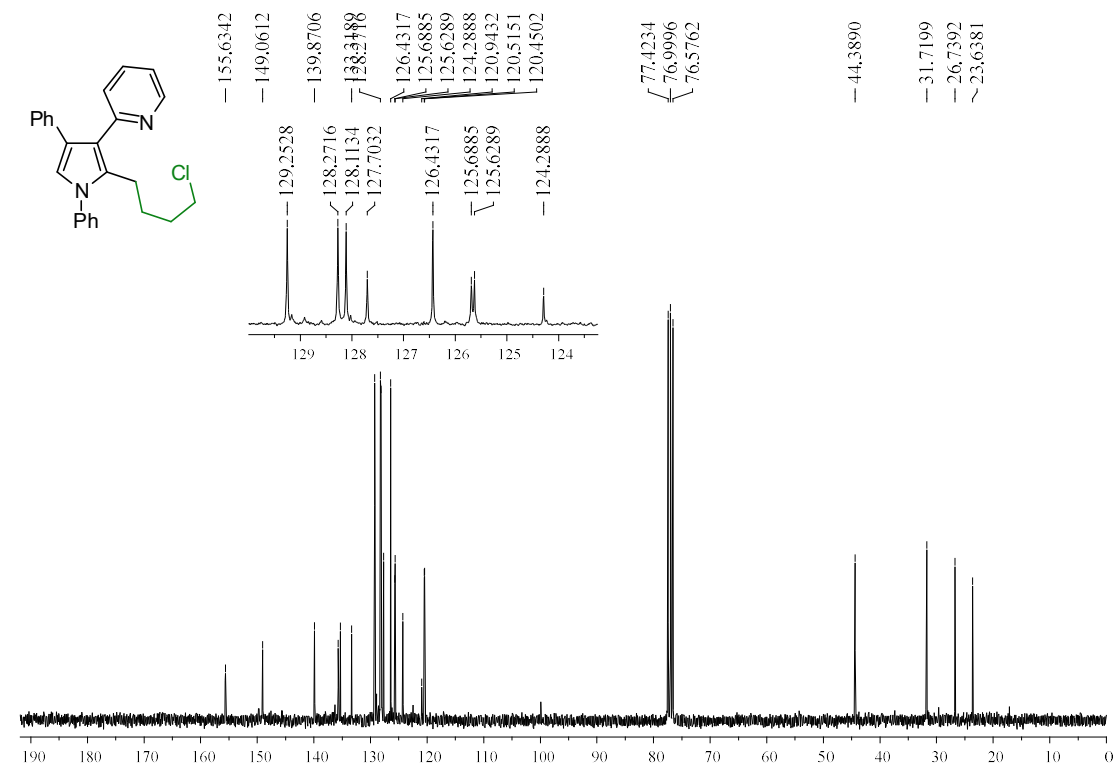
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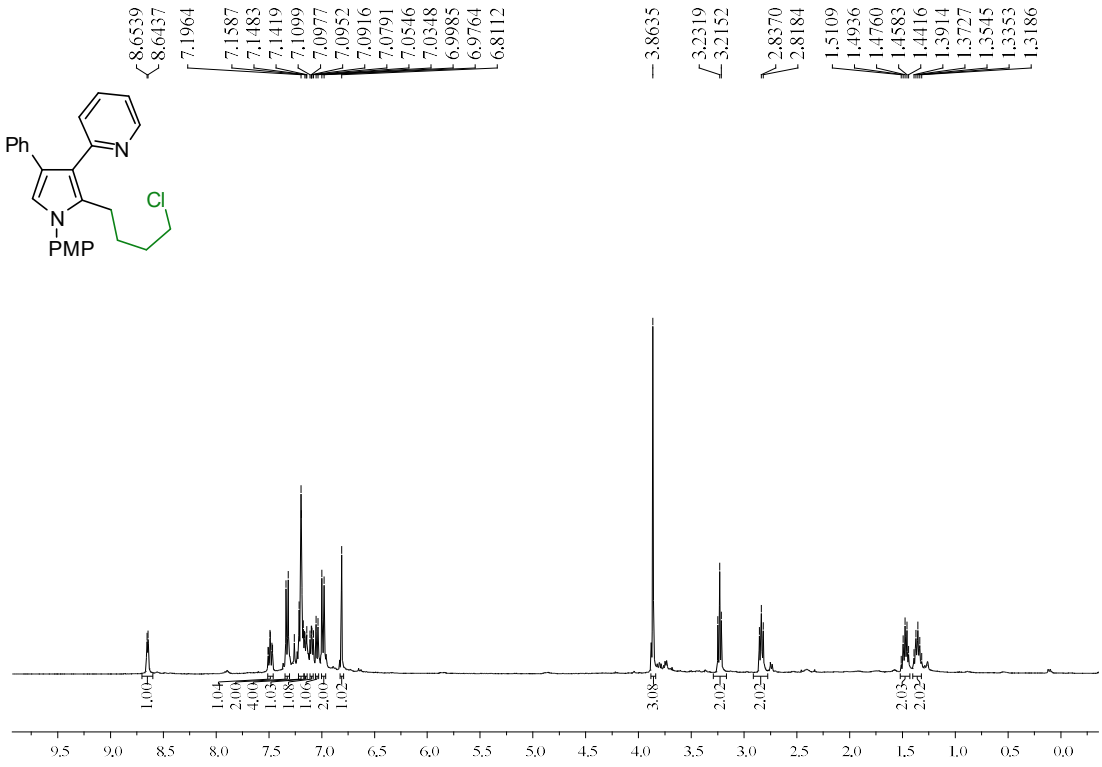
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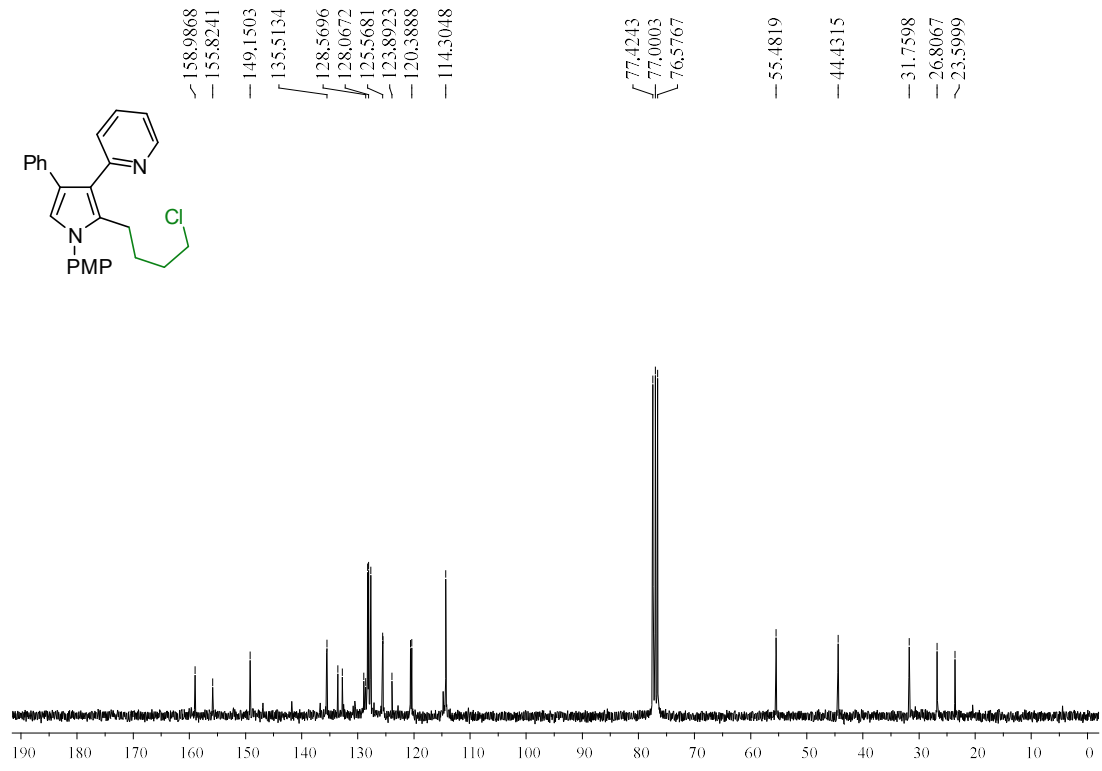
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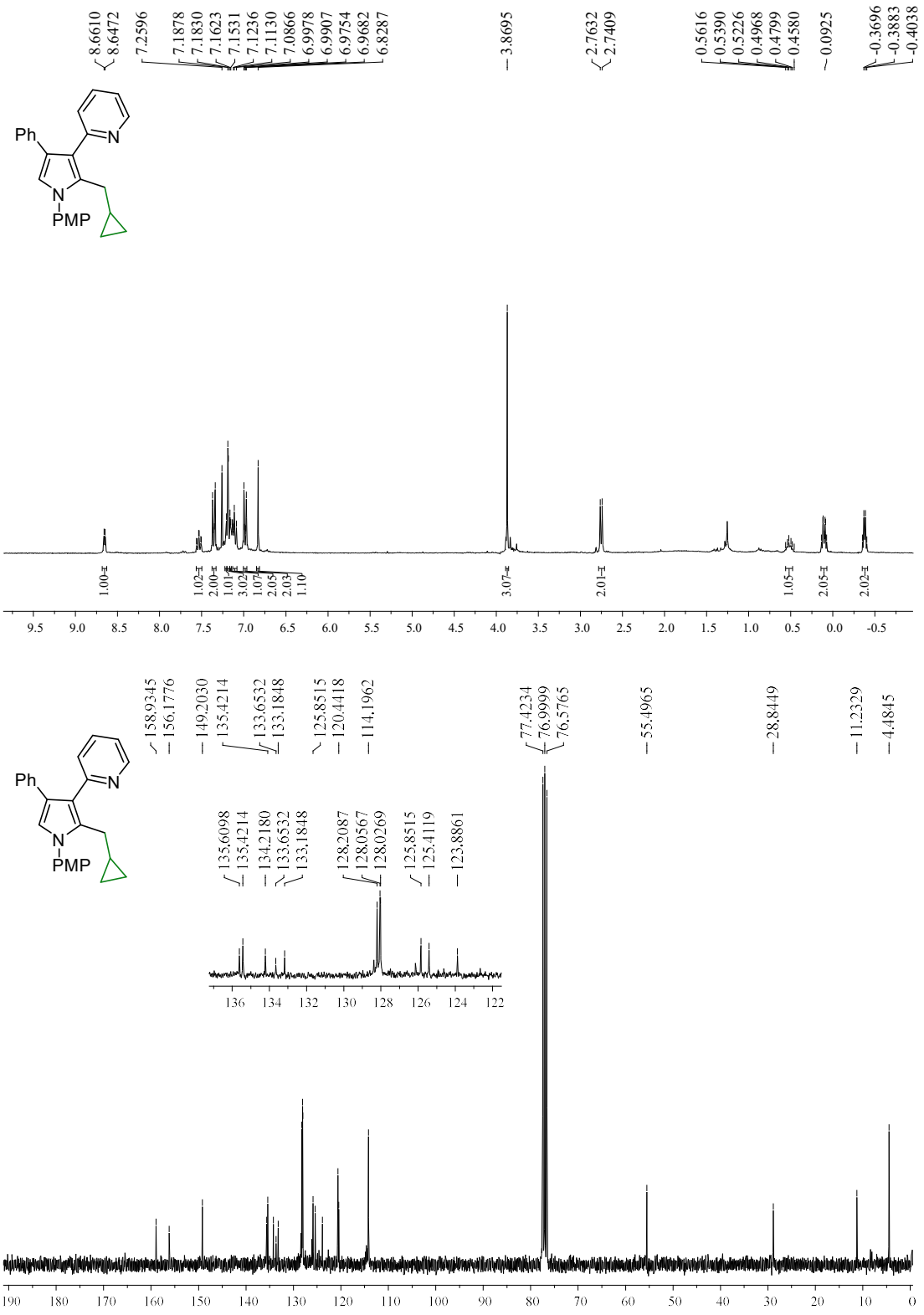
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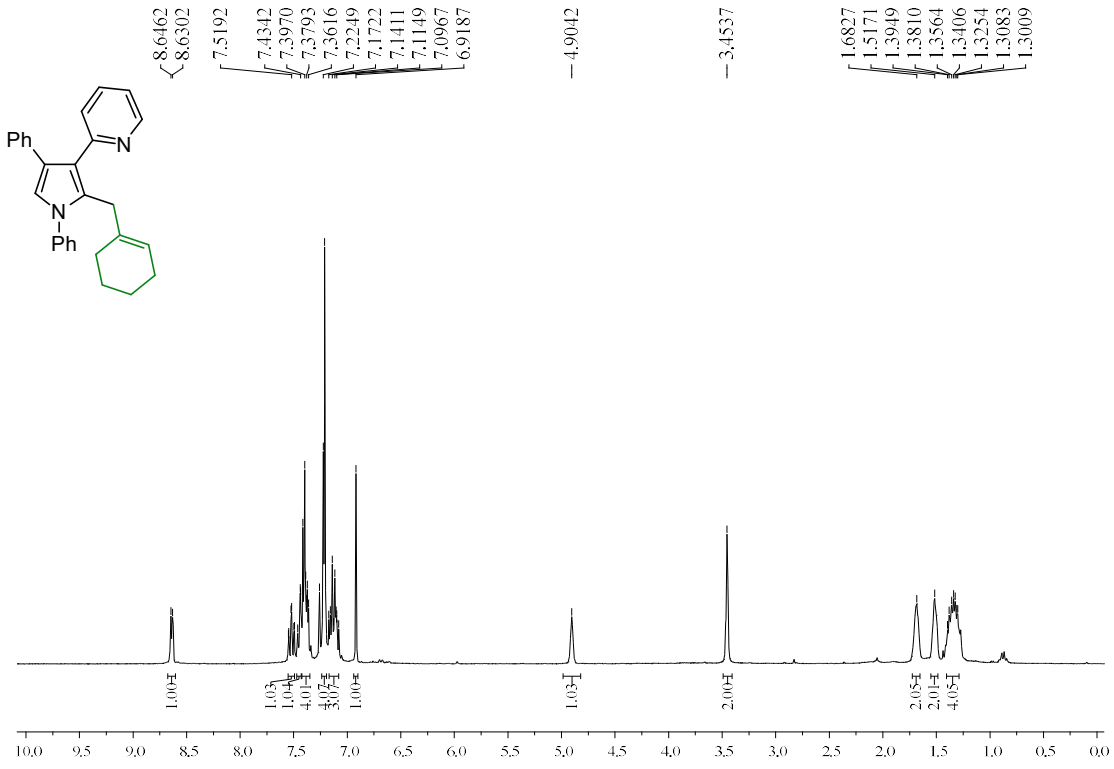
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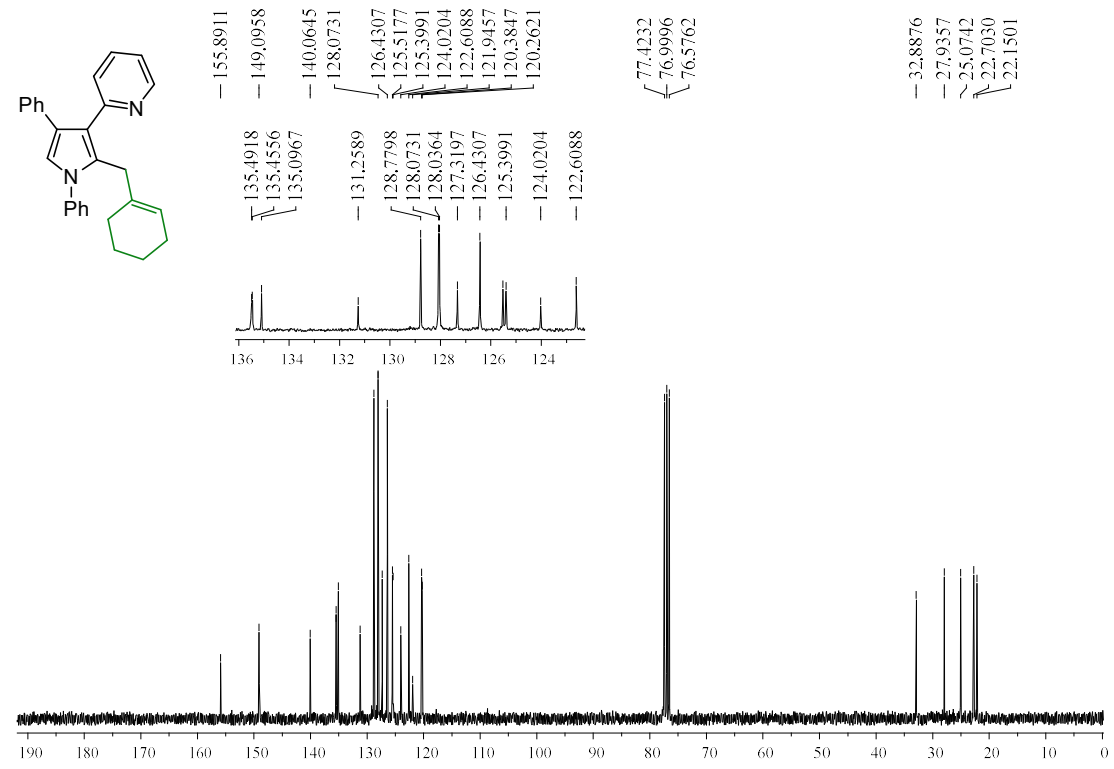
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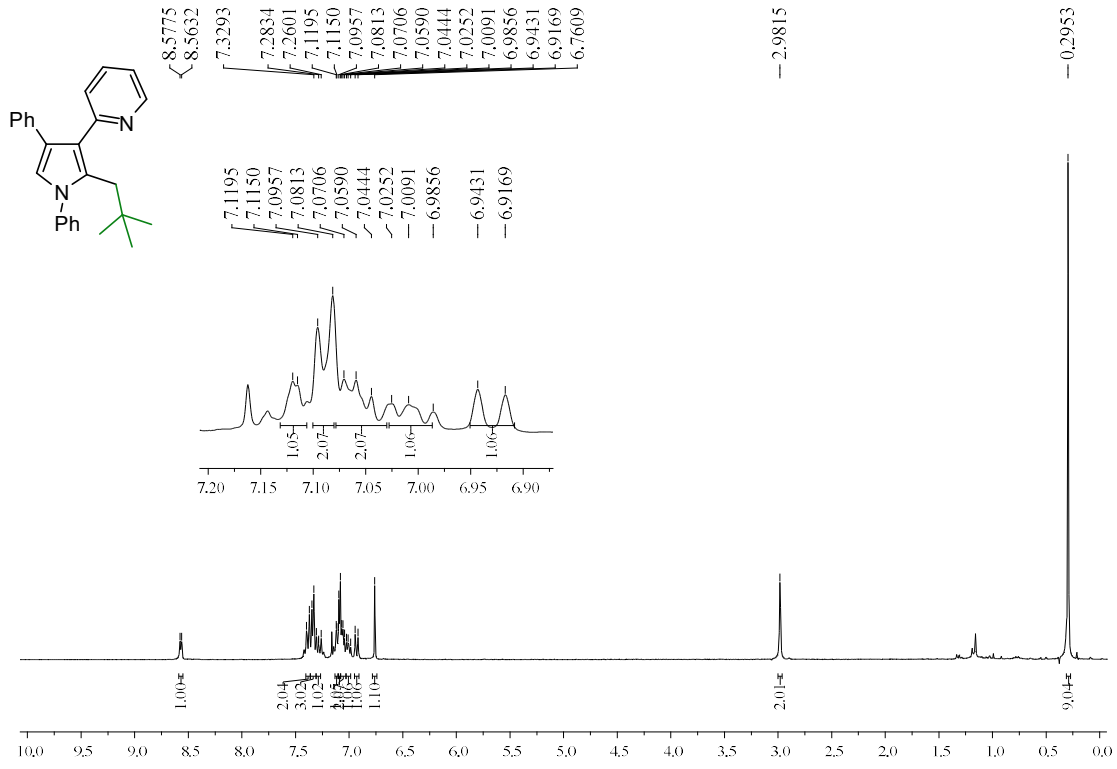
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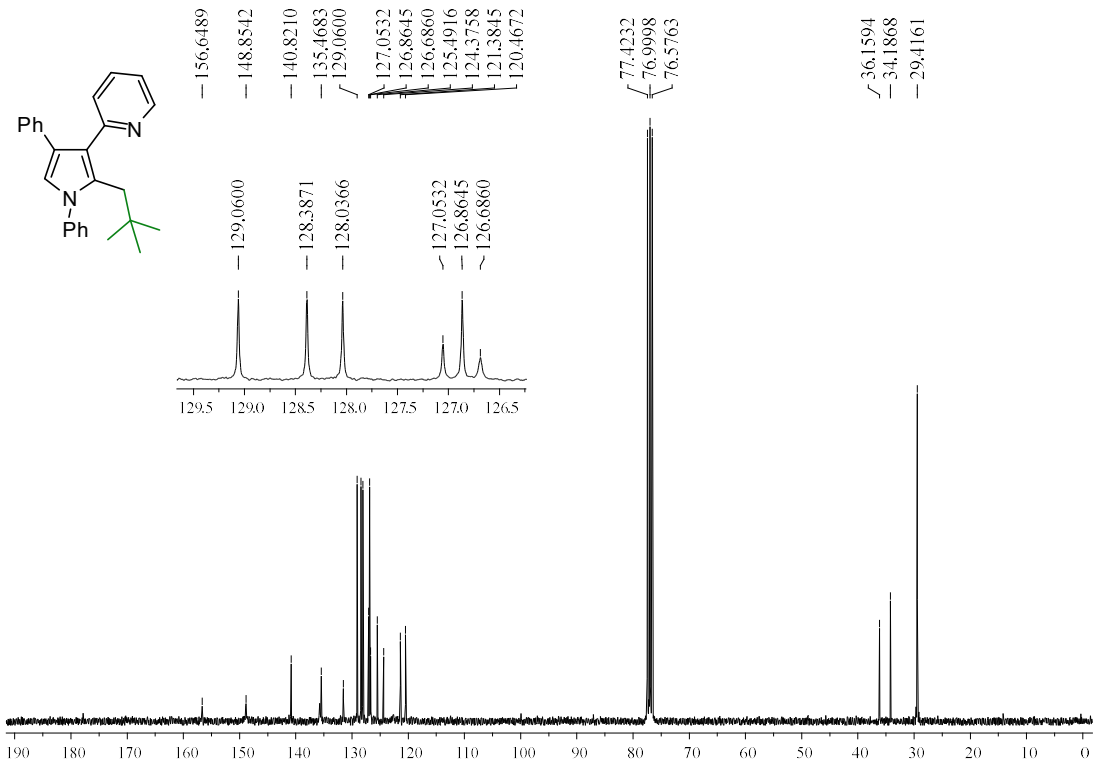
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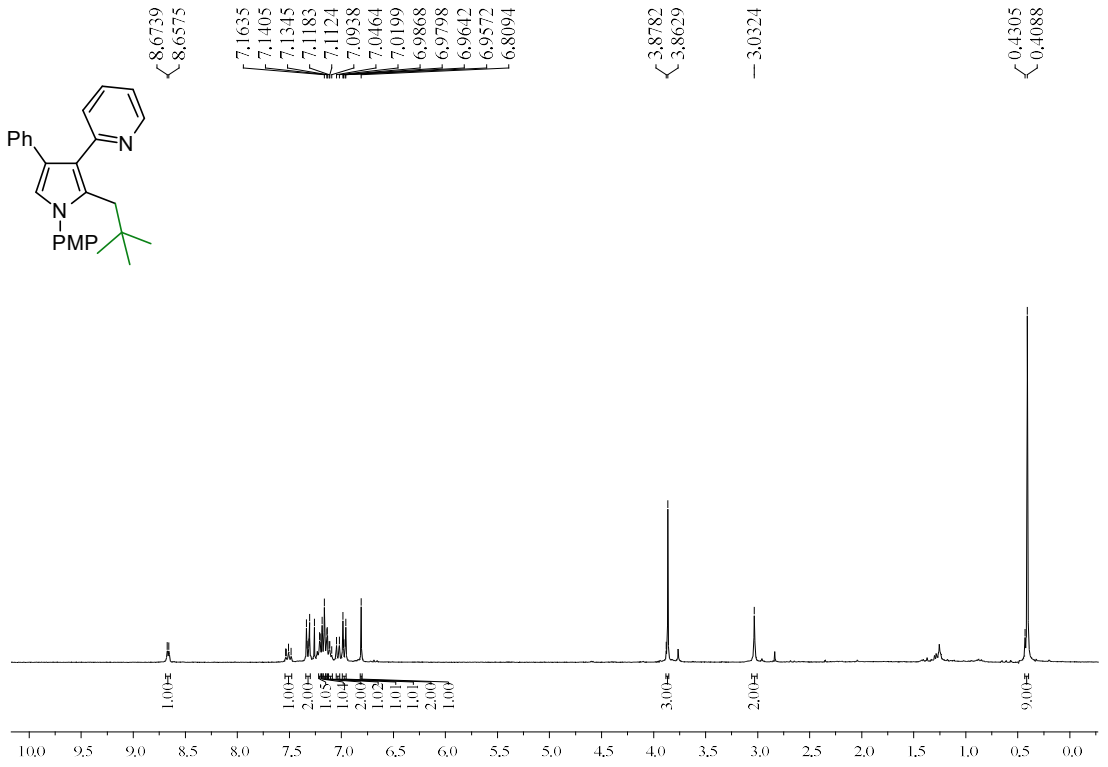
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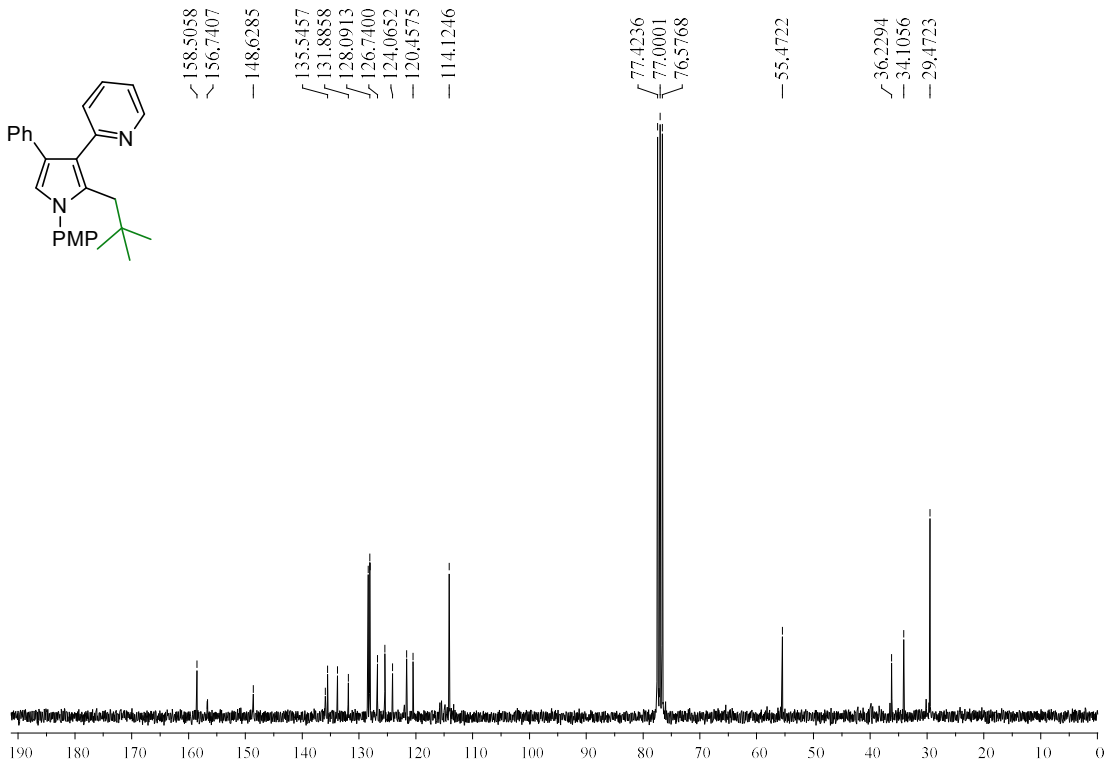
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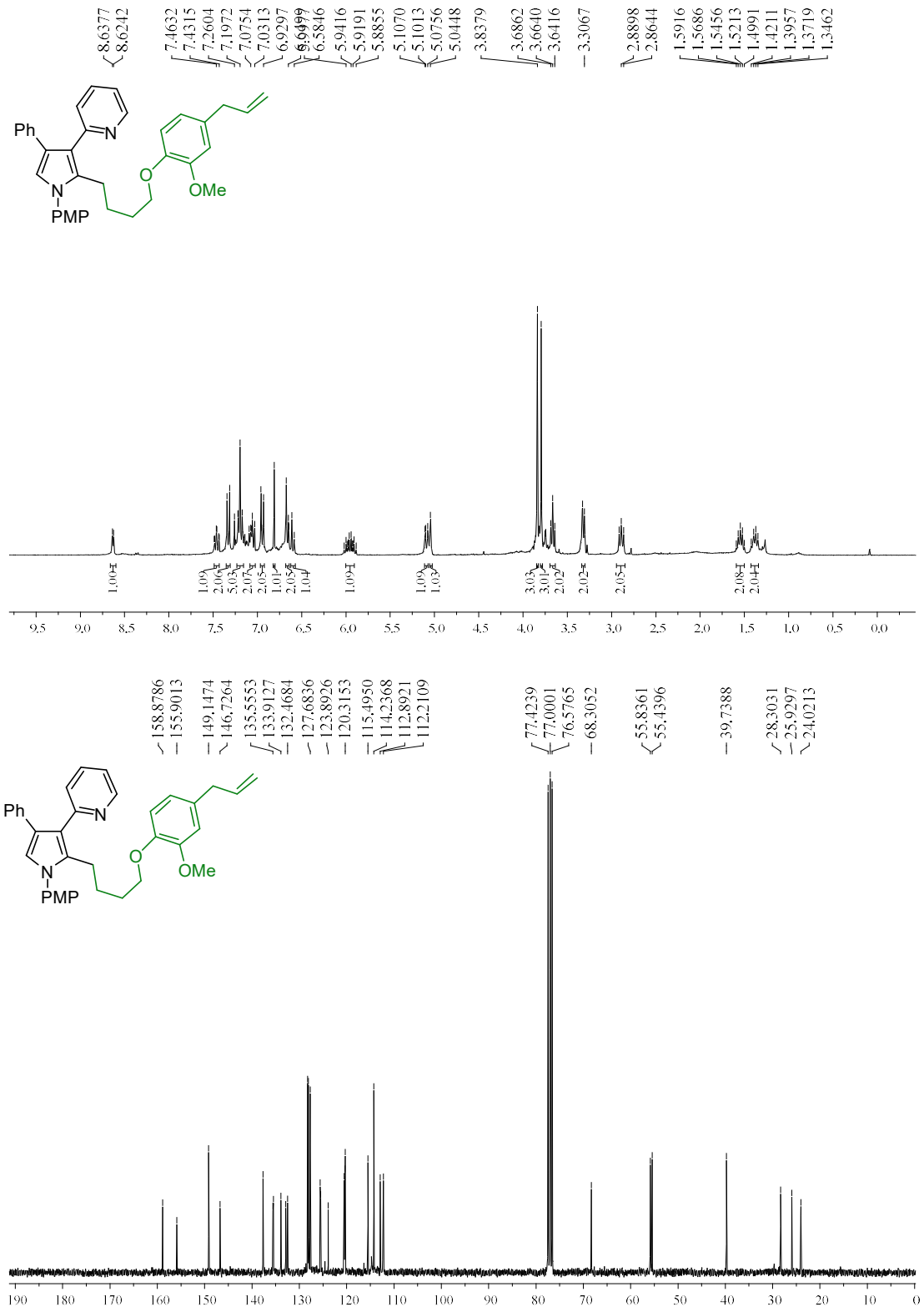
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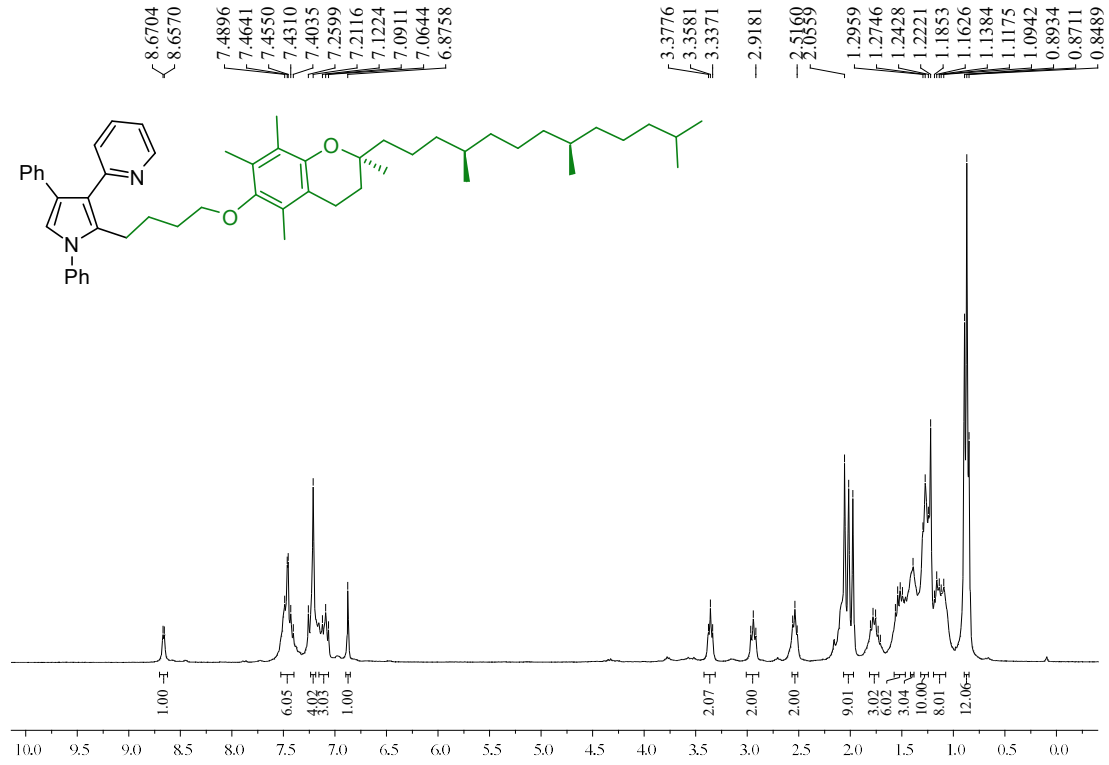
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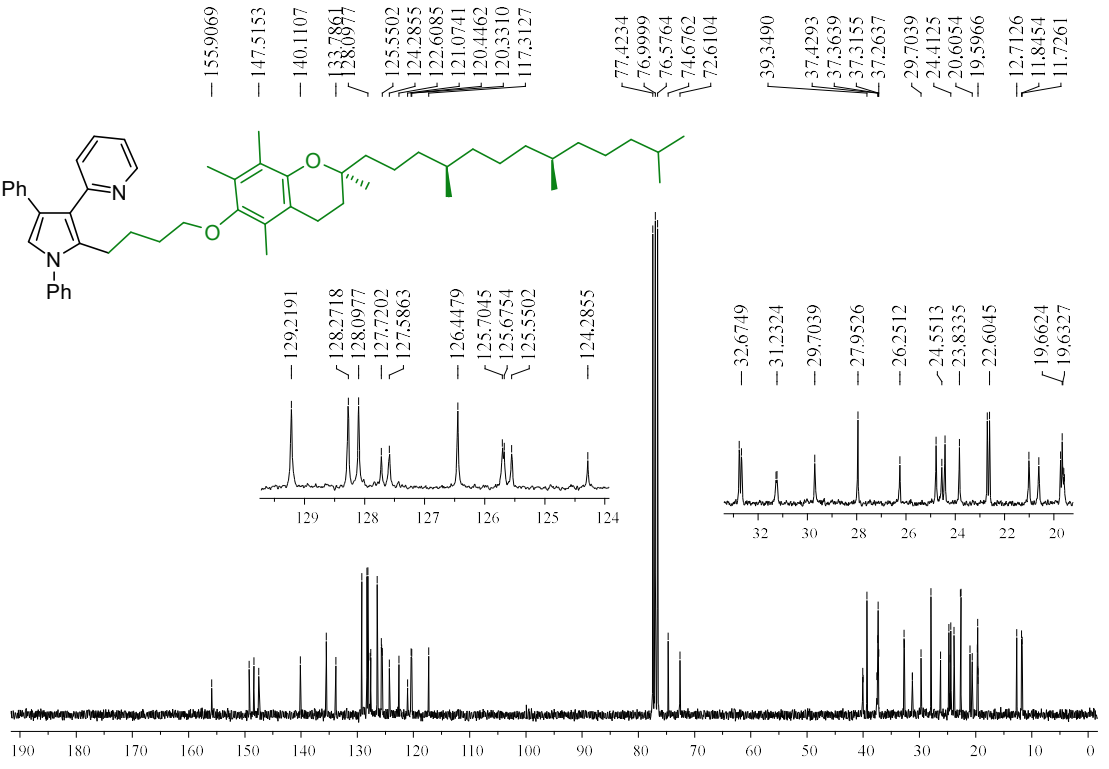
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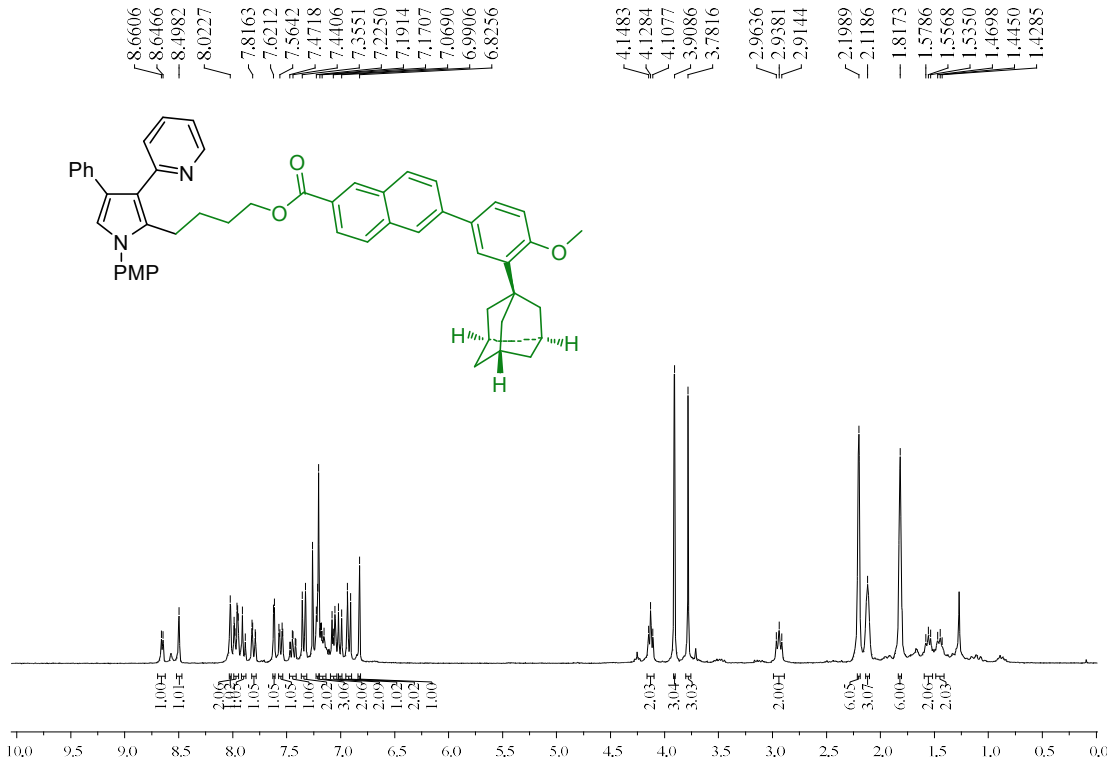
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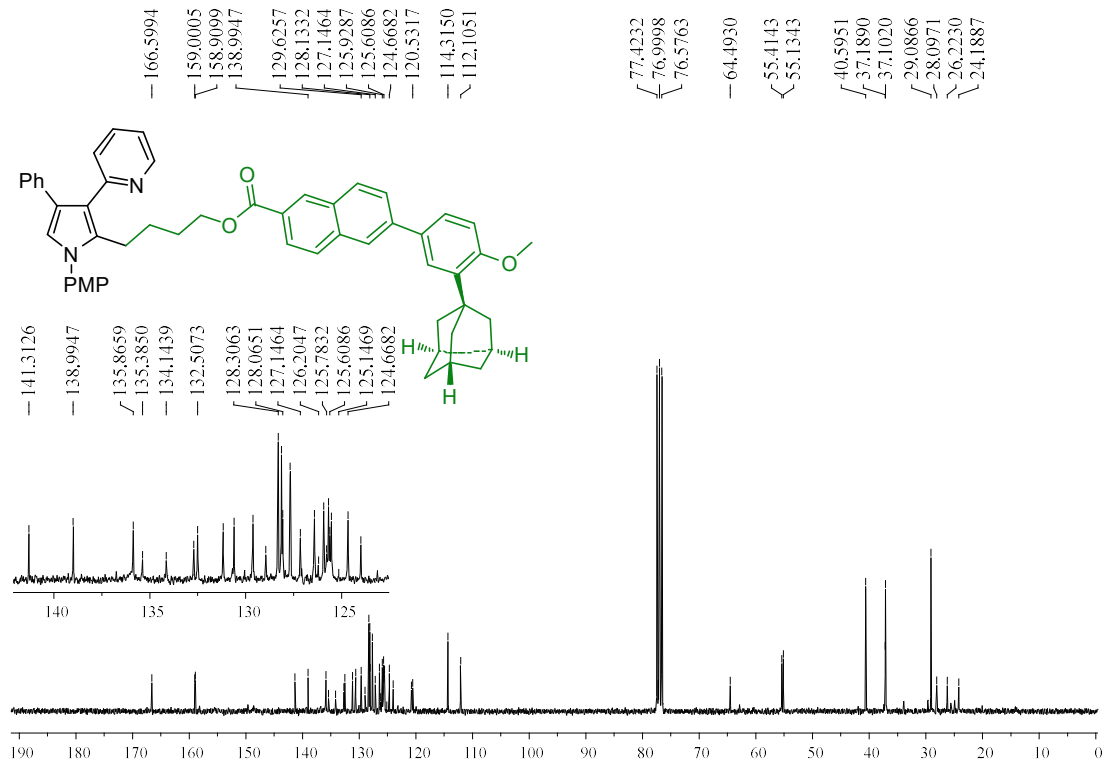
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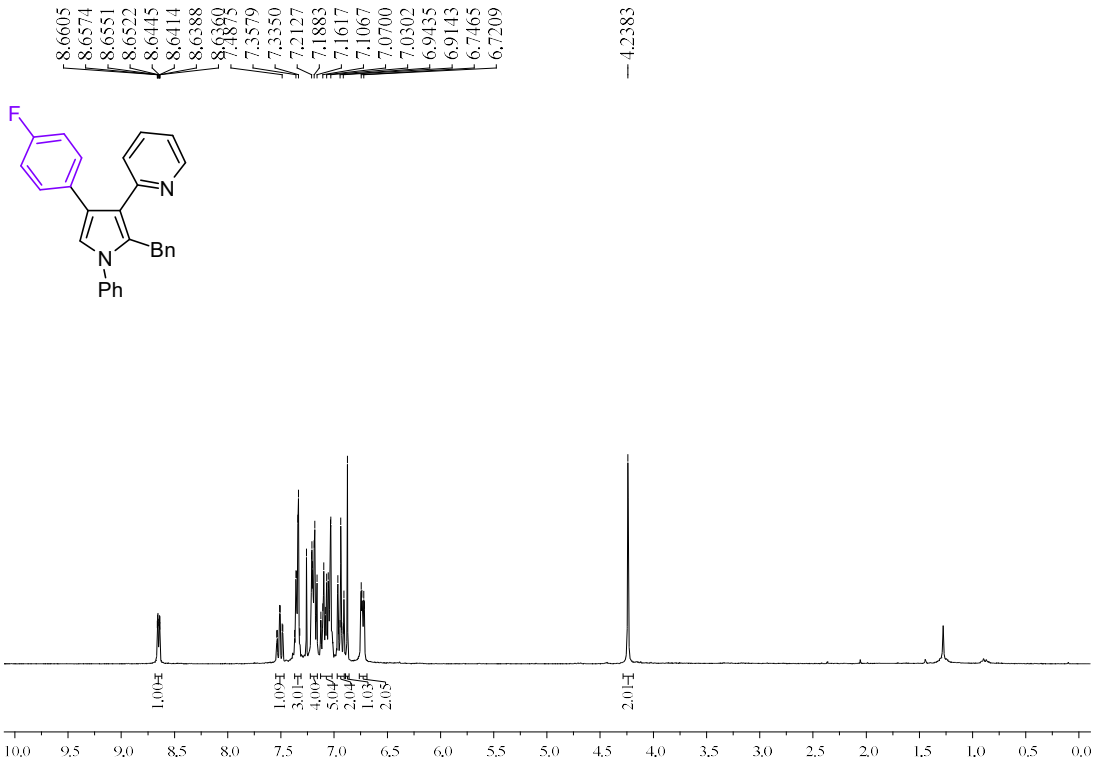
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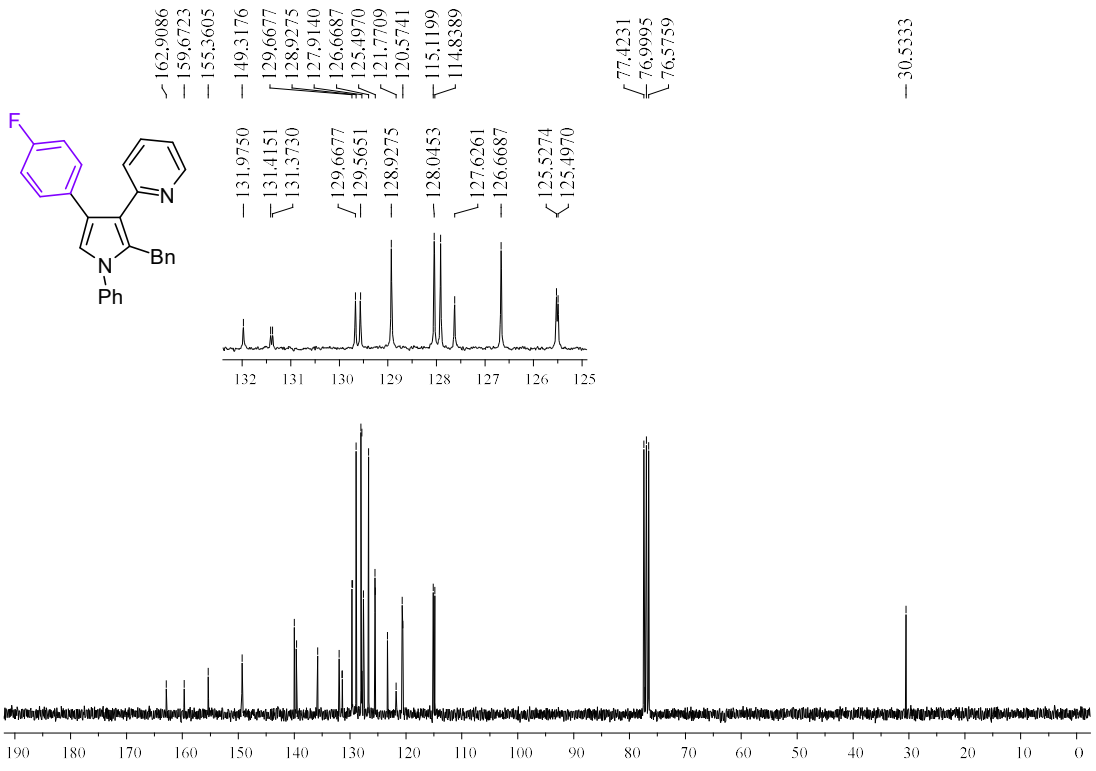
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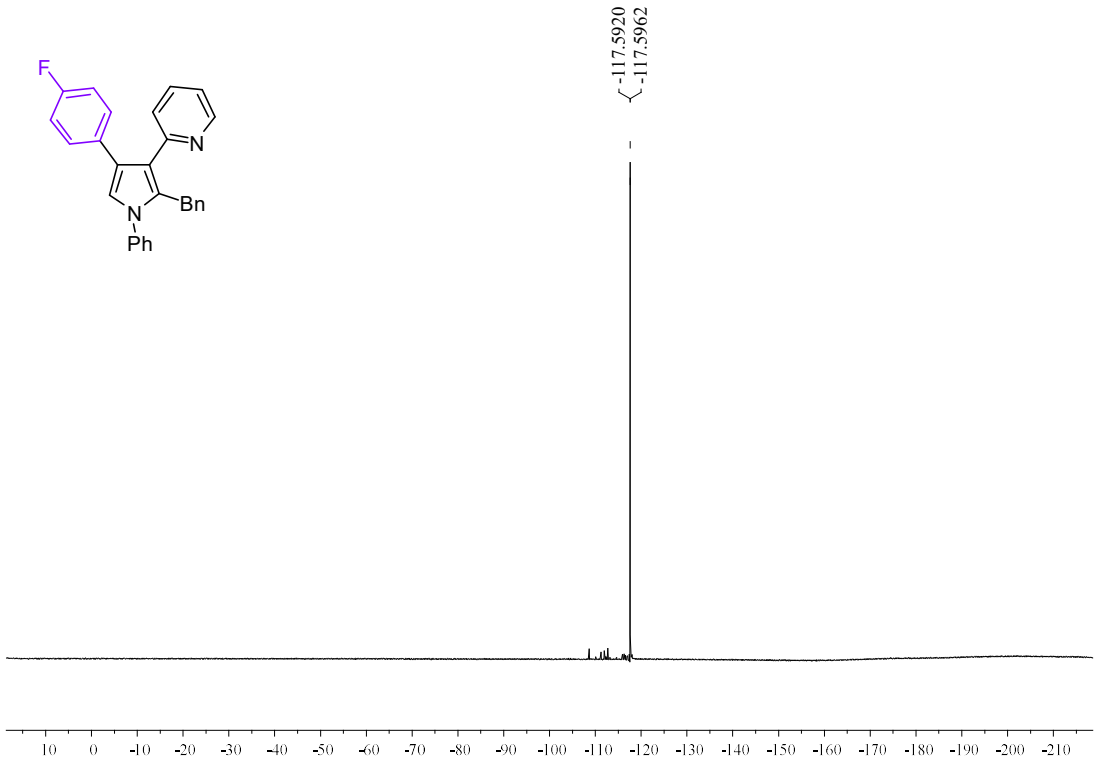
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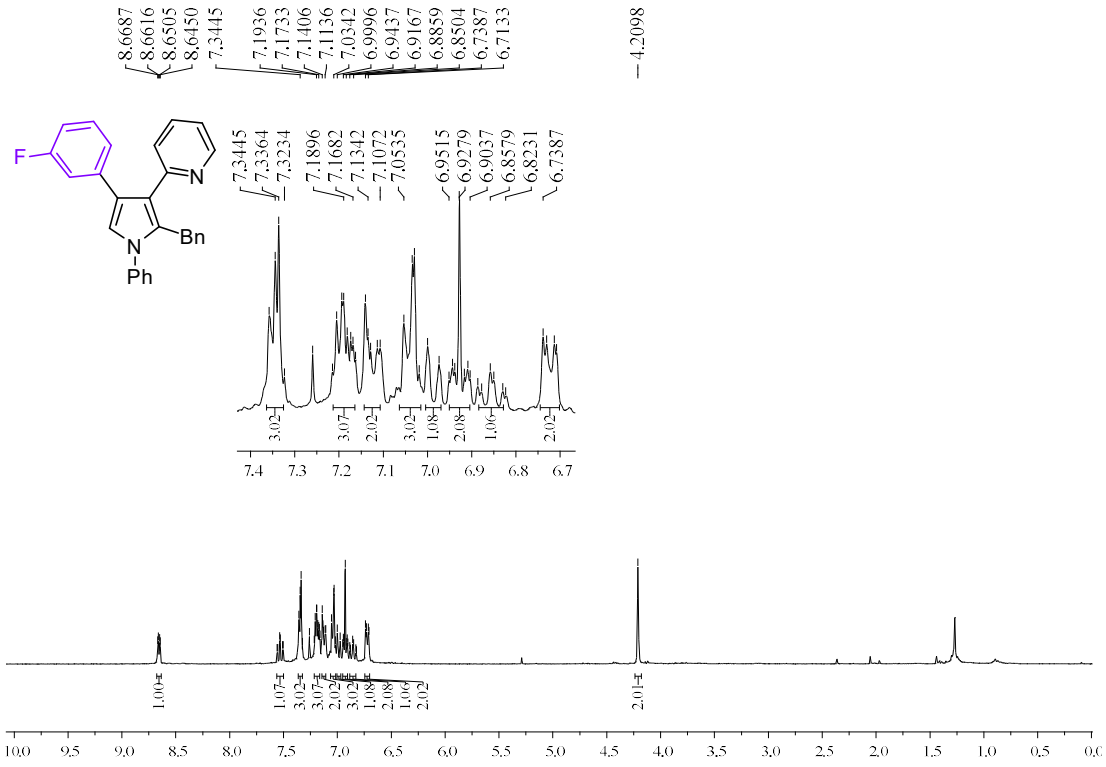
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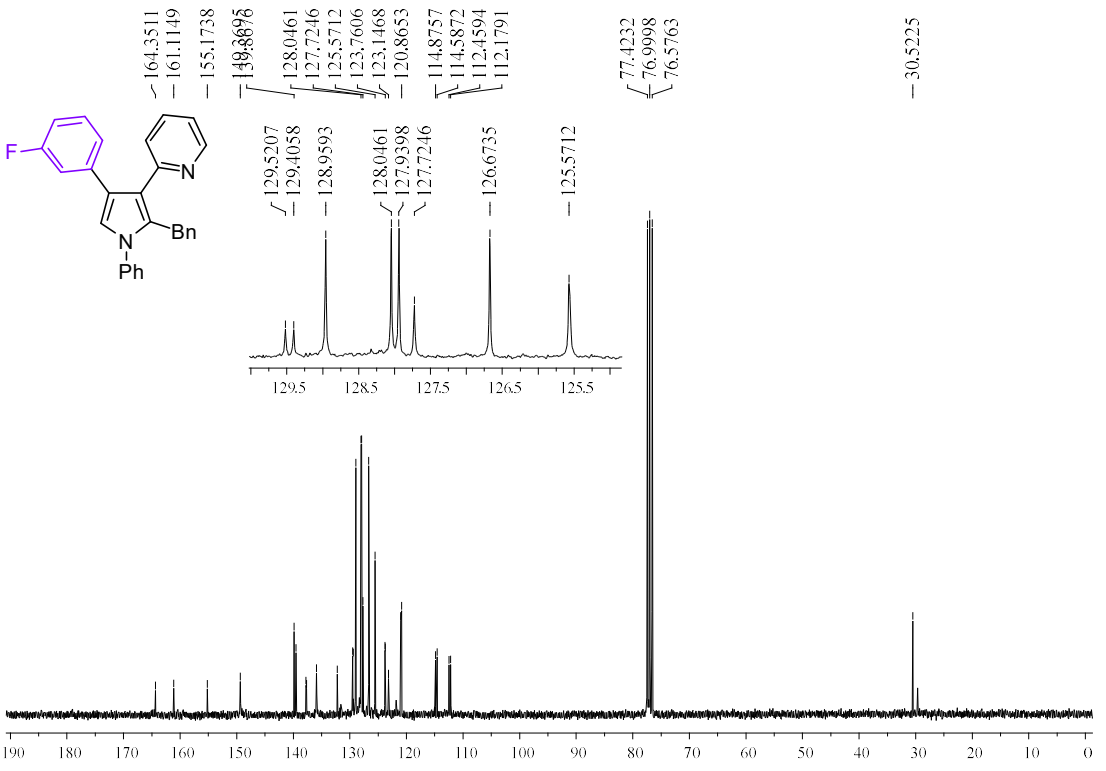
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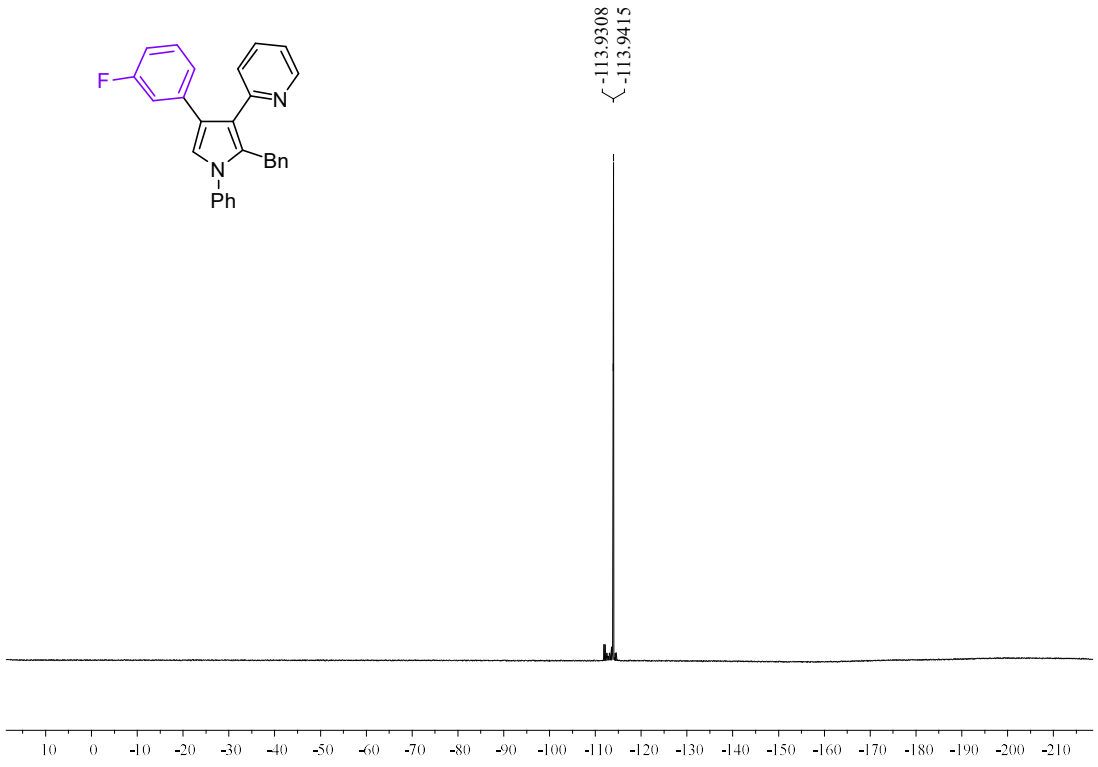
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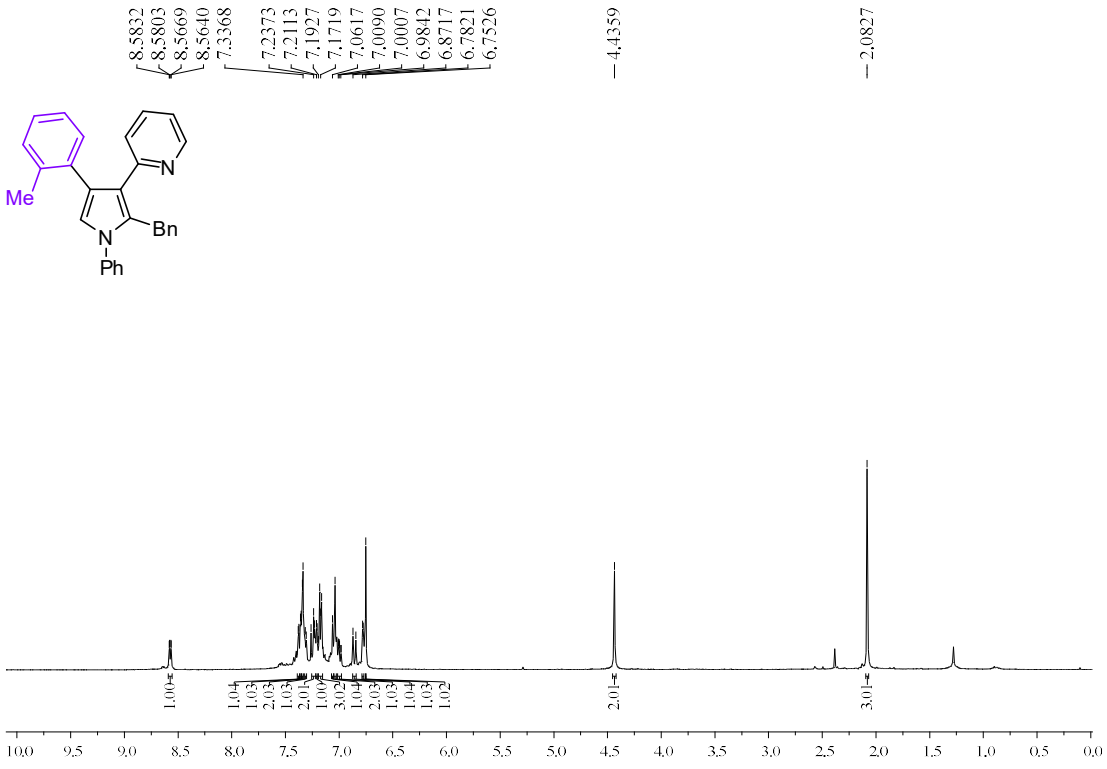
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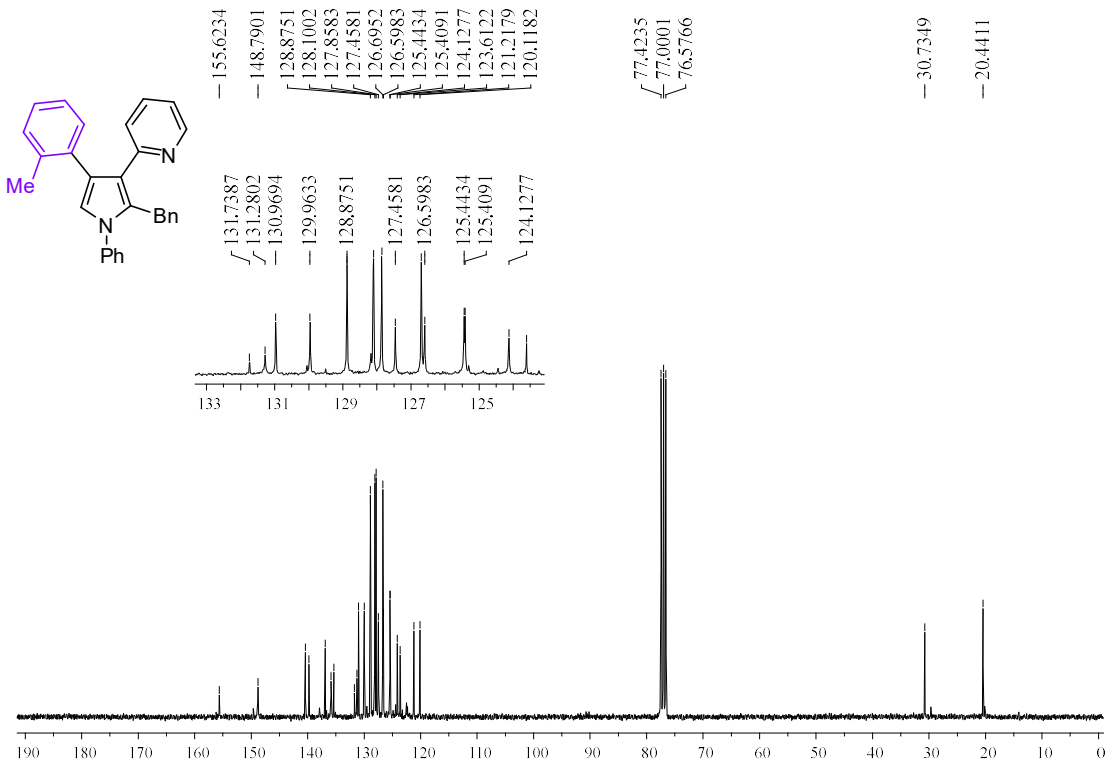
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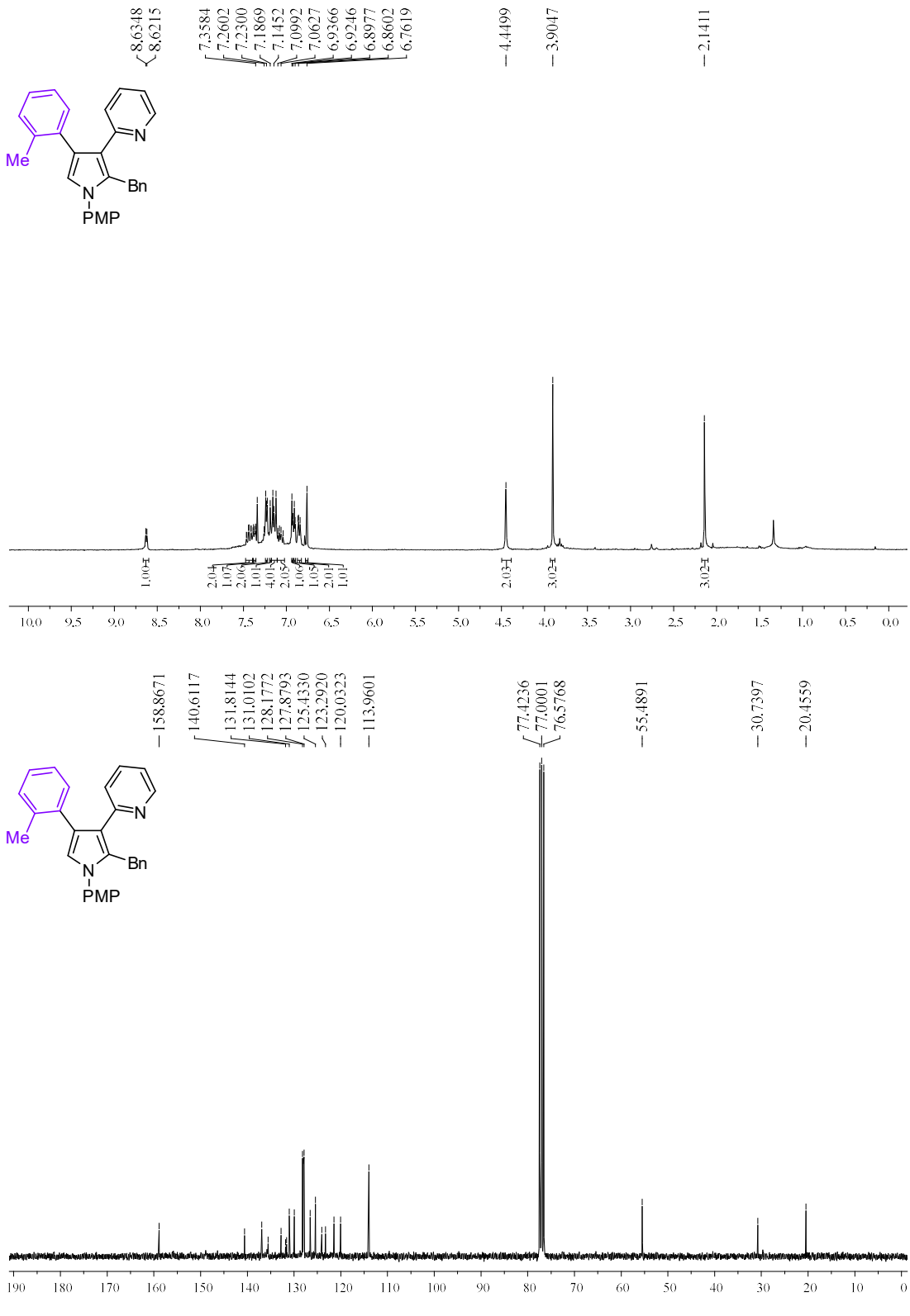
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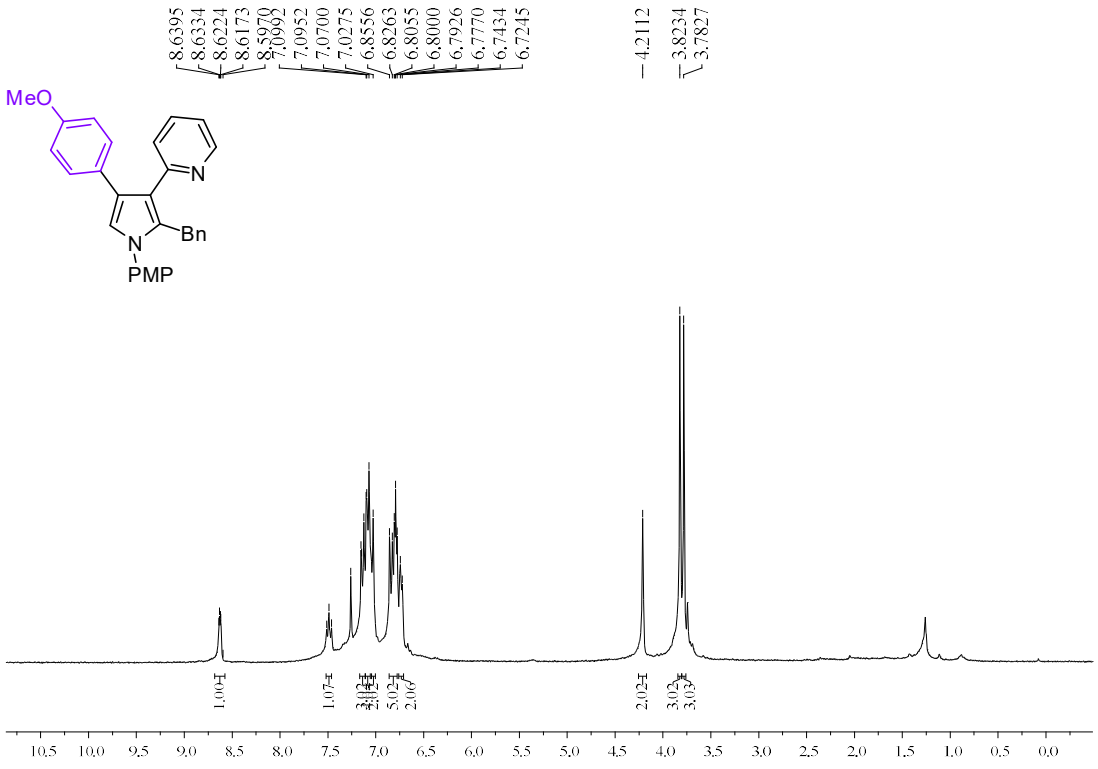
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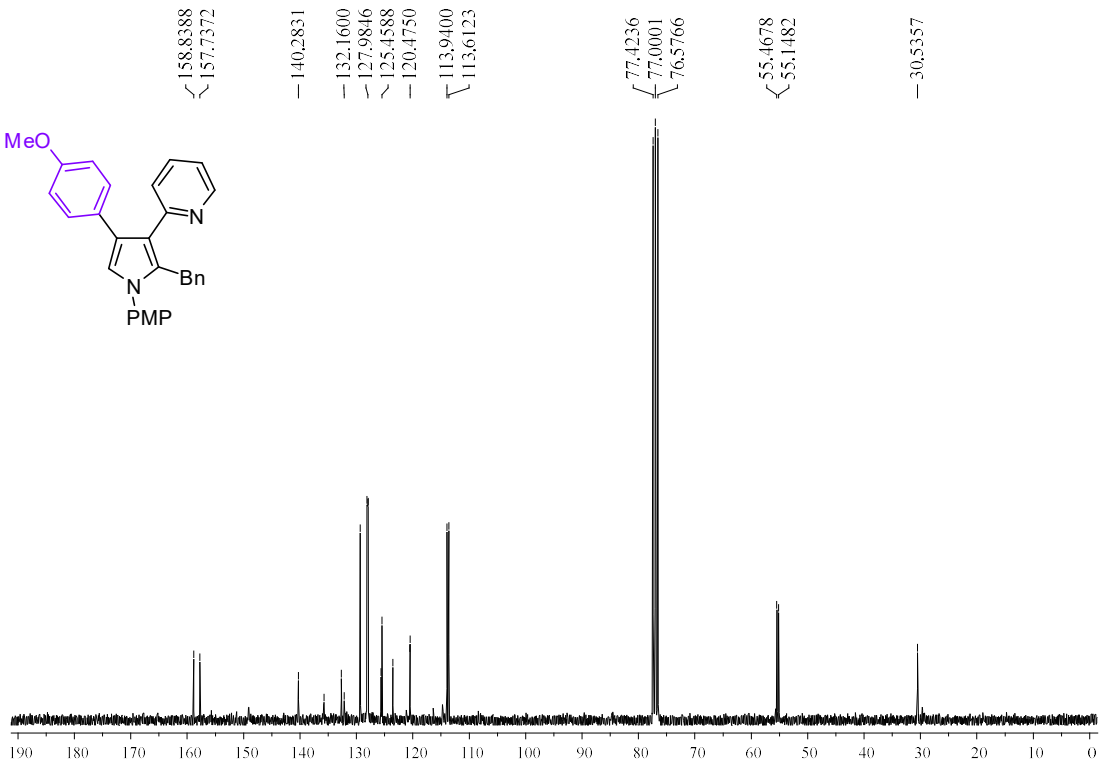
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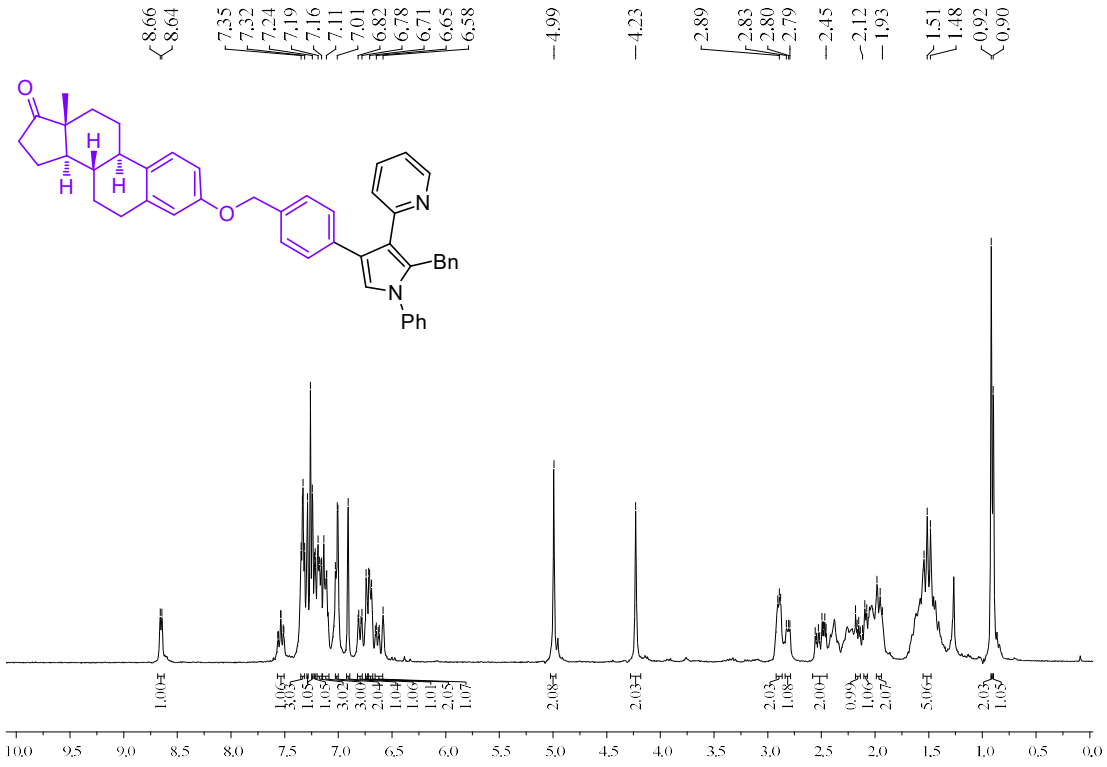
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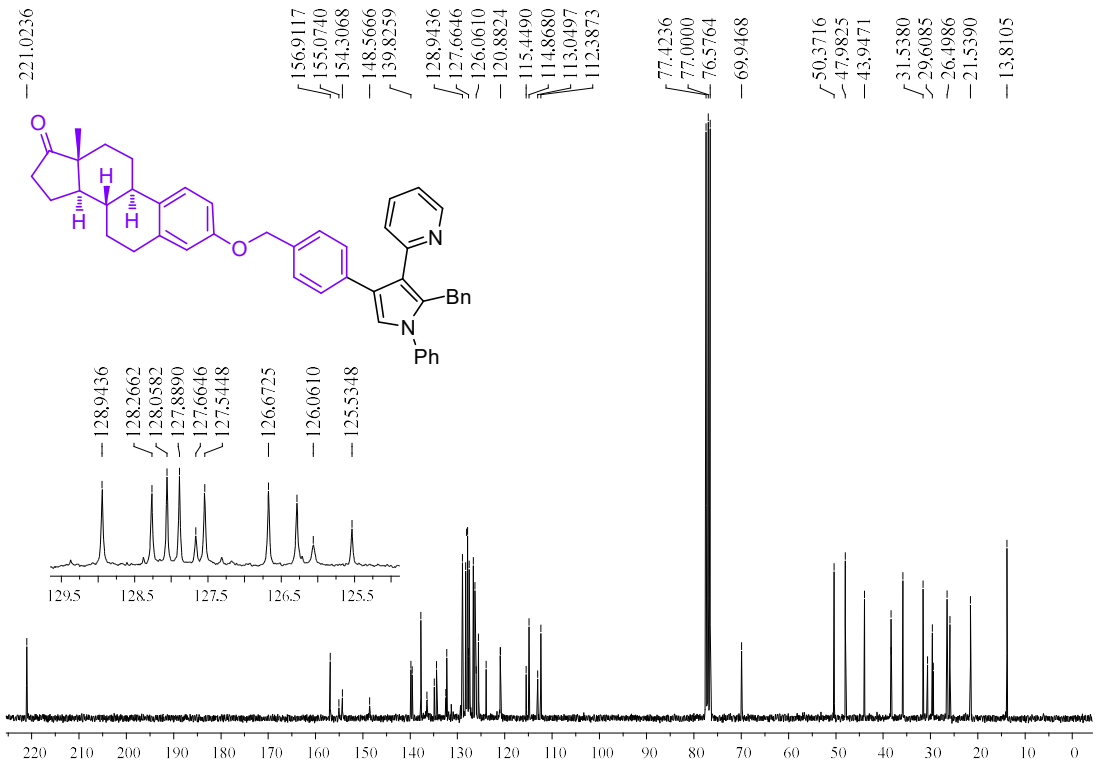
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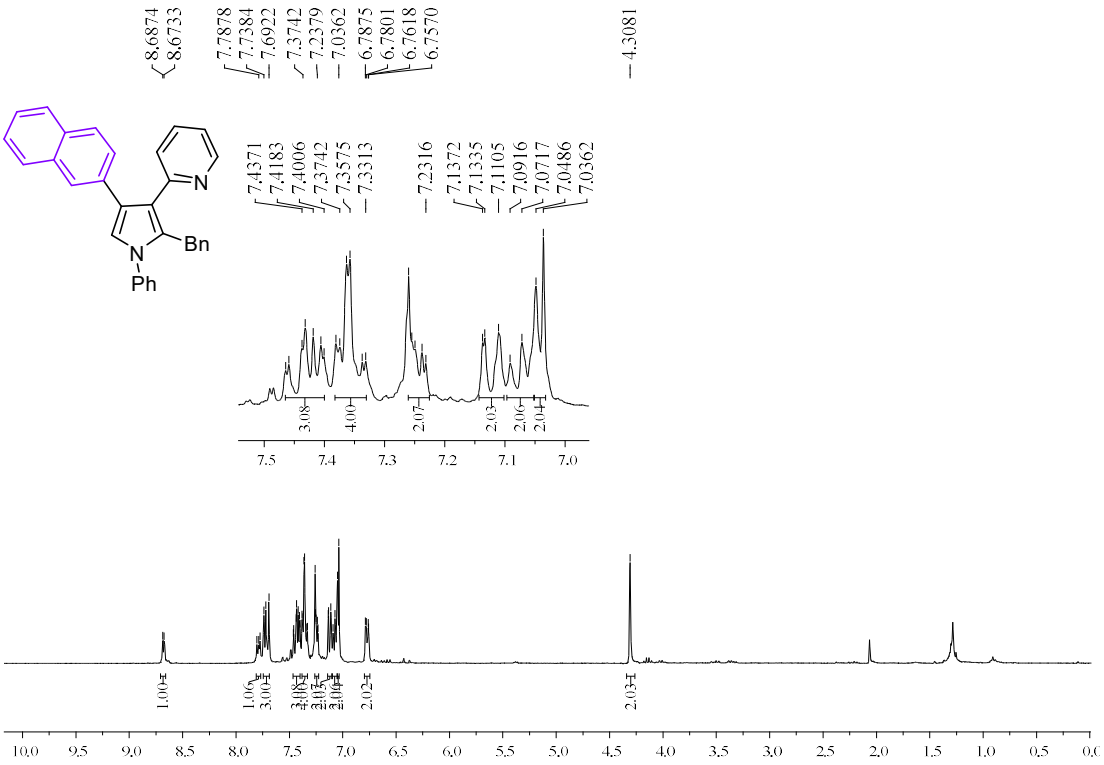
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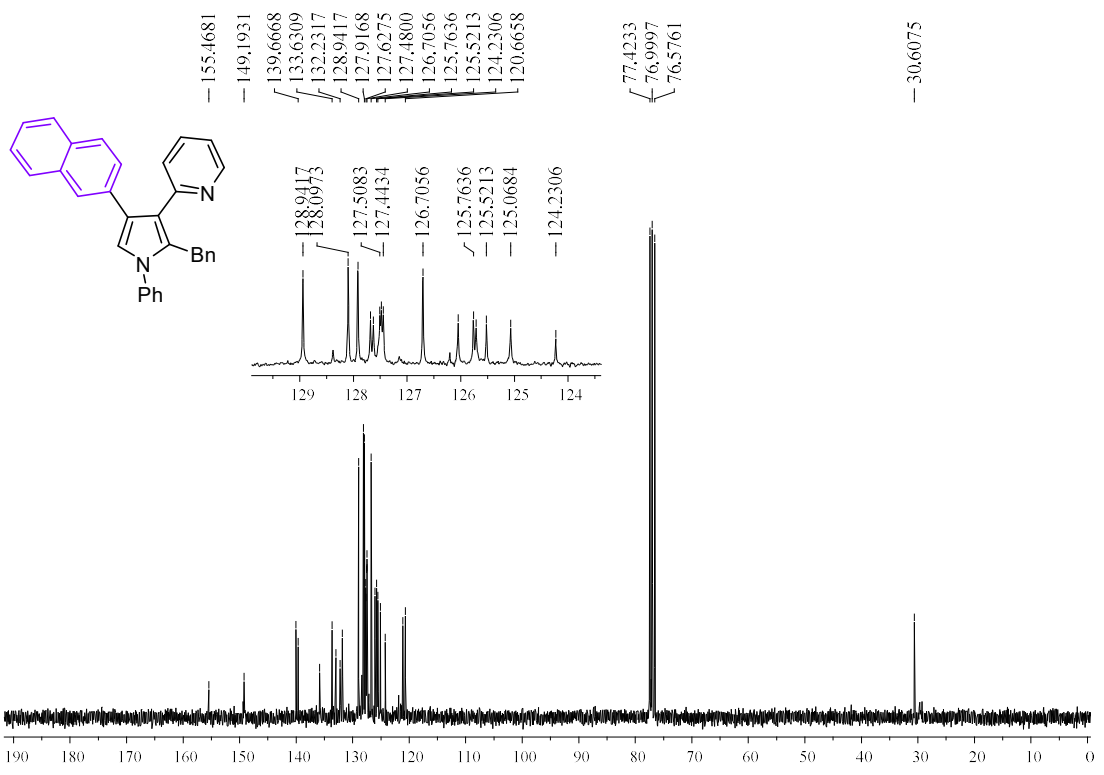
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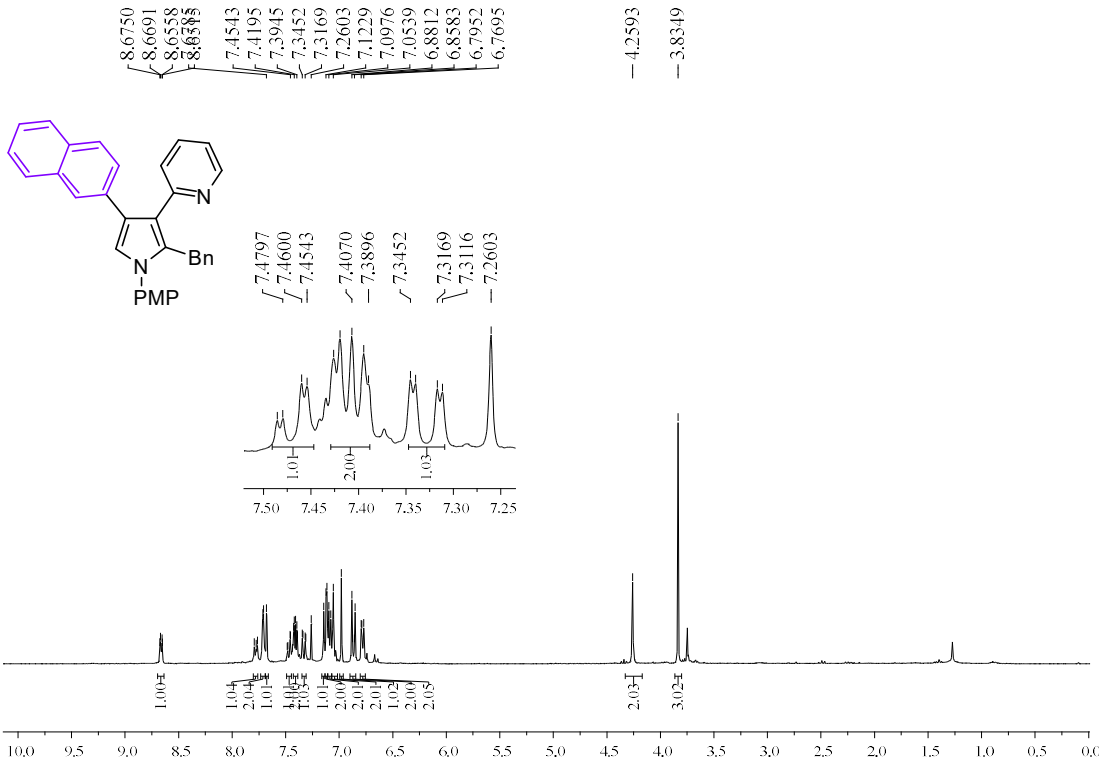
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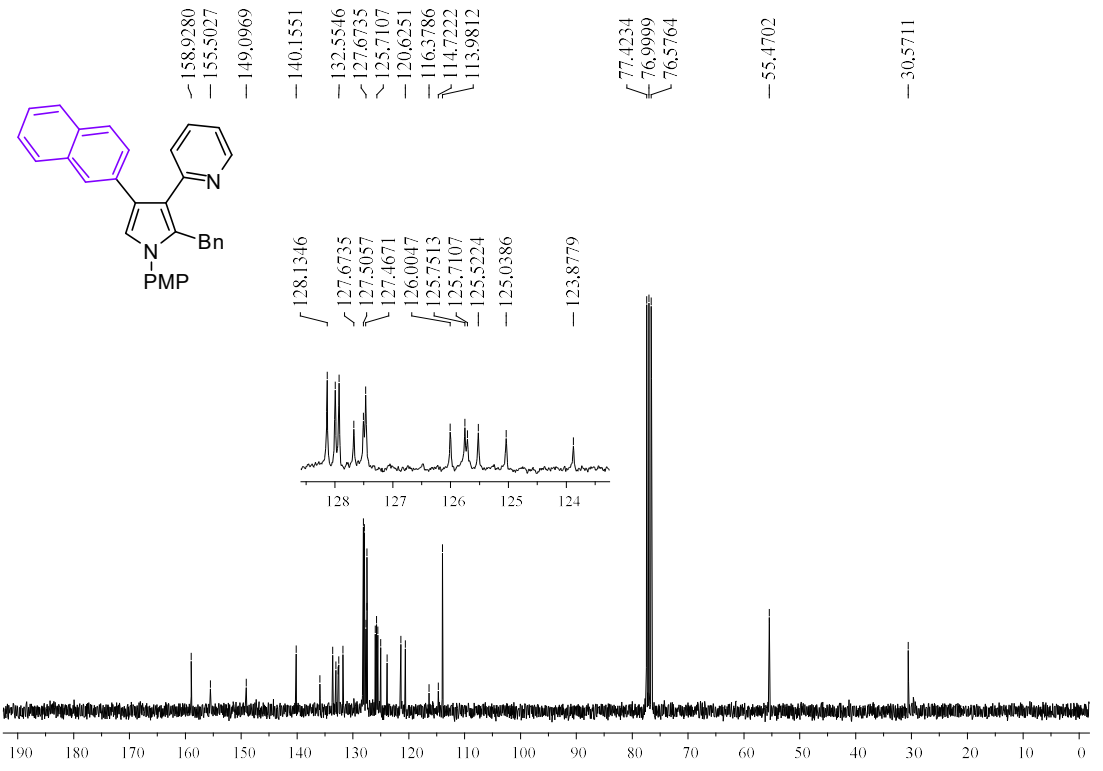
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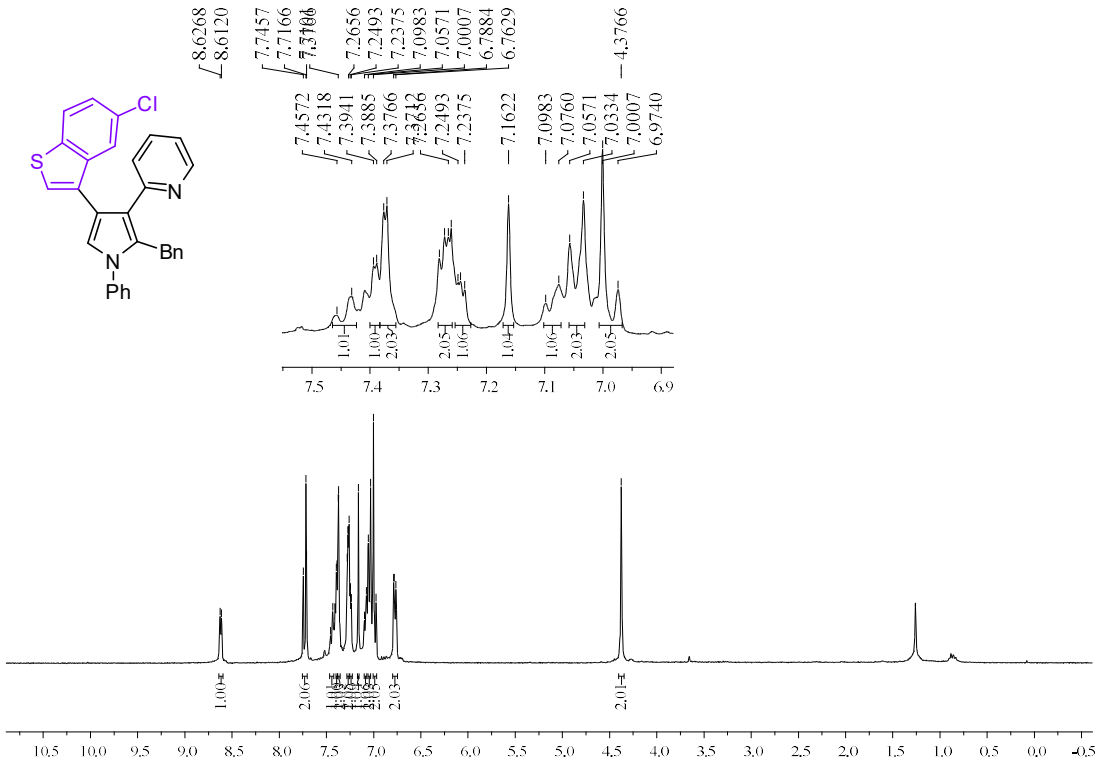
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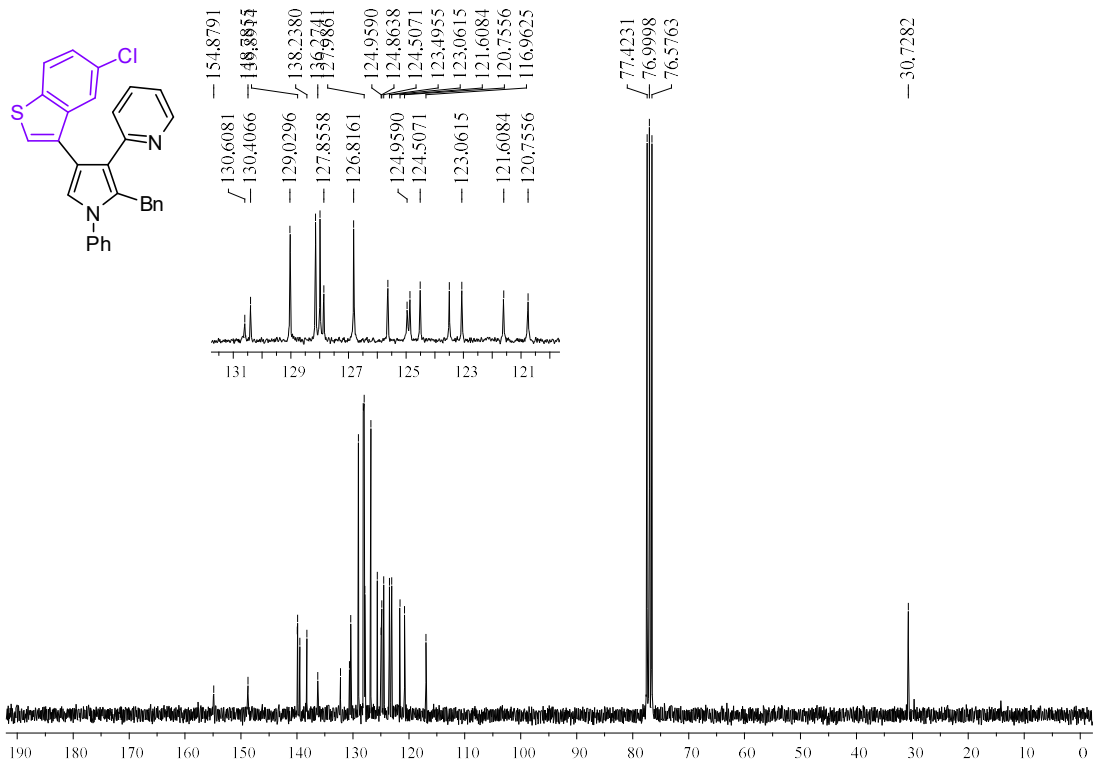
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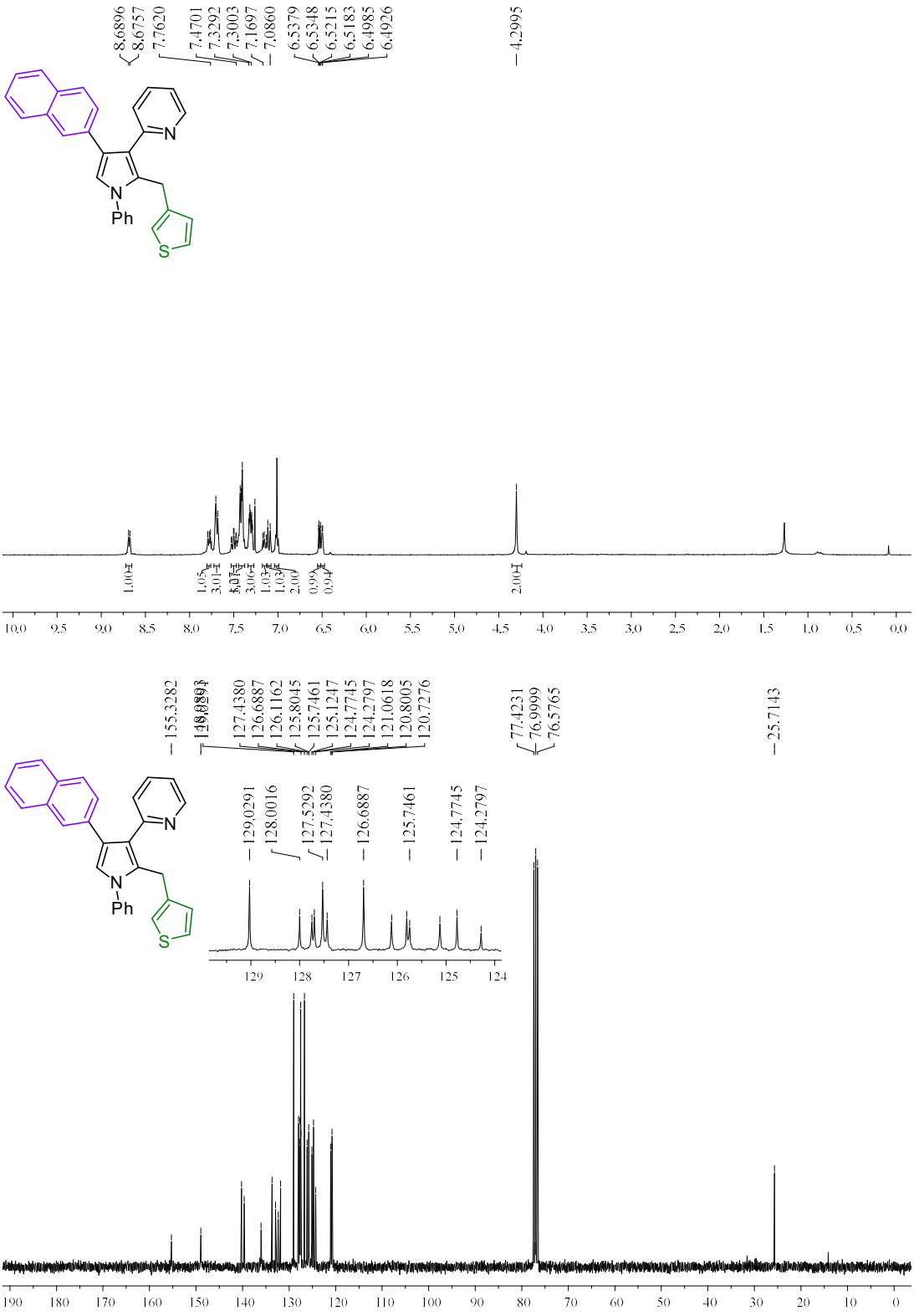
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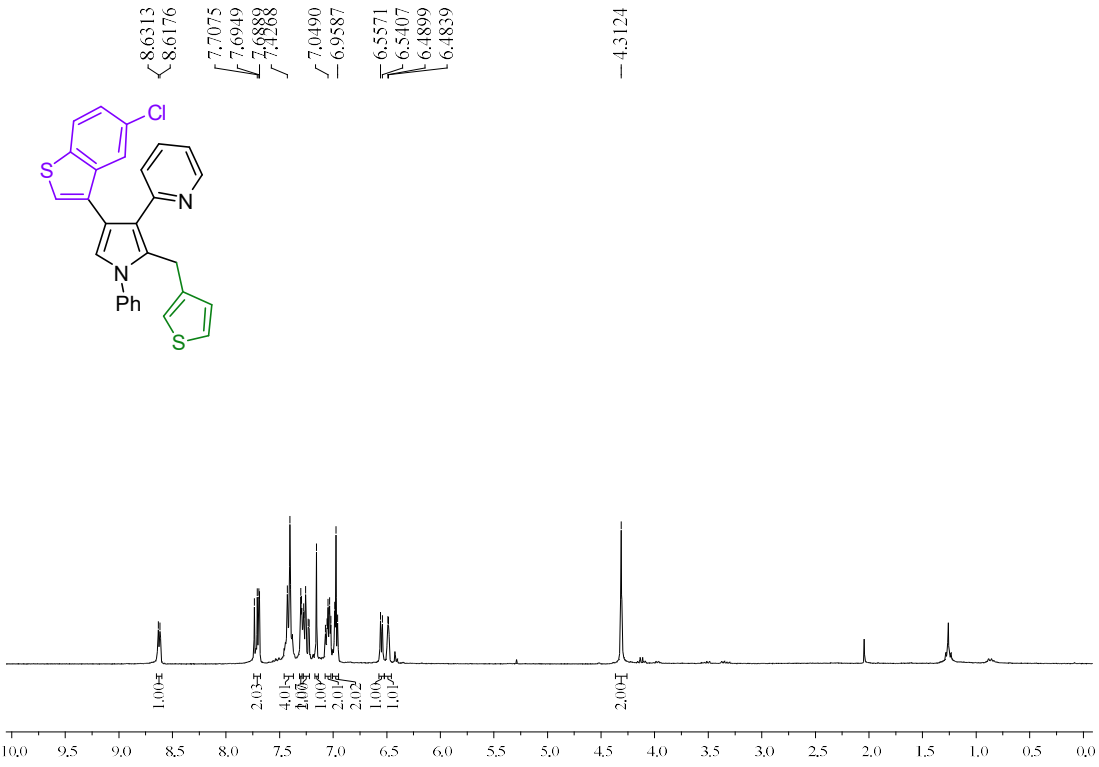
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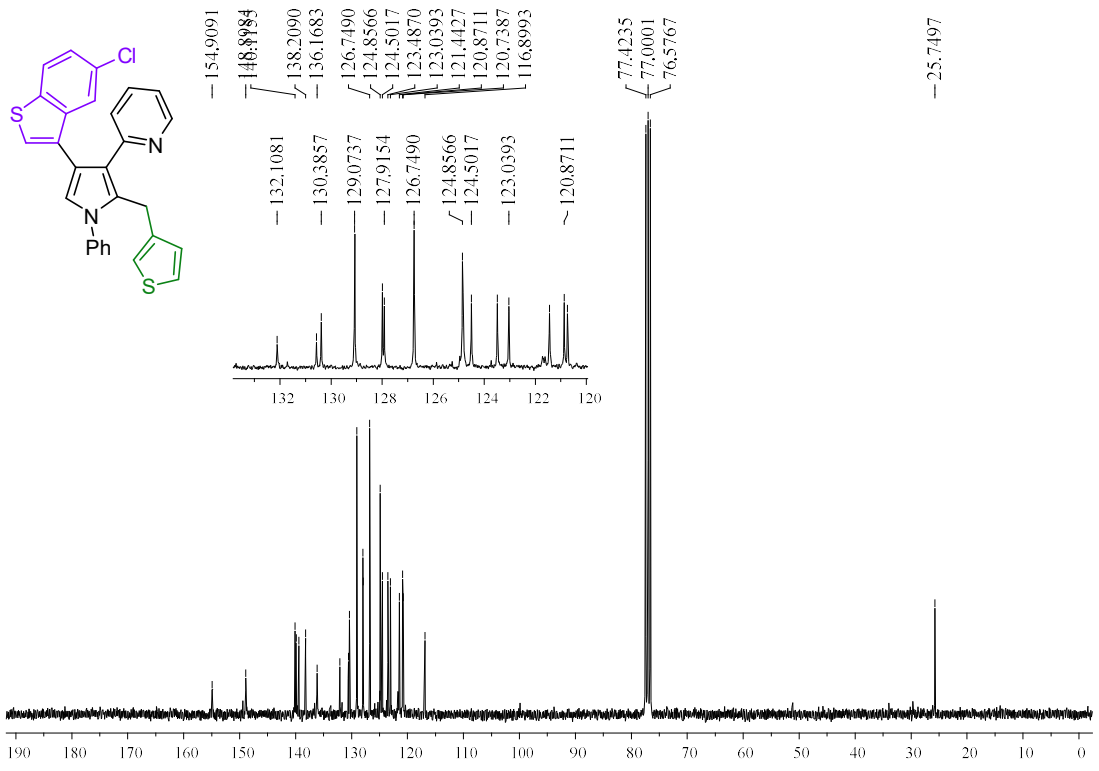
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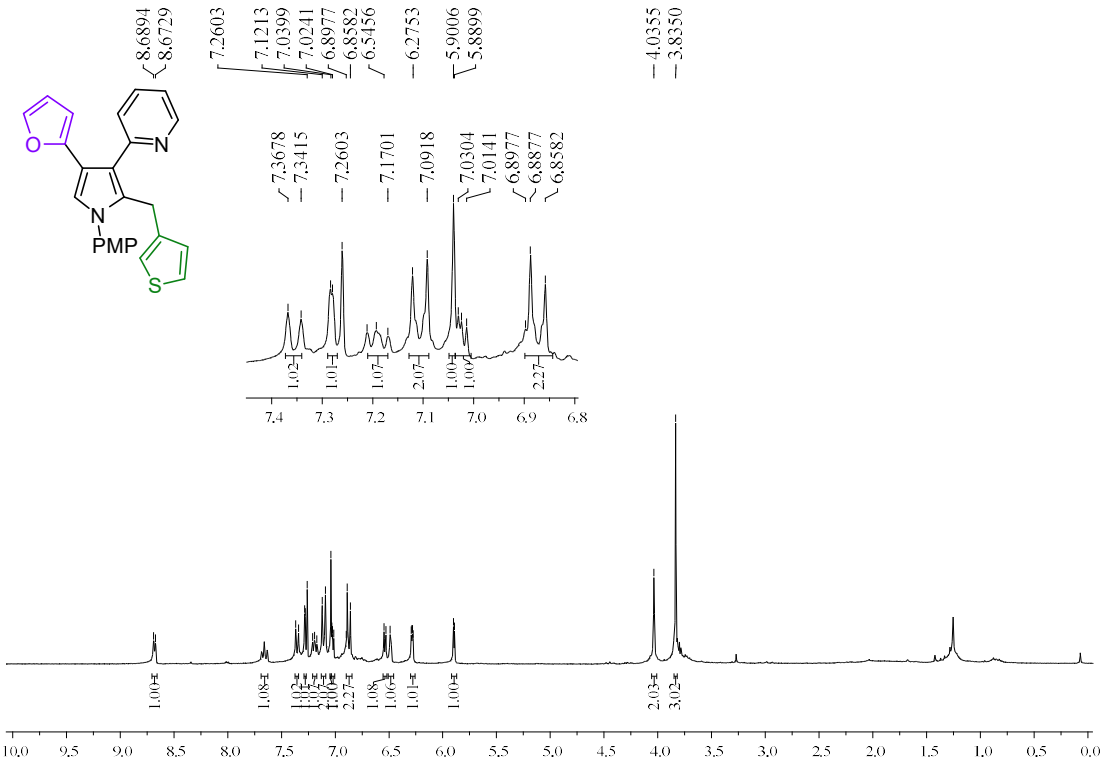
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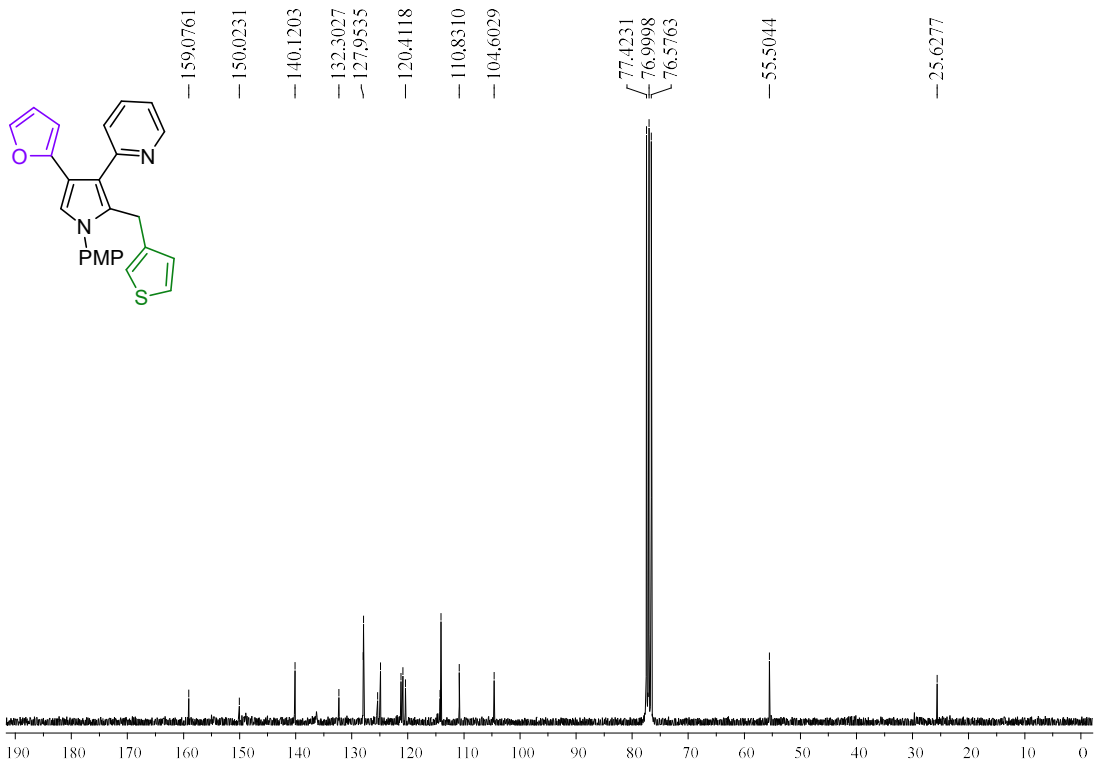
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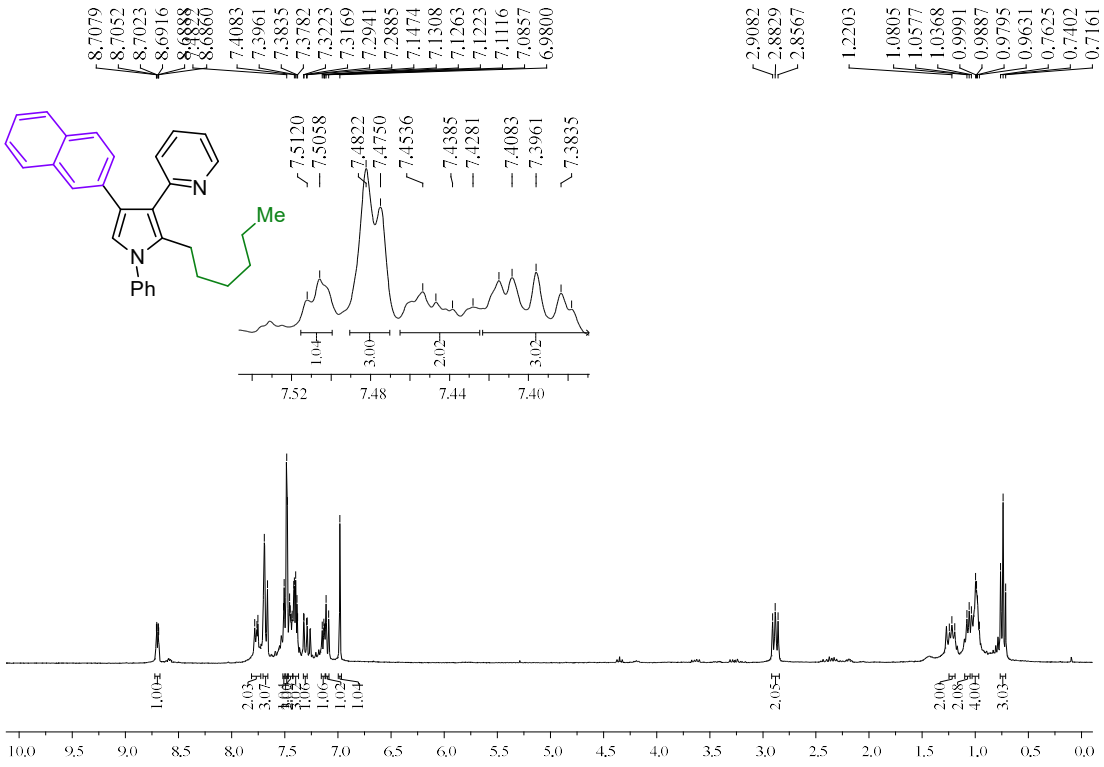
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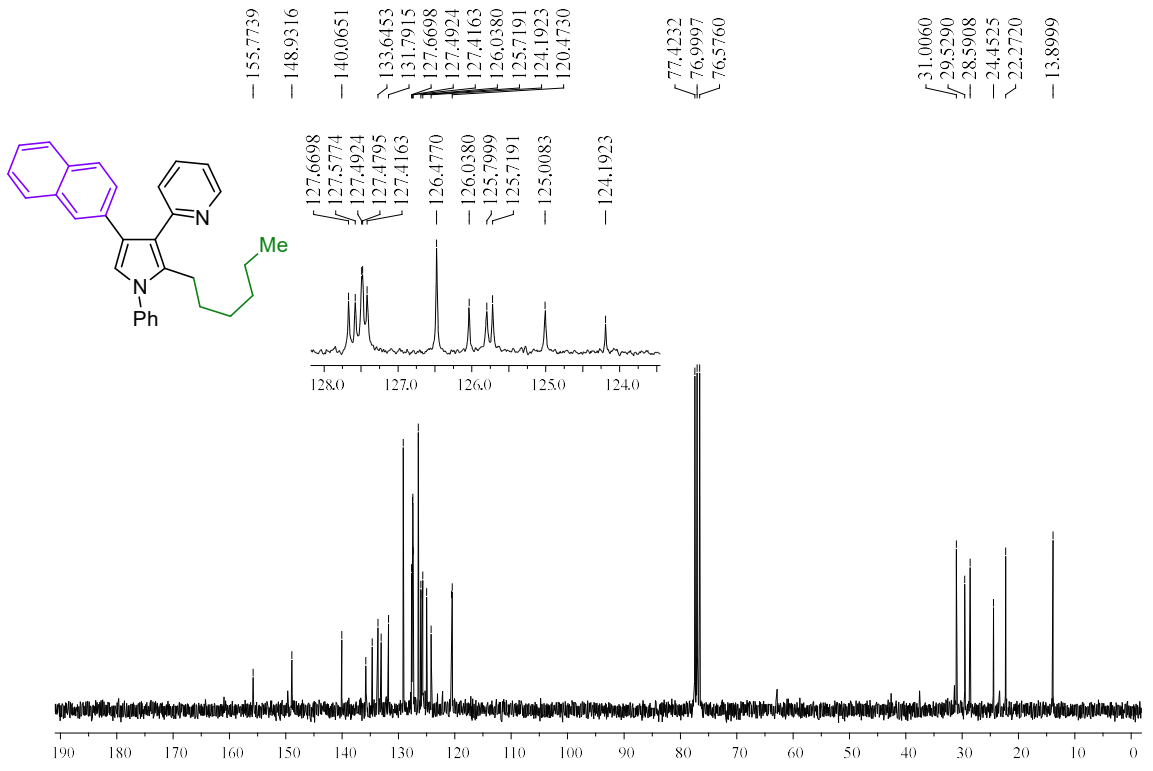
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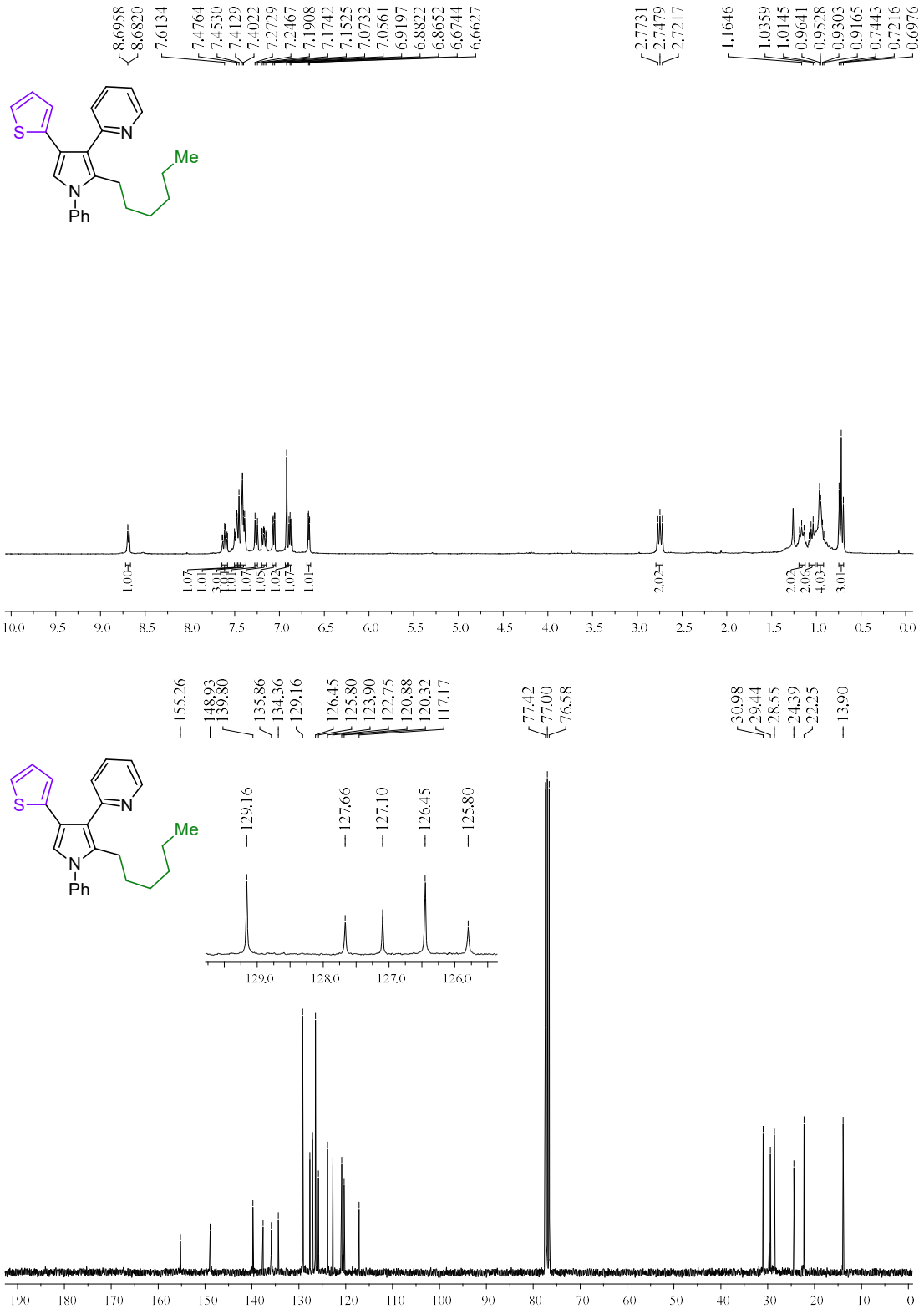
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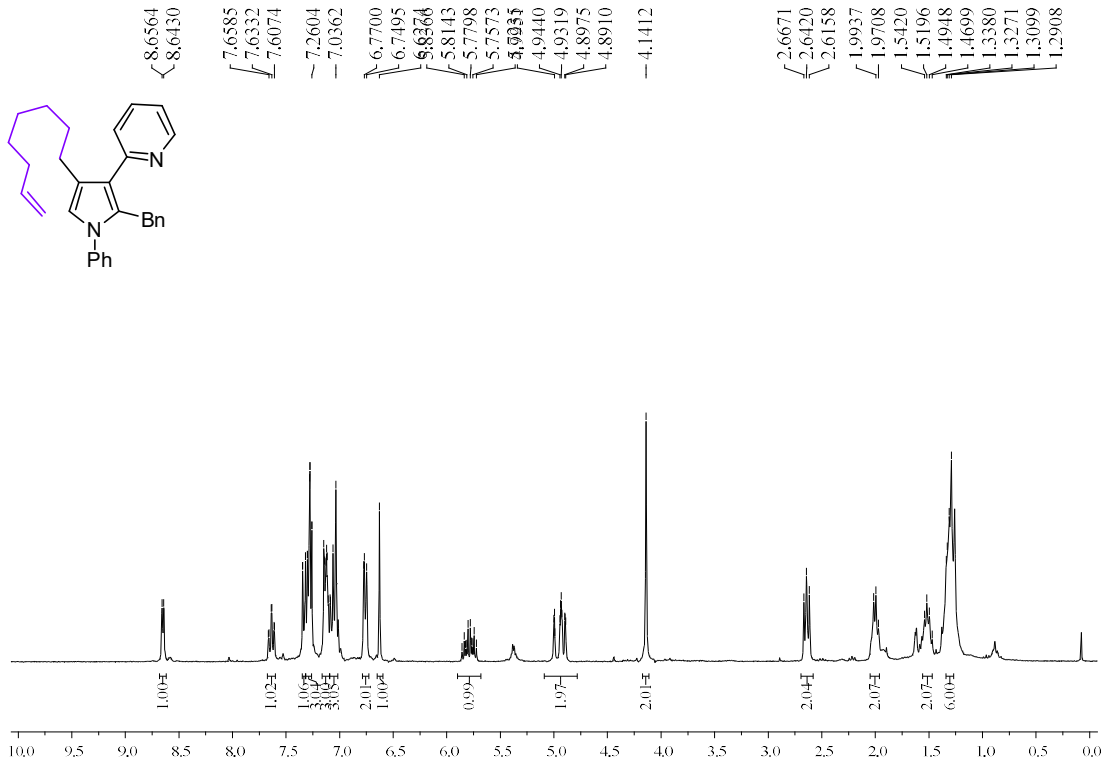
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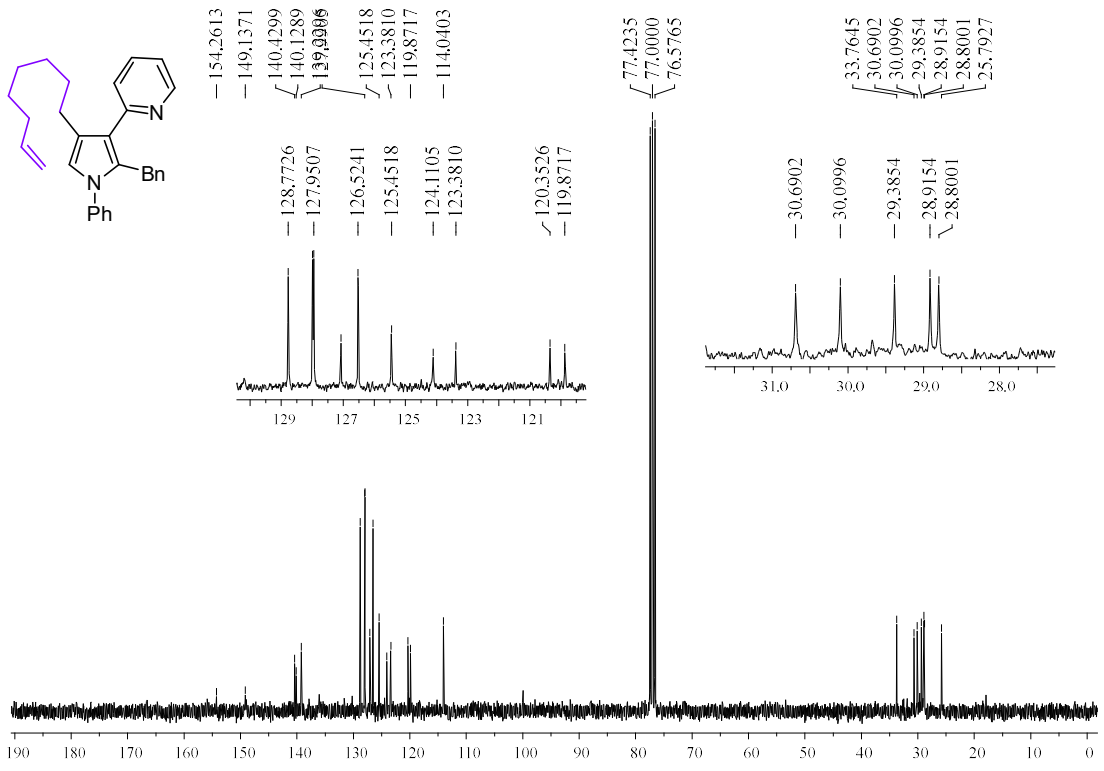
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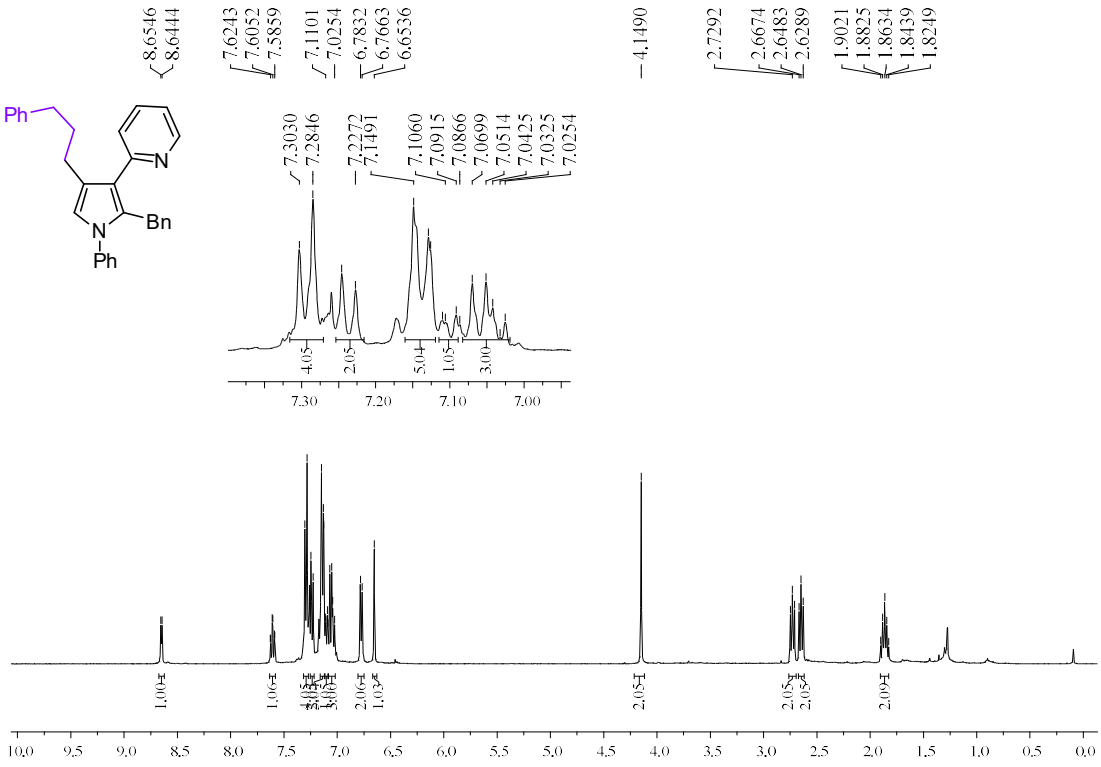
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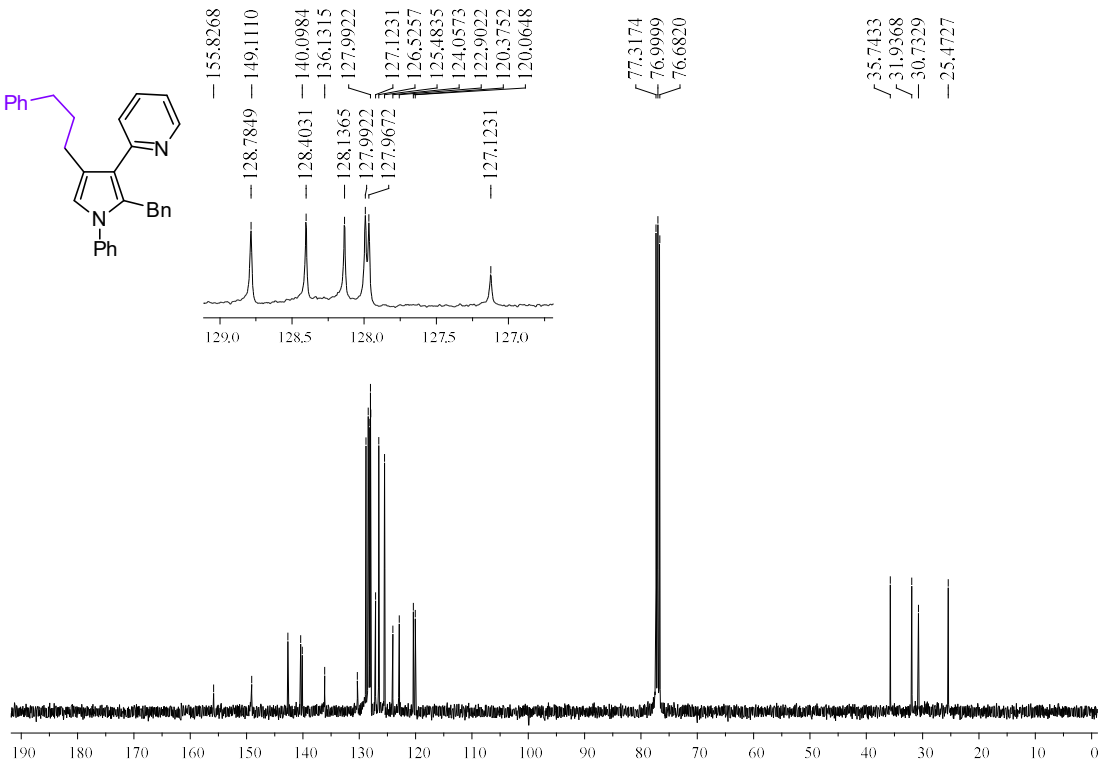
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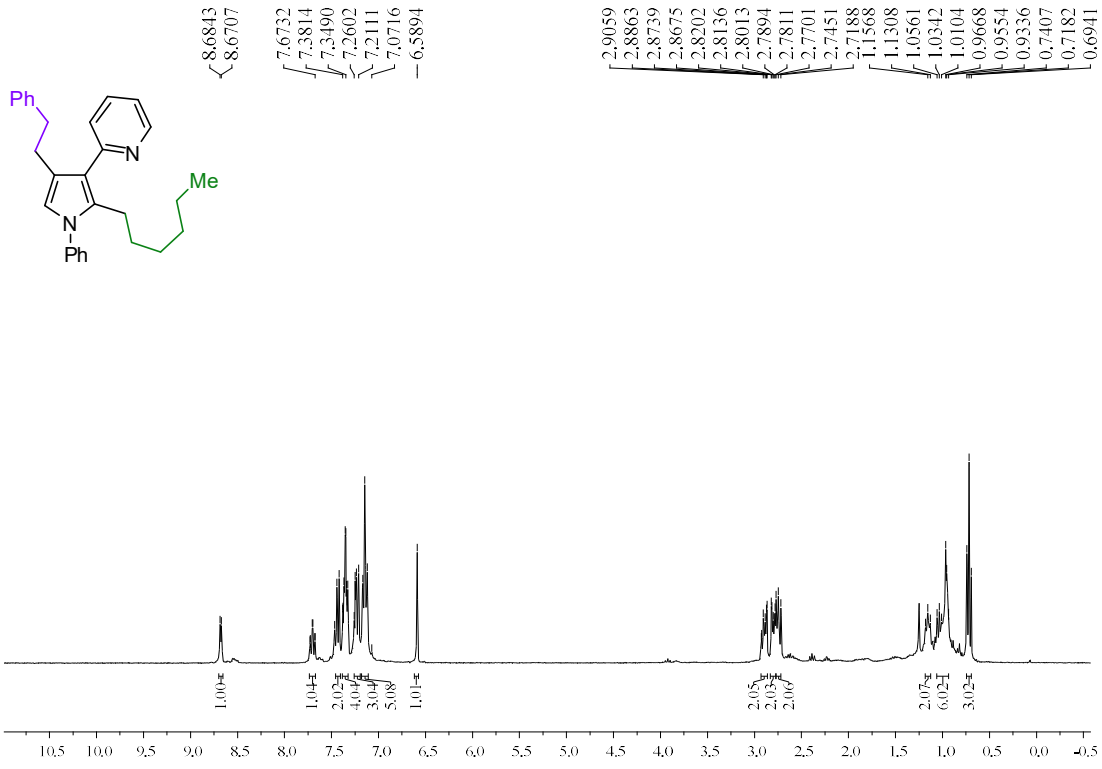
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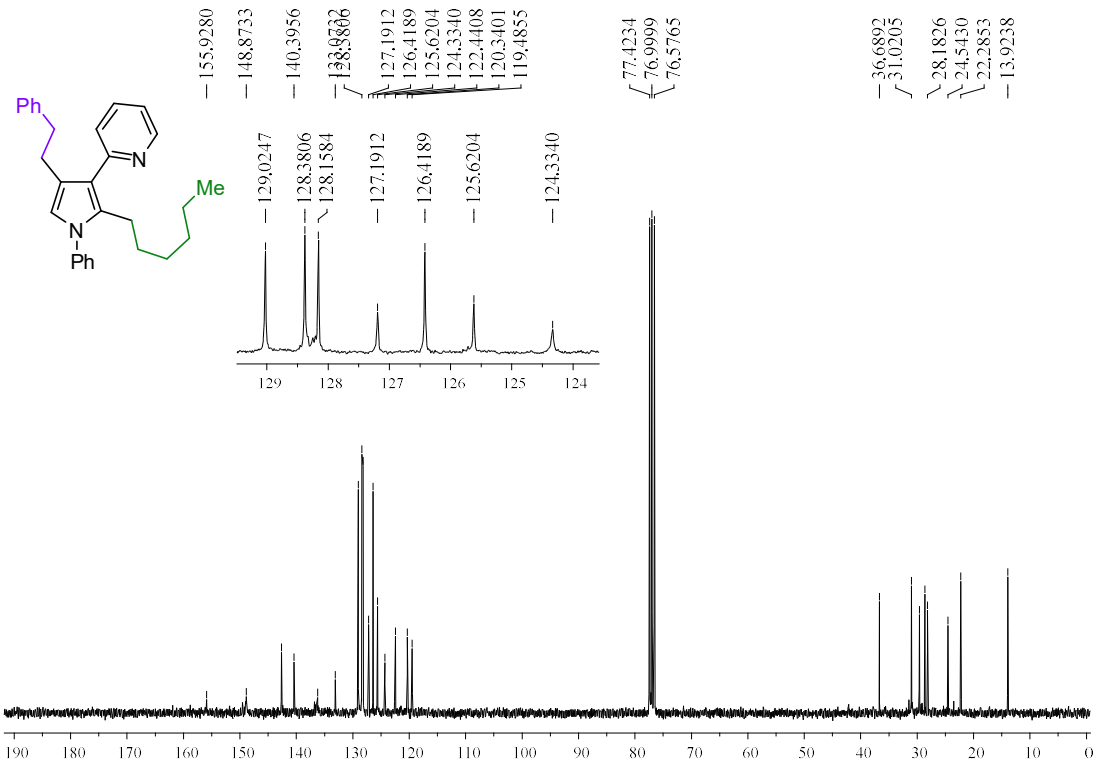
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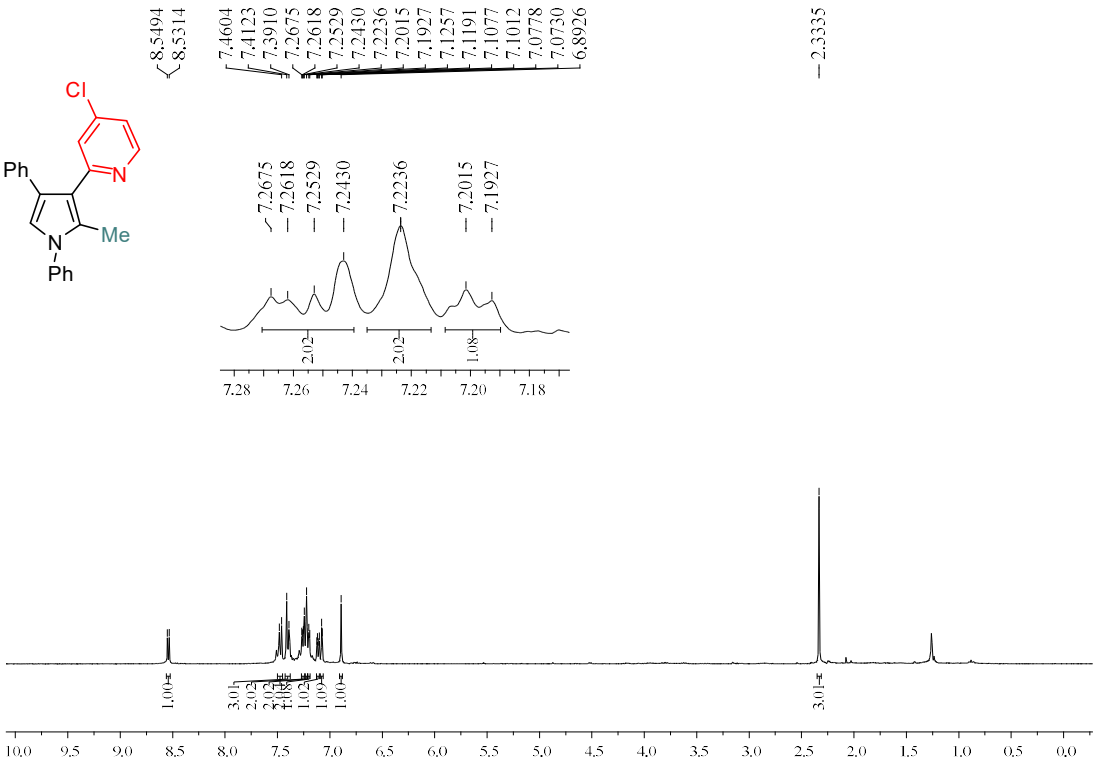
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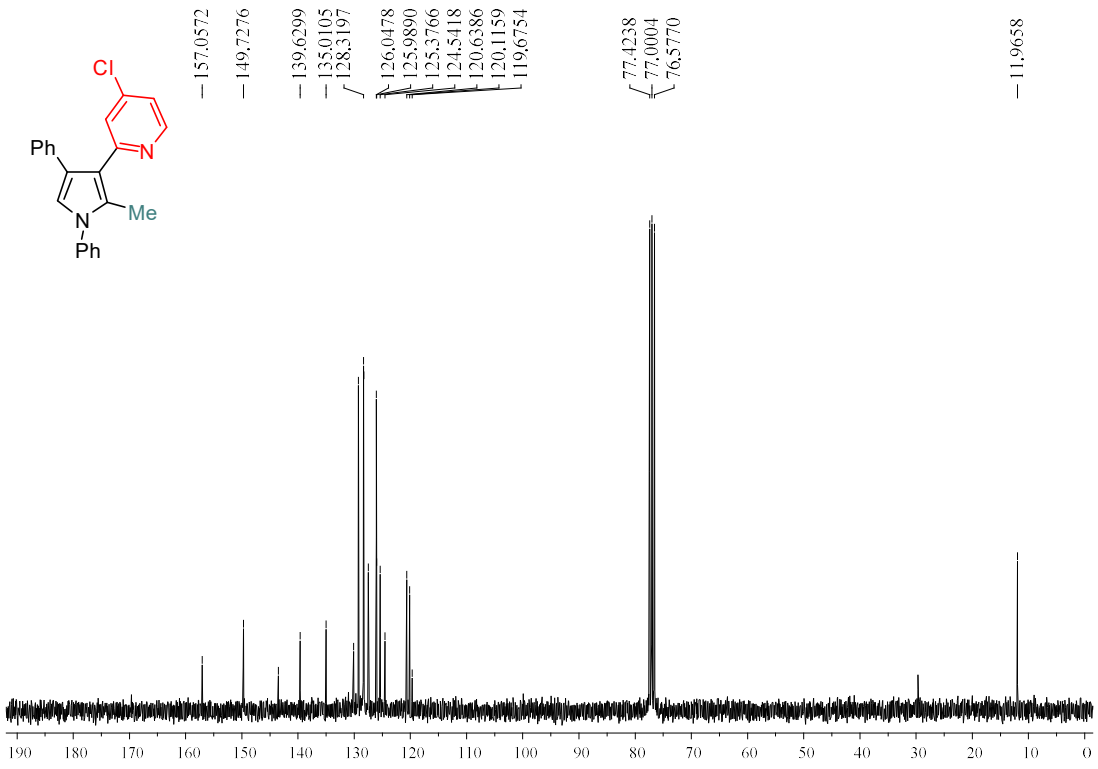
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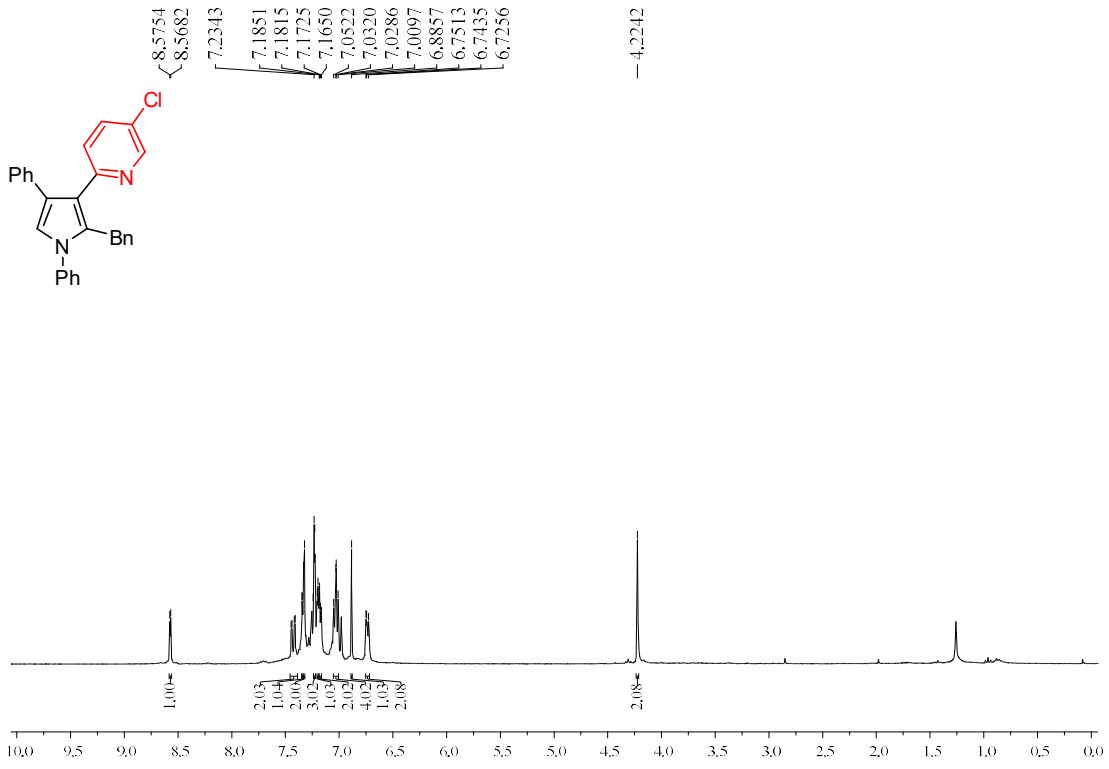
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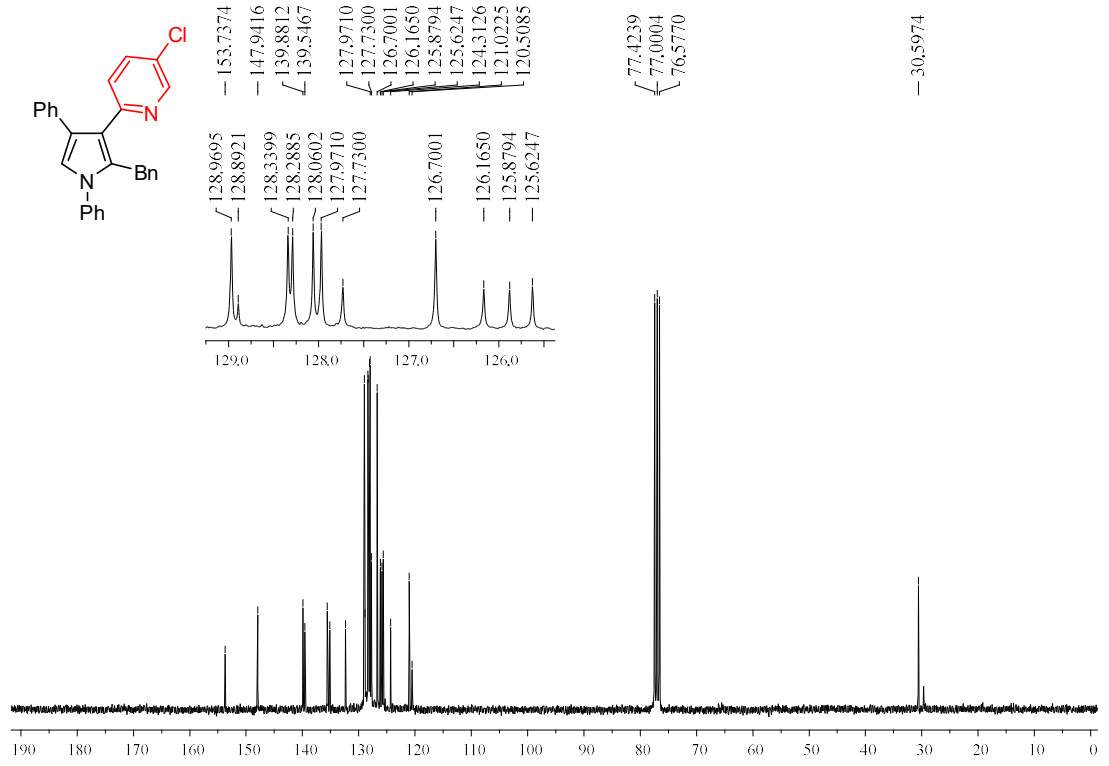
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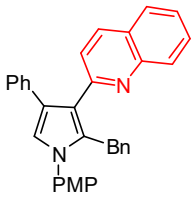
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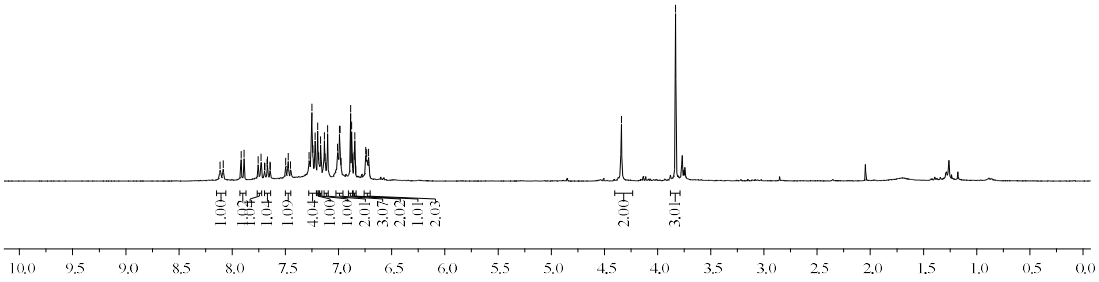
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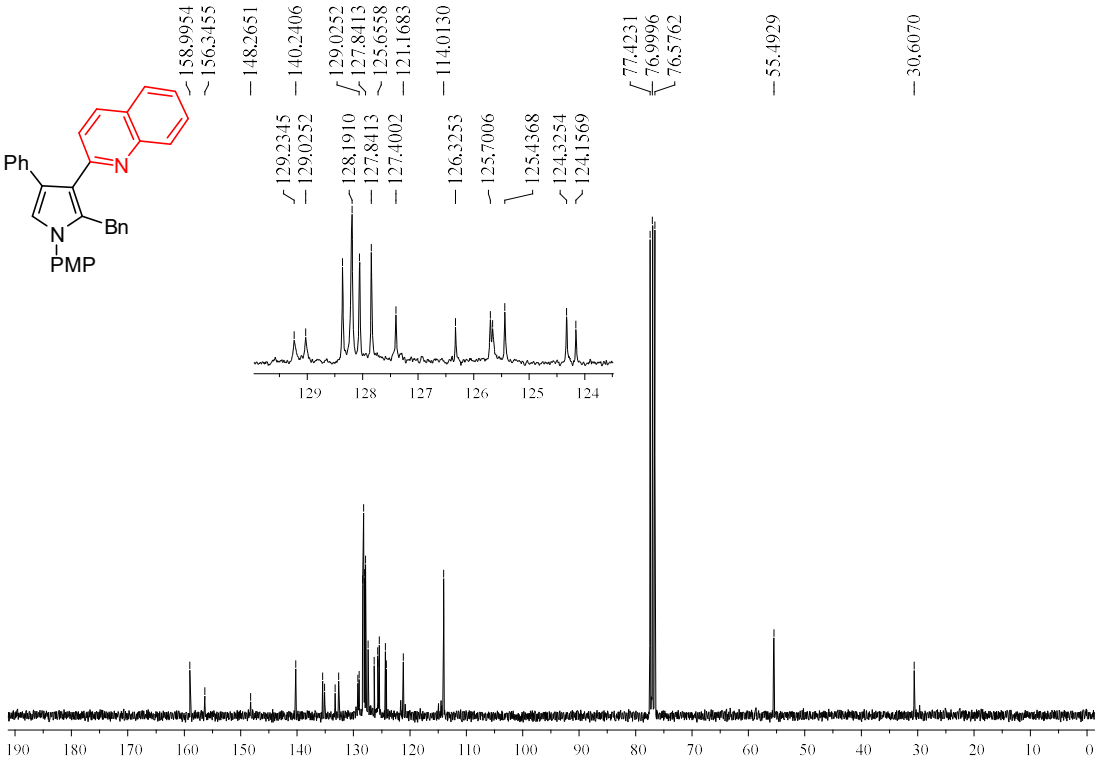
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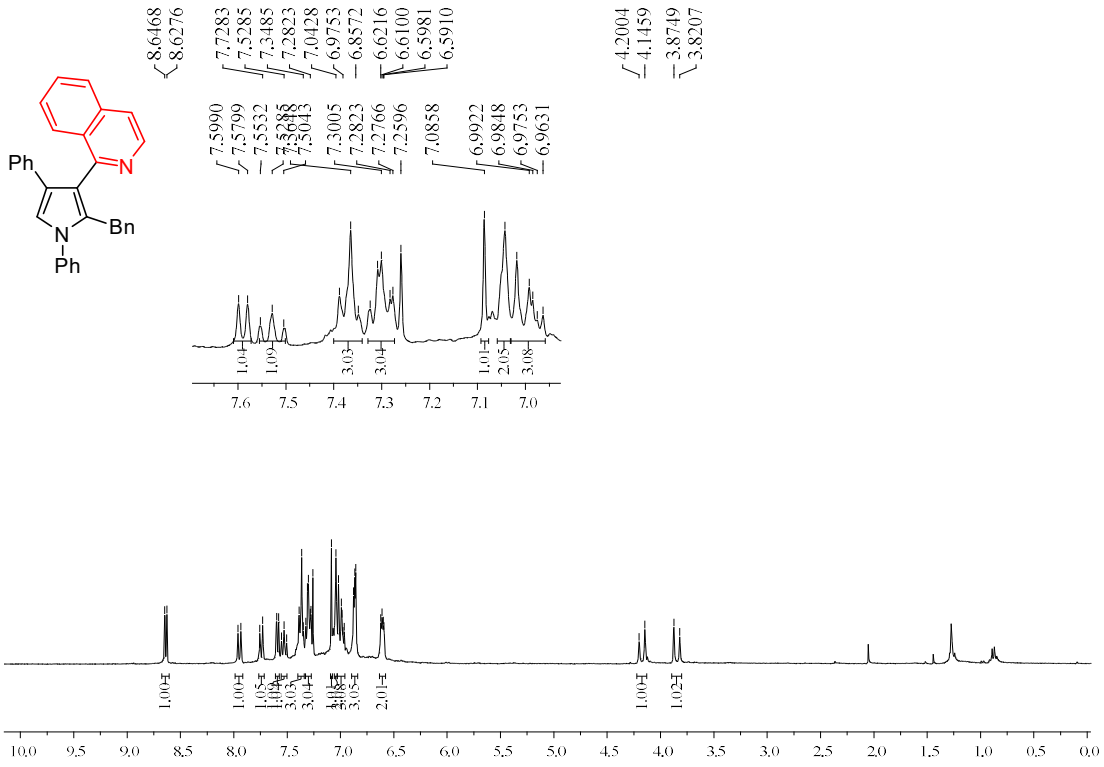
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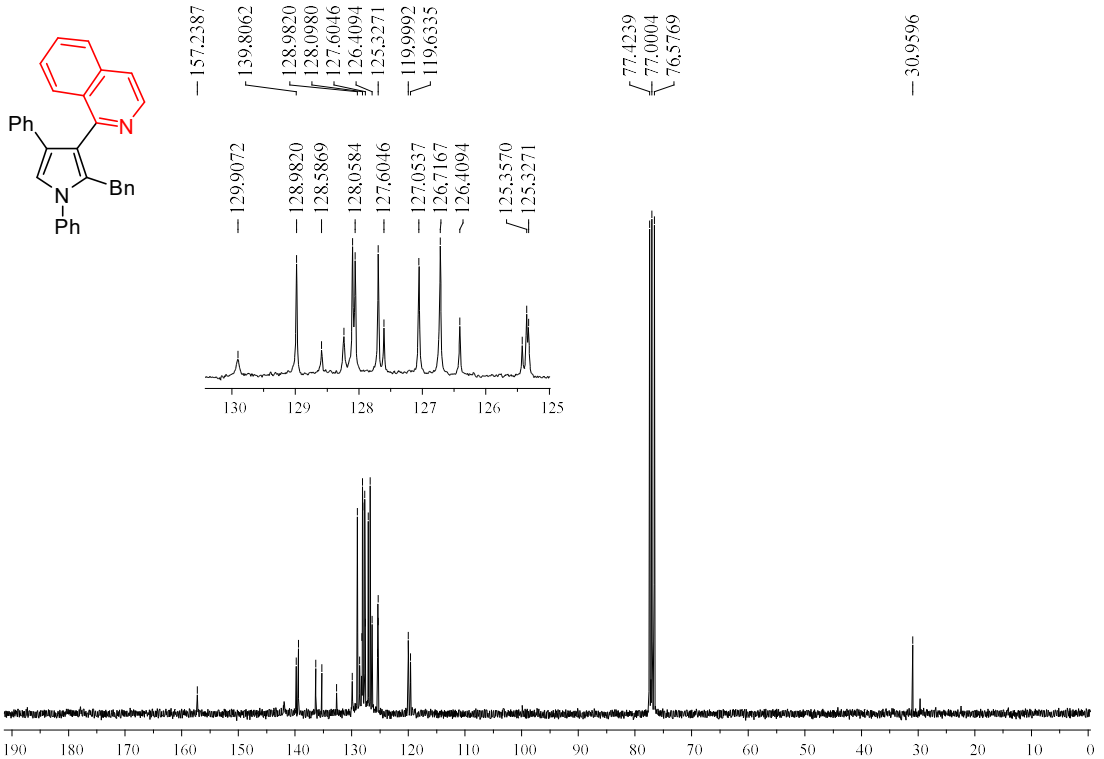
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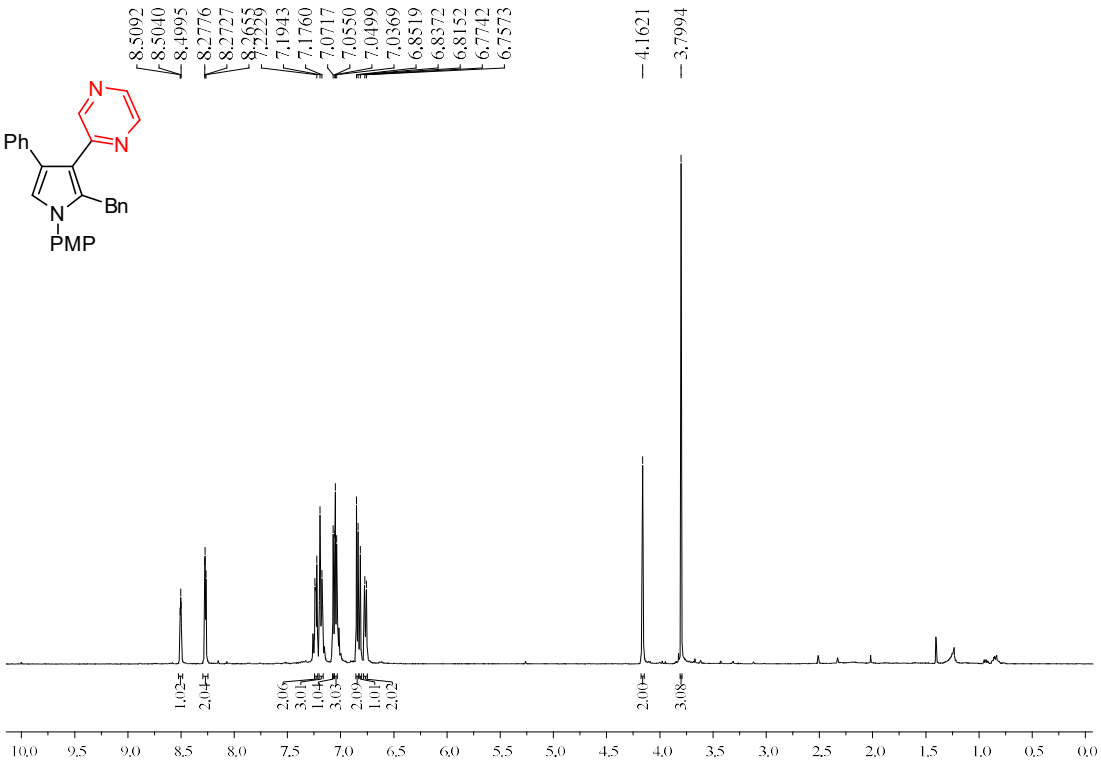
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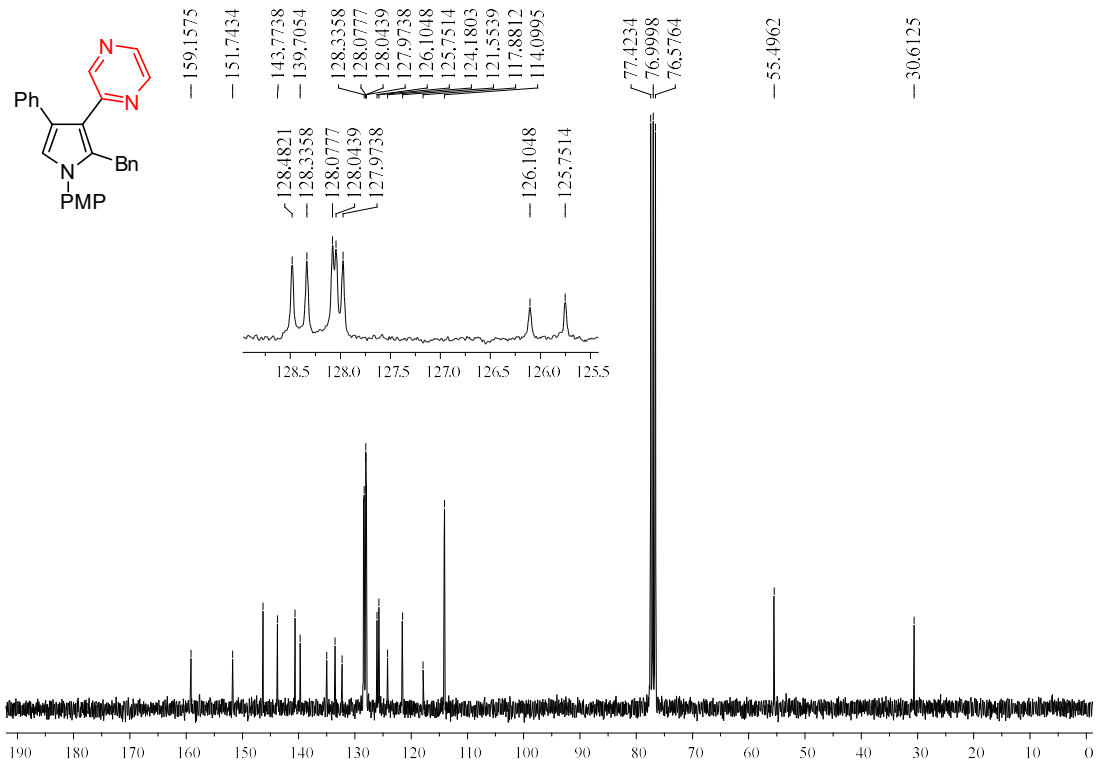
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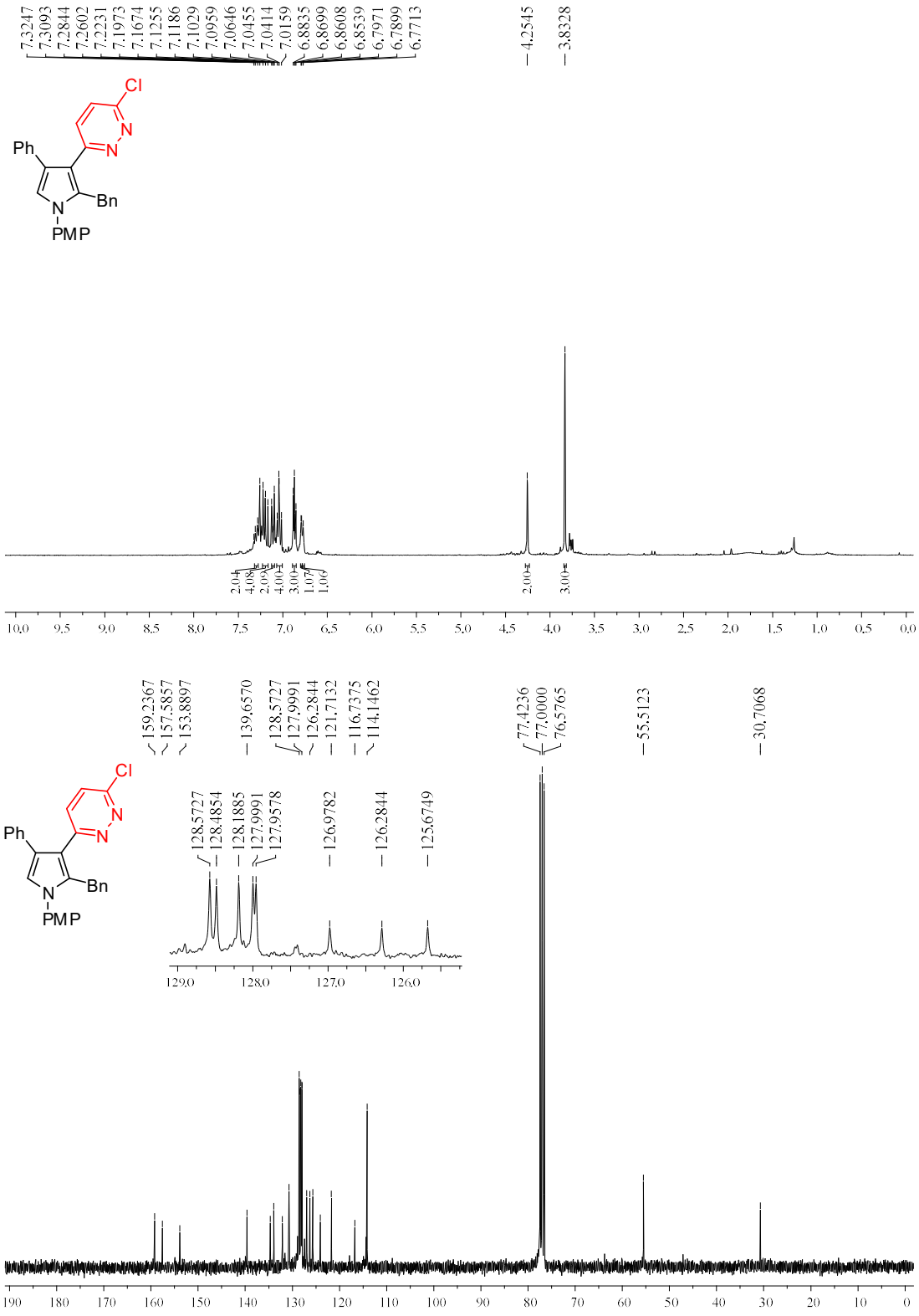
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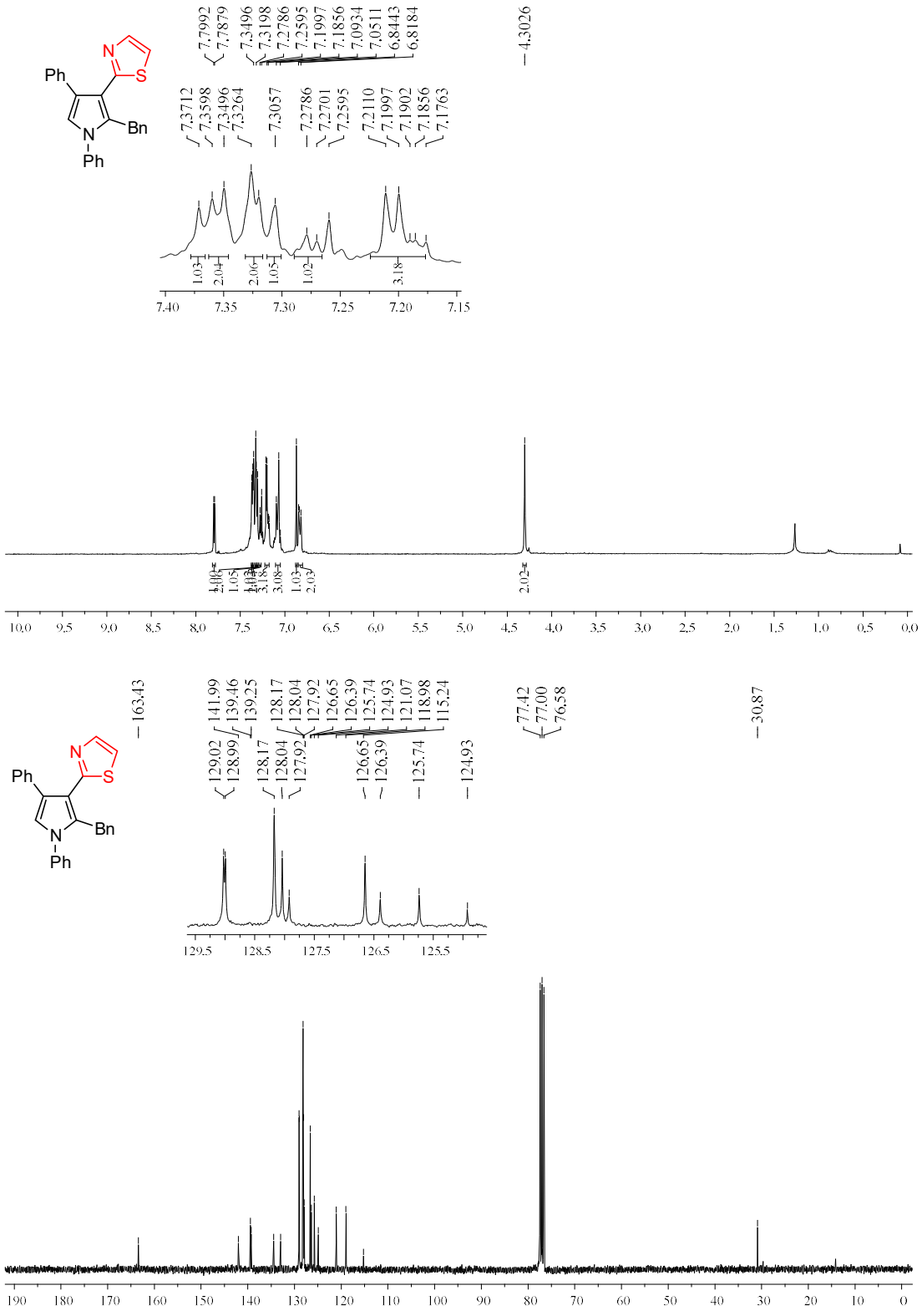
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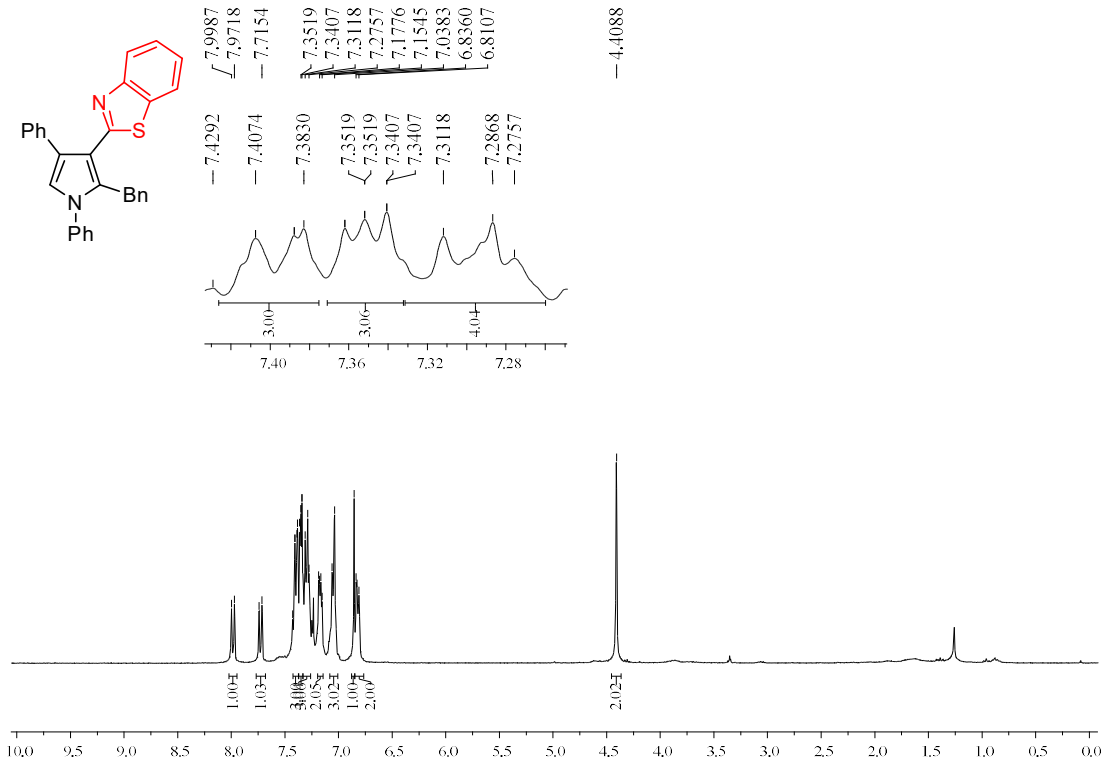
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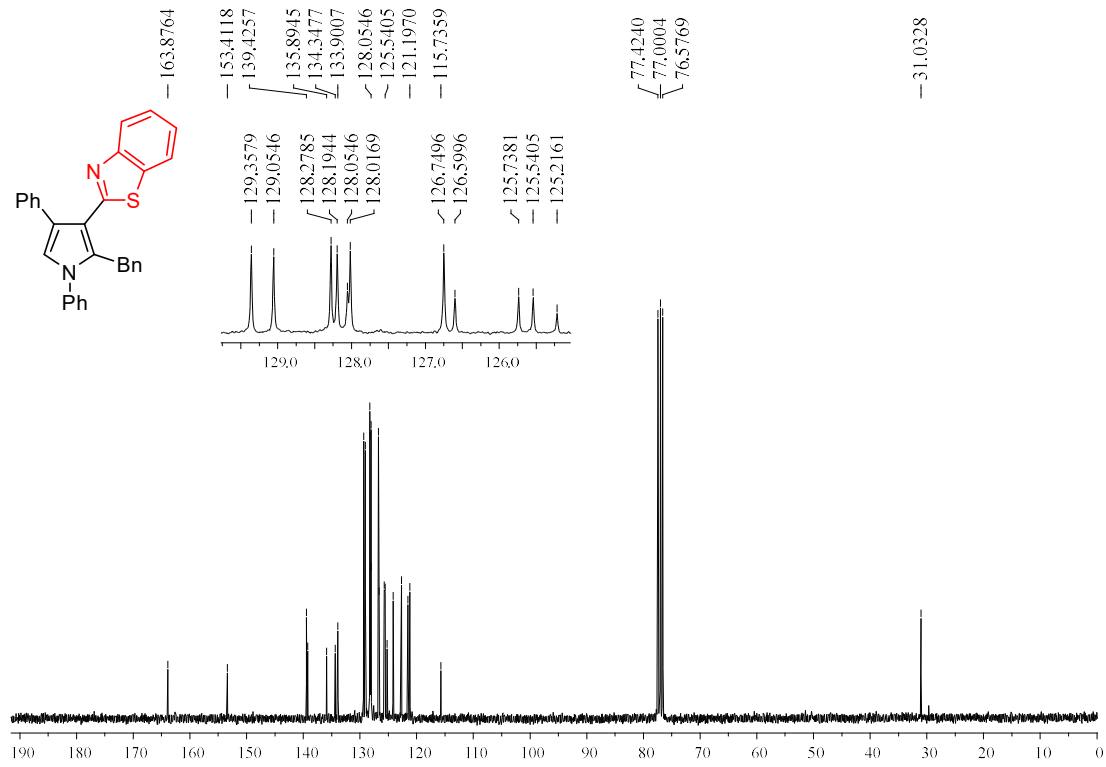
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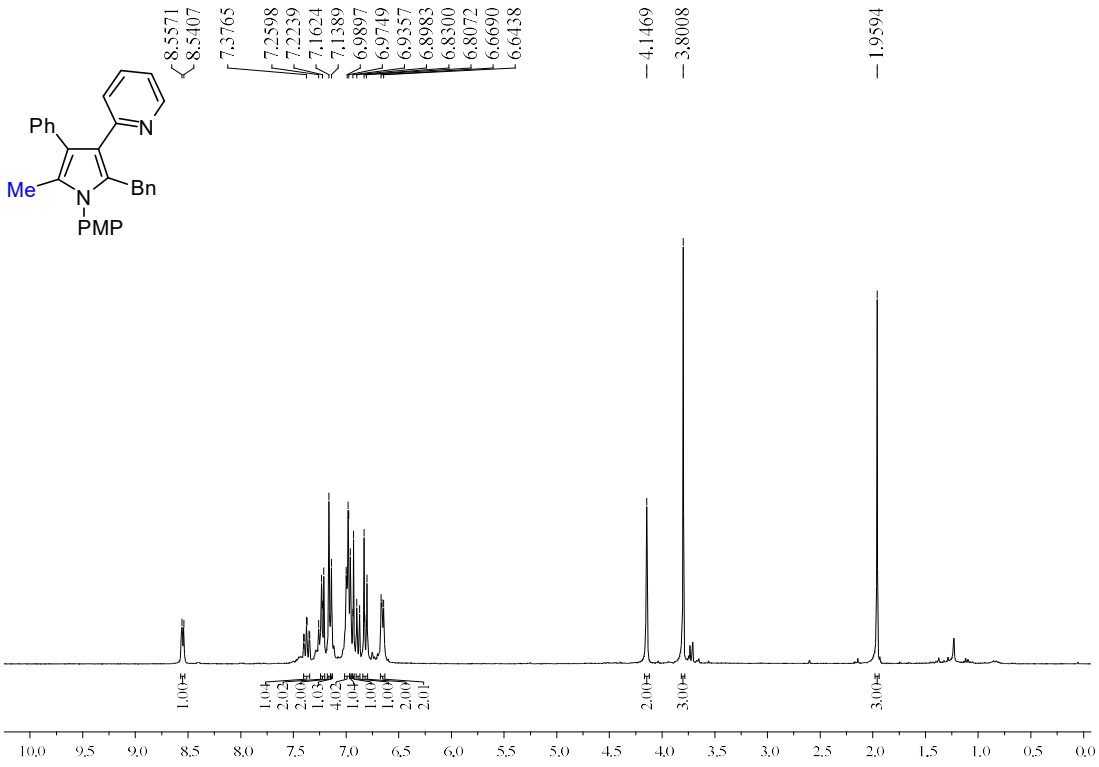
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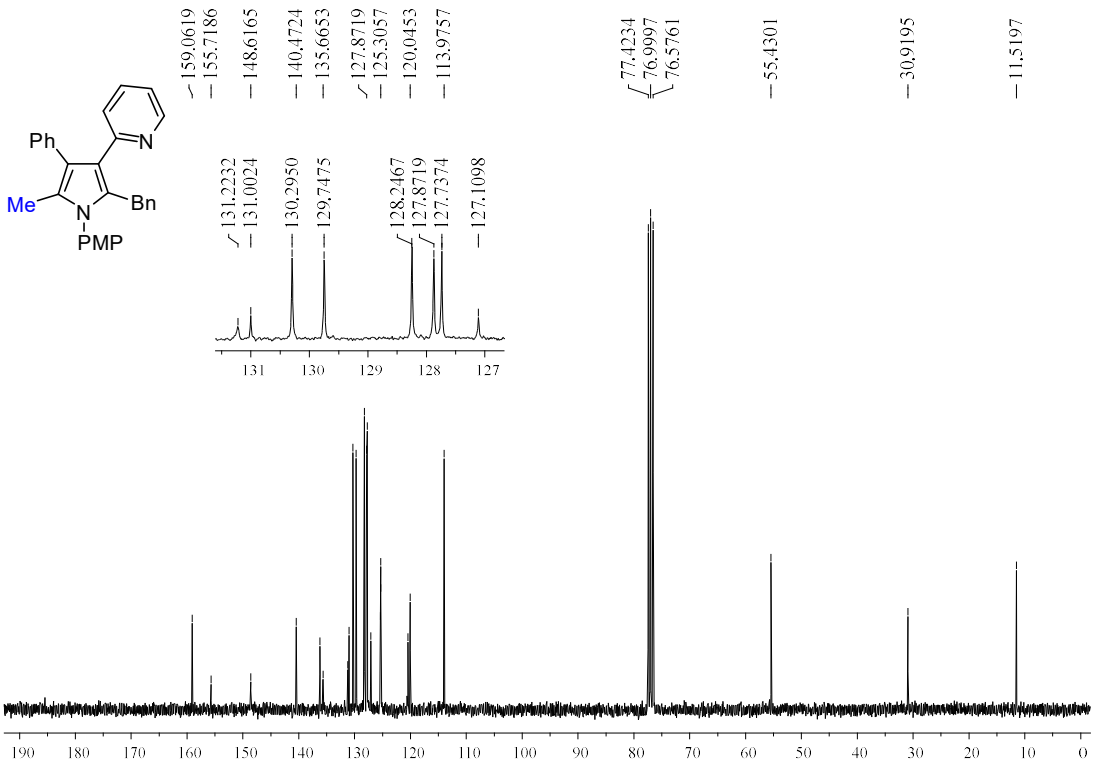
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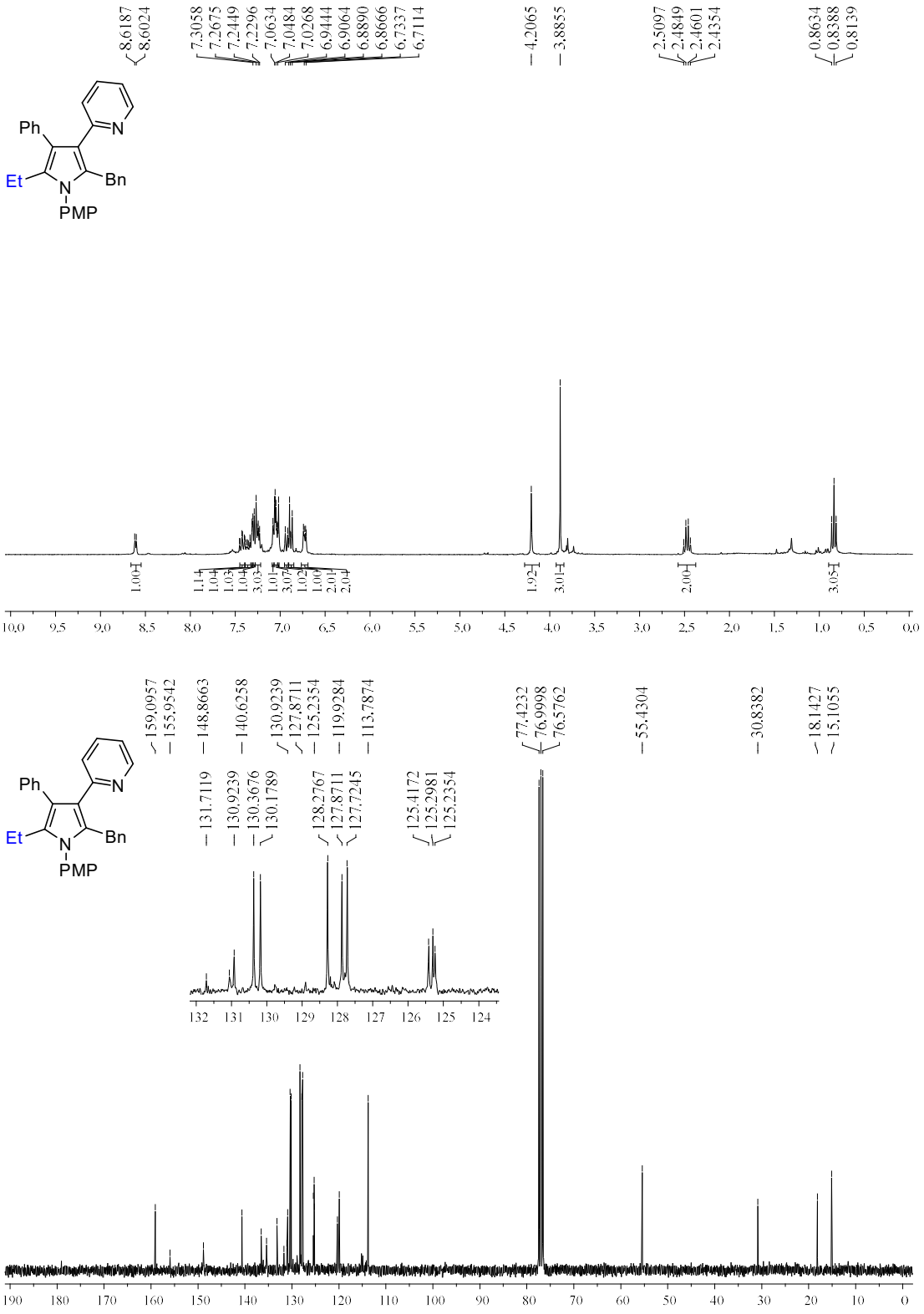
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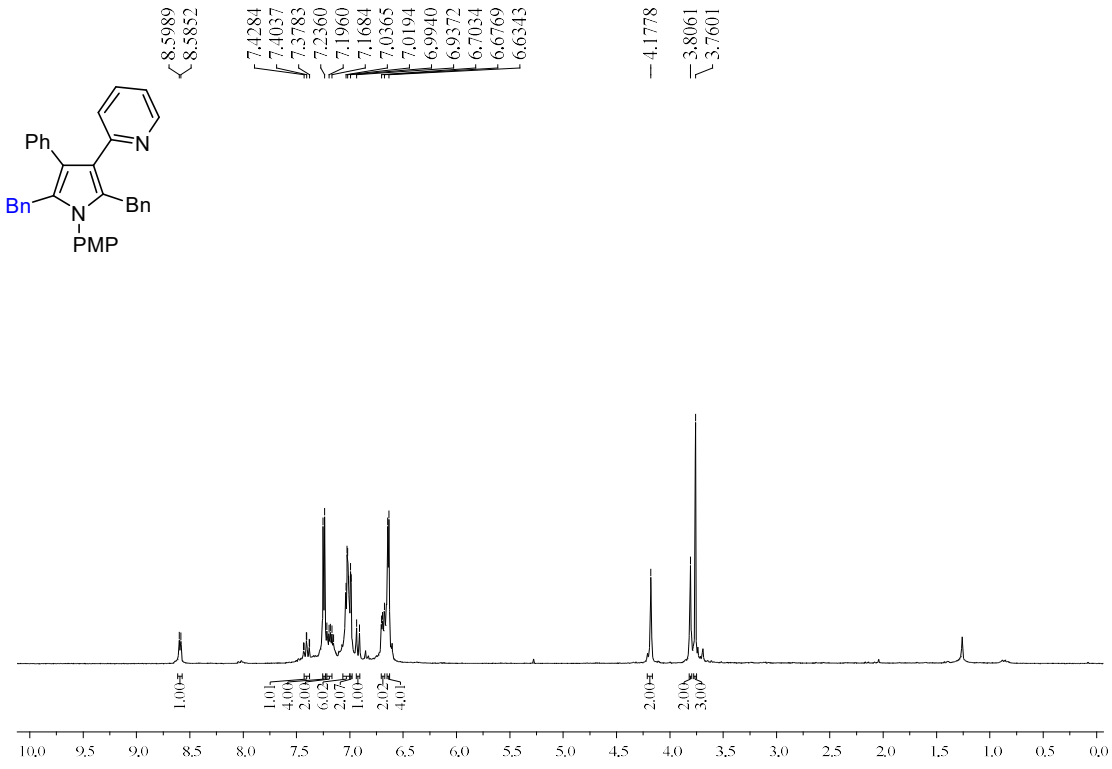
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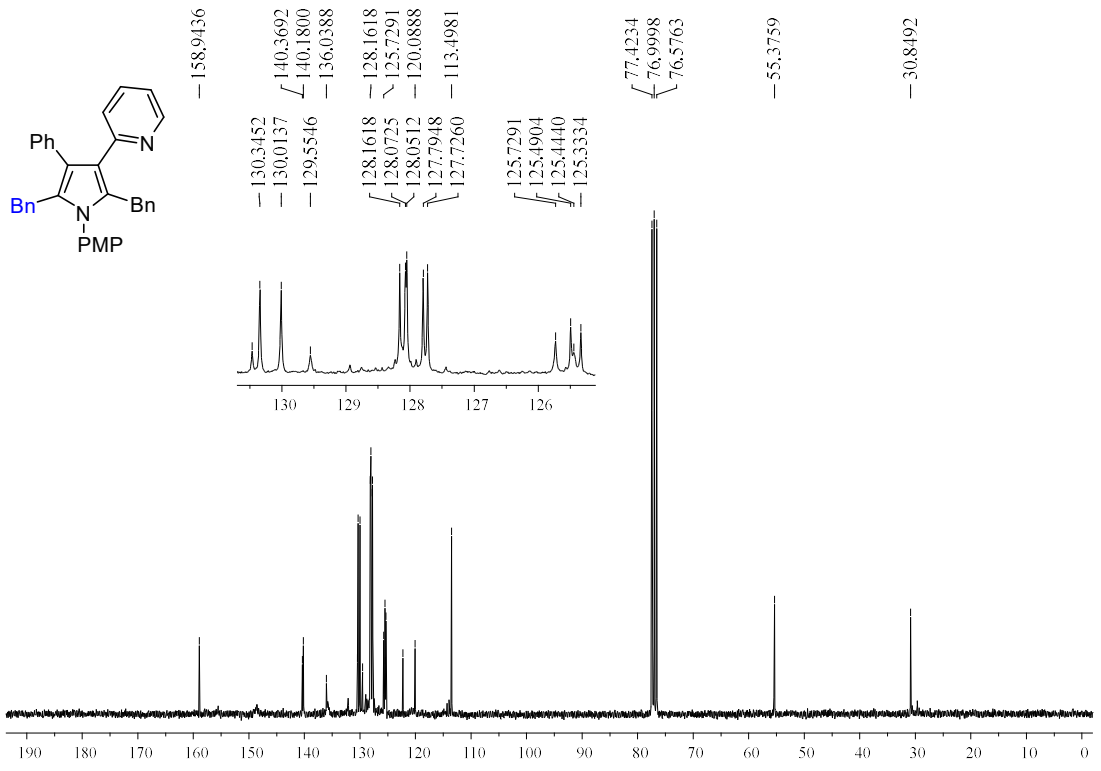
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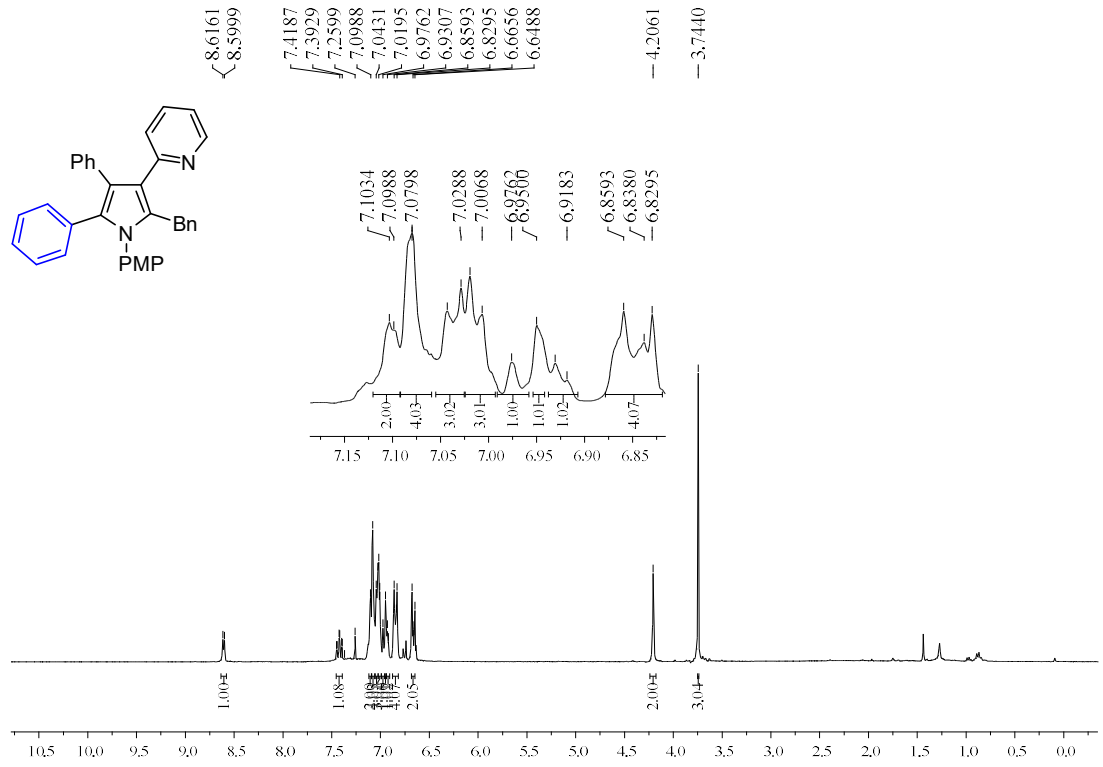
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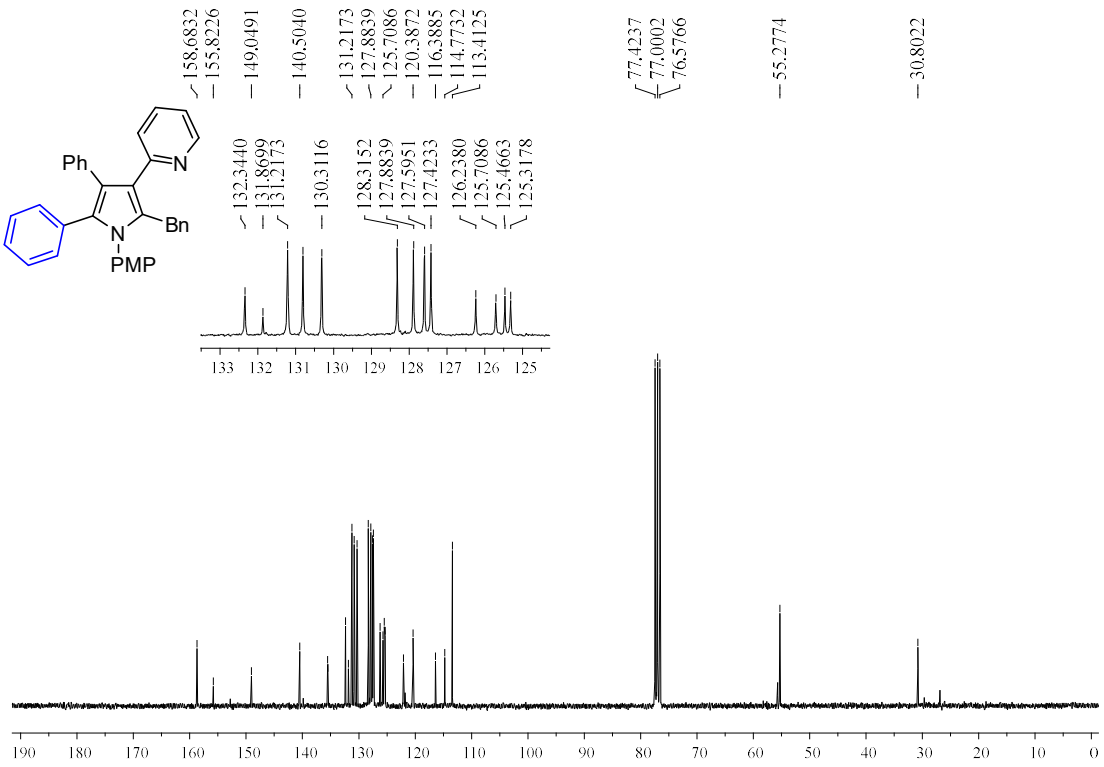
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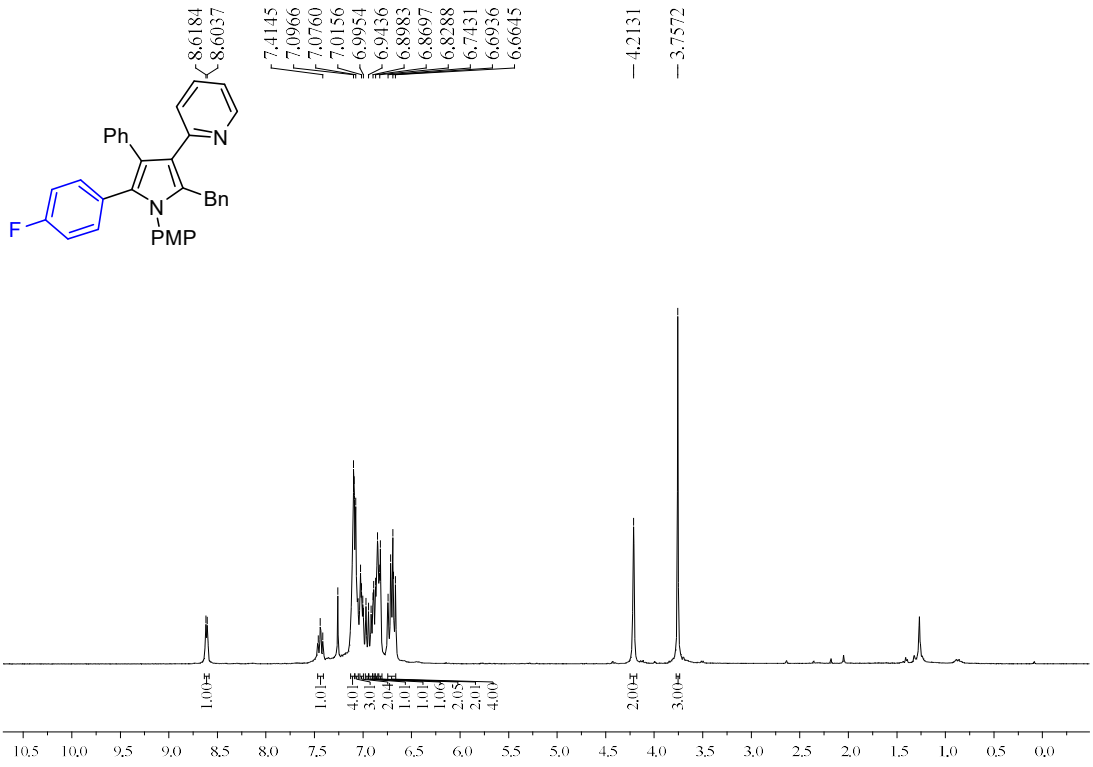
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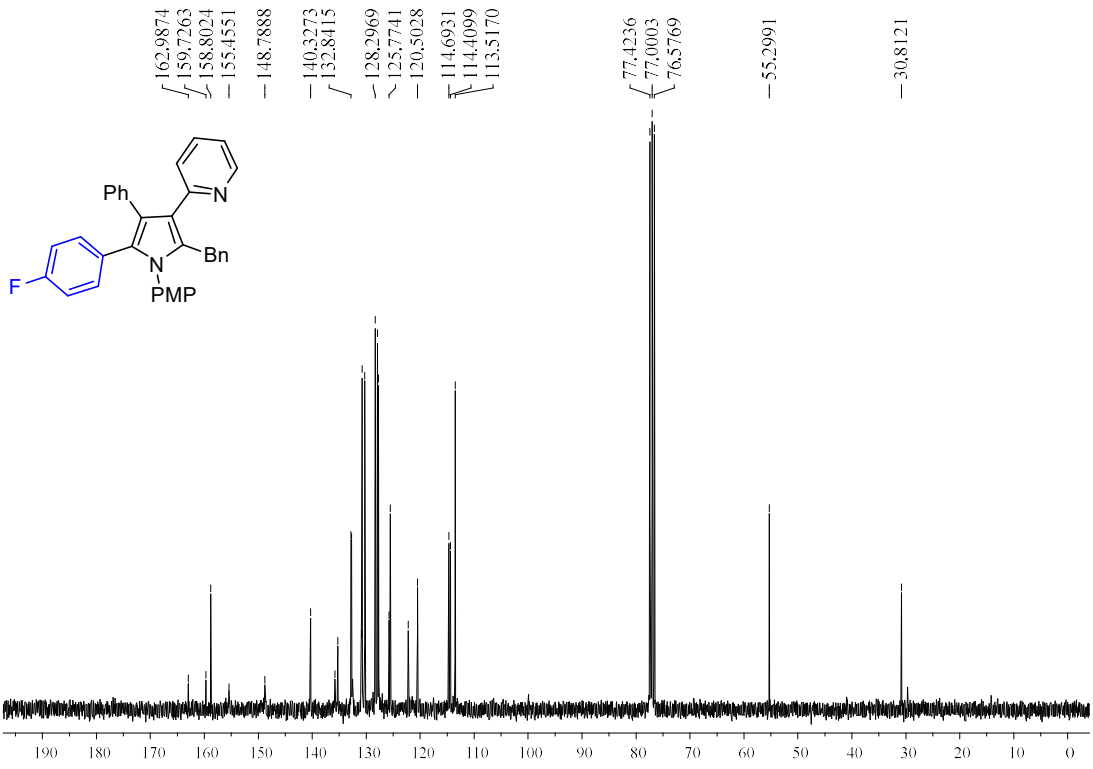
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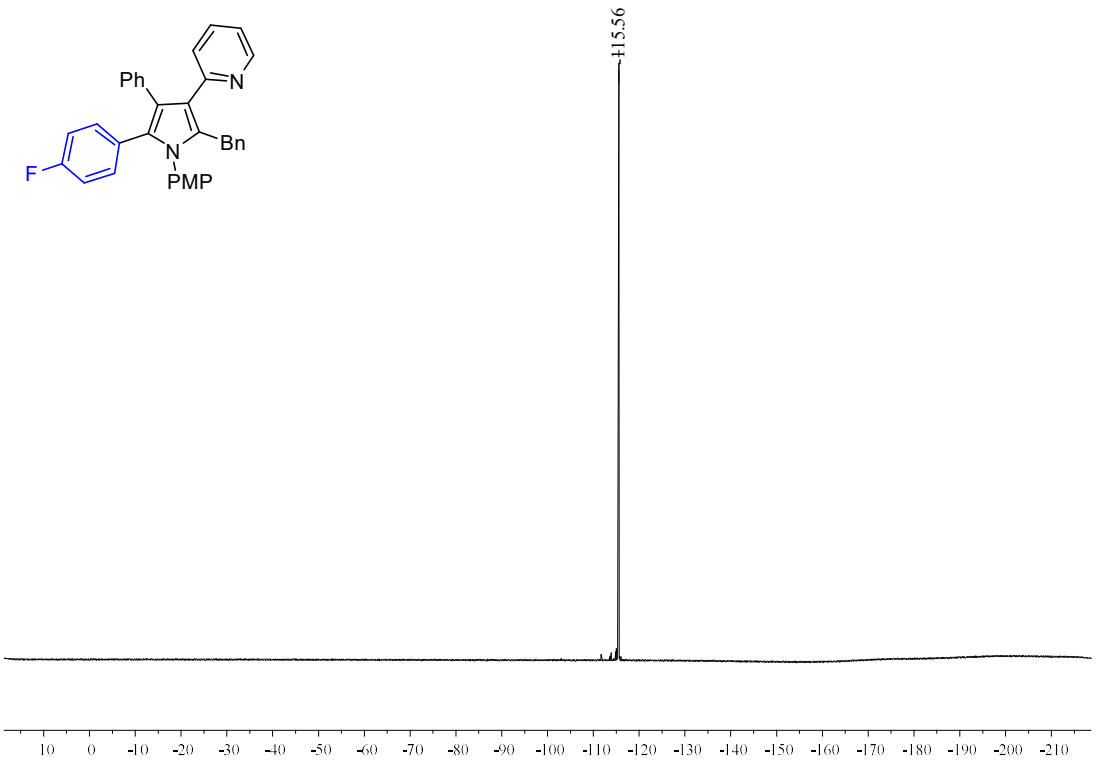
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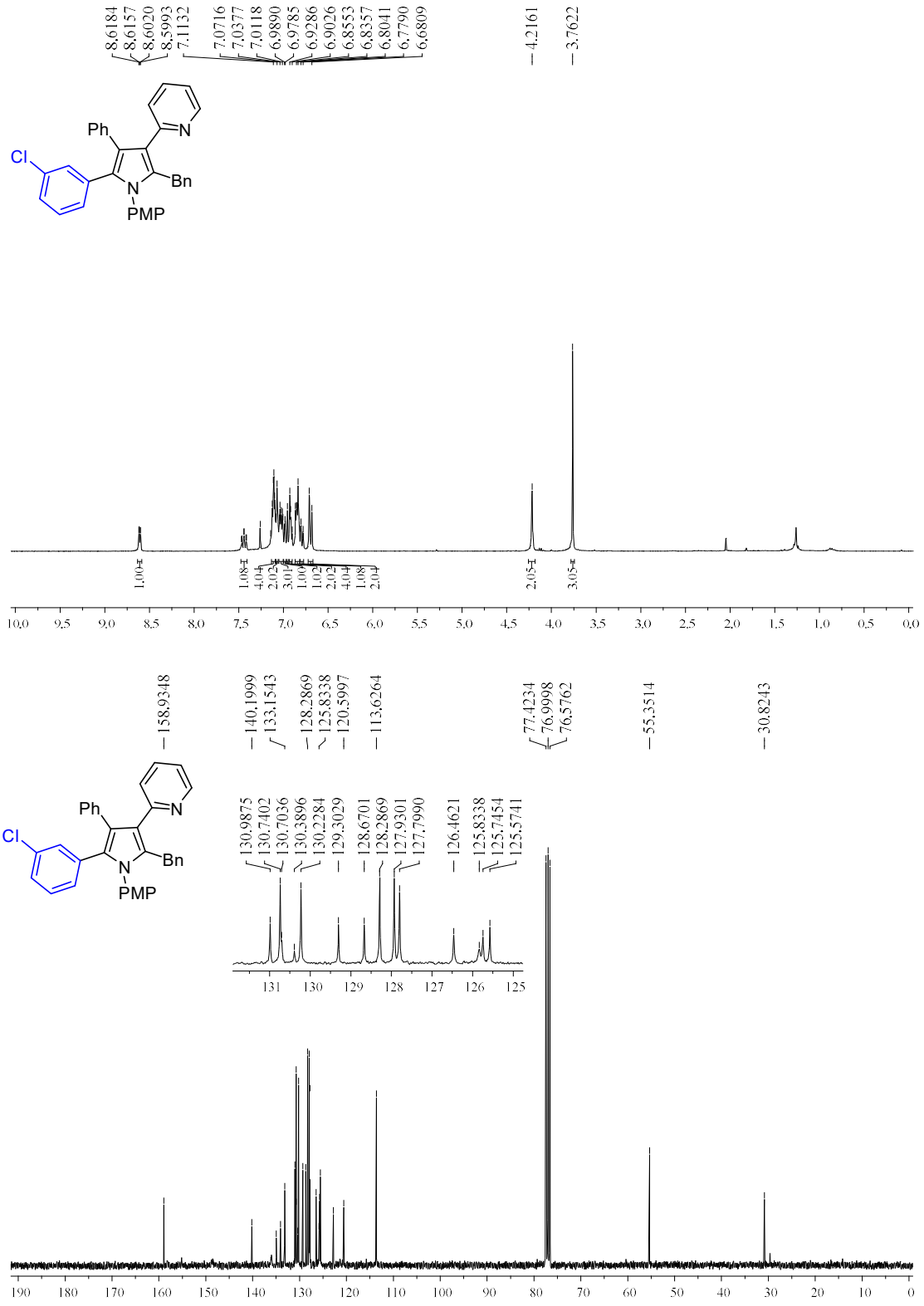
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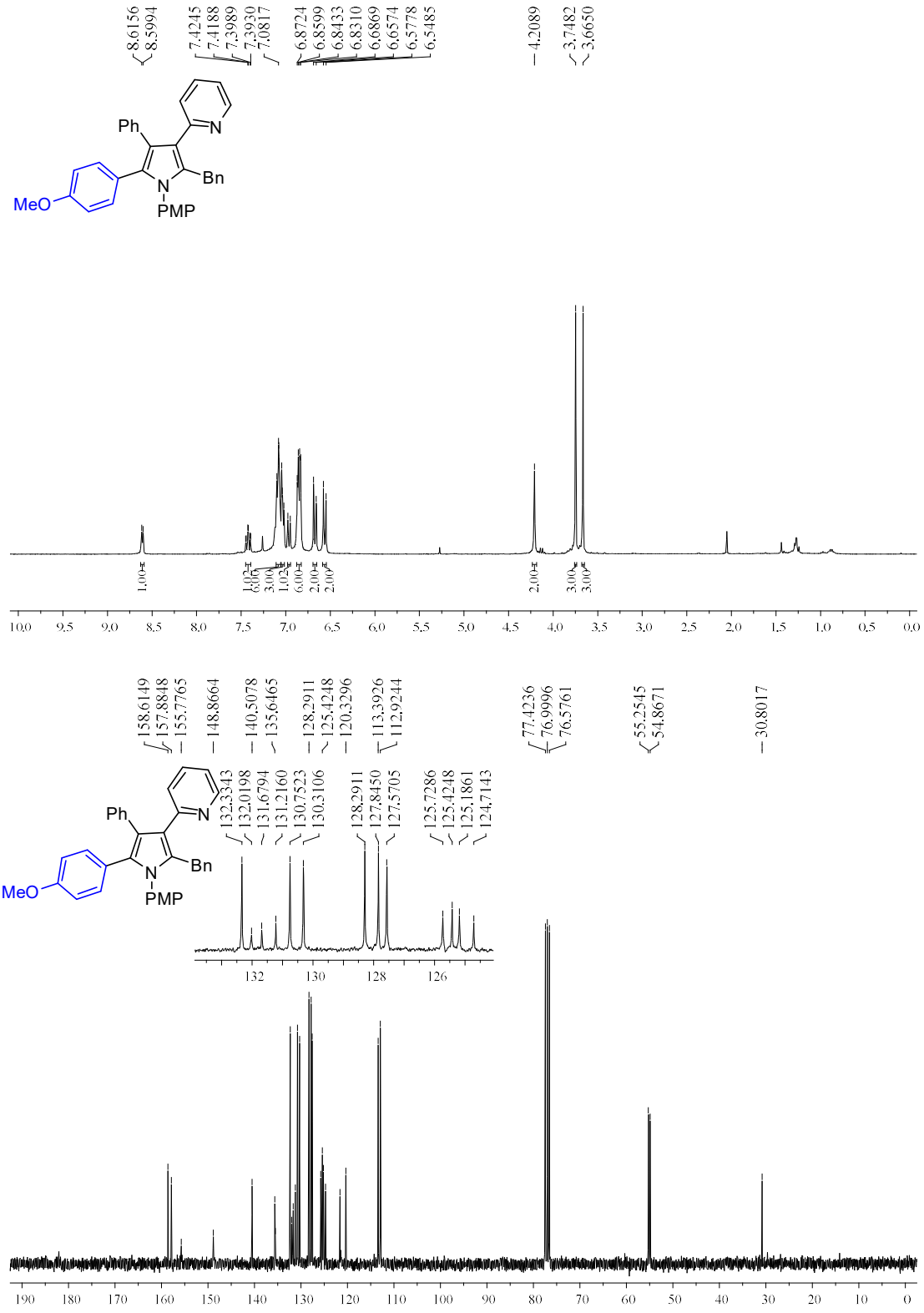
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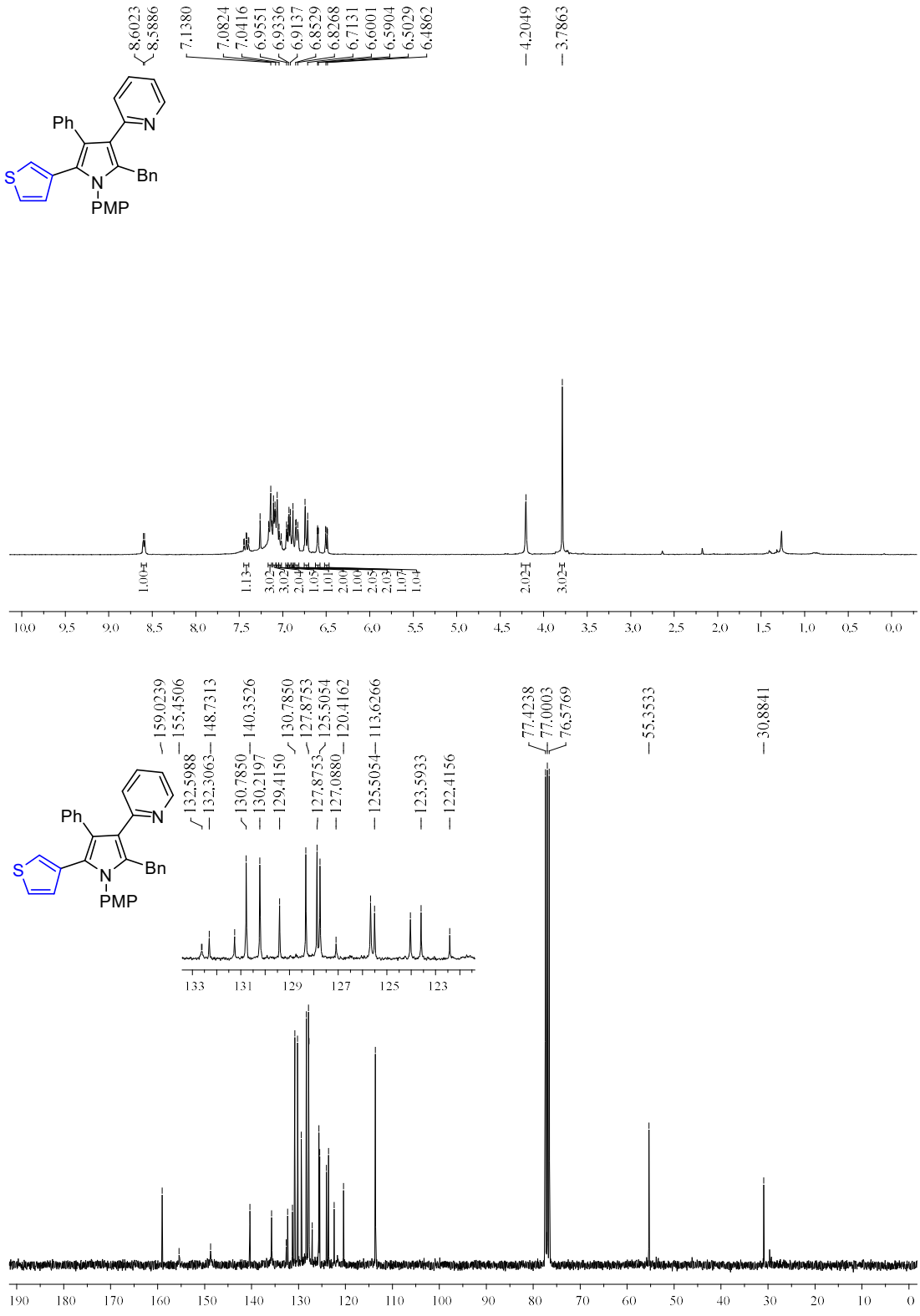
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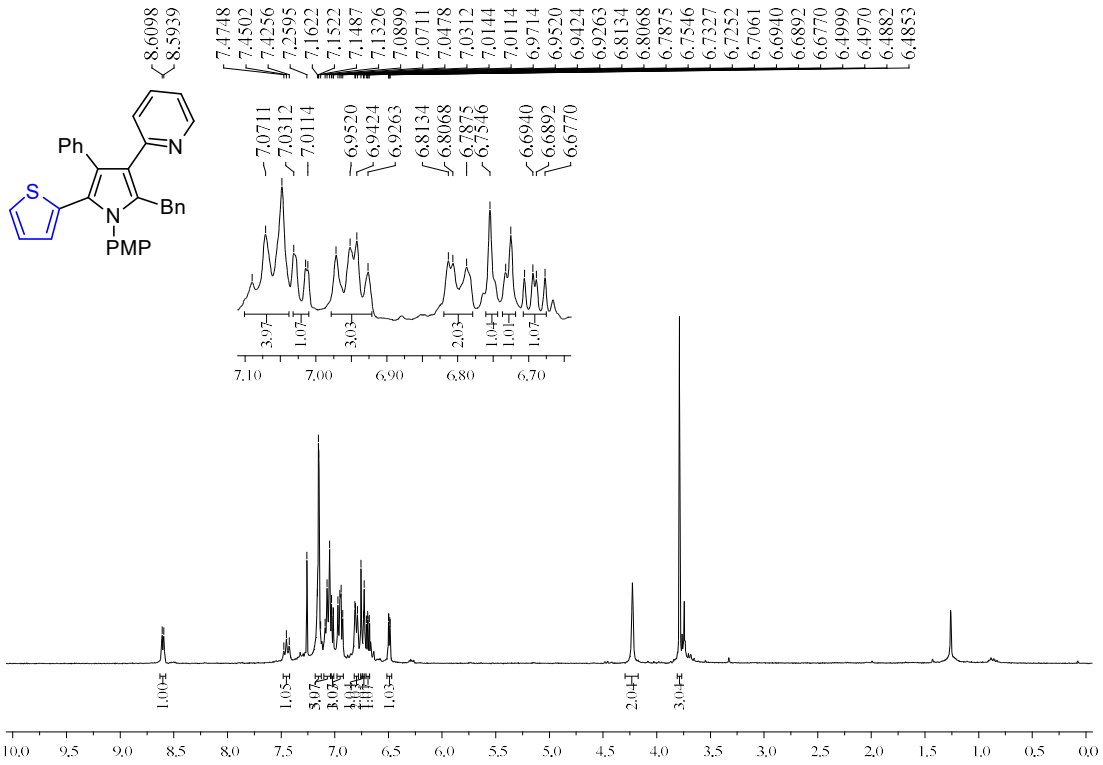
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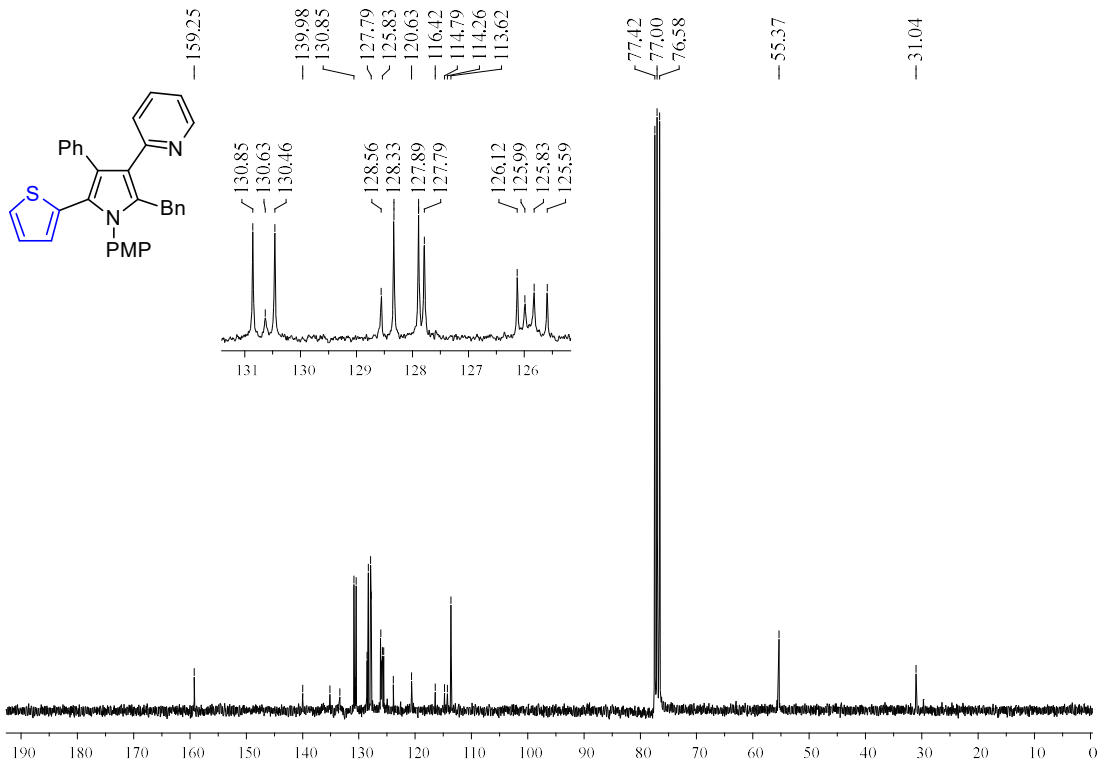
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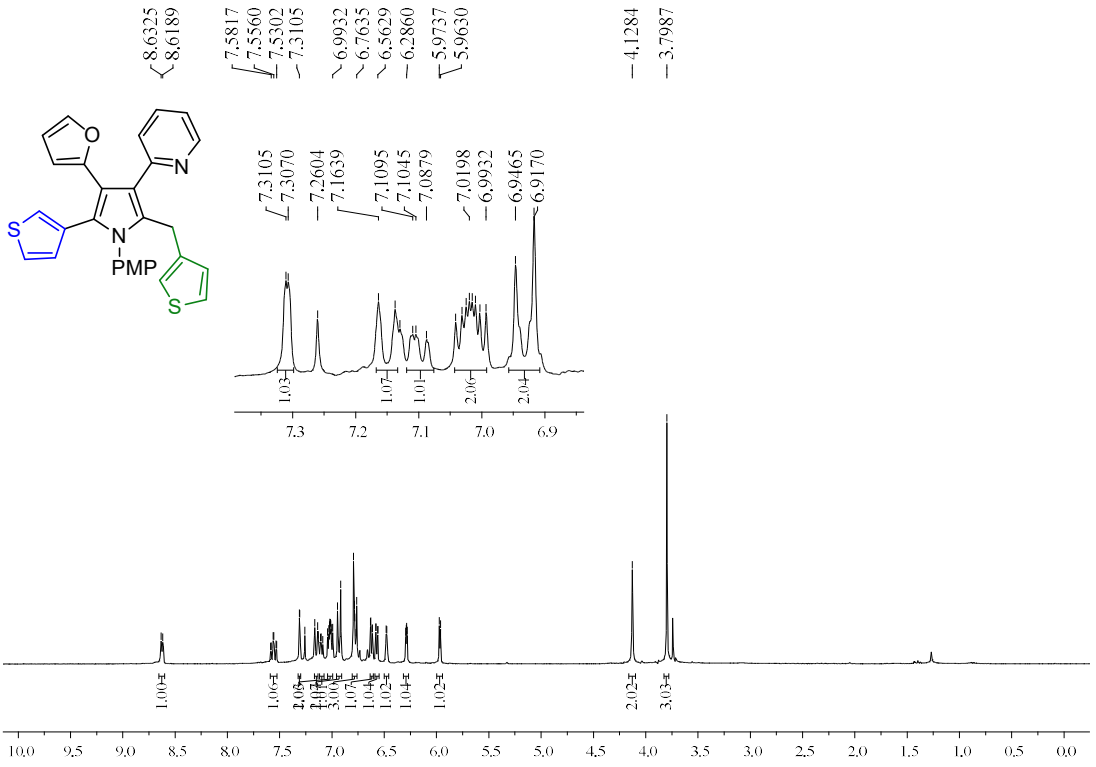
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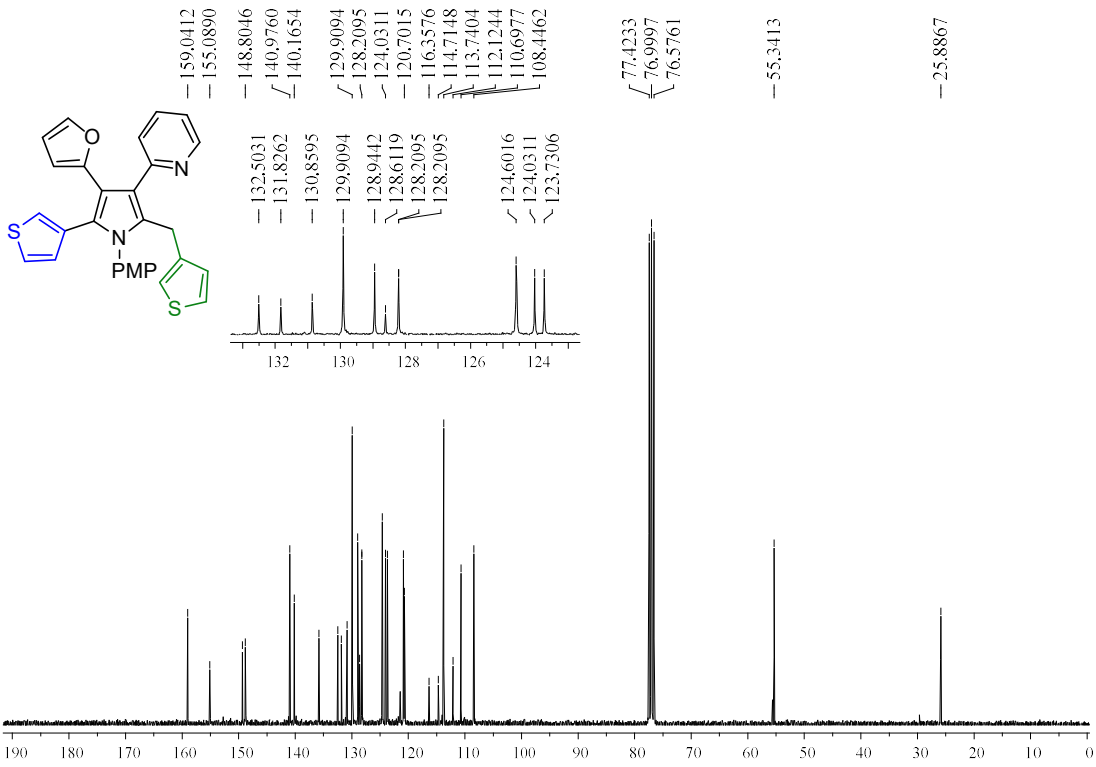
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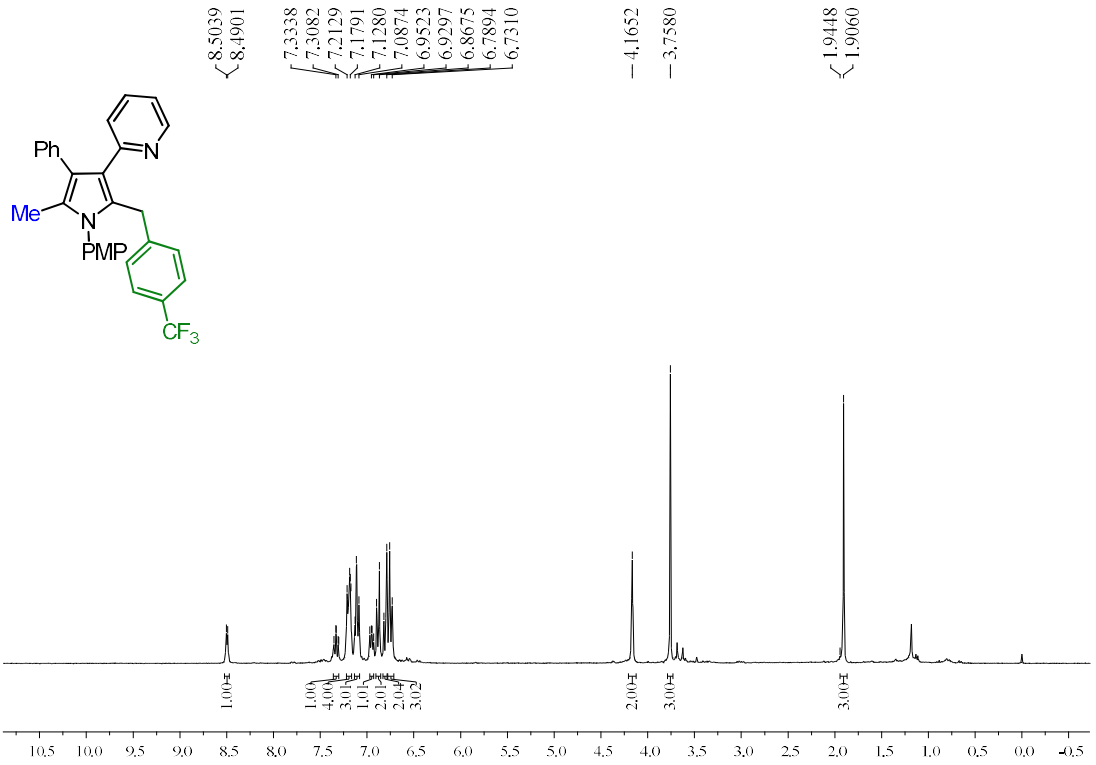
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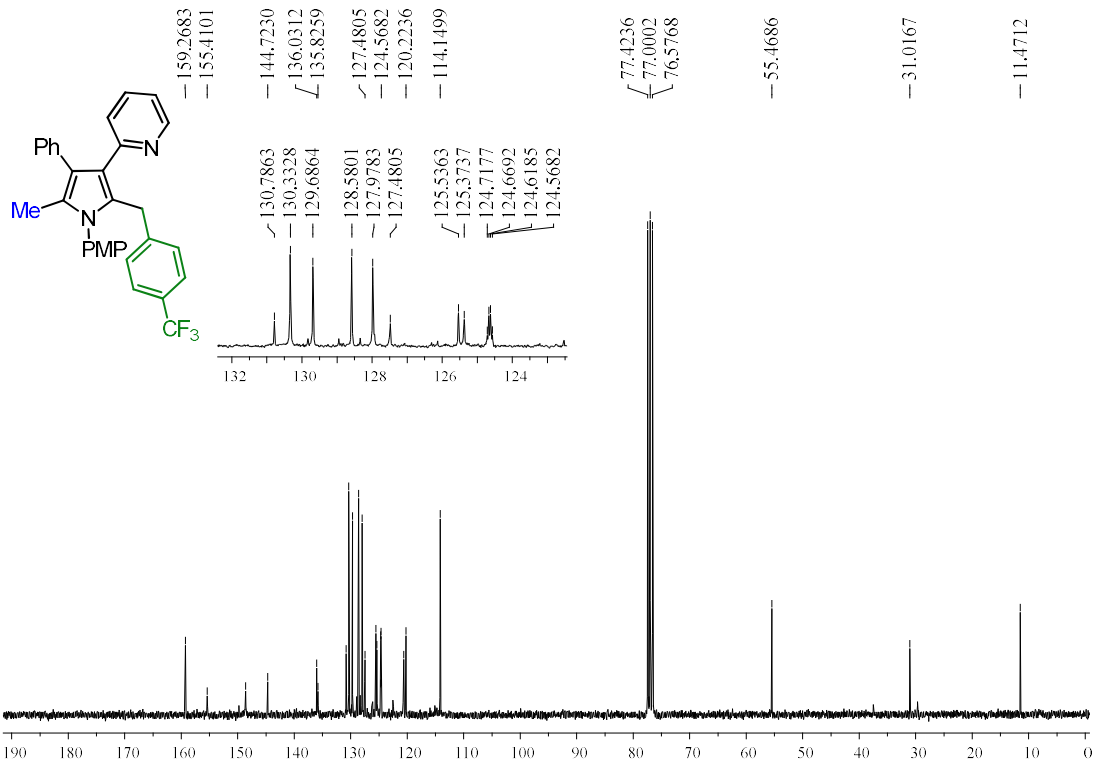
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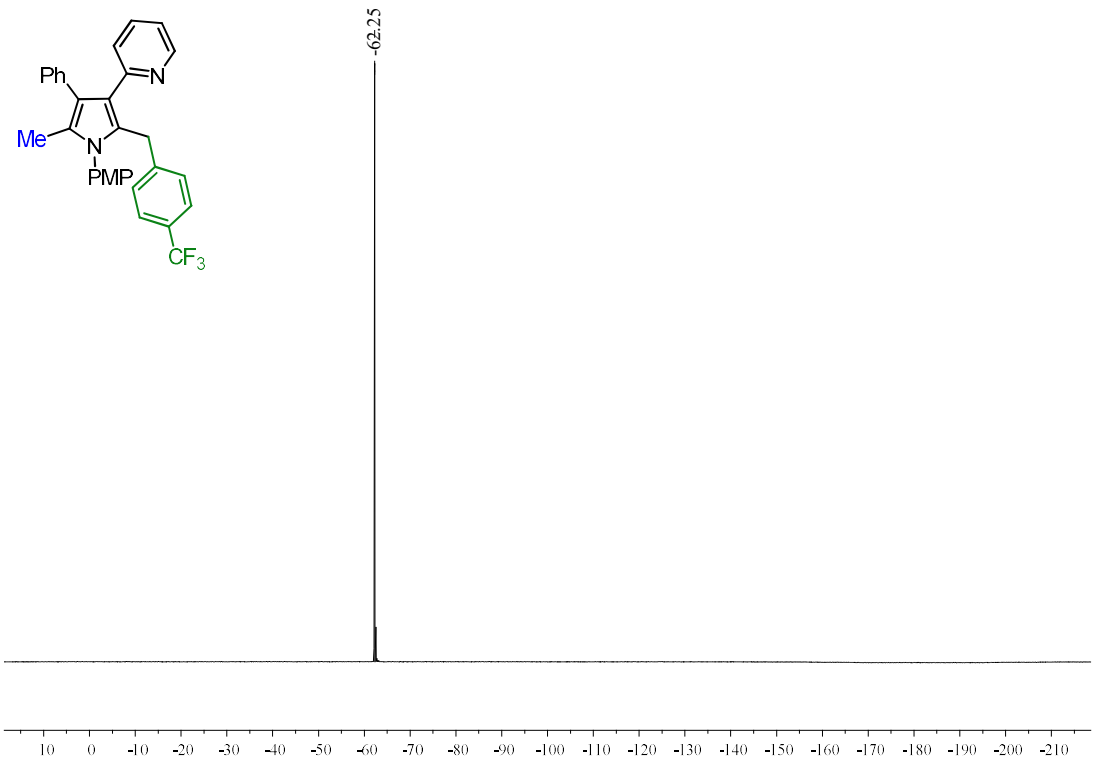
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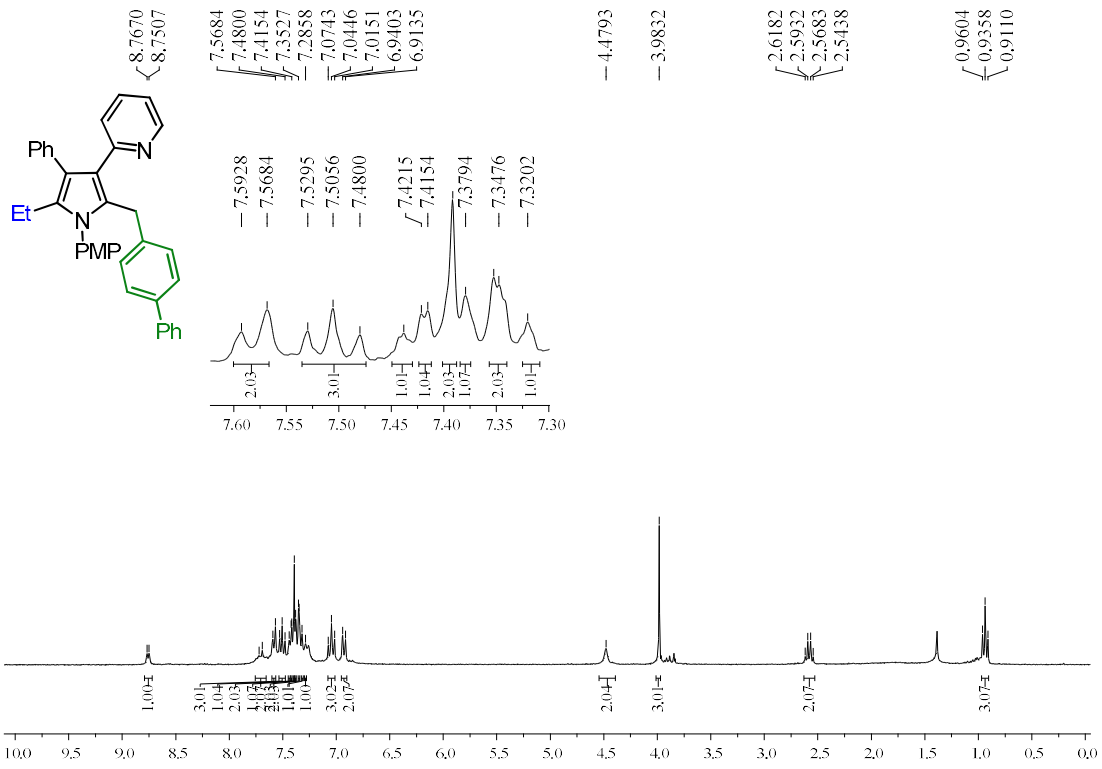
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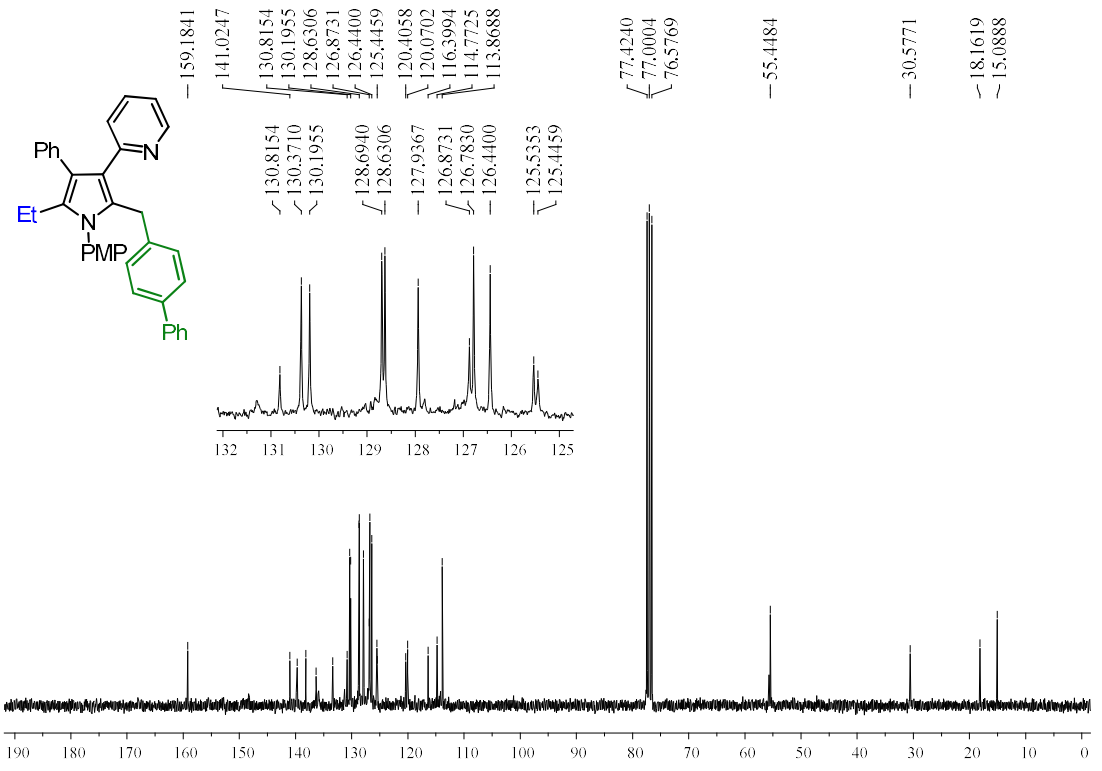
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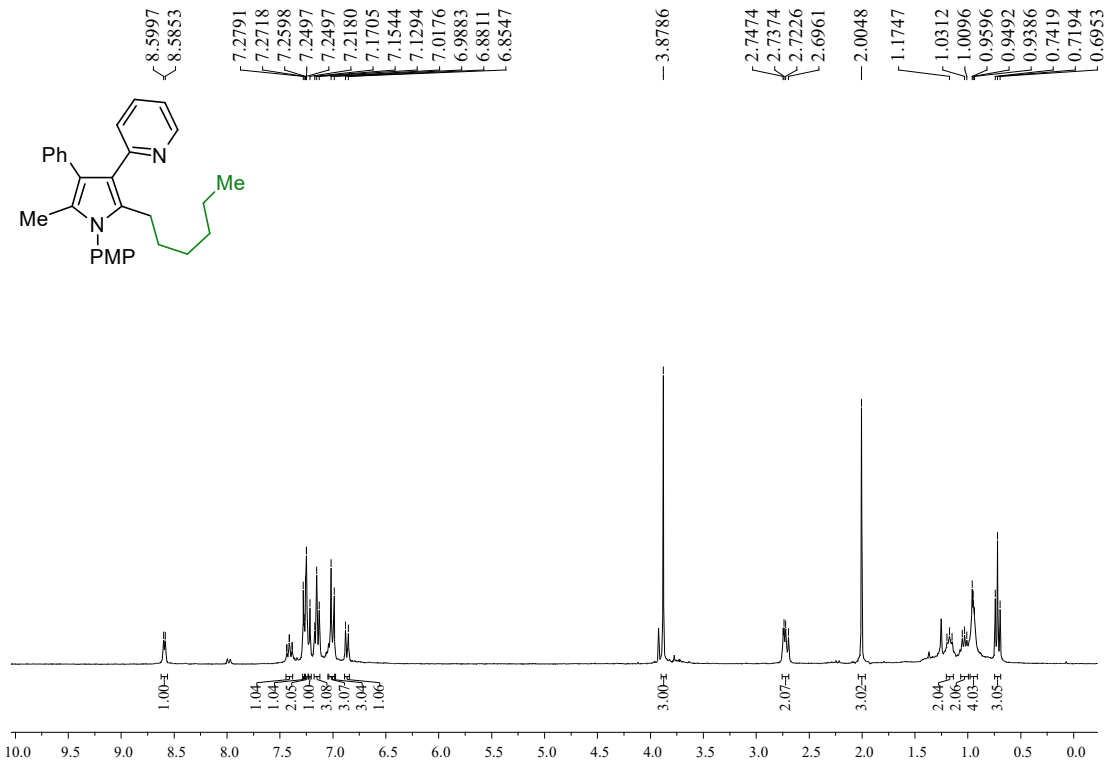
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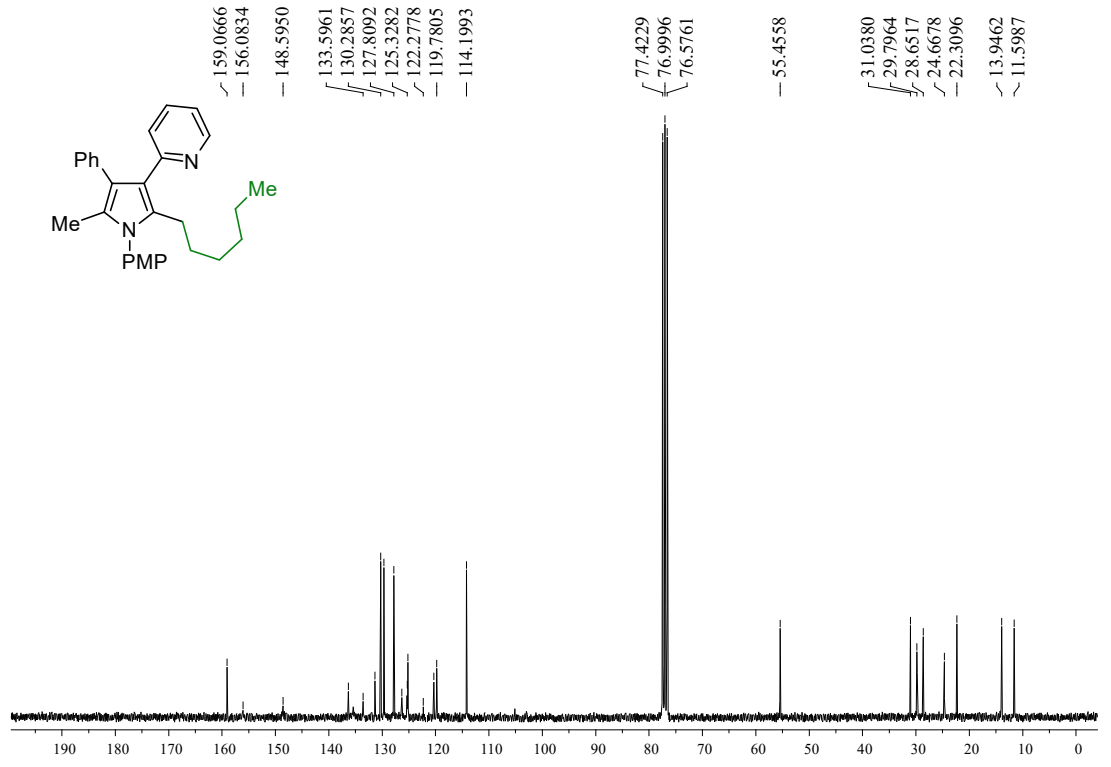
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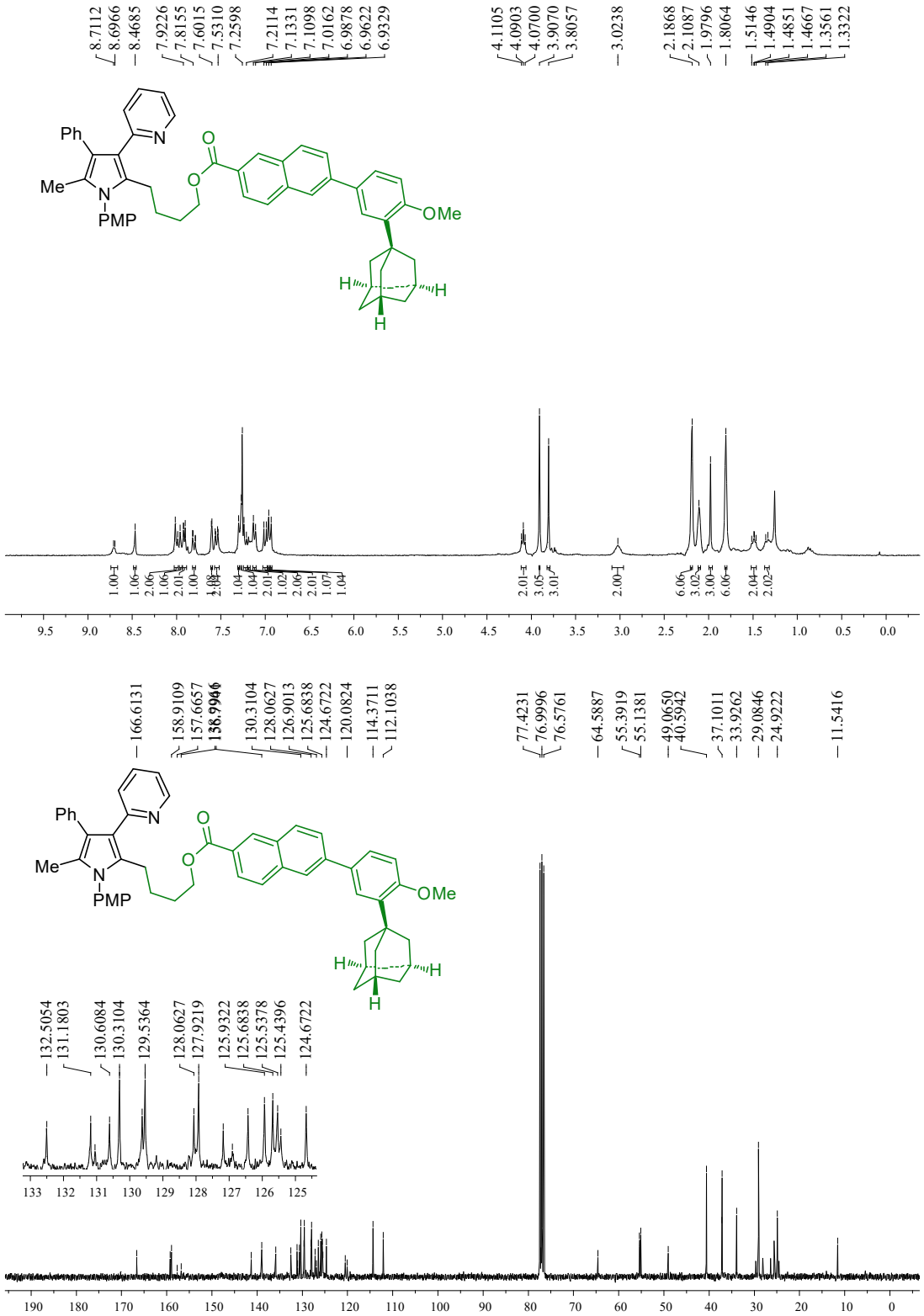
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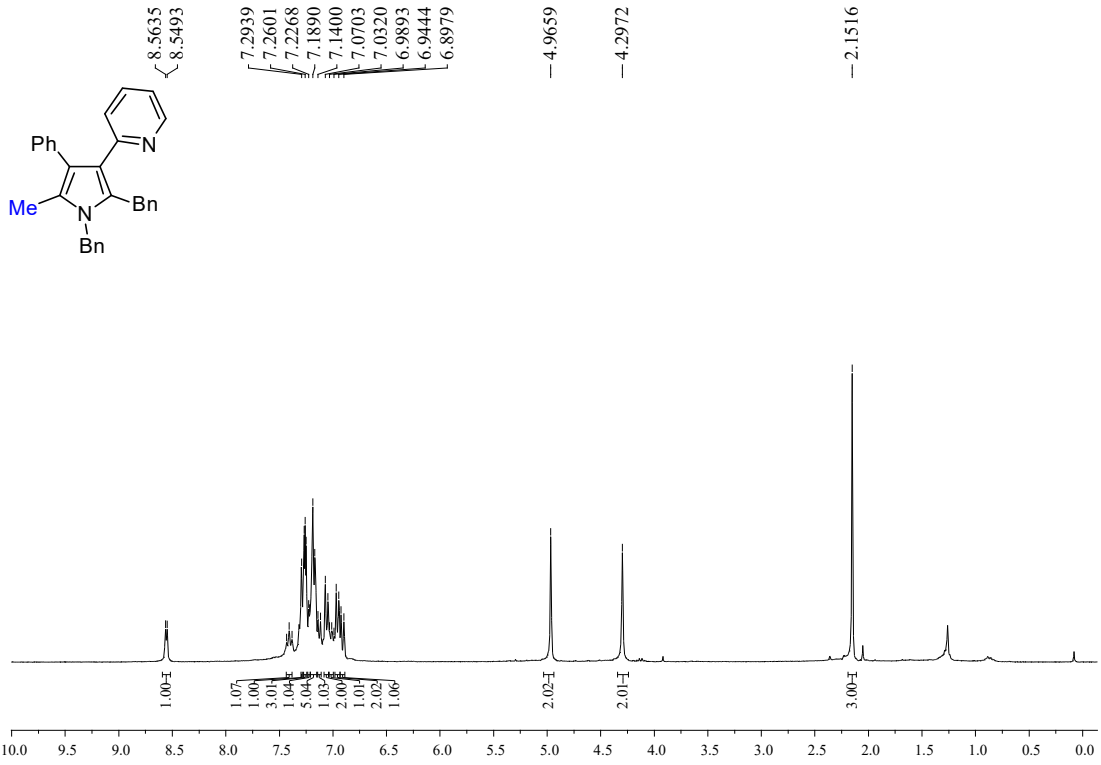
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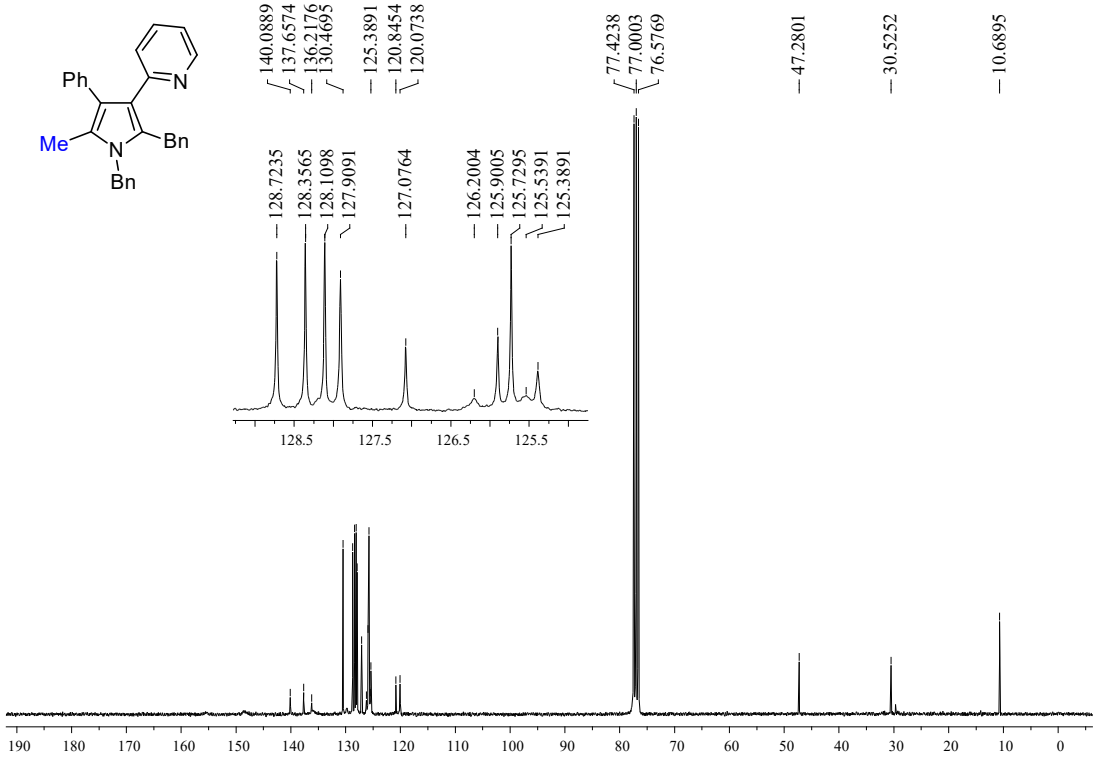
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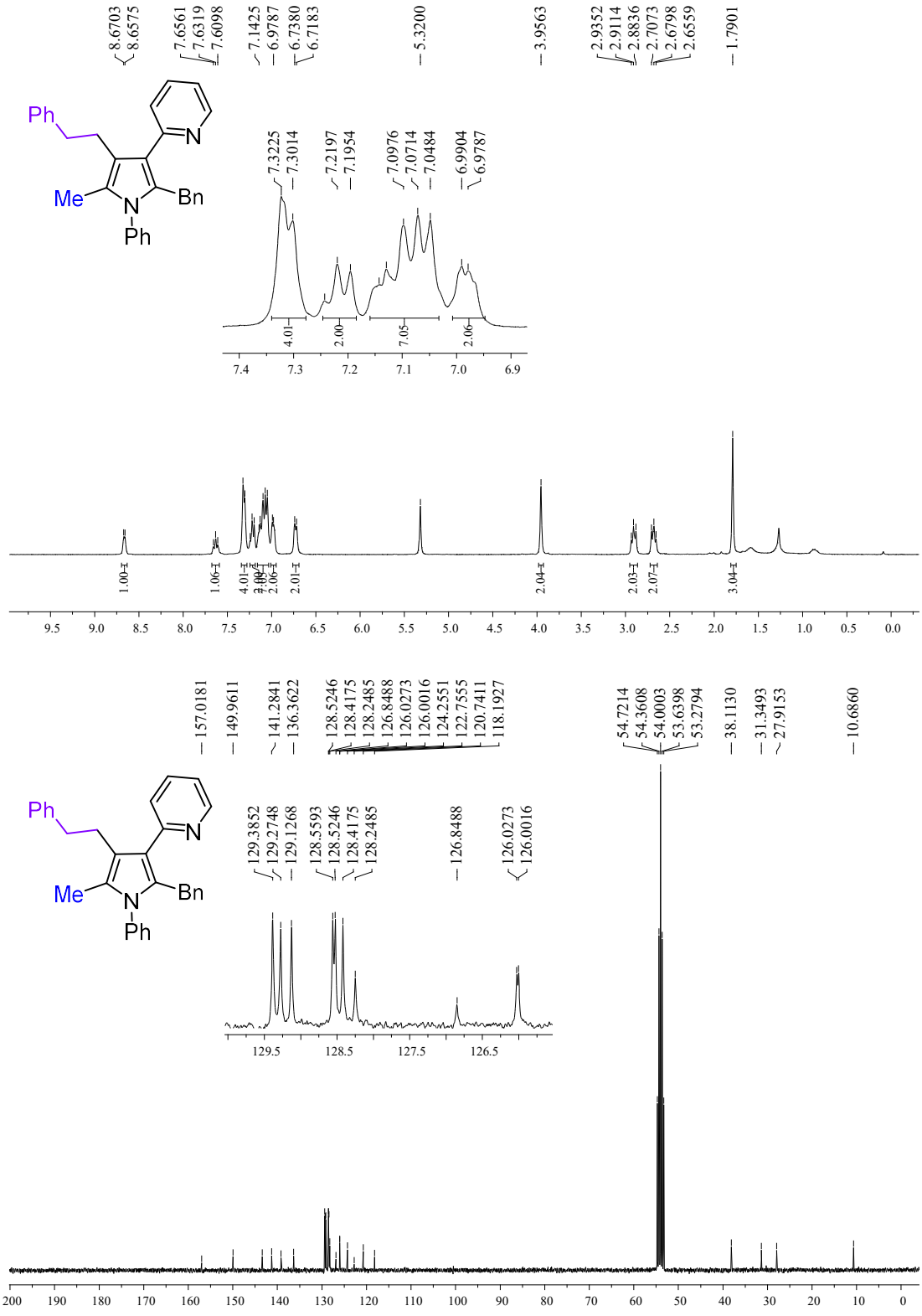
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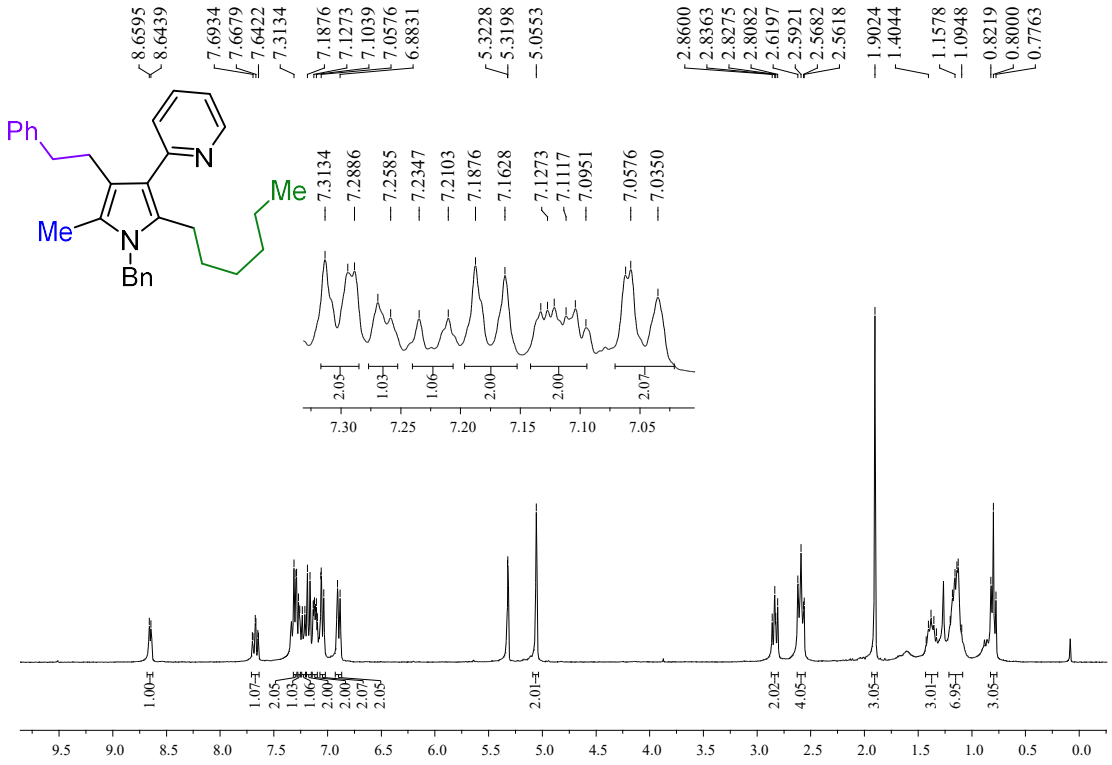
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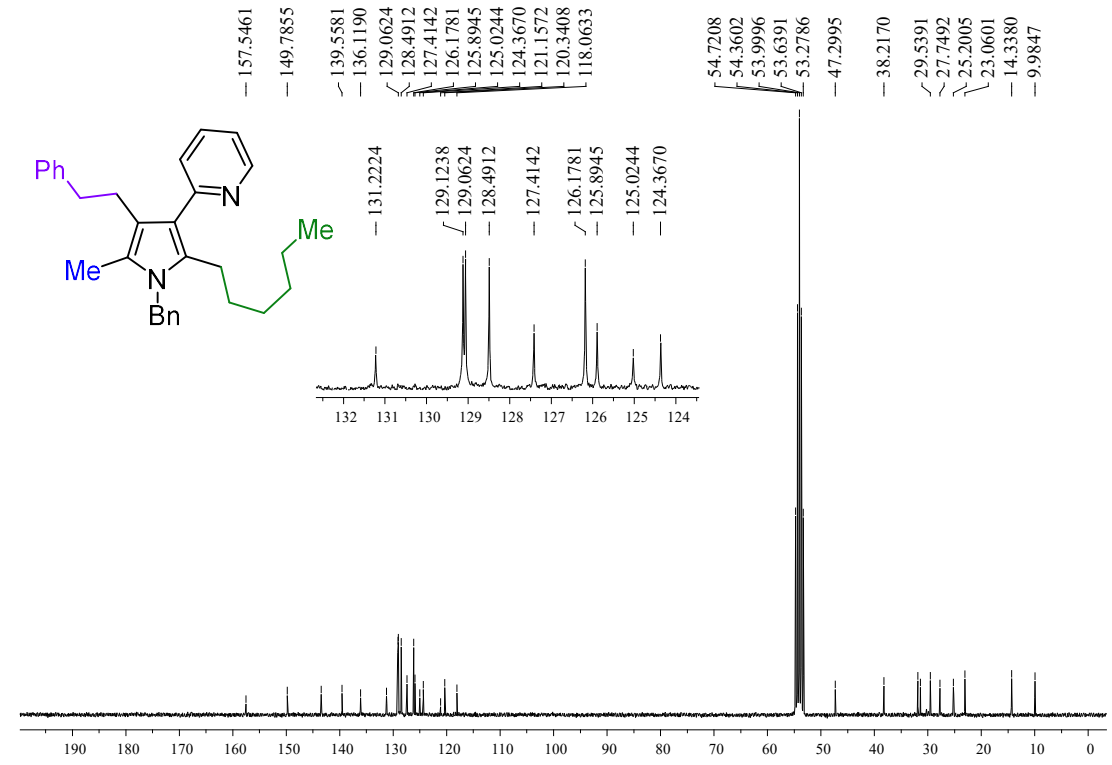
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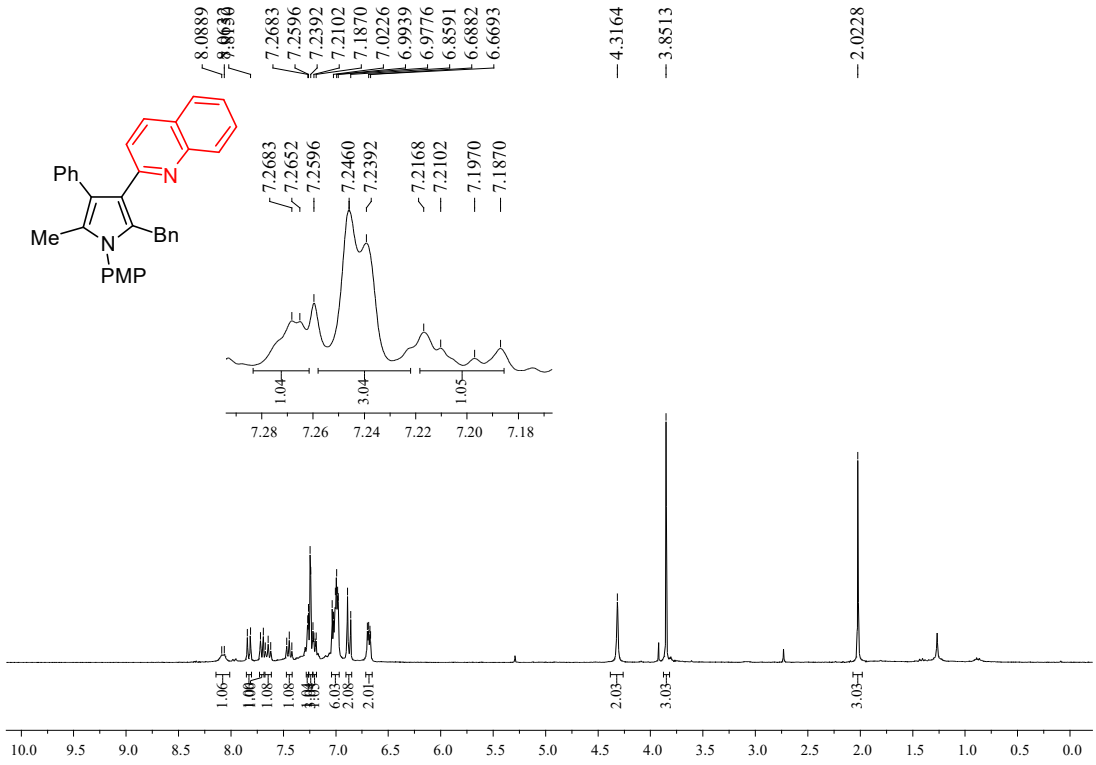
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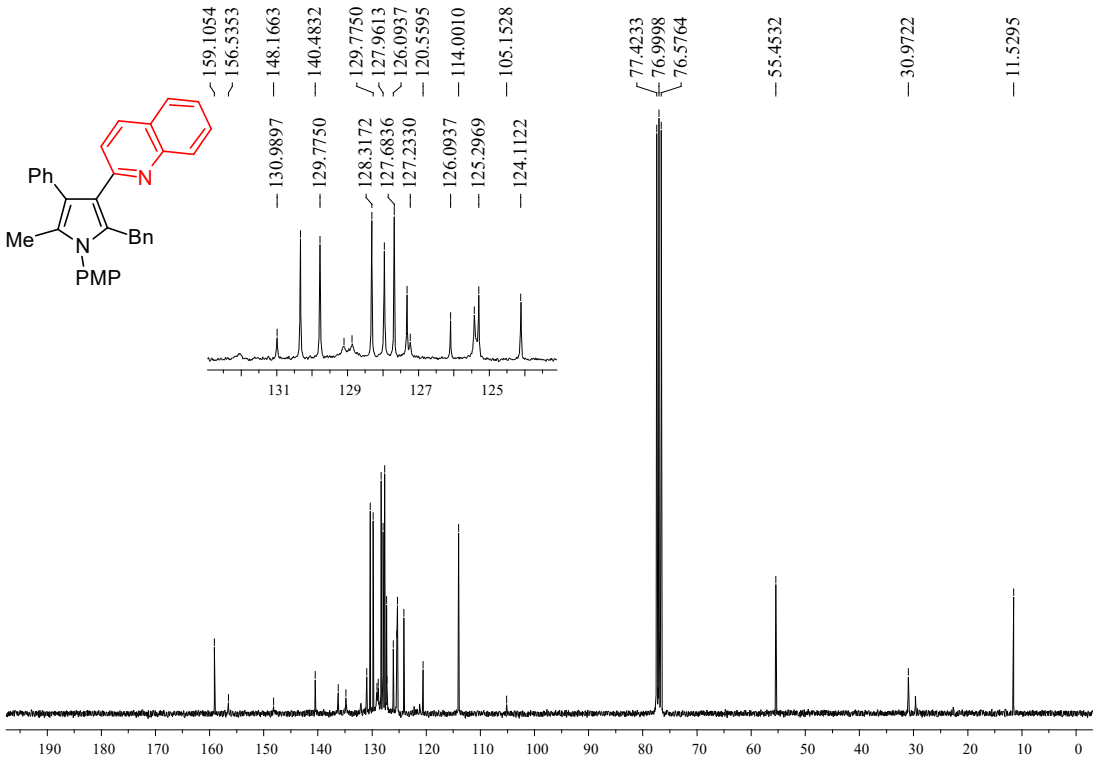
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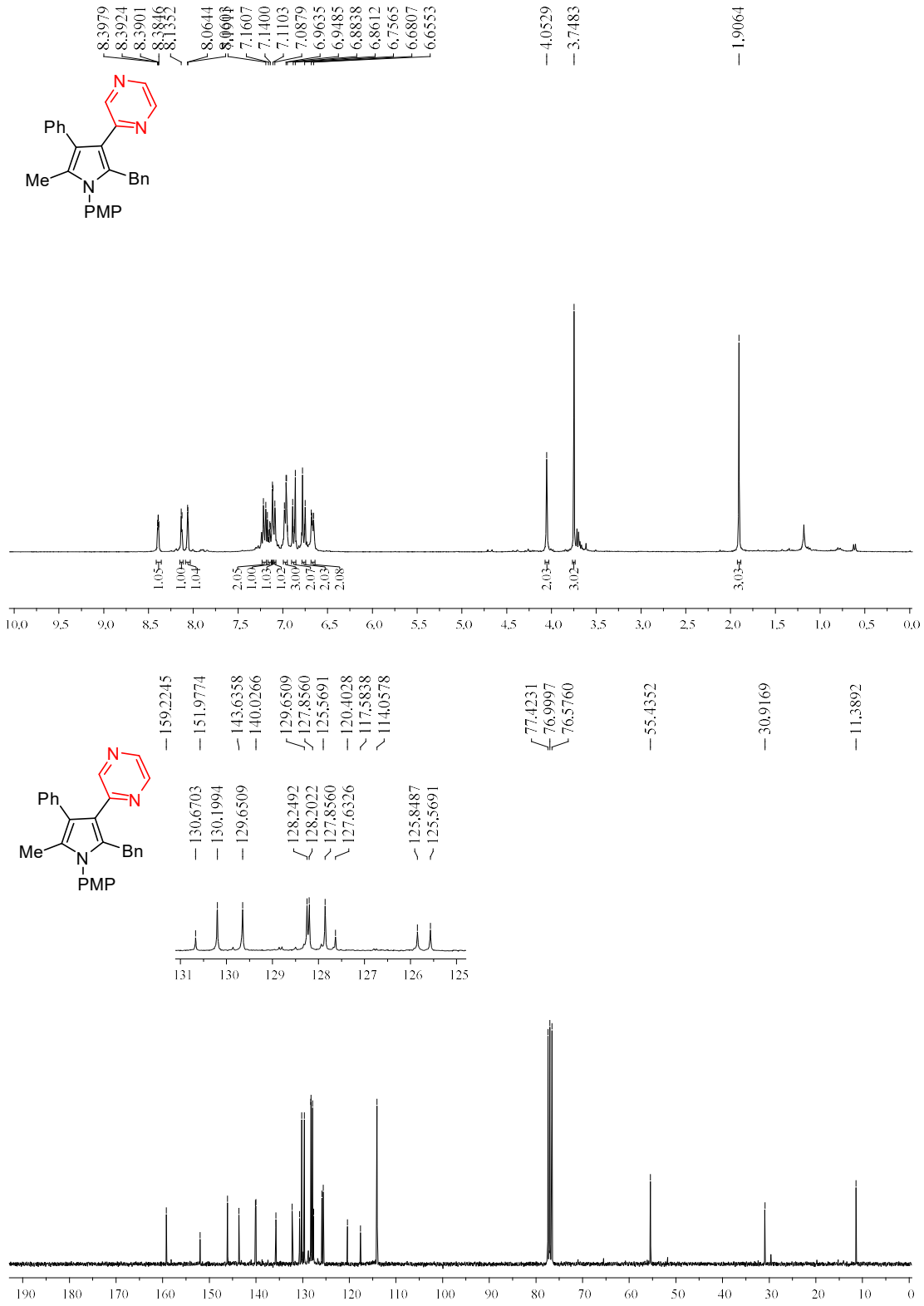
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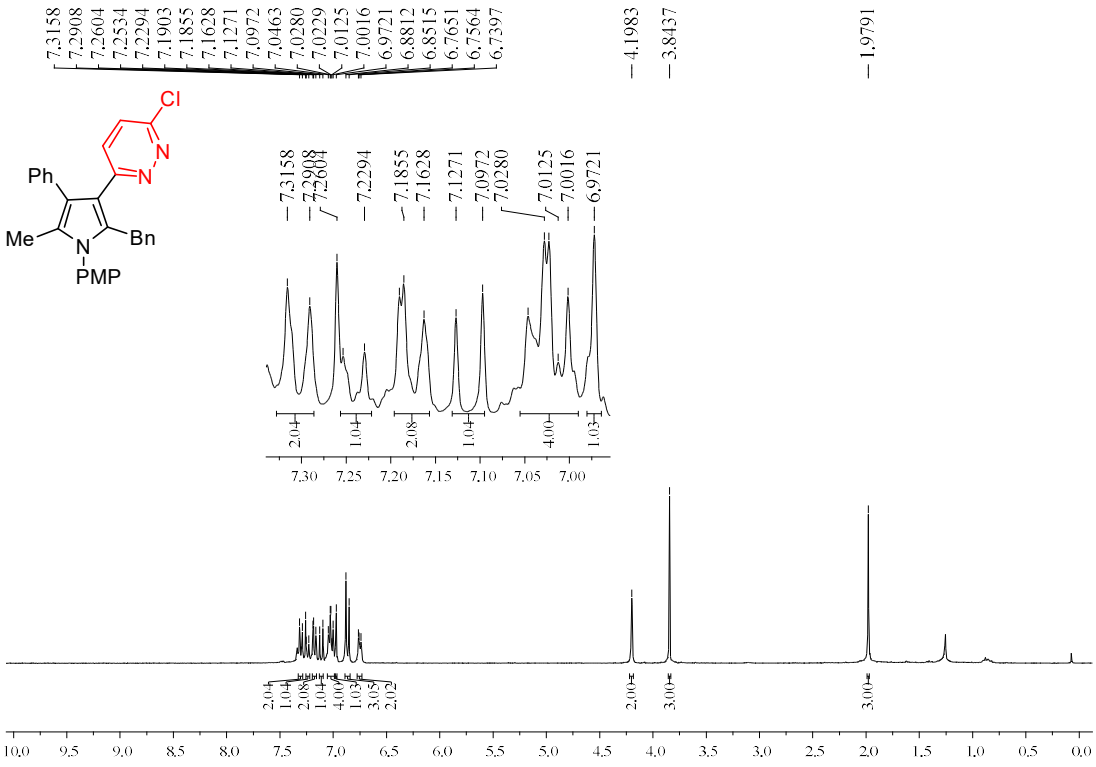
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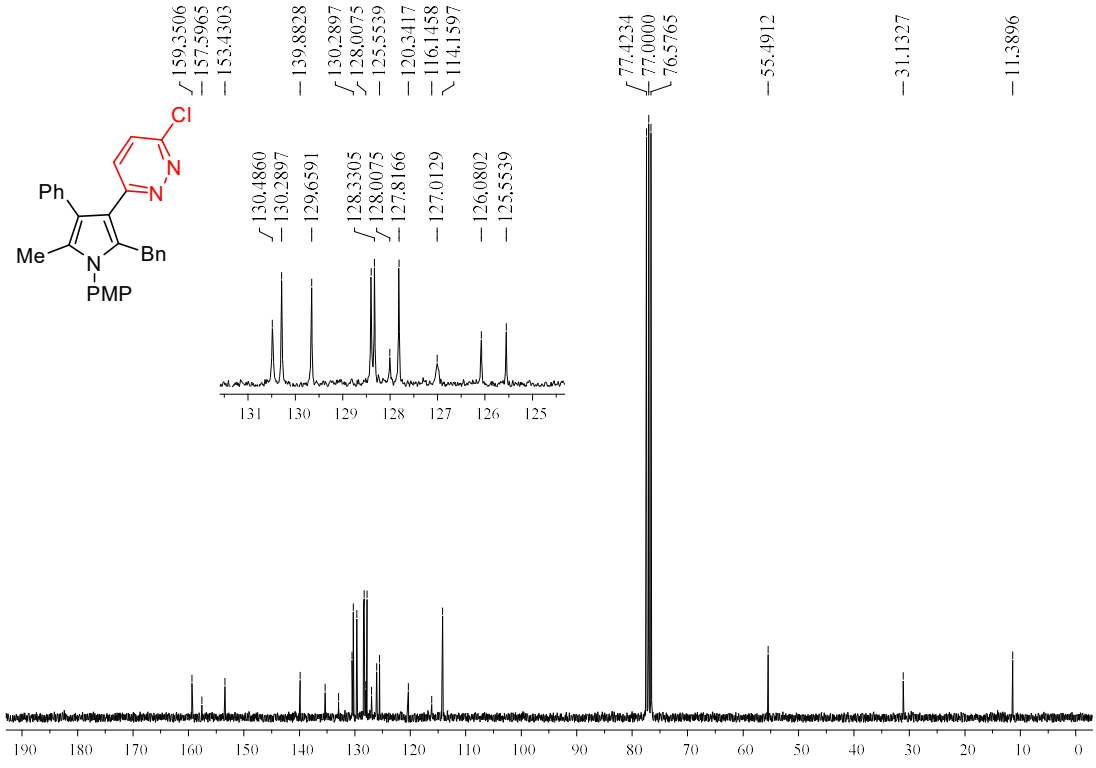
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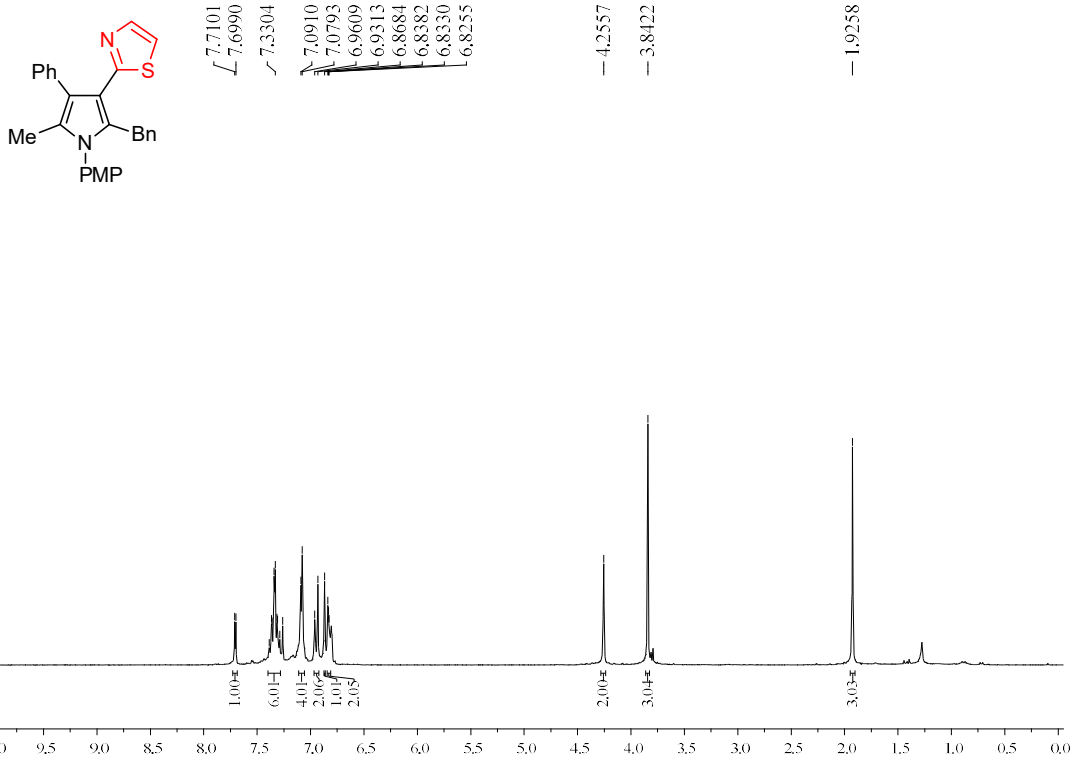
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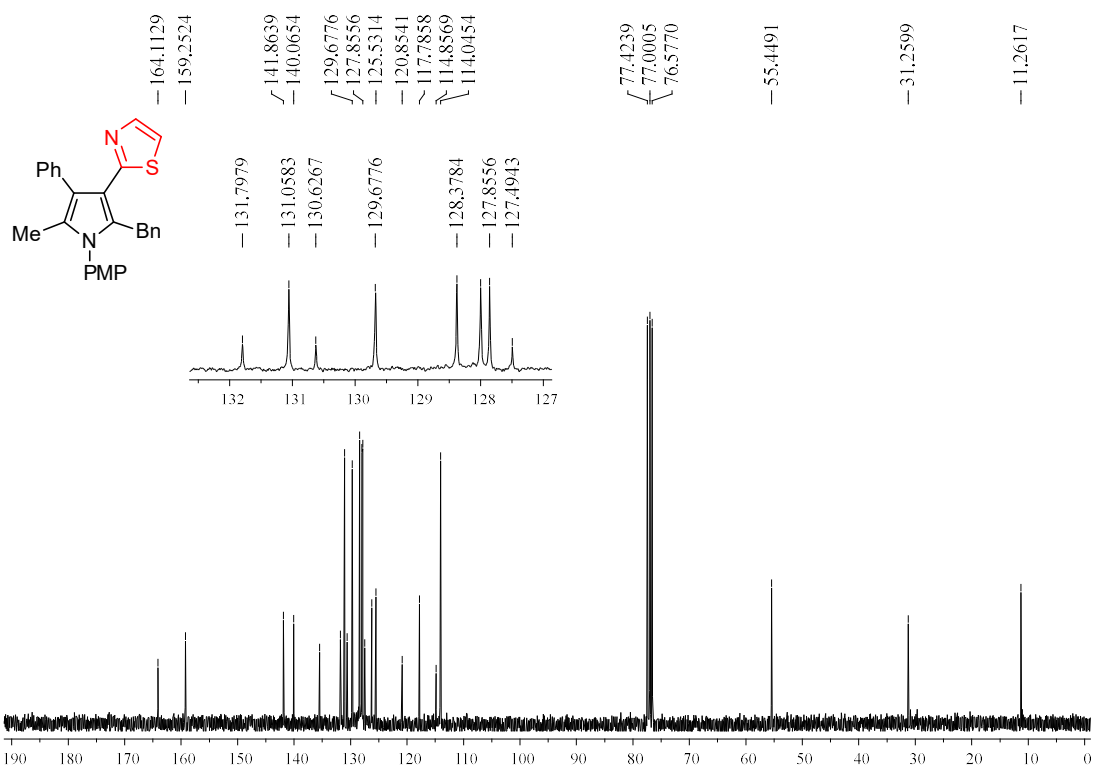
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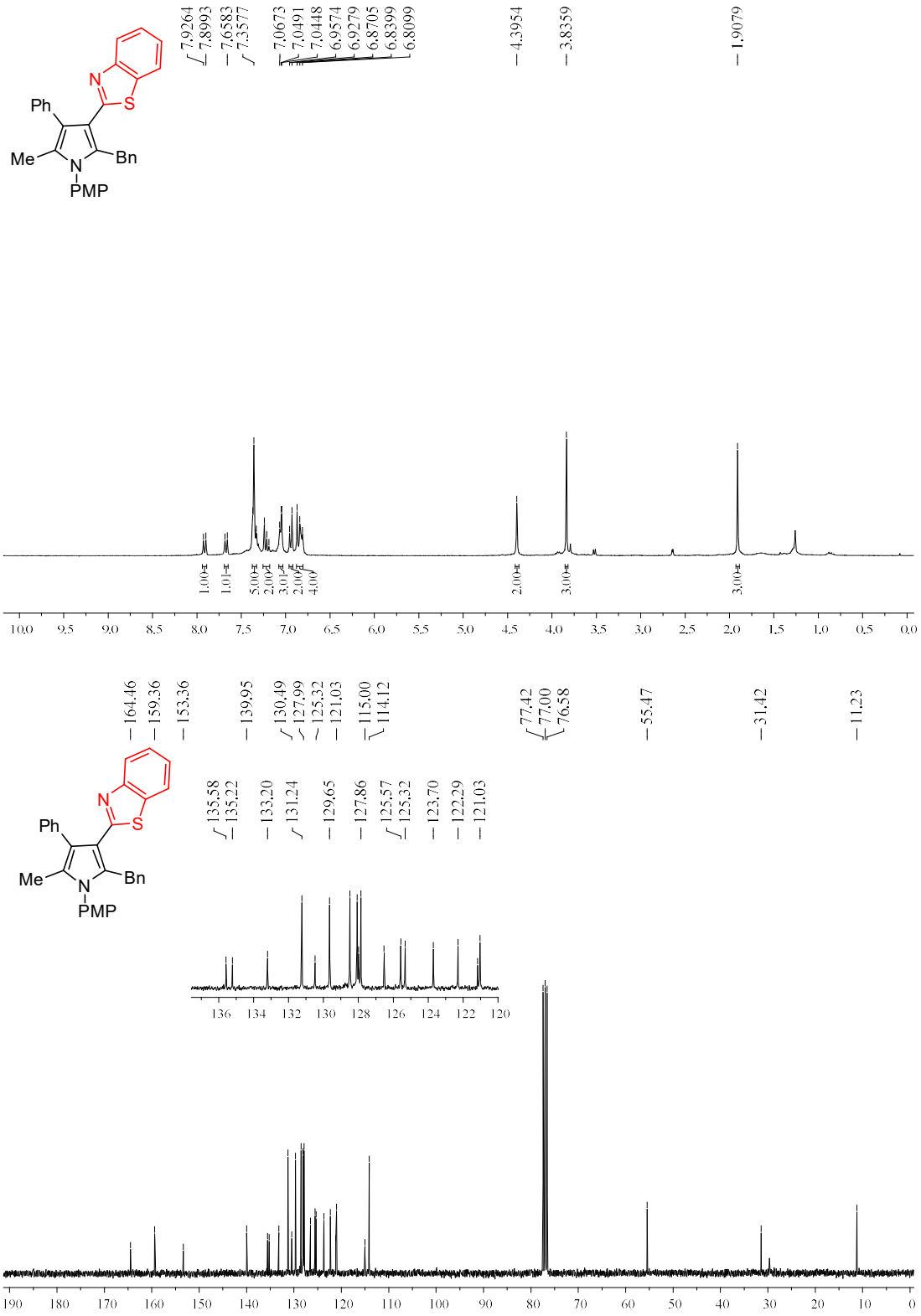
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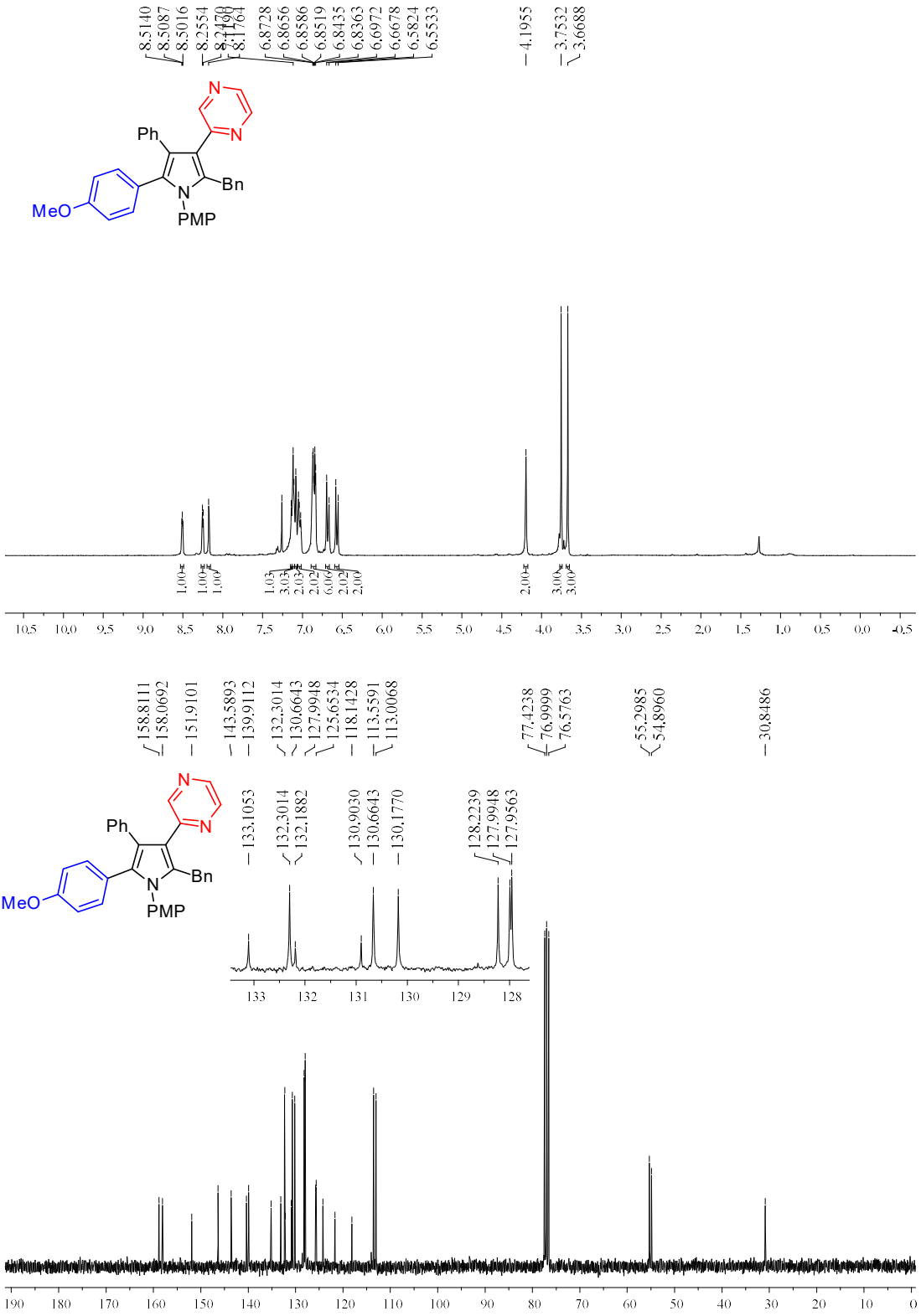
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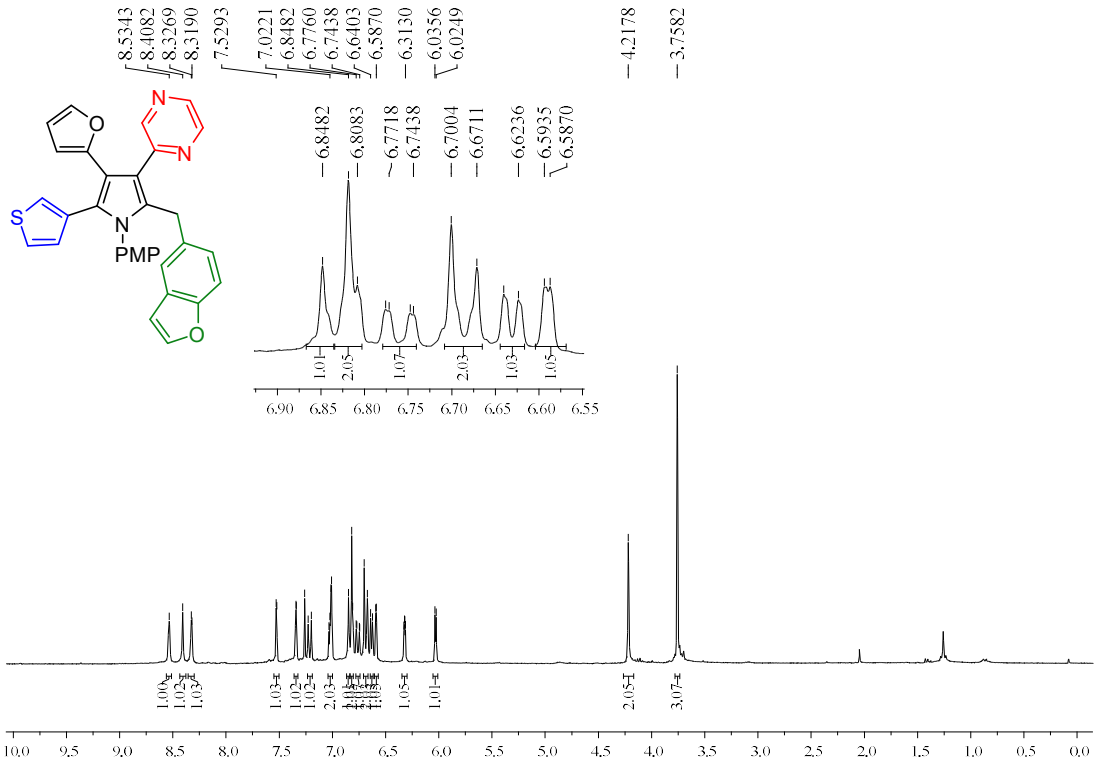
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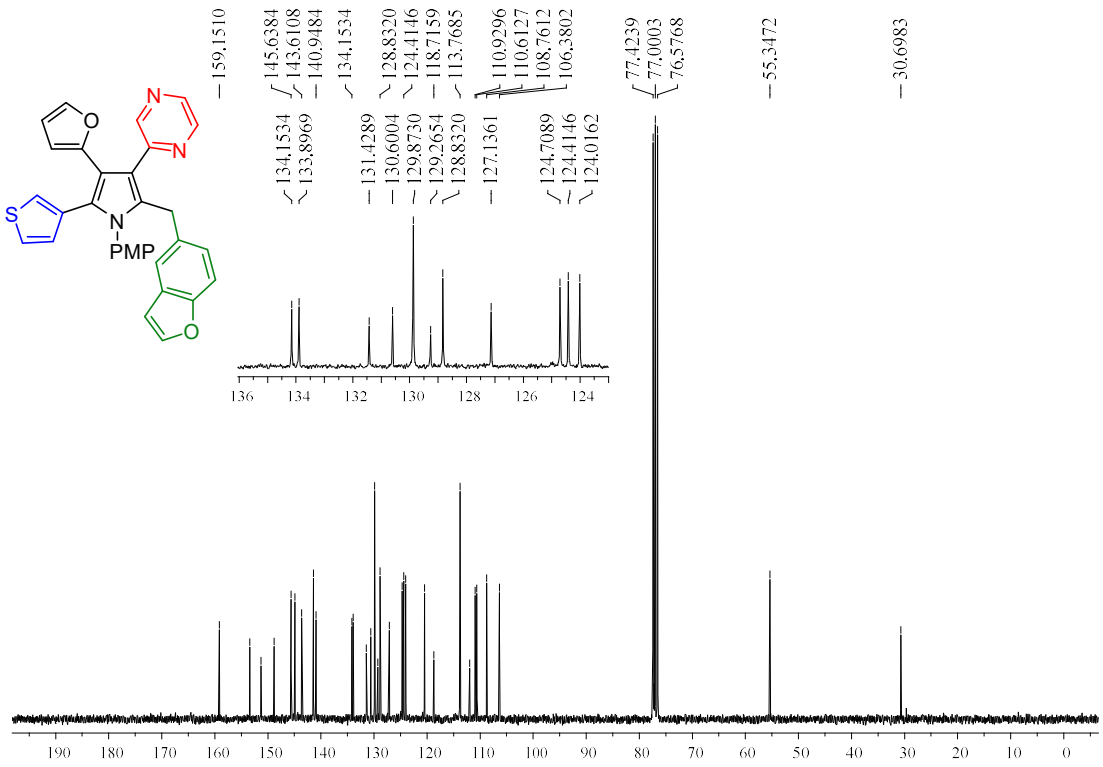
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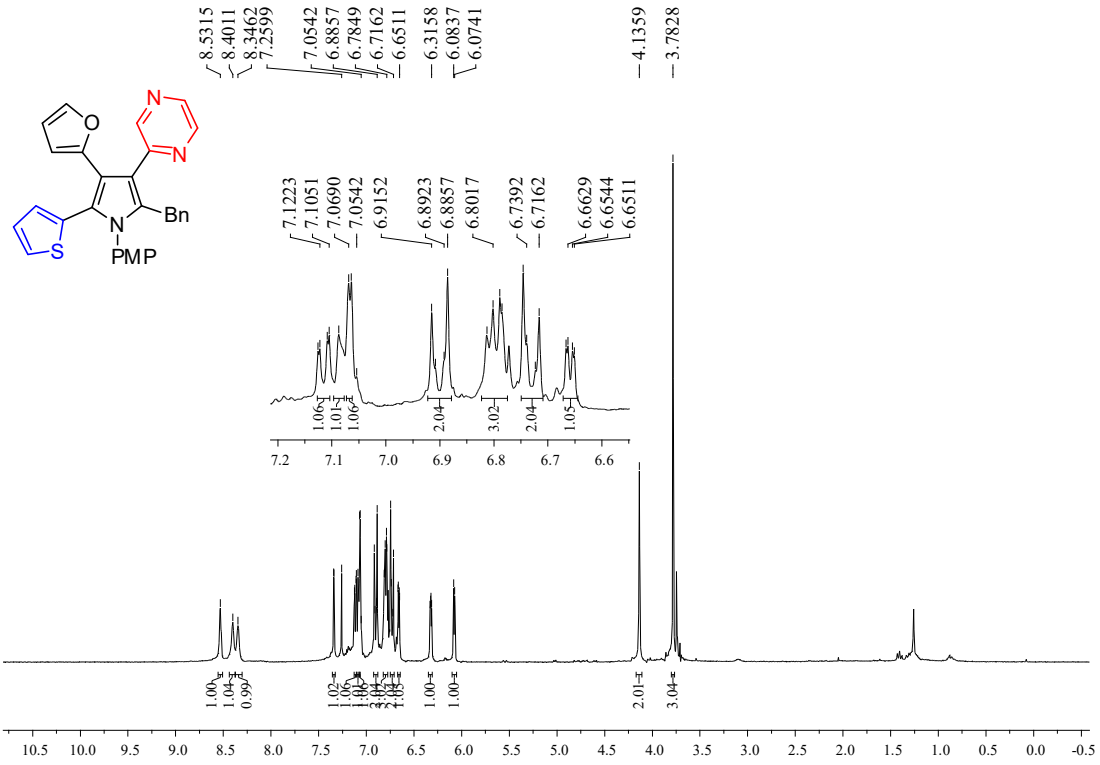
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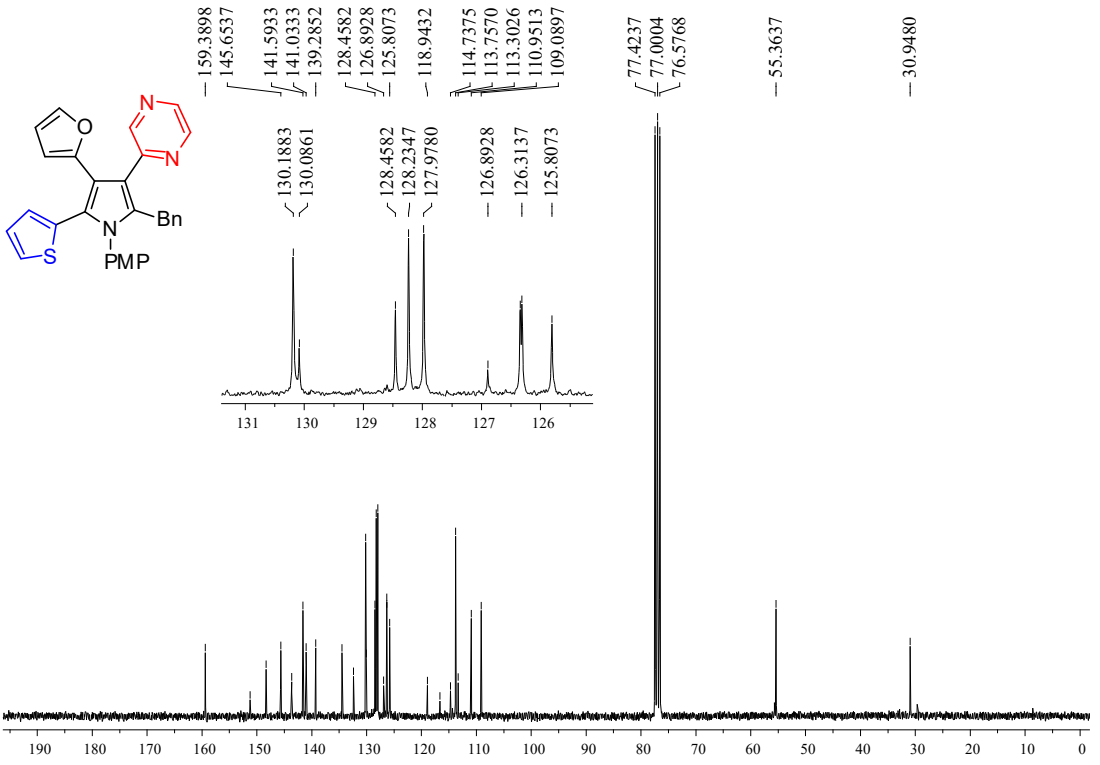
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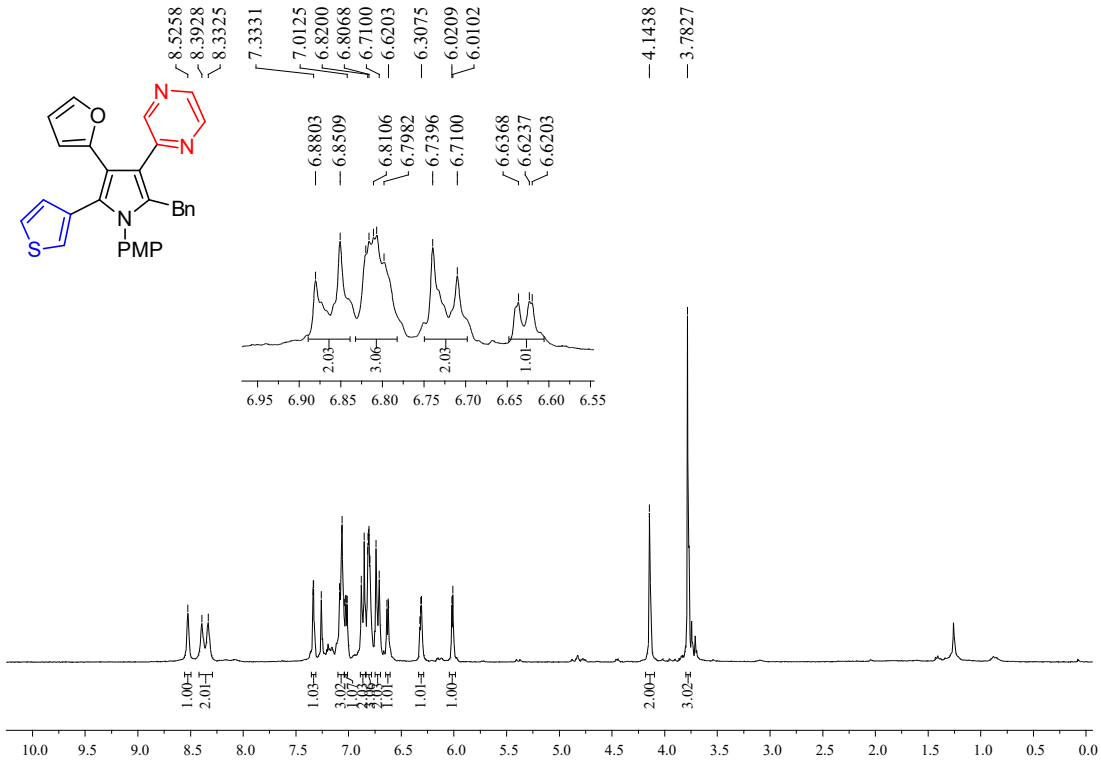
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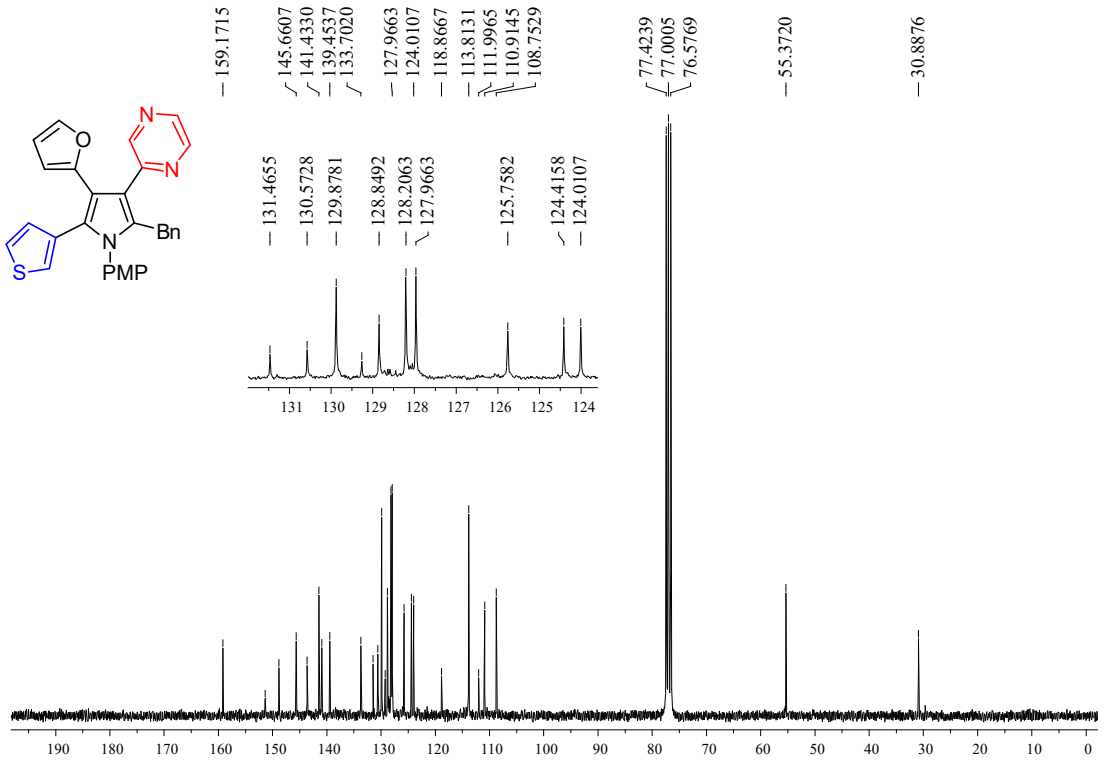
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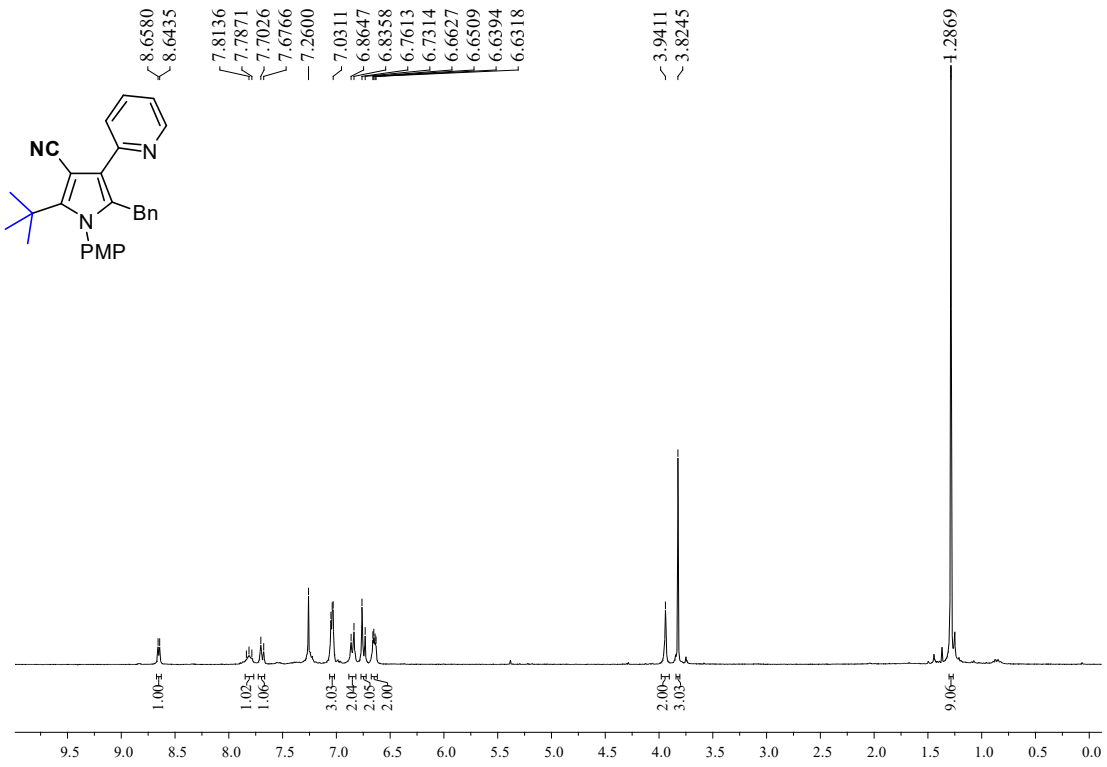
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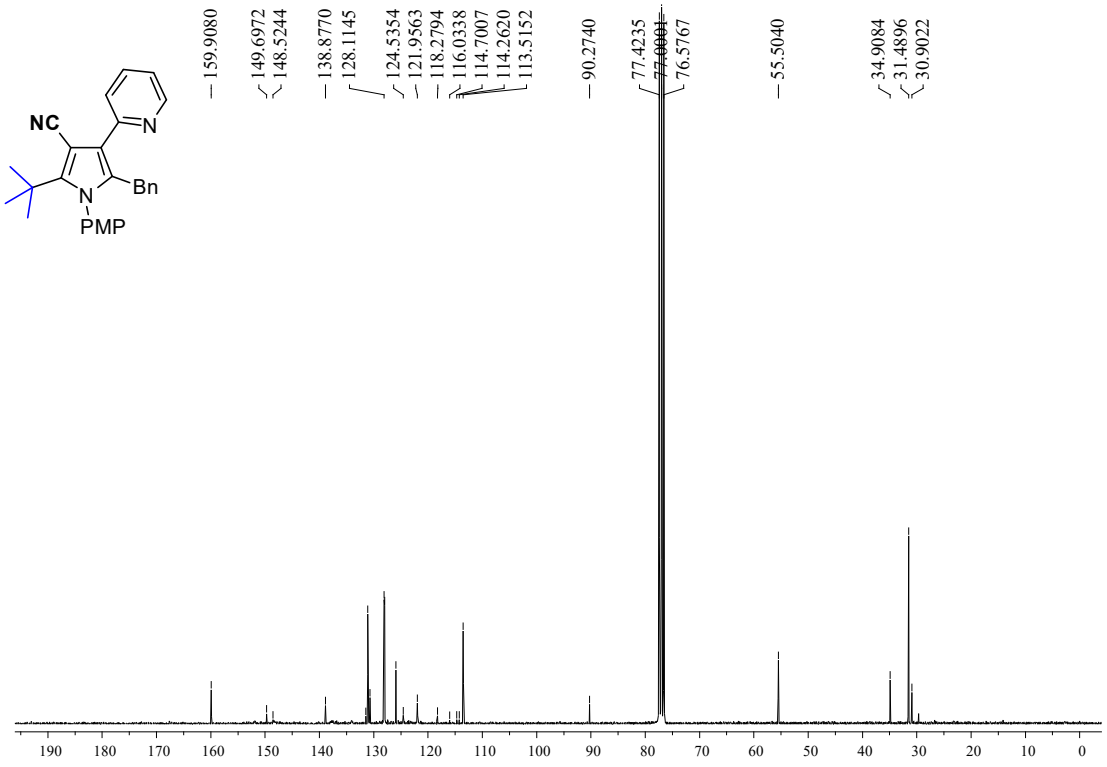
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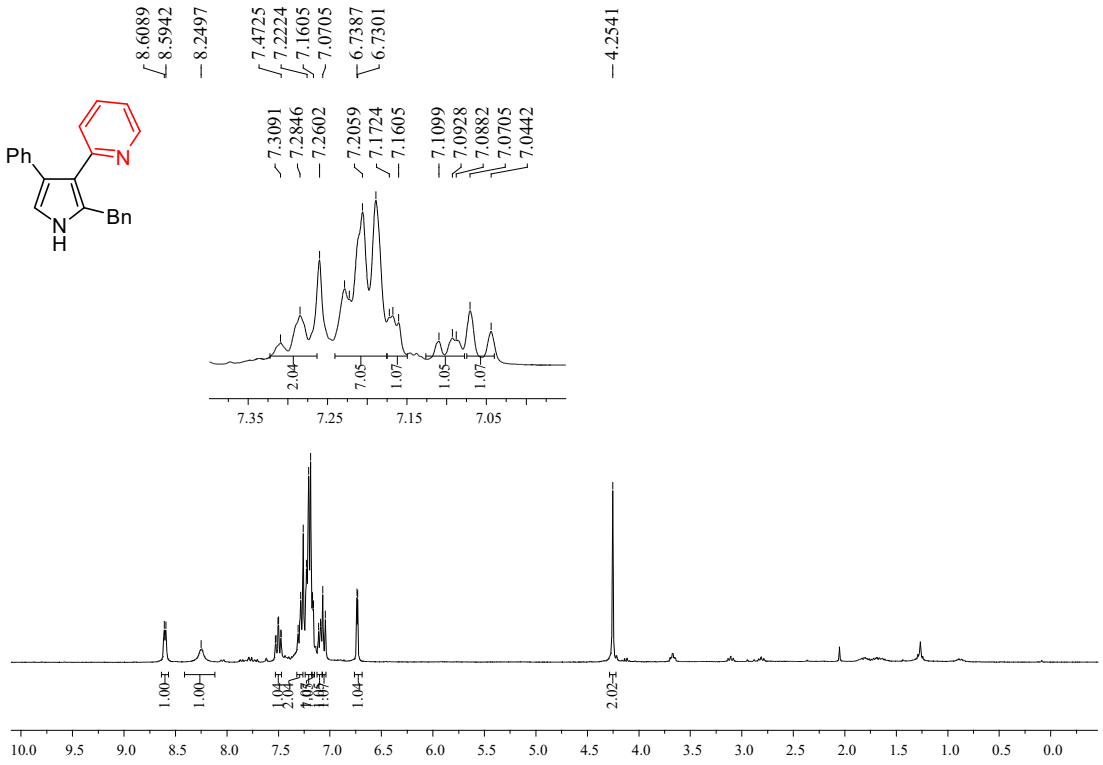
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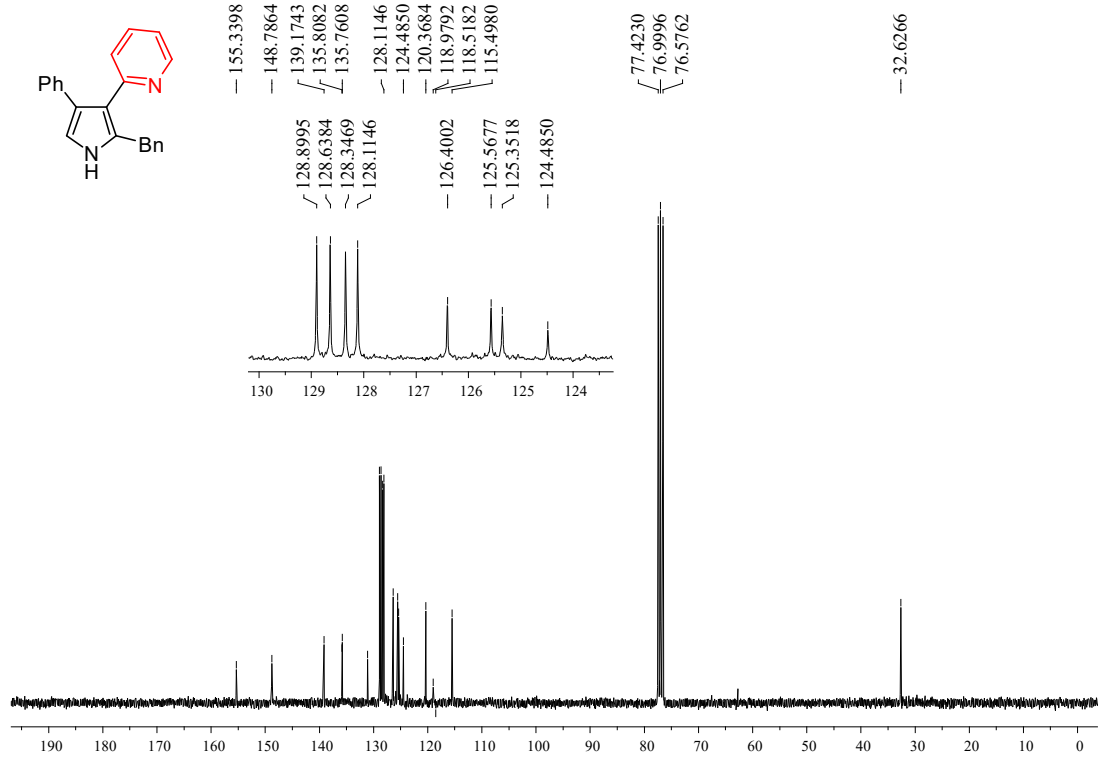
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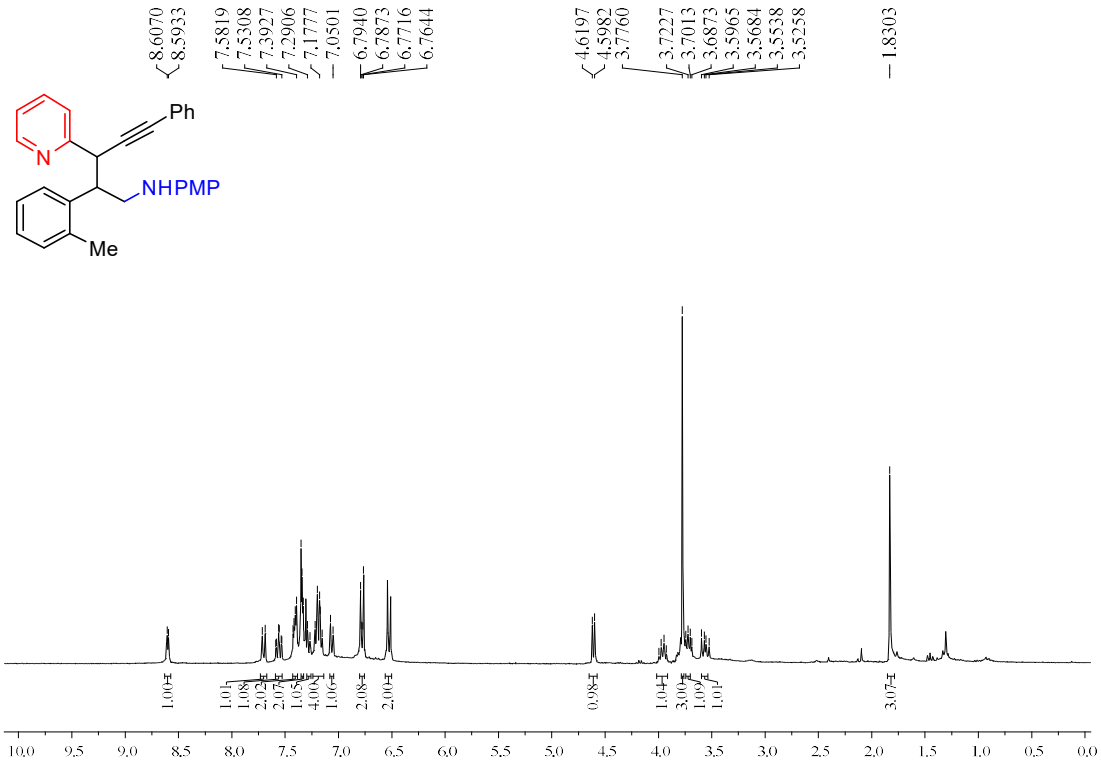
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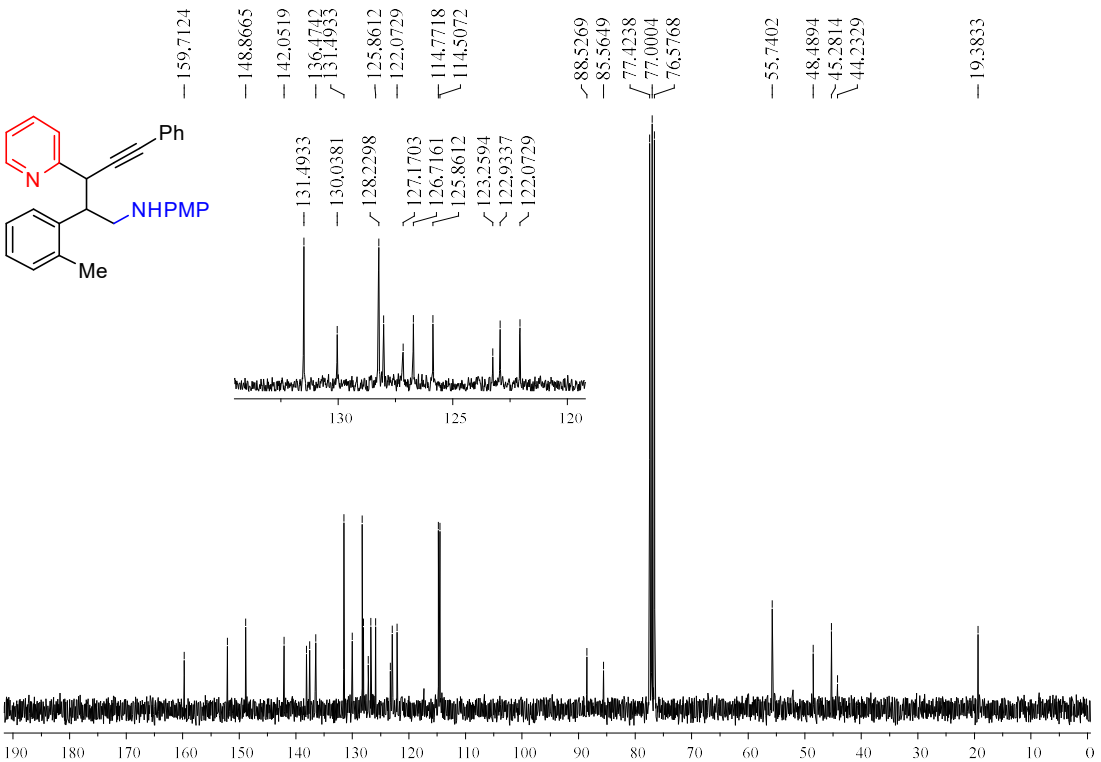
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