Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Regioselective Intramolecular sp^2 C-H Amination: Direct *vs.* Mediated Electrooxidation

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Supporting Information

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1. General Information

^{1}H NMR and ^{13}C NMR were recorded on a Bruker 400 MHz spectrometer (^{1}H NMR: 400MHz, ^{13}C NMR: 100MHz). The chemical shifts (δ) and coupling constants (*J*) were expressed in ppm and Hz respectively. ^{1}H NMR spectra were referenced to the solvent residual peak (TMS, δ 0 ppm) and ^{13}C{1H} NMR spectra were referenced to the solvent residual peak ($CDCl_3$, δ 77.0 ppm). High Resolution mass spectra were obtained using Thermo Scientific LTQ Orbitrap XL mass spectrometer. All solvents were purified and dried according to the standard procedures unless otherwise noted. Commercially substrates were purchased and used directly. Substrates **1a-1al**[1] were prepared according to the literature procedures.

2. General procedures for C-H amination

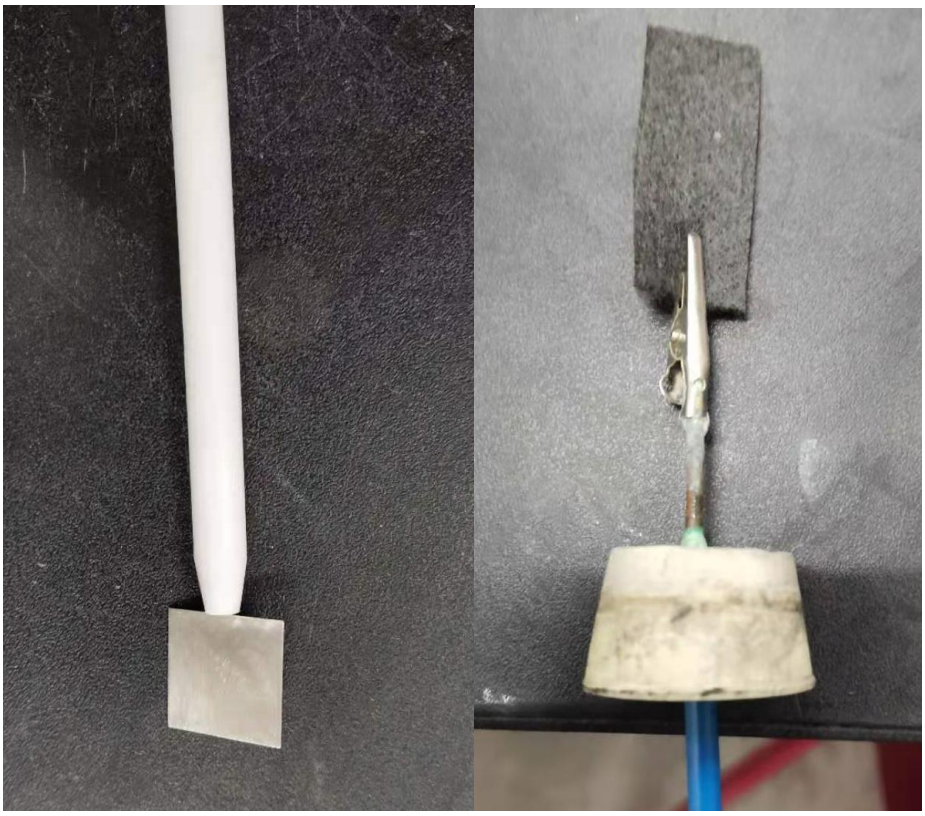
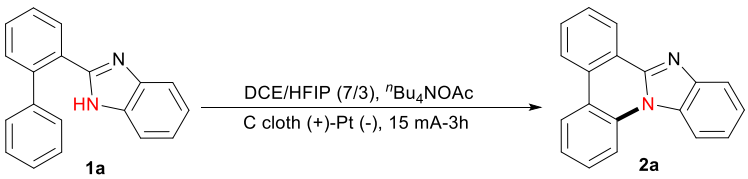


Figure S1. Electrodes (carbon cloth: width 1.5 cm, immergence depth 1.5 cm; platinum plate: width 1.5 cm)

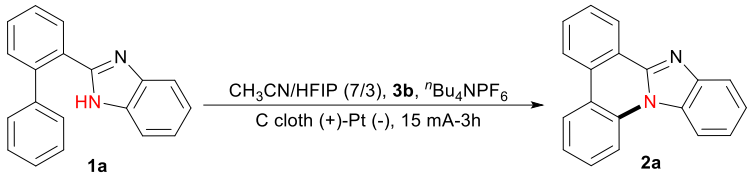
Procedure for direct oxidative C-H amination (Condition A, 1a as an example)



An undivided cell was equipped with a magnet stirrer, carbon cloth (1.5*1.5 cm^2), platinum plate (1.5 *1.5 cm^2), as the working electrode and counter electrode. The substrate 2-([1,1'-

biphenyl]-2-yl)-1H-benzo[d]imidazole **1a** (135 mg, 0.5 mmol), and $^{n}Bu_4NOAc$ (301 mg, 1 mmol) were added to the solvent DCE/HFIP (7/3 mL). The resulting mixture was allowed to stir and electrolyze at constant current conditions (15 mA, *J* = 6.7 mA·cm^{-2}) at room temperature for 3 hours. Then the volatile solvent was removed with a rotary evaporator. The residue was purified by column chromatography (PE/ EA= 10/1-6/1) on silica gel to afford the desired product **2a** (123 mg) in 92% yield.

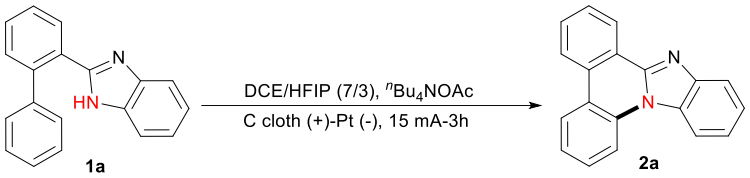
Procedure for indirect oxidative C-H amination (Condition B, 1a as an example)



An undivided cell was equipped with a magnet stirrer, carbon cloth (1.5*1.5 cm^2), platinum plate (1.5 *1.5 cm^2), as the working electrode and counter electrode. The substrate 2-([1,1'-biphenyl]-2-yl)-1H-benzo[d]imidazole **1a** (135 mg, 0.5 mmol), tris(4-bromophenyl)amine **3b** (24 mg, 0.05 mmol), and $^{n}Bu_4NPF_6$ (387 mg, 1 mmol) were added to the solvent CH_3CN/HFIP (7/3 mL). The resulting mixture was allowed to stir and electrolyze at constant current conditions (15 mA, *J* = 6.7 mA·cm^{-2}) at room temperature for 3 hours. Then the volatile solvent was removed with a rotary evaporator. The residue was purified by column chromatography (PE/ EA= 10/1-6/1) on silica gel to afford the desired product **2a** (118 mg) in 88% yield.

3. Procedure for gram scale reaction

Figure S2. Gram-scale electrolysis setup (carbon cloth: width 2.5 cm, immergence depth 3 cm; platinum gauze electrode: width 2.5 cm, immergence depth 3 cm)



An undivided cell was equipped with a magnet stirrer, carbon cloth (2.5*3 cm^2), platinum gauze plate (2.5 *3 cm^2), as the working electrode and counter electrode (the electrolysis setup is shown in Fig. S2). The substrate 2-([1,1'-biphenyl]-2-yl)-1H-benzo[d]imidazole **1a** (1.08 g, 4 mmol), and $^nBu_4NOAc$ (602 mg, 2 mmol) were added to the solvent DCE/HFIP (14/6 mL). The resulting mixture was allowed to stir and electrolyze at constant current conditions (90 mA, J = 12 mA·cm^{-2}) at room temperature for 4 hours. Then the volatile solvent was removed with a rotary evaporator. The residue was purified by column chromatography (PE/ EA= 10/1-6/1) on silica gel to afford the desired product **2a** (954 mg) in 89% yield.

4. Cyclic voltammetric experiments

The electrochemical analysis was demonstrated with Ag wire as a reference electrode, which is not a stable reference electrode. CVs can be calibrated using ferrocene as an external reference. (Figure S3) E_0(Fc/Fc*) = (1.06-0.058)/2 = 0.53 V.

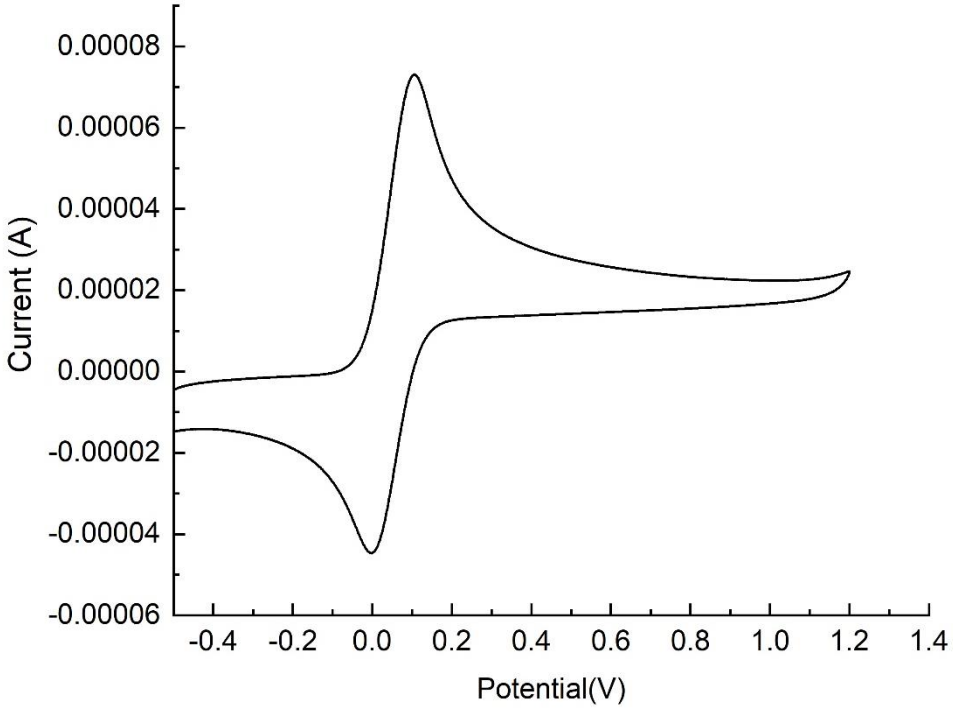


Figure S3. Cyclic voltammograms of ferrocene (5*10^{-3} M) in 0.1 M $LiClO_4/CH_3CN$, using Pt wire working electrode, glassy carbon, and $Ag/AgNO_3$ (0.1 M in CH3CN) as counter and reference electrodes at 100 mV/s scan rate.

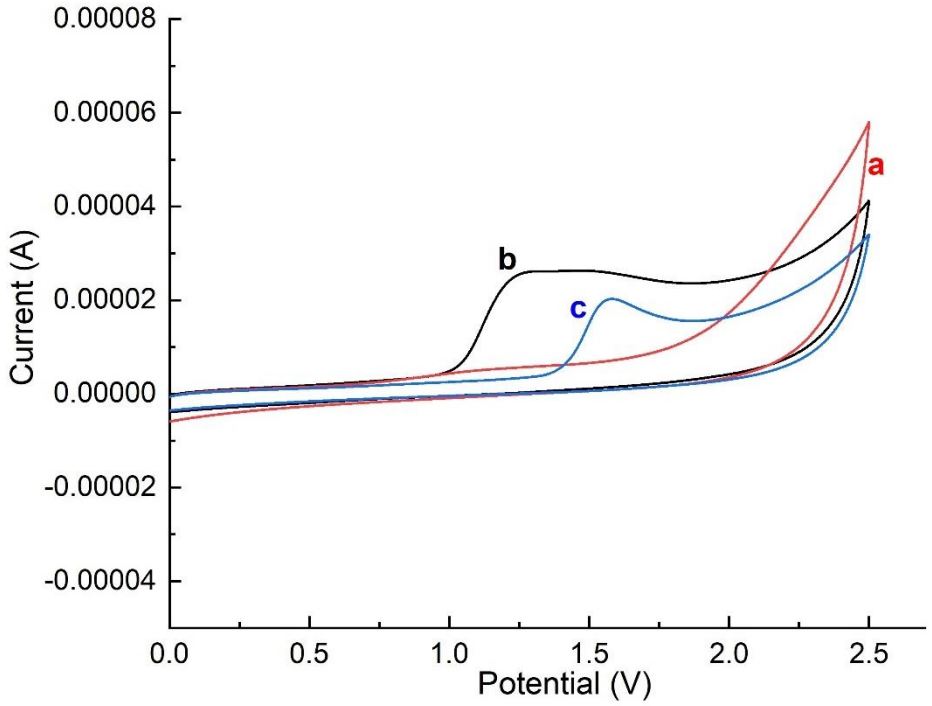


Figure S4. Cyclic voltammograms of substrates and catalyst in 0.1 M $LiClO_4$ (CH_3CN), using Pt wire working electrode, glassy carbon, and $Ag/AgNO_3$ (0.1 M in CH_3CN) as counter and reference electrodes at a 100 $mV{\cdot}s^{-1}$ scan rate: (a) backgroud; (b) 2-phenylbenzimidazole ($5*10^{-3}$ M); (b) biphenyl ($5*10^{-3}$ M).

As shown above, 2-phenylbenzimidazole (with anodic peak at 1.27 V) is more easily oxidized than biphenyl (with anodic peak at 1.57 V), and the anodic peak of 2-phenylbenzimidazole is close to that of substrate **1a** (with anodic peak at 1.14 V). In other word, benzimidazole moiety in the substrate **1a** is more likely to proceed anodic oxidation to afford nitrogen-centered radical.

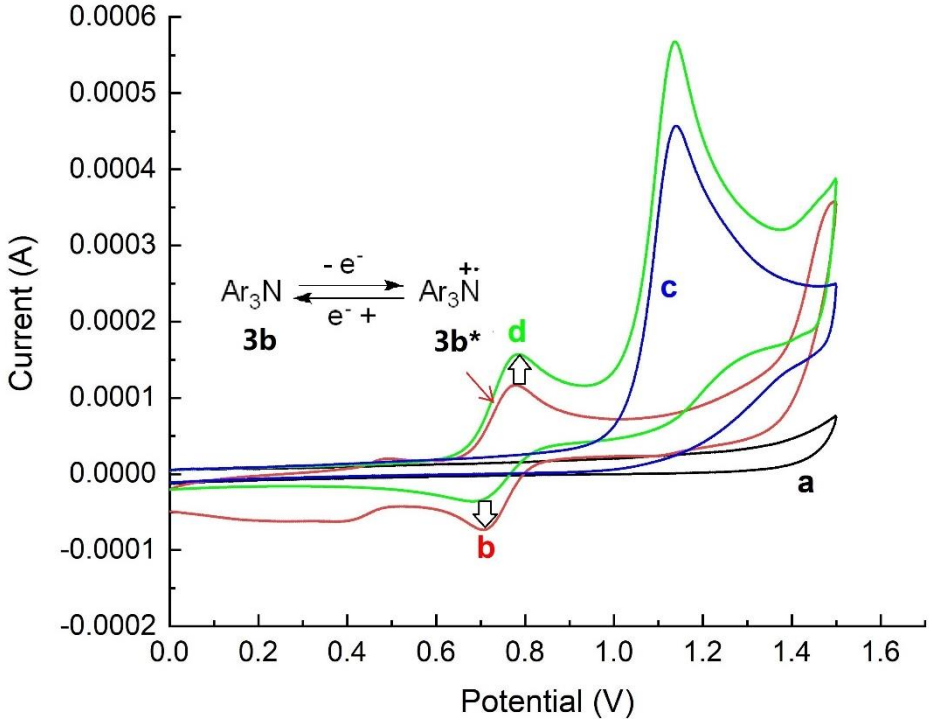
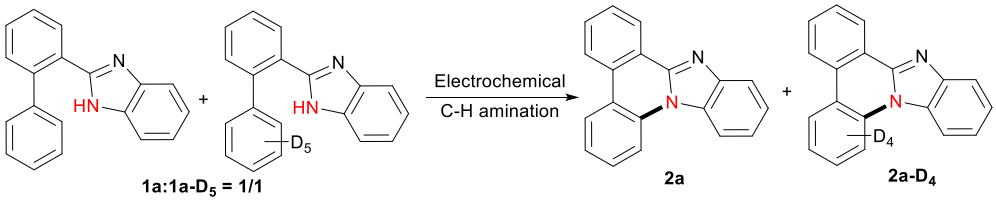


Figure S5. Cyclic voltammograms of substrates and catalyst in 0.1 M $LiClO_4$ (CH_3CN), using Pt wire working electrode, glassy carbon, and $Ag/AgNO_3$ (0.1 M in CH_3CN) as counter and reference electrodes at a 100 $mV{\cdot}s^{-1}$ scan rate: (a) backgroud; (b) **3b** ($1*10^{-3}$ M); (c) **1a** ($5*10^{-3}$ M); (d) **3b** ($1*10^{-3}$ M) + **1a** ($5*10^{-3}$ M).

As shown above, A couple of reversible redox peaks are shown on the spectrum of **3b** (curve b, Figure S5), and the anodic peak is assigned to the oxidation of **3b** to the corresponding cation raidcal species (**3b***). Treating **3b** with 5 equivalents substrate **1a** led to an obvious increase of anodic peak of **3b** and decrease of its cathodic peak (curve d, Figure S5). The increase of anodic peak of **3b** associates with the regeneration of **3b**, which suggests that **3b** serves as a catalyst during the reaction. The decrease of the cathodic peak is attributed to the single electron transfer between substrate **1a** and the cation raidcal **3b*.**

5. Procedure for control experiments

Procedure for KIE study



The mixture **1a** and **1a-D_5** (1/1, 136 mg) were used to replace substrate **1a** under Condition A and Condition B with a shorter reaction time (40 min). The desired products were determined by ^1H NMR (**Figure S5 and Figure S6**).

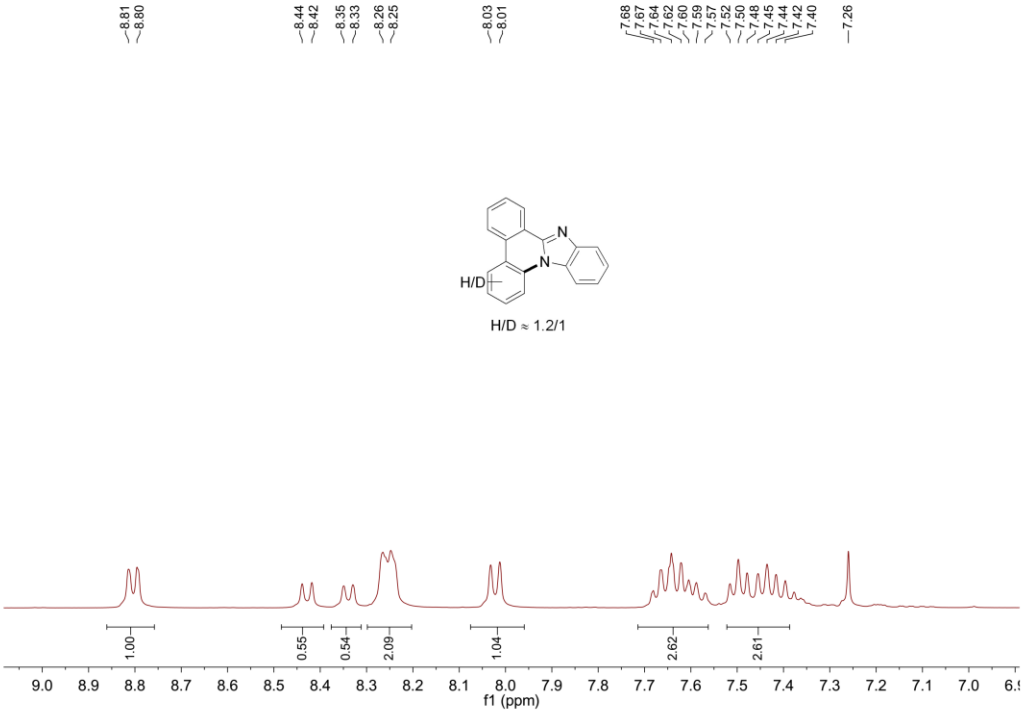


Figure S5. The ^1H NMR spectrum of mixed product under Condition A.

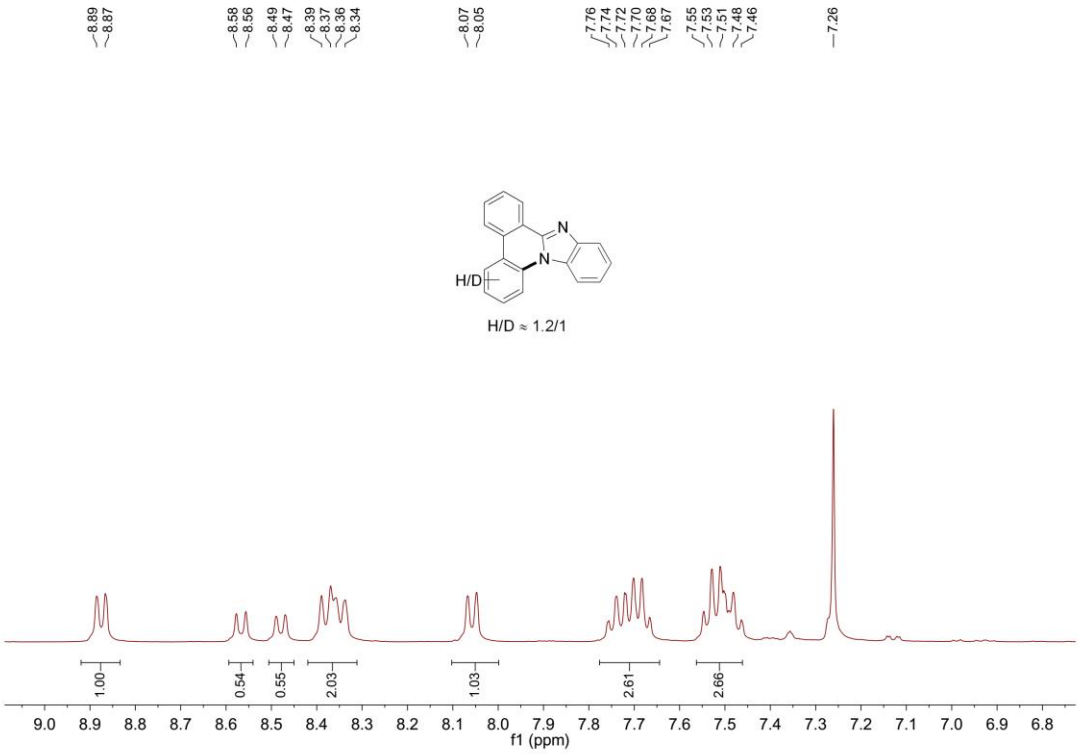
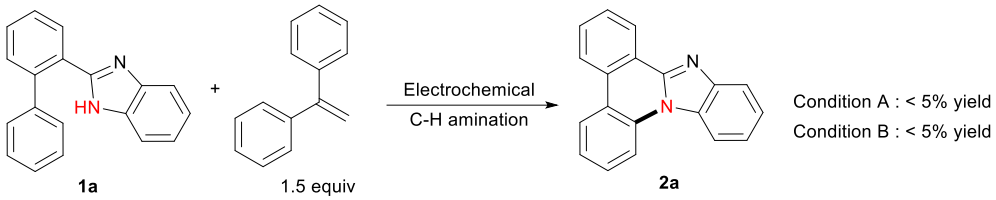


Figure S5. The ^{1}H NMR spectrum of mixed product under Condition B.

Procedure for radical trapping experiments



1,1-Diphenylethylene (1.5 mmol, 270 mg) was introduced to the reaction under Condition A and Condition B. The corresponding products were obtained with 5.2 mg (Condition A) and 5.7 mg (Condition B).

6. Crystal structure of 2z

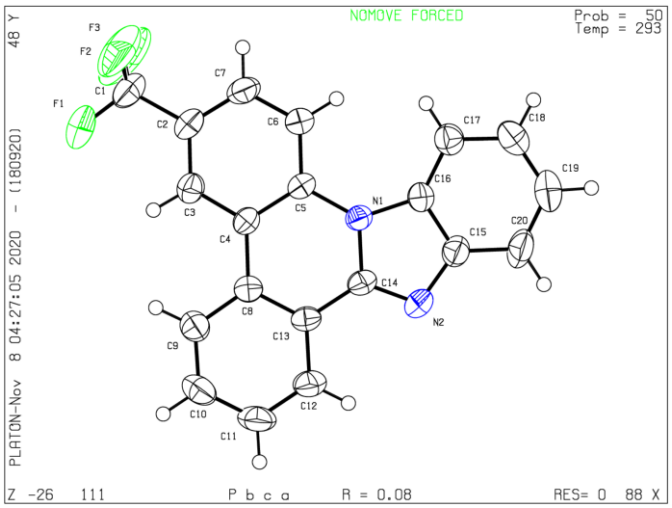


Table S1. Crystal data and structure refinement for 2z.

Identification code	2z
Empirical formula	$C_{20}H_{11}F_3N_2$
Formula weight	336.31
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 9.2360(8) A alpha = 90 deg.
	b = 17.7645(14) A beta = 90 deg.
	c = 18.4265(15) A gamma = 90 deg.
Volume	3023.3(4) A^3
Z, Calculated density	8, 1.478 Mg/m^3
Absorption coefficient	0.114 mm^-1
F(000)	1376
Crystal size	0.25 x 0.21 x 0.14 mm
Theta range for data collection	3.123 to 27.666 deg.
Limiting indices	-12<=h<=11, -23<=k<=22, -23<=l<=24
Reflections collected / unique	45226 / 3506 [R(int) = 0.1677]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6946
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3506 / 0 / 226
Goodness-of-fit on F^2	1.014
Final R indices [I>2sigma(I)]	R_1 = 0.0795, wR_2 = 0.1475
R indices (all data)	R1 = 0.1866, wR2 = 0.1867
Extinction coefficient	n/a
Largest diff. peak and hole	0.260 and -0.309 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2z. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	2900(4)	5597(2)	4824(1)	143(1)
F(3)	3141(4)	6643(2)	5312(1)	136(1)
N(1)	6324(2)	7340(1)	2393(1)	33(1)
F(2)	4763(3)	5856(2)	5414(1)	116(1)
N(2)	6394(3)	7531(2)	1182(1)	48(1)
C(16)	7297(3)	7936(2)	2274(2)	35(1)
C(14)	5844(3)	7125(2)	1705(2)	36(1)
C(8)	4274(3)	6167(2)	2250(1)	34(1)
C(5)	5739(3)	7023(2)	3031(1)	33(1)
C(13)	4847(3)	6510(2)	1629(1)	36(1)
C(4)	4707(3)	6444(2)	2964(1)	33(1)
C(3)	4119(3)	6159(2)	3603(2)	41(1)
C(6)	6139(3)	7291(2)	3711(2)	43(1)
C(7)	5536(4)	6994(2)	4330(2)	49(1)
C(15)	7289(3)	8038(2)	1525(2)	44(1)
C(9)	3286(3)	5574(2)	2150(2)	45(1)
C(17)	8180(3)	8366(2)	2722(2)	45(1)
C(2)	4525(3)	6427(2)	4276(2)	44(1)
C(12)	4455(4)	6260(2)	938(2)	51(1)
C(11)	3495(4)	5682(2)	858(2)	58(1)
C(10)	2899(4)	5342(2)	1467(2)	53(1)
C(18)	9015(4)	8912(2)	2392(2)	55(1)
C(20)	8130(4)	8599(2)	1205(2)	63(1)
C(1)	3839(5)	6128(2)	4944(2)	65(1)
C(19)	8983(4)	9035(2)	1652(2)	66(1)

Table S3. Bond lengths [A] and angles [deg] for 2z.

F(1)-C(1)	1.301(4)
F(3)-C(1)	1.308(4)
N(1)-C(16)	1.406(3)
N(1)-C(14)	1.396(3)
N(1)-C(5)	1.411(3)
F(2)-C(1)	1.309(4)
N(2)-C(14)	1.306(4)
N(2)-C(15)	1.376(4)
C(16)-C(15)	1.393(4)
C(16)-C(17)	1.388(4)
C(14)-C(13)	1.435(4)
C(8)-C(13)	1.401(4)
C(8)-C(4)	1.462(4)
C(8)-C(9)	1.405(4)
C(5)-C(4)	1.407(4)
C(5)-C(6)	1.392(4)
C(13)-C(12)	1.396(4)
C(4)-C(3)	1.391(4)
C(3)-H(3)	0.9300
C(3)-C(2)	1.380(4)
C(6)-H(6)	0.9300
C(6)-C(7)	1.374(4)
C(7)-H(7)	0.9300
C(7)-C(2)	1.376(4)
C(15)-C(20)	1.394(4)
C(9)-H(9)	0.9300
C(9)-C(10)	1.372(4)
C(17)-H(17)	0.9300
C(17)-C(18)	1.380(4)
C(2)-C(1)	1.484(4)
C(12)-H(12)	0.9300
C(12)-C(11)	1.365(4)
C(11)-H(11)	0.9300
C(11)-C(10)	1.387(5)
C(10)-H(10)	0.9300
C(18)-H(18)	0.9300
C(18)-C(19)	1.382(5)
C(20)-H(20)	0.9300
C(20)-C(19)	1.378(5)
C(19)-H(19)	0.9300
C(16)-N(1)-C(5)	132.4(2)
C(14)-N(1)-C(16)	105.5(2)

C(14)-N(1)-C(5)	121.7(2)
C(14)-N(2)-C(15)	104.8(2)
C(15)-C(16)-N(1)	104.4(2)
C(17)-C(16)-N(1)	134.3(3)
C(17)-C(16)-C(15)	121.3(3)
N(1)-C(14)-C(13)	120.0(2)
N(2)-C(14)-N(1)	113.3(3)
N(2)-C(14)-C(13)	126.7(3)
C(13)-C(8)-C(4)	119.1(3)
C(13)-C(8)-C(9)	117.7(3)
C(9)-C(8)-C(4)	123.2(3)
C(4)-C(5)-N(1)	118.6(2)
C(6)-C(5)-N(1)	120.8(3)
C(6)-C(5)-C(4)	120.5(3)
C(8)-C(13)-C(14)	119.6(2)
C(12)-C(13)-C(14)	119.9(3)
C(12)-C(13)-C(8)	120.5(3)
C(5)-C(4)-C(8)	120.6(2)
C(3)-C(4)-C(8)	122.2(3)
C(3)-C(4)-C(5)	117.2(3)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-C(4)	121.9(3)
C(2)-C(3)-H(3)	119.1
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-C(5)	120.6(3)
C(7)-C(6)-H(6)	119.7
C(6)-C(7)-H(7)	120.1
C(6)-C(7)-C(2)	119.8(3)
C(2)-C(7)-H(7)	120.1
N(2)-C(15)-C(16)	111.9(2)
N(2)-C(15)-C(20)	127.5(3)
C(16)-C(15)-C(20)	120.6(3)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-C(8)	120.9(3)
C(10)-C(9)-H(9)	119.5
C(16)-C(17)-H(17)	121.5
C(18)-C(17)-C(16)	117.0(3)
C(18)-C(17)-H(17)	121.5
C(3)-C(2)-C(1)	120.4(3)
C(7)-C(2)-C(3)	120.1(3)
C(7)-C(2)-C(1)	119.5(3)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-C(13)	120.4(3)
C(11)-C(12)-H(12)	119.8

C(12)-C(11)-H(11)	120.1
C(12)-C(11)-C(10)	119.8(3)
C(10)-C(11)-H(11)	120.1
C(9)-C(10)-C(11)	120.5(3)
C(9)-C(10)-H(10)	119.7
C(11)-C(10)-H(10)	119.7
C(17)-C(18)-H(18)	118.9
C(17)-C(18)-C(19)	122.2(3)
C(19)-C(18)-H(18)	118.9
C(15)-C(20)-H(20)	121.0
C(19)-C(20)-C(15)	117.9(3)
C(19)-C(20)-H(20)	121.0
F(1)-C(1)-F(3)	105.5(4)
F(1)-C(1)-F(2)	106.3(3)
F(1)-C(1)-C(2)	113.8(3)
F(3)-C(1)-F(2)	103.6(3)
F(3)-C(1)-C(2)	113.0(3)
F(2)-C(1)-C(2)	113.8(3)
C(18)-C(19)-H(19)	119.6
C(20)-C(19)-C(18)	120.9(3)
C(20)-C(19)-H(19)	119.6

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 2z. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
F(1)	178(3)	190(3)	62(2)	16(2)	30(2)	-116(3)
F(3)	187(3)	144(2)	78(2)	17(2)	86(2)	57(2)
N(1)	33(1)	38(1)	29(1)	0(1)	-1(1)	0(1)
F(2)	120(2)	161(3)	67(2)	65(2)	6(2)	7(2)
N(2)	57(2)	56(2)	31(1)	8(1)	0(1)	-9(2)
C(16)	30(2)	35(2)	40(2)	1(1)	2(1)	2(1)
C(14)	38(2)	43(2)	29(2)	1(1)	-3(1)	3(2)
C(8)	32(2)	35(2)	34(2)	0(1)	-3(1)	5(1)
C(5)	34(2)	37(2)	28(2)	1(1)	1(1)	5(1)
C(13)	38(2)	39(2)	30(2)	-1(1)	-6(1)	4(2)
C(4)	31(2)	35(2)	32(2)	1(1)	4(1)	5(1)
C(3)	39(2)	43(2)	40(2)	2(1)	6(1)	0(2)
C(6)	50(2)	47(2)	33(2)	-1(2)	-2(2)	-7(2)
C(7)	61(2)	55(2)	30(2)	-3(2)	1(2)	1(2)
C(15)	44(2)	46(2)	41(2)	8(2)	2(2)	-3(2)
C(9)	45(2)	42(2)	48(2)	1(2)	-3(2)	-4(2)
C(17)	43(2)	44(2)	48(2)	-1(2)	3(2)	-2(2)
C(2)	49(2)	49(2)	33(2)	5(2)	8(2)	4(2)
C(12)	64(2)	54(2)	35(2)	1(2)	-11(2)	-6(2)
C(11)	73(3)	57(2)	43(2)	-7(2)	-23(2)	-5(2)
C(10)	58(2)	42(2)	60(2)	-6(2)	-15(2)	-8(2)
C(18)	48(2)	48(2)	68(3)	-7(2)	0(2)	-10(2)
C(20)	70(3)	64(2)	54(2)	24(2)	9(2)	-14(2)
C(1)	81(3)	75(3)	39(2)	7(2)	15(2)	-7(2)
C(19)	59(2)	61(2)	79(3)	12(2)	11(2)	-19(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2z.

	x	y	z	U(eq)
H(3)	3432	5777	3576	49
H(6)	6820	7675	3748	52
H(7)	5810	7174	4783	58
H(9)	2889	5336	2553	54
H(17)	8208	8289	3221	54
H(12)	4850	6489	529	61
H(11)	3241	5516	397	69
H(10)	2232	4954	1411	64
H(18)	9619	9208	2679	66
H(20)	8115	8677	706	76
H(19)	9545	9417	1453	80

Table S6. Torsion angles [deg] for 2z.

N(1)-C(16)-C(15)-N(2)	-1.3(3)
N(1)-C(16)-C(15)-C(20)	179.1(3)
N(1)-C(16)-C(17)-C(18)	179.5(3)
N(1)-C(14)-C(13)-C(8)	4.9(4)
N(1)-C(14)-C(13)-C(12)	-175.2(3)
N(1)-C(5)-C(4)-C(8)	1.3(4)
N(1)-C(5)-C(4)-C(3)	-178.1(2)
N(1)-C(5)-C(6)-C(7)	178.2(3)
N(2)-C(14)-C(13)-C(8)	-175.3(3)
N(2)-C(14)-C(13)-C(12)	4.6(5)
N(2)-C(15)-C(20)-C(19)	-178.3(3)
C(16)-N(1)-C(14)-N(2)	-1.2(3)
C(16)-N(1)-C(14)-C(13)	178.6(2)
C(16)-N(1)-C(5)-C(4)	176.5(3)
C(16)-N(1)-C(5)-C(6)	-1.6(4)
C(16)-C(15)-C(20)-C(19)	1.2(5)
C(16)-C(17)-C(18)-C(19)	0.2(5)
C(14)-N(1)-C(16)-C(15)	1.4(3)
C(14)-N(1)-C(16)-C(17)	-176.5(3)
C(14)-N(1)-C(5)-C(4)	3.8(4)
C(14)-N(1)-C(5)-C(6)	-174.3(3)
C(14)-N(2)-C(15)-C(16)	0.6(4)
C(14)-N(2)-C(15)-C(20)	-179.9(3)
C(14)-C(13)-C(12)-C(11)	-179.2(3)
C(8)-C(13)-C(12)-C(11)	0.7(5)
C(8)-C(4)-C(3)-C(2)	-179.6(3)
C(8)-C(9)-C(10)-C(11)	1.0(5)
C(5)-N(1)-C(16)-C(15)	-172.2(3)
C(5)-N(1)-C(16)-C(17)	9.9(5)
C(5)-N(1)-C(14)-N(2)	173.2(2)
C(5)-N(1)-C(14)-C(13)	-7.0(4)
C(5)-C(4)-C(3)-C(2)	-0.2(4)
C(5)-C(6)-C(7)-C(2)	-0.2(5)
C(13)-C(8)-C(4)-C(5)	-3.2(4)
C(13)-C(8)-C(4)-C(3)	176.2(3)
C(13)-C(8)-C(9)-C(10)	0.0(4)
C(13)-C(12)-C(11)-C(10)	0.3(5)
C(4)-C(8)-C(13)-C(14)	0.0(4)
C(4)-C(8)-C(13)-C(12)	-179.9(3)
C(4)-C(8)-C(9)-C(10)	179.0(3)
C(4)-C(5)-C(6)-C(7)	0.2(4)

C(4)-C(3)-C(2)-C(7)	0.2(5)
C(4)-C(3)-C(2)-C(1)	177.9(3)
C(3)-C(2)-C(1)-F(1)	2.1(5)
C(3)-C(2)-C(1)-F(3)	-118.2(4)
C(3)-C(2)-C(1)-F(2)	124.0(4)
C(6)-C(5)-C(4)-C(8)	179.4(3)
C(6)-C(5)-C(4)-C(3)	0.0(4)
C(6)-C(7)-C(2)-C(3)	0.0(5)
C(6)-C(7)-C(2)-C(1)	-177.8(3)
C(7)-C(2)-C(1)-F(1)	179.8(4)
C(7)-C(2)-C(1)-F(3)	59.5(5)
C(7)-C(2)-C(1)-F(2)	-58.3(5)
C(15)-N(2)-C(14)-N(1)	0.4(3)
C(15)-N(2)-C(14)-C(13)	-179.4(3)
C(15)-C(16)-C(17)-C(18)	1.8(4)
C(15)-C(20)-C(19)-C(18)	0.8(6)
C(9)-C(8)-C(13)-C(14)	179.1(3)
C(9)-C(8)-C(13)-C(12)	-0.8(4)
C(9)-C(8)-C(4)-C(5)	177.8(3)
C(9)-C(8)-C(4)-C(3)	-2.8(4)
C(17)-C(16)-C(15)-N(2)	177.0(3)
C(17)-C(16)-C(15)-C(20)	-2.6(5)
C(17)-C(18)-C(19)-C(20)	-1.5(6)
C(12)-C(11)-C(10)-C(9)	-1.1(5)

Symmetry transformations used to generate equivalent atoms:

Table S7. Hydrogen bonds for 2z [A and deg.].

D-H...A				D-H)	d(H...A)	d(D...A)	<(DHA)
C(3)	--H(3)	..F(1)	[ ]	0.93	2.37	2.7067(2)	101
C(6)	--H(6)	..F(3)	[3455.01]	0.93	2.44	3.2010(3)	139
C(11)	--H(11)	..F(1)	[2655.01]	0.93	2.48	3.2325(3)	139

7. Photoluminescence spectra of 2m and 2n

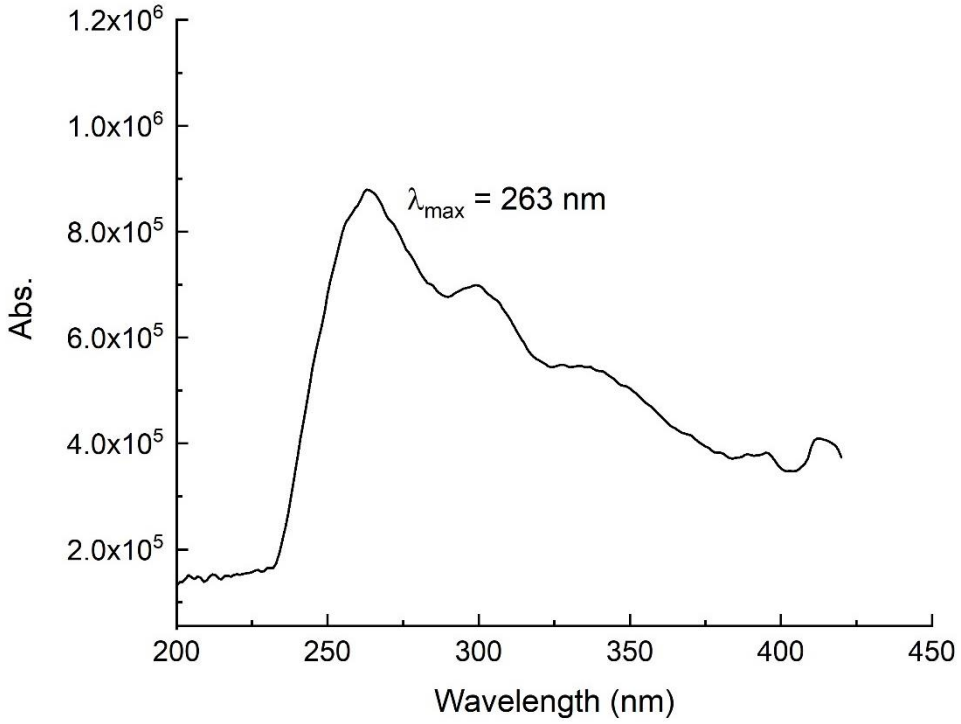


Figure S6. Photoluminescence absorption spectrum of **2m** in solid powders

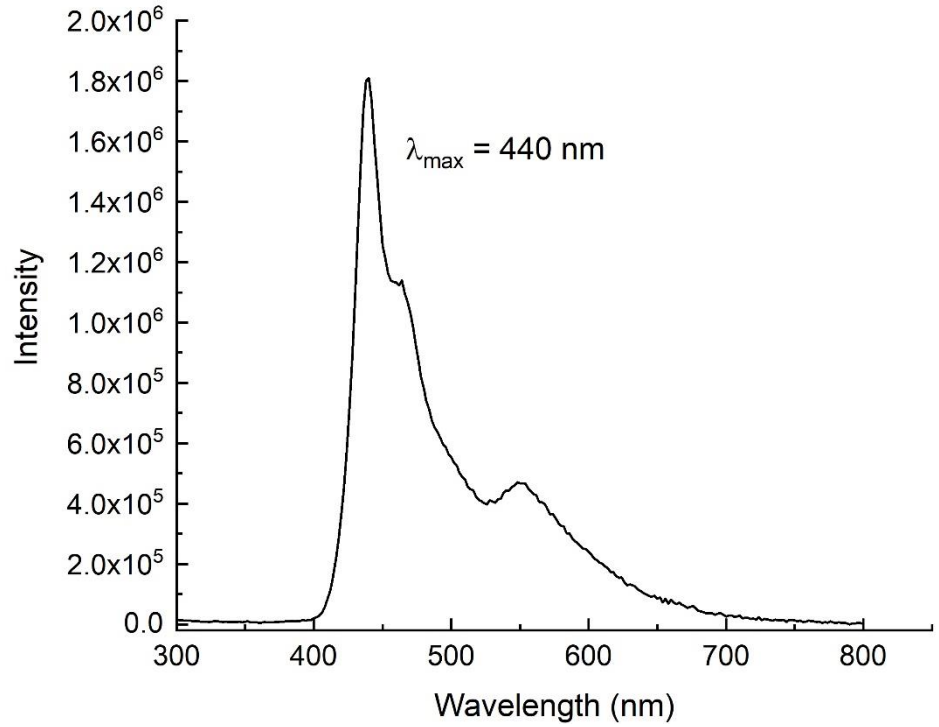


Figure S7. Photoluminescence emission spectrum of **2m** in solid powders upon excitation at 263 nm

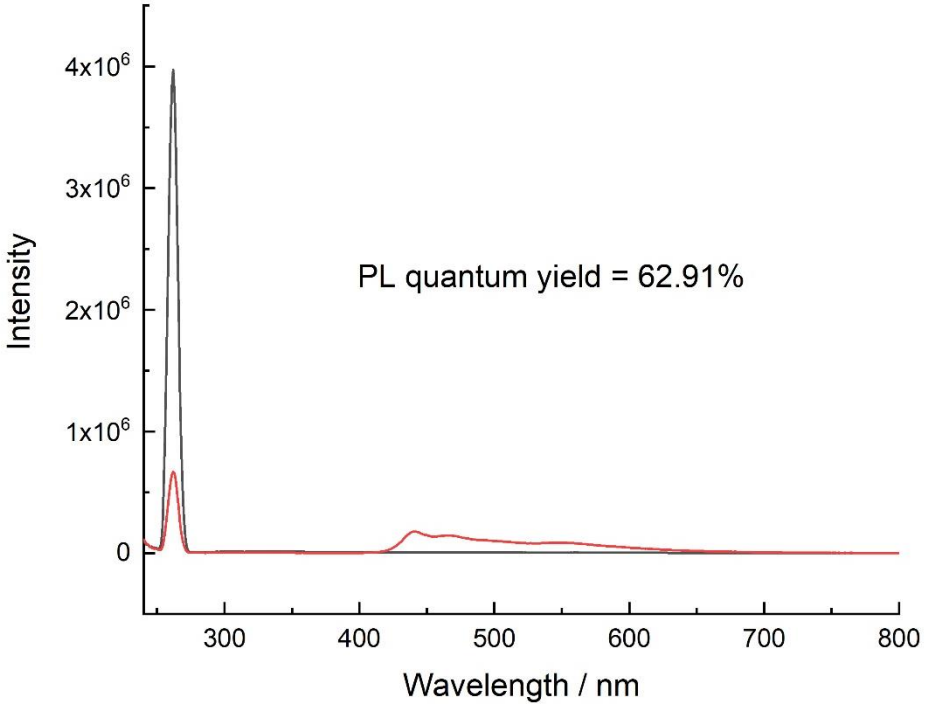


Figure S8. Photoluminescence quantum yield of **2m** in solid powders upon excitation at 263 nm.

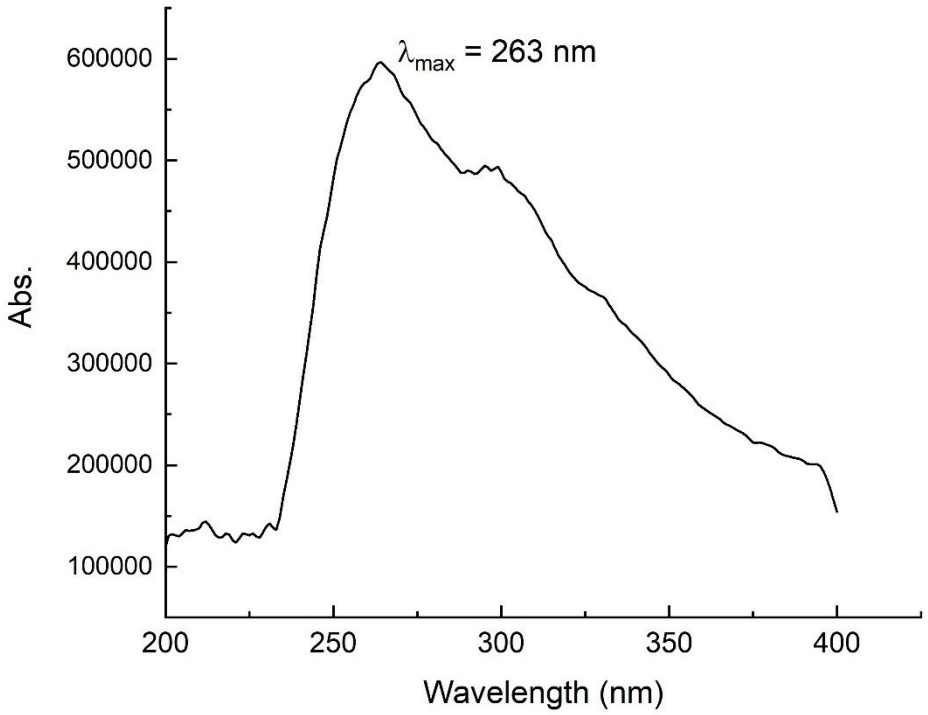


Figure S9. Photoluminescence absorption spectrum of **2n** in solid powders

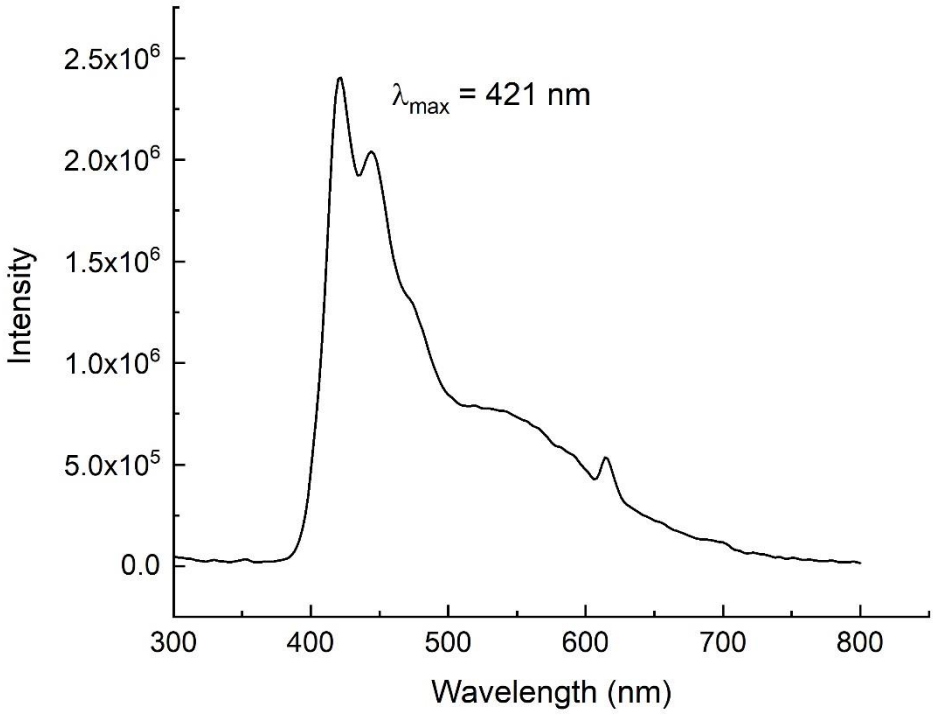


Figure S10. Photoluminescence emission spectrum of **2n** in solid powders upon excitation at 263 nm

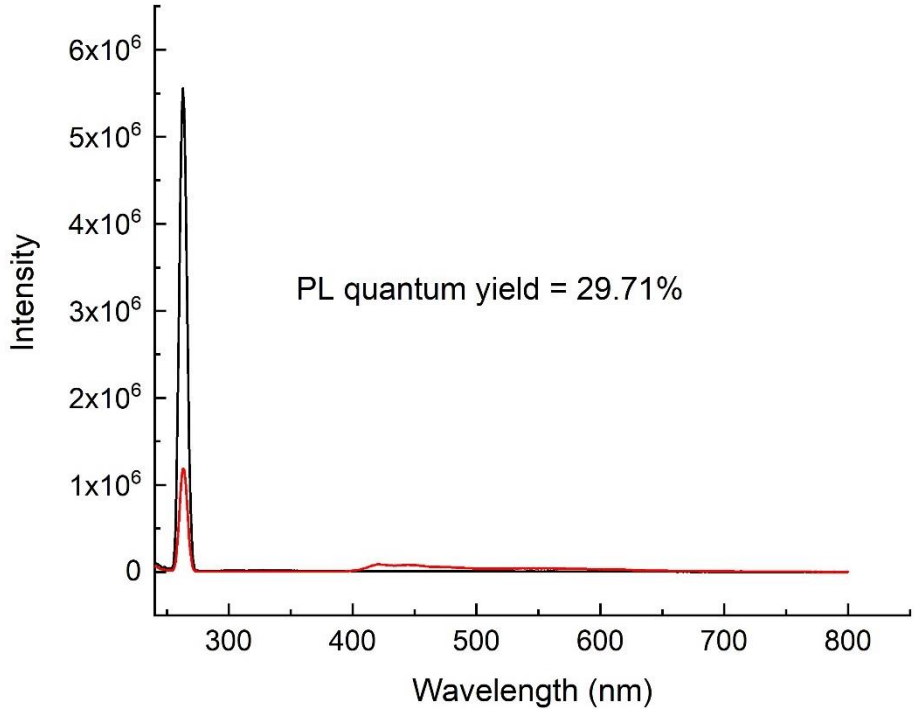
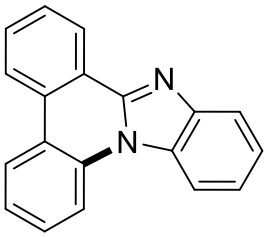
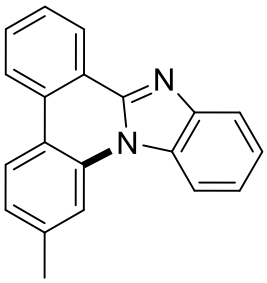


Figure S11. Photoluminescence quantum yield of **2n** in solid powders upon excitation at 263 nm.

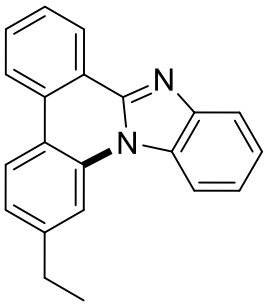
7. Experimental data for C-H amination products



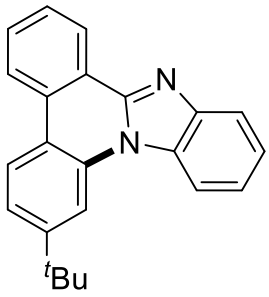
Benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2a**): Condition A: 123 mg, 92% yield; Condition B: 118 mg, 88% yield; white solid, m.p. 156-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.88 (d, *J* = 8 Hz, 1H), 8.57 (d, *J* = 8 Hz, 1H), 8.49 (d, *J* = 8 Hz, 1H), 8.37 (dd, *J* = 12 Hz, *J* = 8 Hz, 2H), 8.06 (d, *J* = 8 Hz, 1H), 7.72 (m, 3H), 7.50 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.4, 144.5, 134.3, 131.8, 130.3, 129.4, 129.0, 128.5, 126.0, 124.3, 124.09, 124.06, 123.4, 122.9, 122.2, 121.6, 120.3, 115.9, 113.9; These data are in accordance with the literature.[2]



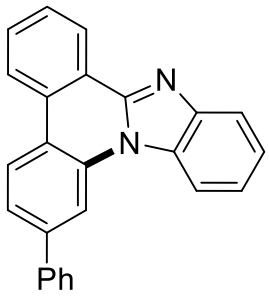
2-Methylbenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2b**): Condition A: 100 mg, 71% yield; Condition B: 130 mg, 92% yield; white solid, m.p. 187-189 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.81 (d, *J* = 8 Hz, 1H), 8.26 (m, 4H), 8.02 (d, *J* = 8 Hz, 1H), 7.64 (m, 2H), 7.48 (m, 2H), 7.22 (d, *J* = 8 Hz, 1H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.4, 144.0, 139.4, 134.0, 131.5, 130.3, 129.5, 127.9, 125.8, 125.4, 124.0, 123.7, 122.7, 122.4, 121.8, 119.8, 118.9, 115.9, 113.9, 21.7; These data are in accordance with the literature.[2]



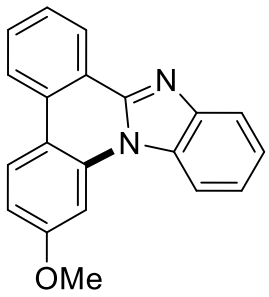
2-Ethylbenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2c**): Condition A: 95 mg, 64% yield; Condition B: 130 mg, 88% yield; white solid, m.p. 158-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.75 (d, *J* = 4Hz, 1H), 8.14 (m, 4H), 7.99 (d, *J* = 8 Hz, 1H), 7.56 (m, 2H), 7.46 (t, *J* = 8 Hz, 1H), 7.40 (t, *J* = 8 Hz, 1H), 7.13 (d, *J* = 8 Hz, 1H), 2.77 (q, *J* = 8 Hz, 2H), 1.33 (t, *J* = 8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.5, 145.6, 144.5, 134.3, 131.8, 130.1, 129.5, 127.9, 125.8, 124.1, 123.9, 122.9, 122.6, 121.8, 120.2, 119.1, 114.8, 113.8, 28.9, 15.3; These data are in accordance with the literature.[1]



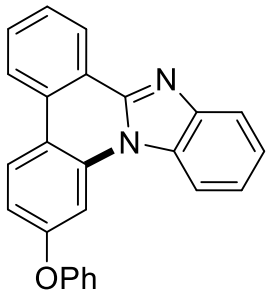
2-(*tert*-Butyl)benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2d**): Condition A: 112 mg, 69% yield; Condition B: 146 mg, 90% yield; white solid, m.p. 144-146 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.85 (d, *J* = 8.0 Hz, 1H), 8.60 (s, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.34 (t, *J* = 6.0 Hz, 2H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.71 (t, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.52 (m, 3H), 1.53 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): 152.9, 147.8, 144.6, 134.4, 131.8, 130.4, 129.6, 128.2, 126.0, 124.0, 123.9, 123.1, 122.9, 122.1, 122.1, 120.4, 119.2, 113.8, 112.9, 35.4, 31.4; HRMS (ESI): calcd for $C_{23}H_{21}N_2^+$ $(M+H)^+$ 325.1699, found 325.1700.



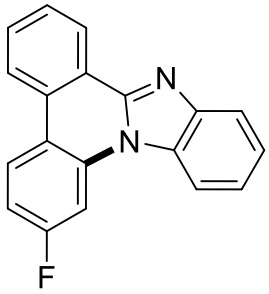
2-Phenylbenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2e**): Condition A: 124 mg, 72% yield; Condition B: 99 mg, 57% yield; white solid, m.p. 233-235 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.76 (d, *J* = 4.0 Hz, 1H), 8.55 (s, 1H), 8.28 (d, *J* = 8 Hz, 1H), 8.20 (t, *J* = 8 Hz, 2H), 7.99 (d, *J* = 8 Hz, 1H), 7.68 (d, *J* = 8 Hz, 2H), 7.56 (m, 5H), 7.44 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.4, 144.5, 141.8, 139.9, 134.6, 131.7, 130.2, 129.1, 128.3, 128.1, 127.2, 125.9, 124.4, 124.0, 123.2, 123.0, 122.8, 122.0, 120.4, 120.3, 114.1, 113.8; HRMS (ESI): calcd for $C_{25}H_{17}N_2^+$ $(M+H)^+$ 345.1386, found 345.1386.



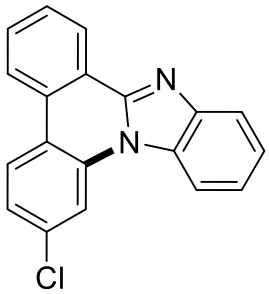
2-Methoxybenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2f**): Condition A: 111 mg, 75% yield; Condition B: 113 mg, 76% yield; white solid, m.p.147-149 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.82 (d, *J* = 8.0 Hz, 1H), 8.32 (t, *J* = 8.0 Hz, 1H), 8.26 (m, 2H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.98 (s, 1H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.60 (t, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 6.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.03 (d, *J* = 8.0 Hz, 1H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 160.2, 147.8, 144.5, 135.3, 131.6, 130.3, 129.6, 127.4, 125.9, 125.2, 124.0, 122.7, 122.1, 121.5, 120.2, 114.8, 113.6, 110.6, 101.1, 55.6; These data are in accordance with the literature.[2]



2-Phenoxybenzo[4,5]imidazo[1,2-f]phenanthridine (**2g**): Condition A: 107 mg, 59% yield; Condition B: 124 mg, 69% yield; white solid, m.p. 238-240 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.85 (d, *J* = 8.0 Hz, 1H), 8.40 (d, *J* = 8.0 Hz, 1H), 8.29 (d, *J* = 8.0 Hz, 1H), 8.15 (s, 1H), 8.03 (q, *J* = 4.0 Hz, 2H), 7.72 (t, *J* = 6.0 Hz, 1H), 7.64 (t, *J* = 8.0 Hz, 1H), 7.49 (m, 3H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 158.7, 156.1, 147.8, 144.6, 135.5, 131.7, 130.5, 130.2, 129.5, 128.0, 126.1, 125.7, 124.5, 124.2, 122.9, 122.7, 121.9, 120.4, 119.9, 116.8, 114.5, 113.6, 105.4; HRMS (ESI): calcd for $C_{25}H_{17}N_2O^+$ $(M+H)^+$ 361.1335, found 361.1335.

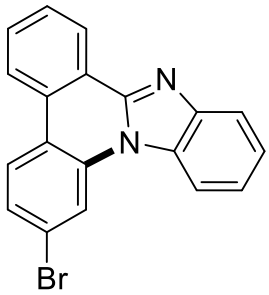


2-Fluorobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2h**): Condition A: 135 mg, 94% yield; Condition B: 118 mg, 82% yield; white solid, m.p. 186-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.84 (d, *J* = 8.0 Hz, 1H), 8.43 (dd, *J* = 8.0 Hz, *J* = 8.0 Hz, 1H), 8.26 (m, 3H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 8.0 Hz, 1H), 7.66 (t, *J* = 8.0 Hz, 1H), 7.52 (m, 2H), 7.22 (m, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): -109.5; ^{13}C NMR (100 MHz, $CDCl_3$): 162.6 (d, $J_{F\text{-}C}$ = 247 Hz), 147.2, 143.8, 134.7(d, $J_{F\text{-}C}$ = 10 Hz), 131.1, 130.6, 128.8, 128.3, 125.82, 125.78, 125.7, 124.6, 123.3, 122.1, 121.8, 120.0, 117.8, 112.0 (d, $J_{F\text{-}C}$ = 22 Hz), 103.0 (d, $J_{F\text{-}C}$ = 27 Hz); These data are in accordance with the literature.[1]

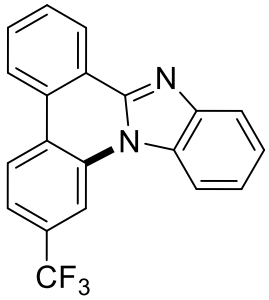


2-Chlorobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2i**): Condition A: 139 mg, 92% yield; Condition B: 109 mg, 72% yield; white solid, m.p. 215-217 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.81 (d, *J* = 8.0 Hz, 1H), 8.46 (s, 1H), 8.31 (d, *J* = 12.0 Hz, 1H), 8.23 (t, *J* = 8.0 Hz, 2H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.67 (m, 2H), 7.51 (m, 2H), 7.42 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.2, 143.7, 135.0, 134.5, 131.2, 130.8, 128.9, 128.7,

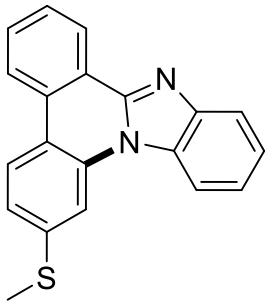
126.0, 125.2, 124.8, 124.7, 123.5, 122.5, 122.1, 120.1, 120.0, 116.0, 113.7; HRMS (ESI): calcd for $C_{19}H_{12}ClN_2^+$ $(M+H)^+$ 303.0684, found 303.0686.



2-Bromobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2j**): Condition A: 125 mg, 72% yield; Condition B: 145 mg, 84% yield; white solid, m.p. 221-223°C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.85 (d, *J* = 4.0 Hz, 1H), 8.68 (s, 1H), 8.29 (m, 3H), 8.05 (d, *J* = 4.0 Hz, 1H), 7.72 (m, 2H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.53 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 146.9, 144.3, 134.6, 131.2, 130.3, 128.7, 128.3, 127.1, 125.8, 125.0, 124.3, 123.1, 122.9, 122.7, 121.8, 120.4, 120.2, 118.5, 113.5; HRMS (ESI): calcd for $C_{19}H_{12}BrN_2^+$ $(M+H)^+$ 347.0178, found 347.0181.

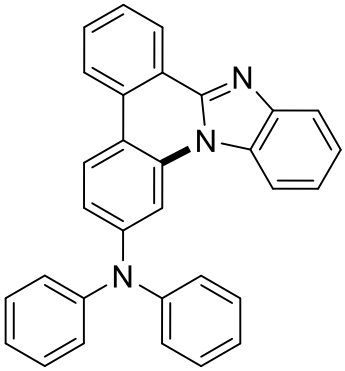


2-(Trifluoromethyl)benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2k**): Condition A: 124 mg, 74% yield; Condition B: trace; white solid, m.p. 217-219 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.80 (d, *J* = 8.0 Hz, 1H), 8.71 (s, 1H), 8.49 (d, *J* = 8.0 Hz, 1H), 8.31 (d, *J* = 8.0 Hz, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.70 (m, 3H), 7.52 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): -62.3; ^{13}C NMR (100 MHz, $CDCl_3$): 147.2, 144.5, 134.2, 131.6, 131.3, 130.8 (q, $J_{F\text{-}C}$ = 33.0 Hz), 130.7, 129.8, 128.2, 126.2, 124.9, 124.6, 124.5, 124.1, 123.8 (q, $J_{F\text{-}C}$ = 270.0 Hz), 123.6, 122.7, 120.7, 113.5, 113.0 (q, $J_{F\text{-}C}$ = 4.0 Hz); These data are in accordance with the literature.[2]

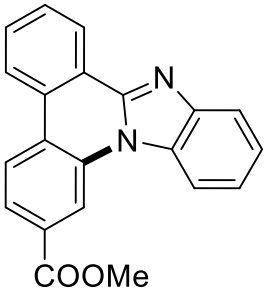


2-(Methylthio)benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2l**): Condition A: 25 mg, 16% yield; Condition B: trace; white solid, m.p. 196-197 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.75 (d, *J* = 8.0 Hz, 1H), 8.16 (m, 4H), 8.00

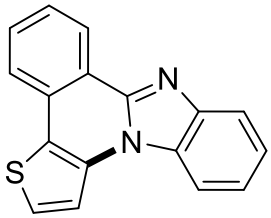
(d, *J* = 8.0 Hz, 1H), 7.60 (m, 2H), 7.46 (m, 2H), 7.18 (d, *J* = 8.0 Hz, 1H), 2.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.6, 144.6, 140.8, 134.7, 131.7, 130.4, 129.3, 128.2, 126.0, 124.3, 124.2, 123.0, 122.9, 122.0, 121.8, 120.4, 118.5, 113.7, 112.7, 15.7; HRMS (ESI): calcd for $C_{20}H_{15}N_2S^+$ $(M+H)^+$ 315.0951, found 315.0952.



N,N-Diphenylbenzo[4,5]imidazo[1,2-*f*]phenanthridin-2-amine (**2m**): Condition A: 118 mg, 54% yield; Condition B: 65 mg, 30% yield; white solid, m.p. 250-251 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.82 (d, *J* = 8.0 Hz, 1H), 8.25 (t, *J* = 8.0 Hz, 2H), 8.15 (d, *J* = 4.0 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.58 (m, 2H), 7.41 (m, 5H), 7.31 (d, *J* = 8.0 Hz, 4H), 7.20 (m, 4H) ; ^{13}C NMR (100 MHz, $CDCl_3$): 149.1, 147.8, 146.8, 144.6, 135.2, 131.7, 130.4, 129.8, 127.4, 126.0, 125.7, 124.97, 124.5, 123.9, 122.6, 122.3, 121.6, 120.2, 117.6, 115.1, 113.4, 108.0; HRMS (ESI): calcd for $C_{31}H_{22}N_3^+$ $(M+H)^+$ 436.1808, found 436.1809.

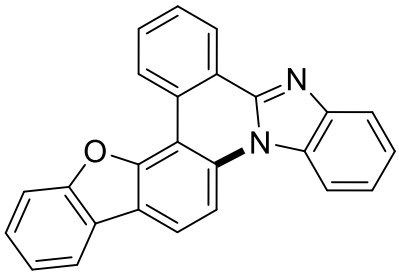


Methyl benzo[4,5]imidazo[1,2-*f*]phenanthridine-2-carboxylate (**2n**): Condition A: 111 mg, 68% yield; Condition B: trace; white solid, m.p. 225-227 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.8 (s, 1H), 8.61 (m, 1H), 8.08 (t, *J* = 8.0 Hz, 2H), 8.00 (m, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.54 (m, 2H), 7.53 (m, 2H), 3.97 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.9, 146.8, 144.3, 133.6, 131.5, 130.3, 129.8, 129.4, 128.2, 125.9, 124.9, 124.5, 124.3, 123.80, 123.76, 123.3, 122.6, 120.4, 116.8, 113.8, 52.6; HRMS (ESI): calcd for $C_{21}H_{15}N_2O_2^+$ $(M+H)^+$ 327.1128, found 327.1128.

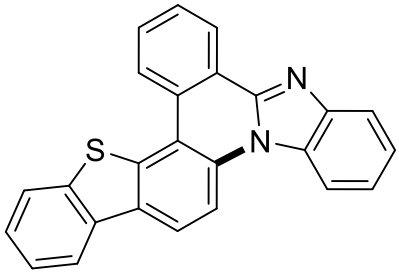


Benzo[4,5]imidazo[2,1-*a*]thieno[3,2-*c*]isoquinoline (**2o**): Condition A: 96 mg, 70% yield; Condition B: 82 mg, 60% yield; white solid, m.p. 108-110 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.76 (d, *J* = 8.0 Hz, 1H), 7.97 (m,

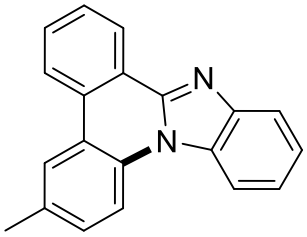
2H), 7.84 (d, *J* = 4 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.57 (m, 3H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.1, 143.3, 133.3, 130.3, 128.1, 127.4, 126.4, 125.9, 124.1, 123.1, 122.5, 122.4, 120.8, 119.9, 116.7, 112.0; HRMS (ESI): calcd for $C_{17}H_{11}N_2S^+$ $(M+H)^+$ 275.0638, found 275.0639.



Benzo[4,5]imidazo[1,2-*f*]benzofuro[2,3-*a*]phenanthridine (**2p**): Condition A: 122 mg, 68% yield; Condition B: 130 mg, 73% yield; white solid, m.p. 247-249 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 9.21 (d, *J* = 8.0 Hz, 1H), 8.79 (d, *J* = 8.0 Hz, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.00 (d, *J* = 8.0 Hz, 1H), 7.85 (m, 2H), 7.62 (m, 3H), 7.42 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): 156.1, 153.4, 147.4, 144.5, 133.5, 131.8, 130.5, 128.4, 127.6, 127.1, 127.0, 125.5, 124.2, 123.4, 123.1, 123.0, 122.8, 120.8, 120.32, 120.26, 114.1, 111.7, 111.0, 108.8; HRMS (ESI): calcd for $C_{25}H_{15}N_2O^+$ $(M+H)^+$ 359.1179, found 359.1178.

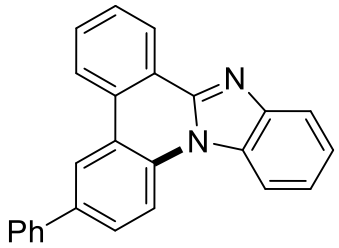


Benzo[4,5]imidazo[1,2-*f*]benzo[4,5]thieno[2,3-*a*]phenanthridine (**2q**): Condition A: 122 mg, 65% yield; Condition B: 127 mg, 68% yield; white solid, m.p. 260-262 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 9.01 (t, *J* = 8.0 Hz, 2H), 8.73 (d, *J* = 8.0 Hz, 1H), 8.42 (t, *J* = 8.0 Hz, 2H), 8.24 (m, 1H), 8.09 (d, *J* = 4.0 Hz, 1H), 7.97 (m, 1H), 7.88 (t, *J* = 8.0 Hz, 1H), 7.75 (t, *J* = 8.0 Hz, 1H), 7.53 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.2, 144.7, 138.6, 136.4, 134.0, 133.8, 133.0, 131.9, 130.2, 129.0, 128.2, 126.8, 126.1, 125.6, 125.0, 124.3, 123.7, 122.8, 122.0, 121.7, 121.2, 120.4, 117.4, 114.2, 113.3; HRMS (ESI): calcd for $C_{25}H_{15}N_2S^+$ $(M+H)^+$ 375.0951, found 375.0950.

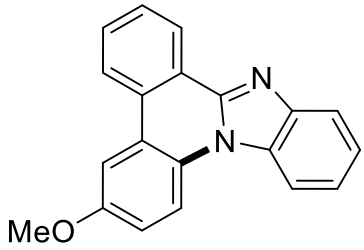


3-Methylbenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2r**): Condition A: 97 mg, 69% yield; Condition B: 109 mg, 77% yield; white solid, m.p. 213-215 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.80 (d, *J* = 4.0 Hz, 1H), 8.23 (m, 3H), 8.07 (s, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.62 (m, 2H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.3, 144.4, 133.9, 132.2, 131.8, 130.2,

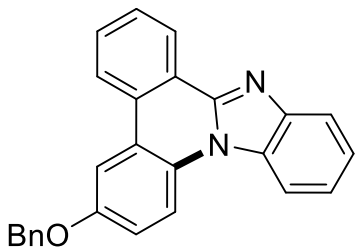
129.9, 129.4, 128.3, 125.9, 124.1, 123.9, 123.4, 122.6, 122.1, 121.4, 120.2, 115.6, 113.8, 21.2; These data are in accordance with the literature.[3]



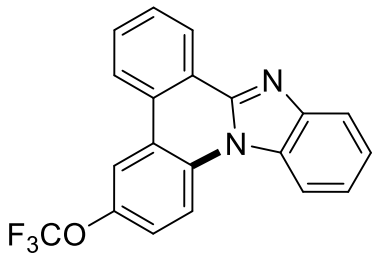
3-Phenylbenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2s**): Condition A: 133 mg, 77% yield; Condition B: 100 mg, 58% yield; white solid, m.p. 237-239 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.91 (d, *J* = 4.0 Hz, 1H), 8.69 (s, 1H), 8.65 (d, *J* = 8.0 Hz, 1H), 8.49 (d, *J* = 8.0 Hz, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.07 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.74 (m, 4H), 7.50 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.3, 144.5, 139.9, 137.0, 133.4, 131.7, 130.3, 129.3, 129.0, 128.6, 127.7, 127.6, 127.1, 126.0, 124.1, 123.4, 122.9, 122.3, 122.1, 121.8, 120.3, 116.2, 113.8; HRMS (ESI): calcd for $C_{25}H_{17}N_2^+$ $(M+H)^+$ 345.1386, found 345.1386.



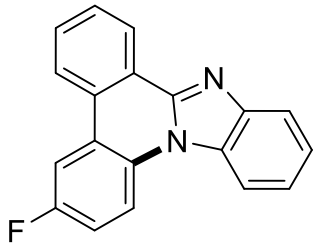
3-Methoxybenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2t**): Condition A: 104 mg, 70% yield; Condition B: 89 mg, 60% yield; white solid, m.p. 149-150 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.75 (m, 1H), 8.20 (d, *J* = 8.0 Hz, 1H), 8.09 (m, 2H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.59 (m, 3H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.03 (dd, *J* = 8.0 Hz, *J* = 4.0 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 156.0, 146.9, 144.3, 131.6, 130.0, 129.1, 128.50, 128.46, 125.9, 123.7, 123.5, 122.8, 122.6, 122.1, 120.2, 116.8, 115.5, 113.5, 107.7, 55.5; These data are in accordance with the literature.[3]



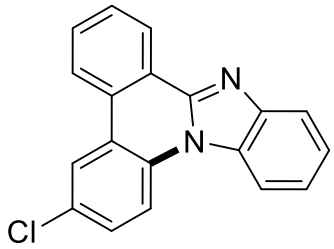
3-(Benzyloxy)benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2u**): Condition A: 117 mg, 62% yield; Condition B: 87 mg, 46% yield; white solid, m.p. 233-234 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.89 (d, *J* = 8.0 Hz, 1H), 8.50 (d, *J* = 8.0 Hz, 1H), 8.30 (m, 2H), 8.04 (m, 2H), 7.71 (m, 2H), 7.44 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): 155.5, 147.2, 144.5, 136.6, 131.8, 130.3, 129.3, 129.0, 128.80, 128.77, 128.3, 127.6, 126.2, 123.9, 123.8, 123.2, 122.8, 122.4, 120.4, 117.2, 116.7, 113.6, 109.6, 70.7; HRMS (ESI): calcd for $C_{26}H_{19}N_2O^+$ $(M+H)^+$ 375.1492, found 375.1492.



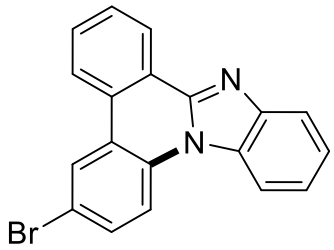
3-(Trifluoromethoxy)benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2v**): Condition A: 127 mg, 72% yield; Condition B: 162 mg, 92% yield; white solid, m.p. 172-174 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.85 (d, *J* = 8.0 Hz, 1H), 8.55 (d, *J* = 8.0 Hz, 1H), 8.27 (m, 3H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.74 (m, 2H), 7.52 (m, 3H); ^{19}F NMR (376 MHz, $CDCl_3$): -57.8; ^{13}C NMR (100 MHz, $CDCl_3$): 146.9, 145.3, 144.2, 132.5, 131.4, 130.5, 129.3, 128.1, 125.9, 124.3, 123.4, 123.2, 123.1, 122.2, 121.5, 120.5 (q, J_{F-C} = 256 Hz), 120.4, 117.0, 116.7, 116.5, 113.3; HRMS (ESI): calcd for $C_{20}H_{12}F_3N_2O^+$ $(M+H)^+$ 353.0896, found 353.0896.



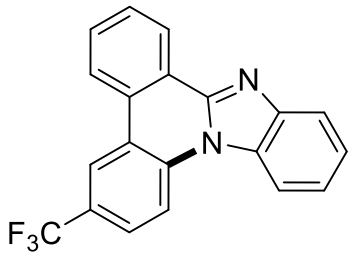
3-Fluorobenzo[4,5]imidazo[1,2-f]phenanthridine (**2w**): Condition A: 115 mg, 80% yield; Condition B: 104 mg, 73% yield; white solid, m.p. 196-198 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.76 (d, *J* = 4.0 Hz, 1H), 8.34 (m, 1H), 8.12 (d, *J* = 8.0 Hz, 2H), 7.97 (m, 2H), 7.64 (m, 2H), 7.45 (m, 2H), 7.28 (t, *J* = 8.0 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): -116.7; ^{13}C NMR (100 MHz, $CDCl_3$): 159.1 (d, J_{F-C} = 243 Hz), 146.9, 144.3, 131.5,130.7, 130.4, 129.2, 128.5, 126.0, 124.1, 123.53, 123.46, 123.01, 122.3, 120.4, 117.3 (d, J_{F-C} = 8 Hz), 116.2 (d, J_{F-C} = 24 Hz), 113.4, 110.2 (d, J_{F-C} = 24 Hz); HRMS (ESI): calcd for $C_{19}H_{12}FN_2^+$ $(M+H)^+$ 287.0979, found 287.0979.



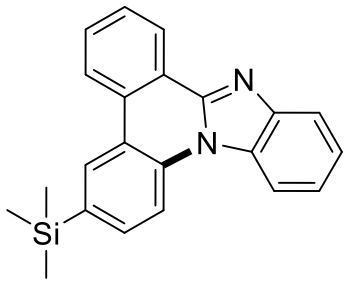
3-Chlorobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2x**): Condition A: 116 mg, 77% yield; Condition B: 110 mg, 73% yield; white solid, m.p. 205-207 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.72 (d, *J* = 8.0 Hz, 1H), 8.25 (d, *J* = 8.0 Hz, 1H), 8.20 (s, 1H), 8.10 (t, *J* = 8.0 Hz, 2H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.63 (m, 2H), 7.48 (t, *J* = 8.0 Hz, 2H), 7.41 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 146.9, 144.4, 132.6, 131.5, 130.4, 129.9, 129.2, 128.8, 128.1, 126.0, 124.3, 123.8, 123.5, 123.1, 123.1, 122.2, 120.5, 117.0, 113.5; HRMS (ESI): calcd for $C_{19}H_{12}ClN_2^+$ $(M+H)^+$ 303.0684, found 303.0681.



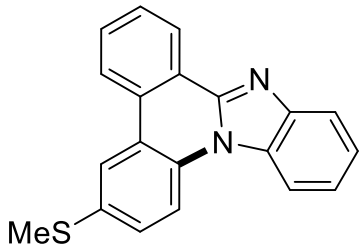
3-Bromobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2y**): Condition A: 125 mg, 72% yield; Condition B: 107 mg, 62% yield; white solid, m.p. 219-220°C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.85 (d, *J* = 4.0 Hz, 1H), 8.68 (s, 1H), 8.29 (m, 3H), 8.05 (d, *J* = 4.0 Hz, 1H), 7.72 (m, 2H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.53 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 146.9, 144.3, 134.6, 131.2, 130.3, 128.7, 128.3, 127.1, 125.8, 125.0, 124.3, 123.1, 122.9, 122.7, 121.8, 120.4, 120.2, 118.54, 113.46; HRMS (ESI): calcd for $C_{19}H_{12}BrN_2^+$ $(M+H)^+$ 347.0178, found 347.0180.



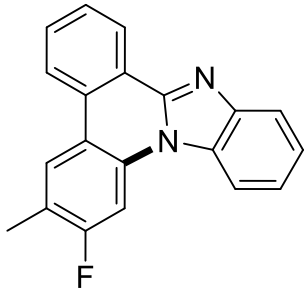
3-(Trifluoromethyl)benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2z**): Condition A: 110 mg, 65% yield; Condition B: 79 mg, 47% yield; white solid, m.p. 211-213 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.69 (d, *J* = 8.0 Hz, 1H), 8.53 (s, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 8.21 (d, *J* = 8.0 Hz, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.65 (m, 2H), 7. 47 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): -61.9; ^{13}C NMR (100 MHz, $CDCl_3$): 147.1, 144.4, 136.1, 131.5, 130.6, 129.4, 128.2, 126.23 (q, $J_{F\text{-}C}$ = 33 Hz), 126.0, 125.4 (q, $J_{F\text{-}C}$ = 3 Hz), 125.6, 123.9 (q, $J_{F\text{-}C}$ = 271 Hz), 123.5, 123.4, 122.2, 121.7, 121.3 (q, $J_{F\text{-}C}$ = 4 Hz), 120.6, 116.1, 113.6; HRMS (ESI): calcd for $C_{20}H_{12}F_3N_2^+$ $(M+H)^+$ 337.0947, found 337.0945.



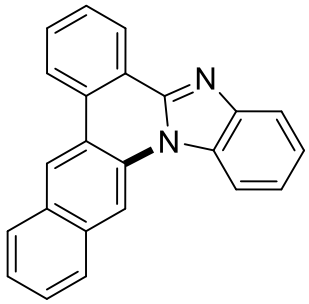
3-(Trimethylsilyl)benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2aa**): Condition A: 109 mg, 64% yield; Condition B: 136 mg, 80% yield; white solid, m.p.198-200 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.82 (d, *J* = 8.0 Hz, 1H), 8.57 (s, 1H), 8.46 (d, *J* = 8.0 Hz, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 8.28 (d, *J* = 8.0 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 8.79 (d, *J* = 8.0 Hz, 1H), 7.71 (t, *J* = 6.0 Hz, 1H), 7.64 (t, *J* = 6.0 Hz, 1H), 7.47 (m, 2H), 0.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.4, 144.5, 136.1, 134.7, 134.0, 131.8, 130.3, 129.5, 129.0, 128.4, 126.0, 124.0, 123.4, 122.8, 122.0, 120.7, 120.3, 115.2, 113.9, -1.0; HRMS (ESI): calcd for $C_{22}H_{21}N_2Si^+$ $(M+H)^+$ 341.1469, found 341.1470.



3-(Methylthio)benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2ab**): Condition A: 28 mg, 18% yield; Condition B: trace; white solid, m.p. 156-158 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.84 (d, *J* = 4.0 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.28 (m, 3H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.69 (m, 2H), 7.5 (m, 3H), 2.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.2, 144.3, 134.5, 132.1, 131.7, 130.5, 128.9, 128.8, 127.9, 126.1, 124.2, 123.5, 123.0, 122.4, 122.3, 122.2, 120.4, 116.5, 113.8, 16.6; HRMS (ESI): calcd for $C_{20}H_{15}N_2S^+$ $(M+H)^+$ 315.0951, found 315.0949.

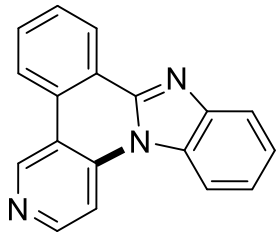


2-Fluoro-3-methylbenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2ac**): Condition A: 119 mg, 80% yield; Condition B: 105 mg, 70% yield; white solid, m.p. 228-230 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.54 (d, *J* = 8.0 Hz, 1H), 8.26 (m, 3H), 8.17 (d, *J* = 12.0 Hz, 1H), 8.05 (d, *J* = 4.0 Hz, 1H), 7.68 (m, 2H), 7.51 (m, 2H); ^{19}F NMR (376 MHz, $CDCl_3$): -113.0; ^{13}C NMR (100 MHz, $CDCl_3$): 161.4 (d, $J_{F\text{-}C}$ = 246 Hz), 147.5, 144.5, 133.2, 131.6, 130.5, 129.0, 128.3, 126.9 (d, $J_{F\text{-}C}$ = 7 Hz), 126.1, 124.3, 123.0, 122.9, 122.1, 121.5, 120.5, 117.9 (d, $J_{F\text{-}C}$ = 2 Hz), 113.5, 102.9 (d, $J_{F\text{-}C}$ = 28 Hz), 14.7 (d, $J_{F\text{-}C}$ = 3 Hz); HRMS (ESI): calcd for $C_{20}H_{14}FN_2^+$ $(M+H)^+$ 301.1136, found 301.1143.

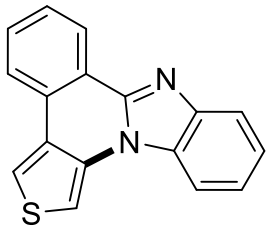


Benzo[*b*]benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2ad**): Condition A: 120 mg, 75% yield; Condition B: 126 mg, 79% yield; white solid, m.p. 214-216 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.87 (d, *J* = 8.0 Hz, 1H), 8.51 (d, *J* = 8.0 Hz, 1H), 8.33 (m, 2H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.68 (m, 2H), 7.60 (t, *J* = 8.0 Hz, 1H), 7.48 (q, *J* = 8.0 Hz, 2H), 7.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 148.8, 144.5, 133.7, 133.4, 130.4, 129.7, 129.4, 128.6, 128.0, 127.2, 125.9, 125.7, 124.8, 124.6, 124.1, 123.8, 123.3, 122.58, 120.62, 120.5, 120.3, 120.1, 115.6; HRMS (ESI): calcd for

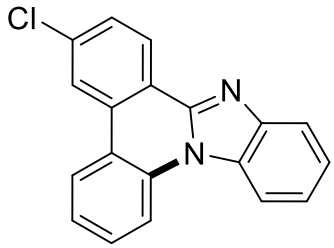
$C_{23}H_{15}N_2^+$ $(M+H)^+$ 319.1230, found 319.1229.



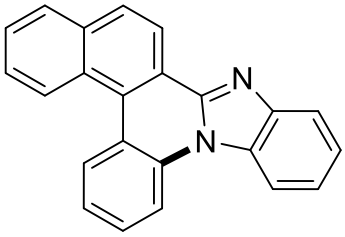
Benzo[*c*]benzo[4,5]imidazo[1,2-*a*][1,6]naphthyridine (**2ae**): Condition A: 79 mg, 59% yield; Condition B: 33 mg, 25% yield; white solid, m.p. 188-190°C; ^{1}H NMR (400 MHz, $CDCl_3$): 9.00 (d, *J* = 8.0 Hz, 1H), 8.69 (m, 1H), 8.57 (d, *J* = 4.0 Hz, 1H), 8.41 (d, *J* = 8.0 Hz, 1H), 8.06 (m, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.58 (m, 2H), 7.47 (m, 2H), 7.24 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 148.14, 148.10, 147.2, 145.8, 143.9, 131.5, 130.2, 129.0, 128.3, 125.8, 124.5, 123.3, 122.2, 119.8, 119.3, 117.1, 116.33, 116.27 ; HRMS (ESI): calcd for $C_{18}H_{12}N_3^+$ $(M+H)^+$ 270.1026, found 270.1026.



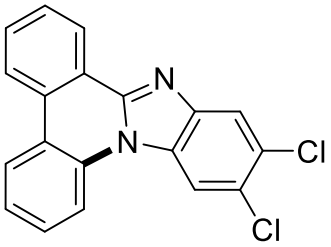
Benzo[4,5]imidazo[2,1-*a*]thieno[3,4-*c*]isoquinoline (**2af**): Condition A: 115 mg, 84% yield; Condition B: 101 mg, 74% yield; white solid, m.p. 195-197 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.77 (d, *J* = 8.0 Hz, 1H), 7.96 (m, 3H), 7.52 (m, 5H), 7.15 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 147.0, 143.4, 134.5, 130.2, 129.8, 128.6, 127.1, 125.7, 124.4, 122.9, 122.8, 122.3, 121.1, 119.8, 117.7, 111.6; HRMS (ESI): calcd for $C_{17}H_{11}N_2S^+$ $(M+H)^+$ 275.0638, found 275.0639.



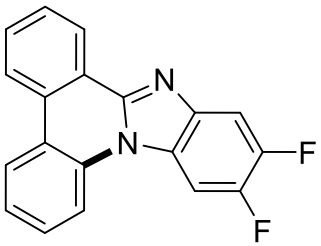
6-Chlorobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2ag**): Condition A: 122 mg, 81% yield; Condition B: trace; white solid, m.p. 210-212 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.61 (d, *J* = 8.0 Hz, 1H), 8.30 (d, *J* = 8.0 Hz, 1H), 8.14 (t, *J* = 6.0 Hz, 2H), 8.09 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.48 (m, 2H), 7.39 (t, *J* = 8.0 Hz, 1H), 7.33 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 146.5, 144.3, 136.7, 134.4, 131.6, 130.6, 129.6, 128.8, 127.4, 124.4, 124.2, 124.0, 123.1, 122.0, 121.5, 120.3, 120.3, 115.8, 113.8; These data are in accordance with the literature.[4]



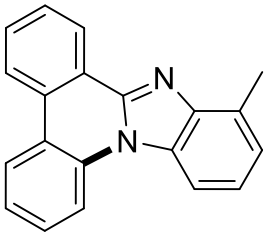
Benzo[*k*]benzo[4,5]imidazo[1,2-*f*]phenanthridine (**2ah**): Condition A: 107 mg, 67% yield; Condition B: 103 mg, 65% yield; white solid, m.p. 155-157 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.76 (d, *J* = 8.0 Hz, 2H), 8.70 (d, *J* = 8.0 Hz, 1H), 8.50 (d, *J* = 12.0 Hz, 1H), 8.26 (d, *J* = 8.0 Hz, 1H), 8.04 (d, *J* = 8.0 Hz, 1H), 7.96 (m, 2H), 7.60 (m, 3H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.43 (q, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 148.0, 145.1, 135.2, 134.3, 131.3, 129.8, 129.4, 129.0, 128.7, 127.4, 127.2, 126.88, 126.85, 124.2, 123.8, 122.8, 122.3, 122.1, 121.9, 120.4, 115.8, 113.9; These data are in accordance with the literature.[4]



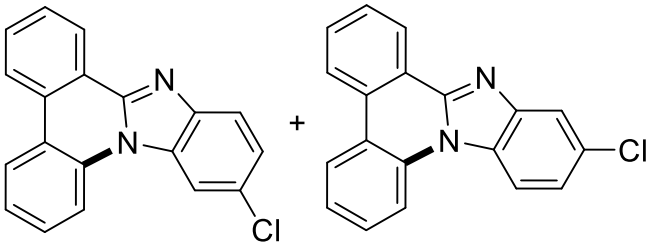
11,12-Dichlorobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2ai**): Condition A: 101 mg, 60% yield; Condition B: 116 mg, 69% yield; white solid, m.p. 242-244 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.71 (d, *J* = 8.0 Hz, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 8.32 (m, 2H), 8.23 (d, *J* = 8.0 Hz, 1H), 7.99 (s, 1H), 7.74 (t, *J* = 8.0 Hz, 1H), 7.67 (m, 2H), 7.51 (t, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 149.0, 143.9, 133.6, 131.0, 130.7, 129.6, 129.4, 128.8, 128.1, 126.4, 126.2, 125.0, 124.4, 122.8, 122.3, 121.7, 121.0, 115.6, 115.0; These data are in accordance with the literature.[1]



11,12-Difluorobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2aj**): Condition A: 58 mg, 38% yield; Condition B: 131 mg, 86% yield; white solid, m.p. 216-218 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.72 (d, *J* = 8.0 Hz, 1H), 8.40 (d, *J* = 8.0 Hz, 1H), 8.30 (d, *J* = 8.0 Hz, 1H), 8.20 (d, *J* = 8.0 Hz, 1H), 8.03 (dd, *J* = 12.0 Hz, *J* = 8.0 Hz, 1H), 7.72 (t, *J* = 10.0 Hz, 2H), 7.65 (m, 2H), 7.48 (t, *J* = 8.0 Hz, 1H); ^{19}F NMR (376 MHz, $CDCl_3$): -140.1 (d, *J* = 18.8 Hz), -140.6 (d, *J* = 18.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): 148.7 (d, $J_{F\text{-}C}$ = 3 Hz), 148.5 (dd, $J_{F\text{-}C}$ = 242 Hz, $J_{F\text{-}C}$ = 13 Hz), 147.5 (dd, $J_{F\text{-}C}$ = 232 Hz, $J_{F\text{-}C}$ = 13 Hz), 140.0 (d, $J_{F\text{-}C}$ = 10 Hz), 133.5, 130.7, 129.2, 128.8, 126.5 (d, $J_{F\text{-}C}$ = 10 Hz), 125.9, 124.9, 124.3, 122.8, 122.2, 121.6, 155.2, 107.1 (d, $J_{F\text{-}C}$ = 19 Hz), 102.2 (d, $J_{F\text{-}C}$ = 24 Hz); HRMS (ESI): calcd for $C_{19}H_{11}F_2N_2^+$ $(M+H)^+$ 305.0885, found 305.0886.



10-Methylbenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2ak**): Condition A: 37 mg, 26% yield; Condition B: 43 mg, 31% yield; white solid, m.p. 193-195 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.89 (d, *J* = 8.0 Hz, 1H), 8.49 (d, *J* = 8.0 Hz, 1H), 8.40 (d, *J* = 8.0 Hz, 1H), 8.30 (d, *J* = 8.0 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 1H), 7.65 (m, 3H), 7.44 (t, *J* = 6.0 Hz, 1H), 7.31 (m, 2H), 2.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 146.7, 143.8, 134.5, 131.5, 130.4, 130.1, 129.3, 129.0, 128.4, 126.1, 124.3, 124.2, 124.1, 123.7, 122.7, 122.1, 121.7, 115.9, 111.3, 17.1; These data are in accordance with the literature.[4]



Mixture of 12-chlorobenzo[4,5]imidazo[1,2-*f*]phenanthridine and 11-chlorobenzo[4,5]imidazo[1,2-*f*]phenanthridine (**2al**) (ratio: 1/1): Condition A: 101 mg, 67% yield; Condition B: 147 mg, 97% yield; white solid, m.p. 165-167 °C; ^{1}H NMR (400 MHz, $CDCl_3$): 8.65 (d, *J* = 8.0 Hz, 1H), 8.12 (m, 4H), 7.84 (m, 1H), 7.58 (m, 3H), 7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 148.3, 147.9, 145.3, 142.9, 133.7, 131.9, 130.8, 130.6, 130.5, 130.2, 129.5, 129.3, 129.2, 129.0, 128.5, 128.2, 125.9, 125.9, 124.6, 124.5, 124.5, 124.0, 122.9, 122.8, 122.10, 122.07, 121.5, 121.4, 120.7, 119.8, 115.5, 114.3, 113.8; HRMS (ESI): calcd for $C_{19}H_{12}ClN_2^+$ $(M+H)^+$ 303.0684, found 303.0682.

6. References

[1] S. K. Bera, M. T. Alam and P. Mal, *J. Org. Chem.,* 2019, **84**, 12009-12020.

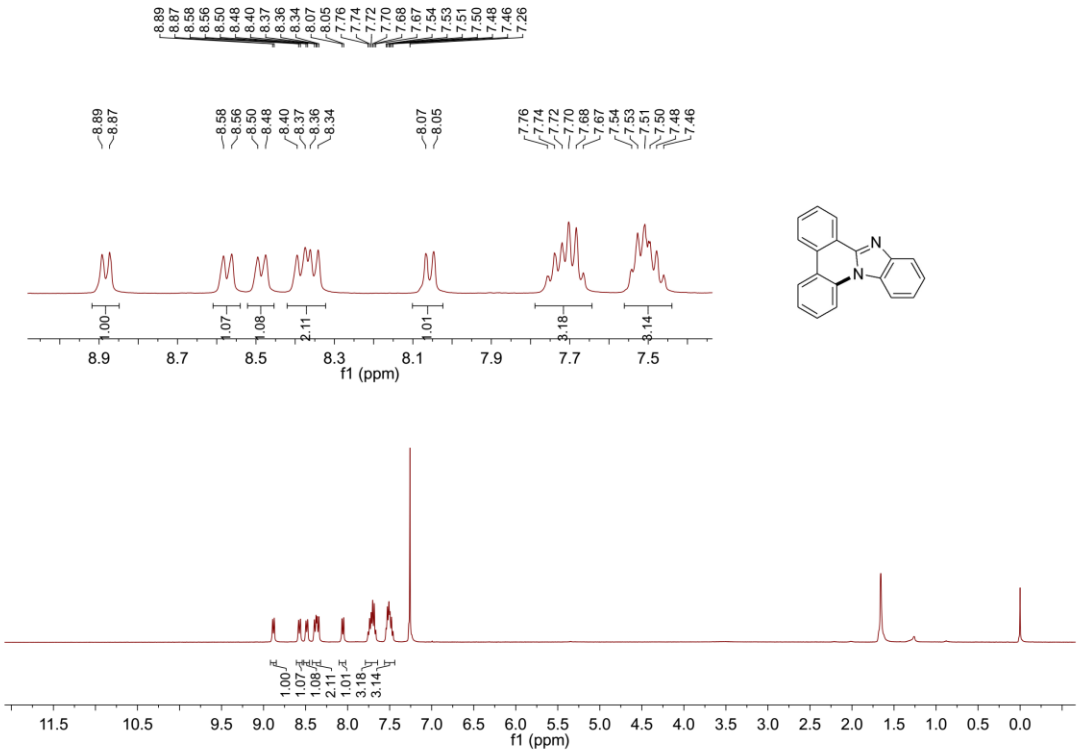
[2] L. Yan, D. Zhao, J. Lan, Y. Cheng, Q. Guo, X. Li, N. Wu and J. You, *Org. Biomol. Chem.,* 2013, **11**, 7966-7977.

[3] G. Zhao, C. Chen, Y. Yue, Y. Yu and J. Peng, *J. Org. Chem.,* 2015, **80**, 2827-2834.

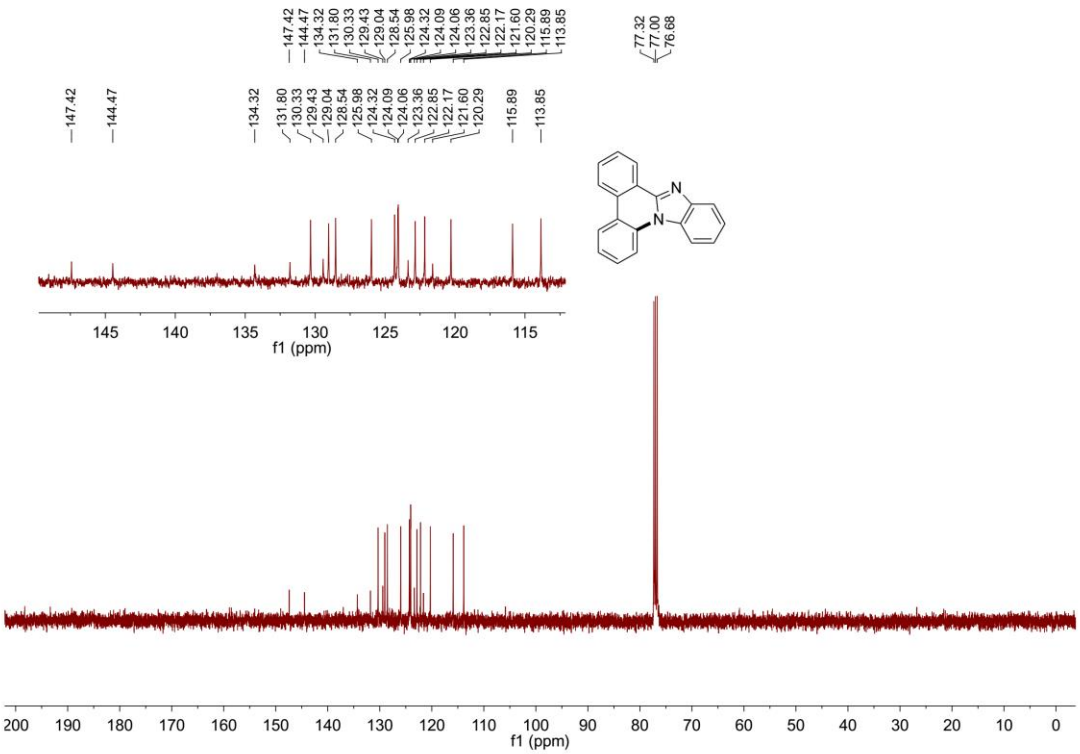
[4] C. Chen, G. Shang, J. Zhou, Y. Yu, B. Li and J. Peng, *Org. Lett.,* 2014, **16**, 1872-1875.

Part II NMR Spectra

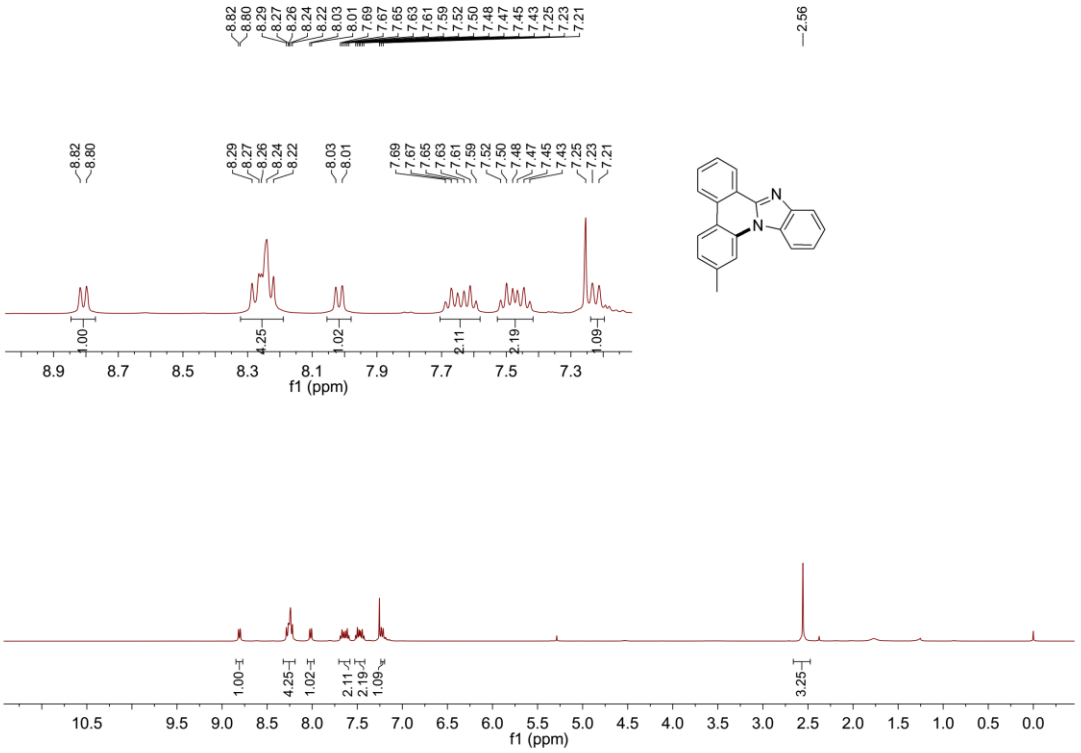
2a ^{1}H NMR



2a ^{13}C NMR



2b ^{1}H NMR



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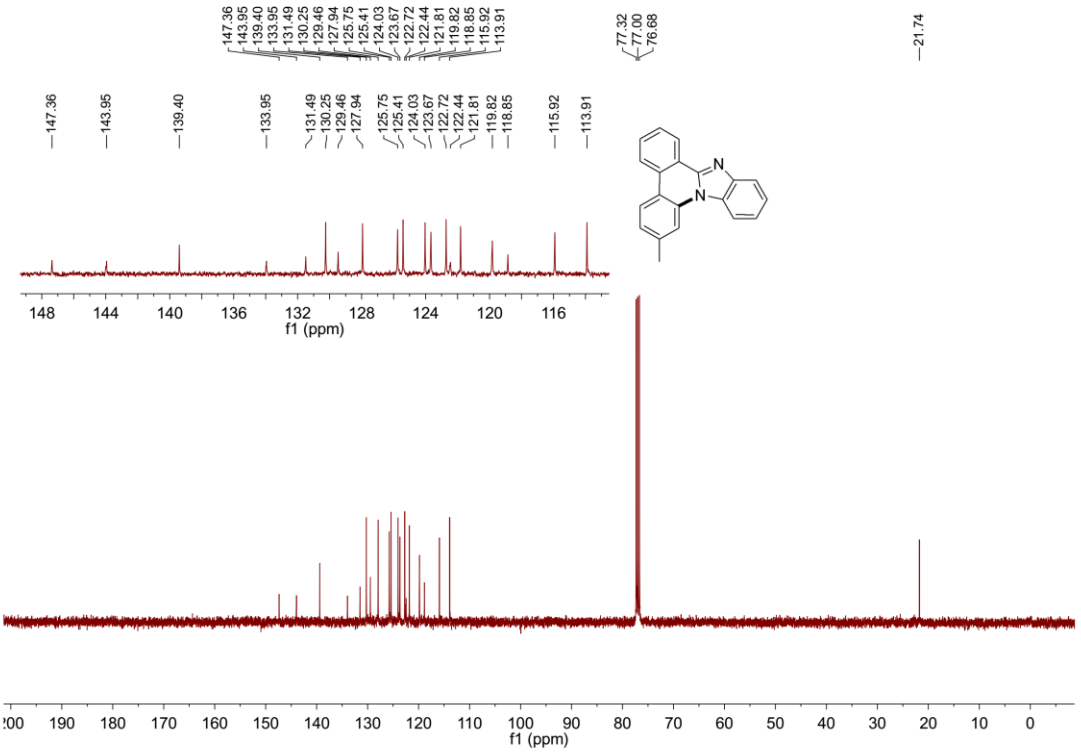

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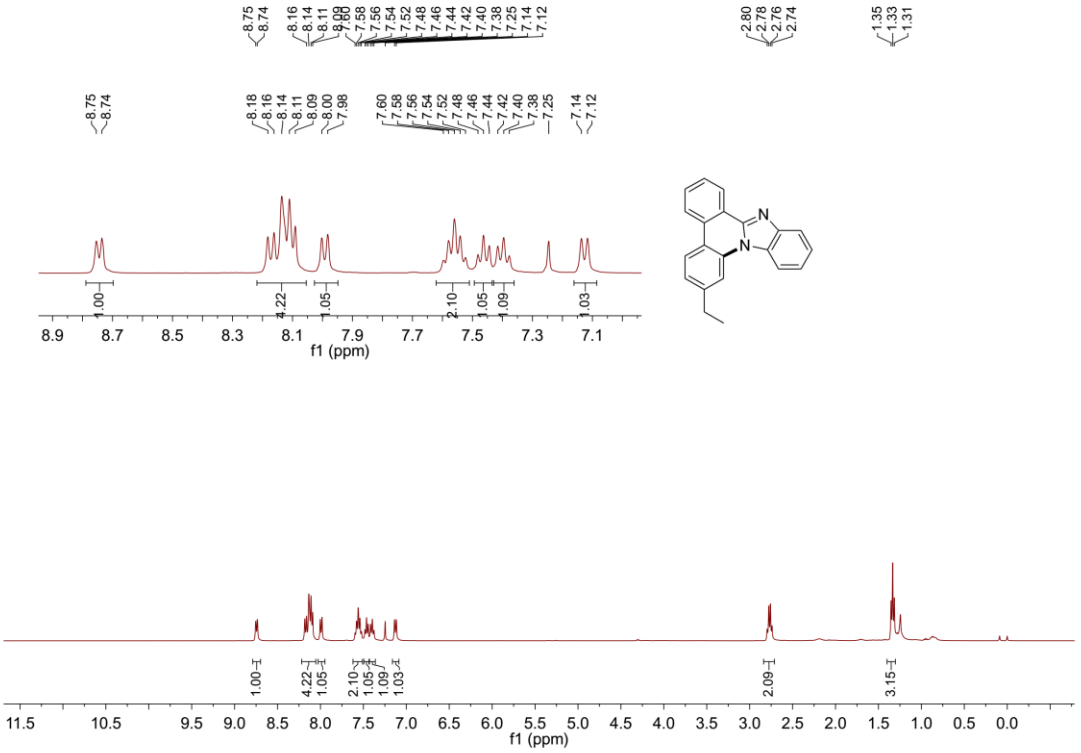

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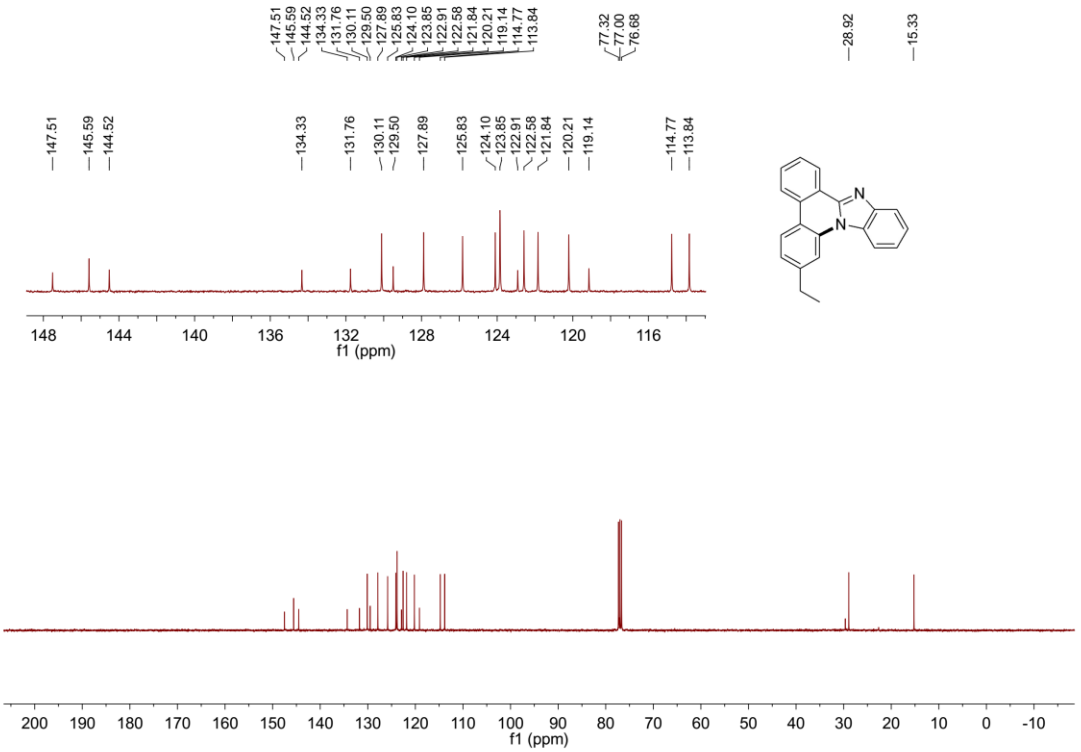
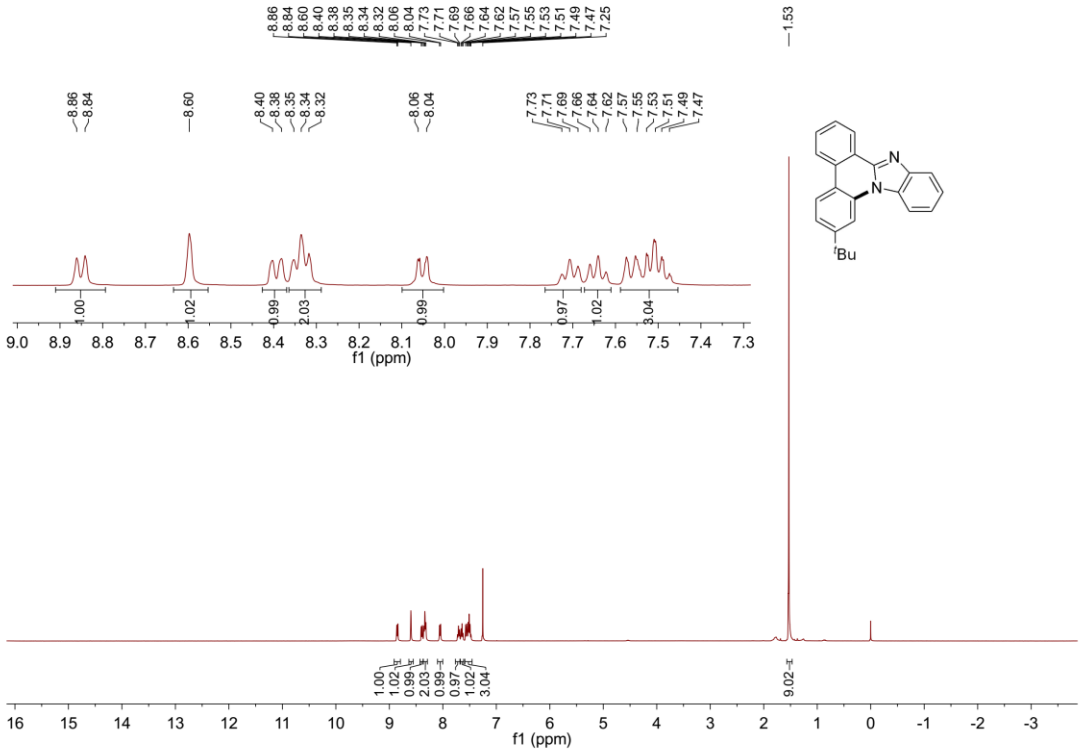
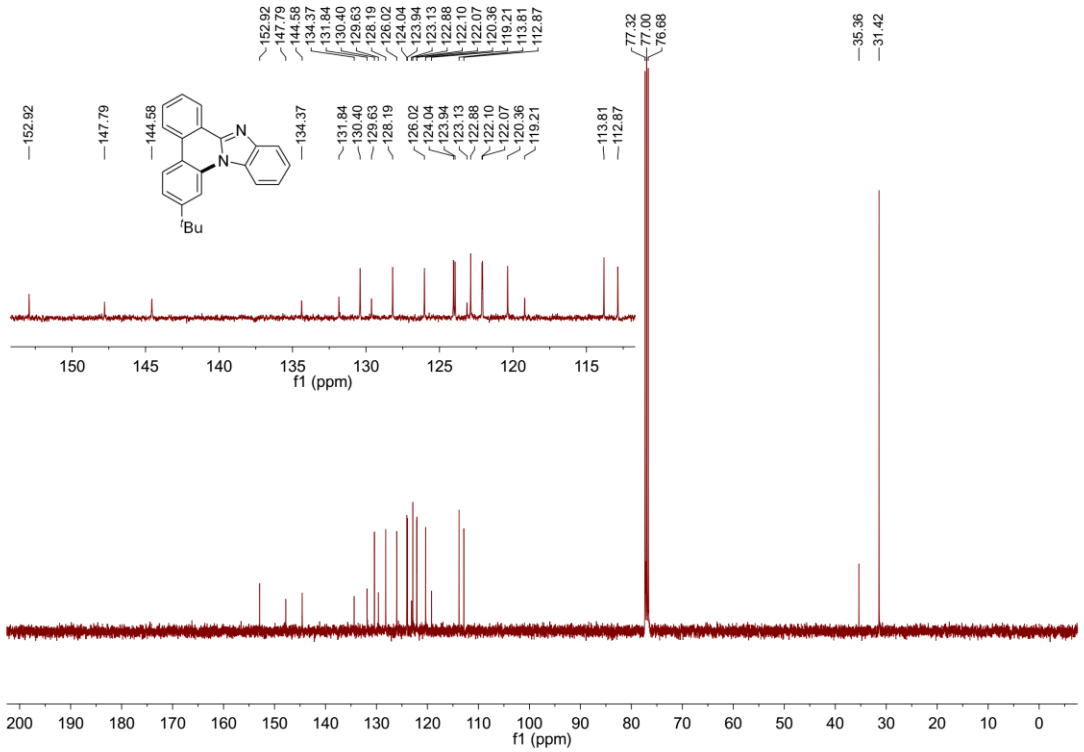


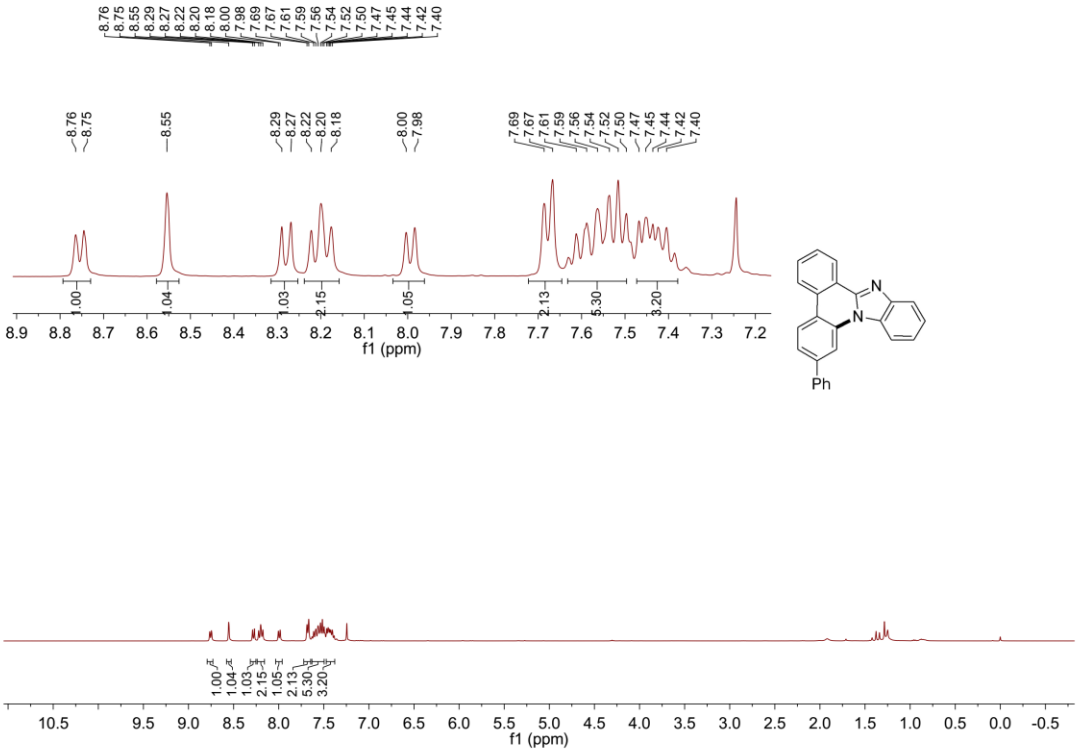
2d ^{1}H NMR



2d ^{13}C NMR



2e ^{1}H NMR



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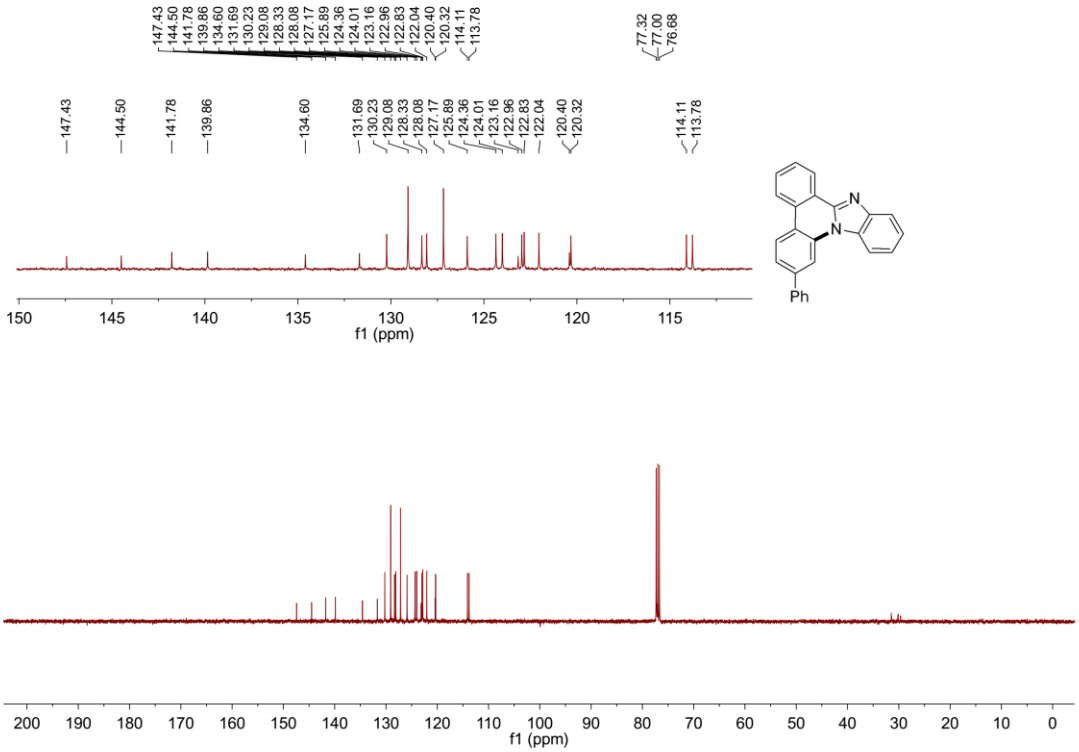
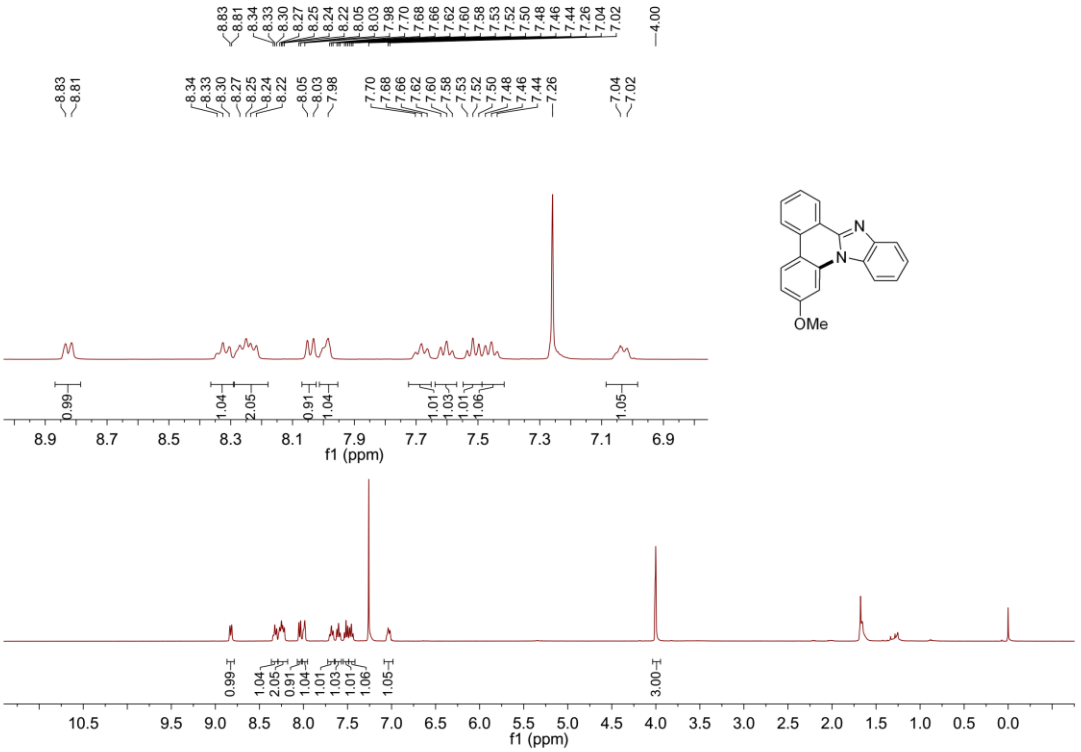
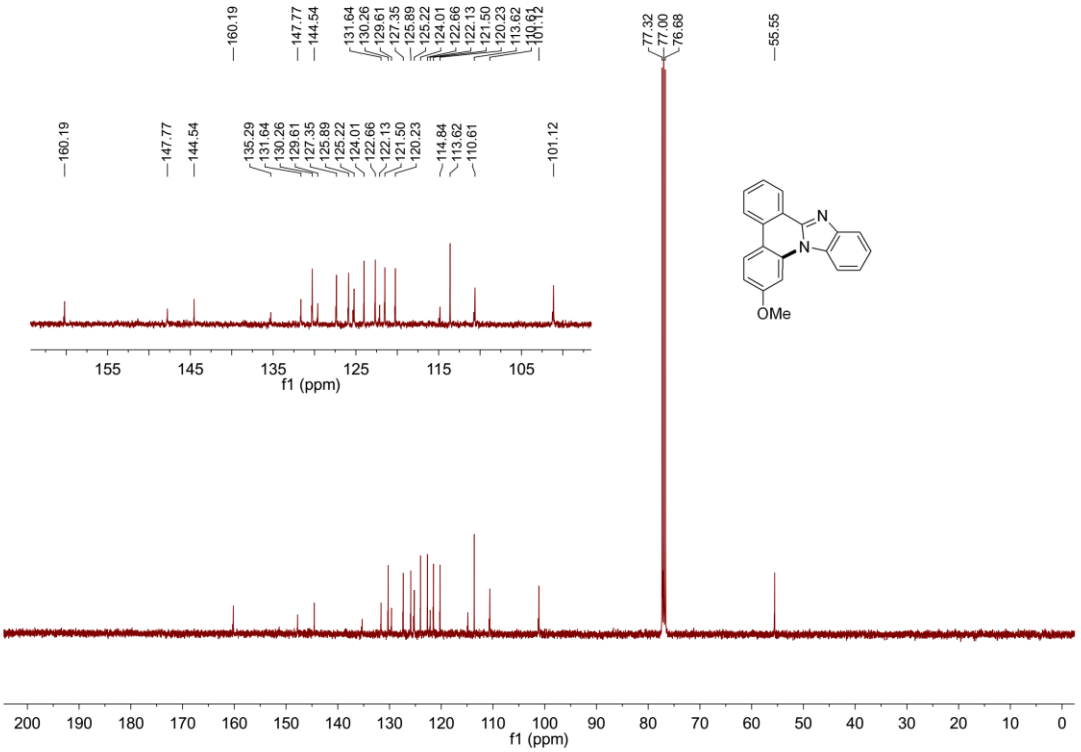


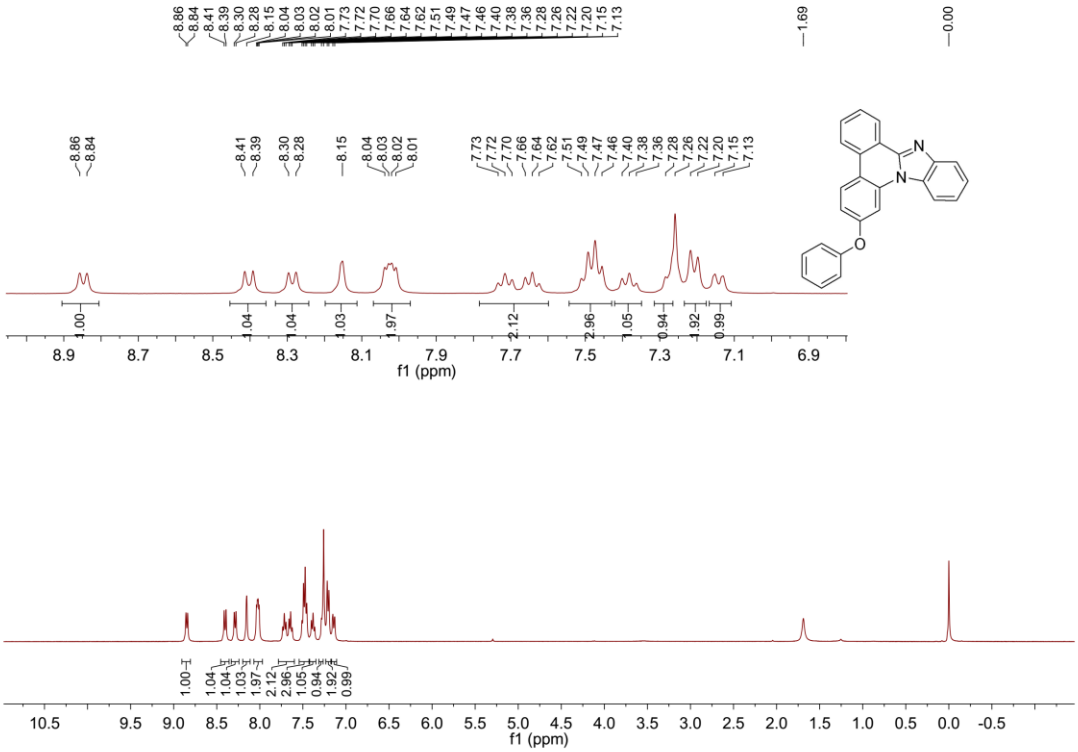
2f ^{1}H NMR



2f ^{13}C NMR



2g ^{1}H NMR



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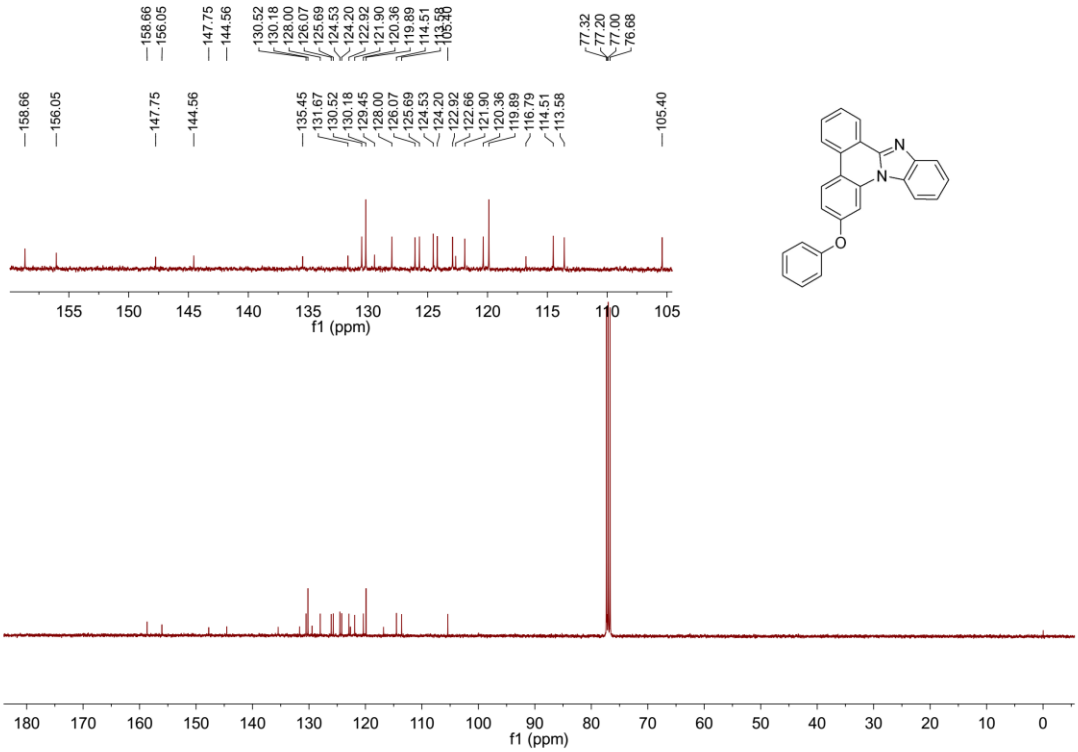
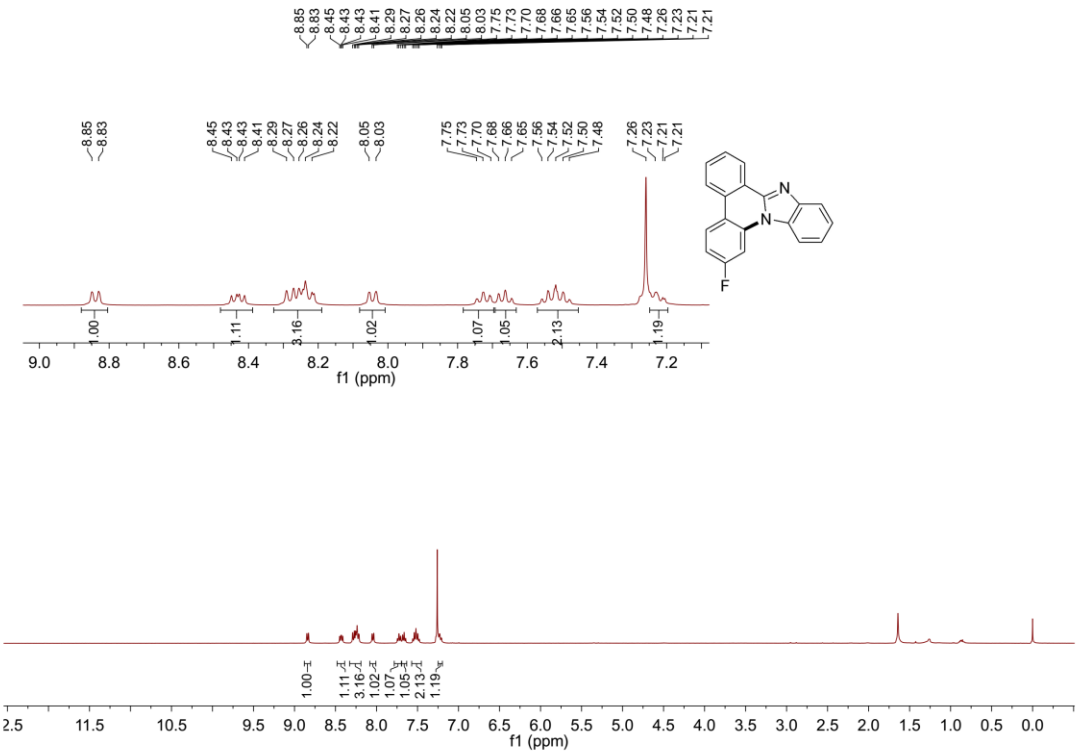
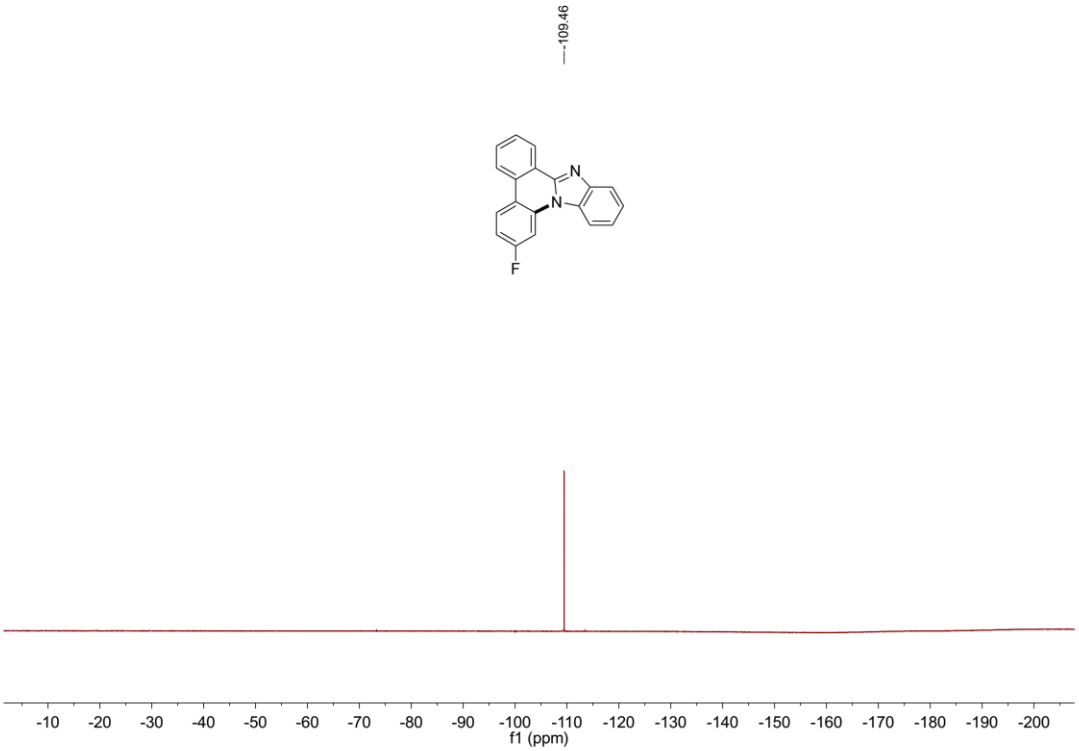


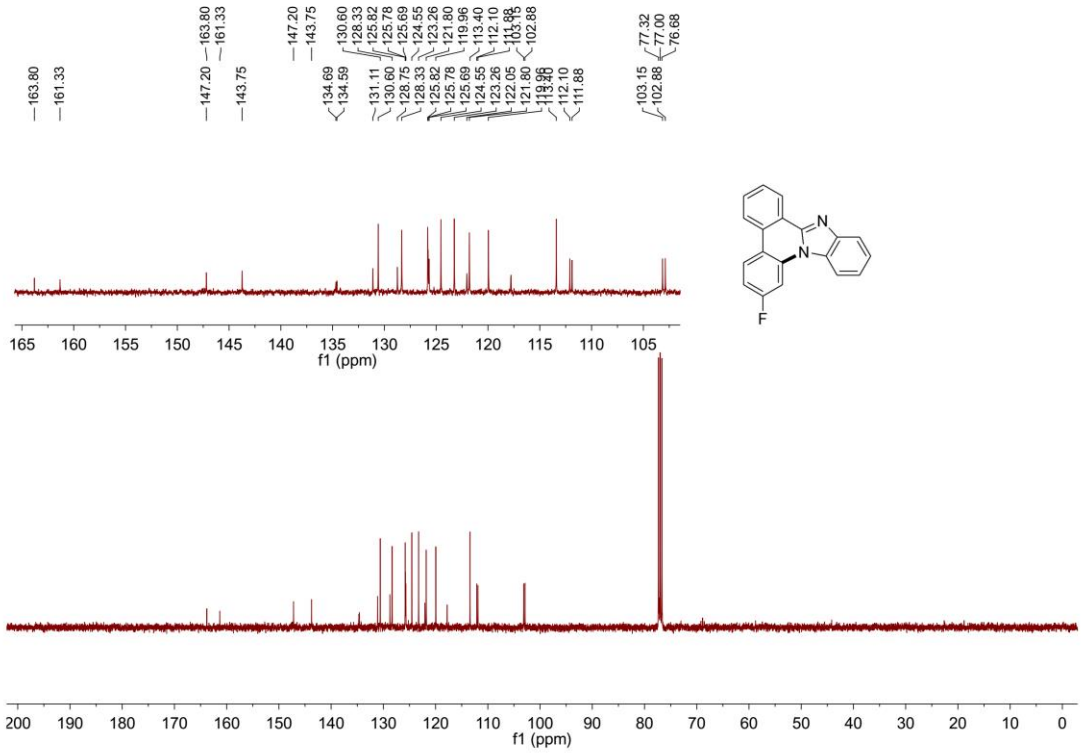
2h ^{1}H NMR



2h ^{19}F NMR



2h ^{13}C NMR



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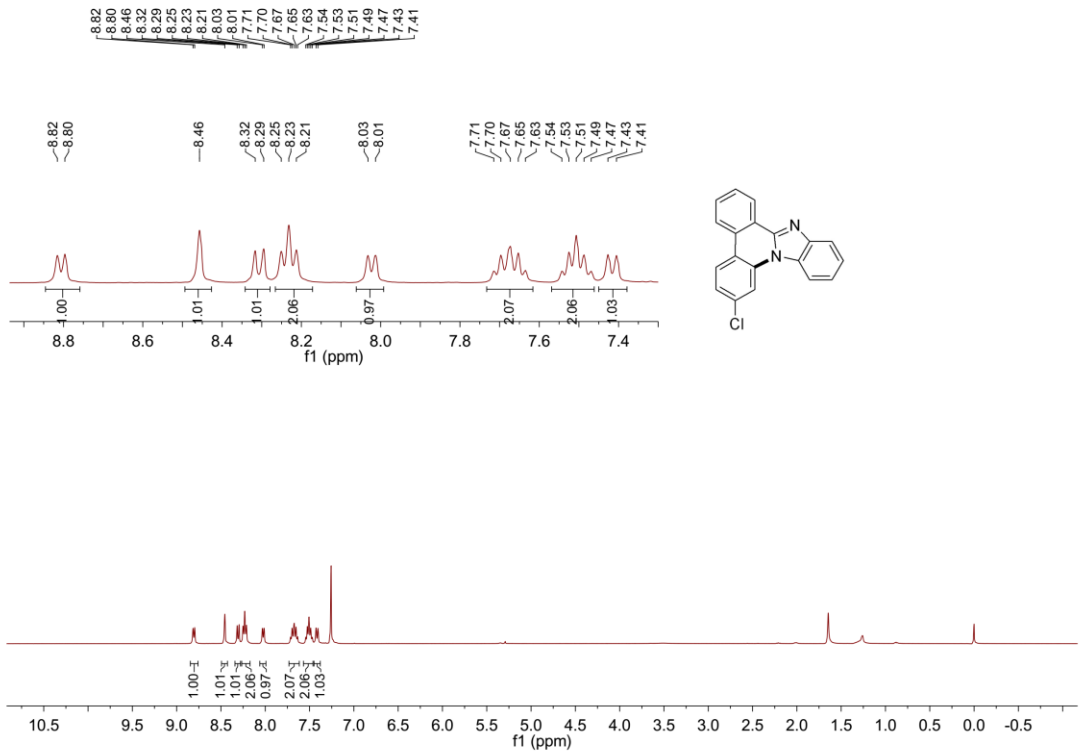

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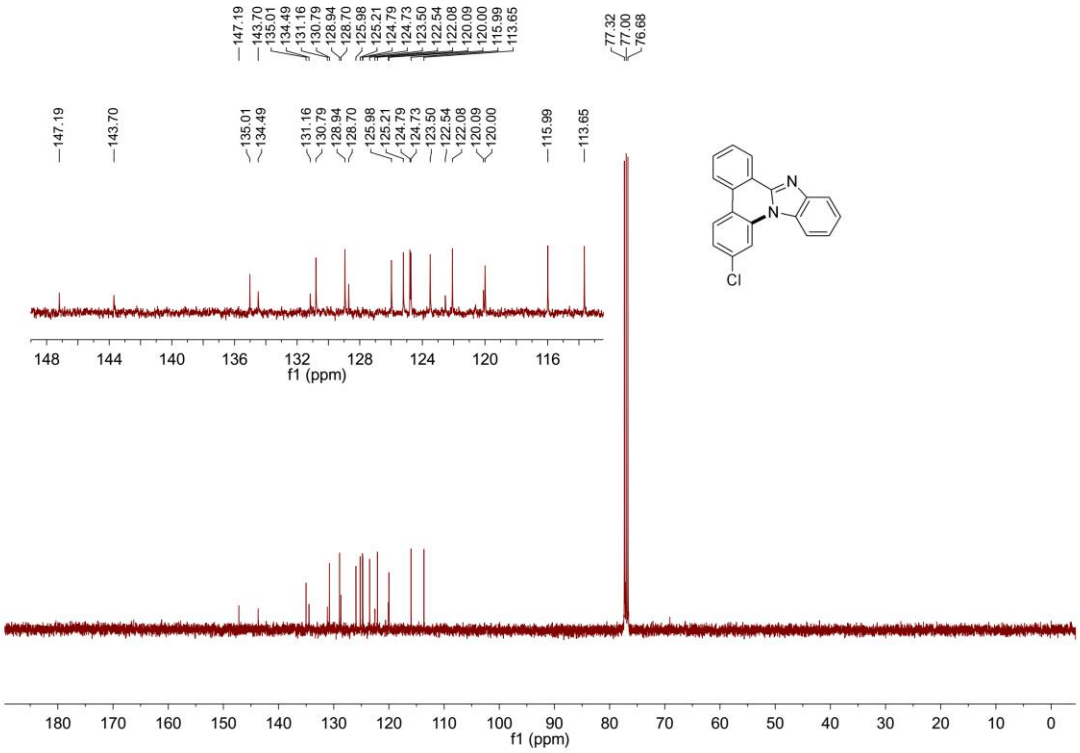

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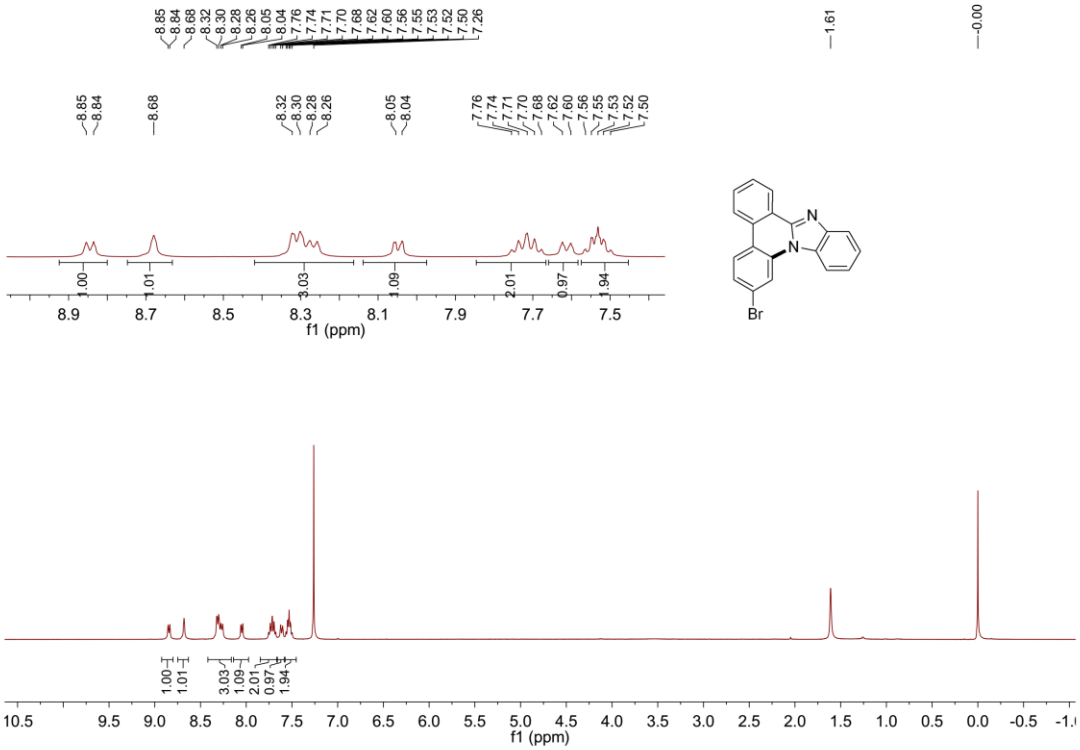

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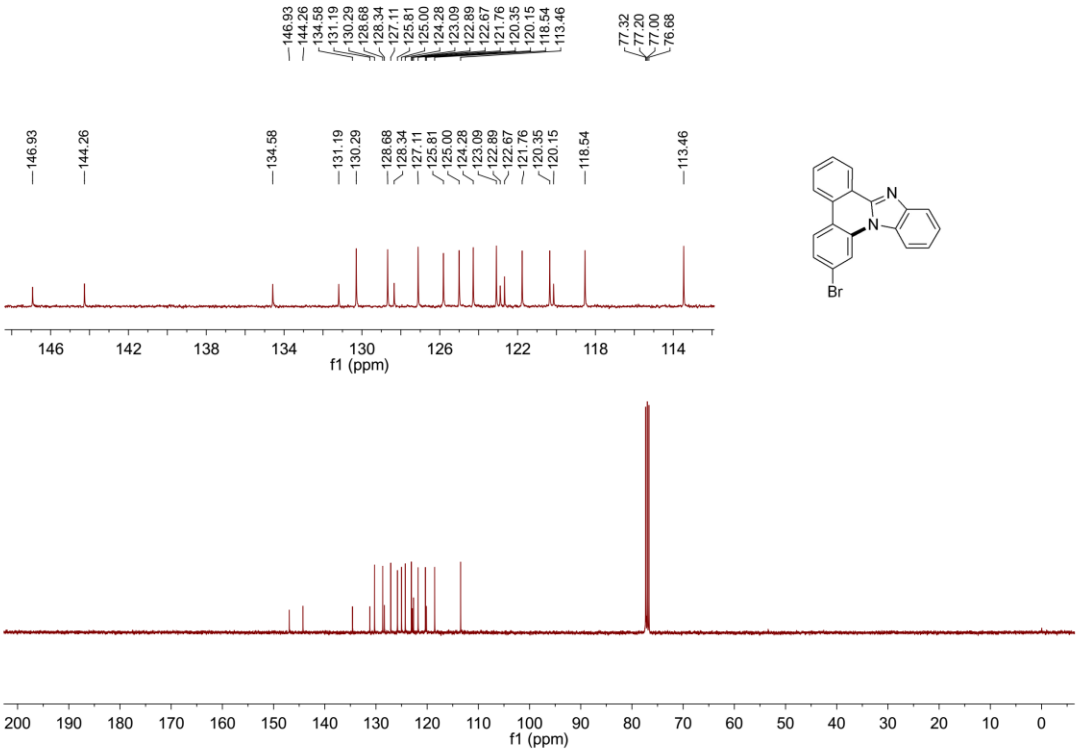

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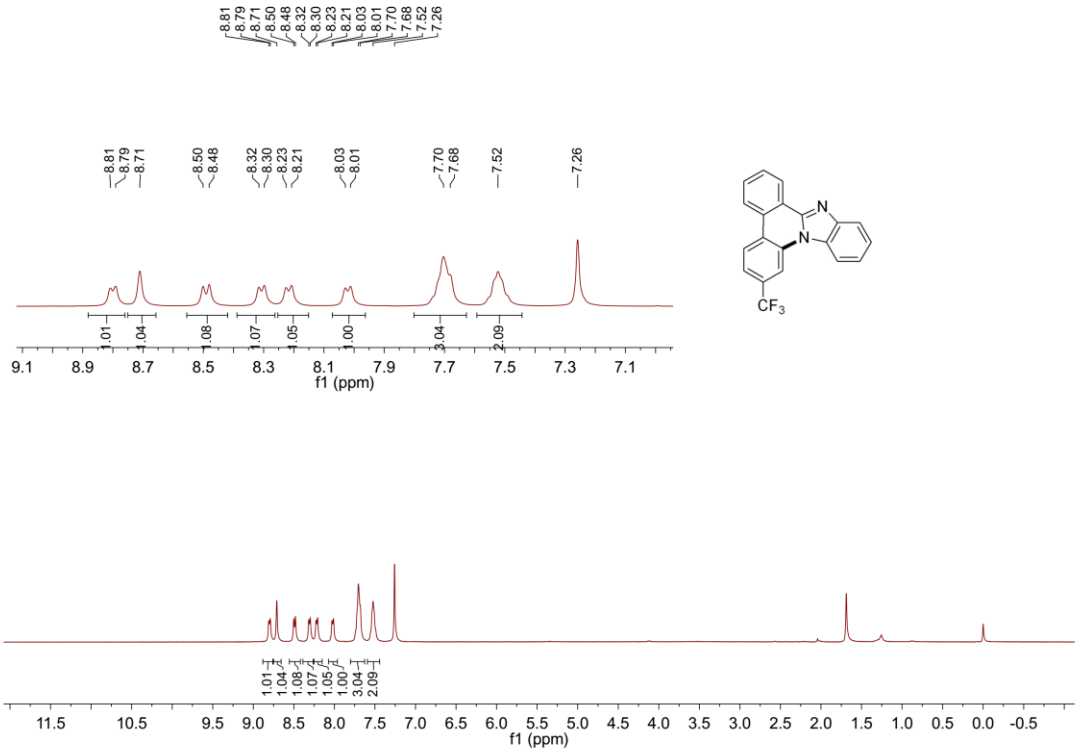

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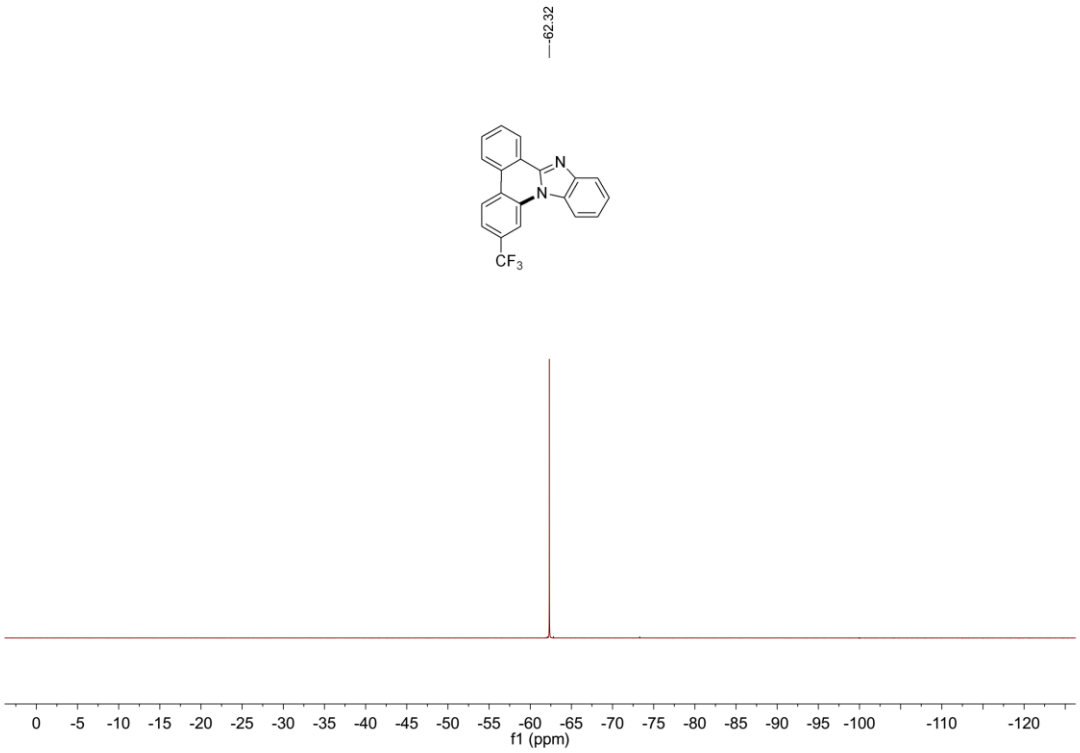

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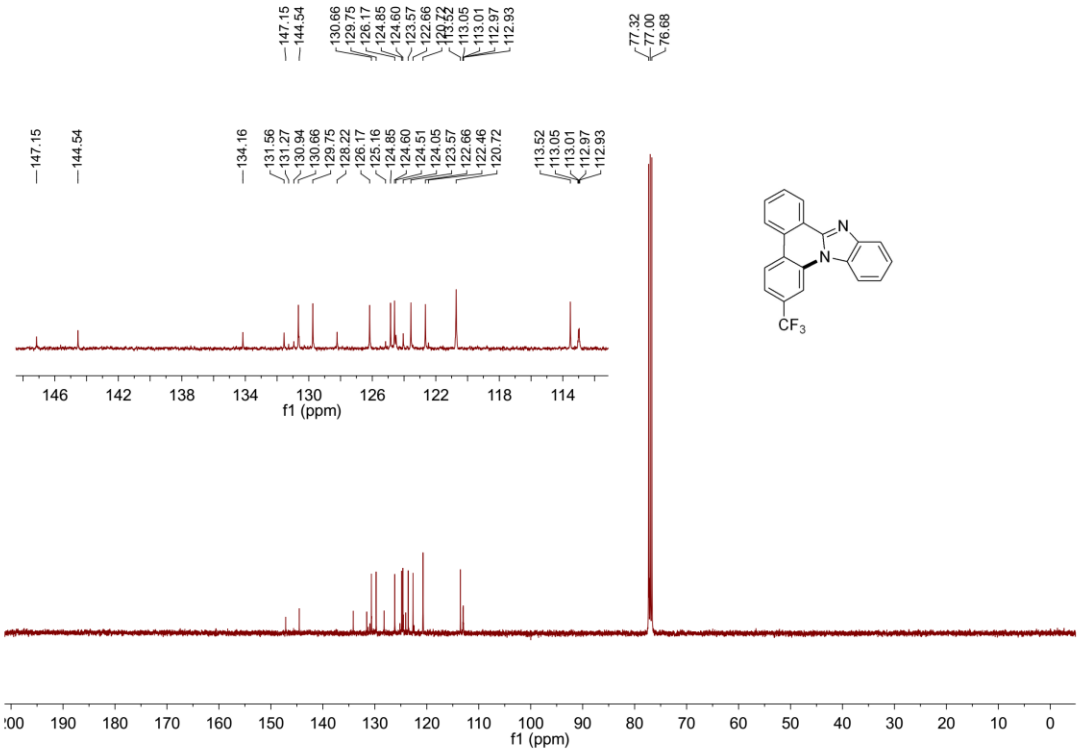

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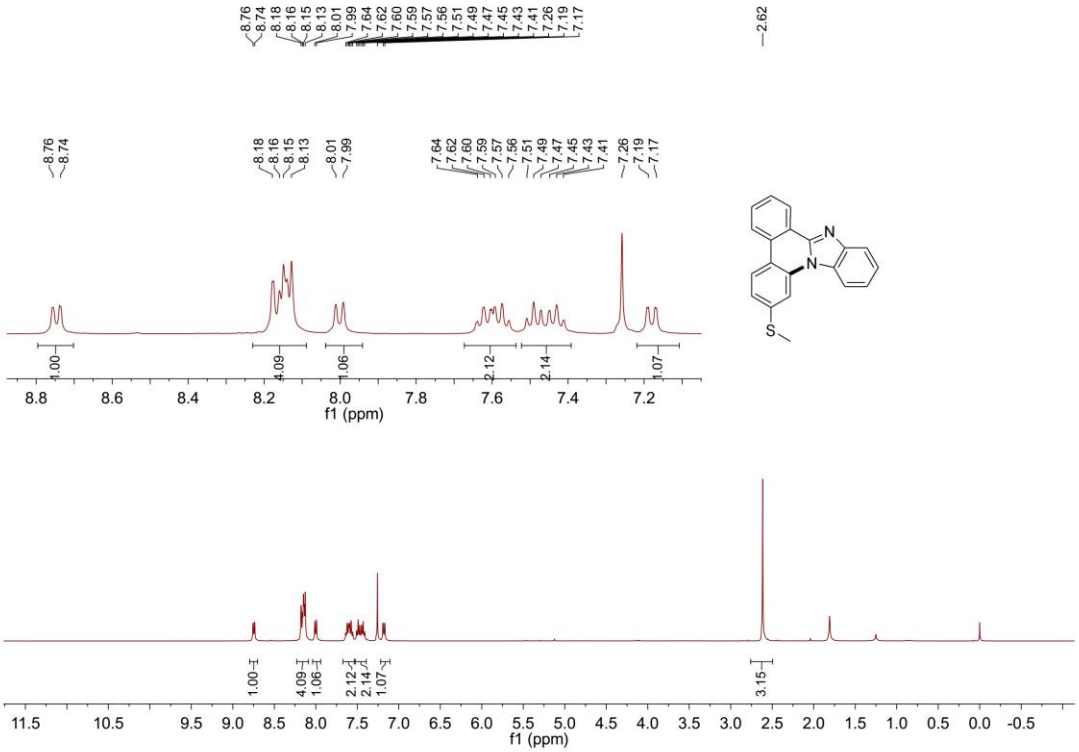

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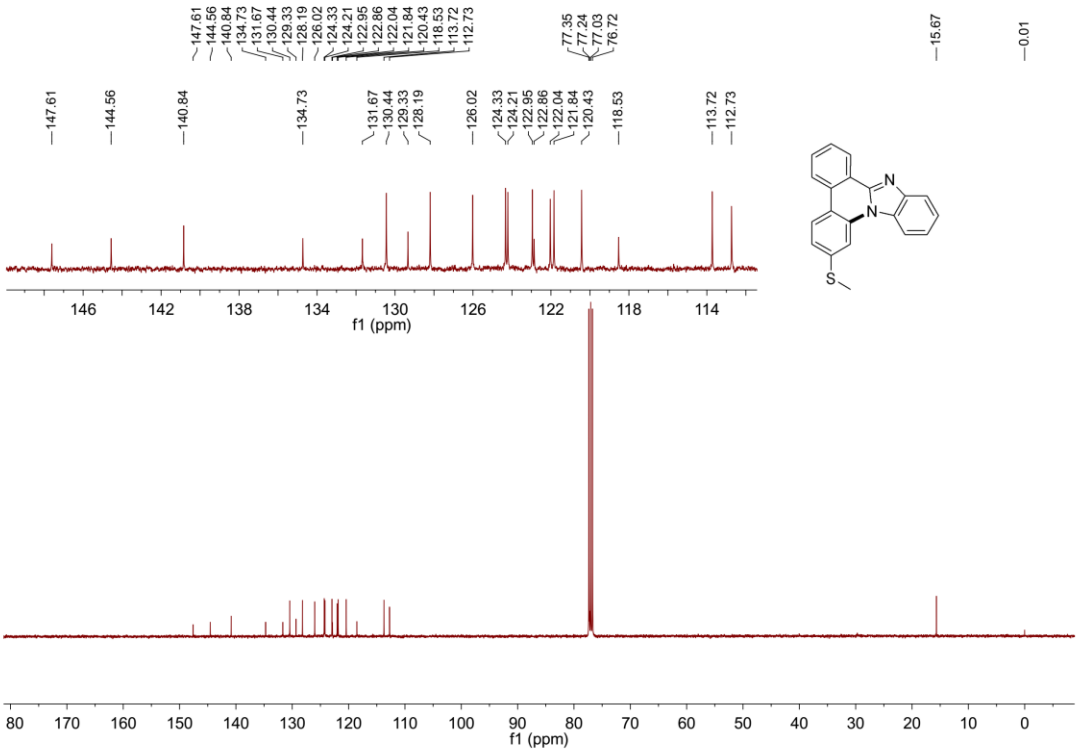

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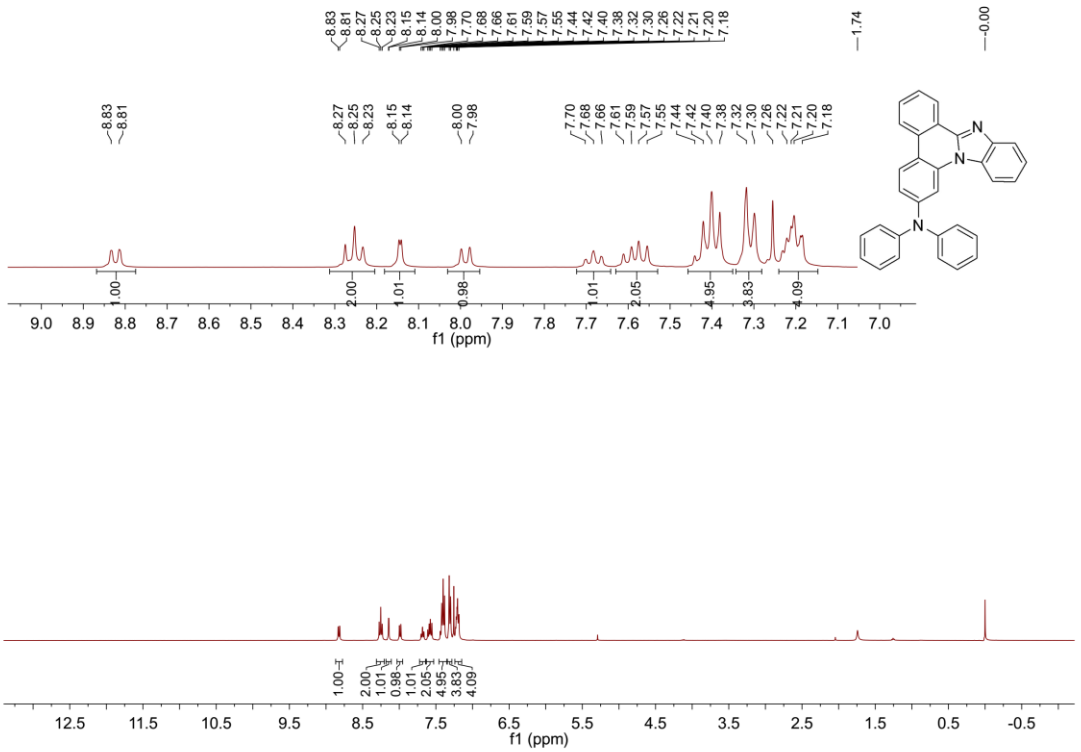

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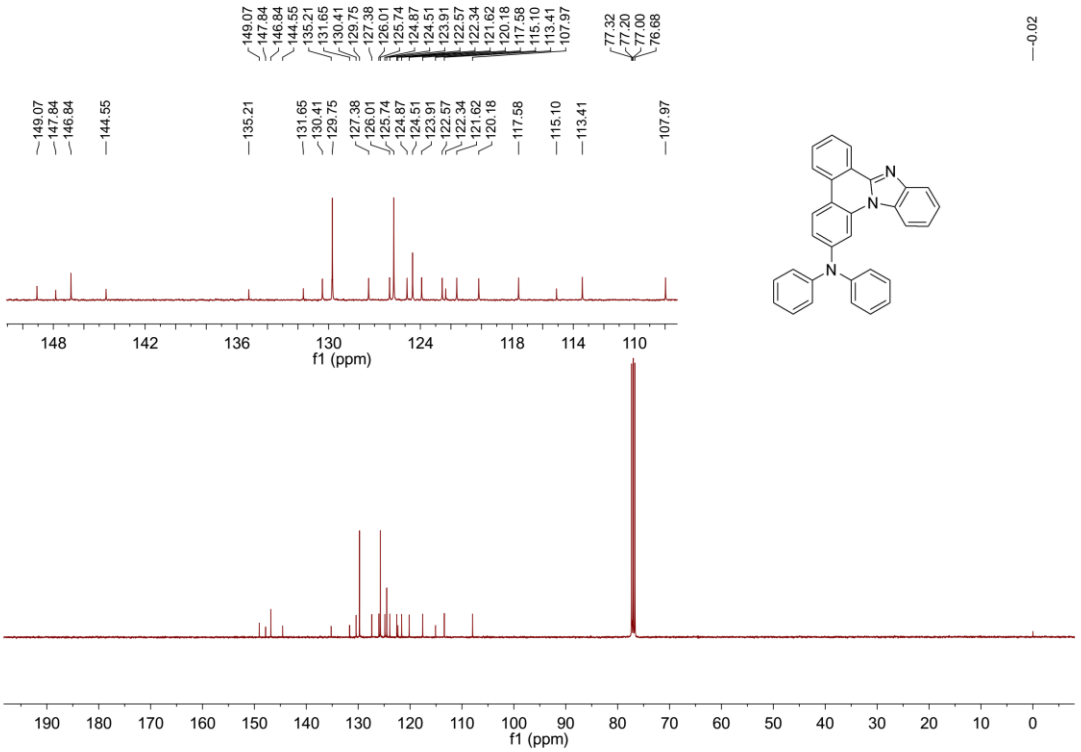

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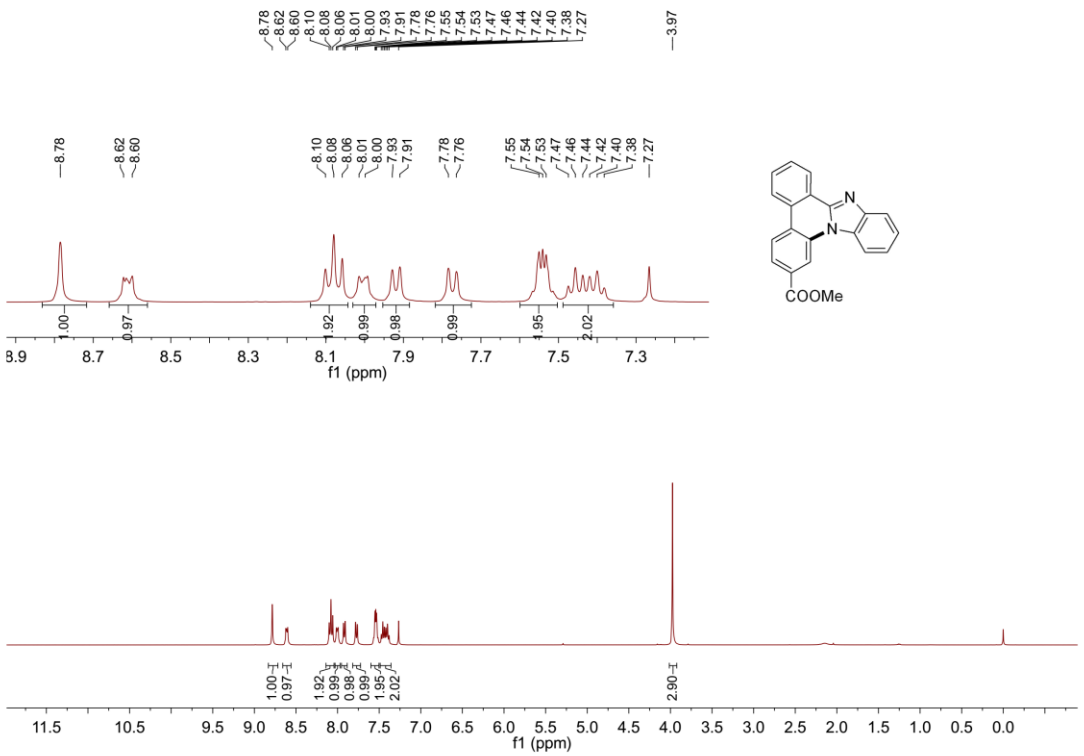

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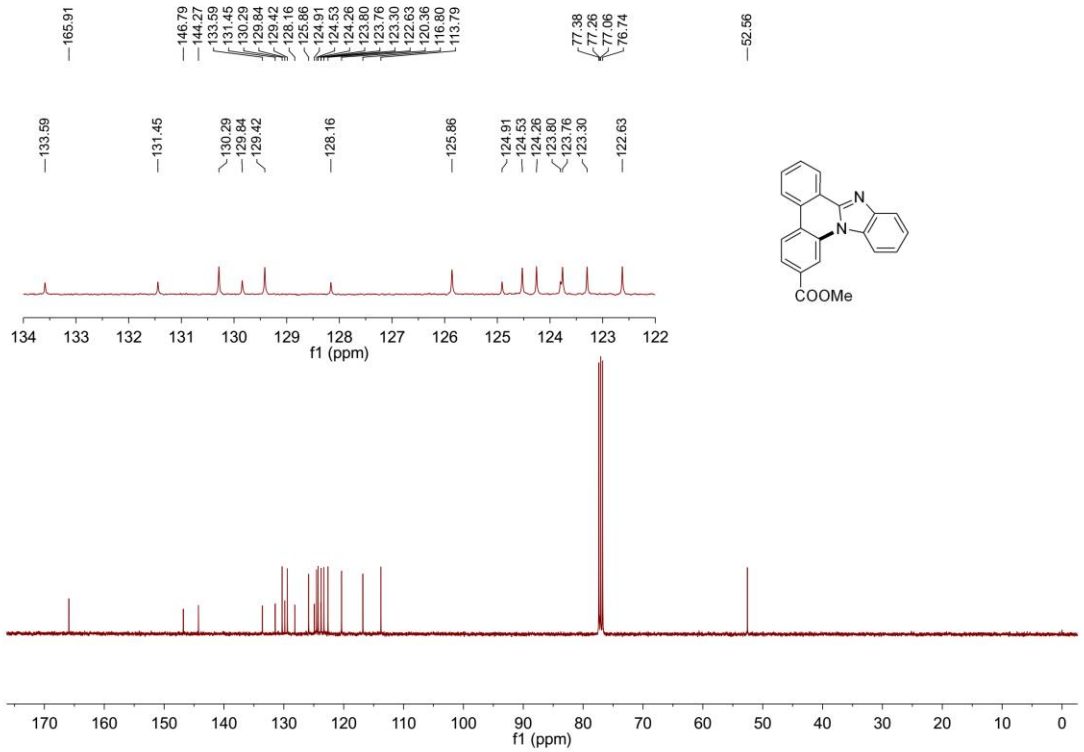

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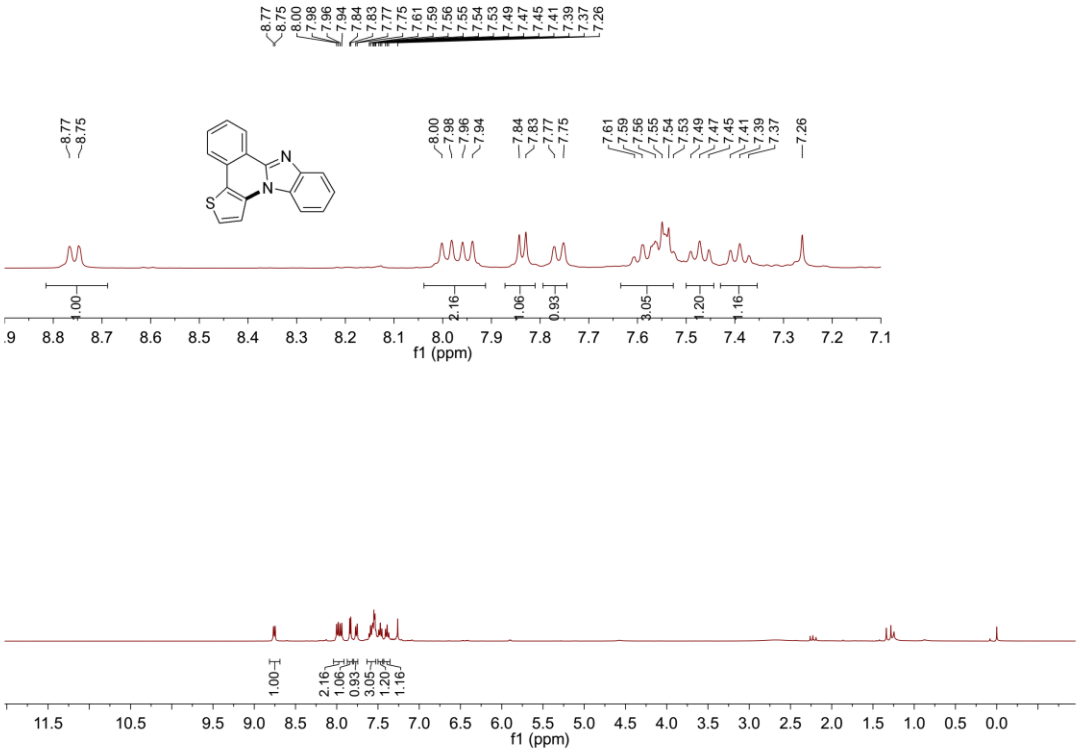

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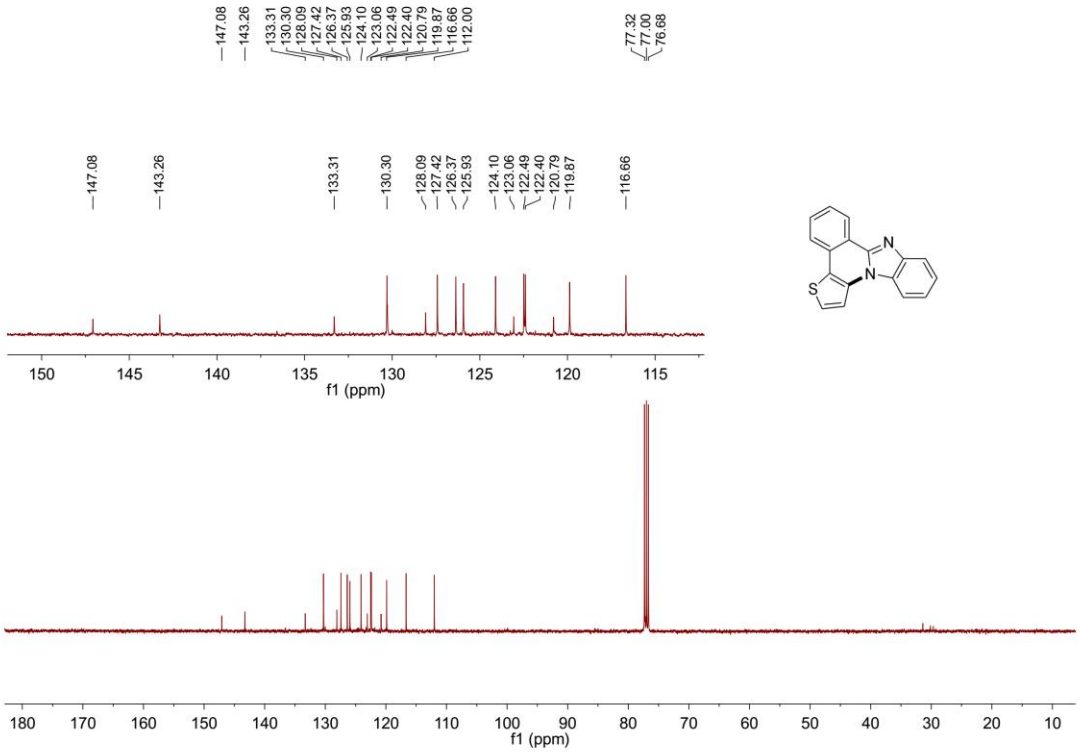
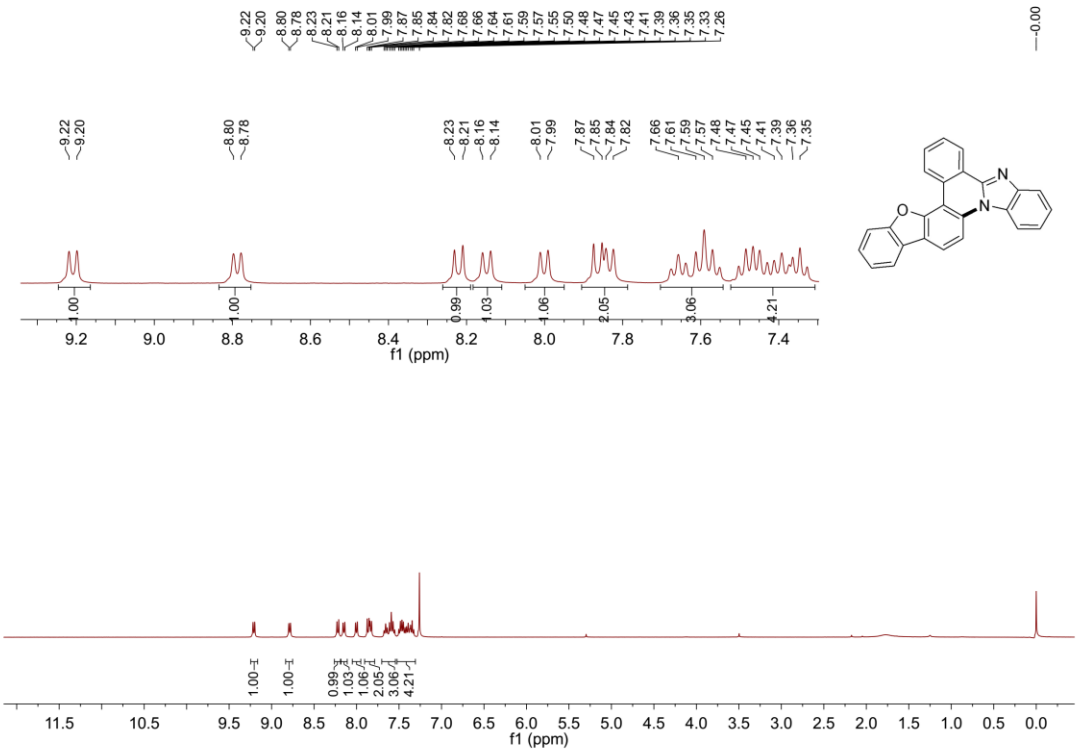


2p ^{1}H NMR



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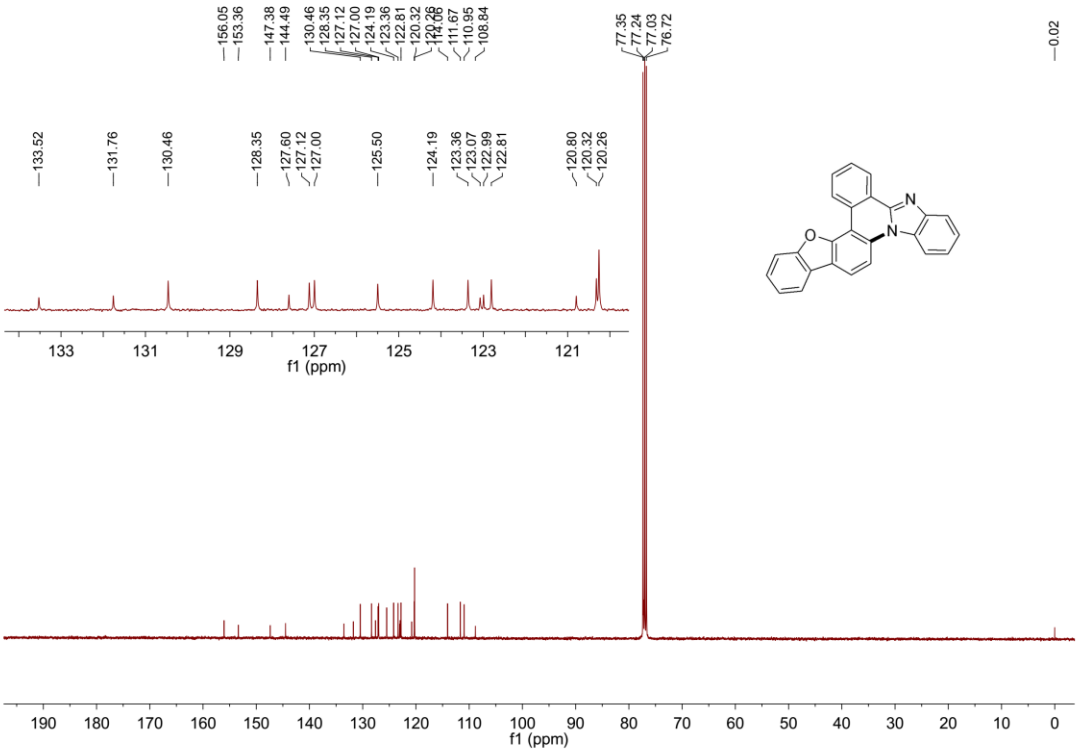

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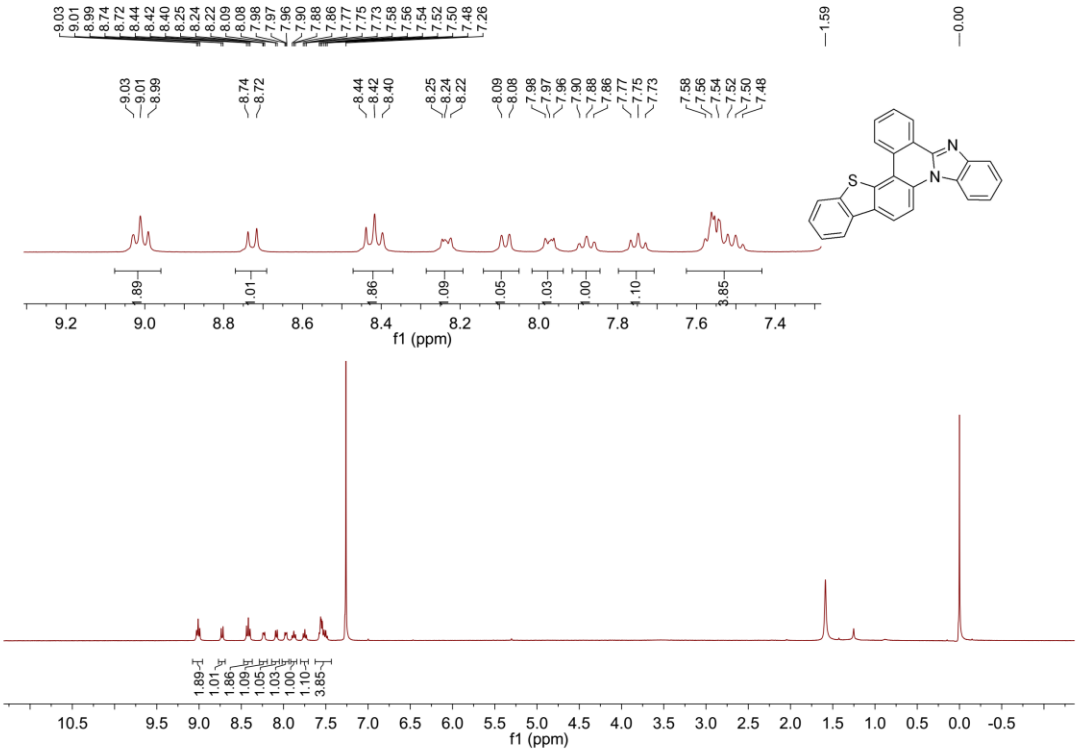

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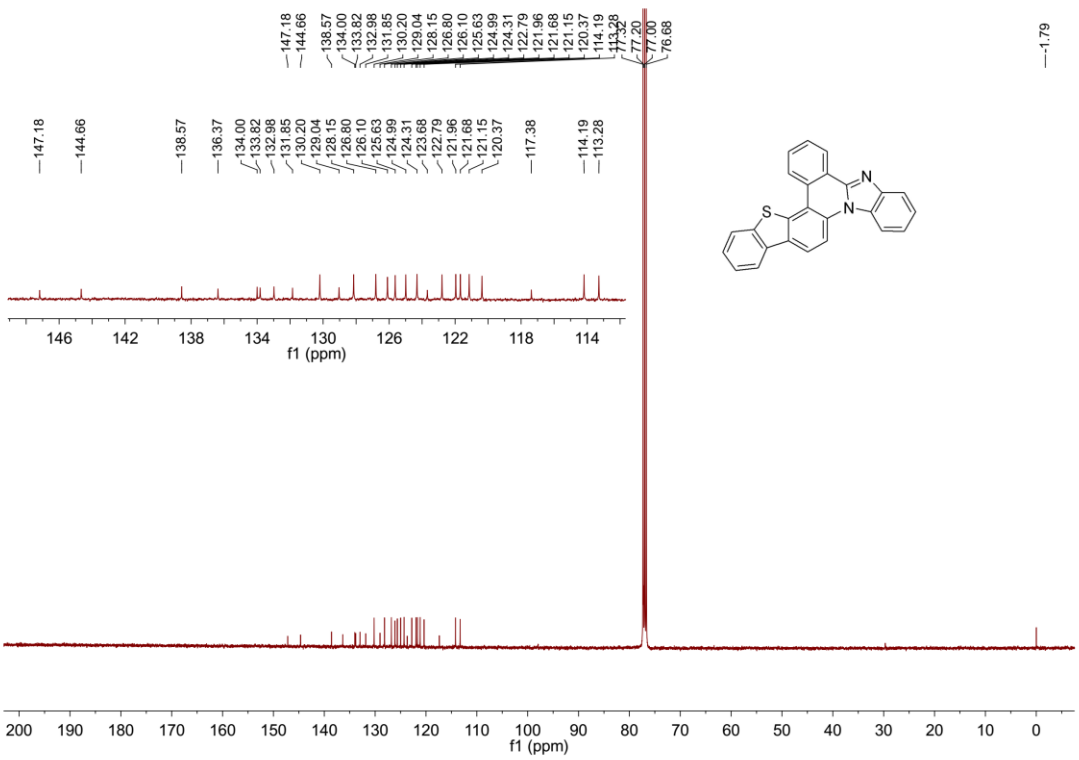

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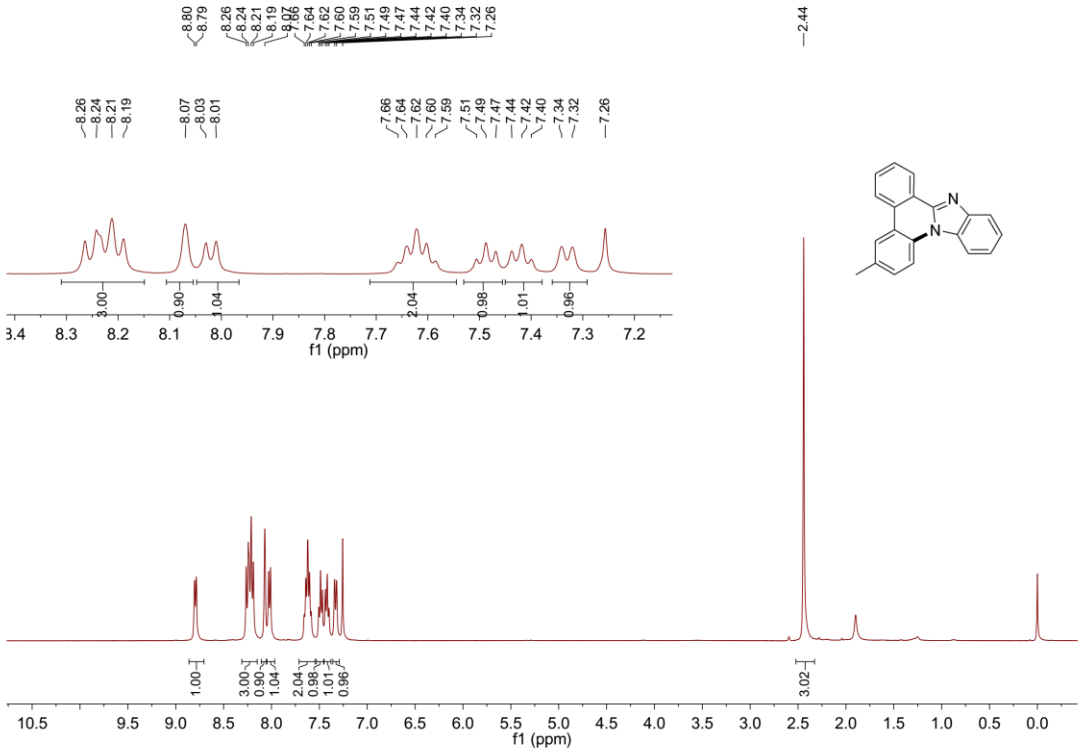

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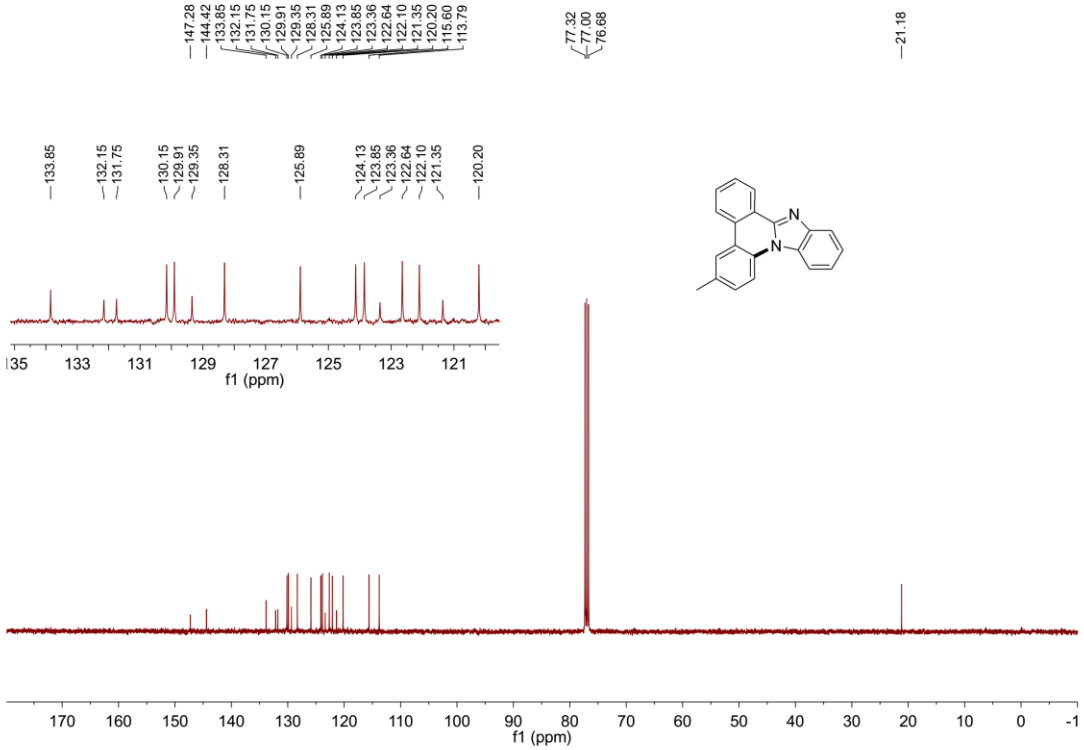

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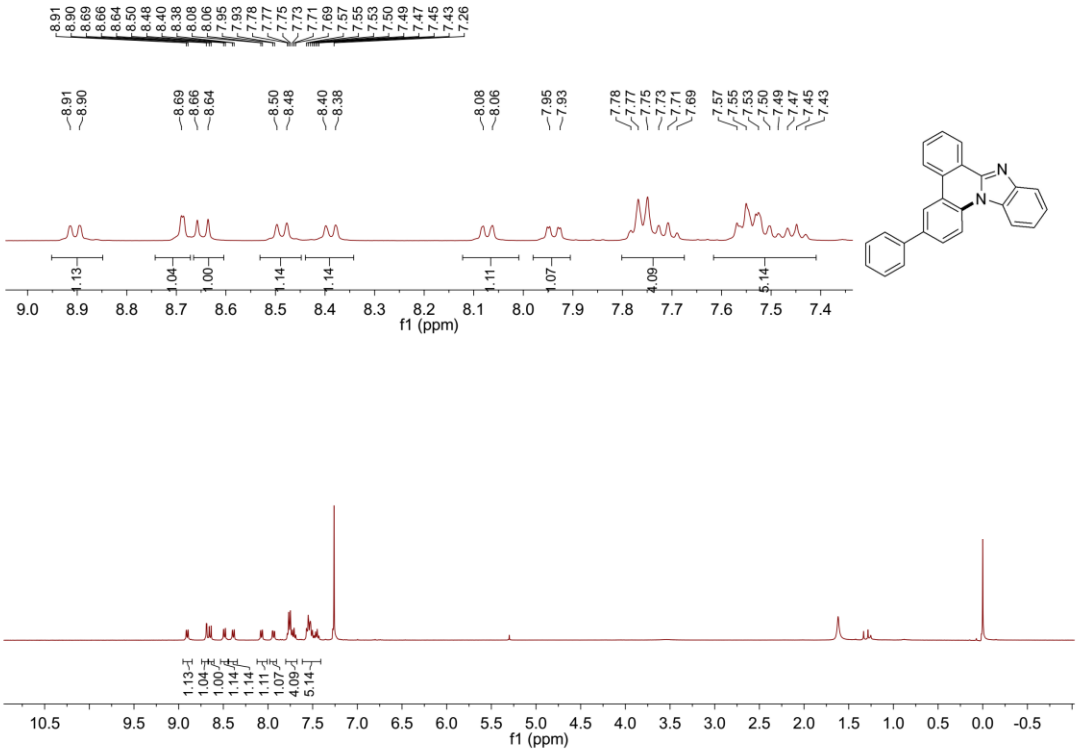

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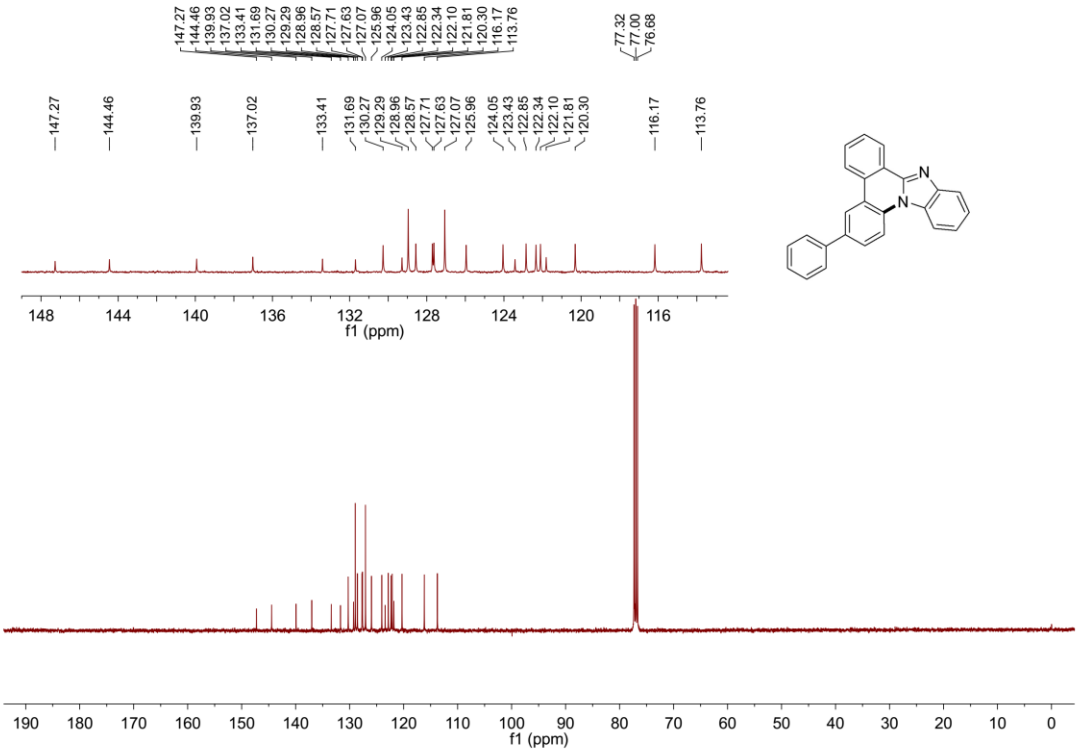

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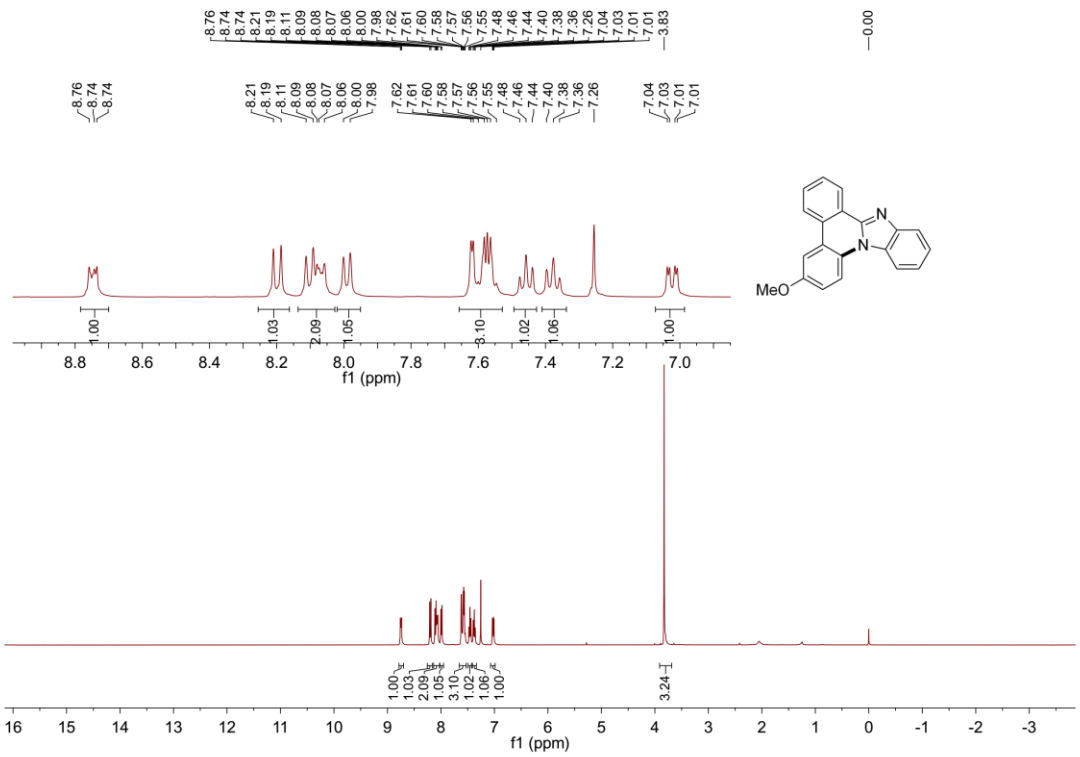

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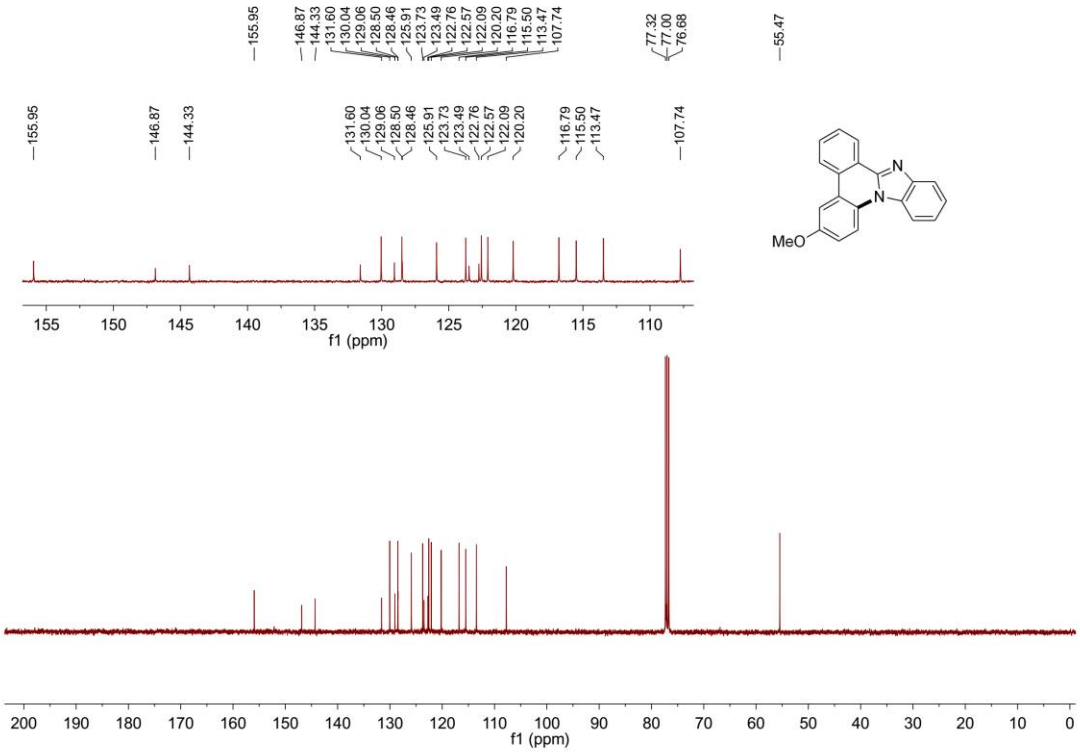

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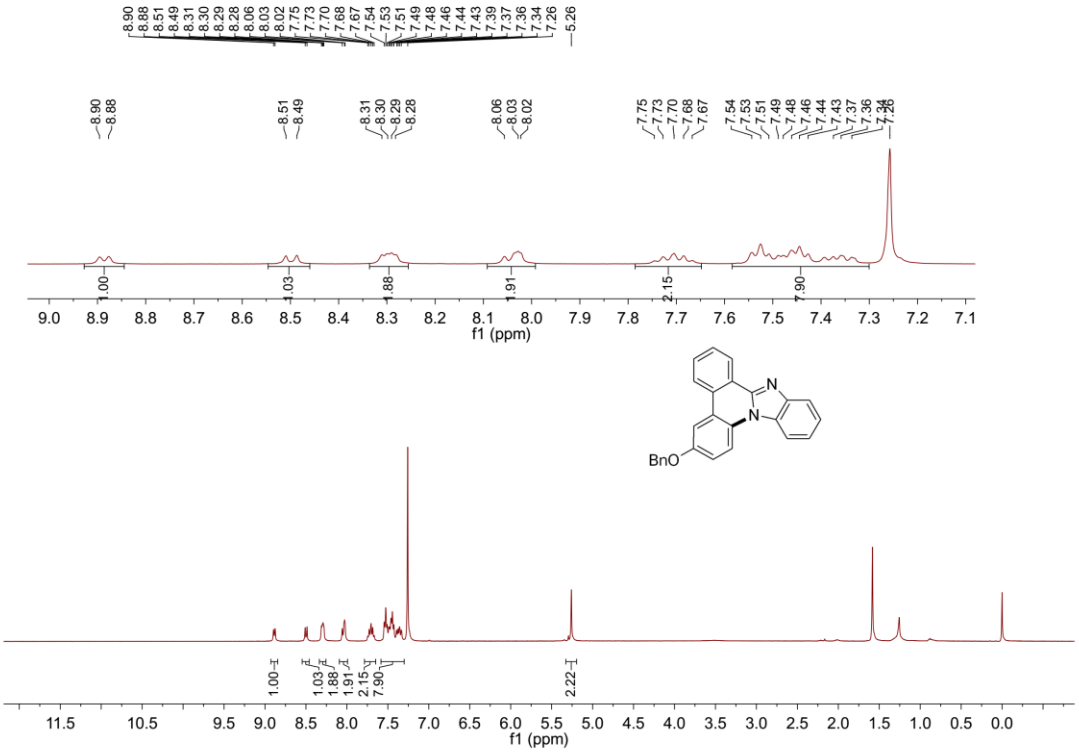

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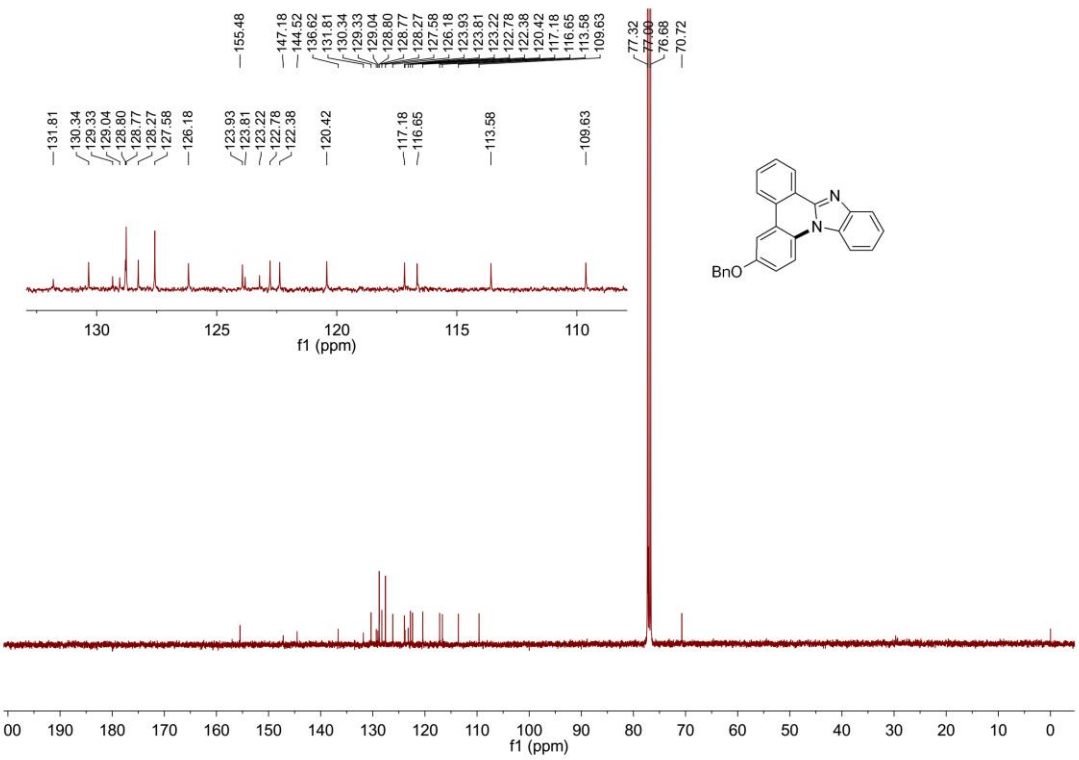

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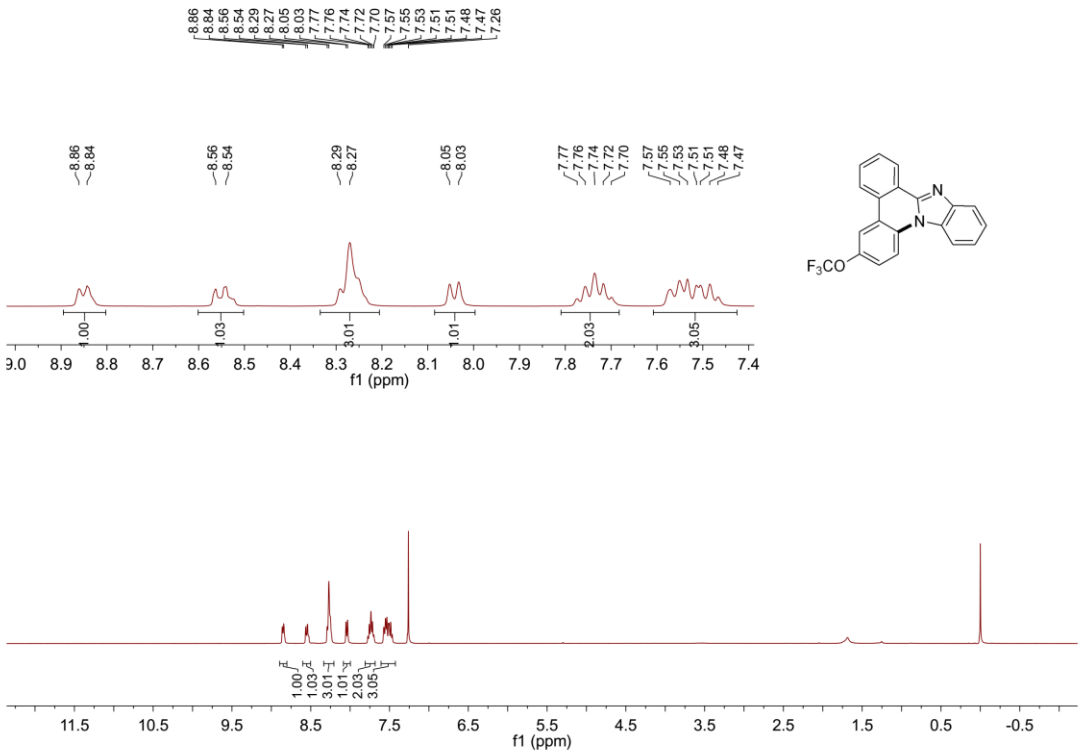

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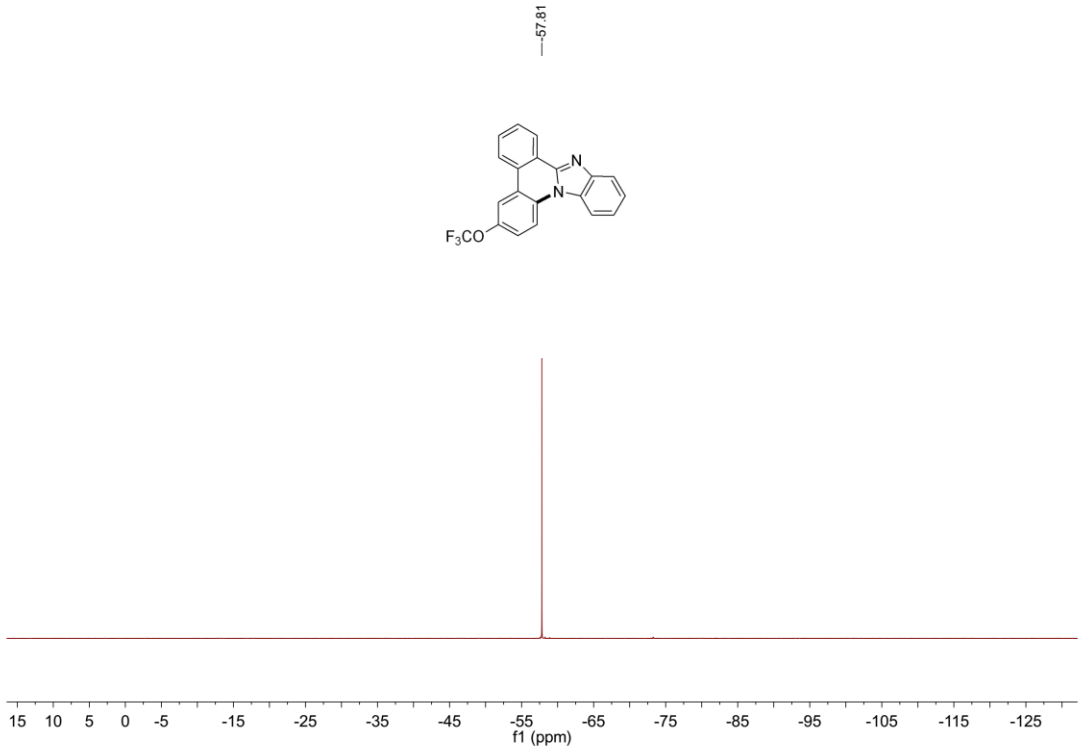

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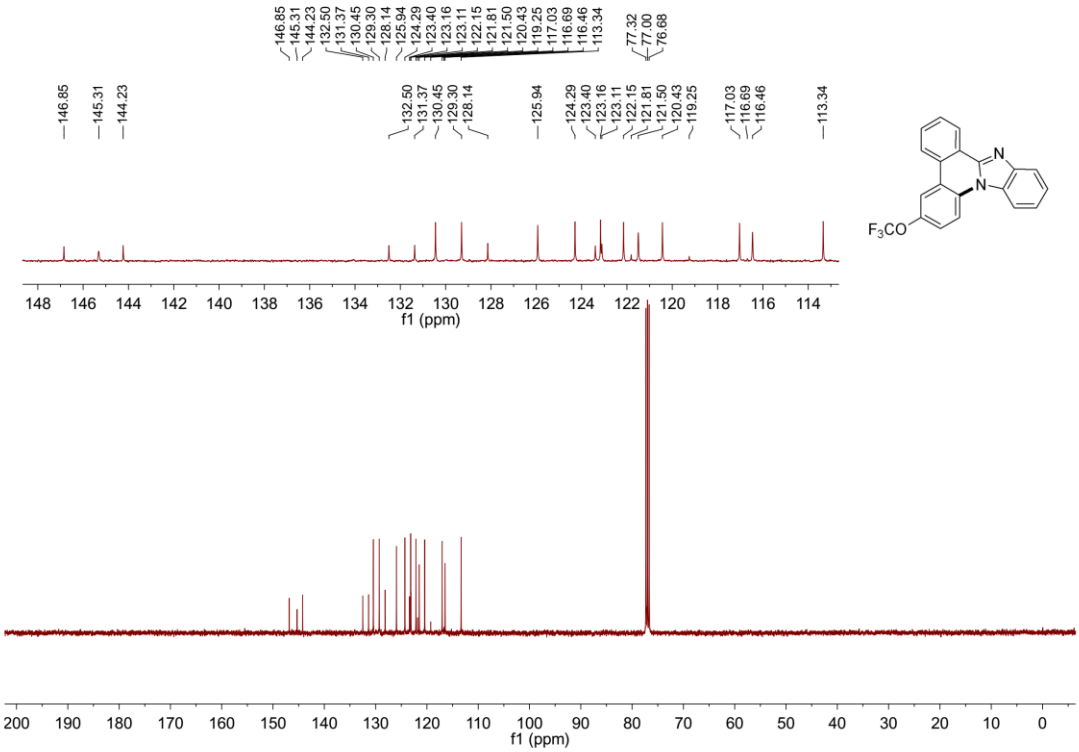

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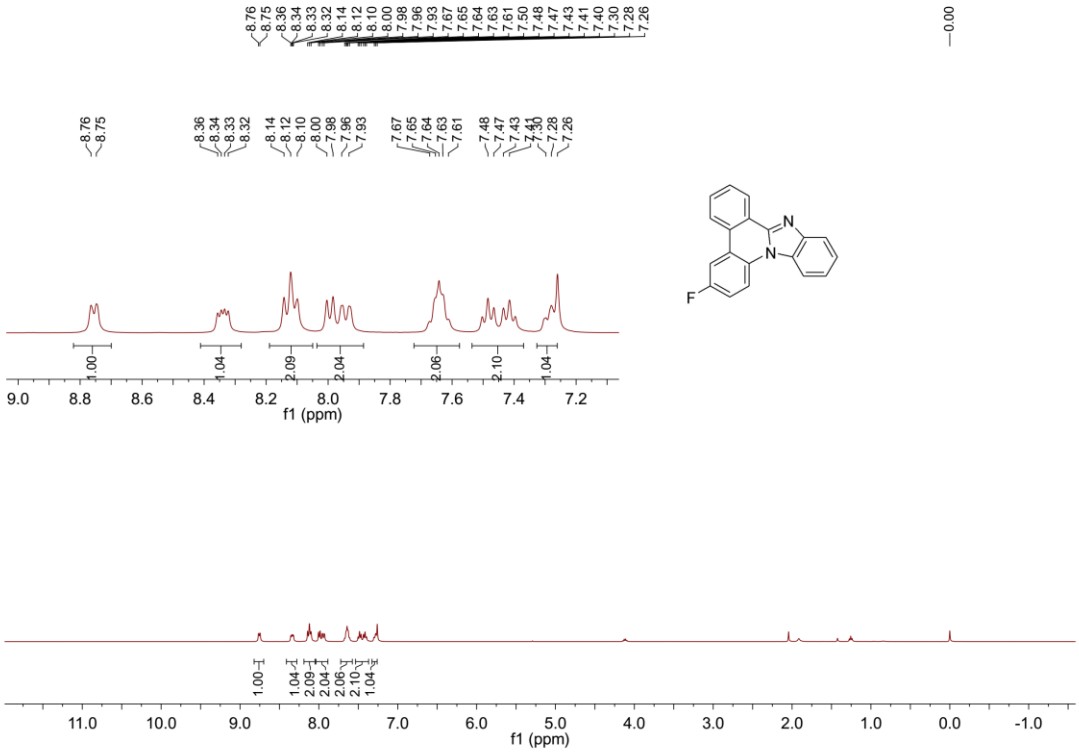

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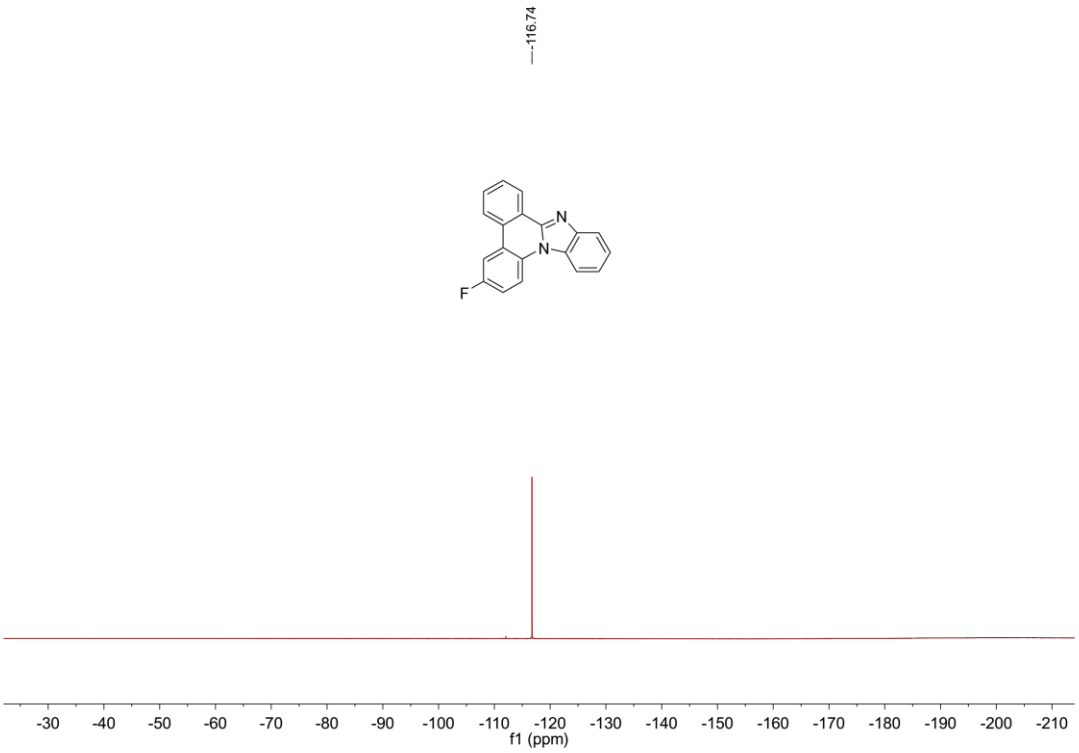

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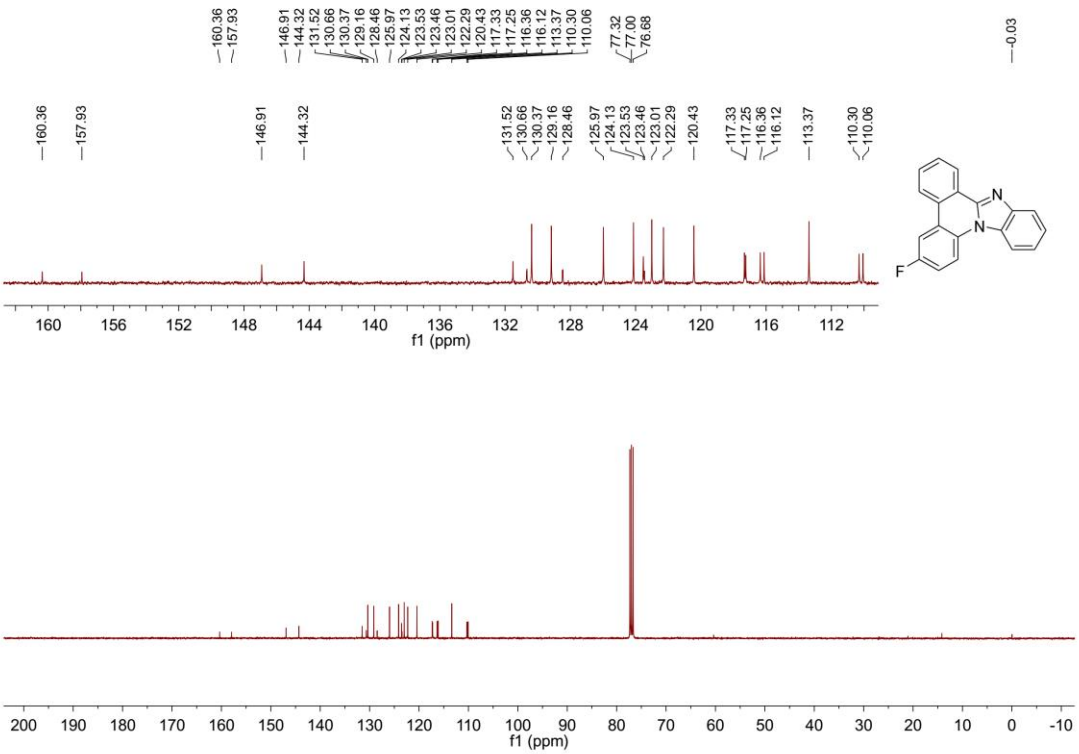

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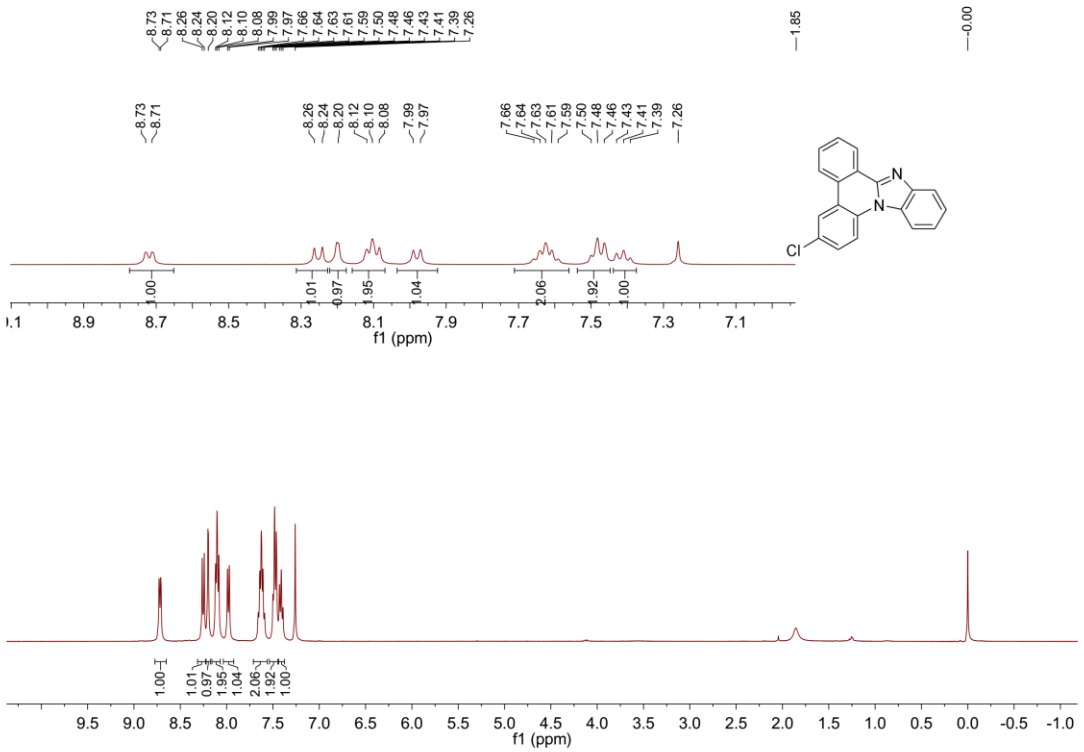

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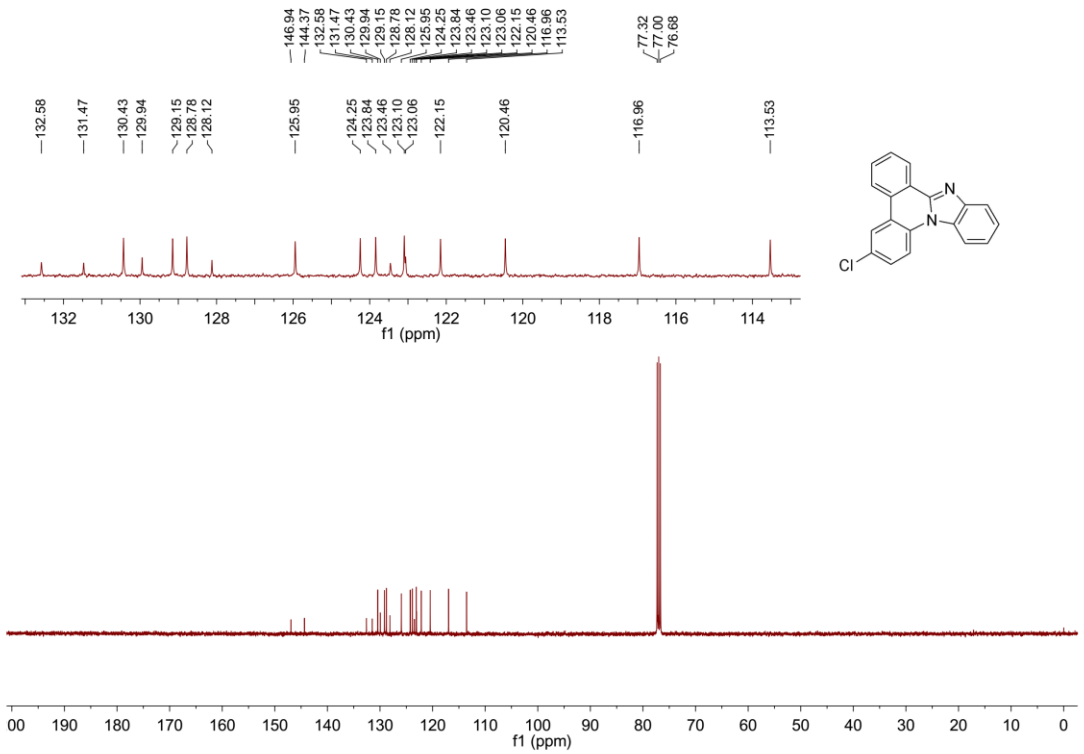

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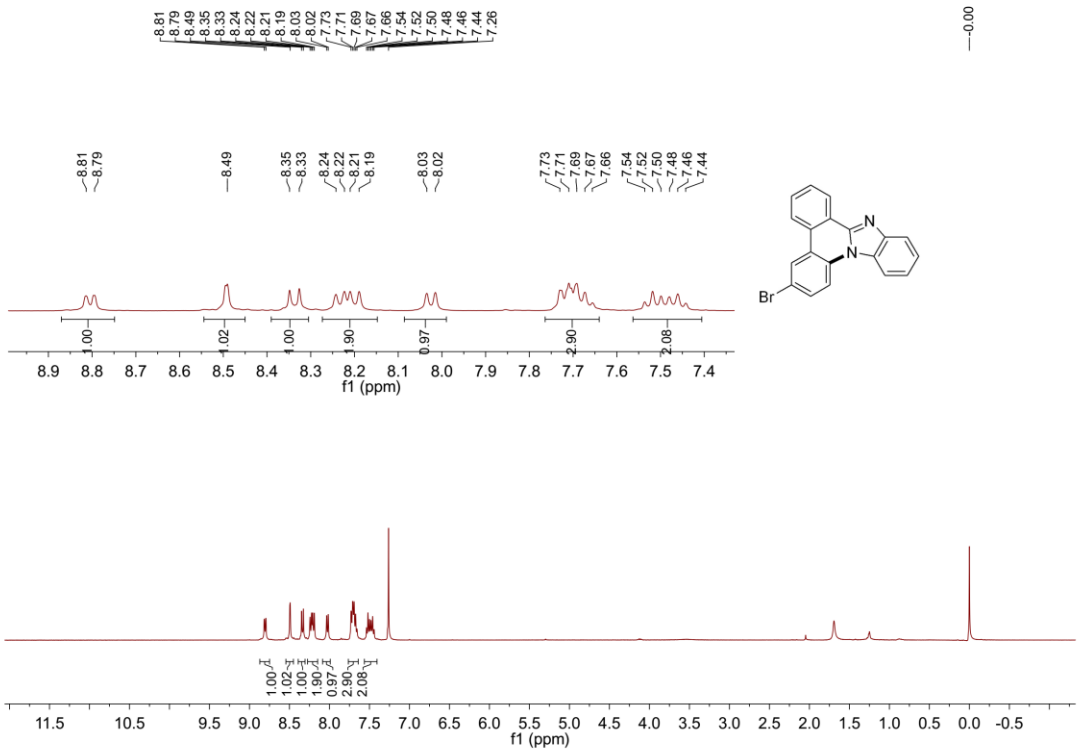

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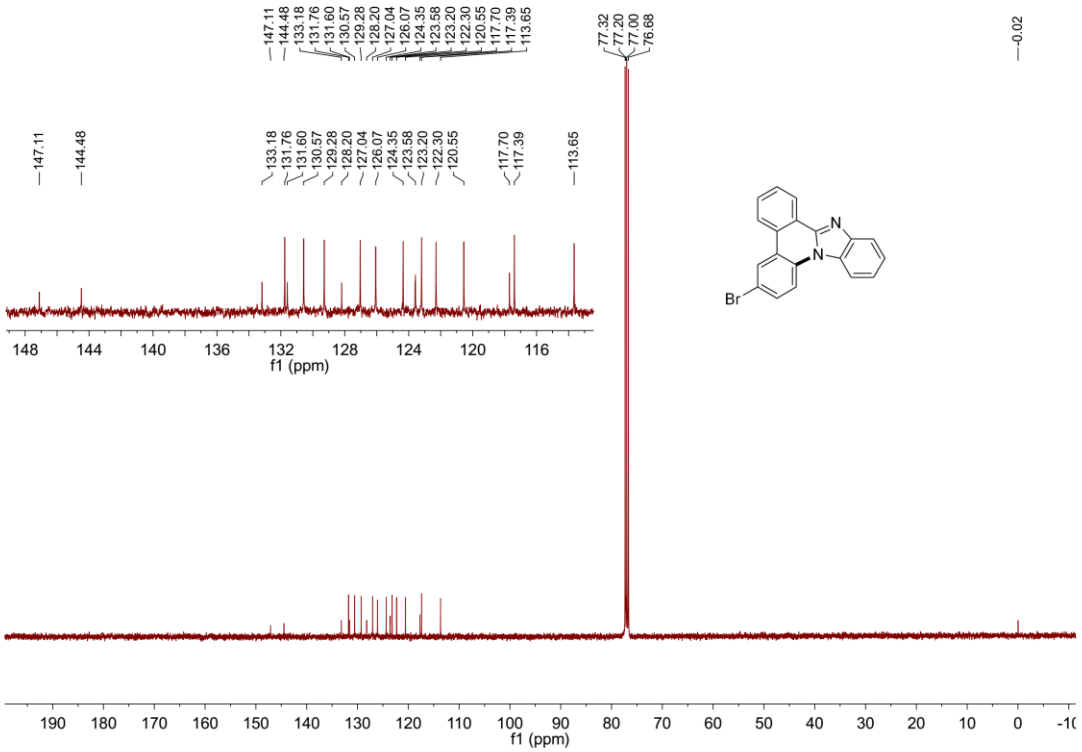

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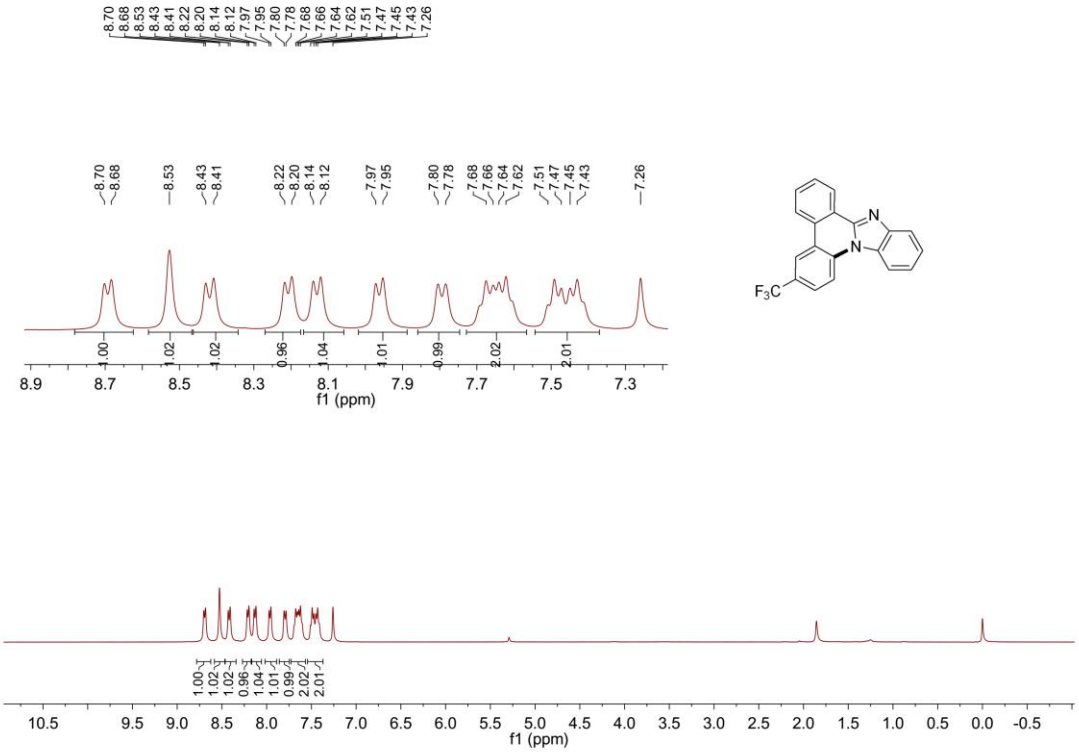

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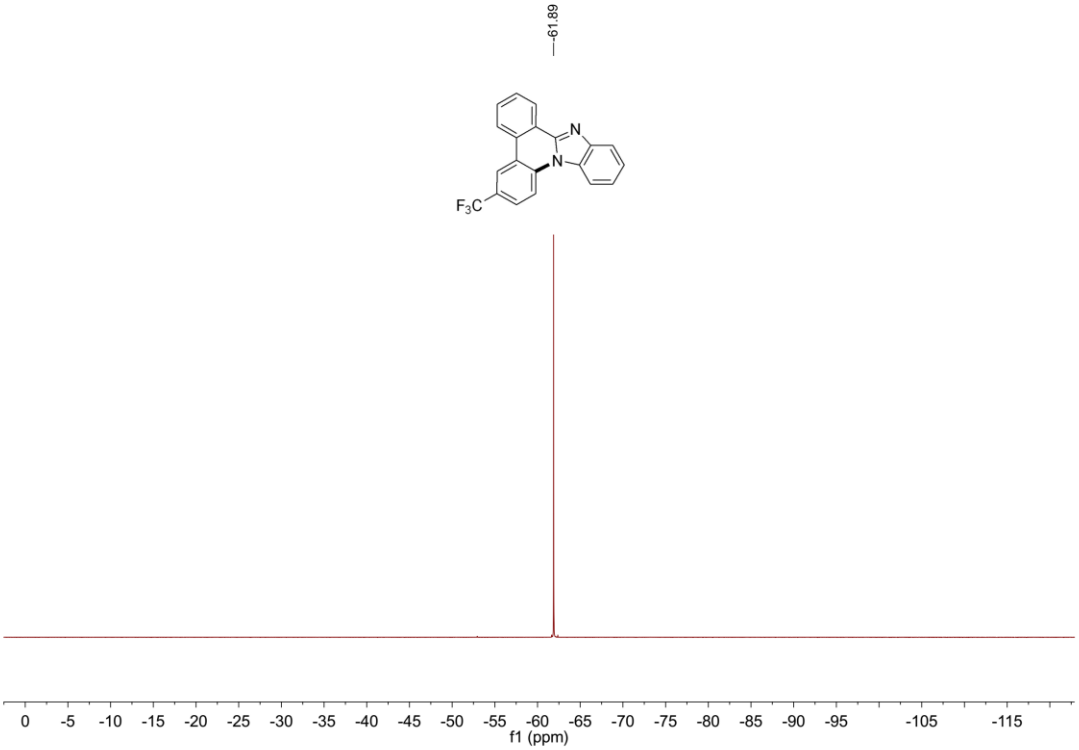

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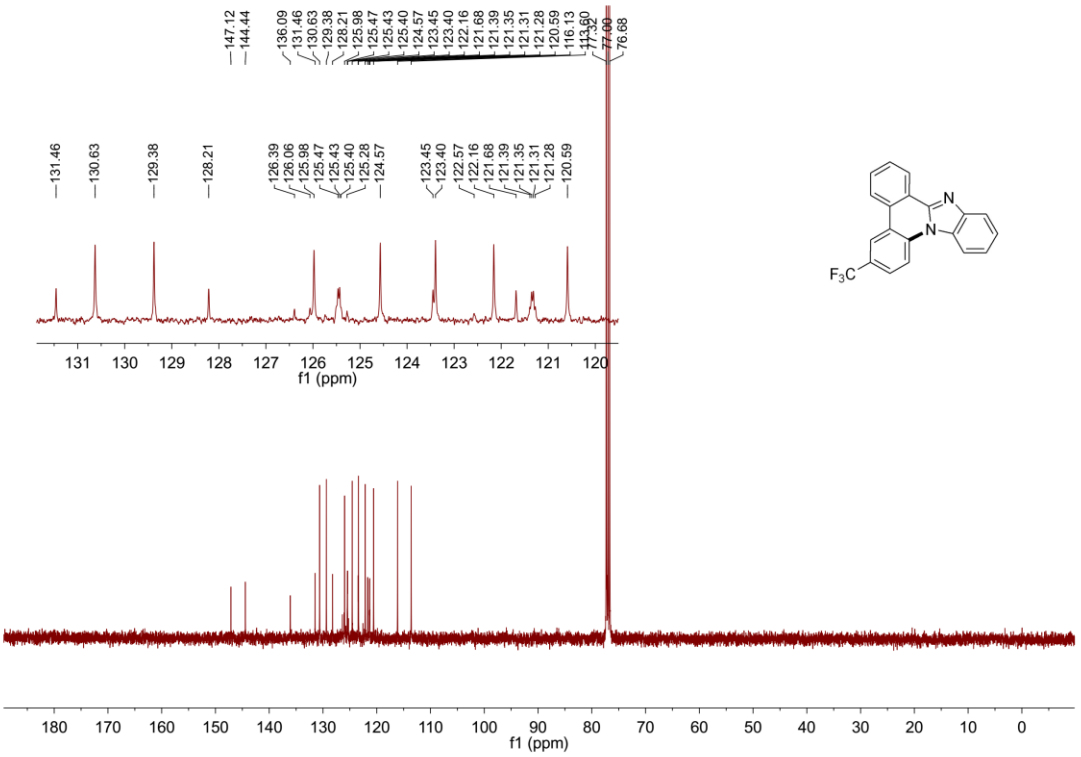

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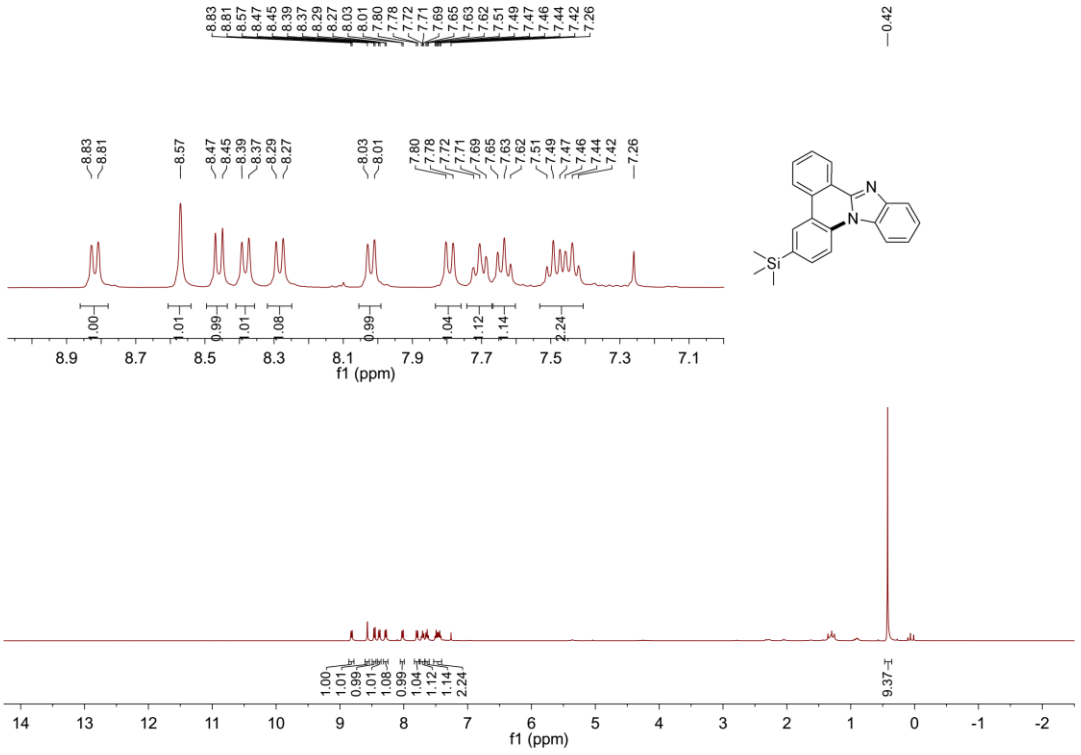

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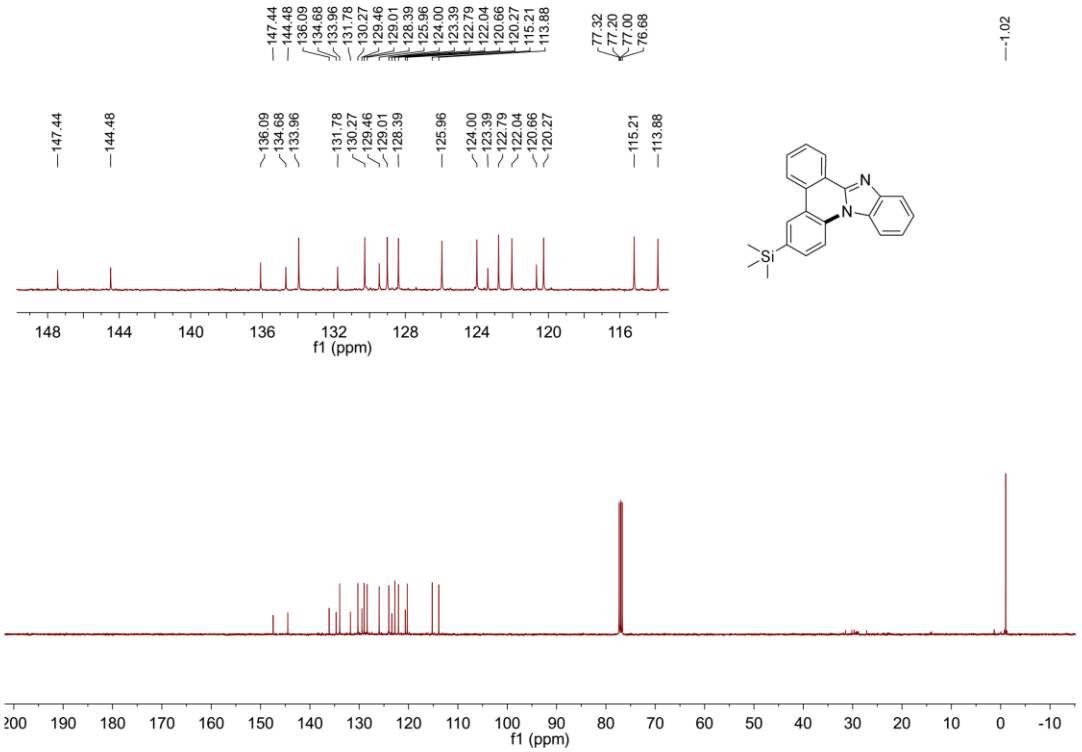

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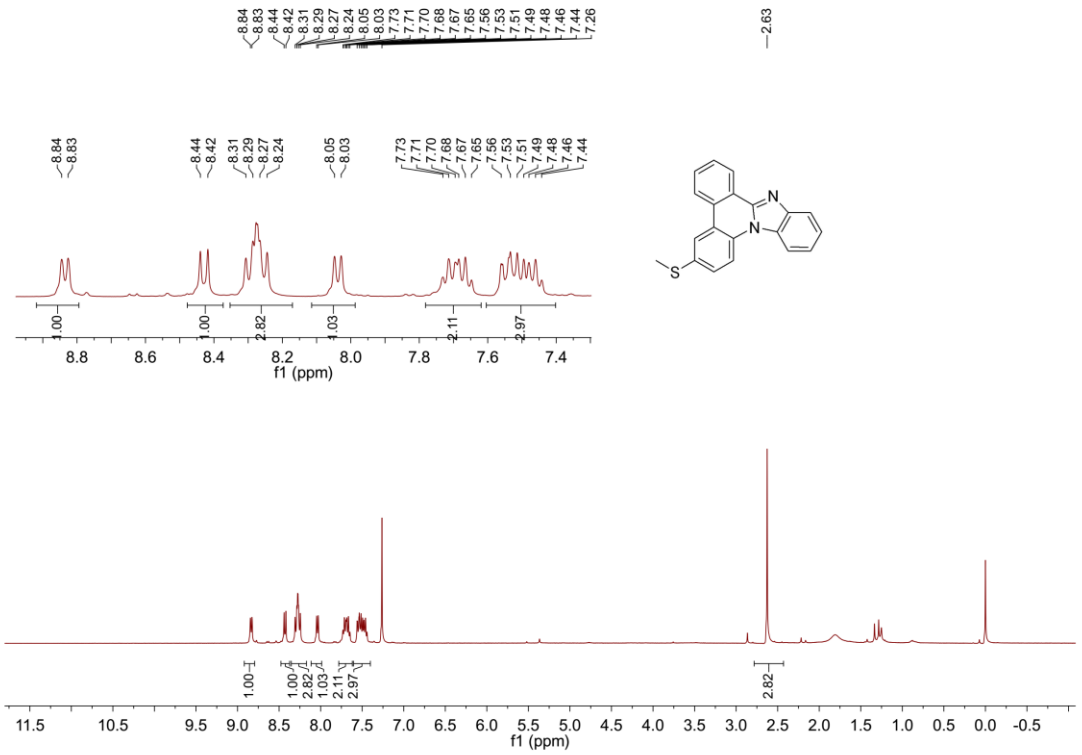

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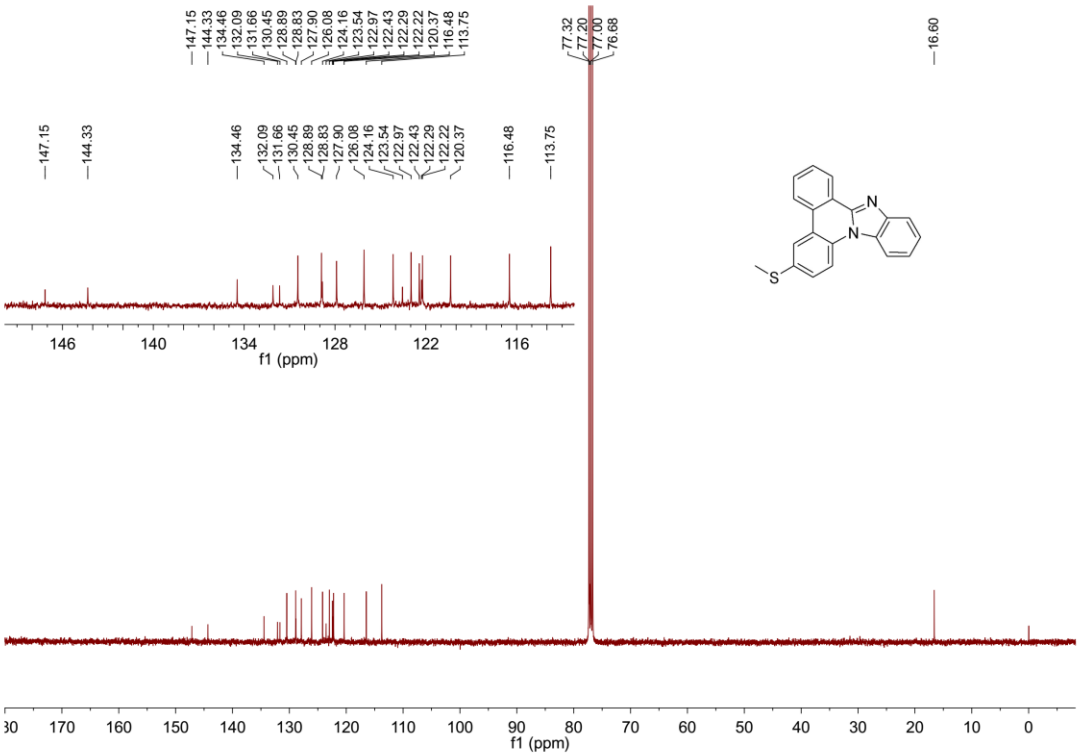

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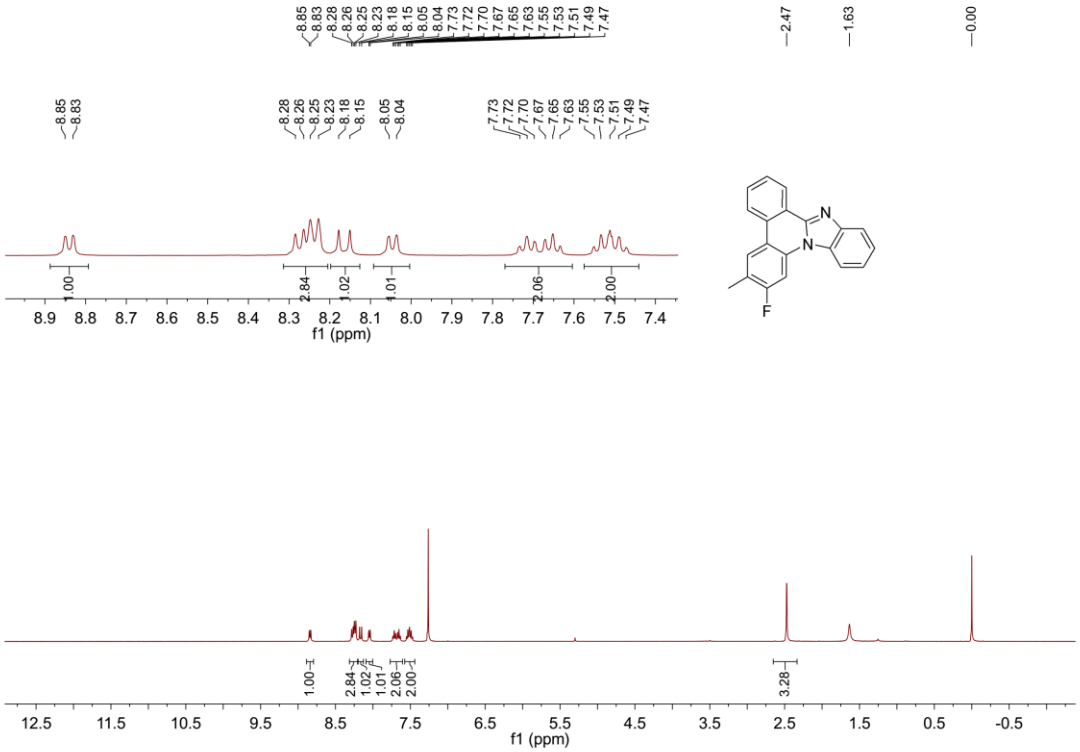

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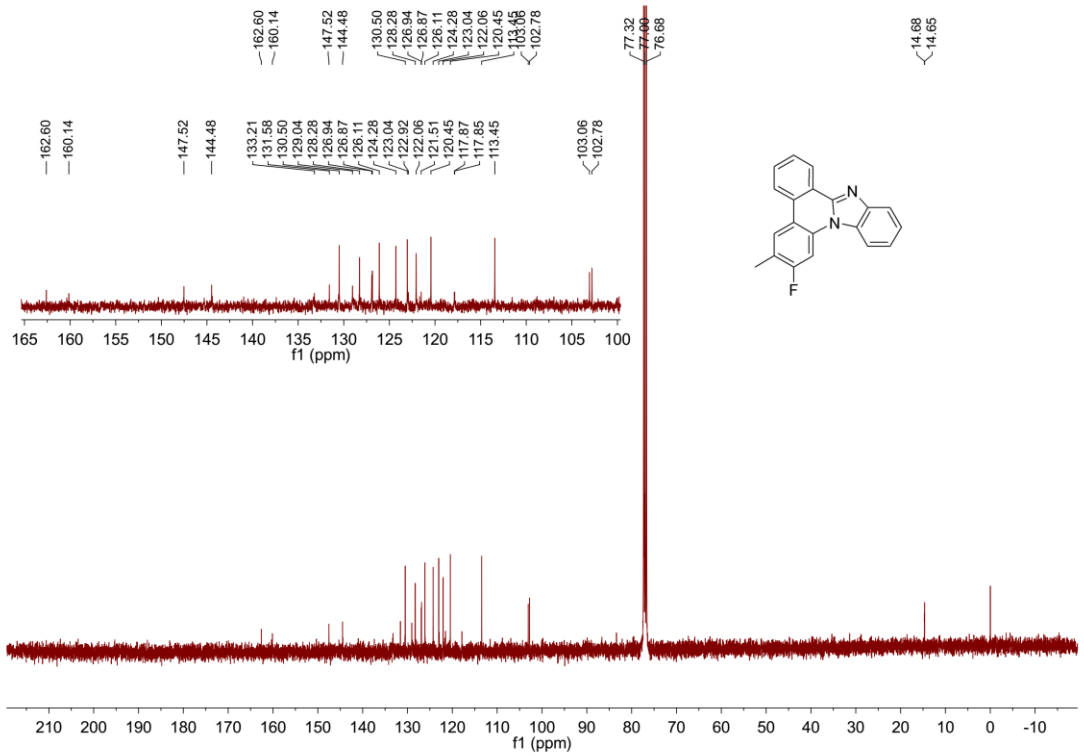

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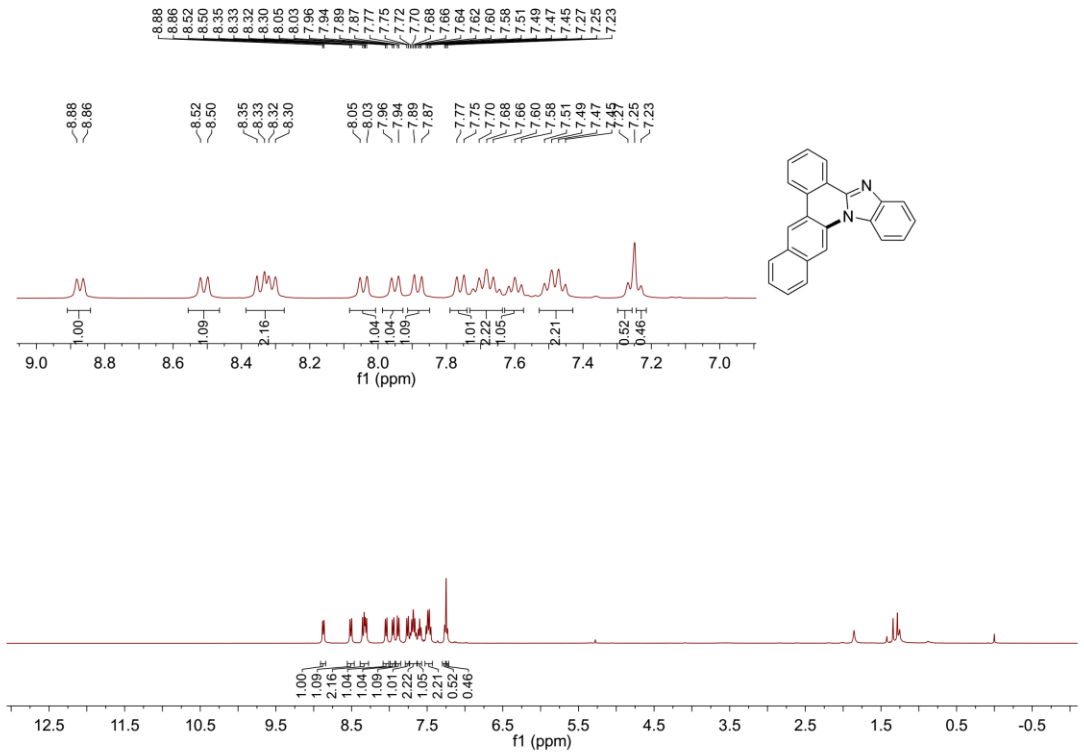

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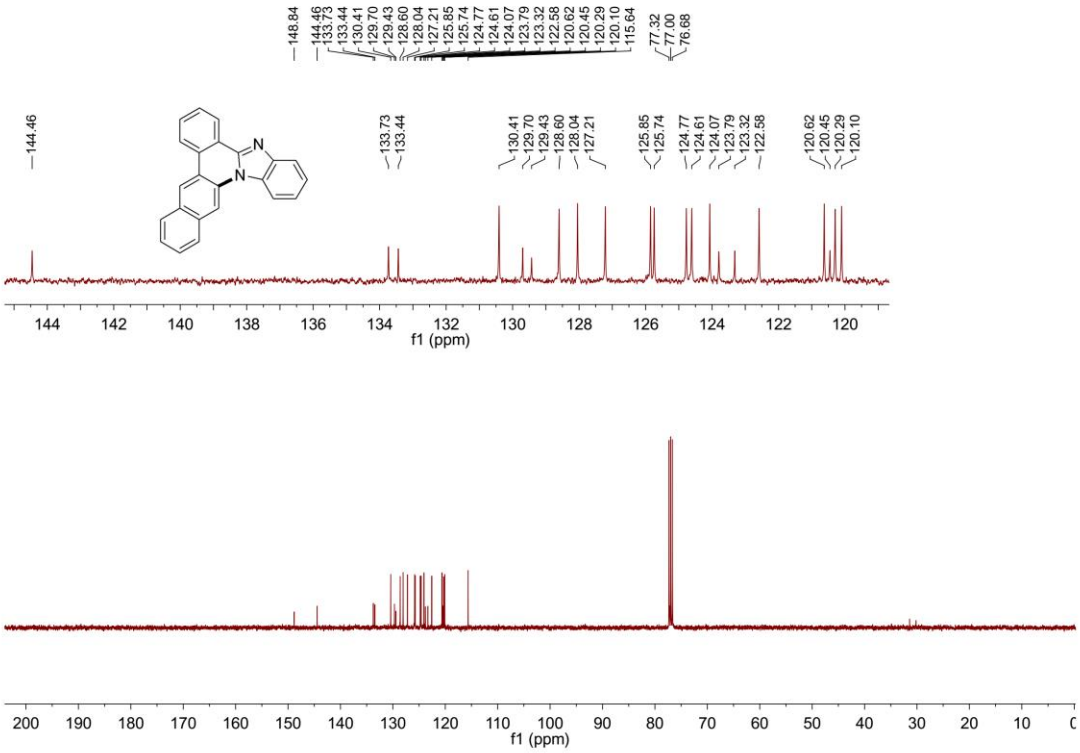

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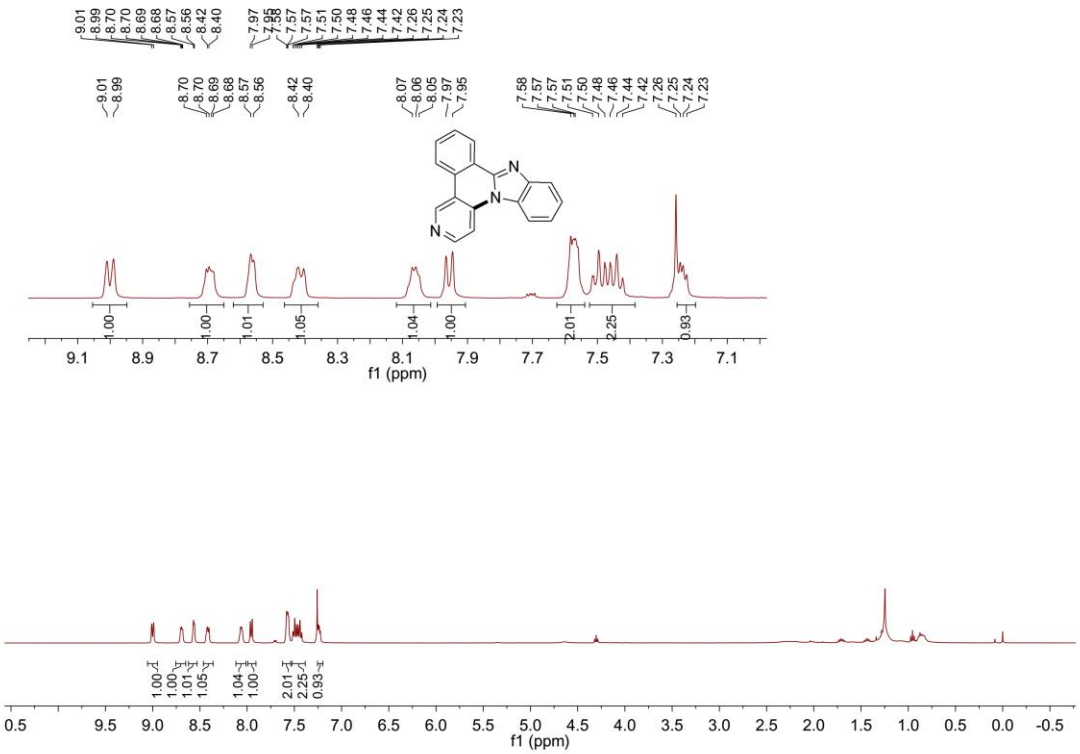

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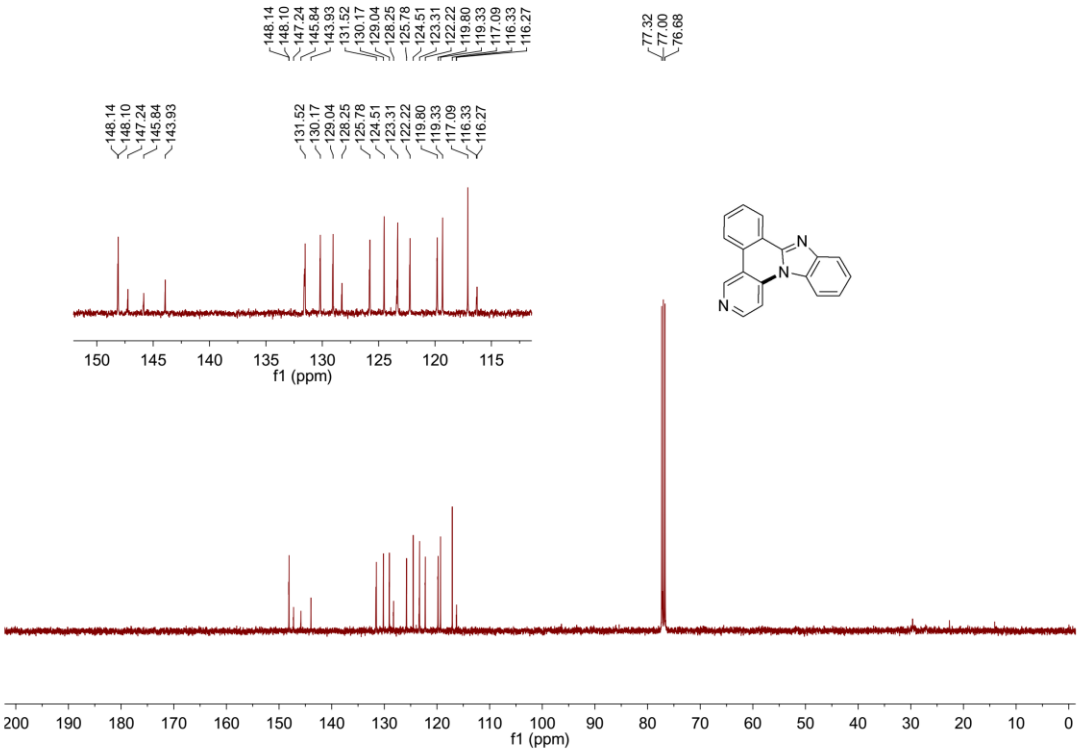

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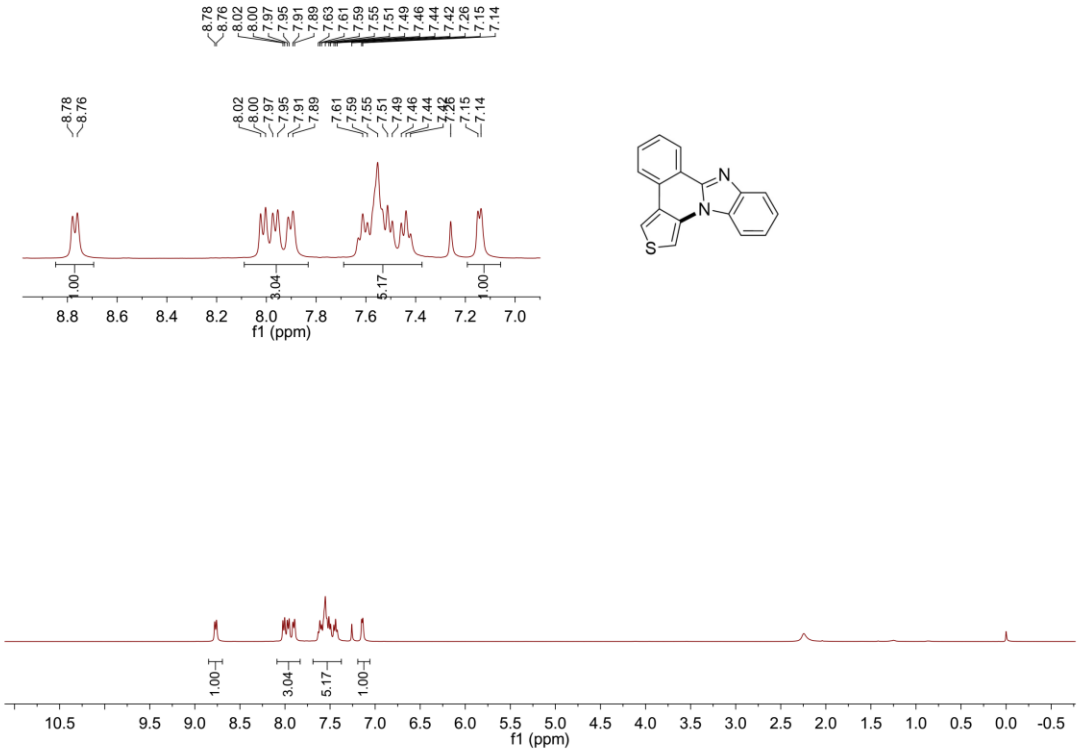

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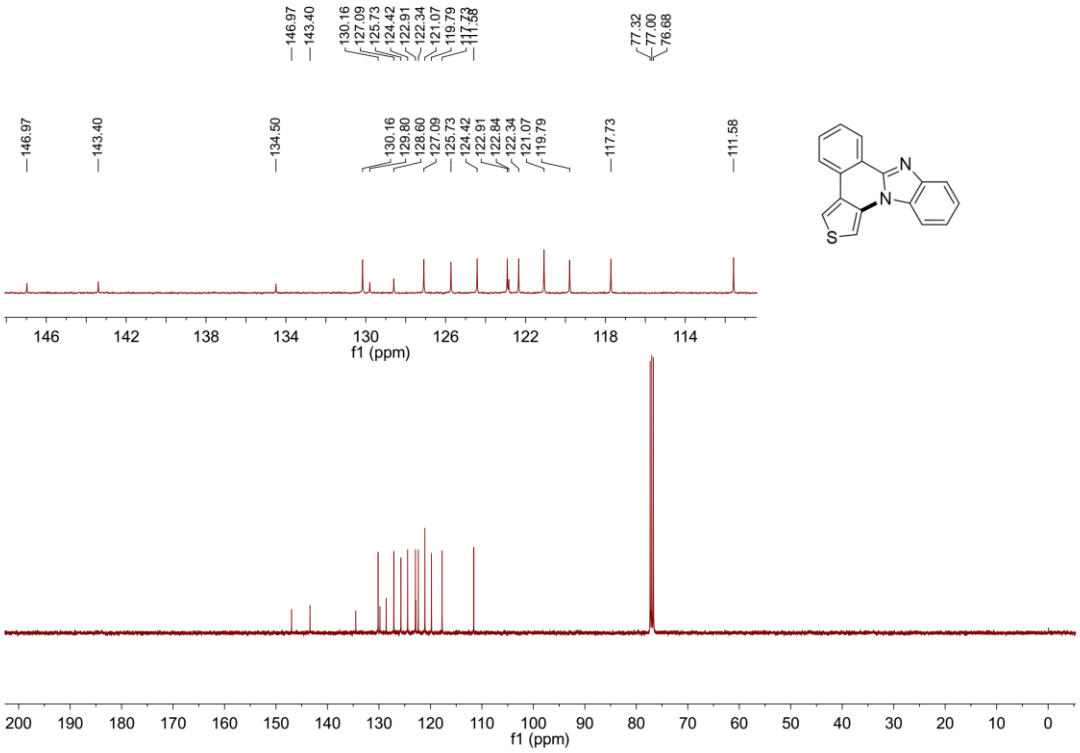

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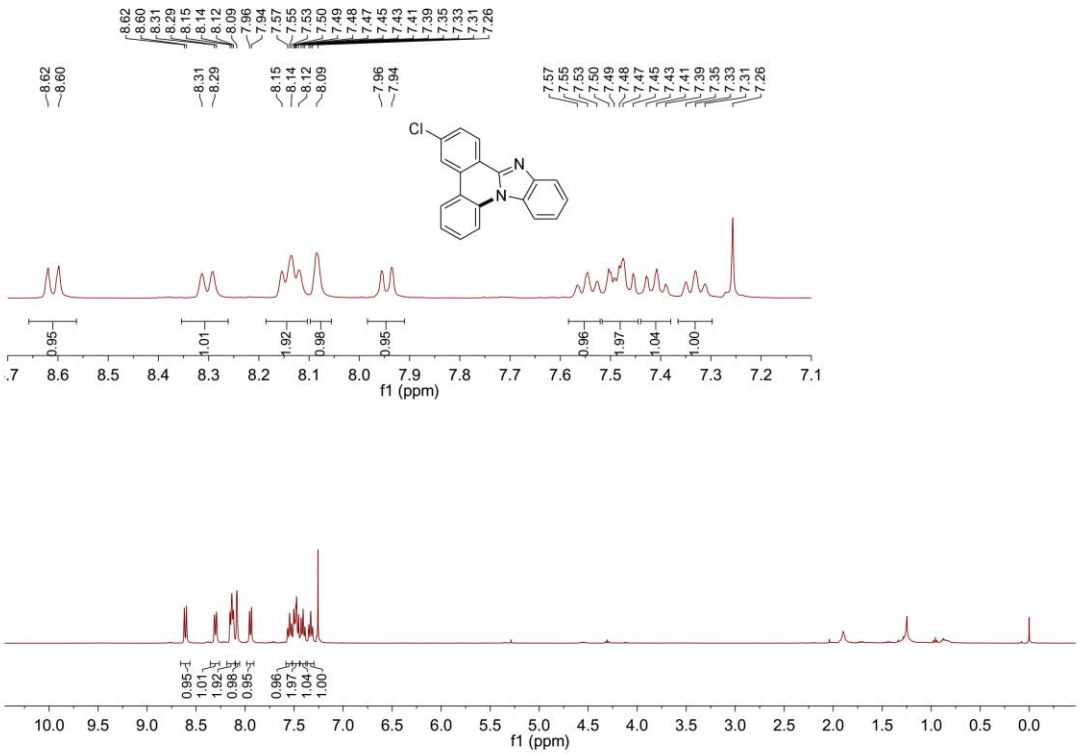

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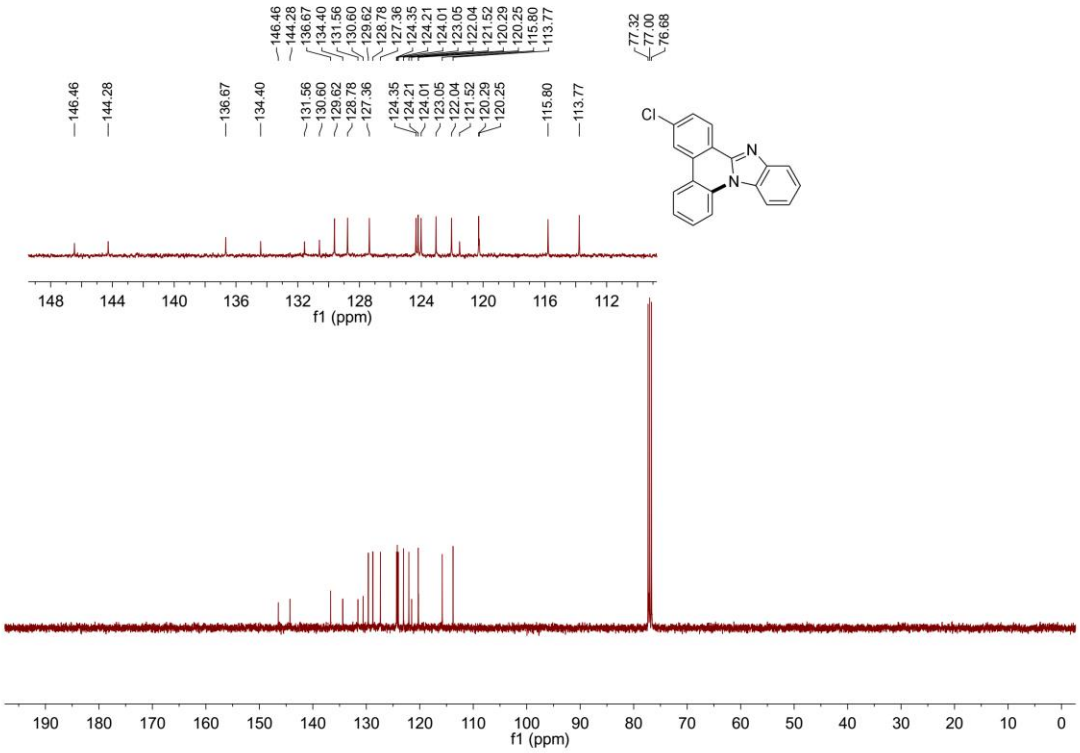

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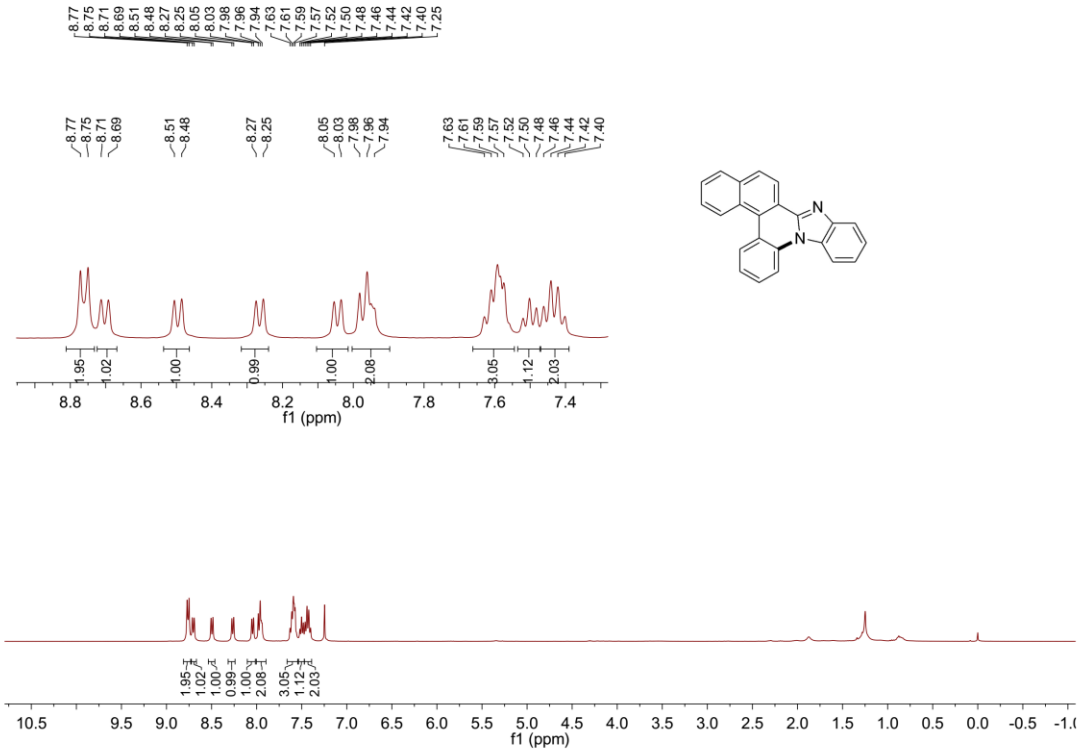

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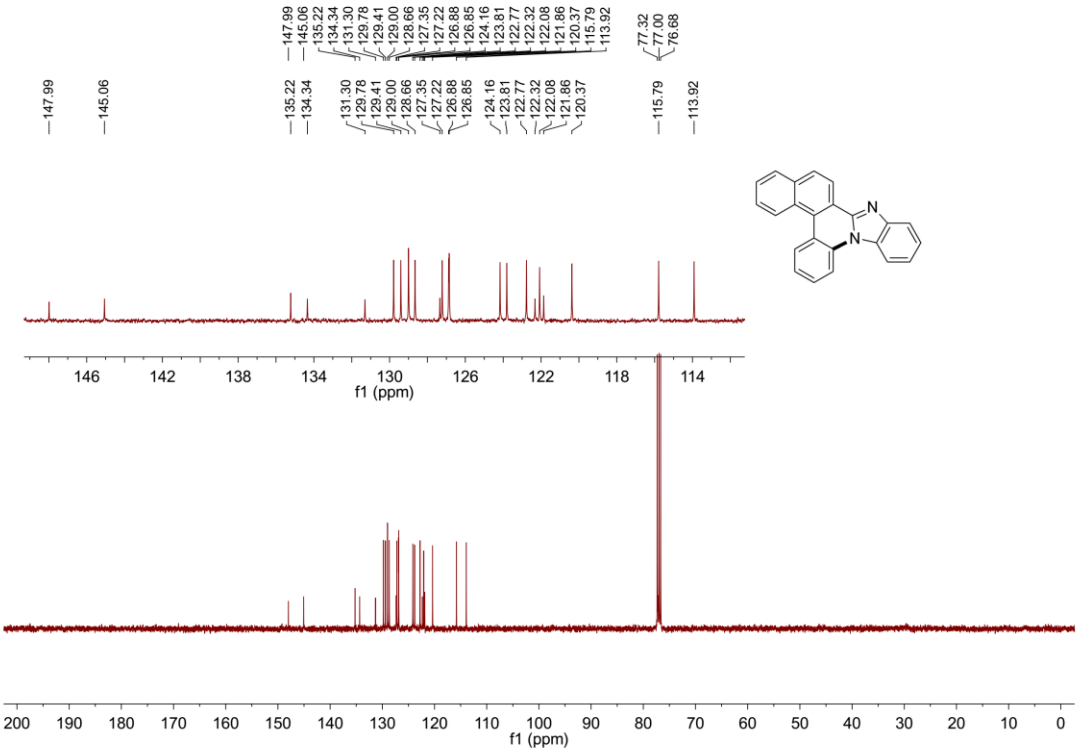

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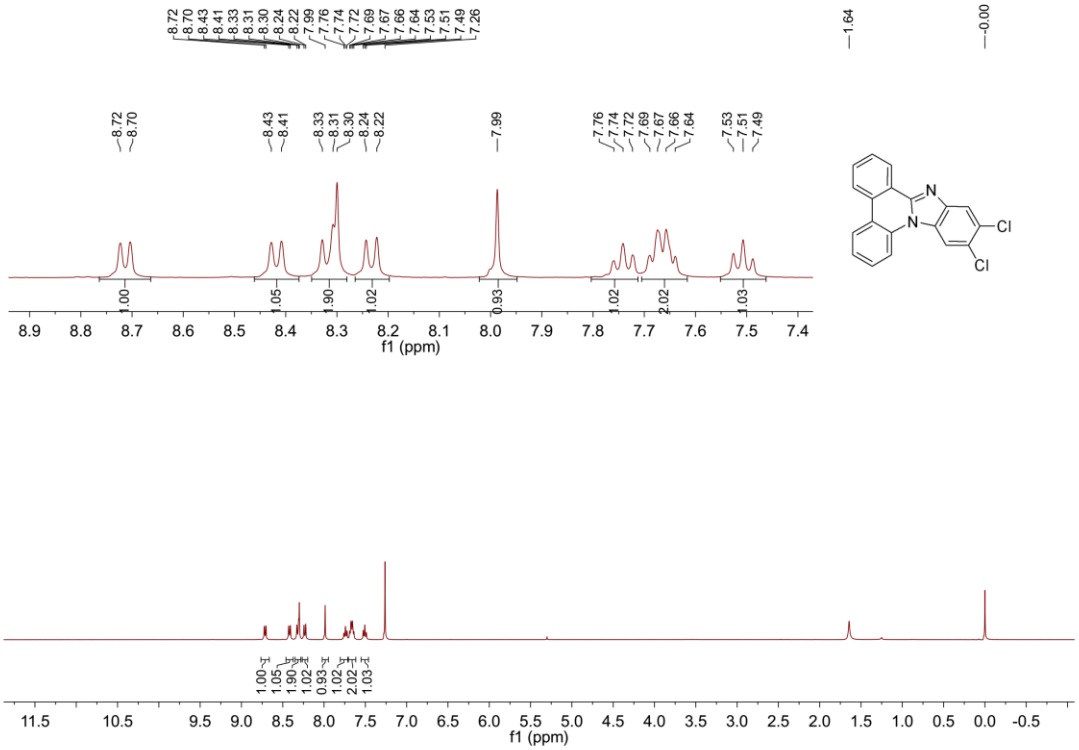
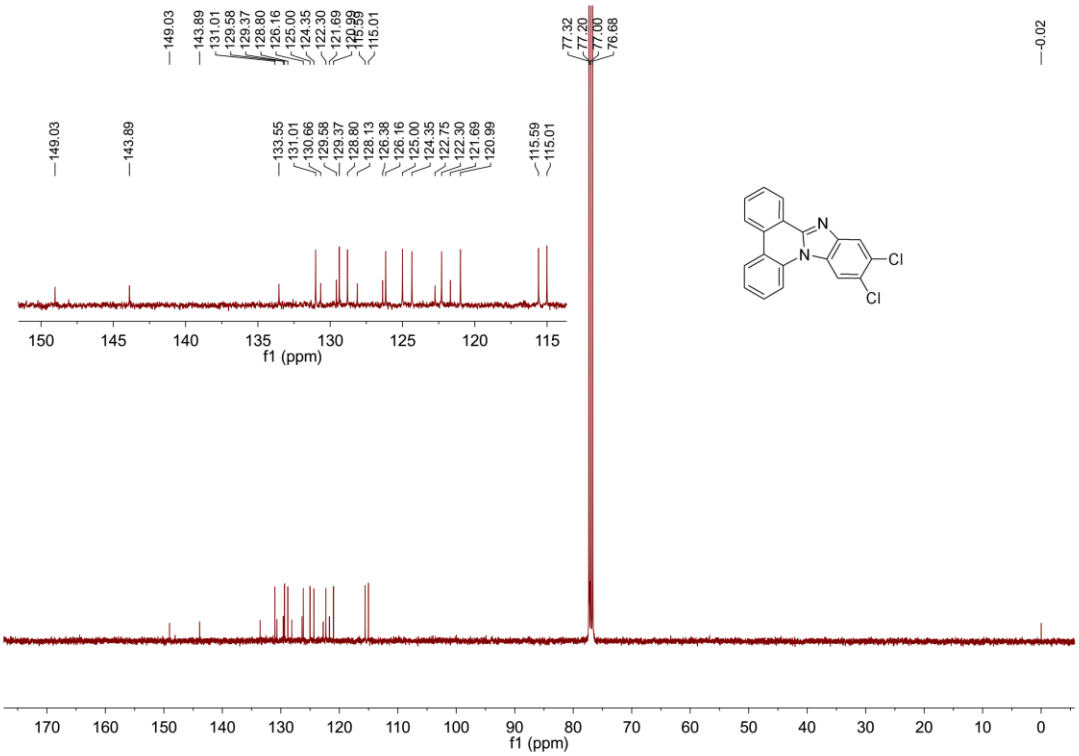
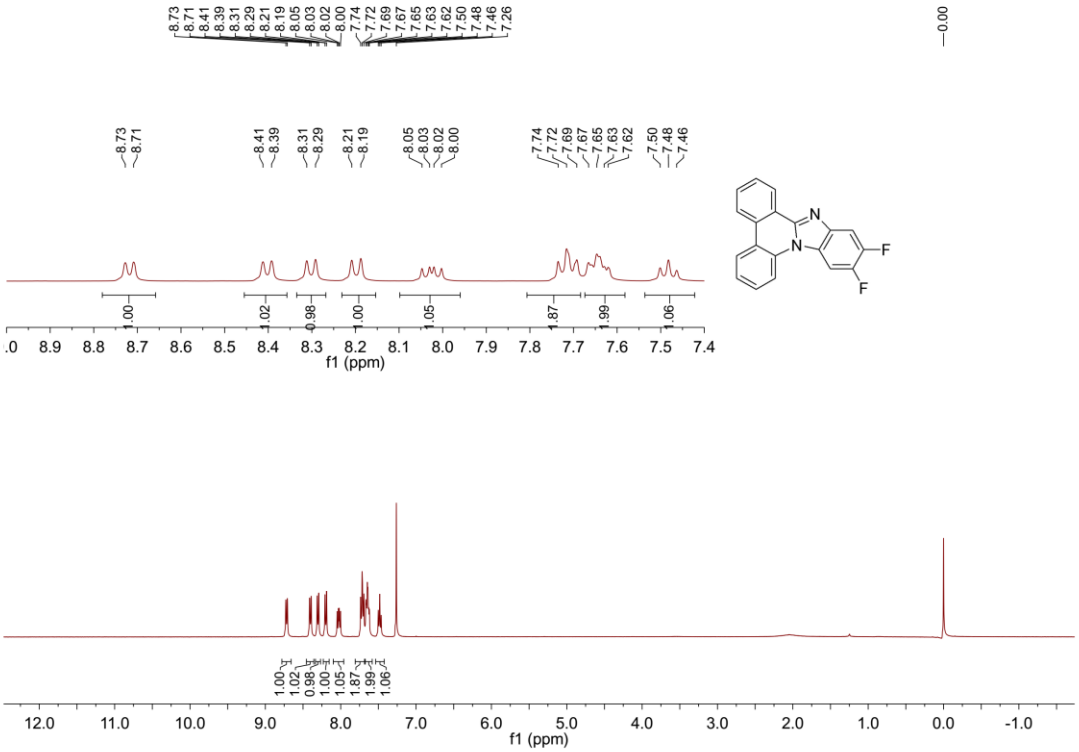


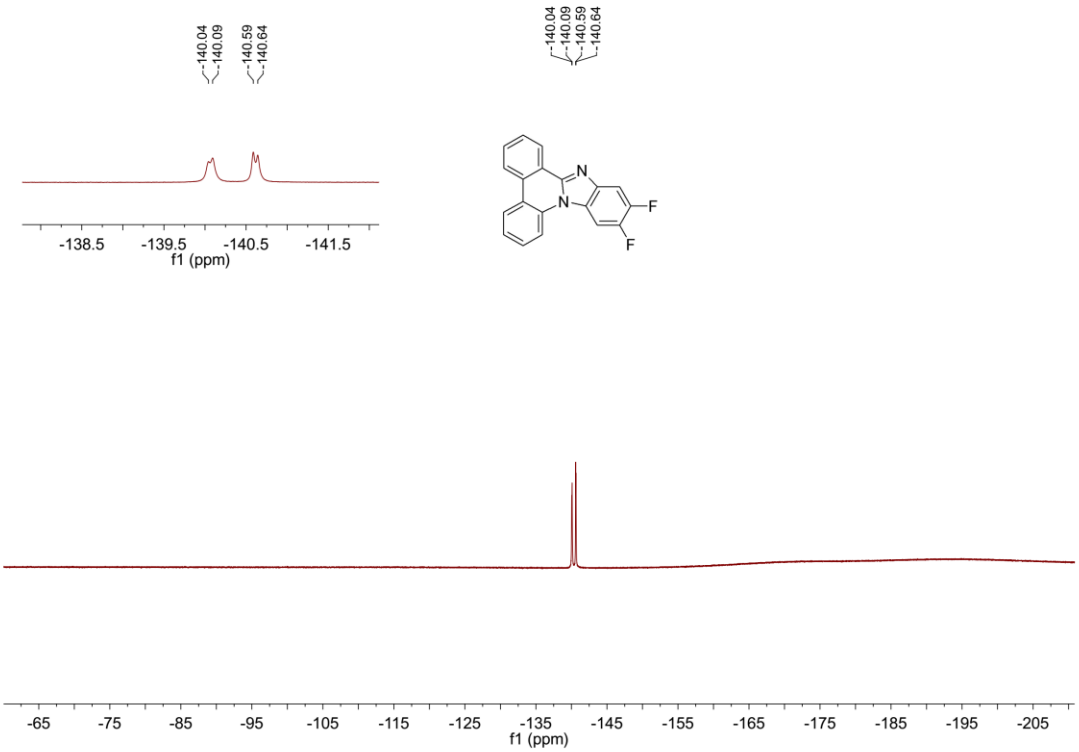
2ai ^{13}C NMR



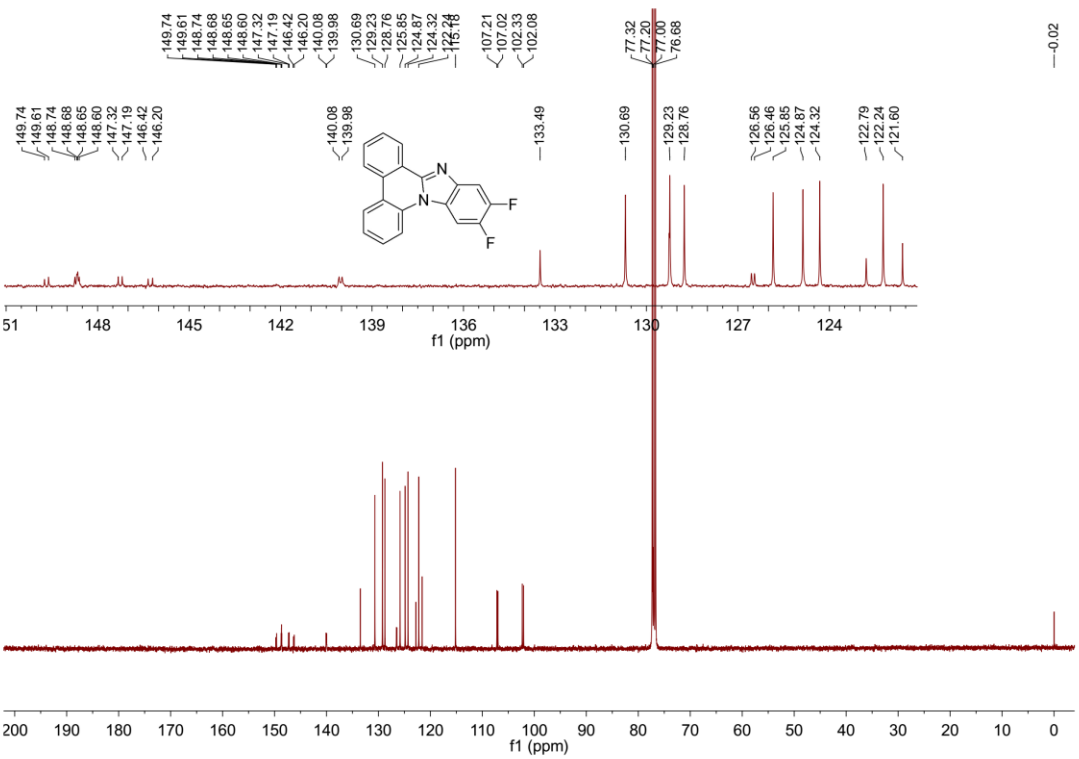
2aj ^{1}H NMR



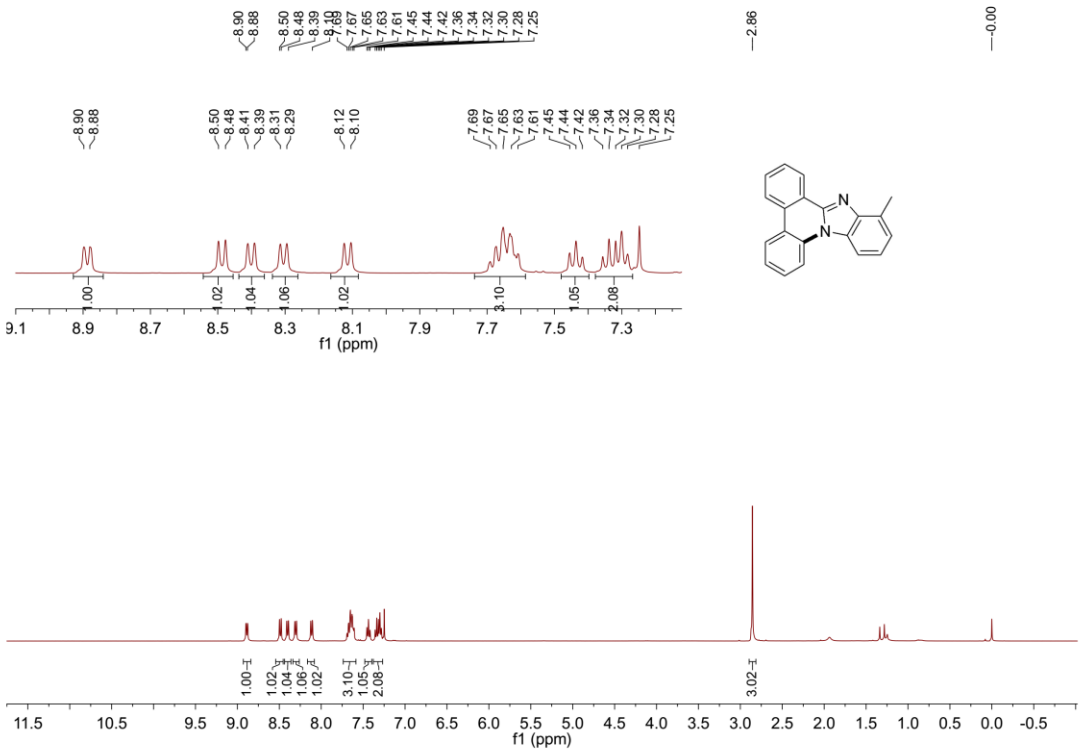
2aj ^{19}F NMR



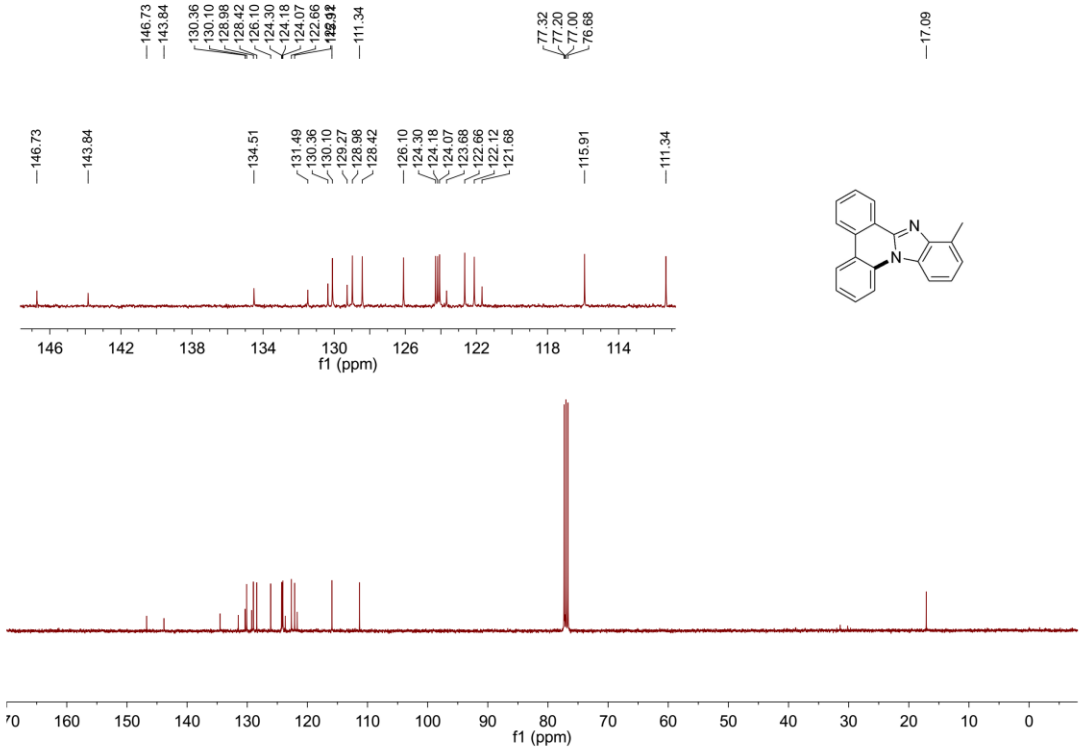
2aj ^{13}C NMR



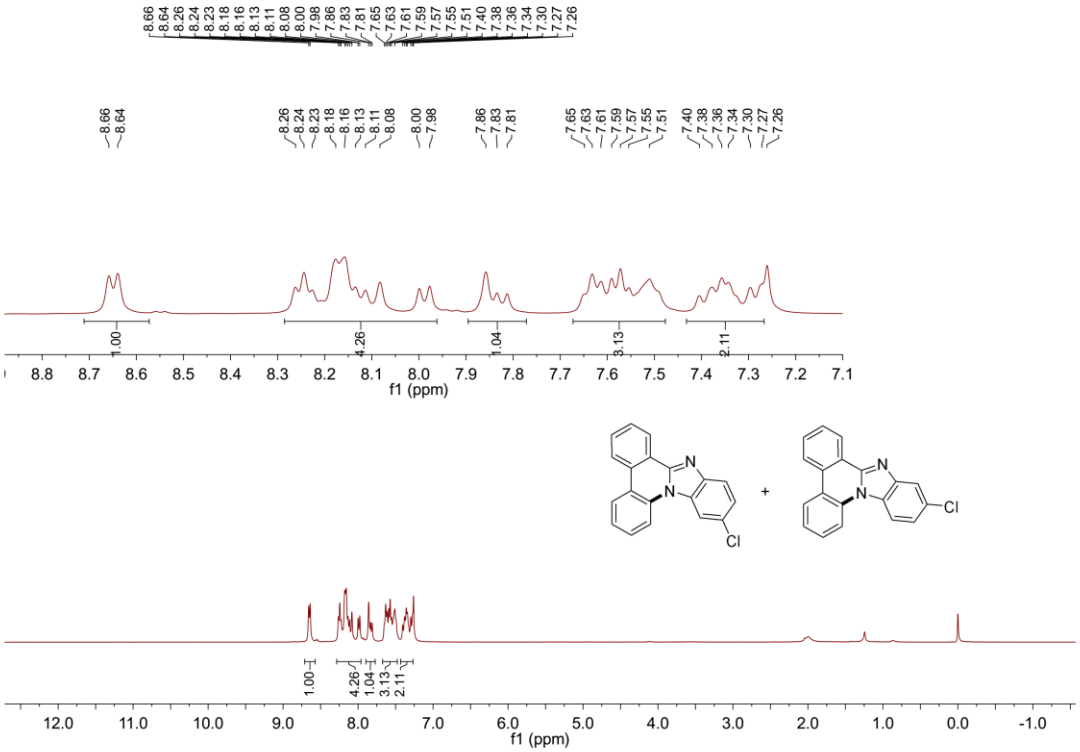
2ak ^{1}H NMR



2ak ^{13}C NMR



2al ^{1}H NMR



2al ^{13}C NMR