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Supporting Information

Ruthenium(II)-catalyzed [5＋1] annulation reaction: a facile and efficient approach to construct 6-ethenyl phenanthridines utilizing primary amine as directing group

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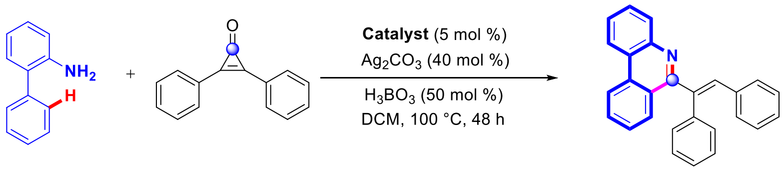
I. General information

Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. Except for the specially mentioned dry solvent, all the solvents were treated according to general methods. All the reactions were monitored by thin-layer chromatography (TLC) and were visualized using UV light. The product purification was done using silica gel column chromatography. Thin-layer chromatography (TLC) characterization was performed with precoated silica gel GF254 (0.2 mm), while column chromatography characterization was performed with silica gel (100-200 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded with tetramethylsilane (TMS, $\delta = 0.00$ ppm) as the internal standard. ^{1}H NMR spectra were recorded at 400 or 600 MHz (Varian) and ^{13}CNMR spectra were recorded at 100 or 150 MHz (Varian). Shifts are reported in ppm downfield from $CDCl_3$ ($\delta = 7.26$ ppm) or DMSO-d_6 ($\delta = 2.50$ ppm; H_2O signal was found at $\delta = 3.34$ ppm) for ^{1}H NMR and chemical shifts for ^{13}C NMR spectra are reported in ppm relative to the central $CDCl_3$ ($\delta = 77.0$ ppm) or DMSO-d_6 ($\delta = 39.6$ ppm). Coupling constants were given in Hz. The following notations were used: br-broad, s-singlet, d-doublet, t-triplet, q-quartet, m-multiplet, dd-doublet of doublet, dt-doublet of triplet, td-triplet of doublet, ddd-doublet of doublet of doublet. Melting points were measured with YRT-3 melting point apparatus (Shantou Keyi Instrument &Equipment Co., Ltd., Shantou, China).

II. Experimental Information

(a) Screening of the Reaction Conditions:

Table S1: Optimization of **Catalyst**[a]

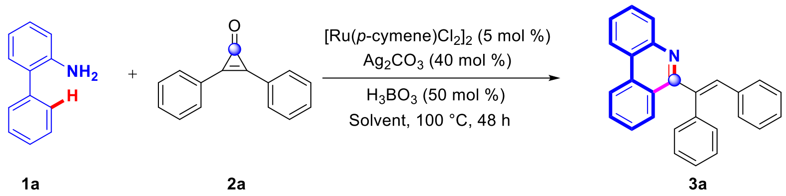


1a **2a** **3a**

Entry	**Catalyst**	Yield[b]
1	$[Cp^*RhCl_2]_2$	N.R.[c]
2	$[Cp^*IrCl_2]_2$	N.R.
3	$Cp^*Co(CO)I_2$	N.R
4	$Co(OAc)_2 \cdot 4H_2O$	N.R.
5	$Pd(OAc)_2$	N.R.
6	$RuCl_3$	<5%
7	$Ru(bpy)_3(Cl)_2$	45%
8	Grubb's catalyst	48%
9	**$[Ru(p\text{-}cymene)Cl_2]_2$**	**73%**
10	-	N.R.

[a] Reaction conditions: **1a** (0.10 mmol), **2a** (0.20 mmol), solvent (1.0 ml) in a sealed tube under air for 48 h. [b] Isolated yields. [c] N.R. = No reaction

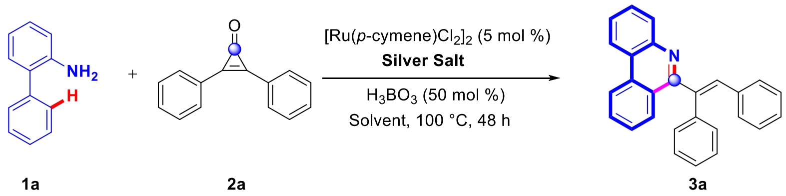
Table S2: Optimization of **Solvent**[a]



Entry	Solvent	Yield[b]
1	toluene	<5%
2	chlorobenzene	<5%
3	MeCN	N.R.
4	THF	N.R.
5	DCE	41%
6	NMP	N.R.
7	H_2O	N.R.
8	H_2O:PEG_{400}(1:1)	N.R.
9	**DCM**	**73%**
10	[BMIM]BF_4	N.R.

[a] Reaction conditions: **1a** (0.10 mmol), **2a** (0.20 mmol), solvent (1.0 ml) in a sealed tube under air for 48 h. [b] Isolated yields. [c] N.R. = No reaction

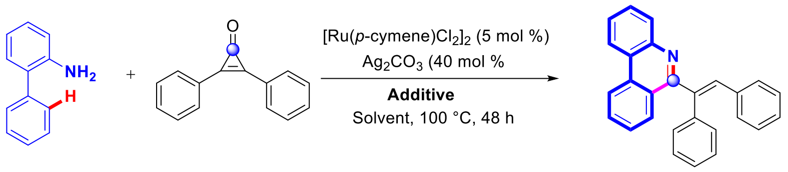
Table S3: Optimization of **Silver Salt**[a]



Entry	**Silver Salt**	Yield[b]
1	Ag_2CO_3 (20 mol %)	63%
2	**Ag_2CO_3 (40 mol %)**	**73%**
3	-	N.R.
4	$AgSbF_6$ (40 mol %)	8%
5	$AgSO_4$ (40 mol %)	25%
6	$AgBF_4$ (40 mol %)	N.R
7	AgF (40 mol %)	N.R
8	$AgNTf_2$ (40 mol %)	<5%
9	AgOTf (40 mol %)	N.R.

[a] Reaction conditions: **1a** (0.10 mmol), **2a** (0.20 mmol), solvent (1.0 ml) in a sealed tube under air for 48 h. [b] Isolated yields. [c] N.R. = No reaction.

Table S4: Optimization of **Additive**[a]



1a **2a** **3a**

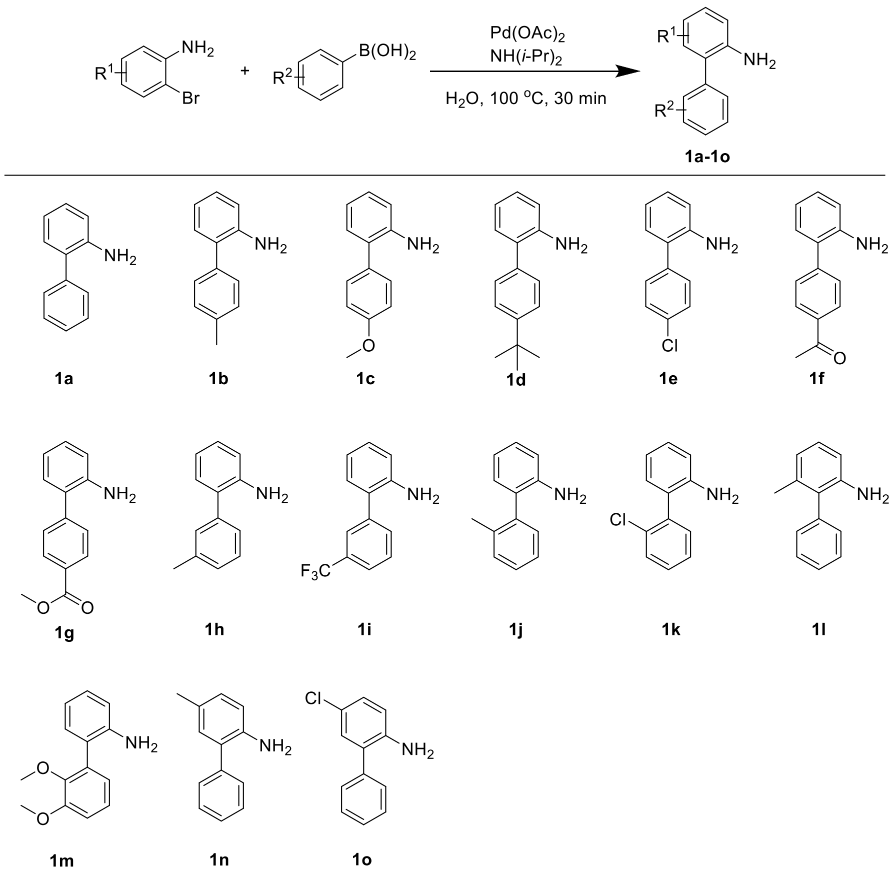
Entry	Additive	Yield[b]
1	$Cu(OAc)_2$ (1.0 eq)	N.R.
2	$Cu(TFA)_2$ (1.0 eq)	N.R.
3	$Mn(OAc)_2{\cdot}4H_2O$ (1.0 eq)	N.R.
4	$PhI(OAc)_2$ (1.0 eq)	<5%
5	NaOAc (1.0 eq)	N.R
6	PivONa (1.0 eq)	N.R
7	PivOH (1.0 eq)	10%
8	1-AdCOOH (1.0 eq)	15%
9	H_3BO_3 (1.0 eq)	65%
10	**H_3BO_3 (0.5 eq)**	**73%**
11	H_3BO_3 (0.2 eq)	29%
12	-	N.R.

[a] Reaction conditions: **1a** (0.10 mmol), **2a** (0.20 mmol), solvent (1.0 ml) in a sealed tube under air for 48 h. [b] Isolated yields. [c] N.R. = No reaction

b) General procedure for the synthesis of substrates 1a-1o[1]

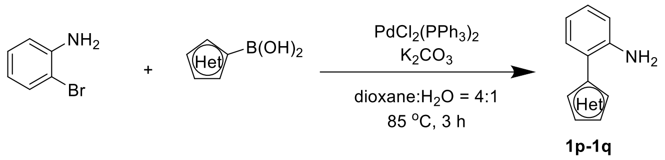
According to the literature procedure, substrates **1a-1p** were prepared by Suzuki–Miyaura coupling between corresponding arylboronic acids and *o*-bromoanilines. All the compounds are known.

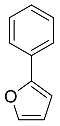
A mixture of *o*-bromoanilines (3.0 mmol), arylboronic acids (4.5 mmol), base (6.0 mmol), $Pd(OAc)_2$ (0.25 mol%, 1.68 mg) and H_2O (6.0 mL) were stirred at 100 °C for 0.5 h. After completion of the reaction, the mixture was added to brine (10 mL) and extracted with ethyl acetate (3 × 20 mL). The solvent was evaporated under vacuum. The residue was purified by column chromatography on silica gel using PE/EA (20:1 - 15:1) as the eluent.



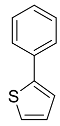
c) General procedure for the synthesis of substrates 1p-1q[1]

$Pd(PPh_3)_2Cl_2$ (105 mg, 0.15 mmol, 5 mol%), *o*-bromoanilines (3.0 mmol, 1 equiv.), corresponding hetero-arylboronic acids (4.5 mmol, 1.5 equiv.), and K_2CO_3 (1.24 g, 9.0 mmol, 3 equiv.) were charged into an oven-dried Schlenk tube to which degassed 1,4-dioxane/H_2O (15 mL, *V/V* = 4/1) was added under argon atmosphere. The reaction was stirred at 85 °C for 3 h. After cooled to room temperature, 1N $NaHCO_3$ (20 mL) was added and the aqueous phase was extracted with EtOAc (20 mL × 3). The combined organic layer was washed with H_2O (20 mL) and brine (10 mL), dried over Na_2SO_4 and evaporated under vacuum. The residue was purified by silica gel column chromatography using PE/EA (20:1) as the eluent to afford products. All the compounds are known.



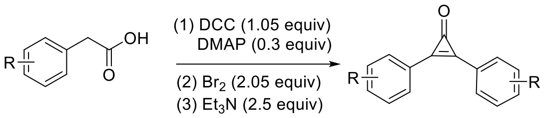


1p



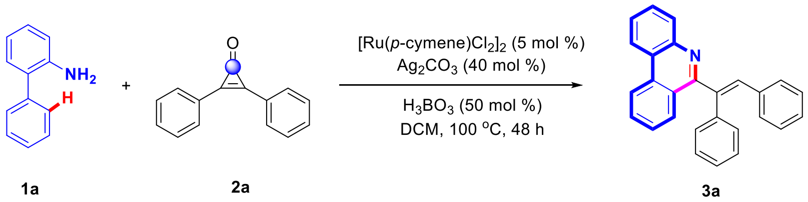
1q

d) General procedure for the synthesis of cyclopropenone 2[2]



Substituted cyclopropenones were prepared in three steps from substituted phenylacetic acid. The diaryl ketone was prepared by adding substituted phenylacetic acid (20 mmol, 1 equiv) to a stirring solution of DCC (1.05 equiv) and DMAP (0.3 equiv) in THF at room temperature. After 60 minutes, the reaction was filtered through Celite. The diaryl ketone was purified by flash chromatography on silica gel. Then a solution of bromine (2.05 equiv) in acetic acid was added to a solution of diaryl ketone in acetic acid over a period of approximately 15 minutes. After 3 hours, the reaction was poured into water while vigorously swirling the receiving flask and the product was collected by filtration. The crude product (dibromoketone) was air dried for several hours, then dissolved in dry dichloromethane, which was added to a stirring solution of triethylamine (2.5 equiv) in dichloromethane, and stirred at room temperature for 1 hour. The reaction mixture was then washed with 1 M HCl, followed by brine, dried with sodium sulfate, and concentrated under reduced pressure. The pure product was obtained by column chromatography on silica gel.

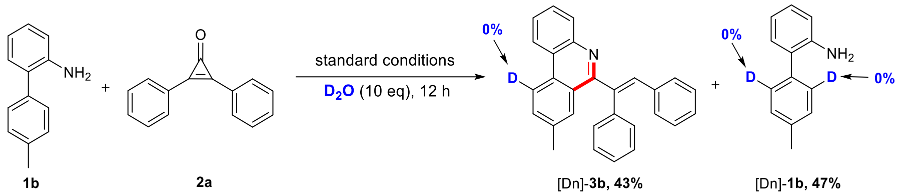
e) General procedure for the synthesis of products 3 (3a as an example)



2-Aminodiphenyl **1a** (0.20 mmol, 1 equiv.), cyclopropenone **2a** (0.40 mmol, 2 equiv.), $[Ru(p\text{-cymene})Cl_2]_2$ (0.01 mmol, 0.05 equiv.), boracic acid (0.10 mmol, 0.5 equiv.) and Ag_2CO_3 (0.04 mmol, 0.4 equiv.) were charged into a pressure tube, to which was added DCM (2.0 mL). The reaction mixture was stirred at 100 °C for 48 h. After cooled to rt, 1N $NaHCO_3$ (20 mL) was added and the aqueous phase was extracted with EtOAc (20 mL × 3). The combined organic layer was washed with H_2O (20 mL) and brine (10 mL), dried over Na_2SO_4 and evaporated under vacuum. The residue was purified by silica gel column chromatography using PE/EA (30:1) as the eluent to afford compound **3a** as yellow oil.

III. Mechanistic Studies

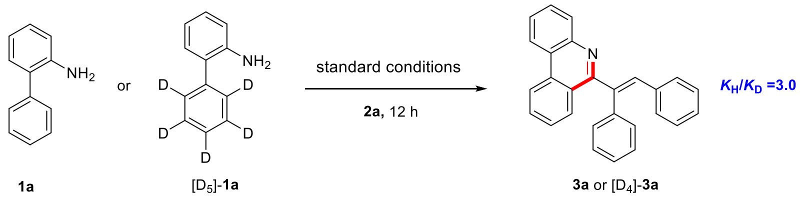
a) H/D Exchange Experiment



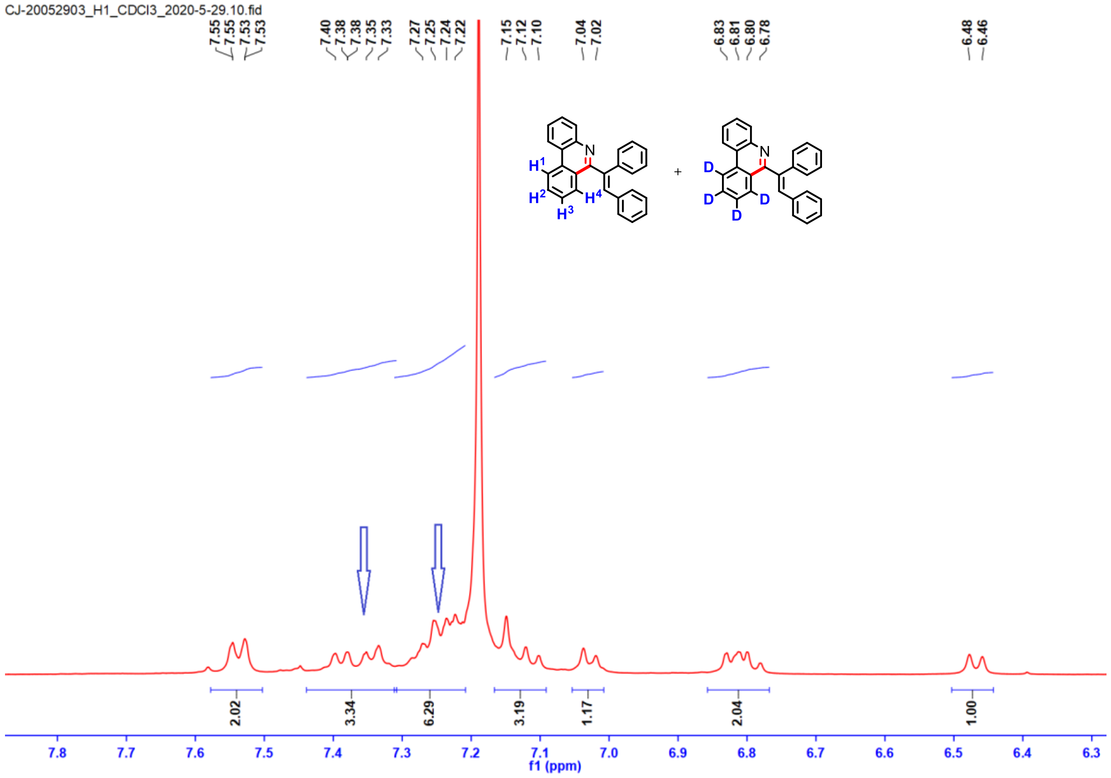
To a stirred solution of **1b** (36.3 mg, 0.20 mmol) in DCM (2.0 mL), **2a** (82.4 mg, 0.40 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (6.2 mg, 0.01 mmol), Ag_2CO_3 (22.0 mg, 0.08 mmol), H_3BO_3 (6.2 mg, 0.1 mmol) and D_2O (36 uL, 10 eq) were added. The reaction mixture was stirred at 100 °C for 12 h. After cooled to room temperature, the solvent was removed under reduced pressure. The residue was purified on a preparative TLC with petroleum ether/ethyl acetate (30/1) as the eluent to furnish the corresponding product **3b** (31.9 mg, 43%) with reisolated **1b** (17.0 mg, 47%). No significant deuterium incorporation was observed, indicating that C-H metalation step was irreversible.

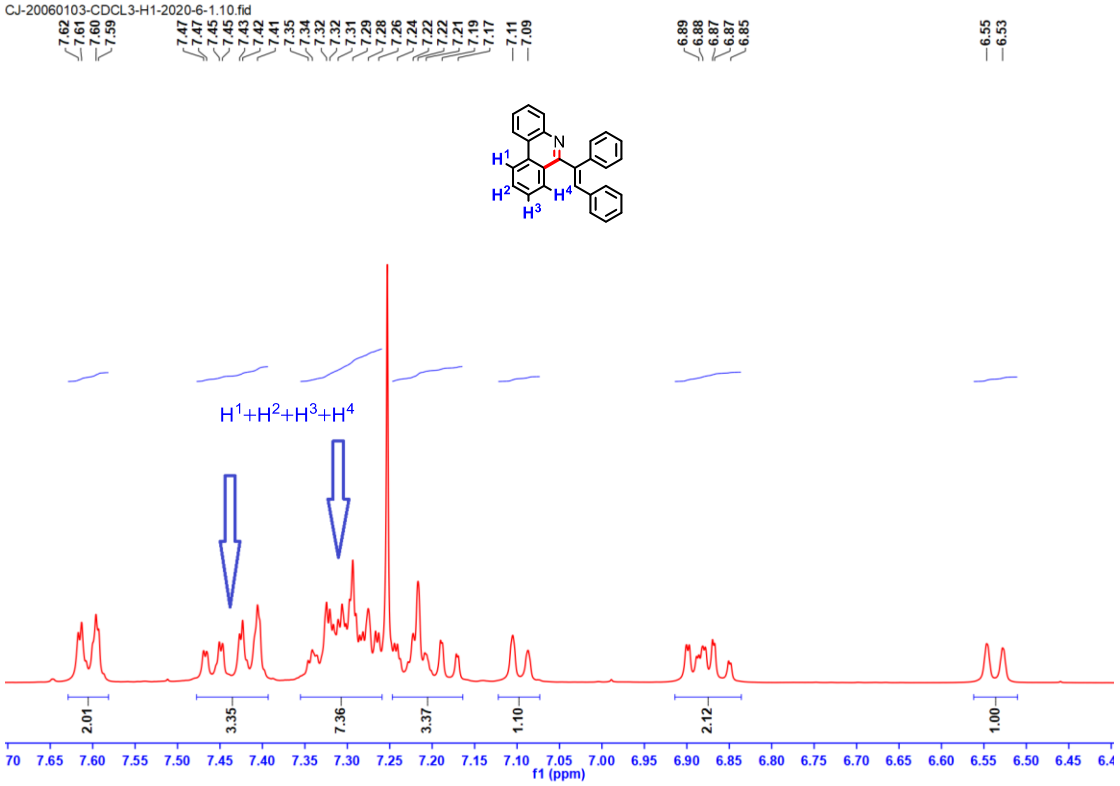
b) Kinetic Isotope Effect (KIE) studies

Two Parallel Reactions

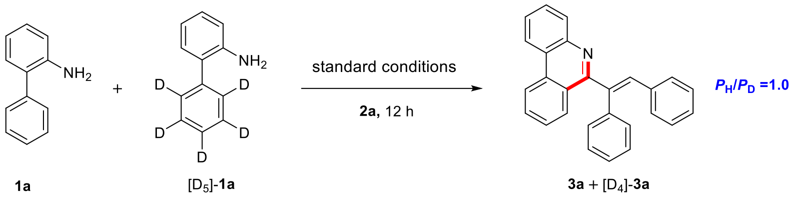


To a stirred solution of **1a** or $[D_5]$-**1a** (0.10 mmol) in DCM (1.0 mL), **2a** (41.2 mg, 0.20 mmol), $[Ru(p\text{-cymene})Cl_2]_2$ (3.1 mg, 0.005 mmol), Ag_2CO_3 (11.0 mg, 0.04 mmol), and H_3BO_3 (3.1 mg, 0.05 mmol) were added. The reaction mixture was stirred at 100 °C for 12 h. After cooled to room temperature, the solvent was removed under reduced pressure. The residue was purified on a preparative TLC with petroleum ether/ethyl acetate (30/1) as the eluent to furnish the corresponding product **3a** or $[D_4]$-**3a**. The ratio of H/D was determined by ^1H NMR spectra in $K_H/K_D = 3.0$.

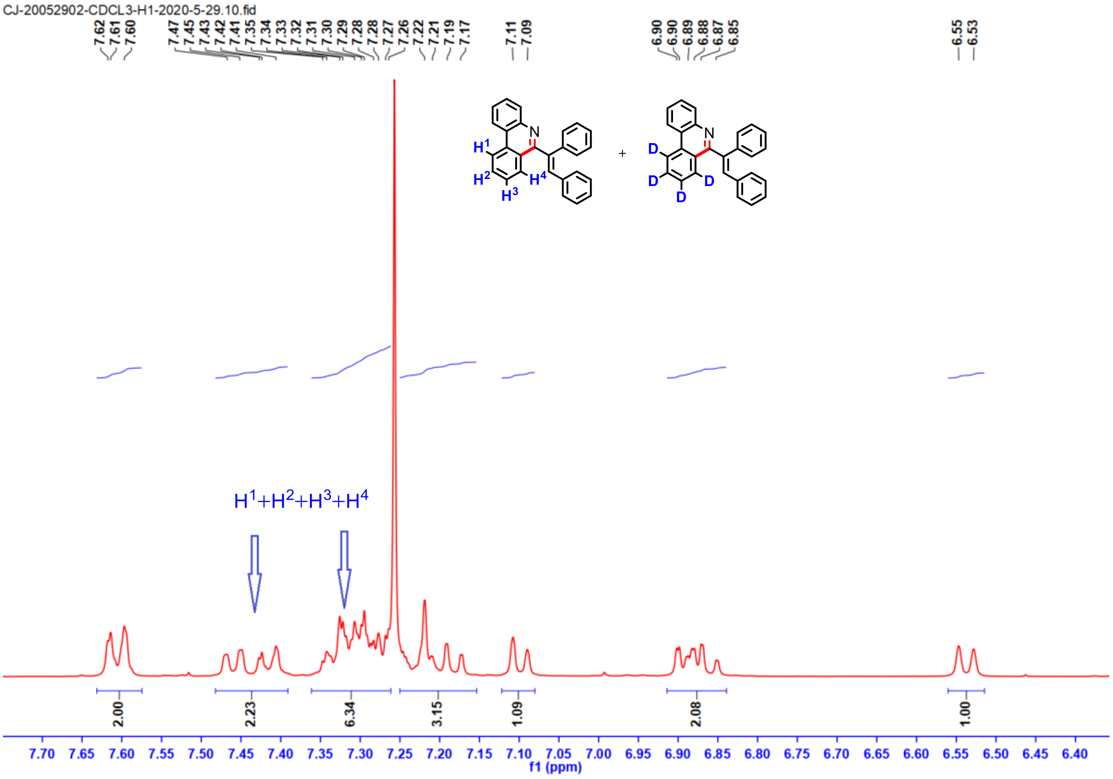


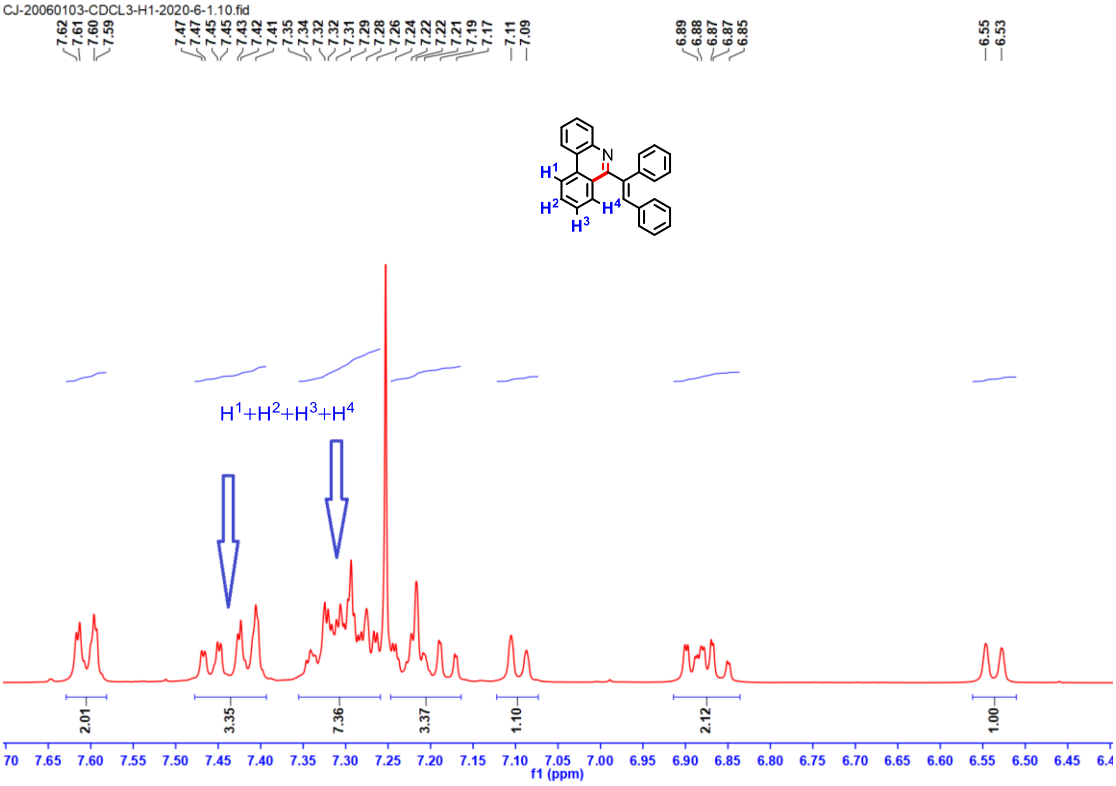


Intermolecular Competition Reactions

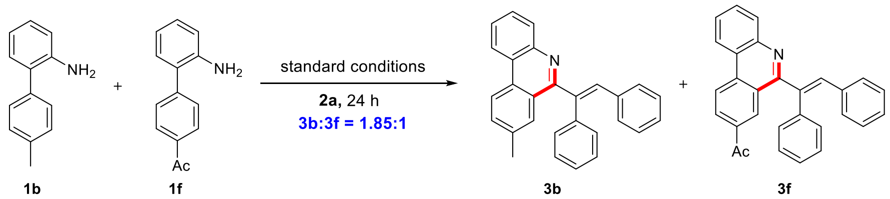


A 15 ml sealed tube equipped with a magnetic stir bar was charged with **1a** (0.10 mmol, 16.9 mg), [D$_5$]-**1a** (0.10 mmol, 18.7 mg), **2a** (41.2 mg, 0.20 mmol), [Ru(*p*-cymene)Cl$_2$]$_2$ (3.1 mg, 0.005 mmol), Ag$_2$CO$_3$ (11.0 mg, 0.04 mmol), and H$_3$BO$_3$ (3.1 mg, 0.05 mmol). The reaction mixture was stirred at 100 °C for 12 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA as the eluent to afford the corresponding compound 3a and [D$_4$]-3a as yellow oil. The ratio of H/D was determined by **^{1}H NMR** spectra in P_H/P_D = 1.0.

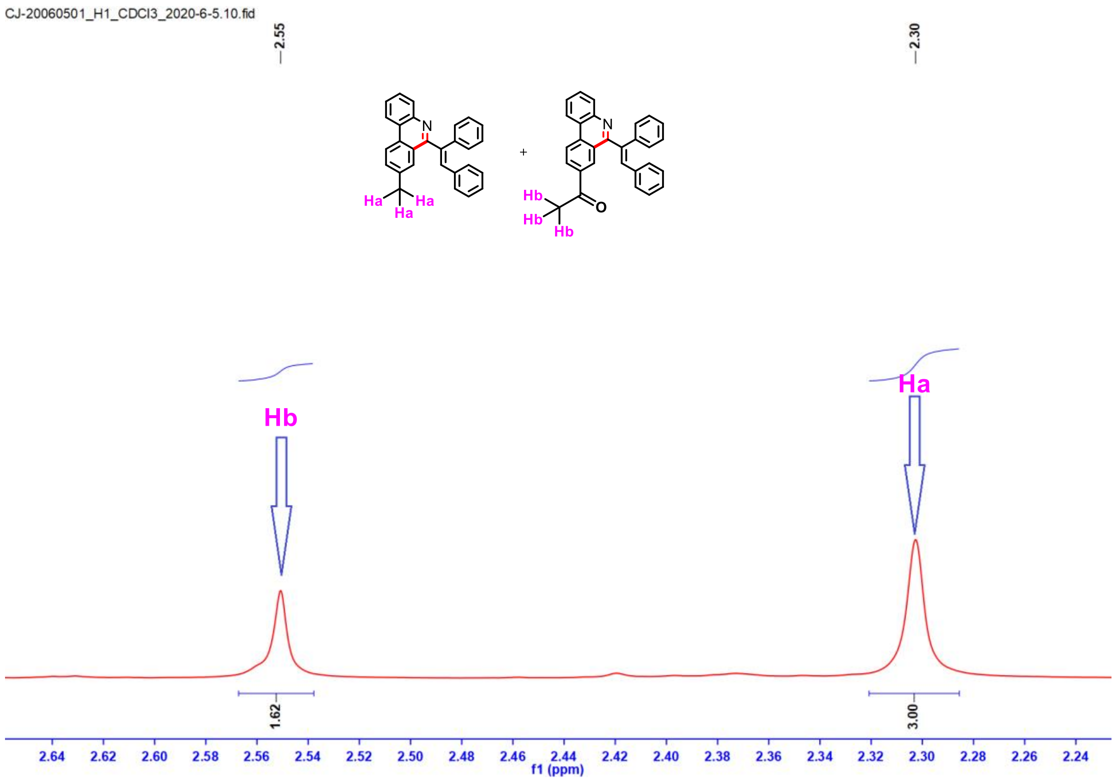




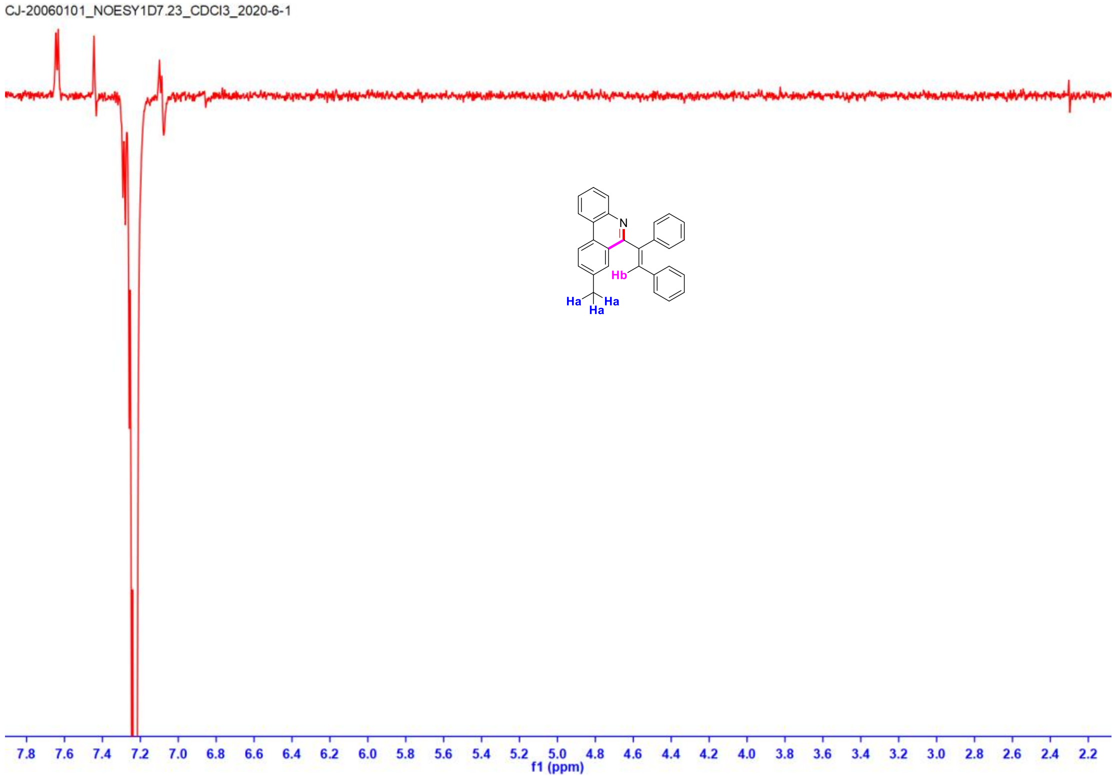
c) Competition Experiment



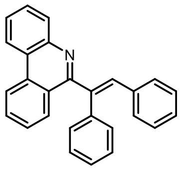
To a stirred solution of **1b** (18.3 mg, 0.10 mmol) and **1f** (21.0 mg, 0.10 mmol) in DCM (2.0 mL), **2a** (41.2 mg, 0.20 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (3.1 mg, 0.005 mmol), Ag_2CO_3 (11.0 mg, 0.04 mmol), and H_3BO_3 (3.1 mg, 0.05 mmol) were added. The reaction mixture was stirred at 100 °C for 24 h. After cooled to room temperature, the solvent was removed under reduced pressure. The residue was purified on a preparative TLC with petroleum ether/ethyl acetate (30/1) as the eluent to furnish the corresponding product **3b** and **3f**. The ratio of **3b**/**3f** was 1.85/1.0, which was determined by **^{1}H NMR**.



IV. The NOESY Spectra of Product 3b

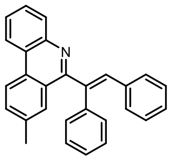


V. Characterization Date of Products



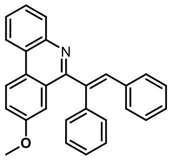
(*E*)-6-(1,2-diphenylvinyl)phenanthridine (3a)

Yield 73%, 52.2 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.60 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.48-7.39 (m, 3H), 7.36-7.26 (m, 7H), 7.25-7.16 (m, 3H), 7.10 (d, *J* = 7.2 Hz, 1H), 6.91-6.84 (m, 2H), 6.54 (d, *J* = 7.5 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.2, 149.2, 144.2, 140.7, 139.6, 136.7, 133.5, 131.2, 130.4, 129.4, 129.1, 128.6, 128.1, 128.1, 127.9, 127.8, 127.0, 126.9, 125.7, 124.6, 121.5, 118.2. **HRMS (ESI): m/z** calculated for $C_{27}H_{20}N$ [M+H]$^+$: 358.1590, found: 358.1591.



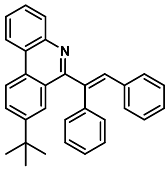
(*E*)-6-(1,2-diphenylvinyl)-8-methylphenanthridine (3b)

Yield 64%, 47.5 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.69-7.63 (m, 2H), 7.49-7.42 (m, 1H), 7.39-7.27 (m, 7H), 7.23 (s, 1H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.15-7.08 (m, 3H), 6.87 (t, *J* = 7.4 Hz, 2H), 6.53 (d, *J* = 7.5 Hz, 1H), 2.31 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.0, 149.3, 144.2, 140.7, 136.7, 136.6, 136.5, 133.5, 131.1, 130.3, 129.2, 129.1, 128.6, 128.6, 128.1, 127.8, 127.8, 127.3, 127.0, 125.7, 124.5, 121.4, 118.1, 21.1. **HRMS (ESI):** m/z calculated for $C_{28}H_{22}N$ [M+H]$^+$: 372.1747, found: 372.1748.



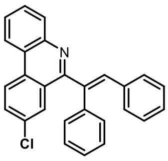
(*E*)-6-(1,2-diphenylvinyl)-8-methoxyphenanthridine (3c)

Yield 62%, 48.0 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.69 – 7.63 (m, 2H), 7.44 (dd, *J* = 7.3, 1.5 Hz, 1H), 7.37 – 7.27 (m, 6H), 7.25 (d, *J* = 4.8 Hz, 2H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.10 (d, *J* = 7.2 Hz, 1H), 6.88 – 6.82 (m, 4H), 6.53 (d, *J* = 7.5 Hz, 1H), 3.77 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.2, 158.7, 149.4, 144.3, 140.8, 136.9, 133.6, 132.2, 131.3, 130.9, 130.5, 130.4, 129.2, 128.7, 128.3, 127.9, 127.8, 127.1, 125.8, 124.7, 121.6, 118.3, 113.5, 55.3. **HRMS (ESI):** m/z calculated for $C_{28}H_{22}NO$ [M+H]$^+$: 388.1696, found: 388.1695.



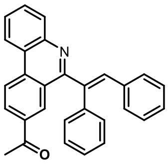
(*E*)-8-(*tert*-butyl)-6-(1,2-diphenylvinyl)phenanthridine (3d)

Yield 54%, 44.6 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.57 (d, *J* = 6.5 Hz, 2H), 7.52-7.46 (m, 1H), 7.38-7.27 (m, 8H), 7.25-7.17 (m, 3H), 7.12 (d, *J* = 7.2 Hz, 1H), 6.88 (t, *J* = 7.6 Hz, 2H), 6.62 (d, *J* = 7.5 Hz, 1H), 1.30 (s, 9H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.3, 150.1, 149.5, 144.7, 141.3, 137.0, 136.9, 133.9, 131.7, 131.5, 130.6, 129.0, 128.4, 127.3, 126.1, 125.1, 124.9, 121.8, 118.5, 34.8, 31.7. **HRMS (ESI):** m/z calculated for $C_{31}H_{28}N$ [M+H]$^+$: 414.2216, found: 414.2215.



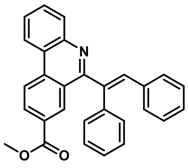
(*E*)-8-chloro-6-(1,2-diphenylvinyl)phenanthridine (3e)

Yield 69%, 54.1 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.64 (d, *J* = 7.1 Hz, 2H), 7.44-7.27 (m, 8H), 7.24-7.16 (m, 4H), 7.10 (d, *J* = 7.1 Hz, 1H), 6.93-6.83 (m, 2H), 6.47 (d, *J* = 7.5 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.4, 149.2, 144.2, 140.5, 138.0, 137.0, 133.4, 132.9, 131.4, 130.6, 130.2, 129.9, 129.0, 128.5, 128.5, 128.2, 128.1, 127.9, 127.1, 125.6, 124.7, 121.6, 118.4. **HRMS (ESI):** m/z calculated for $C_{27}H_{19}ClN$ [M+H]$^+$: 392.1201, found: 392.1202.



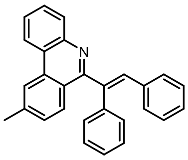
(*E*)-1-(6-(1,2-diphenylvinyl)phenanthridin-8-yl)ethan-1-one (3f)

Yield 81%, 64.7 mg, yellow solid, m.p. 67-70 ℃. **^{1}H NMR (600 MHz, Chloroform-*d*)** δ 7.87 (d, *J* = 8.1 Hz, 2H), 7.65 (d, *J* = 7.5 Hz, 2H), 7.52 (d, *J* = 8.1 Hz, 2H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.42-7.28 (m, 5H), 7.23 (s, 1H), 7.19 (t, *J* = 7.4 Hz, 1H), 7.09 (d, *J* = 7.2 Hz, 1H), 6.93 (d, *J* = 7.8 Hz, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.47 (d, *J* = 7.5 Hz, 1H), 2.55 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 198.2, 166.8, 149.6, 144.9, 144.5, 140.7, 137.4, 135.8, 133.6, 131.8, 130.6, 130.1, 129.8, 129.3, 128.8, 128.5, 128.4, 128.3, 127.4, 125.9, 125.1, 121.9, 118.8, 27.0. **HRMS (ESI):** m/z calculated for $C_{29}H_{22}NO$ [M+H]$^+$: 400.1696, found: 400.1697.

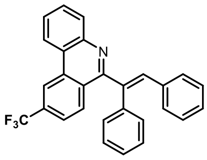


Methyl (*E*)-6-(1,2-diphenylvinyl)phenanthridine-8-carboxylate (3g)

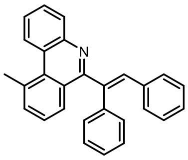
Yield 85%, 70.6 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.95 (d, *J* = 8.3 Hz, 2H), 7.67-7.60 (m, 2H), 7.54-7.42 (m, 3H), 7.40-7.26 (m, 5H), 7.22 (s, 1H), 7.18 (t, *J* = 7.5 Hz, 1H), 7.08 (d, *J* = 7.2 Hz, 1H), 6.92 (d, *J* = 7.1 Hz, 1H), 6.85 (t, *J* = 7.5 Hz, 1H), 6.46 (d, *J* = 7.5 Hz, 1H), 3.87 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 167.0, 166.5, 149.3, 144.4, 144.2, 140.5, 137.1, 133.3, 131.4, 130.3, 130.0, 129.3, 129.2, 129.0, 128.9, 128.5, 128.5, 128.2, 127.9, 127.1, 125.5, 124.7, 121.6, 118.4, 52.0. **HRMS (ESI):** m/z calculated for $C_{29}H_{22}NO_2$ [M+H]$^+$: 416.1645, found: 415.1646.



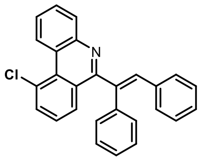
(*E*)-6-(1,2-diphenylvinyl)-9-methylphenanthridine (3h)
Yield 56%, 41.6 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.64 (d, *J* = 7.2 Hz, 2H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.38-7.27 (m, 6H), 7.22-7.16 (m, 4H), 7.09 (d, *J* = 7.2 Hz, 1H), 7.04 (d, *J* = 6.9 Hz, 1H), 6.92-6.83 (m, 2H), 6.49 (d, *J* = 7.5 Hz, 1H), 2.30 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-d)** δ 165.9, 149.3, 144.2, 140.7, 139.5, 137.3, 136.7, 133.5, 131.1, 130.3, 129.1, 128.6, 128.1, 128.0, 127.8, 127.8, 127.6, 127.0, 126.4, 125.7, 124.5, 121.4, 118.1, 21.3. **HRMS (ESI):** m/z calculated for $C_{28}H_{22}N$ $[M+H]^+$: 372.1747, found: 372.1748.



(*E*)-6-(1,2-diphenylvinyl)-9-(trifluoromethyl)phenanthridine (3i)
Yield 49%, 41.7 mg, yellow oil. **^{1}H NMR (600 MHz, Chloroform-*d*)** δ 7.76 (s, 1H), 7.58 (dd, *J* = 19.6, 7.6 Hz, 3H), 7.46 (dd, *J* = 16.8, 7.6 Hz, 2H), 7.42-7.28 (m, 6H), 7.23-7.16 (m, 2H), 7.09 (d, *J* = 7.3 Hz, 1H), 6.93 (d, *J* = 7.8 Hz, 1H), 6.86 (t, *J* = 7.5 Hz, 1H), 6.44 (d, *J* = 7.5 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.9, 149.7, 144.6, 140.9, 140.7, 137.4, 133.6, 132.9, 131.8, 130.7, 130.6, 129.9, 129.3, 129.2, 128.8, 128.7, 128.5, 127.4, 127.1 (q, *J* = 244.0 Hz), 126.4 (q, *J* = 3.7 Hz), 125.1, 124.0 (q, *J* = 3.8 Hz), 121.9, 118.8. **HRMS (ESI):** m/z calculated for $C_{28}H_{19}F_3N$ $[M+H]^+$: 426.1464, found: 426.1465.

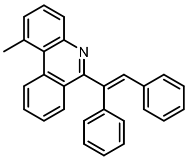


(*E*)-6-(1,2-diphenylvinyl)-10-methylphenanthridine (3j)
Yield 66%, 49.0 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** 7.40 (d, *J* = 7.9 Hz, 1H), 7.31 (m, 5H), 7.22 – 7.07 (m, 8H), 6.89 (t, *J* = 7.8 Hz, 2H), 6.76 (d, *J* = 8.0 Hz, 1H), 6.61 (t, *J* = 8.2 Hz, 1H), 2.22 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** 149.5, 144.4, 140.9, 139.6, 136.3, 133.4, 132.6, 131.2, 130.3, 129.8, 129.6, 128.7, 128.3, 127.9, 127.9, 127.7, 127.3, 126.8, 125.7, 125.2, 124.2, 121.5, 119.4. **HRMS (ESI):** m/z calculated for $C_{28}H_{22}N$ $[M+H]^+$: 372.1747, found: 372.1748.



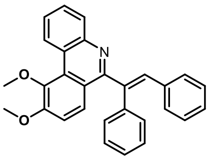
(*E*)-10-chloro-6-(1,2-diphenylvinyl)phenanthridine (3k)
Yield 55%, 43.1 mg, yellow oil. **^{1}H NMR (600 MHz, Chloroform-*d*)** δ 7.60-7.25 (m, 11H), 7.25-7.17 (m, 4H), 7.10 (d, *J* = 7.2 Hz, 1H), 6.95 (d, *J* = 7.8 Hz, 1H), 6.90 (t, *J* = 7.5 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.0, 149.7, 144.7, 141.0, 138.9, 136.9, 133.6, 131.9, 130.9, 129.7, 128.9,

128.4, 128.1, 127.1, 126.5, 124.5, 121.8, 118.3. **HRMS (ESI):** m/z calculated for $C_{27}H_{19}ClN$ $[M+H]^+$: 392.1201, found: 392.1202.



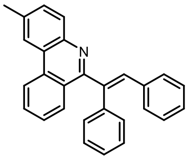
(*E*)-6-(1,2-diphenylvinyl)-1-methylphenanthridine (3l)

Yield 63%, 46.8 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.25 – 7.19 (m, 8H), 7.14 – 7.10 (m, 3H), 6.92 (t, *J* = 8.0 Hz, 1H), 6.70 (m, 2H), 2.20 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 165.2, 149.9, 144.4, 140.9, 138.9, 137.1, 136.2, 133.3, 131.2, 131.1, 129.2, 128.6, 128.00 127.7, 127.6, 126.8, 126.8, 125.8, 125.8, 121.5, 114.9, 20.6. **HRMS (ESI):** m/z calculated for $C_{28}H_{22}N$ $[M+H]^+$: 372.1747, found: 372.1748.



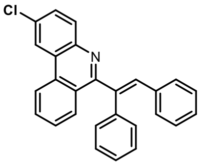
(*E*)-6-(1,2-diphenylvinyl)-9,10-dimethoxyphenanthridine (3m)

Yield 71%, 59.3 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.49-7.36 (m, 3H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.25-7.16 (m, 5H), 7.11 (d, *J* = 7.3 Hz, 1H), 6.99 (t, *J* = 7.9 Hz, 1H), 6.94-6.81 (m, 4H), 6.76 (d, *J* = 7.4 Hz, 1H), 3.85 (s, 3H), 3.51 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 165.3, 152.8, 149.5, 147.0, 144.5, 140.9, 136.3, 134.2, 133.5, 131.1, 131.0, 129.1, 128.8, 128.5, 128.0, 127.9, 127.6, 126.7, 125.9, 124.0, 123.5, 123.2, 121.5, 117.7, 111.9, 60.7, 56.0. **HRMS (ESI):** m/z calculated for $C_{29}H_{24}NO_2$ $[M+H]^+$: 418.1802, found: 418.1803.



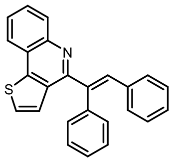
(*E*)-6-(1,2-diphenylvinyl)-2-methylphenanthridine (3n)

Yield 64%, 47.5 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.60 (d, *J* = 7.0 Hz, 2H), 7.41 (d, *J* = 7.3 Hz, 2H), 7.35-7.26 (m, 6H), 7.24-7.15 (m, 3H), 7.14-7.07 (m, 2H), 6.88 (t, *J* = 7.5 Hz, 1H), 6.78 (d, *J* = 7.9 Hz, 1H), 6.63 (d, *J* = 7.5 Hz, 1H), 2.44 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.2, 146.7, 144.3, 140.1, 139.8, 136.6, 134.1, 133.5, 131.2, 131.1, 131.0, 129.4, 129.1, 128.7, 128.6, 128.1, 127.8, 127.7, 126.9, 126.8, 125.7, 121.4, 118.2, 21.0. **HRMS (ESI):** m/z calculated for $C_{28}H_{22}N$ $[M+H]^+$: 372.1747, found: 372.1748.



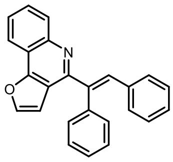
(*E*)-2-chloro-6-(1,2-diphenylvinyl)phenanthridine (3o)

Yield 78%, 61.1 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.59-7.53 (m, 2H), 7.46 (d, *J* = 2.3 Hz, 1H), 7.42-7.36 (m, 2H), 7.35-7.26 (m, 7H), 7.24-7.18 (m, 2H), 7.10 (d, *J* = 7.2 Hz, 1H), 6.96-6.87 (m, 1H), 6.83 (d, *J* = 8.4 Hz, 1H), 6.63 (d, *J* = 7.5 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.8, 147.7, 144.3, 140.7, 138.3, 137.1, 133.3, 133.0, 131.6, 130.2, 129.7, 129.2, 128.9, 128.6, 128.2, 128.1, 128.0, 127.9, 127.5, 127.1, 125.7, 121.7, 119.7. **HRMS (ESI):** m/z calculated for $C_{27}H_{19}ClN$ [M+H]$^+$: 392.1201, found: 392.1202.



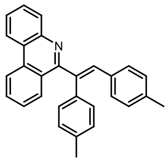
(*E*)-4-(1,2-diphenylvinyl)thieno[3,2-c]quinoline (3p)

Yield 42%, 30.5 mg, yellow oil. **^{1}H NMR (600 MHz, Chloroform-*d*)** δ 7.93 (d, *J* = 7.5 Hz, 2H), 7.74 (d, *J* = 6.9 Hz, 1H), 7.42 – 7.27 (m, 5H), 7.24 (s, 1H), 7.23 – 7.10 (m, 4H), 6.99 – 6.92 (m, 1H), 6.89 (d, *J* = 8.0 Hz, 1H), 6.83 (t, *J* = 7.5 Hz, 1H), 6.49 (d, *J* = 7.5 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** 167.4, 148.1, 143.9, 140.7, 140.1, 137.2, 133.3, 131.3, 128.9, 128.9, 128.5, 128.2, 127.9, 127.8, 127.0, 126.8, 125.7, 125.6, 124.5, 121.4, 118.7. **HRMS (ESI):** m/z calculated for $C_{25}H_{18}NS$ [M+H]$^+$: 364.1154, found: 364.1157.



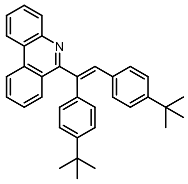
(*E*)-4-(1,2-diphenylvinyl)furo[3,2-c]quinoline (3q)

Yield 47%, 32.6 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.99 (dd, *J* = 10.2, 6.0 Hz, 3H), 7.46 – 7.31 (m, 6H), 7.16 (dt, *J* = 15.8, 7.2 Hz, 3H), 6.93 – 6.86 (m, 1H), 6.81 (t, *J* = 7.4 Hz, 1H), 6.47 (d, *J* = 7.5 Hz, 1H), 6.39 (d, *J* = 3.3 Hz, 1H), 6.34 – 6.28 (m, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** 166.8, 151.1, 147.1, 143.9, 141.5, 139.9, 137.4, 133.4, 131.4, 128.5, 128.4, 128.0, 127.7, 127.2, 126.1, 125.7, 124.5, 121.6, 118.4, 111.9, 109.6. **HRMS (ESI):** m/z calculated for $C_{25}H_{18}NO$ [M+H]$^+$: 348.1383, found: 348.1384.



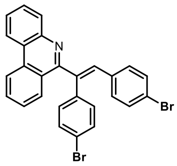
(*E*)-6-(1,2-di-*p*-tolylvinyl)phenanthridine (3r)

Yield 76%, 58.6 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.49 (d, *J* = 8.1 Hz, 2H), 7.46-7.39 (m, 3H), 7.34-7.26 (m, 4H), 7.24-7.19 (m, 1H), 7.12 (d, *J* = 6.2 Hz, 3H), 6.93-6.85 (m, 2H), 6.65 (d, *J* = 7.4 Hz, 1H), 6.39 (d, *J* = 7.4 Hz, 1H), 2.33 (s, 3H), 2.27 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.3, 149.5, 144.8, 141.7, 141.0, 139.7, 137.6, 135.8, 131.3, 130.7, 130.3, 129.4, 128.9, 128.5, 128.1, 127.9, 127.1, 126.8, 126.7, 125.5, 124.4, 122.5, 118.4, 21.7, 21.3. **HRMS (ESI):** m/z calculated for $C_{29}H_{24}NO_2$ [M+H]$^+$: 386.1903, found: 386.1909.



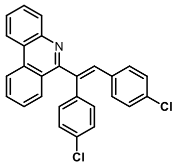
(*E*)-6-(1,2-bis(4-(*tert*-butyl)phenyl)vinyl)phenanthridine (3s)

Yield 72%, 67.6 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.54 (d, *J* = 8.3 Hz, 2H), 7.49-7.42 (m, 3H), 7.37-7.27 (m, 6H), 7.24-7.11 (m, 3H), 6.87 (d, *J* = 7.8 Hz, 2H), 6.44 (d, *J* = 7.8 Hz, 1H), 1.32 (s, 9H), 1.28 (s, 9H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 166.4, 154.9, 150.6, 149.5, 144.5, 140.9, 139.7, 136.4, 131.3, 130.8, 130.1, 129.4, 128.2, 128.0, 127.9, 126.8, 126.7, 125.5, 125.1, 124.4, 123.4, 119.0, 118.5, 35.0, 35.0, 34.3, 34.1. **HRMS (ESI):** m/z calculated for $C_{35}H_{36}N$ [M+H]$^+$: 470.2842, found: 470.2845.



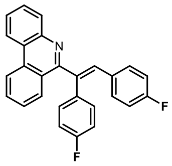
(*E*)-6-(1,2-bis(4-bromophenyl)vinyl)phenanthridine (3t)

Yield 82%, 84.5 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.52-7.41 (m, 5H), 7.39-7.27 (m, 6H), 7.25-7.21 (m, 2H), 7.17 (s, 1H), 7.07-7.00 (m, 1H), 6.86 (d, *J* = 7.2 Hz, 1H), 6.39 (d, *J* = 8.0 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 165.1, 149.0, 146.2, 141.0, 139.7, 135.8, 132.1, 131.7, 131.7, 130.8, 130.5, 130.2, 129.6, 128.5, 128.3, 127.7, 127.4, 127.0, 126.1, 125.4, 125.2, 122.8, 118.3. **HRMS (ESI):** m/z calculated for $C_{27}H_{18}Br_2N$ [M+H]$^+$: 515.9780, found: 515.9777.



(*E*)-6-(1,2-bis(4-chlorophenyl)vinyl)phenanthridine (3u)

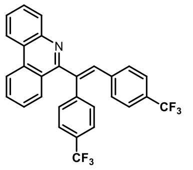
Yield 79%, 67.3 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.54 (d, *J* = 8.5 Hz, 2H), 7.46 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.38-7.32 (m, 3H), 7.33-7.26 (m, 6H), 7.16 (s, 1H), 7.08 (d, *J* = 1.7 Hz, 1H), 6.89-6.83 (m, 2H), 6.45 (d, *J* = 8.1 Hz, 1H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 164.7, 148.7, 145.8, 140.8, 139.4, 137.3, 135.5, 134.2, 131.4, 131.4, 130.5, 129.9, 129.3, 128.4, 128.2, 128.0, 127.0, 126.9, 126.8, 126.4, 125.0, 122.0, 118.0. **HRMS (ESI):** m/z calculated for $C_{27}H_{18}Cl_2N$ [M+H]$^+$: 426.0811, found: 426.0814.



(*E*)-6-(1,2-bis(4-fluorophenyl)vinyl)phenanthridine (3v)

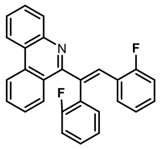
Yield 74%, 58.2 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.62-7.51 (m, 2H), 7.49-7.41 (m, 1H), 7.40-7.26 (m, 6H), 7.25-7.17 (m, 1H), 7.09 (s, 1H), 7.00 (t, *J* = 8.7 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 1H), 6.78 (dd, *J* = 8.2, 1.9 Hz, 1H), 6.56-6.44 (m, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)**

164.9 (d, *J* = 193.0 Hz), 164.7, 162.5 (d, *J* = 190.0 Hz), 148.7, 147.0 (d, *J* = 9.0 Hz), 141.3, 139.5, 134.8, 131.4, 130.5, 130.4 (d, *J* = 10.0 Hz), 129.3, 129.1 (d, *J* = 3.0 Hz), 128.2, 127.9, 127.1, 127.0, 124.9, 124.7 (d, *J* = 3.0 Hz), 118.1, 115.2 (d, *J* = 21.0 Hz), 112.7 (d, *J* = 22.0 Hz), 109.5 (d, *J* = 24.0 Hz). **HRMS (ESI):** m/z calculated for $C_{27}H_{18}F_2N$ $[M+H]^+$: 394.1402, found: 394.1407.



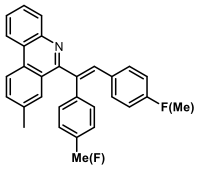
(*E*)-6-(1,2-bis(4-(trifluoromethyl)phenyl)vinyl)phenanthridine (3w)

Yield 77%, 76.0 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.72 (d, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 8.1 Hz, 2H), 7.49 (d, *J* = 7.5 Hz, 1H), 7.41-7.27 (m, 9H), 7.22 (d, *J* = 8.3 Hz, 1H), 6.88 (d, *J* = 7.2 Hz, 1H), 6.68 (d, *J* = 7.8 Hz, 1H). **^{13}C NMR (150 MHz, Chloroform-*d*)** 164.3, 148.4, 144.2, 140.6, 139.1, 136.9, 136.1, 132.9 (q, *J* = 32.2 Hz), 131.3, 131.2, 130.5, 128.8 (q, *J* = 339.0 Hz), 129.1, 128.8, 127.9, 126.8 (q, *J* = 268.0 Hz), 125.5 (q, *J* = 3.7 Hz), 125.3, 124.9, 124.7 (q, *J* = 3.0 Hz), 124.4, 123.1, 122.6, 118.3 (q, *J* = 3.5 Hz), 117.7. **HRMS (ESI):** m/z calculated for $C_{29}H_{18}F_6N$ $[M+H]^+$: 494.1338, found: 494.1336.



(*E*)-6-(1,2-bis(2-fluorophenyl)vinyl)phenanthridine (3x)

Yield 67%, 52.7 mg, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.47-7.38 (m, 5H), 7.38-7.27 (m, 5H), 7.25-7.18 (m, 2H), 7.08 (t, *J* = 9.5 Hz, 1H), 6.99 (t, *J* = 6.6 Hz, 2H), 6.70 (t, *J* = 8.8 Hz, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 162.2 (d, *J* = 8.0 Hz), 160.8 (d, *J* = 248.0 Hz), 156.4 (d, *J* = 259.0 Hz), 150.0 (d, *J* = 2.0 Hz), 147.2 (d, *J* = 5.0 Hz), 140.0, 138.5 (d, *J* = 4.0 Hz), 135.6, 134.0 (d, *J* = 9.0 Hz), 132.7 (d, *J* = 2.0 Hz), 132.2 (d, *J* = 3.0 Hz), 129.7, 129.4, 129.2 (d, *J* = 9.0 Hz), 127.8, 127.3, 126.7, 124.5, 123.5 (d, *J* = 3.0 Hz), 118.5 (d, *J* = 6.0 Hz), 118.1, 116.3 (d, *J* = 25.0 Hz), 115.5 (d, *J* =23.0 Hz). **HRMS (ESI):** m/z calculated for $C_{27}H_{18}F_2N$ $[M+H]^+$: 394.1402, found: 394.1405.



(E)-6-(2-(4-fluorophenyl)-1-(p-tolyl)vinyl)-8-methylphenanthridine (3y+3y')

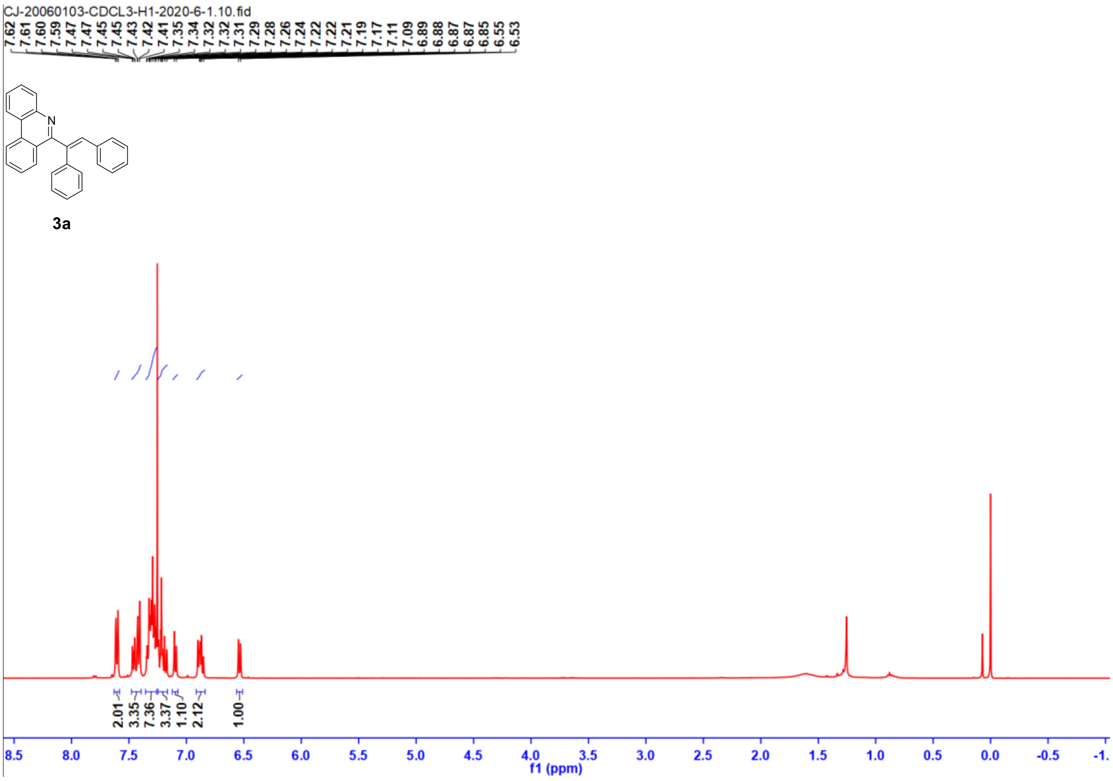
Yield 72%, 58.1 mg, yellow oil, 3y:3y' = 1:1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.64 – 7.58 (m, 2H), 7.55 (d, *J* = 7.8 Hz, 2H), 7.44 (d, *J* = 7.5 Hz, 2H), 7.33 – 7.27 (m, 5H), 7.24 (s, 1H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.14 (s, 1H), 7.10 (d, *J* = 6.8 Hz, 4H), 7.01 (t, *J* = 8.6 Hz, 2H), 6.92 (s, 1H), 6.89 – 6.84 (m, 2H), 6.77 (d, *J* = 7.1 Hz, 1H), 6.67 (d, *J* = 7.6 Hz, 1H), 6.50 (t, *J* = 8.1 Hz, 1H), 6.43 (t, *J* = 8.1 Hz, 2H), 2.36 (s, 3H), 2.31 (s, 6H), 2.28 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 165.9, 164.7, 164.3 (d, *J* = 210.0 Hz), 162.6 (d, *J* = 220.0 Hz), 149.2, 149.0, 147.2 (d, *J* = 7.0 Hz), 144.4, 142.4, 141.8, 139.8, 138.0, 136.7, 136.5, 136.5, 136.2, 134.2, 131.2 (d, *J* = 19.0 Hz), 130.3 (d, *J* = 3.0 Hz), 130.2 (d, J = 6.0 Hz), 129.1, 129.0, 128.9, 128.6, 128.5, 128.5, 127.8, 127.8, 127.3, 127.0 (d, J = 6.0 Hz), 126.4, 125.6, 124.6, 124.5, 122.5, 118.2, 118.1, 115.1, 114.9, 112.5, 112.3, 109.3, 109.1, 21.6, 21.3, 21.1.

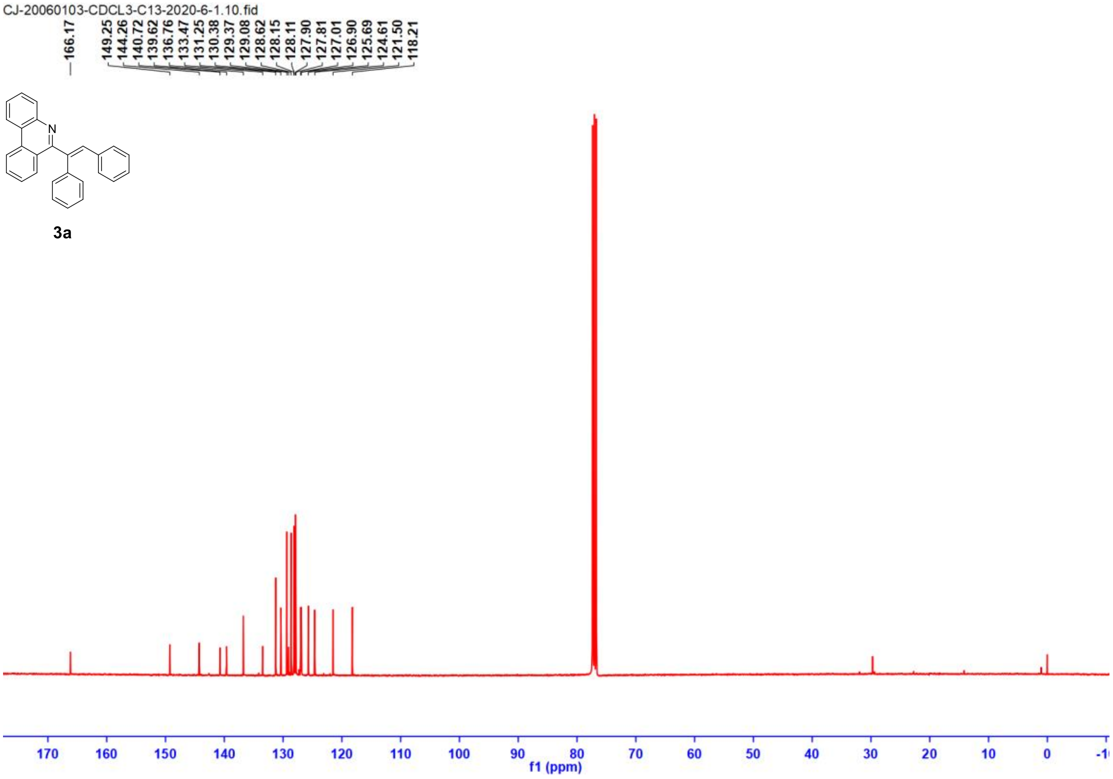
VI. References

1. Yuzhen Gao, Z. C., Shangda Li, and Gang Li, Rhodium(I)-Catalyzed Aryl C−H Carboxylation of 2-Arylanilines with CO_2, *Org. Lett.* 2019, **21**, 3663-3669.

2. (a) Liu, Y.; Tian, Y.; Su, K.; Wang, P.; Guo, X.; Chen, B., Rhodium(iii)-catalyzed [3 + 3] annulation reactions of N-nitrosoanilines and cyclopropenones: an approach to functionalized 4-quinolones. *Org. Chem. Front.* 2019, **6**, 3973-3977; (b) D. N. Eric and H. L. Tristan, Cyclopropenone catalyzed substitution of Alcohols with Mesylate Ion. *Org. Lett.* 2013, **15**, 38-41.

VII. NMR Spectra of Coupled Products





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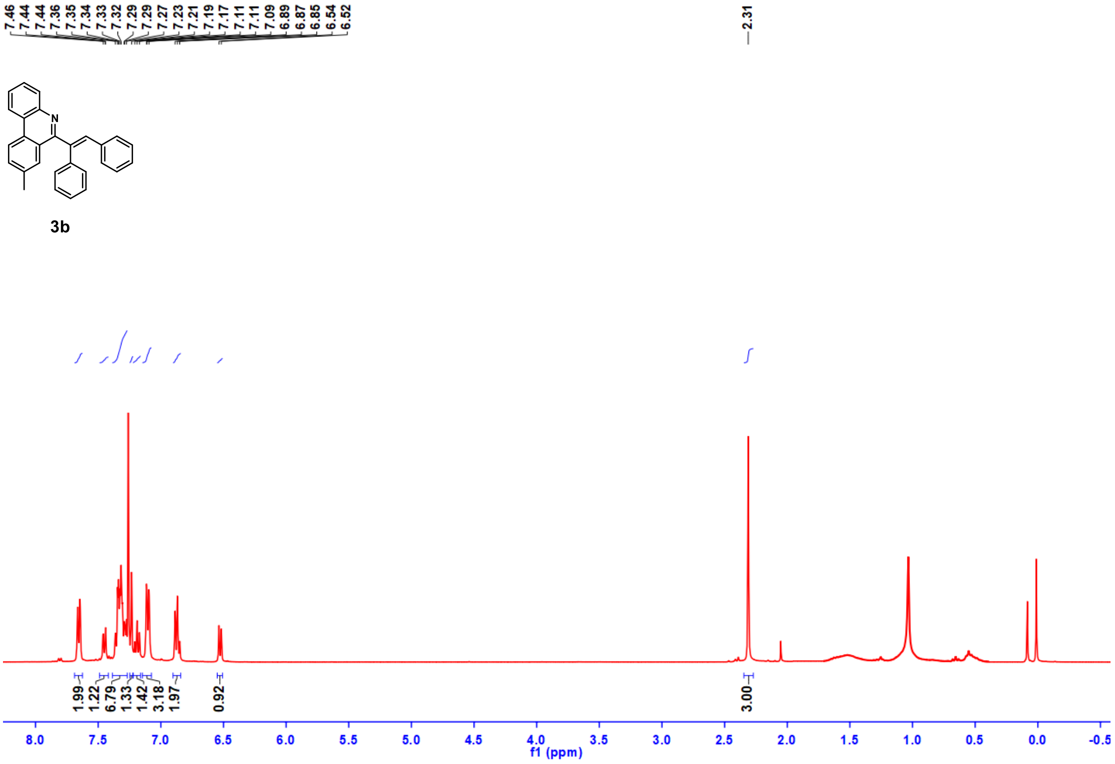

3b

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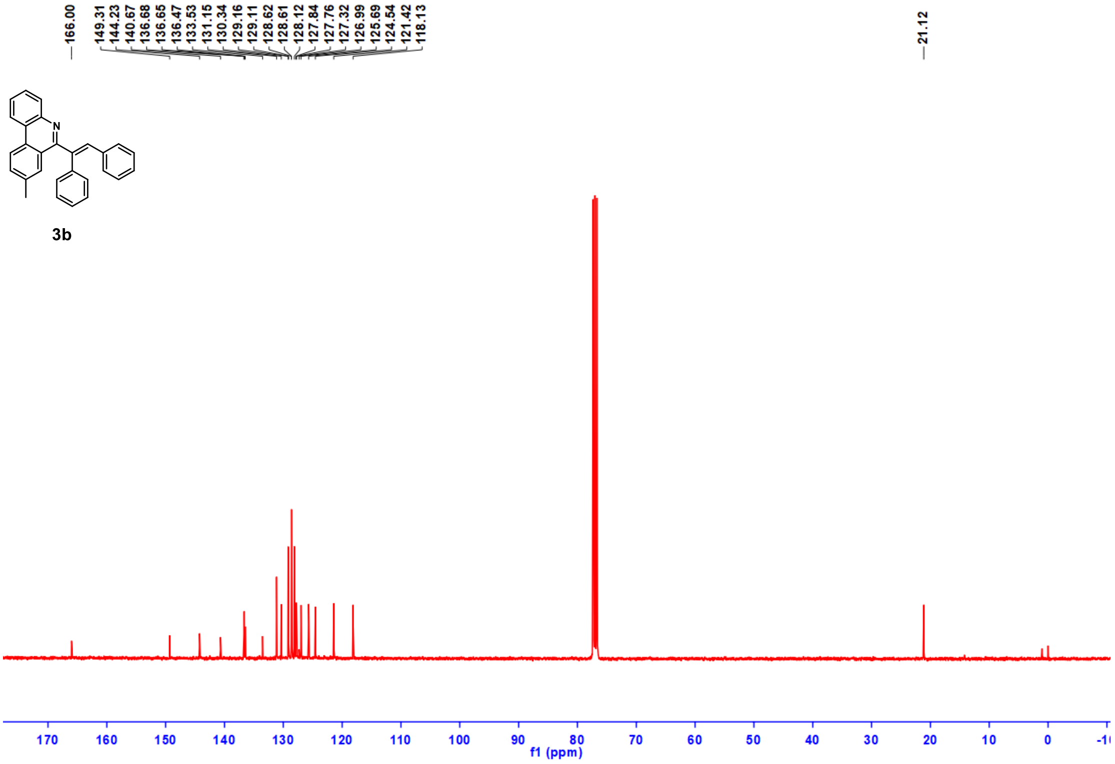

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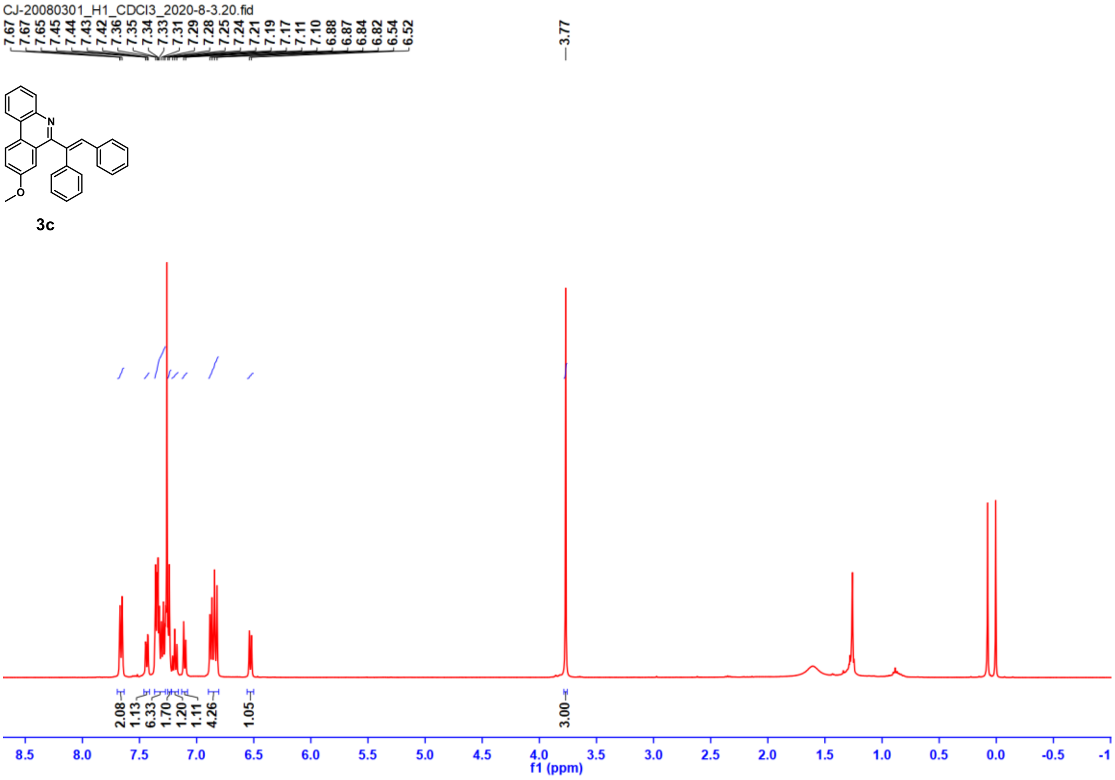
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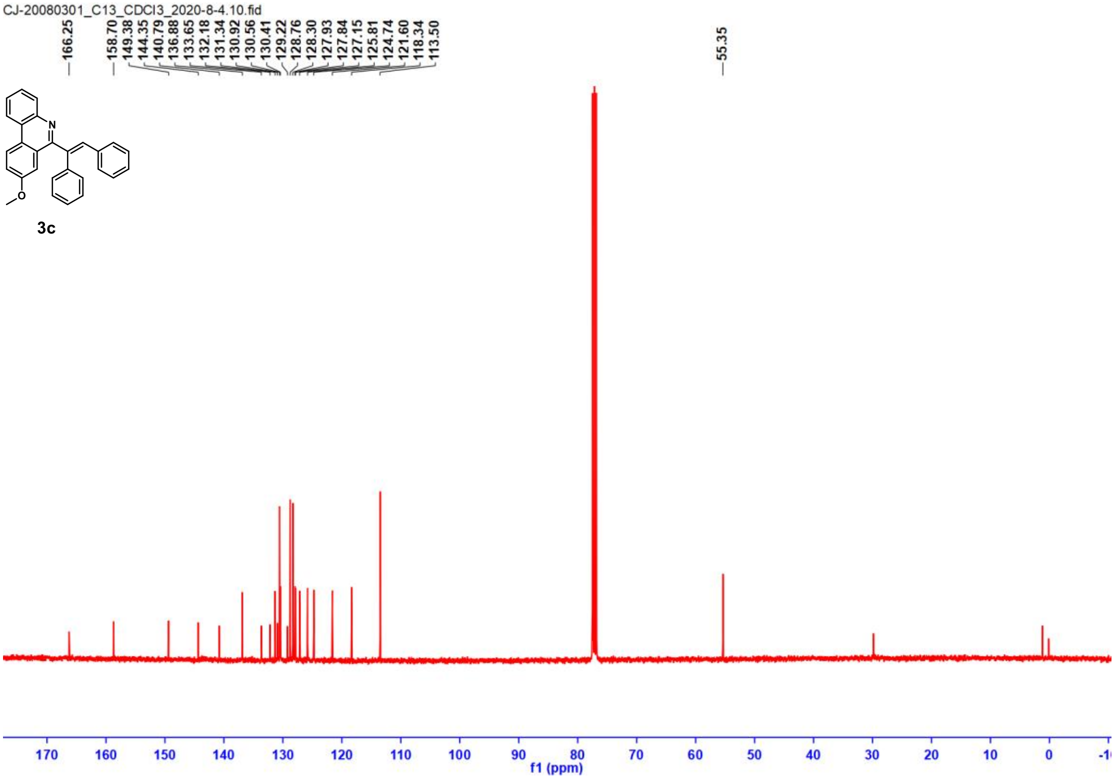
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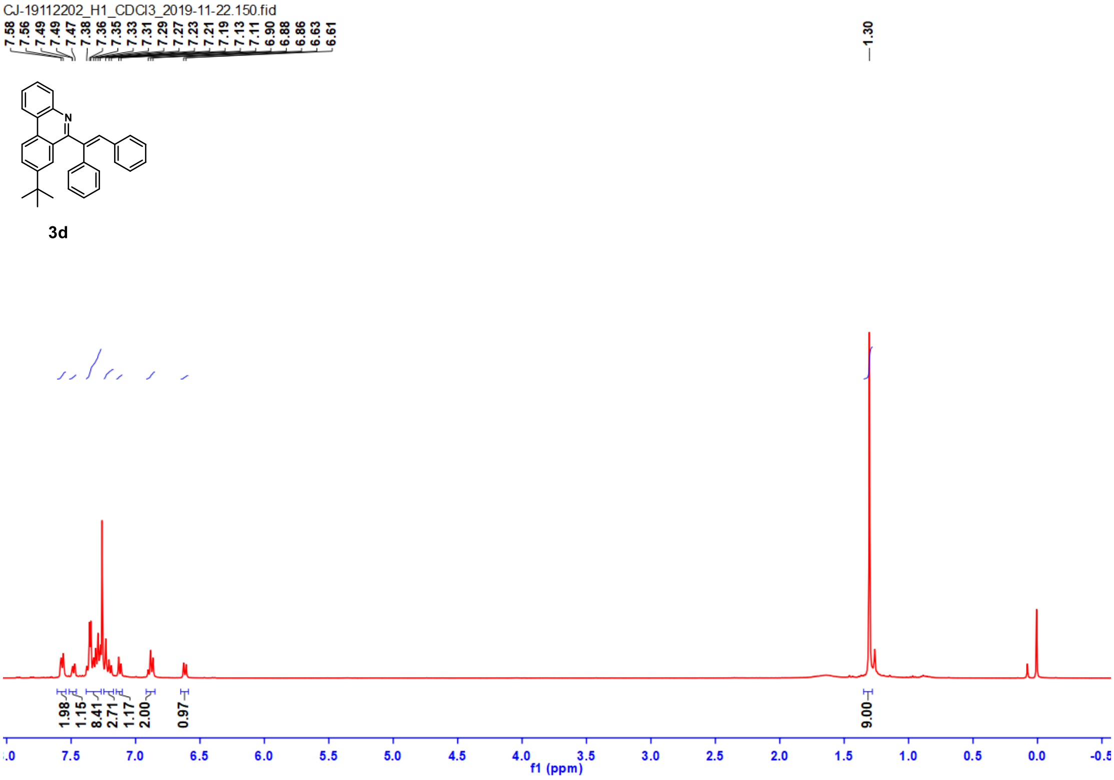
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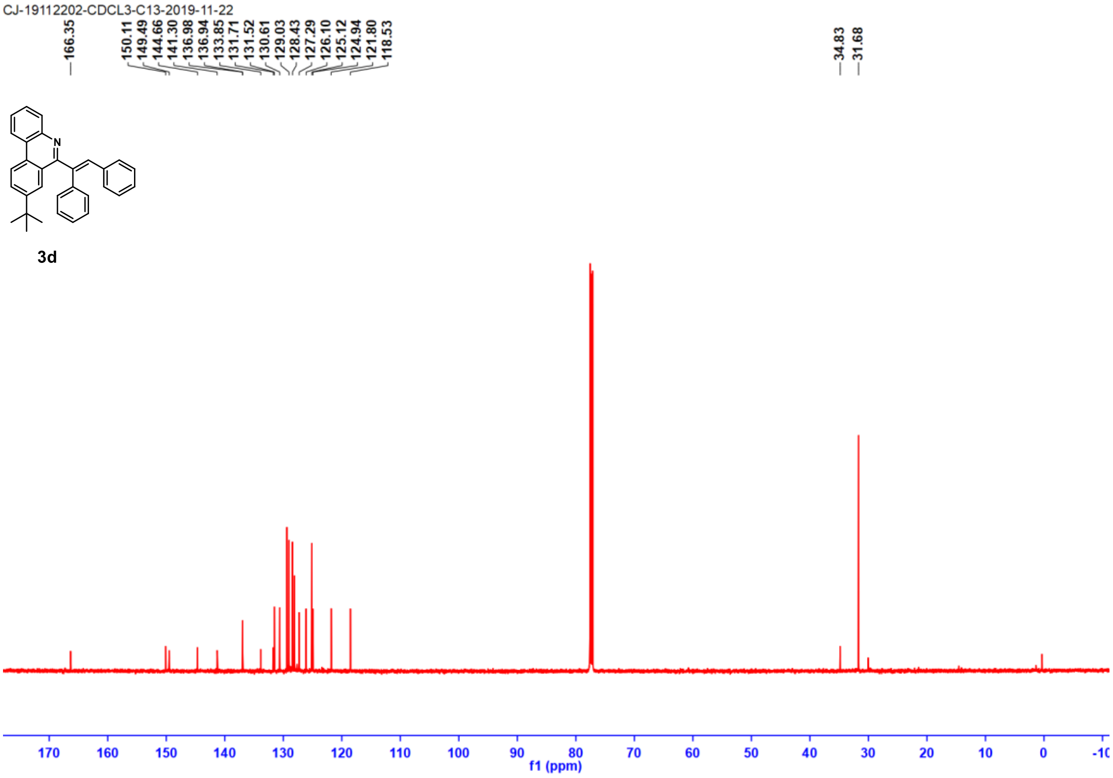
f1 (ppm)

3d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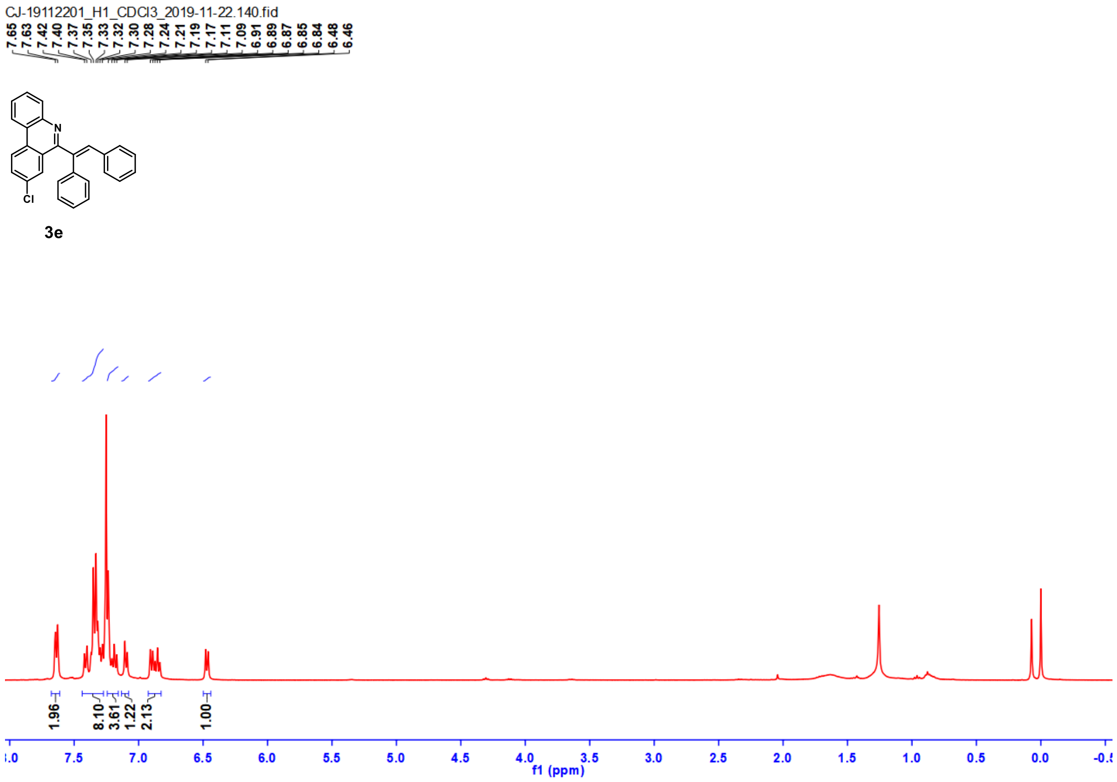
3d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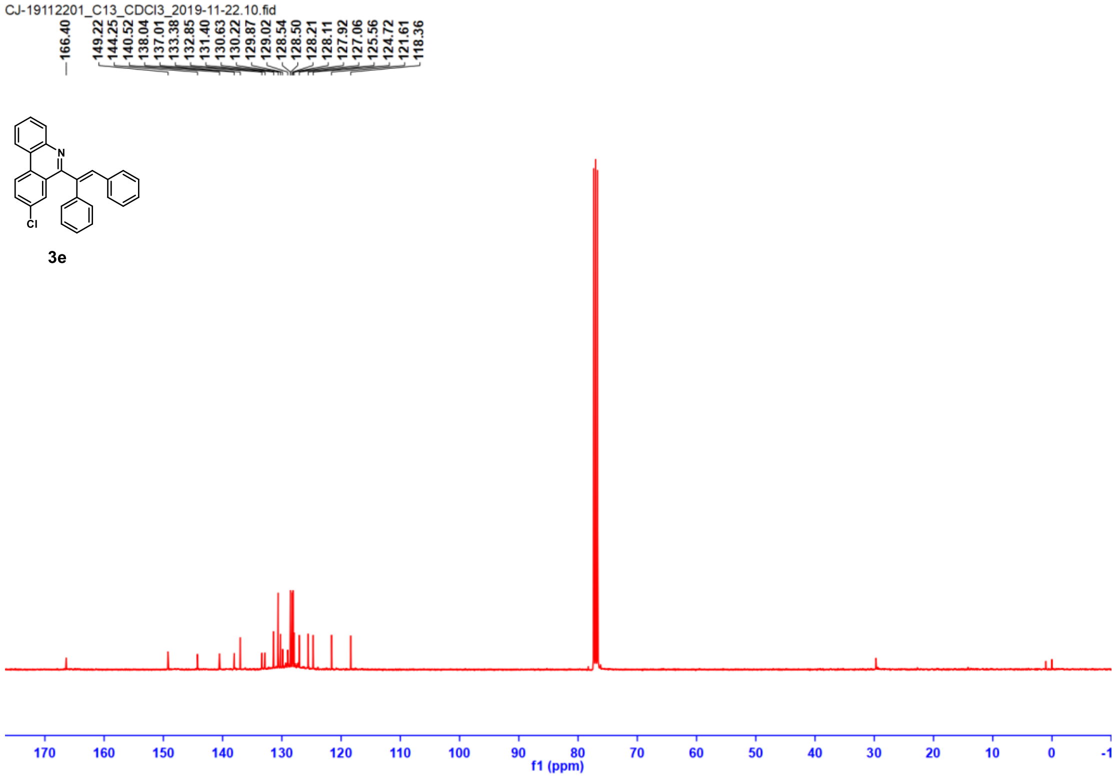
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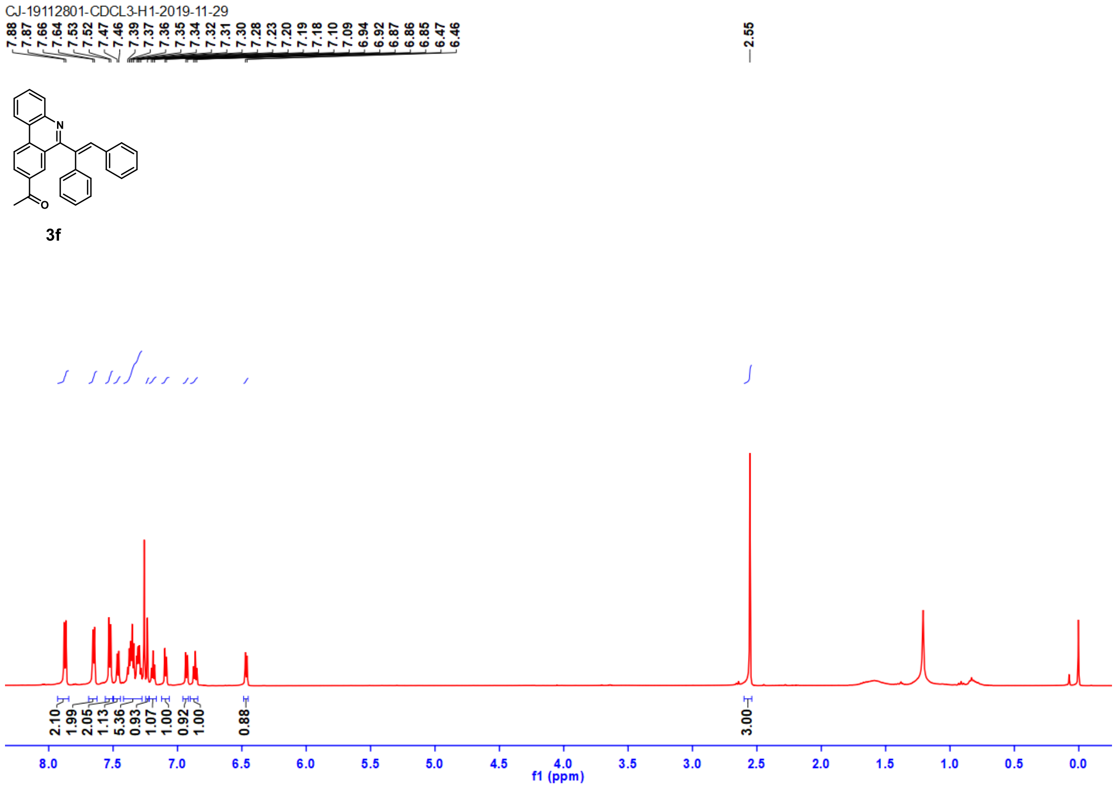
3e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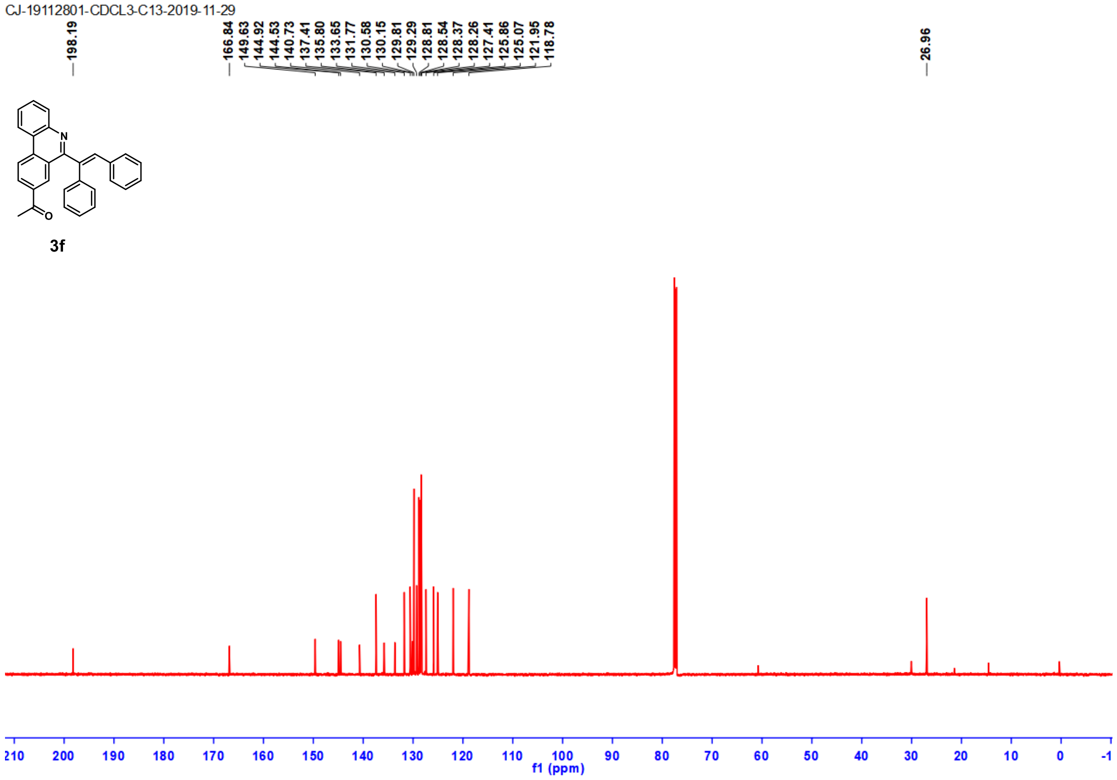
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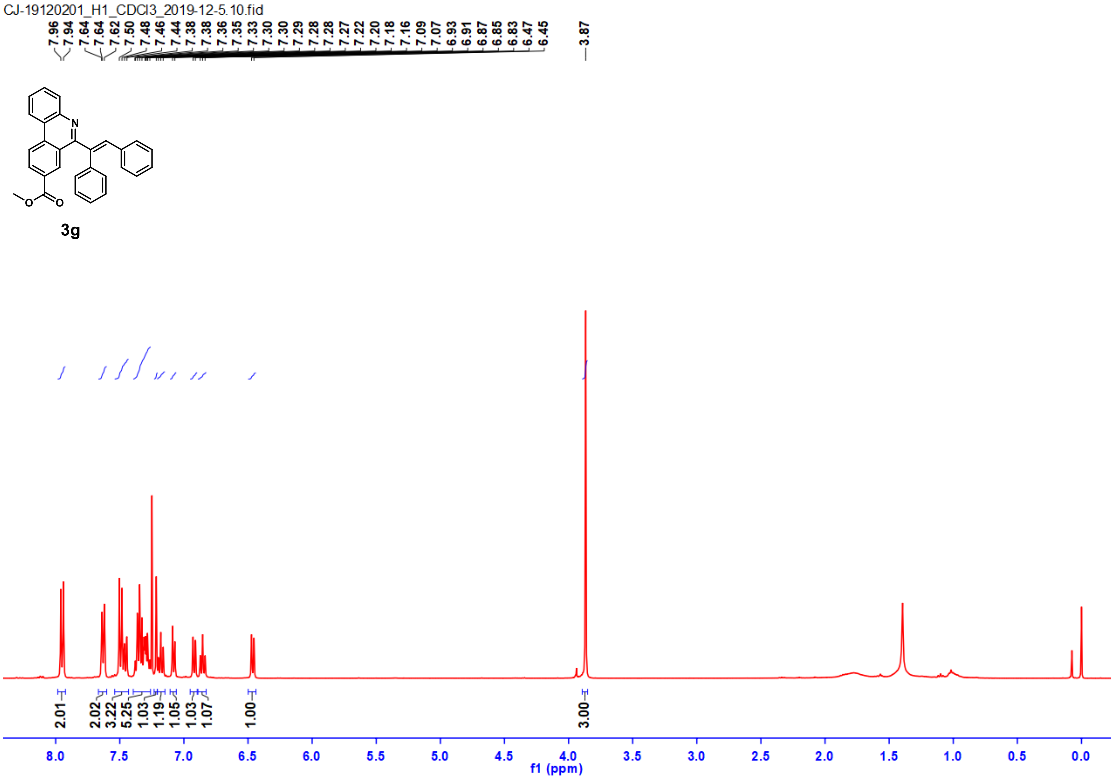
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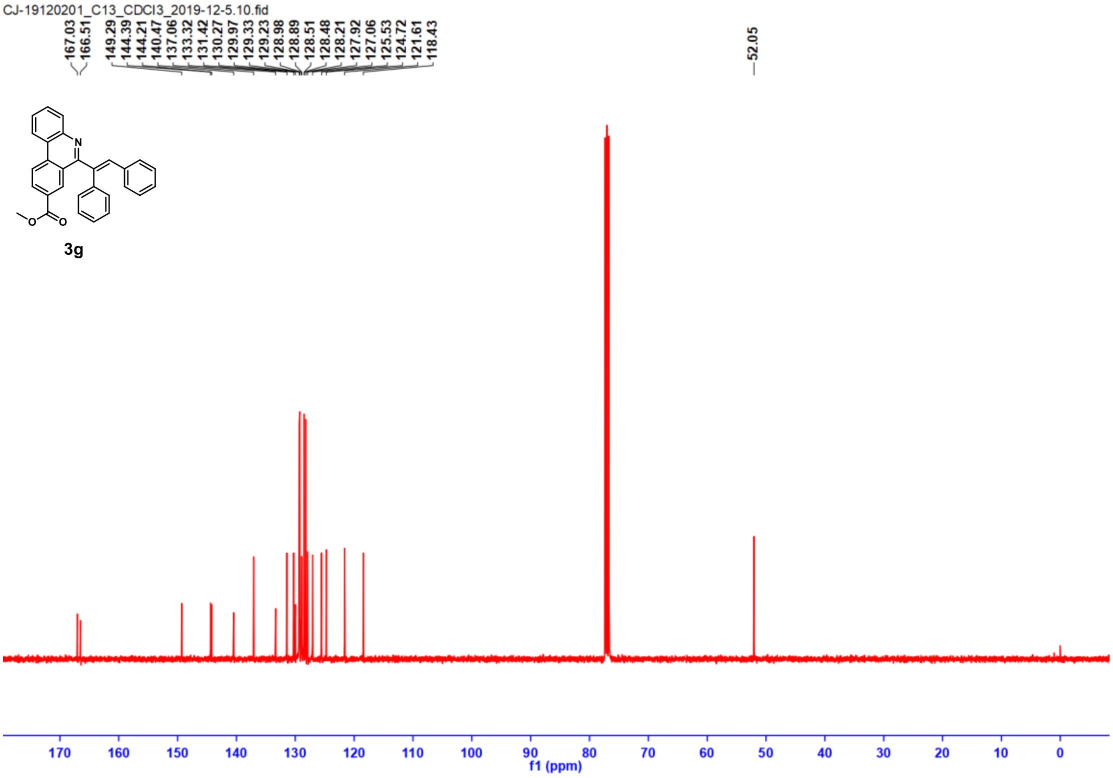
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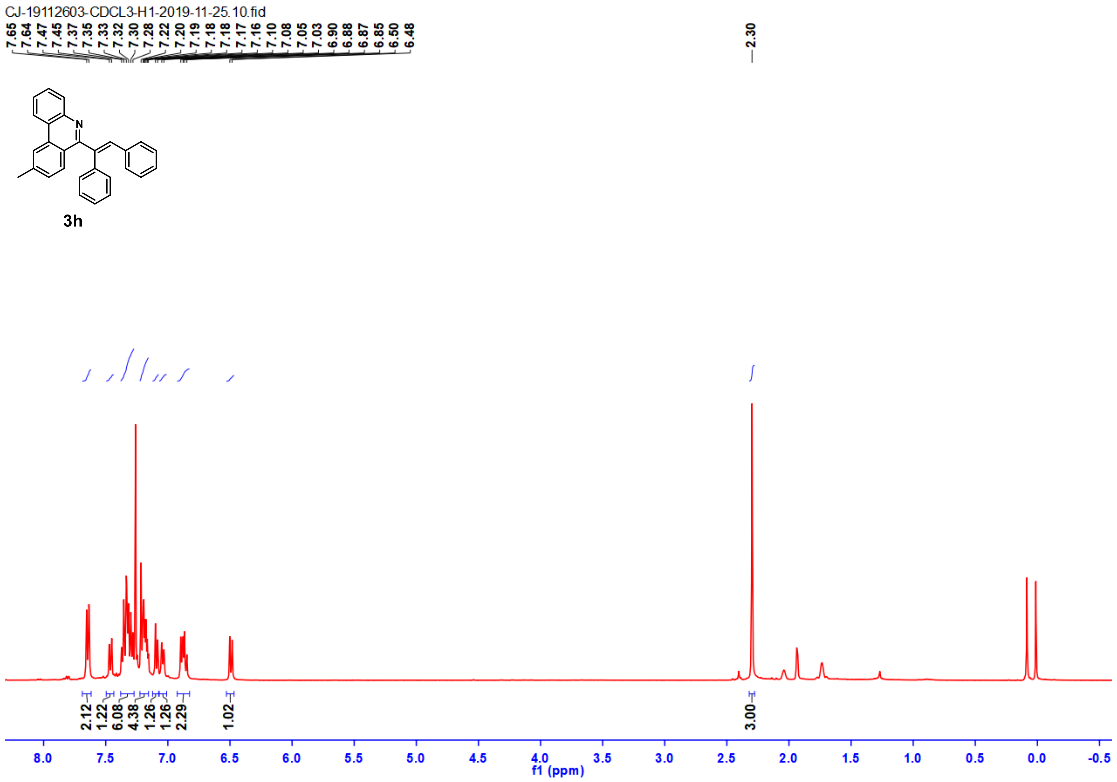
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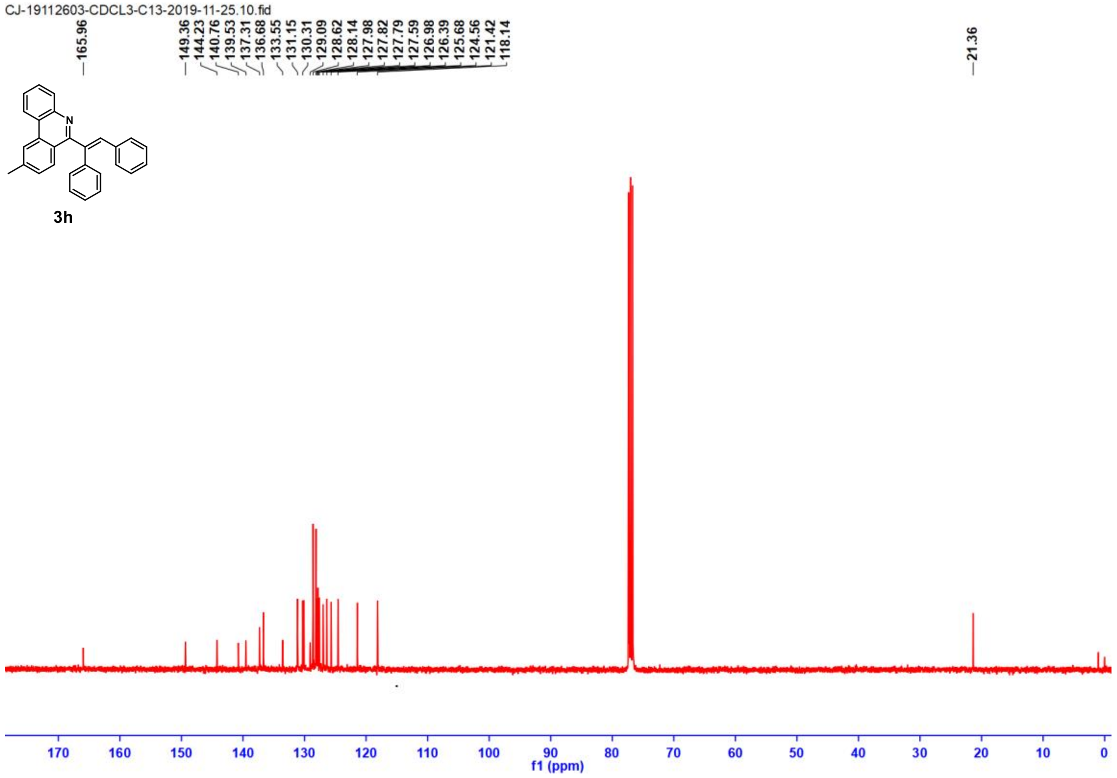
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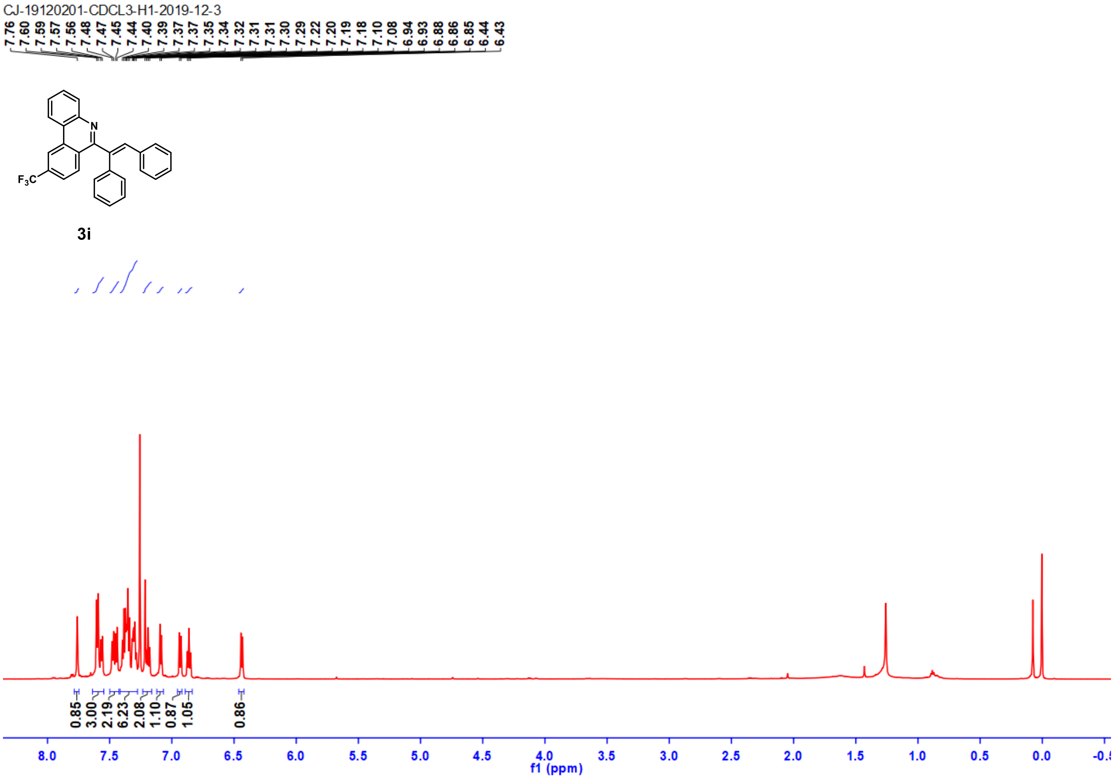
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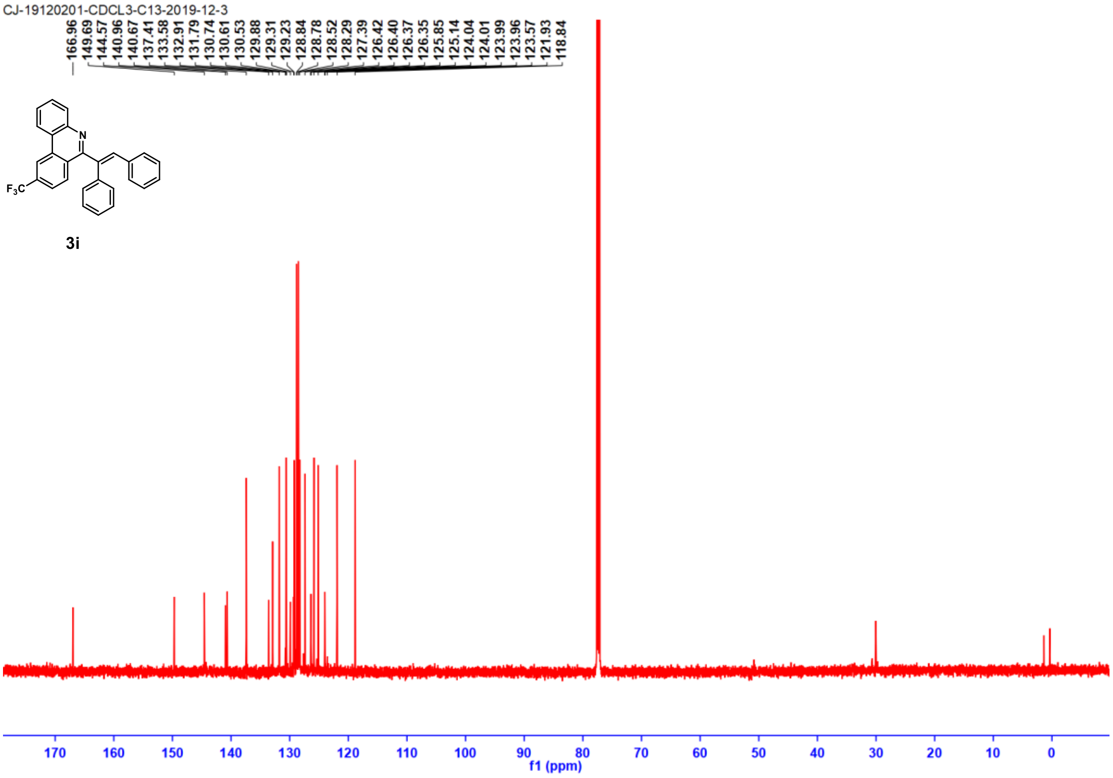
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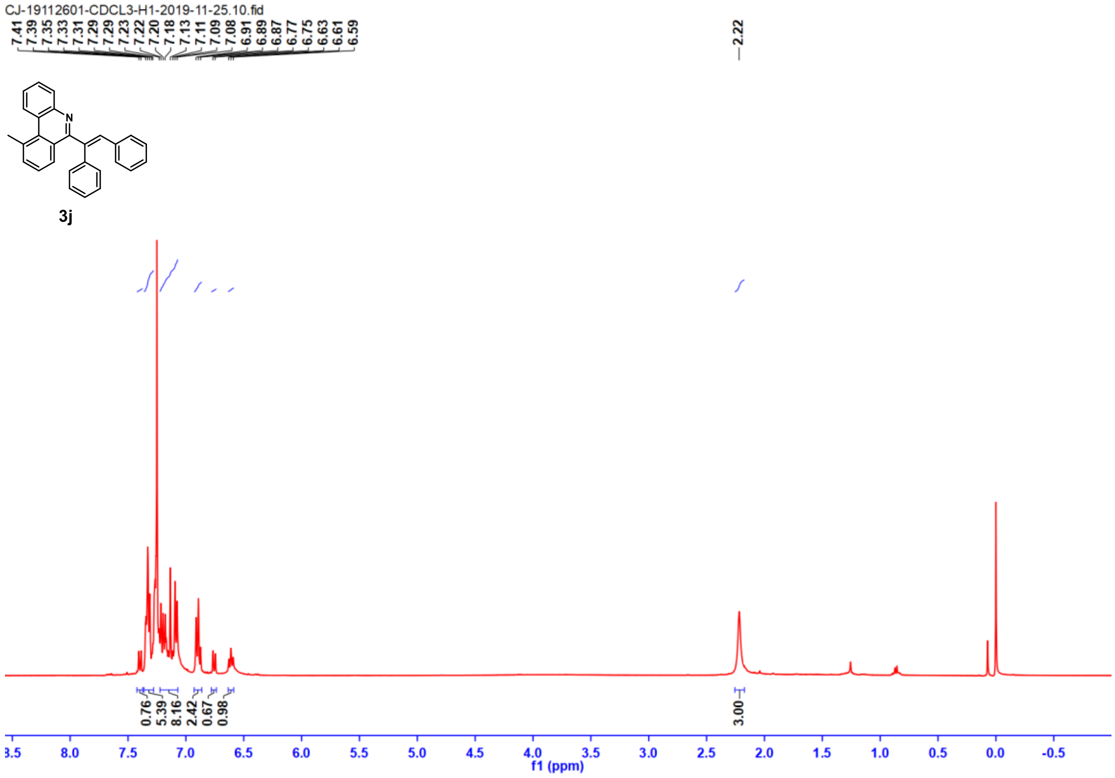
3i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7.13
7.11
7.09
7.08
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6.89
6.87
6.77
6.75
6.63
6.61
6.59
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N
3j
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5.39
8.16
2.42
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6.0
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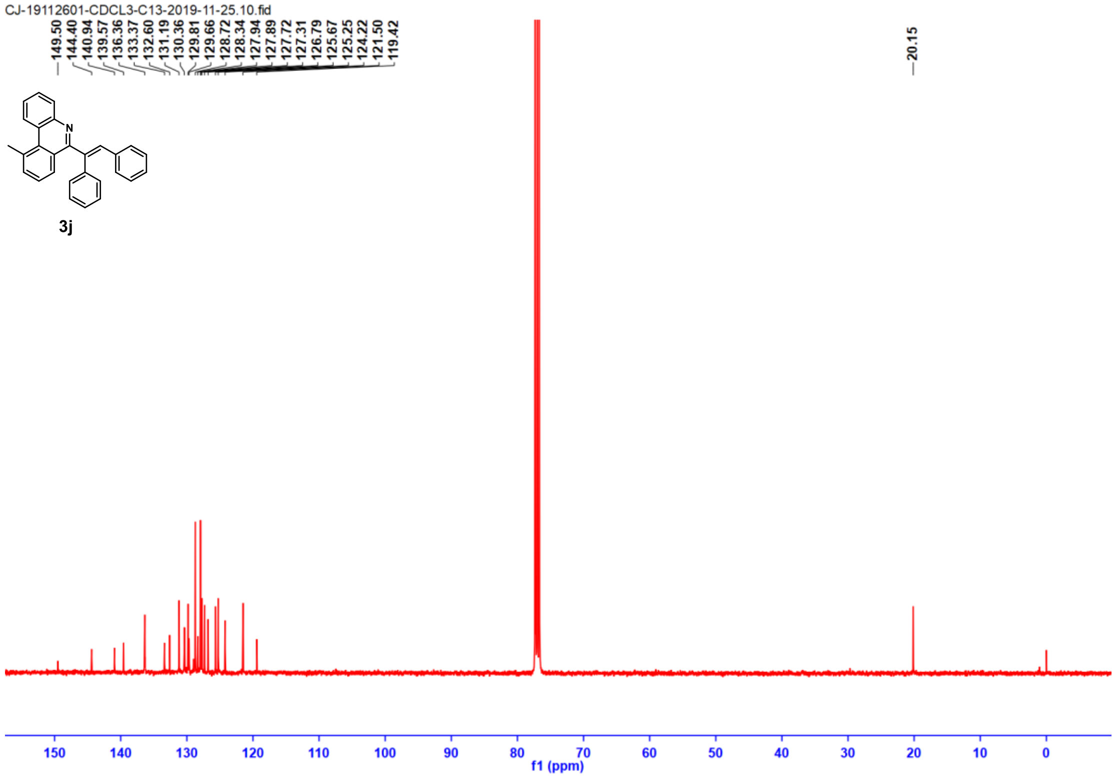
CJ-19112601-CDCL3-C13-2019-11-25.10.fid
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127.89
127.72
127.31
126.79
125.67
125.25
124.22
121.50
119.42
20.15
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90
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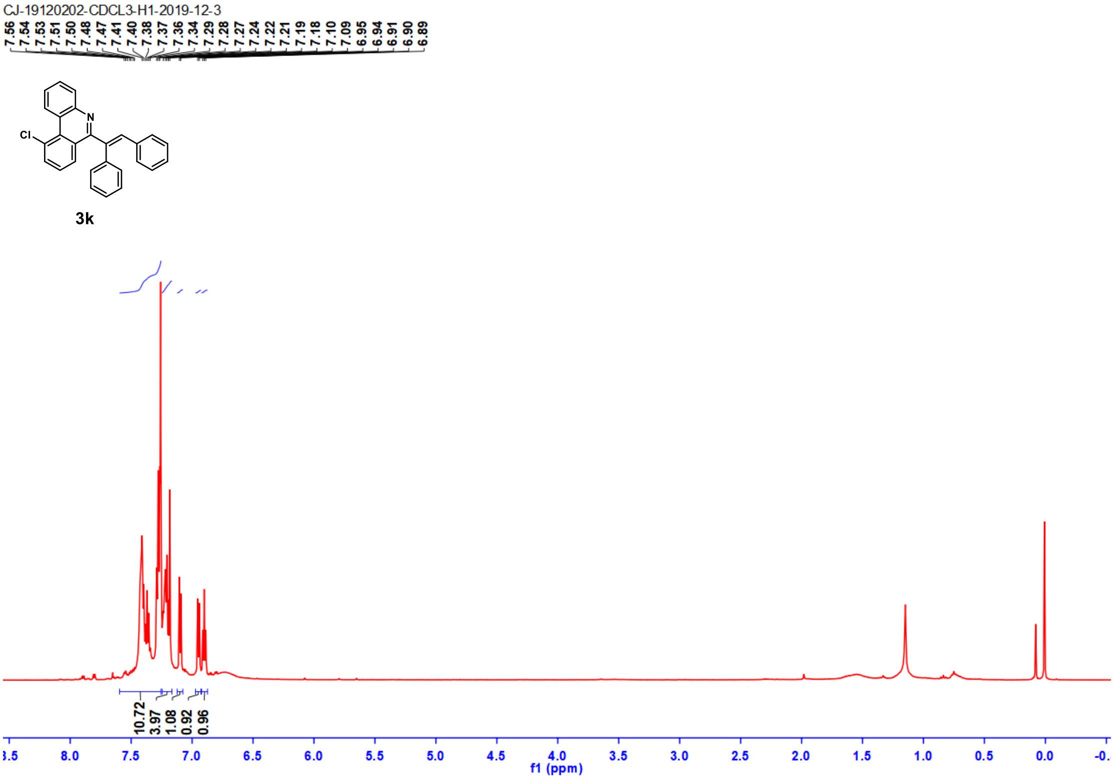
f1 (ppm)


CJ-19120202-CDCL3-H1-2019-12-3
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7.40
7.38
7.37
7.36
7.34
7.29
7.28
7.27
7.24
7.22
7.21
7.19
7.18
7.10
7.09
6.95
6.94
6.91
6.90
6.89
Cl
N
10.72
3.97
1.08
0.92
0.96
8.5
8.0
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7.0
6.5
6.0
5.5
5.0
4.5
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1.5
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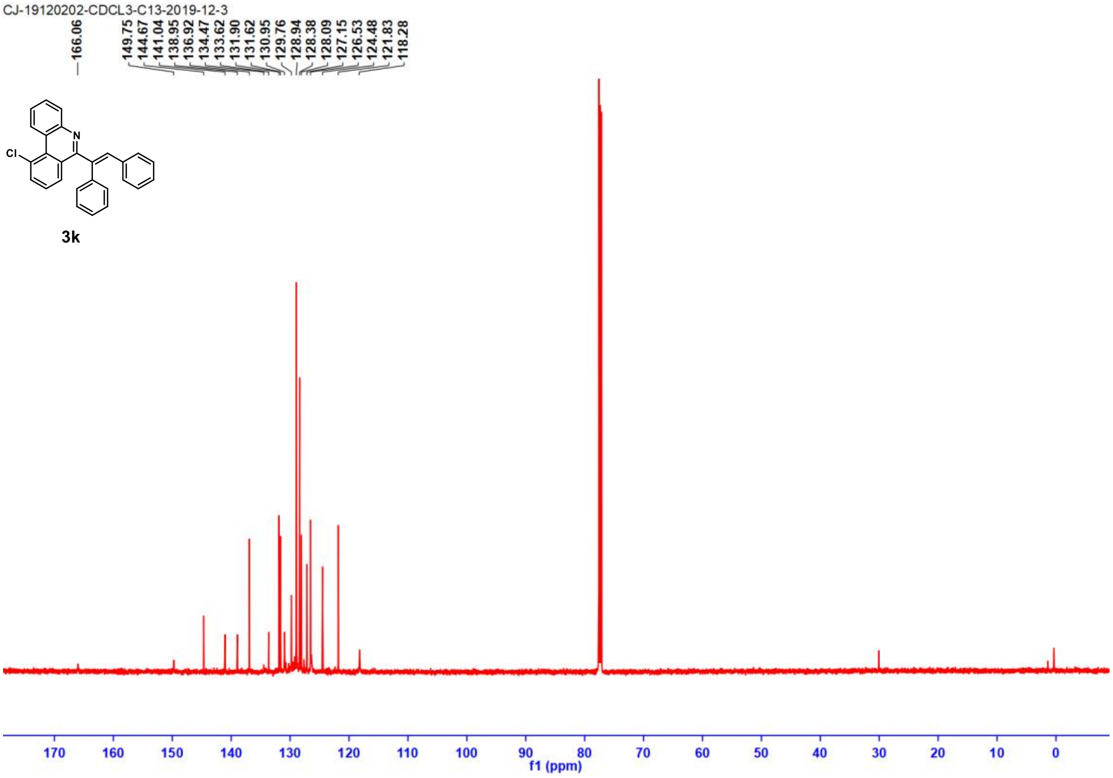
f1 (ppm)

3k


CJ-19120202-CDCL3-C13-2019-12-3
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130.95
129.76
128.94
128.38
128.09
127.15
126.53
124.48
121.83
118.28
Cl
N
170
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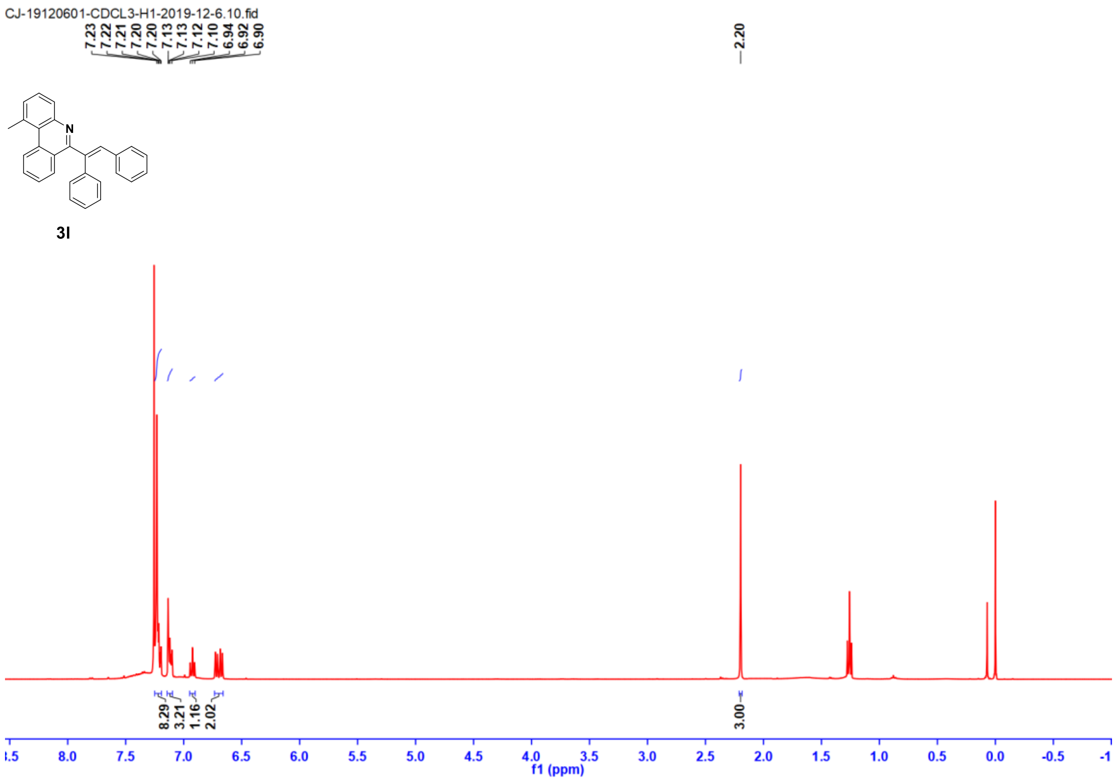
f1 (ppm)

3k


CJ-19120601-CDCL3-H1-2019-12-6.10.fid
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6.90
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3l
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3.21
1.16
2.02
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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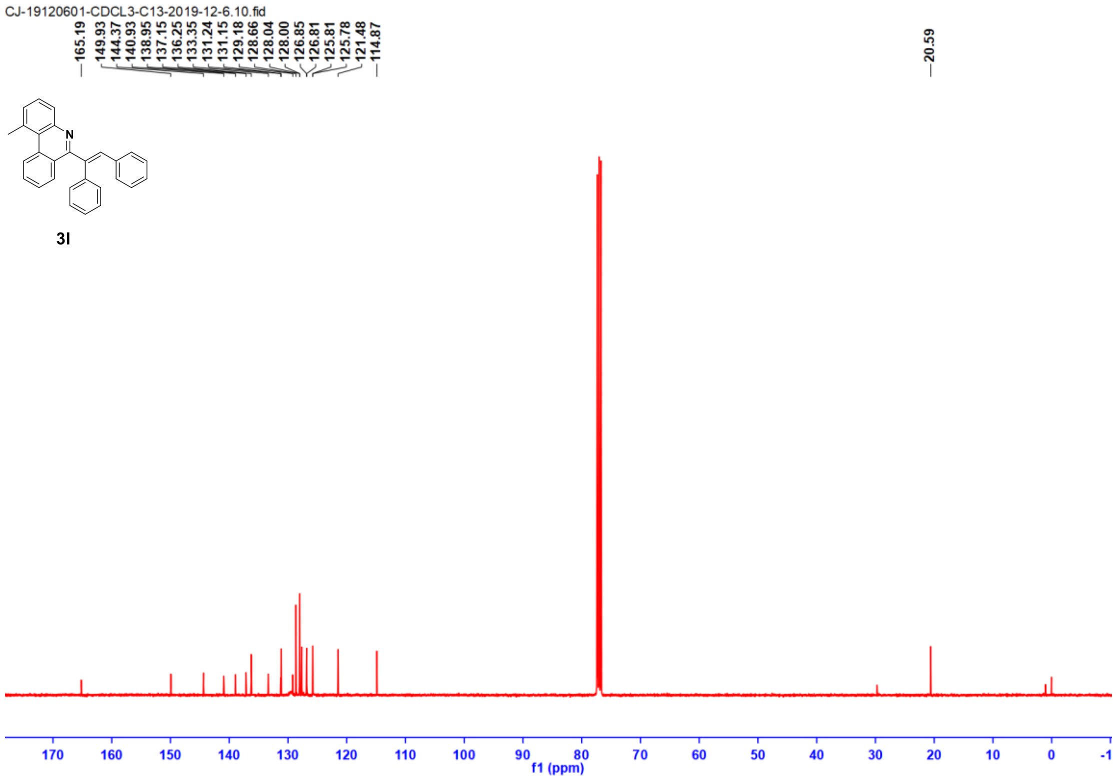
f1 (ppm)


CJ-19120601-CDCL3-C13-2019-12-6.10.fid
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128.00
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126.81
125.81
125.78
121.48
114.87
20.59
N
3l
170
160
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140
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120
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100
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80
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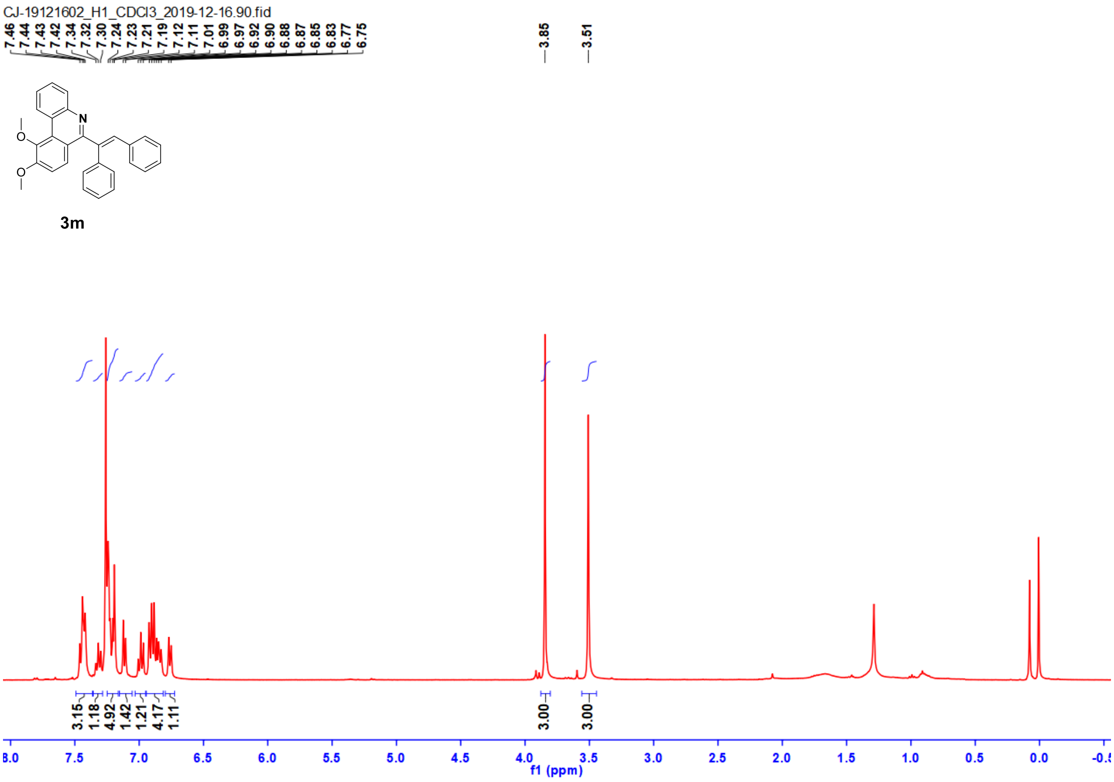
f1 (ppm)


CJ-19121602_H1_CDCl3_2019-12-16.90.fid
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7.19
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7.11
7.01
6.99
6.97
6.92
6.90
6.88
6.87
6.85
6.83
6.77
6.75
3.85
3.51
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O
O
3m
3.15
1.18
4.92
1.42
1.21
4.17
1.11
3.00
3.00
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7.0
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6.0
5.5
5.0
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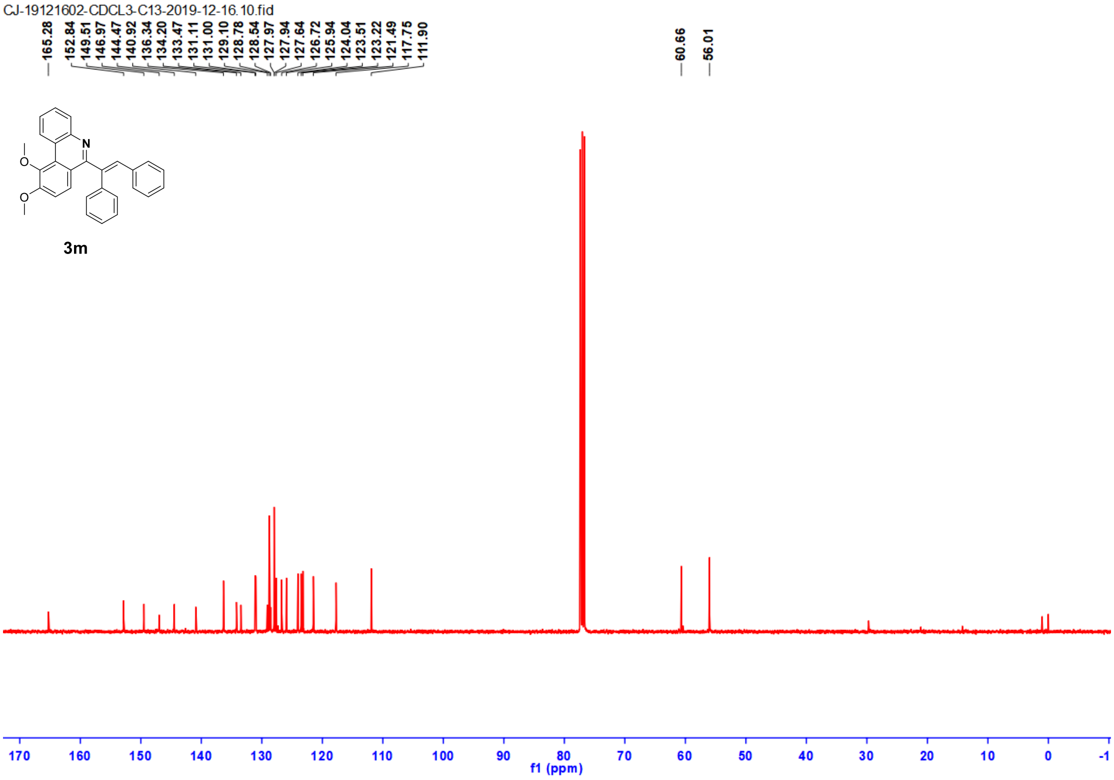
f1 (ppm)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136.34
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133.47
131.11
131.00
129.10
128.78
128.54
127.97
127.94
127.64
126.72
125.94
124.04
123.51
123.22
121.49
117.75
111.90
60.66
56.01
N
O
O
3m
170
160
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140
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120
110
100
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80
70
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40
30
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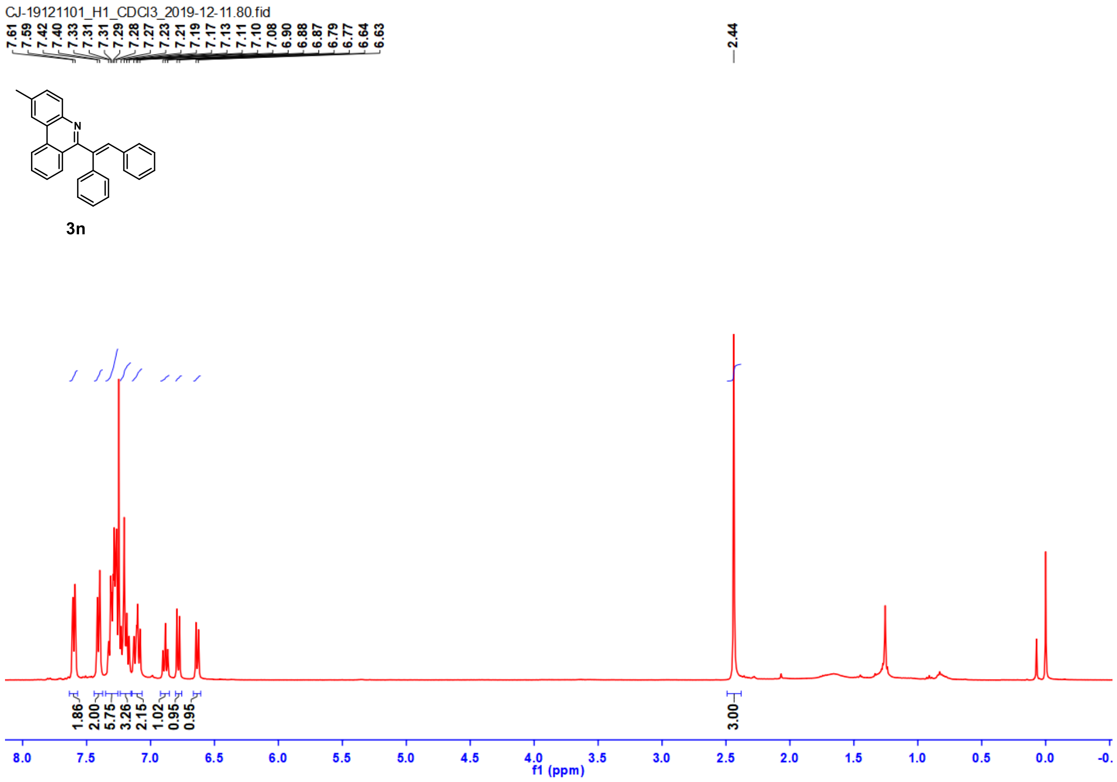
10
0
-1
f1 (ppm)


3n

CJ-19121101_H1_CDCl3_2019-12-11.80.fid
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7.31
7.29
7.28
7.27
7.23
7.21
7.19
7.17
7.13
7.11
7.10
7.08
6.90
6.88
6.87
6.79
6.77
6.64
6.63
2.44
1.86
2.00
5.75
3.26
2.15
1.02
0.95
0.95
3.00
N
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
2.5
2.0
1.5
1.0
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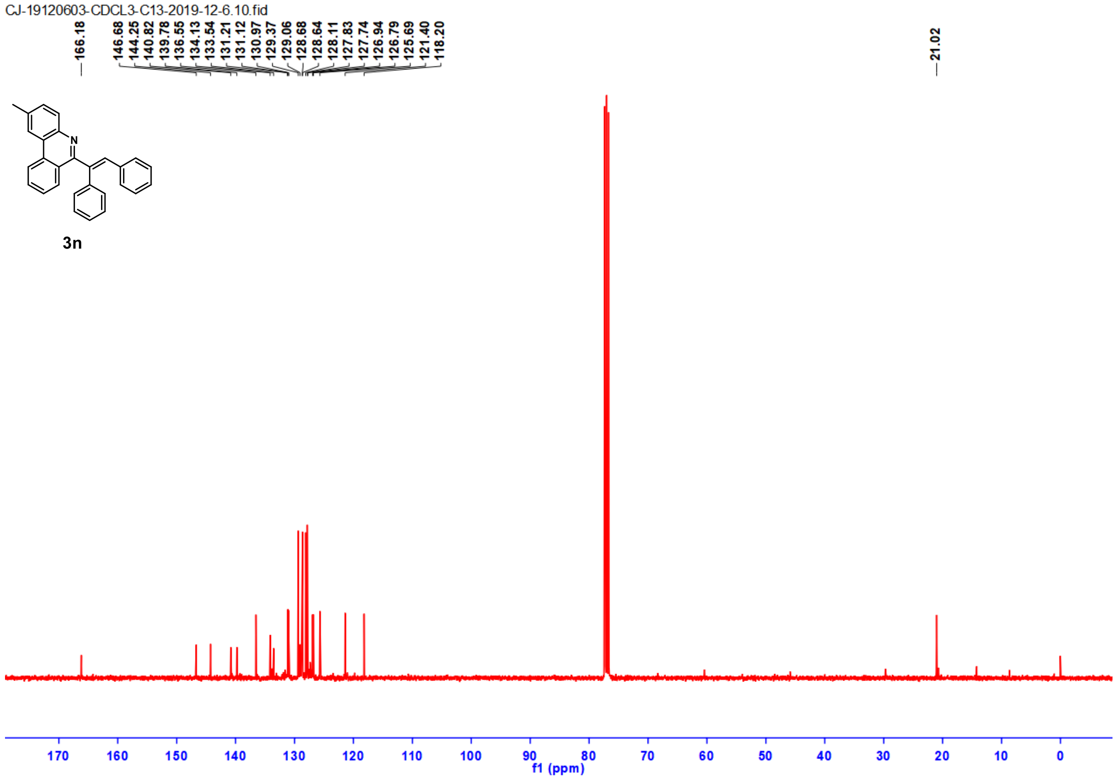
-0.
f1 (ppm)


3n

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139.78
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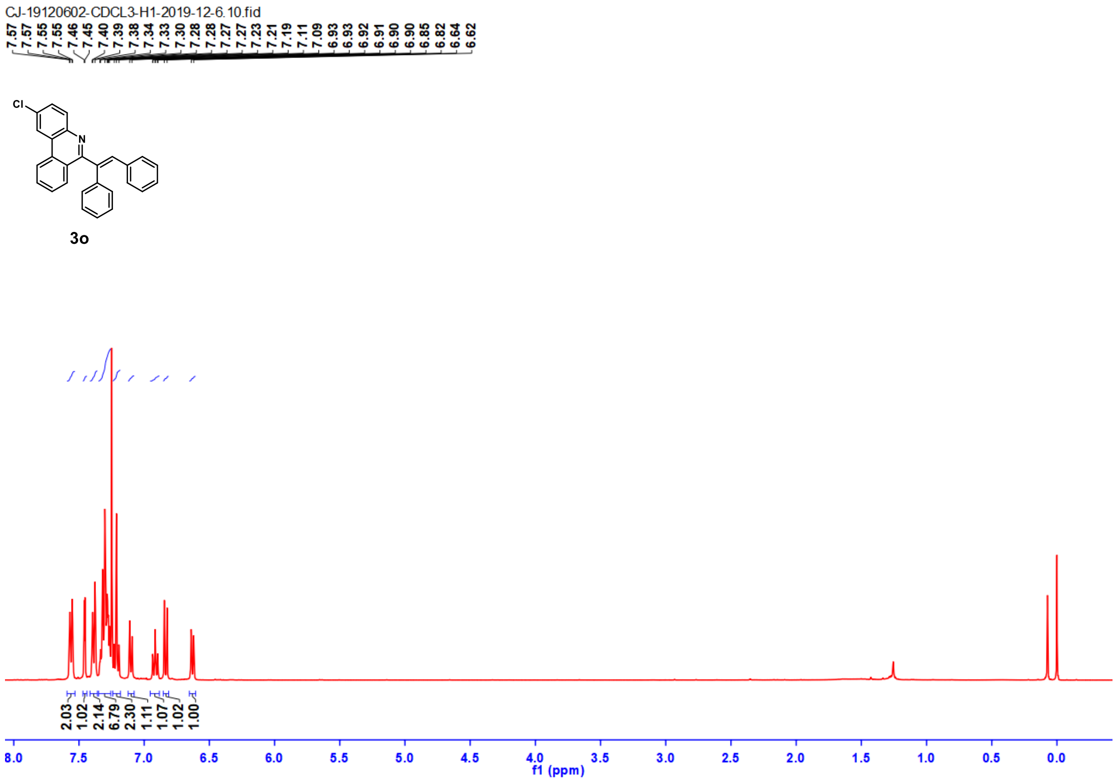
133.54
131.21
131.12
130.97
129.37
129.06
128.68
128.64
128.11
127.83
127.74
126.94
126.79
125.69
121.40
118.20
21.02
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.39
7.38
7.34
7.33
7.30
7.28
7.28
7.27
7.27
7.23
7.21
7.19
7.11
7.09
6.93
6.93
6.92
6.91
6.90
6.90
6.85
6.82
6.64
6.62
Cl
N
2.03
1.02
2.14
6.79
2.30
1.11
1.07
1.02
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
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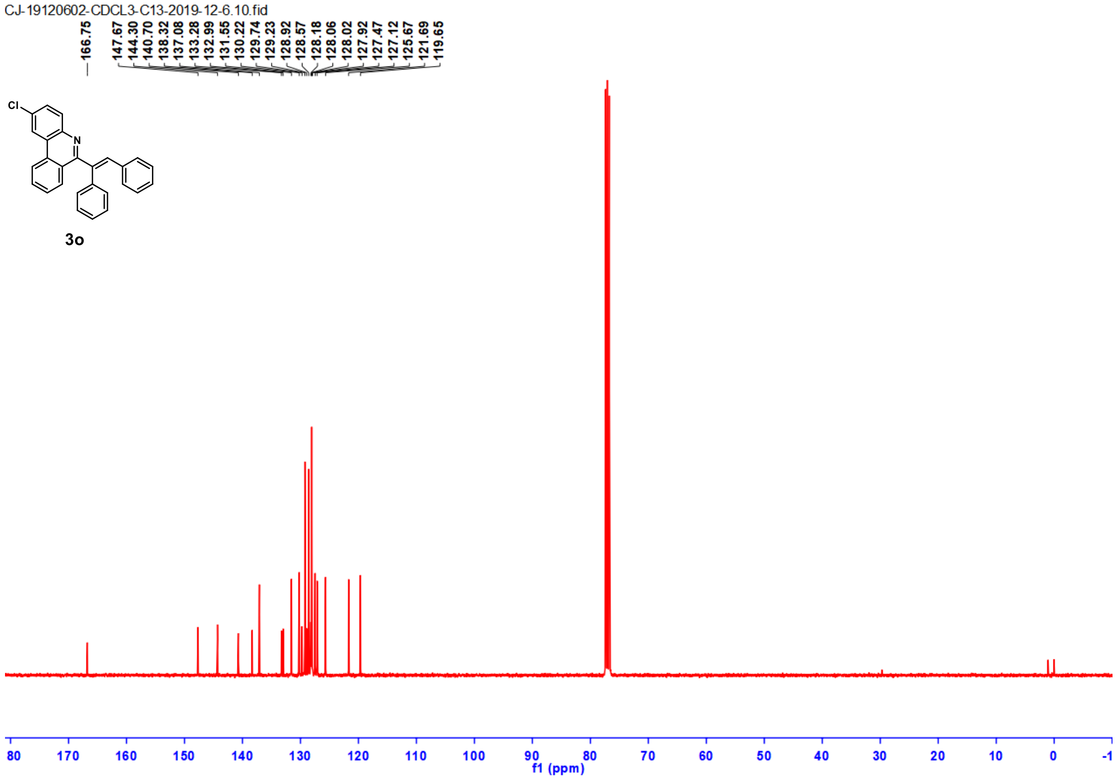
f1 (ppm)

3o


CJ-19120602-CDCL3-C13-2019-12-6.10.fid
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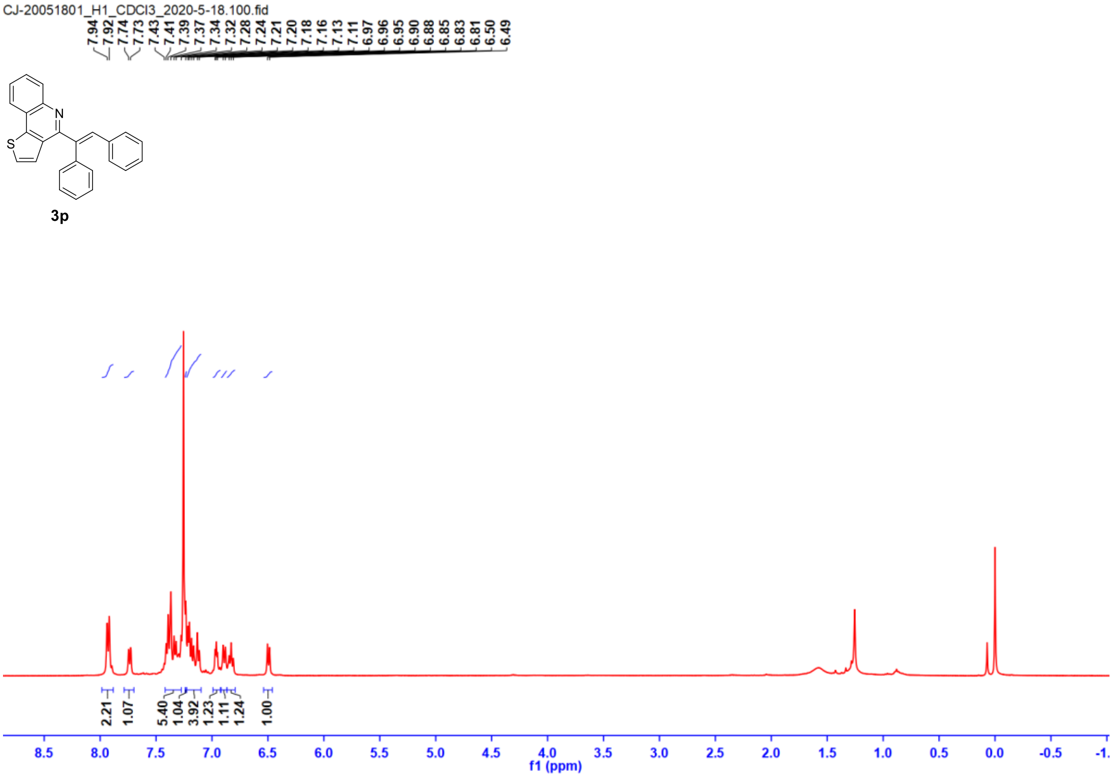
137.08
133.28
132.99
131.55
130.22
129.74
129.23
128.92
128.57
128.18
128.06
128.02
127.92
127.47
127.12
125.67
121.69
119.65
Cl
N
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

3o


CJ-20051801_H1_CDCl3_2020-5-18.100.fid
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7.39
7.37
7.34
7.32
7.28
7.24
7.21
7.20
7.18
7.16
7.13
7.11
6.97
6.96
6.95
6.90
6.88
6.85
6.83
6.81
6.50
6.49
S
N
2.21
1.07
5.40
1.04
3.92
1.23
1.11
1.24
1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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2.0
1.5
1.0
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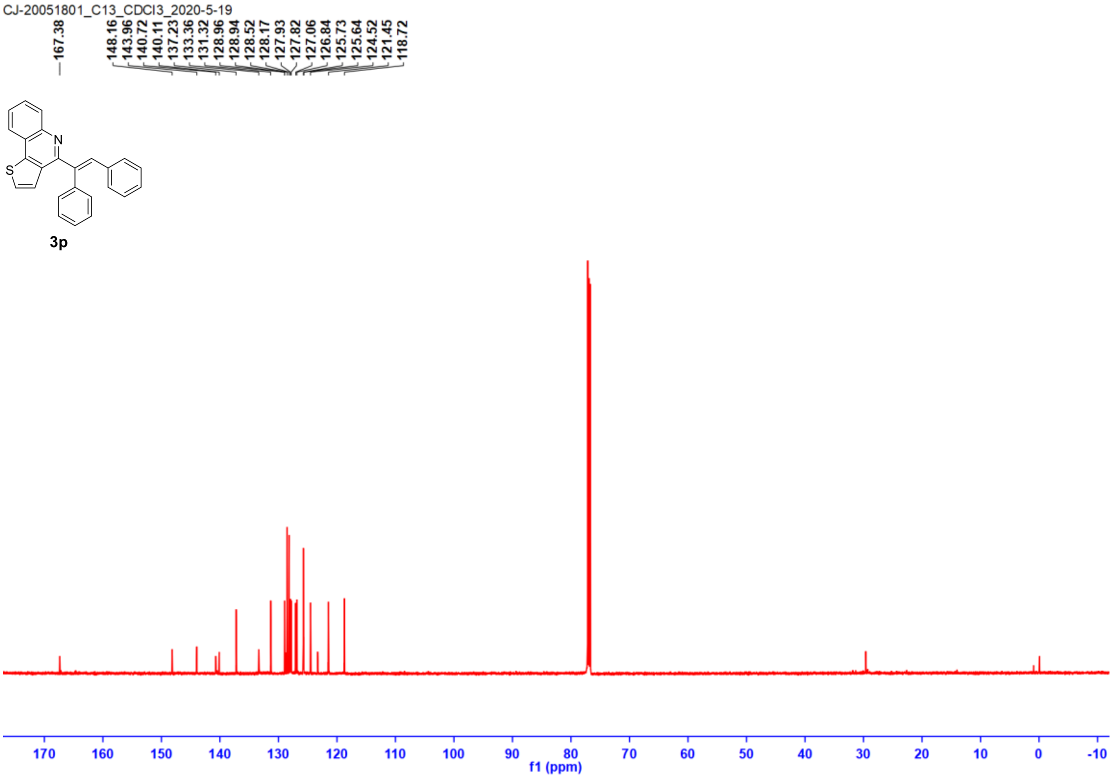
-1.
f1 (ppm)

3p


CJ-20051801_C13_CDCl3_2020-5-19
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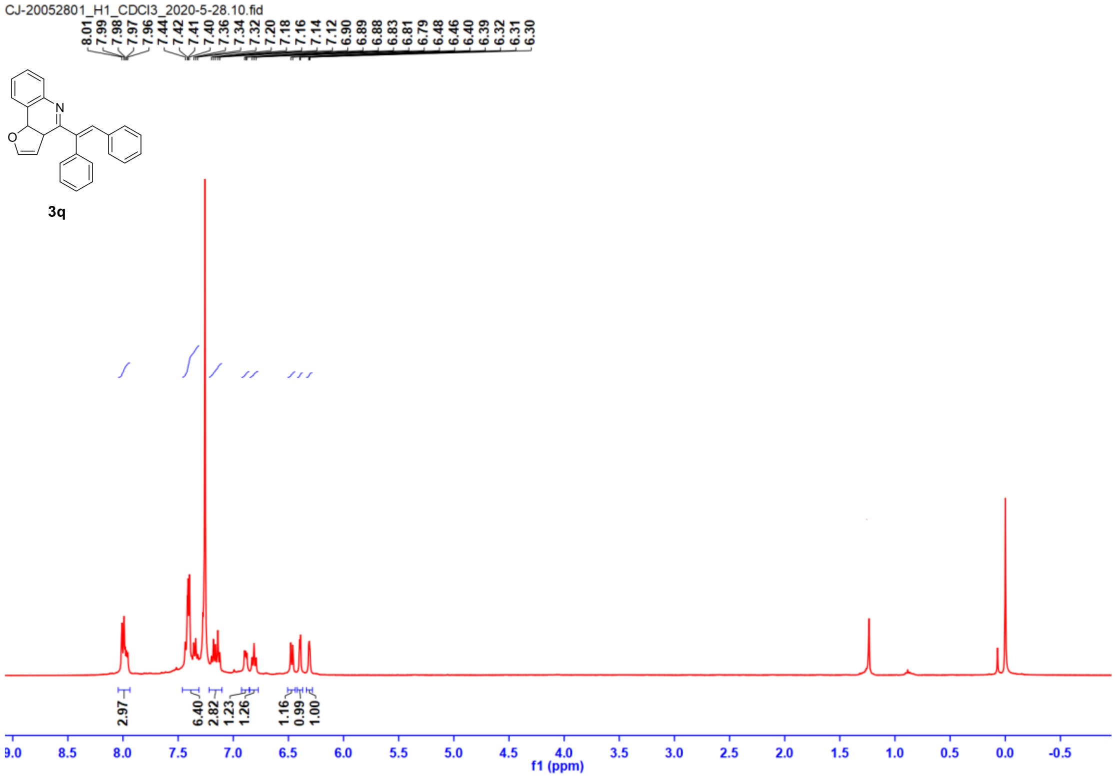
137.23
133.36
131.32
128.96
128.94
128.52
128.17
127.93
127.82
127.06
126.84
125.73
125.64
124.52
121.45
118.72
S
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3p


CJ-20052801_H1_CDCl3_2020-5-28.10.fid
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7.96
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7.41
7.40
7.36
7.34
7.32
7.20
7.18
7.16
7.14
7.12
6.90
6.89
6.88
6.83
6.81
6.79
6.48
6.46
6.40
6.39
6.32
6.31
6.30
N
O
3q
2.97
6.40
2.82
1.23
1.26
1.16
0.99
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
2.5
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1.0
0.5
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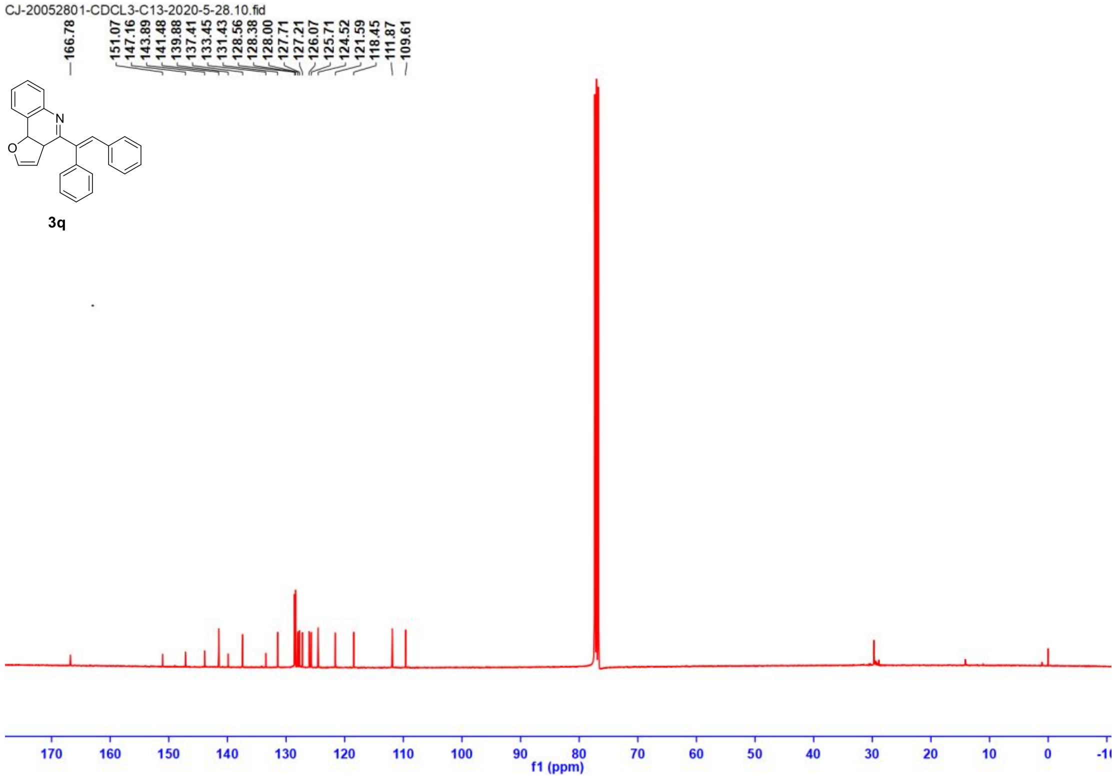
-0.5
f1 (ppm)


CJ-20052801-CDCL3-C13-2020-5-28.10.fid
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141.48
139.88
137.41
133.45
131.43
128.56
128.38
128.00
127.71
127.21
126.07
125.71
124.52
121.59
118.45
111.87
109.61
N
O
3q
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160
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110
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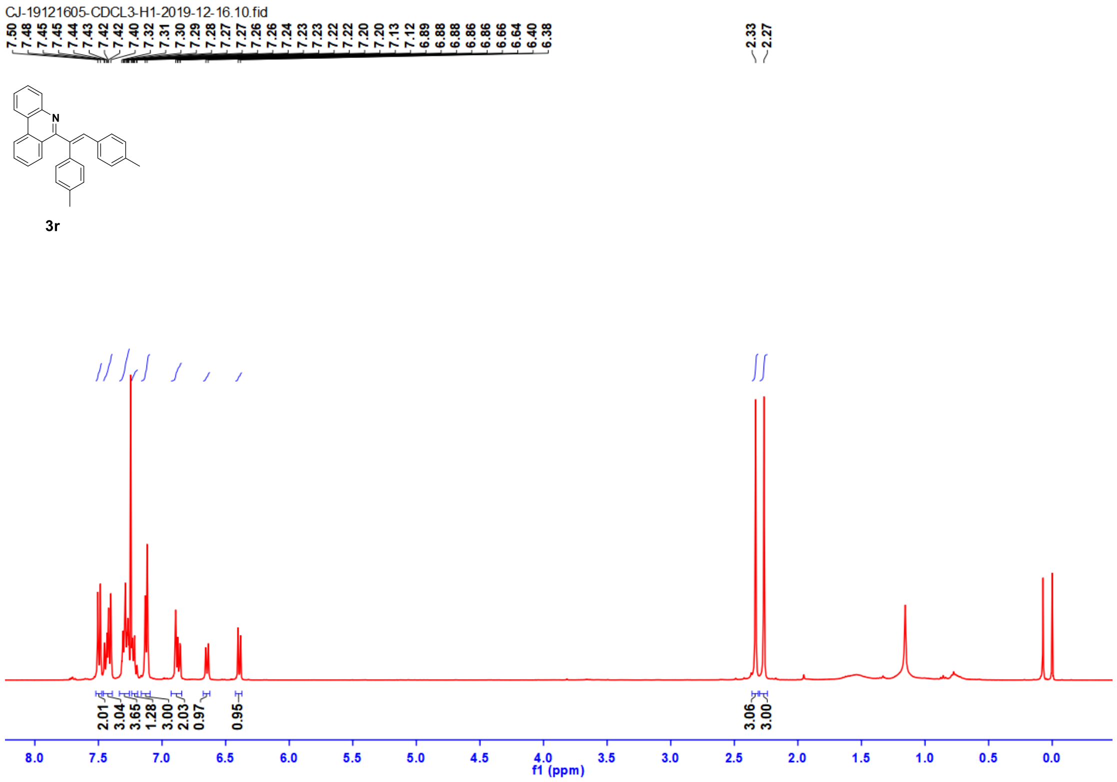
f1 (ppm)


CJ-19121605-CDCL3-H1-2019-12-16.10.fid
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2.33 2.27
N
3r
2.01 3.04 3.65 1.28 3.00 2.03 0.97 0.95
3.06 3.00
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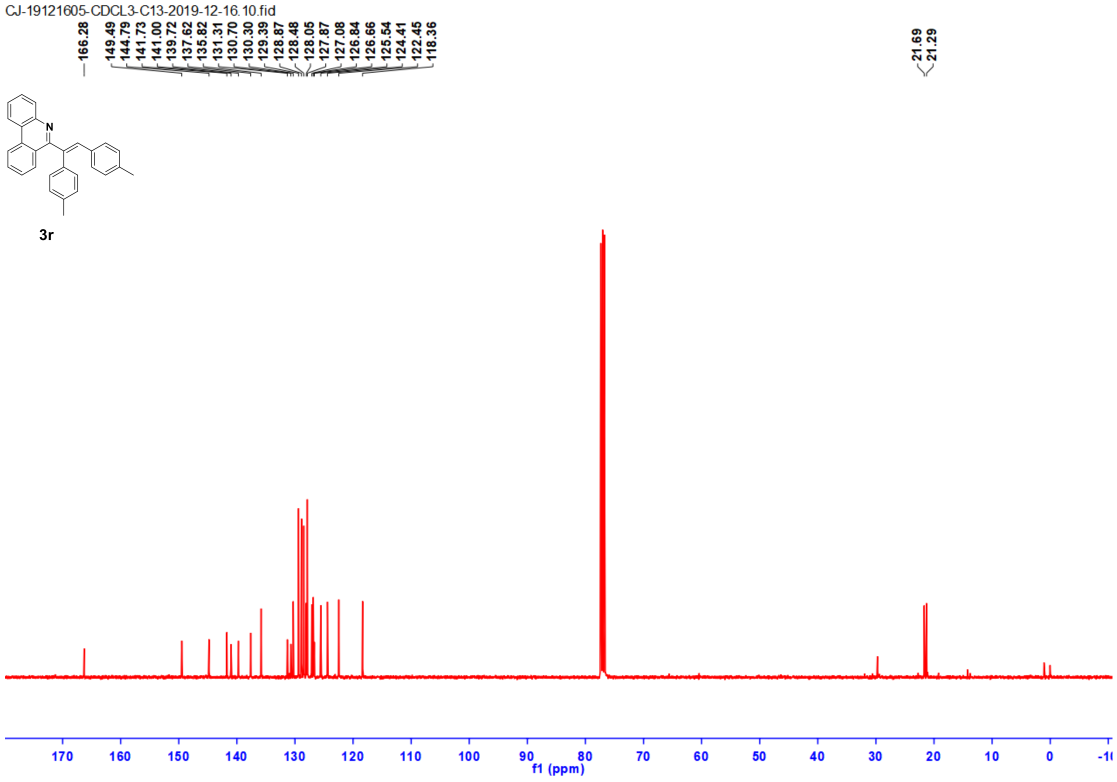
f1 (ppm)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21.69 21.29
N
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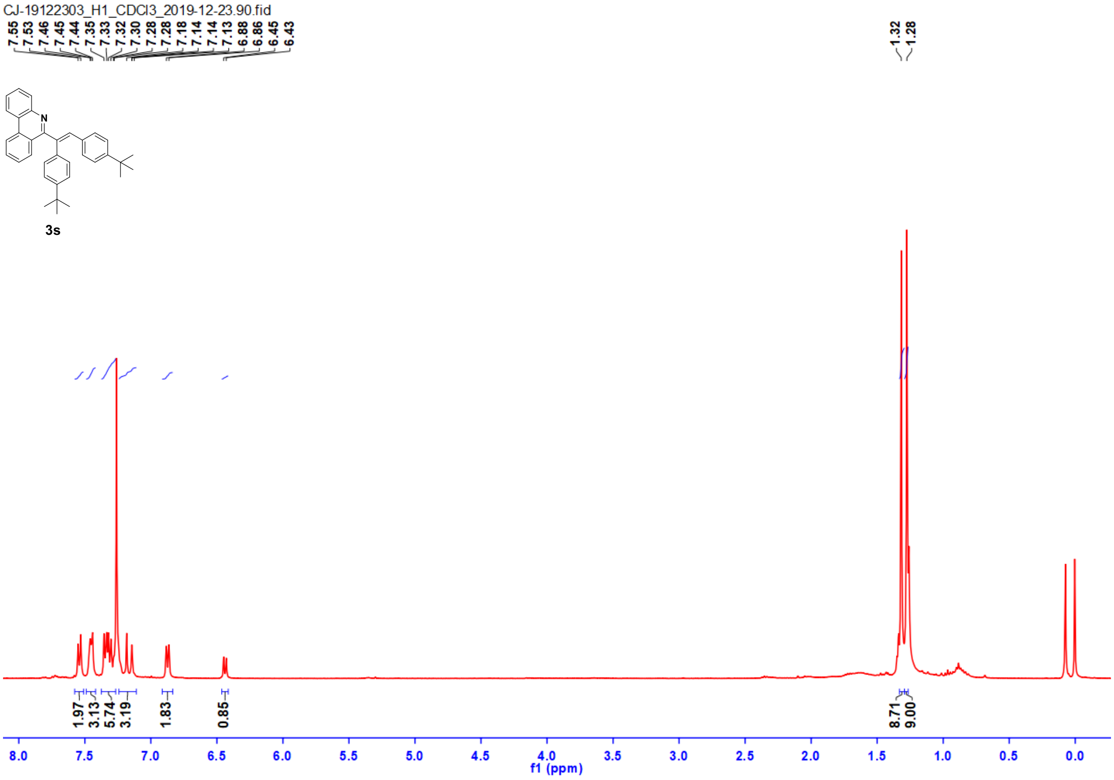
f1 (ppm)


CJ-19122303_H1_CDCl3_2019-12-23.90.fid
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7.30
7.28
7.28
7.18
7.14
7.13
6.88
6.86
6.45
6.43
1.32
1.28
N
3s
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5.74
3.19
1.83
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8.71
9.00
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
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1.0
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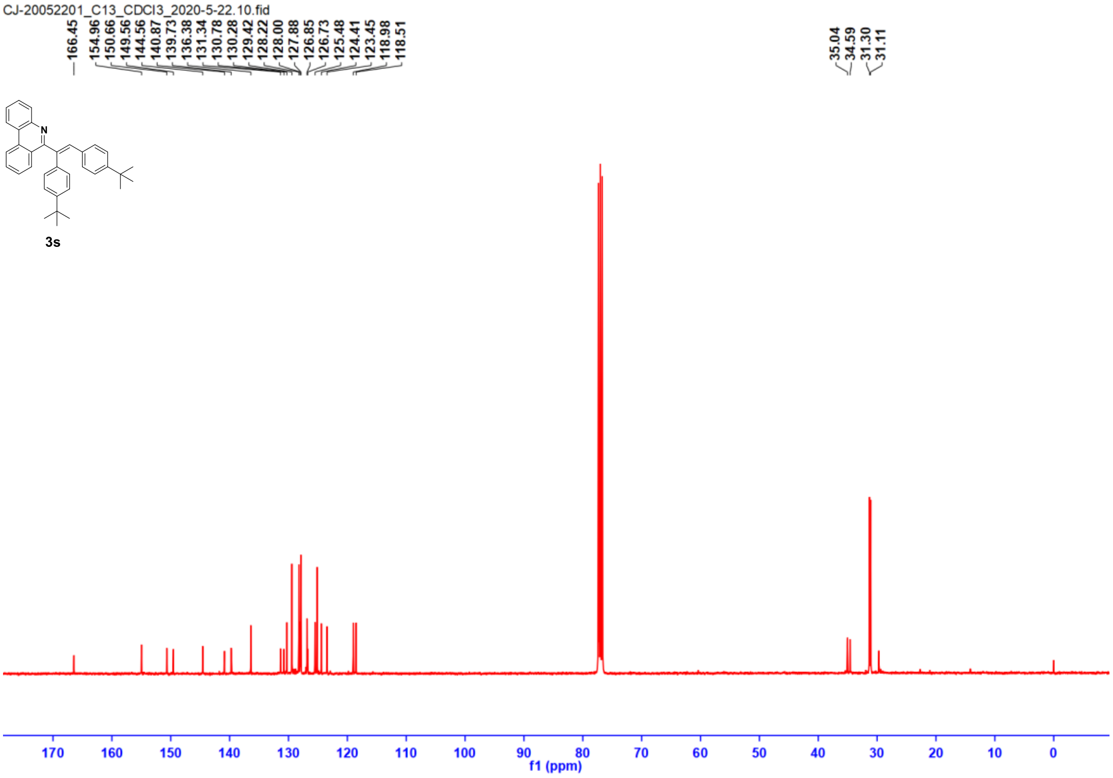
0.0
f1 (ppm)


CJ-20052201_C13_CDCl3_2020-5-22.10.fid
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136.38
131.34
130.78
130.28
129.42
128.22
128.00
127.88
126.85
126.73
125.48
124.41
123.45
118.98
118.51
35.04
34.59
31.30
31.11
N
3s
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120
110
100
90
80
70
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50
40
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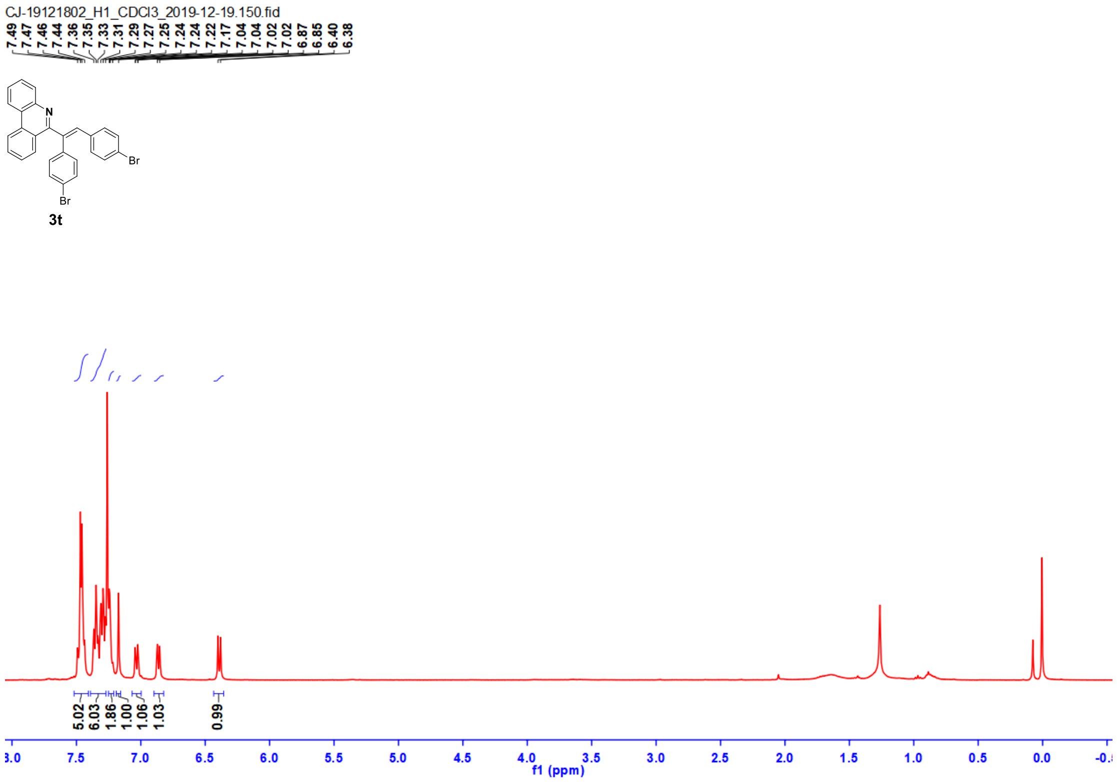
10
0
f1 (ppm)


CJ-19121802_H1_CDCl3_2019-12-19.150.fid
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7.29
7.27
7.25
7.24
7.24
7.22
7.17
7.04
7.04
7.02
7.02
6.87
6.85
6.40
6.38
N
Br
Br
3t
5.02
6.03
1.86
1.00
1.06
1.03
0.99
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
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0.5
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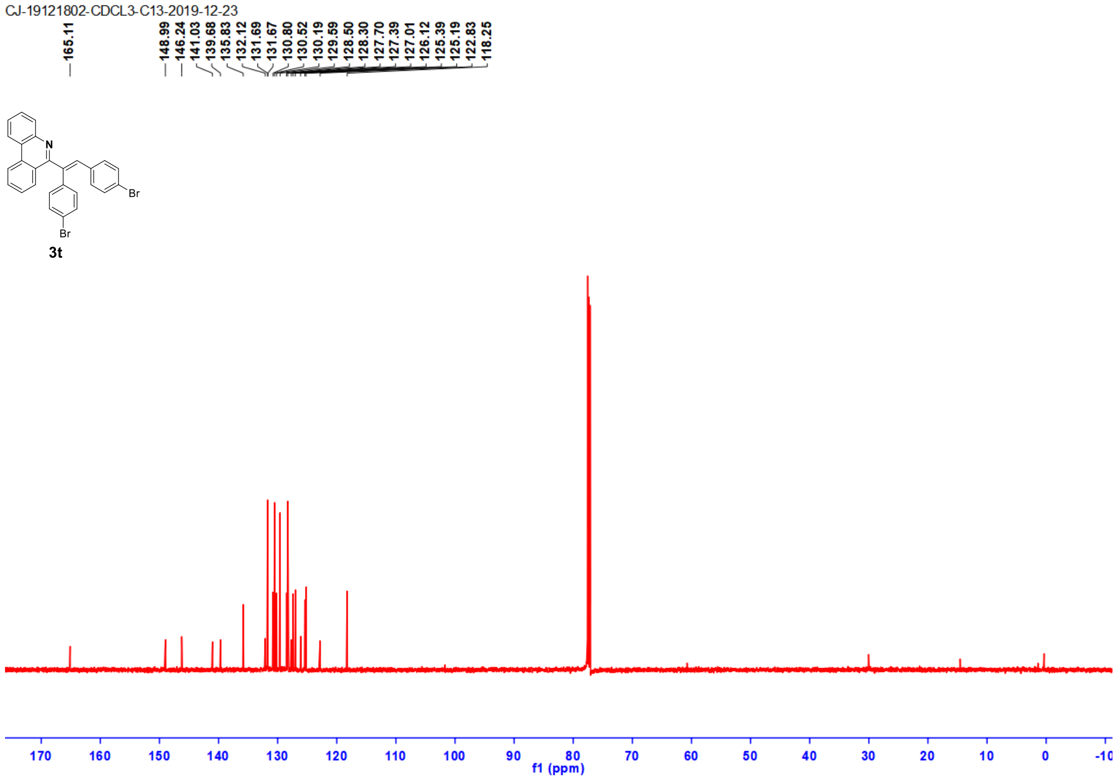
-0.5
f1 (ppm)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130.52
130.19
129.59
128.50
128.30
127.70
127.39
127.01
126.12
125.39
125.19
122.83
118.25
N
Br
Br
3t
170
160
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120
110
100
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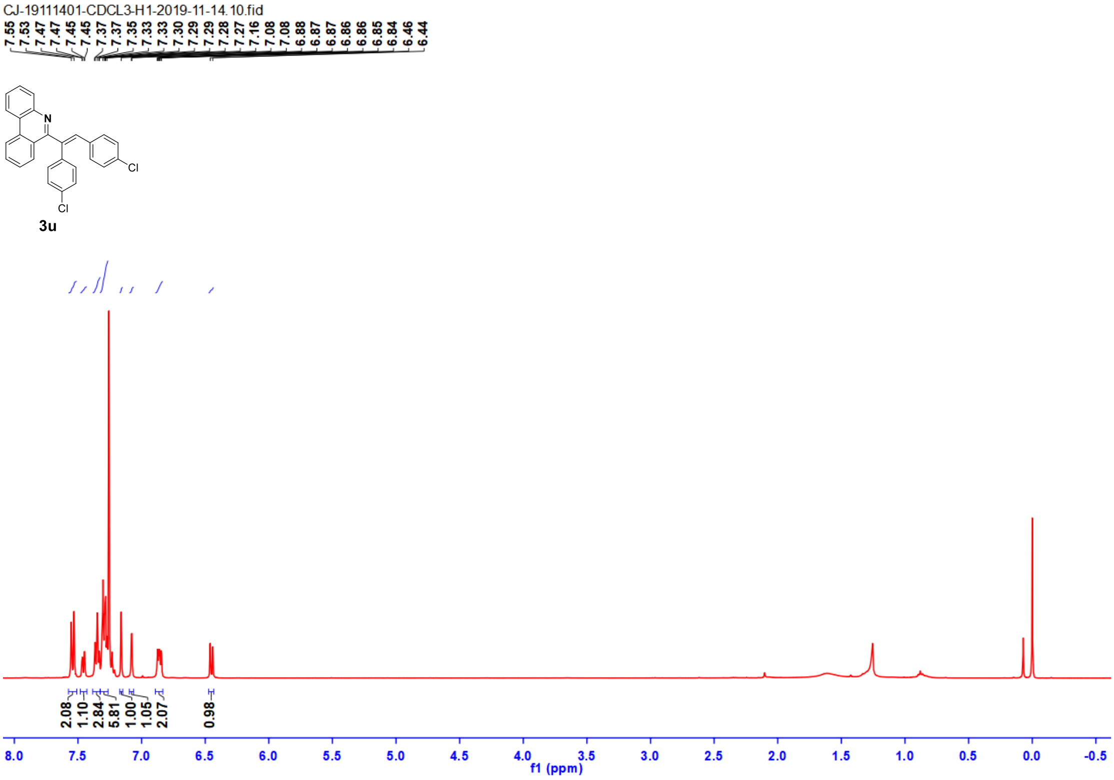
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.27
7.16
7.08
7.08
6.88
6.87
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6.85
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6.46
6.44
N
Cl
Cl
3u
2.08
1.10
2.84
5.81
1.00
1.05
2.07
0.98
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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2.5
2.0
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0.5
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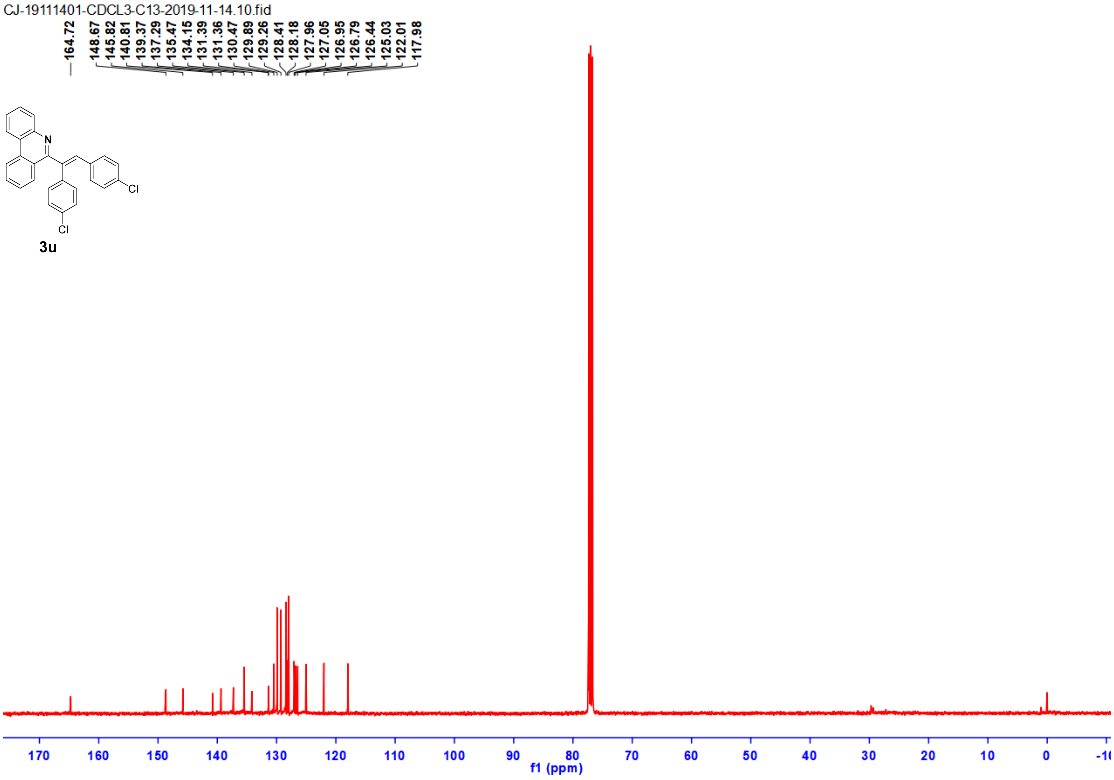
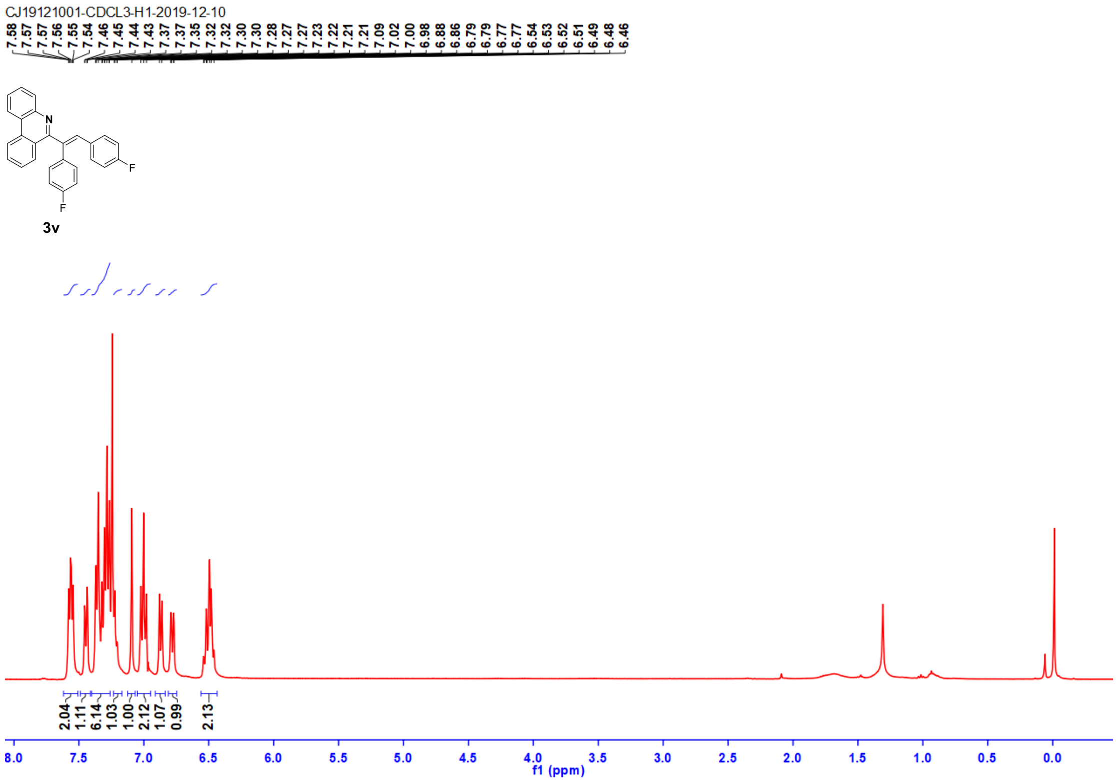
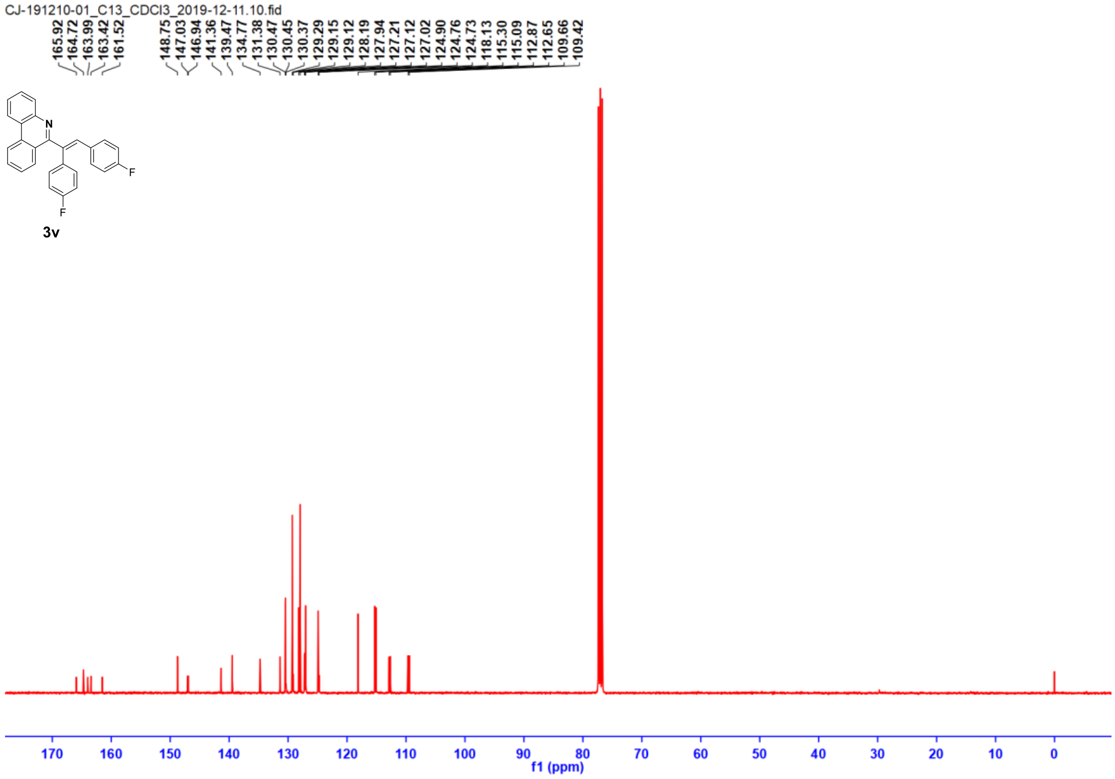
-0.5
f1 (ppm)


CJ-19111401-CDCL3-C13-2019-11-14.10.fid
164.72
148.67
145.82
140.81
139.37
137.29
135.47
134.15
131.39
131.36
130.47
129.89
129.26
128.41
128.18
127.96
127.05
126.95
126.79
126.44
125.03
122.01
117.98
N
Cl
Cl
3u
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


CJ19121001-CDCL3-H1-2019-12-10
7.58
7.57
7.57
7.56
7.55
7.54
7.46
7.45
7.44
7.43
7.37
7.35
7.32
7.32
7.30
7.30
7.28
7.27
7.27
7.23
7.22
7.21
7.21
7.09
7.02
7.00
6.98
6.88
6.86
6.79
6.77
6.77
6.54
6.53
6.52
6.51
6.49
6.48
6.46
N
F
F
3v
2.04
1.11
6.14
1.03
1.00
2.12
1.07
0.99
2.13
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CJ-191210-01_C13_CDCl3_2019-12-11.10.fid
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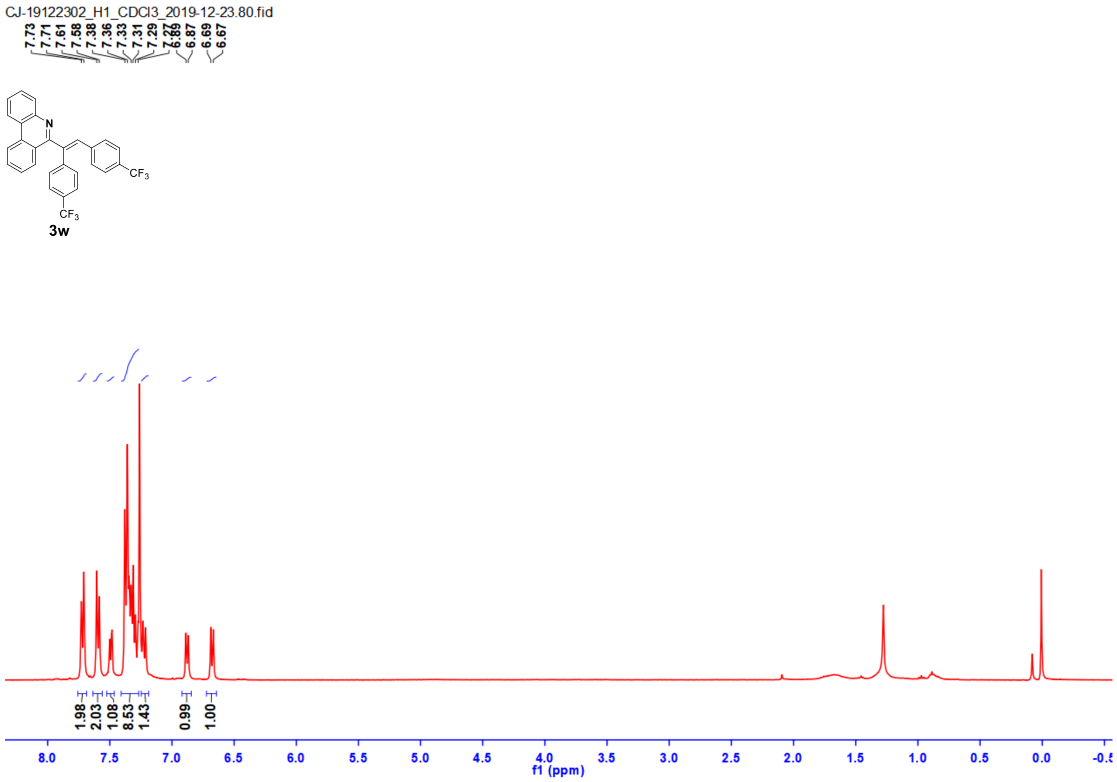
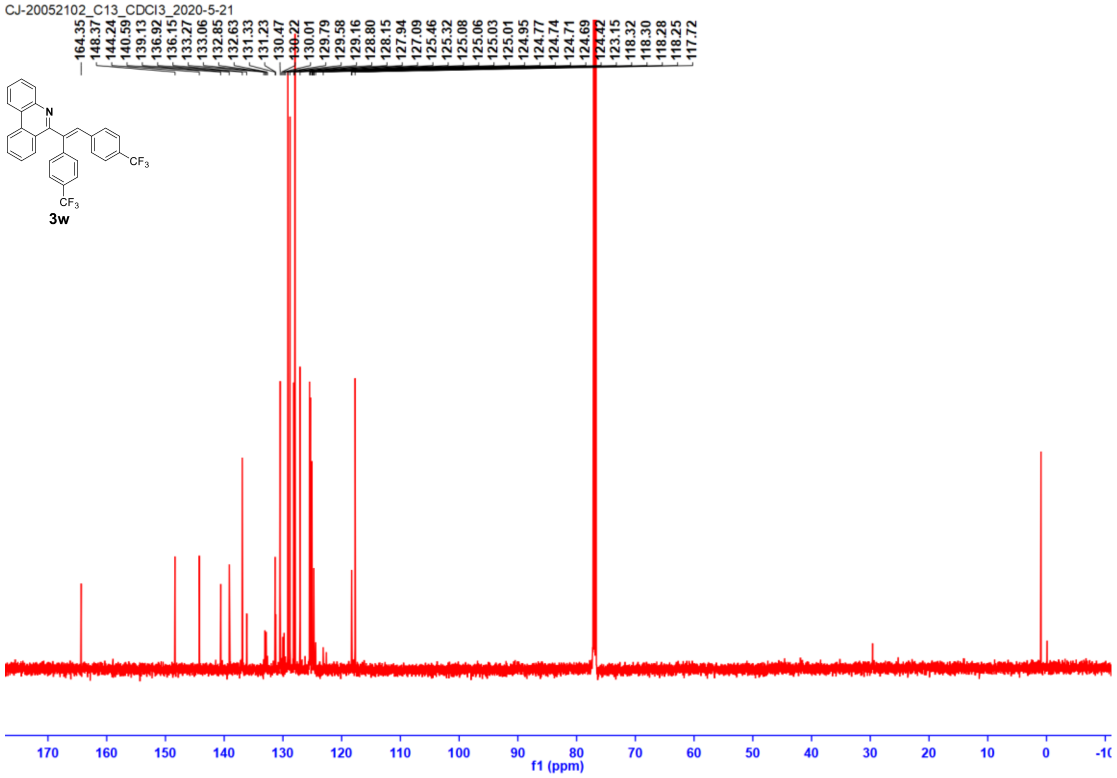
164.72
163.99
163.42
161.52
148.75
147.03
146.94
141.36
139.47
134.77
131.38
130.47
130.45
130.37
129.29
129.15
129.12
128.19
127.94
127.21
127.12
127.02
124.90
124.76
124.73
118.13
115.30
115.09
112.87
112.65
109.66
109.42
N
F
F
3v
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


CJ-19122302_H1_CDCl3_2019-12-23.80.fid
7.73
7.71
7.61
7.58
7.38
7.36
7.33
7.31
7.29
7.27
6.89
6.87
6.69
6.67
N
CF3
CF3
3w
1.98
2.03
1.08
8.53
1.43
0.99
1.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


CJ-20052102_C13_CDCl3_2020-5-21
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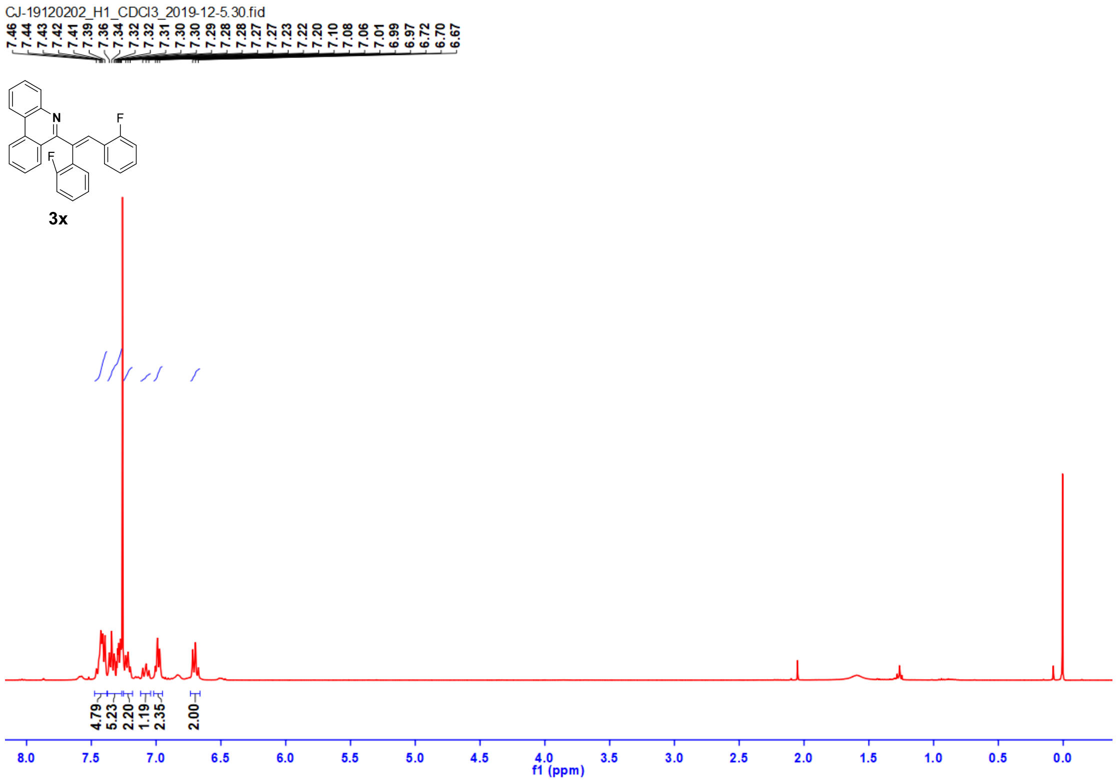
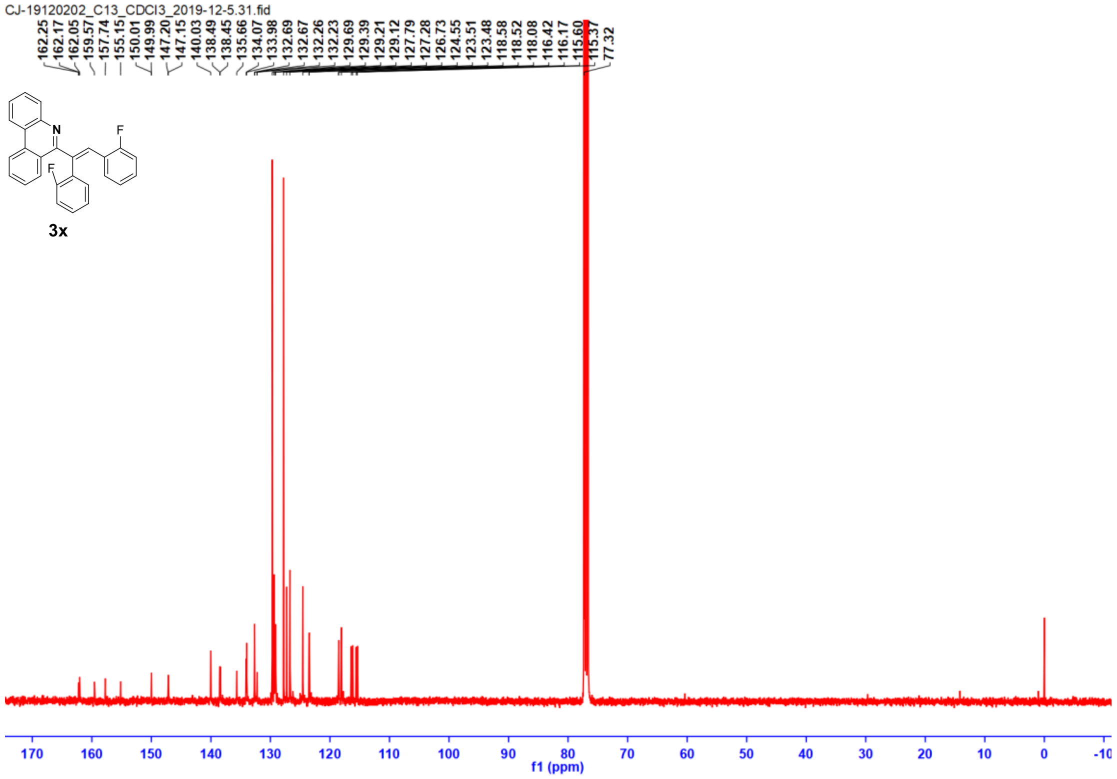
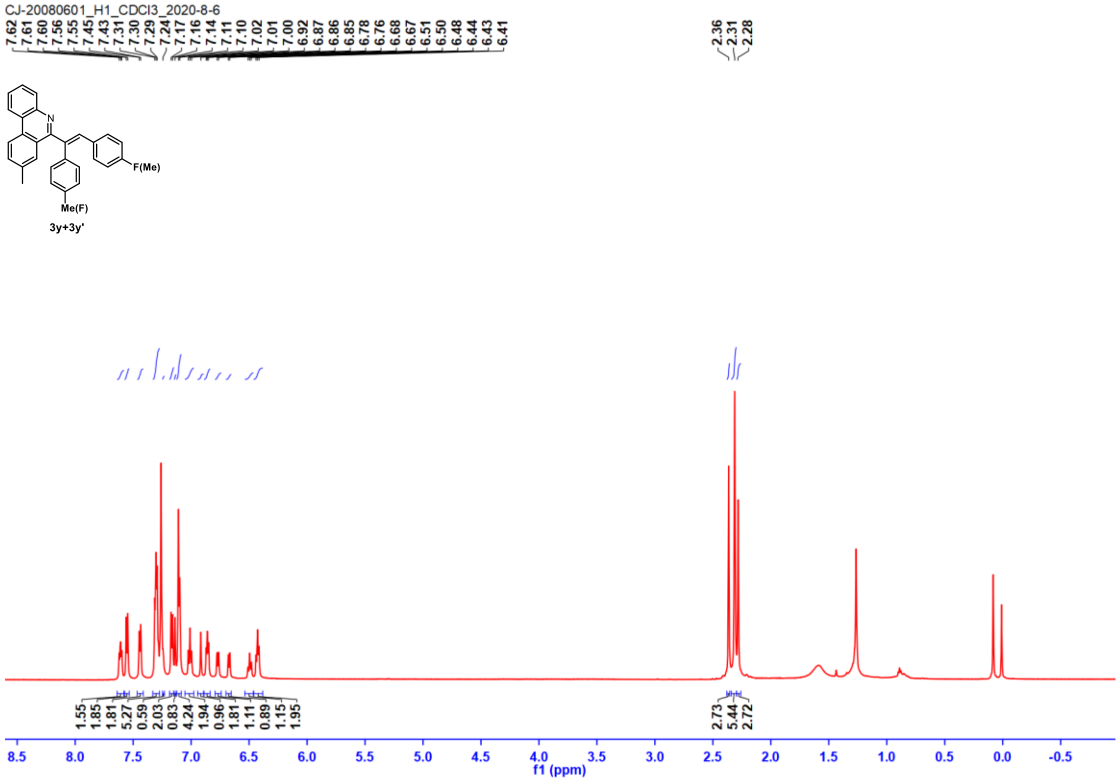
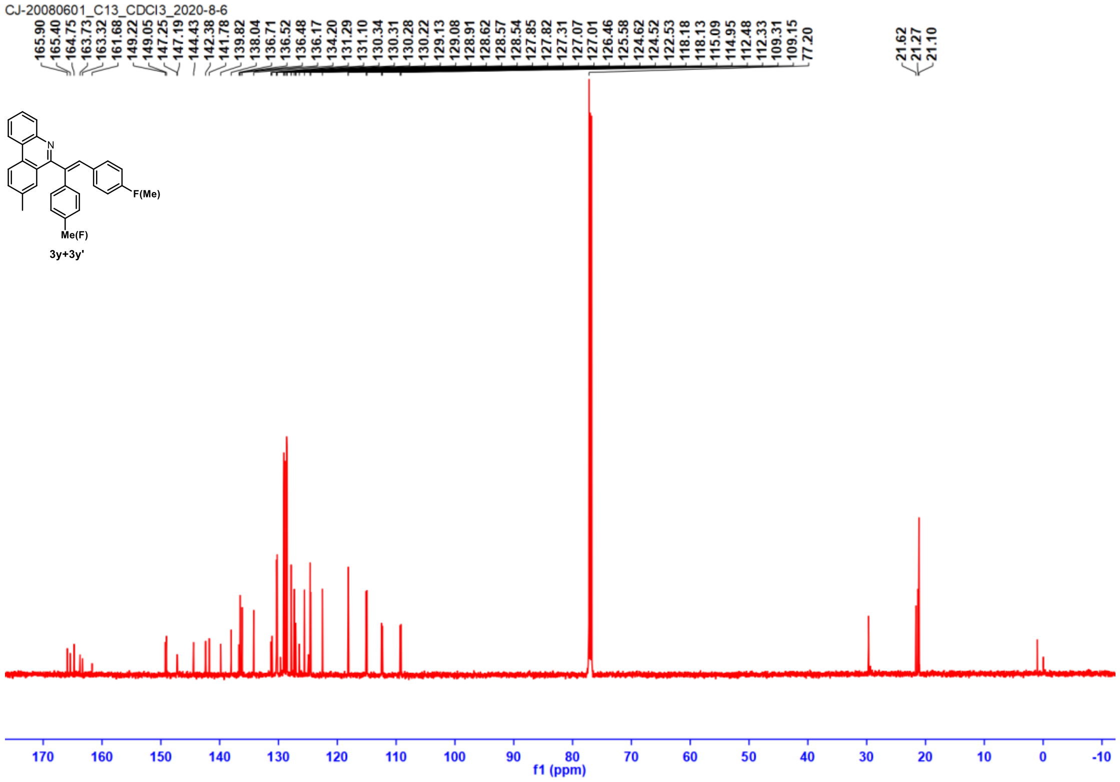
136.92
136.15
133.27
133.06
132.85
132.63
131.33
131.23
130.47
130.22
130.01
129.79
129.58
129.16
128.80
128.15
127.94
127.09
125.46
125.32
125.08
125.06
125.03
125.01
124.95
124.77
124.74
124.71
124.69
124.42
123.15
118.32
118.30
118.28
118.25
117.72
N
CF3
CF3
3w
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CJ-19120202_H1_CDCl3_2019-12-5.30.fid
7.46
7.44
7.43
7.42
7.41
7.39
7.36
7.34
7.32
7.32
7.31
7.30
7.30
7.29
7.28
7.28
7.27
7.27
7.23
7.22
7.20
7.10
7.08
7.06
7.01
6.99
6.97
6.72
6.70
6.67
N
F
F
3x
4.79
5.23
2.20
1.19
2.35
2.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CJ-19120202_C13_CDCl3_2019-12-5.31.fid
162.25
162.17
162.05
159.57
157.74
155.15
150.01
149.99
147.20
147.15
140.03
138.49
138.45
135.66
134.07
133.98
132.69
132.67
132.26
132.23
129.69
129.39
129.21
129.12
127.79
127.28
126.73
124.55
123.51
123.48
118.58
118.52
118.08
116.42
116.17
115.60
115.37
77.32
N
F
F
3x
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


CJ-20080601_H1_CDCl3_2020-8-6
7.62 7.61 7.60 7.56 7.55 7.45 7.43 7.31 7.30 7.29 7.24 7.17 7.16 7.14 7.11 7.10 7.02 7.01 7.00 6.92 6.87 6.86 6.85 6.78 6.76 6.68 6.67 6.51 6.50 6.48 6.44 6.43 6.41
2.36 2.31 2.28
N
F(Me)
Me(F)
3y+3y'
1.55 1.85 1.81 5.27 0.59 2.03 0.83 4.24 1.94 0.96 1.81 1.11 0.89 1.15 1.95
2.73 5.44 2.72
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


CJ-20080601_C13_CDCl3_2020-8-6
165.90 165.40 164.75 163.73 163.32 161.68 149.22 149.05 147.25 147.19 144.43 142.38 141.78 139.82 138.04 136.71 136.52 136.48 136.17 134.20 131.29 131.10 130.34 130.31 130.28 130.22 129.13 129.08 128.91 128.62 128.57 128.54 127.85 127.82 127.31 127.07 127.01 126.46 125.58 124.62 124.52 122.53 118.18 118.13 115.09 114.95 112.48 112.33 109.31 109.15 77.20
21.62 21.27 21.10
N
F(Me)
Me(F)
3y+3y'
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)