Supporting Information

Redox-Neutral Assembly of Diheteroarylalkanes via Transient Directing Group-Enabled C–H Methylenation

Xuemeng Wang, Liqing Xu, KeXin Ma, Yiyan Hong, Chuan Fu, Kai Tan,* and Dong Wang*

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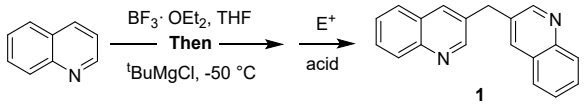
1. General Experimental

All reactions were performed under argon atmosphere in oven dried glassware. THF was distilled from sodium/benzophenone ketyl immediately before use, while other solvents and reagents were used as received from the supplier. All reagents were purchased at the highest commercial quality and used without further purification. Reactions were monitored by thin layer chromatography (TLC) using ultra violet light (UV) and Iodine as the visualizing agent. Metallic heating mantle was used in all of the reactions carried out in this work. Nuclear magnetic resonance spectra (NMR) were recorded on Bruker Avance NEO 600 or VARIAN 400 instruments and were calibrated using residual undeuterated solvent as an internal reference (^{1}H NMR: $CHC1_3$ 7.26 ppm, $(CH_3)_2SO$ 2.50 ppm, ^{13}C NMR: $CHC1_3$ 77.16 ppm, $(CH_3)_2SO$ 39.53 ppm). ^{19}F NMR spectra (proton decoupled) chemical shifts were determined relative to CF_3COOH as standard compound. High resolution mass spectra (HRMS) were recorded on a Thermo Fisher Scientific Ultimate 3000/Q-Exactive mass spectrometer. The X-ray crystallographic data were collected using a Bruker D8 VENTURE diffractometer. Melting points were recorded on an automatic melting point meter (Shang Hai Zhuo Guang) GM30. The ratio of products (**2**, **6** and **42**) and products (**39** and **40**) yielded in the competing experiment was determined by HPLC using an Agilent 1260 Infinity instrument equipped with a Poroshell 120 EC-C18 column (15 cm). The following abbreviations were used to indicate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sex = sextet, sep = septet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets, ddt = doublet of doublet of triplets, m = multiplet).

2. Screening of the Reaction Conditions

Table S1 Reaction Optimization for the synthesis of 1[a]



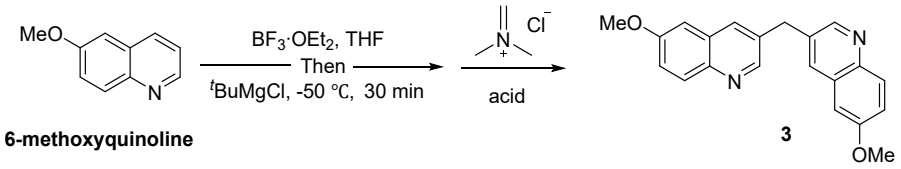
1

Entry	Acid (eq.)	E^+	Molar ratio (quinoline/ES)	Yield (%)
Acid optimization				
1	AcOH (6)	ES	2:1	20
2	TfOH (6)	ES	2:1	0
3	TFA (6)	ES	2:1	34
E^+ optimization				
4[b]	TFA (6)	$(MeO)_2CH_2$	2:1	0
5[c]	TFA (6)	HCHO	2:1	18
6	TFA (6)	$(HCHO)_n$	2:1	15
7	TFA (6)	DMF	2:1	0
8	TFA (6)	DMF-DMA	2:1	0
Molar ratio (quinoline/ES) optimization				
9	TFA (6)	ES	1:1	0
10	TFA (6)	ES	3:1	52
11	TFA (6)	ES	4:1	57
12	TFA (6)	ES	6:1	61
Eq. (TFA) optimization				
13	TFA (1)	ES	4:1	52
14	TFA (2)	ES	4:1	47
15	TFA (3)	ES	4:1	59
16	**TFA (4)**	**ES**	**4:1**	**70**
17	TFA (5)	ES	4:1	52
Molar ratio (quinoline/ES) optimization				
18	TFA (4)	ES	6:1	74
E^+ optimization				

19[c]	TFA (4)	HCHO	4:1	57
20	TFA (4)	$(HCHO)_n$	4:1	trace
Supplementary solvent optimization				
21[d]	TFA (4)	ES	4:1	57
22[e]	TFA (4)	ES	4:1	64
Prolong time before the addition of acid optimization				
23[f]	TFA (4)	ES	4:1	68
24[g]	TFA (4)	ES	4:1	29

[a] Reaction conditions: quinoline (2.32 mmol), $BF_3{\cdot}OEt_2$ (2.55 mmol), THF (4.6 mL) at 0 ℃ for 15 min, followed by ^{t}BuMgCl (2.8 mmol) at -50 ℃ for 30 min, then electrophile and acid at 25 ℃. ES represents Eschenmoser's salt. [b] The reaction was performed at 60 ℃ in the last stage. [c] 40% HCHO in H_2O was employed, and $CaCl_2$ was added to remove the extra water. [d] ES in 0.36 mL of EtOH was employed. [e] ES in 2.32 mL of MeOH was employed. [f] After the addition of Eschenmoser's salt and stirring for 15 minutes, the mixture was treated with TFA. [g] After the addition of Eschenmoser's salt and stirring for 1 hour, the mixture was treated with TFA.

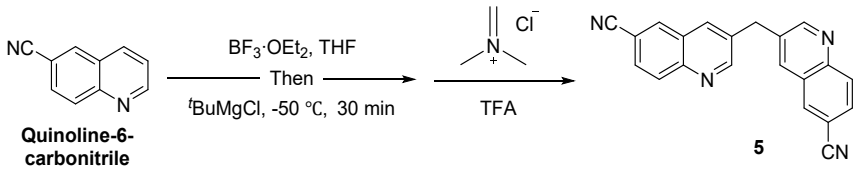
Table S2 Reaction Optimization for the synthesis of 3*



Entry	Acid (eq.)	T (℃)	Time(h)	Yield (%)
		Acid optimization		
1	TFA (4)	r.t.	28	14
2	TfOH (4)	r.t.	17	23
3	AcOH (4)	r.t.	14	16 [a]
		Eq. (BF_3·OEt_2) optimization		
4[b]	TFA (4)	r.t.	15	15
		Temperature optimization		
5[c]	**TFA (4)**	**50**	**14**	**30**

*: 6-methoxyquinoline (369 mg, 2.32 mmol), BF_3·OEt_2 (0.32 mL, 2.55 mmol), THF (4.64 mL) at 0 ℃ for 15 min, followed by ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol) at -50 ℃ for 30 min, then dimethylformiminium chloride (55 mg, 0.58 mmol) and acid (2.32 mmol) were added and warmed up to room temperature. [a]: Yields were determined by HPLC analysis. [b]: BF_3·OEt_2 (0.62 mL, 4.87 mmol) was used. [c]: The reaction mixture was warmed to 50 ℃ after stirring at room temperature for 75 min.

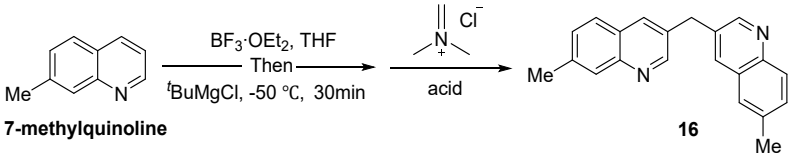
Table S3 Reaction Optimization for the synthesis of 5*



Entry	T (°C)	Time(h)	Yield (%)	Notes
1	50	63	39	The reaction mixture was warm up to 50 °C after stirring at room temperature for 14 h.
2	65	16	20	The reaction mixture was warm up to 65 °C after stirring at room temperature for 15 min.
3	**50**	**16**	**57**	**The reaction mixture was warmed to 50 °C after stirring at room temperature for 75 min.**
4[a]	50	16	54	The reaction mixture was warm up to 50 °C after stirring at room temperature for 135 min.

*: 6-cyanoquinoline (358 mg, 2.32 mmol), $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol), THF (4.64 mL) at 0 °C for 15 min, followed by ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol) at -50 °C for 30 min, then dimethylformiminium chloride (55 mg, 0.58 mmol) and trifluoroacetic acid (177 μL, 2.32 mmol) were added and warmed up to room temperature. [a]: Yields were determined by HPLC analysis.

Table S4 Reaction Optimization for the synthesis of 16[*]

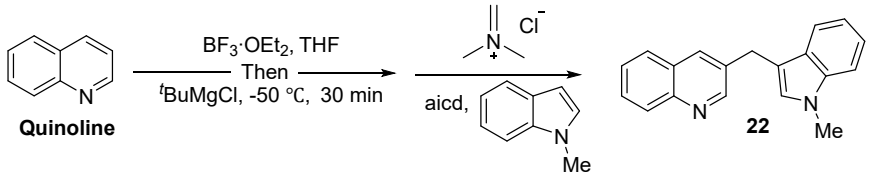


7-methylquinoline **16**

Entry	Acid (eq.)	T (℃)	Time(h)	Yield (%)
Temperature optimization				
1	TFA (4)	r.t.	22	17
2[a]	TFA (4)	50	6	trace
Acid optimization				
3	TfOH (4)	r.t.	15	22
4	AcOH (4)	r.t.	26	10
Eq. (AcOH) optimization				
5	AcOH (6)	r.t.	18	17
6	**AcOH (7)**	**r.t.**	**17**	**40**
7	AcOH (8)	r.t.	24	26
8	AcOH (66)	r.t.	4	34

[*]: 7-methylquinoline (332 mg, 2.32 mmol), $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol), THF (4.64 mL) at 0 ℃ for 15 min, followed by ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol) at -50 ℃ for 30 min, then dimethylformiminium chloride (55 mg, 0.58 mmol) and acid were added and warmed up to room temperature. [a]: The reaction mixture was warmed up to 50 ℃ after stirring at room temperature for 75 min.

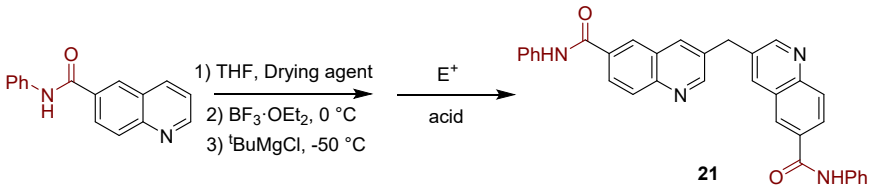
Table S5 Reaction Optimization for the synthesis of 22*



Entry	Acid (eq.)	Quinoline (eq.)	*N*-methylindole (eq.)	T (°C)	Time(h)	Yield (%)
			Eq. (quinoline) optimization			
1	TFA (4)	1	1	23	5	16
2	TFA (4)	1.5	1	24	15	47
3	TFA (4)	2	1	23	20	54
			Acid optimization			
4	TfOH (4)	2	1	27	17	55
5	AcOH (4)	2	1	27	26	64
			Supplementary solvent optimization			
6[a]	TFA (4)	2	1	27	26	74
7[a]	**AcOH (4)**	**2**	**1**	**25**	**14**	**75**
			Eq. (quinoline) optimization			
8[a]	AcOH (4)	1.5	1	25	14	53
			Eq. (AcOH) optimization			
9[a]	AcOH (10)	2	1	26	15	68
			Optimization of the reagent addition sequence			
10[b]	AcOH (4)	2	1	31	15	trace

*: Quinoline (300 mg, 2.32 mmol), $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol), THF (4.64 mL) at 0 °C for 15 min, followed by ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol) at -50 °C for 30 min, then dimethylformiminium chloride (109 mg, 1.16 mmol), acid and *N*-methylindole were added and warmed up to room temperature. The temperatures given are the actual ambient laboratory temperatures, which naturally fluctuate. [a]: *N*-methylindole (0.5 M in MeOH) was used. [b]: A solution of dimethylformiminium chloride and *N*-methylindole in dry MeOH (2.32 mL) was used, followed by adding acetic acid.

Table S6 Reaction Optimization for the synthesis of 21



Entry	Drying agent (eq)	E^+ (eq)	Acid (eq)	Yield
1[a]	/	ES (1 eq)	TFA (4 eq)	N/A
2[a]	/	ES (1 eq)	TfOH (4 eq)	N/A
3[a]	$MgSO_4$ (11 eq)	CH_2O (1 eq)	AcOH (4 eq)	16%
4[a]	$CaCl_2$ (11 eq)	CH_2O (1 eq)	AcOH (4 eq)	20%
5[b]	**$CaCl_2$ (11 eq)**	**CH_2O (1 eq)**	**AcOH (4 eq)**	**22%**
6	/	$(CH_2O)_n$ (1 eq)	AcOH (4 eq)	6%
7	/	CH_2I_2 (1 eq)	AcOH (4 eq)	3%
8	/	$(CH_2O)_3$ (1 eq)	AcOH (4 eq)	N/A
9[c]	$CaCl_2$ (11 eq)	CH_2O (1 eq)	AcOH (4 eq)	19%

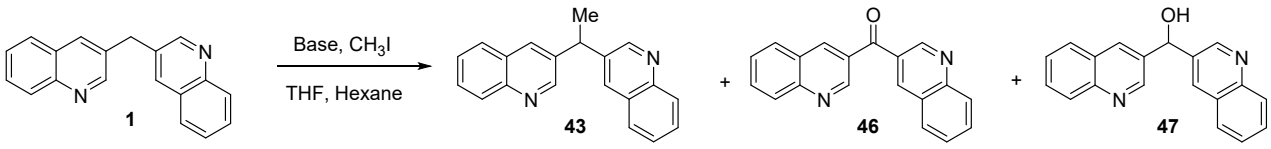
Reaction conditions: N-phenylquinoline-6-carboxamide (2.32 mmol) and drying agent, $BF_3{\cdot}OEt_2$ (2.55 mmol), THF (4.6 mL) at 0 ℃ for 15 min, followed by ^{t}BuMgCl (2.8 mmol) at -50 ℃ for 30 min, then electrophile and acid at 25 ℃.

[a]: A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of a N-phenylquinoline-6-carboxamide (575 mg, 2.32 mmol) in dry THF (4.6 mL) and drying agent (6.25 mmol), and then cooled to 0 ℃. A solution of ^{t}BuMgCl (1.0 M, 2.3 mL, 2.3 mmol) in THF is added dropwise and stirred for 30 min at the same temperature. Then $BF_3{\bullet}OEt_2$ (0.61 mL, 4.87 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 ℃ followed by dropwise addition of a THF solution of ^{t}BuMgCl (1.0 M, 2.8 mL, 2.8 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then, electrophile and acid at 25 ℃.

[b]: R.Y. = 70%

[c]: N-phenylquinoline-6-carboxamide (2.32 mmol) and drying agent, $BF_3{\cdot}OEt_2$ (2.55 mmol), THF (4.6 mL) at 0 ℃ for 15 min, followed by ^{t}BuMgCl (2.8 mmol) at -50 ℃ for 30 min, then add the electrophile and stir at room temperature for 5 minutes, then transfer to a 50 °C oil bath and stir.

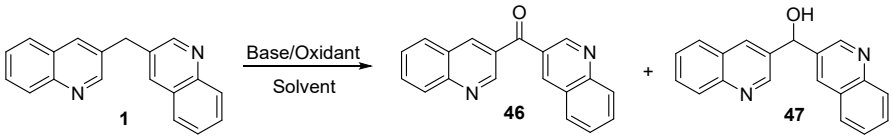
Table S7 Reaction Optimization for the synthesis of 43



Entry	Base (eq.)	T (°C)	CH_3I (eq.)	HMPA (eq.)	Time (h)	Yield (%)	Note
			Eq. (HMPA) and temperature optimization				
1[a]	LDA (2)	r.t.	2	--	--	0	The reaction mixture was warmed up to room temperature after stirred for 2 h at -78 °C.
2[b]	**LDA (2)**	**-78**	**2**	**2**	**18**	**39**	
3[b]	LDA (2)	-30	2	2	--	0	
			Eq. (CH_3I) optimization				
4[b]	LDA (2)	-78	4+4	2	5	21 (**46**: 10[c]; **47**: 13[c])	
			Eq. (LDA/ CH_3I/ HMPA) and temperature optimization				
5[d]	LDA (1.5)	-40	2	--	--	0	
6[d]	LDA (1.5)	0	4	--	19	29	
7[d]	LDA (1.5)	-20	2	2	20	trace	

[a]: A solution of *N*, *N*-diisopropylamine in THF (0.45 M) was added *n*BuLi (1.6 M in Hexane) at -78 °C and stirred for 30 min, followed by substrate **1** (100 mg, 0.37 mmol in 1.8 mL THF) at -78 °C and stirred for 1 h, then iodomethane was added at the same temperature. [b]: Preparing LDA at 0 °C and stirred for 15 min, then HMPA was added and cooled to the corresponding temperature, followed by substrate **1** (100 mg, 0.37 mmol in 1.8 mL THF) and stirred for 20 min, then iodomethane was added. [c]: Yields were determined by HPLC analysis.[d]: Preparing LDA at -78 °C, then warmed up to 0 °C and stirred for 15 min, followed by substrate **1** (100 mg, 0.37 mmol in 1.8 mL THF) at 0 °C for 15 min, then iodomethane was added and cooled to corresponding temperature.

Table S8 Reaction Optimization for the synthesis of 46 and 47



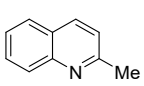
Entry	Base/ Oxidant (eq.)	T (℃)	Solvent (M)	HMPA (eq.)	Time(h)	Yield (%)
Eq. (LiHMDS/ HMPA) and concentration optimization						
1[a]	LiHMDS (2)	-78	THF (0.17)	2	0.083	**46**: 23; **47**: 35
2[b]	LiHMDS (1.6)	-78	THF (0.15)	--	2	**46**: 22[c]; **47**:17[c]
3[d]	LiHMDS (2)	-78	THF (0.15)	--	3	**46**: 9; **47**: 4
4[e]	**LiHMDS (2)**	**-78**	**THF (0.15)**	**2**	**1**	**46**: 38; **47**: 19
Base/oxidant and temperature optimization						
5[f]	LiHMDS (2) + O_2	-78	THF (0.15)	--	3	**46**: 29; **47**: 17
6[g]	LDA (1.1)	r.t.	THF (0.13)	--	16	**46**: 11[c]; **47**: 15[c]
7[h]	SeO_2 (2)	120	1,4-dioxane (0.06)	--	23	0
Eq. (CAN) and solvent optimization						
8[i]	CAN (3)	r.t.	MeOH/CH_3CN (0.2 M)	--	0.5	0
9[i]	CAN (1)	r.t.	CH_3CN (0.2 M)	--	0.5	0
Oxidant and Eq. (HMPA) optimization						
10[j]	LiHMDS (2) + air	-78	THF (0.15)	2	1	**46**: 29; **47**: 18

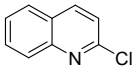
[a]: LiHMDS (1 M in THF) and HMPA (129 μL, 0.74 mmol) at -10 ℃ for 5 min, followed by substrate **1** (100 mg, 0.37 mmol in 1.8 mL THF) at -78 ℃ for 20 min, then iodomethane (46 μL, 0.74 mmol) was added at -78 ℃. [b]: iodomethane (35 μL, 0.56 mmol) was added after the addition of substrate **1** and stirring for 20 min.[c]: Yields were determined by HPLC analysis. [d]: LiHMDS (0.74 mL, 1 M in THF, 0.74 mmol) at -10 ℃ for 5 min, followed

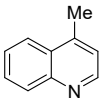
by substrate **1** (100 mg, 0.37 mmol in 1.8 mL THF) at -78 °C. [e]: HMPA (129 μL, 0.74 mmol) was added after the addition of LiHMDS, and stirred for 5 min, iodomethane was not used. [f]: O_2 was introduced after the addition of substrate **1** and stirring for 20 min, iodomethane was not used. [g]: A solution of *N*,*N*-diisopropylamine in THF (0.45 M) and *n*BuLi (1.6 M in Hexane) at -78 °C for 30 min, followed by substrate **1** (100 mg, 0.37 mmol in 1.8 mL THF) at -78 °C for 1 h, then iodomethane (35 μL, 0.56 mmol) was added, the warmed up to room temperature after stirred for 4 h at -78 °C. [h]: SeO_2 (82 mg, 0.74 mmol), 1,4-dioxane (6.32 mL) and substrate **1** (100 mg, 0.37 mmol) were added at room temperature, then warmed up to 120 °C. [i]: CAN, solvent and substrate **1** (100 mg, 0.37 mmol) were added at 0 °C, then warmed to room temperature. [j]: Air was introduced after the addition of substrate **1** and stirring for 20 min, iodomethane was not used.

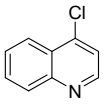
3. Challenges and Limitations

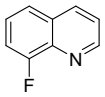
The following substrates did not react under the standard homocoupling conditions. These results indicate that the developed method is incompatible with quinolines substituted at the C2, C4, or C8 positions. The lack of reactivity is likely due to steric encumbrance: substituents at the C2 and C8 positions hinder the boron center, while a substituent at the C4 position clashes with the *tert*-butyl group. In both scenarios, the key intermediate **INT-1** fails to form. Notably, the steric demand of the *tert*-butyl group also affects C5-substituted quinolines, leading to low yields even with a small fluorine atom, as seen in compound **13**.

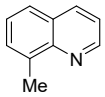


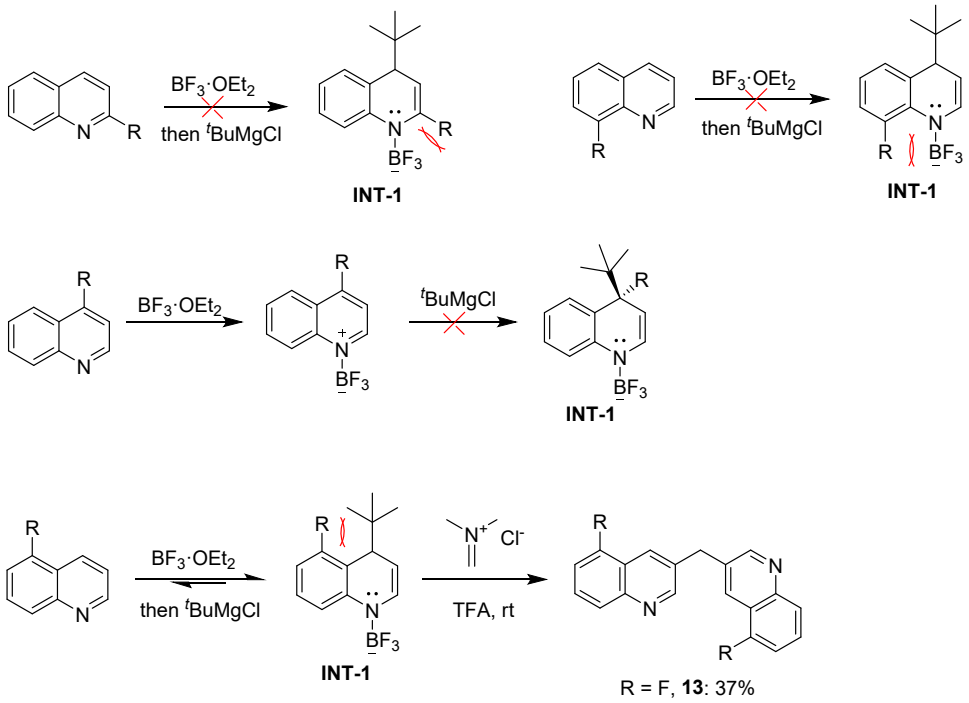












4. General Procedure

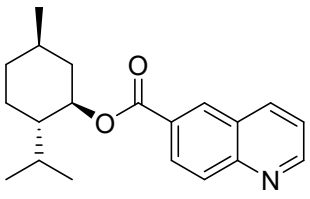
General procedure for the synthesis of diarylmethane (GP1). A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of a quinoline derivative (2.32 mmol, 4.0 eq.) in dry THF (4.6 mL) and cooled to 0 °C. $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol, 4.4 eq.) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.8 mL, 1.0 M in THF, 2.8 mmol, 4.8 eq.), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (55 mg, 0.58 mmol, 1.0 eq.) is added, followed by the addition of trifluoroacetic acid (177 µL, 2.32 mmol, 4.0 eq.). The reaction mixture is then increased to room temperature by removing the cooling bath, and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography furnishes the desired product.

General procedure for the synthesis of 3-((1*H*-indol-3-yl)methyl)quinoline (GP2). A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of a quinoline derivative (2.32 mmol, 2.0 eq.) in dry THF (4.6 mL) and cooled to 0 °C.

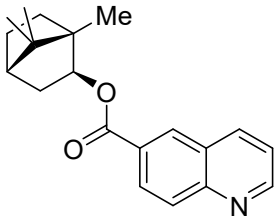
$BF_3 \cdot OEt_2$ (0.32 mL, 2.55 mmol, 2.2 eq.) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.8 mL, 1.0 M in THF, 2.8 mmol, 2.4 eq.), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (109 mg, 1.16 mmol, 1.0 eq.) is added, followed by the addition of acetic acid (266 μL, 4.64 mmol, 4.0 eq.), and a solution of indole derivatives (1.16 mmol, 1.0 eq.) in MeOH (2.32 mL). The reaction mixture is then increased to room temperature by removing the cooling bath, and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography furnishes the desired product.

General procedure for the alkylation of diarylmethane (43-45, GP3). A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of *N*, *N*-diisopropylamine (119 μL, 0.85 mmol, 2.3 eq.) in dry THF (1.5 mL) and cooled to 0 °C. Then a solution of ^{n}BuLi (0.46 mL, 1.6 M in hexane, 0.74 mmol, 2.0 eq.) is added dropwise and stirred for 15 min at the same temperature, followed by the dropwise addition of hexmethylphosphoramide (129 μL, 0.74 mmol, 2.0 eq.). Then the reaction mixture is cooled to -78 °C followed by addition of substrate **1** (100 mg, 0.21 M in THF, 0.37 mmol, 1.0 eq.) and stirred for 20 min. Alkyl halide (0.74 mmol, 2.0 eq.) was added dropwise, and stirred at the same temperature for 5 minutes. The reaction mixture is warmed to rt and quenched with saturated aqueous $NaHCO_3$ (5 mL), then extracted with ethyl acetate three times. The combined organic phases are washed with brine, dried over $MgSO_4$, and concentrated in vacuo to give the crude product. Purification by flash chromatography furnishes the desired product.

5. Preparation Procedure for specific quinolines

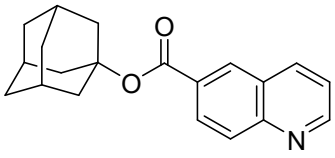


(1S,2R,5S)-2-isopropyl-5-methylcyclohexyl quinoline-6-carboxylate: Add 6-quinolinecarboxylic acid (5.00 g, 29.00 mmol), CH_2Cl_2 (116 mL), DMAP (7.10 g, 58.00 mmol), EDCI (5.60 g, 29.00 mmol), and menthol (3.90 g, 25.00 mmol) into a 250 mL single-neck flask, and stir at room temperature for 16 h. The solution was diluted by the addition of saturated aqueous NH_4Cl solution and CH_2Cl_2 at room temperature. The organic phase was dried with anhydrous Na_2SO_4, and then, filtered. The resulting filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (PE:EA = 15:1~10:1) to give the corresponding product (6.40 g, 82%). The spectroscopic data are consistent with previously reported. The experimental procedure has been partially modified from the known literature.[1] ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.99 (dd, J = 4.2, 1.8 Hz, 1H), 8.57 (d, J = 1.8 Hz, 1H), 8.30 (dd, J = 9.0, 1.8 Hz, 1H), 8.26 (dd, J = 8.4, 1.2 Hz, 1H), 8.13 (d, J = 9.0 Hz, 1H), 7.45 (dd, J = 8.4, 4.2 Hz, 1H), 5.00 (td, J = 10.8, 4.8 Hz, 1H), 2.17 – 2.14 (m, 2H), 2.01 – 1.96 (m, 1H), 1.76 – 1.71 (m, 2H), 1.63 – 1.55 (m, 2H), 1.18 – 1.12 (m, 2H), 0.94 (d, J = 2.4 Hz, 3H), 0.92 (d, J = 3.0 Hz, 3H), 0.81 (d, J = 7.2 Hz, 3H).

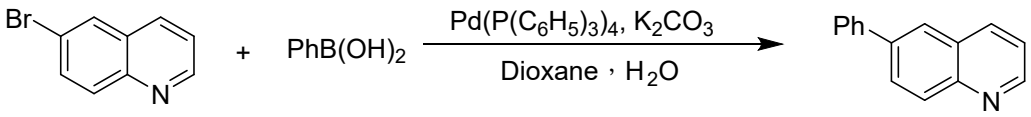


(1S,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl quinoline-6-carboxylate: Add 6-quinolinecarboxylic acid (3.20 g, 18.48 mmol), CH_2Cl_2 (74 mL), DMAP (4.58 g, 37.5 mmol), EDCI (3.59 g, 18.48 mmol), and borneol (2.4 g, 15.7 mmol) into a 250 mL single-neck flask, and stir at room temperature for 16 h. The solution was diluted by the addition of saturated aqueous NH_4Cl solution and CH_2Cl_2 at room temperature. The organic phase was dried with anhydrous Na_2SO_4, and then, filtered. The resulting filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (PE:EA = 15:1) to give the corresponding product (4.13 g, 85%). The spectroscopic data are consistent with previously reported. The experimental procedure has been partially modified from the known literature.[1] ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.98 (d, J = 3.0 Hz, 1H), 8.56 (d, J = 1.2 Hz, 1H), 8.30 (dd, J = 9.0, 1.8 Hz, 1H), 8.26 (d, J = 7.8 Hz, 1H), 8.14 (d, J = 9.0 Hz, 1H), 7.44 (dd, J = 8.4, 4.2 Hz, 1H), 5.18 (dd, J = 7.2, 1.8 Hz, 1H), 2.53 – 2.47 (m, 1H), 2.20 – 2.16

(m, 1H), 1.85 – 1.79 (m, 1H), 1.74 (t, J = 4.2 Hz, 1H), 1.46 – 1.42 (m, 1H), 1.36 – 1.31 (m, 1H), 1.16 (dd, J = 13.8, 3.0 Hz, 1H), 0.97 (s, 3H), 0.93 (s, 3H), 0.91 (s, 3H).

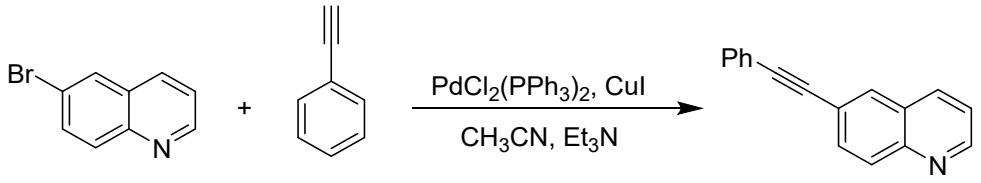


(3s,5s,7s)-adamantan-1-yl quinoline-6-carboxylate: Add 6-quinolinecarboxylic acid (3.20 g, 18.48 mmol), CH_2Cl_2 (74 mL), DMAP (4.58 g, 37.5 mmol), EDCI (3.59 g, 18.48 mmol), and 1-adamantanol (2.81 g, 18.48 mmol) into a 250 mL single-neck flask, and stir at room temperature for 16 h. The solution was diluted by the addition of saturated aqueous NH_4Cl solution and CH_2Cl_2 at room temperature. The organic phase was dried with anhydrous Na_2SO_4, and then, filtered. The resulting filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (PE:EA = 5:1) to give the corresponding product (3.2 g, 56%). The spectroscopic data are consistent with previously reported.[1] ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.97 (dd, J = 4.2, 1.8 Hz, 1H), 8.49 (d, J = 1.8 Hz, 1H), 8.25 – 8.23 (m, 2H), 8.10 (d, J = 8.4 Hz, 1H), 7.43 (dd, J = 4.2 Hz, 1H), 2.30 (s, 6H), 2.23 (s, 3H), 1.76 – 1.68 (s, 6H).

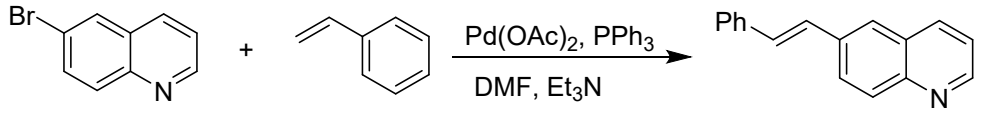


6-phenylquinoline: A solution of 6-bromoquinoline (2.08 g, 10.00 mmol), phenylboronic acid (1.83 g, 15.00 mmol), tetrakis (triphenylphosphine) palladium (0.58 g, 0.5 mmol), and potassium carbonate (2.76 g, 22.00 mmol) in dioxane (40 mL) and water (10 mL) was stirred at 90 °C for 14 h. The reaction mixture was then cooled to room temperature and quenched with saturated sodium bicarbonate solution in water. The resulting aqueous layer was extracted with ethyl acetate and then, the combined organic layer was washed with brine. The resulting mixture was dried over anhydrous Na_2SO_4 and then, filtered. The resulting filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (PE:EA = 10:1) to give the corresponding 6-phenylquinoline (2.01 g, 98%). The spectroscopic data are consistent with previously reported.[2] The experimental operation is consistent with the report literature.[3] ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.00 (dd, J = 4.8, 1.8 Hz, 1H), 8.30 – 8.23 (m, 2H), 8.01 – 8.00 (m, 2H), 7.73 – 7.72 (m, 2H),.7.52 – 7.50 (m, 2H), 7.46 –

7.43 (m, 2H).

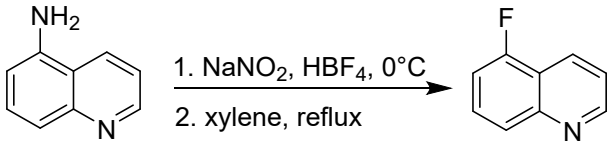


6-(phenylethynyl)quinolone: A solution of 6-bromoquinoline (4.20 g, 20.00 mmol), Phenylacetylene (2.25 g, 22.00 mmol), $PdCl_2(PPh_3)_2$ (0.14 g, 0.20 mmol), CuI (0.11 g, 0.60 mmol), and dry acetonitrile (30 mL) were added to an oven-dried Schlenk tube charged with a magnetic stirrer bar. Dry triethylamine (3.00 g, 30.00 mmol) was added, and the reaction was heated at reflux for 16 h. The reaction mixture was then cooled to room temperature and quenched with water. The resulting aqueous layer was extracted with DCM and then, the combined organic layer was washed with brine. The resulting mixture was dried over anhydrous Na_2SO_4 and then, filtered. The resulting filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (PE:EA = 15:1~5:1) to give the corresponding 6-phenylethynylquinoline (3.85 g, 84%). The spectroscopic data are consistent with previously reported.[4] The experimental operation is consistent with the report literature.[5] ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.92 (s, 1H), 8.13 (dd, J = 8.4, 1.8 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 8.02 (d, J = 2.4 Hz, 1H), 7.82 (dd, J = 9.0, 2.4 Hz, 1H), 7.59 – 7.58 (m, 2H), 7.43 – 7.41 (m, 1H), 7.38 – 7.37 (m, 3H).

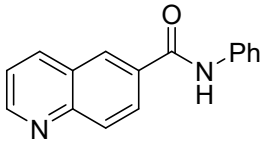


(*E*)-6-styrylquinoline: A solution of 6-bromoquinoline (3.5 g, 16.8 mmol), Phenethylene (2.6 g, 25.2 mmol), $Pd(OAc)_2$ (189 mg, 0.84 mmol), PPh_3 (661 mg, 2.52 mmol), Et_3N (3.4 g, 33.6 mmol), and DMF (28 mL) were added to an oven-dried Schlenk tube charged with a magnetic stirrer bar. The reaction was heated at reflux for 16 h. The reaction mixture was then cooled to room temperature. The resulting filtrate was concentrated under reduced pressure and purified by column chromatography on silica gel (PE:EA = 15:1~5:1) to give the corresponding (*E*)-6-styrylquinoline (2.2 g, 56%). The spectroscopic data are consistent with previously reported.[6] The experimental operation is consistent with the report literature.[7] ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.85 (dd, J = 4.2, 1.8

Hz, 1H), 8.09 – 8.05 (m, 2H), 7.93 (dd, *J* = 9.0, 1.8 Hz, 1H), 7.74 (d, *J* = 1.2 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 2H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.33 (dd, *J* = 7.8, 4.2 Hz, 1H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.22 (s, 2H).



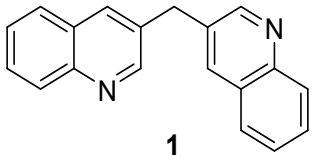
5-fluoroquinoline: To a suspension of 5-aminoquinoline (2.50 g, 17.36 mmol) in 50 % aqueous HBF_4 (20 mL) at 0°C was added sodium nitrite (1.32 g, 19.09 mmol) in several portions. The resulting solution was stirred for 1 hour at 0 °C and then poured into EtOAc:MTBE (1:1, 50 mL). The diazonium tetrafluoroborate salt was collected by filtration, washed with MTBE (100 mL) and dried under vacuum. The tetrafluoroborate salt was added portionwise to xylene (80 mL) heated to reflux and then stirred at reflux for an additional 4 hours before cooling to RT. The xylene was decanted off and the solution was neutralized with $NaHCO_3$ and extracted with EtOAc. The extracts were combined, dried over anhydrous Na_2SO_4, filtered and the solvent removed in vacuo. The residue was purified by column chromatography (PE:EA = 10:1~5:1) to give the corresponding 5-fluoroquinoline (1.17 g, 47 %). The spectroscopic data are consistent with previously reported.[8] The experimental procedure has been partially modified from the known literature.[8] ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (dd, *J* = 4.2, 1.2 Hz, 1H), 8.42 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.44 (dd, *J* = 8.4, 4.2 Hz, 1H), 7.20 (t, *J* = 9.6 Hz, 1H).



N-phenylquinoline-6-carboxamide. 6-quinoxalinecarboxylic acid (3 g, 17.42 mmol), HBTU (9.9 g, 26.13 mmol), aniline (3.24 g, 34.84 mmol) and DIEA (4.5 g, 34.84 mmol) were mixed with THF (58 mL) at room temperature for 16 h. After completion of reaction as indicated by TLC, added 1 M hydrochloric acid to the action mixture to adjust to neutral pH, then extracted with EA three times. The combined organic phases were dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 10:1~1:1) furnishes the desired product (3.24 g, 75% yield) as a yellow solid. The spectroscopic data are consistent with previously reported.[9]

The experimental procedure has been partially modified from the known literature.[10] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (dd, J = 4.4, 2.0 Hz, 1H), 8.34 (d, J = 2.0 Hz, 1H), 8.27 (s, 1H), 8.20 – 8.07 (m, 3H), 7.69 (d, J = 7.6 Hz, 2H), 7.44 (dd, J = 8.4, 4.4 Hz, 1H), 7.37 (t, J = 7.2 Hz, 2H), 7.17 (t, J = 7.2 Hz, 1H).

6. Preparation Procedure for 1-42



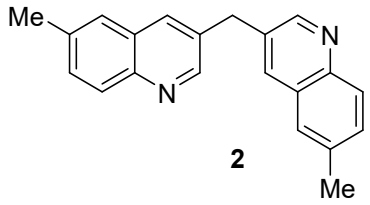
1

Di(quinolin-3-yl) methane (1). Following **GP1**, using quinoline (300 mg, 2.32 mmol), the title compound was obtained (109 mg, 70% yield) as a yellow solid. TLC: R_f = 0.14 (PE:EA = 1: 1). Melting point: 138.8-139.3 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.86 (d, J = 2.4 Hz, 2H), 8.09 (d, J = 9.0 Hz, 2H), 7.90 (d, J = 2.4 Hz, 2H), 7.72 (dd, J = 8.4, 1.2 Hz, 2H), 7.69 – 7.66 (m, 2H), 7.52 – 7.50 (m, 2H), 4.33 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 151.9, 147.2, 135.4, 132.6, 129.4, 129.4, 128.2, 127.6, 127.2, 36.7. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{15}N_2$ 271.1230; found 271.1231.

Gram scale synthesis:

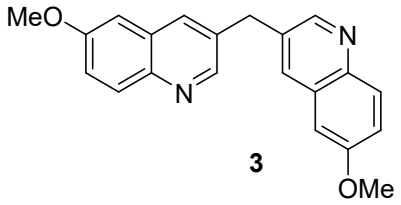
A dry and argon flushed 100 mL 3-necked flask, equipped with a magnetic stirring bar and a dropping funnel is charged with a solution of quinoline (1 g, 7.74 mmol) in dry THF (15.5 mL) and cooled to 0 °C. $BF_3{\cdot}OEt_2$ (1.07 mL, 8.51 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (9.29 mL, 1.0 M in THF, 9.29 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (182 mg, 1.94 mmol) is added, followed by the addition of trifluoroacetic acid (592 µL, 7.74 mmol). The reaction mixture is then increased to room temperature by removing the cooling bath, and continuously stirred overnight (20 h). Finally, it is quenched with 6 M ammonia (15 mL), then extracted with ethyl acetate three times. The

combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA= 5:1-EA) furnishes the desired product (371 mg, 71% yield) as a yellow solid.



2

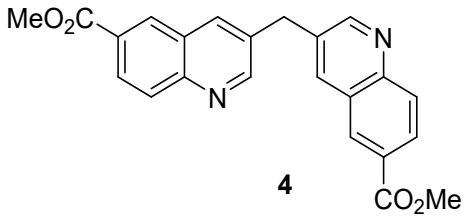
Bis(6-methylquinolin-3-yl)methane (2). Following **GP1**, using 6-methylquinoline (332 mg, 2.32 mmol), the title compound was obtained (77 mg, 44% yield) as a white solid. TLC: R_f = 0.13 (PE:EA = 1: 1). Melting point: 175.7-176.7 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.78 (d, J = 2.4 Hz, 2H), 7.98 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 2.4 Hz, 2H), 7.50 (dd, J = 8.4, 1.8 Hz, 2H), 7.46 (s, 2H), 4.29 (s, 2H), 2.49 (s, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 150.9, 145.7, 136.9, 134.6, 132.6, 131.6, 128.9, 128.2, 126.4, 36.6, 21.7. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{19}N_2$ 299.1543; found 299.1541.



3

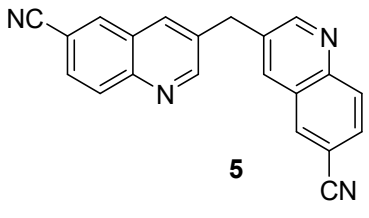
Bis(6-methoxyquinolin-3-yl)methane (3). A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of 6-methoxyquinoline (369 mg, 2.32 mmol) in dry THF (4.6 mL) and cooled to 0 °C. $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (55 mg, 0.58 mmol) is added, followed by the addition of trifluoroacetic acid (177 µL, 2.32 mmol). The reaction mixture is then increased to r.t. by removing the cooling bath for 75 min, then warm up to 50 °C and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then

extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 5: 1~1: 1) furnishes the desired product (57 mg, 30% yield) as a brown solid. TLC: R_f = 0.09 (PE:EA = 1: 1)。Melting point: 175.7-176.7 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.72 (d, J = 2.4 Hz, 2H), 7.98 (d, J = 9.0 Hz, 2H), 7.78 (dd, J = 1.8, 0.6 Hz, 2H), 7.33 (dd, J = 9.6, 3.0 Hz, 2H), 6.98 (d, J = 3.0 Hz, 2H), 4.30 (s, 2H), 3.89 (s, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 158.2, 149.4, 143.3, 134.2, 133.1, 130.7, 129.3, 122.1, 105.0, 55.7, 36.6. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{19}N_2O_2$ 331.1441; found 331.1437.



4

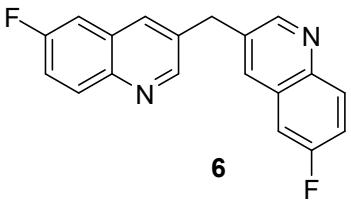
Dimethyl 3,3'-methylenebis(quinoline-6-carboxylate) (4). Following **GP1**, using methyl quinoline-6-carboxylate (434 mg, 2.32 mmol), the title compound was obtained (141 mg, 63% yield) as a white solid. TLC: R_f = 0.10 (PE:EA = 1: 1). Melting point: 149.9-150.2 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (d, J = 2.4 Hz, 2H), 8.52 (d, J = 1.8 Hz, 2H), 8.28 (dd, J = 9.0, 2.4 Hz, 2H), 8.14 (d, J = 9.0 Hz, 2H), 8.03 (t, J = 1.2 Hz, 2H), 4.42 (s, 2H), 3.97 (s, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 166.6, 153.9, 149.1, 136.4, 133.1, 130.8, 129.8, 129.0, 128.7, 127.3, 52.6, 36.6. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{19}N_2O_4$ 387.1339; found 387.1334.



5

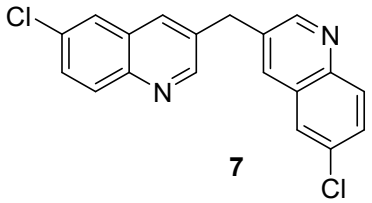
3,3'-methylenebis(quinoline-6-carbonitrile) (5). A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of 6-cyanoquinoline (358

mg, 2.32 mmol) in dry THF (4.6 mL) and cooled to 0 °C. $BF_3 \cdot OEt_2$ (0.32 mL, 2.55 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (55 mg, 0.58 mmol) is added, followed by the addition of trifluoroacetic acid (177 μL, 2.32 mmol). The reaction mixture is then increased to r.t. by removing the cooling bath and stirred for 75 min, then warmed up to 50 ℃ and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA=5:1~1:1) furnishes the desired product (106 mg, 57% yield) as an orange solid. TLC: R_f = 0.08 (PE:EA = 1: 1). Melting point: 159.9-160.9 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 9.10 (d, J = 2.4 Hz, 2H), 8.56 (d, J = 1.8 Hz, 2H), 8.34 (d, J = 2.4 Hz, 2H), 8.15 (d, J = 9.0 Hz, 2H), 7.98 (dd, J = 8.4, 1.8 Hz, 2H), 4.51 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 155.1, 147.3, 135.5, 134.8, 134.7, 130.2, 129.9, 127.2, 118.7, 109.4, 35.1. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{13}N_4$ 321.1135; found 321.1134.



6

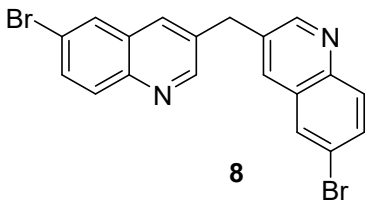
Bis(6-fluoroquinolin-3-yl)methane (6). Following **GP1**, using 6-fluoroquinoline (341 mg, 2.32 mmol), the title compound was obtained (145 mg, 82% yield) as a white solid. TLC: R_f = 0.13 (PE:EA = 1: 1). Melting point: 188.4-190.9 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.82 (d, J = 2.4 Hz, 2H), 8.09 (dd, J = 9.0, 5.4 Hz, 2H), 7.87 (d, J = 1.8 Hz, 2H), 7.46 (td, J = 9.0, 3.0 Hz, 2H), 7.35 (dd, J = 9.0, 3.0 Hz, 2H), 4.35 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.9 (d, $^1J_{C\text{-}F}$ = 249.0 Hz), 151.1 (d, J = 1.5 Hz), 144.4, 134.6 (d, J = 6.0 Hz), 133.2, 131.9 (d, J = 10.5 Hz), 128.9 (d, J = 10.5 Hz), 119.7 (d, J = 27.0 Hz), 110.6 (d, J = 21.0 Hz), 36.6. ^{19}F NMR (564.5 MHz, $CDCl_3$) δ -34.69 (s, 2F). HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{13}F_2N_2$ 307.1041; found 307.1039.



7

Bis(6-chloroquinolin-3-yl)methane (7). Following **GP1**, using 6-chloroquinoline (380 mg, 2.32 mmol), the title compound was obtained (160 mg, 81% yield) as a white solid. TLC: R_f = 0.13 (PE:EA = 1: 1). Melting point: 239.3-240.5 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 8.95 (d, J = 2.4 Hz, 2H), 8.20 (d, J = 2.4 Hz, 2H), 8.07 (d, J = 2.4 Hz, 2H), 8.02 (d, J = 9.0 Hz, 2H), 7.73 (dd, J = 9.0, 2.4 Hz, 2H), 4.43 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 152.6, 144.9, 134.3, 134.2, 131.2, 130.8, 129.6, 128.6, 126.5, 35.3. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{13}Cl_2N_2$ 339.0450 ($^{35}Cl^{35}Cl$), 341.0421 ($^{35}Cl^{37}Cl$) or 343.0391 ($^{37}Cl^{37}Cl$); found 339.0454, 341.0424 or 343.0394.

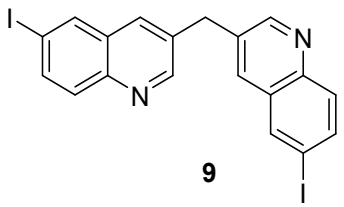
Note: The signal-to-noise ratio (SNR) of ^{13}C NMR is relatively low due to the low solubility of the compound.



8

Bis(6-bromoquinolin-3-yl)methane (8). Following **GP1**, using 6-bromoquinoline (483 mg, 2.32 mmol), the title compound was obtained (177 mg, 71% yield) as a white solid. TLC: R_f = 0.13 (PE:EA = 1: 1). Melting point: 262.9-263.4 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 8.95 (d, J = 1.8 Hz, 2H), 8.23 (d, J = 1.8 Hz, 2H), 8.20 (t, J = 1.2 Hz, 2H), 7.94 (d, J = 9.0 Hz, 2H), 7.83 (dd, J = 8.4, 1.8 Hz, 2H), 4.43 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 152.6, 145.0, 134.2, 134.1, 132.2, 130.9, 129.8, 129.1, 119.8, 35.3. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{13}Br_2N_2$ 426.9440 ($^{79}Br^{79}Br$), 428.9420 ($^{79}Br^{81}Br$) or 430.9399 ($^{81}Br^{81}Br$); found 426.9442, 428.9422 or 430.9402.

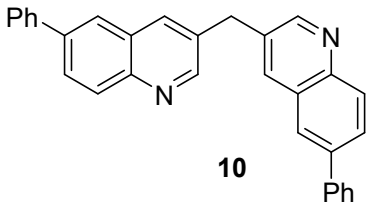
Note: The SNR of ^{13}C NMR is relatively low due to the low solubility of the compound.



9

Bis(6-iodoquinolin-3-yl)methane (9). Following **GP1**, using 6-iodoquinoline (592 mg, 2.32 mmol), the title compound was obtained (224 mg, 74% yield) as a white solid. TLC: R_f = 0.13 (PE:EA = 1: 1). Melting point: 276.4-276.8 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$ + CF_3CO_2D) δ 8.99 (d, J = 1.8 Hz, 2H), 8.44 (d, J = 1.8 Hz, 2H), 8.24 (d, J = 2.4 Hz, 2H), 8.01 (dd, J = 9.0, 2.4 Hz, 2H), 7.81 (d, J = 9.0 Hz, 2H), 4.44 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$ + CF_3CO_2D) δ 151.1, 143.4, 138.0, 136.2, 135.5, 133.7, 129.4, 128.8, 93.0, 34.9. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{13}I_2N_2$ 522.9163; found 522.9162.

Note: The SNR of ^{13}C NMR is relatively low due to the low solubility of the compound.

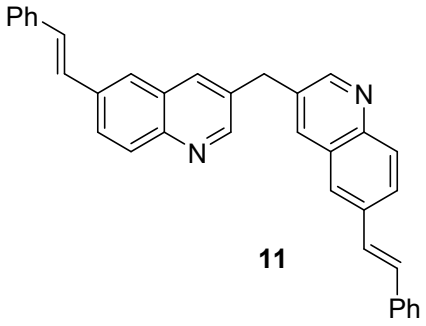


10

Bis(6-phenylquinolin-3-yl)methane (10). Following **GP1**, using 6-phenylquinoline (476 mg, 2.32 mmol), the title compound was obtained (147 mg, 60% yield) as a white solid. TLC: R_f = 0.10 (PE:EA = 1: 1). Melting point: 250.6-251.2 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 8.95 (d, J = 2.4 Hz, 2H), 8.26 (d, J = 28.2 Hz, 4H), 8.07 (q, J = 8.4 Hz, 4H), 7.82 (d, J = 7.8 Hz, 4H), 7.51 (t, J = 7.8 Hz, 4H), 7.41 (t, J = 7.8 Hz, 2H), 4.46 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 151.8, 145.7, 139.2, 138.1, 134.8, 133.6, 129.1, 128.8, 127.9, 127.8, 127.6, 126.8, 124.9, 35.3. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{31}H_{23}N_2$ 423.1856; found 423.1852.

Note: The poor solubility of the compound resulted in a low signal-to-noise ratio (SNR) in the ^{13}C

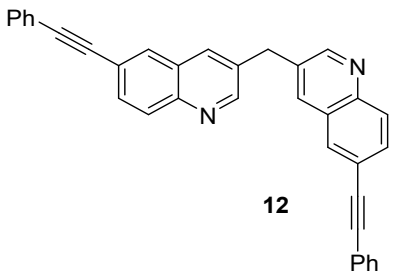
NMR spectrum, and some carbon peaks were not observed.



11

Bis(6-((E)-styryl)quinolin-3-yl)methane (11). A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of (*E*)-6-styrylquinoline (534 mg, 2.32 mmol) in dry THF (4.6 mL) and cooled to 0 °C. $BF_3 \cdot OEt_2$ (0.32 mL, 2.55 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (55 mg, 0.58 mmol) is added, followed by the addition of TfOH (0.20 mL, 2.32 mmol). The reaction mixture is then increased to r.t. by removing the cooling bath and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA= 5: 1~1: 1) furnishes the desired product (103 mg, 37% yield) as a yellow solid. TLC: R_f = 0.24 (PE:EA= 1: 1). Melting point: 271.3-271.8 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.83 (s, 2H), 8.08 (d, J = 8.4 Hz, 2H), 7.95 (d, J = 7.8 Hz, 2H), 7.91 (s, 2H), 7.76 (s, 2H), 7.56 (d, J = 6.6 Hz, 4H), 7.39 (s, 4H), 7.29 (s, 2H), 7.25 (s, 4H), 4.36 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 151.6, 147.3, 137.3, 136.3, 135.1, 133.1, 130.7, 129.9, 129.0, 128.6, 128.2, 128.1, 127.4, 126.9, 125.6, 36.8. HRMS (+ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{35}H_{27}N_2$ 475.2169; found 475.2170.

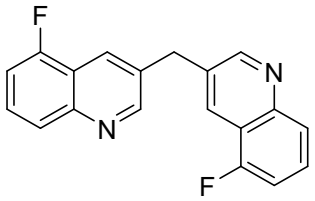
Note: The poor solubility of the compound resulted in a low signal-to-noise ratio (SNR) in the ^{13}C NMR spectrum, and some carbon peaks were not observed.



12

Bis(6-(phenylethynyl)quinolin-3-yl)methane (12). Following **GP1**, using 6-(phenylethynyl)quinoline (531 mg, 2.32 mmol), the title compound was obtained (112 mg, 41% yield) as a white solid. TLC: R_f = 0.12 (PE:EA = 3: 1). Melting point: 230.6-231.4 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.86 (s, 2H), 8.07 (d, J = 8.4 Hz, 2H), 7.94 (s, 2H), 7.89 (s, 2H), 7.79 (d, J = 7.2 Hz. 2H), 7.57 (s, 4H), 7.36 (s, 6H), 4.37 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 152.4, 146.7, 134.9, 133.2, 132.2, 131.9, 130.9, 129.6, 128.8, 128.6, 128.0, 123.1, 122.3, 91.0, 89.1, 36.7. HRMS (+ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{35}H_{23}N_2$ 471.1856; found 471.1852.

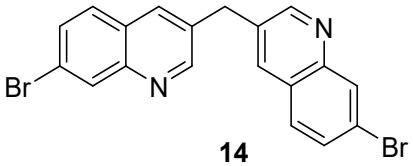
Note: The poor solubility of the compound resulted in a low signal-to-noise ratio (SNR) in the ^{13}C NMR spectrum, and some carbon peaks were not observed.



13

Bis(5-fluoroquinolin-3-yl)methane (13). A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of 5-fluoroquinoline (341 mg, 2.32 mmol) in dry THF (4.6 mL) and cooled to 0 °C. $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (55 mg, 0.58 mmol) is added, followed by the addition of TfOH (0.20 mL, 2.32 mmol). The reaction mixture is then increased to r.t. by removing the cooling bath and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then extracted with ethyl acetate three times. The

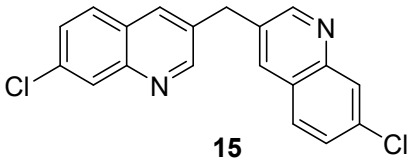
combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 5: 1~1: 1) furnishes the desired product (66 mg, 37% yield) as a white solid. TLC: R_f = 0.41 (EA). Melting point: 181.1-181.5 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.89 (d, J = 1.8 Hz, 2H), 8.22 (s, 2H), 7.90 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 6.0 Hz, 2H), 7.21 (t, J = 9.0 Hz, 2H), 4.40 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 157.8 (d, $^1J_{C\text{-}F}$ = 255.0 Hz), 152.6, 148.0 (d, J = 3.0 Hz), 132.6, 129.0 (d, J = 9.0 Hz), 128.4 (d, J = 4.5 Hz), 125.3 (d, J = 4.5 Hz), 118.9 (d, J = 16.5 Hz), 110.7 (d, J = 19.5 Hz), 37.1. ^{19}F NMR (564.5 MHz, $CDCl_3$) δ -45.10 (s, 2F). HRMS (+ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{13}F_2N_2$ 307.1041; found 307.1035.



14

Bis(7-bromoquinolin-3-yl)methane (14). Following **GP1**, using 7-bromoquinoline (483 mg, 2.32 mmol), the title compound was obtained (187 mg, 75% yield) as a white solid. TLC: R_f = 0.30 (PE:EA = 1: 1). Melting point: 253.2-253.9 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 8.97 (d, J = 2.4 Hz, 2H), 8.27 (d, J = 2.4 Hz, 2H), 8.22 (d, J = 1.8 Hz, 2H), 7.91 (d, J = 9.0 Hz, 2H), 7.73 (dd, J = 8.4, 1.8 Hz, 2H), 4.41 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 152.9, 146.9, 134.8, 133.7, 130.5, 129.7, 129.6, 126.4, 122.0, 35.2. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{13}Br_2N_2$ 426.9440 ($^{79}Br^{79}Br$), 428.9420 ($^{79}Br^{81}Br$) or 430.9399 ($^{81}Br^{81}Br$); found 426.9438, 428.9417 or 430.9391.

Note: The signal-to-noise ratio (SNR) of ^{13}C NMR is relatively low due to the low solubility of the compound.

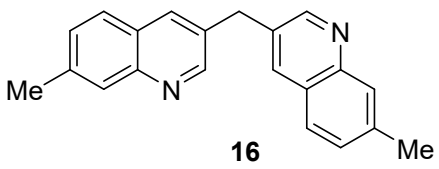


15

Bis(7-chloroquinolin-3-yl)methane (15). Following **GP1**, using 7-chloroquinoline (380 mg, 2.32

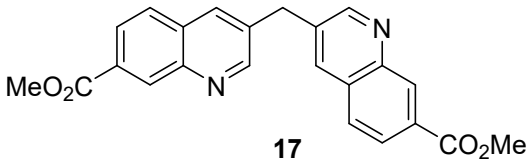
mmol), the title compound was obtained (161 mg, 82% yield) as a white solid. TLC: R_f = 0.22 (PE:EA = 1: 1). Melting point: 240.2-241.2 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 8.98 (d, J = 2.4 Hz, 2H), 8.28 (d, J = 1.8 Hz, 2H), 8.06 (d, J = 2.4 Hz, 2H), 7.99 (d, J = 9.0 Hz, 2H), 7.63 (dd, J = 8.4, 1.8 Hz, 2H), 4.42 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 153.2, 146.7, 134.9, 133.9, 133.6, 129.9, 127.5, 127.4, 126.4, 35.2. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{13}Cl_2N_2$ 339.0450 ($^{35}Cl^{35}Cl$), 341.0421 ($^{35}Cl^{37}Cl$) or 343.0391 ($^{37}Cl^{37}Cl$); found 339.0447, 341.0417 or 343.0390.

Note: The SNR of ^{13}C NMR is relatively low due to the low solubility of the compound.



16

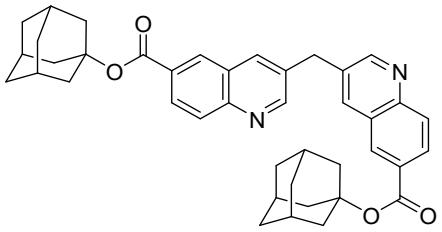
Bis(7-methylquinolin-3-yl)methane (16). A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of 7-methylquinoline (332 mg, 2.32 mmol) in dry THF (4.6 mL) and cooled to 0 °C. $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (55 mg, 0.58 mmol) is added, followed by the addition of acetic acid (232 μL, 4.06 mmol). The reaction mixture is then increased to r.t. by removing the cooling bath, and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 5: 1~1: 1) furnishes the desired product (69 mg, 40% yield) as a white solid. TLC: R_f = 0.12 (PE:EA = 1: 1). Melting point: 205.2-206.2 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.82 (d, J = 2.4 Hz, 2H), 7.87 – 7.86 (m, 4H), 7.62 (d, J = 8.4 Hz, 2H), 7.36 (dd, J = 8.4, 1.8 Hz, 2H), 4.32 (s, 2H), 2.56 (s, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 151.8, 147.4, 139.6, 135.0, 131.9, 129.3, 128.3, 127.2, 126.2, 36.6, 22.0. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{19}N_2$ 299.1543; found 299.1539.



17

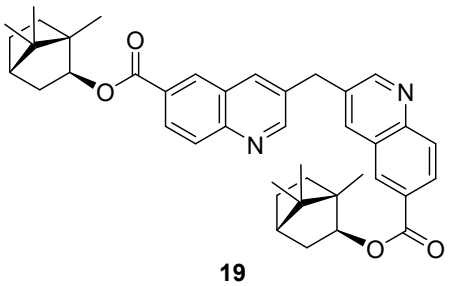
Dimethyl 3,3'-methylenebis(quinoline-7-carboxylate) (17). Following **GP1**, using methyl quinoline-7-carboxylate (434 mg, 2.32 mmol), the title compound was obtained (115 mg, 51% yield) as a white solid. TLC: R_f = 0.10 (PE:EA = 1: 1). Melting point: 255.9-256.2 °C. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 9.07 (d, J = 2.4 Hz, 2H), 8.57 (d, J = 1.2 Hz, 2H), 8.36 (dd, J = 2.4, 1.2 Hz, 2H), 8.06 (t, J = 1.8 Hz, 4H), 4.50 (s, 2H), 3.93 (s, 6H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$ + CF_3CO_2D) δ 165.6, 152.5, 144.5, 135.7, 135.0, 130.3, 130.1, 129.6, 128.4, 125.7, 52.1, 35.2. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{19}N_2O_4$ 387.1339; found 387.1334.

Note: The SNR of ^{13}C NMR is relatively low due to the low solubility of the compound.



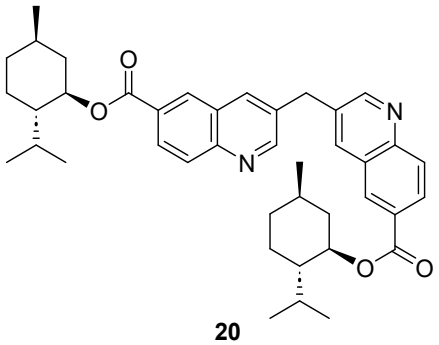
18

Di((3S,5S,7S)-adamantan-1-yl) 3,3'-methylenebis(quinoline-6-carboxylate) (18). Following **GP1**, using (3S,5S,7S)-adamantan-1-yl quinoline-6-carboxylate (712 mg, 2.32 mmol), the title compound was obtained (196 mg, 54% yield) as a yellow solid. Note: The reaction time was extended to 48 hours. TLC: R_f = 0.38 (EA). Melting point: 234.6-235.1 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.91 (d, *J* = 1.8 Hz, 2H), 8.41 (d, *J* = 1.2 Hz, 2H), 8.22 (dd, *J* = 8.4, 2.4 Hz, 2H), 8.09 (d, *J* = 9.0 Hz, 2H), 7.99 (d, *J* = 1.2 Hz, 2H), 4.38 (s, 2H), 2.27 (d, *J* = 3.0 Hz, 12H), 2.21 (s, 6H), 1.70 (q, *J* = 12.0 Hz, 12H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 164.8, 153.6, 148.8, 136.4, 133.0, 130.6, 130.3, 129.4, 129.1, 127.2, 81.8, 41.5, 36.5, 36.3, 31.0. HRMS (+ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{41}H_{43}N_2O_4$ 627.3217; found 627.3210.



19

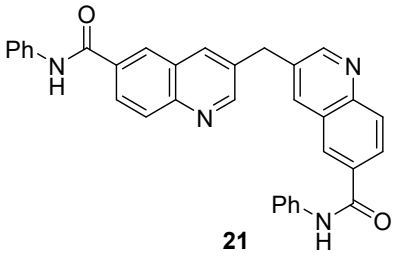
(1R,2R,4R)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 3-((6-((((1S,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)carbonyl)quinolin-3-yl)methyl)quinoline-6-carboxylate (19). Following **GP1**, using (1S,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl quinoline-6-carboxylate (717 mg, 2.32 mmol), the title compound was obtained (210 mg, 57% yield) as a yellow solid. Note: The reaction time was extended to 48 hours. TLC: R_f = 0.14 (PE:EA = 3:1). Melting point: 178.1-178.6 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (s, 2H), 8.49 (s, 2H), 8.28 (dd, J = 9.0, 1.8 Hz, 2H), 8.13 (d, J = 9.0 Hz, 2H), 8.05 (s, 2H), 5.16 (d, J = 9.6 Hz, 2H), 4.40 (s, 2H), 2.50-2.46 (m, 2H), 2.17-2.13 (m, 2H), 1.82-1.77 (m, 2H), 1.73 (s, 2H), 1.43-1.39 (m, 2H), 1.33-1.29 (m, 2H), 1.13 (dd, J = 13.8, 3.0 Hz, 2H), 0.95 (s, 6H), 0.91 (s, 6H), 0.90 (s, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 166.3, 153.8, 149.0, 136.4, 133.1, 130.4, 129.6, 129.4, 129.0, 127.3, 81.2, 49.2, 48.0, 45.1, 37.0, 36.5, 28.2, 27.6, 19.8, 19.0, 13.8. HRMS (+ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{41}H_{47}N_2O_4$ 631.3530; found 631.3522.



20

(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 3-((6-((((1S,2R,5S)-2-isopropyl-5-methylcyclohexyl)oxy)carbonyl)quinolin-3-yl)methyl)quinoline-6-carboxylate (20). Following **GP1**, using (1R,2S,5R)-2-isopropyl-5-methylcyclohexyl quinoline-6-carboxylate (722 mg, 2.32 mmol), the title compound was obtained (192 mg, 52% yield) as a yellow oil. Note: The reaction time

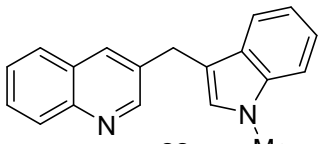
was extended to 48 hours. TLC: R_f = 0.47 (EA). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (d, J = 1.8 Hz, 2H), 8.50 (d, J = 1.8 Hz, 2H), 8.29 (dd, J = 9.0, 1.8 Hz, 2H), 8.14 (d, J = 9.0 Hz, 2H), 8.04 (s, 2H), 4.99 (td, J = 10.8, 4.8 Hz, 2H), 4.42 (s, 2H), 2.15 (d, J = 12.0 Hz, 2H), 2.00-1.95 (m, 2H), 1.76-1.73 (m, 4H), 1.60-1.55 (m, 4H), 1.18-1.11 (m, 4H), 0.93 (t, J = 7.2 Hz, 14H), 0.80 (d, J = 6.6 Hz, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 165.6, 153.7, 149.0, 136.5, 133.1, 130.5, 129.6, 129.4, 129.2, 127.3, 75.5, 47.4, 41.1, 36.6, 34.4, 31.6, 26.7, 23.7, 22.2, 20.9, 16.6. HRMS (+ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{41}H_{51}N_2O_4$ 635.3843; found 635.3838.



21

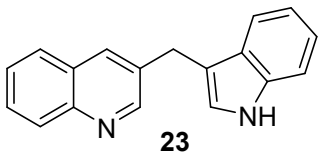
3,3'-Methylenebis(N-phenylquinoline-6-carboxamide) (21). A dry 25 mL flask, equipped with a magnetic stirring bar and a rubber septum, is flushed with argon and charged with N-phenylquinoline-6-carboxamide (575 mg, 2.32 mmol) and calcium chloride (694 mg, 6.25 mmol). Dry THF (4.6 mL) is then added, and the resulting mixture is cooled to 0 °C. $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.8 mL, 1.0 M in THF, 2.8 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then, 40% aqueous formaldehyde solution (44 mg, 0.58 mmol) and acetic acid (139 mg, 2.32 mmol) are added. The reaction mixture is then increased to rt by removing the cooling bath, and continuously stirred overnight. Finally, the reaction mixture is quenched with 6 M dilute ammonia solution and then extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 1:1 - DCM:MeOH = 10:1) furnishes the N-phenylquinoline-6-carboxamide (402 mg, 70% recovery) and desired product as a yellow solid (65 mg, 22% yield). Melting point: 309.6-310.5 °C. TLC: R_f = 0.35 (DCM:MeOH = 20:1). ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 10.44 (s, 2H), 9.07 (d, J = 1.8 Hz, 2H), 8.57 (d, J = 1.2 Hz, 2H), 8.39 (s, 2H), 8.21 (dd, J = 9.0, 1.8 Hz, 2H), 8.12 (d, J = 8.4 Hz, 2H), 7.80 (d, J =

8.4 Hz, 4H), 7.37 (t, J = 7.8 Hz, 4H), 7.12 (t, J = 7.2 Hz, 2H), 4.52 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 165.1, 153.7, 147.5, 139.1, 135.8, 134.3, 133.0, 128.9, 128.7, 128.1, 127.7, 126.9, 123.8, 120.3, 35.2. HRMS (+ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{33}H_{24}N_4O_2Na$ 531.1791; found 531.1784.



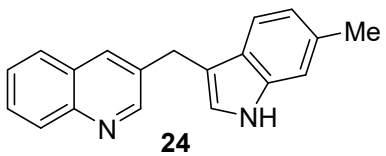
22

3-((1-methyl-1*H*-indol-3-yl)methyl)quinoline (22). Following **GP2**, using *N*-methylindole (145 μL, 1.16 mmol), the title compound was obtained (237 mg, 75% yield) as a yellow solid. TLC: R_f = 0.18 (PE:EA = 5: 1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 (d, J = 2.4 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.98 (d, J = 1.2 Hz, 1H), 7.72 (dd, J = 8.4, 1.2 Hz, 1H), 7.67 – 7.64 (m, 1H), 7.54 - 7.49 (m, 2H), 7.32 (dt, J = 8.4, 0.6 Hz, 1H), 7.26 - 7.23 (m, 1H), 7.10 - 7.07 (m, 1H), 6.80 (s, 1H), 4.29 (s, 2H), 3.75 (s, 3H). The spectroscopic data are consistent with previously reported.[11]



23

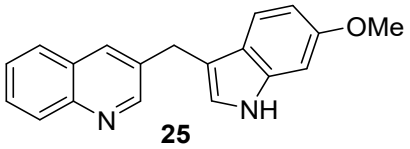
3-((1*H*-indol-3-yl)methyl)quinoline (23). Following **GP2**, using indole (136 mg, 1.16 mmol), the title compound was obtained (210 mg, 70% yield) as a yellow solid. TLC: R_f = 0.21 (PE:EA = 3: 1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 (d, J = 1.8 Hz, 1H), 8.20 (s, 1H), 8.09 (dd, J = 8.4, 0.6 Hz, 1H), 7.97 (dd, J = 1.8, 0.6 Hz, 1H), 7.72 (dd, J = 7.8, 1.2 Hz, 1H), 7.67 -7.64 (m, 1H), 7.54 - 7.48 (m, 2H), 7.39 (dt, J = 7.8, 1.2 Hz, 1H), 7.22 - 7.19 (m, 1H), 7.11 - 7.08 (m, 1H), 6.97 - 6.96 (m, 1H), 4.31 (s, 2H). The spectroscopic data are consistent with previously reported.[12]



24

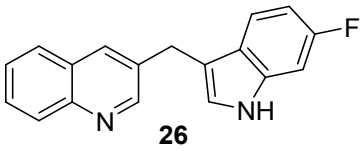
3-((6-methyl-1*H*-indol-3-yl)methyl)quinoline (24). Following **GP2**, using 6-methylindole (152 mg, 1.16 mmol), the title compound was obtained (240 mg, 76% yield) as a yellow solid. TLC:

R_f = 0.25 (PE:EA = 3: 1). Melting point: 142.7-143.9 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.94 (d, J = 2.4 Hz, 1H), 8.43 (s, 1H), 8.12 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 2.4 Hz, 1H), 7.71 (dd, J = 7.8, 1.2 Hz, 1H), 7.67 - 7.64 (m, 1H), 7.51 - 7.49 (m, 1H), 7.41 (d, J = 8.4 Hz, 1H), 7.16 (s, 1H), 6.94 (dd, J = 8.4, 1.8 Hz, 1H), 6.87 (d, J = 1.8 Hz, 1H), 4.28 (s, 2H), 2.46 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 152.2, 146.9, 137.2, 134.7, 134.2, 132.1, 129.1, 128.8, 128.3, 127.6, 126.6, 125.1, 122.2, 121.4, 118.6, 114.1, 111.4, 29.2, 21.8. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{17}N_2$ 273.1386; found 273.1387.



25

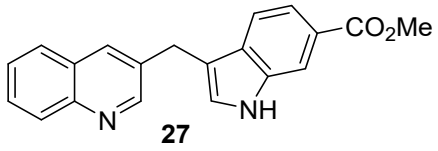
3-((6-methoxy-1*H*-indol-3-yl)methyl)quinoline (25). Following **GP2**, using 6-methoxyindole (171 mg, 1.16 mmol), the title compound was obtained (149 mg, 45% yield) as a yellow solid. TLC: R_f = 0.14 (PE:EA = 3: 1). Melting point: 106.1-107.8 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.92 (d, J = 2.4 Hz, 1H), 8.45 (s, 1H), 8.11 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 2.4 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.66 - 7.64 (m, 1H), 7.51 - 7.48 (m, 1H), 7.37 (d, J = 8.4 Hz, 1H), 6.83 (dd, J = 10.8, 2.4 Hz, 2H), 6.76 (dd, J = 8.4, 1.8 Hz, 1H), 4.25 (s, 2H), 3.80 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 156.8, 152.3, 146.9, 137.5, 134.7, 134.1, 129.1, 128.8, 128.3, 127.6, 126.7, 121.7, 121.6, 119.6, 114.4, 109.6, 94.9, 55.8, 29.3. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{17}N_2O$ 289.1335; found 289.1339.



26

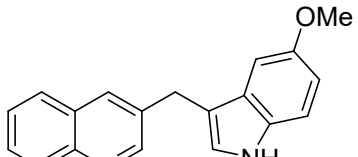
3-((6-fluoro-1*H*-indol-3-yl)methyl)quinoline (26). Following **GP2**, using 6-fluoroindole (157 mg, 1.16 mmol), the title compound was obtained (192 mg, 60% yield) as a white solid. TLC: R_f = 0.19 (PE:EA = 3: 1). Melting point: 210.1-212.0 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 11.02 (s, 1H), 8.89 (d, J = 1.8 Hz, 1H), 8.16 (dd, J = 2.4, 1.2 Hz, 1H), 7.97 (dd, J = 8.4, 1.2 Hz, 1H), 7.87 (dd, J = 7.8, 1.2 Hz, 1H), 7.68 - 7.66 (m, 1H), 7.56 - 7.53 (m, 1H), 7.45 (dd, J = 9.0, 5.4 Hz, 1H), 7.26 (d, J = 2.4 Hz, 1H), 7.14 (dd, J = 10.2, 1.8 Hz, 1H), 6.81 - 6.78 (m, 1H), 4.24 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 159.0 (d, $^1J_{C\text{-}F}$ = 225.0 Hz), 152.1, 146.3, 136.4, 136.3, 134.5, 133.8, 128.6, 127.7, 127.6, 126.6, 124.1 (d, J = 3.0 Hz), 123.7, 119.4 (d, J = 10.5 Hz), 113.2, 107.0 (d, J = 24.0 Hz), 97.5

(d, J = 25.5 Hz), 28.3. ^{19}F NMR (564.5 MHz, $(CD_3)_2SO$) δ -44.27 (s, 1F). HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{14}FN_2$ 277.1136; found 277.1140.



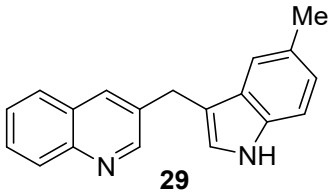
27

Methyl 3-(quinolin-3-ylmethyl)-1*H*-indole-6-carboxylate (27). Following **GP2**, using methyl indole-6-carboxylate (203 mg, 1.16 mmol), the title compound was obtained (236 mg, 64% yield) as a yellow solid. TLC: R_f = 0.12 (PE:EA = 3: 1). Melting point: 139.3-140.4 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.29 (s, 1H), 8.90 (d, J = 2.4 Hz, 1H), 8.15 (d, J = 1.2 Hz, 1H), 8.09 (d, J = 9.0 Hz, 1H), 7.95 (d, J = 3.0 Hz, 1H), 7.77 (dd, J = 8.4, 1.8 Hz, 1H), 7.71 (dd, J = 8.4, 1.8 Hz, 1H), 7.66 - 7.64 (m, 1H), 7.54 - 7.48 (m, 2H), 7.12 (d, J = 2.4 Hz, 1H), 4.29 (s, 2H), 3.91 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 168.4, 152.0, 146.9, 136.0, 134.8, 133.7, 130.8, 129.0, 129.0, 128.3, 127.6, 126.8, 126.4, 123.9, 120.6, 118.5, 114.7, 113.9, 52.1, 29.0. HRMS (+ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{20}H_{16}N_2NaO_2$ 339.1104; found 339.1107.



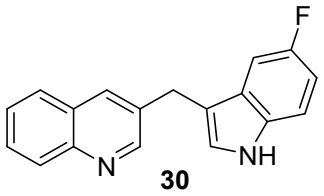
28

3-((5-methoxy-1*H*-indol-3-yl)methyl)quinoline (28). Following **GP2**, using 5-methoxyindole (171 mg, 1.16 mmol), the title compound was obtained (214 mg, 64% yield) as a tan solid. TLC: R_f = 0.17 (PE:EA = 3: 1). Melting point: 146.6-147.2 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.92 (d, J = 2.4 Hz, 1H), 8.28 (s, 1H), 8.09 (dd, J = 8.4, 1.2 Hz, 1H), 7.95 (dd, J = 2.4, 1.2 Hz, 1H), 7.70 (dd, J = 8.4, 1.2 Hz, 1H), 7.66 - 7.63 (m, 1H), 7.50 - 7.48 (m, 1H), 7.25 (d, J = 2.4 Hz, 1H), 6.95 (d, J = 2.4 Hz, 1H), 6.91 (d, J = 2.4 Hz, 1H), 6.86 (dd, J = 9.0, 2.4 Hz, 1H), 4.26 (s, 2H), 3.78 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 154.2, 152.3, 147.0, 134.7, 134.0, 131.8, 129.2, 128.8, 128.3, 127.7, 127.6, 126.7, 123.6, 114.1, 112.5, 112.2, 100.9, 56.0, 29.2. HRMS (+ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{16}N_2NaO$ 311.1155; found 311.1159.



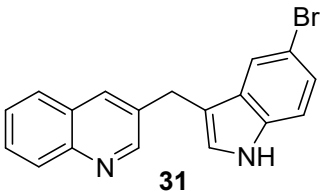
29

3-((5-methyl-1*H*-indol-3-yl)methyl)quinoline (29). Following **GP2**, using 5-methylindole (152 mg, 1.16 mmol), the title compound was obtained (222 mg, 70% yield) as a yellow solid. TLC: R_f = 0.32 (PE:EA = 3: 1). Melting point: 145.0-146.9 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.94 (d, J = 2.4 Hz, 1H), 8.50 (s, 1H), 8.11 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 2.4 Hz, 1H), 7.71 (dd, J = 8.4, 1.2 Hz, 1H), 7.67 - 7.64 (m, 1H), 7.51 - 7.48 (m, 1H), 7.33 (s, 1H), 7.25 (s, 1H), 7.03 (dd, J = 8.4, 1.8 Hz, 1H), 6.89 (d, J = 2.4 Hz, 1H), 4.27 (s, 2H), 2.43 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 152.3, 146.9, 135.0, 134.7, 134.2, 129.1, 128.9, 128.8, 128.3, 127.6, 127.5, 126.6, 124.0, 123.0, 118.6, 113.8, 111.1, 29.1, 21.6. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{17}N_2$ 273.1386; found 273.1389.



30

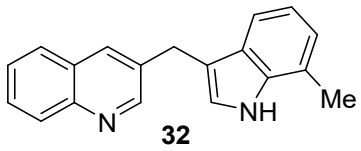
3-((5-fluoro-1*H*-indol-3-yl)methyl)quinoline (30). Following **GP2**, using 5-fluoroindole (157 mg, 1.16 mmol), the title compound was obtained (201 mg, 63% yield) as a white solid. TLC: R_f = 0.18 (PE:EA = 3: 1). Melting point: 221.7-223.9 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 11.05 (s, 1H), 8.90 (d, J = 2.4 Hz, 1H), 8.17 (d, J = 2.4 Hz, 1H), 7.97 (d, J = 8.4 Hz, 1H), 7.88 (dd, J = 8.4, 1.8 Hz, 1H), 7.69 - 7.66 (m, 1H), 7.56 - 7.53 (m, 1H), 7.36 - 7.34 (m, 2H), 7.25 (dd, J = 9.6, 2.4 Hz, 1H), 6.92 - 6.89 (m, 1H), 4.23 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 156.7 (d, $^1J_{C\text{-}F}$ = 240.0 Hz), 152.1, 146.2, 134.6, 133.8, 133.1, 128.7, 127.73, 127.65, 127.04, 126.98, 126.6, 125.6, 113.3 (d, J = 4.5 Hz), 112.5 (d, J = 10.5 Hz),109.3 (d, J = 25.5 Hz), 103.1 (d, J = 24 Hz), 28.2. ^{19}F NMR (564.5 MHz, $(CD_3)_2SO$) δ -47.36 (s, 1F). HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{14}FN_2$ 277.1136; found 277.1139.



31

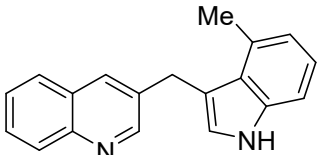
3-((5-bromo-1*H*-indol-3-yl)methyl)quinoline (31). Following **GP2**, using 5-bromoindole (227

mg, 1.16 mmol), the title compound was obtained (223 mg, 57% yield) as a yellow solid. TLC: R_f = 0.18 (PE:EA = 3: 1). Melting point: 191.5-193.0 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 11.19 (s, 1H), 8.90 (d, J = 2.4 Hz, 1H), 8.15 (d, J = 2.4 Hz, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.87 (dd, J = 7.8, 1.2 Hz, 1H), 7.68 - 7.66 (m, 2H), 7.55 - 7.53 (m, 1H), 7.35 - 7.33 (m, 2H), 7.18 (dd, J = 8.4, 1.8 Hz, 1H), 4.24 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 152.1, 146.3, 135.1, 134.5, 133.8, 128.7, 128.7, 128.7, 127.7, 127.6, 126.6, 125.3, 123.6, 120.6, 113.6, 112.8, 111.2, 28.0. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{14}BrN_2$ 337.0335 (^{79}Br) or 339.0314 (^{81}Br); found 337.0337 or 339.0317.



32

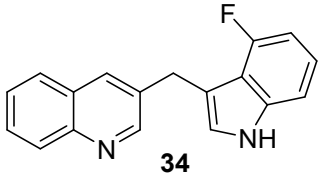
3-((7-methyl-1*H*-indol-3-yl)methyl)quinoline (32). Following **GP2**, using 7-methylindole (152 mg, 1.16 mmol), the title compound was obtained (201 mg, 64% yield) as a yellow solid. TLC: R_f = 0.32 (PE:EA = 3: 1). Melting point: 141.3-142.1 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.95 (d, J = 2.4 Hz, 1H), 8.53 (s, 1H), 8.12 (d, J = 9.0 Hz, 1H), 7.97 (dd, J = 1.8, 0.6 Hz, 1H), 7.71 (dd, J = 8.4, 1.2 Hz, 1H), 7.67 - 7.65 (m, 1H), 7.52 - 7.49 (m, 1H), 7.41 (dd, J = 6.6, 1.8 Hz, 1H), 7.06 - 7.02 (m, 2H), 6.93 (d, J = 2.4 Hz, 1H), 4.30 (s, 2H), 2.49 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 152.3, 146.9, 136.3, 134.7, 134.2, 129.1, 128.8, 128.3, 127.6, 126.8, 126.7, 122.9, 122.5, 120.7, 119.9, 116.7, 114.8, 29.3, 16.8. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{17}N_2$ 273.1386; found 273.1387.



33

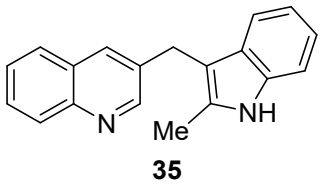
3-((4-methyl-1*H*-indol-3-yl)methyl)quinoline (33). Following **GP2**, using 4-methylindole (152 mg, 1.16 mmol), the title compound was obtained (158 mg, 50% yield) as a yellow solid. TLC: R_f = 0.25 (PE:EA = 3: 1). Melting point: 194.7-195.9 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.91 (d, J = 2.4 Hz, 1H), 8.23 (s, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.85 (dd, J = 2.4, 1.2 Hz, 1H), 7.70 - 7.65 (m, 2H), 7.51 - 7.48 (m, 1H), 7.23 (d, J = 8.4 Hz, 1H), 7.09 (t, J = 7.8 Hz, 1H), 6.84 - 6.83 (m, 2H), 4.49 (s, 2H), 2.57 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 152.3, 147.0, 137.3, 134.9, 134.8, 131.0,

129.3, 128.9, 128.4, 127.7, 126.7, 126.0, 123.6, 122.6, 121.3, 114.8, 109.3, 31.1, 20.3. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{17}N_2$ 273.1386; found 273.1390.



34

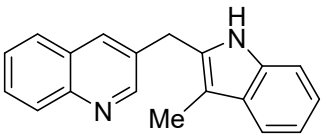
3-((4-fluoro-1*H*-indol-3-yl)methyl)quinoline (34). Following **GP2**, using 4-fluoroindole (157 mg, 1.16 mmol), the title compound was obtained (167 mg, 52% yield) as a yellow solid. TLC: R_f = 0.09 (PE:EA = 3: 1). Melting point: 205.2-206.7 ℃. ^{1}H NMR (600 MHz, $(CD_3)_2SO$) δ 11.26 (s, 1H), 8.87 (s, 1H), 8.06 (s, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.86 (d, J = 8.4 Hz, 1H), 7.67 (t, J = 7.8 Hz, 1H), 7.53 (t, J = 7.8 Hz, 1H), 7.27 - 7.19 (m, 2H), 7.01 (dd, J = 13.2, 7.8 Hz, 1H), 6.67 (dd, J = 11.4, 7.8 Hz, 1H), 4.32 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $(CD_3)_2SO$) δ 156.4 (d, $^1J_{C\text{-}F}$ = 240.0 Hz), 152.0, 146.3, 139.6, 139.5, 134.9, 133.8, 128.6, 127.73, 127.65, 126.6, 124.3, 121.7 (d, J = 7.5 Hz), 115.2 (d, J = 19.5 Hz), 111.2 (d, J = 3.0 Hz), 108.2 (d, J = 3.0 Hz), 103.5 (d, J = 19.5 Hz), 29.4. ^{19}F NMR (564.5 MHz, $(CD_3)_2SO$) δ -46.28 (s, 1F). HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{14}FN_2$ 277.1136; found 277.1141.



35

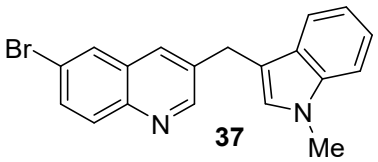
3-((2-methyl-1*H*-indol-3-yl)methyl)quinoline (35). Following **GP2**, using 2-methylindole (152 mg, 1.16 mmol), the title compound was obtained (176 mg, 56% yield) as a yellow solid. TLC: R_f = 0.31 (PE:EA = 3: 1). Melting point: 189.1-190.2 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.90 (d, J = 2.4 Hz, 1H), 8.06 (dd, J = 8.4, 1.2 Hz, 1H), 8.03 (s, 1H), 7.83 (dd, J = 2.4, 1.2 Hz, 1H), 7.67 (dd, J = 7.8, 1.2 Hz, 1H), 7.64 - 7.61 (m, 1H), 7.48 - 7.45 (m, 1H), 7.39 (dd, J = 7.8, 1.2 Hz, 1H), 7.31 (dt, J = 8.4, 0.6 Hz, 1H), 7.14 - 7.11 (m, 1H), 7.04 - 7.02 (m, 1H), 4.25 (s, 2H), 2.43 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 152.2, 146.9, 135.5, 134.5, 134.1, 132.1, 129.2, 128.7, 128.7, 128.4, 127.6, 126.6, 121.4, 119.7, 118.2, 110.4, 109.3, 27.8, 12.0. HRMS (+ESI-TOF) *m/z*: $[M + Na]^+$ calcd for

$C_{19}H_{16}N_2Na$ 295.1206; found 295.1209.



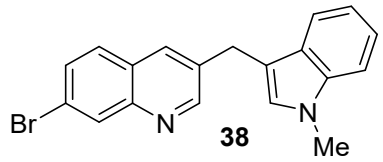
36

3-((3-methyl-1*H*-indol-2-yl)methyl)quinoline (36). Following **GP2**, using 3-methylindole (152 mg, 1.16 mmol), the title compound was obtained (162 mg, 51% yield) as a yellow solid. TLC: R_f = 0.35 (PE:EA = 3: 1). Melting point: 160.9-162.2 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.66 (d, J = 2.4 Hz, 1H), 8.52 (s, 1H), 8.02 (d, J = 9.0 Hz, 1H), 7.77 (d, J = 2.4 Hz, 1H), 7.63 - 7.56 (m, 3H), 7.47 - 7.44 (m, 1H), 7.26 - 7.24 (m, 1H), 7.15 - 7.11 (m, 2H), 4.20 (s, 2H), 2.36 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 151.5, 147.0, 136.0, 134.9, 132.2, 131.8, 129.3, 129.3, 129.0, 128.2, 127.6, 127.0, 121.7, 119.3, 118.6, 110.7, 108.8, 29.8, 8.8. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{17}N_2$ 273.1386; found 273.1391.



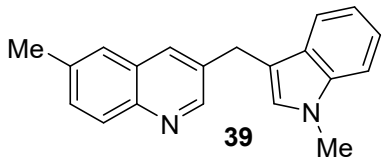
37

6-bromo-3-((1-methyl-1*H*-indol-3-yl)methyl)quinoline (37). Following **GP2**, using 6-bromoquinoline (483 mg, 2.32 mmol) and *N*-methylindole (145 µL, 1.16 mmol), the title compound was obtained (207 mg, 51% yield) as a tan solid. TLC: R_f = 0.14 (PE:EA = 3: 1). Melting point: 142.1-143.5 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.91 (d, J = 2.4 Hz, 1H), 7.94 (d, J = 9.0 Hz, 1H), 7.85 (dd, J = 13.8, 1.8 Hz, 2H), 7.70 (dd, J = 9.0, 2.4 Hz, 1H), 7.49 (dt, J = 7.8, 1.2 Hz, 1H), 7.33 (dt, J = 8.4, 1.2 Hz, 1H), 7.25 - 7.23 (m, 1H), 7.10 - 7.08 (m, 1H), 6.81 (s, 1H), 4.28 (s, 2H), 3.76 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 152.7, 145.5, 137.4, 135.3, 133.5, 132.2, 131.0, 129.6, 129.5, 127.6, 127.5, 122.1, 120.5, 119.3, 119.0, 112.6, 109.5, 32.8, 29.1. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{16}BrN_2$ 351.0491 (^{79}Br) or 353.0471 (^{81}Br); found 351.0496 or 353.0474.



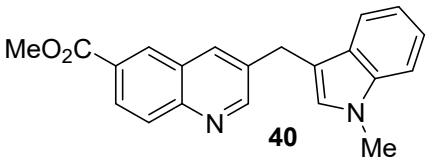
38

7-bromo-3-((1-methyl-1*H*-indol-3-yl)methyl)quinoline (38). Following **GP2**, using 7-bromoquinoline (483 mg, 2.32 mmol) and *N*-methylindole (145 μL, 1.16 mmol), the title compound was obtained (210 mg, 52% yield) as a brown solid. TLC: R_f = 0.29 (PE:EA = 3: 1). Melting point: 134.0-135.2 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.91 (d, J = 2.4 Hz, 1H), 8.27 (d, J = 1.2 Hz, 1H), 8.05 (d, J = 1.8 Hz, 1H), 7.58 - 7.54 (m, 2H), 7.50 (d, J = 8.4 Hz, 1H), 7.32 (d, J = 8.4 Hz, 1H), 7.26 - 7.23 (m, 1H), 7.10 - 7.07 (m, 1H), 6.81 (s, 1H), 4.26 (s, 2H), 3.75 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 153.2, 147.5, 137.4, 134.8, 134.4, 131.6, 130.1, 128.8, 127.6, 127.5, 126.9, 122.6, 122.0, 119.2, 119.0, 112.6, 109.5, 32.8, 29.1. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{16}BrN_2$ 351.0491 (^{79}Br) or 353.0471 (^{81}Br); found 351.0496 or 353.0473.



39

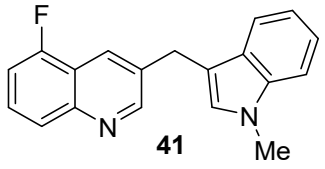
6-methyl-3-((1-methyl-1*H*-indol-3-yl)methyl)quinoline (39). Following **GP2**, using 6-methylquinoline (332 mg, 2.32 mmol) and *N*-methylindole (145 μL, 1.16 mmol), the title compound was obtained (150 mg, 45% yield) as an orange solid. TLC: R_f = 0.22 (PE:EA = 3: 1). Melting point: 132.4-133.5 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.85 (d, J = 1.8 Hz, 1H), 7.98 (d, J = 9.6 Hz, 1H), 7.87 (d, J = 0.6 Hz, 1H), 7.53 (dt, J = 8.4, 0.6 Hz, 1H), 7.49 - 7.47 (m, 2H), 7.32 (dt, J = 8.4, 1.2 Hz, 1H), 7.25 - 7.22 (m, 1H), 7.10 – 7.07 (m, 1H), 6.78 (s, 1H), 4.27 (s, 2H), 3.74 (s, 3H), 2.50 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 151.5, 145.6, 137.4, 136.5, 134.1, 134.0, 131.0, 128.9, 128.4, 127.7, 127.4, 126.5, 122.0, 119.2, 119.1, 113.2, 109.4, 32.8, 29.2, 21.7. HRMS (+ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{20}H_{18}N_2Na$ 309.1362; found 309.1364.



40

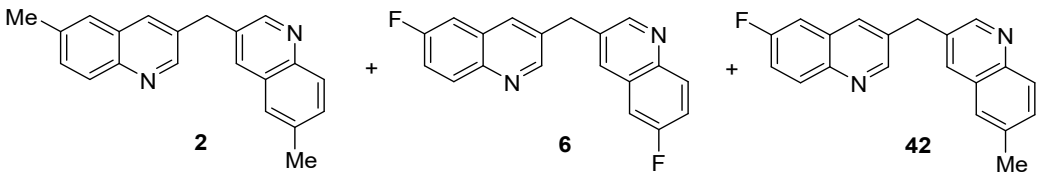
Methyl 3-((1-methyl-1*H*-indol-3-yl)methyl)quinoline-6-carboxylate (40). Following **GP2**,

using methyl quinoline-6-carboxylate (434 mg, 2.32 mmol) and *N*-methylindole (145 μL, 1.16 mmol), the title compound was obtained (160 mg, 42% yield) as an orange solid. TLC: R_f = 0.17 (PE:EA = 5: 1). Melting point: 142.0-143.7 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.99 (d, J = 1.8 Hz, 1H), 8.48 (d, J = 1.8 Hz, 1H), 8.23 (dd, J = 9.0, 1.8 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 8.03 (d, J = 1.2, 1H), 7.50 (dt, J = 8.4, 0.6 Hz, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.25 - 7.23 (m, 1H), 7.10 - 7.07 (m, 1H), 6.82 (s, 1H), 4.30 (s, 2H), 3.97 (s, 3H), 3.75 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 166.8, 154.5, 148.8, 137.4, 135.6, 135.2, 130.8, 129.5, 128.3, 128.1, 127.6, 127.5, 127.5, 122.1, 119.3, 119.0, 112.5, 109.5, 52.4, 32.8, 29.1. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{19}N_2O_2$ 331.1441; found 331.1444.



41

5-fluoro-3-((1-methyl-1*H*-indol-3-yl)methyl)quinoline (41). Following **GP2**, using 5-fluoroquinoine (341 mg, 2.32 mmol) and *N*-methylindole (145 μL, 1.16 mmol), the title compound was obtained (169 mg, 50% yield) as a yellow oil. TLC: R_f = 0.21 (PE:EA = 5: 1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (d, J = 2.4 Hz, 1H), 8.26 (dd, J = 2.0, 1.2 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.33 – 7.31 (m, 1H), 7.25 – 7.22 (m, 1H), 7.20 – 7.16 (m, 1H), 7.12 – 7.07 (m, 1H), 6.81 (s, 1H), 4.31 (s, 2H), 3.75 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 157.8 (d, $^1J_{C\text{-}F}$ = 260.0 Hz), 153.2, 147.8 (d, J = 3.0 Hz), 137.4, 134.6 (d, J = 3.0 Hz), 128.2, 128.1, 127.7 (d, J = 5.0 Hz), 127.6, 127.4, 125.2 (d, J = 4.0 Hz), 122.0, 119.2, 119.0, 112.8, 110.3 (d, J = 19.0 Hz), 109.5, 32.8, 29.4. ^{19}F NMR (564.5 MHz, $CDCl_3$) δ -45.32 (s, 1F). HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{16}FN_2$ 291.1292; found 291.1288.



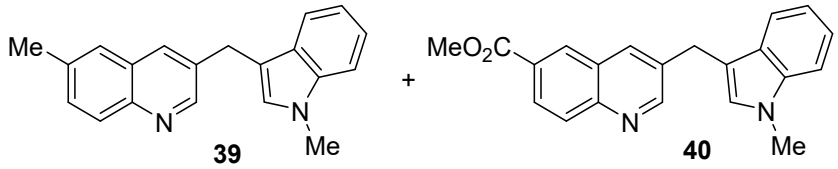
2 **6** **42**

Procedure I: A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of 6-fluoroquinoline (171 mg, 1.16 mmol), 6-methylquinoline (166 mg, 1.16 mmol) in dry THF (4.6 mL) and cooled to 0 °C. $BF_3 \cdot OEt_2$ (0.32mL, 2.55 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.78 mL, 1.0 M in THF, 2.78 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (55 mg, 0.58 mmol) is added, followed by the addition of trifluoroacetic acid (177 μL, 2.32 mmol). The reaction mixture is then increased to r.t. by removing the cooling bath, and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 5: 1~1: 1) to give a mixture of compounds **2**, **6** and **42**, which are further separated by preparation HPLC to afford the product **42** (66 mg, 38% yield) as a white solid. The ratio of compounds **2**, **6** and **42** was determined by Poroshell 120 EC-C18 (15 cm), CH_3CN/H_2O = 40/60-70/30, 1.0 ml/min, 15 min, λ = 234 nm, t_R (**2**) = 9.726 min, t_R (**6**) = 7.902 min, t_R (**42**) = 8.788 min.

Procedure II: A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of 6-fluoroquinoline (171 mg, 1.16 mmol) in dry THF (2.3 mL) and cooled to 0 °C. $BF_3 \cdot OEt_2$ (0.16mL, 1.28 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (1.39 mL, 1.0 M in THF, 1.39 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (55 mg, 0.58 mmol) is added. Meanwhile 6-methylquinoline (166 mg, 1.16 mmol), in dry THF (2.3 mL) and cooled to 0 °C. $BF_3 \cdot OEt_2$ (0.16 mL, 1.28 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (1.39 mL, 1.0 M in THF, 1.39 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then transfer the reaction mixture to the previous one under Ar protection, followed by the addition of trifluoroacetic acid (177 μL, 2.32 mmol). The reaction mixture is then increased to r.t. by removing the cooling bath, and continuously stirred overnight. Finally, it is quenched with 6 M

ammonia (5 mL), then extracted with ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 5: 1~1: 1) to give a mixture of compounds **2**, **6** and **42**, which are further separated by preparation HPLC to afford the products **2** (18 mg, 10% yield), **6** (37 mg, 21% yield) and **42** (46 mg, 26% yield) as white solid.

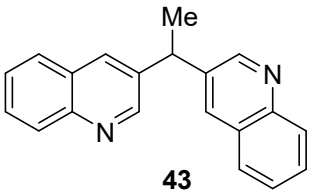
6-Fluoro-3-((6-methylquinolin-3-yl)methyl)quinoline (42). TLC: R_f = 0.15 (PE:EA = 1: 1). Melting point: 165.4-166.4 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.80 (dd, J = 22.2, 1.8 Hz, 2H), 8.08 (dd, J = 9.0, 4.8 Hz, 1H), 7.99 (d, J = 8.4 Hz, 1H), 7.83 (dd, J = 10.2, 2.4 Hz, 2H), 7.53 – 7.50 (m, 2H), 7.46 – 7.43 (m, 1H), 7.33 (dd, J = 9.0, 2.4 Hz, 1H), 4.33 (s, 2H), 2.5 (d, J = 0.6 Hz, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.84 (d, $^1J_{C\text{-}F}$ = 248.1 Hz), 151.3 (d, J = 2.4 Hz), 150.9, 145.9, 144.3, 137.1, 134.7, 134.5 (d, J = 5.4 Hz), 133.7, 132.2, 131.9 (d, J = 9.6 Hz), 131.7, 129.1, 128.9 (d, J = 10.2 Hz), 128.2, 126.4, 119.5 (d, J = 25.1 Hz), 110.6 (d, J = 21.8 Hz), 36.7, 21.7. ^{19}F NMR (564.5 MHz, $CDCl_3$) δ -34.90 (s, 1F). HRMS (+ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{20}H_{16}FN_2$ 303.1292; found 303.1294.



A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a solution of 6-methylquinoline (166 mg, 1.16 mmol) and methyl quinoline-6-carboxylate (217 mg, 1.16 mmol) in dry THF (4.6 mL) and cooled to 0 °C. $BF_3{\cdot}OEt_2$ (0.32 mL, 2.55 mmol) is added dropwise and stirred for 15 min at the same temperature. The reaction mixture is cooled to -50 °C followed by dropwise addition of a solution of ^{t}BuMgCl (2.8 mL, 1.0 M in THF, 2.8 mmol), and stirring the reaction mixture at the same temperature for 30 min. Then dimethylformiminium chloride (109 mg, 1.16 mmol) is added, followed by the addition of acetic acid (266 μL, 4.64 mmol), then *N*-methylindole (145 μL, 1.16 mmol in 2.32 mL MeOH) is added. The reaction mixture is then increased to room temperature by removing the cooling bath, and continuously stirred overnight. Finally, it is quenched with 6 M ammonia (5 mL), then extracted with

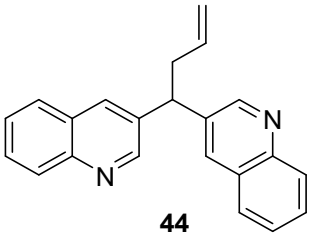
ethyl acetate three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 10: 1~1: 1) to give a mixture of compounds **39** and **40**. The ratio of compounds **39** and **40** was determined by Poroshell 120 EC-C18 (15 cm), MeOH/H_2O = 70/30, 1.0 ml/min, λ_1 = 224 nm, λ_2 = 228 nm, t_R (**39**) = 10.234 min, t_R (**40**) = 7.373 min.

7. Preparation Procedure for 43-50



43

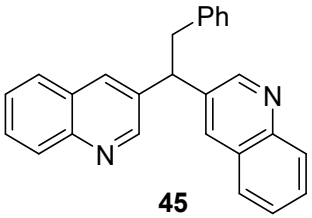
3,3'-(ethane-1,1-diyl)diquinoline (43). Following **GP3**, using iodomethane (92 μL, 0.74 mmol), the title compound was obtained (41 mg, 39% yield) as a brown oil. TLC: R_f = 0.18 (PE:EA = 1: 1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.86 (d, J = 1.8 Hz, 2H), 8.09 (d, J = 8.4 Hz, 2H), 7.96 (d, J = 2.4 Hz, 2H), 7.76 (dd, J = 8.4, 1.8 Hz, 2H), 7.70 – 7.67 (m, 2H), 7.55 – 7.52 (m, 2H), 4.60 (q, J = 7.2 Hz, 1H), 1.88 (d, J = 7.2 Hz, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 151.5, 147.2, 137.7, 133.6, 129.3, 129.3, 128.1, 127.8, 127.1, 40.5, 21.6. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{20}H_{17}N_2$ 285.1386; found 285.1382.



44

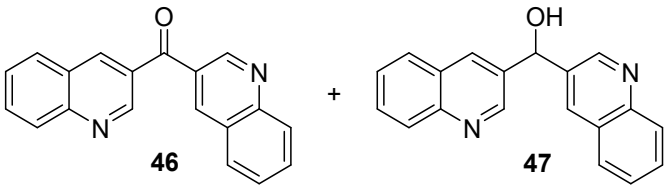
3,3'-(ethane-1,1-diyl)diquinoline (44). Following **GP3**, using allyl bromide (64 μL, 0.74 mmol), the title compound was obtained (107 mg, 93% yield) as a yellow oil. TLC: R_f = 0.33 (PE:EA = 1: 1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.87 (d, J = 2.4 Hz, 2H), 8.08 (d, J = 8.4 Hz, 2H), 8.00 (d, J = 1.8 Hz, 2H), 7.77 (dd, J = 8.4, 1.8 Hz, 2H), 7.70 – 7.67 (m, 2H), 7.55 – 7.52 (m, 2H), 5.82 – 5.76 (m,

1H), 5.11 (dd, J = 16.8, 1.8 Hz, 1H), 5.04 (dd, J = 10.2, 1.2 Hz, 1H), 4.48 (t, J = 7.8 Hz, 1H), 3.06 (t, J = 7.2 Hz, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 151.6, 147.2, 136.0, 135.3, 134.2, 129.4, 129.3, 128.1, 127.8, 127.1, 118.1, 46.5, 39.6. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{19}N_2$ 311.1543; found 311.1539.



45

3,3'-(2-phenylethane-1,1-diyl)diquinoline (45). Following **GP3**, using benzyl bromide (88 µL, 0.74 mmol), the title compound was obtained (48 mg, 36% yield) as a yellow oil. TLC: R_f = 0.33 (PE:EA = 1: 1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.78 (d, J = 2.4 Hz, 2H), 8.07 (dd, J = 8.4, 1.2 Hz, 2H), 7.99 (d, J = 2.4 Hz, 2H), 7.75 (dd, J = 7.8, 1.2 Hz, 2H), 7.69 – 7.66 (m, 2H), 7.54 – 7.51 (m, 2H), 7.20 – 7.18 (m, 2H), 7.16 – 7.14 (m, 1H), 7.08 – 7.07 (m, 2H), 4.69 (t, J = 7.8 Hz, 1H), 3.60 (d, J = 7.8 Hz, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 151.6, 147.2, 138.7, 135.9, 134.2, 129.4, 129.3, 129.2, 128.7, 128.0, 127.8, 127.0, 126.8, 48.6, 41.8. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{26}H_{21}N_2$ 361.1699; found 361.1696.



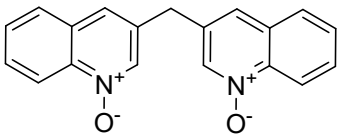
46 **47**

A dry and argon flushed 25 mL flask, equipped with a magnetic stirring bar and a rubber septum is charged with a THF solution of LiHMDS (0.74 mL, 1 M in THF, 0.74 mmol) and cooled to -10 °C, followed by the dropwise addition of hexmethylphosphoramide (129 µL, 0.74 mmol), and stirred for 5 min at the same temperature. Then the reaction mixture is cooled to -78 °C, followed by addition of substrate **1** (100 mg, 0.21 M in THF, 0.37 mmol) and stirred for 1 h. The reaction mixture is

quenched with saturated aqueous $NaHCO_3$ (5 mL), then extracted with ethyl acetate three times and washed with brine one time. The combined organic phases are dried over $MgSO_4$, and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE:EA = 5: 1~EA) furnishes compound **46** (40 mg, 38% yield) as a white solid, and compound **47** (20 mg, 19% yield) as a yellow solid.

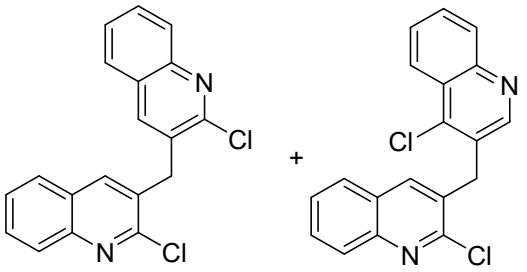
Di(quinolin-3-yl)methanone (46). TLC: R_f = 0.43 (PE:EA = 1: 1). ^1H NMR (600 MHz, $CDCl_3$) δ 9.39 (d, J = 2.4 Hz, 2H), 8.61 (d, J = 2.4 Hz, 2H), 8.22 (d, J = 8.4 Hz, 2H), 7.93 (dd, J = 7.8, 1.2 Hz, 2H), 7.90 – 7.87 (m, 2H), 7.68 – 7.65 (m, 2H). The spectroscopic data are consistent with previously reported.[13]

Di(quinolin-3-yl)methanol (47). TLC: R_f = 0.08 (PE:EA = 1: 1). Melting point: 204.4-205.7 ℃. ^1H NMR (600 MHz, $(CD_3)_2SO$) δ 9.00 (d, J = 1.8 Hz, 2H), 8.40 (d, J = 2.4 Hz, 2H), 8.01 – 7.99 (m, 4H), 7.74 – 7.71 (m, 2H), 7.60 – 7.58 (m, 2H), 6.59 (d, J = 4.2 Hz, 1H), 6.29 (d, J = 4.8 Hz, 1H). ^{13}C $\{^1H\}$ NMR (150 MHz, $(CD_3)_2SO$) δ 150.1, 146.9, 137.4, 132.7, 129.4, 128.7, 128.2, 127.5, 126.9, 70.7. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{15}N_2O$ 287.1179; found 287.1172.



48

3,3'-Methylenebis(quinoline 1-oxide) (48). In a 10 mL sealed tube, compound **1** (100 mg, 0.37 mmol) and DCM (0.3 M) were added, followed by *m*CPBA (181 mg, 0.89 mmol). The mixture was stirred at room temperature for 3 hours. After the reaction was complete, the mixture was concentrated and purified by flash chromatography (PE:EA = 1:1 ~ DCM:MeOH = 10:1) furnishes the desired product as a white solid (67 mg, 60% yield). Melting point: 227.9-228.5 ℃. TLC: R_f = 0.37 (DCM:MeOH = 20:1). ^1H NMR (600 MHz, $CDCl_3$) δ 8.70 (d, J = 8.4 Hz, 2H), 8.53 (s, 2H), 7.80 (d, J = 7.8 Hz, 2H), 7.75 (t, J = 7.8 Hz, 2H), 7.65 (t, J = 7.8 Hz, 2H), 7.59 (s, 2H), 4.17 (s, 2H). ^{13}C $\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 140.6, 136.7, 132.3, 130.6, 130.3, 129.5, 128.1, 125.9, 119.8, 36.5. HRMS (+ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{19}H_{14}N_2O_2Na$ 325.0947; found 325.0945.



49 **50**

In a 25 mL Schlenk flask filled with argon, compound **48** (86 mg, 0.28 mmol) and anhydrous DCM (0.04 M) were added. The mixture was cooled to 0 ℃, and $POCl_3$ (52 mg, 0.34 mmol) was added. Anhydrous DMF (10 mg, 0.14 mmol) was then added dropwise. After stirring for 3 hours at 0 ℃, additional $POCl_3$ (52 mg, 0.34 mmol) and anhydrous DMF (10 mg, 0.14 mmol) were added, and the mixture was stirred for another 2 hours before being allowed to warm to room temperature and stirred overnight. Upon completion of the reaction, the mixture was quenched with saturated aqueous Na_2CO_3 solution and extracted with DCM. The organic layer was subsequently washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure to afford the crude product. Purification by flash column chromatography (PE:EA = 20:1~5:1) yielded **49** (38 mg, 40%) and **50** (22 mg, 23%) as white solids.

bis(2-chloroquinolin-3-yl)methane (49). TLC: R_f = 0.61 (PE:EA = 3:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 8.4 Hz, 2H), 7.85 (s, 2H), 7.75-7.72 (m, 4H), 7.56 (t, J = 8.4 Hz, 2H), 4.51 (s, 2H). The data is consistent with the reported literature.[14]

4-chloro-3-((2-chloroquinolin-3-yl)methyl)quinoline (50). Melting point: 178.5-178.8 ℃. TLC: R_f = 0.35 (PE:EA = 3:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.78 (s, 1H), 8.30 (d, J = 8.4 Hz, 1H), 8.16 (d, J = 8.4 Hz, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.80 (t, J = 7.2 Hz, 1H), 7.69 (t, J = 7.2 Hz, 2H), 7.63-7.62 (m, 2H), 7.49 (t, J = 7.2 Hz, 1H), 4.56 (s, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 152.0, 151.1, 148.3, 146.8, 142.4, 137.8, 130.5, 130.4, 130.3, 129.9, 128.8, 128.4, 128.2, 127.37, 127.36, 127.3, 126.6, 124.4, 34.9. HRMS (+ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{19}H_{13}Cl_2N_2$ 339.0450 ($^{35}Cl^{35}Cl$), 341.0421 ($^{35}Cl^{37}Cl$) or 343.0391 ($^{37}Cl^{37}Cl$); found 339.0446, 341.0416 or 343.0388.

8. X-ray crystallographic analysis

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are summarized in t

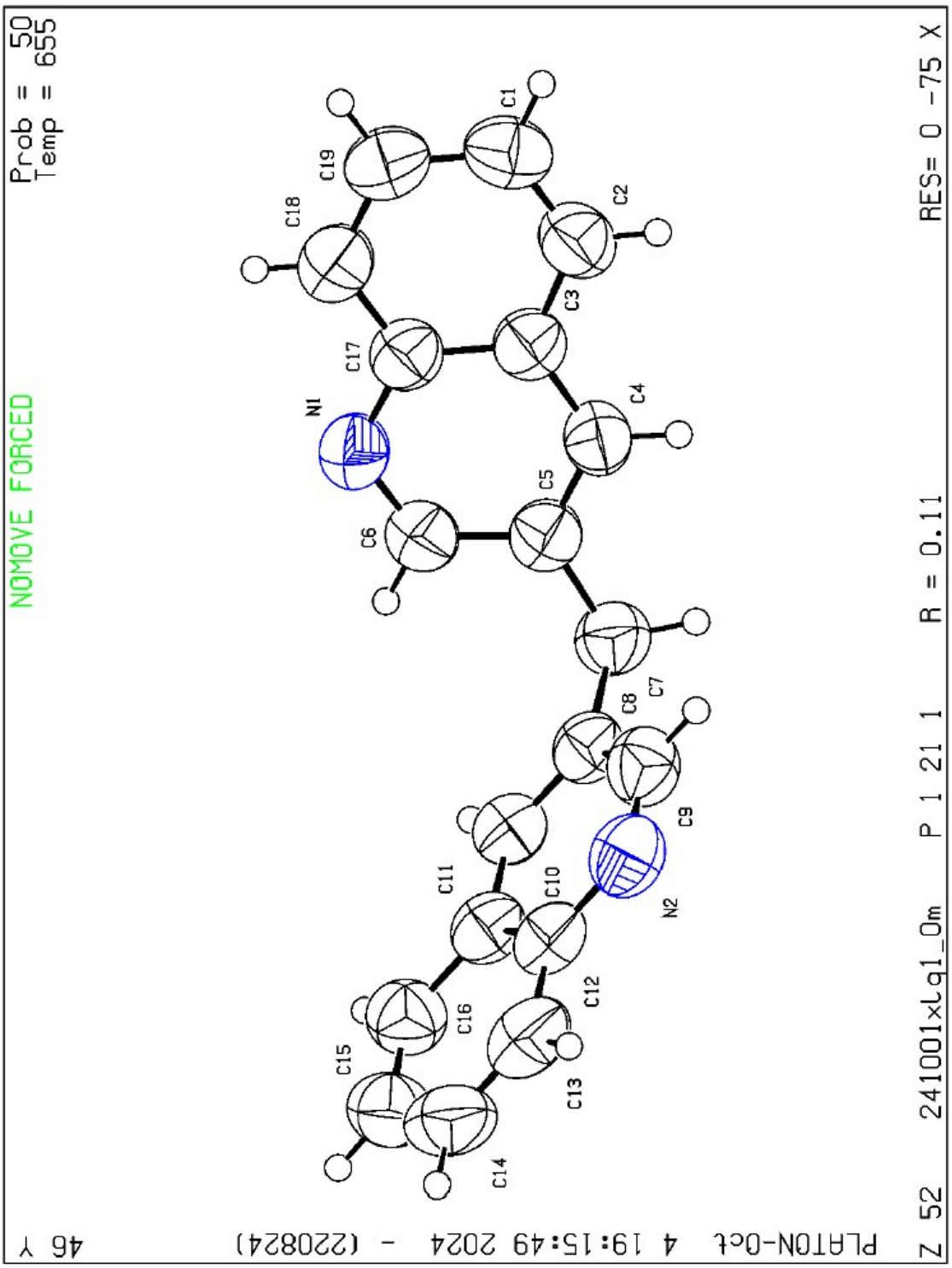


Table S7. Crystal data and structure refinement for **1**.

Crystal data	
Chemical formula	$C_{19}H_{14}N_2$
M_r	270.32
Crystal system, space group	monoclinic, $P2_1$
Temperature (K)	655.00
a, *b*, *c* (Å)	11.1848(4), 4.8073(2), 13.6987(5)
α, β, γ (°)	90, 107.442(2), 90
V (Å^3)	702.69(5)
Z	2
Radiation type	CuKα (λ = 1.54178)
μ (mm^{-1})	0.587
Crystal size (mm)	0.2 × 0.15 × 0.1
Data collection	
Diffractometer	Bruker D8VENTUR
2Θ range for data collection/°	6.764 to 149.864
Index ranges	$-14 \leq h \leq 13$, $-5 \leq k \leq 5$, $-16 \leq l \leq 17$
Reflections collected	8686
Independent reflections	2673 [R_{int} = 0.0404, R_{sigma} = 0.0383]
Refinement	
Data	2673
Restraints	1

Parameters	191

The single cr

and cyclopentan

are summarized

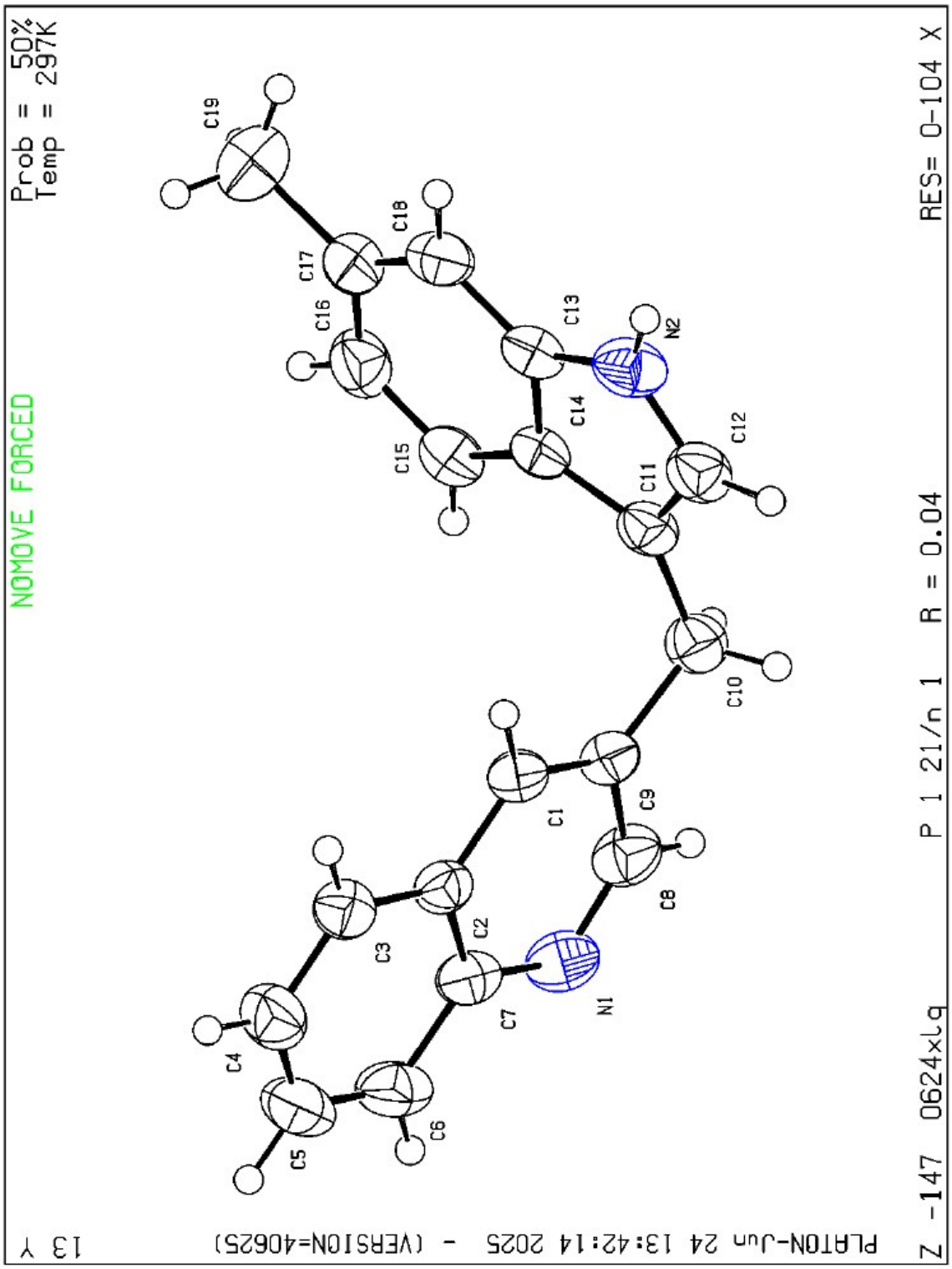


Table S8. Crystal data and structure refinement for **24**.

Crystal data	
Chemical formula	$C_{19}H_{16}N_2$
M_r	272.34
Crystal system, space group	monoclinic, $P2_1/n$
Temperature (K)	297.00
a, *b*, *c* (Å)	14.3089(6), 6.0931(3), 16.8241(9)
α, β, γ (°)	90, 100.837(2), 90
V (Å^3)	1440.66(12)
Z	4
Radiation type	MoKα (λ = 0.71073)
μ (mm^{-1})	0.074
Crystal size (mm)	0.23 × 0.23 × 0.23
Data collection	
Diffractometer	Bruker D8VENTUR
2Θ range for data collection/°	7.422 to 56.58
Index ranges	$-18 \leq h \leq 19$, $-8 \leq k \leq 8$, $-22 \leq l \leq 22$
Reflections collected	44709
Independent reflections	3537 [R_{int} = 0.0635, R_{sigma} = 0.0236]
Refinement	
Data	3537
Restraints	0
Parameters	191

The single crystal of compound **36** (CCDC 2497898) was obtained by vapor diffusion from DCM and cyclopentane. The atoms are depicted with 50% probability ellipsoids. The crystallographic data are summarized in the following table.

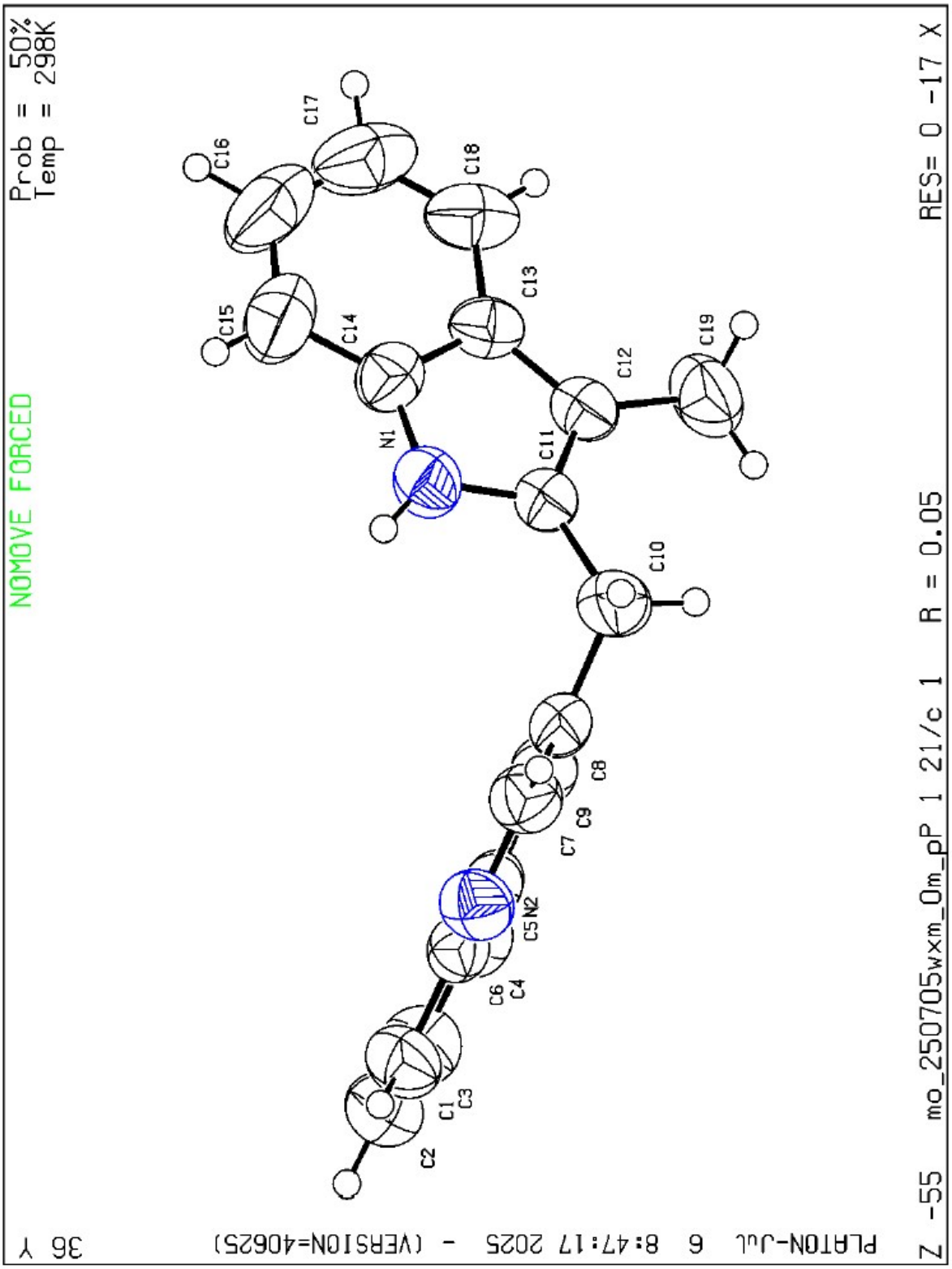

Prob = 50%
Temp = 298K
NOMOVE FORCED
C17
C16
C18
C15
C13
C14
C19
C12
N1
C11
C10
C8
C9
C7
N2
C5
C6
C4
C1
C3
C2
RES= 0 -17 X
Z -55 mo_250705wxm_0m_pP 1 21/c 1 R = 0.05
PLATON-JUL 6 8:47:17 2025 - (VERSION=40625)
36 Y

Table S9. Crystal data and structure refinement for **36**.

Crystal data	
Chemical formula	$C_{19}H_{16}N_2$
M_r	272.34
Crystal system, space group	monoclinic, $P2_1/c$
Temperature (K)	298.15
a, *b*, *c* (Å)	8.4014(4), 11.9943(5), 15.1482(7)
α, β, γ (°)	90, 102.923(3), 90
V (Å^3)	1487.80(12)
Z	4
Radiation type	MoKα (λ = 0.71073)
μ (mm^{-1})	0.072
Crystal size (mm)	0.23 × 0.23 × 0.23
Data collection	
Diffractometer	Bruker D8VENTUR
2Θ range for data collection/°	6.024 to 56.582
Index ranges	-11 ≤ h ≤ 11, -15 ≤ k ≤ 14, -20 ≤ l ≤ 19
Reflections collected	17884
Independent reflections	3684 [R_{int} = 0.0541, R_{sigma} = 0.0392]
Refinement	
Data	3684
Restraints	0
Parameters	191

9. Computational Details

Structure optimizations were carried out with Gaussian 16, Revision A.03 package[15] at the CAM-B3LYP[16] level of theory including Grimme's D3 dispersion corrections with Becke-Johnson damping (D3BJ)[17] with a 6-311G(d, p) basis set. In order to identify each stationary point as either an energy

minimum or a transition state, analytical frequency calculations were carried out at the same level of theory. On the basis of the gas-phase optimized structures, single point energy was calculated at the M06[18] level of theory as implemented in Gaussian 16 with a def2-TZVPP basis set. Solvent effects were considered using self-consistent reaction field with the SMD solvation model.[19] All reported energies are based on gas-phase Gibbs free energies with 6-311G(d, p) basis set for which the electronic energies were corrected to M06 with def2-TZVPP basis set and solvent effects.

10. Reaction Mechanism and Energy Profile

Energy profile is shown in the next page.

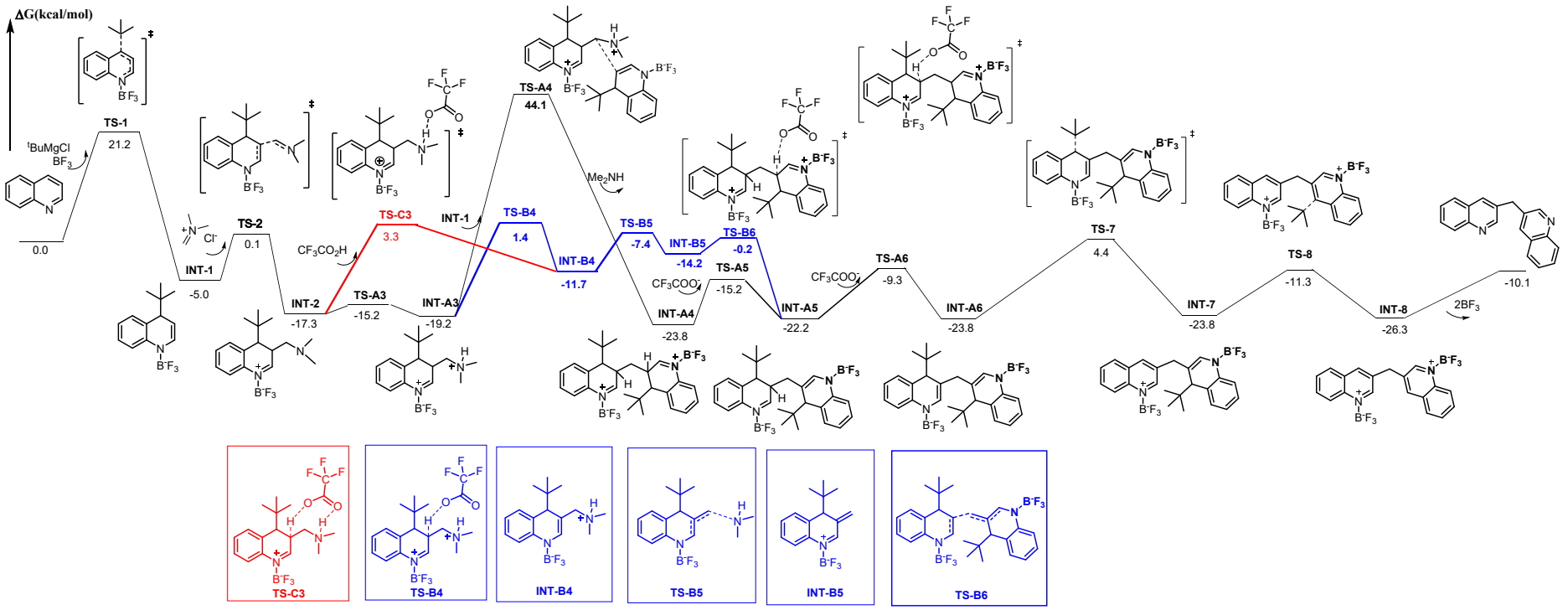
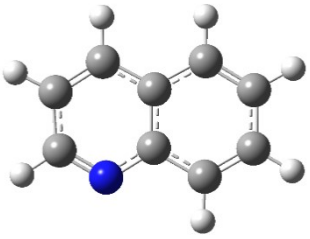


Figure S1 Energy profile of the model reaction. Calculations were performed at the M06-2X-D3/def2tzvpp/SMD (THF)//cam-B3LYP-D3(BJ)/6.311G (d,p)/gas level of theory. The relative Gibbs free energies in THF (DG) are in kcal /mol.

11. Coordinates and geometries of all Stationary Points

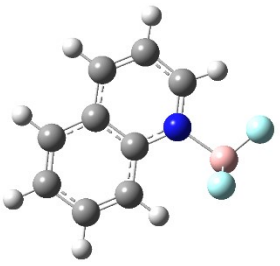
11.1 Standard coordinate and geometry of quinoline:

C	-2.31223800	-0.75963200	-0.00000300
C	-0.02843100	-0.69727400	-0.00000100
C	-0.01435700	0.71977900	0.00000100
C	-1.26092400	1.38532300	0.00000000
C	-2.40905000	0.65046700	-0.00000200
H	1.15915200	-2.47784800	-0.00000200
H	-3.21937900	-1.35828200	-0.00000500
C	1.20131700	-1.39639400	0.00000000
C	1.22687900	1.39907800	0.00000300
H	-1.28672400	2.46945800	0.00000100
H	-3.38350700	1.12181300	-0.00000200
C	2.39844000	0.69805600	0.00000300
C	2.38425800	-0.71470100	0.00000200
H	1.23083200	2.48331600	0.00000400
H	3.34608400	1.22261200	0.00000500
H	3.32231700	-1.25646400	0.00000200
N	-1.18345000	-1.41611700	-0.00000300



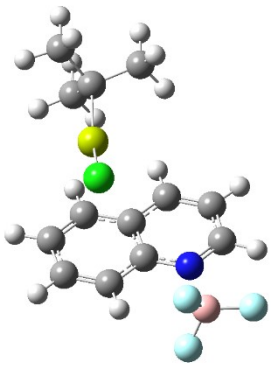
11.2 Standard coordinate and geometry of quinoline-BF_3:

C	0.87750800	1.76693500	-0.00014300
C	-0.52315000	-0.10186600	-0.00005100



C	-1.66347900	0.73612000	-0.00031700
C	-1.47249100	2.13339800	-0.00049400
C	-0.20944200	2.64912300	-0.00040900
H	0.18473100	-2.13815800	0.00032700
H	1.90142100	2.11341200	-0.00006300
C	-0.68715700	-1.50422600	0.00012600
C	-2.95144800	0.15140800	-0.00039700
H	-2.33970700	2.78372000	-0.00069800
H	-0.02662900	3.71438000	-0.00054000
C	-3.09019100	-1.20496300	-0.00022200
C	-1.94725400	-2.03165600	0.00004100
H	-3.81832900	0.80118300	-0.00060100
H	-4.07573300	-1.65306400	-0.00028300
H	-2.07012500	-3.10742800	0.00017700
N	0.72998300	0.45953800	0.00002800
B	2.09349200	-0.48871300	0.00033800
F	2.01887900	-1.24473900	-1.14554200
F	2.01864500	-1.24433100	1.14647300
F	3.14799200	0.39430400	0.00029000

11.3 Standard coordinate and geometry of pre-TS1:

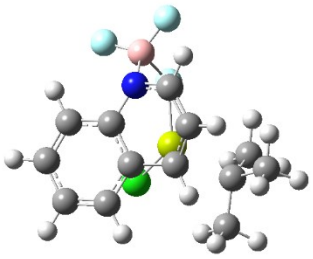


C	1.87779600	-2.02178800	-0.19984400
C	1.34447400	0.07177400	0.67981400
C	0.10848200	-0.42762500	1.15537000
C	0.66471600	-2.57497500	0.23407700
H	2.61257900	1.80373400	0.50046900

H	2.61873800	-2.60323600	-0.73074300
C	1.67880300	1.42826800	0.88704100
C	-0.77013800	0.44860800	1.84783800
H	0.45283100	-3.61467400	0.02845400
C	-0.42383200	1.76047600	2.03274800
C	0.80559000	2.24666000	1.54413300
H	-1.68923800	0.05041000	2.26067500
H	-1.08884000	2.42627500	2.56893600
H	1.05882400	3.28906800	1.68508900
N	2.20402500	-0.76756100	0.01924400
B	3.71606100	-0.24193200	-0.47386200
F	4.33640100	0.15750000	0.68476800
F	3.48670400	0.78777000	-1.34702400
F	4.29540100	-1.34250100	-1.05543000
C	-3.81696000	-0.48037000	-0.22969200
C	-5.00215200	0.29846400	-0.81904900
C	-3.71050200	-1.82192400	-0.96529600
C	-4.11348300	-0.75687400	1.24378400
H	-5.16818600	1.25353800	-0.31038400
H	-4.87571000	0.51215800	-1.88516700
H	-5.93412400	-0.28013000	-0.72066000
H	-2.89791700	-2.44800600	-0.58200500
H	-4.63954700	-2.40265200	-0.85172200
H	-3.54623400	-1.69809800	-2.04023300
H	-5.06255100	-1.30455800	1.35087200
H	-3.34705500	-1.37764900	1.71972100

H	-4.21052700	0.16013200	1.83406900
C	-0.20877100	-1.78544800	0.92158700
H	-1.14922900	-2.18020000	1.28752900
Mg	-2.08756700	0.67206000	-0.62462700
Cl	-0.69189300	1.89384500	-1.81886300

11.4 Standard coordinate and geometry of TS-1:

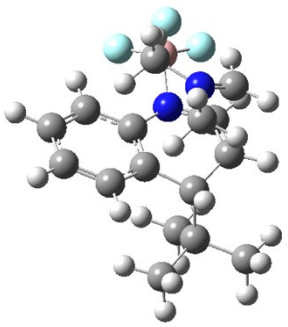


C	-0.79385300	-1.87187400	-1.48639900
C	-1.38616700	0.33766000	-0.88476100
C	-0.15796800	0.80811200	-1.39307800
C	0.36734600	-1.46346400	-2.06565300
H	-3.29796900	0.88533500	-0.08303000
H	-1.10622000	-2.90739500	-1.48788800
C	-2.36927300	1.25460100	-0.49017800
C	0.05397700	2.19295700	-1.52216300
H	0.96477800	-2.16082400	-2.63120200
C	-0.92585900	3.07746000	-1.15193000
C	-2.13386100	2.60215700	-0.62920500
H	1.00305500	2.54382900	-1.90786700
H	-0.75906400	4.14238100	-1.24376700
H	-2.89750200	3.30577500	-0.32356100
N	-1.58699900	-1.04110100	-0.75961100
B	-1.98290000	-1.59328500	0.64167200
F	-3.00781700	-0.93838800	1.23275200
F	-0.70471400	-1.22491700	1.42656300
F	-2.06581500	-2.94597700	0.63289300

C	2.58111100	-0.54131200	-0.00460200
C	2.61218300	-1.04735400	1.45960600
C	3.12698700	-1.65939900	-0.86220300
C	3.40311700	0.72895800	-0.14277900
H	2.33882700	-0.29474000	2.21474300
H	1.99957100	-1.94265700	1.60990000
H	3.64077700	-1.32631900	1.72360000
H	3.22920600	-1.37720400	-1.91292900
H	4.12917700	-1.94522600	-0.51516200
H	2.50335600	-2.55554900	-0.81090100
H	4.44807900	0.54670200	0.14813900
H	3.42561600	1.08728600	-1.17615600
H	3.03463400	1.54537800	0.48345900
C	0.84962900	-0.17147900	-1.74187000
H	1.75076100	0.20032000	-2.20301300
Mg	0.61041600	0.12708700	0.90590500
Cl	0.58425400	2.02843500	2.07147600

11.5 Standard coordinate and geometry of TS-2:

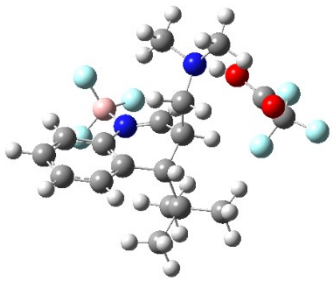
C	-0.36873900	1.24147800	1.14888500
C	-0.41406400	0.16299300	-0.93606000
C	0.82228500	-0.45151600	-0.66140100
H	-2.05637900	0.27125000	-2.30066200
H	-0.91637400	1.86476700	1.84421800
C	-1.12527000	-0.22491400	-2.07666200
C	1.25383100	-1.48701800	-1.48613700



C	0.53502600	-1.88531300	-2.60133100
C	-0.65033100	-1.22903100	-2.90094700
H	2.18996000	-1.98059300	-1.25057800
H	0.90109300	-2.68601200	-3.23189700
H	-1.22264800	-1.50723100	-3.77770000
F	-2.98385200	1.78134000	-1.27934600
F	-3.16696400	0.31406700	0.49167100
F	-2.67978900	2.52103300	0.86610800
B	-2.51060900	1.47028400	-0.02178900
N	-0.96741100	1.10335900	-0.04452700
C	1.67788100	0.00141400	0.50493900
H	2.19318000	-0.87496700	0.91826500
C	2.83085700	0.99101800	0.08919500
C	2.27164700	2.24037800	-0.59393400
H	1.72652200	1.98548400	-1.50436600
H	1.59543200	2.79091200	0.06137300
H	3.08853800	2.91150700	-0.87002700
C	3.80400600	0.29655900	-0.86779900
H	4.64662500	0.95795500	-1.08228400
H	4.20772300	-0.62213800	-0.43114500
H	3.33122300	0.04632700	-1.81726100
C	3.60987900	1.40016900	1.34430800
H	3.96711200	0.52316500	1.89338700
H	4.48304200	1.99476400	1.06699100
H	3.00503900	2.00503400	2.02094200
C	0.77008700	0.59712600	1.54154700

H	1.17562000	0.84531700	2.51332700
C	-0.75760300	-1.11392400	2.34010000
H	-1.63606700	-0.48953500	2.26582400
H	-0.12610200	-1.05895100	3.21246800
C	0.34772400	-3.16400000	1.72020500
H	1.00501800	-2.90162600	2.54636200
H	-0.06735800	-4.15953000	1.88684500
H	0.91566800	-3.16902900	0.78876800
C	-1.71054100	-2.44805000	0.55897200
H	-1.19740300	-2.49221000	-0.40192200
H	-2.20057800	-3.40408700	0.75361000
H	-2.43959800	-1.64200700	0.53250300
N	-0.73556800	-2.19938200	1.61920200

11.6 Standard coordinate and geometry of TS-A3:

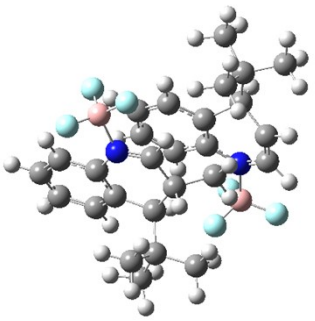


C	0.25354700	-0.57080200	-0.40473300
C	2.53176800	-0.17441500	-0.02398200
C	2.26971000	1.00840000	0.67026600
H	3.97271800	-1.65305000	-0.58623800
H	-0.51271300	-1.10952900	-0.95107600
C	3.80432200	-0.73243900	-0.04927700
C	3.31683600	1.60651900	1.35939800
C	4.59131000	1.06166700	1.33905300
C	4.83376000	-0.10634200	0.63153400
H	3.12661800	2.51240200	1.92188600
H	5.39355300	1.54714700	1.88081900

H	5.82577400	-0.53907900	0.61358600
F	2.71040400	-1.49569500	-2.67151300
F	2.22635900	-3.08300600	-1.07502800
F	0.55866300	-2.26785400	-2.42307400
B	1.76694900	-2.01132500	-1.82385100
N	1.46392400	-0.83814900	-0.70349100
C	0.86774900	1.57693000	0.69559100
H	0.74118700	2.08146700	1.65889100
C	0.57210000	2.66675500	-0.38741500
C	0.55098400	2.09506200	-1.80914200
H	1.48260100	1.58653700	-2.06465300
H	-0.27736600	1.39931500	-1.96256600
H	0.41427900	2.90749700	-2.52564700
C	1.64080300	3.76230900	-0.31538500
H	1.38524400	4.56907500	-1.00489100
H	1.70505300	4.19382700	0.68729500
H	2.62732100	3.38850200	-0.59063700
C	-0.78803000	3.30970200	-0.08208100
H	-0.81269500	3.72165100	0.93033300
H	-0.97212300	4.12999400	-0.77857000
H	-1.62234700	2.61521000	-0.18479100
C	-0.12262400	0.40357300	0.66000600
H	-1.11666500	0.77340200	0.43517900
C	-0.19450600	-0.27202300	2.04603700
H	-0.65460800	0.45192100	2.71619700
H	0.81027300	-0.49081200	2.41837600

C	-1.77346800	-1.59714900	3.34630800
H	-2.46850400	-0.75992300	3.38130400
H	-2.33947500	-2.52814900	3.35207700
H	-1.10513100	-1.57893600	4.21171000
C	-3.35003100	-0.22832100	0.43966000
O	-3.36173500	0.49147100	1.41614900
O	-2.70077600	-1.32504500	0.27838000
H	-1.90938400	-1.44819100	1.16267800
C	-4.07166800	0.22484100	-0.84238200
F	-4.62247900	-0.78433900	-1.51141900
F	-5.01085100	1.12976300	-0.59069900
F	-3.15179900	0.80283100	-1.65124100
N	-1.00847000	-1.51281700	2.08948700
C	-0.20032900	-2.72972600	1.88459300
H	-0.86742000	-3.58675100	1.80196000
H	0.38386200	-2.66314800	0.96972200
H	0.48106200	-2.88093100	2.72656800

11.7 Standard coordinate and geometry of TS-A4:



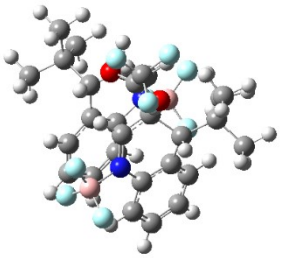
C	-3.32899500	-2.12530200	-2.04993700
H	-3.51871000	-2.90243000	-2.78012300
C	1.84897000	-0.33160000	-1.11165200
C	1.49129300	1.00174500	-0.71423500
C	0.98898900	0.09765000	1.64409800
H	1.21189200	0.88208200	2.35444700
H	1.56241200	-0.80088400	1.79979000

C	0.30784100	1.55275700	-1.25896000
H	-0.00584700	2.54468500	-0.97793800
C	3.52218900	-0.36503300	0.49656800
H	4.16762100	-1.00726600	1.07846600
C	-1.31156500	0.98874100	1.23798500
H	-1.04312900	1.91902900	1.72271300
C	-1.99423100	-1.28865500	-0.20617700
C	-3.84219600	0.01274400	-1.10506700
H	-4.43504200	0.91323500	-1.08201300
C	-2.27062800	-2.25696700	-1.16759600
H	-1.62763900	-3.12175300	-1.23780100
C	-2.76267900	-0.12168700	-0.23542700
C	1.06096400	-1.00961100	-2.07785100
H	1.37486800	-1.98857900	-2.40369100
C	-4.13674300	-0.99935400	-1.99832500
H	-4.97745900	-0.89195000	-2.67153200
C	-0.45290900	0.86213000	-2.15840700
H	-1.36256200	1.31095000	-2.53401300
C	-0.04554800	-0.41270700	-2.60040000
H	-0.63468200	-0.93175600	-3.34446100
N	2.92255200	-0.96064400	-0.55123600
B	3.10964100	-2.56637200	-0.67533900
F	1.93671400	-3.10632200	-0.11777000
F	3.24378000	-2.91012100	-2.00084700
F	4.21385400	-2.89628200	0.07747600
C	2.44624200	3.31370300	0.25655800

C	2.20910000	4.17435300	-0.99520600
H	1.30452700	3.91365800	-1.53921700
H	2.12903700	5.22539000	-0.71028600
H	3.04930100	4.08154600	-1.68788000
C	1.33686500	3.56167700	1.28197200
H	1.49592500	2.98202800	2.19364000
H	1.34107800	4.61471000	1.57122800
H	0.33979400	3.34873200	0.90048300
C	3.77183000	3.79868900	0.86850900
H	3.95179200	3.38662100	1.86254900
H	4.62361300	3.54211400	0.23338400
H	3.75018200	4.88491800	0.97233600
C	-1.19583400	-2.63322200	1.84729000
C	-2.45930300	-2.29278200	2.64279600
H	-3.32613400	-2.19844700	1.98574600
H	-2.67114800	-3.08426800	3.36454400
H	-2.36758700	-1.36223600	3.21026800
C	-1.39355300	-3.99554700	1.17121100
H	-0.54988100	-4.23581800	0.52007400
H	-1.45039900	-4.76970900	1.93908500
H	-2.31692600	-4.04435000	0.59687200
C	0.00304700	-2.80273000	2.79355700
H	0.90399700	-3.05230300	2.22856500
H	0.20543200	-1.92357200	3.40920200
H	-0.19624500	-3.62356800	3.48478500
N	-2.37108800	1.01774200	0.53062300

B	-3.05002900	2.50093000	0.26418200
F	-4.38763500	2.40530900	0.53888200
F	-2.77709300	2.77015400	-1.06512000
F	-2.38366300	3.36920100	1.10848800
C	-0.87422800	-1.50652000	0.78958900
H	-0.00586300	-1.86449400	0.23343200
C	2.62859900	1.82546800	-0.15898200
H	3.35296100	1.88576900	-0.99314300
C	3.25433900	0.92428700	0.85359800
H	3.75182300	1.32285700	1.72658800
C	-0.48229900	-0.19982300	1.50837200
H	-0.71628200	-0.34930700	2.58071400

11.8 Standard coordinate and geometry of TS-A5:



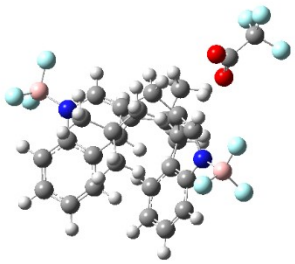
C	-2.66831000	0.38722200	2.95390900
H	-2.60283300	0.24508200	4.02417800
C	-0.31724700	-2.00271200	1.34905300
C	-0.52986800	-2.21803700	-0.02336600
C	0.84960800	0.94512200	-1.28809500
H	1.02013100	0.76210900	-2.34854200
H	1.64603900	1.62453100	-0.97062000
C	-1.68835200	-2.88260800	-0.40489200
H	-1.93953600	-2.99240800	-1.44683200
C	1.12772800	-0.21196900	0.89753000
H	1.66068300	0.63264900	1.32282700
C	-1.62036600	1.15517300	-1.81745500

H	-1.65516100	1.11448200	-2.89851200
C	-1.74460100	1.35008700	0.94211400
C	-3.64721700	-0.15130800	0.83088900
H	-4.35592800	-0.70554800	0.23687300
C	-1.72702100	1.17928800	2.31839700
H	-0.94448500	1.64217700	2.90353400
C	-2.69031400	0.63553200	0.20559500
C	-1.15359200	-2.58172400	2.29691600
H	-0.95233000	-2.42335800	3.34487200
C	-3.64405400	-0.25442700	2.21039400
H	-4.37490600	-0.88760100	2.69716100
C	-2.54604800	-3.43012700	0.53818700
H	-3.43466300	-3.95455600	0.20806400
C	-2.25195500	-3.31665100	1.88645600
H	-2.90199000	-3.76426200	2.62938900
N	0.70493600	-1.11089100	1.76340300
B	1.13932200	-0.98496000	3.29252800
F	0.05959000	-0.48033700	4.03444400
F	1.48484400	-2.24751400	3.74329900
F	2.20325900	-0.09517300	3.33708600
C	0.63445000	-2.17654700	-2.41006700
C	0.54617200	-3.71125200	-2.51347000
H	-0.41703500	-4.11079700	-2.20676000
H	0.72146900	-4.01743900	-3.54824200
H	1.31296100	-4.18017000	-1.89184400
C	-0.47277900	-1.54741200	-3.26589700

H	-0.26412000	-0.49869700	-3.47370600
H	-0.52018700	-2.05244700	-4.23449300
H	-1.46207800	-1.60791800	-2.81688300
C	1.99436700	-1.79970900	-3.01972400
H	2.18067000	-0.72740700	-3.02110400
H	2.81643700	-2.25887400	-2.46849700
H	2.03796500	-2.14701700	-4.05575400
C	-1.26138600	3.78000700	0.26384100
C	-2.49441400	3.98576200	-0.62245800
H	-3.31866200	3.33473100	-0.32458500
H	-2.84149800	5.01892400	-0.54186100
H	-2.28209100	3.80002100	-1.67782500
C	-1.61018600	4.22249200	1.68902100
H	-0.77221800	4.06196600	2.37165200
H	-1.84459400	5.28995400	1.69290600
H	-2.47314900	3.68625500	2.08213900
C	-0.11479600	4.67711100	-0.22319400
H	0.77772400	4.53859000	0.39179900
H	0.16519400	4.48795500	-1.26092700
H	-0.41046200	5.72710600	-0.15820200
N	-2.64095000	0.66845000	-1.22394400
B	-3.88003800	0.10907900	-2.12819600
F	-5.00699900	0.75883400	-1.67615900
F	-3.94231600	-1.26148700	-1.94559200
F	-3.57335400	0.43055700	-3.44013100
C	-0.77738800	2.28690700	0.25699300

H	0.15073200	2.27935900	0.83309500
C	0.62481900	-1.77511300	-0.90805900
H	1.46029300	-2.37046300	-0.51002900
C	1.03843300	-0.34219500	-0.50034800
H	2.42417600	-0.39147700	-0.58836300
C	4.22338100	0.67607300	-0.43596900
O	3.72177400	1.71249700	-0.04894000
O	3.66461500	-0.42424900	-0.76186000
C	5.75561500	0.60897100	-0.61856600
F	6.29081100	-0.43558800	0.02712600
F	6.06628300	0.47500300	-1.92317700
F	6.36481600	1.71234600	-0.17775100
C	-0.45492000	1.78748700	-1.15885400
H	-0.24293300	2.65262300	-1.79198400

11.9 Standard coordinate and geometry of TS-A6:



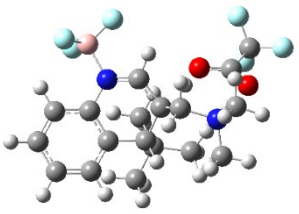
C	4.44495000	-2.06704700	0.46377700
H	4.73309300	-3.07739800	0.73260300
C	-0.70707600	-2.56494600	0.88542000
C	-0.21665600	-1.58997400	1.77060000
C	-0.53192200	1.26519200	-0.44629000
H	-0.65346200	2.22620000	0.05802400
H	-1.07980900	1.35876200	-1.38954000
C	0.87612100	-1.92491100	2.56295000
H	1.32647900	-1.18424400	3.20340600

C	-1.66723400	-0.91930900	-0.46762100
H	-2.07776600	-0.72599700	-1.45260300
C	0.94869100	1.04057200	-0.67841700
C	1.82931800	2.01343800	-0.40389600
H	1.50160800	3.01400100	-0.14978300
C	2.79881300	-0.53545500	-0.44150700
C	4.92985000	0.29292500	0.35615600
H	5.58516400	1.12732700	0.55598000
C	3.19532400	-1.81788600	-0.08000600
H	2.50095300	-2.63512900	-0.23713300
C	3.65052500	0.55281600	-0.16332300
C	-0.17882000	-3.85467700	0.88533800
H	-0.57571800	-4.58436800	0.19719100
C	5.31671300	-0.99877300	0.65492700
H	6.30593200	-1.17109800	1.06879600
C	1.41351400	-3.20250700	2.55640500
H	2.26730300	-3.42690500	3.18470500
C	0.86649700	-4.17401200	1.73385300
H	1.27676600	-5.17785000	1.72096400
N	-1.66048000	-2.19658100	-0.09339400
B	-2.31702200	-3.26715200	-1.04874500
F	-1.31872500	-3.80972700	-1.87558700
F	-2.88889100	-4.27549200	-0.27267500
F	-3.27393100	-2.61463200	-1.81843500
C	-0.67248200	0.78640200	2.85407500
C	-0.85482000	0.16961800	4.25480800

H	-0.13320700	-0.61186600	4.48173600
H	-0.75281300	0.95092000	5.01382000
H	-1.85406900	-0.26447200	4.35258700
C	0.72432500	1.41104800	2.73592200
H	0.78247500	2.09621700	1.89571100
H	0.95012600	1.97939300	3.64389000
H	1.52003100	0.68472900	2.58452600
C	-1.70798200	1.91803000	2.76432300
H	-1.66173600	2.44597800	1.81432200
H	-2.72620700	1.53910600	2.87099100
H	-1.52205100	2.64524800	3.56071300
C	1.62101800	-0.41907500	-2.71762500
C	2.72574200	0.48531300	-3.26830300
H	3.70196200	0.22254500	-2.85845000
H	2.77546900	0.38813700	-4.35847200
H	2.53741600	1.53142500	-3.02467300
C	1.92765900	-1.87765300	-3.07601300
H	1.14304300	-2.54404600	-2.70577100
H	1.98111300	-1.99274200	-4.16379100
H	2.88200900	-2.19904900	-2.65634900
C	0.29935900	-0.03983500	-3.39073800
H	-0.52098800	-0.67017900	-3.04262500
H	0.04317100	1.00339300	-3.20402300
H	0.38128800	-0.17703800	-4.47374700
N	3.19995500	1.84772700	-0.34314700
B	4.12461100	3.08100600	-0.18338800

F	5.21643000	2.96968300	-1.06193200
F	4.62055700	3.17580900	1.13480200
F	3.38054000	4.23388100	-0.47881000
C	1.48689000	-0.28964800	-1.15396500
H	0.79755400	-1.08636600	-0.86192500
C	-1.01022600	-0.29092000	1.78536800
H	-2.01267500	-0.62810800	2.09380900
C	-1.25080200	0.15011600	0.32267400
H	-2.59293100	0.66527800	0.34956300
C	-4.17565000	1.64095500	-0.59333500
O	-3.71697500	1.66262000	-1.71166100
O	-3.69153500	1.16707400	0.49158300
C	-5.56106100	2.28120500	-0.33792700
F	-6.42843300	1.40385100	0.19542900
F	-5.46820300	3.31453800	0.52203200
F	-6.11703100	2.75401600	-1.45962100

11.10 Standard coordinate and geometry of TS-B4:



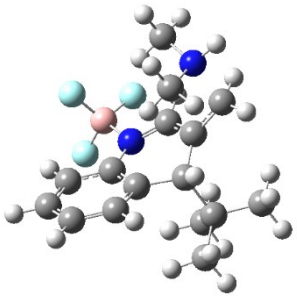
C	0.69034400	0.65923500	-0.99901500
C	2.80488100	0.22650800	-0.11098100
C	2.43278600	-1.08106900	0.20397400
H	4.41483700	1.61708900	-0.34574900
H	0.11553200	1.35263000	-1.60744500
C	4.14760100	0.60044400	-0.10215600

C	3.43197700	-2.02661100	0.41171300
C	4.76917000	-1.66954500	0.39610600
C	5.12010300	-0.34586800	0.16313200
H	3.15012700	-3.05202200	0.62270300
H	5.53326700	-2.41527900	0.57819600
H	6.16201400	-0.05038900	0.16336300
F	2.52967600	3.16074600	0.51239400
F	3.14146100	2.86077000	-1.67784300
F	0.95049200	3.29113700	-1.16374300
B	2.13637600	2.71391100	-0.73365000
N	1.82486300	1.14046200	-0.56883300
C	0.96674400	-1.41585200	0.35390700
H	0.86677900	-2.48595800	0.14255100
C	0.48537900	-1.23468400	1.84117500
C	0.51497400	0.23183400	2.28817600
H	1.50729200	0.66858300	2.17386200
H	-0.19129400	0.85800400	1.74669300
H	0.25113200	0.29115200	3.34686800
C	1.39118900	-2.03259400	2.78784900
H	0.97560900	-2.00769100	3.79781300
H	1.46592300	-3.08167700	2.48629300
H	2.39817400	-1.61995000	2.83105500
C	-0.93041200	-1.80136100	2.00192000
H	-0.92624700	-2.89303100	1.92133000
H	-1.32363600	-1.55661600	2.99052900
H	-1.63606400	-1.40863100	1.27179900

C	0.15882100	-0.61717200	-0.68646900
H	-1.15284600	0.20182900	-0.12240500
C	-0.33386500	-1.30441800	-1.93157100
H	0.40122300	-2.00337900	-2.34729600
H	-0.53879800	-0.55736900	-2.69927000
C	-1.43943300	-3.42625300	-1.16746000
H	-1.04185300	-3.27574400	-0.17127200
H	-2.40503800	-3.92430400	-1.10008000
H	-0.74945100	-4.02818700	-1.75839900
C	-3.15356900	0.37961800	0.03249500
O	-1.97960700	0.84958300	0.20430400
O	-3.46913900	-0.65174000	-0.54091700
H	-2.29647200	-1.55237200	-1.24933400
C	-4.24238400	1.25528400	0.67877000
F	-5.45493400	0.80223500	0.37986900
F	-4.09736200	1.23417700	2.00681100
F	-4.14327300	2.51521700	0.26047600
N	-1.62199300	-2.11360300	-1.82556900
C	-2.25014100	-2.27461000	-3.15759000
H	-3.16587300	-2.85327000	-3.05369300
H	-2.48811700	-1.29147400	-3.55764400
H	-1.55775000	-2.78811500	-3.82403000

11.11 Standard coordinate and geometry of TS-B5:

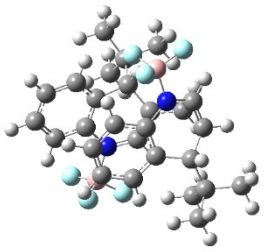
C	-0.42770400	0.94857200	-0.89629100
C	-0.81903300	-0.94083000	0.42400700



C	0.53527500	-1.00741500	0.78217500
H	-2.79308400	-1.67371900	0.80769200
H	-0.88576900	1.74797700	-1.46861000
C	-1.75726300	-1.71837900	1.10558600
C	0.90050700	-1.79138800	1.87340300
C	-0.03183800	-2.54648100	2.56312700
C	-1.36053200	-2.51936200	2.15939500
H	1.94315800	-1.82065600	2.16923500
H	0.27582600	-3.15925200	3.40155300
H	-2.10057700	-3.11445100	2.68036000
F	-3.30240100	-1.08215300	-1.31192800
F	-3.43190400	0.64483400	0.19789100
F	-2.84618800	1.07277100	-1.97731500
B	-2.79715700	0.14840800	-0.93955800
N	-1.25152600	-0.02352900	-0.55892600
C	1.56871300	-0.24497000	-0.01982300
H	2.39300100	0.01538700	0.65386400
C	2.22862500	-1.09511200	-1.16381300
C	1.19706400	-1.57217600	-2.18844700
H	0.42441700	-2.18755100	-1.72534200
H	0.70811300	-0.73555100	-2.68891300
H	1.68879200	-2.17567300	-2.95529800
C	2.93241800	-2.31467200	-0.56169000
H	3.46375600	-2.86209500	-1.34369500
H	3.66701600	-2.01956000	0.19390800
H	2.22411000	-3.00082700	-0.09733300

C	3.27832200	-0.23388400	-1.87223100
H	4.03619300	0.12790600	-1.16958100
H	3.79218900	-0.81875400	-2.63821900
H	2.82353900	0.62710600	-2.36531300
C	0.90996300	1.01491100	-0.53303100
C	1.51820900	2.28045900	-0.53727500
H	1.11132000	3.02124300	-1.22121400
H	2.59872900	2.33206000	-0.43955900
C	1.50412100	2.40024200	2.17914900
H	2.57737000	2.21503300	2.15940300
H	1.23503300	2.89974700	3.11139200
H	0.97465700	1.44875100	2.11691500
C	-0.30212500	3.56450500	1.02859900
H	-0.89139800	2.65108800	0.94275200
H	-0.56982700	4.07231800	1.95649500
H	-0.52761600	4.21008000	0.18087600
H	1.68864600	4.05858700	0.98187100
N	1.12357100	3.21432600	1.01888100

11.12 Standard coordinate and geometry of TS-B6:



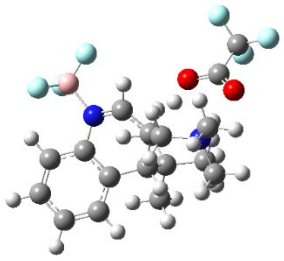
C	3.07054300	1.20125000	-2.28458700
H	3.38193800	1.96126100	-2.99168200
C	-1.51305700	0.93768700	-1.23004100
C	-1.92357600	-0.37469900	-0.92082000
C	-0.72301100	0.14172300	2.34183900
H	-1.17003700	-0.71036100	2.83487800

H	-0.86758300	1.08003500	2.85386600
C	-1.35462900	-1.41520800	-1.64010500
H	-1.56711600	-2.44018400	-1.38459000
C	-2.32748600	1.73094800	0.83228100
H	-2.38494200	2.58050800	1.50071400
C	0.41892100	-0.06680800	1.57683100
C	0.71339100	-1.37550100	1.21186200
H	0.17978100	-2.19520300	1.67013800
C	1.97187200	0.61376900	-0.21048900
C	2.89310400	-1.10684800	-1.64473200
H	3.06447200	-2.15279200	-1.84488000
C	2.37974600	1.56330900	-1.14047900
H	2.11937200	2.59857300	-0.96547100
C	2.18326900	-0.73983300	-0.50094300
C	-0.68237800	1.17356600	-2.31948500
H	-0.39906500	2.18681800	-2.55546100
C	3.34914100	-0.13803100	-2.51893600
H	3.89721400	-0.43726300	-3.40509700
C	-0.47986800	-1.18313800	-2.69325200
H	-0.02351300	-2.02516100	-3.19571400
C	-0.18181900	0.11546600	-3.05779900
H	0.49437800	0.31341200	-3.87952200
N	-1.86929300	2.01713800	-0.38008900
B	-1.43202000	3.50945500	-0.67553200
F	-0.03182100	3.59752100	-0.55503000
F	-1.83064600	3.86293400	-1.95557800

F	-2.03568600	4.31906000	0.28622900
C	-3.52721400	-1.91142500	0.57217600
C	-4.20600300	-2.59209000	-0.62892800
H	-3.52386500	-2.78486000	-1.45282700
H	-4.63834200	-3.54777500	-0.32014500
H	-5.01651700	-1.96600300	-1.01217600
C	-2.47153700	-2.84346000	1.17551200
H	-2.08031200	-2.43626800	2.10807800
H	-2.92875100	-3.80774700	1.41499500
H	-1.62625800	-3.03806000	0.51995100
C	-4.62698400	-1.71705600	1.63004000
H	-4.22451200	-1.37643800	2.58522200
H	-5.37398000	-0.99103200	1.29708700
H	-5.13720900	-2.66632500	1.81263700
C	2.39794900	1.45602600	2.17096200
C	3.34696000	0.29893800	2.48997100
H	3.88877900	-0.02844300	1.60113500
H	4.08235600	0.61051900	3.23751600
H	2.80591400	-0.56074200	2.88965300
C	3.21253500	2.65169400	1.66541300
H	2.55777200	3.47759800	1.37515000
H	3.87911900	3.00661100	2.45678300
H	3.82647900	2.38786500	0.80489900
C	1.69287500	1.89087300	3.45970500
H	0.97465700	2.69265200	3.26476500
H	1.16756500	1.06073800	3.93317600

H	2.42804500	2.26806600	4.17585300
N	1.60494600	-1.74070100	0.31159600
B	1.75828300	-3.28622200	-0.02323100
F	3.10784200	-3.61311600	-0.02675500
F	1.18717100	-3.52802600	-1.27575900
F	1.06598500	-3.99328000	0.96230600
C	1.32551500	1.04049500	1.09206600
H	0.73674400	1.93776900	0.88938500
C	-3.00939200	-0.50741000	0.14419100
H	-3.90192000	-0.06459700	-0.33366700
C	-2.65586400	0.45733800	1.25820000
H	-3.20516900	0.40031200	2.18717600

11.13 Standard coordinate and geometry of TS-C3:

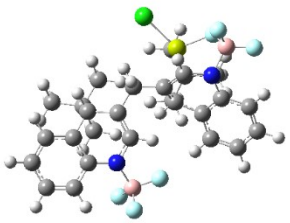


C	0.69032700	0.65923900	-0.99899500
C	2.80488000	0.22652500	-0.11099300
C	2.43279900	-1.08105700	0.20395900
H	4.41482000	1.61712000	-0.34577500
H	0.11550200	1.35263200	-1.60741400
C	4.14759600	0.60047200	-0.10218400
C	3.43200100	-2.02659200	0.41168100
C	4.76919100	-1.66951500	0.39605700
C	5.12011000	-0.34583300	0.16308500
H	3.15016300	-3.05200700	0.62267000
H	5.53329700	-2.41524300	0.57813400
H	6.16201800	-0.05034600	0.16330300

F	2.52966900	3.16075500	0.51240000
F	3.14140800	2.86079700	-1.67785100
F	0.95044700	3.29114500	-1.16370100
B	2.13634500	2.71392500	-0.73363800
N	1.82484700	1.14047300	-0.56882500
C	0.96676300	-1.41585400	0.35390800
H	0.86680400	-2.48596000	0.14255100
C	0.48541400	-1.23469400	1.84118200
C	0.51499800	0.23182400	2.28818800
H	1.50731000	0.66858200	2.17386500
H	-0.19128200	0.85798900	1.74671600
H	0.25116600	0.29113400	3.34688300
C	1.39124300	-2.03259600	2.78784400
H	0.97567400	-2.00770100	3.79781300
H	1.46598700	-3.08167800	2.48628400
H	2.39822300	-1.61994000	2.83104100
C	-0.93037000	-1.80138600	2.00194300
H	-0.92619400	-2.89305500	1.92135000
H	-1.32358500	-1.55664700	2.99055700
H	-1.63603400	-1.40866100	1.27183000
C	0.15882000	-0.61717600	-0.68645400
H	-1.15285800	0.20180700	-0.12236900
C	-0.33386600	-1.30441900	-1.93155700
H	0.40122700	-2.00337000	-2.34729100
H	-0.53881000	-0.55736700	-2.69925100
C	-1.43941300	-3.42626100	-1.16743900

H	-1.04184300	-3.27574100	-0.17124900
H	-2.40501100	-3.92432500	-1.10006400
H	-0.74941800	-4.02818900	-1.75837000
C	-3.15358200	0.37958600	0.03252100
O	-1.97962000	0.84955000	0.20434900
O	-3.46914300	-0.65177000	-0.54089700
H	-2.29647100	-1.55239100	-1.24932300
C	-4.24240200	1.25527400	0.67875600
F	-5.45494600	0.80209600	0.38002700
F	-4.09727200	1.23440100	2.00678700
F	-4.14340900	2.51514500	0.26024000
N	-1.62198600	-2.11361600	-1.82555500
C	-2.25012800	-2.27463700	-3.15757700
H	-3.16585500	-2.85330500	-3.05368100
H	-2.48811200	-1.29150500	-3.55763800
H	-1.55773000	-2.78813800	-3.82401300

11.14 Standard coordinate and geometry of TS-7:



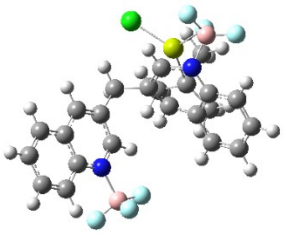
C	-6.29835700	-1.01183700	-1.52914200
H	-7.14958600	-1.59297400	-1.86434900
C	2.93747300	1.65443600	-0.68136300
C	1.80121600	1.64001400	0.14660900
C	-0.20876400	-1.19079100	-1.36365600
H	-0.06665300	-2.19350500	-0.95573600
H	-0.20925600	-1.32952600	-2.45090600
C	1.44883700	2.78690300	0.87509800

H	0.50275900	2.80417500	1.40124200
C	2.09569000	-0.24126400	-1.82364000
H	2.22617900	-0.86982500	-2.69614900
C	-1.52654200	-0.63170200	-0.88066200
C	-1.74413600	0.68543000	-0.76020400
H	-0.95408400	1.41008200	-0.90847300
C	-3.96305100	-0.89928600	-0.89283500
C	-5.33300900	1.09835700	-0.87991800
H	-5.40762800	2.16718800	-0.73470400
C	-5.06703600	-1.61811000	-1.33868600
H	-4.95824100	-2.68403500	-1.51168900
C	-4.08091200	0.49121900	-0.71866400
C	3.79092500	2.76292800	-0.66252000
H	4.68385000	2.75371600	-1.26864700
C	-6.42574300	0.34981300	-1.27121300
H	-7.38493000	0.83927300	-1.40149600
C	2.26899800	3.88983100	0.84536100
H	1.99183100	4.78370000	1.38921900
C	3.45364700	3.85920200	0.10034100
H	4.10347700	4.72636500	0.09242500
N	3.16292400	0.57169400	-1.52718600
B	4.52901800	-0.14413300	-1.60862700
F	5.59802600	0.65237400	-1.35083300
F	4.41074800	-1.12236500	-0.42365700
F	4.62885400	-0.91021300	-2.72969100
C	2.23125900	-0.54088200	2.19339800

C	3.49583100	0.28365600	2.35927100
H	3.36151300	1.31378200	2.03048600
H	3.76788300	0.32509100	3.42441200
H	4.35626100	-0.12483700	1.82331600
C	1.10883500	0.01471900	3.04250200
H	0.17995900	-0.54685200	2.92932700
H	1.39271100	-0.03582000	4.10347500
H	0.90089900	1.06231100	2.82569500
C	2.49071000	-1.99122400	2.65594800
H	1.62739200	-2.64624500	2.52400900
H	3.35627500	-2.48400700	2.18697900
H	2.73218300	-1.97650800	3.72772600
C	-2.63472300	-2.05702000	0.97147900
C	-2.86376800	-0.89727900	1.94396900
H	-3.83464200	-0.42489800	1.79713300
H	-2.81753200	-1.26456500	2.97406500
H	-2.11126600	-0.11725600	1.82784600
C	-3.72653400	-3.10895100	1.19042900
H	-3.60177100	-3.95659500	0.50921800
H	-3.67745800	-3.49256300	2.21360900
H	-4.72087500	-2.69045800	1.03490100
C	-1.28523900	-2.70589700	1.29411500
H	-1.04887500	-3.53173800	0.61867700
H	-0.47249800	-1.98130800	1.23494000
H	-1.29478700	-3.10215400	2.31368100
N	-2.95434600	1.25281500	-0.45287900

B	-3.00333500	2.60957100	0.29943400
F	-3.72501100	2.44639700	1.48656800
F	-3.59520200	3.61217400	-0.47657200
F	-1.66300500	2.96641200	0.60165400
C	-2.65662200	-1.57610700	-0.52998900
H	-2.56418900	-2.49007400	-1.13167600
C	0.99753800	-0.33803300	-1.01741500
C	1.05590500	0.41518300	0.21317700
H	0.18464300	0.38294000	0.84342200
Mg	2.62228000	-1.63973700	0.23292800
Cl	2.19331600	-3.76456700	-0.36168600

11.15 Standard coordinate and geometry of TS-8:

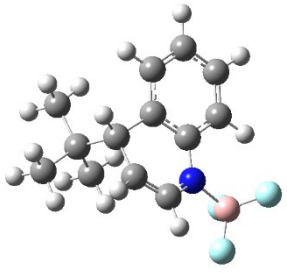


C	1.44100300	3.91681500	-0.83865900
H	1.22257500	4.95580400	-0.62981000
C	-4.35497700	-0.46859200	-0.11285300
C	-3.97408700	-1.80126600	-0.39318300
C	-0.31336200	-1.68356200	0.71805500
H	-0.10944600	-2.70092200	0.38510500
H	-0.14492500	-1.68153300	1.79793900
C	-4.92872700	-2.68652300	-0.94463800
H	-4.63215200	-3.70626000	-1.15834100
C	-2.20757700	-0.01870000	0.67313400
H	-1.56365500	0.73911700	1.09216500
C	0.64491900	-0.72573800	0.05581500
C	1.22188000	-0.99666600	-1.15694300

H	1.16853200	-1.97932800	-1.61004600
C	1.32162200	1.59045100	-0.23421100
C	2.34947400	2.24632900	-2.33457800
H	2.83449300	1.97133800	-3.25843900
C	1.06146300	2.94163100	0.04924400
H	0.53169400	3.19783900	0.95741600
C	1.91553400	1.24286900	-1.46190200
C	-5.67133900	-0.03997800	-0.38202700
H	-5.95145800	0.97803700	-0.16250000
C	2.11031600	3.56383200	-2.01702000
H	2.42051500	4.33787500	-2.70794300
C	-6.19822500	-2.25634400	-1.19911600
H	-6.92883300	-2.93493500	-1.62075700
C	-6.56617900	-0.92521000	-0.91402200
H	-7.57728100	-0.59753300	-1.12020200
N	-3.42784500	0.39178100	0.42104300
B	-3.79202800	1.97678100	0.74199700
F	-4.17051600	2.52223300	-0.45942800
F	-4.80374400	1.95202900	1.66905100
F	-2.62076600	2.52441800	1.23571600
C	2.96445400	0.41711200	2.30242300
C	4.43577500	-0.06477500	2.24552900
H	4.98229600	0.34254900	1.38899700
H	4.95991500	0.28121500	3.14582900
H	4.56669300	-1.15843300	2.26916700
C	2.98223100	1.92186700	2.36155400

H	1.98985500	2.34470600	2.52252400
H	3.60263300	2.25537200	3.20506800
H	3.39711700	2.37187800	1.45691600
C	2.25961100	-0.19005100	3.50411000
H	1.22659900	0.15816600	3.58870400
H	2.24577800	-1.28236800	3.48332800
H	2.76685800	0.10820600	4.43338600
N	2.02531100	-0.10478200	-1.79796800
B	3.37631300	-0.71693700	-2.28099000
F	4.06424700	-0.91216700	-0.91447900
F	4.14662000	0.12950000	-2.99591400
F	3.18950900	-1.95434300	-2.80285300
C	0.99867200	0.52152800	0.66732900
H	0.56369400	0.77362300	1.62214100
C	-2.64818900	-2.20136600	-0.11800800
H	-2.35086500	-3.22054900	-0.34119400
C	-1.75037300	-1.32200000	0.41764100
Mg	3.01021200	-1.17509600	0.71347700
Cl	2.69067600	-3.29446700	1.35984600

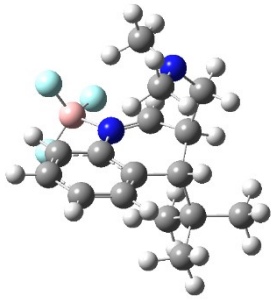
11.16 Standard coordinate and geometry of INT-1:



C	-0.52500000	-1.44410700	-1.08706300
C	-0.57756200	0.73536800	-0.20764400
C	0.77580100	0.91597000	-0.56231300
C	0.76393700	-1.36455800	-1.44081700
H	-2.34616800	1.70944500	0.50532200

H	-1.14963300	-2.27274600	-1.39165000
C	-1.31495500	1.85261900	0.22055600
C	1.29856800	2.20577000	-0.59439500
H	1.18300100	-2.11716300	-2.09623900
C	0.55810300	3.30825100	-0.20301100
C	-0.75028600	3.11139100	0.22865800
H	2.32555100	2.33716300	-0.92033000
H	0.99284400	4.30113600	-0.22692800
H	-1.34831800	3.95618000	0.55453800
N	-1.18319000	-0.50204100	-0.33276400
B	-2.61881300	-0.78850300	0.20035800
F	-3.56456100	0.02035500	-0.45620400
F	-2.66155500	-0.51300600	1.57466000
F	-2.90915200	-2.13842300	-0.03868300
C	2.47819200	-0.78549800	0.36697800
C	1.56167800	-1.15340000	1.53527100
C	3.28318800	-2.01966100	-0.05176400
C	3.45961400	0.29704300	0.82401100
H	0.99395100	-0.28791000	1.88058200
H	0.84498300	-1.92182800	1.24464700
H	2.15328800	-1.53133200	2.37553600
H	3.92655800	-1.79655500	-0.90972600
H	3.92268200	-2.35732400	0.76948100
H	2.62251000	-2.84255700	-0.32748900
H	4.08355900	-0.07918000	1.64079800
H	4.12364800	0.59969900	0.00745300

H	2.93631000	1.18437400	1.18099800
C	1.64462300	-0.28603400	-0.87184900
H	2.39363100	0.01614300	-1.61710700

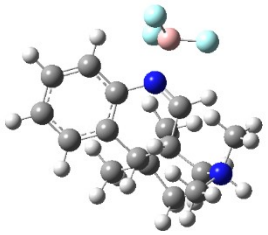


11.17 Standard coordinate and geometry of INT-2:

C	0.47968400	-0.17520500	1.45542600
C	0.48857100	-0.29157900	-0.88675000
C	-0.82997700	0.15310100	-0.97363400
H	2.31196800	-0.72945400	-1.91884500
H	0.99049100	-0.41586000	2.38146700
C	1.28945900	-0.40032800	-2.01856700
C	-1.32149300	0.50144100	-2.22587300
C	-0.53666800	0.39073900	-3.36159200
C	0.76982500	-0.06351300	-3.25576500
H	-2.33393900	0.87718700	-2.30651700
H	-0.94184200	0.66797300	-4.32691400
H	1.39337900	-0.14759000	-4.13661900
F	2.26617500	-2.57854700	-0.22859900
F	3.43598100	-0.61292300	0.01220900
F	2.61414900	-1.69006100	1.86351200
B	2.45169600	-1.44201900	0.51758300
N	1.04884400	-0.59364800	0.39206800
C	-1.67451000	0.27861000	0.27298300
H	-2.35235700	1.12528600	0.12404000
C	-2.59924500	-0.96391800	0.52843500
C	-1.79627100	-2.21983400	0.88391800

H	-1.06415800	-2.46878500	0.11353400
H	-1.26770300	-2.11998500	1.83459500
H	-2.47131600	-3.07248000	0.98347200
C	-3.43727600	-1.26324500	-0.71964800
H	-4.14515400	-2.06523500	-0.50069700
H	-4.01529000	-0.38976900	-1.03324900
H	-2.82055500	-1.58420200	-1.55857900
C	-3.57503700	-0.63998400	1.66776500
H	-4.15677400	0.25850000	1.44447100
H	-4.27727600	-1.46549400	1.80018700
H	-3.07797400	-0.49139100	2.62779600
C	-0.77489200	0.60844000	1.47426900
H	-1.29330500	0.32653500	2.39225600
C	-0.45958000	2.13562300	1.71238400
H	-0.07610400	2.21002400	2.73516000
H	-1.43579900	2.63131500	1.70765200
C	-0.00476500	3.29025800	-0.44366800
H	-1.08118400	3.47414600	-0.43582900
H	0.49104300	4.23075900	-0.70369600
H	0.21094600	2.56883300	-1.24178700
C	1.85328600	2.65374800	0.99995800
H	2.25165200	1.82389900	0.40162300
H	2.38369100	3.56061400	0.69574600
H	2.10218700	2.46433800	2.04638300
N	0.42879800	2.86630400	0.86571700

11.18 Standard coordinate and geometry of INT-A3:

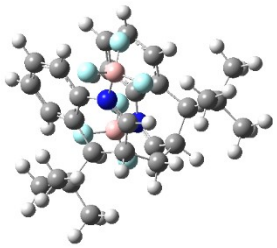


C	0.50987500	0.99254500	-0.26272900
C	-1.40683600	0.07181600	0.69004300
C	-0.81244800	-1.19027400	0.79759800
H	-3.06254900	1.33822100	1.16908500
H	0.94153800	1.75671600	-0.89989100
C	-2.63393700	0.35248600	1.27728100
C	-1.46936700	-2.15951300	1.54167600
C	-2.69023800	-1.88736300	2.14210300
C	-3.27292600	-0.63582800	2.00572100
H	-1.02378400	-3.14042300	1.65116200
H	-3.18730600	-2.65719600	2.71852400
H	-4.22762100	-0.42509900	2.46934900
F	-2.47448800	1.61904200	-1.63254500
F	-2.16124500	3.05886700	0.13759200
F	-0.61516900	2.97469700	-1.55425500
B	-1.59372200	2.30558600	-0.85142000
N	-0.74060000	1.08414600	-0.06043600
C	0.52048000	-1.45791100	0.11775500
H	1.03803900	-2.22109900	0.70619600
C	0.39158600	-2.03753300	-1.33260500
C	-0.19513200	-1.04683000	-2.34394300
H	-1.17452000	-0.66882300	-2.04983700
H	0.45809300	-0.18778000	-2.52205200
H	-0.31755200	-1.54822200	-3.30541600
C	-0.52452100	-3.26872000	-1.27882700

H	-0.55149100	-3.74215500	-2.26106800
H	-0.16154400	-4.01277600	-0.56502800
H	-1.54658100	-3.00544500	-1.01079700
C	1.75997400	-2.51481300	-1.84238600
H	2.26318800	-3.16127700	-1.11723700
H	1.62490700	-3.09961600	-2.75300600
H	2.42743600	-1.69393900	-2.10971900
C	2.76718800	-0.12640600	-0.11769000
H	2.88615600	0.20528200	-1.14854800
H	3.20500700	-1.11787000	-0.02602300
C	3.84914800	0.29691500	2.11682700
H	4.16045400	-0.74506200	2.09067100
H	4.61577400	0.90414100	2.59347500
H	2.91632600	0.39678700	2.66498700
C	3.26039100	2.22662800	0.68679000
H	2.30926000	2.34823900	1.19902400
H	4.02626500	2.80592300	1.19806100
H	3.17564800	2.55515100	-0.34668900
H	4.57351800	0.72882900	0.26700500
N	3.65733600	0.78382100	0.71564700
C	1.30830300	-0.13116600	0.31808500
H	1.27166900	0.00614700	1.40708300

11.19 Standard coordinate and geometry of INT-A4:

C	2.35457700	-2.18960300	-2.16600300
H	3.21202000	-2.16753600	-2.82734500



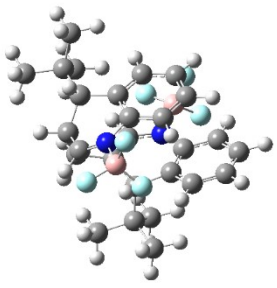
C	0.24919100	1.57398600	-1.26454000
C	-1.09696100	1.43015300	-0.88748500
C	-0.35254700	0.92227100	2.34387900
H	-1.28505500	0.84821000	2.90627600
H	0.40675000	1.19371000	3.08164900
C	-1.89812300	0.62339100	-1.68103900
H	-2.92608400	0.43856200	-1.41851300
C	0.83699600	2.49888700	0.81164000
H	1.60526300	2.96572100	1.41881800
C	-1.11724400	-1.21547500	1.23487800
H	-2.08814200	-1.13866600	1.70560100
C	1.29703300	-1.45075600	-0.11755300
C	0.13040300	-2.91726000	-1.66495400
H	-0.76108500	-3.46430900	-1.92609500
C	2.37172200	-1.44070100	-1.00154200
H	3.22262200	-0.81357200	-0.78564600
C	0.15283600	-2.14999200	-0.50468700
C	0.74724700	0.99924500	-2.42404400
H	1.78254800	1.13967300	-2.69001200
C	1.24433400	-2.95698200	-2.48154600
H	1.22770000	-3.55963400	-3.38077800
C	-1.39776700	0.01560700	-2.82398400
H	-2.04447400	-0.63513300	-3.39644300
C	-0.08677900	0.22491600	-3.21031100
H	0.30305900	-0.24119800	-4.10522400
N	1.14845500	2.28245800	-0.40742700

B	2.68185100	2.68020200	-0.87963300
F	3.37376400	1.47657200	-0.88711700
F	2.58544100	3.25570800	-2.11477500
F	3.15421000	3.53316200	0.09290100
C	-3.04009700	2.30365800	0.73256300
C	-3.86410100	2.89359500	-0.42555900
H	-3.86463900	2.26634800	-1.31381200
H	-4.90164000	3.02323900	-0.11107900
H	-3.47871300	3.87484100	-0.71389400
C	-3.65766200	0.97010000	1.17118900
H	-3.25243100	0.63437700	2.12623200
H	-4.73038900	1.10700400	1.32387300
H	-3.53993000	0.16121300	0.45460200
C	-3.17755700	3.28379200	1.90906900
H	-2.71893000	2.90430500	2.82464700
H	-2.73219400	4.25542300	1.67758600
H	-4.23414700	3.44984200	2.12674300
C	2.34524200	-1.50583500	2.22880900
C	1.82118800	-2.91687800	2.51256400
H	1.76338600	-3.50619500	1.59574700
H	2.49425700	-3.43371600	3.19967600
H	0.83060700	-2.91958400	2.97444400
C	3.77252600	-1.61896500	1.68017300
H	4.16056600	-0.64668700	1.36677600
H	4.42907900	-2.00499900	2.46274500
H	3.83525900	-2.30256600	0.83571400

C	2.44299600	-0.70559000	3.53626000
H	2.82053500	0.30342600	3.34880000
H	1.49481300	-0.62352200	4.07147700
H	3.14236800	-1.19626000	4.21535300
N	-1.05621500	-2.01353900	0.24390500
B	-2.43979300	-2.79707900	-0.20154800
F	-2.14928500	-4.13554800	-0.17166500
F	-2.76302000	-2.33774600	-1.46304700
F	-3.38899200	-2.42464100	0.73381200
C	1.40126000	-0.74401400	1.22221200
H	1.88951300	0.21380200	1.03918400
C	-1.54323300	2.26506500	0.29928500
H	-1.38377600	3.29552400	-0.05344400
C	-0.48236800	2.15282100	1.41184000
H	-0.67836600	2.96729100	2.11297200
C	0.01432900	-0.50476500	1.86956000
H	0.02997600	-1.03856500	2.82887500

11.20 Standard coordinate and geometry of INT-A5:

C	-1.92259100	-2.76812600	-2.08087800
H	-1.77902600	-3.64356800	-2.70353300
C	1.67961300	-0.16402600	-1.20901200
C	1.36404800	1.16966900	-0.90709300
C	0.83720000	0.53871100	2.27362200
H	0.60565100	1.48101000	2.77368500
H	1.13083000	-0.15333300	3.06844500

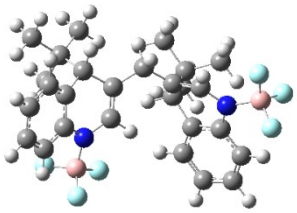


C	0.42075900	1.79525900	-1.70405000
H	0.07460200	2.78933800	-1.47656000
C	2.64087700	-0.51083100	0.90780300
H	3.18434100	-1.18358600	1.56161200
C	-0.38241300	0.05168000	1.54075100
C	-1.27720700	0.95369600	1.10658600
H	-1.21682000	1.98350300	1.41830700
C	-1.34966600	-1.49942900	-0.09583200
C	-2.99491900	-0.65484400	-1.65554400
H	-3.69323300	0.11739200	-1.94013900
C	-1.18152100	-2.60568300	-0.92302700
H	-0.43772300	-3.34481300	-0.65103100
C	-2.22809900	-0.47399400	-0.49433900
C	1.14083300	-0.81160100	-2.30784800
H	1.39261500	-1.84224900	-2.49940000
C	-2.85127800	-1.79194400	-2.42511200
H	-3.45542700	-1.90484100	-3.31921900
C	-0.16160500	1.13821500	-2.78021800
H	-0.95103700	1.63629900	-3.32537600
C	0.22125600	-0.14889000	-3.10274800
H	-0.24353300	-0.67006600	-3.92861000
N	2.49001200	-0.91477300	-0.29632600
B	3.13173400	-2.35825300	-0.71180900
F	2.08303000	-3.25958300	-0.78050000
F	3.76453000	-2.18196000	-1.92012000
F	4.01738500	-2.68833700	0.30290500

C	1.99672900	3.29827400	0.57885200
C	2.47071600	4.09681300	-0.64830800
H	1.83044200	3.95114200	-1.51541400
H	2.48120700	5.16440400	-0.41455700
H	3.48574300	3.80498000	-0.93234600
C	0.60959200	3.80001300	1.00068300
H	0.32109600	3.40996000	1.97570800
H	0.64208700	4.88958100	1.09046500
H	-0.18903300	3.55407500	0.30623200
C	2.96805700	3.63144600	1.72322300
H	2.64997700	3.19353100	2.67125900
H	3.98143500	3.28105300	1.50504200
H	3.01279000	4.71383600	1.86509100
C	-1.38629400	-2.17016700	2.37834700
C	-2.81662500	-1.64954400	2.53156300
H	-3.39732300	-1.81467900	1.62323600
H	-3.31808200	-2.16788800	3.35494000
H	-2.82585000	-0.57973800	2.74301100
C	-1.42941000	-3.67016100	2.07004200
H	-0.42247300	-4.07426700	1.92835800
H	-1.89687700	-4.20990800	2.89924200
H	-2.00473200	-3.87651900	1.16792200
C	-0.65262700	-1.98369400	3.70992100
H	0.38958300	-2.31086900	3.63977300
H	-0.67079400	-0.94074300	4.02938800
H	-1.13502200	-2.57921200	4.49041400

N	-2.28903500	0.71944300	0.21553000
B	-3.11518200	1.94277700	-0.28560900
F	-4.46676300	1.60968700	-0.38766600
F	-2.64405200	2.35847200	-1.55318400
F	-2.93071700	2.99710300	0.62472000
C	-0.61901300	-1.40916600	1.22978100
H	0.33402500	-1.94047800	1.12239000
C	2.13464100	1.78047200	0.25094500
H	3.18084900	1.72205300	-0.08937800
C	2.12817400	0.78422300	1.43019200
H	2.88402600	1.11262900	2.14848500

11.21 Standard coordinate and geometry of INT-A6:



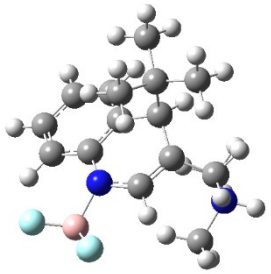
C	-5.49455500	-0.02426700	2.59967100
H	-6.24575700	0.28204400	3.31978000
C	3.35998800	-0.85761700	0.22550900
C	2.44197300	-0.76894000	-0.83954200
C	-0.04834700	1.65857700	0.64554700
H	-0.13302400	2.60783500	0.10510300
H	-0.06076400	1.93901300	1.70790400
C	2.30954400	-1.84025900	-1.71612700
H	1.53032600	-1.79958800	-2.46957600
C	2.17949900	0.83547600	1.34718700
H	2.02498100	1.25940200	2.33160800
C	-1.29904900	0.84721600	0.37245000
C	-1.29947100	-0.44960500	0.03994400

H	-0.38776500	-0.98252800	-0.18888400
C	-3.57650500	0.51286800	1.21562400
C	-4.49553800	-1.72676200	1.21087800
H	-4.43882800	-2.74964700	0.86728700
C	-4.54017700	0.87514900	2.14978800
H	-4.55571600	1.90185000	2.50425600
C	-3.49969400	-0.82859300	0.78813300
C	4.23571000	-1.95358300	0.27175300
H	4.94666000	-2.01072900	1.08308500
C	-5.47469000	-1.32329200	2.09655500
H	-6.22100100	-2.04197900	2.42186800
C	3.14706300	-2.94155700	-1.64152600
H	3.02877600	-3.76695100	-2.33439500
C	4.13124400	-2.97057800	-0.65756000
H	4.80545100	-3.81926500	-0.58955700
N	3.34045000	0.09358300	1.22962200
B	4.51886600	0.30359300	2.20990100
F	4.76600900	-0.84819300	2.98785300
F	5.68527900	0.60022600	1.47761700
F	4.20198400	1.37506700	3.06097200
C	2.43665400	1.56085200	-1.89751100
C	3.78276100	1.96012500	-1.28843300
H	4.45092200	1.10655300	-1.17614300
H	4.27463500	2.69678300	-1.93443600
H	3.65366600	2.40198800	-0.30055800
C	2.67829200	0.96853400	-3.29038500

H	1.73602200	0.66646700	-3.75810100
H	3.15580900	1.71161200	-3.93822800
H	3.32455600	0.09175100	-3.24194100
C	1.58581600	2.82268500	-2.06157900
H	0.60394100	2.58575500	-2.47927100
H	1.44003800	3.32556800	-1.10526000
H	2.07968600	3.52638500	-2.74038800
C	-3.26413400	2.16730500	-0.70997800
C	-3.55223500	1.12419400	-1.79267000
H	-4.26251700	0.36817000	-1.45896900
H	-3.96902100	1.61841600	-2.67765500
H	-2.64234100	0.60244900	-2.08797400
C	-4.57043200	2.88534100	-0.35313800
H	-4.40729600	3.63912800	0.42486100
H	-4.97037600	3.39513400	-1.23584800
H	-5.32513400	2.18599700	0.00718800
C	-2.29663000	3.20405400	-1.28530900
H	-2.03032700	3.96187400	-0.54187600
H	-1.37938600	2.73124700	-1.63114300
H	-2.75465600	3.71403900	-2.13941200
N	-2.44017600	-1.24236600	0.01501200
B	-2.51447200	-2.49840800	-0.89027700
F	-3.62995600	-2.37329000	-1.74589500
F	-2.67391000	-3.67741800	-0.13212200
F	-1.33656200	-2.56990600	-1.64254200
C	-2.64211400	1.52034400	0.58650700

H	-2.51106700	2.35485700	1.29039600
C	1.28263200	1.00902100	0.36495900
C	1.65770200	0.51171100	-1.01673600
H	0.74818300	0.28316500	-1.58129600

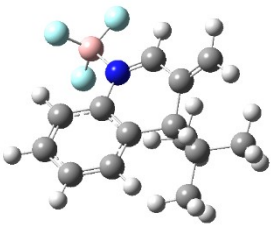
11.22 Standard coordinate and geometry of INT-B4:



C	0.56445200	-0.85553900	-0.87394500
C	0.56235400	1.22461800	0.18534800
C	-0.73934000	0.99000300	0.66546900
H	2.27266500	2.50382600	0.30277900
H	1.19134800	-1.59761500	-1.35453900
C	1.28734800	2.30790300	0.69549500
C	-1.23056000	1.78176000	1.70215500
C	-0.49824800	2.83275900	2.22267500
C	0.75827200	3.10151400	1.69408100
H	-2.22215300	1.57372000	2.08919000
H	-0.90561200	3.44298800	3.01938600
H	1.34327300	3.93009900	2.07505800
F	3.28249500	1.49358200	-1.19265700
F	3.23449500	-0.29706000	0.26154400
F	2.96264200	-0.63204200	-1.98790000
B	2.72994700	0.25392100	-0.93716800
N	1.15573700	0.34346100	-0.73767300
C	-1.59429200	-0.10506700	0.06180900
H	-2.26435700	-0.47891200	0.84670600
C	-2.55029100	0.38673600	-1.08110000

C	-1.77142700	1.02968400	-2.22971900
H	-1.21116100	1.90189200	-1.89010200
H	-1.06592500	0.32964100	-2.67819100
H	-2.46245200	1.35755000	-3.01047500
C	-3.54681600	1.40575400	-0.52217100
H	-4.26016300	1.69662900	-1.29708200
H	-4.11698000	0.98968200	0.31447100
H	-3.04470000	2.30891500	-0.17512700
C	-3.33366300	-0.81629700	-1.61497400
H	-3.90030500	-1.30838200	-0.81704900
H	-4.04912300	-0.49735100	-2.37614600
H	-2.66930400	-1.55072100	-2.07518000
C	-0.65789200	-1.19840800	-0.38809200
C	-0.89661300	-2.61771500	-0.14365200
H	-0.45686600	-3.27167800	-0.89886800
H	-1.94331500	-2.88421000	0.00864500
C	-0.65298400	-2.30735100	2.36741000
H	-1.73621600	-2.37407800	2.44644400
H	-0.18430600	-2.69457400	3.27014000
H	-0.35625000	-1.27251500	2.20486000
C	1.28941000	-3.11098200	1.11045200
H	1.65997300	-2.09391200	0.99050900
H	1.68811300	-3.54469700	2.02603500
H	1.59189500	-3.70690800	0.25199200
H	-0.50185300	-4.06981500	1.33794700
N	-0.19872300	-3.10570800	1.20026000

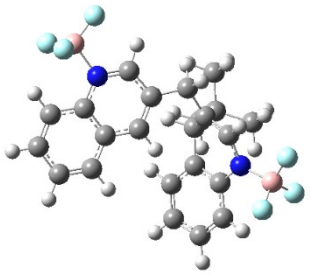
11.23 Standard coordinate and geometry of INT-B5:



C	-0.42729500	-1.45375400	-0.79534800
C	-0.69206300	0.82102700	-0.28536500
C	0.65855600	1.08906400	-0.51664100
H	-2.64705300	1.61407800	0.06839300
H	-0.87207600	-2.44113300	-0.84300500
C	-1.60739900	1.85063700	-0.09769400
C	1.05890800	2.41557400	-0.60783300
C	0.15320000	3.44935100	-0.43049000
C	-1.17758000	3.16412300	-0.16384500
H	2.09778300	2.63885100	-0.81724700
H	0.48712900	4.47696100	-0.50317400
H	-1.89084800	3.96583800	-0.02158000
F	-2.53134100	-0.46834200	1.66347200
F	-3.59333300	-0.31106600	-0.36783000
F	-2.67772900	-2.30699000	0.28847400
B	-2.61480600	-0.93268700	0.37328300
N	-1.16022100	-0.52736800	-0.30006300
C	1.64568500	-0.04801600	-0.65441800
H	2.44007100	0.26625900	-1.33578100
C	2.35892400	-0.42299500	0.70242400
C	1.37846600	-0.98327500	1.73777300
H	0.54960300	-0.30199500	1.93694000
H	0.96182600	-1.94500700	1.43157300
H	1.90156200	-1.14768300	2.68201300

C	3.03466800	0.82150300	1.28592000
H	3.61563100	0.54053800	2.16663500
H	3.72187300	1.27868900	0.56877100
H	2.30882000	1.57420400	1.59263100
C	3.44362400	-1.46601000	0.41837100
H	4.17304300	-1.09325800	-0.30638400
H	3.98127300	-1.69982500	1.33941200
H	3.02731200	-2.39843200	0.03559000
C	0.93272800	-1.22868900	-1.25916700
C	1.44652800	-2.06757100	-2.15636500
H	0.88464500	-2.92461900	-2.50925500
H	2.43491600	-1.91668200	-2.57249900

11.24 Standard coordinate and geometry of INT-7:



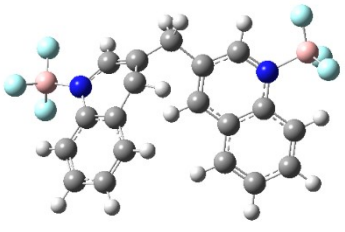
C	-2.65863500	-2.37682300	2.41226800
H	-2.51844100	-3.00380500	3.28510900
C	3.64628200	-0.85008000	-0.10402500
C	2.34496400	-1.39332900	-0.03799700
C	0.26439600	1.72408500	-0.83400000
H	0.24943500	1.94994800	-1.90575300
H	0.49476600	2.66661200	-0.32555700
C	2.18274500	-2.76371200	0.27491100
H	1.17710700	-3.16261700	0.33150100
C	2.73858800	1.24308200	-0.60266200
H	2.95784600	2.28216800	-0.81026400
C	-1.06428000	1.16435100	-0.42664300

C	-1.93811400	0.71913300	-1.34671300
H	-1.81482600	0.94302100	-2.39955400
C	-2.09408900	-0.38552500	1.15092800
C	-3.75454000	-1.93215000	0.30994600
H	-4.44132300	-2.22141500	-0.47114500
C	-1.91943300	-1.21709800	2.25423600
H	-1.20233200	-0.92484100	3.01483900
C	-2.97749000	-0.77730300	0.12659000
C	4.76473500	-1.67895500	0.13229700
H	5.75578600	-1.25832900	0.07712000
C	-3.59694800	-2.71035100	1.43872900
H	-4.19910000	-3.60558800	1.55057300
C	3.27362900	-3.55040500	0.50239400
H	3.14899900	-4.59925500	0.74186300
C	4.56972000	-2.99902300	0.42703400
H	5.42918300	-3.63314900	0.60797500
N	3.79708900	0.48502400	-0.39201900
B	5.28304900	1.16797200	-0.46658400
F	5.85969900	0.99078400	0.77578400
F	5.97361500	0.50136300	-1.45946700
F	5.08179300	2.49990000	-0.76815200
C	-2.17465800	2.12652600	1.69602600
C	-3.56762500	2.28924100	1.08344100
H	-4.17641100	1.39535600	1.22251500
H	-4.08491000	3.12919300	1.55747900
H	-3.51019100	2.48415400	0.01262500

C	-2.31689700	1.87208500	3.19956300
H	-1.33851700	1.74963100	3.67544000
H	-2.81841500	2.71778600	3.67883900
H	-2.90484200	0.97547300	3.39784200
C	-1.39509100	3.43001500	1.49800500
H	-0.37702800	3.35070600	1.89259200
H	-1.33808300	3.69544600	0.44120900
H	-1.89246000	4.25151300	2.02123700
N	-3.01919700	-0.07279900	-1.06533100
B	-4.11181000	-0.32564700	-2.15220700
F	-5.37072600	-0.12739100	-1.57622100
F	-4.02502300	-1.64163100	-2.63709700
F	-3.88698600	0.58076400	-3.19412900
C	-1.37992600	0.94260400	1.03585700
H	-0.44200300	0.87433900	1.60424300
C	1.23886500	-0.55320100	-0.28040400
H	0.23512500	-0.96073900	-0.23045300
C	1.41678000	0.77234700	-0.56666900

11.25 Standard coordinate and geometry of INT-8:

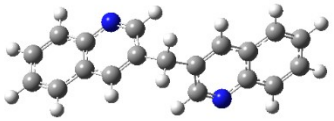
C	-2.65863500	-2.37682300	2.41226800
H	-2.51844100	-3.00380500	3.28510900
C	3.64628200	-0.85008000	-0.10402500
C	2.34496400	-1.39332900	-0.03799700
C	0.26439600	1.72408500	-0.83400000
H	0.24943500	1.94994800	-1.90575300



H	0.49476600	2.66661200	-0.32555700
C	2.18274500	-2.76371200	0.27491100
H	1.17710700	-3.16261700	0.33150100
C	2.73858800	1.24308200	-0.60266200
H	2.95784600	2.28216800	-0.81026400
C	-1.06428000	1.16435100	-0.42664300
C	-1.93811400	0.71913300	-1.34671300
H	-1.81482600	0.94302100	-2.39955400
C	-2.09408900	-0.38552500	1.15092800
C	-3.75454000	-1.93215000	0.30994600
H	-4.44132300	-2.22141500	-0.47114500
C	-1.91943300	-1.21709800	2.25423600
H	-1.20233200	-0.92484100	3.01483900
C	-2.97749000	-0.77730300	0.12659000
C	4.76473500	-1.67895500	0.13229700
H	5.75578600	-1.25832900	0.07712000
C	-3.59694800	-2.71035100	1.43872900
H	-4.19910000	-3.60558800	1.55057300
C	3.27362900	-3.55040500	0.50239400
H	3.14899900	-4.59925500	0.74186300
C	4.56972000	-2.99902300	0.42703400
H	5.42918300	-3.63314900	0.60797500
N	3.79708900	0.48502400	-0.39201900
B	5.28304900	1.16797200	-0.46658400
F	5.85969900	0.99078400	0.77578400
F	5.97361500	0.50136300	-1.45946700

F	5.08179300	2.49990000	-0.76815200
N	-3.01919700	-0.07279900	-1.06533100
B	-4.11181000	-0.32564700	-2.15220700
F	-5.37072600	-0.12739100	-1.57622100
F	-4.02502300	-1.64163100	-2.63709700
F	-3.88698600	0.58076400	-3.19412900
C	-1.37992600	0.94260400	1.03585700
H	-0.44200300	0.87433900	1.60424300
C	1.23886500	-0.55320100	-0.28040400
H	0.23512500	-0.96073900	-0.23045300
C	1.41678000	0.77234700	-0.56666900

11.26 Standard coordinate and geometry of product:



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H	-6.52309900	-1.54066900	-0.49750200
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C	3.44191600	0.37450500	0.33009000
C	0.00000000	-0.00000100	1.93522900
H	0.15604500	0.86222800	2.58915000
H	-0.15604500	-0.86223100	2.58914900
C	4.58738100	1.20320000	0.31653600
H	4.60951200	2.07920400	0.95504100
C	1.31452300	-1.32855900	0.22434800
H	0.46791000	-2.00956100	0.16860500

C	2.31158200	0.62849500	1.14095500
H	2.30993800	1.49684200	1.79250100
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H	-2.30993800	-1.49684300	1.79250000
C	1.23901400	-0.21321100	1.10106800
C	-1.23901400	0.21321000	1.10106800
C	-1.31452300	1.32855900	0.22435000
H	-0.46791000	2.00956000	0.16860700
C	-3.44191600	-0.37450500	0.33009000
C	-4.51828900	1.05732100	-1.32608800
H	-4.46105000	1.93898300	-1.95116500
C	-4.58738100	-1.20320100	0.31653500
H	-4.60951200	-2.07920400	0.95503900
C	-3.40716400	0.76957800	-0.50198400
C	4.51828900	-1.05732000	-1.32608900
H	4.46105000	-1.93898200	-1.95116600
C	-5.61266300	0.23951800	-1.31974500
H	-6.46157700	0.46397000	-1.95398000
C	5.64805000	0.90235100	-0.49033600
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C	5.61266300	-0.23951700	-1.31974500
H	6.46157700	-0.46396800	-1.95398100

12. Table of the computed energies (hartree)

Reaction species	Structure	△△G(298.15K)	Electronic Energy	Total Gibbs Free Energy	△G (kcal/mol)
reaction species	**quinoline**	0.105923	-401.9182447	-401.8123217	
$CH_2=N(CH_3)_2$	**BF_3**	-0.011987	-324.6104202	-324.6224072	
	quin-BF_3	0.115496	-726.5774921	-726.4619961	-17.1
	HCl	-0.011097	-460.8038346	-460.8149316	
	MgClR	0.087651	-818.1701262	-818.0824752	
	MgCl	-0.020865	-660.2001552	-660.2210202	
	$MgCl_2$	-0.023363	-1120.644091	-1120.667454	
	NitroCl	0.08263	-634.0709273	-633.9882973	
	Nitro	0.083928	-173.6841897	-173.6002617	
	HB	0.008423	-526.8588662	-526.8504432	
	B	-0.005238	-526.3974843	-526.4027223	
	Me_2NH	0.067461	-135.1490937	-135.0816327	
	pre-TS1	0.220743	-1544.752604	-1544.531861	
add of ^{t}Bu	**TS-1**	0.227997	-1544.72606	-1544.498063	21.2
	pro-TS1	0.230282	-1544.809227	-1544.578945	
	INT-1	0.230552	-884.5347455	-884.3041935	-5.0
	pre-TS2	0.337676	-1058.241266	-1057.90359	
C=N	**TS-2**	0.339637	-1058.235121	-1057.895484	5.1
	INT-2	0.340298	-1058.263529	-1057.923231	-17.4
PATH A	**TS-A3**	0.367827	-1585.154759	-1584.786932	-2.1
	INT-A3	0.35723	-1058.709664	-1058.352434	-4.0
	TS-A'4	0.607648	-1943.163456	-1942.555808	63.3

	INT-A4	0.525522	-1808.107904	-1807.582382	-67.9
	TS-A5	0.534263	-2334.503568	-2333.969305	8.6
	INT-A5	0.537344	-2334.517853	-2333.980509	-7.0
	TS-A6	0.515248	-2334.026655	-2333.511407	12.9
	INT-6A	0.490763	-1807.179635	-1806.688872	
	TS-7	0.490932	-2467.387977	-2466.897045	28.2
	INT-7	0.37443	-1649.234036	-1648.859606	-12.5
	TS-8	0.370107	-2309.42758	-2309.057473	12.5
	INT-8	0.256522	-1491.277359	-1491.020837	
	product	0.237772	-841.9603203	-841.7225483	-10.1
PATH B	**TS-B4**	0.368961	-1585.119993	-1584.751032	20.6
	INT-B4	0.342765	-1058.264289	-1057.921524	-13.1
	TS-B5	0.339187	-1058.253791	-1057.914604	4.3
	INT-B5	0.248815	-923.0926139	-922.8437989	-6.8
	TS-B6	0.506954	-1807.613379	-1807.106425	14.0
PATH C	**TS-2C**	0.368961	-1585.119993	-1584.751032	20.6

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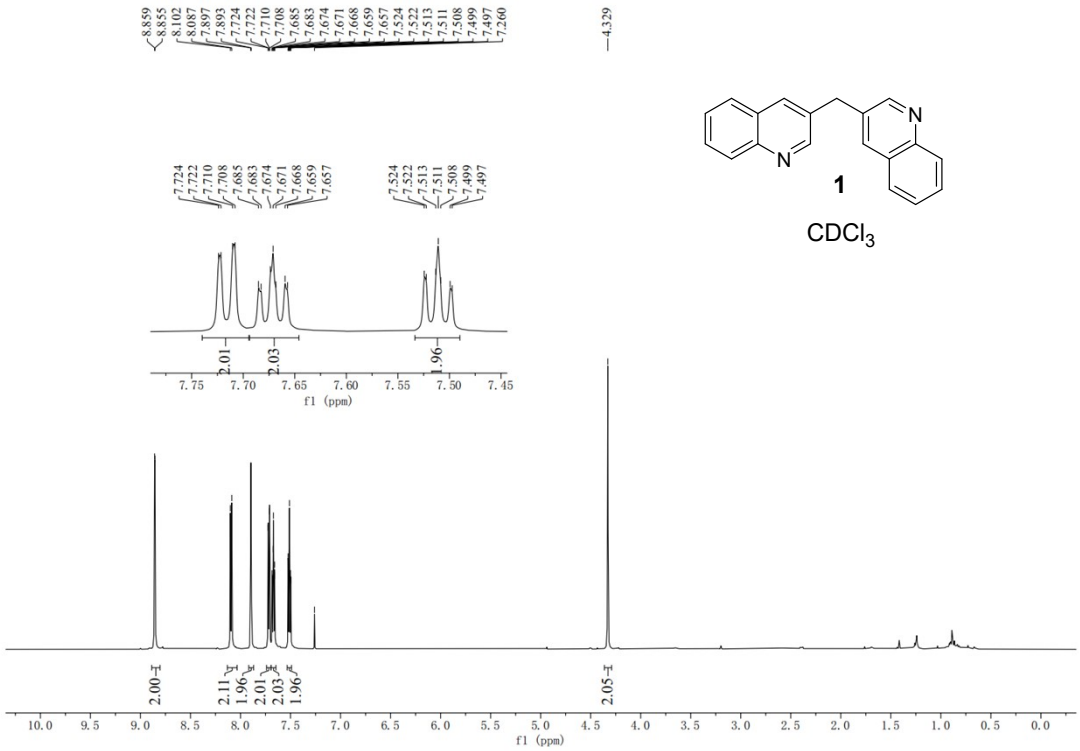
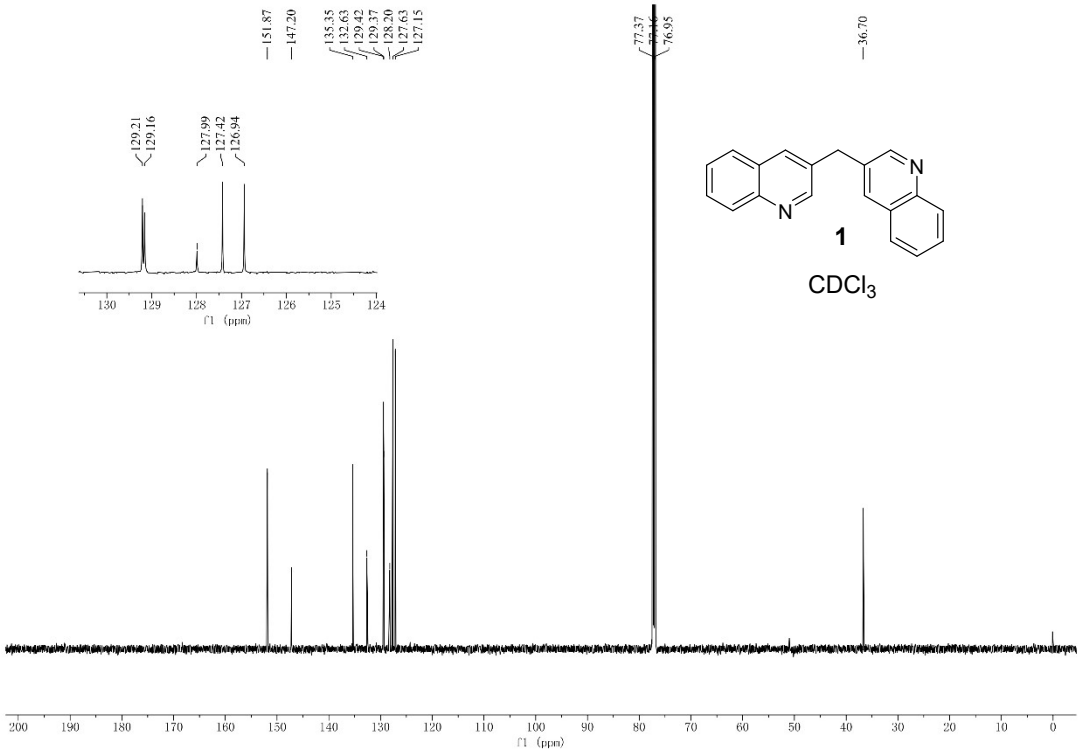
14. Spectra Data

Spectra data are shown from the next page.

^{1}H NMR (600 MHz, $CDCl_3$):



^{13}C NMR (150 MHz, $CDCl_3$):



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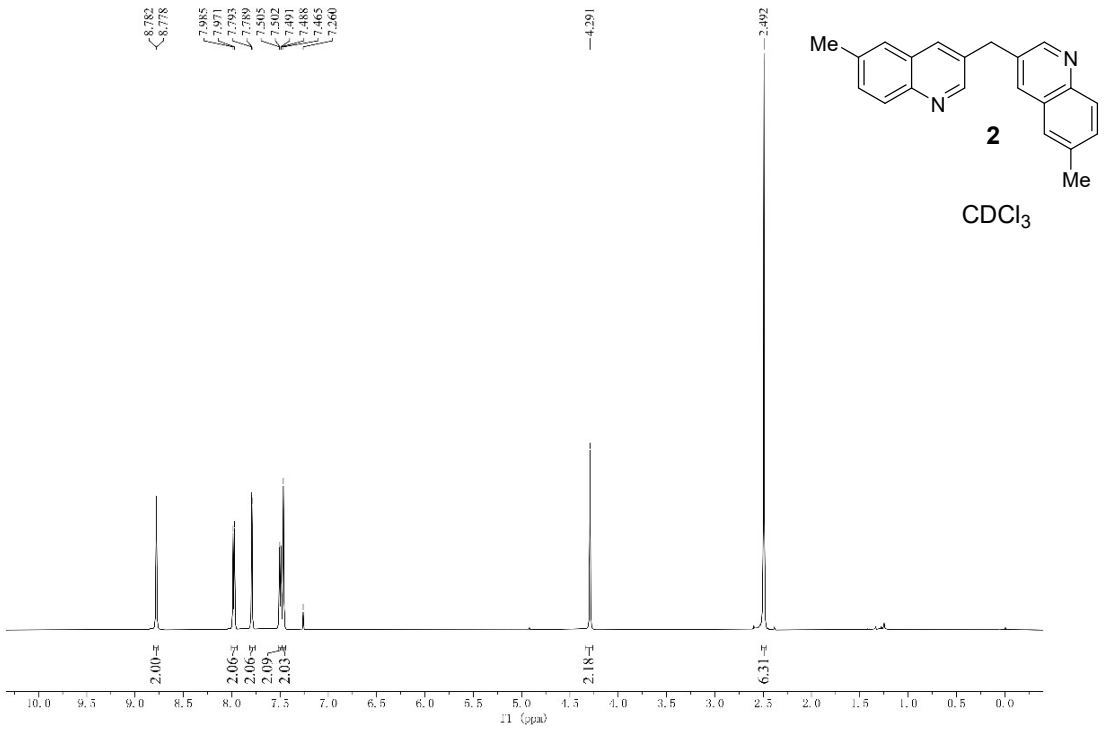

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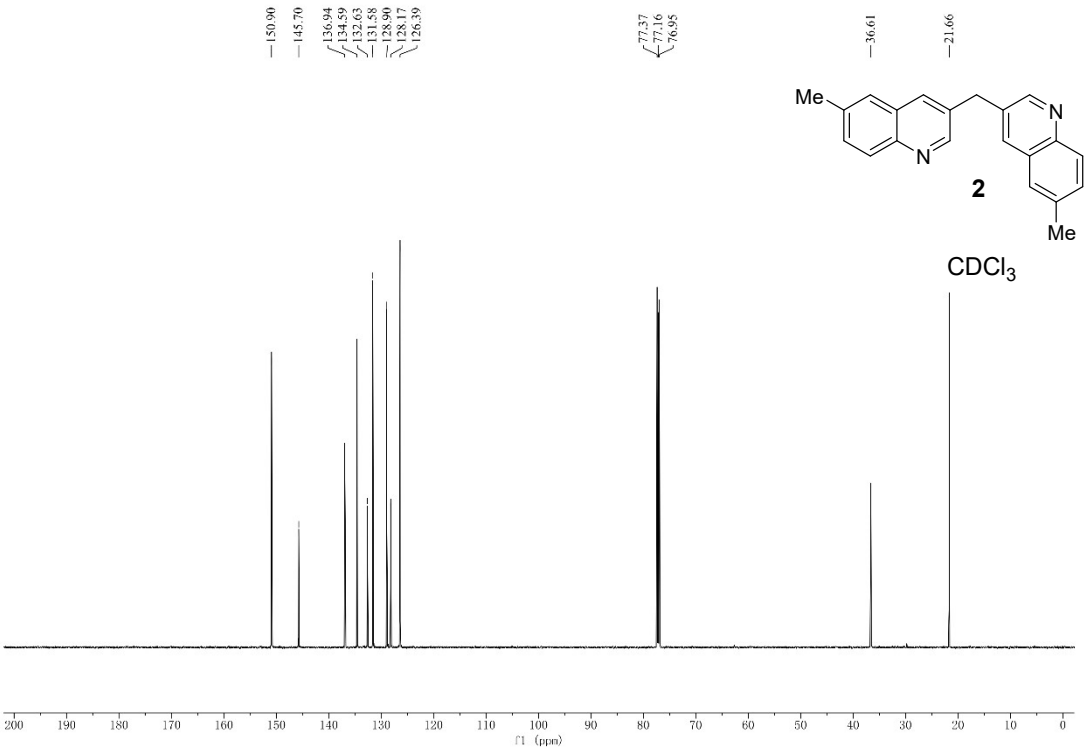

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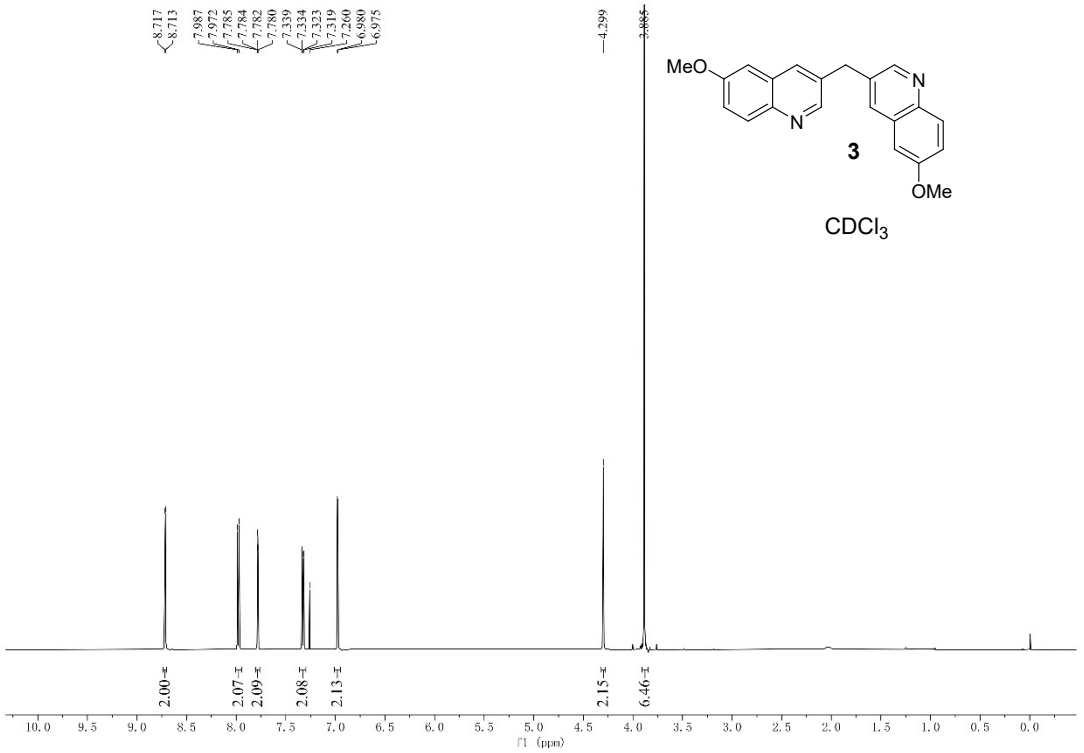

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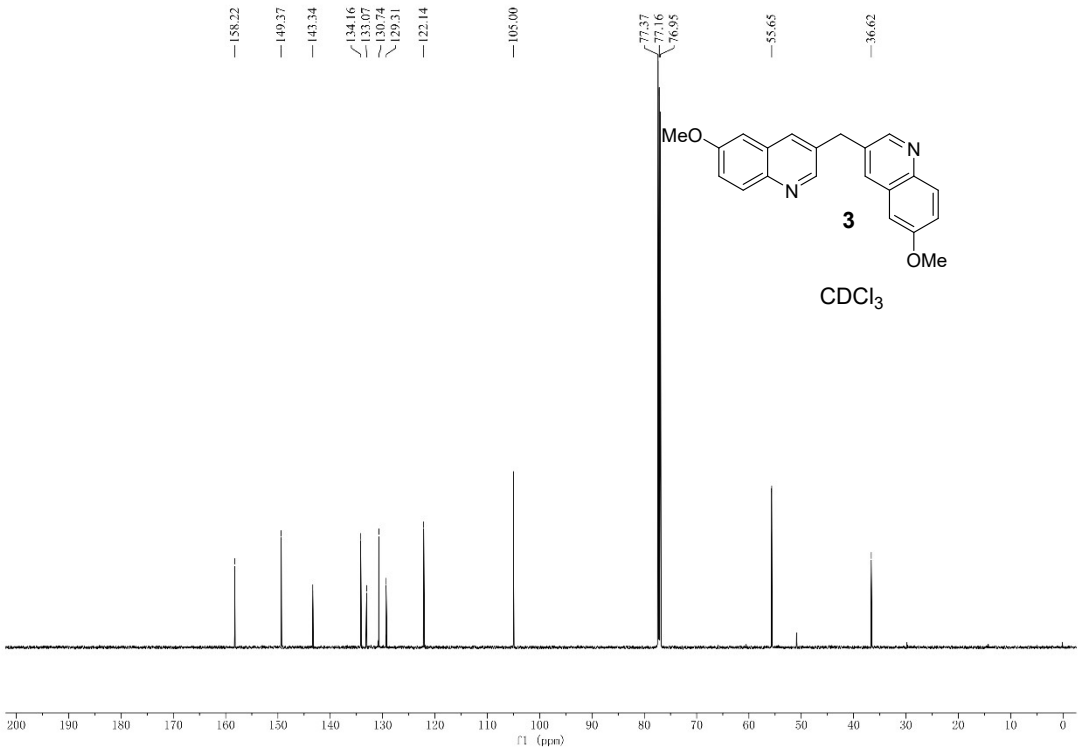

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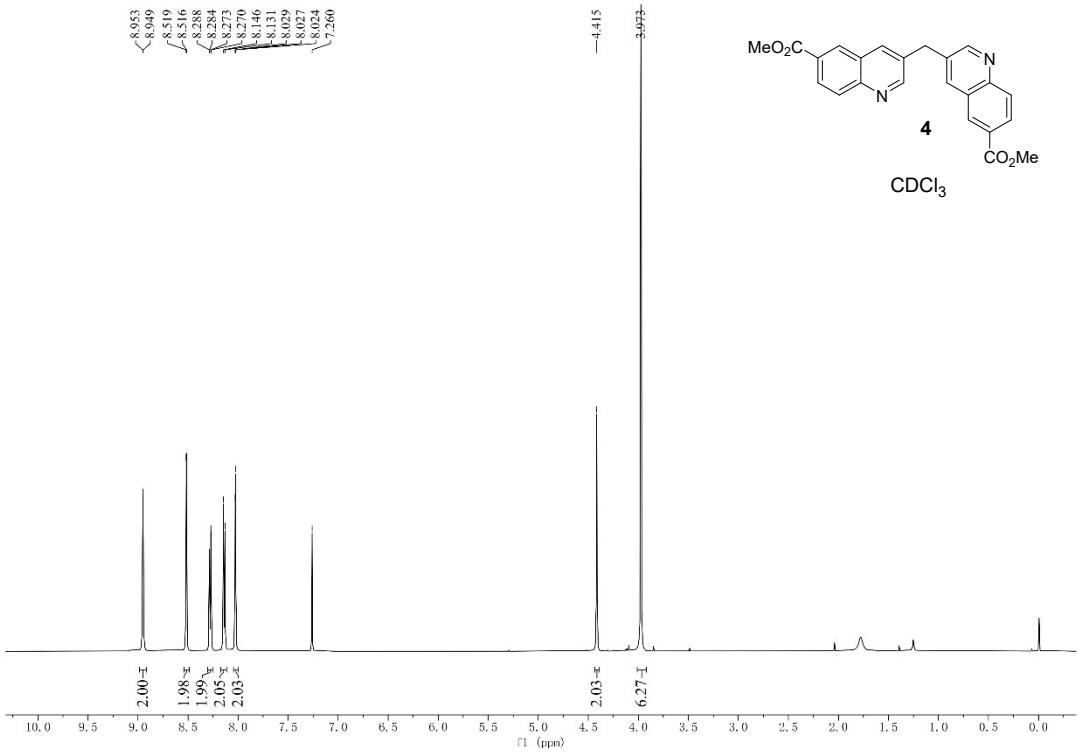

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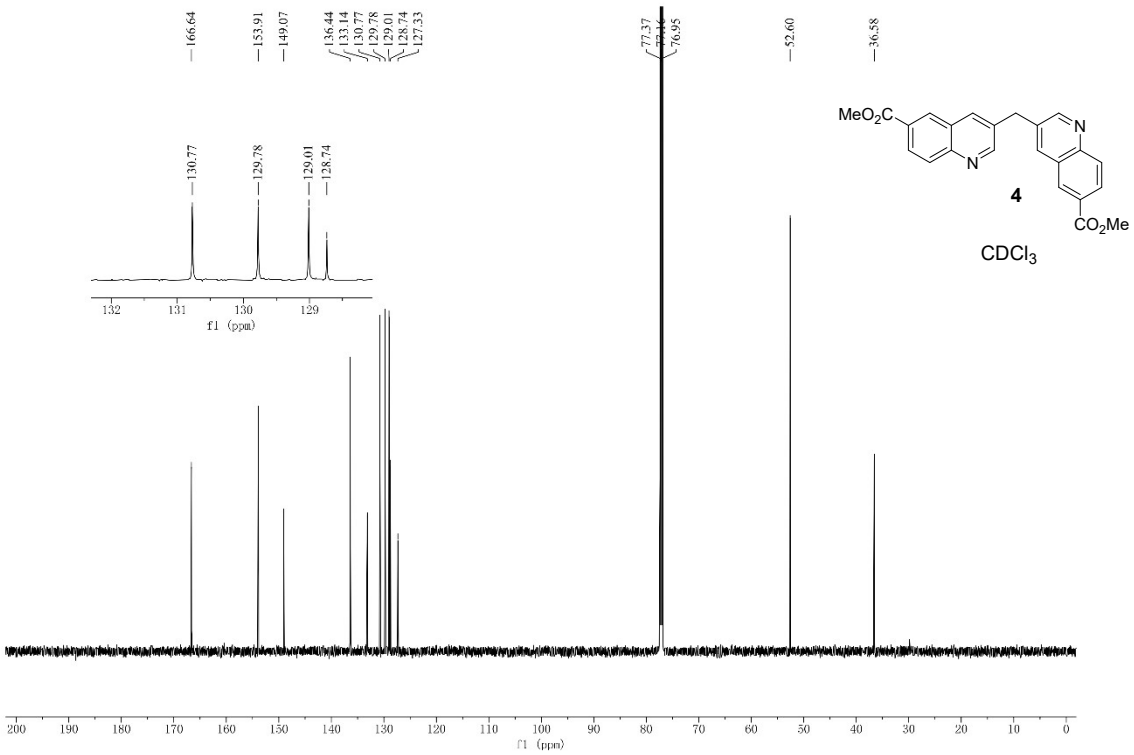

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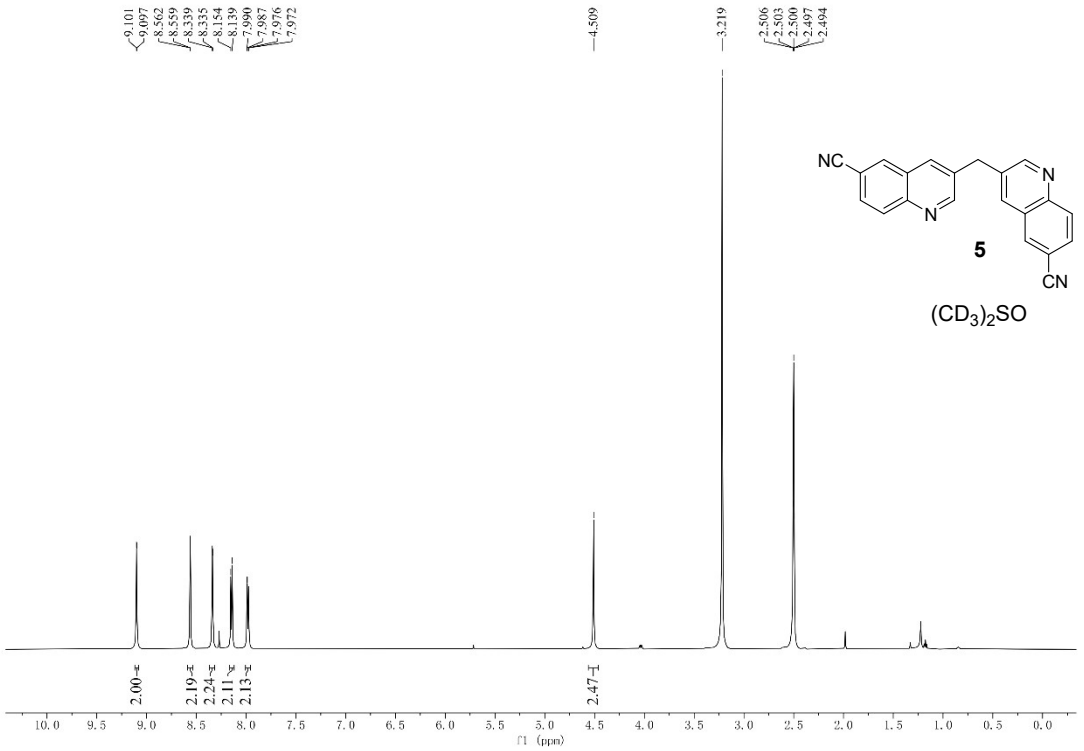

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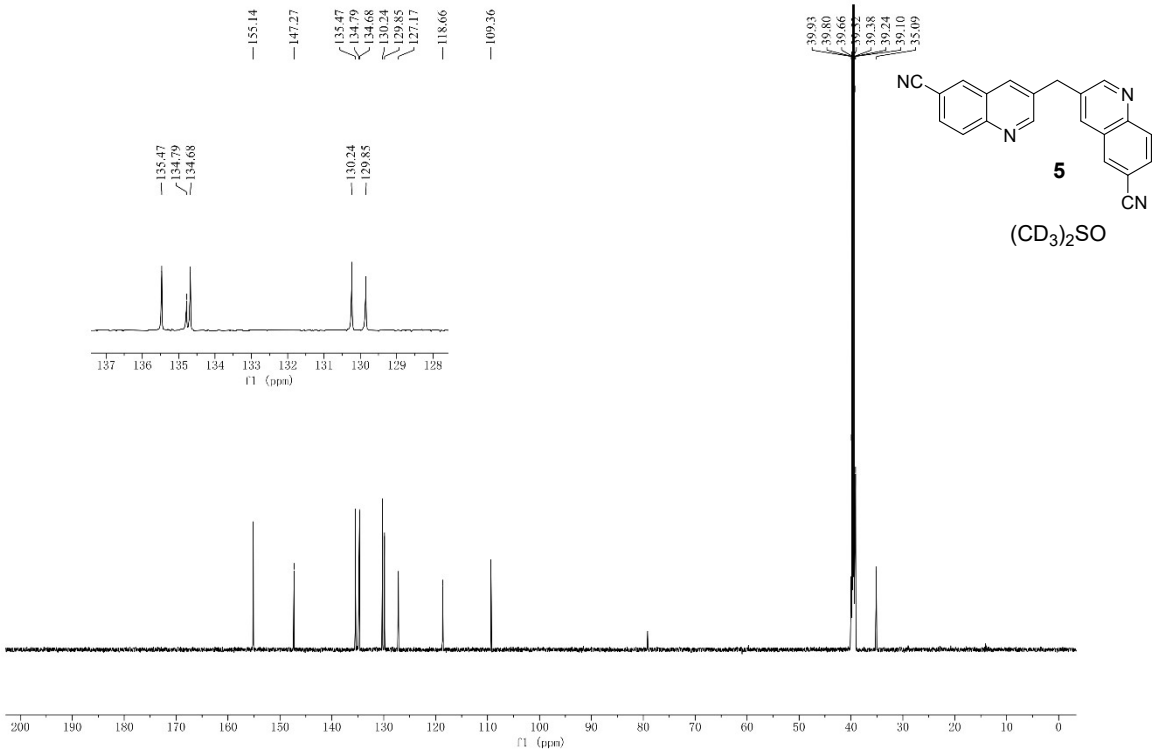

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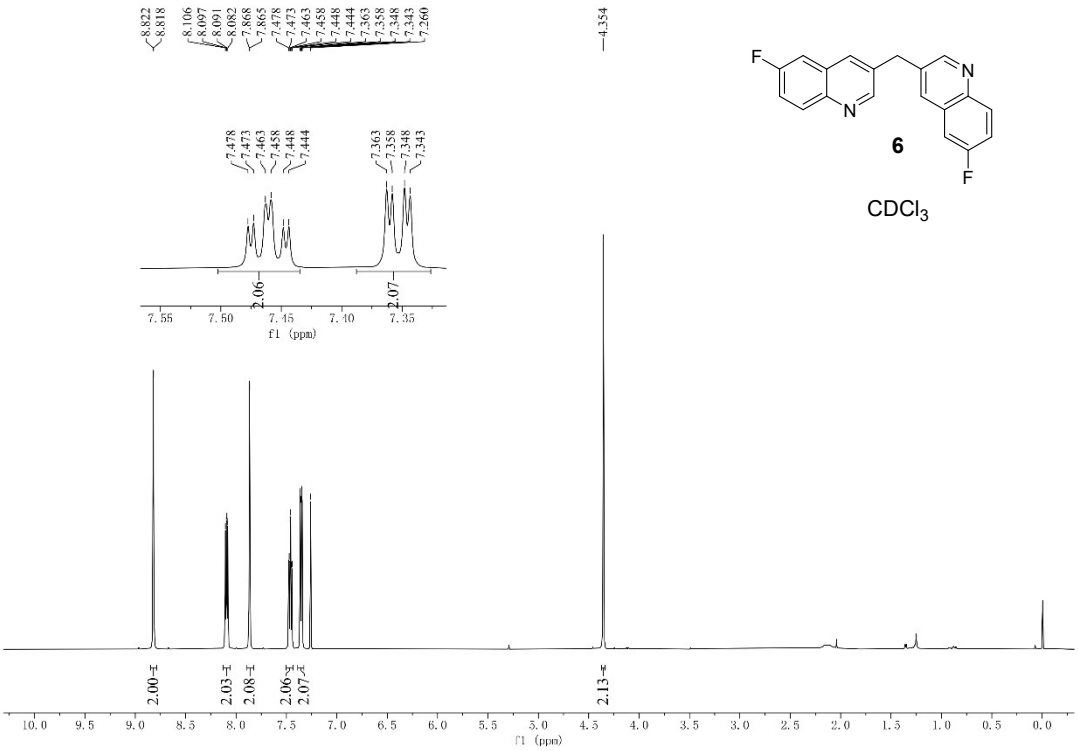

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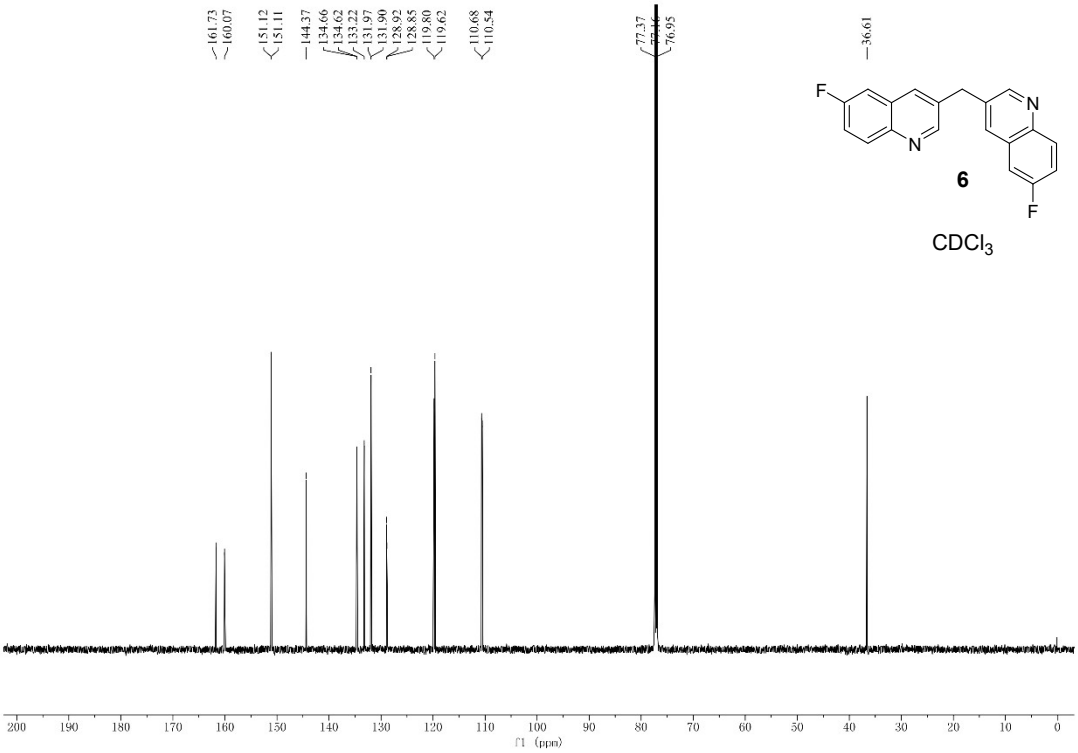

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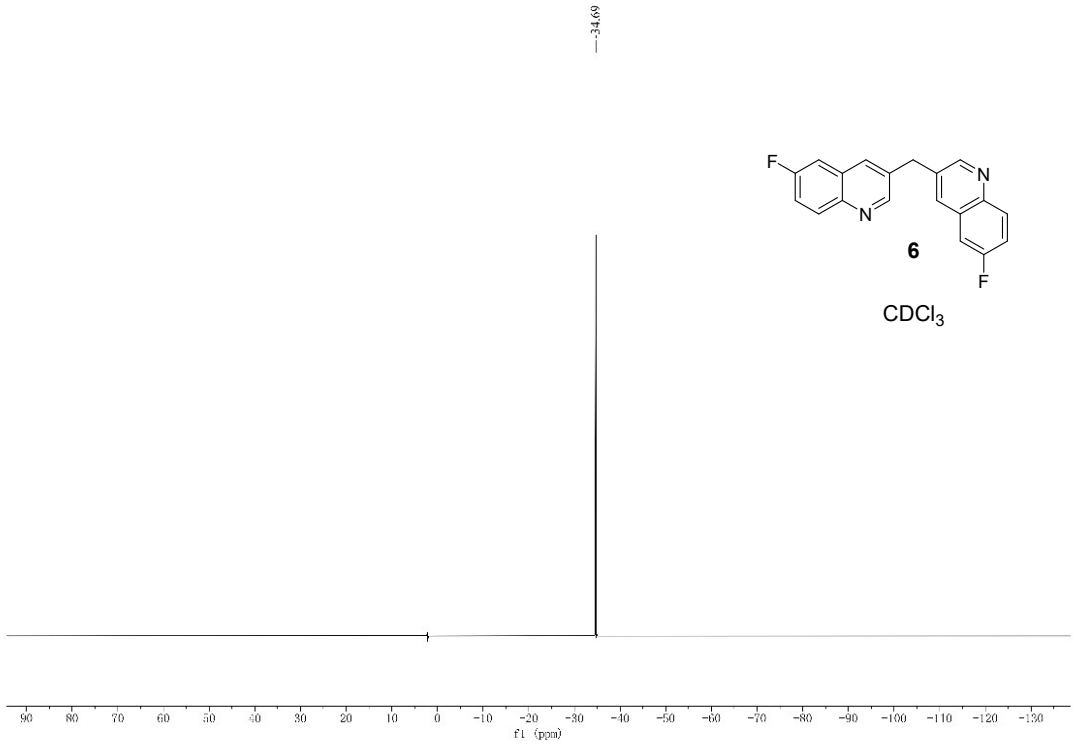

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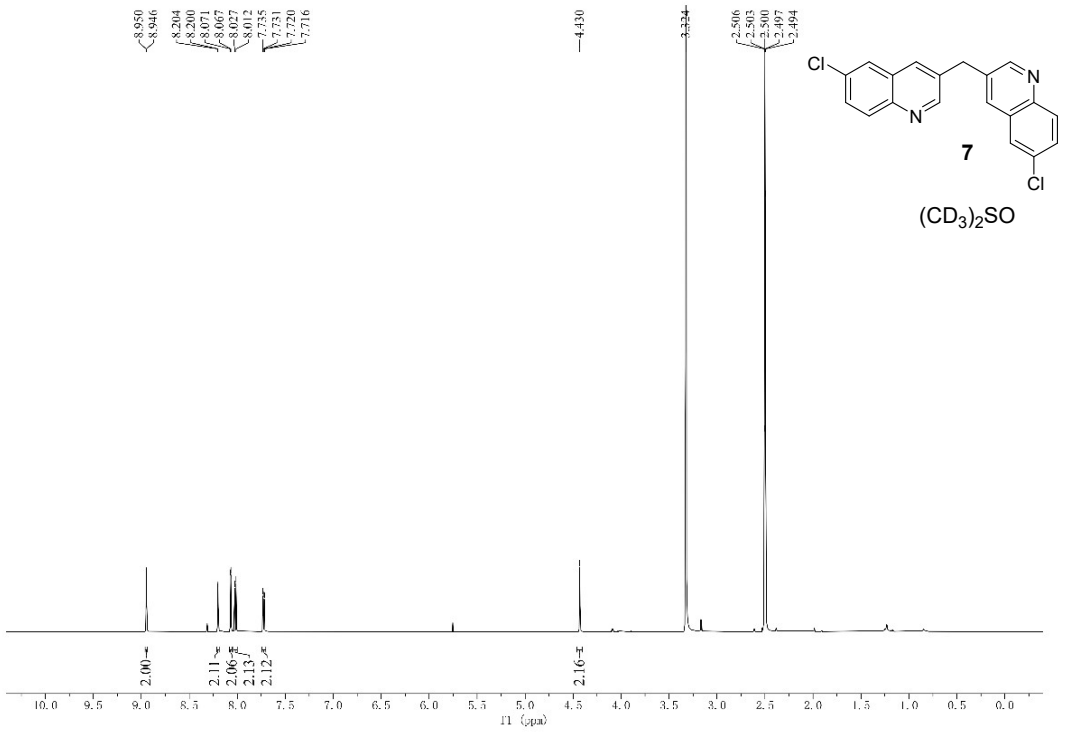

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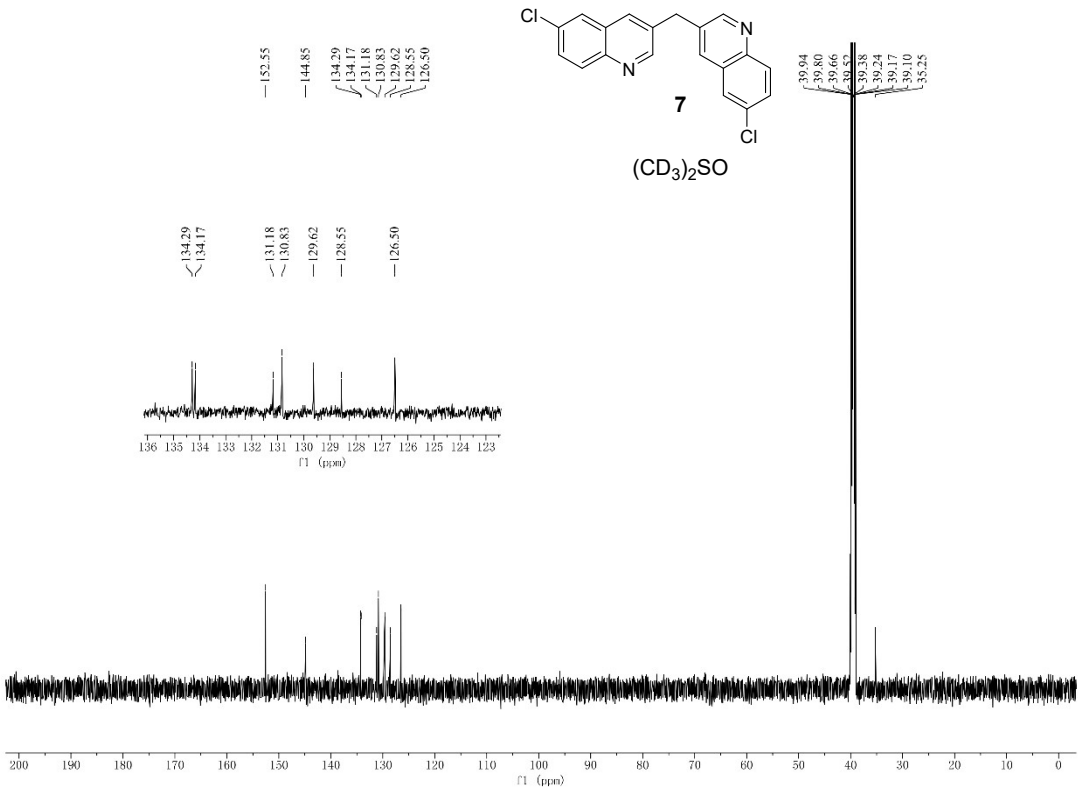

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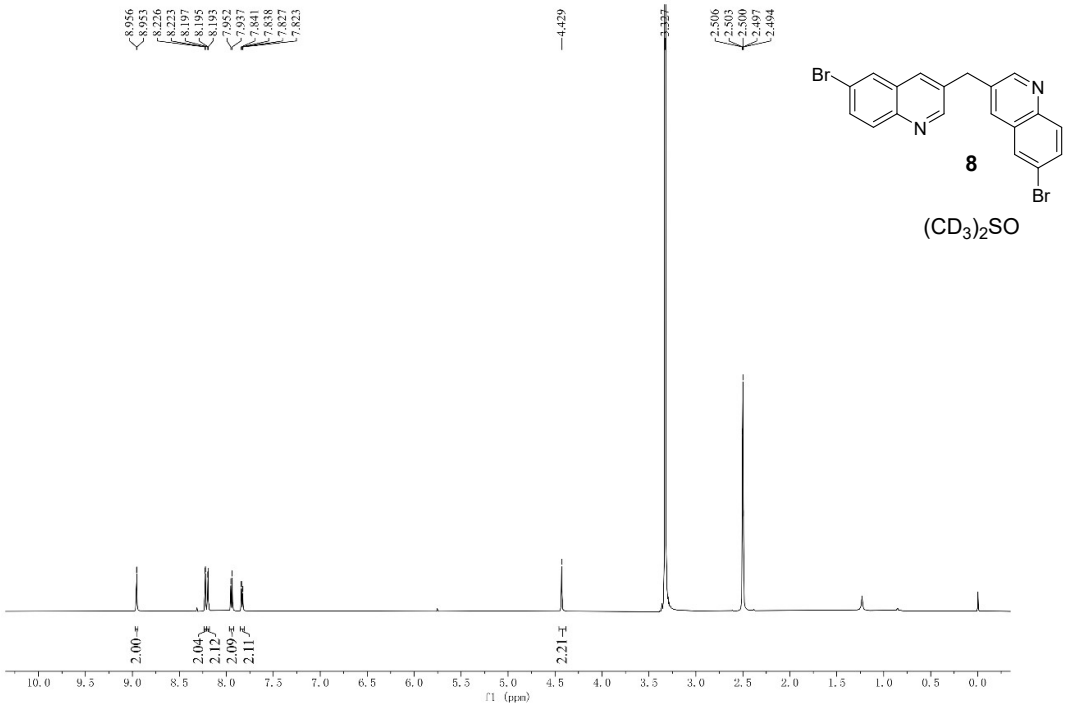

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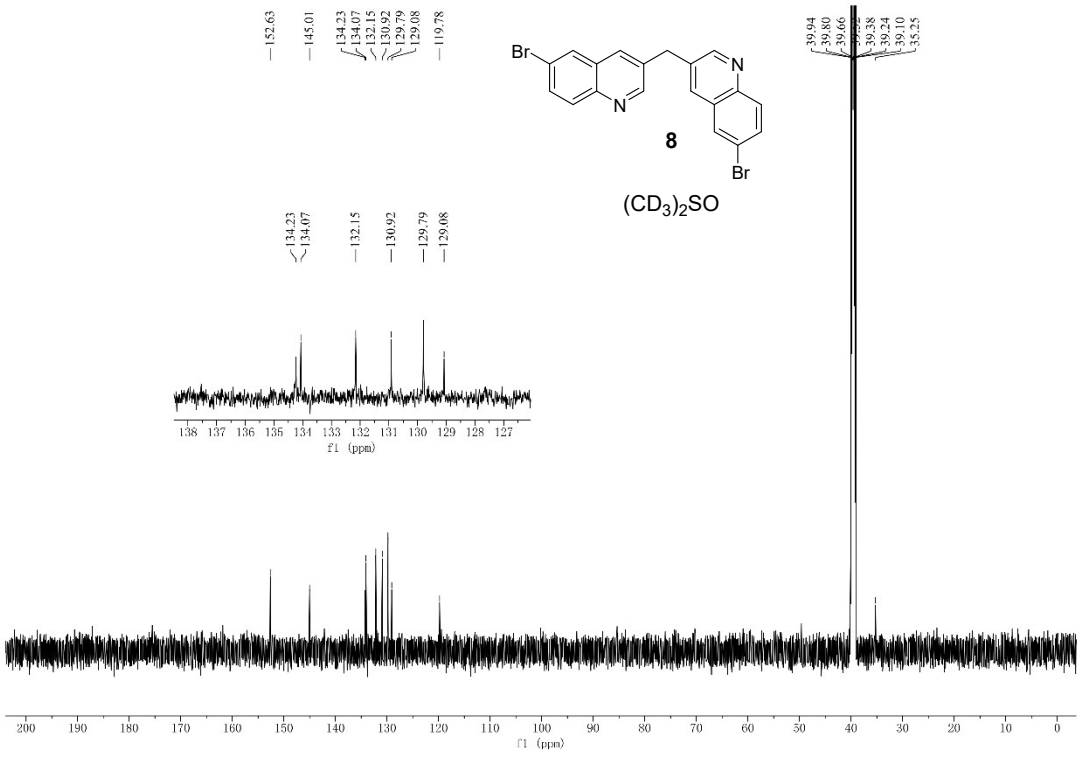

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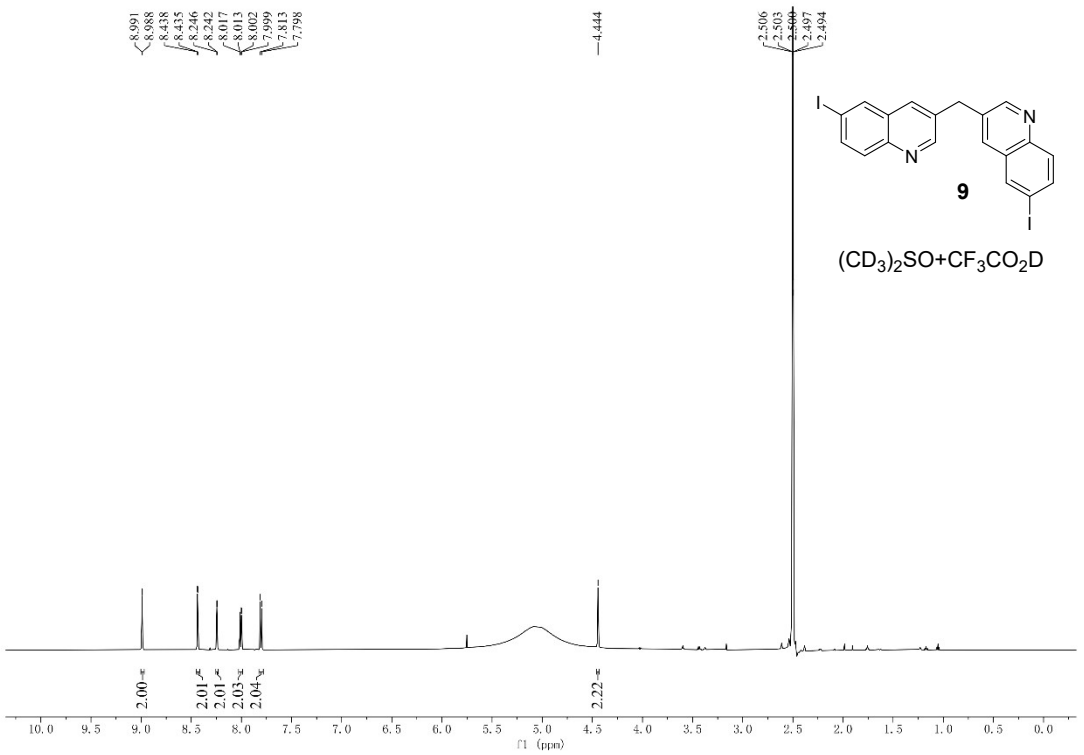

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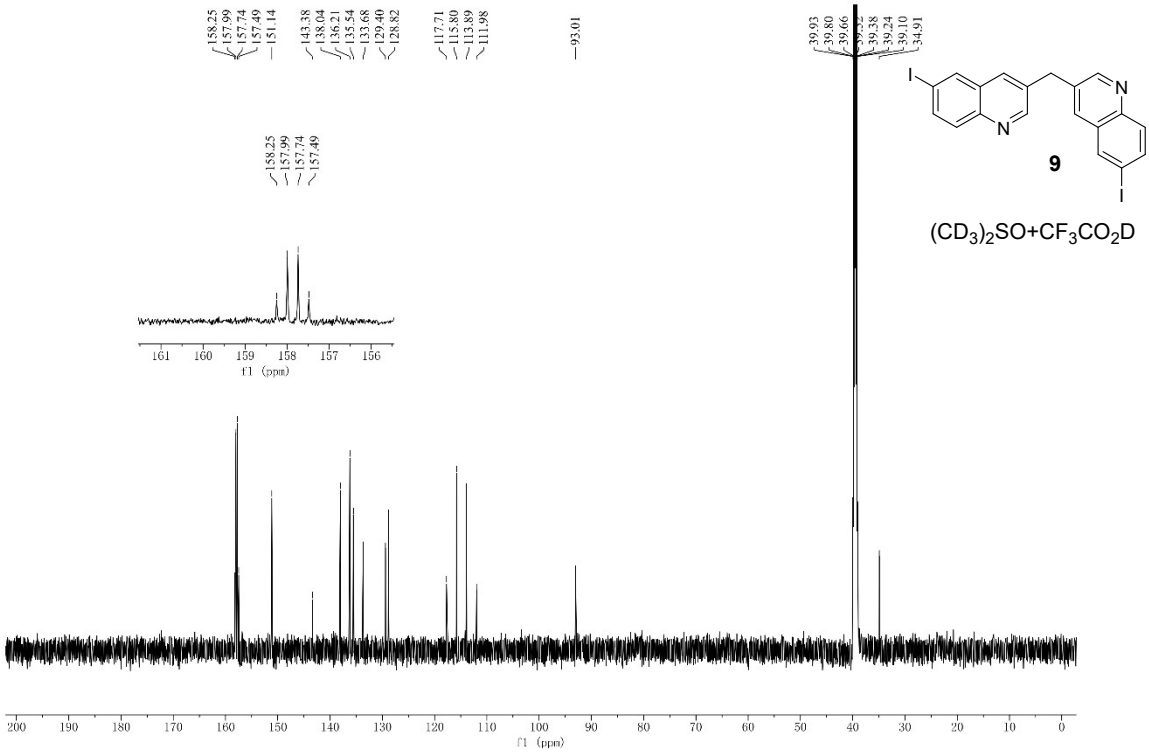
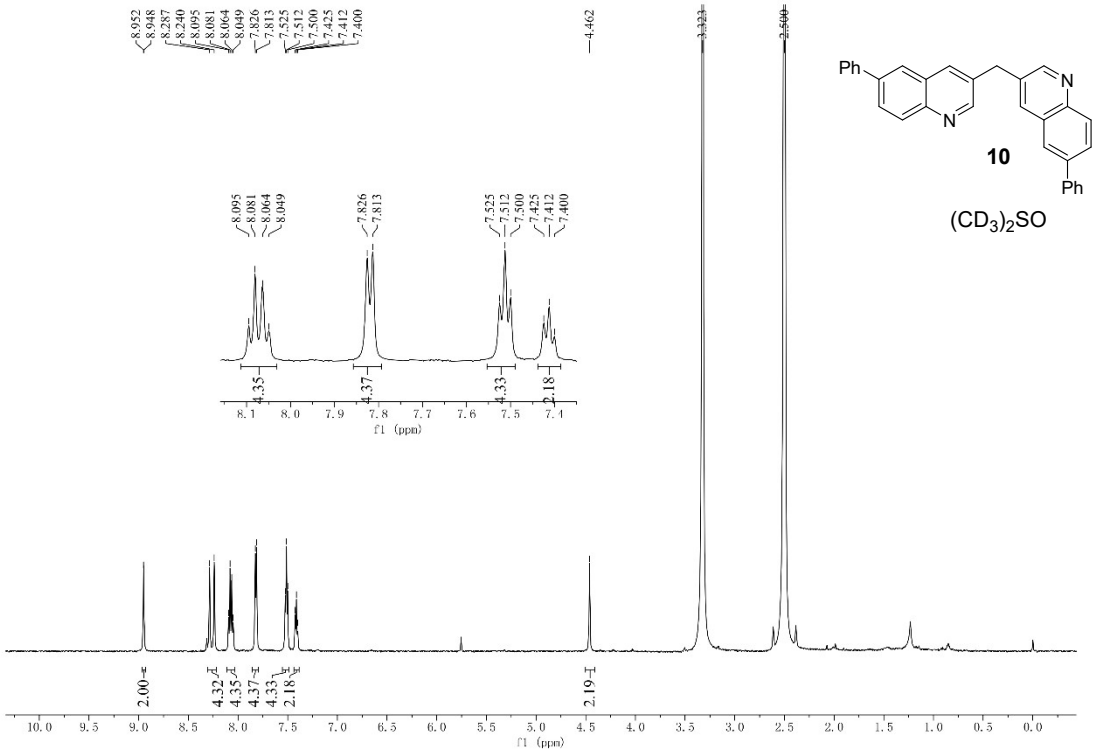
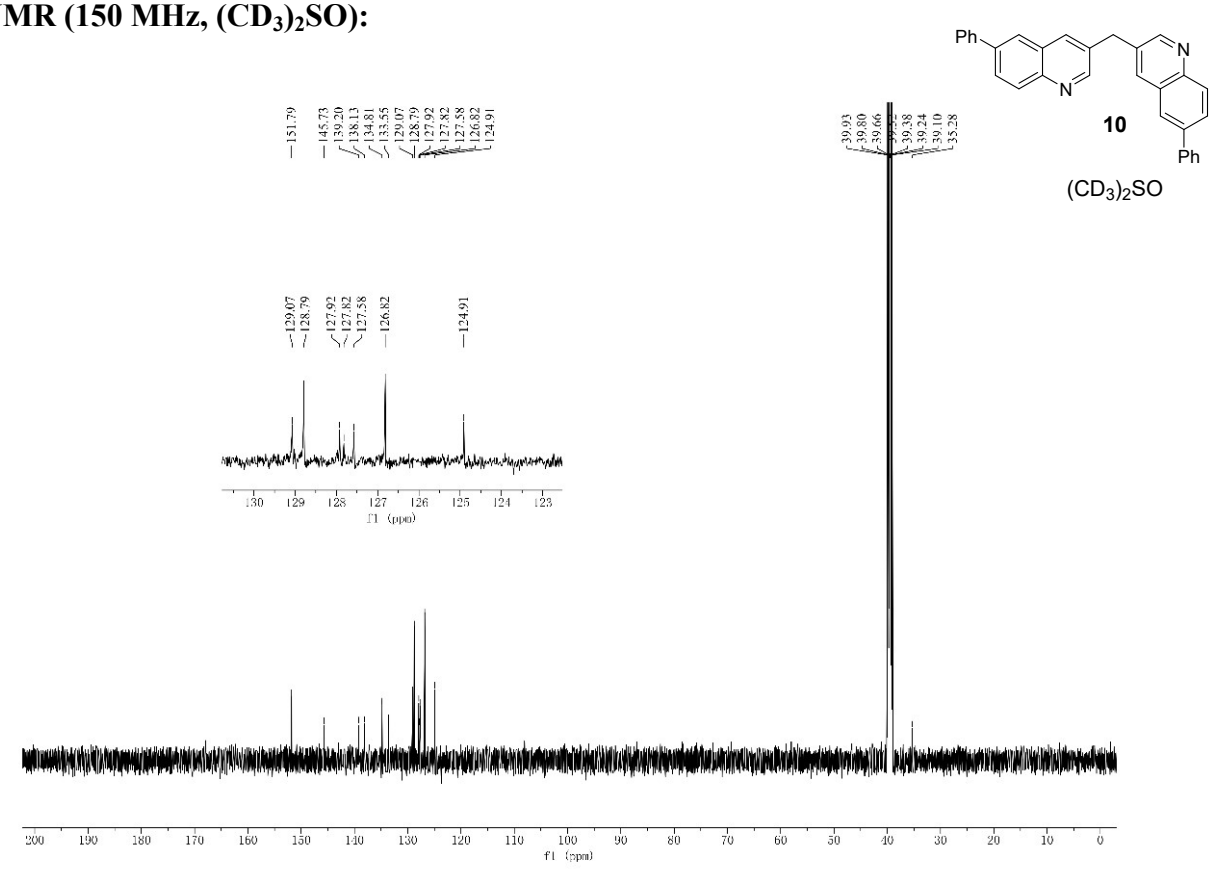


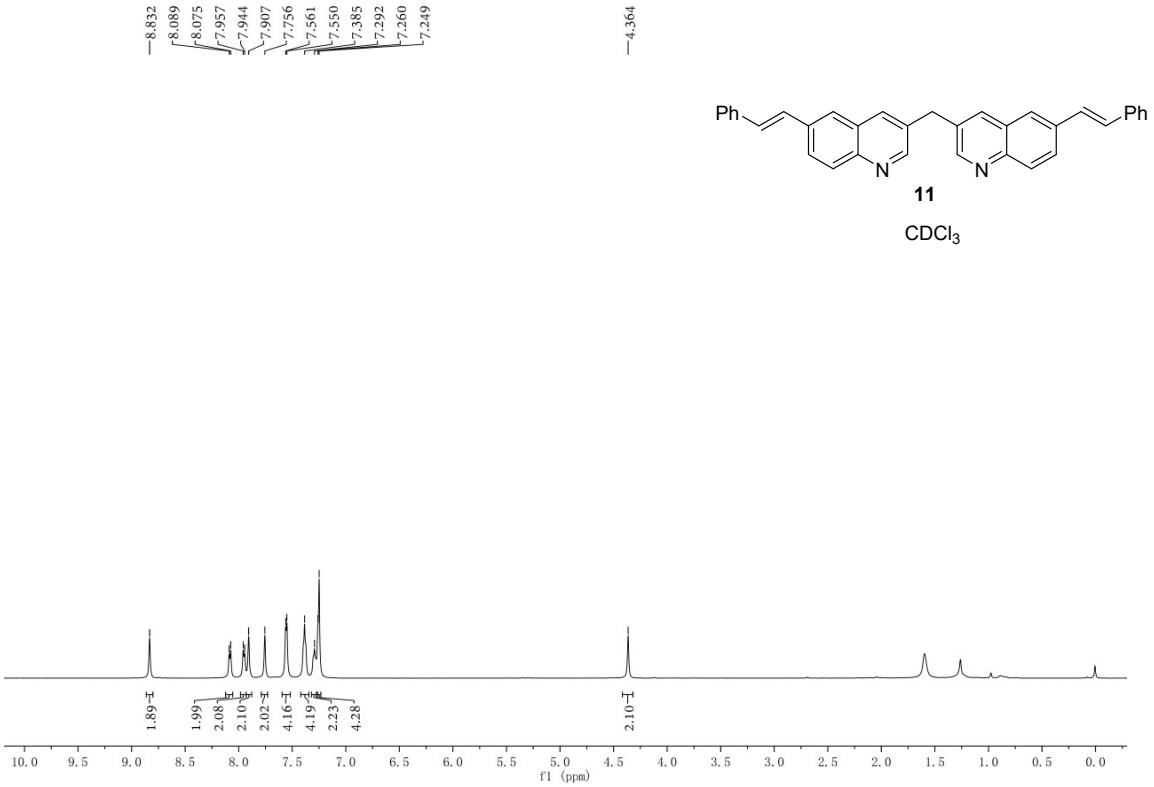
^{1}H NMR (600 MHz, $(CD_3)_2SO$):



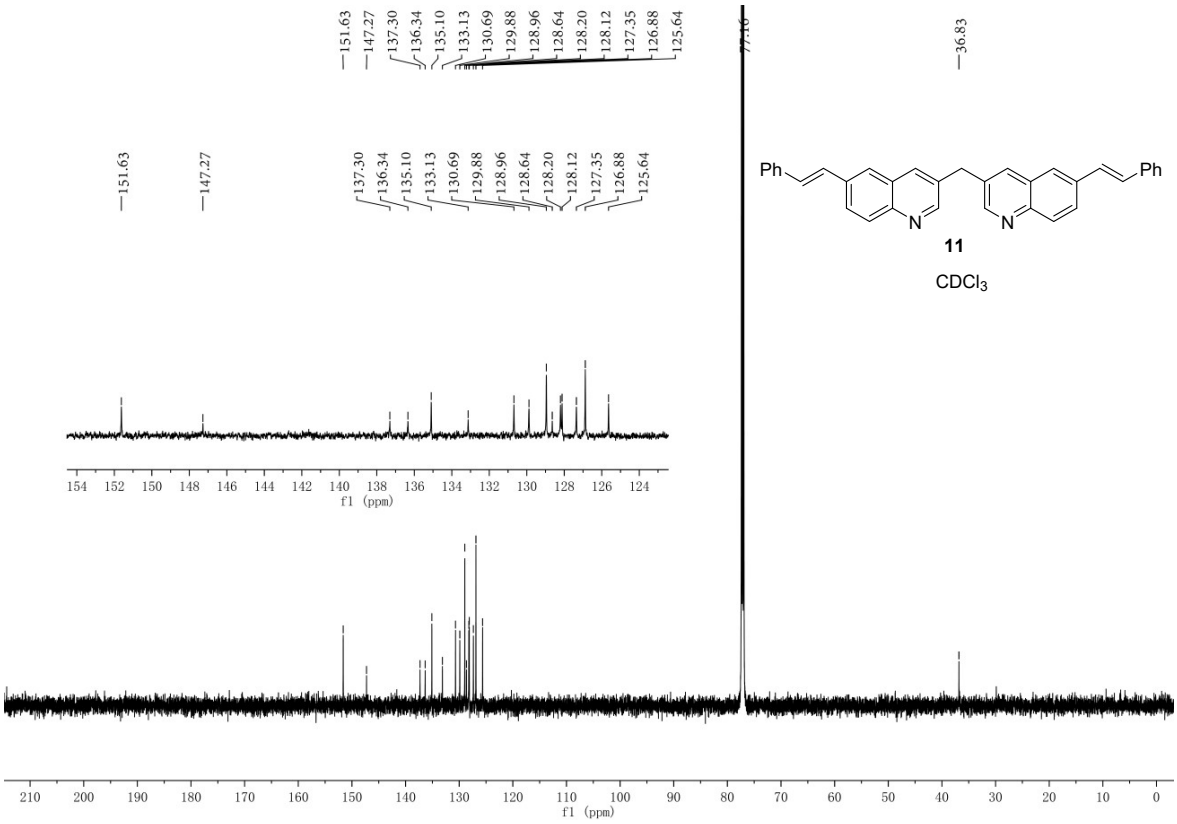
^{13}C NMR (150 MHz, $(CD_3)_2SO$):



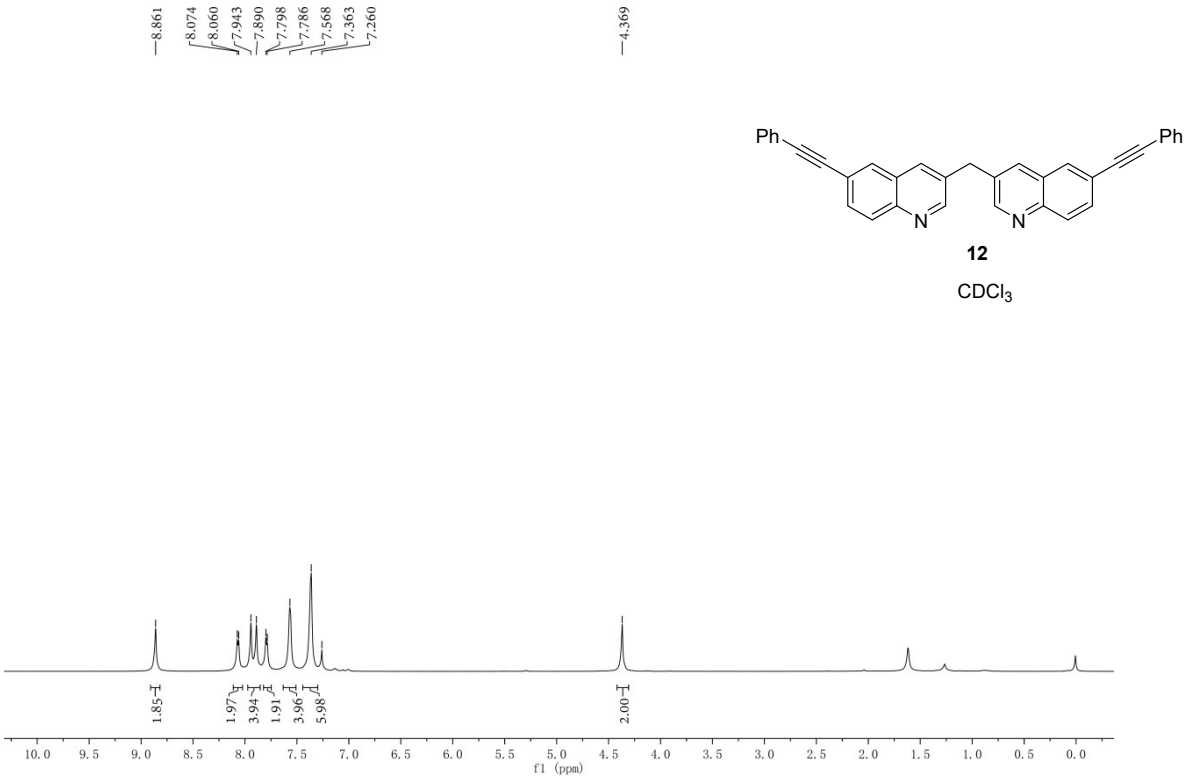
^{1}H NMR (600 MHz, $CDCl_3$):



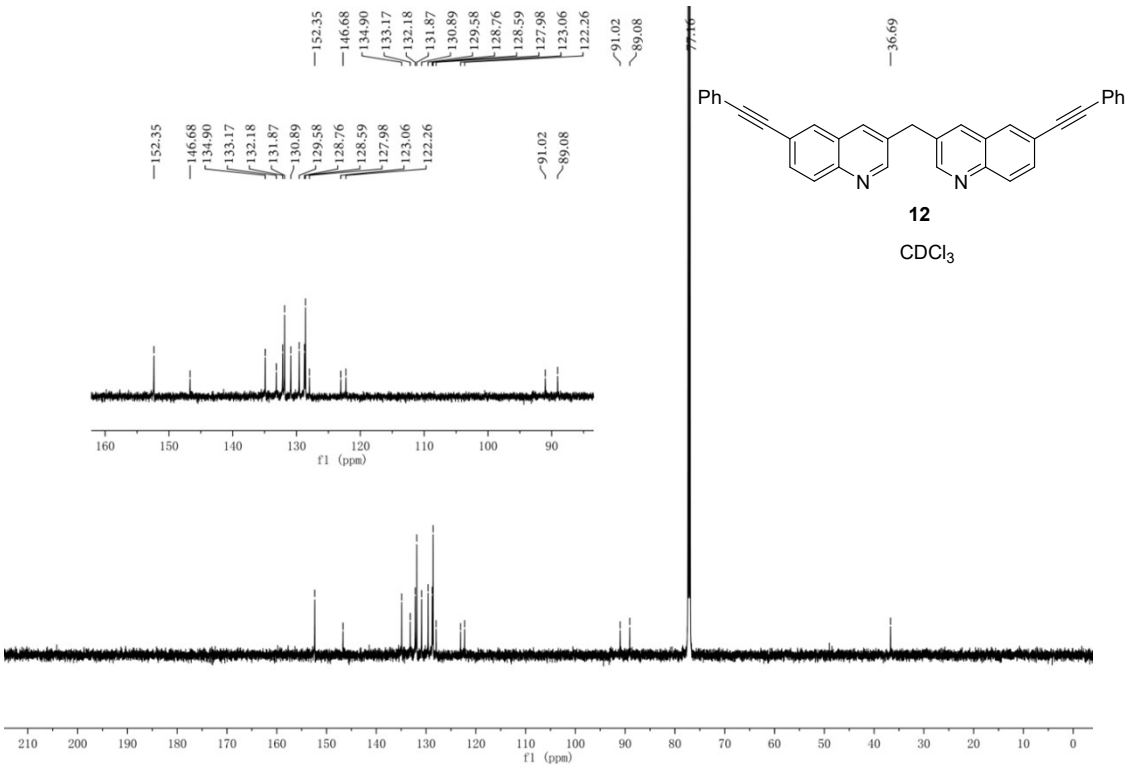
^{13}C NMR (150 MHz, $CDCl_3$):



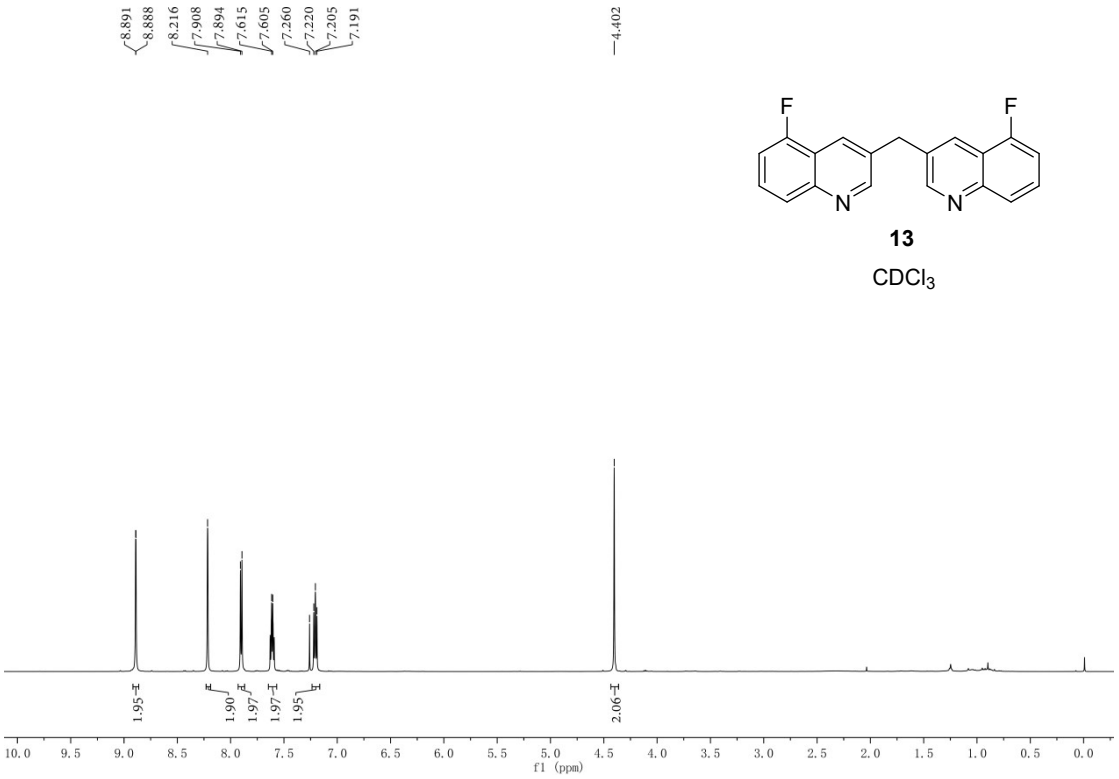
^{1}H NMR (600 MHz, $CDCl_3$):



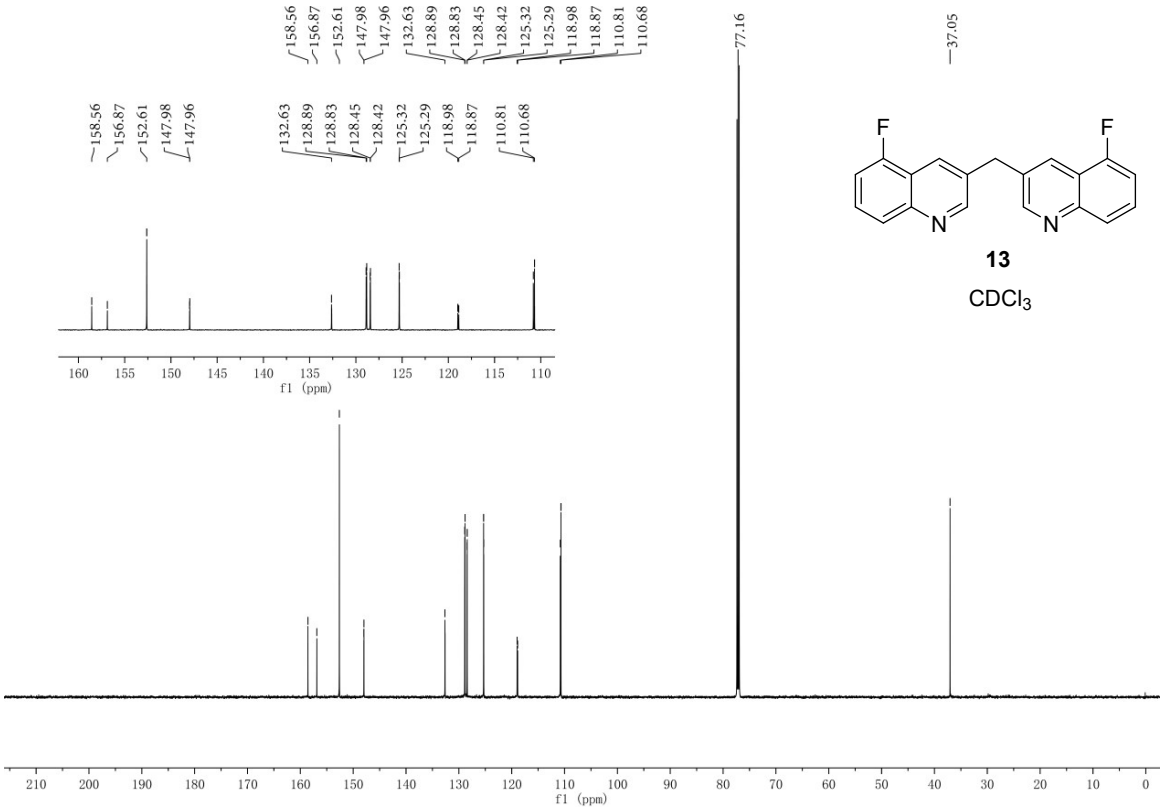
^{13}C NMR (150 MHz, $CDCl_3$):



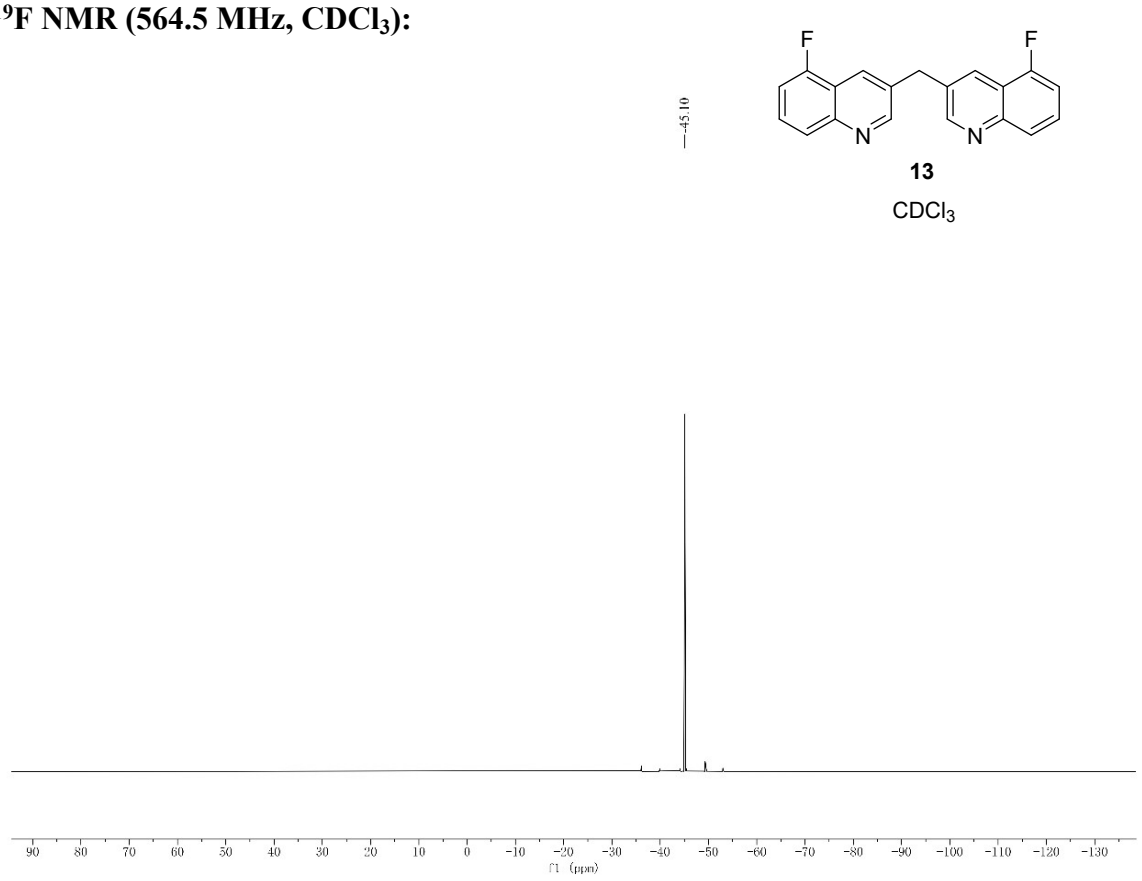
^{1}H NMR (600 MHz, $CDCl_3$):



^{13}C NMR (150 MHz, $CDCl_3$):

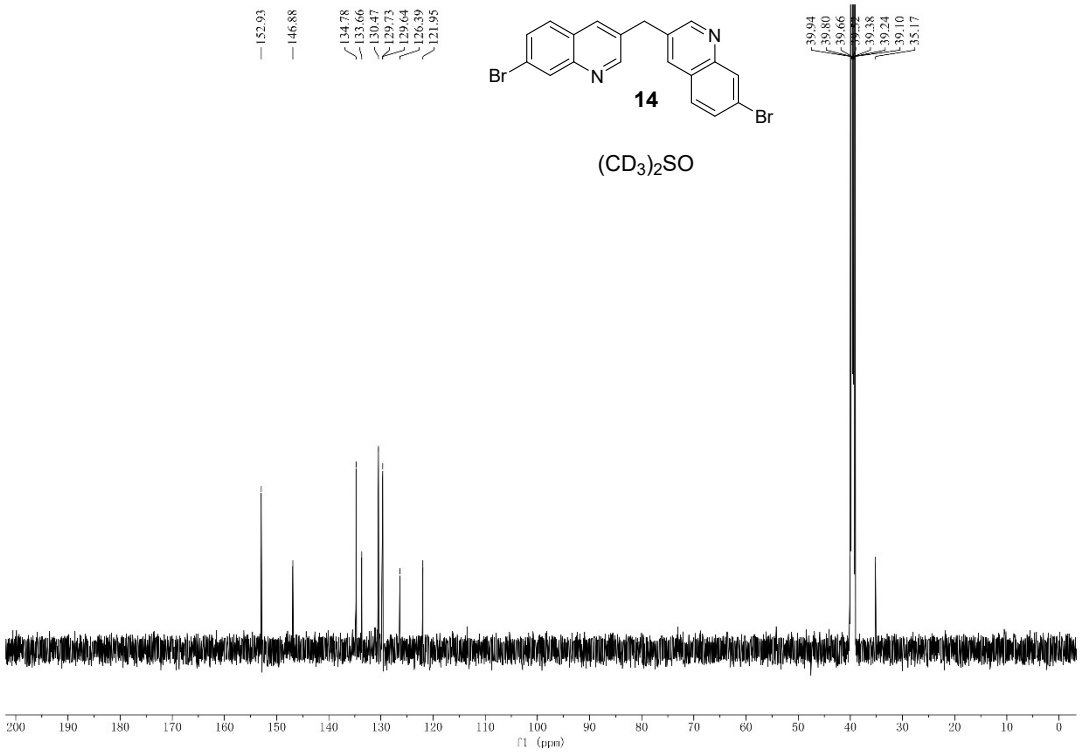


^{19}F NMR (564.5 MHz, $CDCl_3$):

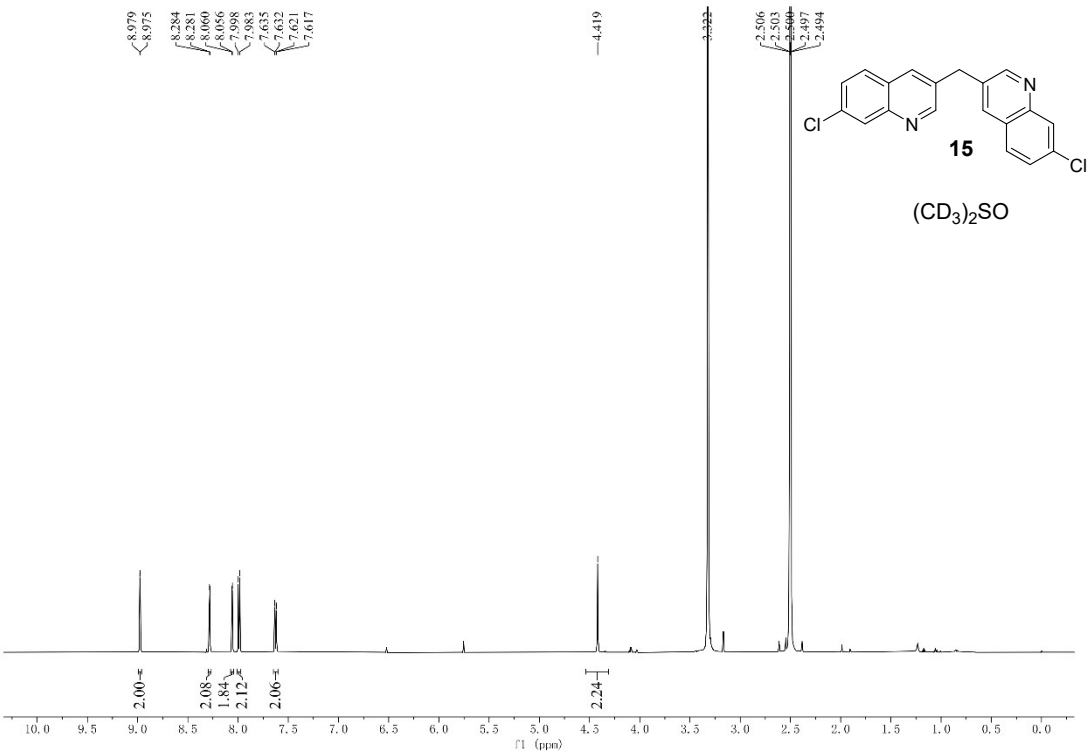


^{1}H NMR (600 MHz, $(CD_3)_2SO$):

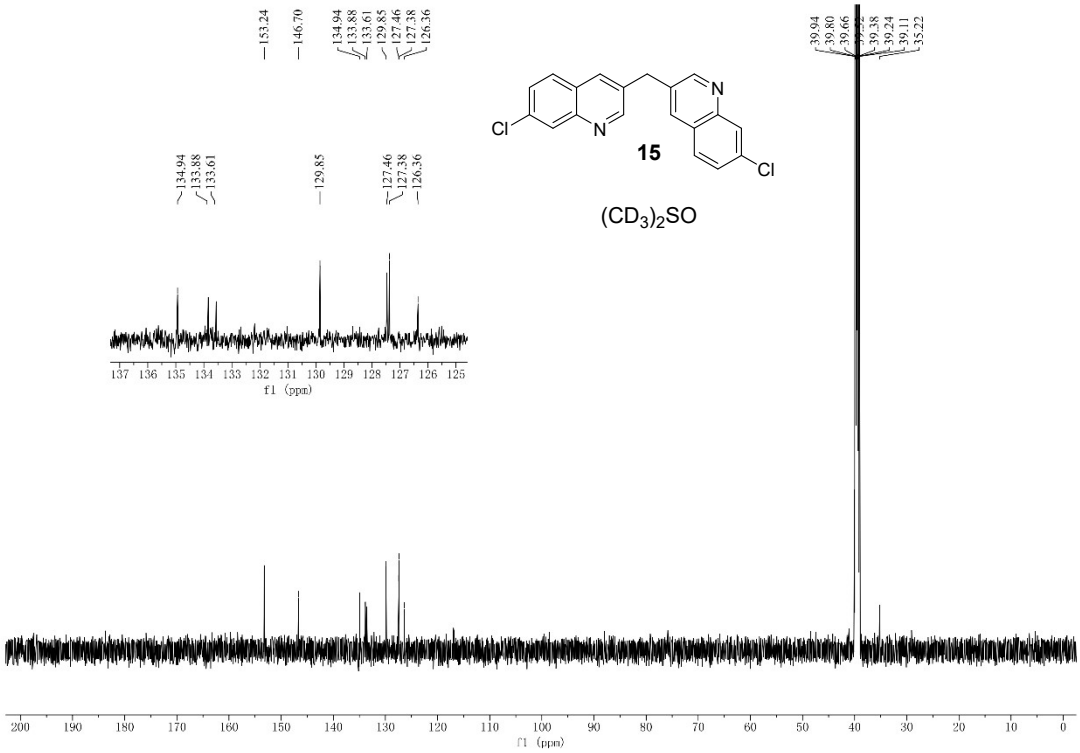
^{13}C NMR (150 MHz, $(CD_3)_2SO$):



^{1}H NMR (600 MHz, $(CD_3)_2SO$):

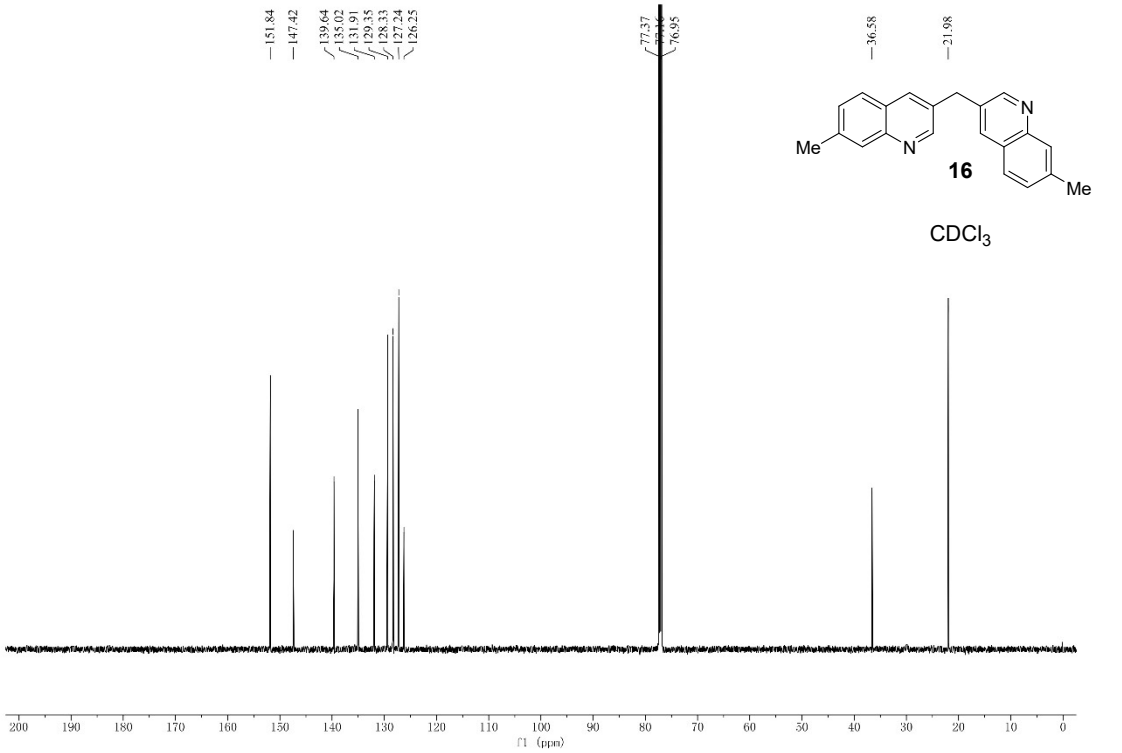


^{13}C NMR (150 MHz, $(CD_3)_2SO$):

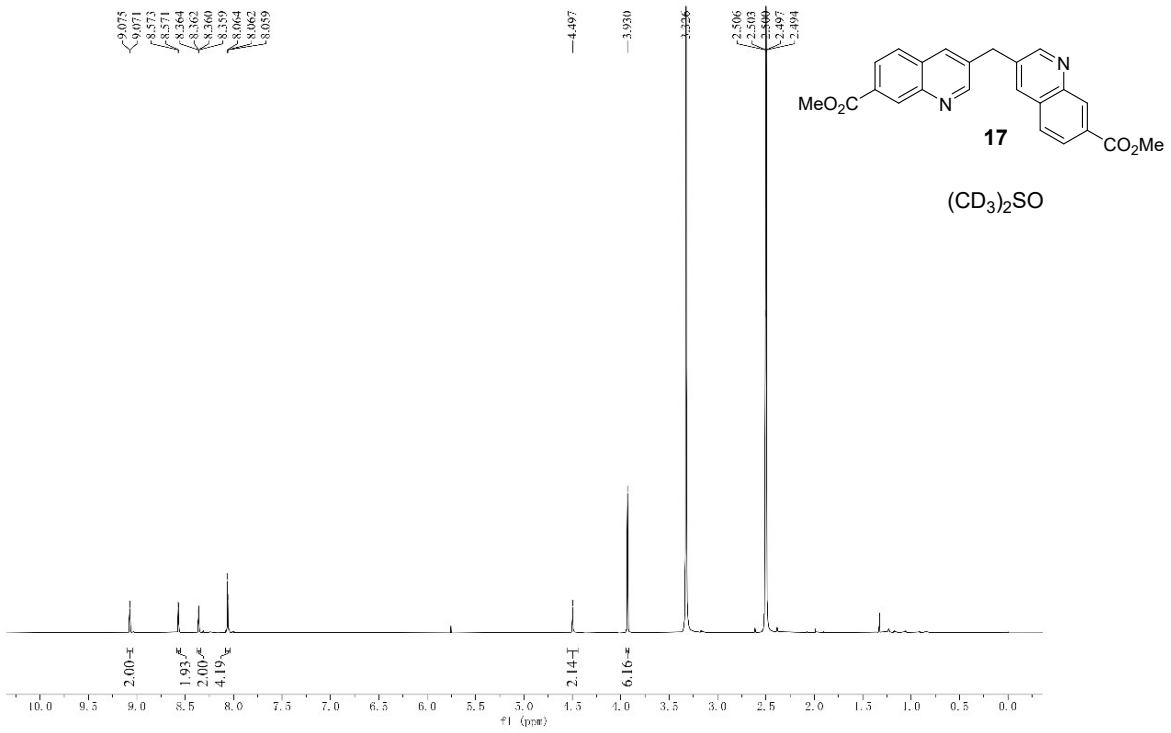


^{1}H NMR (600 MHz, $CDCl_3$):

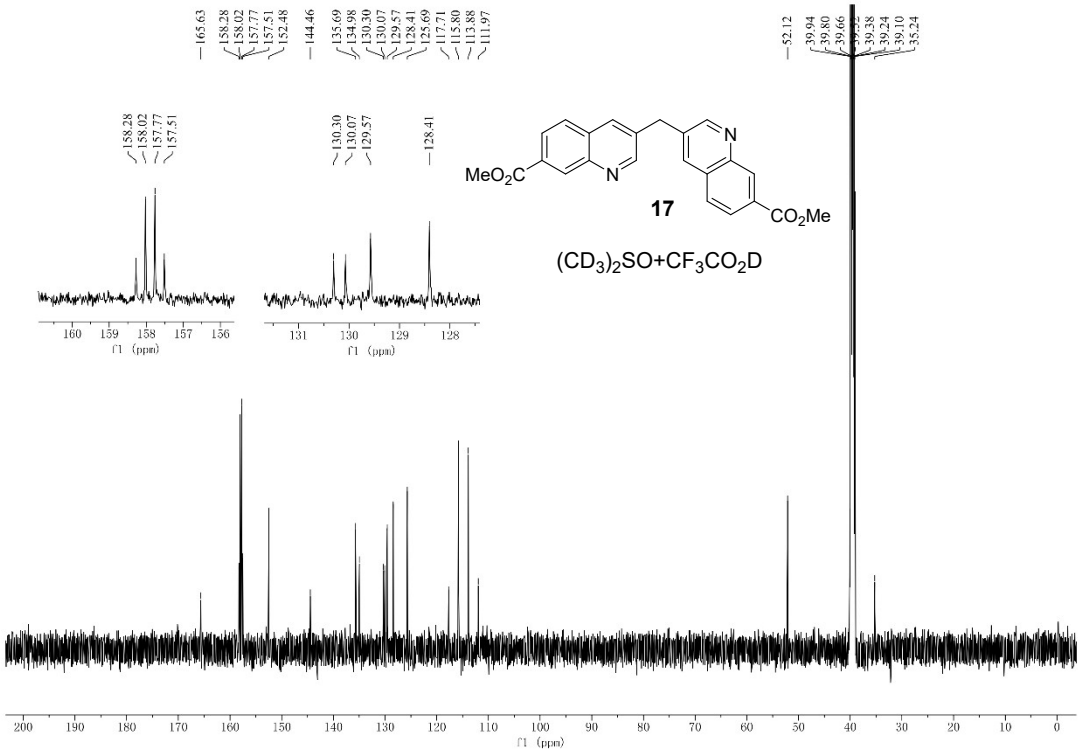
^{13}C NMR (150 MHz, $CDCl_3$):



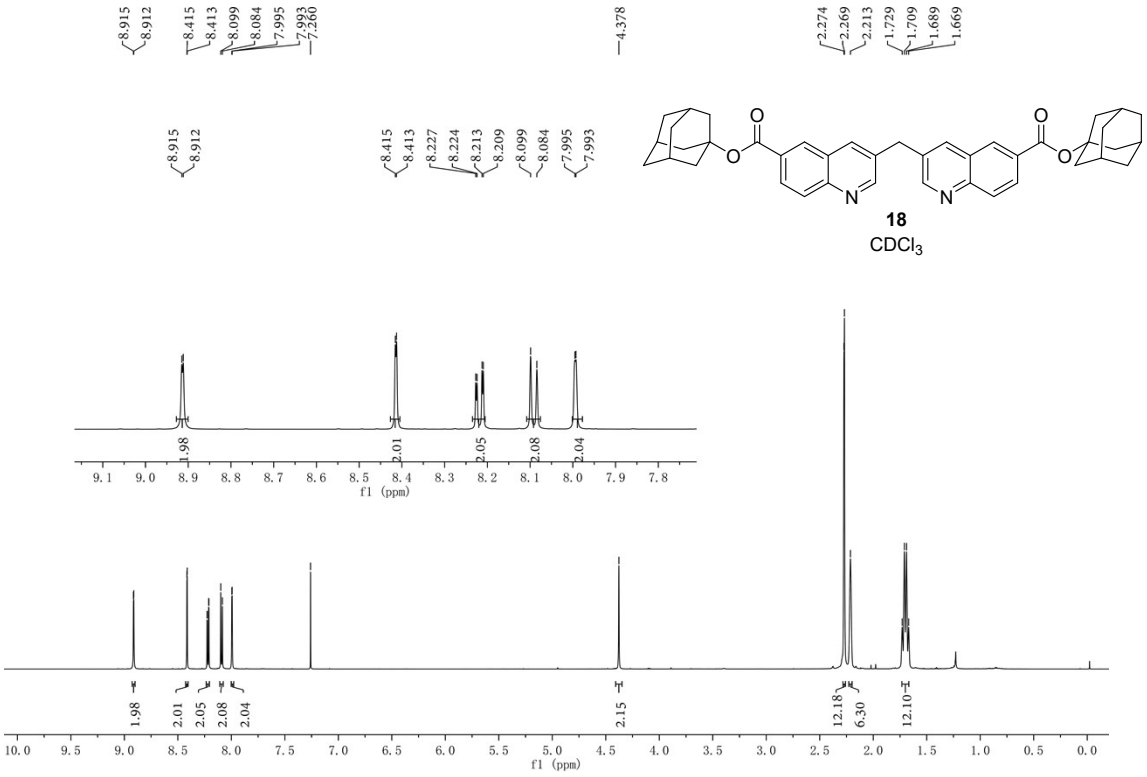
^{1}H NMR (600 MHz, $(CD_3)_2SO$):



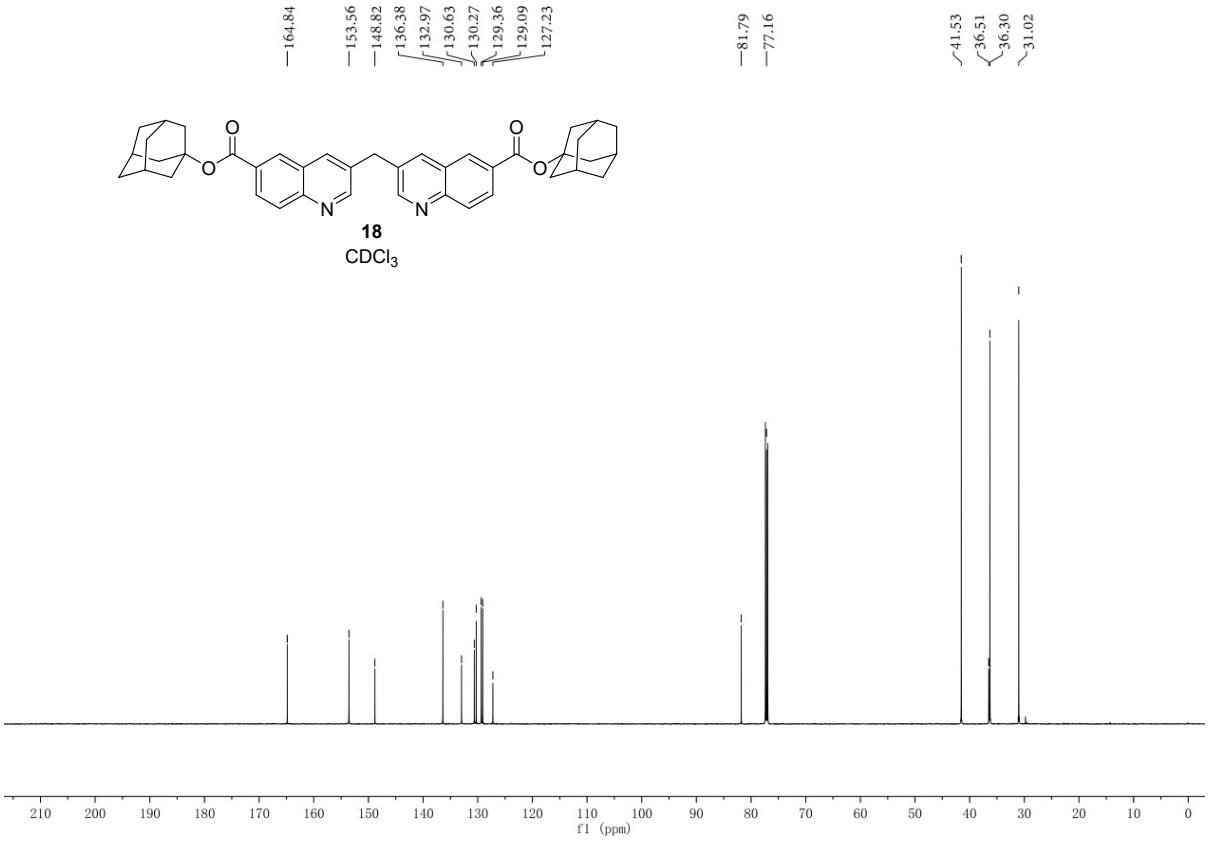
^{13}C NMR (150 MHz, $(CD_3)_2SO+CF_3CO_2D$):



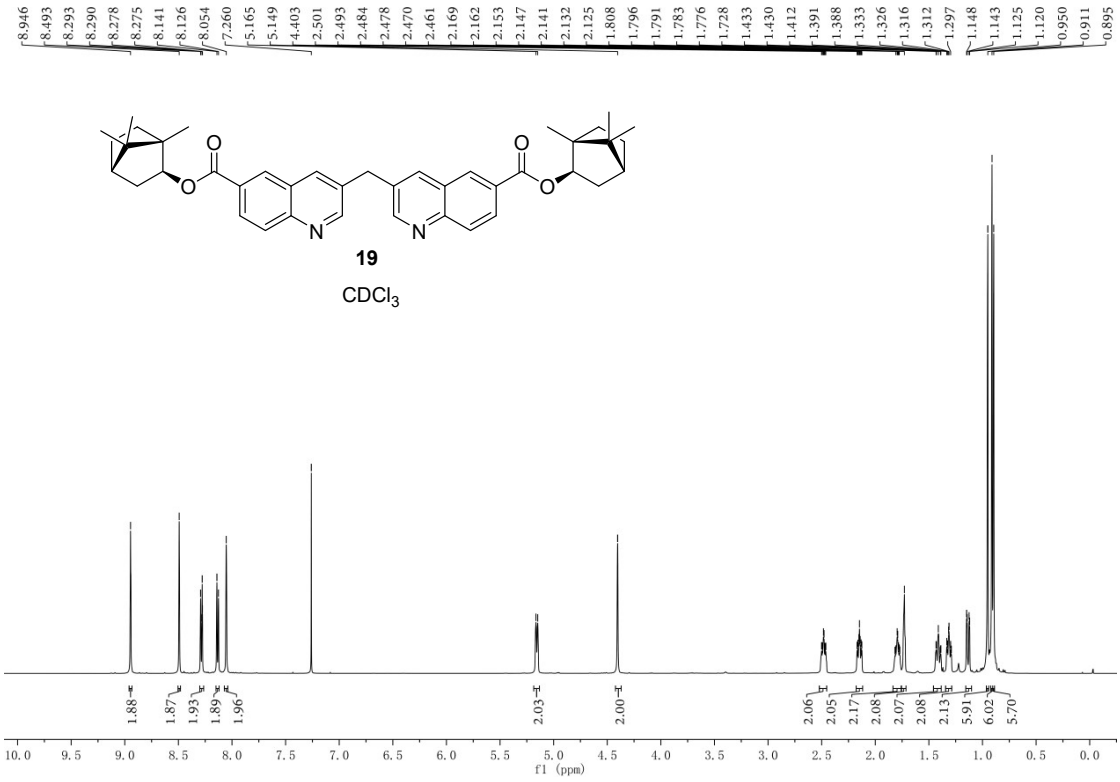
^{1}H NMR (600 MHz, $CDCl_3$):



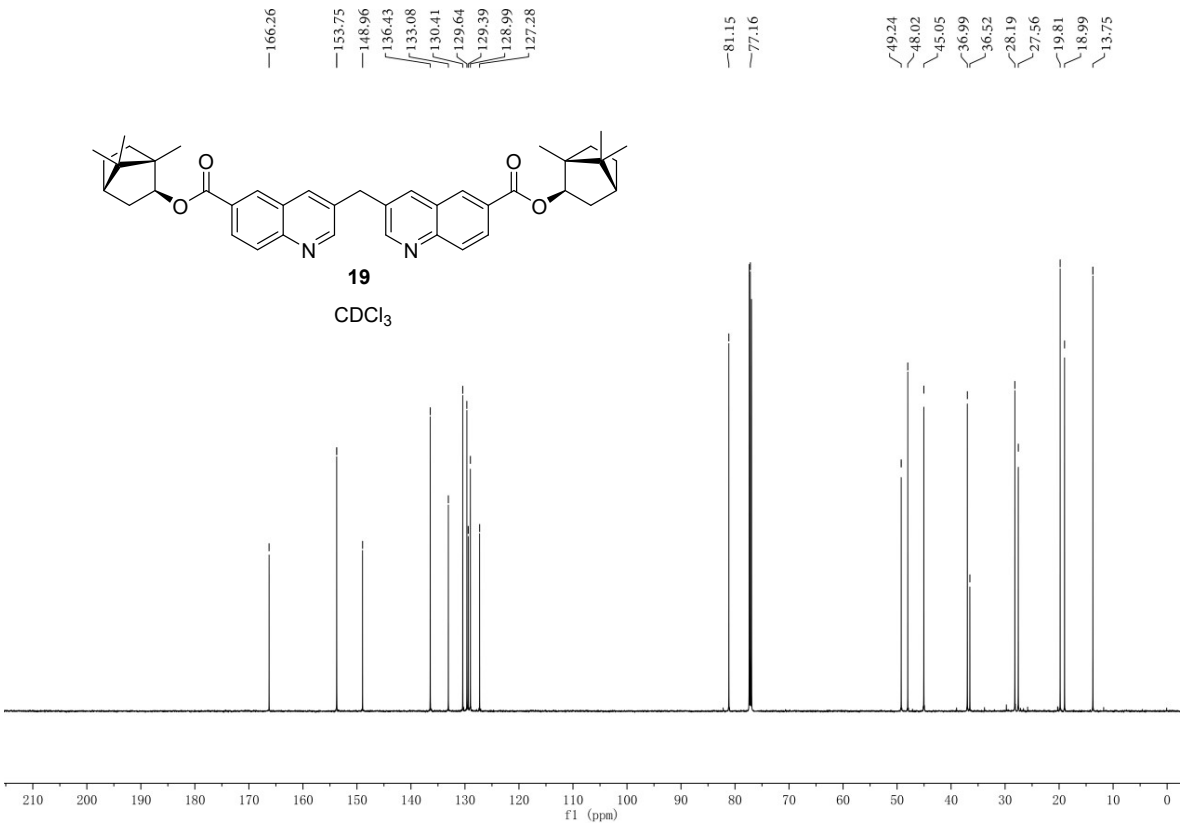
^{13}C NMR (150 MHz, $CDCl_3$):



^{1}H NMR (600 MHz, $CDCl_3$):

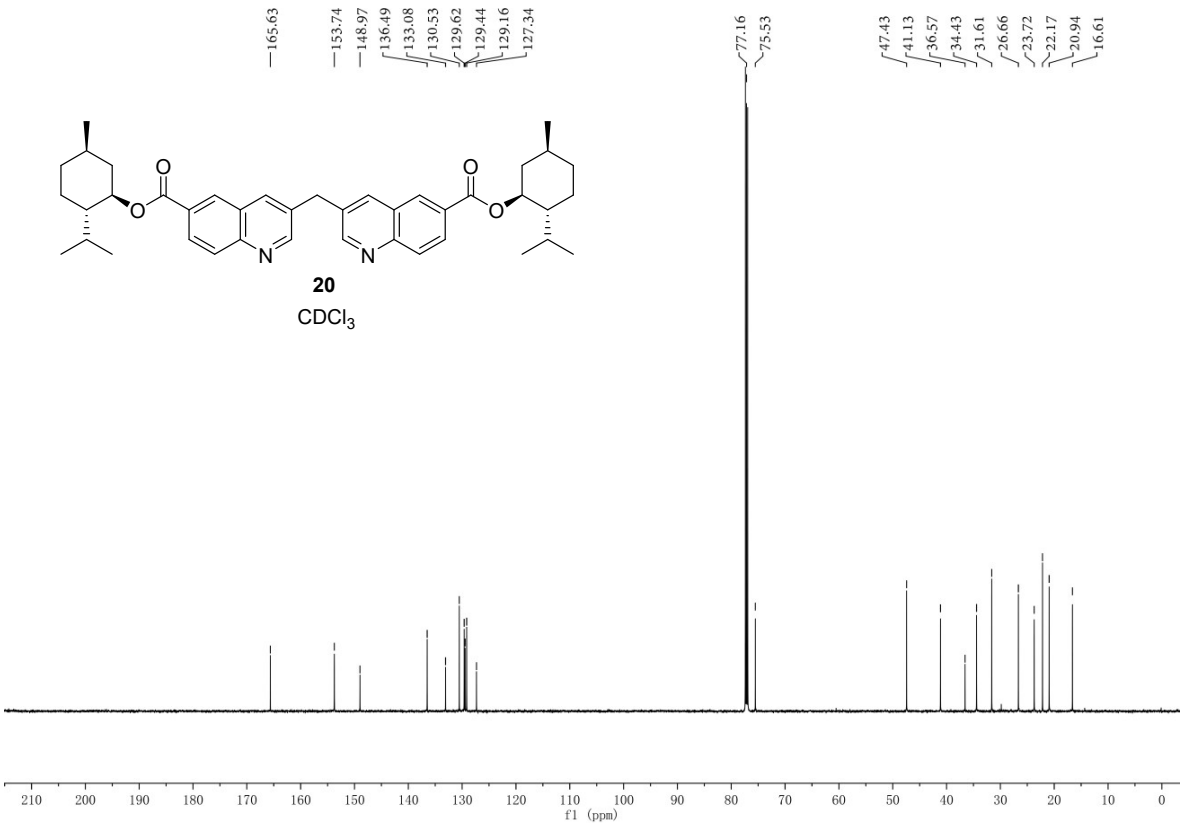


^{13}C NMR (150 MHz, $CDCl_3$):

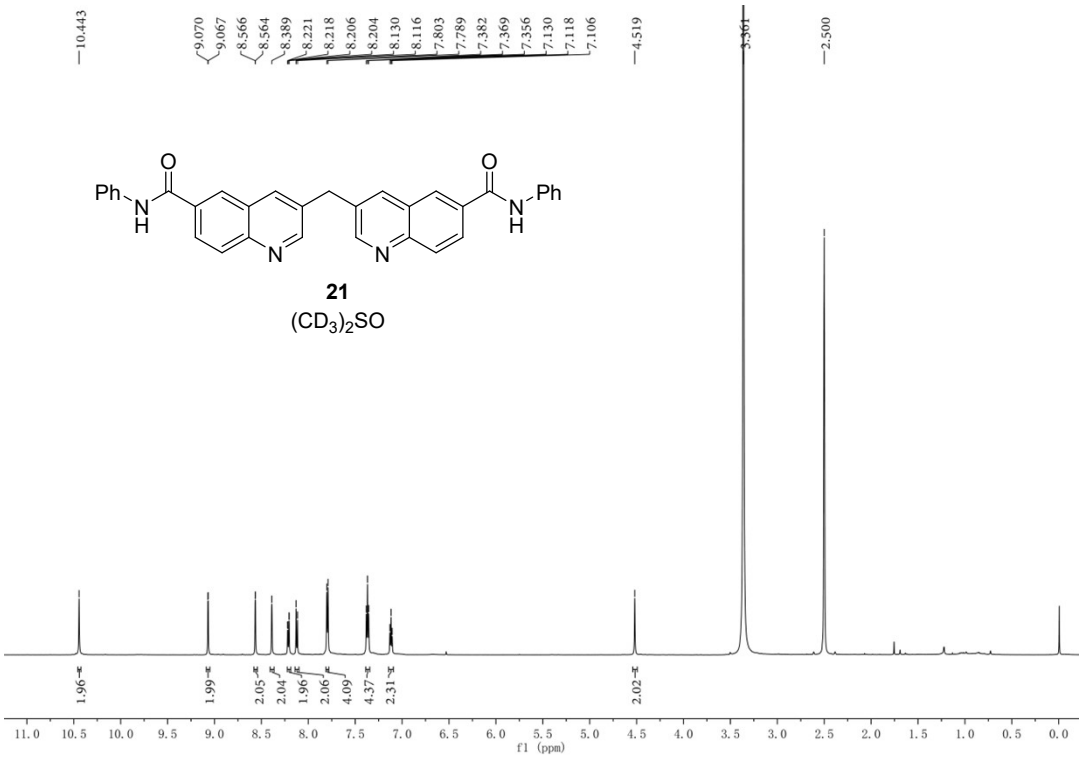


^{1}H NMR (600 MHz, $CDCl_3$):

^{13}C NMR (150 MHz, $CDCl_3$):

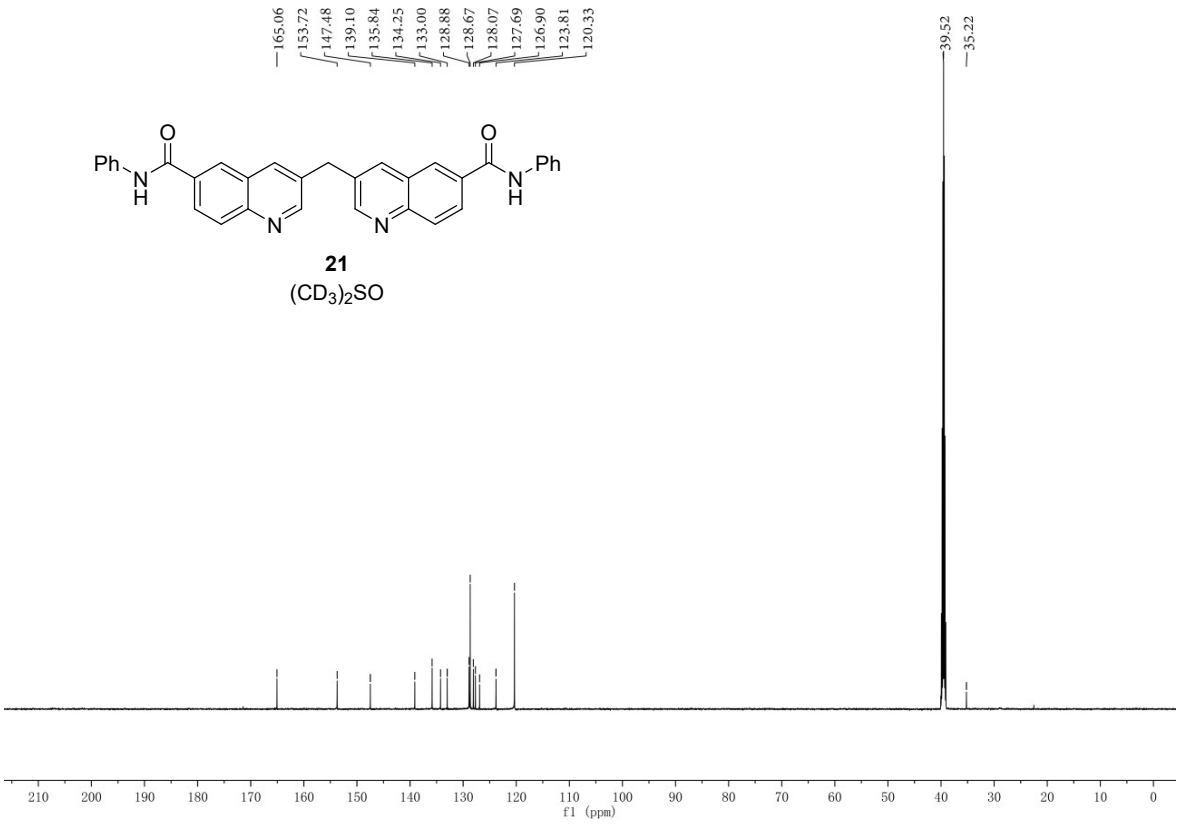


^{1}H NMR (600 MHz, $(CD_3)_2SO$):



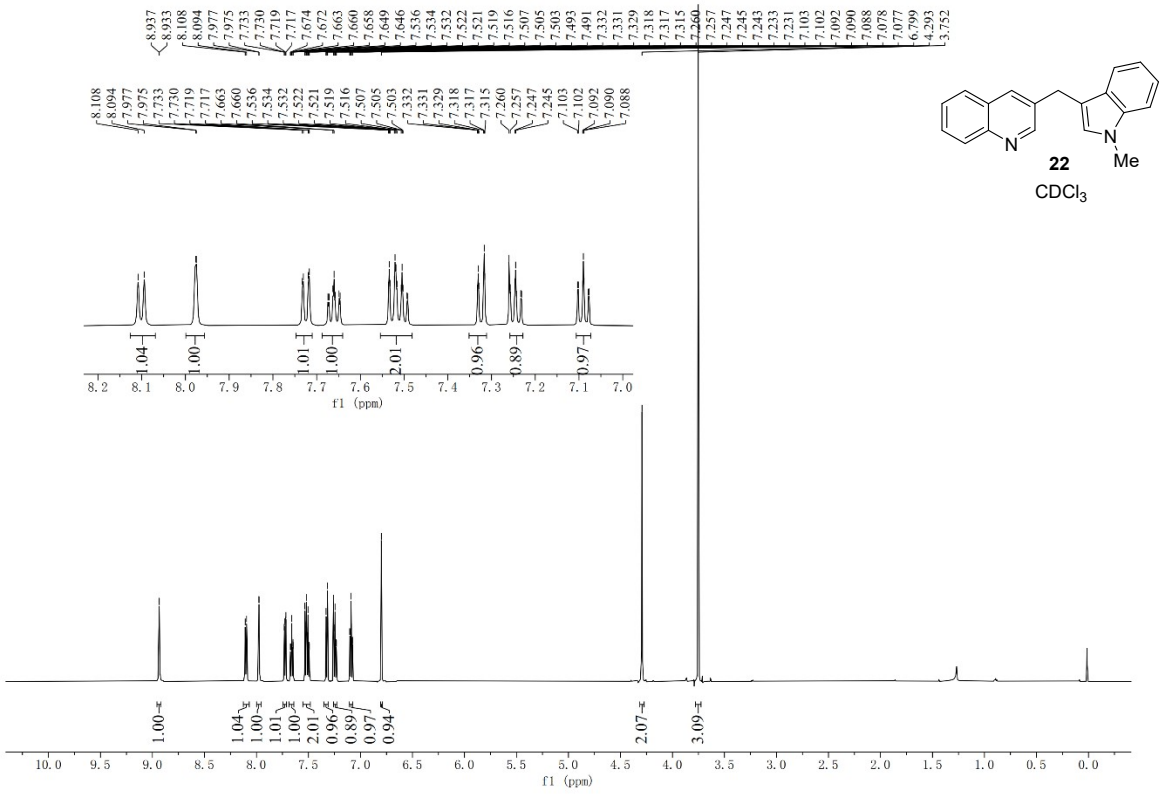
21
$(CD_3)_2SO$

^{13}C NMR (150 MHz, $(CD_3)_2SO$):

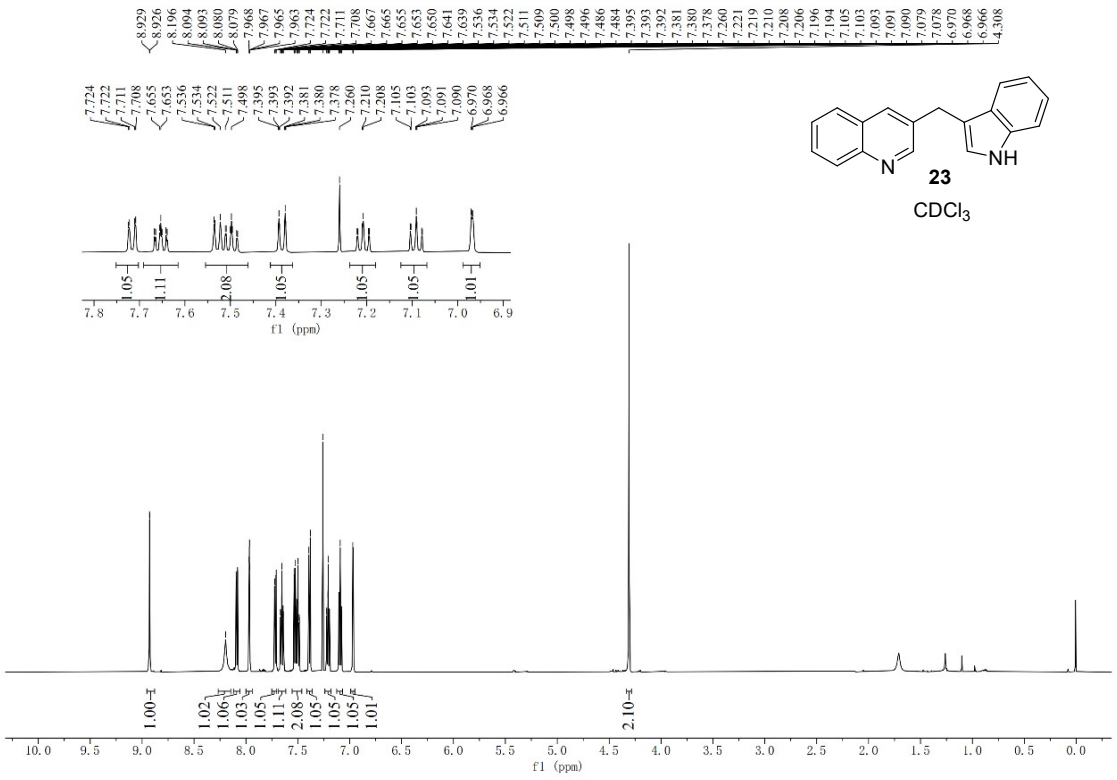


21
$(CD_3)_2SO$

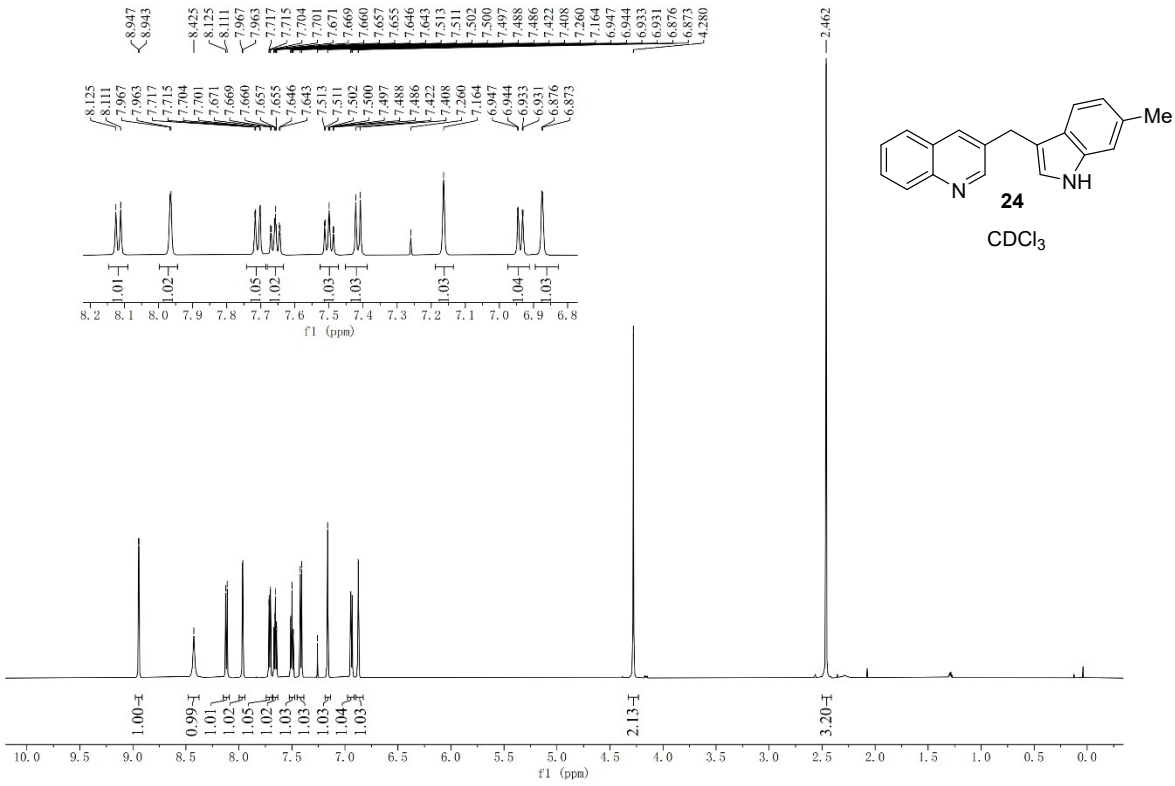
^{1}H NMR (600 MHz, $CDCl_3$):



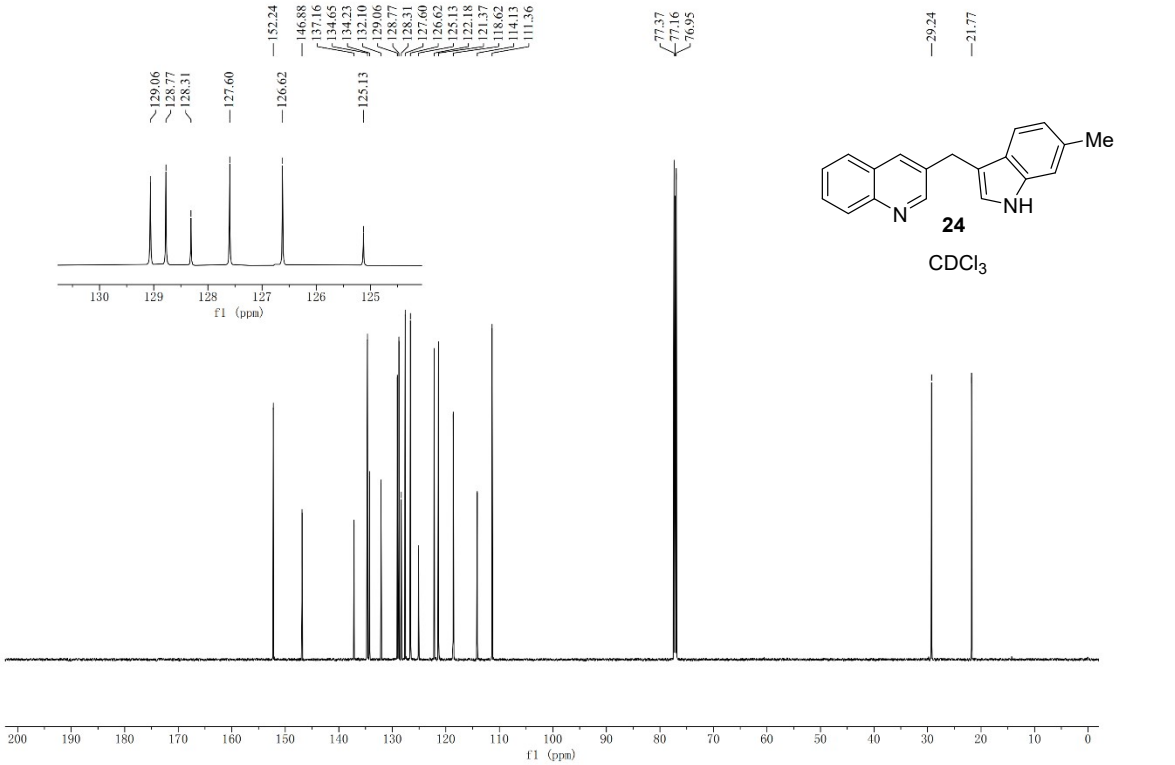
^{1}H NMR (600 MHz, $CDCl_3$):



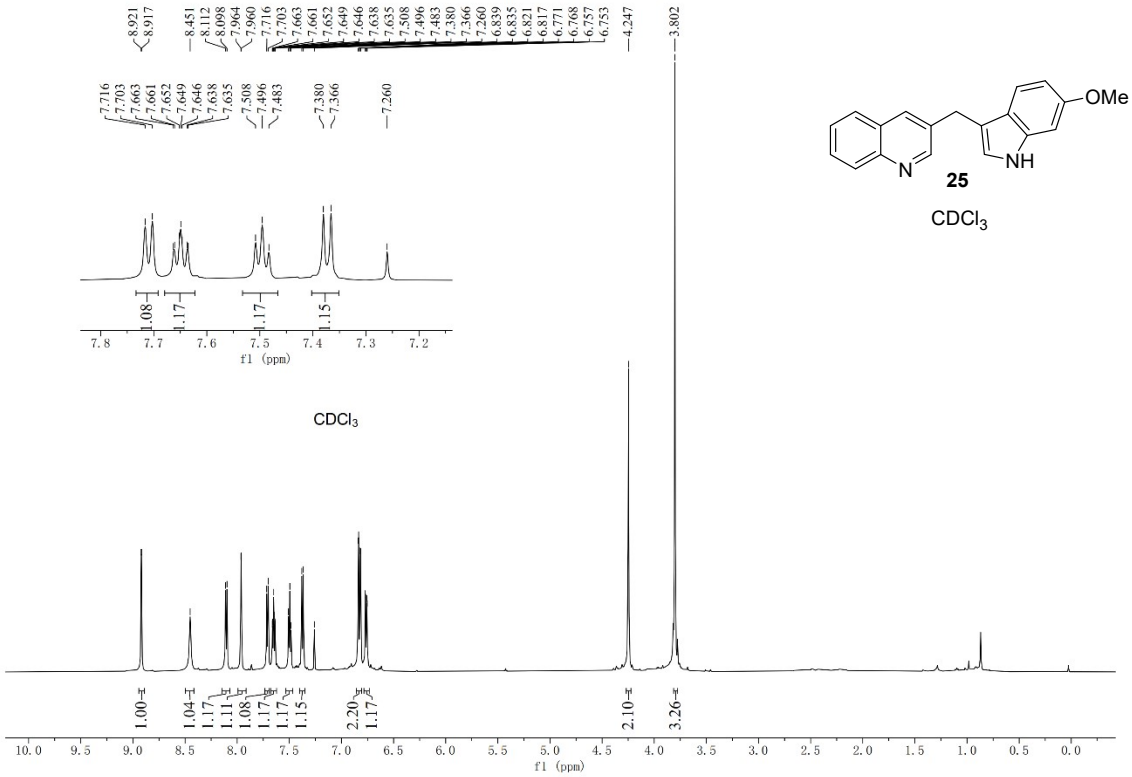
^{1}H NMR (600 MHz, $CDCl_3$):



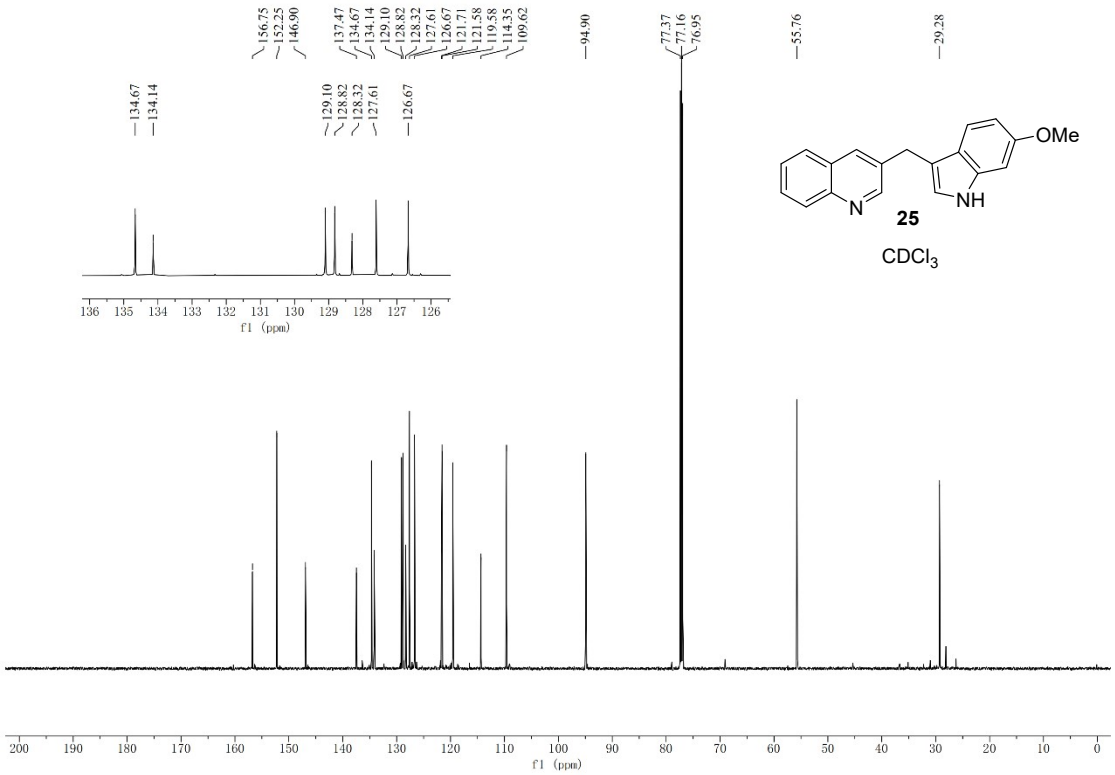
^{13}C NMR (150 MHz, $CDCl_3$):



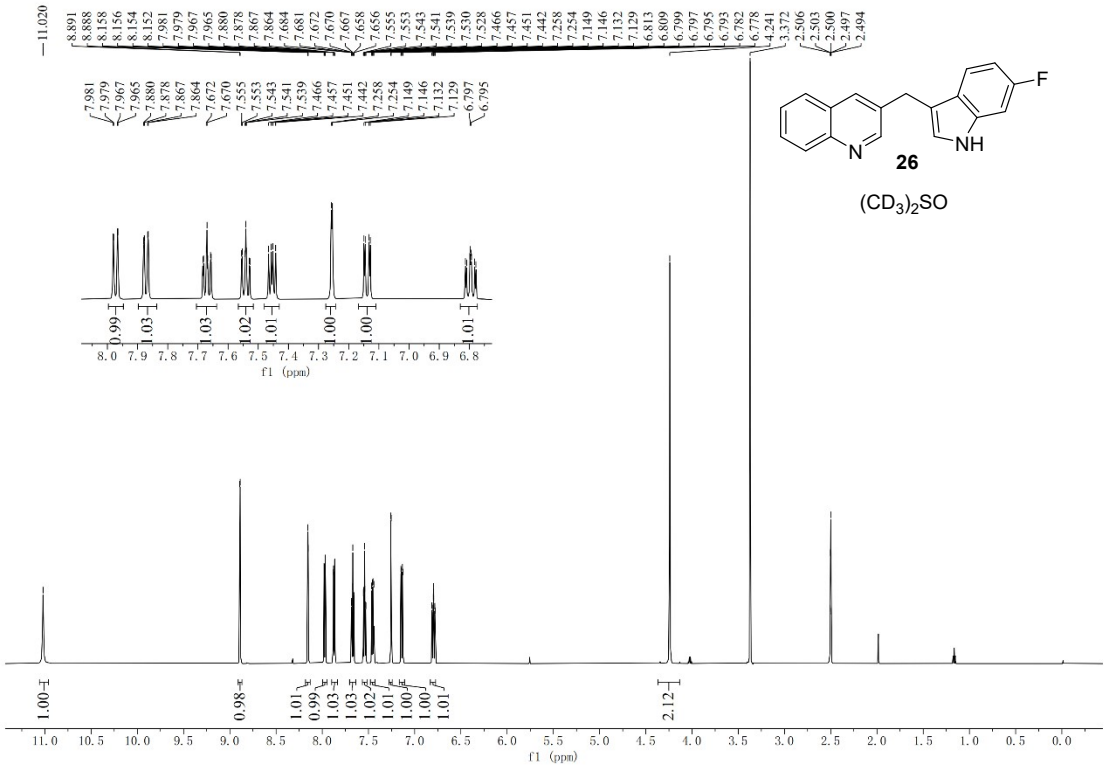
^{1}H NMR (600 MHz, $CDCl_3$):



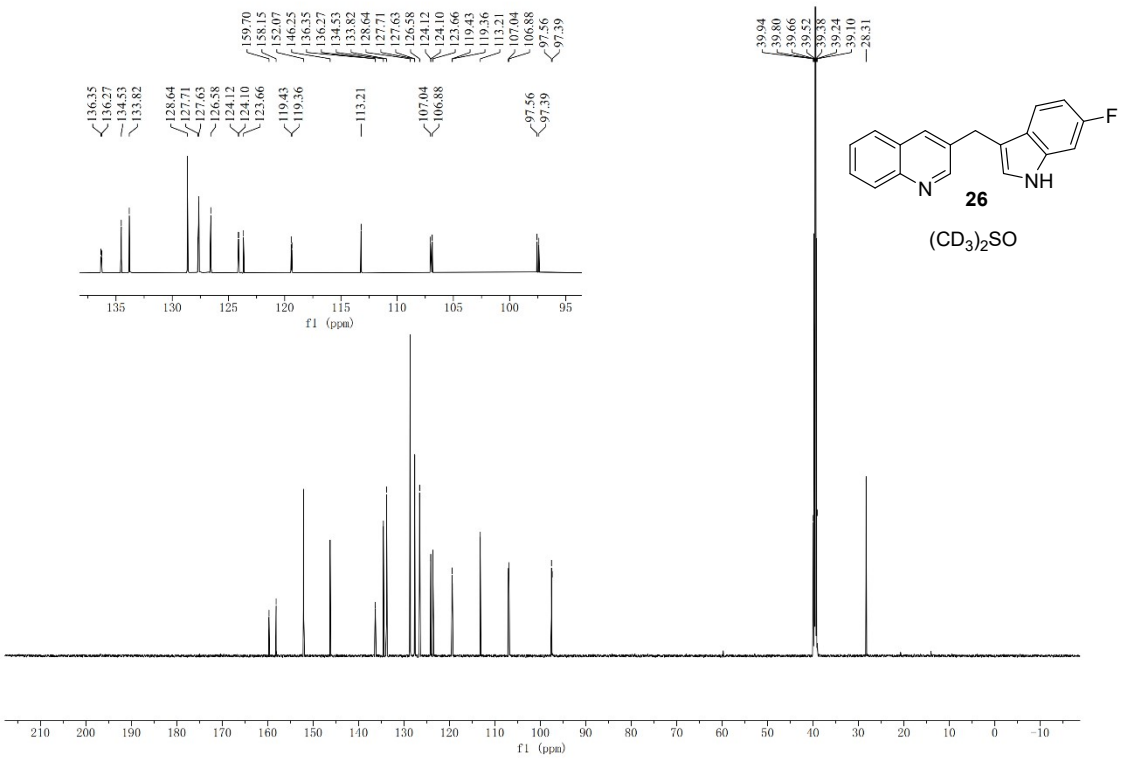
^{13}C NMR (150 MHz, $CDCl_3$):



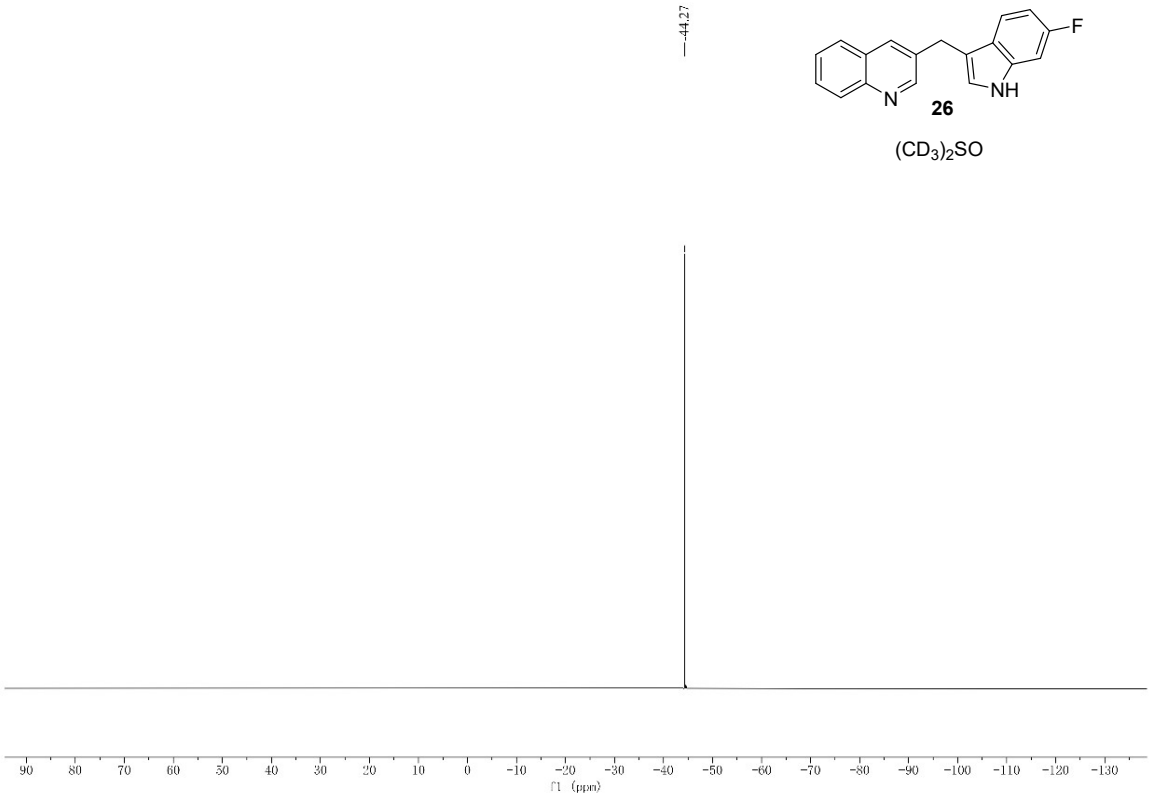
^{1}H NMR (600 MHz, $(CD_3)_2SO$):



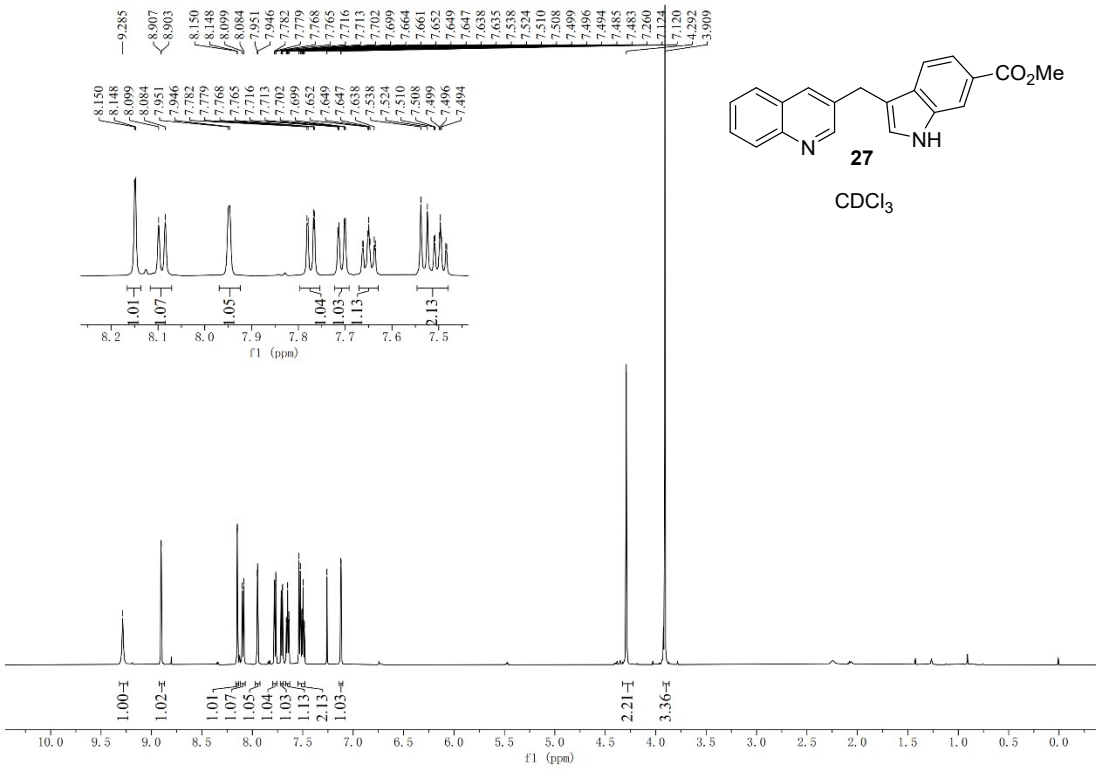
^{13}C NMR (150 MHz, $(CD_3)_2SO$):



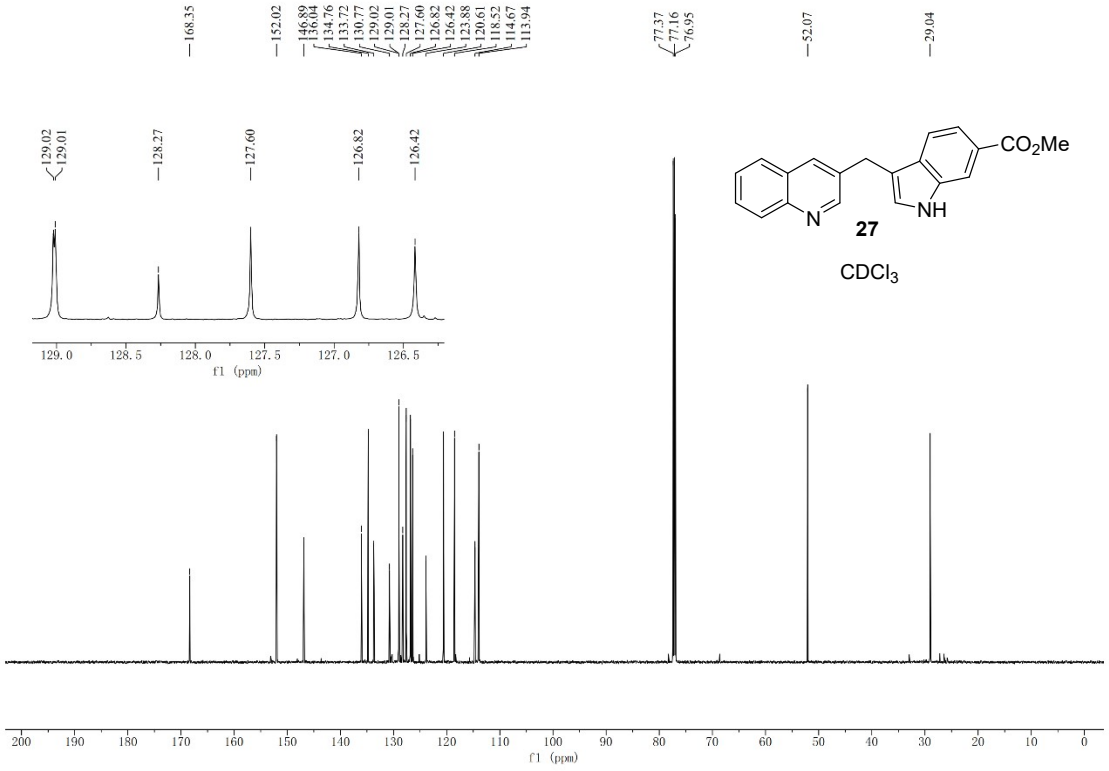
^{19}F NMR (564.5 MHz, $(CD_3)_2SO$):



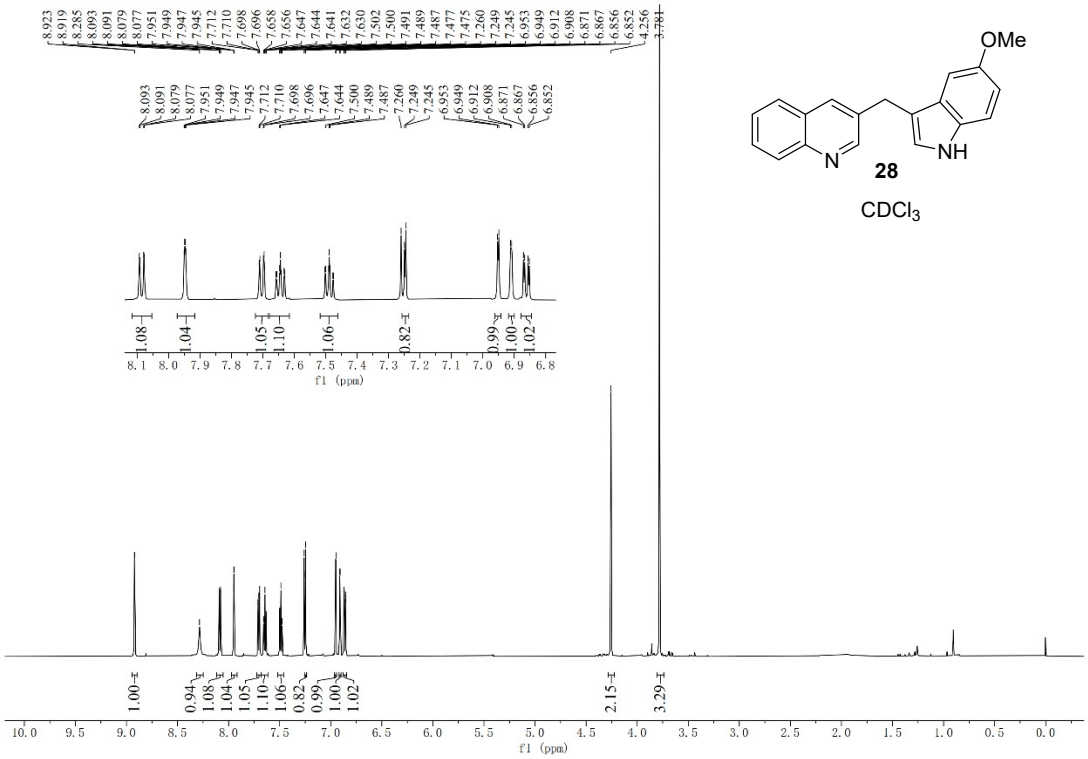
^{1}H NMR (600 MHz, $CDCl_3$):



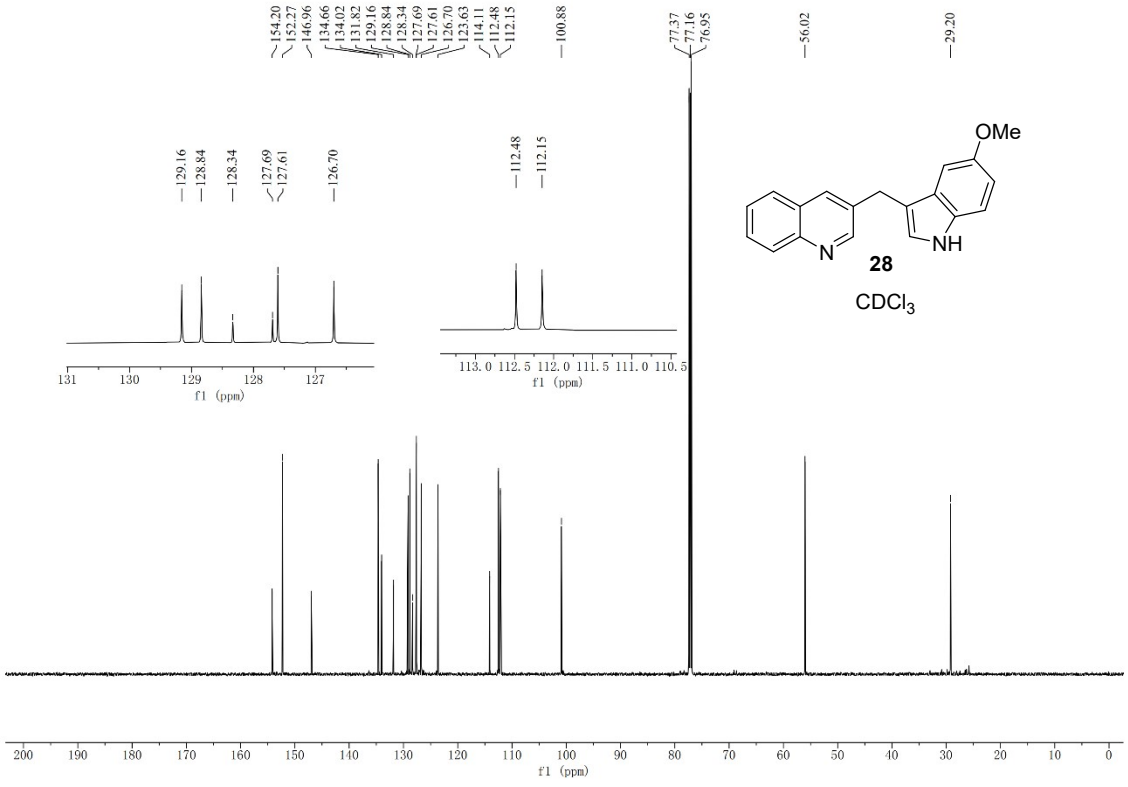
^{13}C NMR (150 MHz, $CDCl_3$):



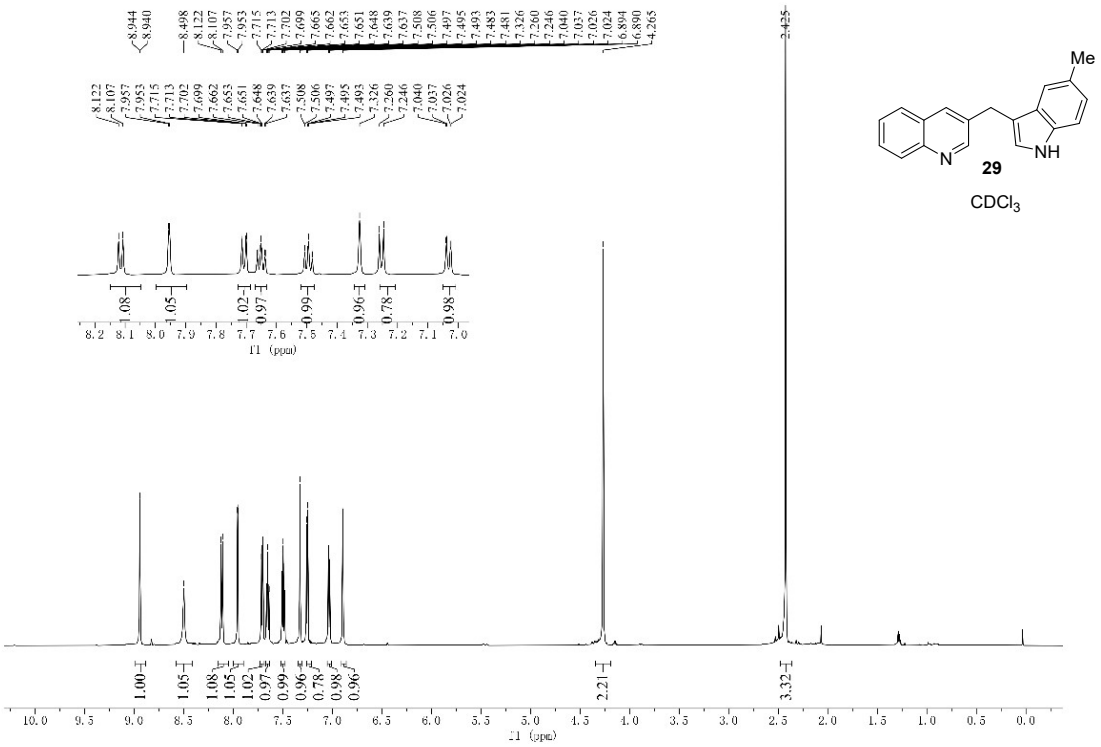
^{1}H NMR (600 MHz, $CDCl_3$):



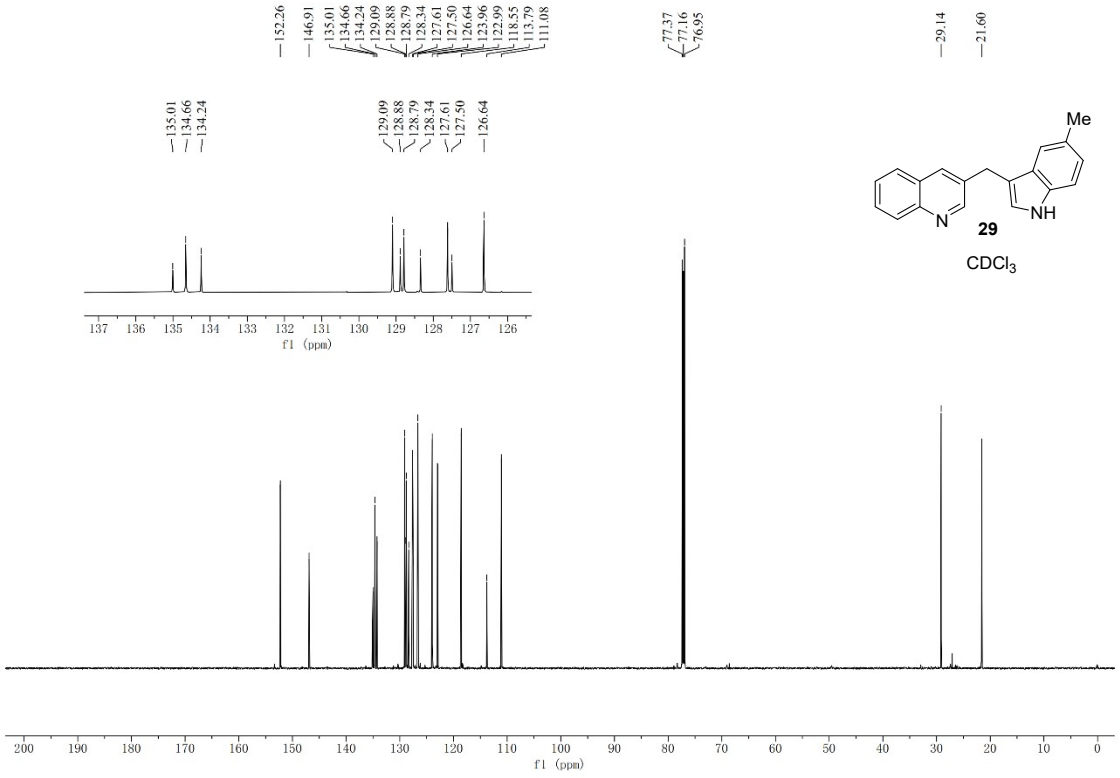
^{13}C NMR (150 MHz, $CDCl_3$):



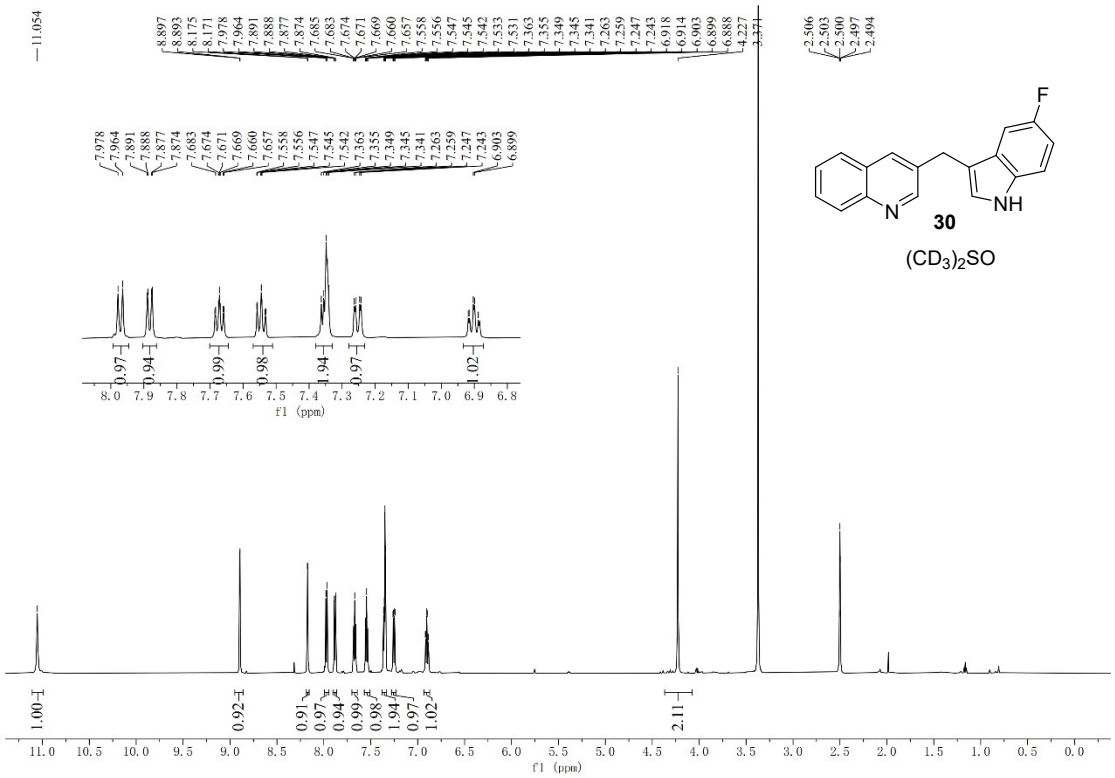
^{1}H NMR (600 MHz, $CDCl_3$):



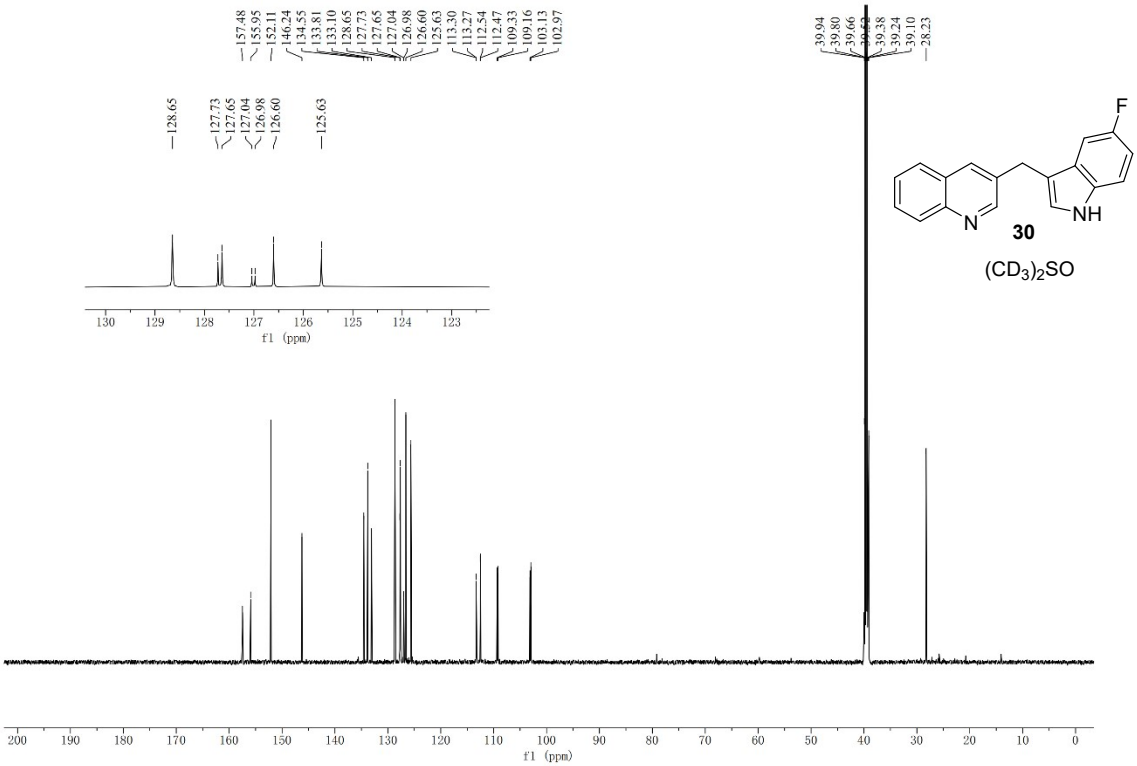
^{13}C NMR (150 MHz, $CDCl_3$):



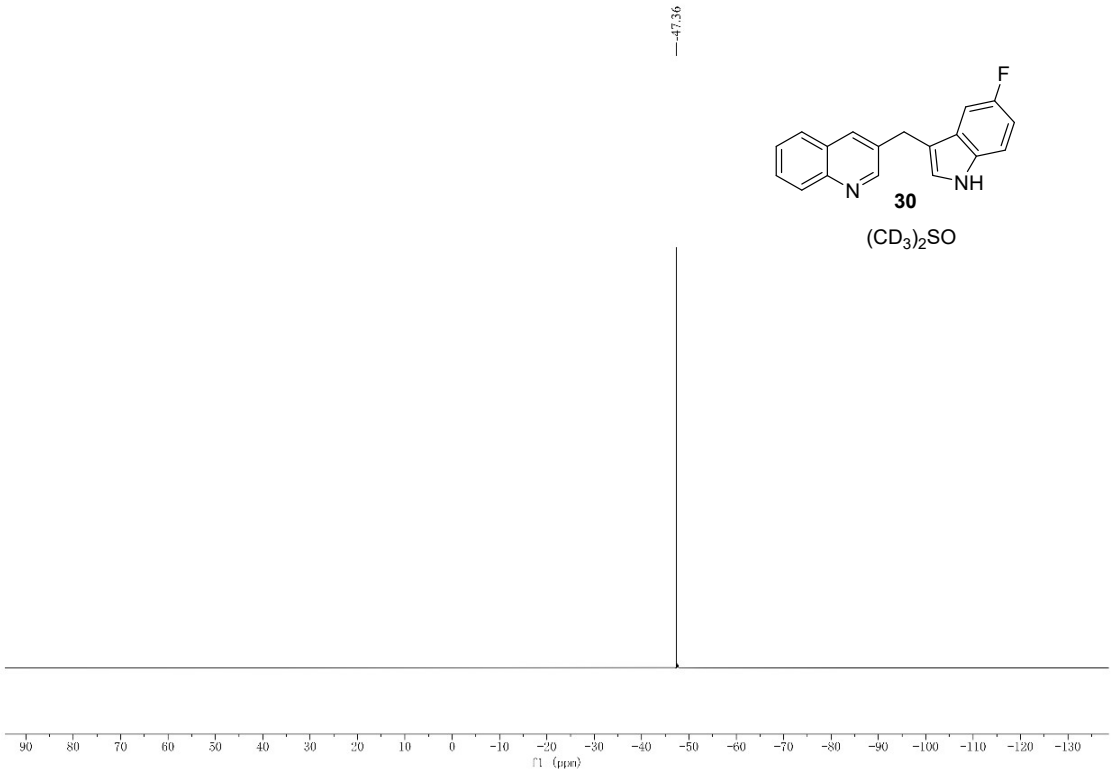
^{1}H NMR (600 MHz, $(CD_3)_2SO$):



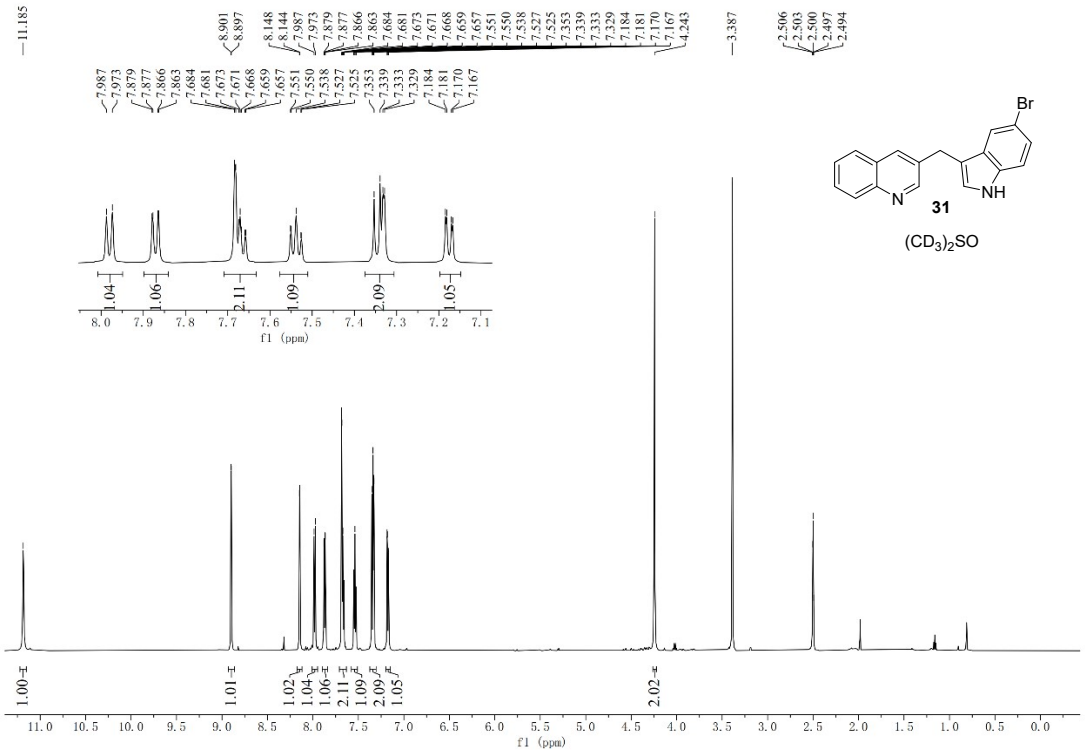
^{13}C NMR (150 MHz, $(CD_3)_2SO$):



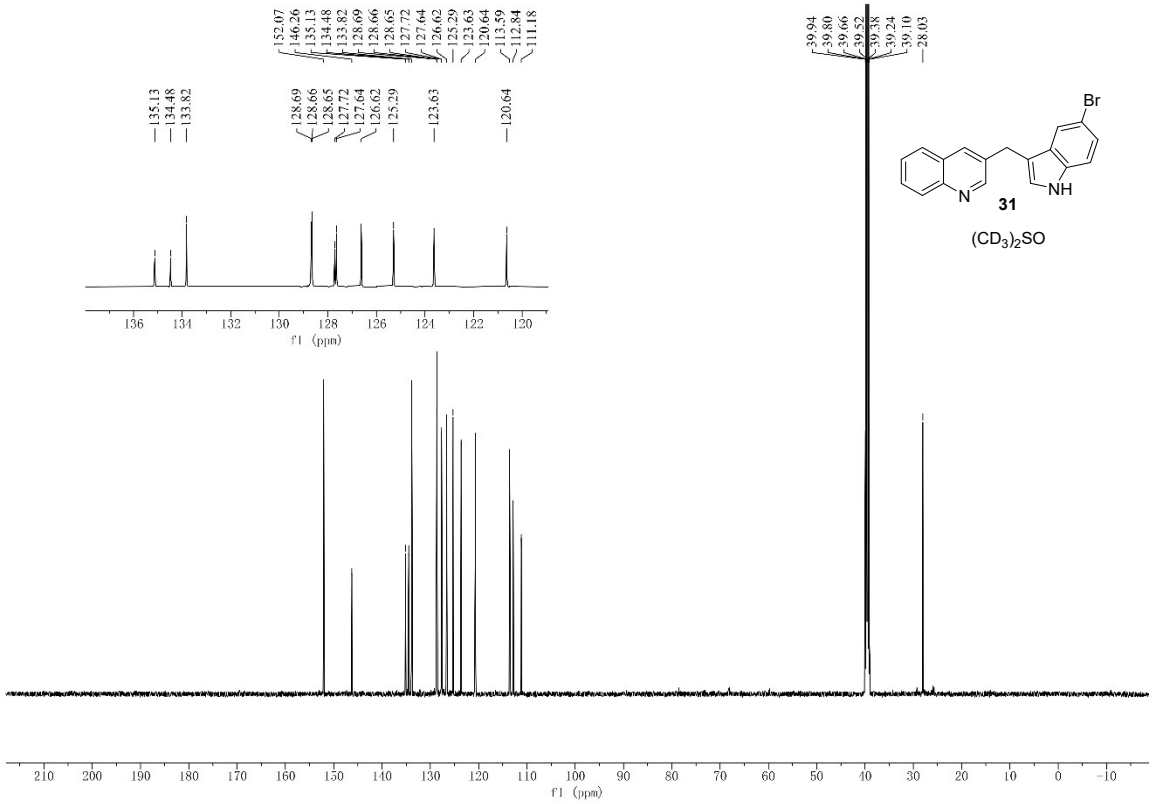
^{19}F NMR (564.5 MHz, $(CD_3)_2SO$):



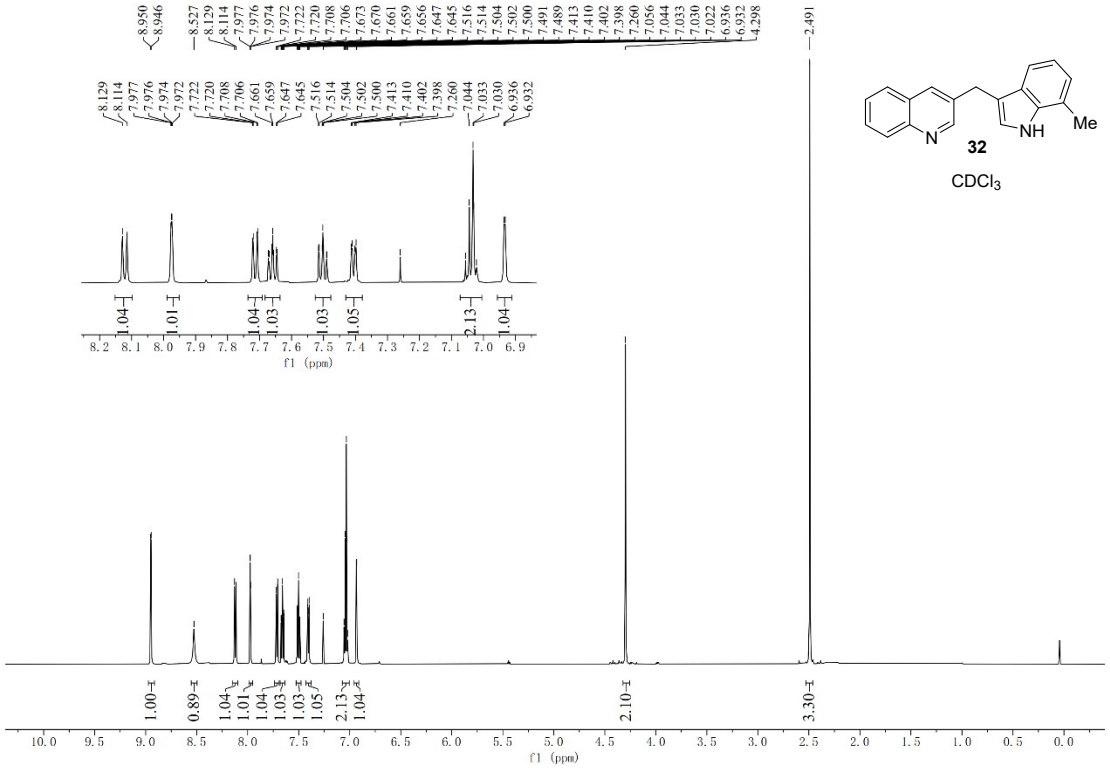
^{1}H NMR (600 MHz, $(CD_3)_2SO$):



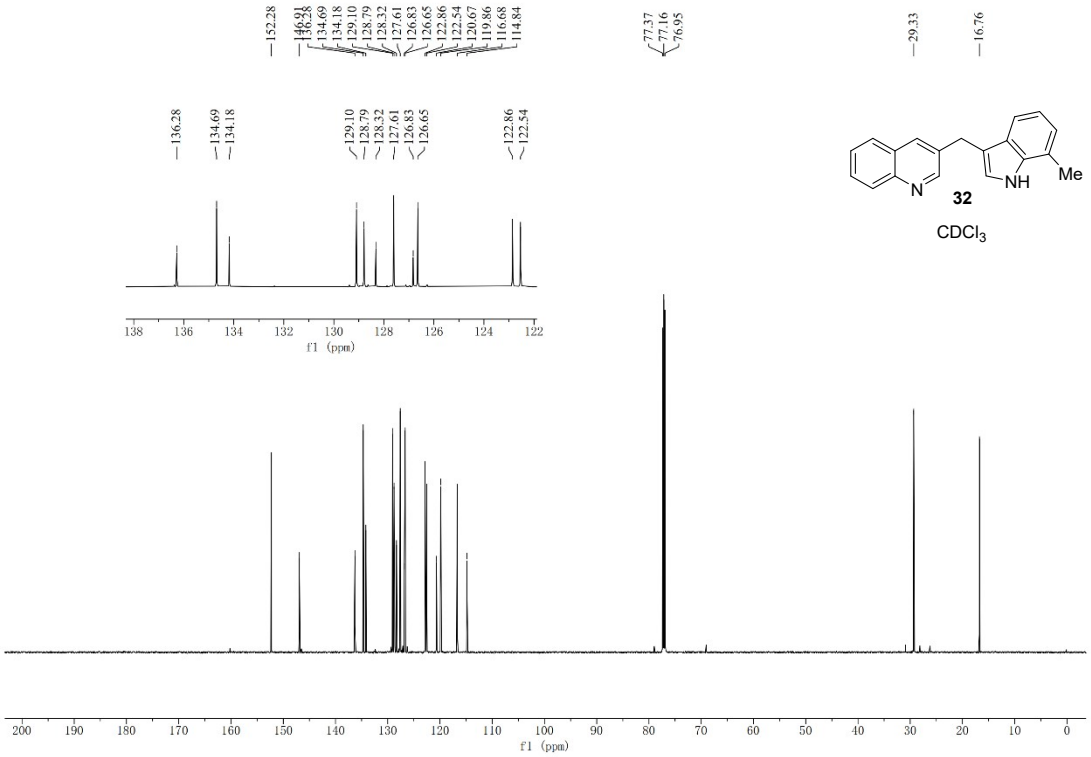
^{13}C NMR (150 MHz, $(CD_3)_2SO$):



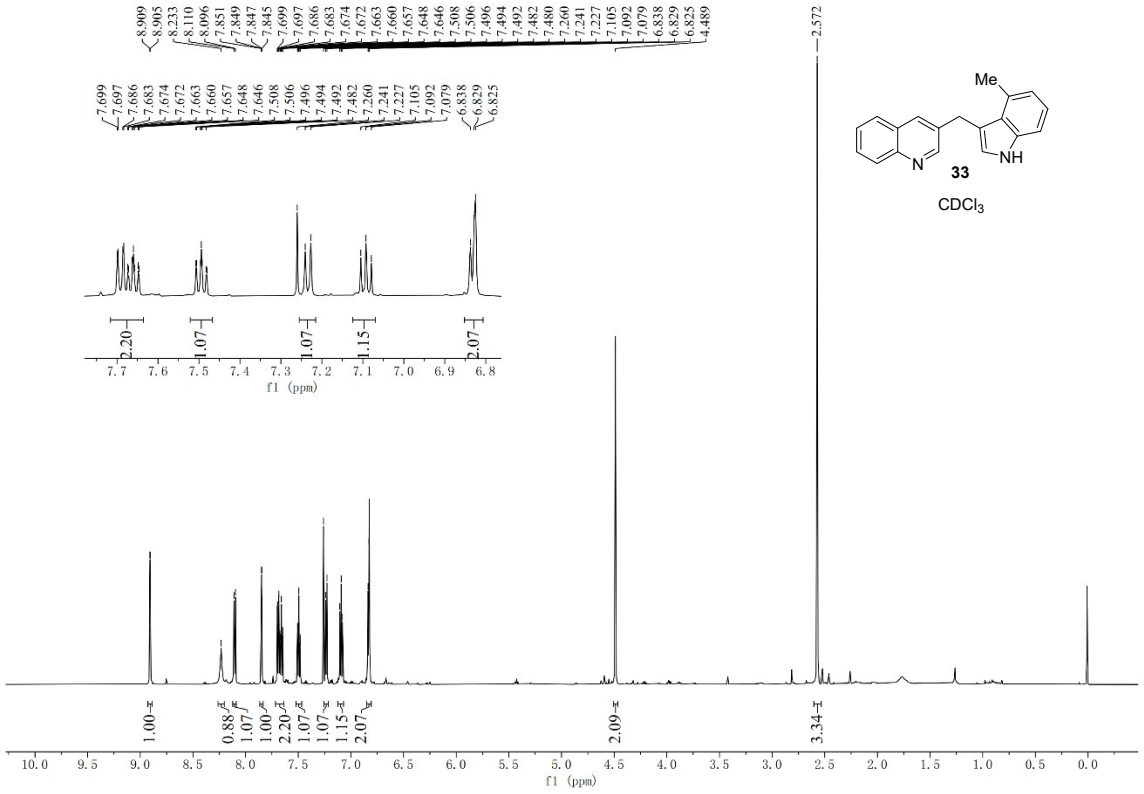
^{1}H NMR (600 MHz, $CDCl_3$):



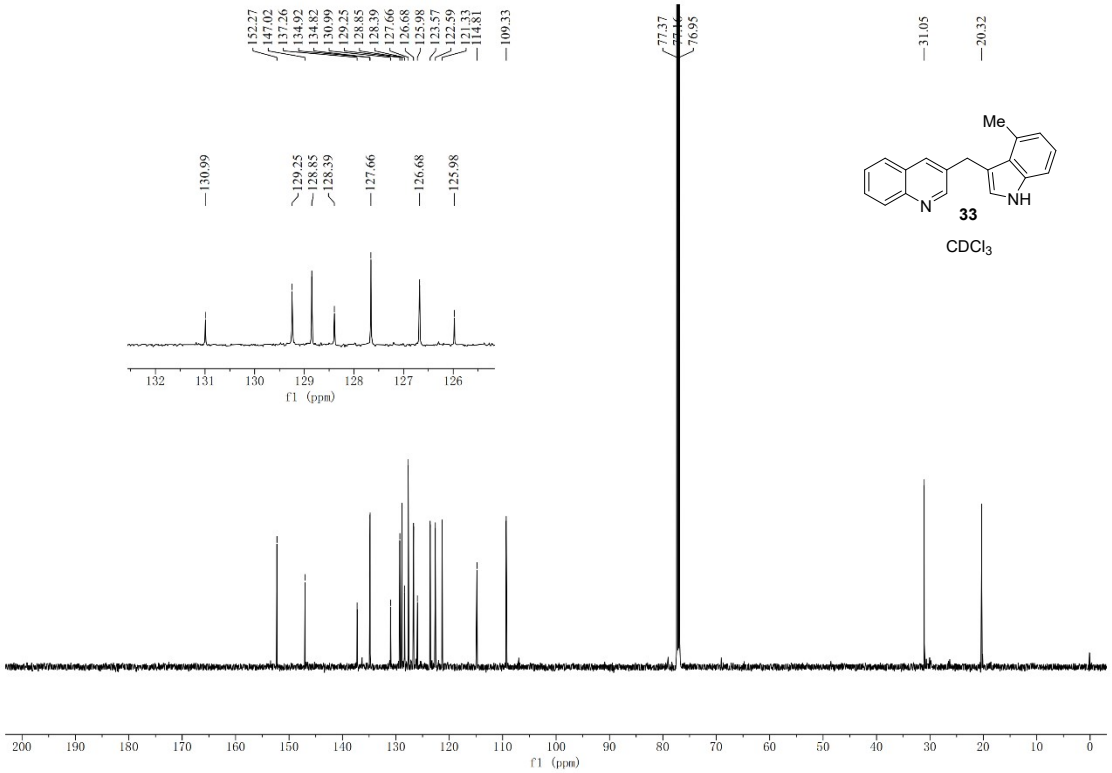
^{13}C NMR (150 MHz, $CDCl_3$):



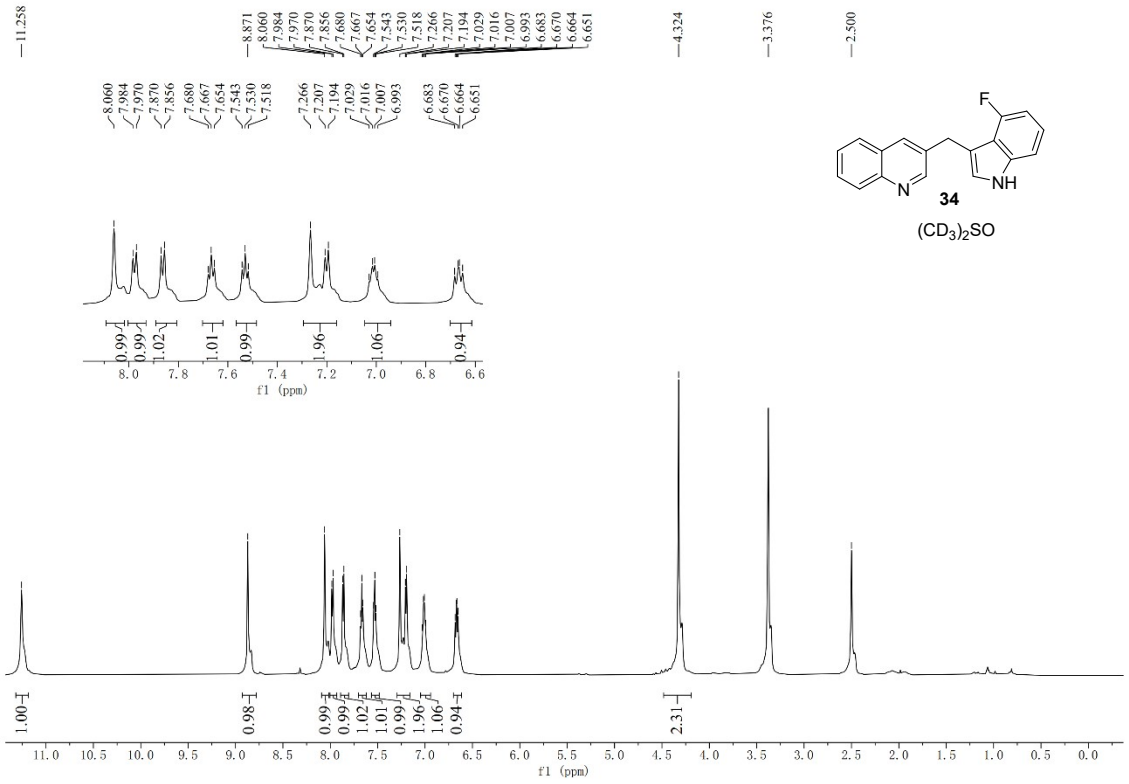
^{1}H NMR (600 MHz, $CDCl_3$):



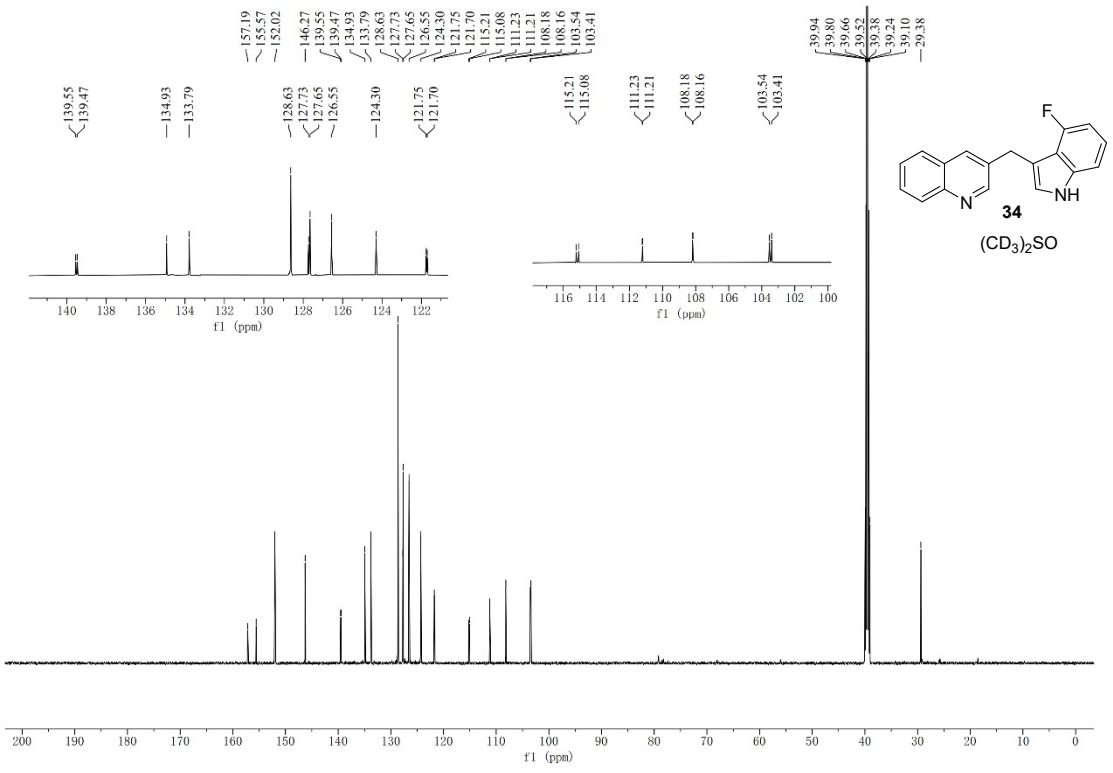
^{13}C NMR (150 MHz, $CDCl_3$):



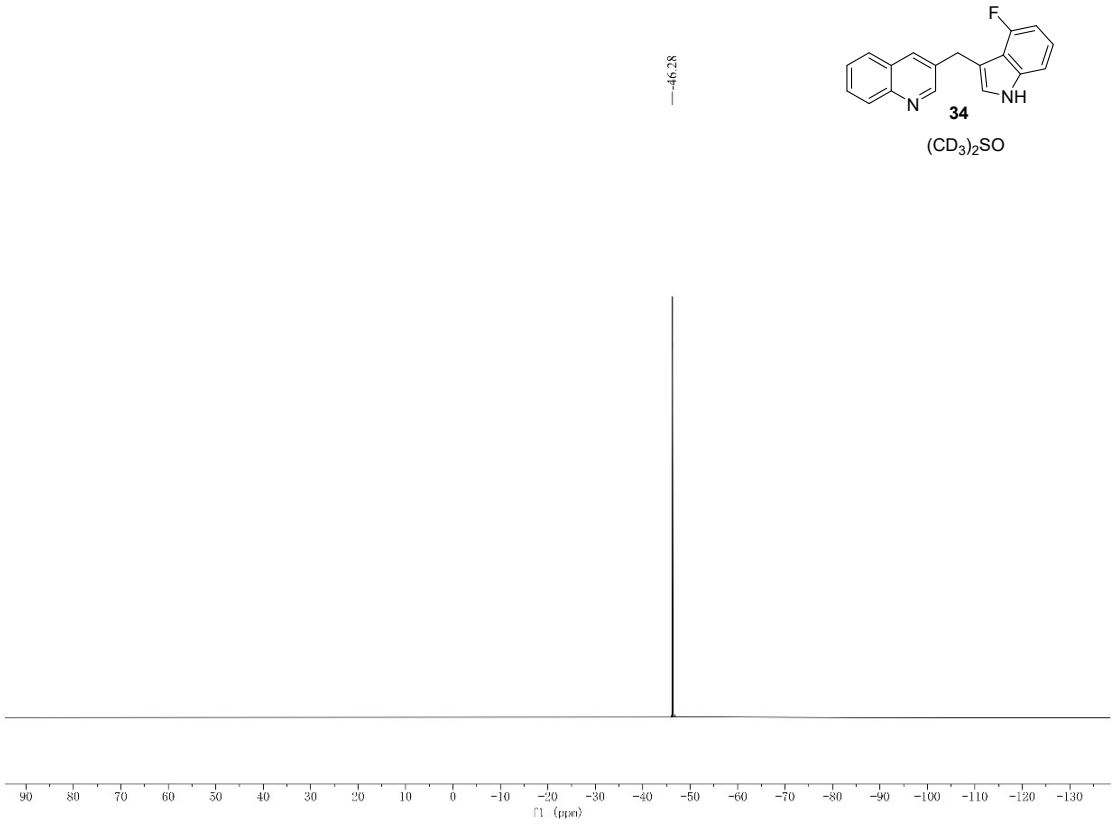
^{1}H NMR (600 MHz, $(CD_3)_2SO$):



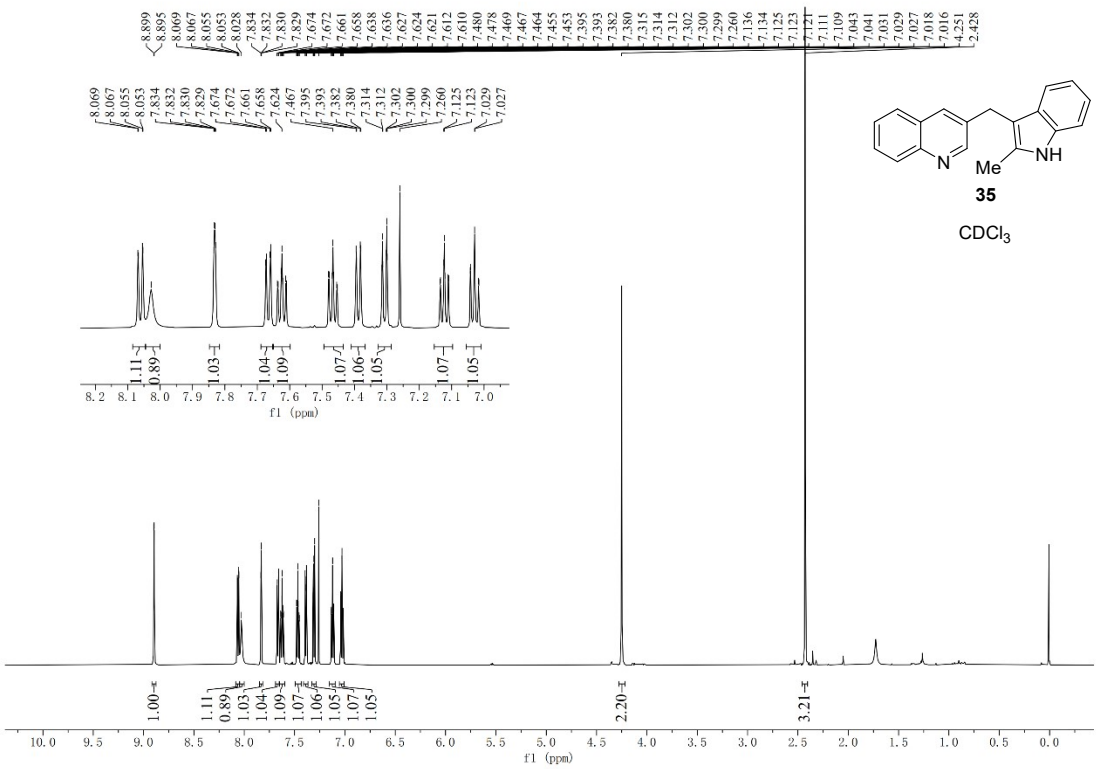
^{13}C NMR (150 MHz, $(CD_3)_2SO$):



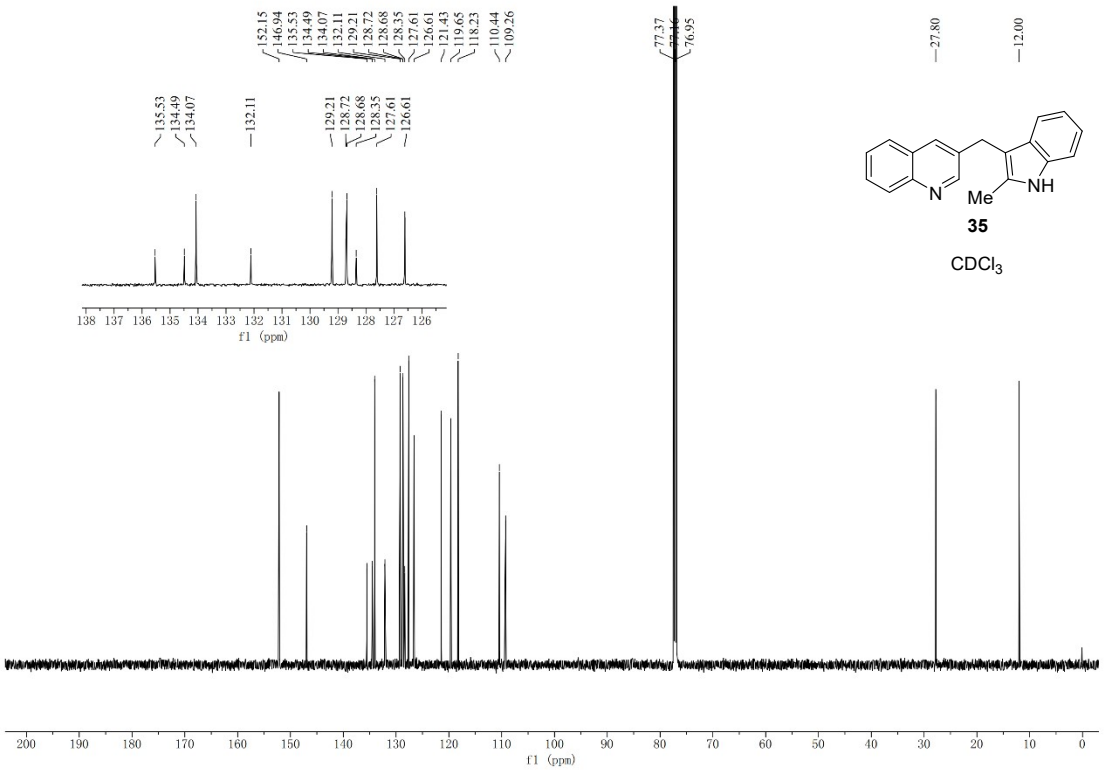
^{19}F NMR (564.5 MHz, $(CD_3)_2SO$):



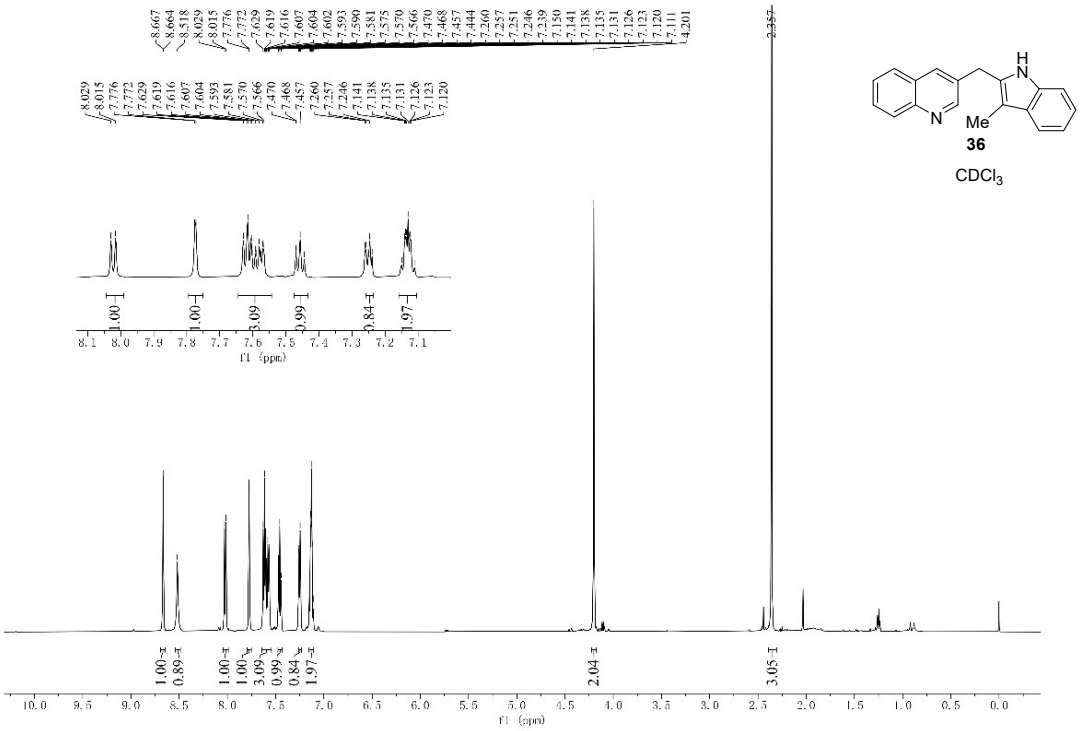
^{1}H NMR (600 MHz, $CDCl_3$):



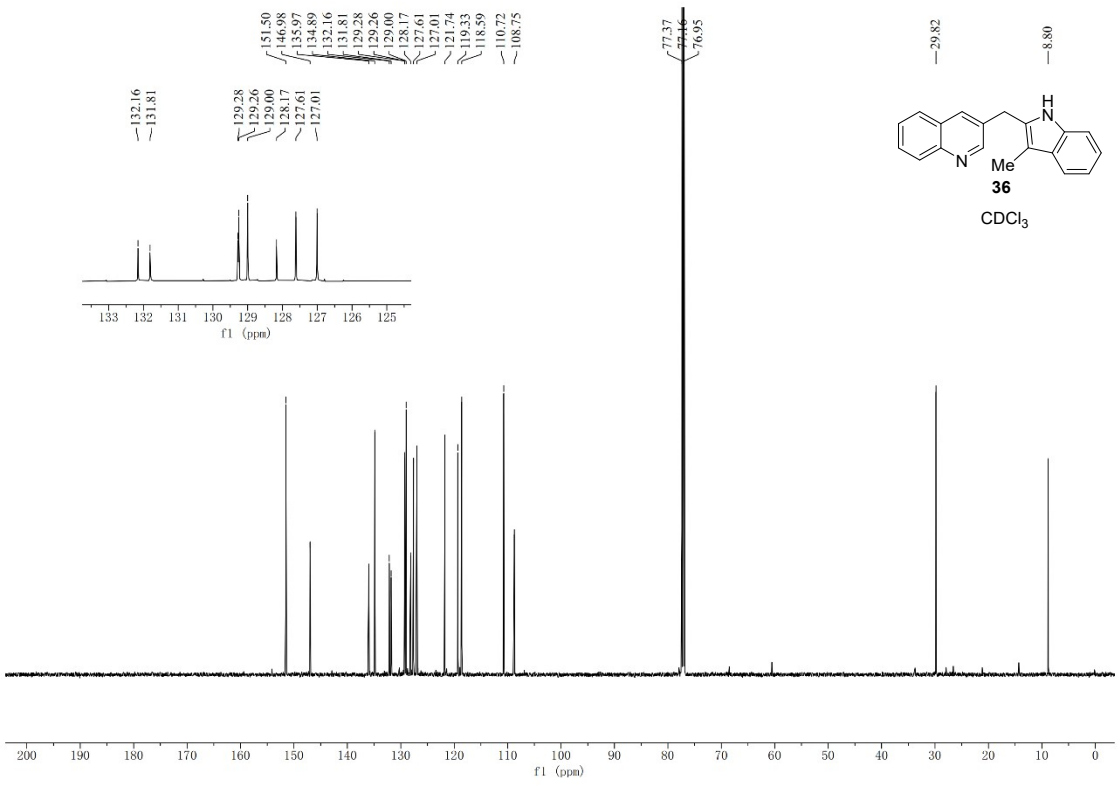
^{13}C NMR (150 MHz, $CDCl_3$):



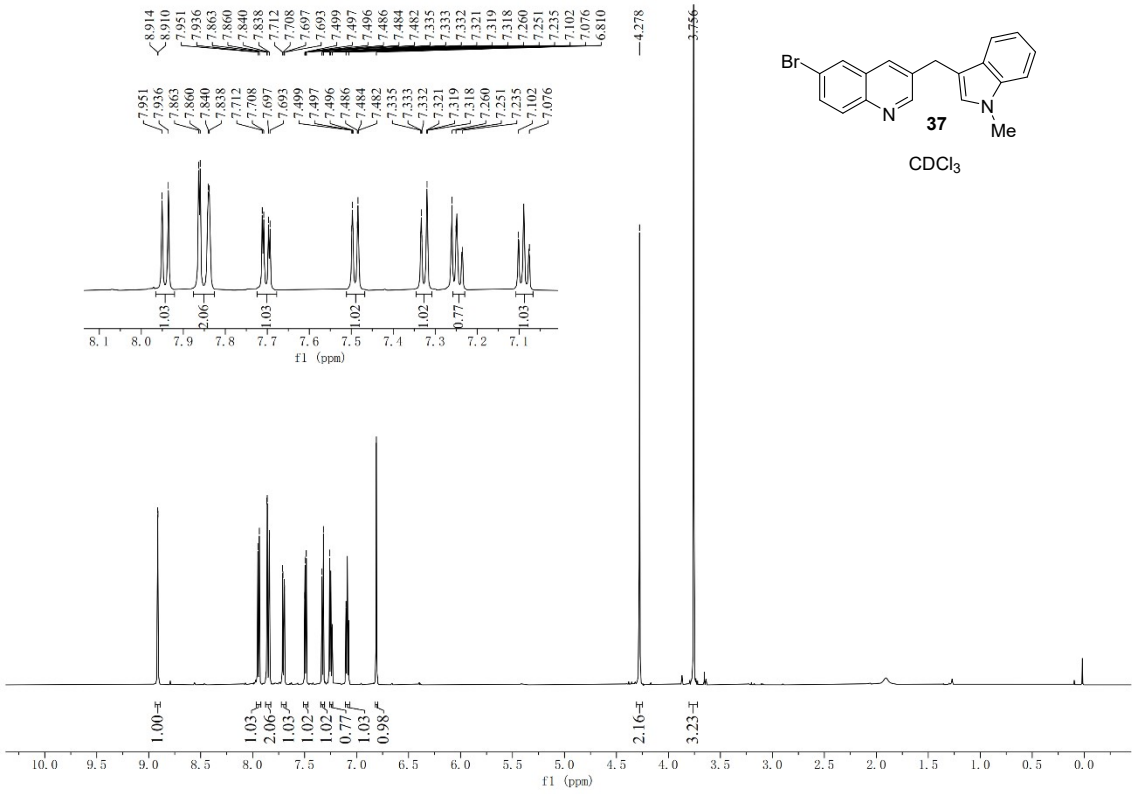
^{1}H NMR (600 MHz, $CDCl_3$):



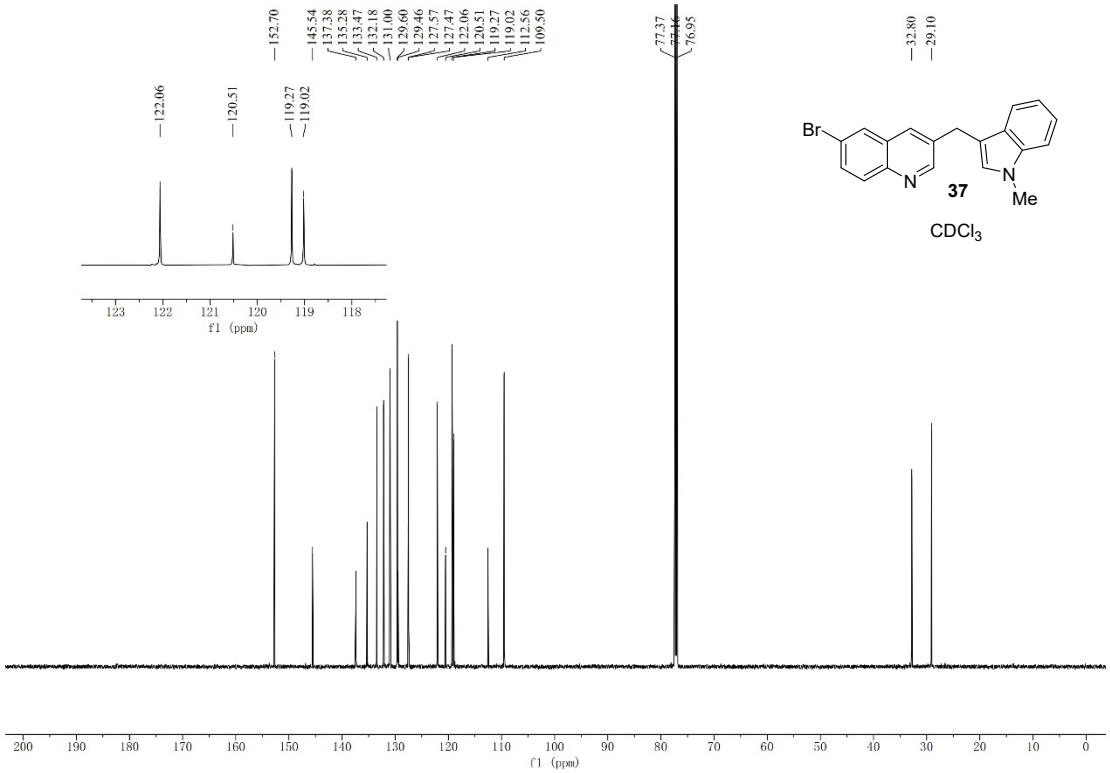
^{13}C NMR (150 MHz, $CDCl_3$):



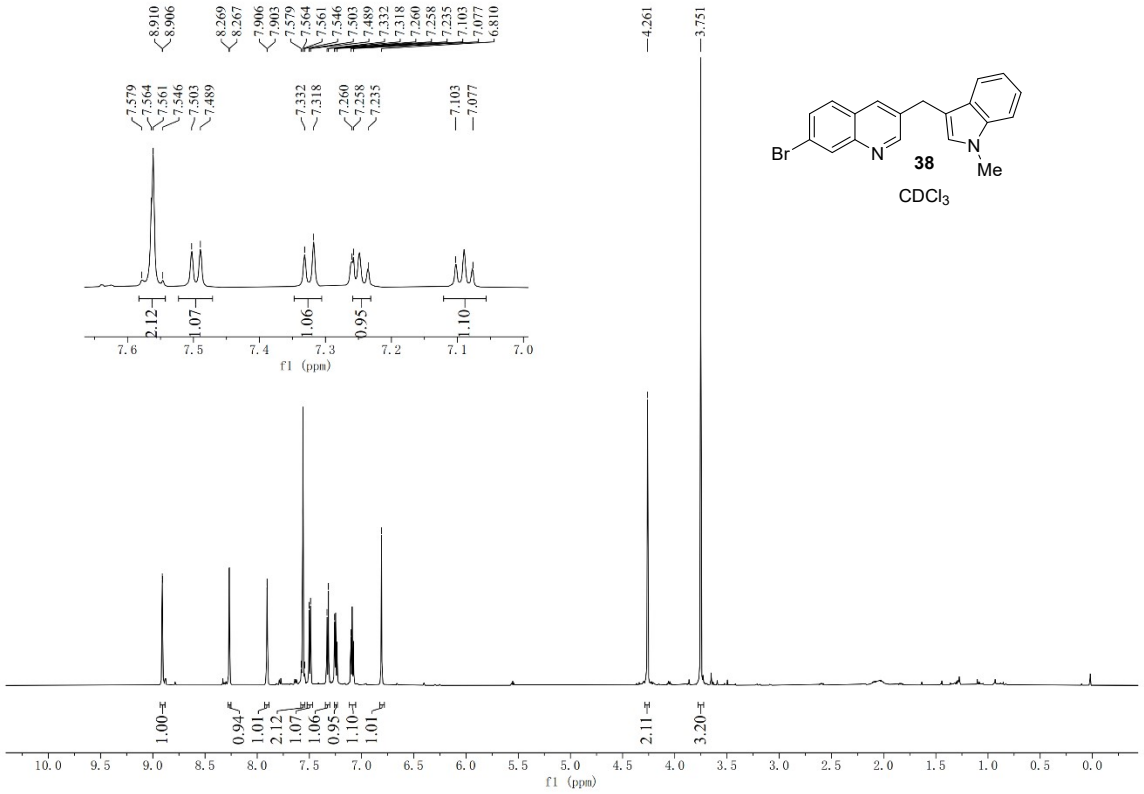
^{1}H NMR (600 MHz, $CDCl_3$):



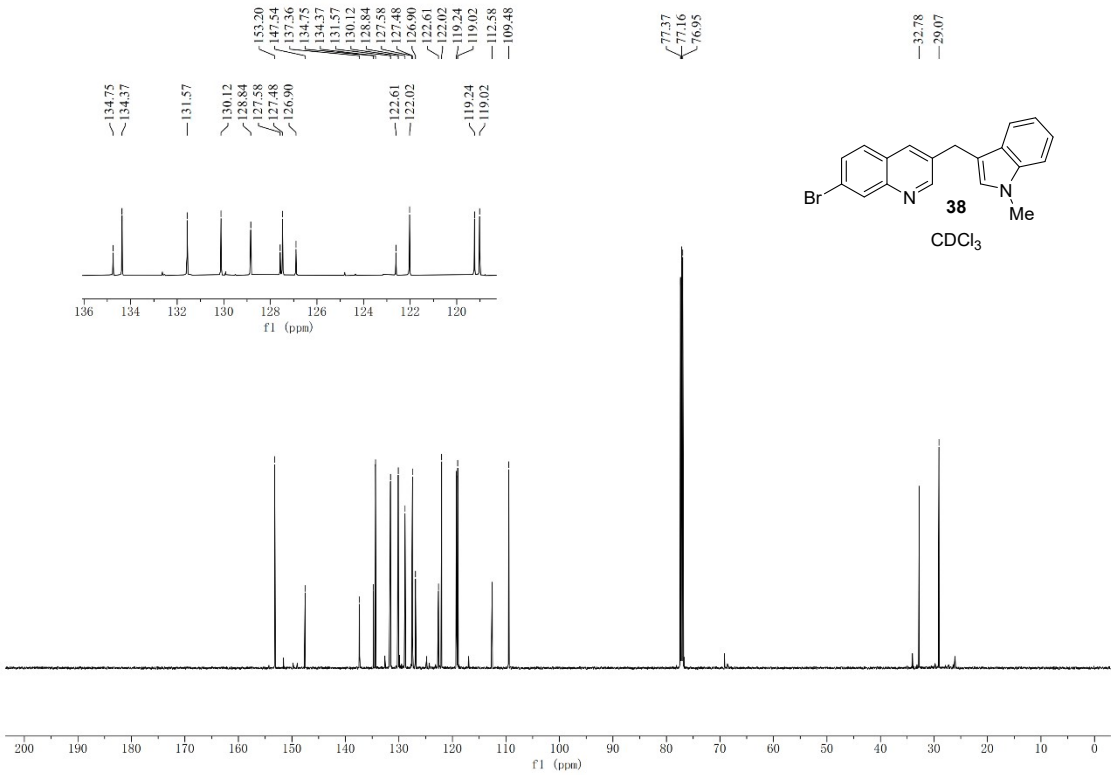
^{13}C NMR (150 MHz, $CDCl_3$):



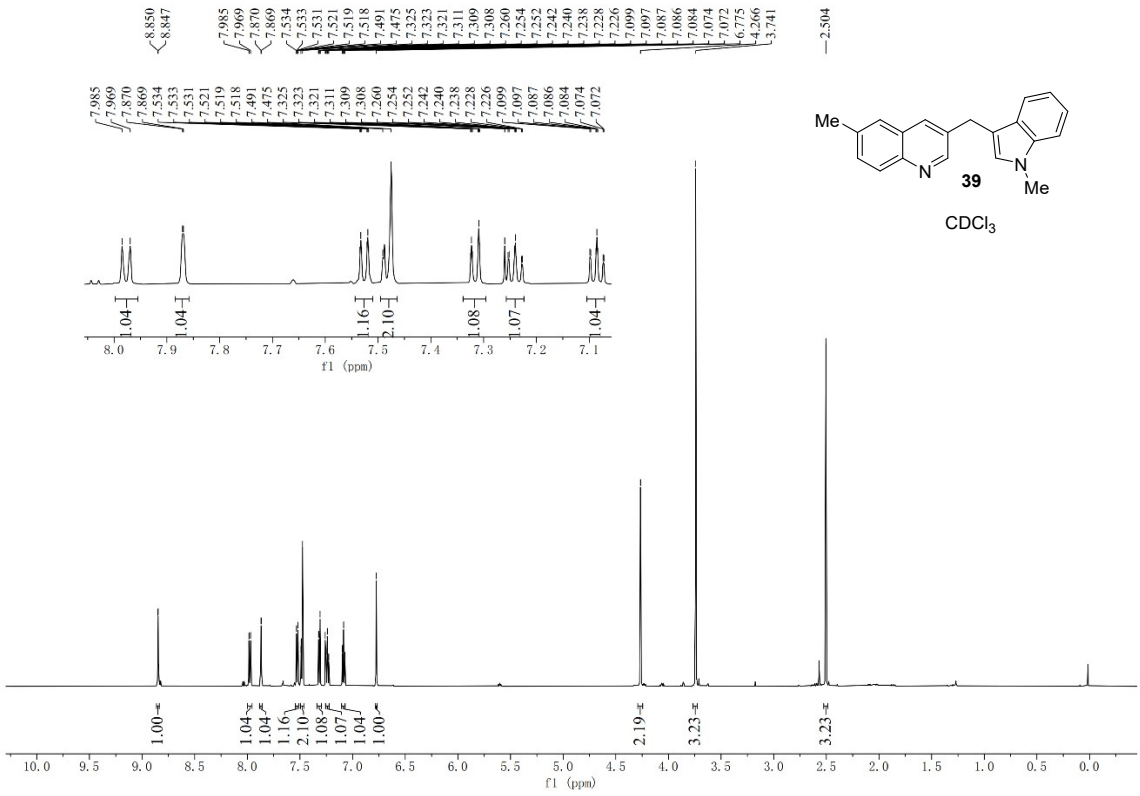
^{1}H NMR (600 MHz, $CDCl_3$):



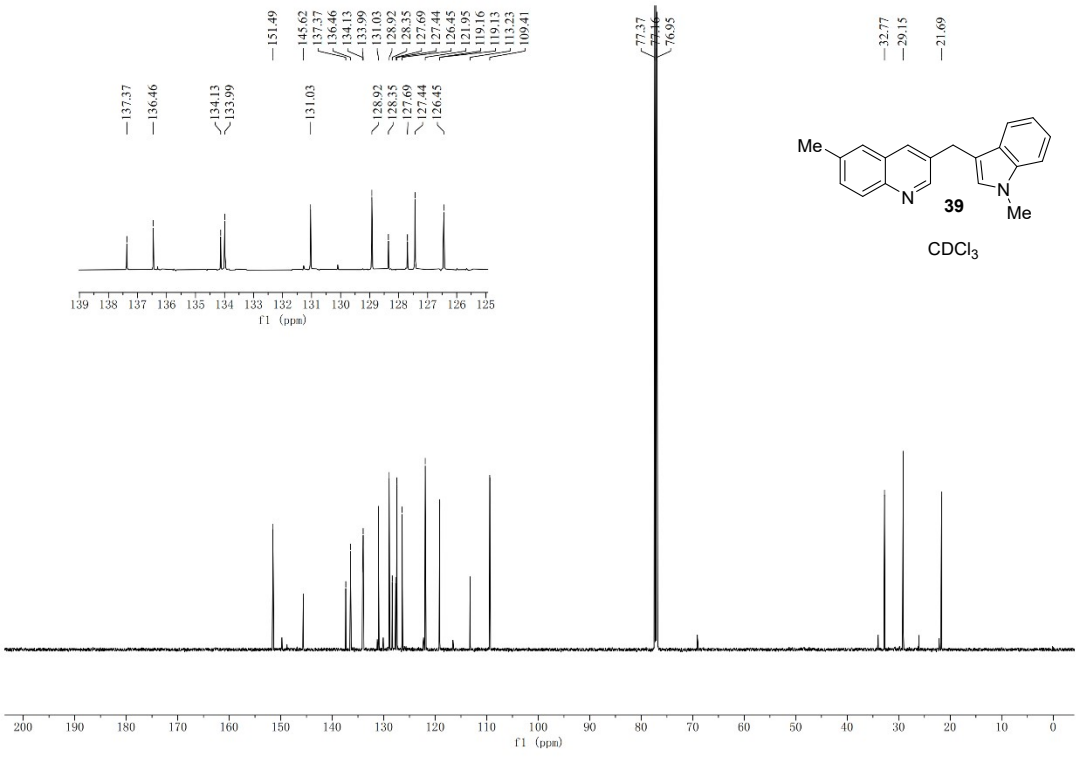
^{13}C NMR (150 MHz, $CDCl_3$):



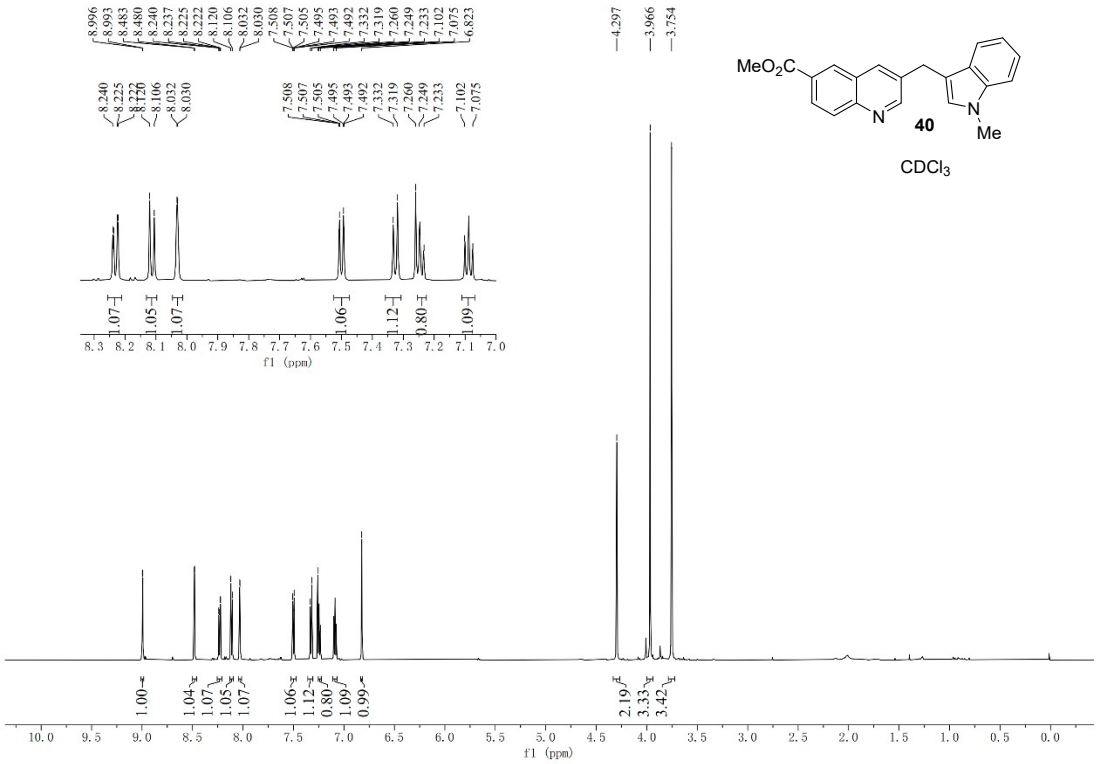
^{1}H NMR (600 MHz, $CDCl_3$):



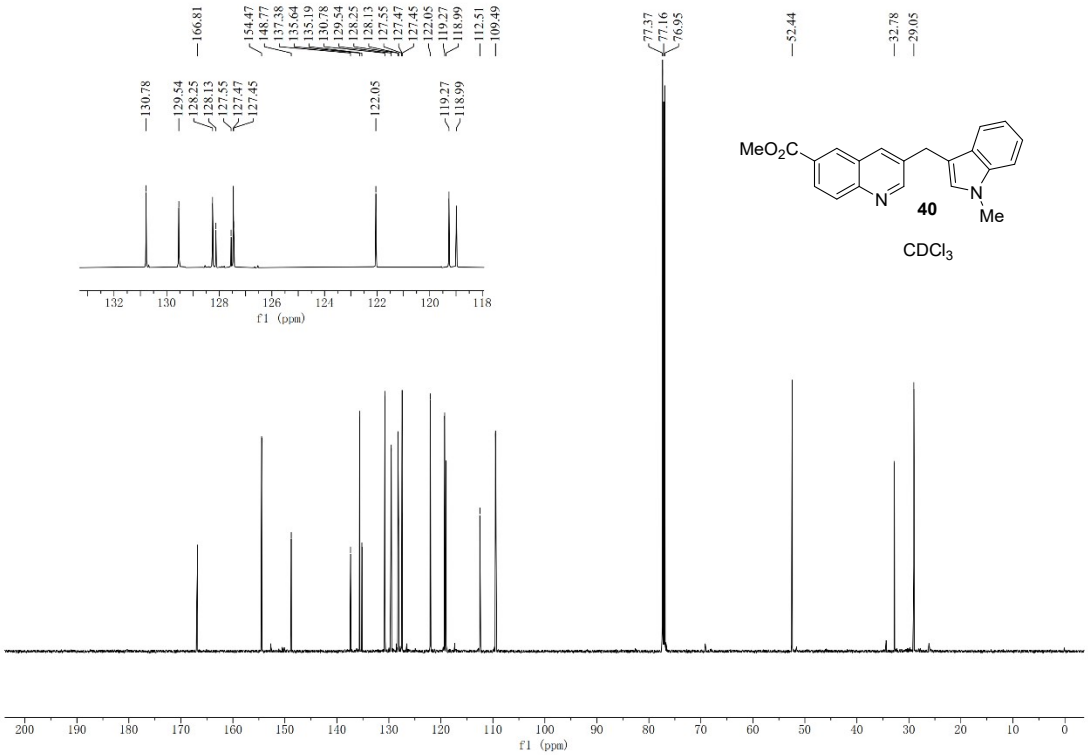
^{13}C NMR (150 MHz, $CDCl_3$):



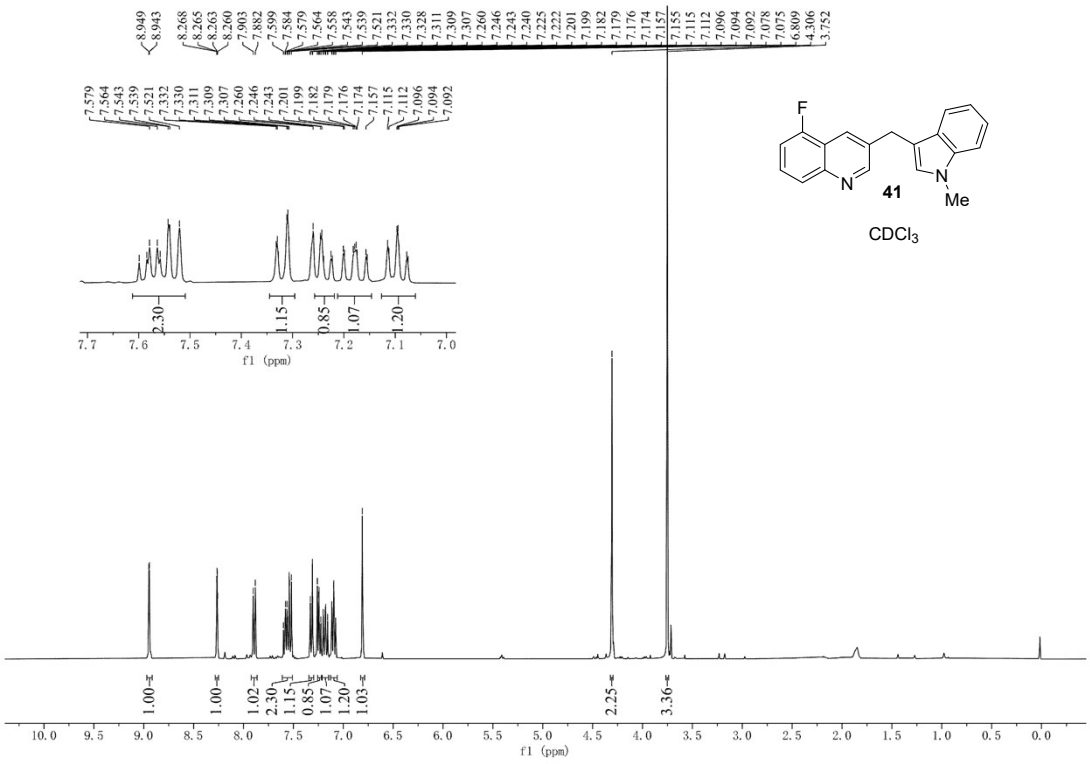
^{1}H NMR (600 MHz, $CDCl_3$):



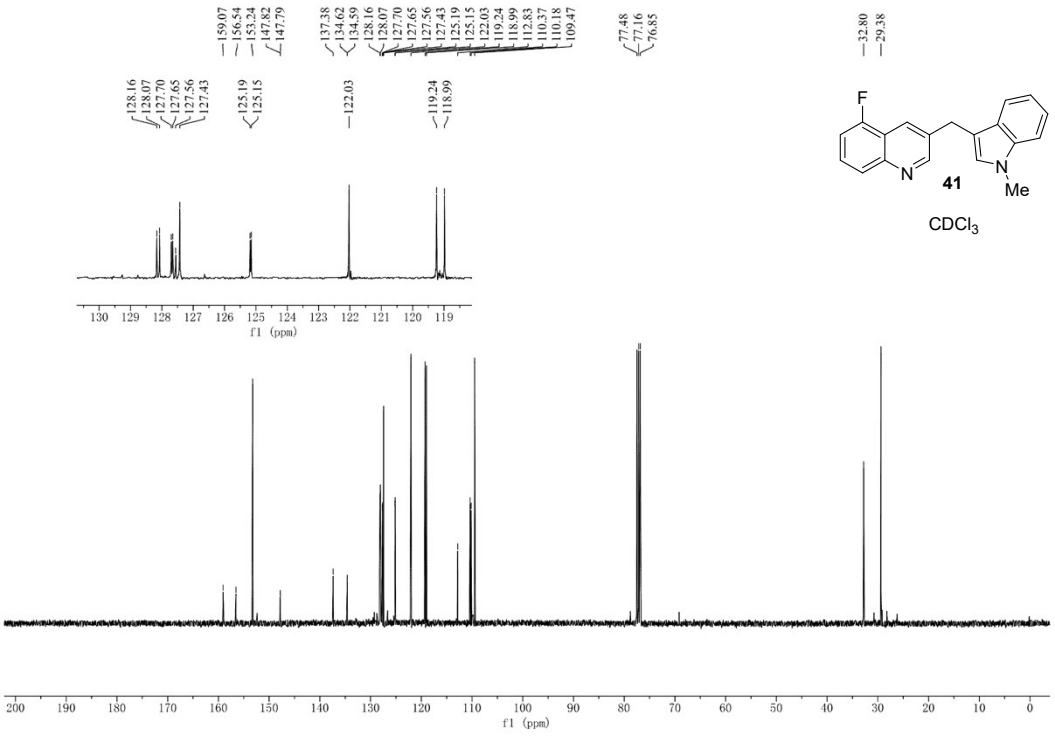
^{13}C NMR (150 MHz, $CDCl_3$):



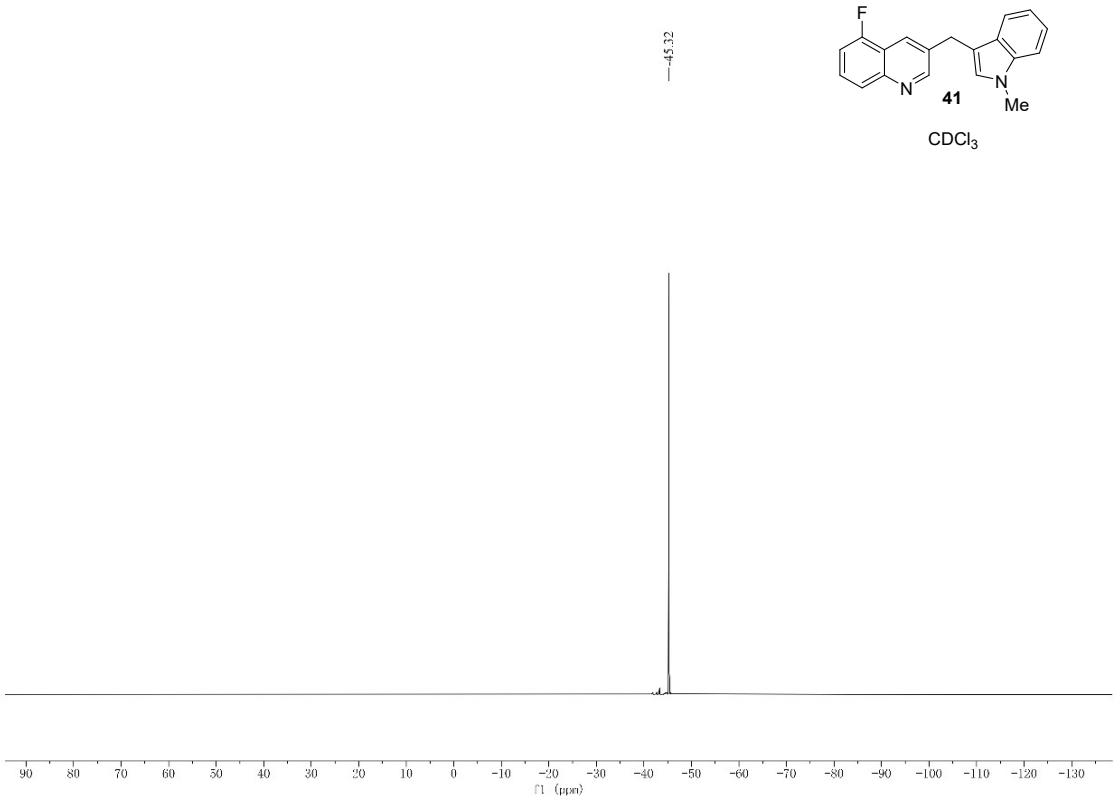
^{1}H NMR (400 MHz, $CDCl_3$):



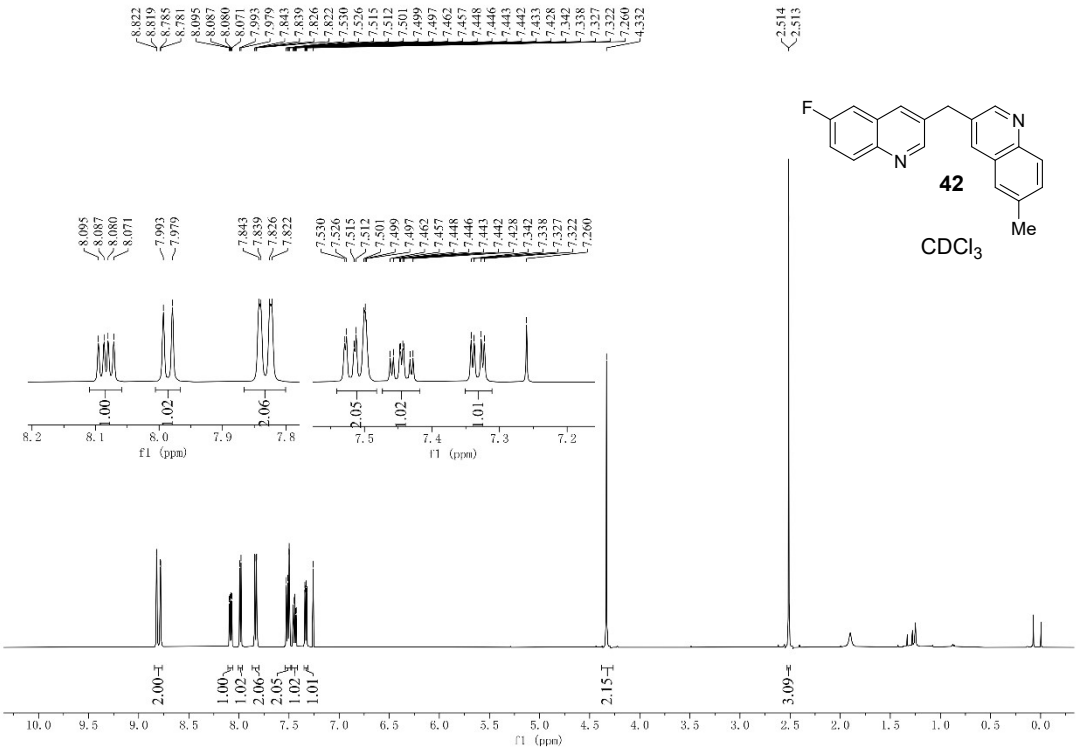
^{13}C NMR (100 MHz, $CDCl_3$):



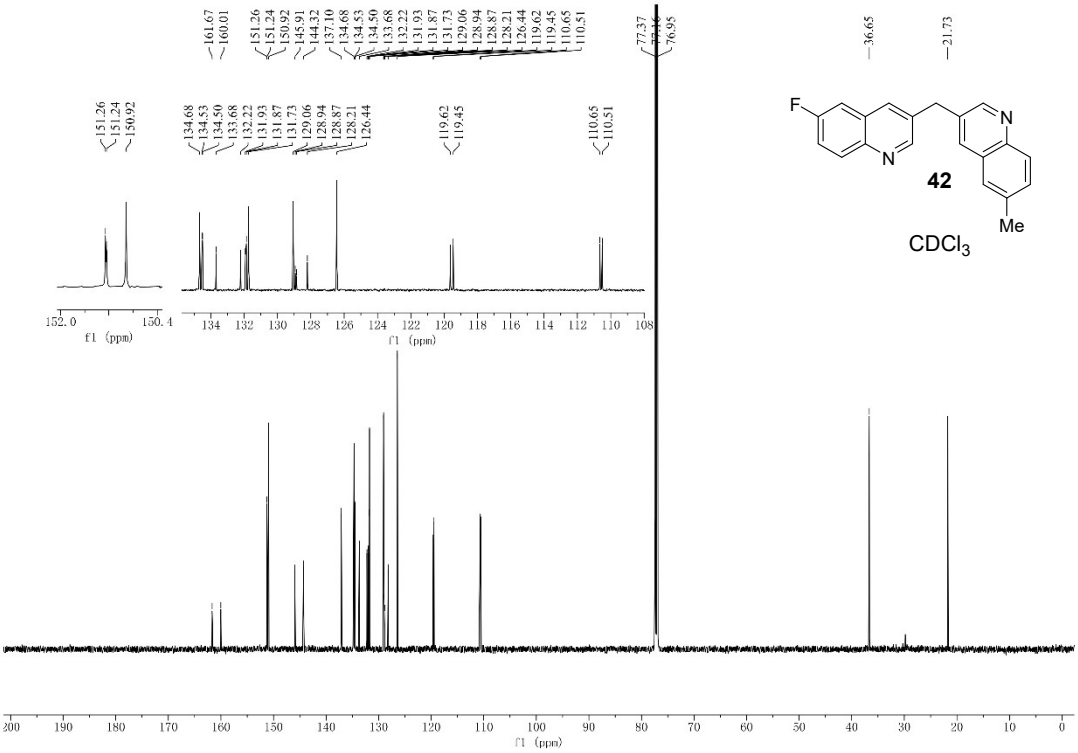
^{19}F NMR (564.5 MHz, $CDCl_3$):



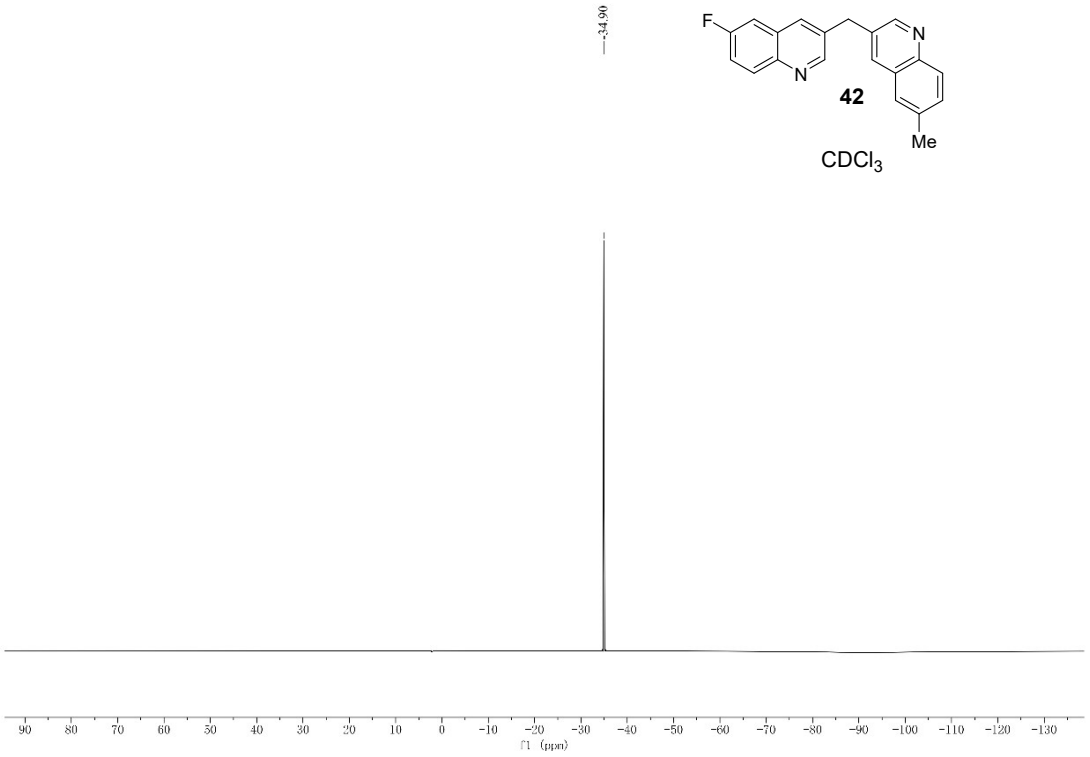
^{1}H NMR (600 MHz, $CDCl_3$):



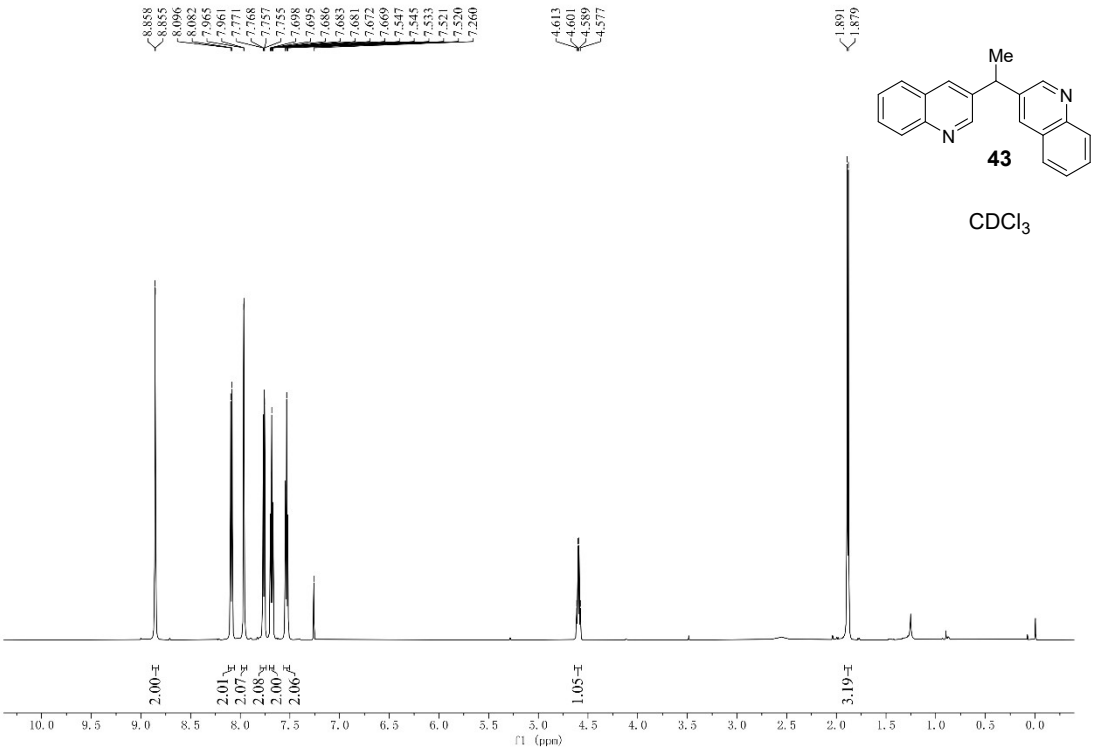
^{13}C NMR (150 MHz, $CDCl_3$):



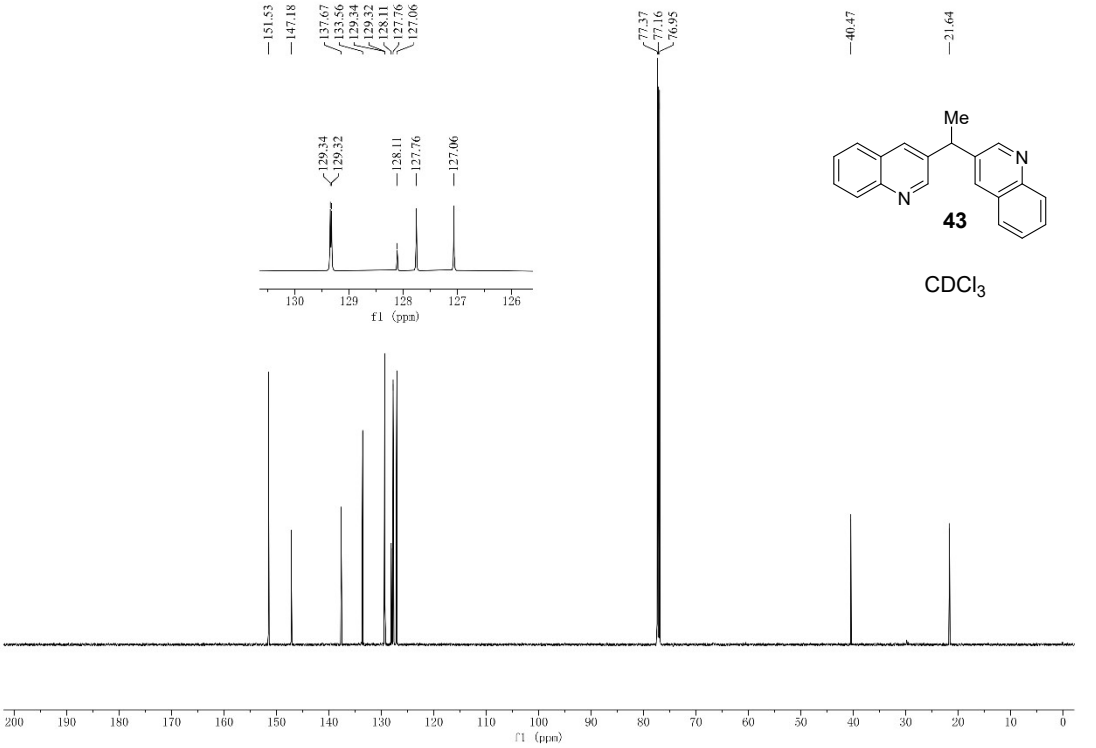
^{19}F NMR (564.5 MHz, $CDCl_3$):



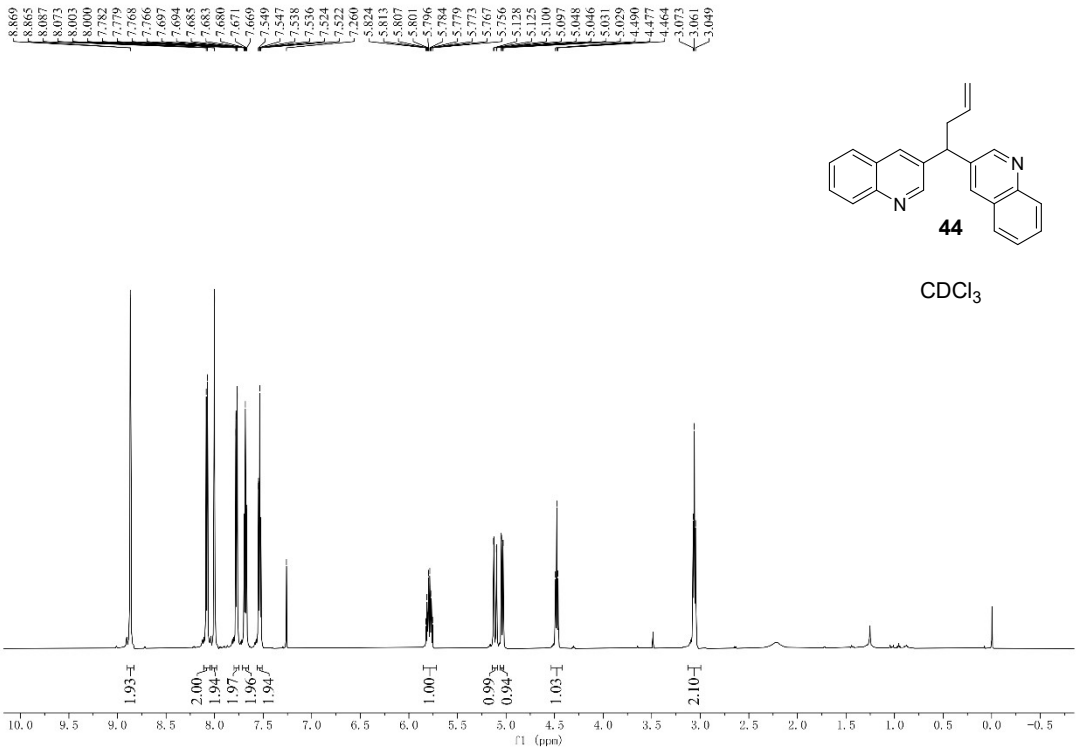
^{1}H NMR (600 MHz, $CDCl_3$):



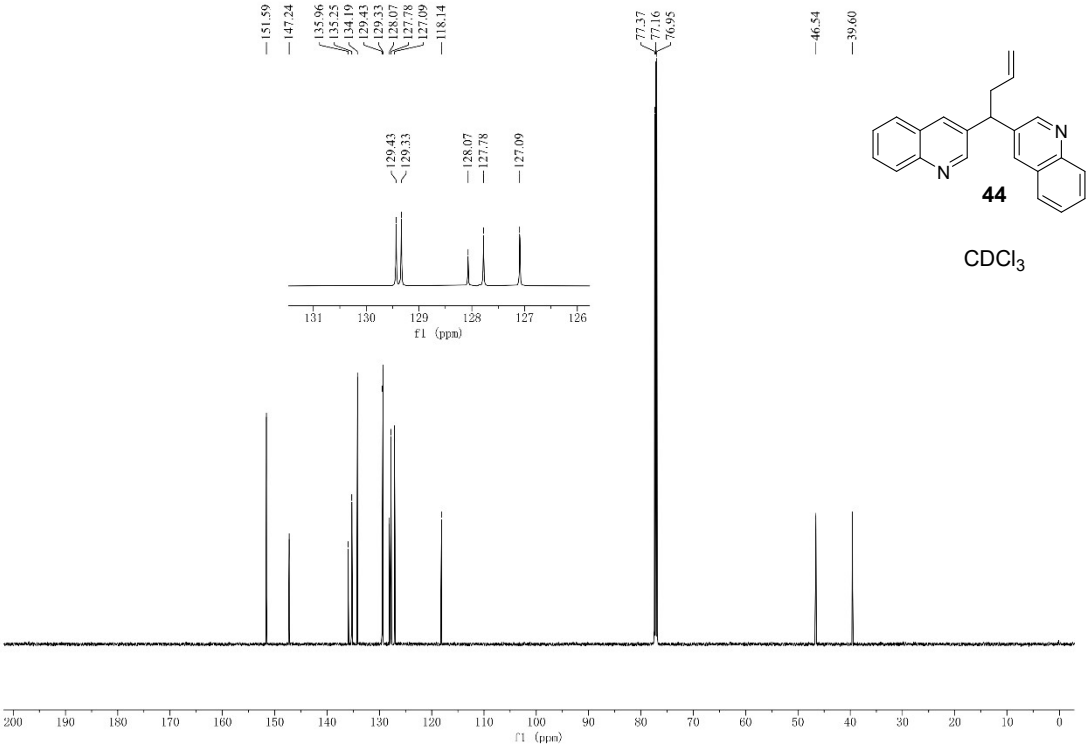
^{13}C NMR (150 MHz, $CDCl_3$):



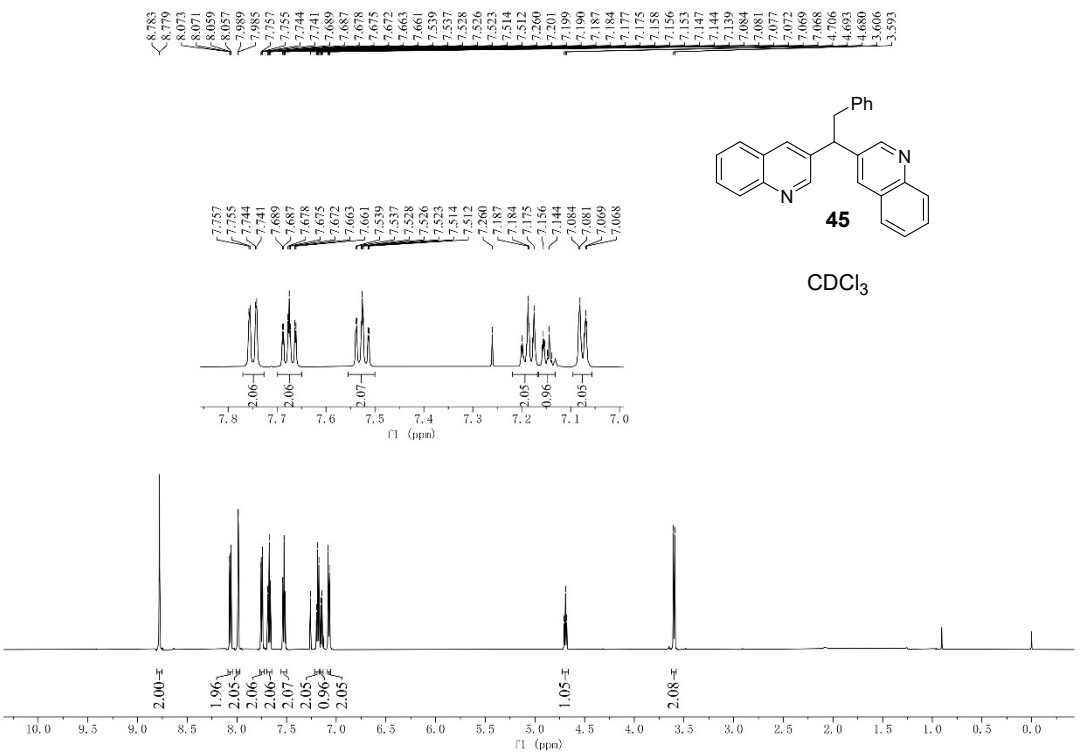
^{1}H NMR (600 MHz, $CDCl_3$):



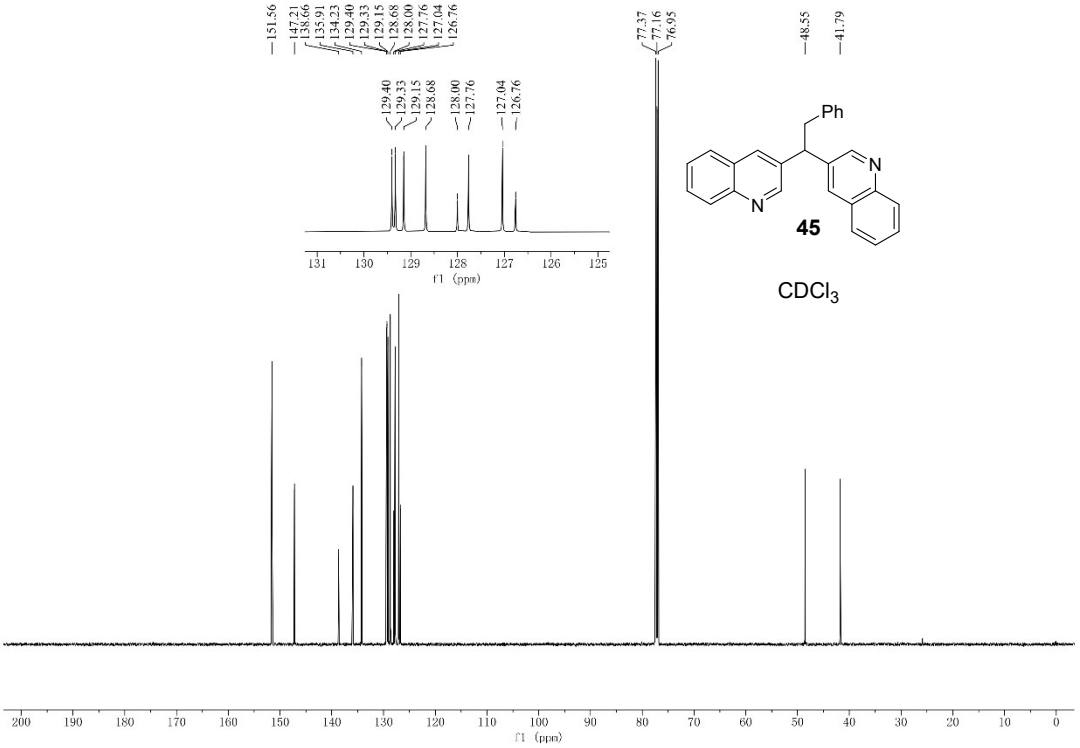
^{13}C NMR (150 MHz, $CDCl_3$):



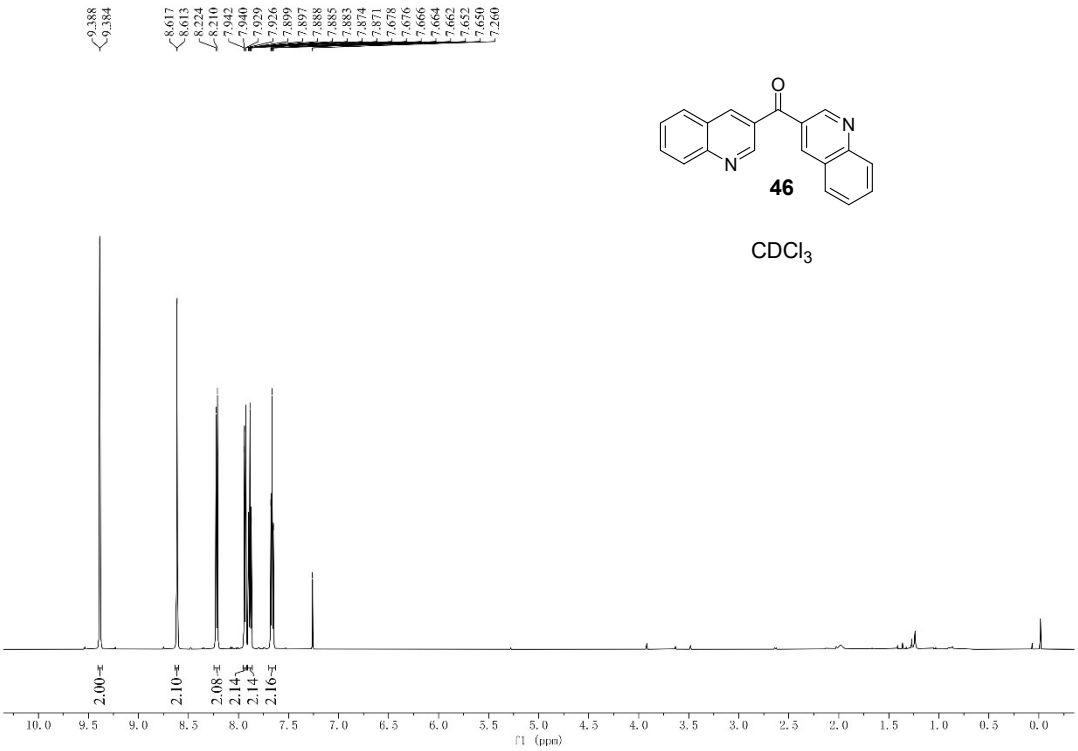
^{1}H NMR (600 MHz, $CDCl_3$):



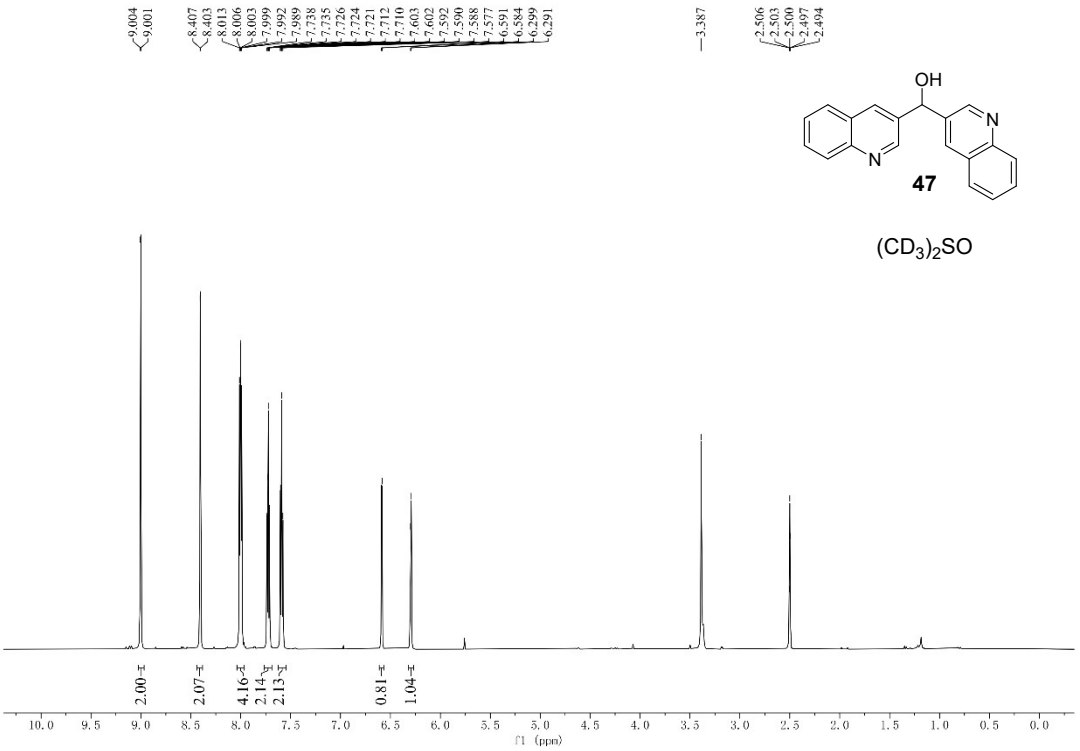
^{13}C NMR (150 MHz, $CDCl_3$):



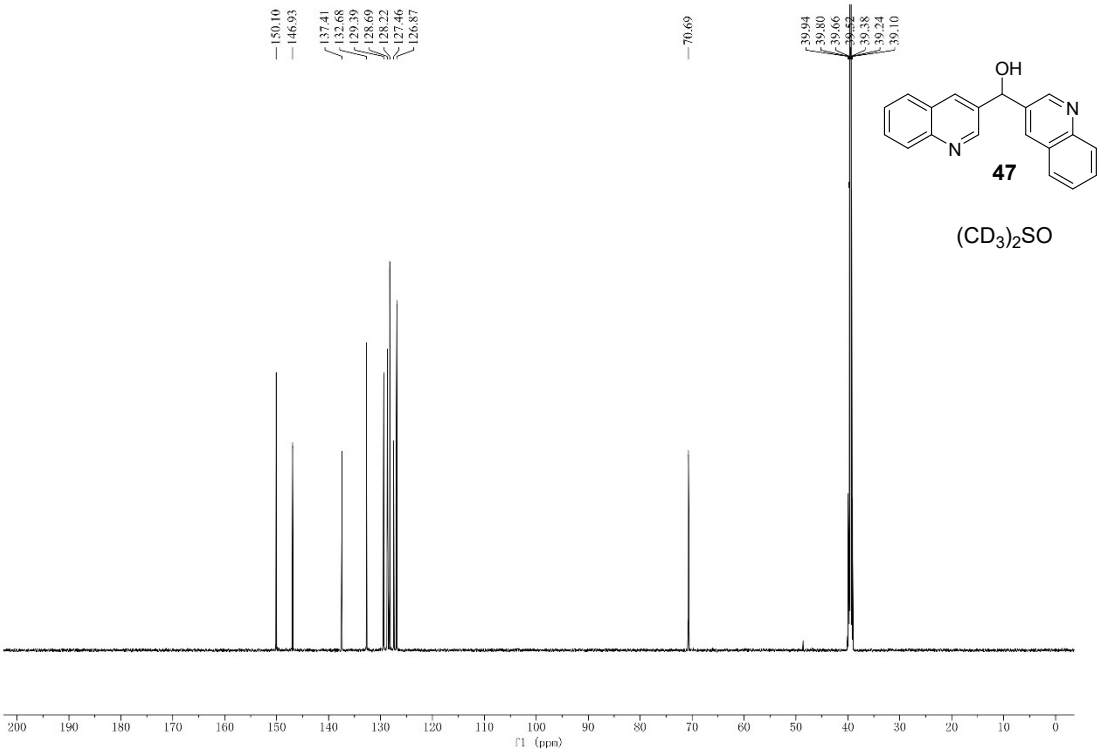
^{1}H NMR (600 MHz, $CDCl_3$):



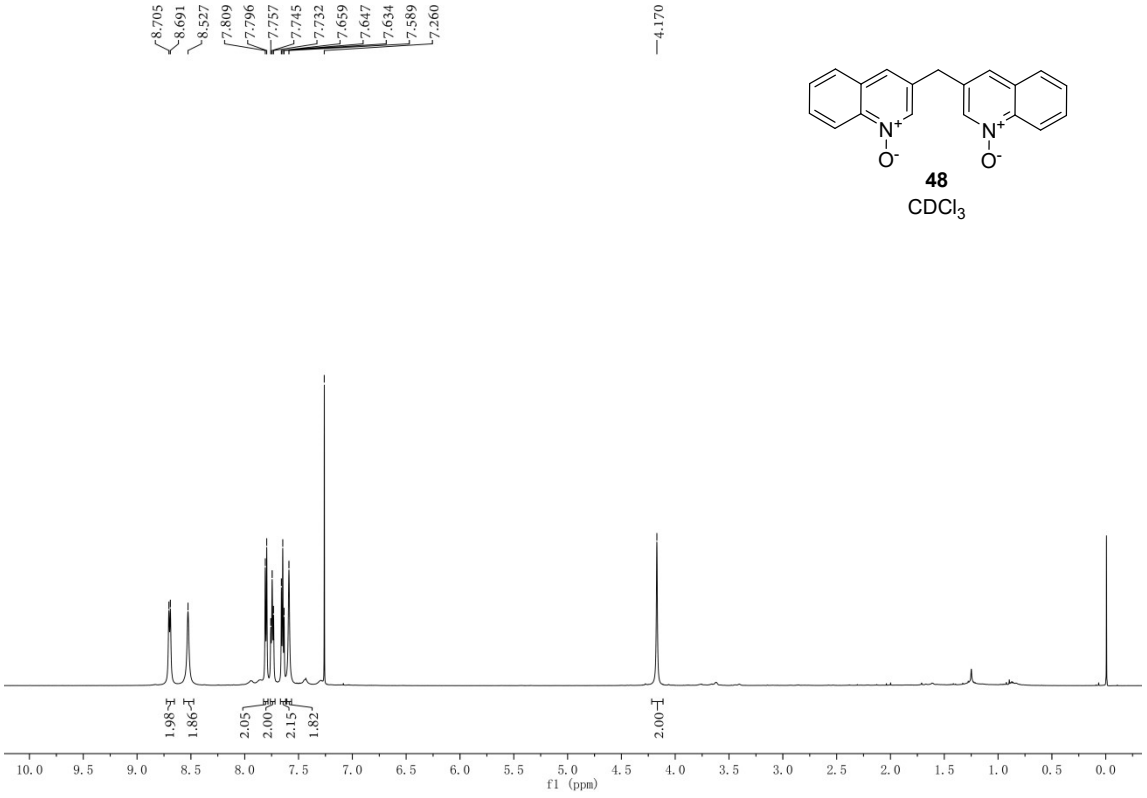
^{1}H NMR (600 MHz, $(CD_3)_2SO$):



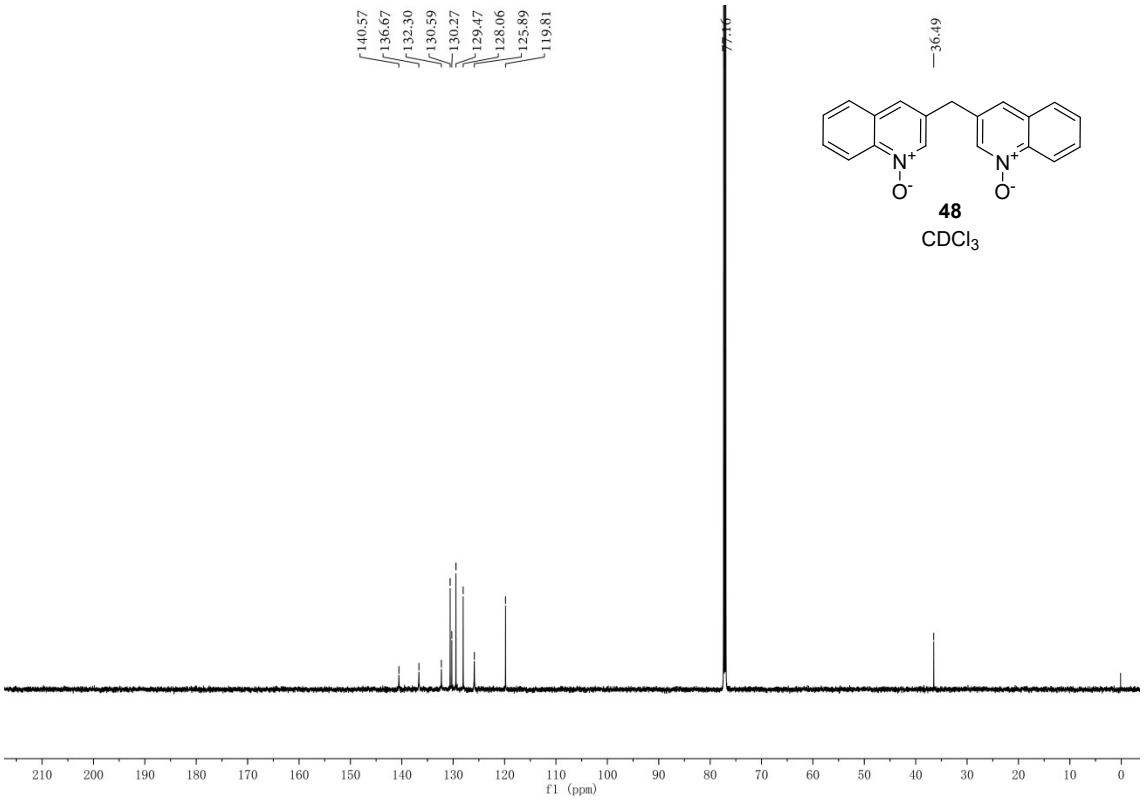
^{13}C NMR (150 MHz, $(CD_3)_2SO$):



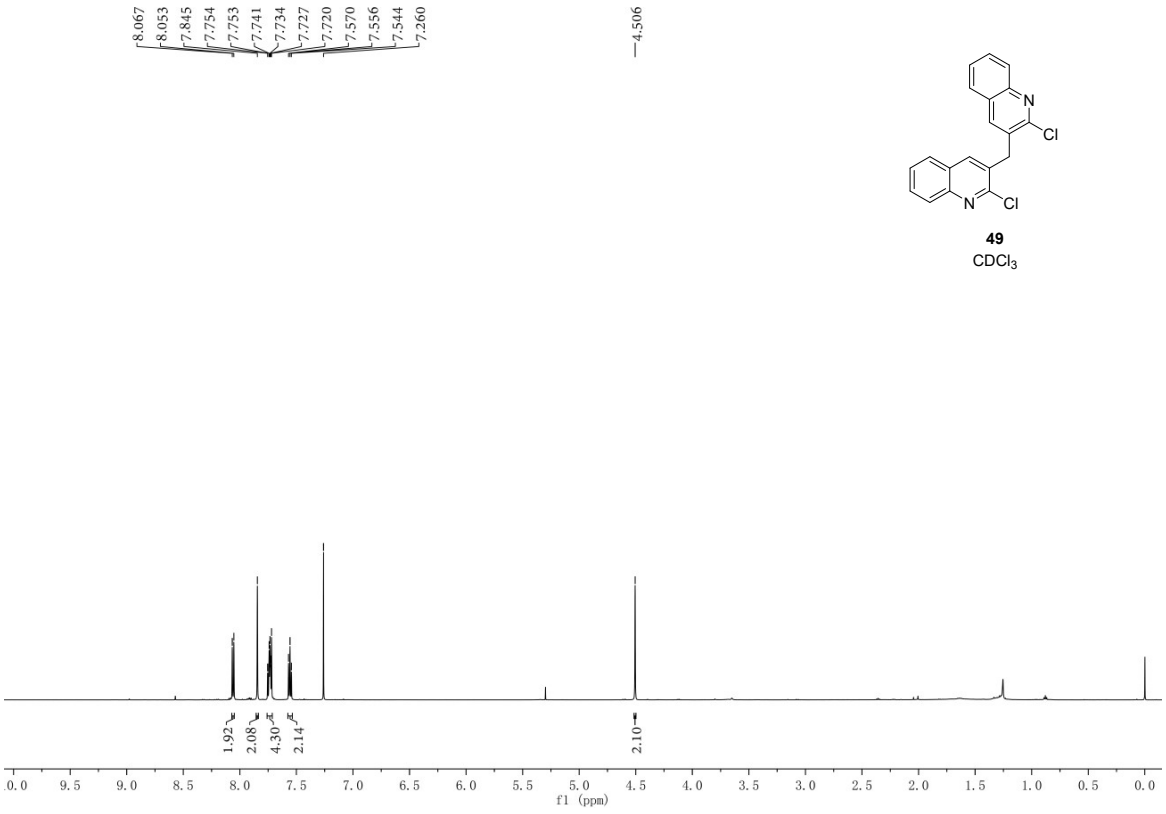
^{1}H NMR (600 MHz, $CDCl_3$):



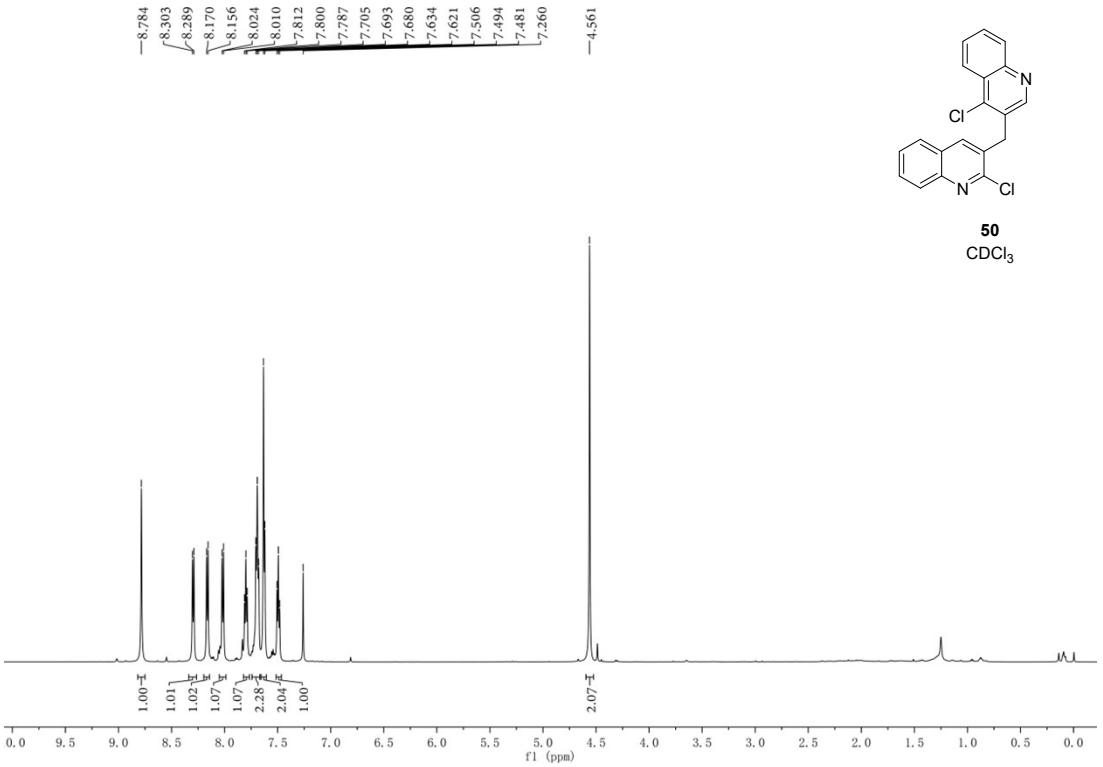
^{13}C NMR (150 MHz, $CDCl_3$):



^{1}H NMR (600 MHz, $CDCl_3$):

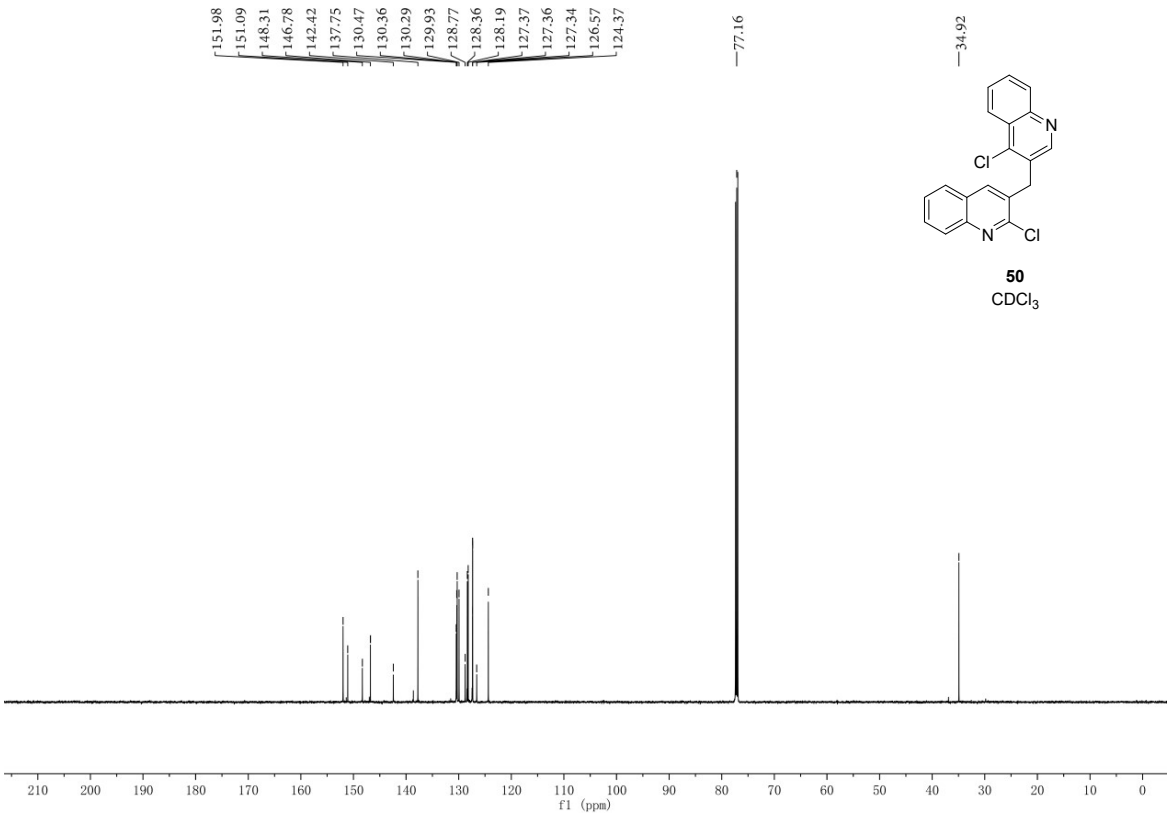


^{1}H NMR (600 MHz, $CDCl_3$):



50
$CDCl_3$

^{13}C NMR (150 MHz, $CDCl_3$):



50
$CDCl_3$