Supporting Information

Divergent C-H Activation Synthesis of Chalcones, Quinolones and Indoles

Yuesen Shi, Huimin Xing, Tianle Huang, Xuexin Liu, Jian Chen, Xiaoyu Guo, Guo-Bo Li* and Yong Wu*

Key Laboratory of Drug-Targeting and Drug Delivery System of the Education Ministry and Sichuan Province, Sichuan Engineering Laboratory for Plant-Sourced Drug and Sichuan Research Center for Drug Precision Industrial Technology, West China School of Pharmacy, Sichuan University, Chengdu 610041, China
Email: wyong@scu.edu.cn (Y. Wu); liguobo@scu.edu.cn (G.-B. Li)

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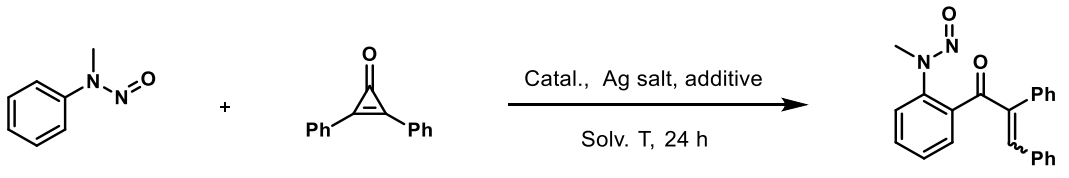
I. General Information

Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. Except for the specially mentioned dry solvent, all the solvents were treated according to general methods. All the reactions were monitored by thin-layer chromatography (TLC) and were visualized using UV light. The product purification was done using silica gel column chromatography. Thin-layer chromatography (TLC) characterization was performed with precoated silica gel GF254 (0.2 mm), while column chromatography characterization was performed with silica gel (100-200 mesh). ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded with tetramethylsilane (TMS, δ = 0.00 ppm) as the internal standard. ^{1}H NMR spectra were recorded at 400 or 600 MHz (Varian), ^{13}C NMR spectra were recorded at 100 or 150 MHz (Varian) .Chemical shifts are reported in ppm downfield from $CDCl_3$ (δ = 7.26 ppm) or DMSO-d_6 (δ = 2.50 ppm; H_2O signal was found at δ = 3.34 ppm) for ^{1}H NMR and chemical shifts for ^{13}C NMR spectra are reported in ppm relative to the central $CDCl_3$ (δ = 77.0 ppm) or DMSO-d_6 (δ = 39.6 ppm). Coupling constants were given in Hz. The following notations were used: br–broad, s–singlet, d– doublet, t–triplet, q–quartet, m–multiplet, dd–doublet of doublet, dt–doublet of triplet, td–triplet of doublet, ddd–doublet of doublet of doublet. Melting points were measured with YRT-3 melting point apparatus (Shantou Keyi Instrument & Equipment Co., Ltd., Shantou, China). X-ray analysis was performed with a single-crystal X-ray diffractometer. N-nitrosoanilines[1] and cyclopropenones[2] were prepared according to literatures.

II. Experimental Information

(a) Optimization of chalcones synthesis



1a 2a 3a

1) Optimization of catalysts [a]

Entry	Catal.	Ag salt	additive	Solv.	Temp.	**y** Yield [b]
1	**$[RhCp^*Cl_2]_2$**	**$AgSbF_6$**	**4 ÅMS**	**DCM**	100 °C	**70%**
2	$[Ru(p\text{-cymene})Cl_2]_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	<5%
3	$[IrCp^*Cl_2]_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	5%
4	$CoCp^*(CO)I_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	<5%
5	$[CoCp^*Cl_2]_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	-
6	$[CoCp^*(OAc)_2]_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	-
7	$CoCp^*(MeCN)_3(SbF_6)_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	-

8	$Pd(OAc)_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	5%
9	$Ni(COD)_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	-
10	$Mn(acac)_3$	$AgSbF_6$	4 ÅMS	DCM	100 °C	-

[a] Reaction conditions: **1a** (0.12 mmol), **2a** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %), 4 ÅMS (60 mg), in DCM (1.0 mL) at 100 °C under air in sealed tube for 24 h; [b] Isolated yields.

2) Optimization of Rh catalyst [a]

Entry	Catal.	Ag salt	additive	Temp.	time	**y** Yield [b]
1	$[RhCp^*Cl_2]_2$	$AgSbF_6$	4 ÅMS	100 °C	24h	70%
2	**$[RhCp^*(OAc)_2]_2$**	**$AgSbF_6$**	**4 ÅMS**	100 °C	**24h**	**76%**
3	$[Rh(COD)Cl]_2$	$AgSbF_6$	4 ÅMS	100 °C	24h	<5%
4	$RhCp^*(MeCN)_3(SbF_6)_2$	--	4 ÅMS	100 °C	24h	75%
5	$[Rh(OAc_2)]_2$	$AgSbF_6$	4 ÅMS	100 °C	24h	6%
6	$[RhCp^*Cl_2]_2$	$AgSbF_6$	--	100 °C	24h	<5%
7	--	$AgSbF_6$	4 ÅMS	100 °C	24h	<5%

[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %), 4 ÅMS (60 mg), in DCM (1.0 mL) at 100 °C under air in sealed tube for 24 h; [b] Isolated yields.

3) Optimization of Ag salts [a]

Entry	Cat.	Ag salt	Add.	Solv.	yield
1	$[RhCp^*(OAc)_2]_2$	$AgSbF_6$	4 ÅMS	DCM	76%
2	**$[RhCp^*(OAc)_2]_2$**	**$AgBF_4$**	**4 ÅMS**	**DCM**	**85%**
3	$[RhCp^*(OAc)_2]_2$	AgOAc	4 ÅMS	DCM	<5%
4	$[RhCp^*(OAc)_2]_2$	Ag_2CO_3	4 ÅMS	DCM	<5%
5	$[RhCp^*(OAc)_2]_2$	$AgNTf_2$	4 ÅMS	DCM	67%
6	$[RhCp^*(OAc)_2]_2$	$AgNO_3$	4 ÅMS	DCM	<5%
7	$[RhCp^*(OAc)_2]_2$	AgOTf	4 ÅMS	DCM	53%
8	$[RhCp^*(OAc)_2]_2$	-	4 ÅMS	DCM	<5%

[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %), 4 ÅMS (60 mg), in DCM (1.0 mL) at 100 °C under air in sealed tube for 24 h; [b] Isolated yields.

4) Optimization of sovlents [a]

Entry	**Cat.**	**Ag salt**	**Add.**	**Solv.**	**yield**
1	**$[RhCp^*(OAc)_2]_2$**	**$AgBF_4$**	**4 ÅMS**	**DCM**	**85%**
2	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	DCE	80%
3	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	Tol	<5%
4	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	PhCl	0%
5	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	EtOH	60%
6	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	THF	<5%
7	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	HFIP	65%
8	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	MeCN	65%
9	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	PEG/H_2O(v/v=1:3)	32%

[a] Reaction conditions: **1a** (0.12 mmol), **2a** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %), 4 ÅMS (60 mg) at 100 °C under air in sealed tube for 24 h; [b] Isolated yields.

5) Optimization of additive [a]

Entry	Cat.	Ag salt	Add.	Solv.	Temp.	time	yield
1	**$[RhCp^*(OAc)_2]_2$**	**$AgBF_4$**	4 ÅMS	**DCM**	**100 °C**	**24h**	**85%**
2	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	SiO_2	DCM	100 °C	24h	65%
3	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	Al_2O_3	DCM	100 °C	24h	60%
4	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	SBA-15 [c]	DCM	100 °C	24h	<5%
6	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	BN-OH	DCM	100 °C	24h	<5%
7	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	GO	DCM	100 °C	24h	<5%
	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	-	DCM	100 °C	24h	<5%

[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %), addictive (60 mg), in DCM (1.0 mL) at 100 °C under air in sealed tube for 24 h; [b] Isolated yields; [c] Titanium doped silica mesoporous SBA-15, <150 mum particle size, pore size 4 nm, Hexagonal pore morphology.

6) Optimization of equivalents [a]

Entry	1a:2a	Cat.	Ag salt	4 ÅMS	yield
1	**1.2:1**	**0.05eq**	**0.2eq**	**60mg**	**85%**
2	1:1	0.05eq	0.2eq	60mg	60%
3	1:1.2	0.05eq	0.2eq	60mg	60%
4	1:1.2	0.04eq	0.16eq	60mg	70%
5	1:1.2	0.02eq	0.08eq	60mg	65%
6	1:1.2	0.05eq	0.2eq	20mg	<5%
7	1:1.2	0.05eq	0.2eq	40mg	<5%
8	1:1.2	0.05eq	0.2eq	80mg	55%
9	1:1.2	0.05eq	0.2eq	90mg	50%

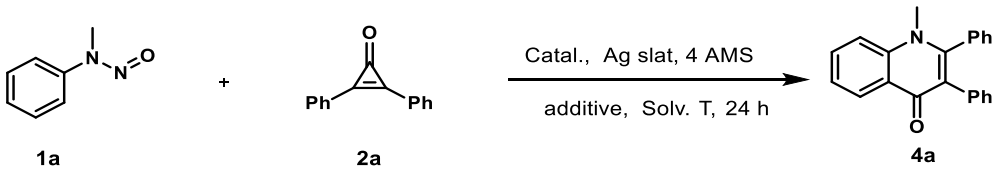
[a] Reaction conditions: **1a**, **2a**, Catal. (5 mol %), $AgBF_4$ (20 mol %), 4 ÅMS in DCM (1.0 mL) at 100 °C under air in sealed tube for 24 h; [b] Isolated yields.

7) Optimization of Temperature [a]

Entry	Cat.	Ag salt	Add.	Solv.	Temp.	time	yield
1	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	DCM	100 °C	24h	85%
2	**$[RhCp^*(OAc)_2]_2$**	**$AgBF_4$**	**4 ÅMS**	**DCM**	**80 °C**	**24h**	**91%**
3	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	DCM	60 °C	24h	79%
4	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	DCM	45 °C	24h	40%
6	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	DCM	30 °C	24h	<5%
7	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	DCM	120 °C	24h	80%

[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %), 4 ÅMS (60 mg), in DCM (1.0 mL) under air in sealed tube for 24 h; [b] Isolated yields.

(b) Optimization of the reaction quinolone [a]

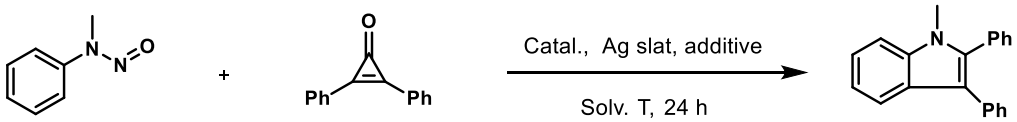


1a 2a 4a

Entry	Cat.	Ag salt	Add.	Solv.	Temp.	Time	Yield [b]
1	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	$Cu(OAc)_2$	DCM	100°C	24h	<5%
2	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	Cs_2CO_3	DCM	100°C	24h	<5%
3	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	AdCOOH	DCM	100°C	24h	<5%
4	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	HOAc	DCM	100°C	24h	<5%
5	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	HOPiv	DCM	100°C	24h	<5%
6	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	NaOAc	DCM	100°C	24h	<5%
7	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	$ZnCl_2$	DCM	100°C	24h	<5%
8	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	NaF	DCM	100°C	24h	<5%
9	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	$AlCl_3$	DCM	100°C	24h	<5%
10	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	NaOPiv	DCM	100 °C	24h	<5%
11	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	-	DCM	120 °C	24h	11%
12	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	-	DCM	120 °C	48h	13%
13	$[RhCp^*(OAc)_2]_2$	$AgSb_6$	-	DCM	120°C	24h	<5%
14	$[RhCp^*(OAc)_2]_2$	$AgNTf_2$	-	DCM	120°C	24h	63%
15	$[RhCp^*(OAc)_2]_2$	$AgNO_3$	-	DCM	120°C	24h	<5%
16	$[RhCp^*(OAc)_2]_2$	AgOTf	-	DCM	120°C	24h	<5%
17	**$[RhCp^*(OAc)_2]_2$**	**$AgNTf_2$**	-	**DCE**	**120°C**	**24h**	**83%**
18	$[RhCp^*(OAc)_2]_2$	$AgNTf_2$		Tol	120 °C	24h	<5%
19	$[RhCp^*(OAc)_2]_2$	$AgNTf_2$	NaOPiv	DCE	120 °C	24h	75%
20	$[RhCp^*(OAc)_2]_2$	$AgNTf_2$	HOPiv	DCE	120 °C	24h	74%
21	$[RhCp^*(OAc)_2]_2$	$AgNTf_2$	CsOAc	DCE	120 °C	24h	69%

Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %),4 ÅMS (60 mg), addictive (0.2eq),solvent (1.0 mL) under air in sealed tube; [b] Isolated yields;

(c) Optimization of the indoles synthesis



1a **2a** **5a**

1) Optimization of catalyst [a]

Entry	Cat.	Ag salt	Add.	Solv.	Temp.	Time	Yield [b]
1	$[RhCp^*Cl_2]_2$	$AgBF_4$	4 ÅMS	DCM	100 °C	24h	<5%
2	$[RhCp^*(OAc)_2]_2$	$AgBF_4$	4 ÅMS	DCM	100 °C	24h	<5%
3	**$[Rh(COD)Cl]_2$**	**$AgBF_4$**	**4 ÅMS**	**DCM**	**100 °C**	**24h**	**15%**
4	$RhCp^*(MeCN)_3(SbF_6)_2$	$AgBF_4$	4 ÅMS	DCM	100 °C	24h	<5%
6	$[Ru_3(CO)_{12}]$	$AgBF_4$	4 ÅMS	DCM	100 °C	24h	<5%

[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %),4 ÅMS (60 mg), in DCM (2.0mL) under air in sealed tube; [b] Isolated yields;

2) Optimization of Ag slats [a]

Entry	Cat.	Ag salt	Add.	Solv.	Temp.	Time	Yield [b]
1	$[Rh(COD)Cl]_2$	$AgNTf_2$	4 ÅMS	DCM	100 °C	24h	<5%
2	$[Rh(COD)Cl]_2$	$AgOTf_2$	4 ÅMS	DCM	100 °C	24h	<5%
3	$[Rh(COD)Cl]_2$	AgOAc	4 ÅMS	DCM	100 °C	24h	<5%
4	$[Rh(COD)Cl]_2$	Ag_2CO_3	4 ÅMS	DCM	100 °C	24h	<5%
6	$[Rh(COD)Cl]_2$	$AgSbF_6$	4 ÅMS	DCM	100 °C	24h	15%
7	**$[Rh(COD)Cl]_2$**	**$AgSbF_6$(0.1eq)**	**4 ÅMS**	**DCM**	**100 °C**	**24h**	**15%**
8	$[Rh(COD)Cl]_2$	$AgSbF_6$(0.3eq)	4 ÅMS	DCM	100 °C	24h	12%
9	$[Rh(COD)Cl]_2$	$AgSbF_6$(0.3eq)	-	DCM	100 °C	24h	<5%

[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %), 4 ÅMS (60 mg), in DCM (2.0 mL) under air in sealed tube; [b] Isolated yields;

4) Optimization of temperature [a]

Entry	Cat.	Ag salt	Add.	Solv.	Temp.	Yield [b]
1	$[Rh(COD)Cl]_2$	$AgSbF_6$	4 ÅMS	DCM	80 °C	<5%
2	$[Rh(COD)Cl]_2$	$AgSbF_6$	4 ÅMS	DCM	110 °C	19%
3	**$[Rh(COD)Cl]_2$**	**$AgSbF_6$**	**4 ÅMS**	**DCM**	**120 °C**	**35%**
4	$[Rh(COD)Cl]_2$	$AgSbF_6$	4 ÅMS	DCM	130 °C	28%
6	$[Rh(COD)Cl]_2$	$AgSbF_6$	4 ÅMS	DCM	150 °C	18%

[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (20 mol %),4 ÅMS (60 mg), in DCM (2.0 mL) under air in sealed tube; [b] Isolated yields;

5) Optimization of addictive and solvents [a]

Entry	Cat.	Ag salt	Add.	Solv.	Temp.	Time	Yield [b]
1	$[Rh(COD)Cl]_2$	$AgSbF_6$	Cs_2CO_3	DCM	80 °C	24h	<5%

2	$[Rh(COD)Cl]_2$	$AgSbF_6$	$Cu(OAc)_2.H_2O$	DCM	120 °C	24h	10%
3	$[Rh(COD)Cl]_2$	$AgSbF_6$	PivOH	DCM	120 °C	24h	16%
4	$[Rh(COD)Cl]_2$	$AgSbF_6$	NaOAc	DCM	120 °C	24h	8%
6	$[Rh(COD)Cl]_2$	$AgSbF_6$	CsF	DCM	120 °C	24h	11%
7	$[Rh(COD)Cl]_2$	$AgSbF_6$	Al_2O_3	DCM	120 °C	24h	14%
8	$[Rh(COD)Cl]_2$	$AgSbF_6$		DCM	120 °C	24h	15%
9	$[Rh(COD)Cl]_2$	$AgSbF_6$	-	DCE	120 °C	24h	14%
10	$[Rh(COD)Cl]_2$	$AgSbF_6$	-	MeOH	120 °C	24h	<5%
11	$[Rh(COD)Cl]_2$	$AgSbF_6$	-	Tol	120 °C	24h	<5%

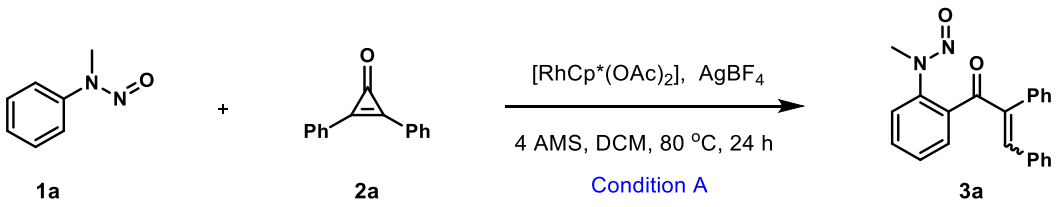
[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catal. (5 mol %), Ag salt (10 mol %),4 ÅMS (60 mg), addictive (0.2eq) in solvent(2.0 mL) under air in sealed tube; [b] Isolated yields;

6) Optimization of mixture catalysts [a]

Entry	Cat.1	Cat.2	Add.	Solv.	Temp.	time	yield
1	$[RhCp^*Cl_2]_2$	$Pd(OAc)_2$	4 ÅMS	DCM	120 °C	24h	<5%
2	$[RhCp^*Cl_2]_2$	Al_2O_3	4 ÅMS	DCM	120 °C	24h	<5%
3	$[RhCp^*Cl_2]_2$	$Ru_3(CO)_{12}$	4 ÅMS	DCM	120 °C	24h	45%
4	$[RhCp^*Cl_2]_2$	uv(200-400nm)	4 ÅMS	DCM	120 °C	24h	45%
5	$[RhCp^*Cl_2]_2$	$[Rh(COD)Cl]_2$	4 ÅMS	DCM	120 °C	24h	65%
6	$[RhCp^*Cl_2]_2$	COD	4 ÅMS	DCM	120 °C	24h	<5%
7	Cp*	$[Rh(COD)Cl]_2$	4 ÅMS	DCM	120 °C	24h	18%
8[c]	$[RhCp^*Cl_2]_2$	$[Rh(COD)Cl]_2$	4 ÅMS	DCM	120 °C	24h	37%
9	**$[RhCp^*Cl_2]_2$**	**$[Rh(COD)Cl]_2$**	**4 ÅMS**	**DCM**	**120 °C**	**36h**	**73%**
10[d]	-	$[Rh(COD)Cl]_2$	4 ÅMS	DCM	120 °C	24h	42%
11[e]	-	$[Rh(COD)Cl]_2$	4 ÅMS	DCM	120 °C	24h	41%

[a] Reaction conditions: **1a** (0.12 mmol), **2** (0.1 mmol), Catalyst 1 (5 mol %), Catalyst 2 (5 mol %), Ag salt (10 mol %),4 ÅMS (60 mg), addictive (0.2eq) in solvent (2.0 mL) under air in sealed tube; [b] Isolated yields; [c] $[RhCp^*Cl_2]_2$ (2.5 mol %), $[Rh(COD)Cl]_2$ (2.5 mol %); [d] $[Rh(COD)Cl]_2$ (10 mol %); [e]$[Rh(COD)Cl]_2$ (20 mol %).

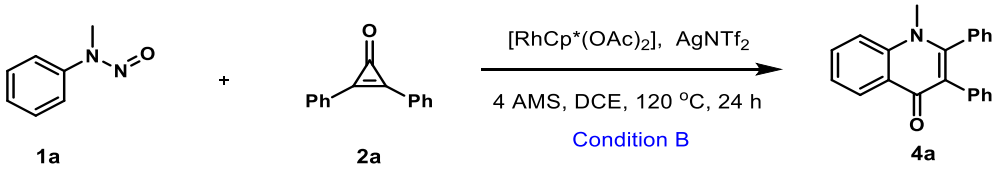
(d) General procedure for the synthesis of products 3 (3a as an example).



1a 2a 3a

N-nitrosoaniline **1a** (0.12 mmol), diphenylcyclopropenone **2a** (0.10 mmol), $[RhCp^*(OAc)_2]_2$ (0.005 mmol), 4 ÅMS (60 mg) and $AgBF_4$ (0.02 mmol) were charged into a pressure tube, to which was added DCM (1.0 mL) under air. The test tube was sealed with a rubber septum and the reaction mixture was stirred at 80 ℃ for 24 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford compound **3a** as yellow oil.

(e) General procedure for the synthesis of products 4 (4a as an example).



1a **2a** **4a**

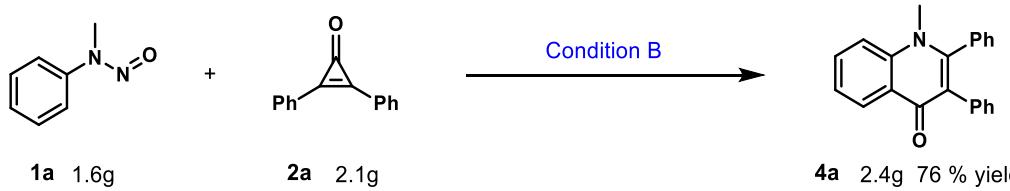
N-nitrosoaniline **1a** (0.12 mmol), diphenylcyclopropenone **2a** (0.10 mmol), $[RhCp^*(OAc)_2]_2$ (0.005 mmol), 4 ÅMS (60 mg) and $AgNTf_2$ (0.02 mmol) were charged into a pressure tube, to which was added DCE (1.0 mL) under air. The test tube was sealed with a rubber septum and the reaction mixture was stirred at 120 ℃ for 24 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford compound **4a** as a yellow solid.

(f) General procedure for the synthesis of products 5 (5a as an example).

1a **2a** **Condition C** **5a**

N-nitrosoaniline **1a** (0.12 mmol), diphenylcyclopropenone **2a** (0.10 mmol), $[Cp^*RhCl_2]_2$ (0.005 mmol), $[Rh(COD)Cl]_2$ (0.005 mmol), 4 ÅMS (60 mg) and $AgSbF_6$ (0.01 mmol) were charged into a pressure tube, to which was added DCM (2.0 mL) under air. The test tube was sealed with a rubber septum and the reaction mixture was stirred at 120 ℃ for 36 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford compound **5a** as a yellow solid.

(g) Gram-scale production of quinolone 4a



1a 1.6g **2a** 2.1g **4a** 2.4g 76 % yield

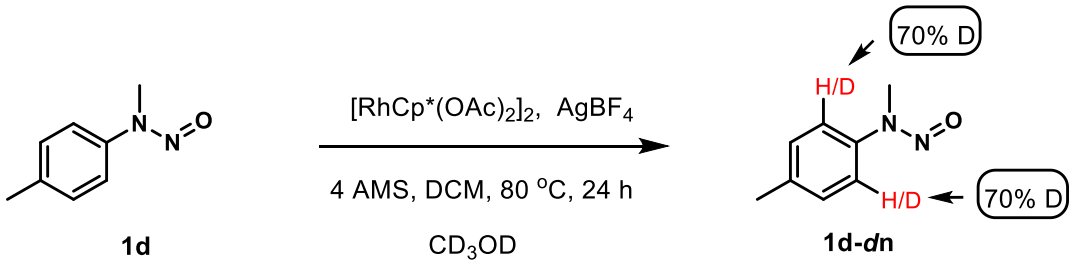
N-nitrosoaniline **1a** (12 mmol, 1.6 g), diphenylcyclopropenone **2a** (10 mmol, 2.1 g), $[RhCp^*(OAc)_2]_2$ (0.5 mmol, 0.33 g), 4 ÅMS (6.0 g) and $AgNTf_2$ (2 mmol, 0.77 g) were charged into a pressure tube, to which was added DCE (100 mL) under air. The test tube was sealed with a rubber septum and the reaction mixture was stirred at 120 ℃ for 28 h. After cooled to room

temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford compound **4a** as a yellow solid in 76% yield.

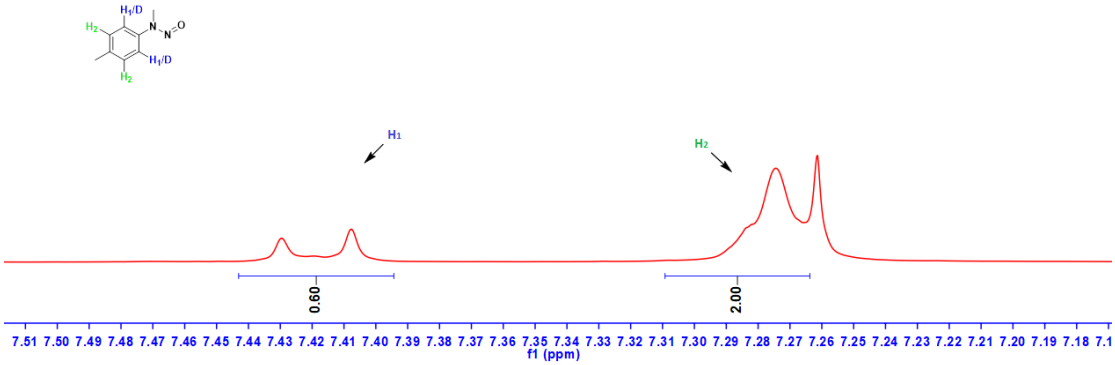
III. Mechanistic Studies

(a) The mechanistic studies of chalcones synthesis

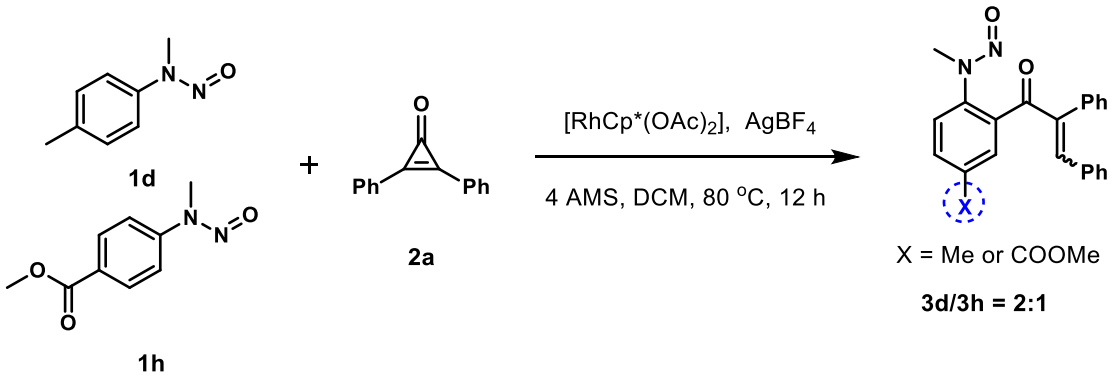
1) Deuterium exchange experiments



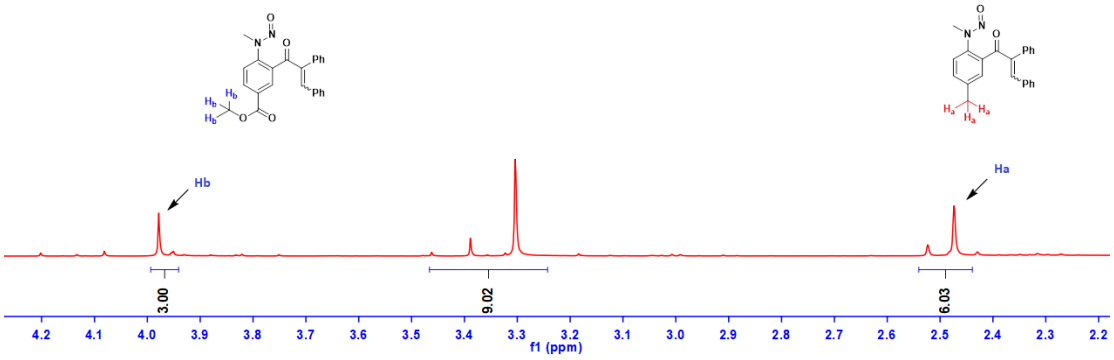
N-nitrosoaniline **1d** (0.10 mmol), [Cp*Rh (OAc) $_2$]$_2$ (0.005 mmol), 4 AMS (60 mg) and $AgBF_4$ (0.02 mmol) were charged into a pressure tube, to which was added CD_3OD (0.1mL) and DCM (0.9 mL) . The reaction mixture was stirred at 80 ℃ for 24 h. After cooled to rt, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford compound **1d-*d*$_n$** as yellow oil. The deuterium incorporation was determined to be 70% by ^{1}H NMR method. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.42 (d, *J* = 8.8 Hz, 0.6H), 7.28 (d, *J* = 8.8 Hz, 2H), 3.44 (s, 3H), 2.40 (s, 3H).



2) Competition experiments

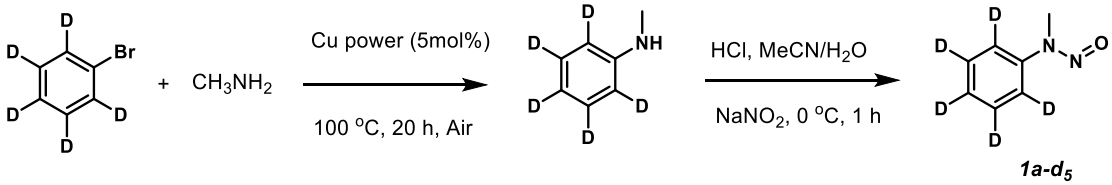


A mixture of **1d** (0.1 mmol), **1h** (0.1 mmol), cyclopropenone **2a** (0.2 mmol), $[Cp^*Rh(OAc)_2]_2$ (5 mol %), $AgBF_4$ (20 mol%), 4 Å MS (60 mg) were dissolved in DCM (1 mL) in a pressure tube under air. The reaction mixture was stirred at 80 ℃ for 12 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford **3d** and **3h**, which were characterized by **^{1}H NMR** spectroscopy.



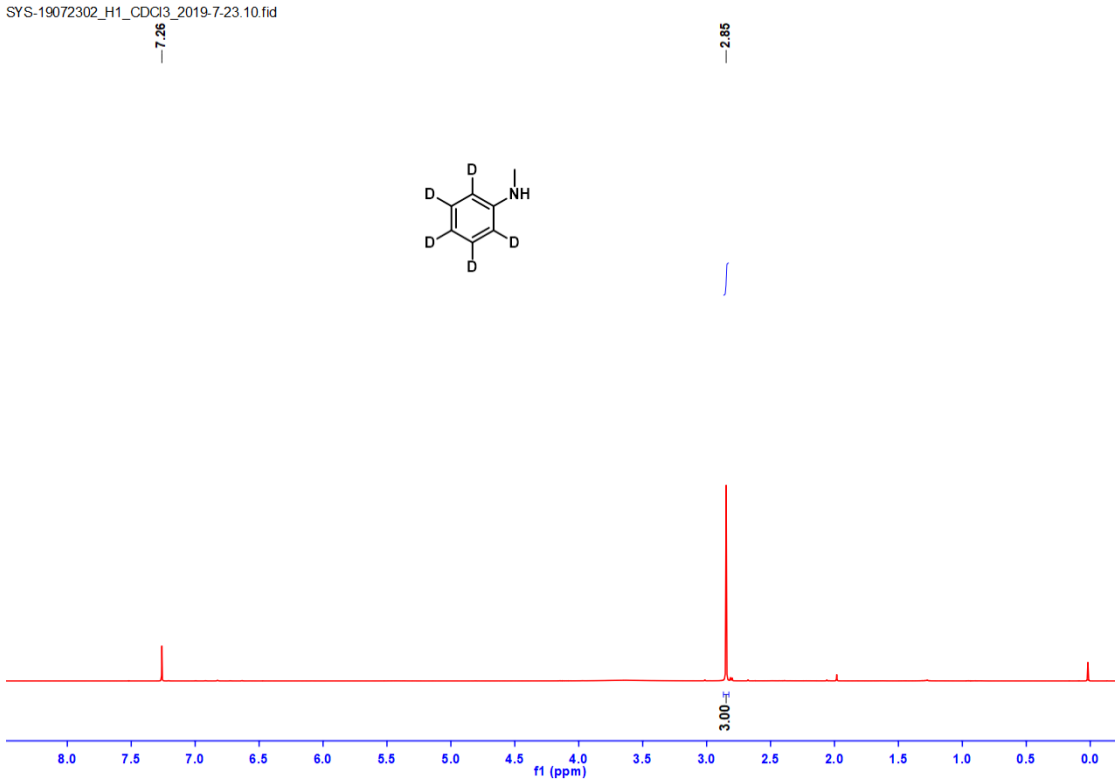
3) Kinetic isotope effect of the transformation

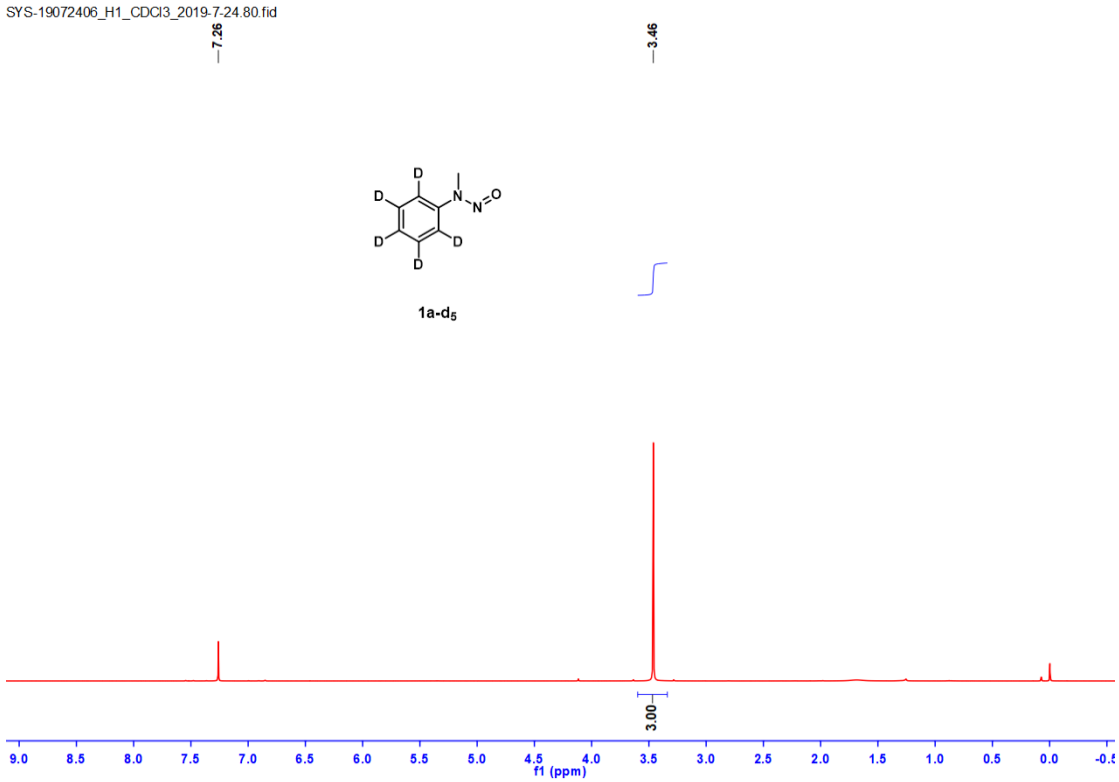
i) Experimental procedure for the synthesis of 1a-d_5



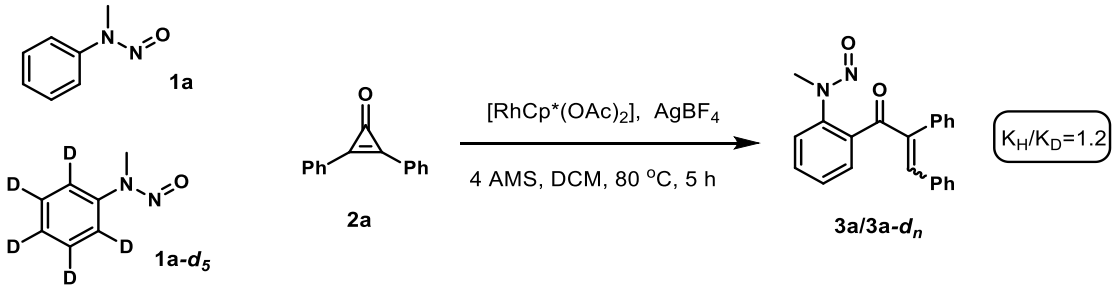
Bromobenzene-d_5 (5 mmol, 0.805 g), 30 % aqueous methylamine solution (2.7 mL, 25 mmol), copper power (0.016 g, 5 mol %) was combined in a 30 mL screwed sealed tube and placed in an oil bath under Air atmosphere. The reaction mixture was magnetically stirred and heated to 100 ℃ for 12 h. When the reaction completed or underwent to the time, the reaction mixture was cooled

to room temperature and ethyl acetate (20 mL) was added to extract the product. The organic layer was separated and the aqueous layer was extracted by ethyl acetate (3×10 mL). The combined organic phase was washed with brine and dried over Mg_2SO_4. The organic layer was evaporated in vacuum and the crude product was purified by flash column chromatography (Petroleum ether /EtOAc = 10:1) to give N-methylbenzen-d5-amine (600 mg) in 85% yield, **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 2.85 (s, 3H). **1a-d_5** was prepared according to literatures[1]: red-brown oil, yield 84%, **^{1}H NMR (400 MHz, Chloroform-*d*) δ** 3.46 (s, 3H).

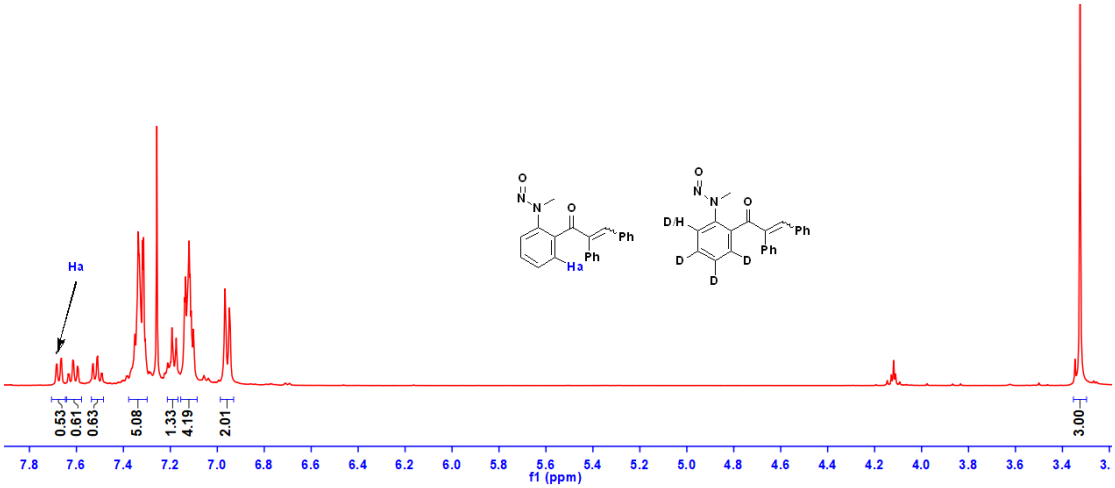




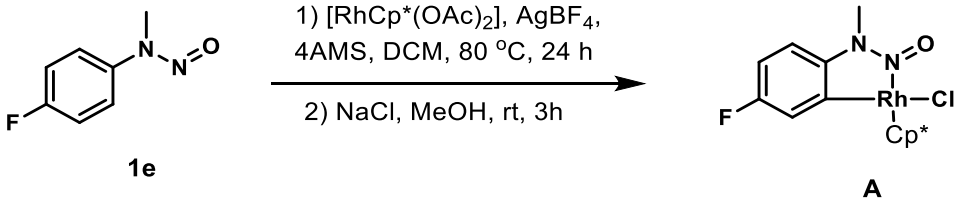
ii) Kinetic isotope effect



Two pressure tubes were separately charged with **1a** and **1a-*d*$_5$** (0.12 mmol), and to each tube was added cyclopropenone **2a** (0.1 mmol), $[Cp^*Rh(OAc)_2]_2$ (5 mol %), $AgBF_4$ (20 mol%), 4 Å M.S. (60 mg), DCM (1 mL). The two reaction mixtures were stirred side by side in an oil bath preheated at 80 °C for 5h. The resulting mixtures in the two tubes were rapidly combined and the solvent was rapidly removed under reduced pressure. The resulting residue was purified by silica gel chromatography using EA/PE to afford the mixture products. The KIE value was determined to be *k*H/*k*D= 1.2 on the basis of **^{1}H NMR** analysis.

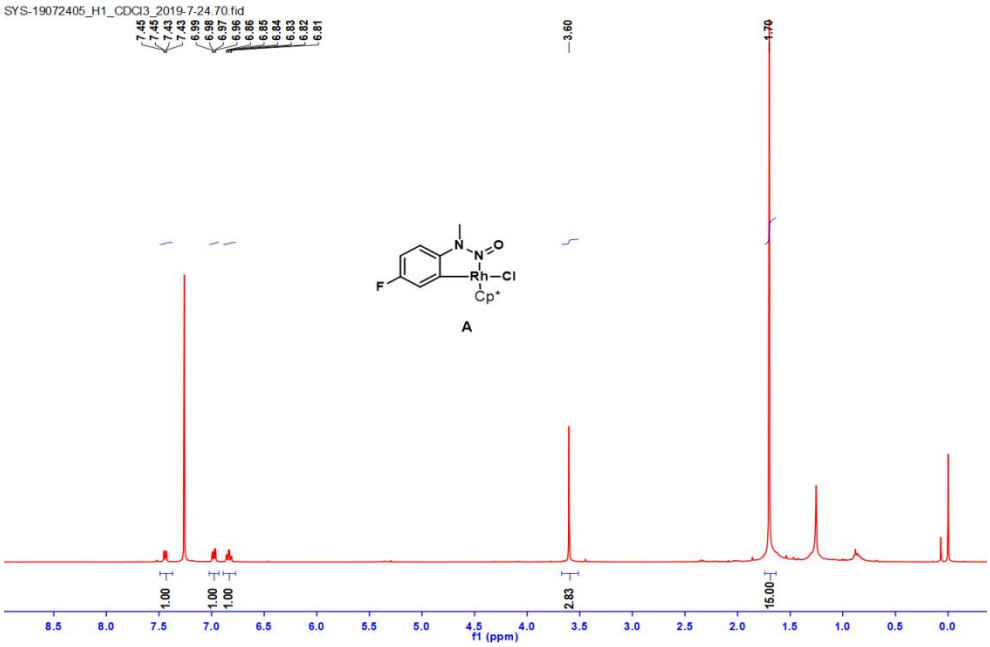


4) The synthesis of Rh(III) specie A

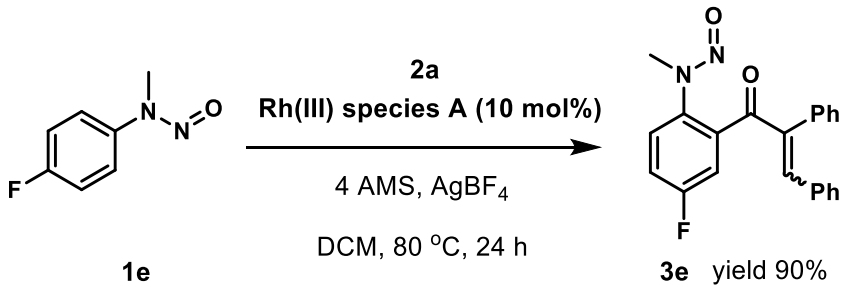


1e **A**

$[RhCp^*(OAc)_2]_2$ (0.1 mmol), $AgBF_4$ (0.2 mmol), 4 ÅMS (60mg) and **1f** (0.05 mmol) were dissolved in DCM (1 mL) in a pressure tube under air. The reaction mixture was stirred at 80 ℃ for 24 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford **Rh(III) specie A**, which was characterized by ^{1}H NMR spectroscopy. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.4 (d, *J* = 8.0, 1H), 7.0 (d, *J* = 8.0, 1H), 6.8 (d, *J* = 8.0, 1H), 3.6 (s, 3H), 1.7 (s, 15H).



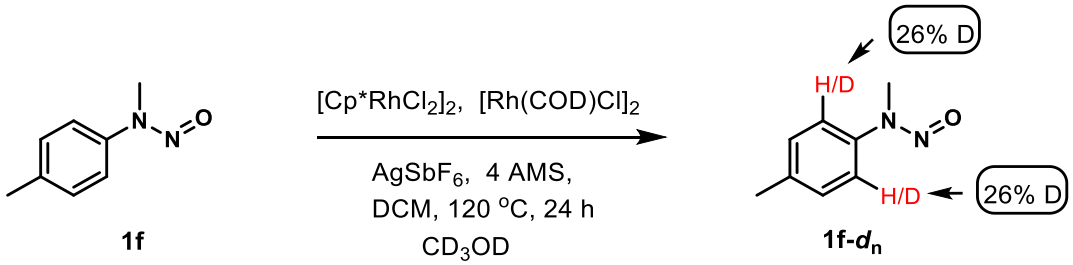
5) The catalytic activity study of Rh(III) specie A



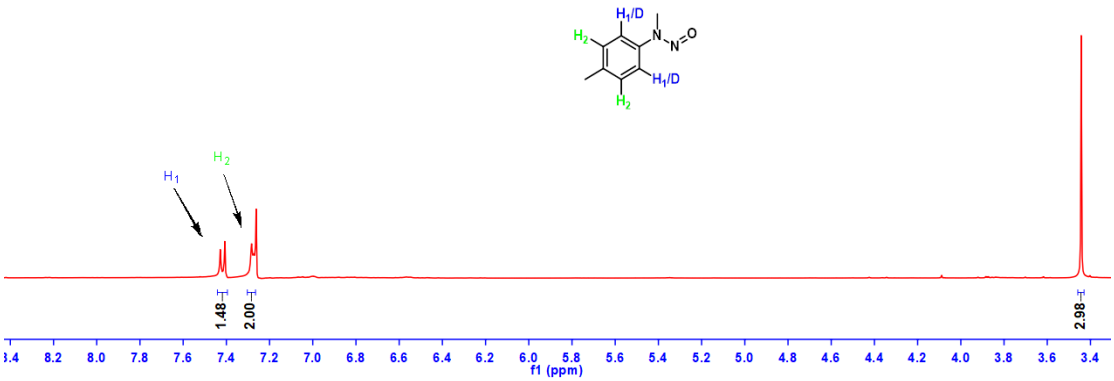
N-nitrosoaniline **1e** (0.12 mmol), diphenylcyclopropenone **2a** (0.10 mmol), **Rh(III) specie A** (0.01 mmol), 4 ÅMS (60 mg) and $AgBF_4$ (0.02 mmol) were charged into a pressure tube, to which was added DCM (1.0 mL) under air. The test tube was sealed with a rubber septum and the reaction mixture was stirred at 80 ℃ for 24 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford compound **3e** in 90% yield.

(b) The mechanistic studies of indoles synthesis

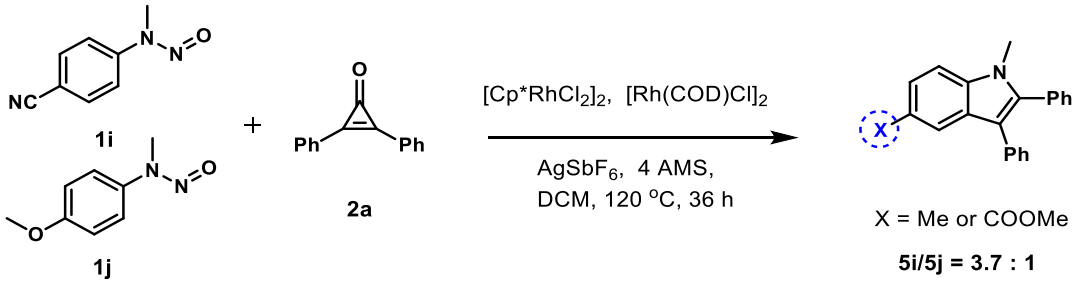
1) Deuterium exchange experiments



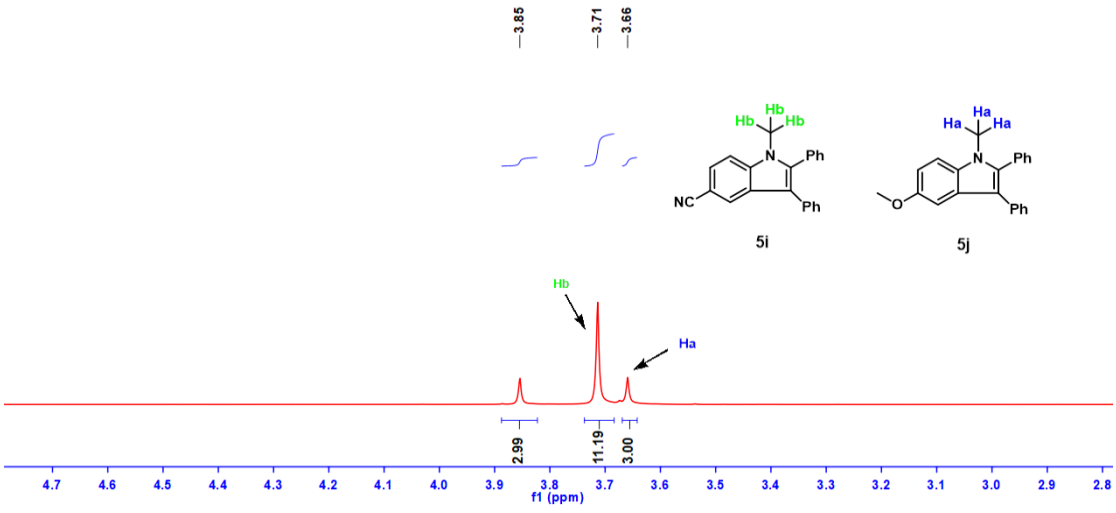
N-nitrosoaniline **1f** (0.10 mmol), $[Cp^*RhCl_2]_2$ (0.005 mmol), $[Rh(COD)Cl]_2$ (0.005 mmol), 4 ÅMS (60 mg), $AgSbF_6$ (0.01 mmol) were charged into a pressure tube, to which was added CD_3OD (0.1mL) and DCM (1.9 mL). The reaction mixture was stirred at 120 ℃ for 24 h. After cooled to rt, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford compound **1f-d_n** as a yellow oil. The deuterium incorporation was determined to be 26% by **^{1}H NMR** method, confirming that the initial *ortho*-C-H metalation was reversible.



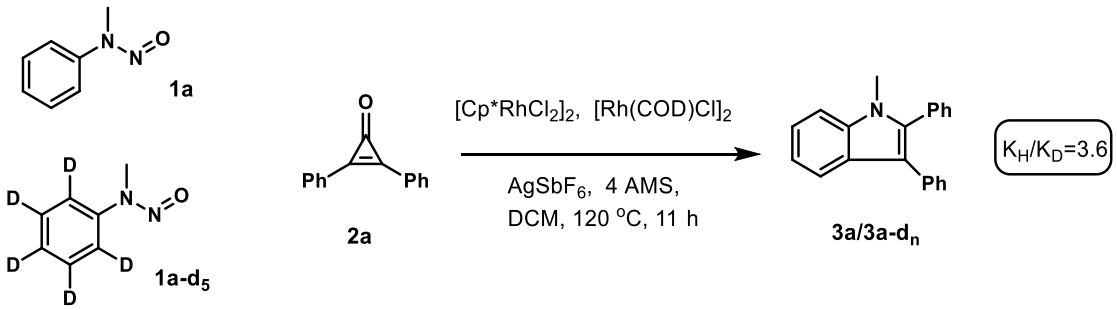
2) Competition experiments



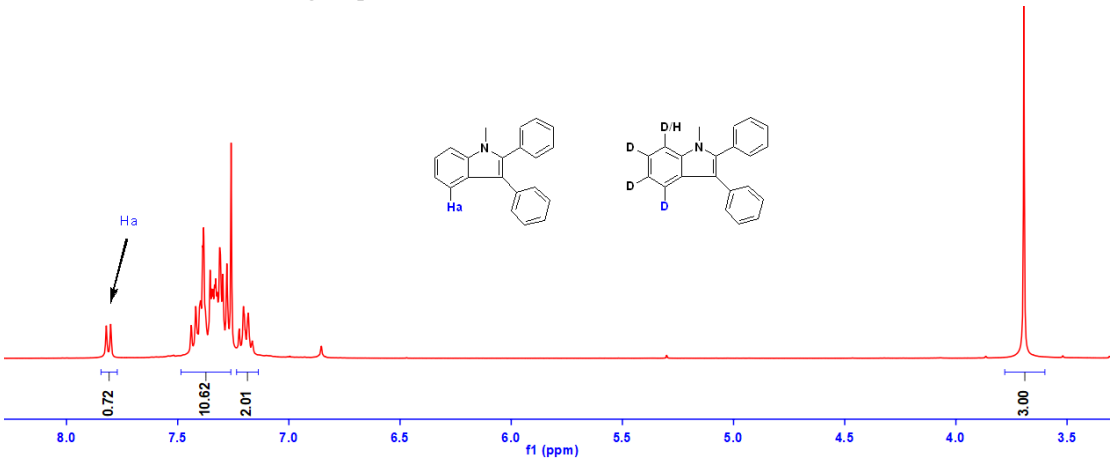
A mixture of **1i** (0.1 mmol), **1j** (0.1 mmol), cyclopropenone **2a** (0.2 mmol), $[Cp^*RhCl_2]_2$ (0.005 mmol), $[Rh(COD)Cl]_2$ (0.005 mmol), 4 ÅMS (60 mg), $AgSbF_6$ (0.01 mmol) and DCM (2.0 mL) were charged into a pressure tube under air. The reaction mixture was stirred at 120 ℃ for 36 h. After that, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford **5i** and **5j**, which were characterized by **^{1}H NMR** spectroscopy. The competition reaction determined the reaction favored the electron-withdrawing N-nitrosoaniline.



3) Kinetic isotope effect of the transformation



Two pressure tubes were separately charged with **1a** and **1a-*d*$_5$** (0.12 mmol), and to each tube was added cyclopropenone **2a** (0.1 mmol), $[Cp^*RhCl_2]_2$ (0.005 mmol), $[Rh(COD)Cl]_2$ (0.005 mmol), 4 ÅMS (60 mg), $AgSbF_6$ (0.01 mmol) and DCM (2.0 mL)were charged into a pressure tube. The two reaction mixtures were stirred side by side in an oil bath preheated at 120 ^oC for 11h. The resulting mixtures in the two tubes were rapidly combined and the solvent was rapidly removed under reduced pressure. The resulting residue was purified by silica gel chromatography using EA/PE to afford the mixture products. The KIE value was determined to be *k*H/*k*D= 3.6 on the basis of ^1H NMR analysis, suggesting that the C–H cleavage of N-nitrosoaniline was probably involved in the rate-limiting step.

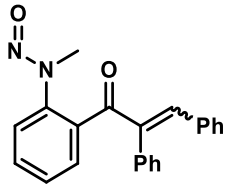


4) The catalytic activity study of Rh(III) specie A

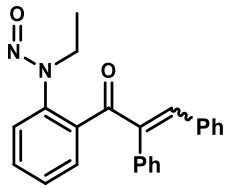
N-nitrosoaniline **1g** (0.12 mmol), diphenylcyclopropenone **2a** (0.10 mmol), **Rh(III) specie A**

(0.01 mmol), $[Rh(COD)Cl]_2$ (0.005 mmol), 4 ÅMS (60 mg), $AgSbF_6$ (0.01 mmol) and DCM (2.0 mL) were charged into a pressure tube under air. The test tube was sealed with a rubber septum and the reaction mixture was stirred at 120 ℃ for 36 h. After cooled to room temperature, the solvent was removed under reduced pressure and the residue was purified by silica gel chromatography using PE/EA to afford compound **5g** in 77% yield, demonstrating that such rhodacycles **A** could be involved in the catalytic formation of indole product.

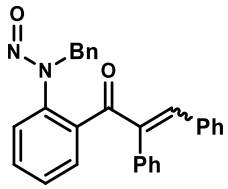
IV. Characterization Date of Products



N-(2-(2,3-diphenylacryloyl)phenyl)-N-methylnitrous amide (3a): yield 91%, yellow oil. *E/Z* = 12 : 1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.68 (d, *J* = 7.7 Hz, 1H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.37-7.31 (m, 5H), 7.23-7.17 (m, 1H), 7.16-7.09 (m, 4H), 6.96 (d, *J* = 7.5 Hz, 2H), 3.33 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 196.1, 143.7, 140.8, 140.3, 135.3, 135.1, 134.5, 131.2, 130.8, 130.3, 130.1, 129.6, 128.8, 128.4, 128.1, 128.1, 122.7, 34.4. **HRMS (ESI):** m/z calculated for $C_{22}H_{19}N_2O_2$ $[M+H]^+$: 343.1441, found: 343.1443.

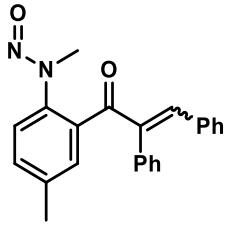


N-(2-(2,3-diphenylacryloyl)phenyl)-N-ethylnitrous amide (3b): yield 84%, yellow oil. *E/Z* = 5 : 1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.67-7.59 (m, 2H), 7.51 (t, *J* = 7.1 Hz, 1H), 7.40-7.29 (m, 6H), 7.17-7.13 (m, 6H), 7.03 (d, *J* = 7.4 Hz, 1H), 6.95 (d, *J* = 7.5 Hz, 2H), 3.93 (q, *J* = 7.2 Hz, 2H), 1.13 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 196.2, 144.1, 140.9, 139.3, 135.5, 135.5, 134.5, 131.0, 130.8, 130.3, 130.0, 129.6, 128.8, 128.3, 128.1, 128.0, 123.1, 41.7, 11.7. **HRMS (ESI):** m/z calculated for $C_{23}H_{21}N_2O_2$ $[M+H]^+$: 357.1598, found: 357.1599.

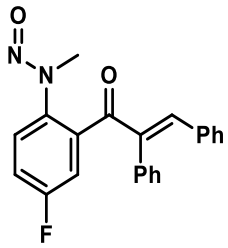


N-benzyl-N-(2-(2,3-diphenylacryloyl)phenyl)nitrous amide (3c): yield 92%, yellow oil. *E/Z* =

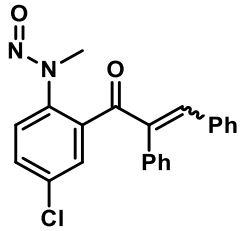
5 : 1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.66-7.62 (m, 1H), 7.47-7.44 (m, 2H), 7.42-7.38 (m, 1H), 7.37-7.29 (m, 6H), 7.23-7.15 (m, 7H), 7.15-7.10 (m, 3H), 7.07 (dd, *J* = 6.7, 2.8 Hz, 2H), 6.95 (d, *J* = 7.5 Hz, 2H), 5.07 (s, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 196.1, 143.7, 140.7, 139.2, 135.3, 134.8, 134.3, 134.1, 130.8, 130.7, 130.1, 129.9, 129.5, 129.1, 128.7, 128.7, 128.2, 128.0, 127.8, 127.7, 123.0, 49.3. **HRMS (ESI):** m/z calculated for $C_{28}H_{23}N_2O_2$ $[M+H]^+$: 419.1754, found: 419.1756.



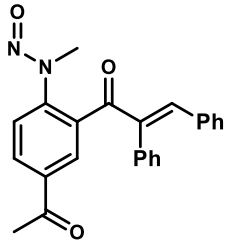
N-(2-(2,3-diphenylacryloyl)-4-methylphenyl)-N-methylnitrous amide (3d): yield 92%, yellow solid, m.p. 92 - 94°C. *E/Z* = 14 : 1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.47 (s, 1H), 7.43-7.39 (m, 1H), 7.35-7.30 (m, 4H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.19 (t, *J* = 7.3 Hz, 1H), 7.15-7.09 (m, 4H), 6.95 (d, *J* = 7.4 Hz, 2H), 3.30 (s, 3H), 2.47 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 196.3, 143.7, 141.0, 138.5, 137.9, 135.3, 134.9, 134.4, 131.8, 130.7, 130.7, 130.0, 129.6, 128.7, 128.3, 128.1, 122.8, 34.6, 21.2. **HRMS (ESI):** m/z calculated for $C_{23}H_{21}N_2O_2$ $[M+H]^+$: 357.1598, found: 357.1599.



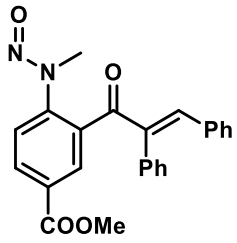
N-(2-(2,3-diphenylacryloyl)-4-fluorophenyl)-N-methylnitrous amide (**3e**): yield 89%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.42-7.32 (m, 7H), 7.26-7.20 (m, 1H), 7.18-7.12 (m, 4H), 6.99 (d, *J* = 7.4 Hz, 2H), 3.32 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 194.6 (d, *J* = 1.0 Hz), 161.6 (d, *J* = 251.2 Hz)., 144.4, 140.3, 137.2 (d, *J* = 6.7 Hz), 136.4 (d, *J* = 3.2 Hz), 135.0, 134.2, 130.9, 130.0, 130.0, 128.9, 128.4, 128.3, 125.1 (d, *J* = 8.4 Hz), 118.1 (d, *J* = 22.9 Hz), 117.2 (d, *J* = 24.0 Hz), 34.7. **HRMS (ESI):** m/z calculated for $C_{22}H_{18}FN_2O_2$ $[M+H]^+$: 361.1347, found: 361.1349.



N-(4-chloro-6-(2,3-diphenylacryloyl)phenyl)-N-methylnitrous amide (3f): yield 53%, yellow oil. *E/Z* = 5: 1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.65 (d, *J* = 2.4 Hz, 1H), 7.58 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.36-7.31 (m, 5H), 7.29 (s, 1H), 7.23-7.06 (m, 7H), 6.99-6.94 (m, 2H), 3.28 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 194.4, 144.1, 140.1, 136.1, 134.8, 133.9, 131.0, 130.8, 130.1, 129.9, 129.7, 129.1, 128.7, 128.3, 128.2, 127.3, 123.6, 34.0. **HRMS (ESI):** m/z calculated for $C_{22}H_{18}ClN_2O_2$ $[M+H]^+$: 377.1051, 379.1022 (isotopic peak), found: 377.1054, 379.1031.

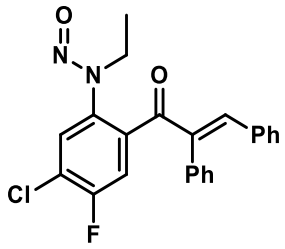


N-(4-acetyl-2-(2,3-diphenylacryloyl)phenyl)-N-methylnitrous amide (3g): yield 93%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.20 (d, *J* = 2.0 Hz, 1H), 8.16 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.39-7.35 (m, 2H), 7.33-7.28 (m, 3H), 7.22-7.17 (m, 1H), 7.14-7.07 (m, 4H), 6.95 (d, *J* = 7.3 Hz, 2H), 3.29 (s, 3H), 2.66 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 196.3, 195.0, 143.4, 143.2, 140.2, 135.9, 135.2, 134.3, 134.1, 130.8, 130.8, 130.6, 130.0, 129.7, 128.7, 128.4, 128.2, 121.3, 33.1, 26.8. **HRMS (ESI):** m/z calculated for $C_{24}H_{21}N_2O_3$ $[M+H]^+$: 385.1547, found: 385.1549.

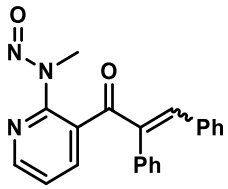


methyl4-(2,3-diphenylacryloyl)-3-(methyl(nitroso)amino) benzoate (3h): yield 88%, yellow solid, m.p. 146 - 148^{o}C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.33 (d, *J* =2.0 Hz, 1H), 8.25 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.39-7.34 (m, 2H), 7.31 (dd, *J* = 5.0, 1.9 Hz, 3H), 7.24-7.16 (m, 1H), 7.15-7.07 (m, 4H), 7.00-6.92 (m, 2H), 3.97 (s, 3H), 3.30 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 194.9, 165.5, 143.5, 143.2, 140.1, 135.0, 134.2, 134.0, 132.1, 131.5, 130.7, 129.9, 129.6, 129.2, 128.6, 128.2 128.1, 121.1, 52.6, 33.1. **HRMS (ESI):** m/z calculated for

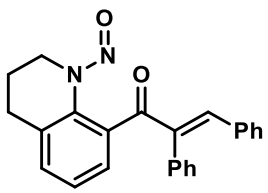
$C_{24}H_{21}N_2O_4$ $[M+H]^+$: 401.1496, found: 401.1498.



N-(5-chloro-2-(2,3-diphenylacryloyl)-4-fluorophenyl)-N-methylnitrous amide (3i): yield 58%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.45-7.30 (m, 7H), 7.22-7.11 (m, 6H), 3.87 (q, *J* = 7.2 Hz, 2H), 1.11 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 193.6, 157.0 (d, *J* = 253.6 Hz), 144.6, 135.9 (d, *J* = 3.7 Hz), 134.8, 134.0, 131.1, 130.8, 129.9, 129.8, 128.9, 128.8, 128.3, 128.2, 125.5, 123.5 (d, *J* = 19.1 Hz), 118.0 (d, *J* = 23.4 Hz), 41.7, 11.5. **HRMS (ESI):** m/z calculated for $C_{23}H_{19}ClFN_2O_2$ $[M+Na]^+$: 431.0933, 433.0904 (isotopic peak)，found: 431.0936, 433.0912.

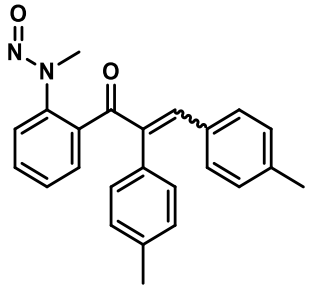


N-(3-(2,3-diphenylacryloyl)pyridin-2-yl)-N-methylnitrous amide (3j): yield 54%, yellow oil. *E/Z* = 3 : 2. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.44 (d, *J* = 3.7 Hz, 1H), 8.11-8.03 (m, 2H), 7.76 (t, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 7.5 Hz, 2H), 7.54-7.49 (m, 3H), 7.45-7.29 (m, 10H), 7.20-7.02 (m, 5H), 6.98-6.91 (m, 2H), 6.67 (s, 1H), 6.59 (d, *J* = 8.1 Hz, 1H), 3.43 (s, 3H), 3.33 (s, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 171.1, 170.5, 148.1, 148.0, 137.8, 137.6, 137.4, 137.3, 137.0, 136.5, 135.9, 135.6, 129.2, 129.1, 128.9, 128.7, 128.7, 128.5, 128.5, 128.4, 128.4, 128.3, 128.1, 127.7, 126.6, 126.0, 121.3, 121.0, 120.2, 119.3, 35.5, 34.8. **HRMS (ESI):** m/z calculated for $C_{21}H_{18}N_3O_2$ $[M+H]^+$: 344.1394, found: 344. 1395.

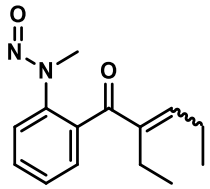


1-(1-nitroso-1,2,3,4-tetrahydroquinolin-8-yl)-2,3-diphenylprop-2-en-1-one (3k): yield 85%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.53-7.47 (m, 2H), 7.32 (t, *J* = 7.5 Hz, 1H),

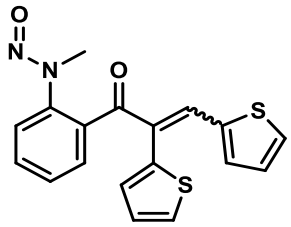
7.29-7.26 (m, 1H), 7.25-7.20 (m, 3H), 7.19-7.14 (m, 1H), 7.13-7.07 (m, 2H), 7.01-6.93 (m, 4H), 3.62 (t, *J* = 6.4 Hz, 2H), 2.77-2.58 (m, 2H), 1.71 (m, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 195.4, 141.0, 140.0, 136.0, 135.0, 134.4, 131.7, 130.7, 130.3, 130.2, 129.1, 129.1, 128.8, 128.4, 128.2, 127.8, 126.3, 43.8, 27.8, 21.0. **HRMS (ESI):** m/z calculated for $C_{24}H_{21}N_2O_2$ $[M+H]^+$: 369.1598, found: 369.1604.



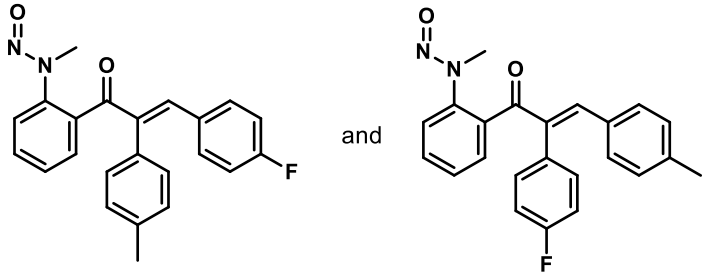
N-(2-(2,3-di-p-tolylacryloyl)phenyl)-N-methylnitrous amide (3m): yield 87%, yellow solid, m.p. 145 - 147°C. *E/Z* = 20 : 1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.66 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.60 (m, 1H), 7.50 (m, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.27-7.25 (m, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.97-6.91 (m, 2H), 6.87 (d, *J* = 8.2 Hz, 2H), 3.32 (s, 3H), 2.35 (s, 3H), 2.25 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 196.3, 143.8, 140.2, 140.0, 139.9, 137.7, 135.3, 132.3, 131.6, 131.0, 130.8, 130.2, 129.8, 129.4, 129.0, 128.0, 122.9, 34.5, 21.4, 21.4. **HRMS (ESI):** m/z calculated for $C_{24}H_{23}N_2O_2$ $[M+H]^+$: 371.1754, found: 371.1758.



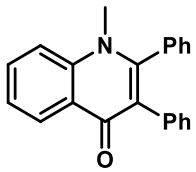
N-(2-(2-ethylpent-2-enoyl)phenyl)-N-methylnitrous amide (3n): yield 78%, yellow oil. *E/Z* = 5 : 1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.58 (m, 1H), 7.51-7.42 (m, 2H), 7.37 (d, *J* = 7.9 Hz, 1H), 6.19 (t, *J* = 7.6 Hz, 1H), 3.31 (s, 3H), 2.37 (q, *J* = 7.5 Hz, 2H), 2.25-2.17 (m, 2H), 1.01-0.93 (m, 6H)**. ^{13}C NMR (100 MHz, Chloroform-*d*)** δ 197.1, 150.7, 142.9, 140.2, 135.7, 130.7, 129.9, 128.2, 124.0, 35.1, 22.4, 19.0, 13.8, 13.4. **HRMS (ESI):** m/z calculated for $C_{14}H_{19}N_2O_2$ $[M+H]^+$: 247.1441, found: 247.1442.



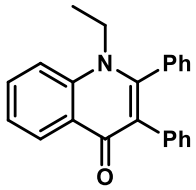
N-(2-(2,3-di(thiophen-2-yl)acryloyl)phenyl)-N-methylnitrous amide (**3o**): yield 74%, yellow oil. *E/Z* = 22 : 1. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.69 (s, 1H), 7.62 (t, *J* = 7.6 Hz, 2H), 7.52-7.48 (m, 2H), 7.37 (t, *J* = 6.6 Hz, 2H), 7.17-7.09 (m, 2H), 7.00-6.91 (m, 2H), 3.37 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 194.3, 140.2, 139.6, 138.2, 135.3, 134.8, 134.4, 132.8, 131.1, 130.3, 129.9, 129.5, 128.5, 128.1, 127.7, 127.0, 123.1, 34.4. **HRMS (ESI):** m/z calculated for $C_{18}H_{15}N_2O_2S_2$ $[M+H]^+$:355.0569, found: 355.0571.



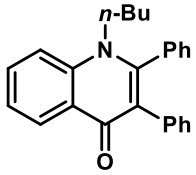
(E)-N-(2-(3-(4-fluorophenyl)-2-(p-tolyl)acryloyl)phenyl)-N-methylnitrous amide(3p) and (E)-N-(2-(2-(4-fluorophenyl)-3-(p-tolyl)acryloyl)phenyl)-N-methylnitrous amide(3p`)**: yield 88%, **3p**:**3p`= 1.5:1, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.70-7.57 (m, 3H), 7.56-7.47 (m, 2H), 7.35 (t, *J* = 8.9 Hz, 2H), 7.27 (s, 2H), 7.17-6.93 (m, 10H), 6.87-6.78 (m, 3H), 3.35 (s, 2H), 3.32 (s, 3H), 2.36 (s, 3H), 2.27 (s, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 196.1, 196.0, 163.7, 161.8, 161.3, 144.2, 142.1, 140.4, 140.4, 140.3, 140.2, 140.1, 139.0, 138.0, 135.1, 134.9, 132.7, 132.6, 131.9, 131.8, 131.8, 131.3, 131.3, 131.1, 131.1, 130.7, 130.7, 129.7, 129.6, 129.2, 128.1, 128.0, 122.8, 122.7, 115.9, 115.7, 115.5, 115.3, 34.3, 21.4, 21.4. m/z: 375.1503 **HRMS (ESI):** m/z calculated for $C_{23}H_{20}FN_2O_2$+ $[M+H]^+$: 375.1503, found: 375.1513.



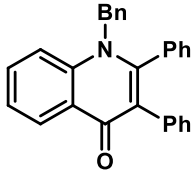
1-Methyl-2,3-diphenylquinolin-4(1*H*)-one (4a)[3]: yield 83%, yellow solid, m.p. 237-239 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.60 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.78-7.69 (m, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.47-7.40 (m, 1H), 7.31-7.26 (m, 3H), 7.17-7.02 (m, 7H), 3.55 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.3, 152.2, 141.4, 135.9, 135.0, 132.3, 131.4, 129.6, 128.7, 128.3, 127.5, 127.3, 126.6, 126.1, 124.3, 123.6, 115.9, 37.7. **HRMS (ESI):** m/z calculated for $C_{22}H_{18}NO$ $[M+H]^+$: 312.1383, found: 312.1384.



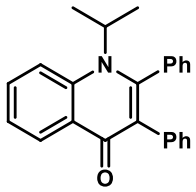
1-Ethyl-2,3-diphenylquinolin-4(1*H*)-one (4b): yield 76%, yellow solid, m.p. 185-187 ^{o}C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.60 (d, *J* = 8.1 Hz, 1H), 7.71 (t, *J* = 8.1 Hz, 1H), 7.60 (d, *J* = 8.1 Hz, 1H), 7.42 (t, *J* = 8.1 Hz, 1H), 7.32-7.26 (m, 3H), 7.22-7.17 (m, 2H), 7.14-7.07 (m, 2H), 7.06-6.99 (m, 3H), 4.07 (q, *J* = 7.1 Hz, 2H), 1.29 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.3, 152.0, 140.0, 136.0, 135.0, 132.3, 131.4, 129.4, 128.8, 128.4, 127.9, 127.6, 127.2, 126.3, 124.8, 123.6, 116.1, 43.7, 14.5. **HRMS (ESI):** m/z calculated for $C_{23}H_{20}NO$ $[M+H]^+$: 326.1539, found: 326.1538.



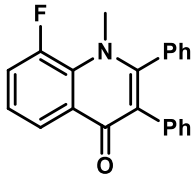
1-Butyl-2,3-diphenylquinolin-4(1*H*)-one (4c): yield 75%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.59 (d, *J* = 8.0 Hz, 1H), 7.75-7.67 (m, 1H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.30-7.26 (m, 3H), 7.18-6.99 (m, 7H), 3.98-3.94 (m, 2H), 1.80-1.59 (m, 2H), 1.19-1.11 (m, 2H), 0.76 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.3, 152.1, 140.3, 136.0, 134.9, 132.3, 131.4, 129.5, 128.7, 128.3, 127.8, 127.5, 127.1, 126.2, 124.6, 123.6, 116.2, 48.7, 30.9, 19.9, 13.5. **HRMS (ESI):** m/z calculated for $C_{25}H_{24}NO$ $[M+H]^+$: 354.1852, found: 354.1858.



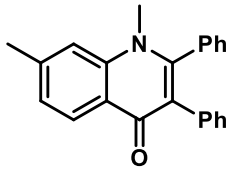
1-Benzyl-2,3-diphenylquinolin-4(1*H*)-one (4d): yield 69%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.60 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.61-7.50 (m, 1H), 7.43-7.35 (m, 2H), 7.33-7.26 (m, 3H), 7.17-6.99 (m, 12H), 5.25 (s, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.7, 152.7, 140.8, 136.6, 135.9, 134.6, 132.4, 131.5, 129.3, 129.1, 128.9, 128.2, 127.7, 127.6, 127.6, 127.0, 126.4, 125.6, 124.9, 123.9, 117.2, 52.7. **HRMS (ESI):** m/z calculated for $C_{28}H_{22}NO$ $[M+H]^+$: 388.1696, found: 388.1695.



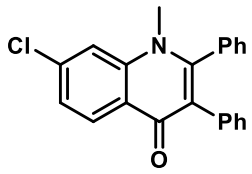
1-Isopropyl-2,3-diphenylquinolin-4(1*H*)-one (4e): yield 58%, yellow solid, m.p. 199-201 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.60 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.87 (d, *J* = 8.8 Hz, 1H), 7.69-7.61 (m, 1H), 7.42-7.37 (m, 1H), 7.26-6.97 (m, 10H), 4.65 (m, 1H), 1.62 (d, *J* = 7.2 Hz, 6H). **^{13}CMR (100 MHz, Chloroform-*d*)** δ 176.1, 152.7, 139.6, 136.1, 135.8, 131.3, 130.8, 129.0, 128.5, 128.3, 127.9, 127.9, 127.4, 126.0, 124.5, 123.2, 118.5, 53.7, 21.2. **HRMS (ESI):** m/z calculated for $C_{24}H_{22}NO$ $[M+H]^+$: 340.1696, found: 340.1694.



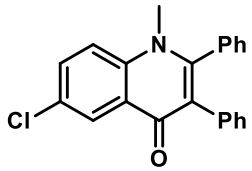
8-Fluoro-1-methyl-2,3-diphenylquinolin-4(1*H*)-one (4g): yield 85%, yellow solid, m.p. 159-162 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.35-8.31 (m, 1H), 7.46-7.38 (m, 1H), 7.36-7.30 (m, 1H), 7.30-7.26 (m, 3H), 7.21-7.02 (m, 7H), 3.62 (d, *J* = 8.2 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 175.6 (d, *J* = 2.4 Hz), 154.2, 152.7 (d, *J* = 248.7 Hz), 135.2, 134.7, 132.4 (d, *J* = 6.7 Hz), 131.5, 130.1, 129.7, 129.1, 128.6, 127.6, 126.4, 124.4, 123.9 (d, *J* = 8.2 Hz), 123.1 (d, *J* = 3.6 Hz), 118.9 (d, *J* = 22.7 Hz), 42.5 (d, *J* = 15.4 Hz). **HRMS (ESI):** m/z calculated for $C_{22}H_{17}FNO$ $[M+H]^+$: 330.1289, found: 330.1288.



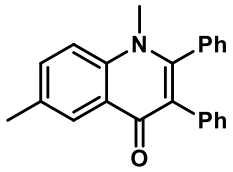
1,7-Dimethyl-2,3-diphenylquinolin-4(1*H*)-one (4h): yield 61%, yellow solid, m.p. 276-278 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.46 (d, *J* = 8.2 Hz, 1H), 7.35 (s, 1H), 7.30-7.26 (m, 4H), 7.17-6.99 (m, 7H), 3.52 (s, 3H), 2.56 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.3, 152.0, 143.1, 141.8, 136.0, 135.3, 131.6, 129.7, 128.8, 128.4, 127.5, 127.5, 126.2, 125.4, 124.7, 124.4, 115.6, 37.7, 22.5. **HRMS (ESI):** m/z calculated for $C_{23}H_{20}NO$ $[M+H]^+$: 326.1539, found: 326.1539.



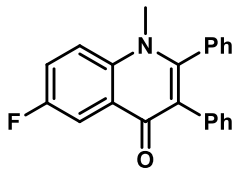
7-Chloro-1-methyl-2,3-diphenylquinolin-4(1*H*)-one (4i): yield 53%, yellow solid, m.p. 250-252 ^{o}C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.49 (d, *J* = 8.6 Hz, 1H), 7.57 (d, *J* = 1.8 Hz, 1H), 7.38 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.30-7.27 (m, 2H), 7.17-6.98 (m, 8H), 3.51 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 175.9, 152.5, 142.2, 138.8, 135.4, 134.8, 131.3, 129.6, 129.3, 129.0, 128.6, 127.6, 126.5, 125.1, 125.0, 124.4, 115.8, 37.9. **HRMS (ESI):** m/z calculated for $C_{22}H_{17}ClNO$ $[M+H]^+$: 346.0993, 348.0964 (isotopic peak), found: 346.0995, 348.0969.



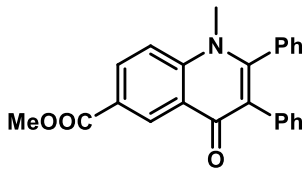
6-Chloro-1-methyl-2,3-diphenylquinolin-4(1*H*)-one (4j): yield 85%, yellow solid, m.p. 229-231 ^{o}C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.52 (d, *J* = 2.6 Hz, 1H), 7.65 (dd, *J* = 9.1, 2.6 Hz, 1H), 7.52 (d, *J* = 9.1 Hz, 1H), 7.30-7.27 (m, 3H), 7.16-7.00 (m, 7H), 3.53 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 175.3, 152.5, 140.0, 135.5, 134.8, 132.6, 131.4, 130.0, 129.6, 129.0, 128.5, 127.8, 127.7, 126.8, 126.5, 124.8, 117.8, 38.0. **HRMS (ESI):** m/z calculated for $C_{22}H_{17}ClNO$ $[M+H]^+$: 346.0993, 348.0964 (isotopic peak), found: 346.0998, 348.0967.



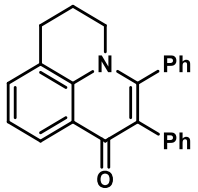
1,6-Dimethyl-2,3-diphenylquinolin-4(1*H*)-one (4k): yield 80%, yellow solid, m.p. 237-239 ^{o}C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.37 (s, 1H), 7.55 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.48 (d, *J* = 8.8 Hz, 1H), 7.33-7.26 (m, 3H), 7.20-6.90 (m, 7H), 3.53 (s, 3H), 2.51 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.2, 151.9, 139.6, 136.1, 135.2, 133.8, 133.6, 131.6, 129.7, 128.8, 128.4, 127.5, 126.9, 126.6, 126.2, 124.1, 115.8, 37.7, 21.0. **HRMS (ESI):** m/z calculated for $C_{23}H_{20}NO$ $[M+H]^+$: 326.1539, found: 326.1537.



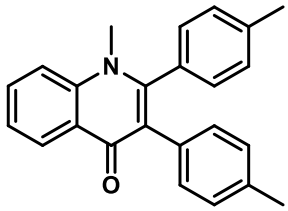
6-Fluoro-1-methyl-2,3-diphenylquinolin-4(1*H*)-one (4l): yield 84%, yellow solid, m.p. 238-240 ^{o}C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.20 (dd, *J* = 8.9, 3.1 Hz, 1H), 7.57 (dd, *J* = 9.3, 4.1 Hz, 1H), 7.50-7.37 (m, 1H), 7.31-7.26 (m, 3H), 7.18-6.98 (m, 7H), 3.55 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 175.5, 159.3 (d, *J* = 245.1 Hz), 152.4, 138.0, 135.6, 134.8, 131.4, 129.6, 129.0, 128.5, 128.2 (d, *J* = 6.6 Hz), 127.6, 126.4, 123.8, 120.8 (d, *J* = 25.0 Hz), 118.3 (d, *J* = 7.5 Hz), 111.9 (d, *J* = 22.4 Hz), 38.1. **HRMS (ESI):** m/z calculated for $C_{22}H_{17}FNO$ $[M+H]^+$: 330.1289, found: 330.1287.



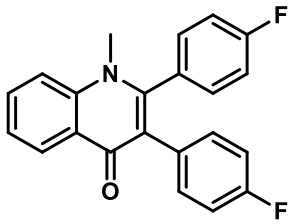
Methyl 1-methyl-4-oxo-2,3-diphenyl-1,4-dihydroquinoline-6-carboxylate (4m): yield 51%, yellow solid, m.p. 247-249 ^{o}C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 9.21 (d, *J* = 2.1 Hz, 1H), 8.34 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.60 (d, *J* = 8.9 Hz, 1H), 7.31-7.28 (m, 2H), 7.19-6.98 (m, 8H), 3.97 (s, 3H), 3.56 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.3, 166.7, 152.6, 144.2, 135.3, 134.7, 132.8, 131.3, 130.1, 129.6, 129.1, 128.6, 127.7, 126.5, 126.1, 125.5, 125.3, 116.2, 52.4, 38.1. **HRMS (ESI):** m/z calculated for $C_{24}H_{20}NO_3$ $[M+H]^+$: 370.1438, found: 370.1439.



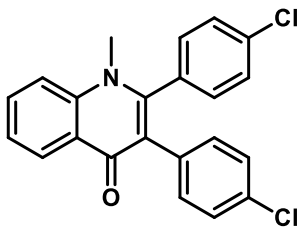
2,3-Diphenyl-6,7-dihydro-1*H*,5*H*-pyrido[3,2,1-*ij*]quinolin-1-one (4n): yield 57%, yellow solid, m.p. 266-268 ^{o}C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.43 (d, *J* = 7.7 Hz, 1H), 7.46 (d, *J* = 6.8 Hz, 1H), 7.36-7.29 (m, 2H), 7.27 (d, *J* = 2.1 Hz, 2H), 7.18-6.97 (m, 7H), 3.87-3.73 (m, 2H), 3.07 (t, *J* = 6.1 Hz, 2H), 2.09 (m, 2H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.2, 151.5, 138.2, 135.9, 134.8, 131.6, 131.6, 129.5, 128.7, 128.5, 127.6, 126.9, 126.8, 126.3, 125.6, 124.1, 123.6, 50.3, 28.0, 22.1. **HRMS (ESI):** m/z calculated for $C_{24}H_{20}NO_3$ $[M+H]^+$: 338.1539, found: 338.1536.



1-Methyl-2,3-di-*p*-tolylquinolin-4(1*H*)-one (4o): yield 85%, yellow solid, m.p. 211-213 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.56 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.73-7.66 (m, 1H), 7.54 (d, *J* = 8.6 Hz, 1H), 7.44-7.37 (m, 1H), 7.08 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 8.2 Hz, 2H), 6.93-6.91 (m, 4H), 3.51 (s, 3H), 2.31 (s, 3H), 2.21 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.5, 152.3, 141.5, 138.6, 135.5, 132.9, 132.3, 132.2, 131.2, 129.5, 129.1, 128.3, 127.5, 126.6, 124.3, 123.5, 115.9, 37.7, 21.4, 21.3. **HRMS (ESI):** m/z calculated for $C_{24}H_{21}NO$ $[M+H]^+$: 339.1623, found: 339.1626.

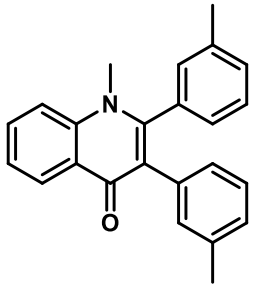


2,3-Bis(4-fluorophenyl)-1-methylquinolin-4(1*H*)-one (4p): yield 79%, yellow solid, m.p. 277-279 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.55 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.77-7.70 (m, 1H), 7.57 (d, *J* = 8.6 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.13 (dd, *J* = 8.5, 5.4 Hz, 2H), 7.04-6.94 (m, 4H), 6.87-6.78 (m, 2H), 3.55 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.3, 162.7 (d, *J* = 248.0 Hz), 161.4 (d, *J* = 244.0 Hz), 151.3, 141.5, 133.0 (d, *J* = 8.0 Hz), 132.6, 131.6 (d, *J* = 8.2 Hz), 131.0 (d, *J* = 3.7 Hz), 130.1 (d, *J* = 9.0 Hz), 127.4, 126.6, 124.0, 123.6, 116.0, 115.9 (d, *J* = 19.0 Hz), 114.7 (d, *J* = 21.0 Hz), 37.8. **HRMS (ESI):** m/z calculated for $C_{22}H_{16}F_2NO$ $[M+H]^+$: 348.1194, found: 348.1193.

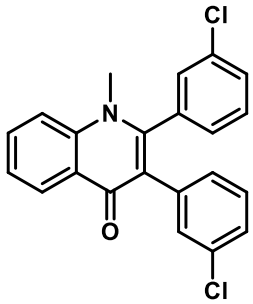


2,3-Bis(4-chlorophenyl)-1-methylquinolin-4(1*H*)-one (4q): yield 61%, yellow solid, m.p. 220-222 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.55 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.77-7.71(m, 1H), 7.57 (d, *J* = 8.6 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.15-7.07 (m, 4H), 6.98-6.92 (m, 2H), 3.54 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.1, 151.1, 141.5,

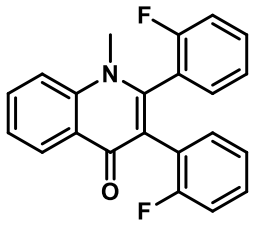
135.4, 134.0, 133.3, 132.8, 132.8, 132.5, 131.0, 129.1, 128.1, 127.6, 126.6, 124.2, 123.3, 116.0, 37.9. **HRMS (ESI):** m/z calculated for $C_{22}H_{16}Cl_2NO$ $[M+H]^+$: 402.0423, 404.0393 (isotopic peak), found: 402.0417, 404.0398.



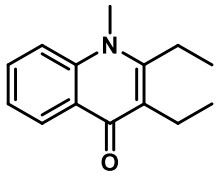
1-Methyl-2,3-di-*m*-tolylquinolin-4(1*H*)-one (4r): yield 71%, yellow solid, m.p.176-179 ^oC. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.58 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.72 (t, *J* = 8.0, 1H), 7.57 (d, *J* = 8.0Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.15 (t, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 7.7 Hz, 1H), 7.01-6.91 (m, 3H), 6.90-6.83 (m, 2H), 6.80 (d, *J* = 7.7 Hz, 1H), 3.55 (s, 3H), 2.27 (s, 3H), 2.18 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.4, 152.4, 141.5, 138.1, 136.7, 135.8, 135.0, 132.3, 132.2, 130.2, 129.5, 128.4, 128.2, 127.6, 127.4, 127.0, 126.7, 126.7, 124.5, 123.6, 115.8, 37.8, 21.4, 21.4. **HRMS (ESI):** m/z calculated for $C_{24}H_{22}NO$ $[M+H]^+$: 340.1696, found: 340.1695.



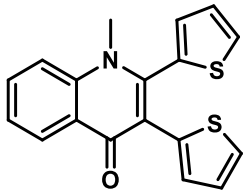
2,3-Bis(3-chlorophenyl)-1-methylquinolin-4(1*H*)-one (4s): yield 83%, yellow solid, m.p. 190-192 ^oC. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.54 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.79-7.71 (m, 1H), 7.58 (d, *J* = 8.6 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 1H), 7.32-7.26 (m, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.21-7.16 (m, 1H), 7.10-7.01 (m, 4H), 6.95-6.85 (m, 1H), 3.56 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.0, 150.7, 141.4, 137.3, 136.3, 134.8, 133.5, 132.8, 131.5, 130.0, 129.7, 129.6, 129.4, 129.0, 127.8, 127.5, 126.8, 126.7, 124.2, 123.1, 116.0, 37.9. **HRMS (ESI):** m/z calculated for $C_{22}H_{16}Cl_2NO$ $[M+Na]^+$: 402.0423, 404.0393 (isotopic peak), found: 402.0411, 404.0396.



2,3-Bis(2-fluorophenyl)-1-methylquinolin-4(1*H*)-one (4t): yield 73%, yellow solid, m.p. 169-172 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.60-8.53 (m, 1H), 7.80-7.68 (m, 1H), 7.59 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.35-7.27 (m, 1H), 7.24-6.74 (m, 7H), 3.65-3.56 (m, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 175.7, 163.5 (d, *J* = 243.0 Hz), 159.0 (d, *J* = 246.0 Hz), 147.2, 141.4, 133.5, 132.5, 132.0 (d, *J* = 3.5 Hz), 131.7 (d, *J* = 8.0 Hz), 131.5 (d, *J* = 3.1 Hz), 130.4 (d, *J* = 2.2 Hz), 129.1 (d, *J* = 8.2 Hz), 127.4, 124.5 (d, *J* = 3.6 Hz), 123.9, 123.7 (d, *J* = 3.6 Hz), 123.3 – 123.0 (m), 115.9, 115.8, 115.4 (d, *J* = 21.0 Hz), 114.9 (d, *J* = 22.3 Hz), 36.7. **HRMS (ESI):** m/z calculated for $C_{22}H_{16}F_2NO$ $[M+H]^+$: 348.1149, found: 348.1148.

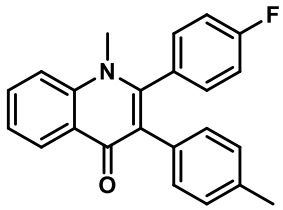


2,3-Diethyl-1-methylquinolin-4(1*H*)-one (4u): yield 46%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.51 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.67-7.60 (m, 1H), 7.50 (d, *J* = 8.7 Hz, 1H), 7.37-7.31 (m, 1H), 3.81 (s, 3H), 2.92 (q, *J* = 7.6 Hz, 2H), 2.74 (q, *J* = 7.4 Hz, 2H), 1.33 (t, *J* = 7.6 Hz, 3H), 1.16 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.6, 152.6, 141.3, 131.8, 127.2, 125.2, 123.3, 123.1, 115.2, 34.9, 23.8, 19.7, 14.4, 13.5. **HRMS (ESI):** m/z calculated for $C_{14}H_{18}NO$ $[M+H]^+$:216.1383, found: 216.1385.

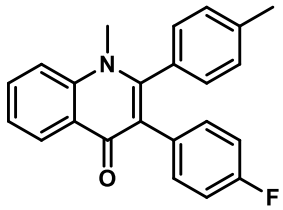


1-Methyl-2,3-di(thiophen-2-yl)quinolin-4(1*H*)-one (4v): yield 56%, yellow solid, m.p. 174-176 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.56 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.76-7.69 (m, 1H), 7.57 (d, *J* = 8.6 Hz, 1H), 7.49-7.40 (m, 2H), 7.21 (d, *J* = 5.1 Hz, 1H), 7.06-7.04 (m, 2H), 6.84 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.74 (d, *J* = 3.6 Hz, 1H), 3.66 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 175.8, 145.7, 141.4, 136.3, 135.3, 132.7, 130.7, 128.9, 128.5, 127.7, 127.3, 126.4, 126.0, 125.9,

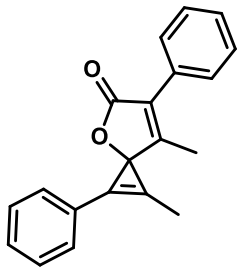
124.2, 119.2, 116.1, 38.1. **HRMS (ESI):** m/z calculated for $C_{18}H_{14}S_2NO$ $[M+H]^+$: 324.0511, found: 324.0510.



2-(4-Fluorophenyl)-1-methyl-3-(p-tolyl)quinolin-4(1H)-one (4x): yellow solid, m.p. 177-180 ^oC. yield 54%. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.57 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.73 (dd, *J* = 8.5, 6.9 Hz, 1H), 7.57 (d, *J* = 8.5 Hz, 1H), 7.48-7.40 (m, 1H), 7.19-7.11 (m, 2H), 6.99 (t, *J* = 8.4 Hz, 2H), 6.94 (d, *J* = 7.8 Hz, 2H), 6.89 (d, *J* = 7.8 Hz, 2H), 3.54 (s, 3H), 2.23 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.4, 162.5 (d, *J* = 249.8 Hz), 150.9, 141.5, 135.8, 132.5, 132.3, 131.5 (d, *J* = 8.3 Hz), 131.3 (d, *J* = 3.7 Hz), 131.1, 128.4, 127.5, 126.6, 124.6, 123.6, 115.7, 115.6 (d, *J* = 21.9 Hz), 37.6, 21.2. **HRMS (ESI):** m/z calculated for $C_{23}H_{19}FNO$ $[M+H]^+$: 344.1445, found: 344.1448.



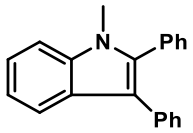
3-(4-fluorophenyl)-1-methyl-2-(p-tolyl)quinolin-4(1H)-one (4x`): yellow solid, m.p. 227-229 ^oC. yield 30%. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.58 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.73 (dd, *J* = 8.6, 7.0 Hz, 1H), 7.58 (d, *J* = 8.6 Hz, 1H), 7.44 (dd, *J* = 8.0, 7.0 Hz, 1H), 7.10 (d, *J* = 8.3 Hz, 2H), 7.05-6.96 (m, 4H), 6.87-6.77 (m, 2H), 3.55 (s, 3H), 2.33 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 176.2, 161.3 (d, *J* = 244.5 Hz), 152.5, 141.5, 138.9, 133.0 (d, *J* = 7.9 Hz), 132.3, 132.0, 131.8 (d, *J* = 3.5 Hz), 129.4, 129.2, 127.4, 126.6, 123.7, 123.3, 115.8, 114.4 (d, *J* = 21.4 Hz), 37.7, 21.3. **HRMS (ESI):** m/z calculated for $C_{23}H_{19}FNO$ $[M+H]^+$: 344.1445, found: 344.1447.



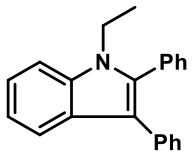
For the synthesis of chalcone or quinolone product, methylphenylcyclopropenone was observed to be more active to react with itself than to produce the desired product, resulting spirolactone product:

1,7-dimethyl-2,6-diphenyl-4-oxaspiro[2.4]hepta-1,6-dien-5-one[4], yield 78%, yellow solid, m.p. 168-170 ^oC. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.45-7.40 (m, 5H), 7.35-7.28 (m, 3H),

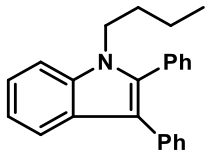
7.12-7.06 (m, 2H), 2.27 (s, 3H), 2.07 (s, 3H).



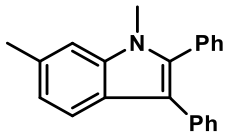
1-Methyl-2,3-diphenyl-1*H*-indole (5a) [1]: white solid, yield 73%, m.p. 139-141°C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.80 (d , *J* = 8.2 Hz, 1H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.40-7.27 (m, 10H), 7.20 (t, *J* = 8.2 Hz, 2H), 3.69 (s, 3H). **^{13}C NMR (150 MHz, Chloroform-*d*)** δ 137.9, 137.5, 135.4, 132.1, 131.3, 130.0, 128.5, 128.3, 128.2, 127.1, 125.6, 122.3, 120.3, 119.7, 115.25, 109.07, 31.1. **HRMS (ESI)**: m/z calculated for $C_{21}H_{17}NNa^+$ $[M+Na]^+$: 306.1253, found: 306.1257.



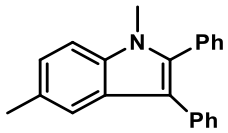
1-Ethyl-2,3-diphenyl-1*H*-indole (5b) [1]**:** yield 78%, yellow solid, m.p. 116-118°C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.81 (d, *J* = 8.2 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.42-7.26 (m, 10H), 7.21-7.14 (m, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 1.30 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 137.4, 136.2, 135.3, 132.4, 131.2, 129.9, 128.6, 128.2, 128.2, 127.4, 125.5, 122.2, 120.2, 119.9, 115.4, 109.9, 38.8, 15.5. **HRMS (ESI)**: m/z calculated for $C_{19}H_{22}NNa^+$ $[M+Na]^+$: 320.1410, found: 320.1411.



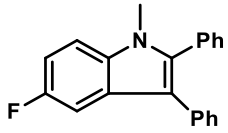
1-Butyl-2,3-diphenyl-1*H*-indole (5c)[5]: yield 82%, white solid, m.p. 91-93°C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 8.2 Hz, 1H), 7.43 (d, *J* = 8.2 Hz, 1H), 7.40-7.24 (m, 10H), 7.19-7.15 (m, 2H), 4.12-4.04 (m, 2H), 1.65(q, *J* = 7.7 Hz, 2H), 1.22-1.15 (m, 2H), 0.79 (t, *J* = 7.7 Hz, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 137.7, 136.6, 135.4, 132.5, 131.3, 130.0, 128.5, 128.2, 128.2, 127.3, 125.5, 122.1, 120.2, 119.9, 115.39, 110.1, 43.8, 32.2, 20.2, 13.8. **HRMS (ESI)**: m/z calculated for $C_{24}H_{23}NNa^+$ $[M+Na]^+$: 348.1723, found: 348.1725.



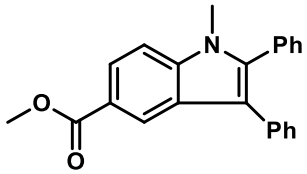
1,6-Dimethyl-2,3-diphenyl-1*H*-indole (5e) [5]**:** yield 72%, white solid, m.p. 99-101°C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 8.1 Hz, 1H), 7.41-7.28 (m, 7H), 7.26 (s, 2H), 7.21 (s, 1H), 7.19-7.14 (m, 1H), 7.05-7.01 (m, 1H), 3.65 (s, 3H), 2.55 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 137.9, 137.2, 135.6, 132.2, 132.2, 131.3, 129.9, 128.5, 128.3, 128.0, 125.5, 125.0, 122.0, 119.4, 115.1, 109.7, 31.0, 22.1. **HRMS (ESI)**: m/z calculated for $C_{22}H_{19}NNa^+$ $[M+Na]^+$: 320.1410, found: 320.1413.



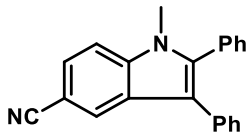
1,5-Dimethyl-2,3-diphenyl-1*H*-indole (5f)[1]**:** yield 68%, white solid, m.p. 103-105°C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.57 (s, 1H), 7.40-7.26 (m, 10H), 7.19-7.12 (m, 2H), 3.66 (s, 3H), 2.47 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 138.0, 136.0, 135.6, 132.21, 131.3, 130.1, 129.6, 128.5, 128.3, 128.1, 127.4, 125.5, 123.9, 119.3, 114.8, 109.4, 31.1, 21.7. **HRMS (ESI)**: m/z calculated for $C_{22}H_{19}NNa^+$ $[M+Na]^+$: 320.1410, found: 320.1411.



5-Fluoro-1-methyl-2,3-diphenyl-1*H*-indole (5g)[1]**:** yield 81%, yellow solid, m.p. 128-130°C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.44 (dd, *J* = 9.9, 2.5 Hz, 1H), 7.40-7.26 (m, 10H), 7.20 – 7.17 (m, 1H), 7.04 (td, *J* = 9.9, 2.5 Hz, 1H), 3.67 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 158.7 (d, *J* = 234.8 Hz), 139.4, 134.9, 134.2, 131.8, 131.2, 129.8, 128.6, 128.4, 128.4, 127.4 (d, *J* = 9.7 Hz), 125.8, 115.3 (d, *J* = 4.7 Hz), 110.6 (d, *J* = 26.3 Hz), 110.4 (d, *J* = 9.6 Hz), 104.6 (d, *J* = 24.0 Hz), 31.3. **HRMS (ESI)**: m/z calculated for $C_{21}H_{16}FNNa^+$ $[M+Na]^+$: 324.1159, found: 301.1159.

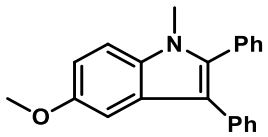


Methyl 1-methyl-2,3-diphenyl-1*H*-indole-5-carboxylate (5h)[1]**:** yield 76%, white solid, m.p. 166-168°C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.53 (d, *J* = 1.6 Hz, 1H), 8.02 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.44-7.38 (m, 4H), 7.35-7.30 (m, 6H), 7.21-7.19 (m, 1H), 3.93 (s, 3H), 3.71 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 168.2, 139.7, 138.9, 134.3, 131.3, 131.0, 129.9, 128.5, 128.4, 128.3, 126.6, 125.9, 123.6, 122.6, 122.1, 116.5, 109.2, 51.8, 31.2. **HRMS (ESI)**: m/z calculated for $C_{23}H_{19}NO_2Na^+$ $[M+Na]^+$: 364.1308, found: 364.1303.

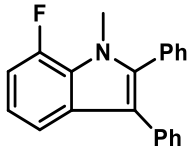


1-Methyl-2,3-diphenyl-1*H*-indole-5-carbonitrile (5i)[6]**:** yield 85%, white solid, m.p. 178-180°C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.16-8.03 (m, 1H), 7.51 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.44 (d, *J* = 8.5 Hz, 1H), 7.43-7.37 (m, 3H), 7.34-7.27 (m, 4H), 7.25-7.19 (m, 3H), 3.70 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 139.9, 138.8, 133.8, 131.1, 130.8, 129.8, 128.8, 128.7, 128.6, 127.1,

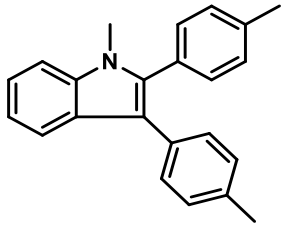
126.5, 125.5, 125.1, 121.0, 116.1, 110.6, 103.2, 31.4. **HRMS (ESI)**: m/z calculated for $C_{22}H_{16}N_2Na^+$ $[M+Na]^+$: 331.1206, found: 331.1191.



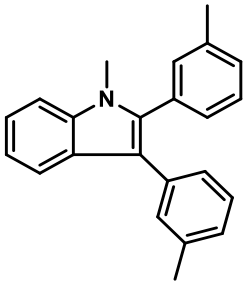
5-Methoxy-1-methyl-2,3-diphenyl-1*H*-indole (5j)[1]: yield 67%, white solid, m.p. 132-134°C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.41-7.27 (m, 10H), 7.25 (s, 1H), 7.21-7.16 (m, 1H), 6.97 (dd, *J* = 8.8, 2.5 Hz, 1H), 3.86 (s, 3H), 3.66 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 154.9, 138.5, 135.5, 132.9, 132.1, 131.2, 129.9, 128.5, 128.4, 128.1, 127.3, 125.6, 114.9, 112.6, 110.5, 101.4, 56.2, 31.2. **HRMS (ESI)**: m/z calculated for $C_{21}H_{16}NONa^+$ $[M+Na]^+$: 336.1359, found: 336.1353.



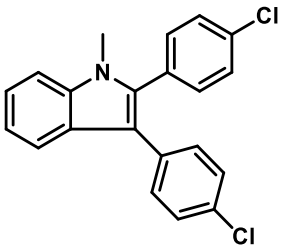
7-Fluoro-1-methyl-2,3-diphenyl-1*H*-indole (5k): yield 53%, white solid, m.p. 120-122°C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.4 (dd, *J* = 9.9, 2.5 Hz, 1H), 7.4-7.3 (m, 10H), 7.2-7.2 (m, 1H), 7.0 (td, *J* = 9.0, 2.5 Hz, 1H), 3.7 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 158.7 (d, *J* = 234.8 Hz), 139.4, 134.9, 134.1, 131.8, 131.2, 129.8, 128.6, 128.4, 128.3, 127.5 (d, *J* = 4.2 Hz), 125.8, 115.3 (d, *J* = 4.7 Hz), 110.56 (d, *J* = 26.3 Hz), 110.35 (d, *J* = 9.6 Hz), 104.6 (d, *J* = 24.0 Hz), 31.3. **HRMS (EI)** m/z Calcd. for $C_{21}H_{16}NFNa^+$: [M+Na]+ , 324.1159, Found: 324.1157.



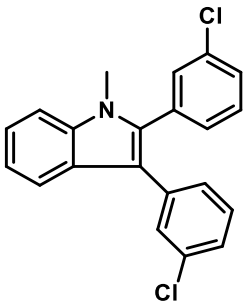
1-Methyl-2,3-di-p-tolyl-1*H*-indole (5m)[1]: yield 87%, yellow solid, m.p. 108-110 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.77 (d, *J* = 8.2 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.30-7.25 (m, 1H), 7.23-7.13 (m, 7H), 7.08 (d, *J* = 8.0 Hz, 2H), 3.65 (s, 3H), 2.38 (s, 3H), 2.32 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 137.9, 137.7, 137.4, 135.0, 132.4, 131.1, 129.8, 129.2, 129.1, 129.1, 127.2, 122.1, 120.1, 119.7, 109.6, 31.0, 21.5, 21.3. **HRMS (ESI)**: m/z calculated for $C_{23}H_{21}NNa^+$ $[M+Na]^+$: 334.1566, found: 344.1566.



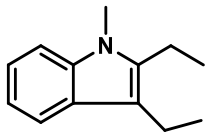
1-Methyl-2,3-di-m-tolyl-1*H*-indole (5n)[5]**:** yield 71%, white solid, 93-95 °C. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.79 (d, *J* = 8.2 Hz, 1H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.30 (t, *J* = 8.2 Hz, 1H), 7.26 (t, *J* = 8.2 Hz, 1H), 7.20-7.10 (m, 6H), 7.05 (d, *J* = 7.7 Hz, 1H), 6.98 (d, *J* = 7.4 Hz, 1H), 3.66 (s, 3H), 2.34 (s, 3H), 2.28 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 137.9, 137.9, 137.5, 137.3, 135.2, 131.9, 131.6, 130.5, 128.8, 128.3, 128.2, 128.0, 127.1, 127.0, 126.2, 122.0, 120.0, 119.7, 115.0, 109.5, 30.9, 21.5, 21.5. **HRMS (ESI)**: m/z calculated for $C_{23}H_{21}NNa^+$ $[M+Na]^+$: 344.1566, found: 344.1569.



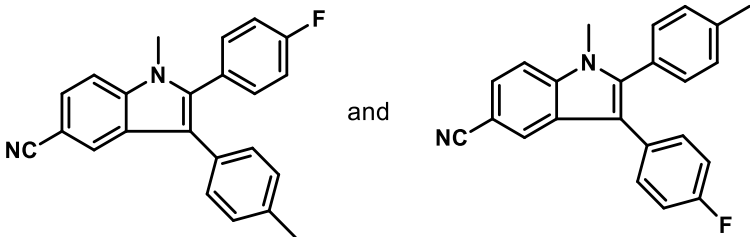
2,3-Bis(4-chlorophenyl)-1-methyl-1*H*-indole (5p)[6]**:** yield 54%, yellow solid, m.p. 96-98°C.
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.40-7.35 (m, 2H), 7.35-7.30 (m, 1H), 7.26-7.18 (m, 7H), 3.67 (s, 3H). **^{13}C NMR** (100 MHz, Chloroform-d) δ 136.4, 135.4, 133.4 132.4, 131.3, 130.4, 130.0, 129.0, 127.8, 127.5, 125.6, 121.6, 119.5, 118.3, 113.3, 108.7, 30.0. **HRMS (ESI)**: m/z calculated for $C_{21}H_{15}Cl_2NNa^+$ $[M+Na]^+$: 374.0474, 376.0444 (isotopic peak), Found: 374.0475, 376.0450.



2,3-Bis(3-chlorophenyl)-1-methyl-1*H*-indole (5q): yield 86%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.75 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.39-7.28 (m, 5H), 7.24-7.15 (m, 4H), 7.11-7.05 (m, 1H), 3.67 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-d)** δ 137.5, 136.9, 136.5, 134.5, 134.2, 133.5, 130.9, 130.0, 129.7, 129.7, 129.5, 128.7, 128.1, 126.7, 126.0, 122.9, 120.8, 119.6, 114.5, 109.9, 31.2. **HRMS (EI)** m/z calculated for $C_{21}H_{15}Cl_2NNa^+$: $[M+Na]^+$, 374.0474, 376.0444 (isotopic peak), Found: 374.0474, 376.0448.

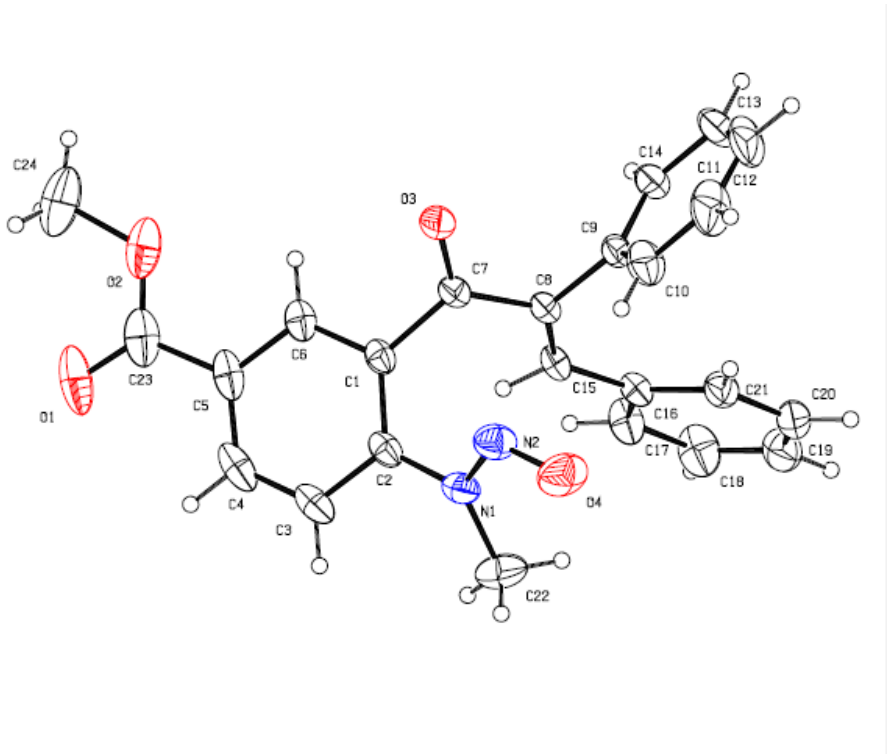


2,3-diethyl-1-methyl-1*H*-indole (5r)[7]: yield 45%, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.24 (s, 1H), 7.18-7.12 (m, 1H), 7.06 (t, *J* = 7.8 Hz, 1H), 3.67 (s, 3H), 2.80-2.71 (m, 4H), 1.25-1.19 (m, 6H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 138.1, 136.8, 127.6, 120.6, 118.7, 118.3, 112.8, 108.7, 17.8, 17.8, 16.4, 15.1. **HRMS (ESI):** m/z calculated for C13H17NNa^{+} [M+Na]$^{+}$: 210.1253, Found: 210.1255.



2-(4-fluorophenyl)-1-methyl-3-(p-tolyl)-1H-indole-5-carbonitrile (5s) and 3-(4-fluorophenyl)-1-methyl-2-(p-tolyl)-1H-indole-5-carbonitrile (5s`):** yield 52%, **3S**:**3S`= 1:1, yellow oil. **^{1}H NMR (400 MHz, Chloroform-*d*)** δ 8.08 (s, 1H), 8.03 (s, 1H), 7.52 (d, *J* = 8.1 Hz, 2H), 7.44 (d, *J* = 8.6 Hz, 2H), 7.34-7.28 (m, 3H), 7.26-7.07 (m, 13H), 7.00 (t, *J* = 8.6 Hz, 2H), 3.70 (s, 3H),3.69 (s, 6H), 2.41 (s, 3H), 2.35 (s, 3H). **^{13}C NMR (100 MHz, Chloroform-*d*)** δ 164.1, 161.6, 160.3, 140.0, 138.8, 138.7, 138.6, 138.4, 136.2, 132.8, 132.8, 131.2, 131.1, 130.9, 130.8, 130.4, 129.9, 129.8, 129.5, 129.5, 129.3, 128.9, 127.5, 127.0, 125.5, 125.1, 125.0, 125.0, 122.0, 116.0, 115.8, 115.6, 115.4, 110.4, 110.4, 103.1, 31.2, 31.2, 21.4, 21.2. **HRMS (ESI):** m/z calculated for $C_{22}H_{18}NNa^{+}$ [M+Na]$^{+}$: 363.1268, Found: 363.1266.

V. X-Ray Crystallographic Data



Single-crystal X-ray Structure of 3h

The structure of 3aa was determined by the X-ray diffraction. Recrystallized from CH_2Cl_2/hexane. Further information can be found in the CIF file. This crystal was deposited in the Cambridge Crystallographic Data Centre and assigned as CCDC 1957755.

Table 1 Crystal data and structure refinement for 3h.

Identification code	3h
Empirical formula	$C_{24}H_{20}N_2O_4$
Formula weight	400.42
Temperature/K	293.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.2065(14)
b/Å	8.0264(5)
c/Å	17.9481(17)
α/°	90
β/°	116.108(11)
γ/°	90
Volume/Å^3	2096.5(3)

Z	4
ρ_{calc}g/cm^3	1.269
μ/mm^{-1}	0.087
F(000)	840.0
Crystal size/mm^3	0.35 × 0.3 × 0.25
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.772 to 58.988
Index ranges	$-20 \leq h \leq 21$, $-10 \leq k \leq 10$, $-17 \leq l \leq 24$
Reflections collected	13664
Independent reflections	4974 [R_{int} = 0.0253, R_{sigma} = 0.0429]
Data/restraints/parameters	4974/0/273
Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0569, wR_2 = 0.1205
Final R indexes [all data]	R_1 = 0.1060, wR_2 = 0.1409
Largest diff. peak/hole / e Å^{-3}	0.17/-0.17

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

Atom	*x*	*y*	*z*	U(eq)
O1	6796.5(13)	5456(3)	5673.3(11)	111.1(7)
O2	6159.2(11)	7971(3)	5340.1(10)	89.7(6)
O3	3847.7(9)	9210.0(15)	2553.3(8)	56.9(4)
O4	3108.7(14)	5110(2)	701.7(10)	85.3(5)
N1	3706.3(11)	4392.8(17)	1982.2(10)	47.6(4)
N2	3614.6(13)	5520.3(19)	1417.4(12)	59.3(5)
C1	4233.6(11)	6503(2)	3069.5(11)	40.5(4)
C2	4259.1(12)	4875(2)	2807.0(12)	44.3(4)
C3	4868.6(14)	3732(3)	3348.1(15)	59.2(6)
C4	5472.8(15)	4212(3)	4123.1(16)	67.1(7)
C5	5500.1(13)	5845(3)	4382.7(13)	58.4(6)
C6	4870.6(12)	6978(2)	3850.4(12)	49.5(5)
C7	3563.0(12)	7818(2)	2564.1(11)	40.5(4)
C8	2562.7(11)	7458(2)	2142.6(10)	37.5(4)
C9	2009.1(12)	8705(2)	1511.2(11)	43.6(4)
C10	2058.1(16)	8845(3)	768.0(13)	65.4(6)
C11	1549(2)	10034(4)	199.9(16)	91.6(9)
C12	997(2)	11077(3)	369(2)	102.8(11)
C13	955.6(17)	10981(3)	1100(2)	89.4(9)

C14	1460.4(13)	9807(2)	1677.2(14)	59.9(6)
C15	2220.0(12)	6196(2)	2406.8(10)	41.1(4)
C16	1274.7(12)	5593(2)	2108.7(11)	41.8(4)
C17	1057.5(14)	4668(3)	2649.4(13)	59.6(6)
C18	192.8(16)	4013(3)	2402.1(17)	76.5(7)
C19	-463.1(16)	4240(3)	1614.1(17)	70.2(6)
C20	-263.8(14)	5133(2)	1062.5(14)	61.6(6)
C21	599.9(13)	5805(2)	1309.2(12)	51.6(5)
C22	3239.9(18)	2802(2)	1752.8(16)	78.8(7)
C23	6215.7(16)	6354(4)	5191.7(15)	77.1(7)
C24	6883(2)	8690(5)	6071.3(17)	123.9(12)

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	63.0(11)	174(2)	65.7(12)	46.0(12)	0.1(10)	24.6(12)
O2	61.4(11)	139.2(17)	47.9(10)	5.7(10)	5.2(8)	-13.6(11)
O3	52.5(8)	38.4(7)	66.1(9)	7.1(6)	13.4(7)	-0.6(6)
O4	119.4(15)	75.4(11)	56.1(10)	-12.4(8)	33.9(11)	-3.3(10)
N1	50.7(10)	35.2(8)	62.5(11)	3.8(7)	29.9(9)	3.6(7)
N2	78.0(13)	47.0(9)	56.8(12)	3.8(9)	33.1(11)	2.6(9)
C1	32.1(9)	43.7(9)	46.8(11)	10.9(8)	18.4(9)	4.6(7)
C2	37.0(10)	43.3(10)	57.7(12)	16.3(9)	25.6(10)	8.0(8)
C3	53.4(13)	53.9(11)	76.7(16)	25.1(11)	34.5(13)	21.3(10)
C4	49.5(13)	80.0(16)	77.4(17)	41.2(13)	33.1(13)	27.8(12)
C5	34.2(10)	91.8(16)	48.1(12)	25.8(11)	17.2(10)	7.9(10)
C6	37.4(10)	62.3(12)	47.0(12)	11.7(9)	17.0(10)	2.3(9)
C7	42.9(10)	37.4(9)	40.8(10)	5.3(8)	17.8(9)	6.3(8)
C8	38.0(9)	37.8(9)	36.5(9)	4.8(7)	16.2(8)	8.6(7)
C9	36.7(10)	37.7(9)	47.4(11)	9.1(8)	10.3(9)	2.0(8)
C10	65.6(14)	72.0(14)	52.5(13)	20.8(11)	20.5(12)	8.5(11)
C11	83.9(19)	103(2)	63.9(17)	41.2(15)	10.4(15)	-7.4(17)
C12	63.1(17)	72.1(17)	121(3)	53.5(18)	-7.1(18)	2.0(14)
C13	54.2(15)	48.9(13)	135(3)	17.2(15)	13.9(17)	16.6(11)
C14	44.3(11)	44.6(11)	79.0(15)	2.9(10)	16.4(11)	8.0(9)
C15	37.0(9)	46.1(9)	38.5(10)	11.2(8)	15.1(8)	11.8(8)
C16	38.8(10)	42.2(9)	46.2(11)	8.9(8)	20.3(9)	9.3(8)
C17	45.3(12)	75.4(14)	58.9(13)	21.6(11)	23.6(11)	5.9(10)

C18	57.5(15)	94.2(17)	86.4(18)	27.3(14)	39.5(15)	-0.6(13)
C19	45.4(12)	67.6(14)	97.6(19)	6.6(13)	31.4(14)	-1.3(11)
C20	48.4(12)	54.1(12)	65.7(15)	5.9(10)	9.9(11)	0.9(10)
C21	49.7(12)	47.0(10)	53.0(12)	9.1(9)	17.9(10)	2.3(9)
C22	98.1(19)	45.1(12)	101(2)	-10.1(12)	51.6(17)	-17.9(12)
C23	48.0(14)	125(2)	56.5(15)	23.3(16)	21.2(13)	1.1(15)
C24	89(2)	192(4)	59.9(18)	-14(2)	5.2(16)	-27(2)

Table 4 Bond Lengths for 3h.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C23	1.199(3)	C7	C8	1.485(2)
O2	C23	1.336(3)	C8	C9	1.482(2)
O2	C24	1.441(3)	C8	C15	1.338(2)
O3	C7	1.2124(19)	C9	C10	1.375(3)
O4	N2	1.226(2)	C9	C14	1.377(3)
N1	N2	1.317(2)	C10	C11	1.375(3)
N1	C2	1.406(2)	C11	C12	1.354(4)
N1	C22	1.448(2)	C12	C13	1.343(4)
C1	C2	1.396(2)	C13	C14	1.373(3)
C1	C6	1.379(2)	C15	C16	1.465(2)
C1	C7	1.500(2)	C16	C17	1.385(2)
C2	C3	1.384(3)	C16	C21	1.380(3)
C3	C4	1.358(3)	C17	C18	1.375(3)
C4	C5	1.385(3)	C18	C19	1.356(3)
C5	C6	1.387(3)	C19	C20	1.371(3)
C5	C23	1.462(3)	C20	C21	1.379(3)

Table 5 Bond Angles for 3h.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C23	O2	C24	118.1(2)	C15	C8	C9	125.19(16)
N2	N1	C2	115.15(15)	C10	C9	C8	121.53(17)

N2	N1	C22	121.25(18)	C10	C9	C14	118.42(18)
C2	N1	C22	123.57(16)	C14	C9	C8	119.99(17)
O4	N2	N1	114.74(17)	C11	C10	C9	120.2(2)
C2	C1	C7	125.15(16)	C12	C11	C10	120.2(3)
C6	C1	C2	118.79(16)	C13	C12	C11	120.3(2)
C6	C1	C7	116.06(16)	C12	C13	C14	120.5(3)
C1	C2	N1	120.88(15)	C13	C14	C9	120.3(2)
C3	C2	N1	118.92(18)	C8	C15	C16	130.62(16)
C3	C2	C1	120.11(19)	C17	C16	C15	117.95(17)
C4	C3	C2	120.1(2)	C21	C16	C15	124.19(16)
C3	C4	C5	120.99(19)	C21	C16	C17	117.75(17)
C4	C5	C6	119.0(2)	C18	C17	C16	121.1(2)
C4	C5	C23	119.5(2)	C19	C18	C17	120.3(2)
C6	C5	C23	121.5(2)	C18	C19	C20	119.8(2)
C1	C6	C5	120.89(19)	C19	C20	C21	120.1(2)
O3	C7	C1	118.59(16)	C20	C21	C16	120.90(18)
O3	C7	C8	120.59(15)	O1	C23	O2	122.8(3)
C8	C7	C1	120.64(14)	O1	C23	C5	125.1(3)
C9	C8	C7	114.59(14)	O2	C23	C5	112.1(2)
C15	C8	C7	119.80(15)				

Table 6 Torsion Angles for 3h.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O3	C7	C8	C9	19.0(2)	C7	C8	C15	C16	179.59(17)
O3	C7	C8	C15	-153.86(17)	C8	C9	C10	C11	-178.8(2)
N1	C2	C3	C4	173.53(17)	C8	C9	C14	C13	179.09(19)
N2	N1	C2	C1	38.1(2)	C8	C15	C16	C17	-158.06(19)
N2	N1	C2	C3	-138.53(17)	C8	C15	C16	C21	25.8(3)
C1	C2	C3	C4	-3.1(3)	C9	C8	C15	C16	7.5(3)
C1	C7	C8	C9	-166.03(15)	C9	C10	C11	C12	0.1(4)
C1	C7	C8	C15	21.1(2)	C10	C9	C14	C13	1.9(3)
C2	N1	N2	O4	-177.85(17)	C10	C11	C12	C13	1.3(4)
C2	C1	C6	C5	-2.9(2)	C11	C12	C13	C14	-1.1(4)
C2	C1	C7	O3	-135.73(18)	C12	C13	C14	C9	-0.5(4)
C2	C1	C7	C8	49.2(2)	C14	C9	C10	C11	-1.7(3)
C2	C3	C4	C5	-0.8(3)	C15	C8	C9	C10	-116.8(2)
C3	C4	C5	C6	2.8(3)	C15	C8	C9	C14	66.1(2)
C3	C4	C5	C23	-174.25(18)	C15	C16	C17	C18	-177.7(2)

C4	C5	C6	C1	-0.9(3)	C15	C16	C21	C20	176.85(17)
C4	C5	C23	O1	-0.9(3)	C16	C17	C18	C19	1.1(4)
C4	C5	C23	O2	178.56(19)	C17	C16	C21	C20	0.7(3)
C6	C1	C2	N1	-171.64(15)	C17	C18	C19	C20	-0.3(4)
C6	C1	C2	C3	4.9(2)	C18	C19	C20	C21	-0.3(3)
C6	C1	C7	O3	43.9(2)	C19	C20	C21	C16	0.1(3)
C6	C1	C7	C8	-131.16(17)	C21	C16	C17	C18	-1.3(3)
C6	C5	C23	O1	-177.9(2)	C22	N1	N2	O4	0.3(3)
C6	C5	C23	O2	1.5(3)	C22	N1	C2	C1	-140.06(19)
C7	C1	C2	N1	8.0(3)	C22	N1	C2	C3	43.3(3)
C7	C1	C2	C3	-175.49(16)	C23	C5	C6	C1	176.11(17)
C7	C1	C6	C5	177.46(16)	C24	O2	C23	O1	6.5(3)
C7	C8	C9	C10	70.8(2)	C24	O2	C23	C5	-173.0(2)
C7	C8	C9	C14	-106.32(19)					

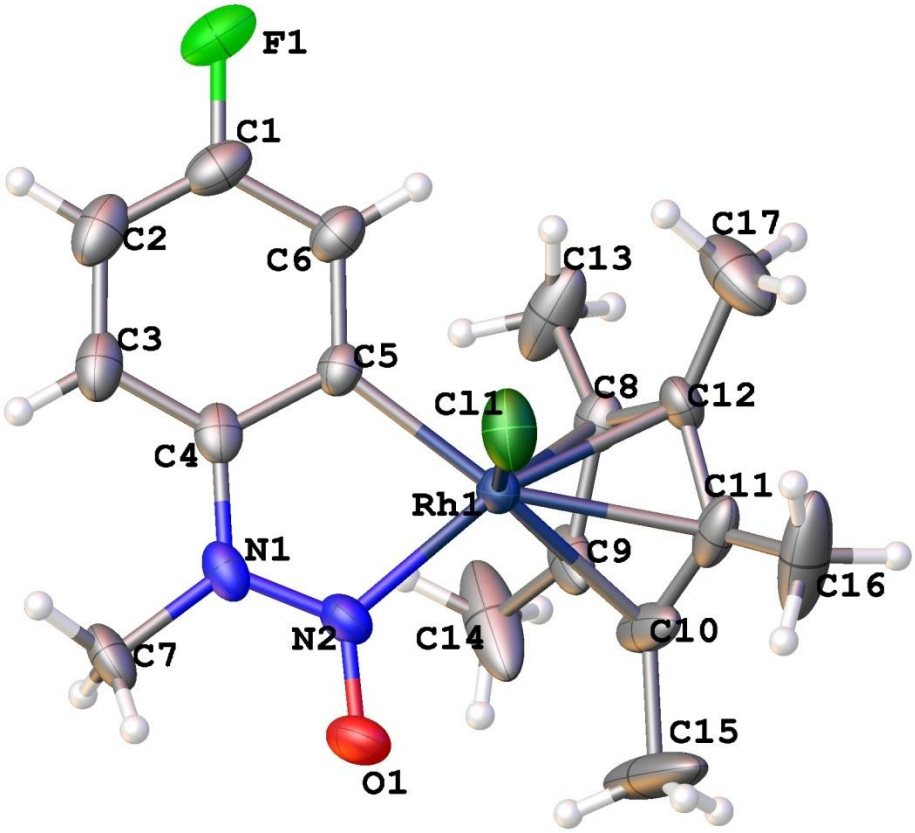
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 3h.

Atom	*x*	*y*	*z*	U(eq)
H3	4864	2634	3181	71
H4	5874	3433	4485	81
H6	4878	8073	4022	59
H10	2437	8132	649	78
H11	1584	10121	-302	110
H12	644	11864	-22	123
H13	583	11715	1215	107
H14	1432	9757	2183	72
H15	2653	5605	2853	49
H17	1504	4488	3189	72
H18	57	3412	2777	92
H19	-1046	3791	1448	84
H20	-712	5285	521	74
H21	729	6411	931	62
H22A	2588	2981	1472	118
H22B	3386	2149	2243	118
H22C	3436	2221	1391	118
H24A	6824	9881	6048	186
H24B	7468	8386	6097	186
H24C	6840	8281	6556	186

Crystal structure determination of 3h

Crystal Data for $C_{24}H_{20}N_2O_4$ (M =400.42 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 16.2065(14) Å, b = 8.0264(5) Å, c = 17.9481(17) Å, β = 116.108(11) °, V = 2096.5(3) Å^3, Z = 4, T = 293.15 K, μ(MoKα) = 0.087 mm^{-1}, $Dcalc$ = 1.269 g/cm^3, 13664 reflections measured (6.772° ≤ 2Θ ≤ 58.988°), 4974 unique (R_{int} = 0.0253, R_{sigma} = 0.0429) which were used in all calculations. The final R_1 was 0.0569 (I > 2σ(I)) and wR_2 was 0.1409 (all data).

b) X-Ray Crystallographic Data of species A



Single-crystal X-ray Structure of **species A**

The structure of 3aa was determined by the X-ray diffraction. Recrystallized from CH_2Cl_2/hexane. Further information can be found in the CIF file. This crystal was deposited in the Cambridge Crystallographic Data Centre and assigned as CCDC 1960116.

Table 1 Crystal data and structure refinement for species A.

Identification code	specie A
Empirical formula	$C_{17}H_{21}ClN_2ORhF$
Formula weight	426.72
Temperature/K	123.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.543(4)

b/Å	14.111(6)
c/Å	14.684(7)
α/°	90
β/°	92.284(7)
γ/°	90
Volume/$Å^3$	1768.7(14)
Z	4
$\rho_{calc}g/cm^3$	1.602
μ/mm^{-1}	1.131
F(000)	864.0
Crystal size/mm^3	0.2 × 0.18 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/ °	5.424 to 55.714
Index ranges	$-11 \leq h \leq 11$, $-18 \leq k \leq 18$, $-19 \leq l \leq 19$
Reflections collected	20794
Independent reflections	4209 [R_{int} = 0.0438, R_{sigma} = 0.0322]
Data/restraints/parameters	4209/0/213
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0573, wR_2 = 0.1736
Final R indexes [all data]	R_1 = 0.0619, wR_2 = 0.1788
Largest diff. peak/hole / e $Å^{-3}$	0.74/-1.44

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

Atom	*x*	*y*	*z*	U(eq)
Rh1	3027.4(4)	7254.1(3)	6221.1(2)	23.59(16)
Cl1	5147(2)	7616.3(11)	5274.0(12)	45.6(4)
F1	7306(4)	5222(3)	8254(3)	51.7(10)
O1	1222(5)	6326(3)	4709(3)	41.8(10)
N1	2848(5)	5369(3)	5438(3)	30.6(9)
N2	2248(5)	6218(3)	5330(3)	31.2(9)
C1	6212(6)	5246(5)	7550(4)	37.7(13)
C2	5911(7)	4434(4)	7064(5)	42.2(14)
C3	4781(7)	4449(4)	6350(4)	37.8(13)
C4	3988(6)	5290(4)	6168(4)	29.2(10)
C5	4292(6)	6123(3)	6668(3)	25.6(9)

C6	5447(6)	6089(4)	7356(4)	32.2(11)
C7	2308(7)	4575(4)	4859(4)	38.9(13)
C8	2343(7)	7750(4)	7552(4)	30.6(11)
C9	976(7)	7533(4)	7001(5)	42.2(15)
C10	909(8)	8201(5)	6251(5)	51.9(19)
C11	2255(8)	8772(4)	6320(4)	40.4(14)
C12	3176(6)	8478(4)	7104(4)	30.7(10)
C13	2835(12)	7321(5)	8443(5)	63(2)
C14	-248(10)	6837(6)	7247(9)	100(5)
C15	-426(14)	8259(10)	5551(8)	129(6)
C16	2697(16)	9544(5)	5684(6)	94(4)
C17	4651(9)	8937(6)	7459(6)	67(2)

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Rh1	23.5(2)	23.0(2)	24.3(2)	-4.13(13)	1.37(15)	2.26(12)
Cl1	55.1(9)	33.8(7)	49.7(9)	-2.5(6)	26.3(7)	-3.3(6)
F1	41(2)	63(2)	51(2)	13.6(19)	-2.4(16)	18.2(18)
O1	37(2)	50(2)	38(2)	-13.7(19)	-9.0(17)	1.3(18)
N1	30(2)	27(2)	35(2)	-10.8(18)	10.2(17)	-5.9(17)
N2	30(2)	33(2)	31(2)	-9.4(18)	-0.9(17)	-3.6(18)
C1	26(3)	49(3)	38(3)	11(3)	5(2)	9(2)
C2	35(3)	35(3)	58(4)	13(3)	17(3)	7(2)
C3	34(3)	25(2)	56(4)	1(2)	17(2)	0(2)
C4	23(2)	26(2)	39(3)	-2(2)	14(2)	-3.4(18)
C5	23(2)	24(2)	30(2)	0.2(18)	7.1(18)	3.2(17)
C6	29(3)	35(3)	32(2)	4(2)	7(2)	8(2)
C7	37(3)	31(3)	50(3)	-18(2)	11(2)	-13(2)
C8	35(3)	30(3)	28(2)	-2.5(19)	11(2)	7(2)
C9	25(3)	31(3)	72(4)	-23(3)	16(3)	1(2)
C10	45(3)	61(4)	48(3)	-30(3)	-18(3)	33(3)
C11	65(4)	30(3)	27(2)	-1(2)	9(2)	23(3)
C12	37(3)	24(2)	32(2)	-8.2(19)	0(2)	-3(2)
C13	100(6)	57(4)	35(3)	15(3)	27(4)	44(4)
C14	49(4)	57(5)	200(13)	-63(7)	68(6)	-22(4)
C15	106(8)	164(12)	109(8)	-91(8)	-85(7)	96(8)
C16	199(13)	37(4)	51(4)	15(3)	45(6)	38(6)
C17	45(4)	71(5)	86(6)	-40(5)	17(4)	-21(4)

Table 4 Bond Lengths for species A.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Rh1	Cl1	2.3822(17)	C2	C3	1.397(9)
Rh1	N2	2.056(4)	C3	C4	1.387(8)
Rh1	C5	2.022(5)	C4	C5	1.405(7)
Rh1	C8	2.177(5)	C5	C6	1.385(7)
Rh1	C9	2.167(6)	C8	C9	1.427(9)
Rh1	C10	2.251(6)	C8	C12	1.425(8)
Rh1	C11	2.247(5)	C8	C13	1.487(9)
Rh1	C12	2.160(5)	C9	C10	1.449(11)
F1	C1	1.366(7)	C9	C14	1.489(10)
O1	N2	1.249(6)	C10	C11	1.405(11)
N1	N2	1.310(6)	C10	C15	1.507(9)
N1	C4	1.423(7)	C11	C12	1.429(8)
N1	C7	1.469(6)	C11	C16	1.493(10)
C1	C2	1.368(9)	C12	C17	1.492(8)
C1	C6	1.382(8)			

Table 5 Bond Angles for species A.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	Rh1	Cl1	90.87(14)	C4	C3	C2	118.4(5)
N2	Rh1	C8	135.1(2)	C3	C4	N1	121.8(5)
N2	Rh1	C9	102.6(2)	C3	C4	C5	122.4(5)
N2	Rh1	C10	101.2(2)	C5	C4	N1	115.8(4)
N2	Rh1	C11	129.1(2)	C4	C5	Rh1	113.9(4)
N2	Rh1	C12	163.9(2)	C6	C5	Rh1	128.3(4)
C5	Rh1	Cl1	87.13(14)	C6	C5	C4	117.6(5)
C5	Rh1	N2	78.5(2)	C1	C6	C5	119.9(5)
C5	Rh1	C8	97.0(2)	C9	C8	Rh1	70.5(3)
C5	Rh1	C9	113.9(2)	C9	C8	C13	127.4(7)
C5	Rh1	C10	151.8(3)	C12	C8	Rh1	70.2(3)
C5	Rh1	C11	152.3(2)	C12	C8	C9	107.8(5)
C5	Rh1	C12	114.7(2)	C12	C8	C13	124.8(6)
C8	Rh1	Cl1	133.82(16)	C13	C8	Rh1	125.6(4)
C8	Rh1	C10	63.1(2)	C8	C9	Rh1	71.2(3)
C8	Rh1	C11	62.97(19)	C8	C9	C10	107.3(5)
C9	Rh1	Cl1	156.79(19)	C8	C9	C14	124.8(8)

C9	Rh1	C8	38.4(2)	C10	C9	Rh1	74.0(4)
C9	Rh1	C10	38.2(3)	C10	C9	C14	127.3(8)
C9	Rh1	C11	63.1(2)	C14	C9	Rh1	126.8(4)
C10	Rh1	Cl1	121.0(2)	C9	C10	Rh1	67.7(3)
C11	Rh1	Cl1	93.75(18)	C9	C10	C15	124.1(10)
C11	Rh1	C10	36.4(3)	C11	C10	Rh1	71.7(3)
C12	Rh1	Cl1	98.69(16)	C11	C10	C9	108.1(5)
C12	Rh1	C8	38.4(2)	C11	C10	C15	127.8(10)
C12	Rh1	C9	64.4(2)	C15	C10	Rh1	127.3(5)
C12	Rh1	C10	62.7(2)	C10	C11	Rh1	71.9(3)
C12	Rh1	C11	37.8(2)	C10	C11	C12	108.3(5)
N2	N1	C4	114.5(4)	C10	C11	C16	126.9(8)
N2	N1	C7	121.0(5)	C12	C11	Rh1	67.8(3)
C4	N1	C7	124.4(5)	C12	C11	C16	124.8(8)
O1	N2	Rh1	125.3(4)	C16	C11	Rh1	124.9(4)
O1	N2	N1	117.4(4)	C8	C12	Rh1	71.5(3)
N1	N2	Rh1	117.3(3)	C8	C12	C11	108.2(5)
F1	C1	C2	118.9(5)	C8	C12	C17	125.6(6)
F1	C1	C6	118.7(6)	C11	C12	Rh1	74.4(3)
C2	C1	C6	122.4(5)	C11	C12	C17	125.8(6)
C1	C2	C3	119.2(5)	C17	C12	Rh1	125.8(4)

Table 6 Torsion Angles for species A.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Rh1	C5	C6	C1	-178.5(4)	C8	C9	C10	Rh1	63.9(4)
Rh1	C8	C9	C10	-65.8(4)	C8	C9	C10	C11	3.3(6)
Rh1	C8	C9	C14	122.3(6)	C8	C9	C10	C15	-175.2(6)
Rh1	C8	C12	C11	65.9(4)	C9	C8	C12	Rh1	-60.7(4)
Rh1	C8	C12	C17	-121.3(6)	C9	C8	C12	C11	5.2(6)
Rh1	C9	C10	C11	-60.6(4)	C9	C8	C12	C17	178.0(6)
Rh1	C9	C10	C15	120.9(6)	C9	C10	C11	Rh1	58.1(4)
Rh1	C10	C11	C12	-58.2(4)	C9	C10	C11	C12	-0.1(6)
Rh1	C10	C11	C16	120.6(6)	C9	C10	C11	C16	178.7(6)
Rh1	C11	C12	C8	-64.0(3)	C10	C11	C12	Rh1	60.8(4)
Rh1	C11	C12	C17	123.2(6)	C10	C11	C12	C8	-3.2(6)
F1	C1	C2	C3	179.3(5)	C10	C11	C12	C17	-175.9(6)
F1	C1	C6	C5	-177.7(5)	C12	C8	C9	Rh1	60.5(4)
N1	C4	C5	Rh1	-0.3(5)	C12	C8	C9	C10	-5.2(6)
N1	C4	C5	C6	-177.0(4)	C12	C8	C9	C14	-177.2(6)

N2	N1	C4	C3	-177.3(5)	C13	C8	C9	Rh1	-120.4(6)
N2	N1	C4	C5	0.6(6)	C13	C8	C9	C10	173.8(5)
C1	C2	C3	C4	-0.8(8)	C13	C8	C9	C14	1.9(9)
C2	C1	C6	C5	2.3(8)	C13	C8	C12	Rh1	120.2(5)
C2	C3	C4	N1	178.4(5)	C13	C8	C12	C11	-173.9(5)
C2	C3	C4	C5	0.6(8)	C13	C8	C12	C17	-1.0(9)
C3	C4	C5	Rh1	177.6(4)	C14	C9	C10	Rh1	-124.5(7)
C3	C4	C5	C6	0.9(7)	C14	C9	C10	C11	175.0(6)
C4	N1	N2	Rh1	-0.6(5)	C14	C9	C10	C15	-3.5(10)
C4	N1	N2	O1	-178.8(4)	C15	C10	C11	Rh1	-123.4(7)
C4	C5	C6	C1	-2.3(7)	C15	C10	C11	C12	178.4(6)
C6	C1	C2	C3	-0.6(9)	C15	C10	C11	C16	-2.8(10)
C7	N1	N2	Rh1	177.2(4)	C16	C11	C12	Rh1	-118.0(6)
C7	N1	N2	O1	-1.0(7)	C16	C11	C12	C8	178.0(6)
C7	N1	C4	C3	4.9(7)	C16	C11	C12	C17	5.2(9)
C7	N1	C4	C5	-177.1(5)					

Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for species A.

Atom	*x*	*y*	*z*	U(eq)
H2	6464.86	3866.79	7210.75	51
H3	4561.12	3896.77	5998.3	45
H6	5712.42	6643.88	7694.35	39
H7A	1407.3	4269.92	5129.86	58
H7B	3157.4	4113.16	4809.82	58
H7C	1999.86	4812.53	4250.74	58
H13A	2557.32	6646.79	8441.44	95
H13B	2300.43	7643.77	8933.04	95
H13C	3970.63	7388.64	8541.65	95
H14A	-1015.23	6769.33	6737.32	150
H14B	-777.48	7062.58	7786.49	150
H14C	241.75	6222.11	7380.72	150
H15A	-66.77	8571.42	5001.38	193
H15B	-1286.36	8624.51	5799.25	193
H15C	-793.26	7618.34	5397.52	193
H16A	3835.2	9544.37	5624.01	142
H16B	2366.82	10156.49	5926.32	142
H16C	2178.55	9438.24	5085.67	142
H17A	4983.83	9414.5	7022.19	101

H17B	4465.41	9241.65	8044.26	101
H17C	5471.35	8456	7542.42	101

Crystal structure determination of species A

Crystal Data for $C_{17}H_{21}ClN_2ORhF$ (M =426.72 g/mol): monoclinic, space group $P2_1/n$ (no. 14), a = 8.543(4) Å, b = 14.111(6) Å, c = 14.684(7) Å, β = 92.284(7) °, V = 1768.7(14) Å^3, Z = 4, T = 123.15 K, μ(MoKα) = 1.131 mm^{-1}, *Dcalc* = 1.602 g/cm^3, 20794 reflections measured (5.424 ° ≤ 2Θ ≤ 55.714 °), 4209 unique (R_{int} = 0.0438, R_{sigma} = 0.0322) which were used in all calculations. The final R_1 was 0.0573 (I > 2σ(I)) and wR_2 was 0.1788 (all data).

VI. References

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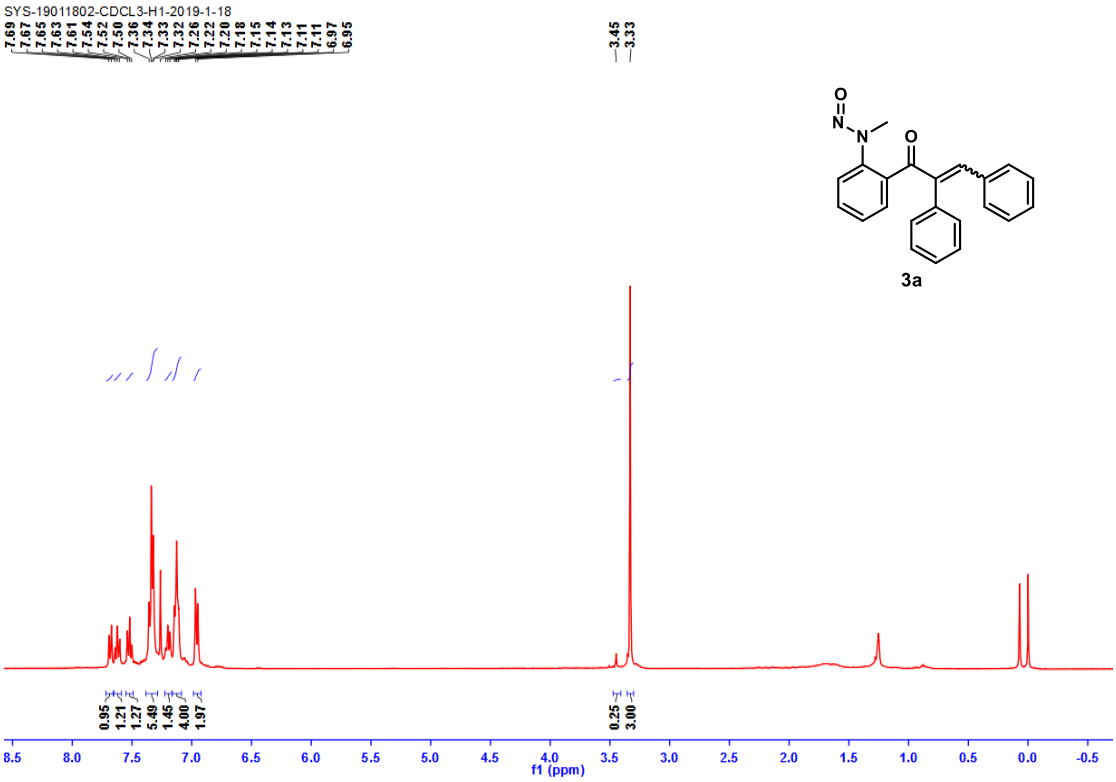
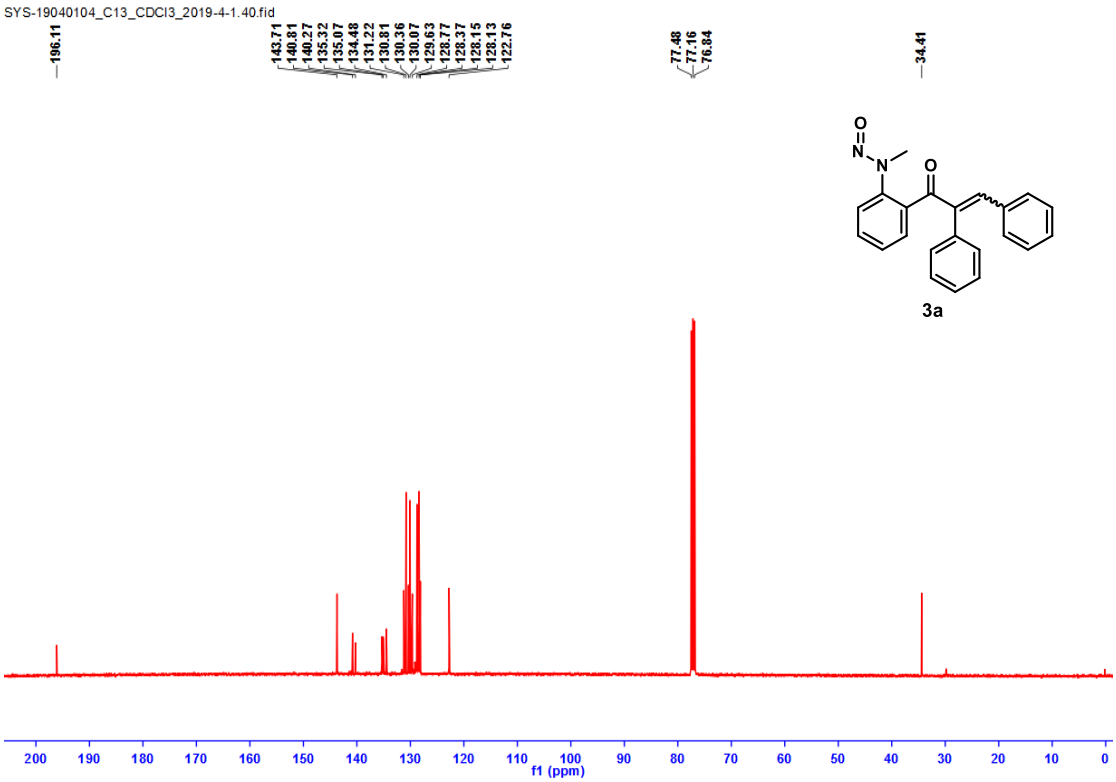
VII. NMR Spectra of Products





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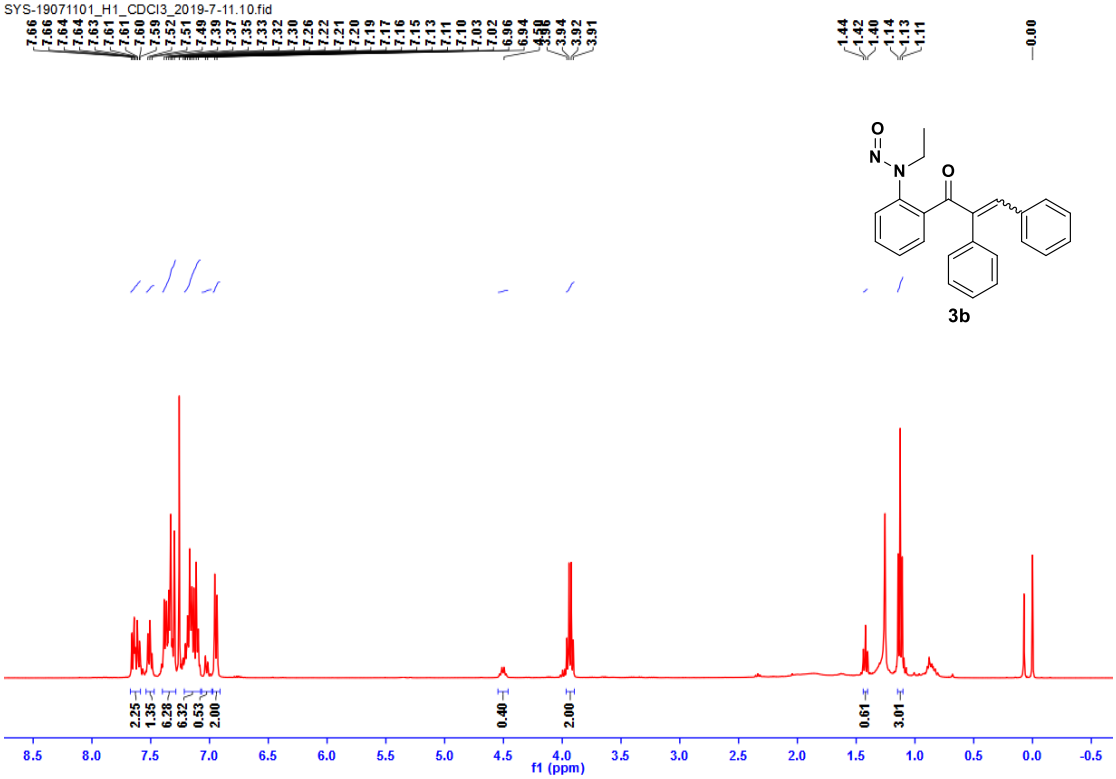

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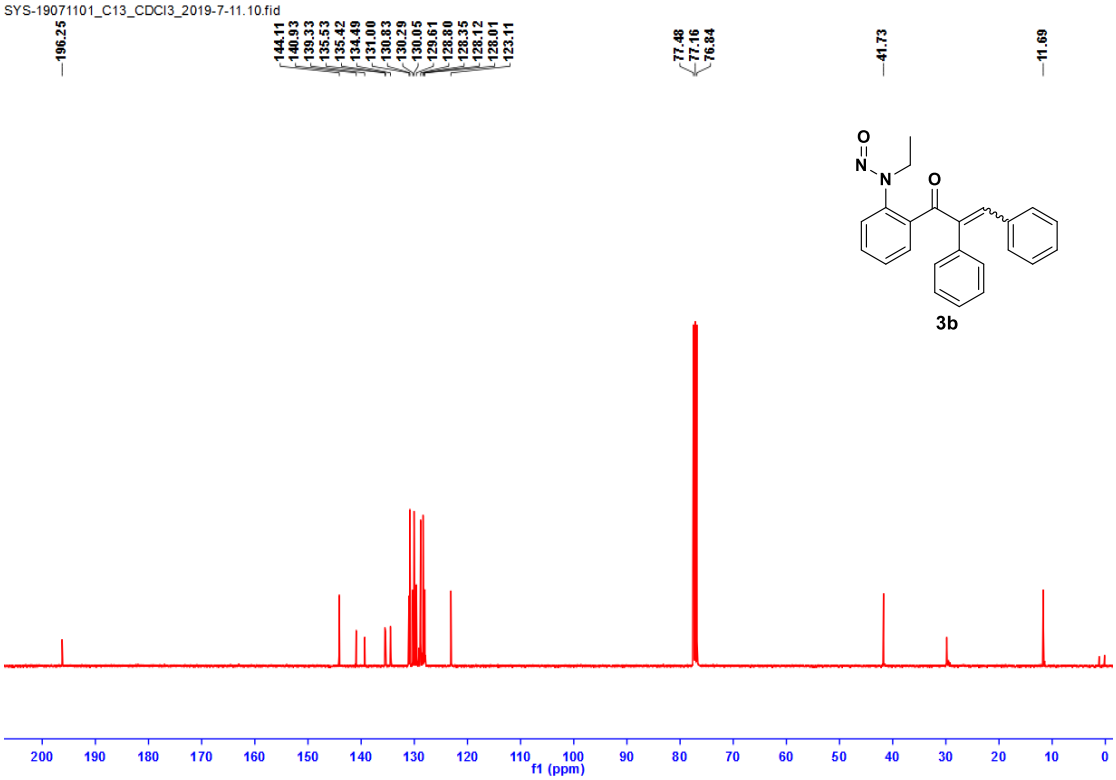

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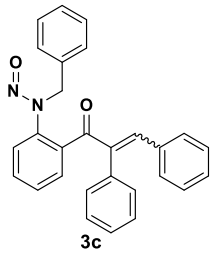

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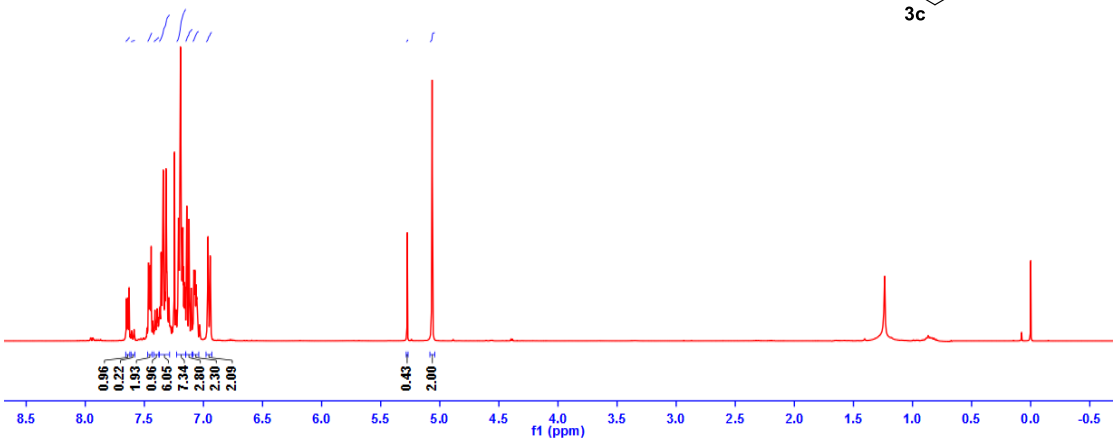

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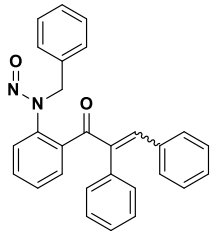

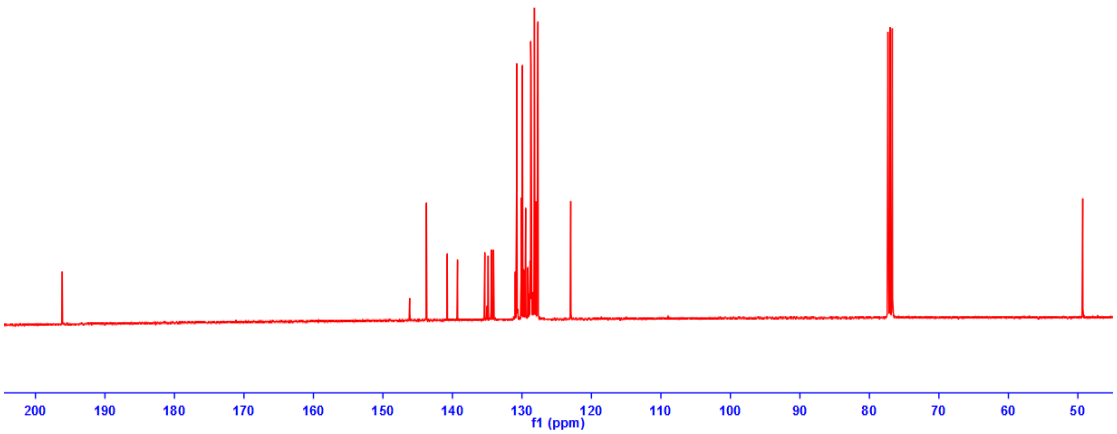

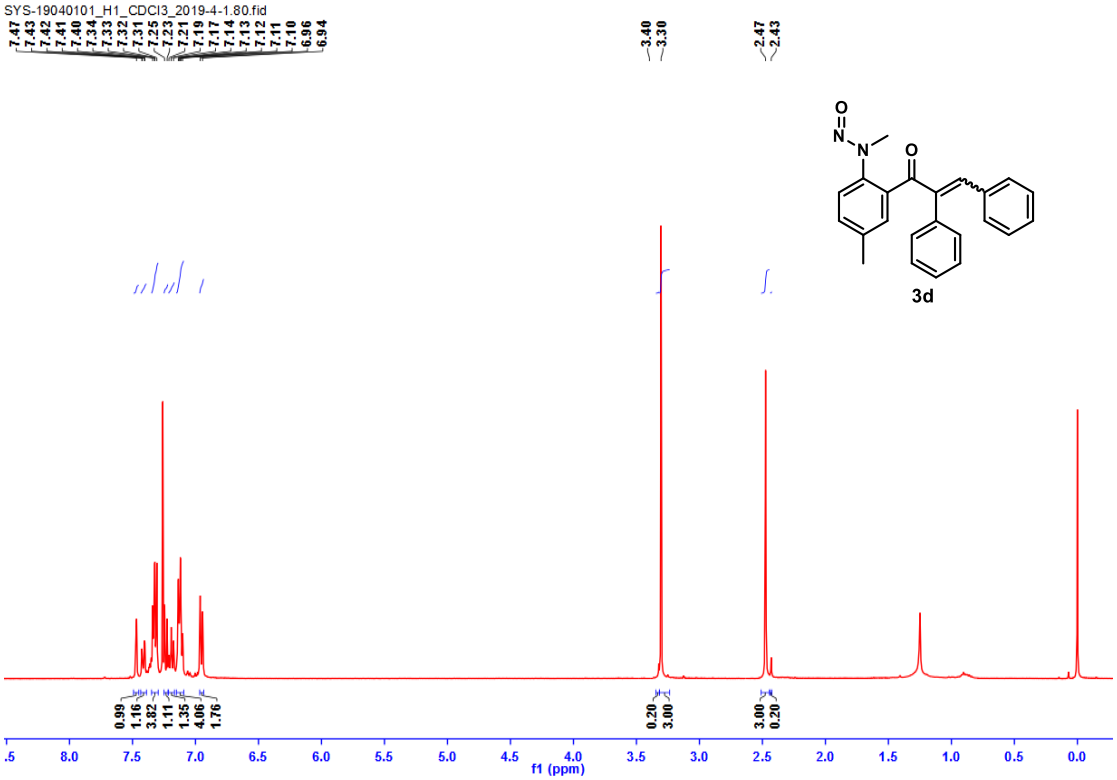
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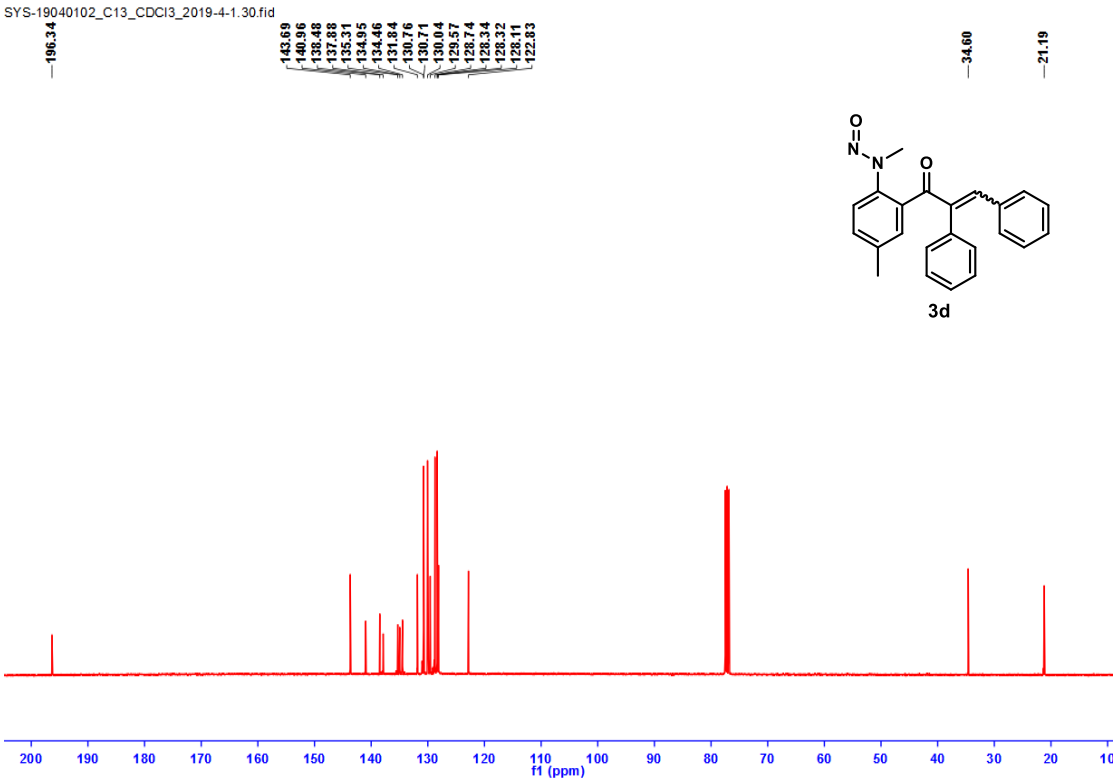
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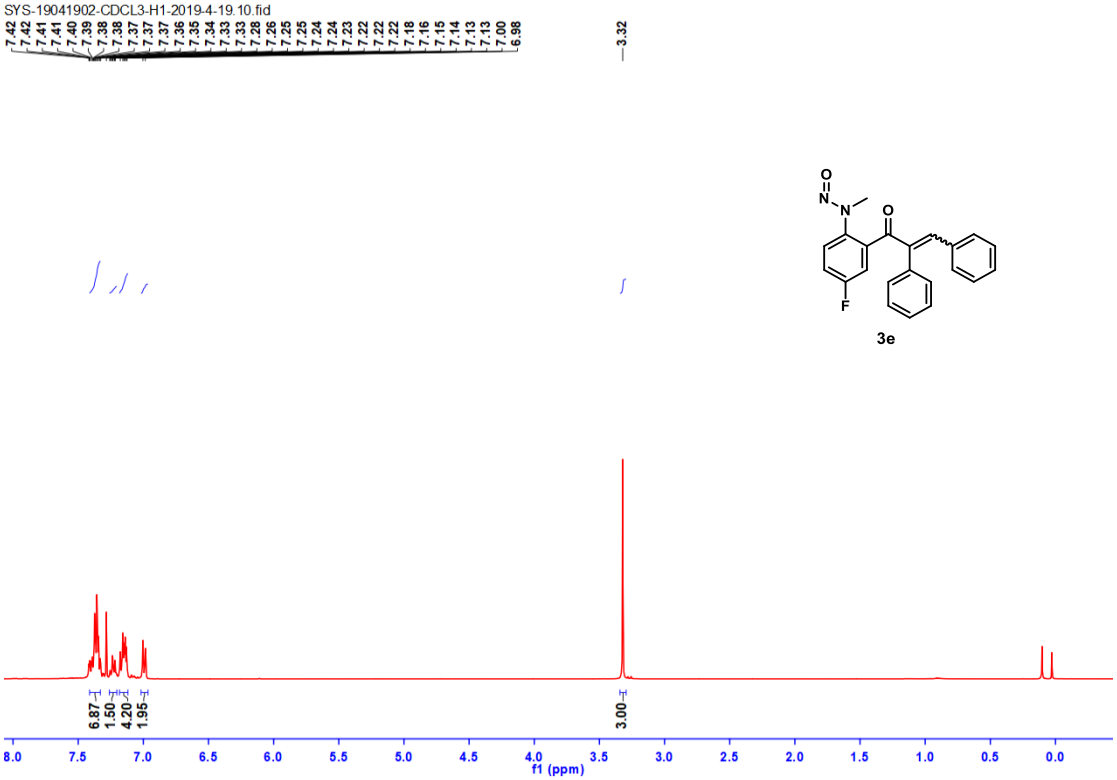

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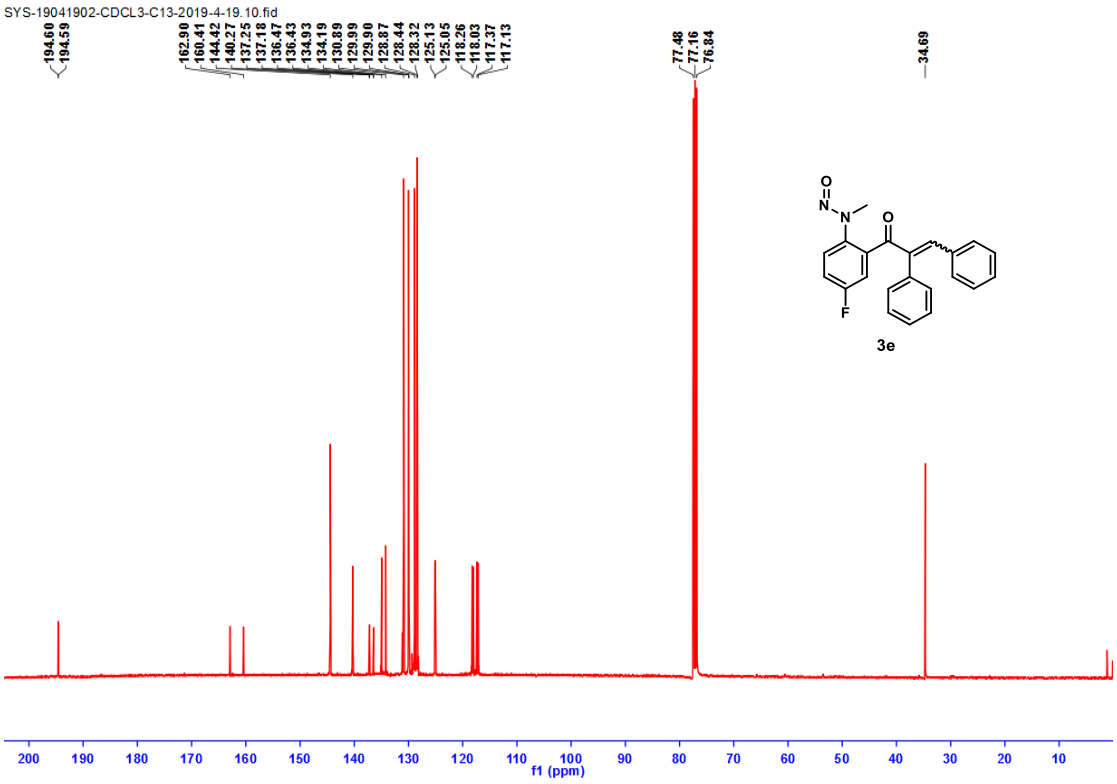

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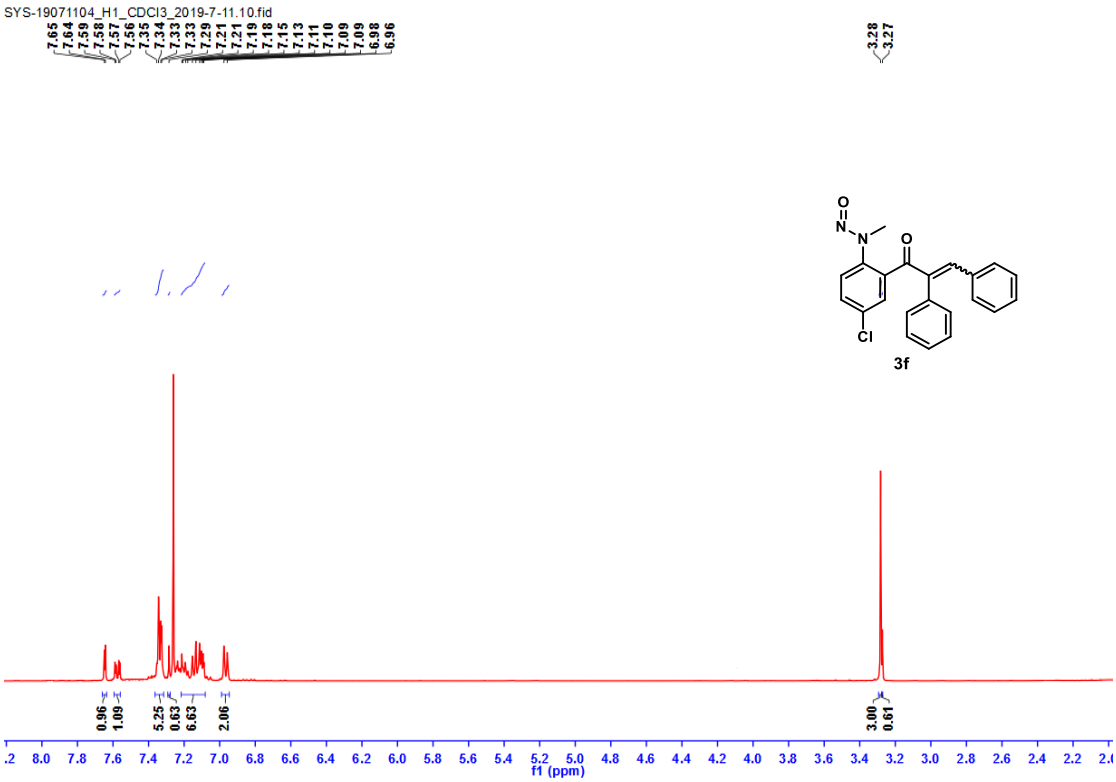
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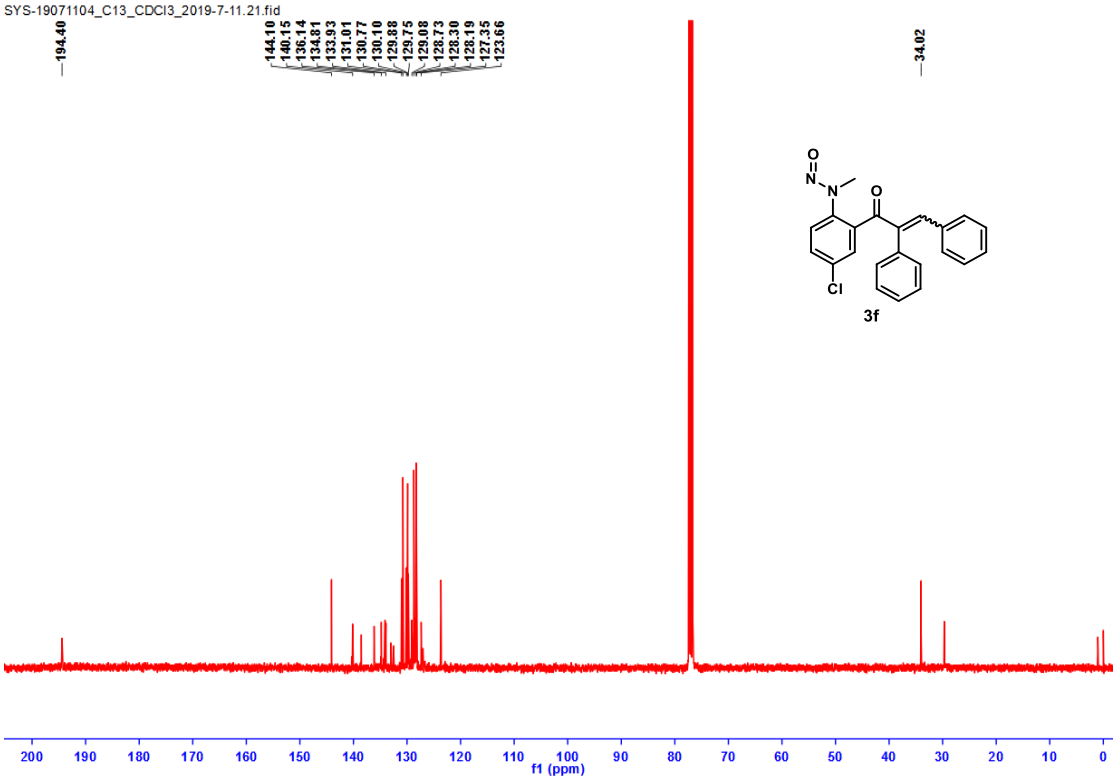
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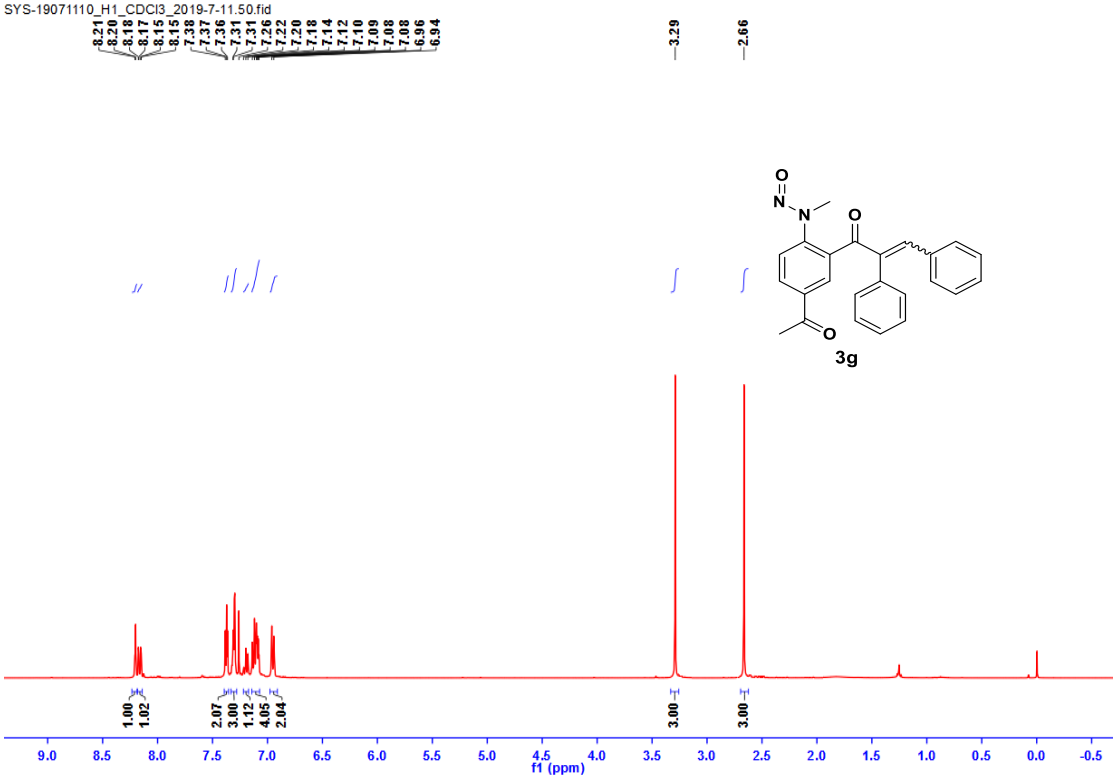

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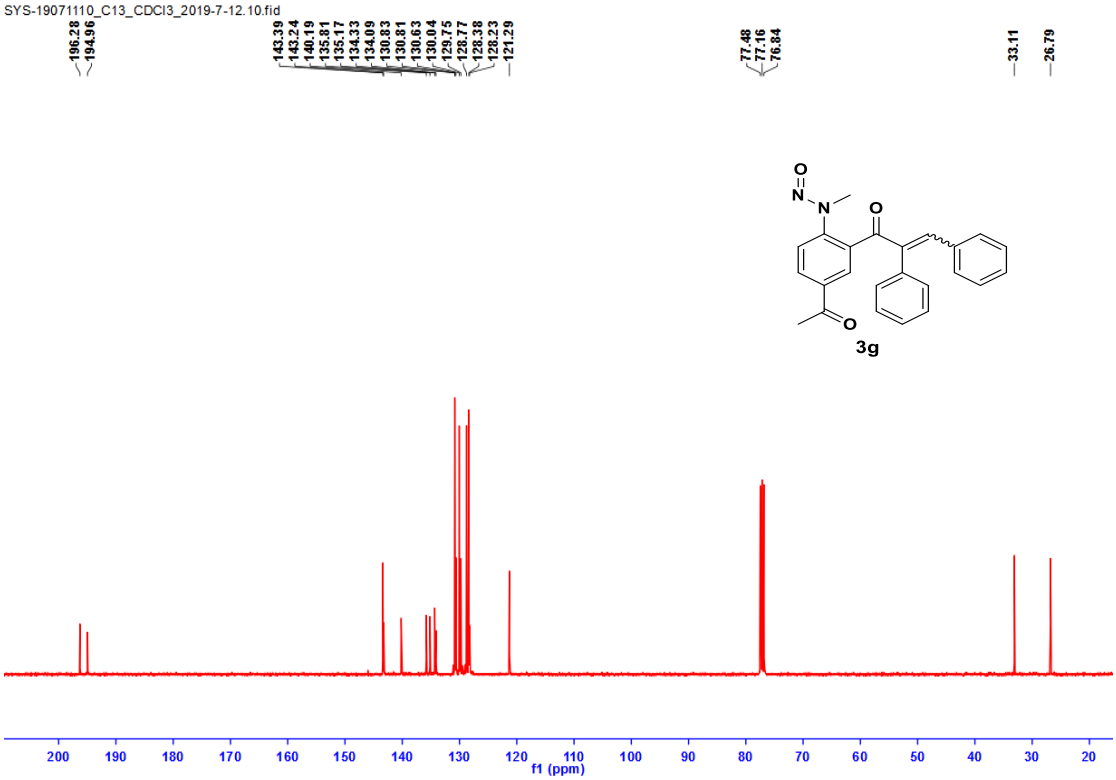

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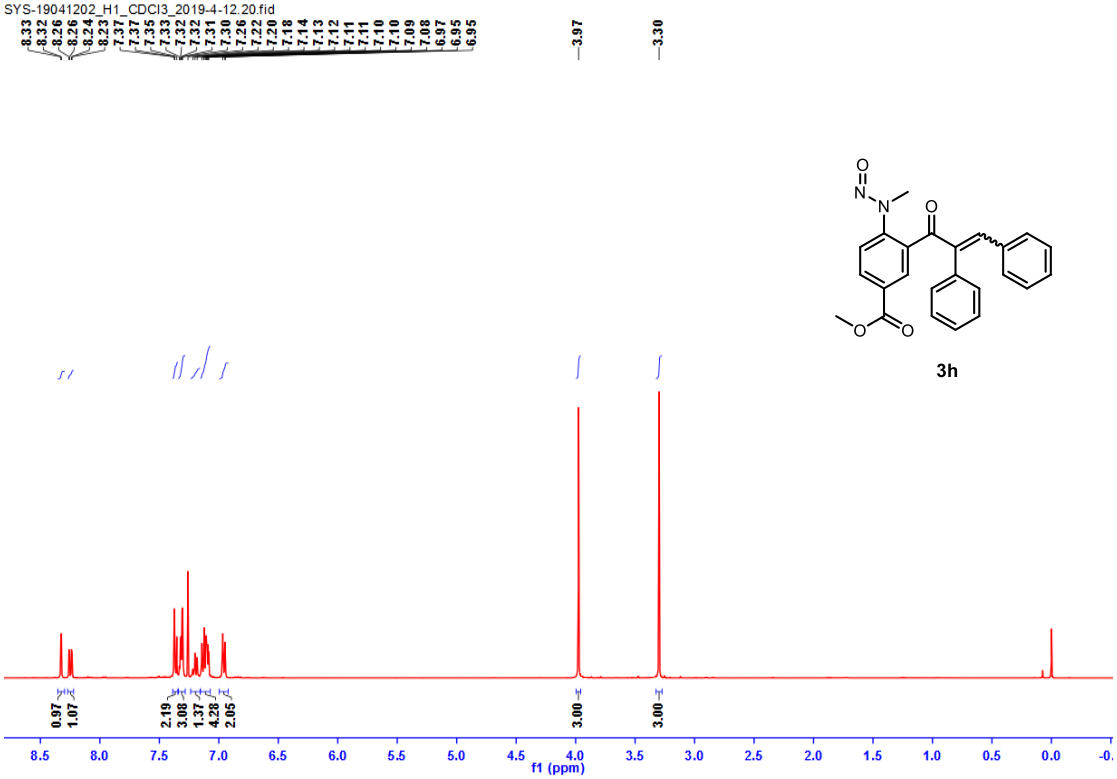

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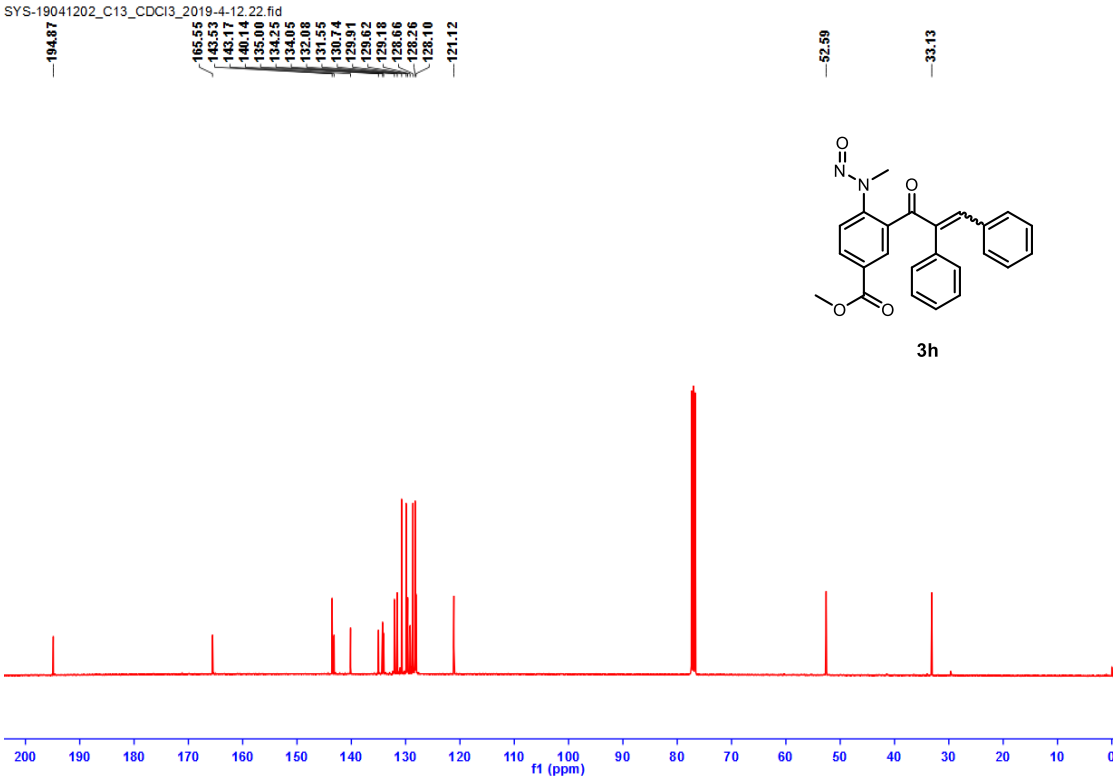

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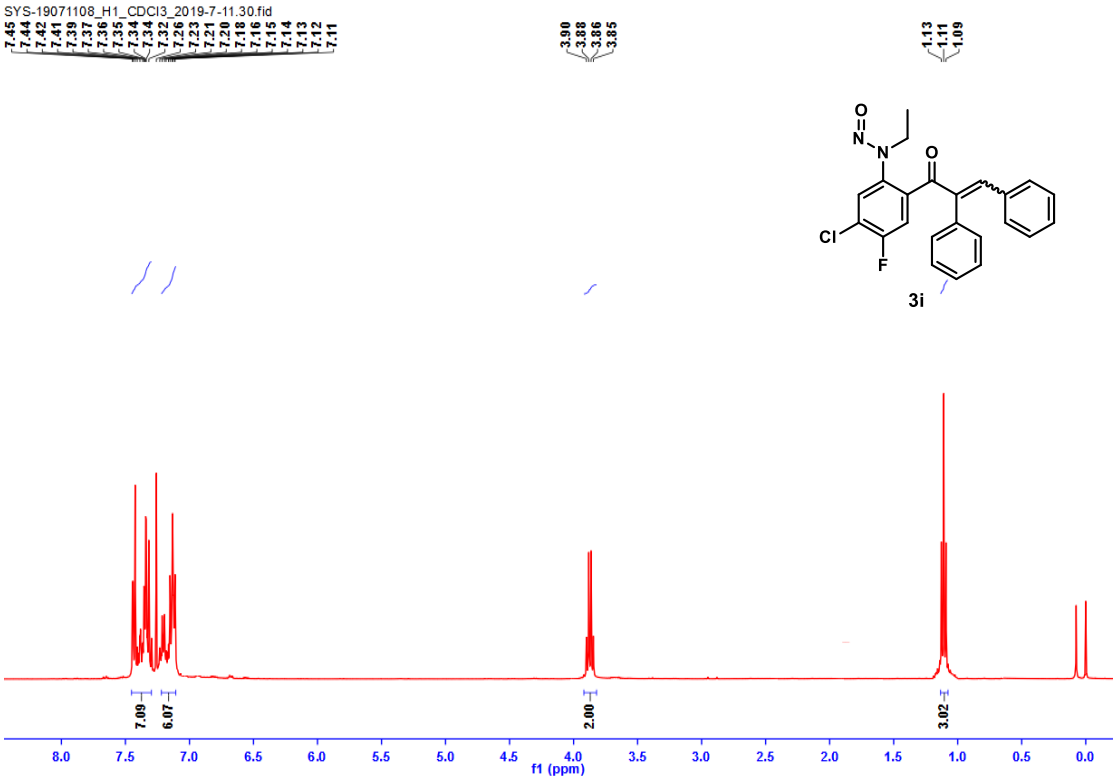
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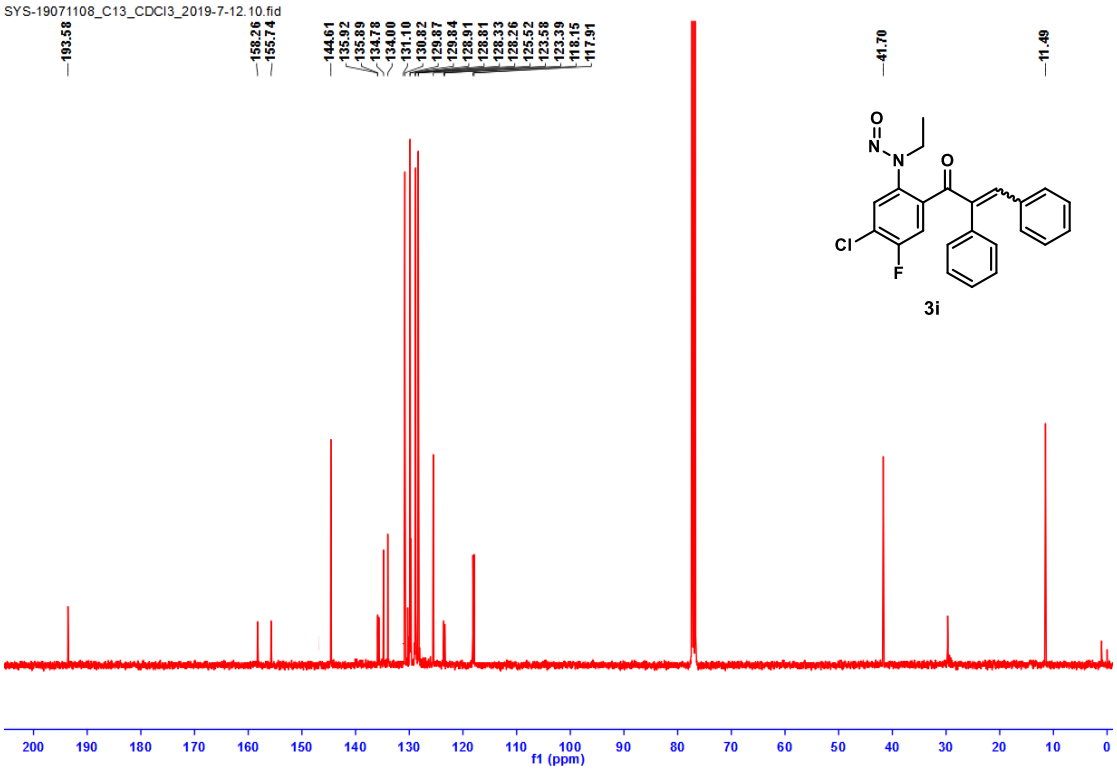
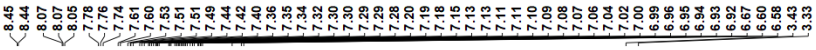
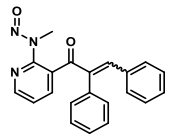
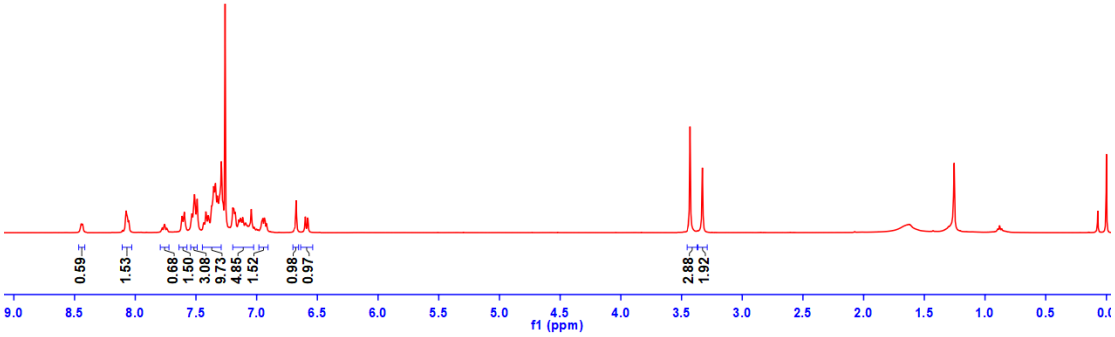
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


SYS-19071108_C13_CDCl3_2019-7-12.10.fid
193.58
158.26
155.74
144.61
135.92
135.89
134.78
134.00
131.10
130.82
129.87
129.84
128.91
128.81
128.33
128.26
125.52
123.58
123.39
118.15
117.91
41.70
11.49
O
N
N
O
Cl
F
3i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

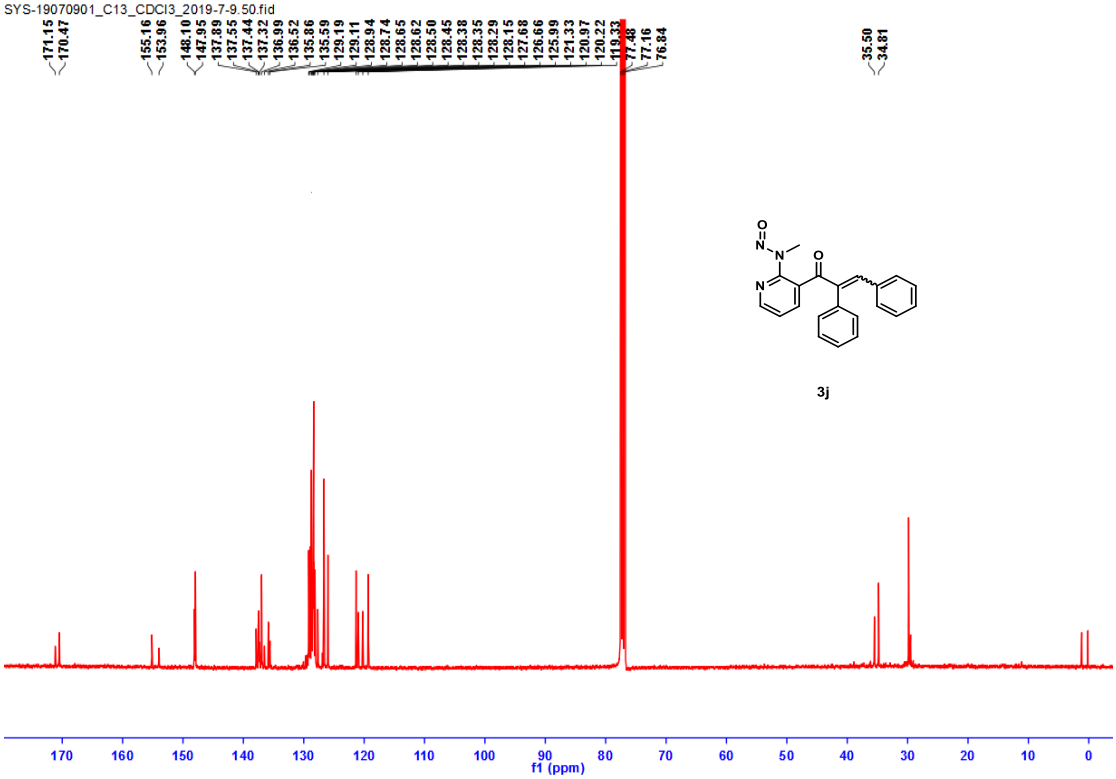




3j



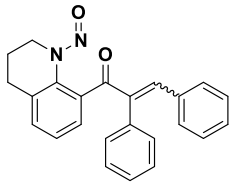
SYS-19070901_C13_CDCl3_2019-7-9.50.fid



3j

SYS-19041903-CDCL3-H1-2019-4-19.10.fid

7.51 7.51 7.50 7.49 7.49 7.34 7.32 7.31 7.28 7.28 7.26 7.24 7.23 7.23 7.22 7.22 7.21 7.19 7.18 7.18 7.17 7.17 7.16 7.15 7.15 7.15 7.12 7.11 7.10 7.08 7.08 6.99 6.99 6.98 6.98 6.97 6.95 6.95 3.63 3.62 3.60 2.70 2.68 2.67 1.74 1.72 1.71 1.69 1.68



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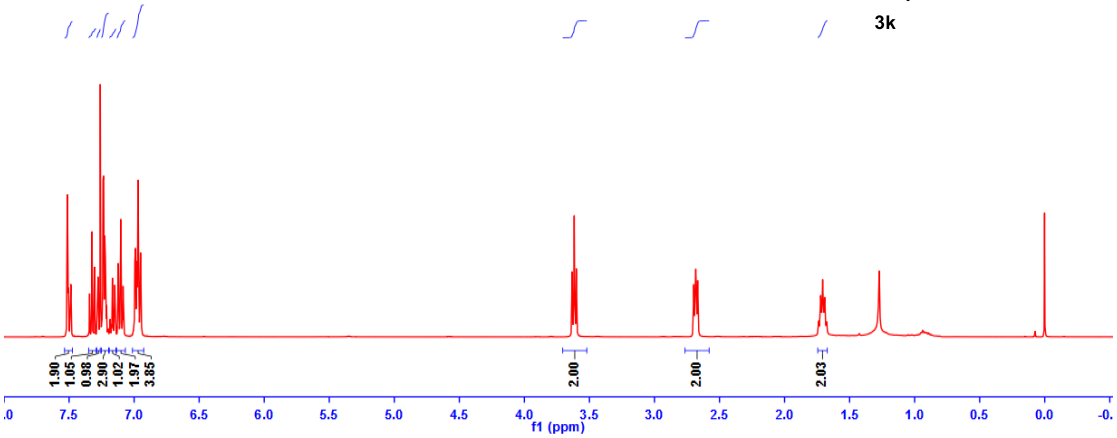
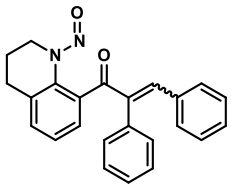


SYS-19041903-CDCL3-C13-2019-4-19.10.fid

195.41 141.04 140.00 135.92 135.03 134.46 131.72 130.72 130.30 130.21 129.17 129.12 128.81 128.40 128.24 127.80 126.28 77.48 77.16 76.84 43.82 27.85 20.98



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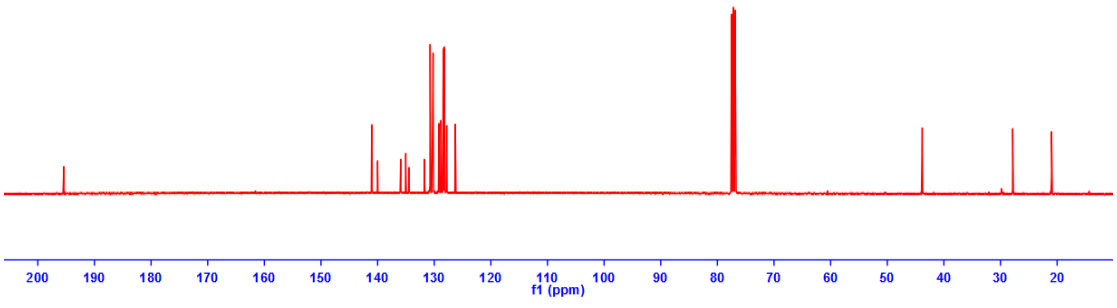
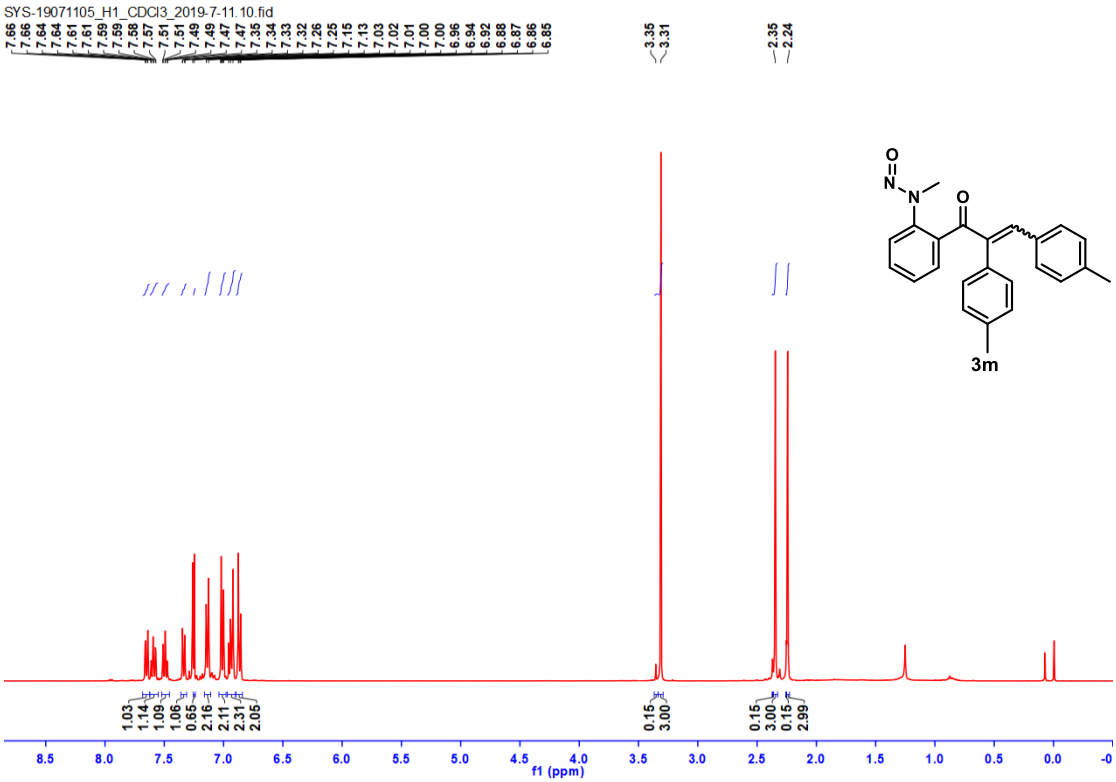
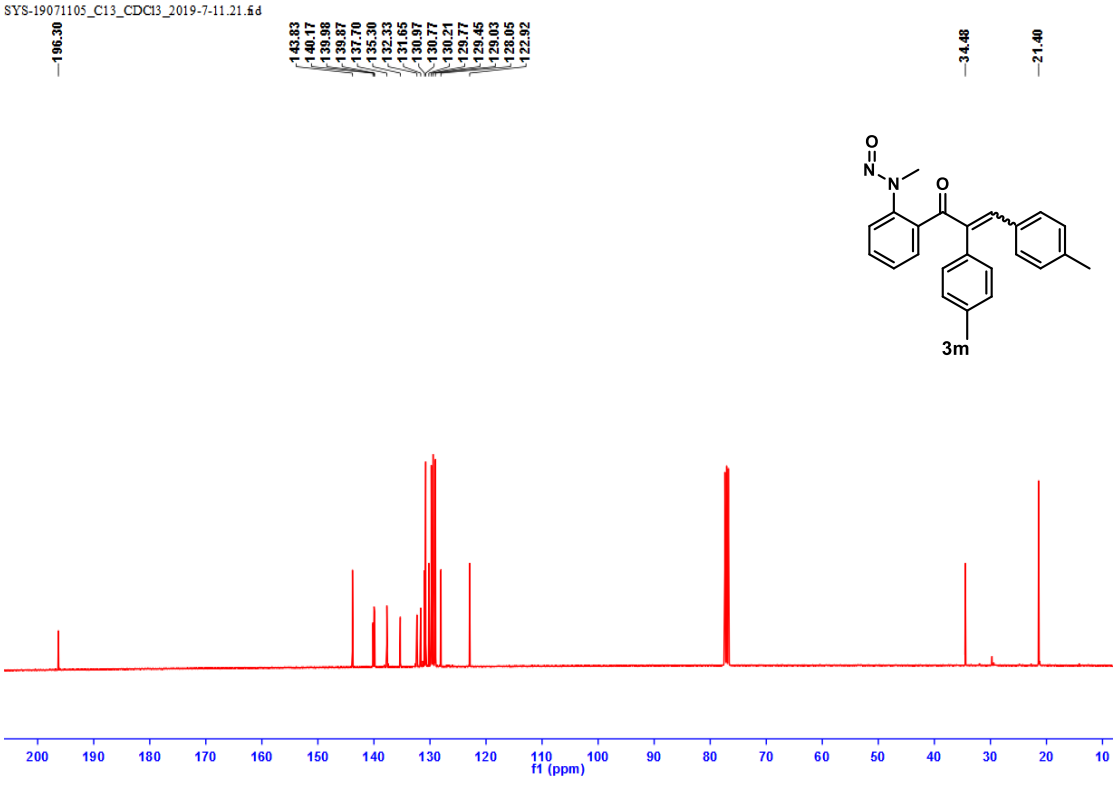
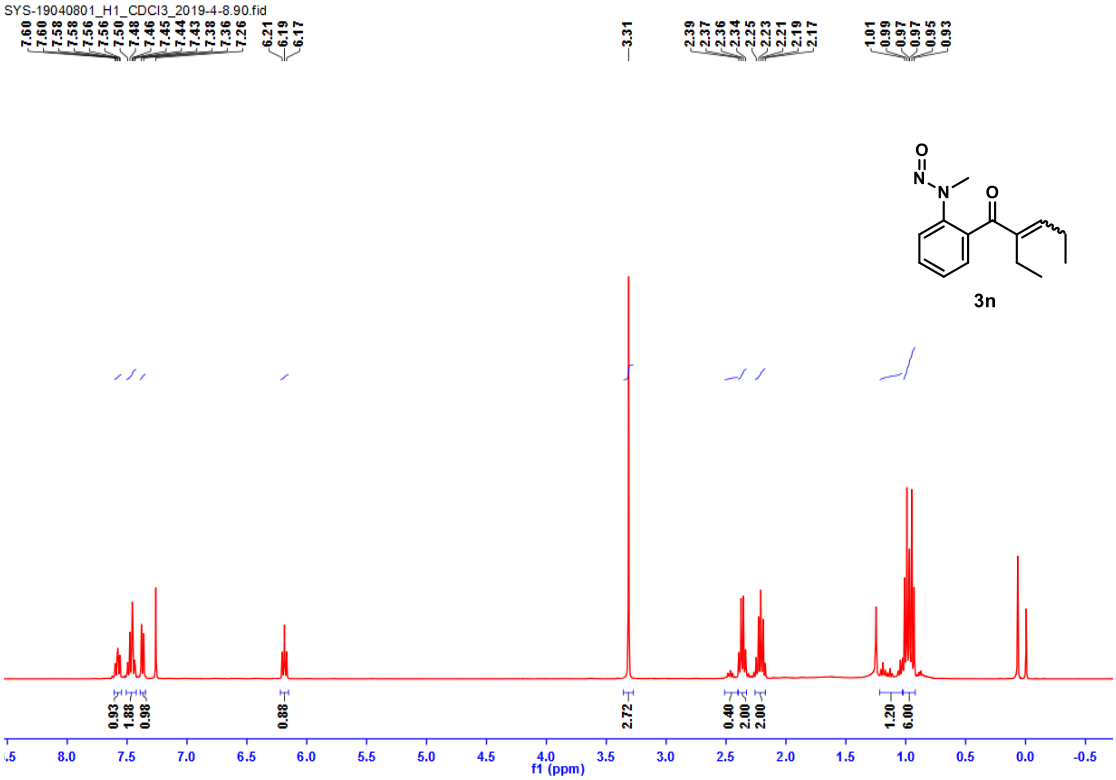
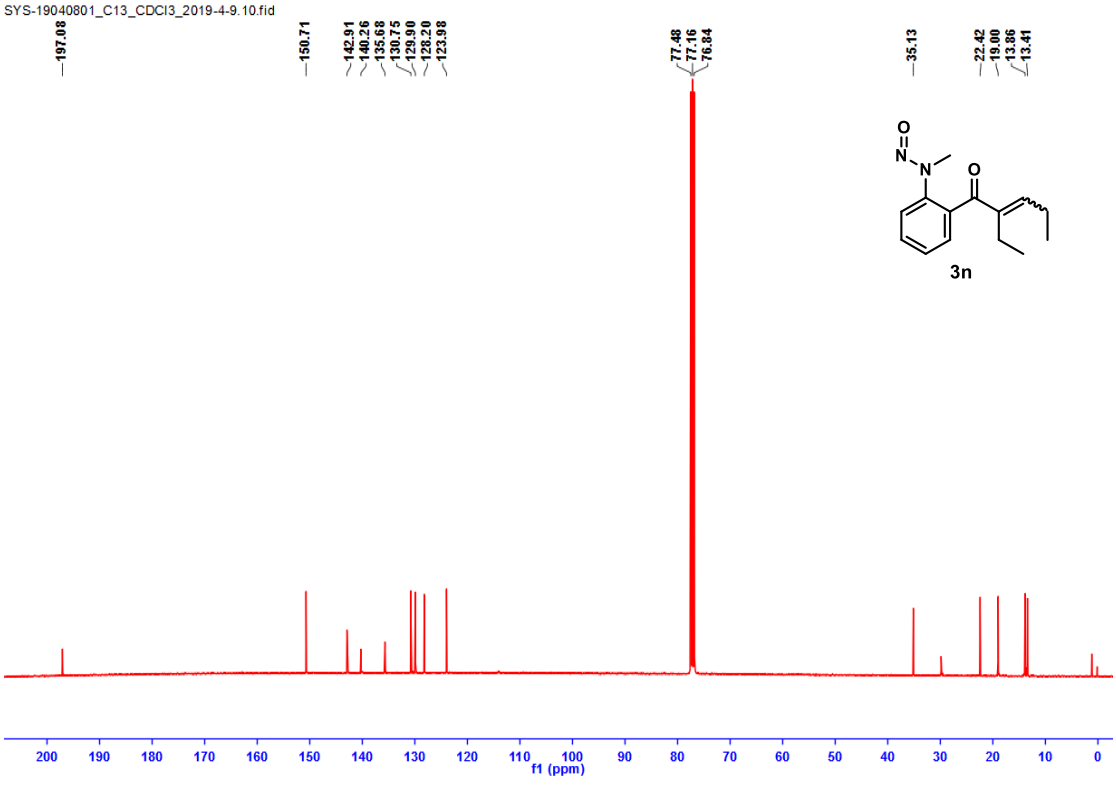


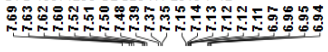

SYS-19071105_H1_CDCl3_2019-7-11.10.fid
7.66 7.66 7.64 7.64 7.61 7.61 7.59 7.59 7.58 7.57 7.51 7.51 7.49 7.49 7.47 7.47 7.35 7.34 7.33 7.32 7.26 7.25 7.15 7.13 7.03 7.02 7.01 7.00 7.00 6.96 6.94 6.92 6.88 6.87 6.86 6.85
3.35 3.31
2.35 2.24
3m
1.03 1.14 1.09 1.06 0.65 2.16 2.11 2.31 2.05
0.15 3.00
0.15 3.00 0.15 2.99
f1 (ppm)

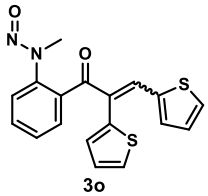

SYS-19071105_C13_CDCl3_2019-7-11.21.fid
196.30
143.83 140.17 139.98 139.87 137.70 135.30 132.33 131.65 130.97 130.77 130.21 129.77 129.45 129.03 128.05 122.92
34.48
21.40
3m
f1 (ppm)


SYS-19040801_H1_CDCl3_2019-4-8.90.fid
7.60
7.60
7.58
7.58
7.56
7.56
7.50
7.48
7.46
7.45
7.44
7.43
7.38
7.36
7.26
6.21
6.19
6.17
3.31
2.39
2.37
2.36
2.34
2.25
2.23
2.21
2.19
2.17
1.01
0.99
0.97
0.97
0.95
0.93
3n
0.93
1.88
0.98
0.88
2.72
0.40
2.00
2.00
1.20
6.00
f1 (ppm)

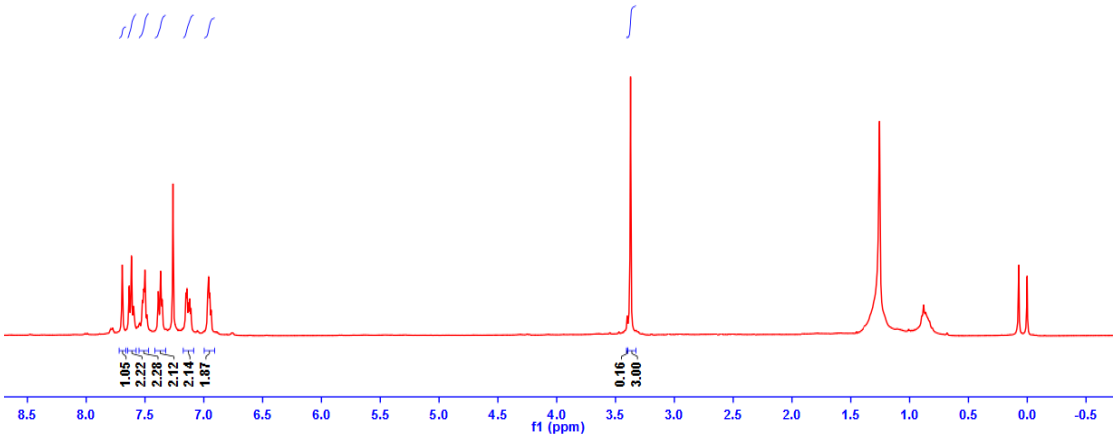

SYS-19040801_C13_CDCl3_2019-4-9.10.fid
197.08
150.71
142.91
140.26
135.68
130.75
129.90
128.20
123.98
77.48
77.16
76.84
35.13
22.42
19.00
13.86
13.41
3n
f1 (ppm)

SYS-19071203-CDCL3-H1-2019-7-12





3o



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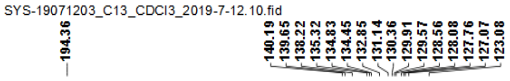

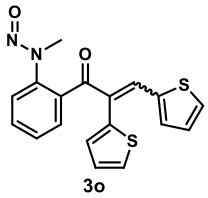

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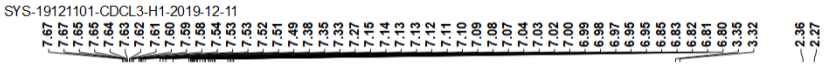
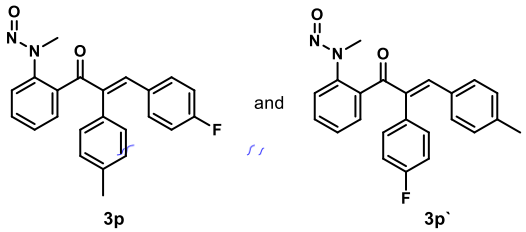
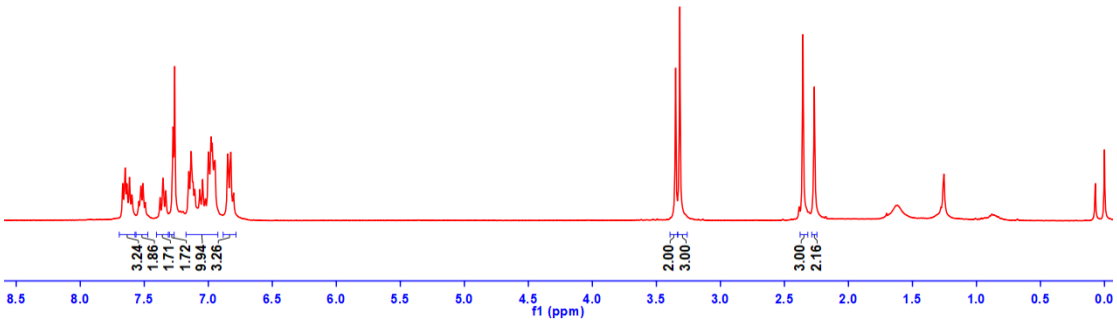
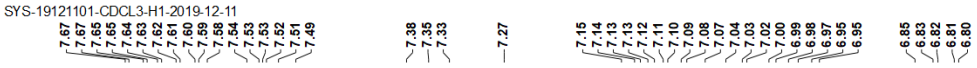

SYS-19121101-CDCL3-H1-2019-12-11


and
3p
3p`


3.24
1.86
1.71
1.72
9.94
3.26
2.00
3.00
3.00
2.16
f1 (ppm)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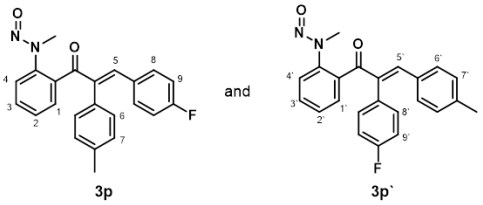
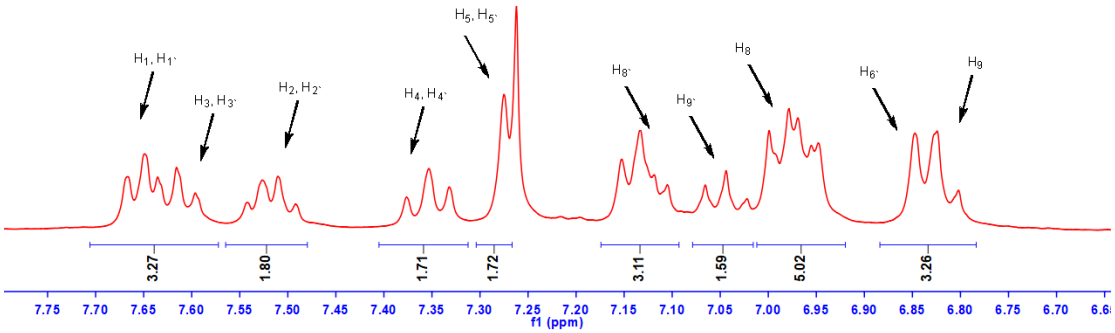
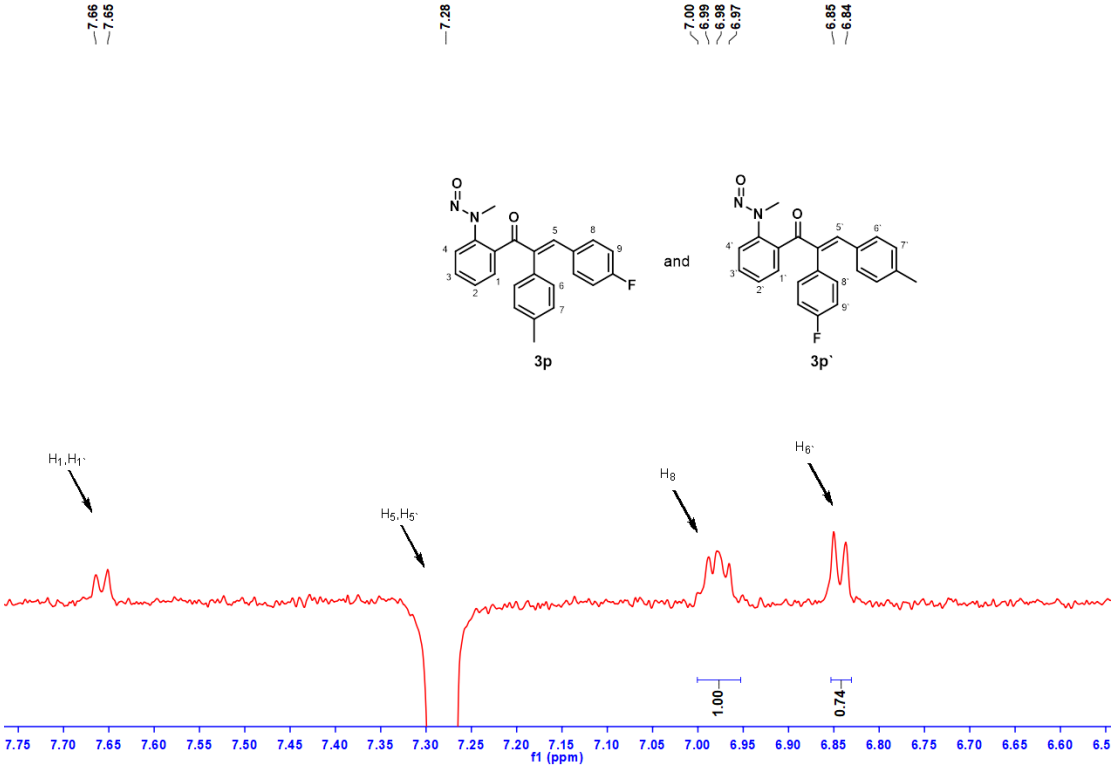
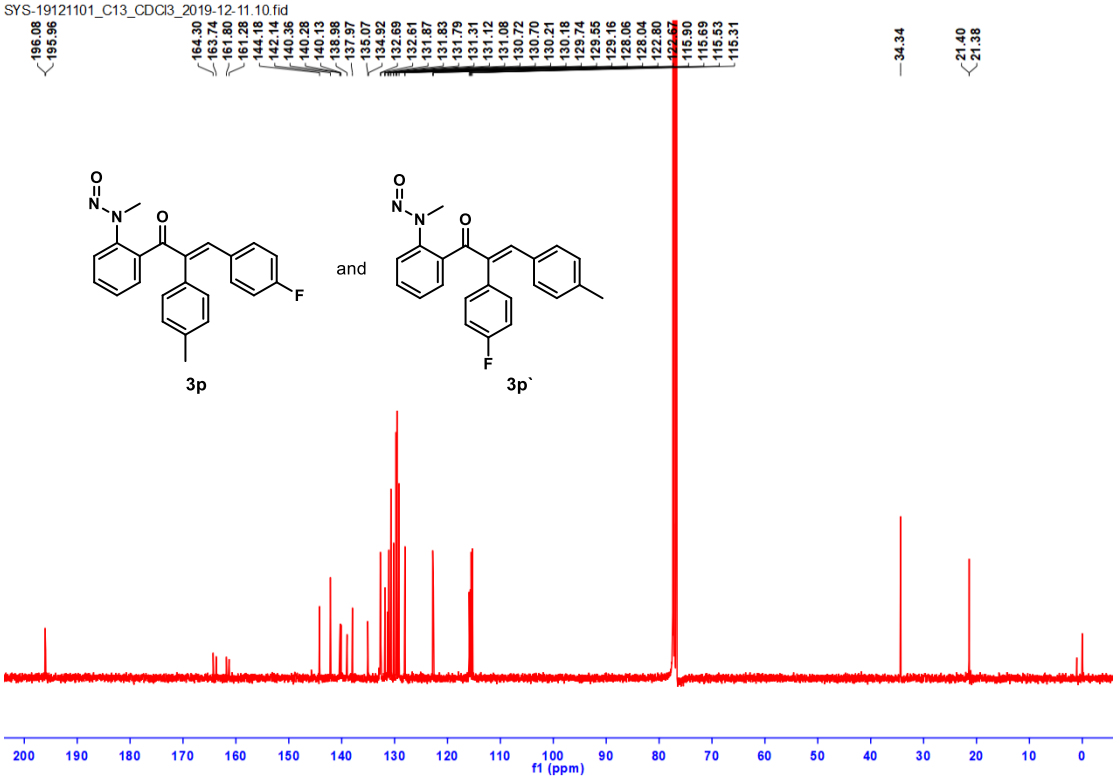

and
3p
3p`


H1, H1`
H3, H3`
H2, H2`
H4, H4`
H5, H5`
H8`
H9`
H8
H6`
H9
3.27
1.80
1.71
1.72
3.11
1.59
5.02
3.26
f1 (ppm)

SYS-19121101-CDCL3-NOESY 1D7.28-2019-12-12

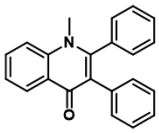


SYS-19121101_C13_CDCl3_2019-12-11.10.fid

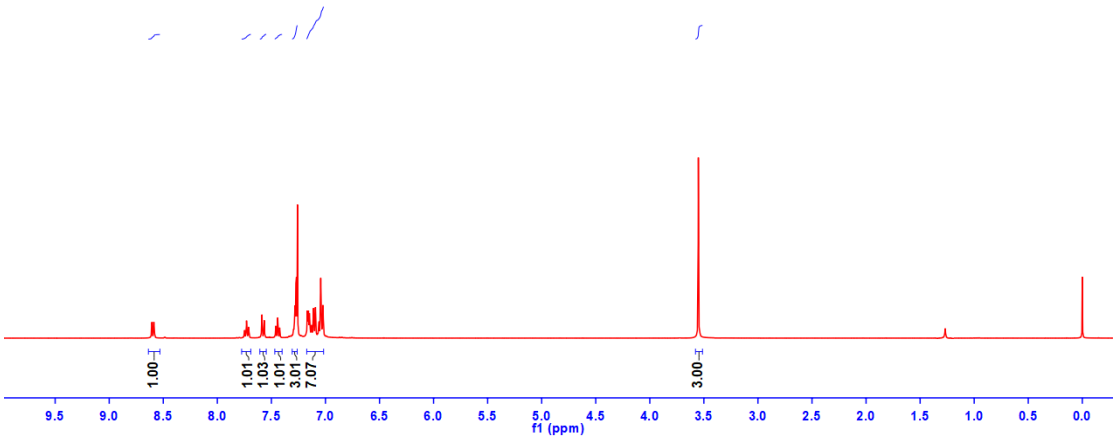


SYS-19061401-CDCL3-H1-2019-6-14.10.fid

8.61 8.60 8.59 8.58 7.75 7.75 7.73 7.73 7.71 7.71 7.59 7.57 7.46 7.46 7.44 7.44 7.42 7.42 7.29 7.28 7.27 7.26 7.17 7.16 7.15 7.14 7.13 7.13 7.11 7.09 7.06 7.06 7.04 7.04 7.03 7.02 3.55

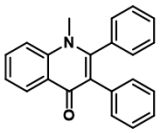


4a

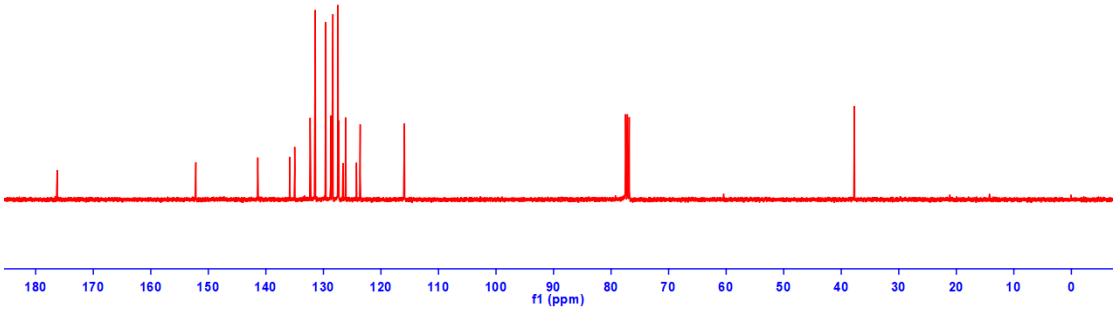


2019-06-20 shiyueseng-SYS-19061401.1.fid

176.25 152.17 141.40 135.85 134.99 132.30 131.40 129.58 128.75 128.35 127.46 127.31 126.60 126.13 124.25 123.61 115.91 37.71



4a



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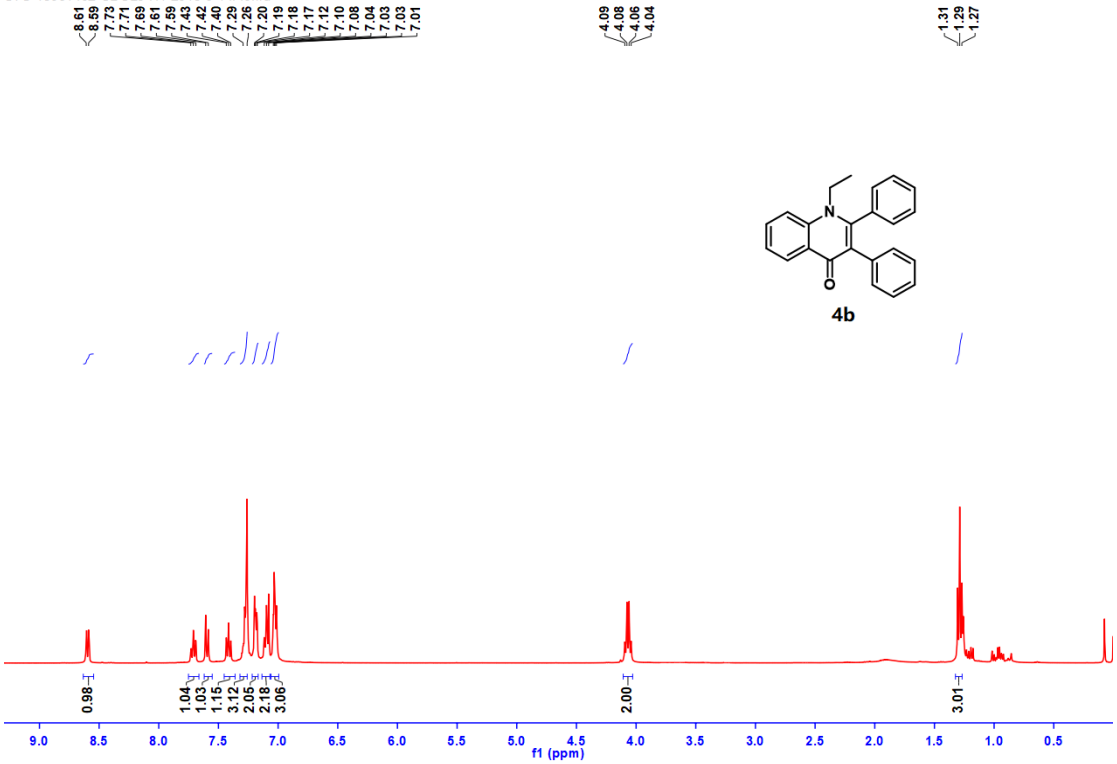
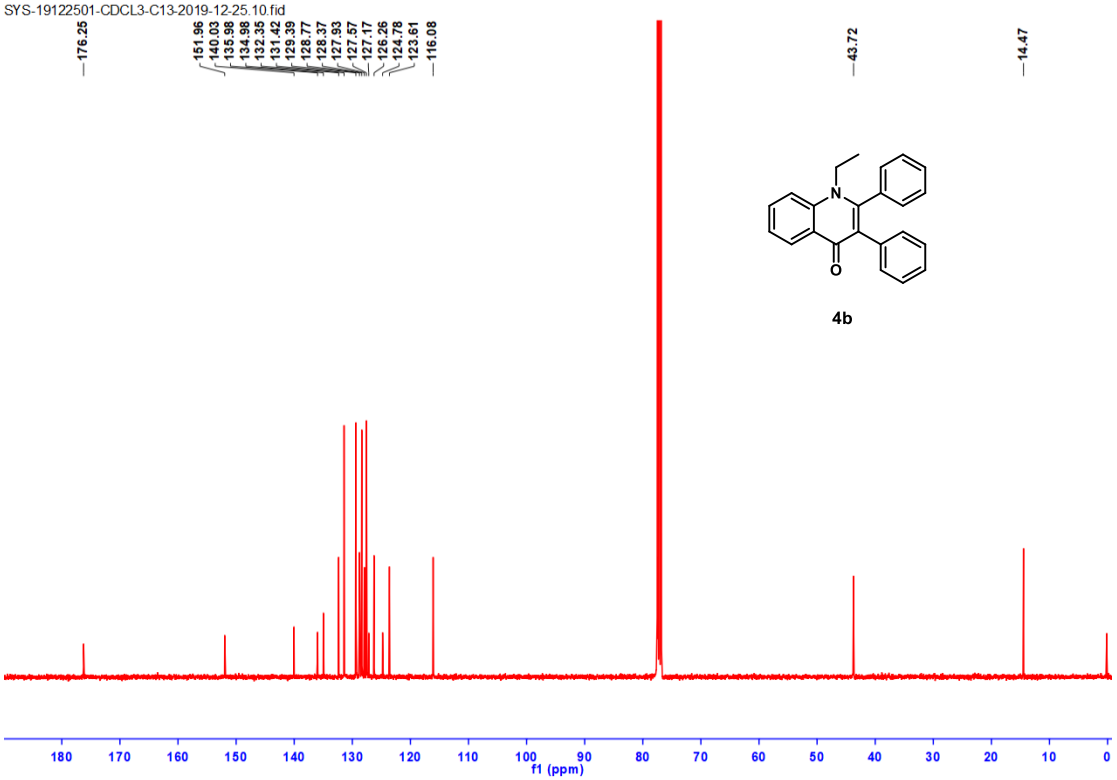
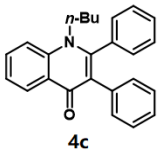


SYS-19122501-CDCL3-C13-2019-12-25.10.fid



SYS-19061403-CDCL3-H1-2019-6-14.50.fid



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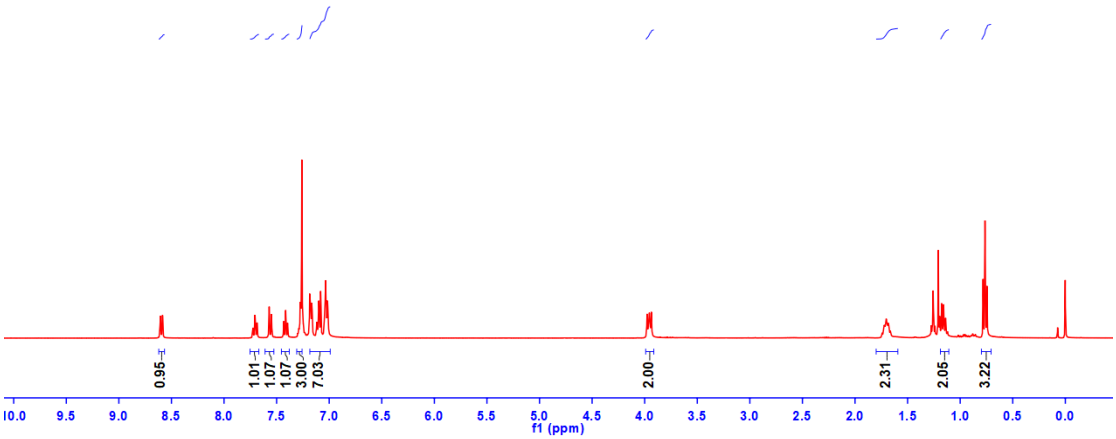
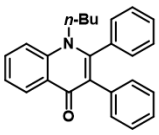
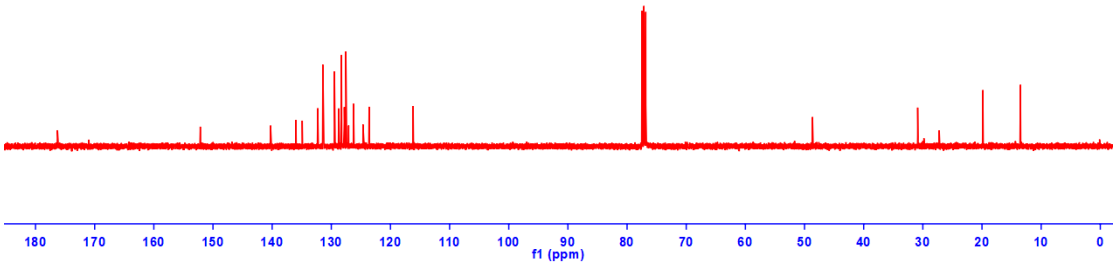


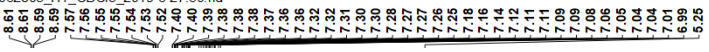
2019-06-20 shiyueseng-SYS-19061403.1.fid

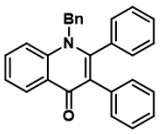


4c

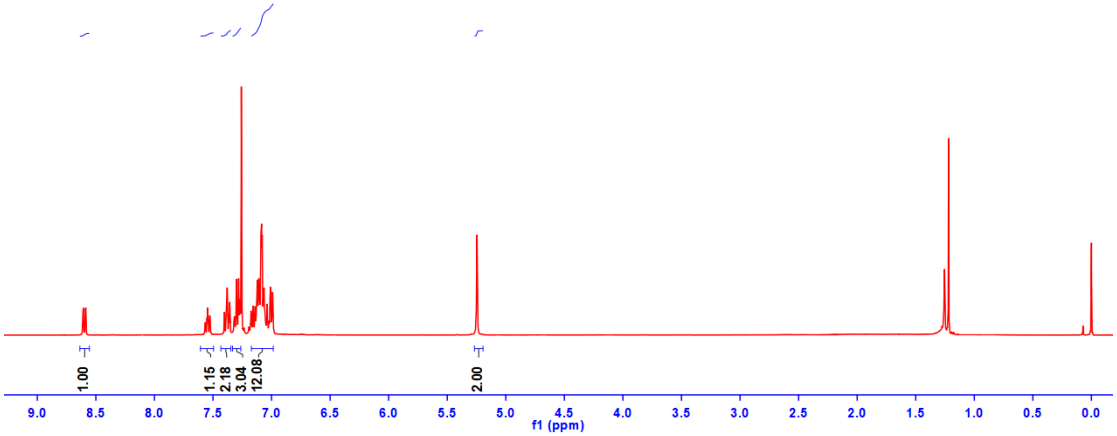


SYS-19062805_H1_CDCl3_2019-6-27.50.fid

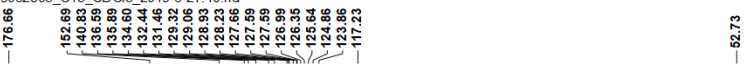


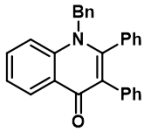


4d

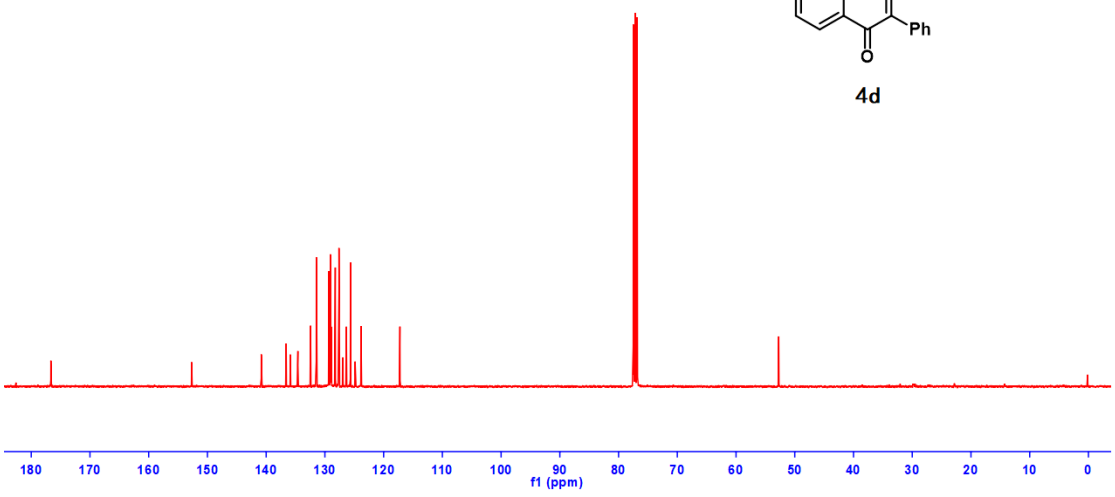


SYS-19062805_C13_CDCl3_2019-6-27.10.fid

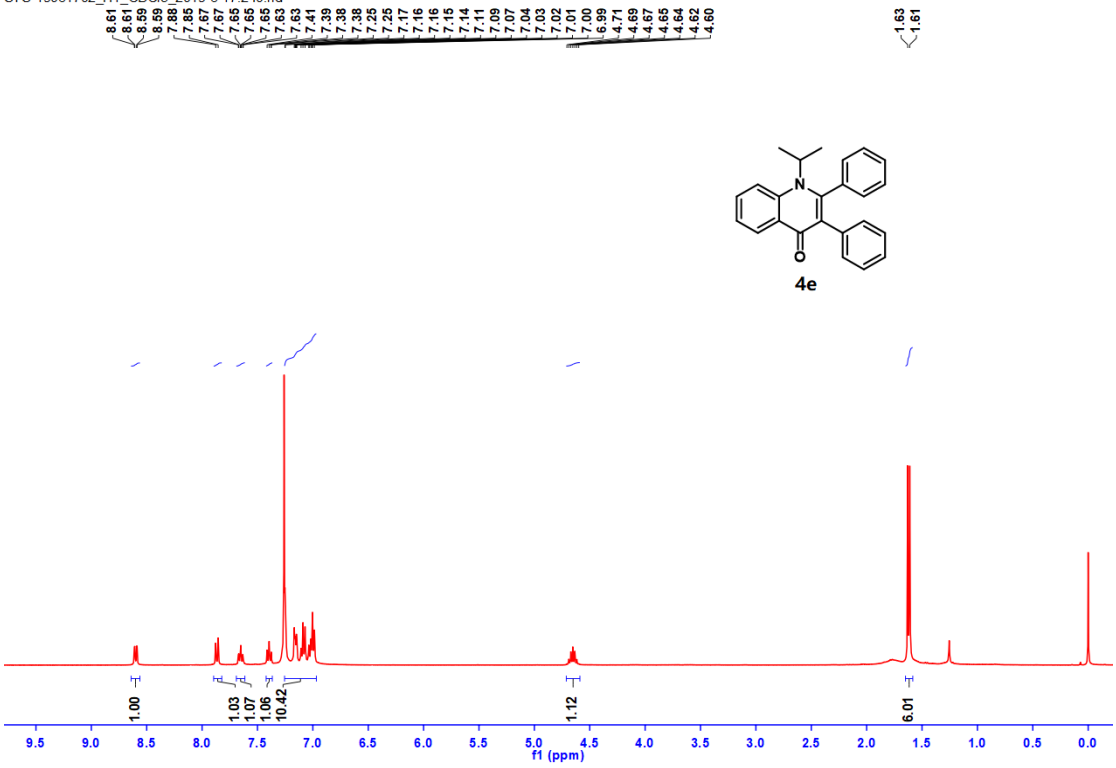




4d

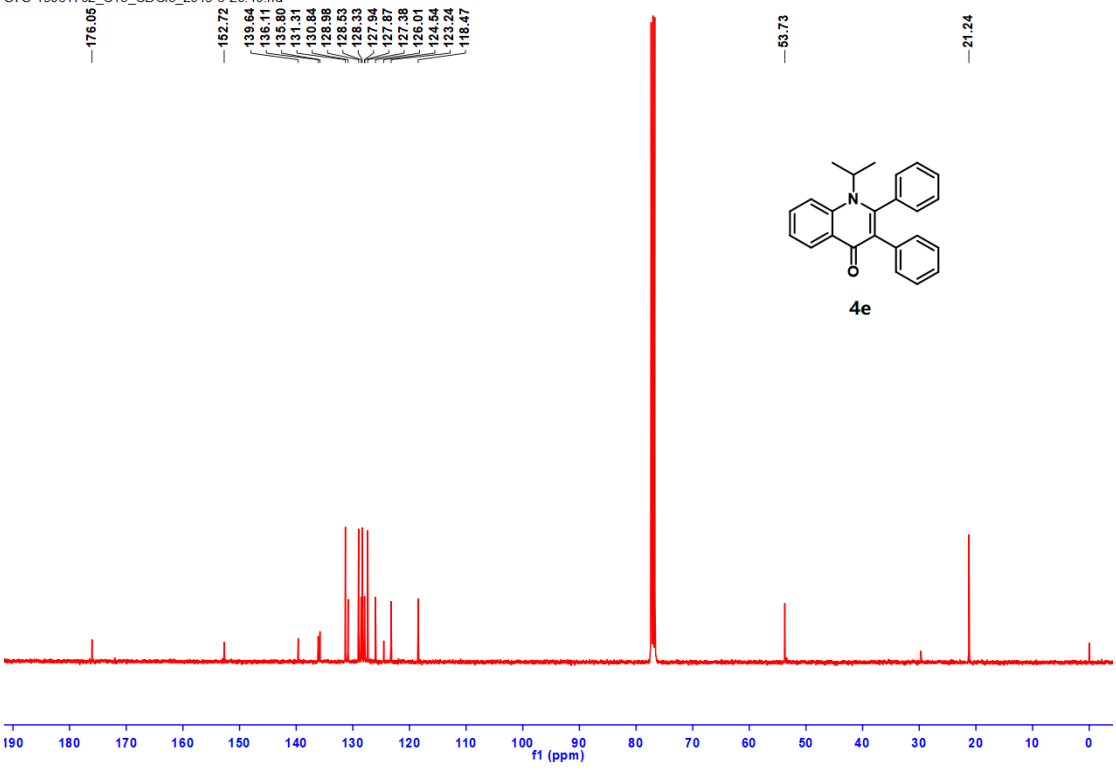


SYS-19061702_H1_CDCl3_2019-6-17.240.fid



4e

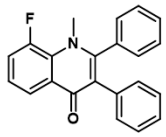
SYS-19061702_C13_CDCl3_2019-6-20.10.fid



4e

SYS-19062804_H1_CDCl3_2019-6-27.40.fid

8.34 8.34 8.34 8.33 8.32 8.32 8.32 8.31 7.45 7.43 7.43 7.42 7.41 7.40 7.39 7.36 7.35 7.34 7.33 7.32 7.31 7.29 7.28 7.27 7.27 7.26 7.20 7.19 7.18 7.18 7.17 7.15 7.14 7.14 7.13 7.12 7.11 7.11 7.09 7.08 7.08 7.07 7.06 7.05 7.04 7.04 7.03 3.63 3.61

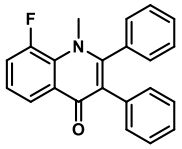


4g

175.61

154.24 154.02 151.55 135.25 134.79 132.43 132.37 131.51 130.06 129.74 129.14 128.57 127.59 126.43 124.48 123.96 123.88 123.13 123.10 119.05 118.82

42.63 42.48



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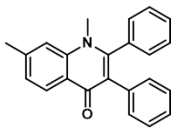

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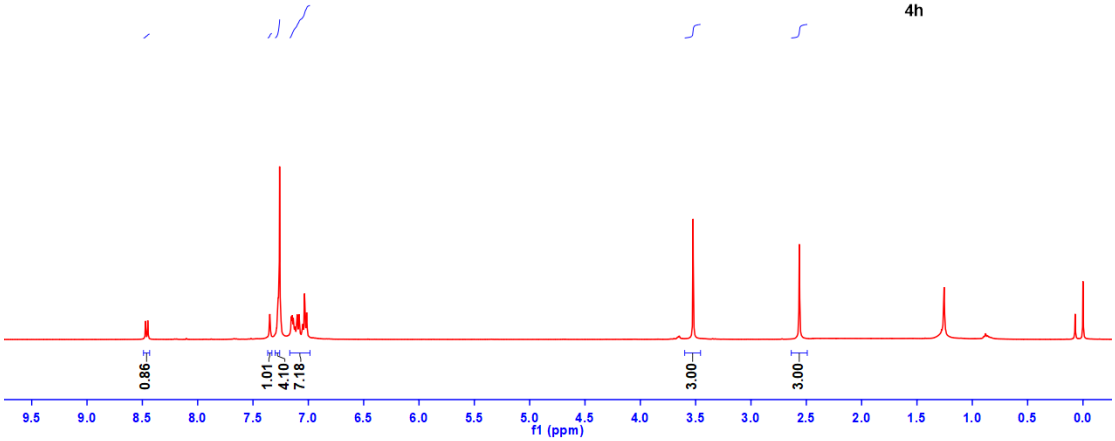

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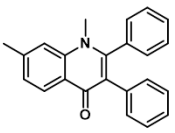

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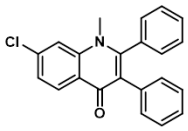

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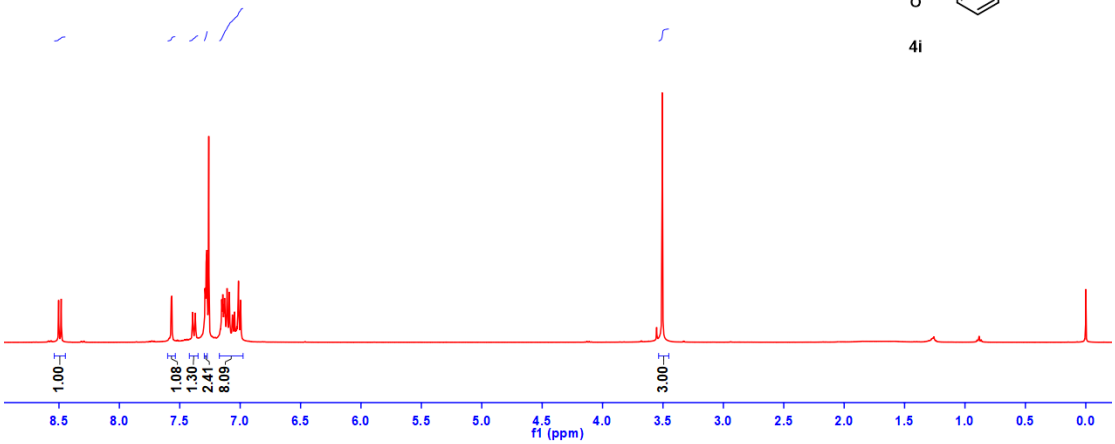

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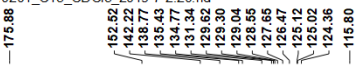

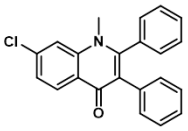

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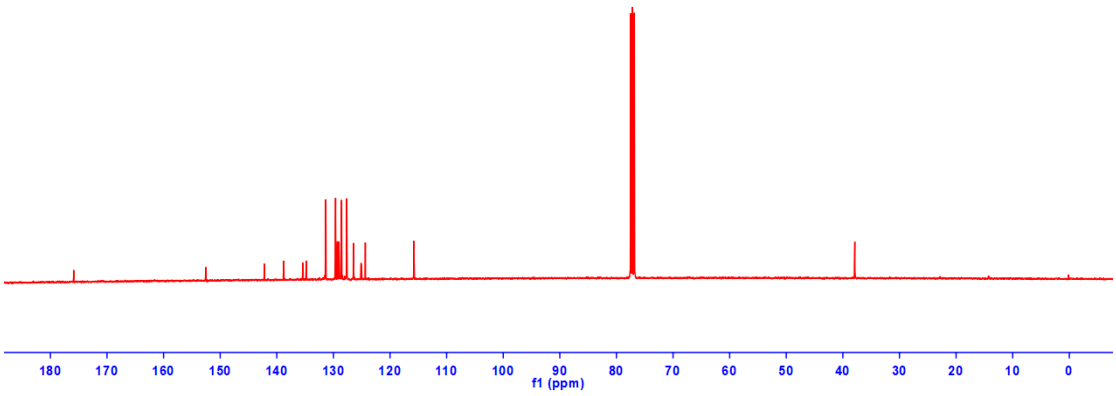

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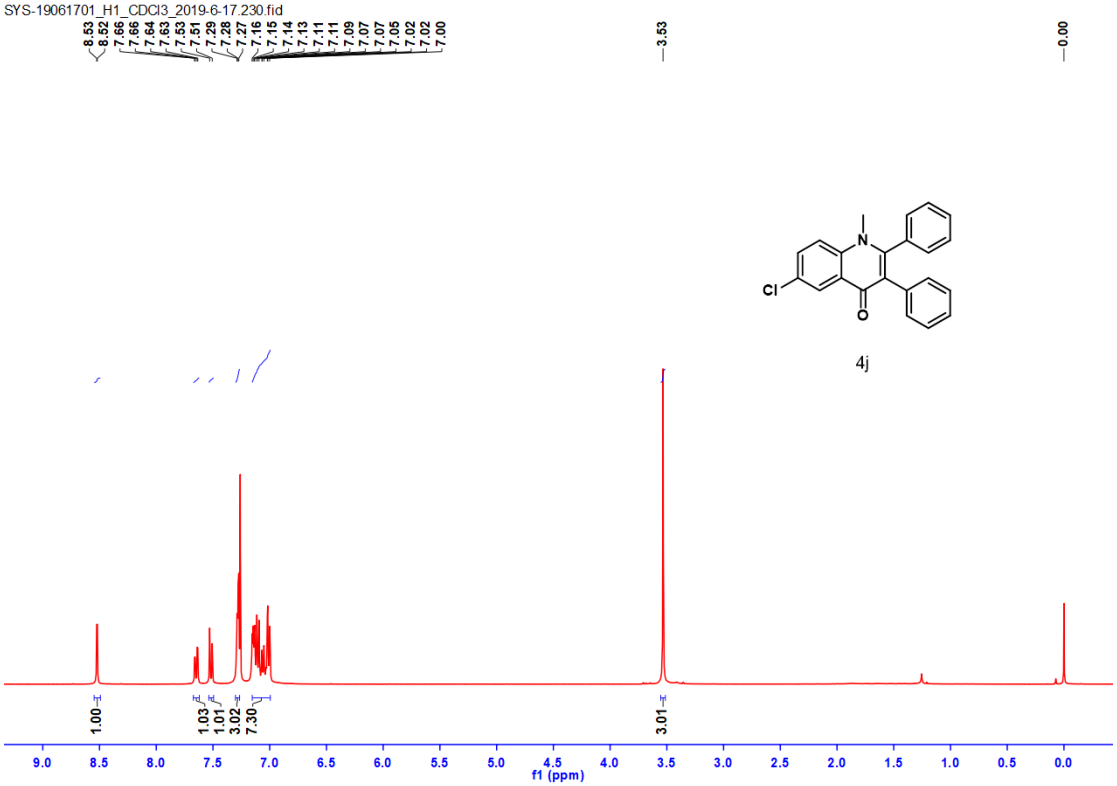

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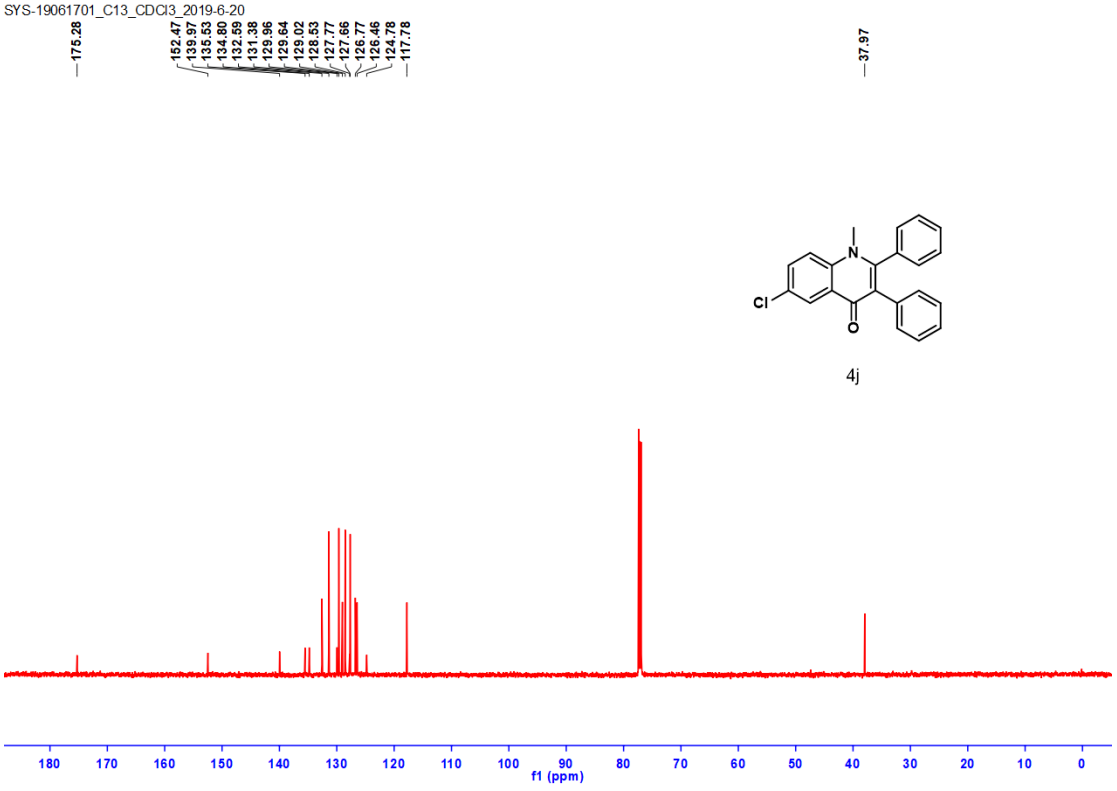

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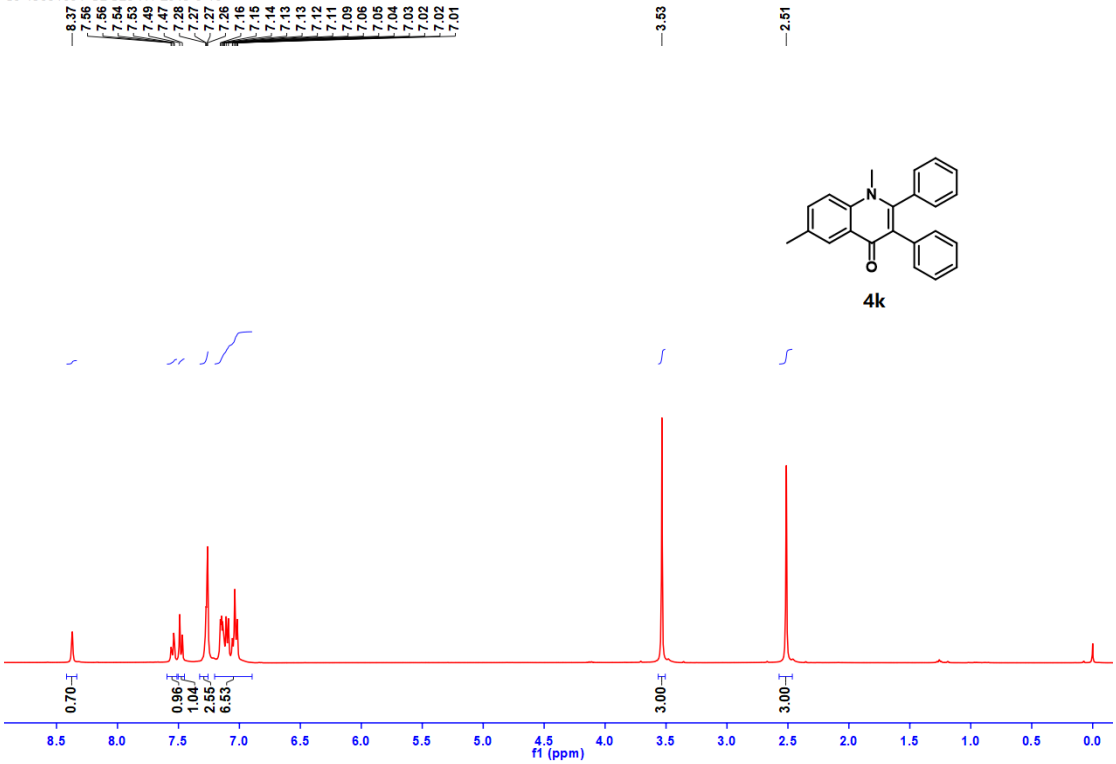

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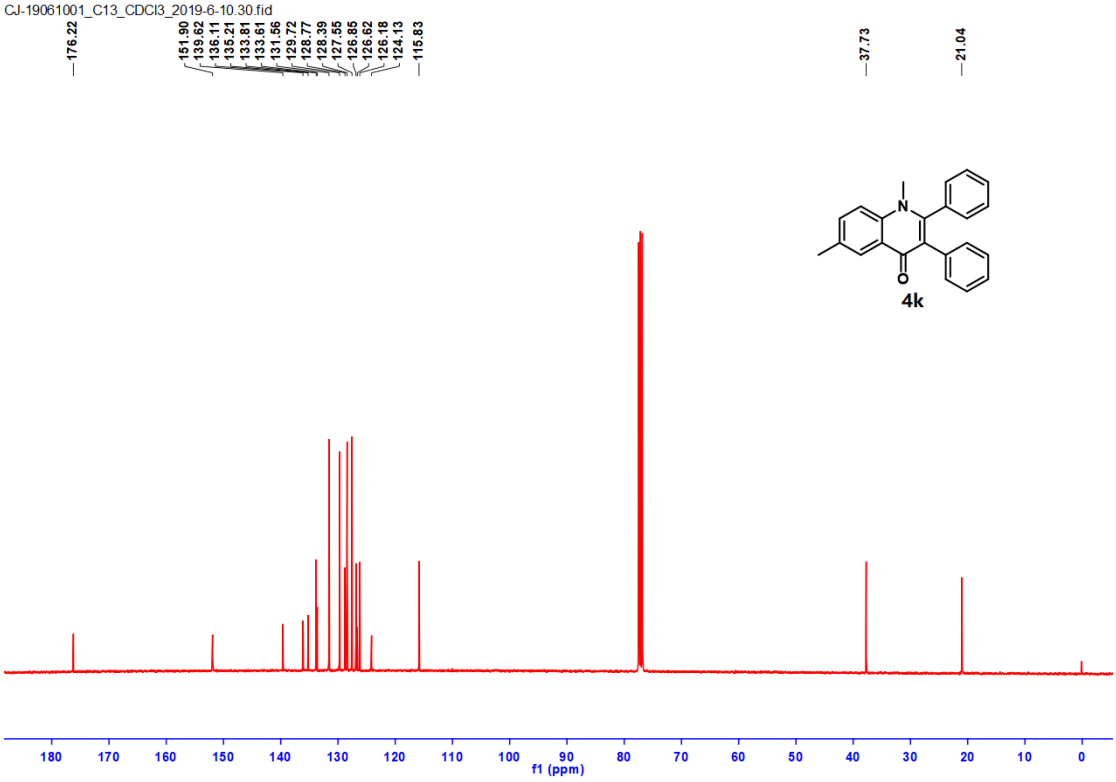

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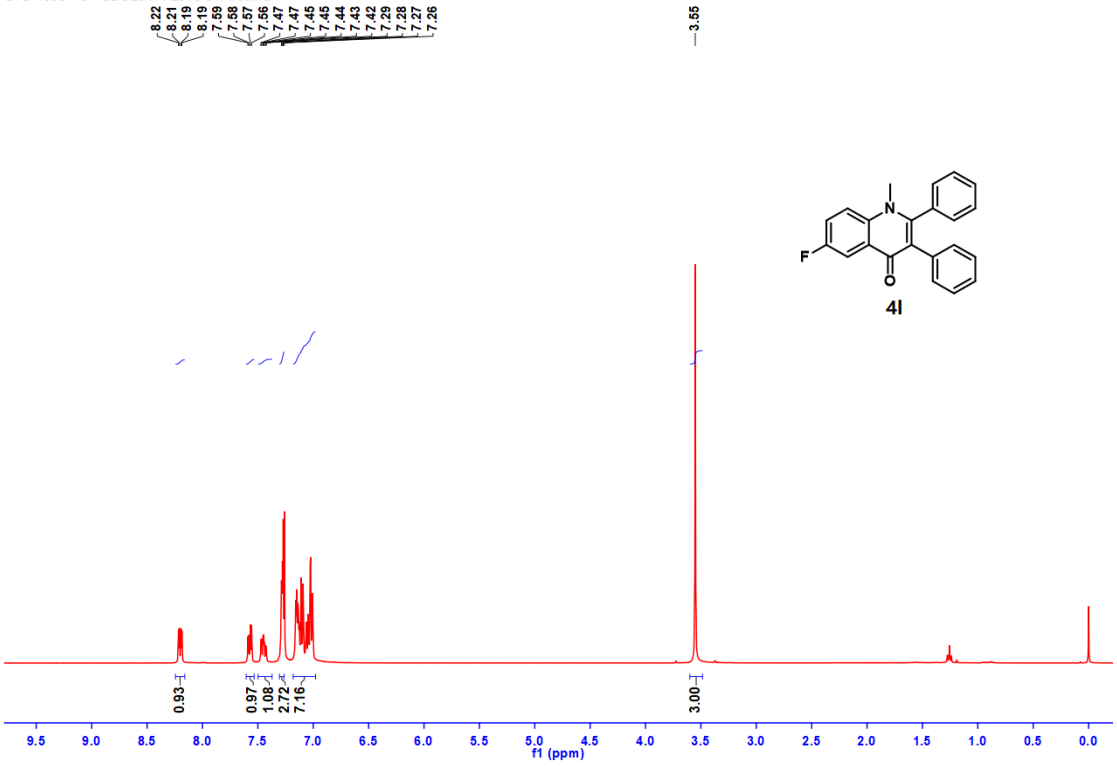

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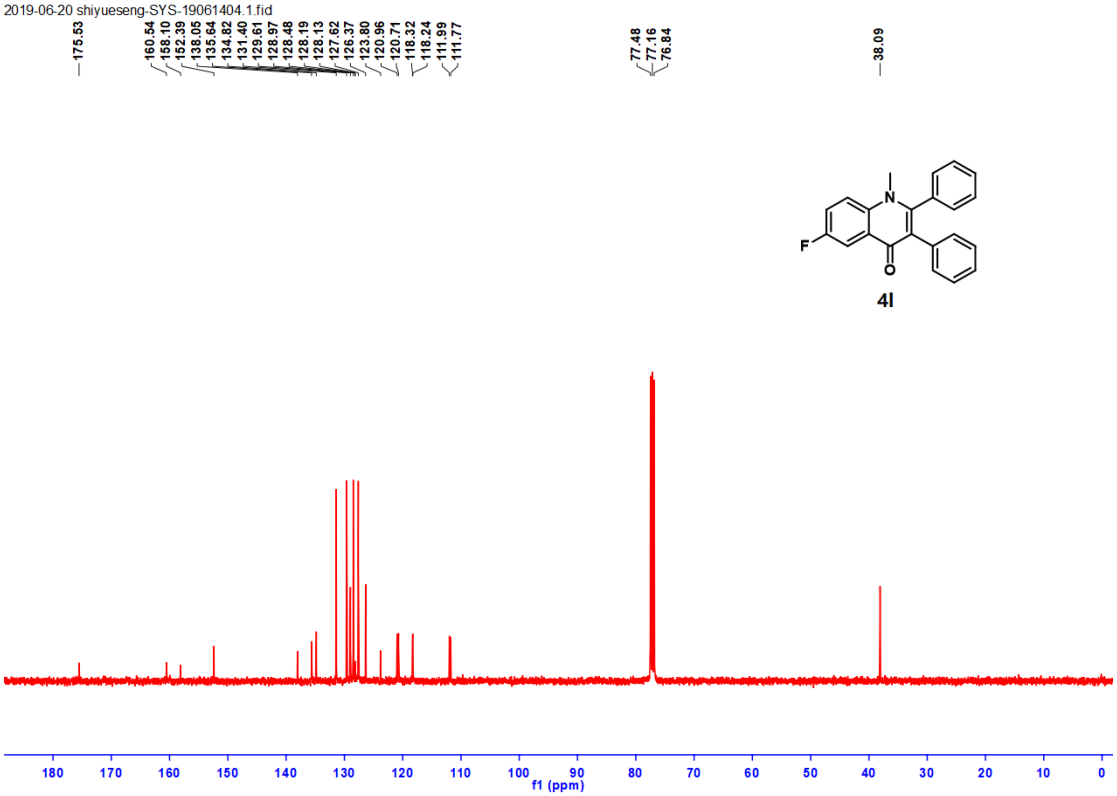
2019-06-20 shiyueseng-SYS-19061404.1.fid



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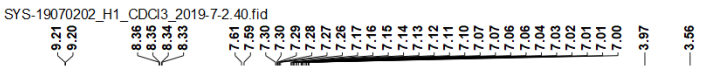

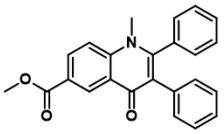

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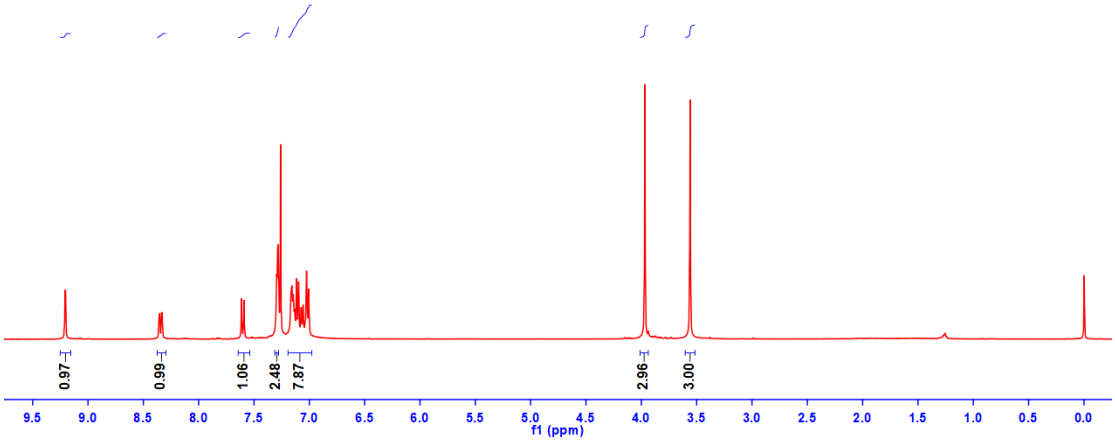

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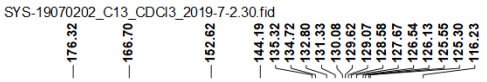

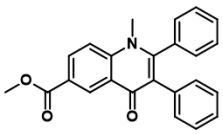

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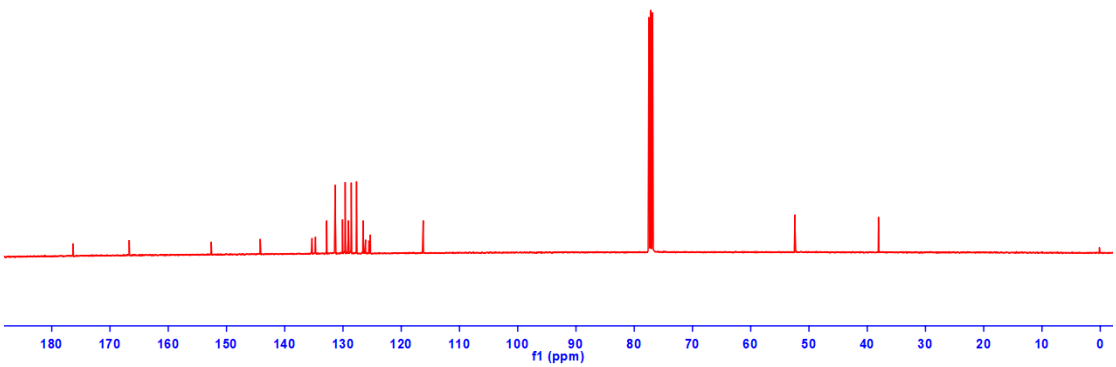

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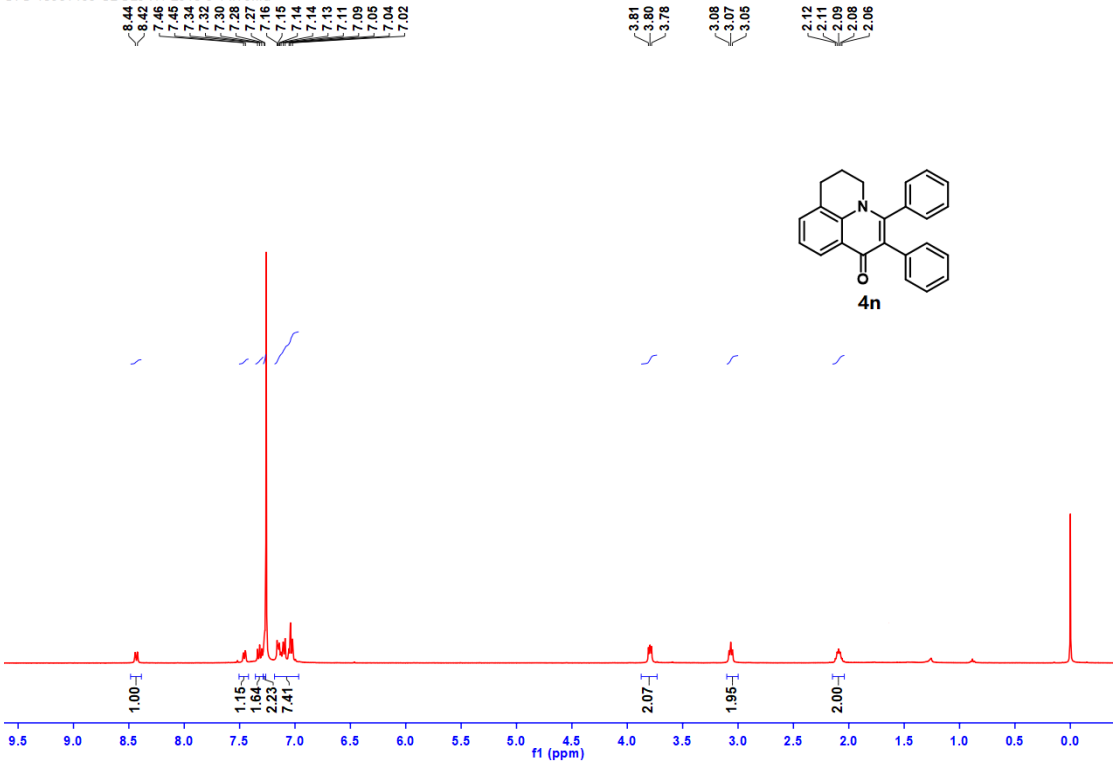

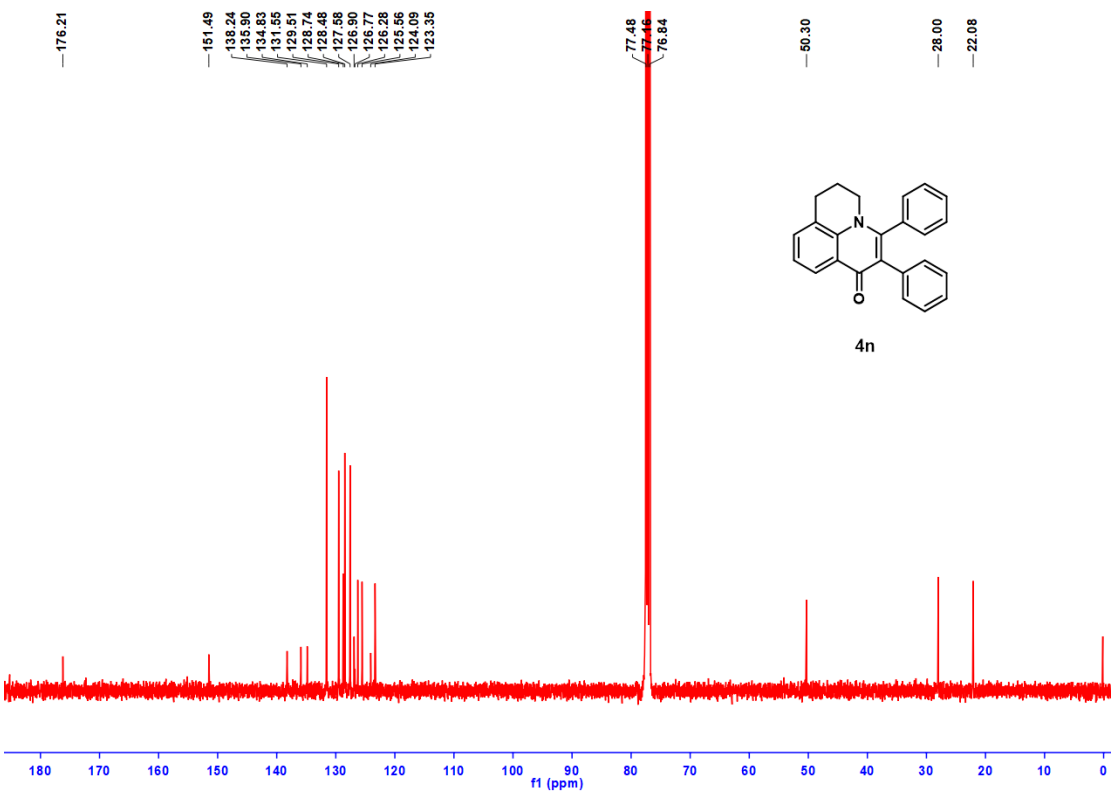

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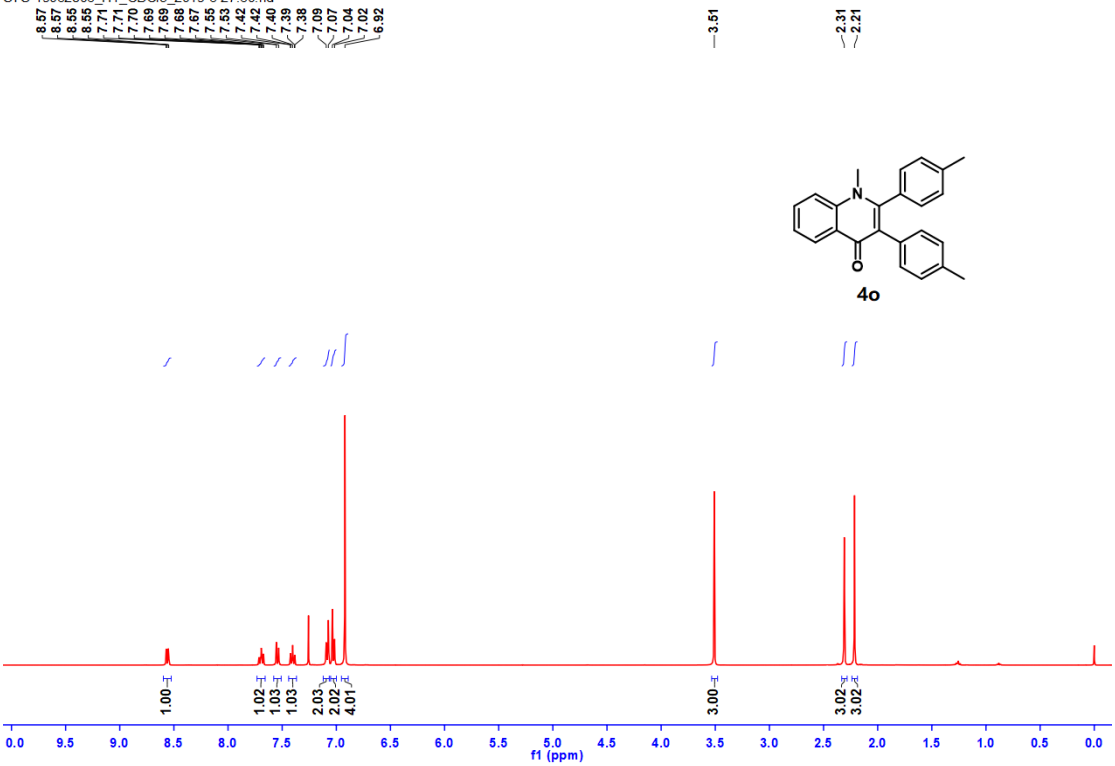

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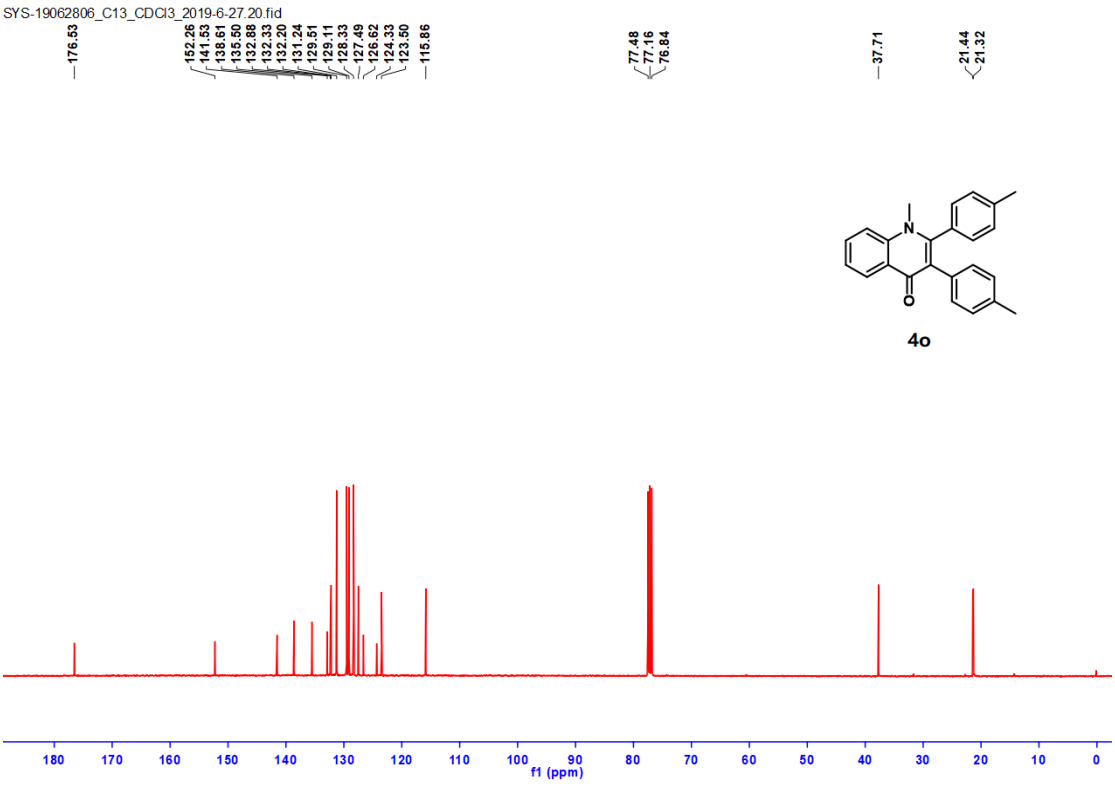

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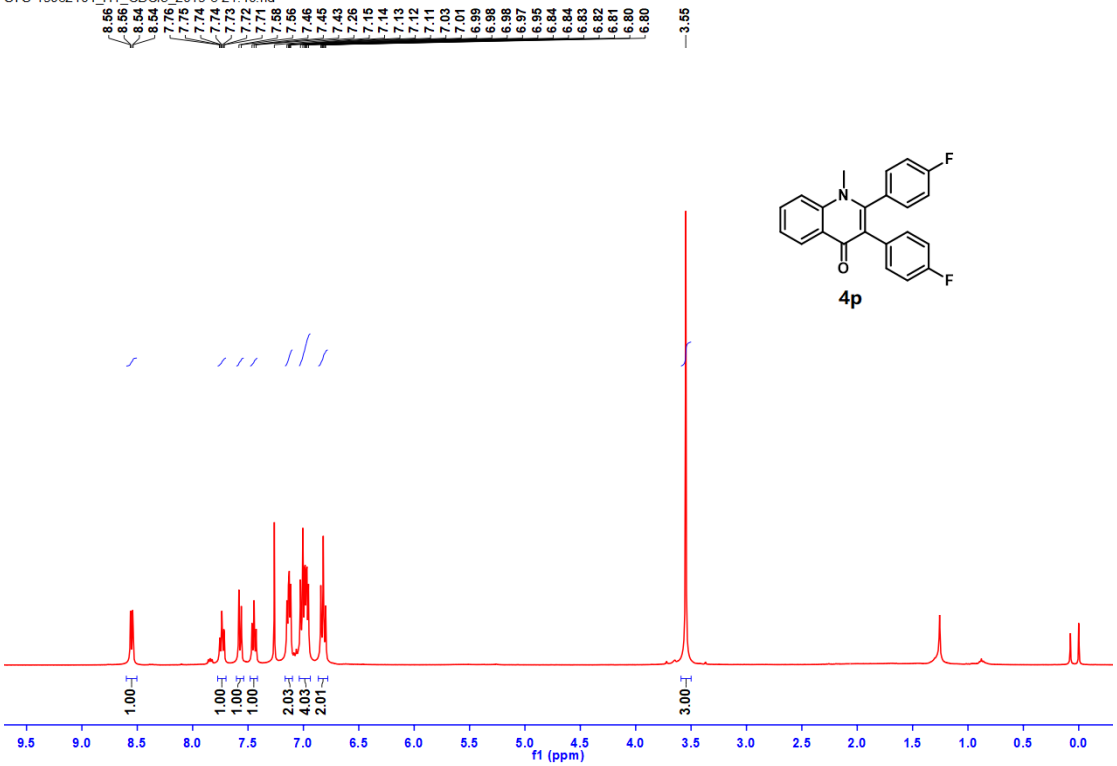

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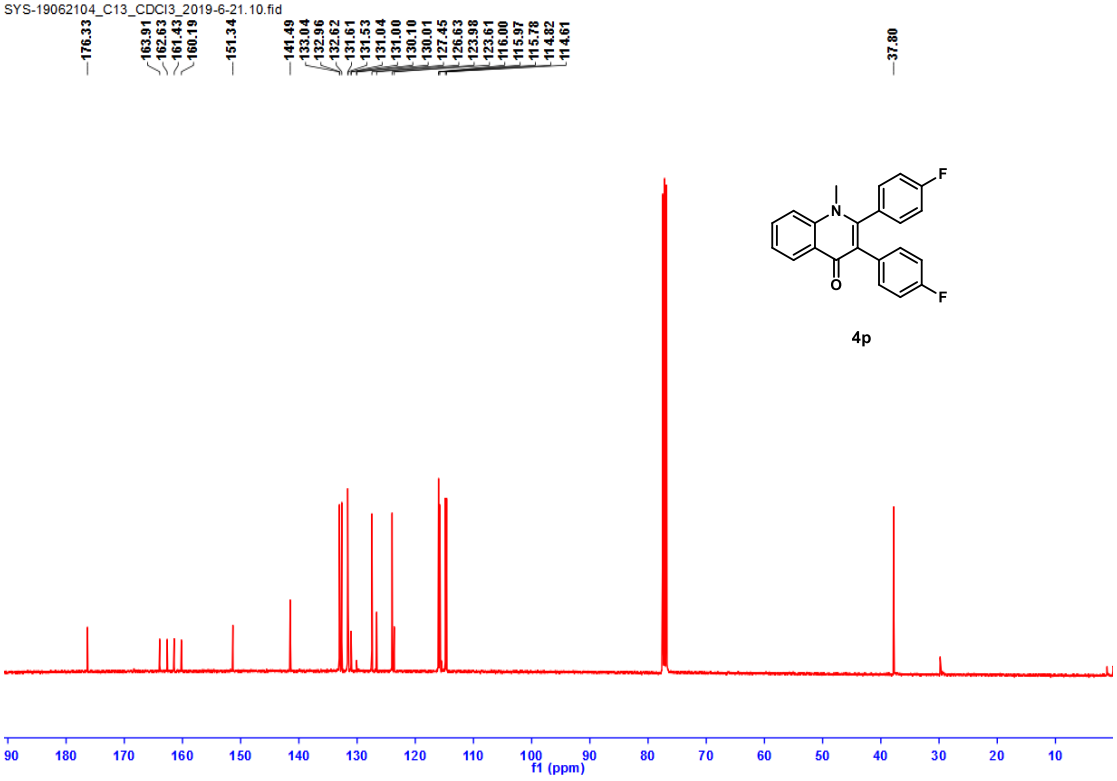

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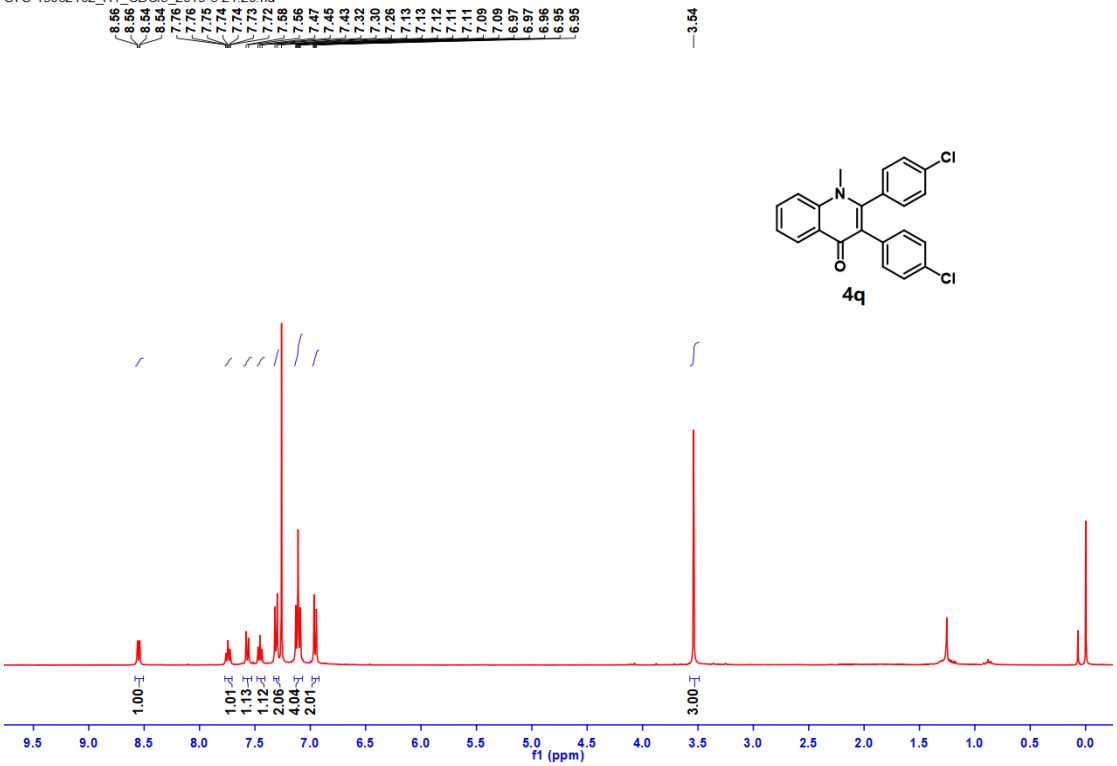

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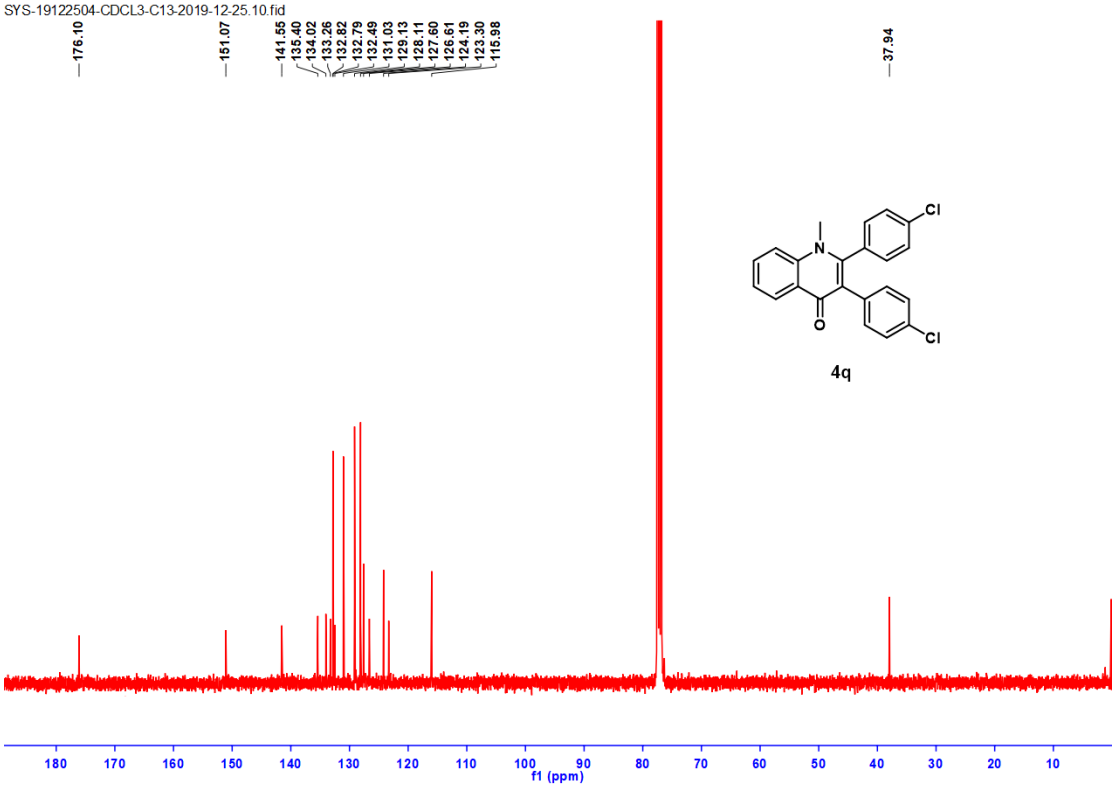
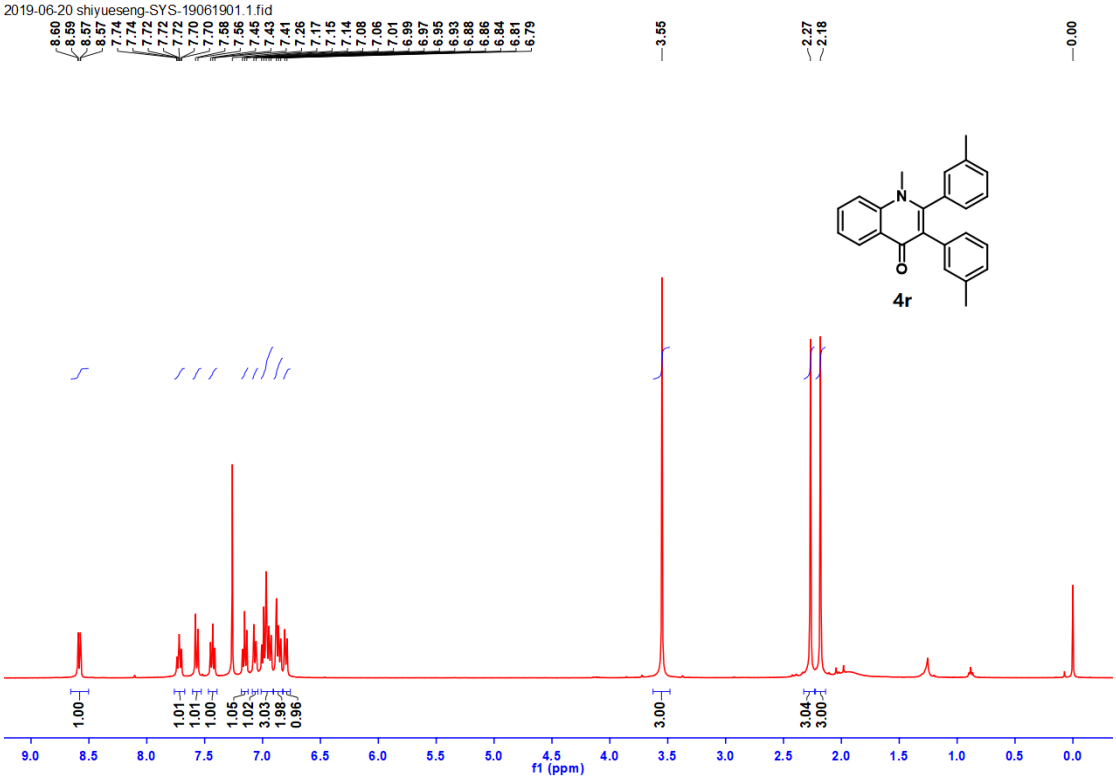


2019-06-20 shiyueseng-SYS-19061901.1.fid



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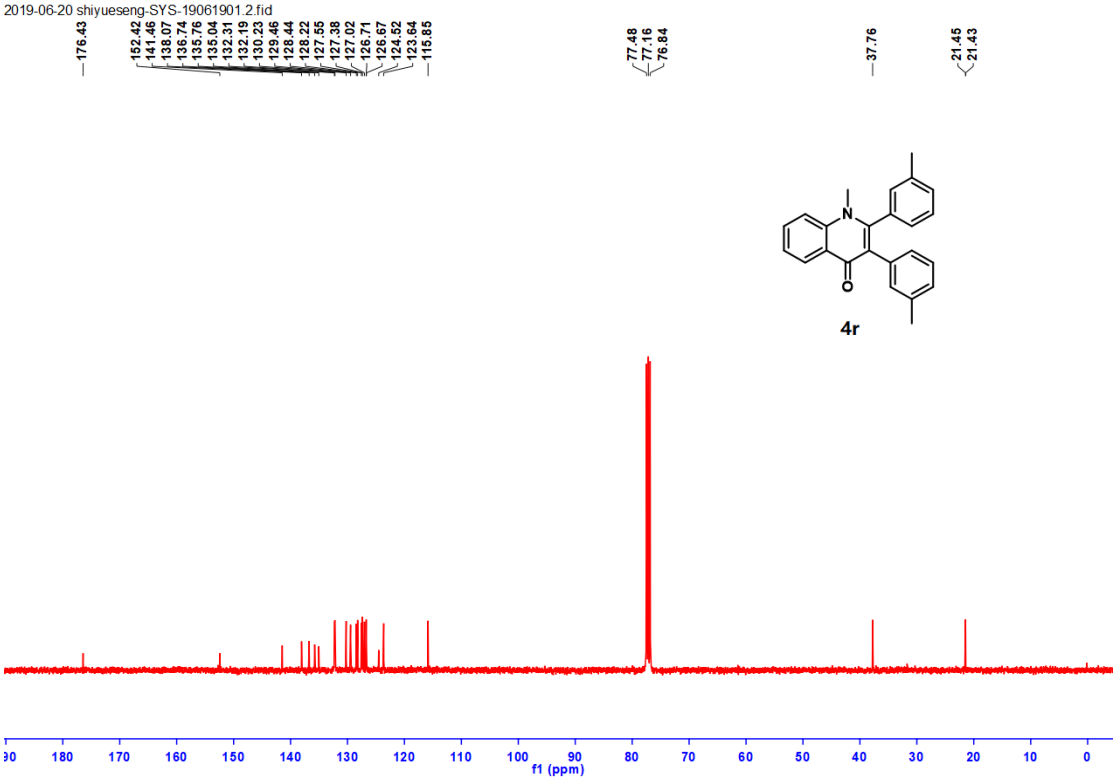

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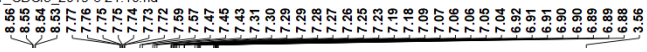

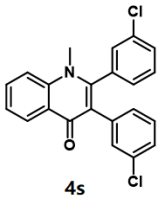

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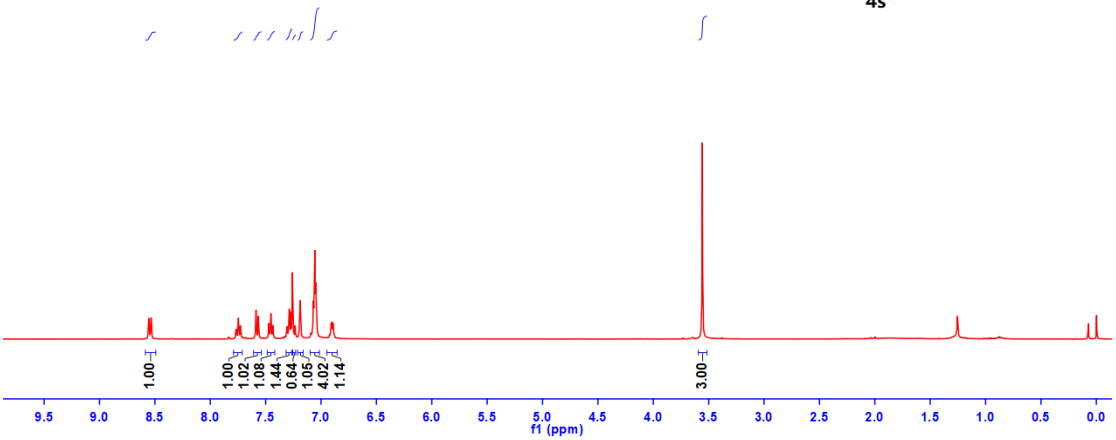

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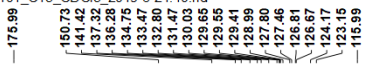

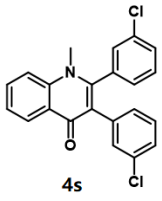

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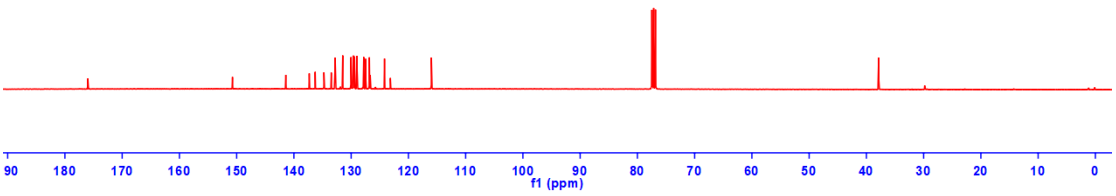

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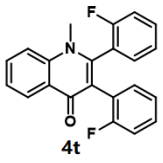

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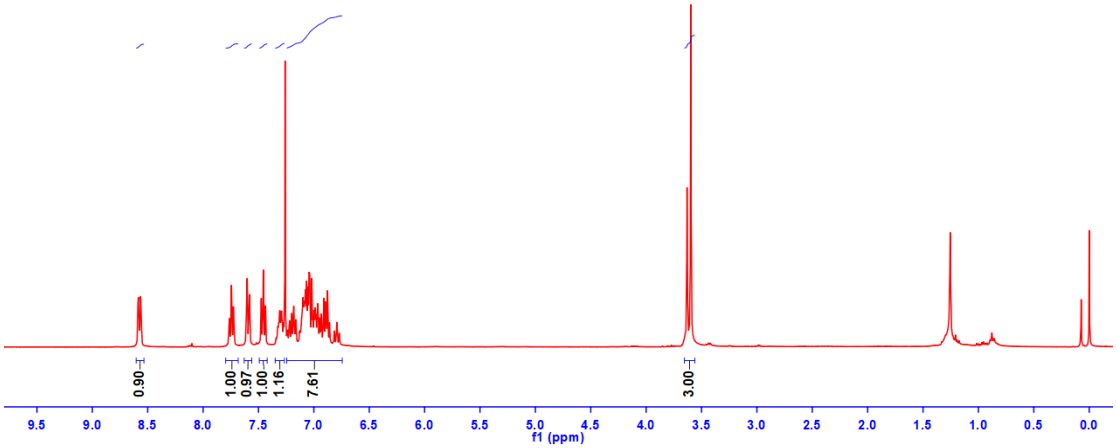

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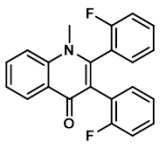

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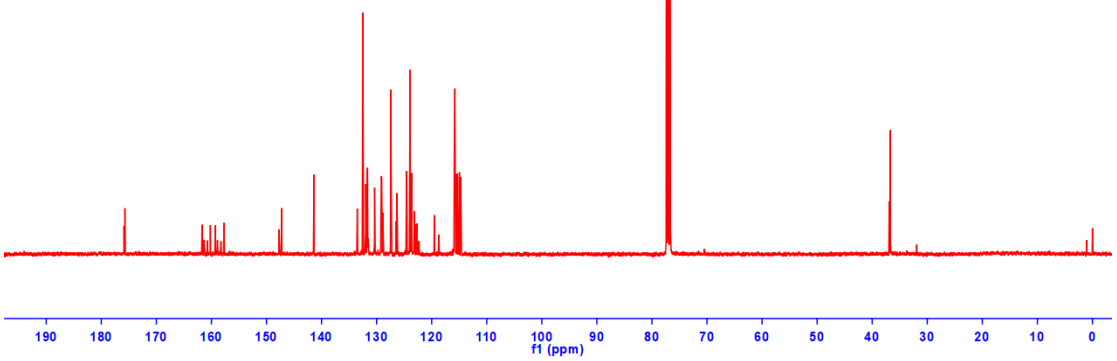

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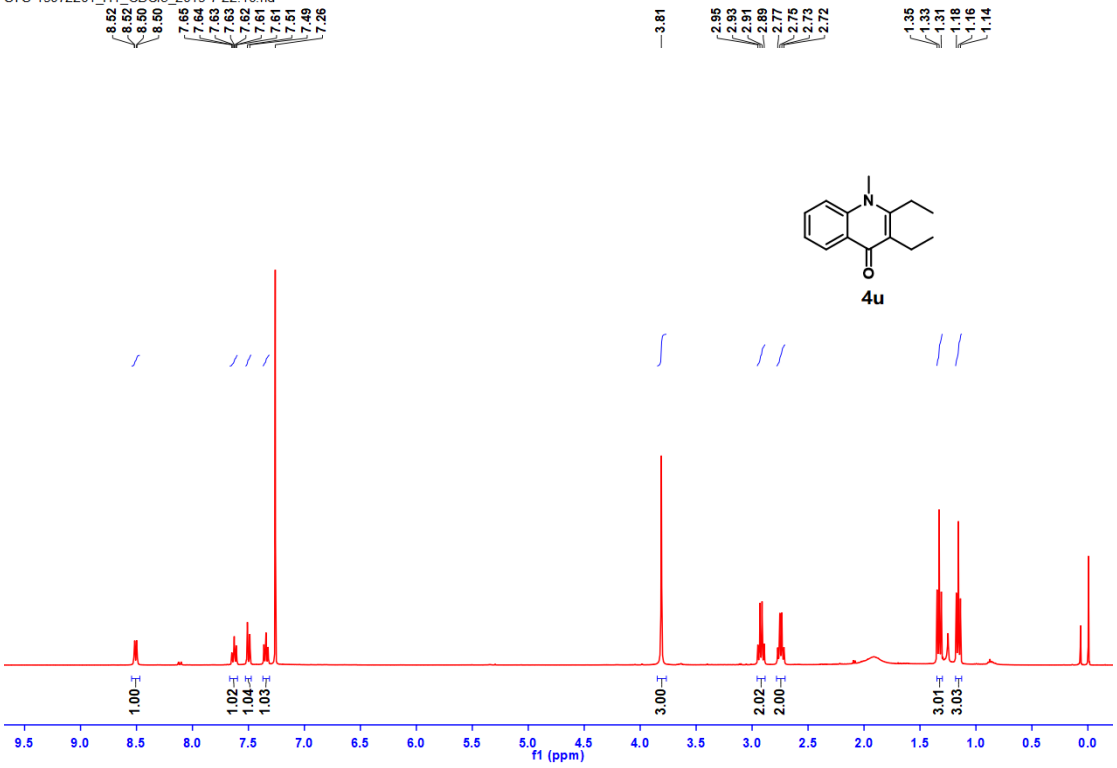

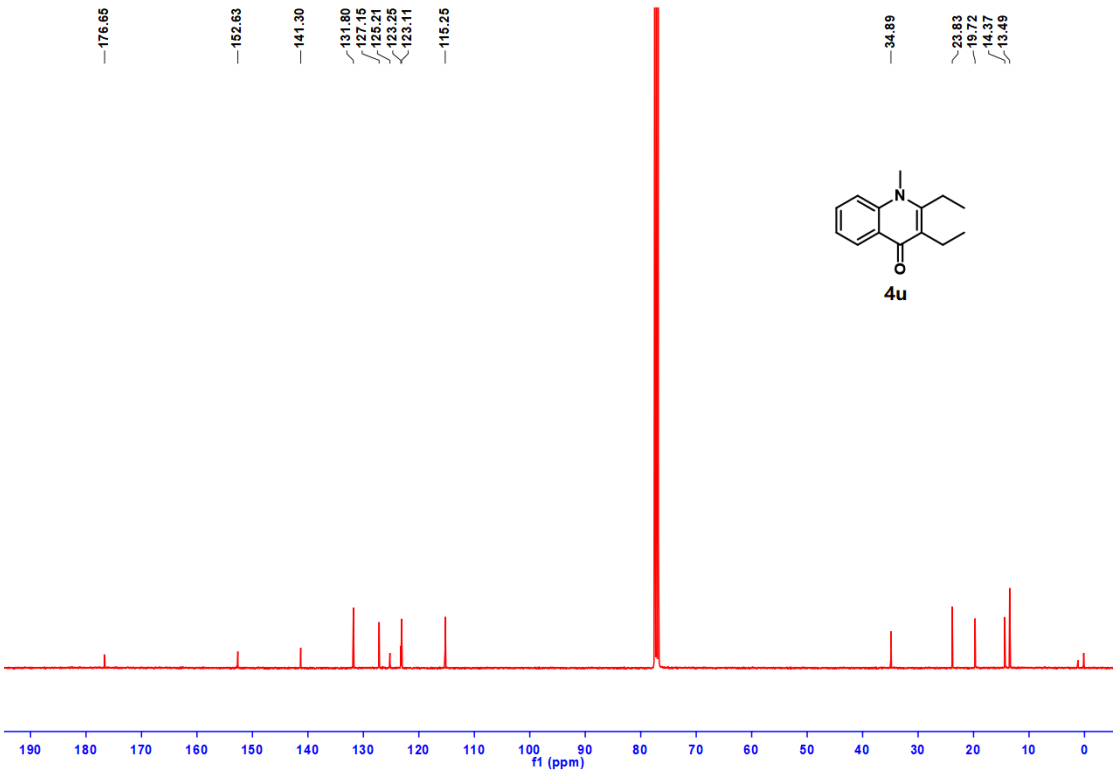

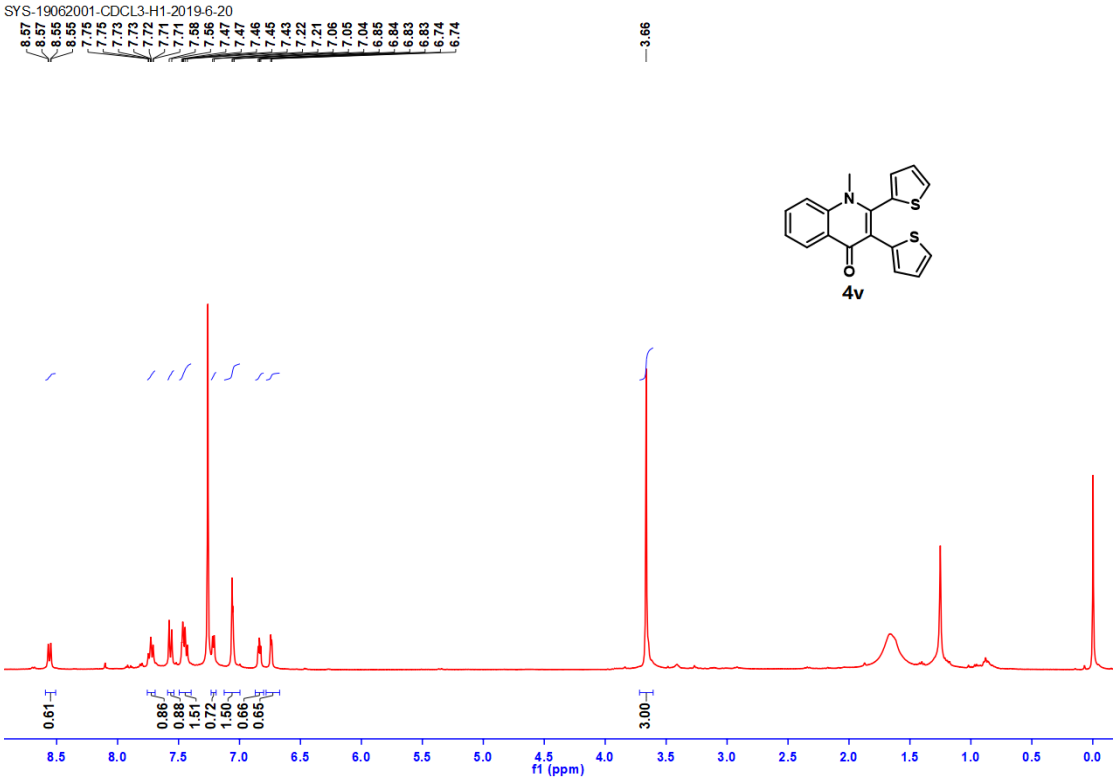
SYS-19062001-CDCL3-H1-2019-6-20
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6.83
6.74
6.74
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4v
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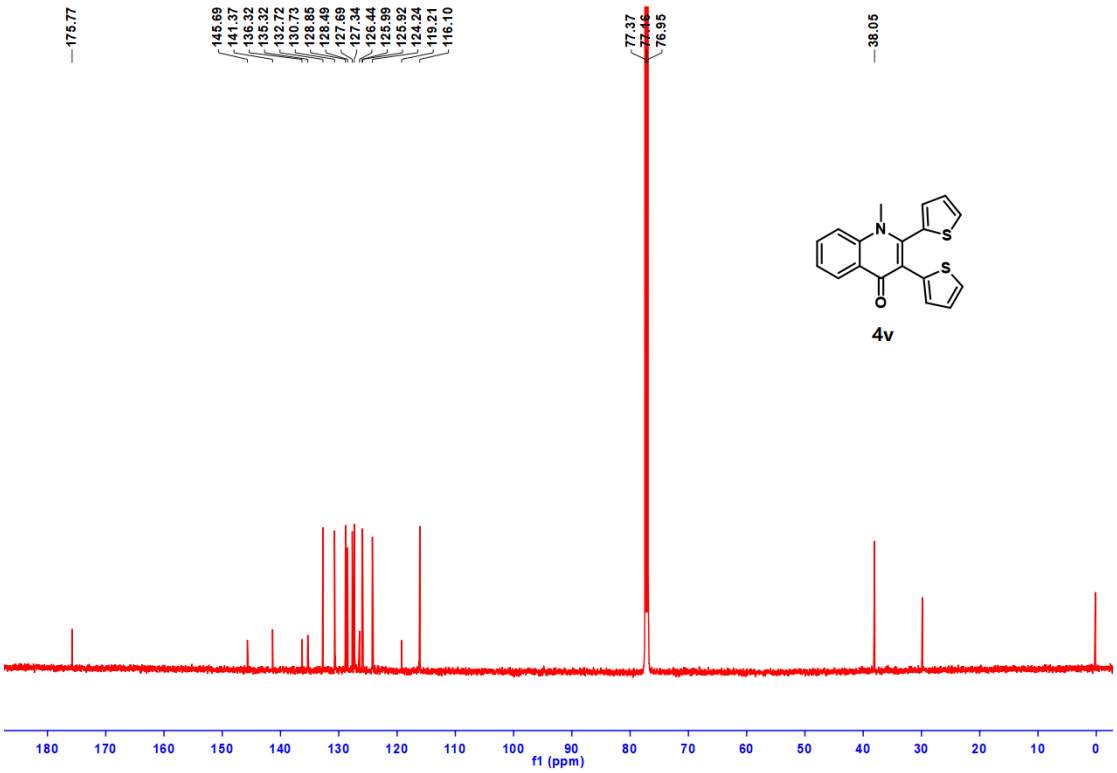
0.72
1.50
0.66
0.65
3.00
f1 (ppm)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125.92
124.24
119.21
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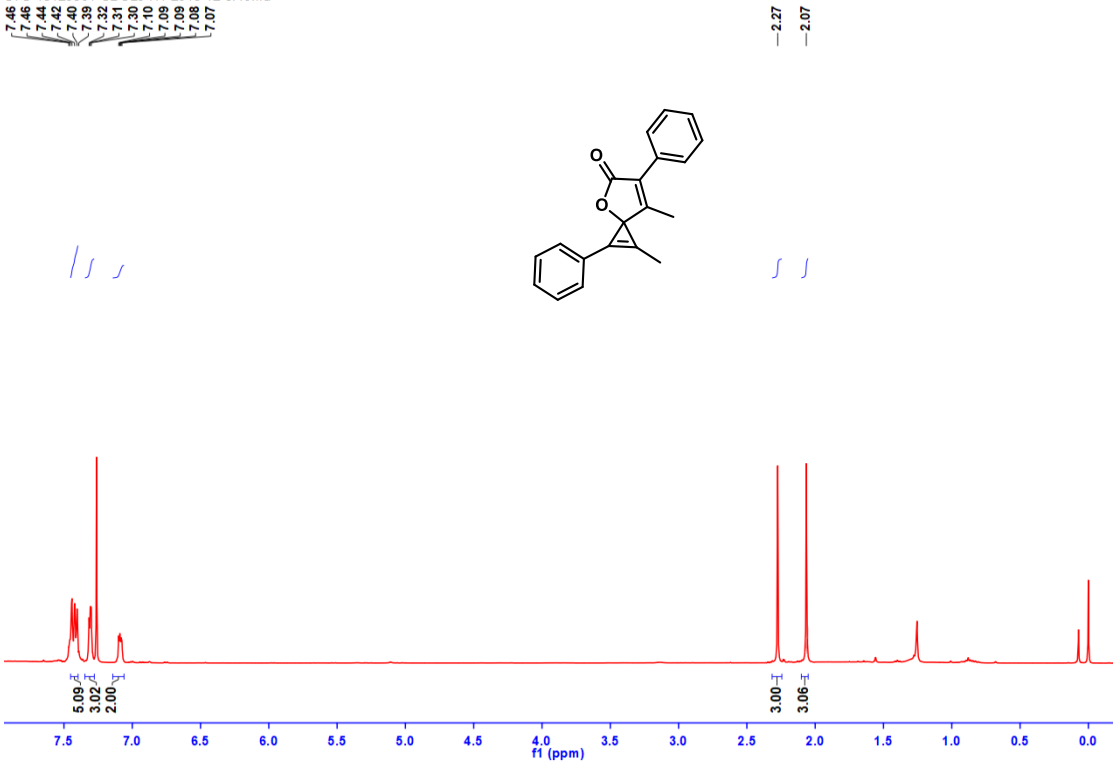
38.05
4v
f1 (ppm)

SYS-19120901-CDCL3-H1-2019-12-9.10.fid



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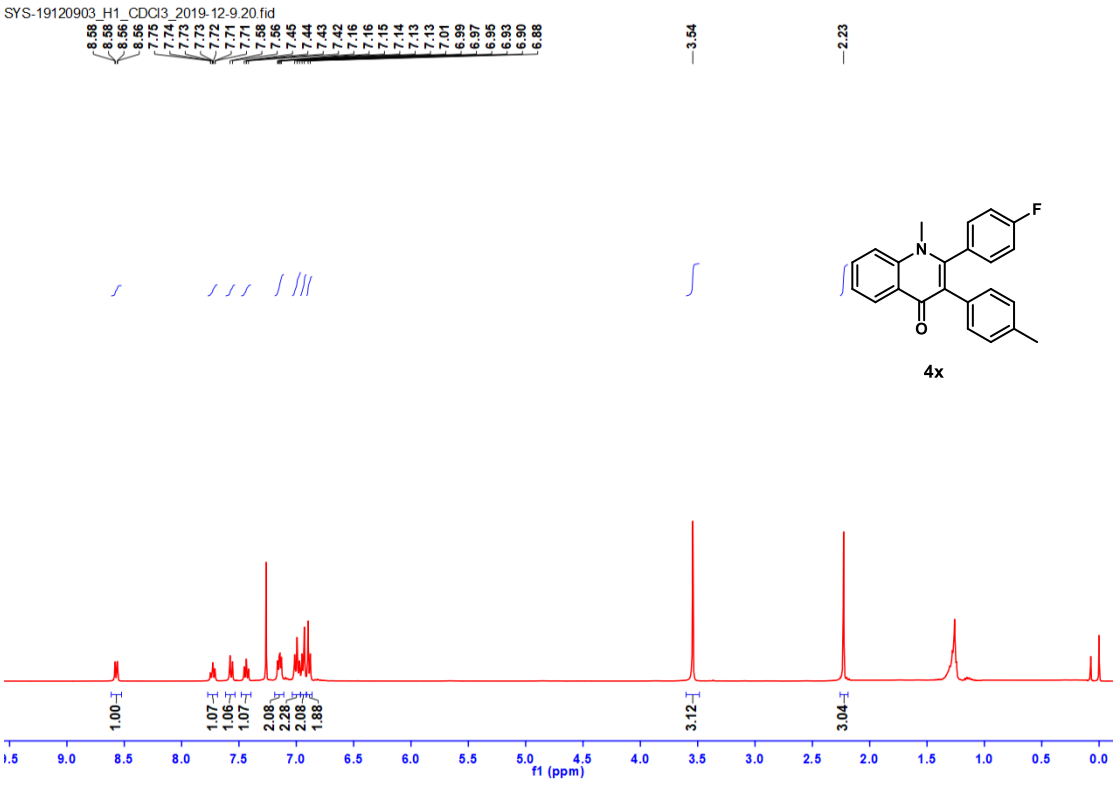
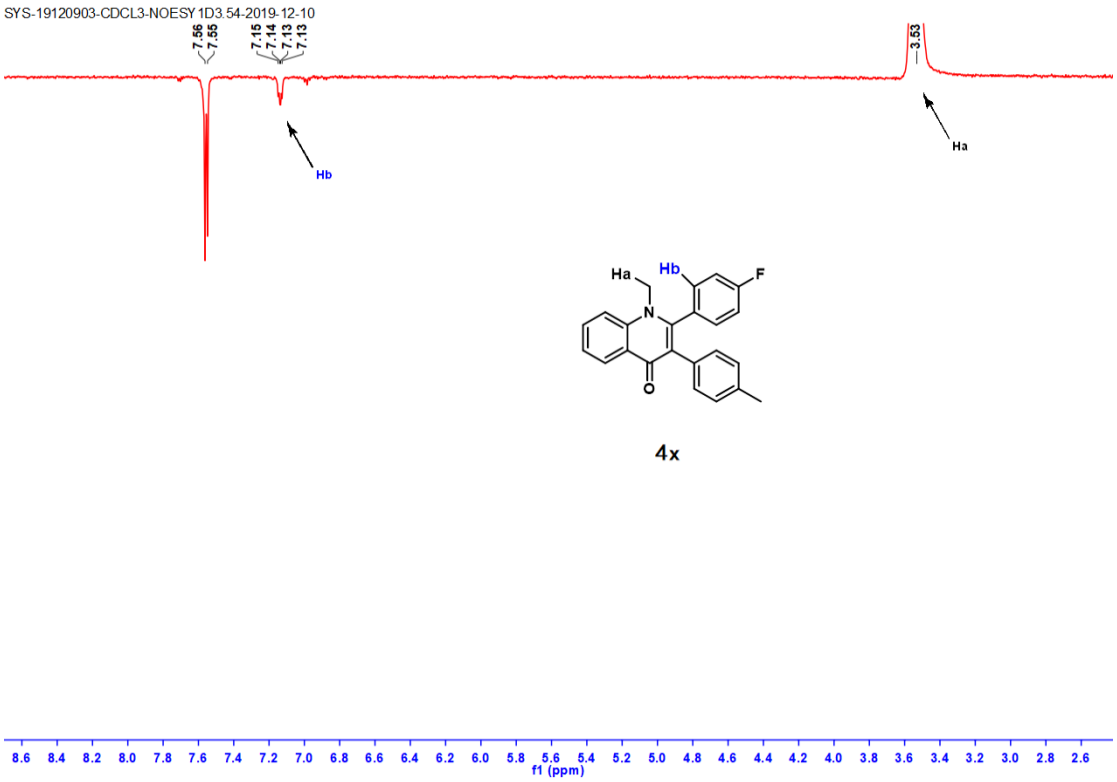
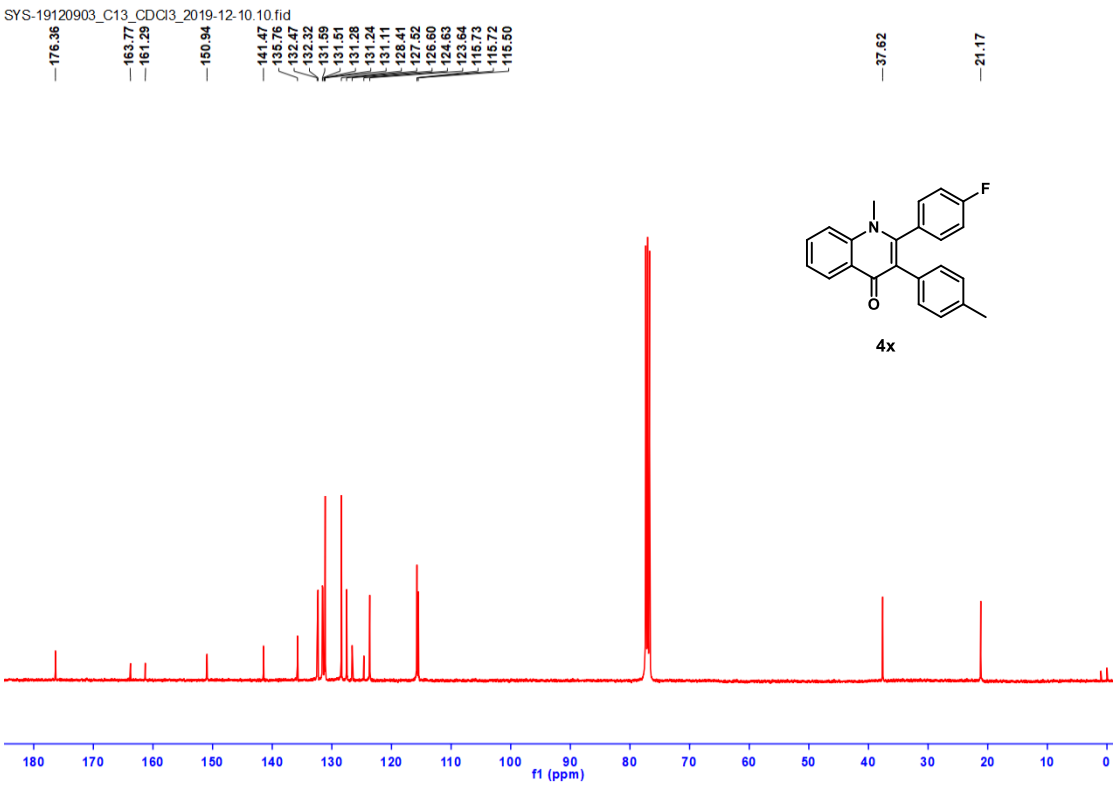


4x


SYS-19120903-CDCL3-NOESY1D3.54-2019-12-10
7.56
7.55
7.15
7.14
7.13
7.13
3.53
Hb
Ha
Ha
Hb
F
N
O

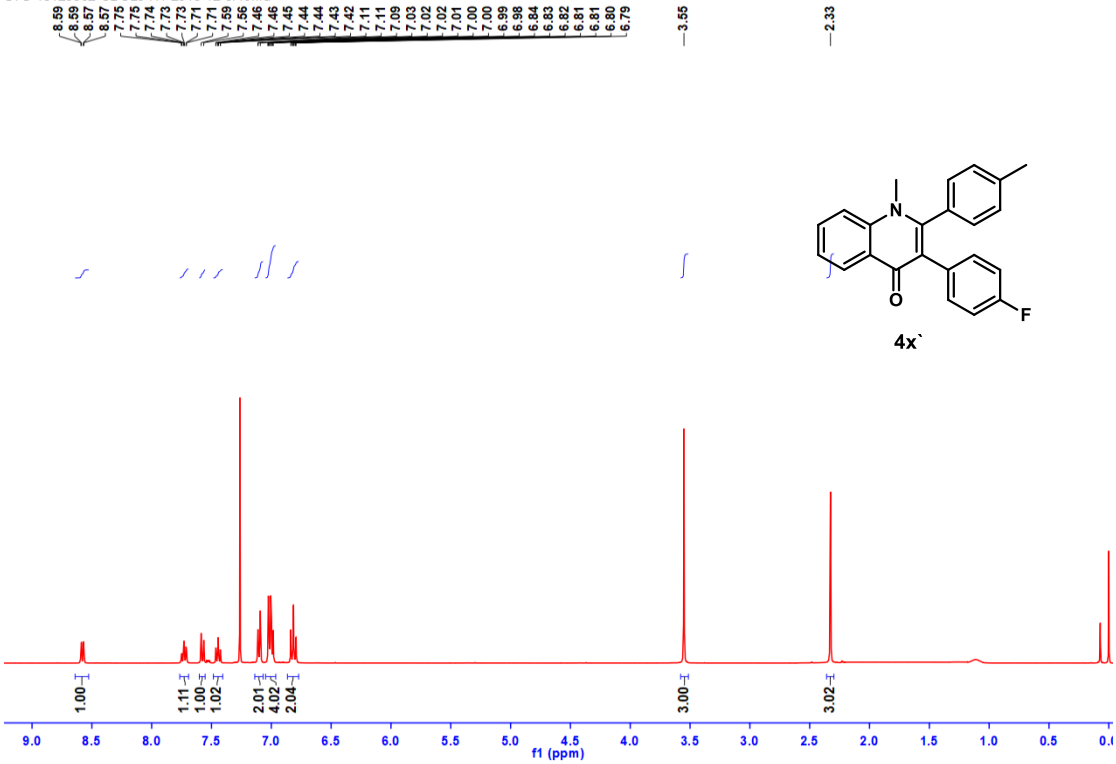
4x

8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6
f1 (ppm)


SYS-19120903_C13_CDCl3_2019-12-10.10.fid
176.36
163.77
161.29
150.94
141.47
135.76
132.47
132.32
131.69
131.51
131.28
131.24
131.11
128.41
127.52
126.60
124.63
123.64
115.73
115.72
115.50
37.62
21.17
F
N
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

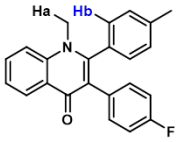
4x

SYS-19120902-CDCL3-H1-2019-12-9.10.fid

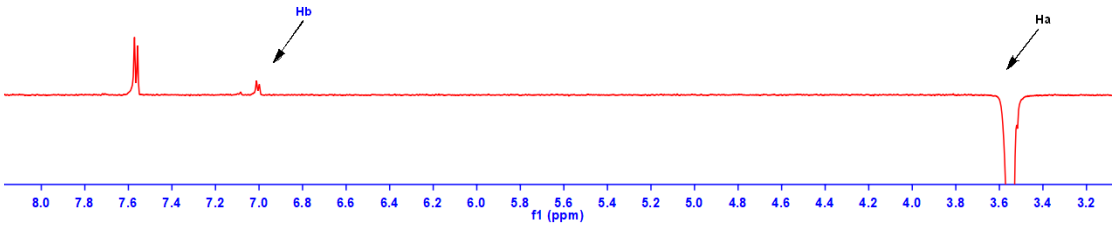


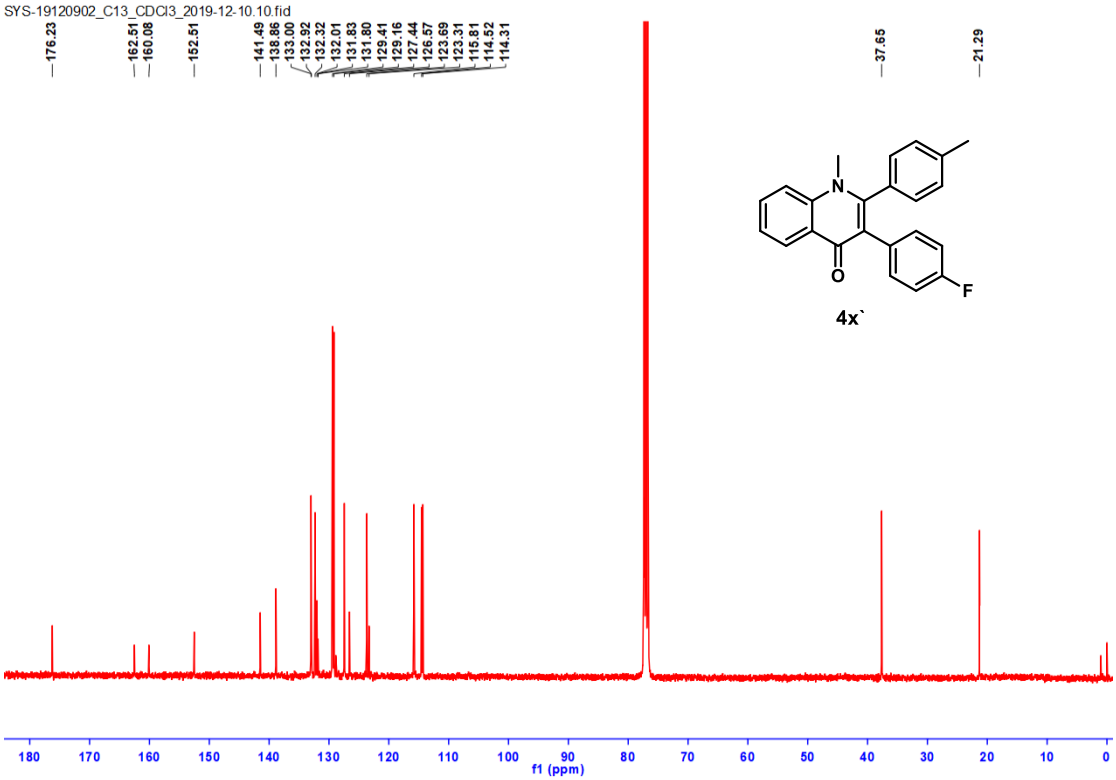
4x`

SYS-19120902-CDCL3-NOESY1D3.55-2019-12-10

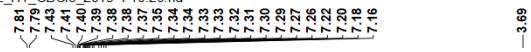


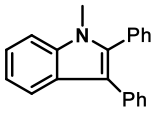
4x`



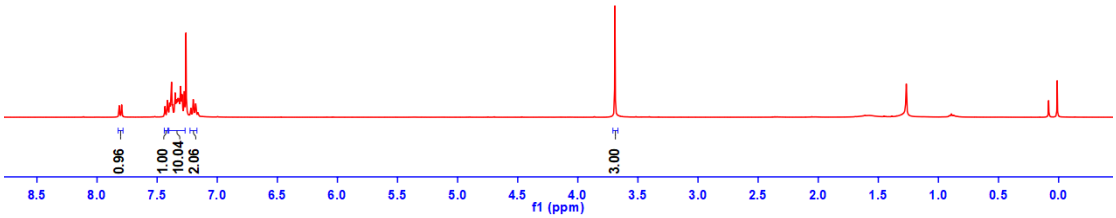

SYS-19120902_C13_CDCl3_2019-12-10.10.fid
176.23
162.51
160.08
152.51
141.49
138.86
133.00
132.92
132.32
132.01
131.83
131.80
129.41
129.16
127.44
126.57
123.69
123.31
115.81
114.52
114.31
37.65
21.29
N
O
F
4x`
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

SYS-19041002_H1_CDCl3_2019-4-10.20.fid

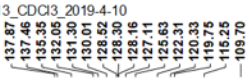


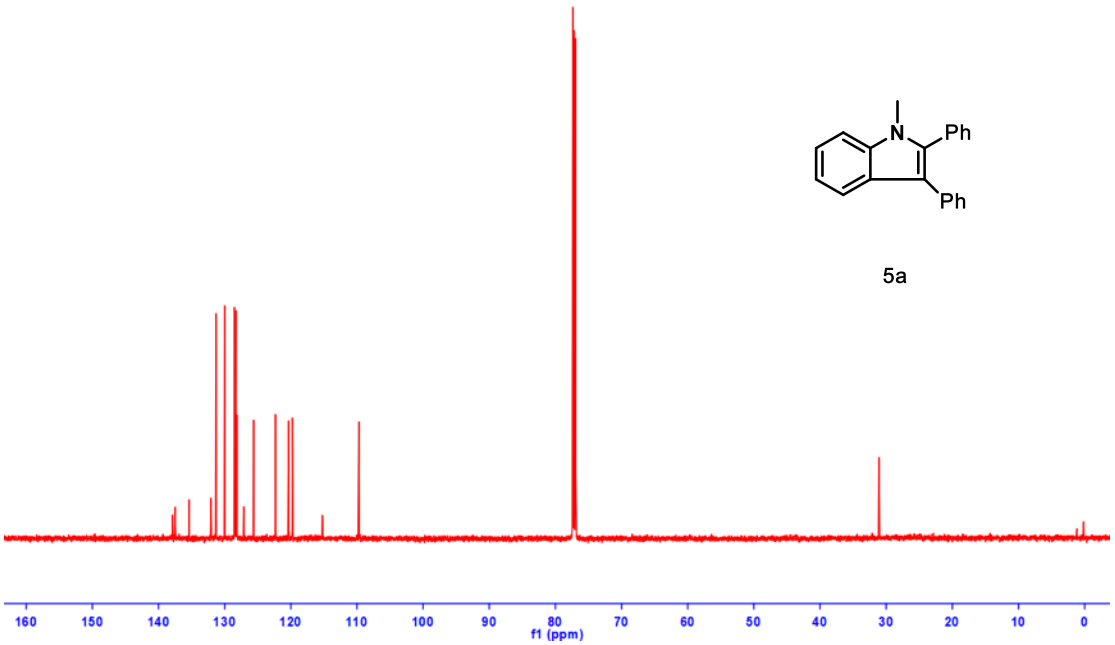


5a

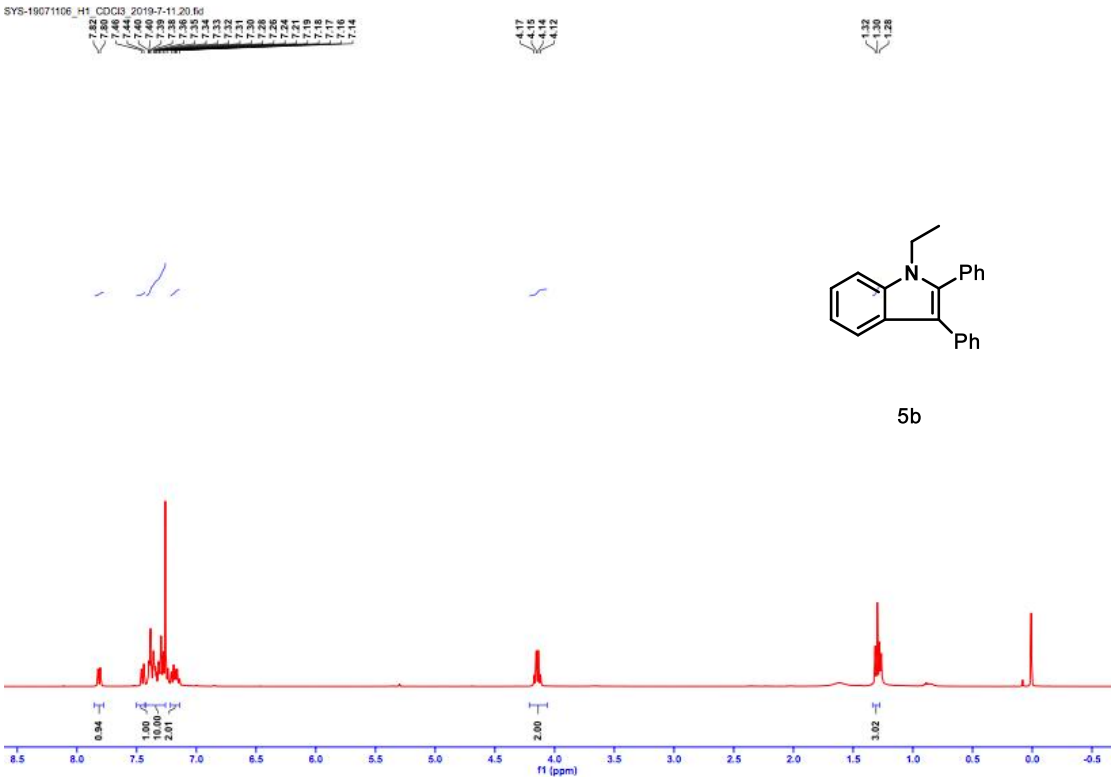


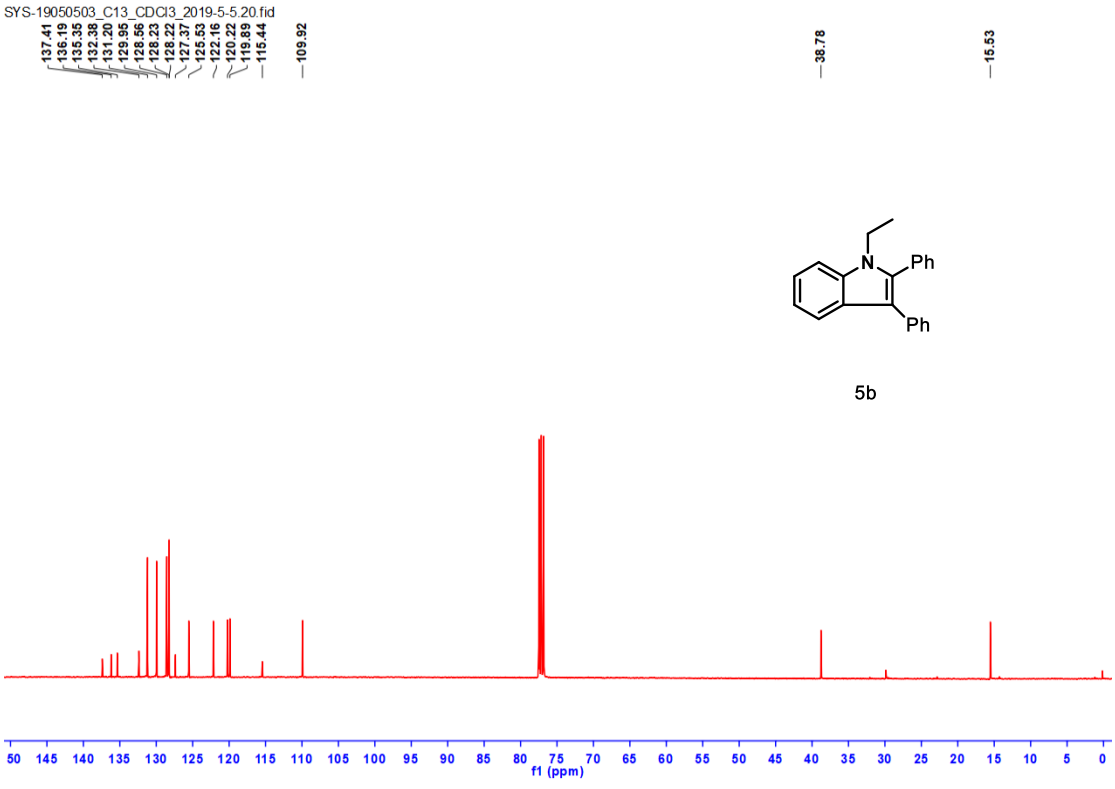
SYS-19041002_C13_CDCl3_2019-4-10

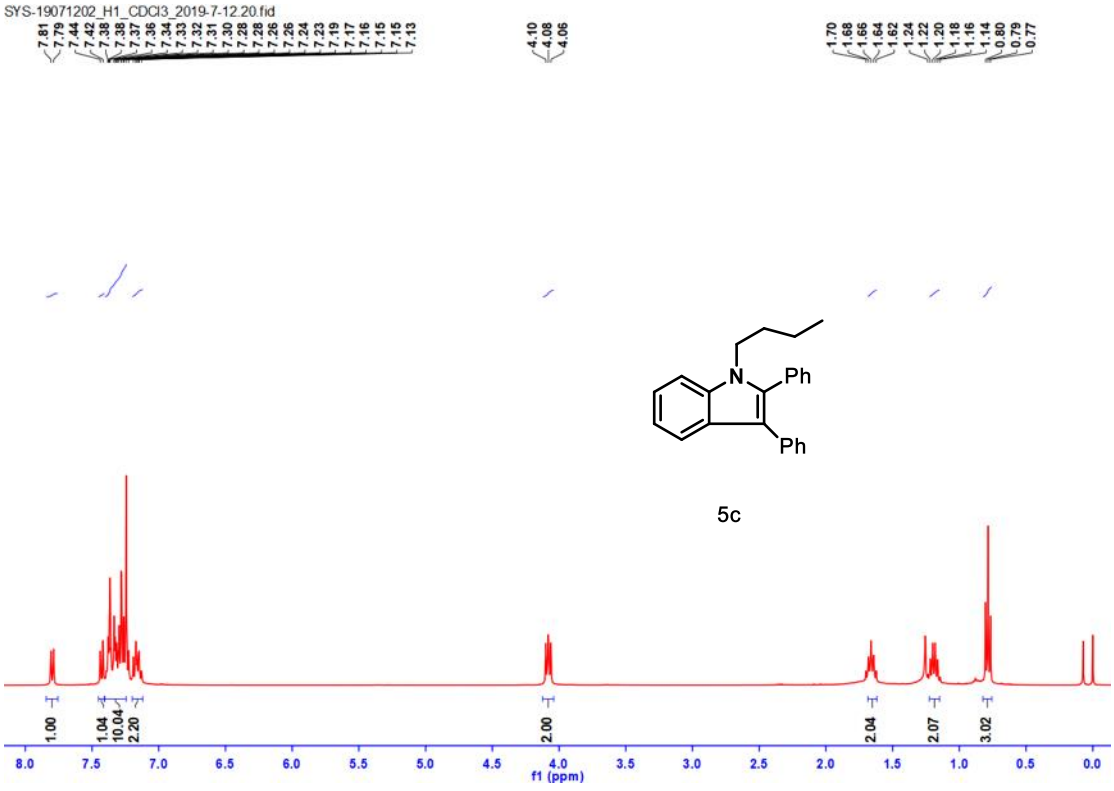


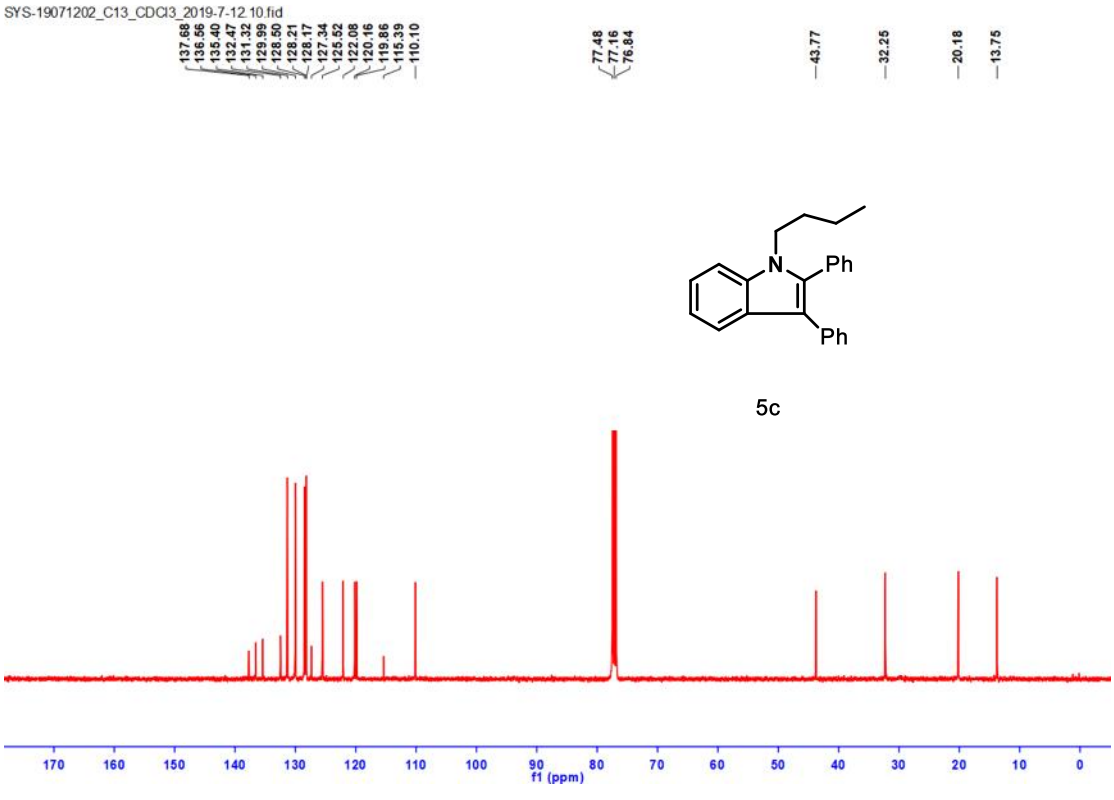


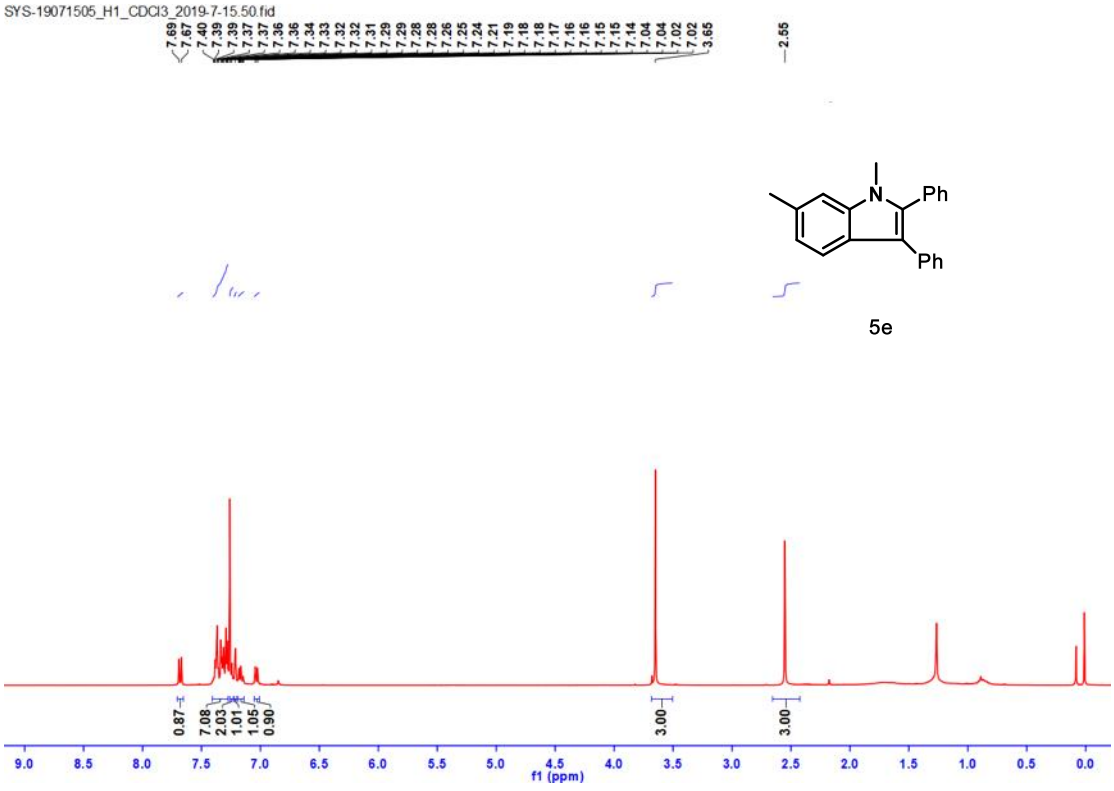
5a


SYS-19071106_H1_CDCl3_2019-7-11.20.fid
7.82
7.80
7.46
7.44
7.40
7.39
7.38
7.36
7.35
7.34
7.33
7.32
7.31
7.30
7.28
7.26
7.24
7.21
7.19
7.18
7.17
7.16
7.14
4.17
4.15
4.14
4.12
1.32
1.30
1.28
N
Ph
Ph
5b
0.84
1.00
10.00
2.01
2.00
3.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

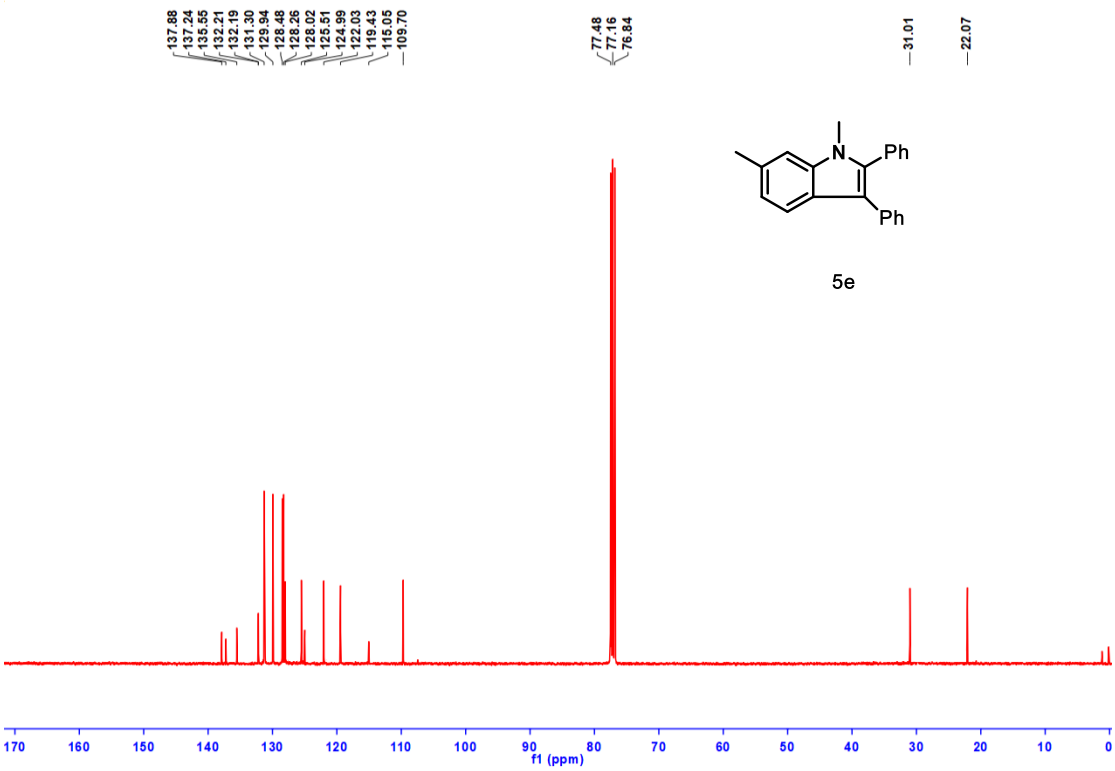

SYS-19050503_C13_CDCl3_2019-5-5.20.fid
137.41
136.19
135.35
132.38
131.20
129.95
128.56
128.23
128.22
127.37
125.53
122.16
120.22
119.89
115.44
109.92
38.78
15.53
N
Ph
Ph
5b
50
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


SYS-19071202_H1_CDCl3_2019-7-12 20.fid
7.81 7.79 7.44 7.42 7.38 7.38 7.37 7.36 7.34 7.33 7.32 7.31 7.30 7.28 7.28 7.26 7.24 7.23 7.19 7.17 7.16 7.15 7.15 7.13
4.10 4.08 4.06
1.70 1.68 1.66 1.64 1.62 1.24 1.22 1.20 1.18 1.16 1.14 0.80 0.79 0.77
N
Ph
Ph
5c
1.00 1.04 10.04 2.20 2.00 2.04 2.07 3.02
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

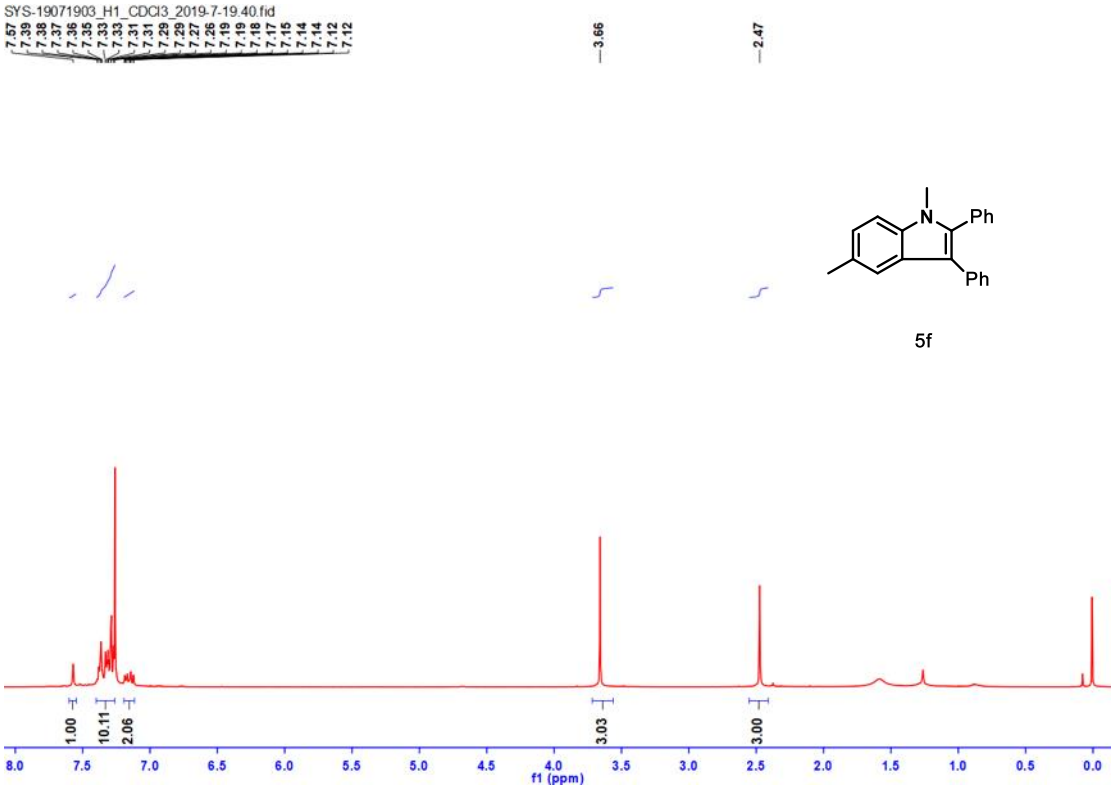

SYS-19071202_C13_CDCl3_2019-7-12 10.fid
137.68 136.56 135.40 132.47 131.32 129.99 128.50 128.21 128.17 127.34 125.52 122.08 120.16 119.86 115.39 110.10
77.48 77.16 76.84
43.77
32.25
20.18
13.75
N
Ph
Ph
5c
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


SYS-19071505_H1_CDCl3_2019-7-15.50.fid
7.69
7.67
7.40
7.39
7.39
7.37
7.37
7.36
7.36
7.34
7.33
7.32
7.32
7.31
7.29
7.29
7.28
7.28
7.26
7.25
7.24
7.21
7.19
7.18
7.18
7.17
7.16
7.16
7.15
7.15
7.14
7.04
7.04
7.02
7.02
3.65
2.55
N
Ph
Ph
0.87
7.08
2.03
1.01
1.05
0.90
3.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

5e


137.88
137.24
135.55
132.21
132.19
131.30
129.94
128.48
128.26
128.02
125.51
124.99
122.03
119.43
115.05
109.70
77.48
77.16
76.84
31.01
22.07
N
Ph
Ph
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5e


SYS-19071903_H1_CDCl3_2019-7-19.40.fid
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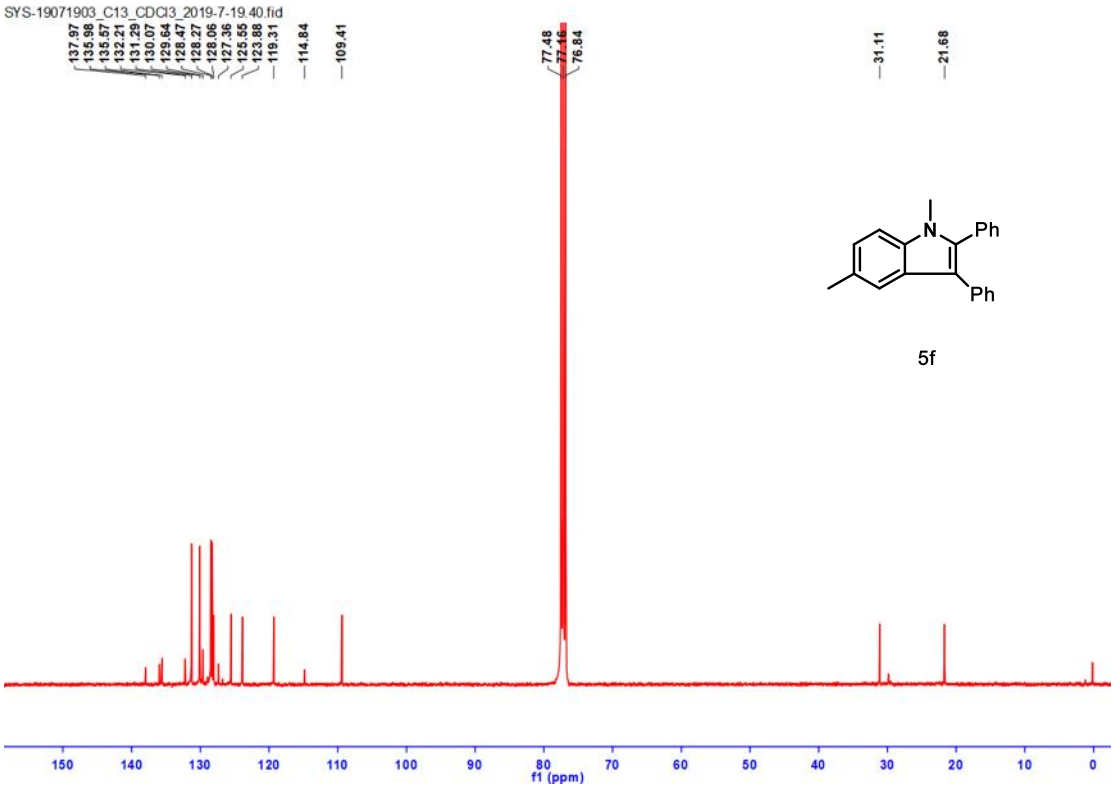
7.39
7.38
7.37
7.36
7.35
7.33
7.33
7.31
7.31
7.29
7.29
7.27
7.26
7.19
7.19
7.18
7.17
7.15
7.14
7.14
7.12
7.12
3.66
2.47
N
Ph
Ph
1.00
10.11
2.06
3.03
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

5f


SYS-19071903_C13_CDCl3_2019-7-19.40.fid
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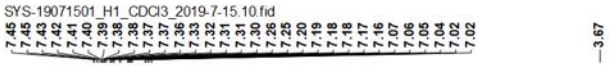
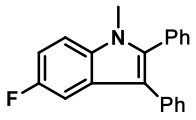
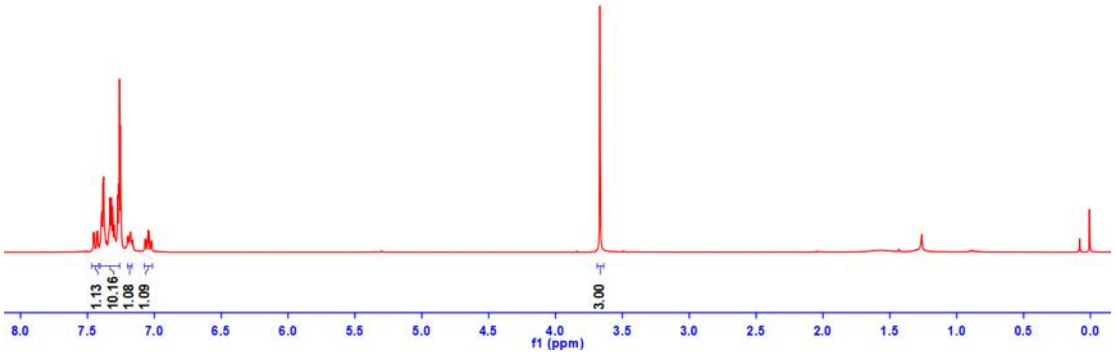
135.98
135.57
132.21
131.29
130.07
129.64
128.47
128.27
128.06
127.36
125.55
123.88
119.31
114.84
109.41
77.48
77.16
76.84
31.11
21.68
N
Ph
Ph
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

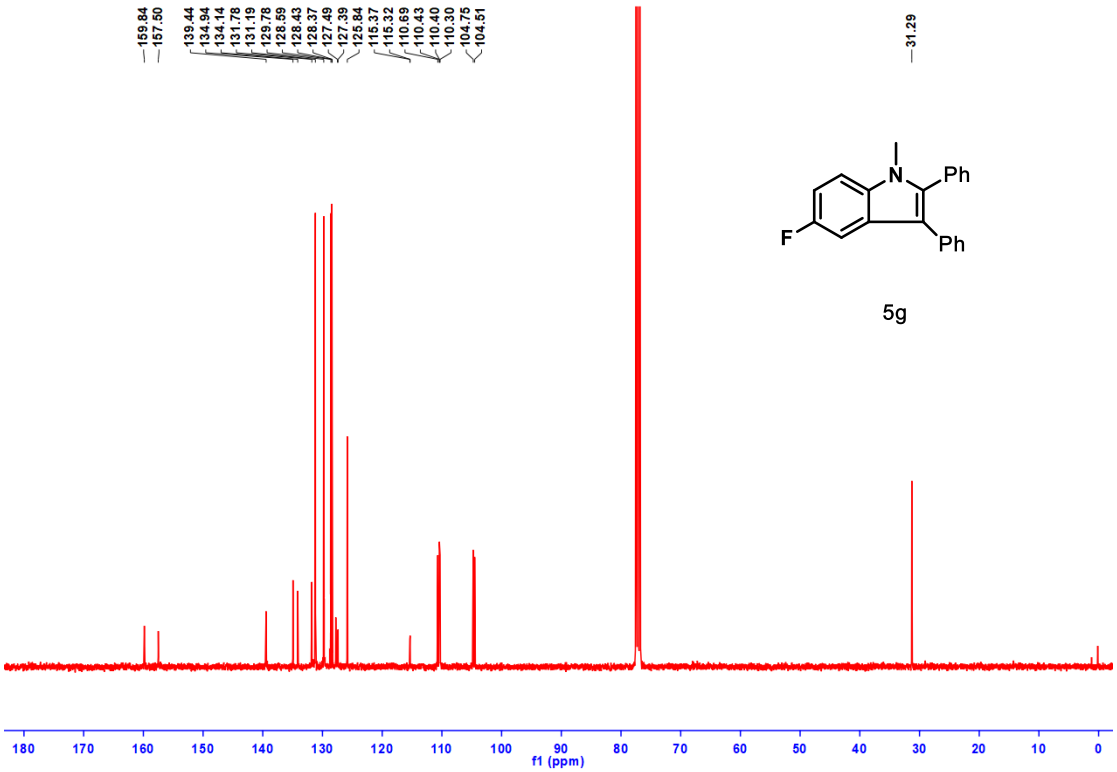
5f


SYS-19071501_H1_CDCl3_2019-7-15.10.fid
7.45
7.45
7.43
7.42
7.41
7.40
7.39
7.38
7.38
7.37
7.37
7.36
7.33
7.32
7.31
7.31
7.30
7.26
7.25
7.20
7.19
7.18
7.18
7.17
7.16
7.07
7.06
7.05
7.04
7.02
7.02
3.67


N
Ph
F
Ph

5g

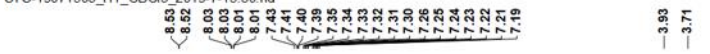

1.13
10.16
1.08
1.09
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

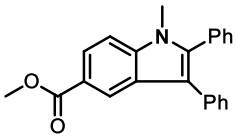

159.84
157.50
139.44
134.94
134.14
131.78
131.19
129.78
128.59
128.43
128.37
127.49
127.39
125.84
115.37
115.32
110.69
110.43
110.40
110.30
104.75
104.51
31.29
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

N
Ph
F
Ph

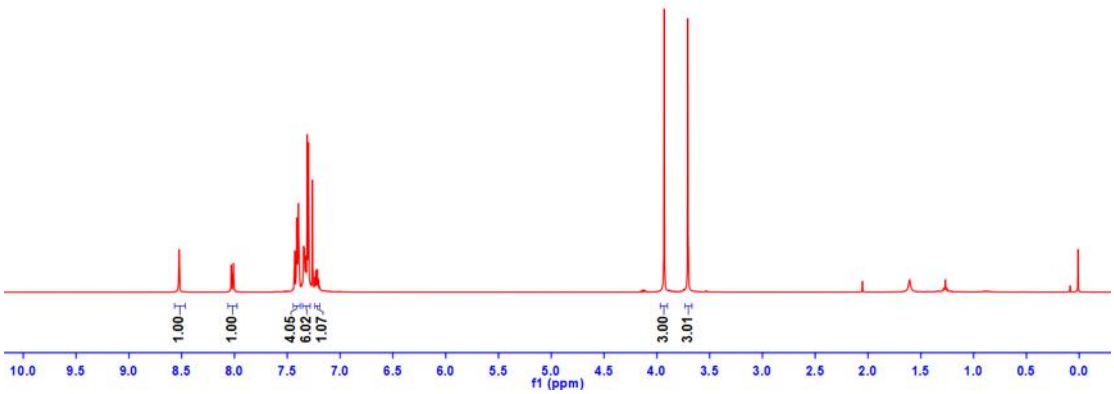
5g

SYS-19071503_H1_CDCl3_2019-7-15.30.fid

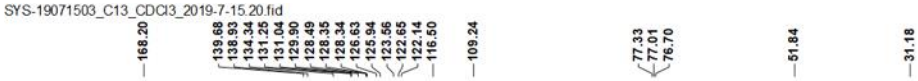


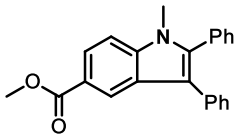


5h

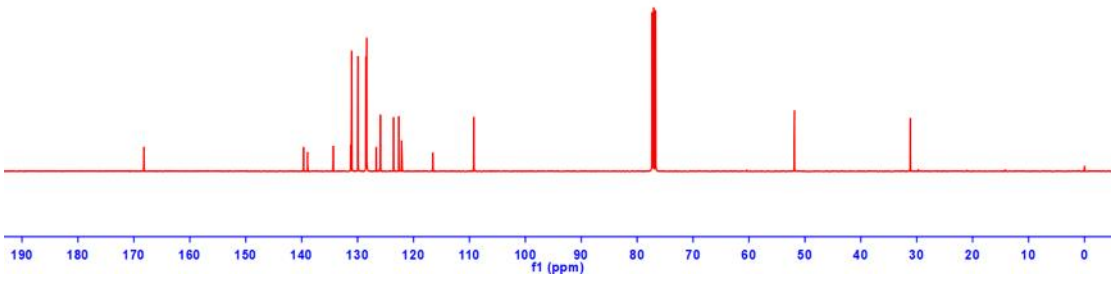


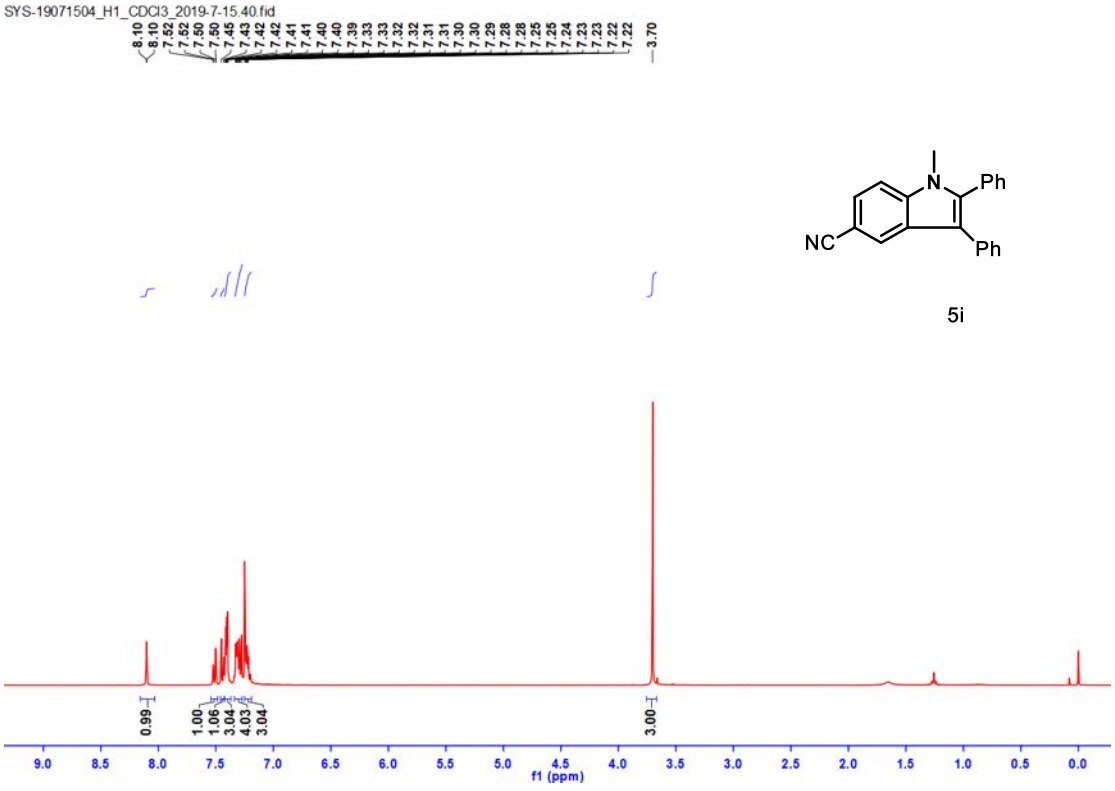
SYS-19071503_C13_CDCl3_2019-7-15.20.fid



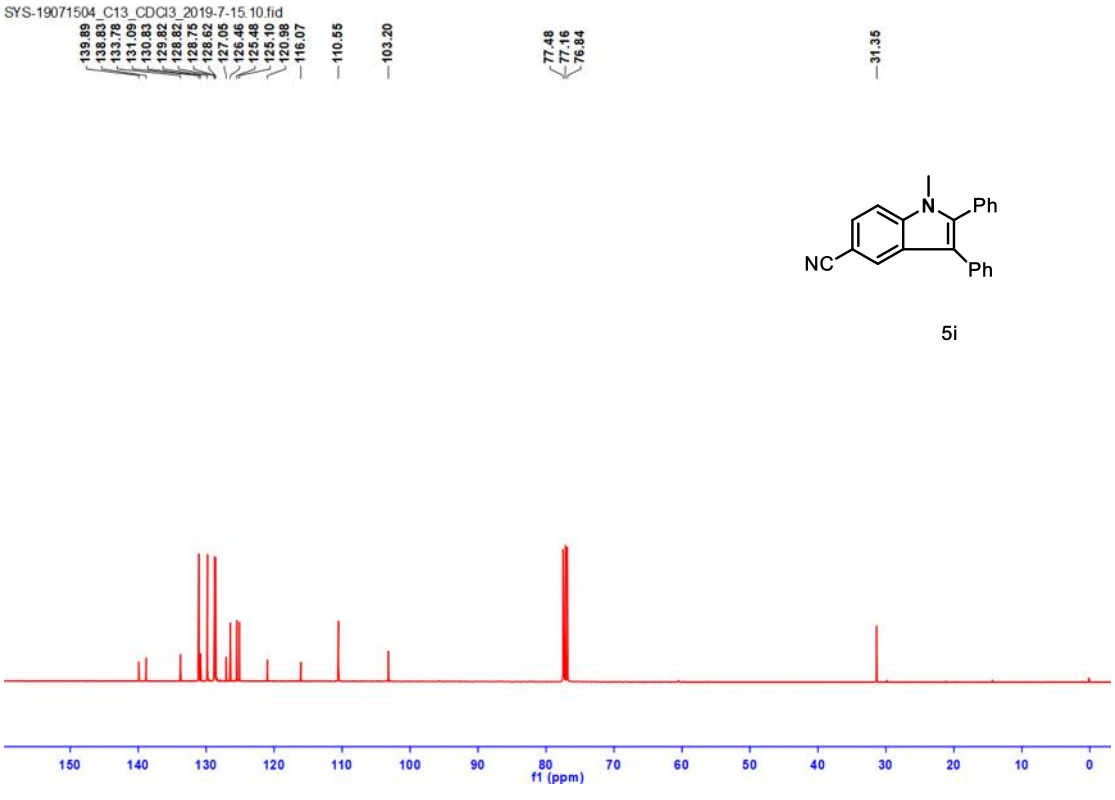


5h

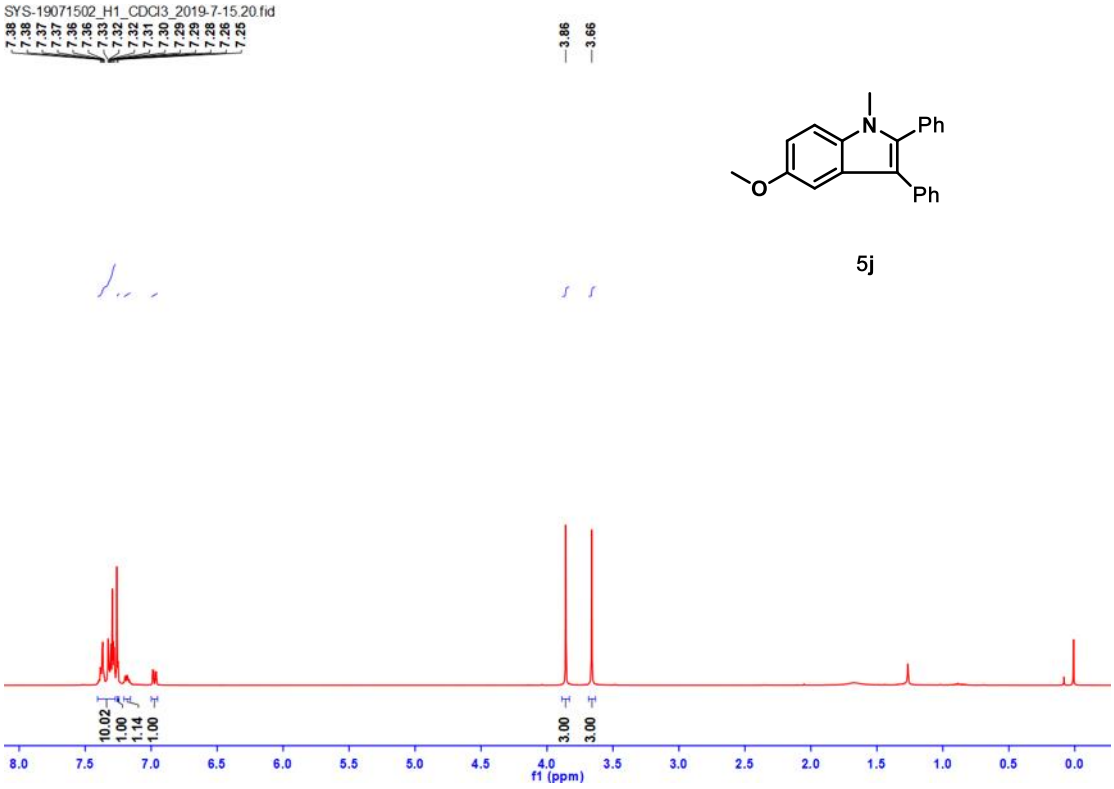



SYS-19071504_H1_CDCl3_2019-7-15.40.fid
8.10
8.10
7.52
7.52
7.50
7.50
7.45
7.43
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.29
7.28
7.28
7.25
7.25
7.24
7.23
7.23
7.22
7.22
3.70
N
Ph
Ph
NC
0.99
1.00
1.06
3.04
4.03
3.04
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

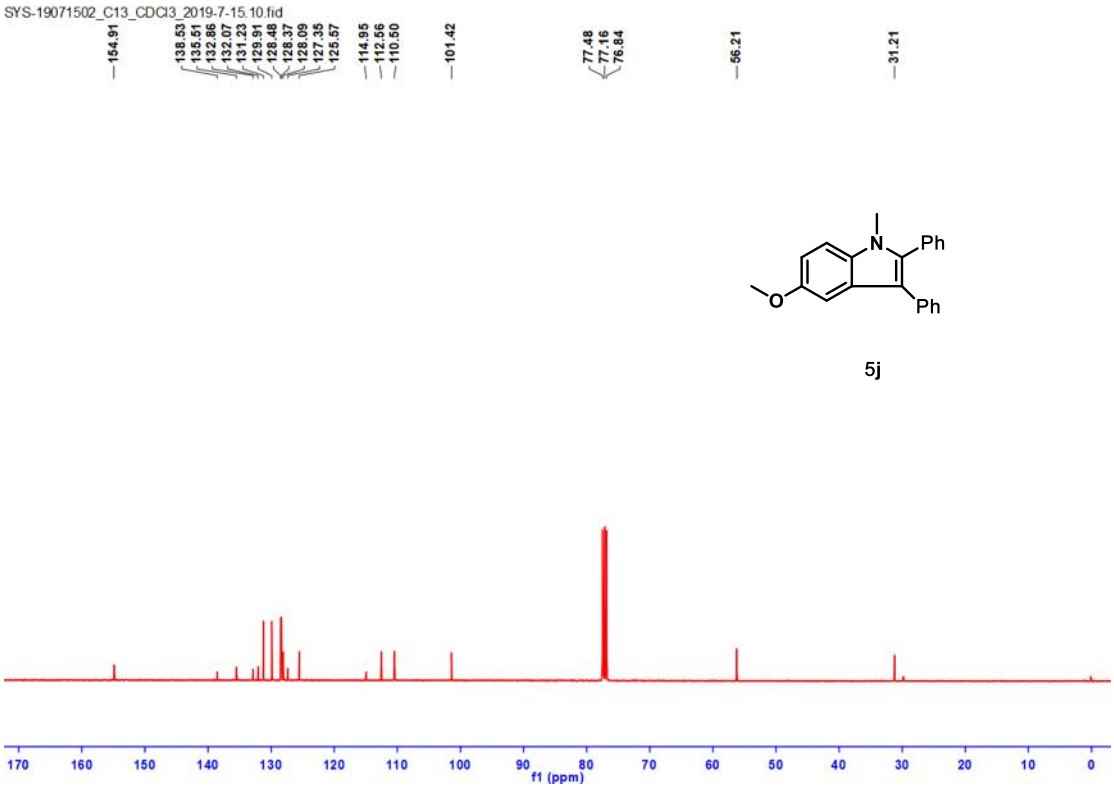
5i


SYS-19071504_C13_CDCl3_2019-7-15.10.fid
139.89
138.83
133.78
131.09
130.83
129.82
128.82
128.75
128.62
127.05
126.46
125.48
125.10
120.98
116.07
110.55
103.20
77.48
77.16
76.84
31.35
N
Ph
Ph
NC
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

5i


SYS-19071502_H1_CDCl3_2019-7-15.20.fid
7.38
7.38
7.37
7.37
7.36
7.36
7.33
7.32
7.32
7.31
7.30
7.29
7.29
7.28
7.26
7.25
3.86
3.66
N
Ph
Ph
O
10.02
1.00
1.14
1.00
3.00
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

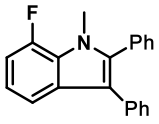
5j


SYS-19071502_C13_CDCl3_2019-7-15.10.fid
154.91
138.53
135.51
132.86
132.07
131.23
129.91
128.48
128.37
128.09
127.35
125.57
114.95
112.56
110.50
101.42
77.48
77.16
76.84
56.21
31.21
N
Ph
Ph
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

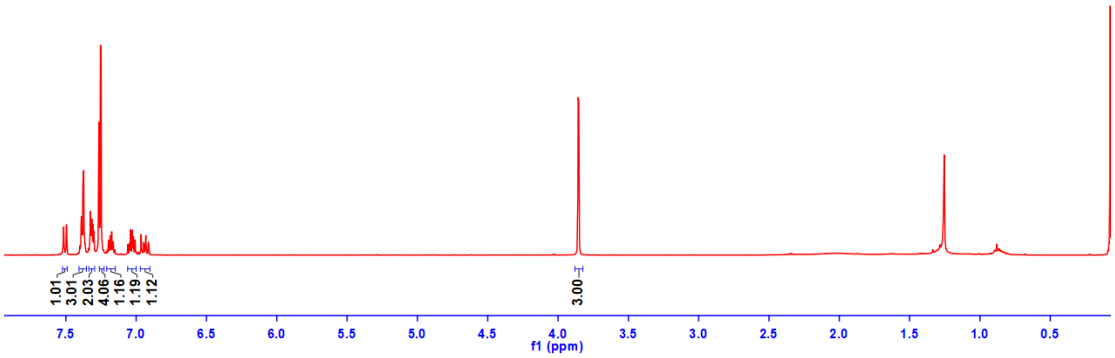
5j

SYS-19093004_H1_CDCl3_2019-9-30.40.fid

7.52 7.50 7.40 7.39 7.39 7.38 7.37 7.34 7.32 7.32 7.31 7.30 7.26 7.25 7.25 7.21 7.20 7.18 7.17 7.16 7.15 7.06 7.05 7.04 7.02 7.01 6.96 6.95 6.93 6.91



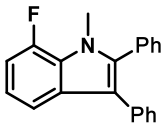
5k



SYS19093004_C13_CDCl3_2019-9-30.10.fid

151.65 149.23 139.25 134.91 131.37 131.33 131.03 130.98 129.98 128.58 128.42 128.33 125.91 125.49 125.40 120.26 120.20 116.11 116.09 115.51 115.47 107.99 107.81

33.73 33.67



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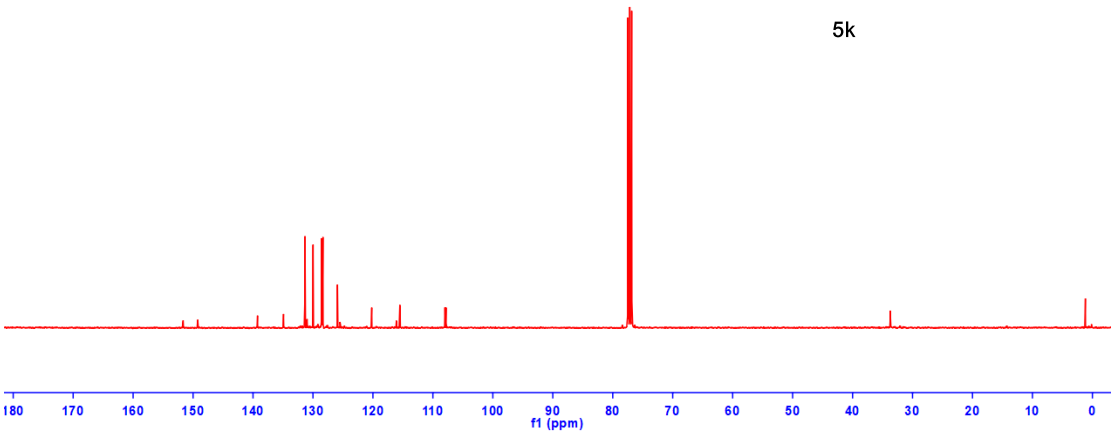

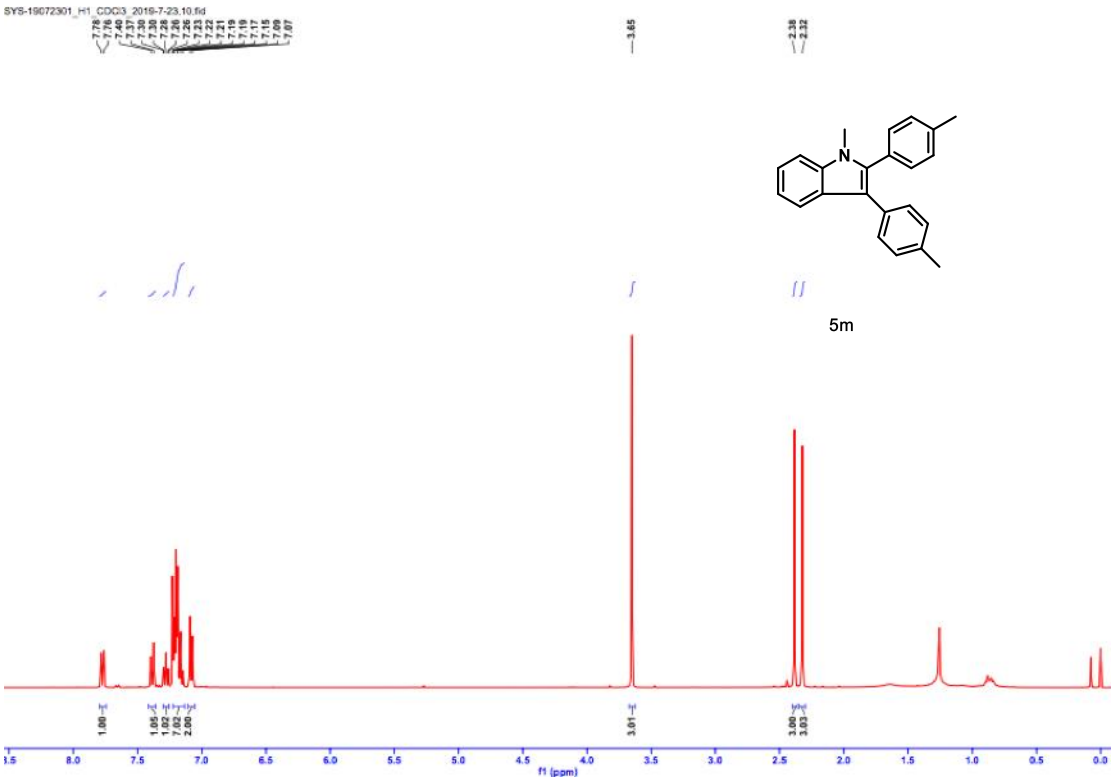
SYS-19072301_H1_CDCl3_2019-7-23.10.fid
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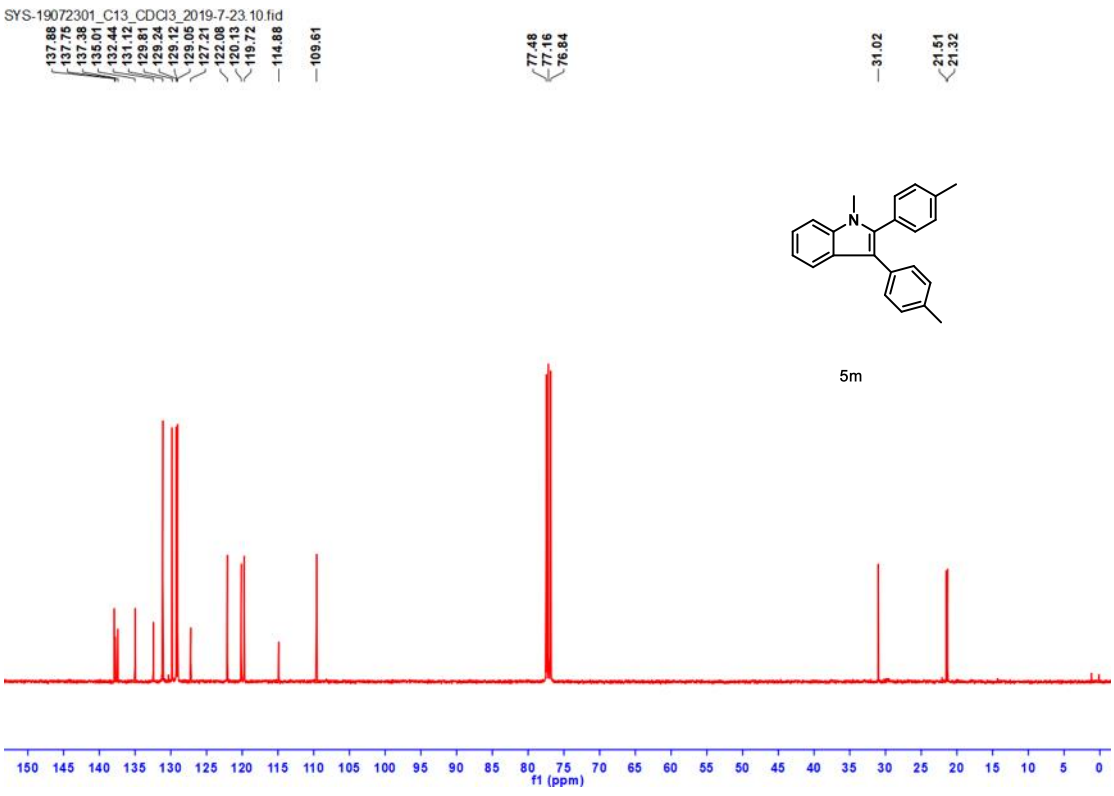
7.76
7.40
7.37
7.30
7.28
7.26
7.23
7.21
7.19
7.17
7.15
7.09
7.07
3.65
2.38
2.32
N
5m
1.00
1.05
1.02
7.02
2.00
3.01
3.00
3.03
f1 (ppm)


SYS-19072301_C13_CDCl3_2019-7-23.10.fid
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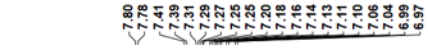
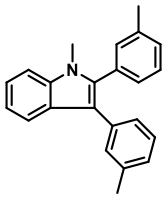
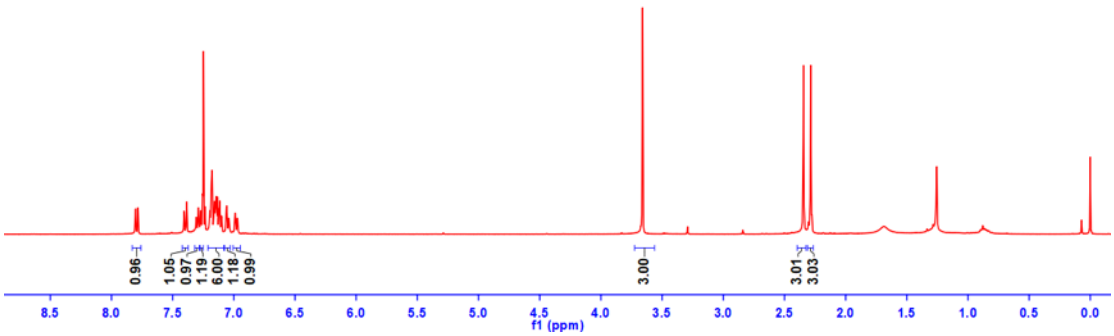
137.75
137.38
135.01
132.44
131.12
129.81
129.24
129.12
129.05
127.21
122.08
120.13
119.72
114.88
109.61
77.48
77.16
76.84
31.02
21.51
21.32
N
5m
f1 (ppm)

NDW-ZC-SYS-01.1.fid

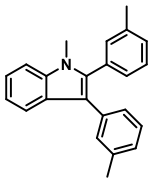




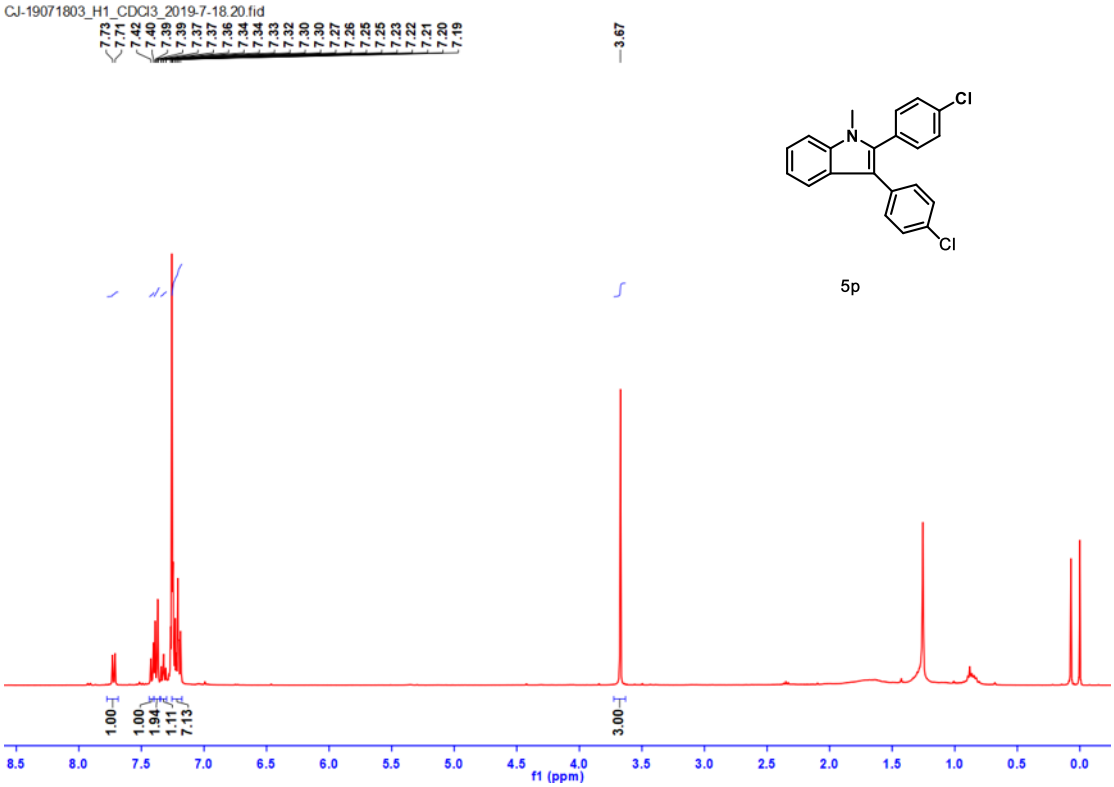
5n



NDW-ZC-SYS-01.2.fid



5n


CJ-19071803_H1_CDCl3_2019-7-18.20.fid
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7.71
7.42
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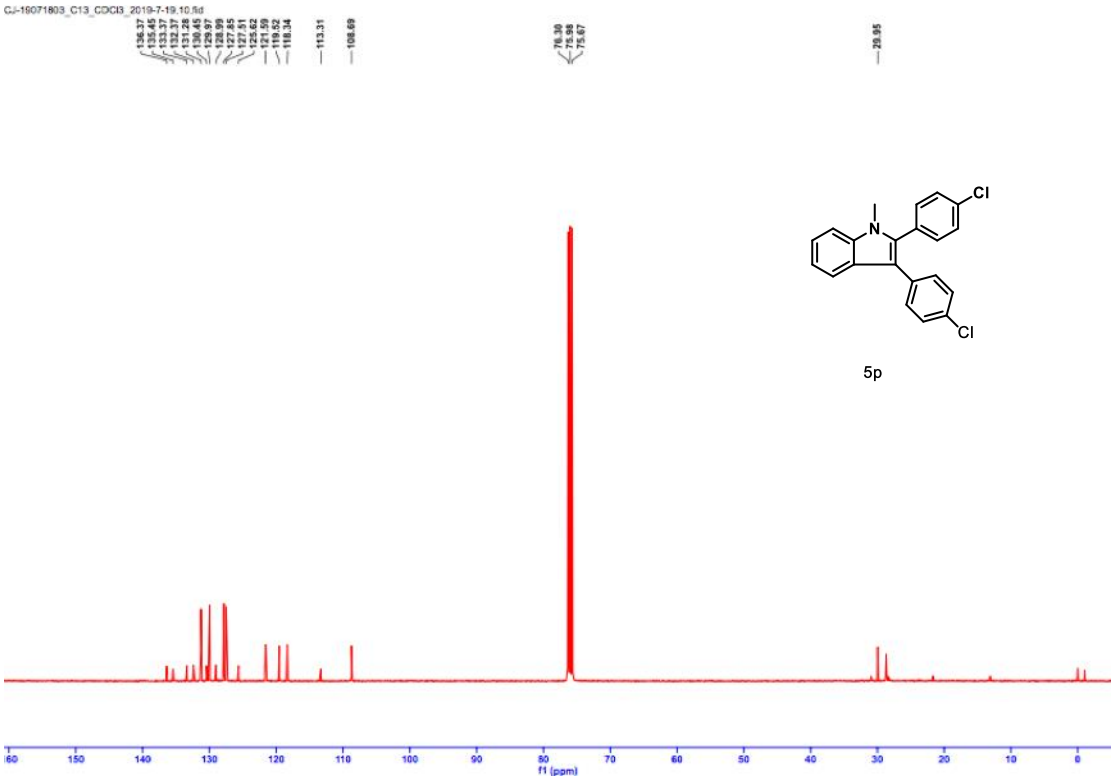
7.39
7.39
7.37
7.37
7.36
7.34
7.34
7.33
7.32
7.30
7.30
7.27
7.26
7.25
7.23
7.22
7.21
7.20
7.19
3.67
Cl
N
Cl
5p
1.00
1.00
1.94
1.11
7.13
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


CJ-19071803_C13_CDCl3_2019-7-19.10.fid
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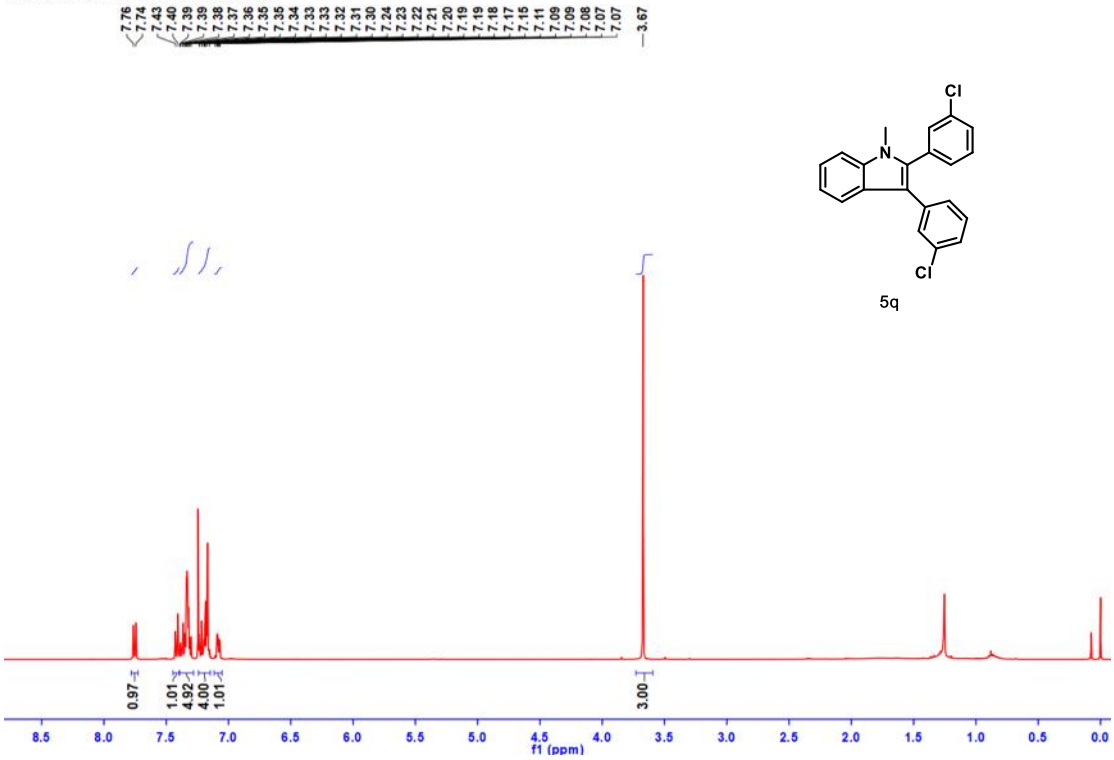
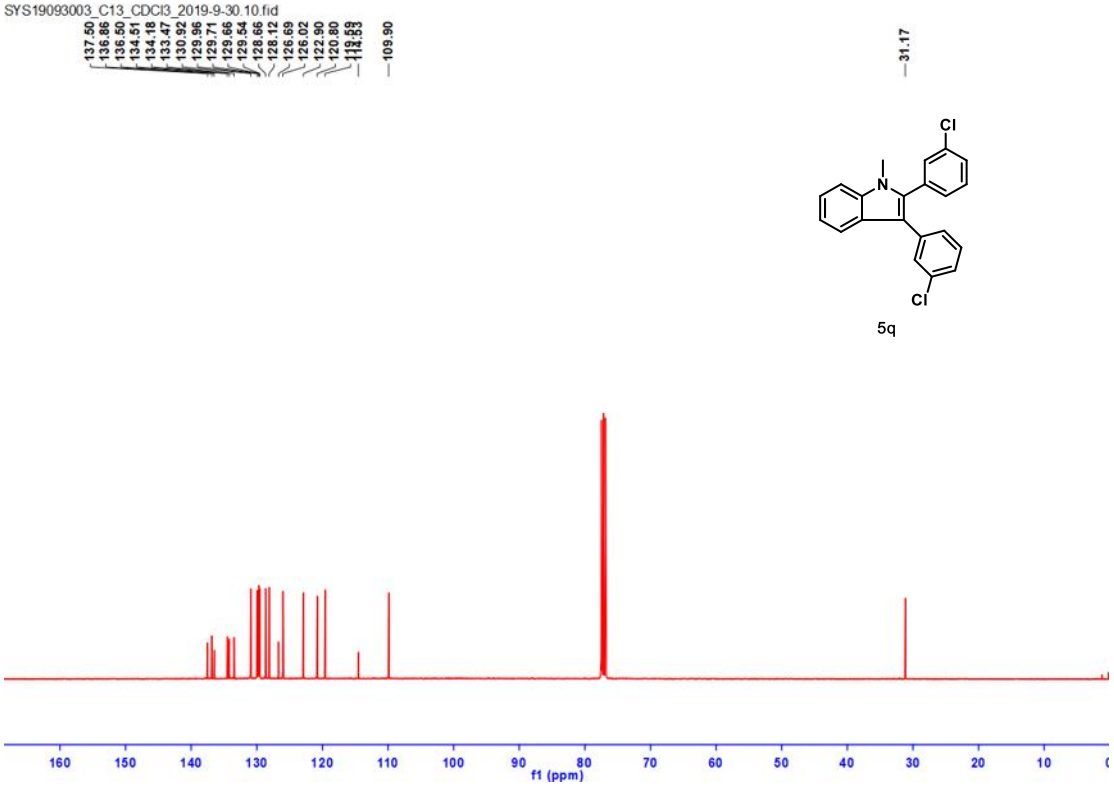
135.45
133.37
132.37
131.26
130.40
129.97
128.99
127.85
127.61
125.65
121.59
119.52
118.34
113.31
108.69
76.30
75.98
75.67
29.95
Cl
N
Cl
5p
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

SYS-19093003_H1_CDCl3_2019-9-30.30.fid



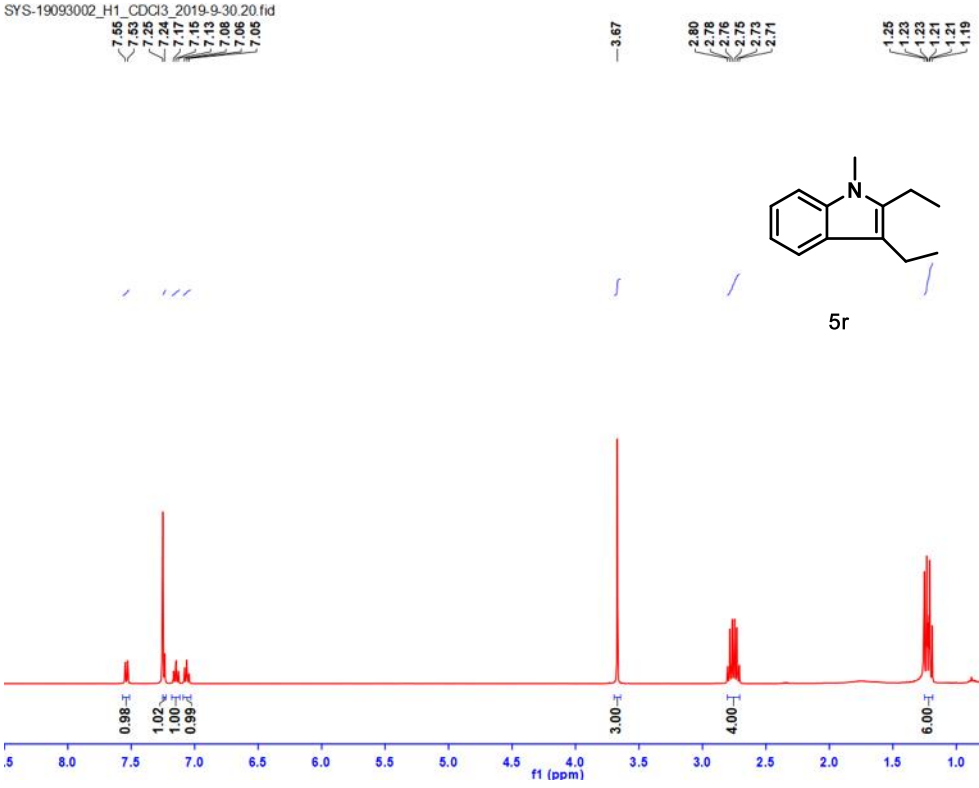
5q

SYS19093003_C13_CDCl3_2019-9-30.10.fid



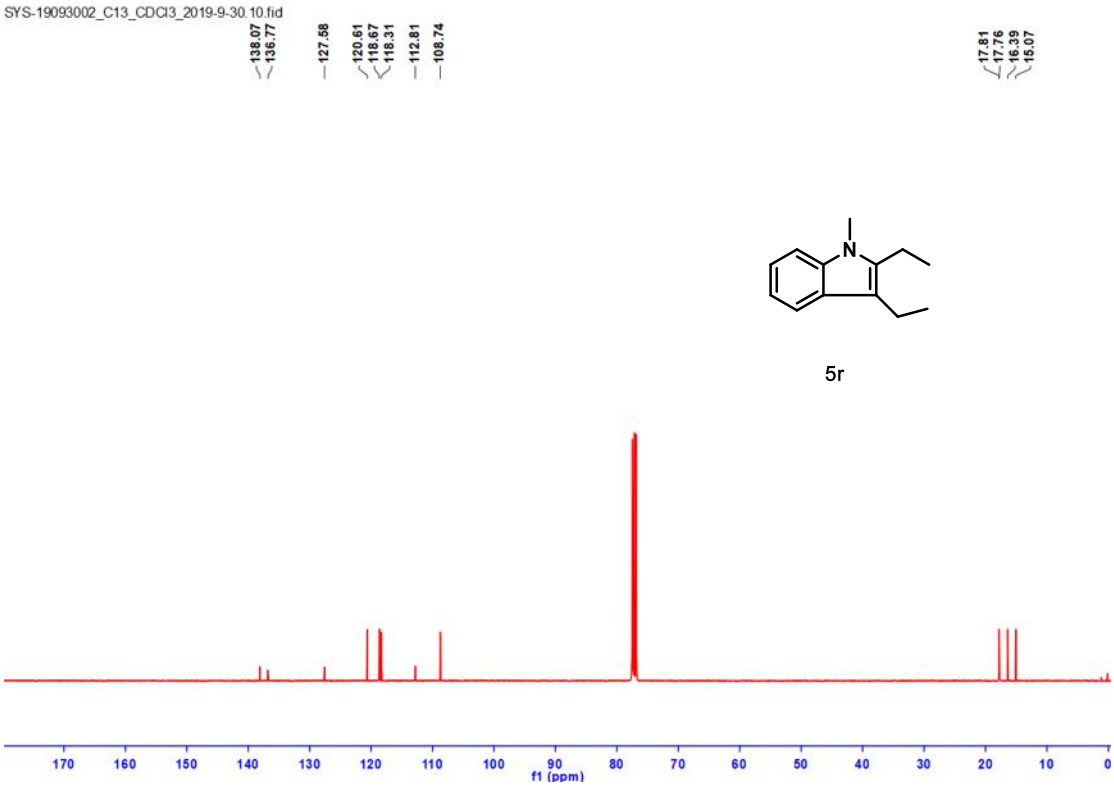
5q

SYS-19093002_H1_CDCl3_2019-9-30.20.fid



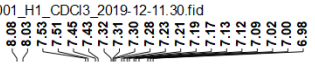
5r

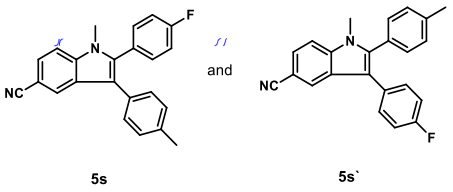
SYS-19093002_C13_CDCl3_2019-9-30.10.fid



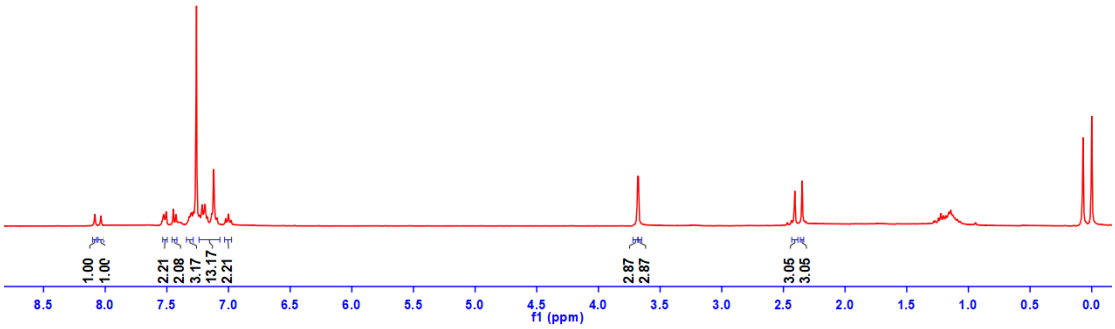
5r

SYS-19121001_H1_CDCl3_2019-12-11.30.fid





5s and 5s`



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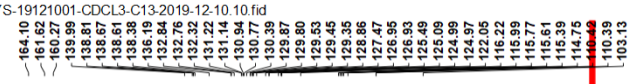

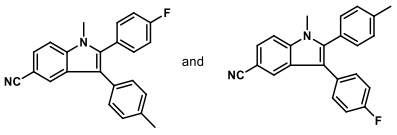

5s and 5s`