Supplementary Information

Sustainable Synthesis of Heteroaryl Ethers from Azine *N*-Oxides via Phosphoramide Catalysis

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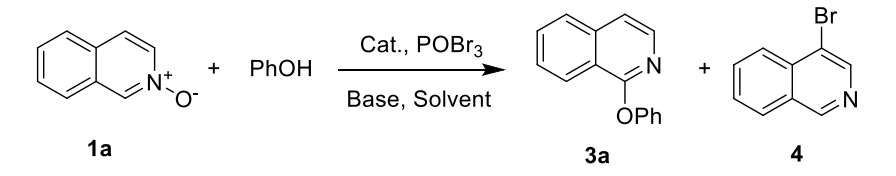
1. General Experimental

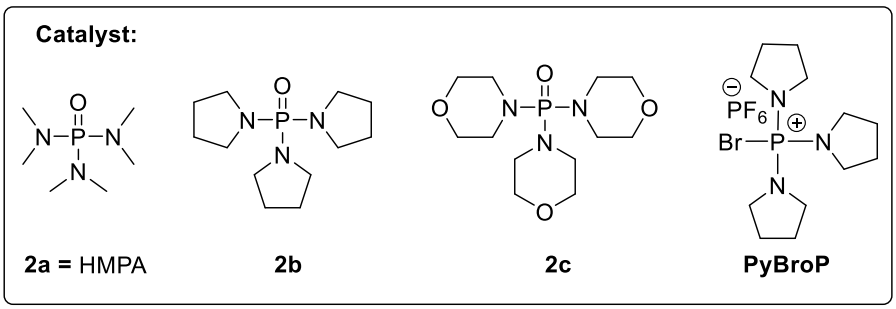
The preparation experiments were performed under air or an argon atmosphere in oven dried glassware. Solvents used as reaction media were distilled immediately before use: THF was distilled from Na/benzophenone ketyl, DCM and DCE were distilled from calcium hydride, DMF was obtained from vacuum distillation. All reagents were purchased at the highest commercial quality and used without further purification. Reactions were monitored by thin layer chromatography (TLC) using ultra violet light (UV) as the visualizing agent. Metallic heating mantle was used in all of the reactions carried out in this work. Nuclear magnetic resonance spectra (NMR) were recorded on Bruker Bruker Avance NEO 600 instruments and were calibrated using residual undeuterated solvent as an internal reference (^{1}H NMR: $CHC1_3$ 7.26 ppm, ^{13}C NMR: $CHC1_3$ 77.16 ppm). High resolution mass spectra (HRMS) were recorded on a Thermo Fisher Scientific Ultimate 3000/Q-Exactive mass spectrometer. Melting points were recorded on an automatic melting point meter (Shang Hai Zhuo Guang) GM50. The following abbreviations were used to indicate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sex = sextet, sep = septet, dd = doublet of doublets, dt = doublet of triplets, ddd = doublet of doublet of doublets, ddt = doublet of doublet of triplets, m = multiplet).

2. Optimization of the Aryloxylation

Table S1 Optimization of the phenoxylation of isoquinoline *N*-oxide.[a]



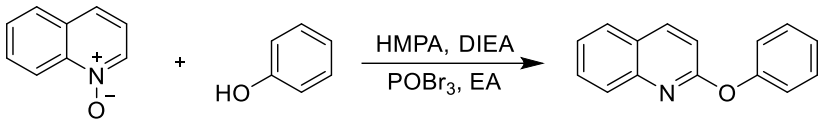
1a **3a** **4**



Entry	Solvent	Base (eq.)	Cat. (eq.)	Phenol/eq.	Y/% (3a)	Y/% (4)
			Catalyst screen			
1	EA	DIEA (2)	HMPA (0.2)	2	61	23
2	EA	DIEA (2)	**2b** (0.2)	2	53	16
3	EA	DIEA (2)	**2c** (0.2)	2	33	9
4	EA	DIEA (2)	PyBroP (0.2)	2	20	trace
5	EA	DIEA (2)	HMPA (0)	2	40	13
			Solvent screen			
6	DCM	DIEA (2)	HMPA (0.2)	2	56	28
7	CH_3CN	DIEA (2)	HMPA (0.2)	2	47	18
8	THF	DIEA (2)	HMPA (0.2)	2	41	20
9	toluene	DIEA (2)	HMPA (0.2)	2	44	23
			Temperature screen			
10 [b]	EA	DIEA (2)	HMPA (0.2)	2	42	33
11 [c]	EA	DIEA (2)	HMPA (0.2)	2	49	trace
			Concentration screen			
12 [d]	EA	DIEA (2)	HMPA (0.2)	2	55	20
13 [e]	EA	DIEA (2)	HMPA (0.2)	2	33	24
			Ag Additive screen			
14 [f]	EA	DIEA (2)	HMPA (0.2)	2	39	26
15 [g]	EA	DIEA (2)	HMPA (0.2)	2	23	10
			Equivalent and base screen			
16 [h]	EA	DIEA (2)	HMPA (0.2)	2	55	23
17 [i]	EA	DIEA (2)	HMPA (0.2)	2	trace	trace
18	EA	DIEA (2)	HMPA (0.1)	2	48	26
19	EA	DIEA (2)	HMPA (0.4)	2	66	22
20	EA	DIEA (2)	HMPA (0.6)	2	54	23
21	EA	DIEA (2)	HMPA (0.8)	2	56	27
22	EA	DIEA (2)	HMPA (1.0)	2	56	18
23	EA	DIEA (1)	HMPA (0.4)	2	41	trace
24	EA	DIEA (1.5)	HMPA (0.4)	2	60	trace
25	EA	DIEA (3)	HMPA (0.4)	2	40	trace
26	EA	Na_2CO_3 (2)	HMPA (0.4)	2	0	trace
27	EA	Et_3N (2)	HMPA (0.4)	2	41	trace
28	EA	DBU (2)	HMPA (0.4)	2	31	trace
29	EA	DABCO (2)	HMPA (0.4)	2	14	trace
30	EA	TMG (2)	HMPA (0.4)	2	20	trace
31	EA	DMAP (2)	HMPA (0.4)	2	0	trace
32	EA	DIEA (2)	HMPA (0.4)	1.5	44	19
33	**EA**	**DIEA (2)**	**HMPA (0.4)**	**3**	**72**	**10**
34	EA	DIEA (2)	HMPA (0.4)	4	75	14
35	EA	DIEA (2)	HMPA (0.2)	3	36	trace

[a] Unless otherwise noted, all reactions were conducted with isoquinoline *N*-oxide (100 mg, 0.69 mmol), phenol, base, catalyst and $POBr_3$ (2.0 equiv) in solvent (0.5 M) at room temperature and stirred for 5 minutes. [b] Reacted at 0 ℃. [c] Reacted at 60 ℃. [d] 0.25 M concentration. [e] 0.75 M concentration. [f] 1.0 equiv of Ag_2CO_3 was used. [g] 1.0 equiv of $AgBF_4$ was used. [h] 1.2 equiv of $POBr_3$ was used. [i] 3.0 equiv of $POBr_3$ was used.

Table S2 Optimization of the phenoxylation of quinoline *N*-oxide.[a]

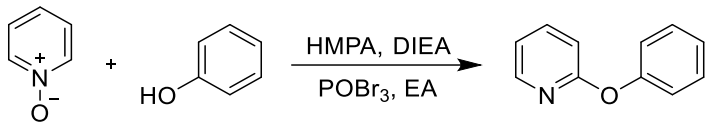


5a **6a**

Entry	DIEA/eq	HMPA/eq	Phenol/eq	$POBr_3$/eq	Y/% (6a)
1	2	0.4	3	2	74
2	2	0.4	2	2	69
3	2	0.2	2	2	65
4	1	0.2	2	2	27
5	2	0.2	2	1	68
6	2	0.1	2	2	64
7	2	0.1	2	1.5	71
8	2	0.1	2	1	70
9 [b]	2	0.1	2	0.5	52
10	**2**	**0.1**	**1.5**	**1**	**69**
11	2	0.1	1	1	48
12 [c]	2	0.1	1.5	1	62
13 [d]	2	0.1	1.5	1	57

[a] Unless otherwise noted, all reactions were conducted with quinoline *N*-oxide (100 mg, 0.69 mmol), phenol, DIEA, HMPA and $POBr_3$ in EA (0.5 M) at room temperature and stirred for 5 minutes. [b] Reacted for 12 h. [c] 0.75 M concentration. [d] 0.25 M concentration.

Table S3 Optimization of the phenoxylation of pyridine *N*-oxide.[a]

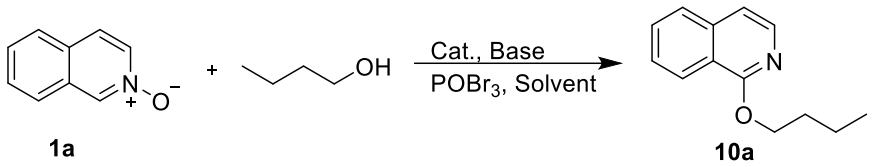


7a

Entry	DIEA/eq	HMPA/eq	Phenol/eq	$POBr_3$/eq	Y/% (7a)
1	2	0.4	3	2	56
2	2	0.8	3	2	60
3	2	0.2	3	2	59
4	2	0	3	2	50
5	2	0.2	**2**	**2**	**58**
6	2	0.2	1	2	31
7 [b]	2	0.2	2	2	51
8 [c]	2	0.2	2	2	40
9 [d]	2	0.2	2	2	50
10 [e]	2	0.2	2	2	43
11 [f]	2	0.2	2	2	51
12	2	0.2	2	0.5	45
13	2	0.2	2	1	50
14	2	0.2	2	4	46
15	4	0.2	2	2	54
16	1	0.2	2	2	47

[a] Unless otherwise noted, all reactions were conducted with pyridine *N*-oxide (100 mg, 1.0 mmol), phenol, DIEA, HMPA and $POBr_3$ in EA (0.5 M) at room temperature and stirred for 5~8 hours. [b] 0.75 M concentration. [c] 0.25 M concentration. [d] 0.1 M concentration. [e] Reacted at 60 ℃. [f] Reacted at 80 ℃.

Table S4 Optimization of the alkoxylation of isoquinoline *N*-oxide.[a]



1a **10a**

Entry	M	Solvent	Base(eq)	Cat.(eq)	Time	Y/%
1	0.5	EA	DIEA (2)	HMPA (0.4)	0.5 h	trace
2[b]	0.25	DCM	Na_2CO_3 (2)	PyBroP (0.6)	12 h	5
3	0.25	DCM	Na_2CO_3 (2)	HMPA (0.4)	12 h	N/A
4	0.25	DCM	DIEA (2)	PyBroP (0.6)	0.5 h	12
5	**0.5**	**EA**	**DIEA (2)**	**PyBroP (0.4)**	**0.5 h**	**14**

[a] Unless otherwise noted, all reactions were conducted with isoquinoline *N*-oxide (100 mg, 0.69 mmol), *n*-BuOH (3.0 equiv), base and catalyst in solvent at room temperature and stirred for 30 minutes, then $POBr_3$ (2.0 equiv) was added dropwise at 0 °C. The reaction was then warmed to room temperature. [b] This condition was referred to *Org. Lett.* 2016, 18, 1362−1365. 4Å molecular sieve was added to the reaction mixture.

3. General Procedure

General Procedure 1: Aryloxylation of Isoquinoline *N*-oxide. To a solution of an isoquinoline *N*-oxide derivative (1.0 mmol) in dry EA (1.0 mL) is added ArOH (3.0 mmol), DIEA (2.0 mmol) and HMPA (0.4 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of a solution of $POBr_3$ (2.0 mmol) in EA (1.0 mL). The reaction mixture is then warmed to room temperature and stirred for 5 minutes (the reaction is complete as indicated by TLC). The reaction was quenched with a saturated potassium carbonate solution and the organic phase was separated. The aqueous phase was extracted once with EA. The organic phase was combined, dried over Na_2SO_4 and concentrated in vacuo to give the crude product. Purification by flash column chromatography (PE : EA = 200:1-100:1) furnishes the desired product.

General Procedure 2: Aryloxylation of Quinoline *N*-oxide. To a solution of a quinoline *N*-oxide derivative (1.0 mmol) in dry EA (1.0 mL) is added ArOH (1.5 mmol), DIEA (2.0 mmol) and HMPA (0.1 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of a solution of $POBr_3$ (1.0 mmol) in EA (1.0 mL). The reaction mixture is then warmed to room temperature and stirred for 5 minutes (the reaction is complete as indicated by TLC). The reaction was quenched with

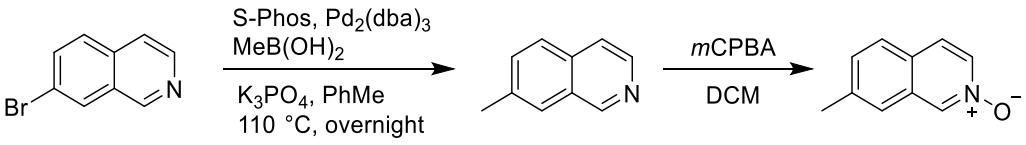
a saturated potassium carbonate solution and the organic phase was separated. The aqueous phase was extracted once with EA. The organic phase was combined, dried over Na_2SO_4 and concentrated in vacuo to give the crude product. Purification by flash column chromatography (PE : EA = 200:1-100:1) furnishes the desired product.

General Procedure 3: Aryloxylation of Pyridine *N*-oxide. To a solution of a pyridine *N*-oxide derivative (1.0 mmol) in dry EA (1.0 mL) is added ArOH (2.0 mmol), DIEA (2.0 mmol) and HMPA (0.2 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of a solution of $POBr_3$ (2.0 mmol) in EA (1.0 mL). The reaction mixture is then warmed to room temperature and stirred for 5-24 hours (the reaction is complete as indicated by TLC). The reaction was quenched with a saturated potassium carbonate solution and the organic phase was separated. The aqueous phase was extracted once with EA. The organic phase was combined, dried over Na_2SO_4 and concentrated in vacuo to give the crude product. Purification by flash column chromatography (PE : EA = 200:1-100:1) furnishes the desired product.

General Procedure 4: Alkoxylation of azine *N*-oxide. To a solution of an azine *N*-oxide derivative (1.0 mmol) in dry EA (1.0 mL) is added ROH (3.0 mmol), DIEA (2.0 mmol) and PyBroP (0.4 mmol). The resulting solution is stirred for 30 minutes at room temperature. Then the resulting solution is cooled to 0 °C, followed by the dropwise addition of a solution of $POBr_3$ (2.0 mmol) in EA (1.0 mL). The reaction mixture is then warmed to room temperature and stirred for 30 minutes (the reaction is complete as indicated by TLC). The reaction was quenched with a saturated potassium carbonate solution and the organic phase was separated. The aqueous phase was extracted once with EA. The organic phase was combined, dried over Na_2SO_4 and concentrated in vacuo to give the crude product. Purification by flash column chromatography (PE : EA = 200:1) furnishes the desired product.

4. Preparation of Azine *N*-oxides

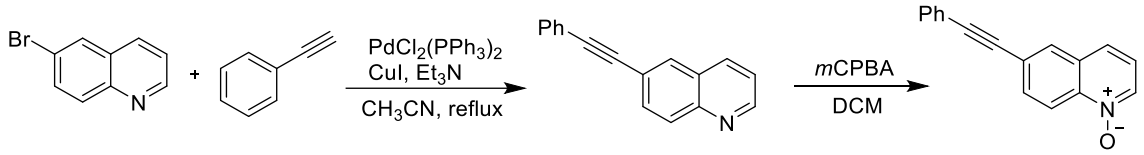
All *N*-oxides were prepared following the reported procedure.[1]



7-methylisoquinoline 2-oxide. In a 2-necked round bottom flask, 7-bromoisoquinoline (1.5 g, 7.2

mmol), methylboronic acid (0.86 g, 14.4 mmol), K_3PO_4 (6.1 g, 28.8 mmol) and S-Phos (1 mol%) were combined and taken up in PhMe (72 mL). Argon was bubbled through for 10 min, then $Pd_2(dba)_3$ (0.5 mol%) was added and the mixture was heated to 110 ℃ for 8-18 h. The reaction was cooled to room temperature and water was added. The layers were separated, and the aqueous phase was extracted with EtOAc once. The combined organic phases were dried over $MgSO_4$, filtered, and concentrated in vacuo. Purification by flash column chromatography (PE : EA = 8:1-4:1) afforded the product 7-methylisoquinoline as a white solid (989 mg, 96%).[2]

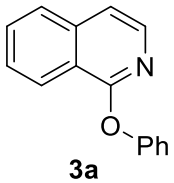
7-Methylisoquinoline (500 mg, 3.5 mmol) was dissolved in DCM (11.6 mL) and *m*CPBA (725 mg, 4.2 mmol) was added and stirred at room temperature overnight until the reaction was complete as indicated by TLC. The reaction mixture was concentrated in vacuo and chromatographed (DCM: MeOH = 100:1-50:1) to afford the product 7-methylisoquinoline 2-oxide as a white solid (350 mg, 63%).



6-(phenylethynyl)quinoline 1-oxide. 6-Bromoquinoline (4.2 g, 20 mmol), phenylacetylene (2.2 g, 22 mmol), $PdCl_2(PPh_3)_2$ (140 mg, 1 mol %), CuI (114 mg, 3 mol %), and dry acetonitrile (30 mL) were added to an oven-dried Schlenk tube charged with a magnetic stirrer bar. Dry triethylamine (3.0 g, 30 mmol) was added, and the reaction was heated at reflux for 16 h. On completion, the reaction mixture was washed with H_2O, extracted with DCM, dried over $MgSO_4$, and filtered and the solvent removed in vacuo. Purification by flash column chromatography (PE : EA = 15:1-5:1) afforded the product 6-(phenylethynyl)quinoline as a red solid (3.85 g, 84%).[3]

6-(Phenylethynyl)quinoline (500 mg, 2.2 mmol) was dissolved in DCM (2.2 mL) and *m*CPBA (530 mg, 2.6 mmol) was added and stirred at room temperature overnight until the reaction was complete as indicated by TLC. The reaction mixture was concentrated in vacuo and chromatographed (DCM : MeOH = 40:1-20:1) afforded the product as a red-brown solid (430 mg, 80%).

5. Preparation Procedure



3a

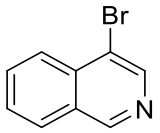
1-phenoxyisoquinoline (3a). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (110 mg, 72% yield) as a white solid. Additionally, 4-bromoisoquinoline was isolated (14 mg, 10% yield) as a yellow solid. The spectroscopic data of the major product are consistent with previously reported.[4] TLC: R_f = 0.75 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (d, J = 7.8 Hz, 1H), 7.88 (d, J = 5.4 Hz, 1H), 7.71-7.70 (m, 1H), 7.63 (t, J = 7.8 Hz, 1H), 7.53 (t, J = 7.8 Hz, 1H), 7.36 (t, J =7.8 Hz, 2H), 7.22 (d, J = 6.0 Hz, 1H), 7.18-7.15 (m, 3H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{110}{153} \times 1 = 72\%$$

Gram scale synthesis:

In a 2-necked 50 mL round bottom flask equipped with a magnetic stir bar was added isoquinoline *N*-oxide (1.0 g, 6.9 mmol) and dry EA (7 mL), followed by PhOH (1.95 g, 20.7 mmol), DIEA (1.78 g, 13.8 mmol) and HMPA (0.50 g, 2.8 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of $POBr_3$ (3.96 g, 13.8 mmol) in dry EA (7 mL). The reaction mixture is then warmed to room temperature and stirred for 30 minutes. The reaction was quenched with a saturated potassium carbonate solution (5 mL) and the organic phase was separated. The aqueous phase was extracted once with EA (15 mL). The organic phase was combined, dried over Na_2SO_4 and concentrated in vacuo to give the crude product. Purification by flash chromatography (PE : EA = 150:1-100:1) furnishes the desired pure product (967 mg, 63%). Additionally, 4-bromoisoquinoline was isolated (187 mg, 13% yield) as a yellow solid.

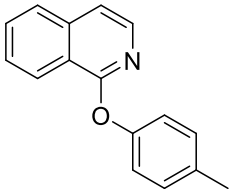
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{0.97}{1.53} \times 1 = 63\%$$



4

4-bromoisoquinoline (4). The spectroscopic data are consistent with previously reported.[5] TLC: R_f = 0.50 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.72 (s, 1H), 8.17-8.15 (m, 1H), 7.98 (d, J = 7.8 Hz, 1H), 7.84-7.81 (m, 1H), 7.70-7.67(m, 1H).

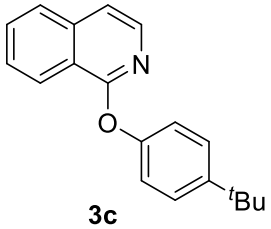
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{14}{144} \times 1 = 10\%$$



3b

1-(p-tolyloxy)isoquinoline (3b). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (105 mg, 65% yield) as a white solid. Additionally, 4-bromoisoquinoline was isolated (36 mg, 25% yield). **3b**: TLC: R_f = 0.74 (PE : EA = 10:1). Melting point: 77.0-77.2 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, J = 8.4 Hz, 1H), 7.96 (d, J = 6.0 Hz, 1H), 7.78 (d, J = 8.4 Hz, 1H), 7.72-7.69 (m, 1H), 7.62-7.59 (m, 1H), 7.28 (d, J = 5.4 Hz, 1H), 7.25-7.24 (m, 2H), 7.14-7.13 (m, 2H), 2.38 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.1, 151.7, 140.1, 138.6, 134.7, 130.9, 130.3, 127.2, 126.4, 124.4, 121.8, 120.0, 116.2, 21.1. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}NO$ 236.1070; found 236.1066.

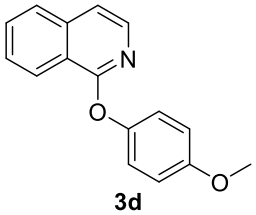
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{105}{162} \times 1 = 65\%$$



3c

1-(4-(tert-butyl)phenoxy)isoquinoline (3c). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (82 mg, 43% yield) as a yellow solid. The spectroscopic data are consistent with previously reported.[4] TLC: R_f = 0.74 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, J = 8.4 Hz, 1H), 7.99 (d, J = 6.0 Hz, 1H), 7.80 (d, J = 7.8 Hz, 1H), 7.73 (t, J = 7.8 Hz, 1H), 7.62 (t, J = 7.8 Hz, 1H), 7.47-7.46 (m, 2H), 7.31 (d, J = 6.0 Hz, 1H), 7.20-7.19 (m, 2H), 1.36 (s, 9H).

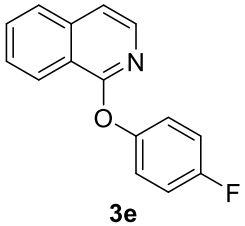
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{82}{191} \times 1 = 43\%$$



3d

1-(4-methoxyphenoxy)isoquinoline (3d). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (90 mg, 52% yield) as a white solid. Additionally, 4-bromoisoquinoline was isolated (29 mg, 20% yield). The spectroscopic data of major product are consistent with previously reported.[6] TLC: R_f = 0.70 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (d, J = 9.6 Hz, 1H), 7.97 (d, J = 6.0 Hz, 1H), 7.80-7.79 (m, 1H), 7.74-7.71 (m, 1H), 7.64-7.61 (m, 1H), 7.30 (d, J = 6.6 Hz, 1H), 7.20-7.18 (m, 2H), 7.00-6.98 (m, 2H), 3.84 (s, 3H).

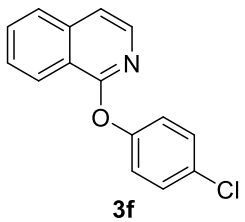
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{90}{173} \times 1 = 52\%$$



3e

1-(4-fluorophenoxy)isoquinoline (3e). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (111 mg, 67% yield) as a colorless solid. Additionally, 4-bromoisoquinoline was isolated (36 mg, 25% yield). The spectroscopic data of major product are consistent with previously reported.[7] TLC: R_f = 0.64 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 5.4 Hz, 1H), 7.82-7.81 (d, J = 7.8 Hz, 1H), 7.76-7.73 (m, 1H), 7.66-7.63 (m, 1H), 7.33 (d, J = 5.4 Hz, 1H), 7.25-7.22 (m, 2H), 7.16-7.13 (m, 2H).

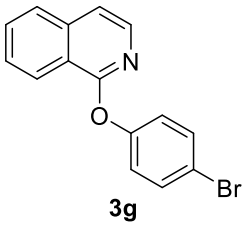
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{111}{165} \times 1 = 67\%$$



3f

1-(4-chlorophenoxy)isoquinoline (3f). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (123 mg, 70% yield) as a white solid. Additionally, 4-bromoisoquinoline was isolated (35 mg, 24% yield). The spectroscopic data of major product are consistent with previously reported.[6] TLC: R_f = 0.64 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (d, J = 9.6 Hz, 1H), 7.97 (d, J = 6.0 Hz, 1H), 7.80 (d, J = 7.8 Hz, 1H), 7.76-7.73 (m, 1H), 7.65-7.63 (m, 1H), 7.42-7.41 (m, 2H), 7.34 (d, J = 6.6 Hz, 1H), 7.22-7.21 (m, 2H).

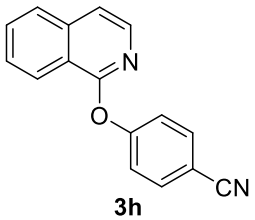
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{123}{176} \times 1 = 70\%$$



3g

1-(4-bromophenoxy)isoquinoline (3g). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (93 mg, 45% yield) as a colorless oil. Additionally, 4-bromoisoquinoline was isolated (29 mg, 20% yield). **3g**: TLC: R_f = 0.64 (PE : EA = 10:1). Melting point: 119.4-119.7 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (d, J = 9.0 Hz, 1H), 7.97 (d, J = 6.0 Hz, 1H), 7.82-7.81 (m, 1H), 7.76-7.73 (m, 1H), 7.65-7.63 (m, 1H), 7.57-7.56 (m, 2H), 7.34 (d, J = 6.6Hz, 1H), 7.17-7.16 (m, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.4, 153.1, 139.8, 138.7, 132.8, 131.1, 127.4, 126.5, 124.2, 123.9, 119.8, 118.1, 116.9. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrNO$ 300.0019; found 300.0017.

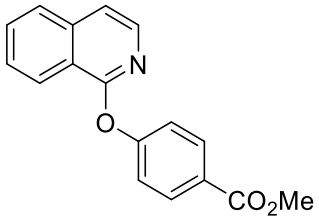
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{93}{207} \times 1 = 45\%$$



3h

4-(isoquinolin-1-yloxy)benzonitrile (3h). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (77 mg, 45% yield) as a yellow solid. Additionally, 4-bromoisoquinoline was isolated (27 mg, 19% yield). The spectroscopic data of major product are consistent with previously reported.[6] TLC: R_f = 0.68 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (d, J = 8.4 Hz, 1H), 7.98 (d, J = 6.0 Hz, 1H), 7.85-7.84 (m, 1H), 7.78-7.75 (m, 1H), 7.74-7.73 (m, 2H), 7.67-7.65 (m, 1H), 7.41 (d, J = 6.0 Hz, 1H), 7.39-7.38 (m, 2H).

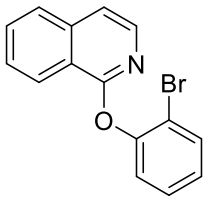
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{77}{170} \times 1 = 45\%$$



3i

methyl 4-(isoquinolin-1-yloxy)benzoate (3i). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (77 mg, 40% yield) as a yellow solid. TLC: R_f = 0.45 (PE : EA = 10:1). Melting point: 89.8-90.2 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, J = 7.8 Hz, 1H), 8.15-8.14 (m, 2H), 7.99 (d, J = 6.0 Hz, 1H), 7.84-7.82 (m, 1H), 7.76-7.74 (m,1H), 7.66-7.63 (m, 1H), 7.38 (d, J = 5.4 Hz, 1H), 7.34-7.32 (m, 2H), 3.93 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 166.7, 160.1, 158.1, 139.8, 138.8, 131.6, 131.2, 127.5, 126.7, 126.5, 124.2, 121.6, 120.0, 117.2, 52.2. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{17}H_{14}NO_3$ 280.0968; found 280.0965.

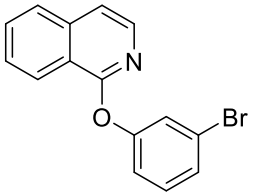
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{77}{193} \times 1 = 40\%$$



3j

1-(2-bromophenoxy)isoquinoline (3j). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (95 mg, 46% yield) as a yellow oil. Additionally, 4-bromoisoquinoline was isolated (36 mg, 25% yield). **3j**: TLC: R_f = 0.60 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, J = 7.8 Hz, 1H), 7.95 (d, J = 5.4 Hz, 1H), 7.83-7.82 (m, 1H), 7.77-7.74 (m, 1H), 7.70-7.66 (m, 2H), 7.44-7.41 (m, 1H), 7.36-7.34 (m, 2H), 7.18-7.15 (m, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 159.9, 151.2, 139.8, 138.7, 133.8, 131.1, 128.7, 127.4, 126.8, 126.4, 124.6, 124.5, 119.6, 116.9 116.8. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrNO$ 300.0019; found 300.0016.

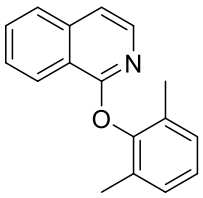
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{95}{207} \times 1 = 46\%$$



3k

1-(3-bromophenoxy)isoquinoline (3k). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (89 mg, 43% yield) as a yellow oil. Additionally, 4-bromoisoquinoline was isolated (35 mg, 24% yield). **3k**: TLC: R_f = 0.66 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.40 (d, J = 8.4 Hz, 1H), 7.98 (d, J = 5.4 Hz, 1H), 7.83-7.82 (m, 1H), 7.76-7.73 (m, 1H), 7.65-7.63 (m, 1H), 7.46-7.45 (m, 1H), 7.40-7.38 (m, 1H), 7.36 (d, J = 5.4 Hz, 1H), 7.32 (t, J = 8.4 Hz, 1H), 7.23-7.21 (m, 1H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.2, 154.7, 139.8, 138.7, 131.2, 130.8, 128.3, 127.5, 126.5, 125.5, 124.2, 122.8, 120.8, 119.9, 117.0. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrNO$ 300.0019; found 300.0016.

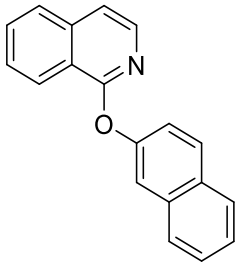
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{89}{207} \times 1 = 43\%$$



3l

1-(2,6-dimethylphenoxy)isoquinoline (3l). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (98 mg, 57% yield) as a yellow solid. Additionally, 4-bromoisoquinoline was isolated (30 mg, 21% yield). **3l**: TLC: R_f = 0.66 (PE : EA = 10:1). Melting point: 46.1-46.3 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.54 (d, J = 9.6 Hz, 1H), 7.95 (d, J = 6.0 Hz, 1H), 7.83 (d, J = 8.4 Hz, 1H), 7.77-7.74 (m, 1H), 7.67-7.65 (m, 1H), 7.29 (d, J = 6.0 Hz, 1H), 7.18-7.17 (m, 2H), 7.15-7.12 (m, 1H), 2.17 (s, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 159.6, 150.7, 140.3, 138.6, 131.2, 130.9, 128.8, 127.2, 126.5, 125.6, 124.4, 119.3, 115.9, 16.7. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{17}H_{16}NO$ 250.1226; found 250.1223.

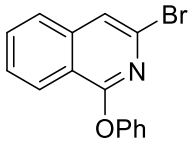
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{98}{172} \times 1 = 57\%$$



3m

1-(naphthalen-2-yloxy)isoquinoline (3m). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (85 mg, 45% yield) as a yellow solid. Additionally, 4-bromoisoquinoline was isolated (26 mg, 18% yield). The spectroscopic data of major product are consistent with previously reported.[4] TLC: R_f = 0.63 (PE: EA = 10:1). ^{1}H NMR (600 MHz,$CDCl_3$) δ 8.64 (d, J = 9.6 Hz, 1H), 7.97 (d, J = 9.8 Hz, 1H), 7.93-7.91 (m, 2H), 7.87-7.85 (m, 1H), 7.80-7.77 (m, 2H), 7.72-7.69 (m, 1H), 7.57 (t, J = 7.8 Hz, 1H), 7.52-7.49 (m, 1H), 7.44-7.40 (m, 2H), 7.34 (d, J = 6.6 Hz, 1H).

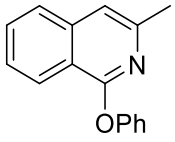
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{85}{187} \times 1 = 45\%$$



3n

3-bromo-1-phenoxyisoquinoline **(3n)**. Following **GP 1**, using 3-bromoisoquinoline *N*-oxide (154 mg, 0.69 mmol), the title compound was obtained (157 mg, 76% yield) as a yellow solid. TLC: R_f = 0.69 (PE : EA = 10:1). Melting point: 66.3-67.1 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.44 (d, J = 8.4 Hz, 1H), 8.13-8.10 (m, 2H), 7.85-7.82 (m, 1H), 7.69-7.67 (m, 1H), 7.46-7.43 (m, 2H), 7.27-7.23 (m, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.3, 153.7, 141.2, 136.9, 132.2, 129.8, 128.2, 126.1, 125.4, 124.8, 121.9, 121.1, 113.1. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrNO$ 300.0019; found 300.0015.

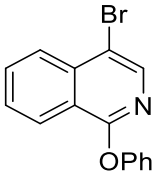
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{157}{207} \times 1 = 76\%$$



3o

3-methyl-1-phenoxyisoquinoline (3o). Following **GP 1**, using 3-methylisoquinoline *N*-oxide (110 mg, 0.69 mmol), the title compound was obtained (70 mg, 43% yield) as a colorless oil. TLC: R_f = 0.65 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (d, J = 8.4 Hz, 1H), 7.72-7.66 (m, 2H), 7.55-7.52 (m, 1H), 7.45-7.42 (m, 2H), 7.30-7.28 (m, 2H), 7.24-7.21 (m, 1H), 7.18 (s, 1H), 2.48 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 159.5, 154.6, 149.3, 139.5, 130.8, 129.4, 126.2, 125.8, 124.4, 124.3, 121.4, 118.3, 114.5, 24.1. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}NO$ 236.1070; found 236.1066.

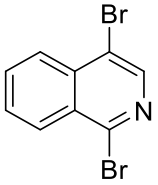
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{70}{162} \times 1 = 43\%$$



3p

4-bromo-1-phenoxyisoquinoline (3p). Following **GP I**, using 4-bromoisoquinoline *N*-oxide (154 mg, 0.69 mmol), the title compound was obtained (110 mg, 53% yield) as a yellow solid. Purification by flash column chromatography (PE : DCM = 5:1-1:1) furnishes the desired pure product. Additionally, 1,4-dibromoisoquinoline (**4-bis**) was isolated (42 mg, 21% yield) as a yellow solid. **3p**: TLC: R_f = 0.78 (PE : DCM = 1:1). Melting point: 66.7-67.3 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, J = 8.4 Hz, 1H), 8.15-8.12 (m, 2H), 7.86-7.84 (m, 1H), 7.71-7.68 (m, 1H), 7.47-7.44 (m, 2H), 7.29-7.26 (m, 1H), 7.25-7.24 (m, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.3, 153.7, 141.2, 136.9, 132.2, 129.8, 128.2, 126.1, 125.5, 124.8, 122.0, 121.1, 113.1. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrNO$ 300.0019; found 300.0015.

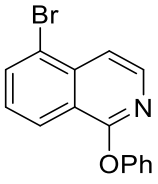
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{110}{207} \times 1 = 53\%$$



4-bis

1,4-dibromoisoquinoline (4-bis). The spectroscopic data are consistent with previously reported.[8] TLC: R_f = 0.71 (PE : DCM = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.31 (d, J = 8.4 Hz, 1H), 8.18 (d, J = 8.4 Hz, 1H), 7.87 (t, J = 7.8 Hz, 1H), 7.77 (t, J = 7.8 Hz, 1H).

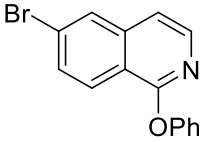
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{42}{198} \times 1 = 21\%$$



3q

5-bromo-1-phenoxyisoquinoline (3q). Following **GP 1**, using 5-bromoisoquinoline *N*-oxide (154 mg, 0.69 mmol), the title compound was obtained (128 mg, 62% yield) as a yellow solid. TLC: R_f = 0.66 (PE : EA = 10:1). Melting point: 94.8-95.4 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.43 (d, J = 8.4 Hz, 1H), 8.05 (d, J = 6.0 Hz, 1H), 7.99-7.98 (m, 1H), 7.64-7.63 (m, 1H), 7.47-7.43 (m, 3H), 7.27-7.23 (m, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.9, 153.8, 141.4, 137.8, 134.8, 129.8, 127.6, 125.4, 124.1, 122.0, 121.4, 121.2, 115.4. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrNO$ 300.0019; found 300.0017.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{128}{207} \times 1 = 62\%$$

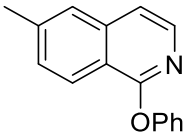


3r

6-bromo-1-phenoxyisoquinoline (3r). Following **GP 1**, using 6-bromoisoquinoline *N*-oxide (154 mg, 0.69 mmol), the title compound was obtained (68 mg, 33% yield) as a yellow solid. The spectroscopic data are consistent with previously reported.[9] TLC: R_f = 0.71 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (d, J = 9.0 Hz, 1H), 7.99-7.98 (m, 2H), 7.72-7.70 (m, 1H), 7.46 (t, J

= 7.8 Hz, 2H), 7.29-7.27 (m, 1H), 7.26-7.22 (m, 3H).

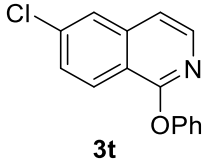
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{68}{207} \times 1 = 33\%$$



3s

6-methyl-1-phenoxyisoquinoline (3s). Following **GP 1**, using 6-methylisoquinoline *N*-oxide (110 mg, 0.69 mmol), the title compound was obtained (105 mg, 65% yield) as a yellow solid. TLC: R_f = 0.51 (PE : EA = 10:1). Melting point: 87.9-88.2 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (d, J = 8.4 Hz, 1H), 7.93 (d, J = 6.0 Hz, 1H), 7.56 (s, 1H), 7.45-7.43 (m, 3H), 7.25-7.21 (m, 4H), 2.55 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.7, 154.1, 141.4, 140.1, 139.0, 129.7, 129.4, 125.5, 125.0, 124.2, 122.0, 118.2, 116.1, 22.0. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}NO$ 236.1070; found 236.1065.

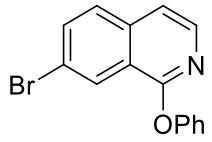
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{105}{162} \times 1 = 65\%$$



3t

6-chloro-1-phenoxyisoquinoline (3t). Following **GP 1**, using 6-chloroisoquinoline *N*-oxide (123 mg, 0.69 mmol), the title compound was obtained (88 mg, 50% yield) as a white solid. TLC: R_f = 0.72 (PE : EA = 10:1). Melting point: 85.7-86.3 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (d, J = 9.0 Hz, 1H), 7.97 (d, J = 6.0 Hz, 1H), 7.78 (d, J = 1.8 Hz, 1H), 7.55 (dd, J = 9.0 Hz, 2.4 Hz, 1H), 7.47-7.44 (m, 2H), 7.27-7.21 (m, 4H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.8, 153.7, 141.4, 139.5, 137.4, 129.8, 128.2, 126.3, 125.4, 125.3, 122.0, 118.2, 115.6. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}ClNO$ 256.0524; found 256.0522.

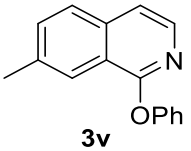
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{88}{176} \times 1 = 50\%$$



3u

7-bromo-1-phenoxyisoquinoline (3u). Following **GP 1**, using 7-bromoisoquinoline *N*-oxide (154 mg, 0.69 mmol), the title compound was obtained (104 mg, 50% yield) as a yellow solid. The spectroscopic data are consistent with previously reported.[9] TLC: R_f = 0.55 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.61 (s, 1H), 7.98 (d, J = 6.0 Hz, 1H), 7.80-7.79 (m, 1H), 7.68-7.66 (m, 1H), 7.47-7.44 (m, 2H), 7.28-7.27 (m, 2H), 7.25-7.24 (m, 2H).

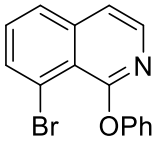
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{104}{207} \times 1 = 50\%$$



3v

7-methyl-1-phenoxyisoquinoline (3v). Following **GP 1**, using 7-methylisoquinoline *N*-oxide (110 mg, 0.69 mmol), the title compound was obtained (62 mg, 38% yield) as a yellow solid. The spectroscopic data are consistent with previously reported.[10] TLC: R_f = 0.63 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.91 (d, J = 6.0 Hz, 1H), 7.71-7.70 (m, 1H), 7.57-7.55 (m, 1H), 7.46-7.44 (m, 2H), 7.28 (d, J = 6.0 Hz, 1H), 7.26-7.24 (m, 3H), 2.58 (s, 3H).

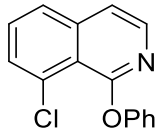
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{62}{162} \times 1 = 38\%$$



3w

8-bromo-1-phenoxyisoquinoline (3w). Following **GP 1**, using 8-bromoisoquinoline *N*-oxide (154 mg, 0.69 mmol), the title compound was obtained (112 mg, 54% yield) as a white solid. TLC: R_f = 0.58 (PE : EA = 10:1). Melting point: 78.5-78.8 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, J = 6.0 Hz, 1H), 7.93-7.92 (m, 1H), 7.74-7.72 (m, 1H), 7.47-7.44 (m, 3H), 7.32 (d, J = 5.4 Hz, 1H), 7.26-7.23 (m, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 159.4, 153.6, 141.4, 140.4, 134.4, 130.9, 129.8, 126.6, 125.0, 121.9, 119.1, 118.7, 117.2. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}BrNO$ 300.0019; found 300.0017.

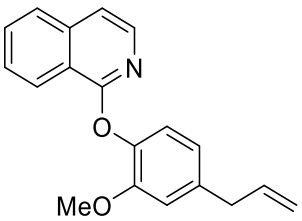
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{112}{207} \times 1 = 54\%$$



3x

8-chloro-1-phenoxyisoquinoline (3x). Following **GP 1**, using 8-chloroisoquinoline *N*-oxide (123 mg, 0.69 mmol), the title compound was obtained (128 mg, 73% yield) as a white solid. TLC: R_f = 0.52 (PE : EA = 10:1). Melting point:105.7-105.8 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, J = 5.4 Hz, 1H), 7.69-7.66 (m, 2H), 7.57-7.54 (m, 1H), 7.47-7.44 (m, 2H), 7.31 (d, J = 5.4 Hz, 1H), 7.26-7.24 (m, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 159.8, 153.8,141.4, 140.5, 131.5, 130.5, 130.3, 129.7, 125.8, 125.0, 121.9, 117.9, 117.0. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{15}H_{11}ClNO$ 256.0524; found 256.0521.

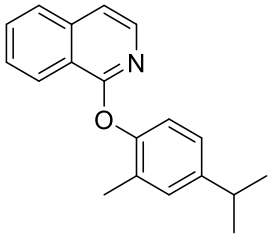
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{128}{176} \times 1 = 73\%$$



3y

1-(4-allyl-2-methoxyphenoxy)isoquinoline (3y). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (94 mg, 47% yield) as a white solid. TLC: R_f = 0.49 (PE : EA = 10:1). Melting point: 88.7-88.8 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.49 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 6.0 Hz, 1H), 7.80-7.78 (m, 1H), 7.73-7.70 (m, 1H), 7.63-7.60 (m, 1H), 7.28 (d, J = 6.0 Hz, 1H), 7.16 (d, J = 7.8 Hz, 1H), 6.89-6.86 (m, 2H), 6.06-6.00 (m, 1H), 5.17-5.11 (m, 2H), 3.73 (s, 3H), 3.44 (d, J = 6.6 Hz, 2H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.7, 151.7, 141.0, 140.1, 138.5, 138.3, 137.4, 130.8, 127.0, 126.3, 124.7, 123.3, 121.2, 119.7, 116.2, 116.1, 113.5, 56.1, 40.3. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{19}H_{18}NO_2$ 292.1332; found 292.1328.

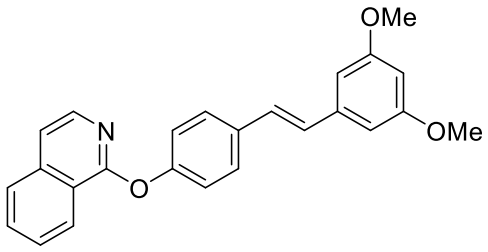
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{94}{201} \times 1 = 47\%$$



3z

1-(4-isopropyl-2-methylphenoxy)isoquinoline (3z). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (124 mg, 65% yield) as a yellow oil. TLC: R_f = 0.63 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.49 (d, J = 7.2 Hz, 1H), 7.97 (d, J = 6.0 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.75-7.72 (m, 1H), 7.65-7.62 (m, 1H), 7.29 (d, J = 4.8 Hz, 1H), 7.24 (d, J = 8.4 Hz, 1H), 7.09-7.07 (m, 1H), 7.05 (s, 1H), 2.96-2.90 (m, 1H), 2.15 (s, 3H), 1.27 (d, J = 7.2 Hz, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.5, 152.2, 148.3, 140.2, 138.6, 131.2, 130.9, 128.1, 127.2, 126.4, 124.5, 123.8, 120.5, 119.7, 116.0, 33.8, 24.1, 16.2. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{19}H_{20}NO$ 278.1539; found 278.1538.

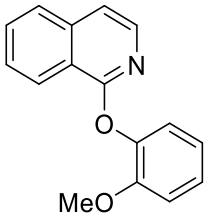
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{124}{191} \times 1 = 65\%$$



3aa

(E)-1-(4-(3,5-dimethoxystyryl)phenoxy)isoquinoline (3aa). Following **GP 1**, using isoquinoline 2-oxide (100 mg, 0.69 mmol), the title compound was obtained (116 mg, 44% yield) as a white solid. TLC: R_f = 0.66 (PE : EA = 10:1). Melting point:142.8-143.3 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.46 (d, J = 8.4 Hz, 1H), 8.01 (d, J = 6.0 Hz, 1H), 7.83-7.81 (m, 1H), 7.76-7.73 (m, 1H), 7.66-7.63 (m, 1H), 7.61 (d, J = 8.4 Hz, 2H), 7.34 (d, J = 6.0 Hz, 1H), 7.30-7.28 (m, 2H), 7.16-7.13 (m, 1H), 7.05-7.02 (m, 1H), 6.71 (d, J = 1.8 Hz, 2H), 6.43 (t, J = 2.4 Hz, 1H), 3.86 (s, 6H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.1, 160.7, 153.6, 139.9, 139.5, 138.6, 134.2, 131.0, 128.6, 128.5, 127.9, 127.3, 126.4, 124.3, 122.2, 119.9, 116.6, 104.6, 100.1, 55.4. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{25}H_{22}NO_3$ 384.1594; found 384.1594.

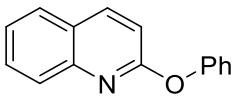
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{116}{265} \times 1 = 44\%$$



3ab

1-(2-methoxyphenoxy)isoquinoline (3ab). Following **GP 1**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (69 mg, 40% yield) as a white solid. TLC: R_f = 0.37 (PE : EA = 10:1). Melting point: 105.9-106.1°C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.50 (d, J = 8.4 Hz, 1H), 7.94 (d, J = 6.0 Hz, 1H), 7.79-7.78 (m, 1H), 7.72-7.69 (m, 1H), 7.63-7.60 (m, 1H), 7.28 (d, J = 6.0 Hz, 1H), 7.26-7.23 (m, 2H), 7.06-7.03 (m, 2H), 3.73 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.6, 152.0, 144.8, 140.1, 138.5, 130.8, 127.0, 126.3, 124.6, 123.6, 121.2, 119.6, 116.1, 113.1, 56.0. HRMS (+ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{16}H_{14}NO_2$ 252.1019; found 252.1018.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{69}{173} \times 1 = 40\%$$



6a

2-phenoxyquinoline (6a). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (106 mg, 69% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.70 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.74 (d, J = 7.8 Hz, 1H), 7.60 (t, J = 7.8 Hz, 1H), 7.43-7.39 (m, 3H), 7.26-7.21 (m, 3H), 7.06 (d, J = 8.4 Hz, 1H).

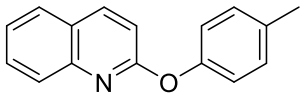
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{106}{153} \times 1 = 69\%$$

Gram scale synthesis:

In a 2-necked 50 mL round bottom flask equipped with a magnetic stir bar was added isoquinoline *N*-oxide (1.0 g, 6.9 mmol) and dry EA (7 mL), followed by PhOH (0.98 g, 10.4 mmol), DIEA (1.78 g, 13.8 mmol) and HMPA (0.12 g, 0.69 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of $POBr_3$ (1.98 g, 6.9 mmol) in dry EA (7 mL). The reaction mixture is then warmed to room temperature and stirred for 30 minutes. The reaction was quenched with a saturated potassium carbonate solution (5 mL) and the organic phase was separated. The aqueous phase was extracted once with EA (15 mL). The organic phase was combined, dried over Na_2SO_4 and

concentrated in vacuo to give the crude product. Purification by flash chromatography (PE : EA = 150:1-100:1) furnishes the desired pure product (950 mg, 62%).

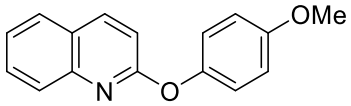
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{0.95}{1.53} \times 1 = 62\%$$



6b

2-(p-tolyloxy)quinoline (6b). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (141 mg, 87% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.50 (PE : acetone = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, J = 9.0 Hz, 1H), 7.82 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.63-7.60 (m, 1H), 7.42 (t, J = 7.2 Hz, 1H), 7.24-7.23 (m, 2H), 7.16-7.15 (m, 2H), 7.07 (d, J = 9.0 Hz, 1H), 2.40 (s, 3H).

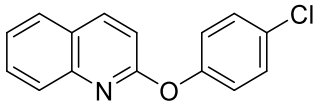
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{141}{162} \times 1 = 87\%$$



6c

2-(4-methoxyphenoxy)quinoline (6c). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (137 mg, 79% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.50 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, J = 9.0 Hz, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 7.8 Hz, 1H), 7.61 (t, J = 7.2 Hz, 1H), 7.41 (t, J = 7.2 Hz, 1H), 7.20-7.18 (m, 2H), 7.05 (d, J = 9.0 Hz, 1H), 6.97-6.95 (m, 2H), 3.84 (s, 3H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{137}{173} \times 1 = 79\%$$

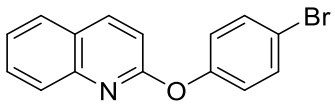


6d

2-(4-chlorophenoxy)quinoline (6d). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69

mmol), the title compound was obtained (111 mg, 63% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.74 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, J = 9.0 Hz, 1H), 7.79-7.76 (m, 2H), 7.64-7.61 (m, 1H), 7.44 (t, J = 7.8 Hz, 1H), 7.40-7.38 (m, 2H), 7.23-7.21 (m, 2H), 7.09 (d, J = 9.0 Hz, 1H).

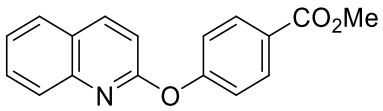
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{111}{176} \times 1 = 63\%$$



6e

2-(4-bromophenoxy)quinoline (6e). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (114 mg, 55% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.60 (PE : acetone = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (d, J = 9.0 Hz, 1H), 7.78 (t, J = 9.0 Hz, 2H), 7.64-7.61 (m, 1H), 7.55-7.52 (m, 2H), 7.44 (t, J = 7.2 Hz, 1H), 7.18-7.15 (m, 2H), 7.09 (d, J = 9.0 Hz, 1H).

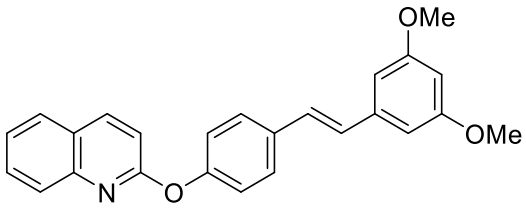
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{114}{207} \times 1 = 55\%$$



6f

methyl 4-(quinolin-2-yloxy)benzoate (6f). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (100 mg, 52% yield) as a white solid. TLC: R_f = 0.50 (PE : EA = 10:1). Melting point: 63.9-64.1 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.16 (d, J = 9.0 Hz, 1H), 8.12-8.11 (m, 2H), 7.79 (t, J = 7.8 Hz, 2H), 7.64 (t, J = 8.4 Hz, 1H), 7.46 (t, J = 7.2 Hz, 1H), 7.33-7.32 (m, 2H), 7.13 (d, J = 9.0 Hz, 1H), 3.93 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 166.8, 161.0, 158.0, 146.4, 140.2, 131.5, 130.1, 128.1, 127.5, 126.4, 126.1, 125.4, 121.0, 113.1, 52.2. HRMS (+ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{17}H_{14}NO_3$ 280.0968; found 280.0966.

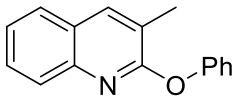
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{100}{193} \times 1 = 52\%$$



6g

(E)-2-(4-(3,5-dimethoxystyryl)phenoxy)quinoline (6g). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (180 mg, 68% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.45 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, J = 9.0 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.62 (t, J = 8.4 Hz, 1H), 7.56 (d, J = 9.0 Hz, 2H), 7.43 (t, J = 7.2 Hz, 1H), 7.26-7.25 (m, 2H), 7.13-7.09 (m, 2H), 7.03-7.00 (m, 1H), 6.68 (d, J = 2.4 Hz, 2H), 6.41-6.40 (m, 1H), 3.84 (s, 6H).

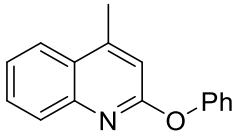
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{180}{265} \times 1 = 68\%$$



6h

3-methyl-2-phenoxyquinoline (6h). Following **GP 2**, using 3-methylquinoline *N*-oxide (110 mg, 0.69 mmol), the title compound was obtained (66 mg, 41% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.45 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.70 (dd, J = 16.2 Hz, 8.4 Hz, 2H), 7.52-7.50 (m, 1H), 7.43-7.41(m, 2H), 7.38-7.36 (m, 1H), 7.26-7.25 (m, 2H), 7.23-7.20 (m, 1H), 2.50 (s, 3H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{66}{162} \times 1 = 41\%$$

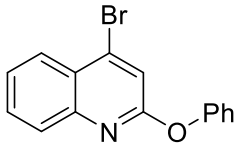


6i

4-methyl-2-phenoxyquinoline (6i). Following **GP 2**, using 4-methylquinoline *N*-oxide (110 mg, 0.69 mmol), the title compound was obtained (87 mg, 54% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.80 (PE : EA = 10:1). ^{1}H NMR (600 MHz,

$CDCl_3$) δ 7.90 (d, J = 8.4 Hz, 1H), 7.81 (d, J = 8.4 Hz, 1H), 7.61-7.59 (m, 1H), 7.44-7.40 (m, 3H), 7.24-7.23 (m, 2H), 7.22-7.20 (m, 1H), 6.91 (s, 1H), 2.66 (s, 3H).

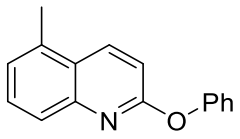
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{87}{162} \times 1 = 54\%$$



6j

4-bromo-2-phenoxyquinoline (6j). Following **GP 2**, using 4-bromoquinoline *N*-oxide (154 mg, 0.69 mmol), the title compound was obtained (130 mg, 63% yield) as a white solid. The spectroscopic data are consistent with previously reported.[12] TLC: R_f = 0.80 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, J = 9.6 Hz, 1H), 7.78-7.77 (m, 1H), 7.65-7.63 (m, 1H), 7.51-7.48 (m, 1H), 7.44-7.42 (m, 2H), 7.40 (s, 1H), 7.25-7.23 (m, 3H).

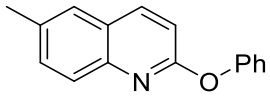
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{130}{207} \times 1 = 63\%$$



6k

5-methyl-2-phenoxyquinoline (6k). Following **GP 2**, using 5-methylquinoline *N*-oxide (110 mg, 0.69 mmol), the title compound was obtained (87 mg, 54% yield) as a white solid. TLC: R_f = 0.80 (PE : EA = 10:1). Melting point: 94.8-95.1 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.29 (d, J = 9.0 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.50 (t, J = 7.2 Hz, 1H), 7.42 (t, J = 7.8 Hz, 2H), 7.26-7.22 (m, 4H), 7.08 (d, J = 9.0 Hz, 1H), 2.66 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.5, 154.2, 146.9, 136.6, 134.6, 129.8, 129.7, 126.3, 125.8, 125.1, 124.8, 121.4, 112.1, 18.9. HRMS (+ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{16}H_{14}NO$ 236.1070; found 236.1067.

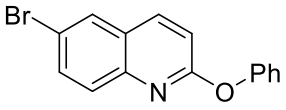
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{87}{162} \times 1 = 54\%$$



6l

6-methyl-2-phenoxyquinoline (6l). Following **GP 2**, using 6-methylquinoline *N*-oxide (110 mg, 0.69 mmol), the title compound was obtained (92 mg, 57% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.80 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, J = 8.4 Hz, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.53 (s, 1H), 7.46 (dd, J = 9.0 Hz, 2.4 Hz, 1H), 7.43-7.41 (m, 2H), 7.26-7.21 (m, 3H), 7.04 (d, J = 9.0 Hz, 1H), 2.50 (s, 3H).

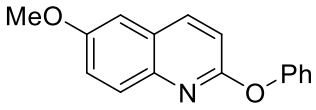
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{92}{162} \times 1 = 57\%$$



6m

6-bromo-2-phenoxyquinoline (6m). Following **GP 2**, using 6-bromoquinoline *N*-oxide (154 mg, 0.69 mmol), the title compound was obtained (148 mg, 71% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.50 (PE : acetone = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, J = 9.0 Hz, 1H), 7.91 (d, J = 1.8 Hz, 1H), 7.69-7.65 (m, 2H),7.44 (t, J = 8.4 Hz, 2H), 7.27-7.24 (m, 3H), 7.11 (d, J = 9.0 Hz, 1H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{148}{207} \times 1 = 71\%$$

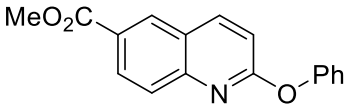


6n

6-methoxy-2-phenoxyquinoline (6n). Following **GP 2**, using 6-methoxyquinoline *N*-oxide (121 mg, 0.69 mmol), the title compound was obtained (100 mg, 58% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.50 (PE : DCM = 1:3). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, J = 9.0 Hz, 1H), 7.73 (d, J = 9.0 Hz, 1H), 7.41 (t, J = 8.4 Hz, 2H), 7.29 (dd, J = 3.0 Hz, 9.6 Hz, 1H), 7.24-7.20 (m, 3H), 7.08 (d, J = 3.0 Hz, 1H), 7.05 (d, J = 9.0 Hz,

1H), 3.91 (s, 3H).

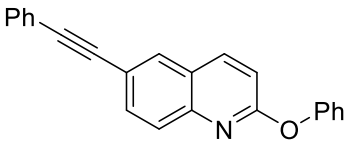
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{100}{173} \times 1 = 58\%$$



6o

methyl 2-phenoxyquinoline-6-carboxylate (6o). Following **GP 2**, using 6-(methoxycarbonyl) quinoline *N*-oxide (140 mg, 0.69 mmol), the title compound was obtained (119 mg, 62% yield) as a white solid. The spectroscopic data are consistent with previously reported.[11] TLC: R_f = 0.30 (PE : DCM = 1:3). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, J = 1.8 Hz, 1H), 8.21-8.19 (m, 2H), 7.79 (d, J = 8.4 Hz, 1H), 7.45 (t, J = 7.8 Hz, 2H), 7.27-7.26 (m, 3H), 7.14 (d, J = 8.4 Hz, 1H), 3.97 (s, 3H).

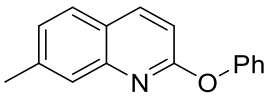
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{119}{193} \times 1 = 62\%$$



6p

2-phenoxy-6-(phenylethynyl)quinoline (6p). Following **GP 2**, using 6-(phenylethynyl)quinoline *N*-oxide (169 mg, 0.69 mmol), the title compound was obtained (93 mg, 42% yield) as a white solid. TLC: R_f = 0.50 (PE : DCM = 5:1). Melting point: 164.1-164.3 °C.^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, J = 9.0 Hz, 1H), 7.98 (s, 1H), 7.78-7.73 (m, 2H), 7.59-7.56 (m, 2H), 7.46 (t, J = 7.8 Hz, 2H), 7.40-7.36 (m, 3H), 7.29-7.27 (m, 3H), 7.12 (d, J = 9.0 Hz, 1H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) 162.3, 153.8, 146.2, 139.6, 132.8, 131.8, 130.8, 129.7, 128.6, 128.2, 125.6, 125.0, 123.3, 121.7, 119.9, 113.6, 90.1, 89.3. HRMS (+ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{23}H_{16}NO$ 322.1226; found 322.1224.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{93}{222} \times 1 = 42\%$$

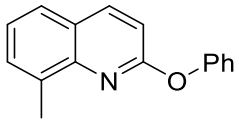


6q

7-methyl-2-phenoxyquinoline. (6q). Following **GP 2**, using 7-methylquinoline *N*-oxide (110 mg,

0.69 mmol), the title compound was obtained (88 mg, 54% yield) as a white solid. TLC: R_f = 0.80 (PE : EA = 10:1). Melting point: 45.4-45.6 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, J = 9.0 Hz, 1H), 7.65 (d, J = 8.4 Hz,1H), 7.61 (s, 1H), 7.44-7.41 (m, 2H), 7.27-7.22 (m, 4H), 7.01 (d, J = 9.0 Hz, 1H), 2.49 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.9, 154.2, 146.8, 140.4, 139.6, 129.7, 127.3, 127.1, 124.7, 123.8, 121.5, 111.8, 21.9. HRMS (+ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{16}H_{14}NO$ 236.1070; found 230.1067.

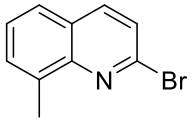
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{88}{162} \times 1 = 54\%$$



6r

8-methyl-2-phenoxyquinoline (6r). Following **GP 2**, using 8-methylquinoline *N*-oxide (110 mg, 0.69 mmol), the title compound was obtained (49 mg, 30% yield) as a white solid. Additionally, 2-bromo-8-methylquinoline (**6r-bis**) was isolated (44 mg, 29% yield) as a white solid. **6r**: TLC: R_f = 0.40 (PE : DCM= 5:1). Melting point: 64.0-64.2 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, J = 8.4 Hz, 1H), 7.60 (d, J = 7.8 Hz, 1H), 7.48 (d, J = 6.6 Hz, 1H), 7.44-7.41 (m, 2H), 7.33-7.31 (m, 3H), 7.23 (t, J = 7.8 Hz, 1H), 7.06 (d, J = 8.4 Hz, 1H). 2.55 (s, 3H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.9, 154.2, 145.4, 140.2, 136.0, 130.2, 129.5, 125.7, 125.3, 124.6, 121.6, 112.2, 17.6. HRMS (+ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{16}H_{14}NO$ 236.1070; found 230.1066.

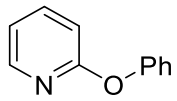
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{49}{162} \times 1 = 30\%$$



6r-bis

2-bromo-8-methylquinoline (6r-bis). The spectroscopic data are consistent with previously reported.[8] TLC: R_f = 0.60 (PE : DCM = 5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (d, J = 8.4 Hz, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.57 (d, J = 7.2 Hz, 1H), 7.49 (d, J = 8.4 Hz, 1H), 7.45 (t, J = 7.2 Hz, 1H), 2.77 (s, 3H).

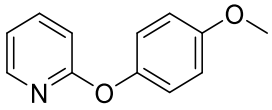
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{44}{153} \times 1 = 29\%$$



7a

2-phenoxypyridine (7a). Following **GP 3**, using pyridine *N*-oxide (100 mg, 1.05 mmol), the title compound was obtained (104 mg, 58% yield) as a white solid. The spectroscopic data are consistent with previously reported.[13] TLC: R_f = 0.50 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22-8.21 (m, 1H), 7.69-7.67 (m, 1H), 7.44-7.39 (m, 2H), 7.22-7.19 (m, 1H), 7.16-7.14 (m, 2H), 7.00-6.98 (m, 1H), 6.91 (d, J = 8.4 Hz, 1H).

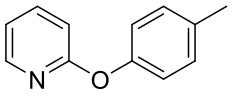
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{104}{180} \times 1 = 58\%$$



7b

2-(4-methoxyphenoxy)pyridine (7b). Following **GP 3**, using pyridine *N*-oxide (100 mg, 1.05 mmol), the title compound was obtained (99 mg, 47% yield) as a white solid. The spectroscopic data are consistent with previously reported.[13] TLC: R_f = 0.35 (PE : EA= 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19-8.18 (m, 1H), 7.67-7.64 (m, 1H), 7.08-7.07 (m, 2H), 6.96-6.92 (m, 3H), 6.86 (d, J = 8.4 Hz, 1H), 3.81 (s, 3H).

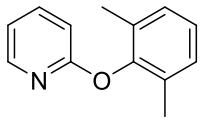
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{99}{211} \times 1 = 47\%$$



7c

2-(p-tolyloxy)pyridine (7c). Following **GP 3**, using pyridine *N*-oxide (100 mg, 1.05 mmol), the title compound was obtained (81 mg, 42% yield) as a white solid. The spectroscopic data are consistent with previously reported.[14] TLC: R_f = 0.70 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.16 (d, J = 7.2 Hz, 1H), 7.59 (t, J = 6.6 Hz, 1H), 7.16 (d, J = 8.4 Hz, 2H), 7.01 (d, J = 8.4 Hz, 2H), 6.91-6.89 (m, 1H), 6.84 (d, J = 7.8 Hz, 1H), 2.32 (s, 3H).

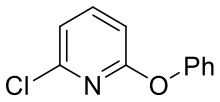
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{81}{194} \times 1 = 42\%$$



7d

2-(2,6-dimethylphenoxy)pyridine (7d). Following **GP 3**, using pyridine *N*-oxide (100 mg, 1.05 mmol), the title compound was obtained (92 mg, 44% yield) as a white solid. The spectroscopic data are consistent with previously reported.[15] TLC: R_f = 0.70 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.18 (d, J = 7.2 Hz, 1H), 7.67-7.64 (m, 1H), 7.14-7.09 (m, 3H), 6.95-6.93 (m, 1H), 6.84 (d, J = 7.8 Hz, 1H), 2.16 (s, 6H)

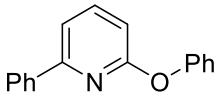
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{92}{209} \times 1 = 44\%$$



7e

2-chloro-6-phenoxypyridine (7e). Following **GP 3**, using 2-chloropyridine *N*-oxide (136 mg, 1.05 mmol), the title compound was obtained (90 mg, 42% yield) as a white solid. The spectroscopic data are consistent with previously reported.[16] TLC: R_f= 0.69 (PE : EA= 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (t, J = 7.8 Hz, 1H), 7.42-7.39 (m, 2H), 7.22 (t, J = 7.2 Hz, 1H), 7.15-7.14 (m, 2H), 7.03 (d, J = 7.8 Hz, 1H), 6.74 (d, J = 7.8 Hz, 1H).

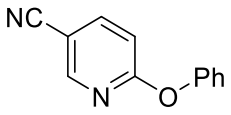
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{90}{216} \times 1 = 42\%$$



7f

2-phenoxy-6-phenylpyridine (7f). Following **GP 3**, using 2-phenylpyridine *N*-oxide (180 mg, 1.05 mmol), the title compound was obtained (163 mg, 63% yield) as a colorless oil. The spectroscopic data are consistent with previously reported.[17] TLC: R_f = 0.70 (PE : EA= 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79-7.78 (m, 2H), 7.52 (t, J = 7.8 Hz, 1H), 7.29 (d J = 7.8 Hz, 1H), 7.27-7.23 (m, 4H), 7.21-7.18 (m, 1H), 7.09-7.04 (m, 3H), 6.61 (d, J = 7.8 Hz, 1H).

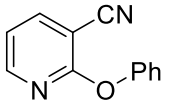
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{163}{260} \times 1 = 63\%$$



7g-1

6-phenoxynicotinonitrile (7g-1). Following **GP 3**, using 3-cyanopyridine *N*-oxide (126 mg, 1.05 mmol), 6-phenoxynicotinonitrile (**7g-1**) and 2-phenoxynicotinonitrile (**7g-2**) were obtained. The title compound was obtained (81 mg, 39% yield) as a white solid. The spectroscopic data are consistent with previously reported.[18] TLC: R_f = 0.50 (PE : EA= 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.47 (d, J = 2.4 Hz, 1H), 7.91 (dd, J = 8.4 Hz, 2.4 Hz, 1H), 7.46-7.44 (m, 2H), 7.30-7.28 (m, 1H), 7.15-7.14 (m, 2H), 7.02 (d, J = 8.4 Hz, 1H).

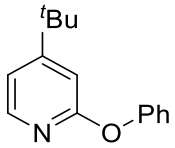
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{81}{206} \times 1 = 39\%$$



7g-2

2-phenoxynicotinonitrile (7g-2). The title compound was obtained (54 mg, 26% yield) as a white solid. The spectroscopic data are consistent with previously reported.[19] TLC: R_f = 0.30 (PE:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.31 (dd, J = 4.8 Hz, 2.4 Hz, 1H), 8.01 (dd, J = 7.2 Hz, 1.8 Hz, 1H), 7.46-7.43 (m, 2H), 7.30-7.27 (m, 1H), 7.21-7.18 (m, 2H), 7.10-7.08 (m, 1H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{54}{206} \times 1 = 26\%$$

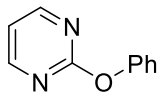


7h

4-(tert-butyl)-2-phenoxypyridine (7h). Following **GP 3**, using 4-(tert-butyl)pyridine *N*-oxide (159 mg, 1.05 mmol), the title compound was obtained (105 mg, 44% yield) as a white solid. TLC: R_f = 0.60 (PE : EA= 10:1). Melting point: 37.5-37.6 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, J = 5.4 Hz, 1H), 7.41-7.38 (m, J = 7.8 Hz, 2H), 7.18 (t, J = 7.8 Hz, 1H), 7.14 (d, J = 7.2 Hz, 2H), 7.00

(dd, J = 5.4 Hz, 1.2 Hz, 1H), 6.93 (d, J = 1.8 Hz, 1H), 1.32 (s, 9H). ^{13}C {^{1}H} NMR (150 MHz, $CDCl_3$) δ 164.3, 164.2, 154.5, 147.4, 129.7, 124.6, 121.1, 116.3, 108.6, 35.0, 30.6.HRMS (+ESI-TOF) m/z: $[M + H]^+$ calcd for $C_{15}H_{18}NO$ 228.1383; found 228.1382.

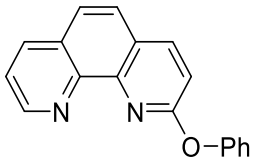
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{105}{239} \times 1 = 44\%$$



8

2-phenoxypyrimidine (8). Following **GP 1**, using pyrimidine *N*-oxide (100 mg, 1.04 mmol), the title compound was obtained (119 mg, 66% yield) as a white solid. Purification by flash column chromatography (PE : EA = 10:1-5:1) furnishes the desired pure product. The spectroscopic data are consistent with previously reported.[20] TLC: R_f = 0.68 (PE : EA = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.56 (d, J = 4.8 Hz, 2H), 7.45-7.42 (m, 2H), 7.27-7.25 (m, 1H), 7.21-7.20 (m, 2H), 7.03 (t, J = 4.8 Hz, 1H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{119}{179} \times 1 = 66\%$$

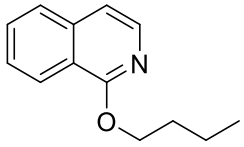


9

2-phenoxy-1,10-phenanthroline (9). To a solution of a 1,10-phenanthroline *N*-oxide (135 mg, 0.69 mmol) in dry EA (0.7 mL) is added PhOH (198 mg, 2.1 mmol), DIEA (181 mg, 1.4 mmol) and HMPA (13 mg, 0.07 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of a solution of $POBr_3$ (198 mg, 0.69 mmol) in EA (0.7 mL). The reaction mixture is then warmed to room temperature and stirred for 20 minutes (the reaction is complete as indicated by TLC). Finally, it is quenched with saturated potassium carbonate solution and extracted with EA one time. The combined organic phases are dried over Na_2SO_4 and concentrated in vacuo to give the crude product. Purification by flash column chromatography (PE : EA = 10:1-5:1) furnishes the desired product (41 mg, 22% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[21] TLC: R_f = 0.50 (PE : EA= 1:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.12 (dd, J = 4.2 Hz, 1.8 Hz, 1H), 8.23 (dd, J = 7.8 Hz, 1.8 Hz, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.76-7.75 (m, 1H), 7.72-7.70 (m,

1H), 7.59 (dd, *J* = 7.8 Hz, 4.2 Hz, 1H), 7.40-7.38 (m, 2H), 7.27-7.26 (m, 2H), 7.18 (t, *J* = 7.8 Hz, 1H), 7.13 (t, *J* = 8.4 Hz, 1H)**.**

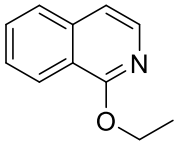
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{41}{188} \times 1 = 22\%$$



10a

1-butoxyisoquinoline (10a). Following **GP 4**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (20 mg, 14% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[22] TLC: R_f = 0.71 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (d, *J* = 7.8 Hz, 1H), 7.98 (d, *J* = 6.0 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.66-7.63 (m, 1H), 7.54-7.51 (m, 1H), 7.19 (d, *J* = 6.0 Hz, 1H), 4.51 (t, *J* = 6.6 Hz, 2H), 1.91-1.87 (m, 2H), 1.61-1.55 (m, 2H), 1.03 (t, *J* = 7.2 Hz, 3H).

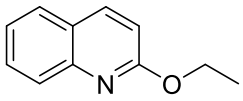
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{20}{139} \times 1 = 14\%$$



10b

1-ethoxyisoquinoline (10b). Following **GP 4**, using isoquinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (20 mg, 17% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[22] TLC: R_f = 0.71 (PE : EA = 10:1).^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (d, *J* = 7.2 Hz, 1H), 7.90 (d, *J* = 6.0 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.57-7.54 (m, 1H), 7.45-7.42 (m, 1H), 7.10 (d, *J* = 5.4 Hz, 1H), 4.48 (q, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{20}{120} \times 1 = 17\%$$



10d

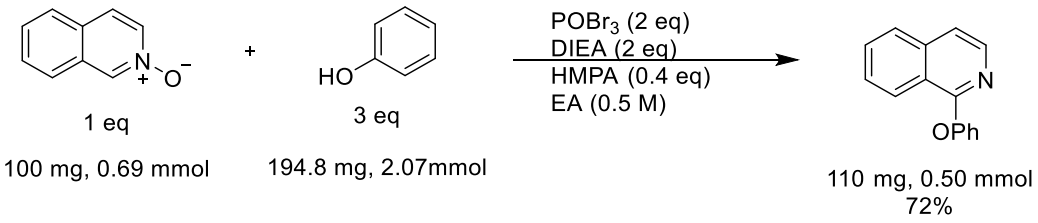
2-ethoxyquinoline (10d). Following **GP 4**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (27 mg, 23% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[23] TLC: R_f = 0.70 (PE : EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 9.0 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.63-7.60 (m, 1H), 7.38-7.35 (m, 1H), 6.89 (d, *J* = 9.0 Hz, 1H), 4.54 (q, *J* = 7.2 Hz, 2H), 1.46 (t, *J* = 7.2 Hz, 3H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{27}{120} \times 1 = 23\%$$

6. Green Chemistry Metrics Analysis

The following formula were used for calculating Atom Economy (AE)

$$\mathrm{AE} = \frac{Molecular\ weight\ of\ product}{Total\ molecular\ weight\ of\ reactants} \times 100\%$$



$$\mathrm{AE}\ (\mathbf{3a}) = \frac{221.26}{145.16 + 94.11} X\ 100\% = 92.47$$

7. References

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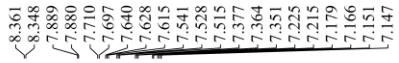
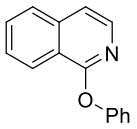
8. NMR Spectra

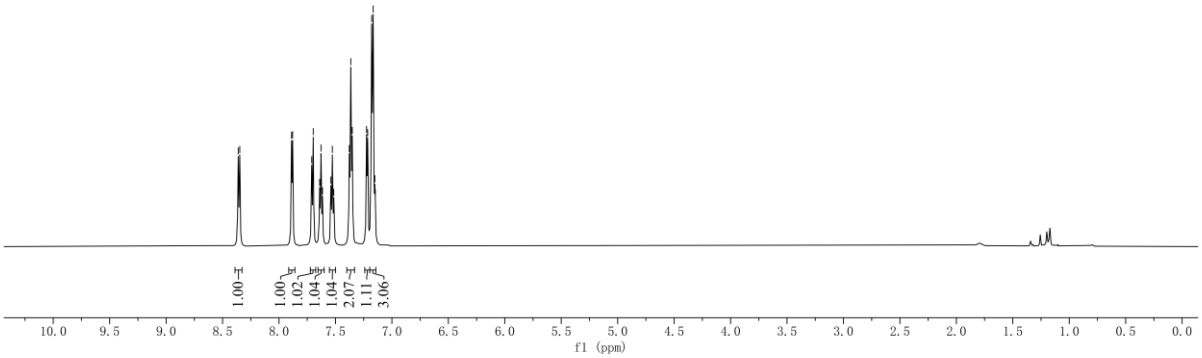
Spectra data are shown from the next page.





3a

$CDCl_3$



4

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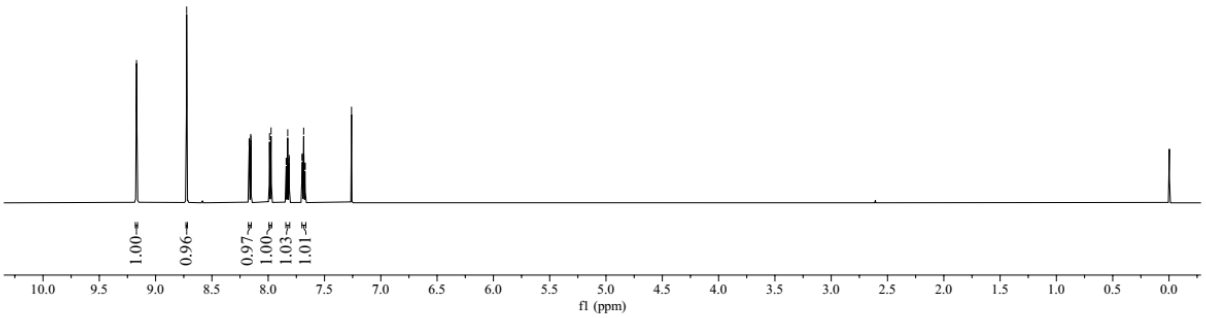

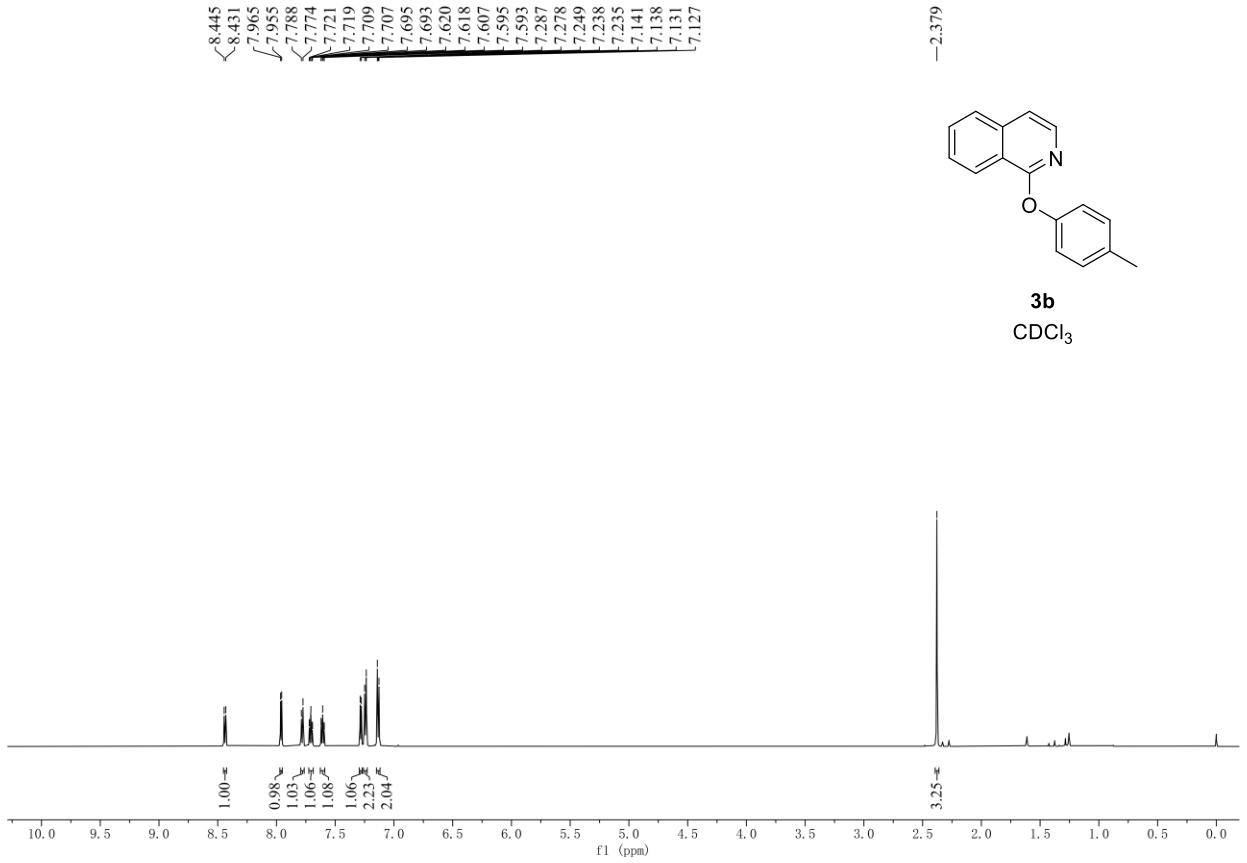
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7.774
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7.719
7.709
7.707
7.695
7.693
7.620
7.618
7.607
7.595
7.593
7.287
7.278
7.249
7.238
7.235
7.141
7.138
7.131
7.127
2.379
N
O
3b
CDCl3
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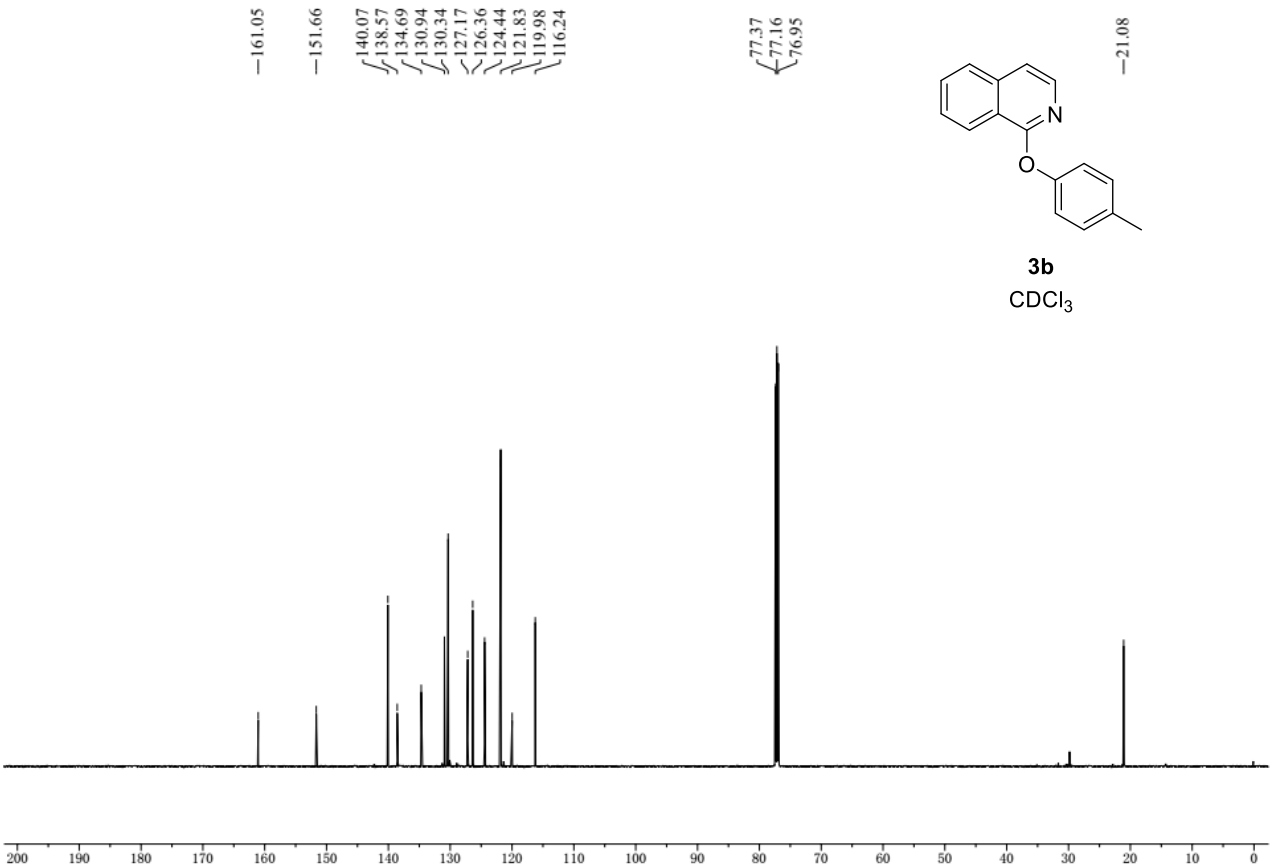
0.98
1.03
1.06
1.08
1.06
2.23
2.04
3.25
f1 (ppm)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130.34
127.17
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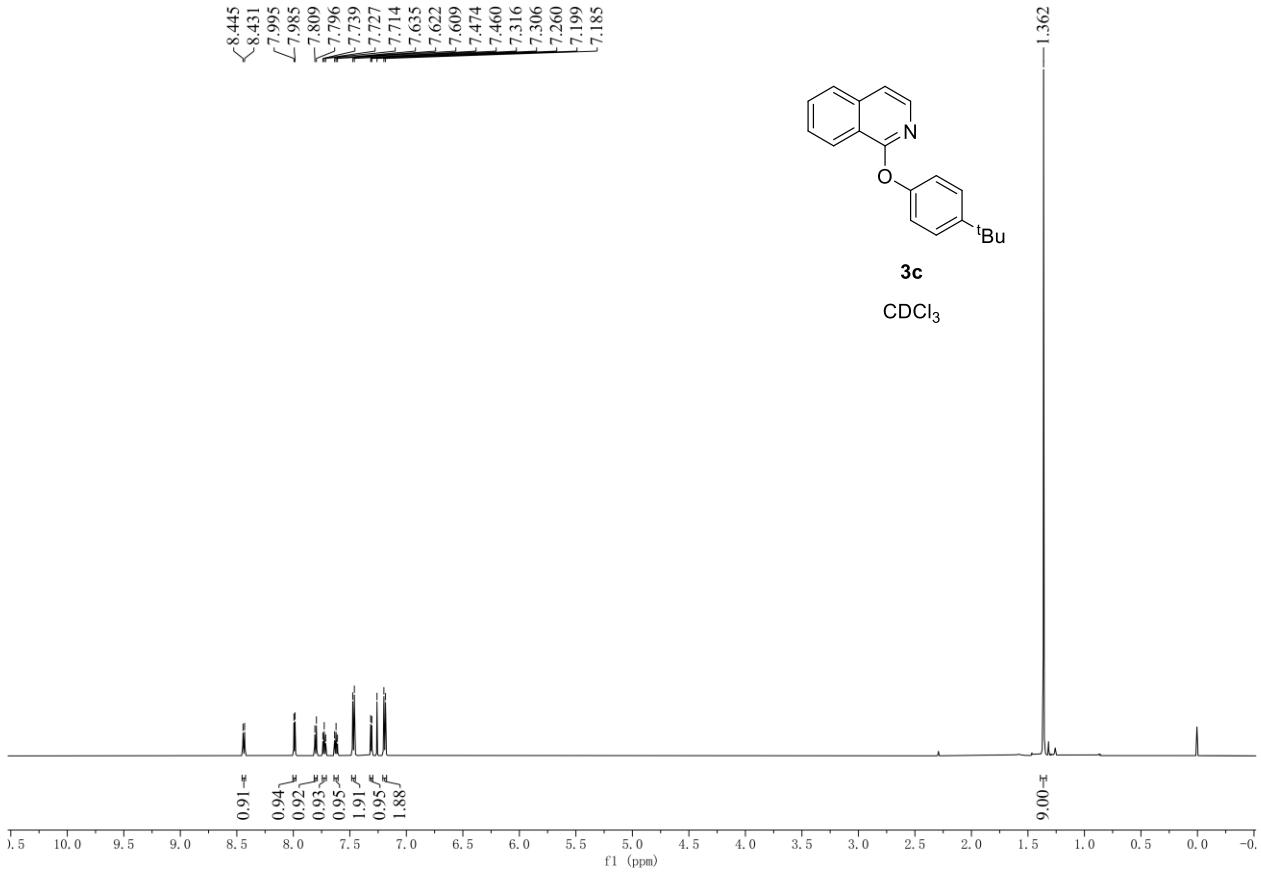
21.08
N
O
3b
CDCl3
f1 (ppm)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7.260
7.199
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O
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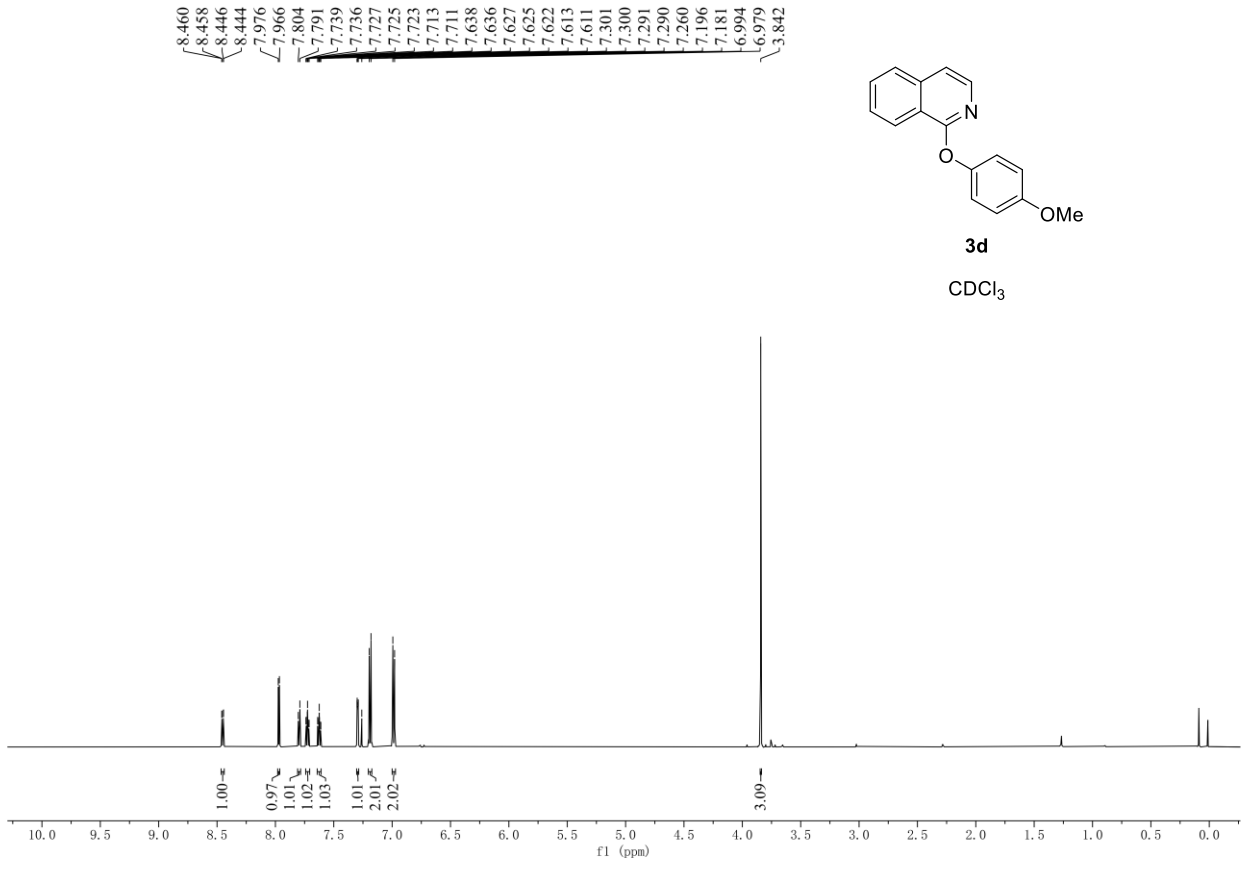
9.00
f1 (ppm)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7.622
7.613
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7.301
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7.181
6.994
6.979
3.842
N
O
OMe
3d
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1.02
1.03
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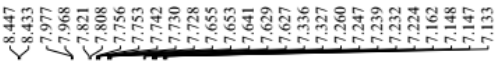
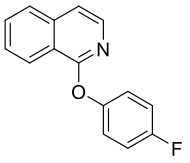
3.09
f1 (ppm)





3e

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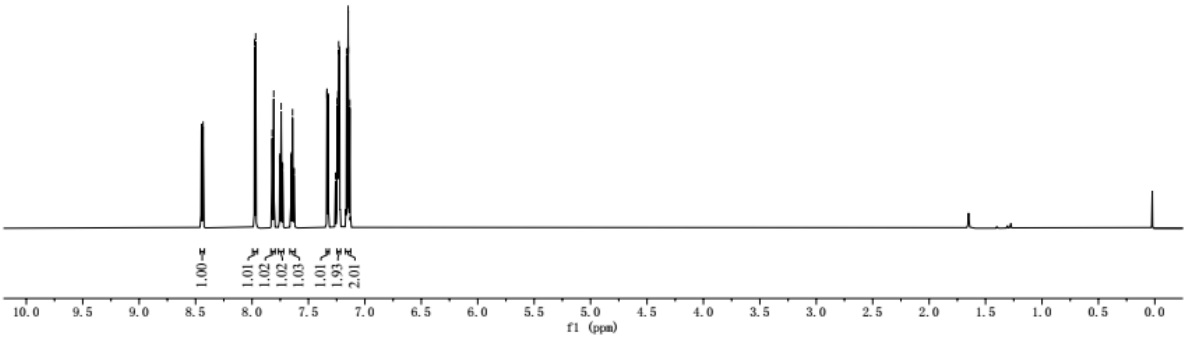
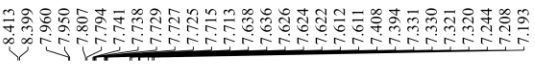
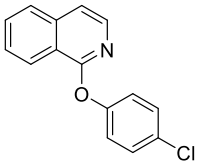
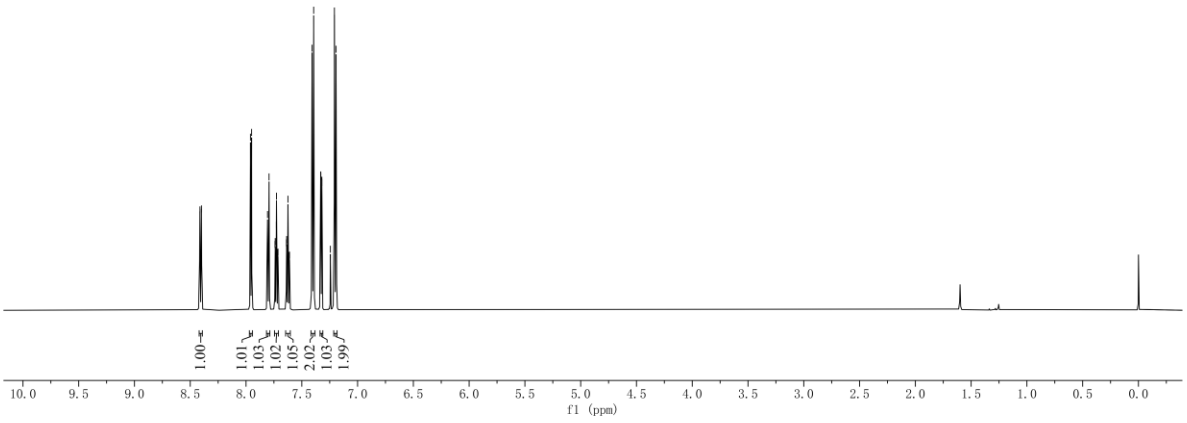


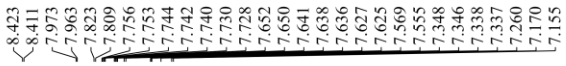


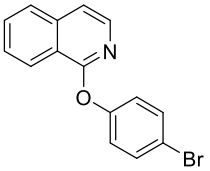


3f

$CDCl_3$

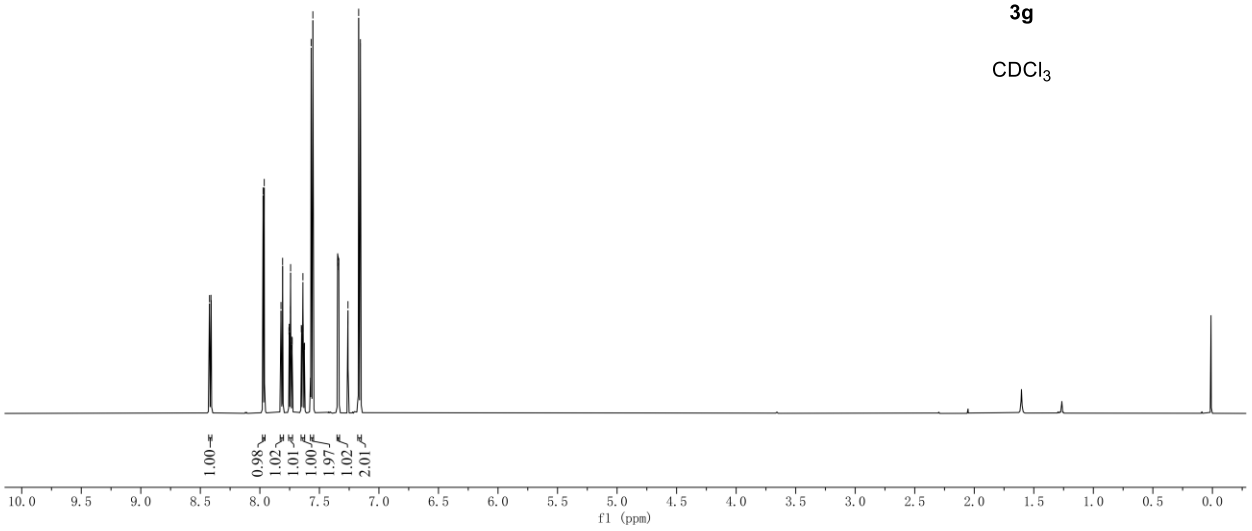


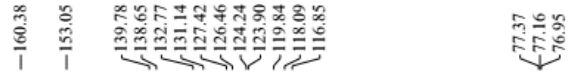


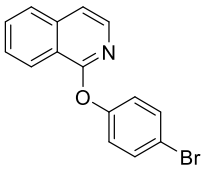


3g

$CDCl_3$

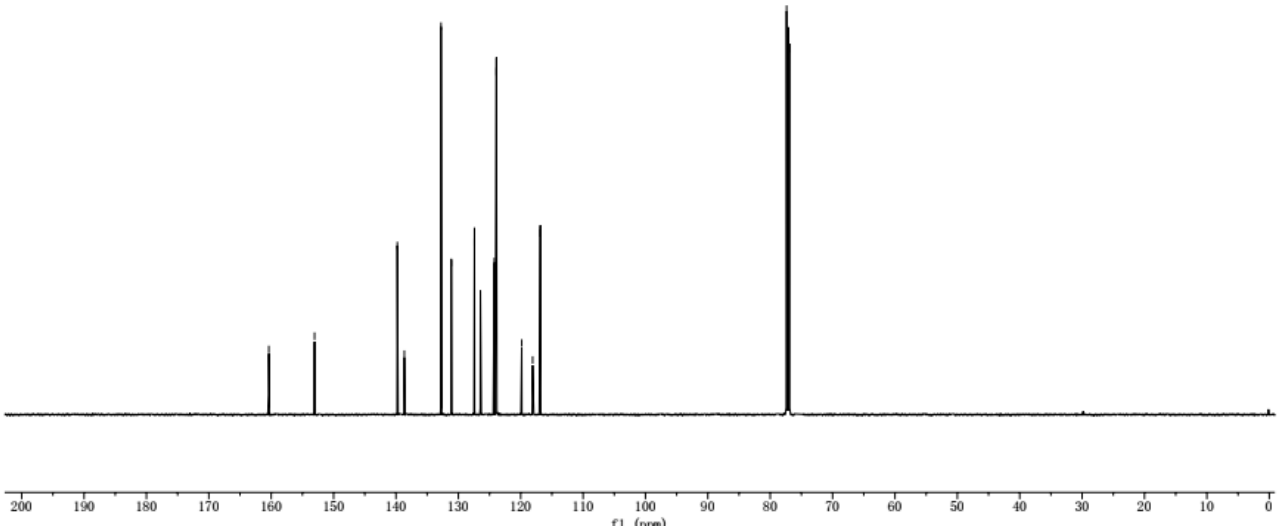


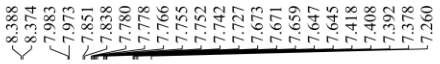


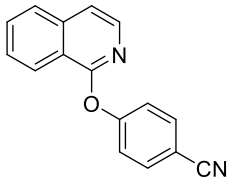


3g

$CDCl_3$







3h

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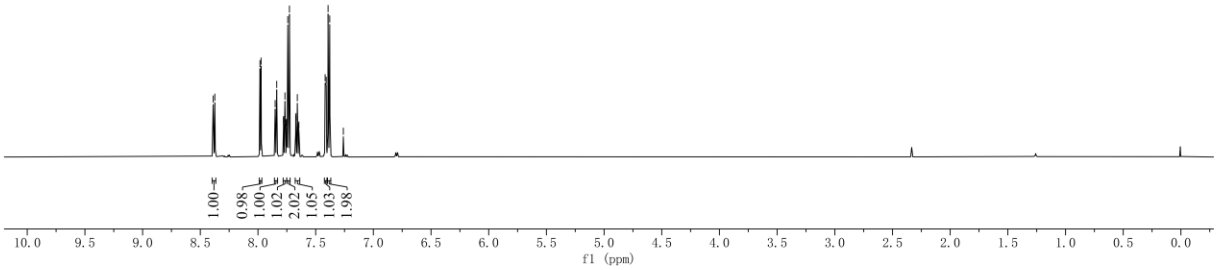

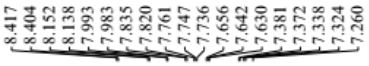

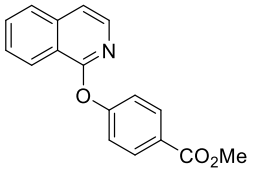

3i

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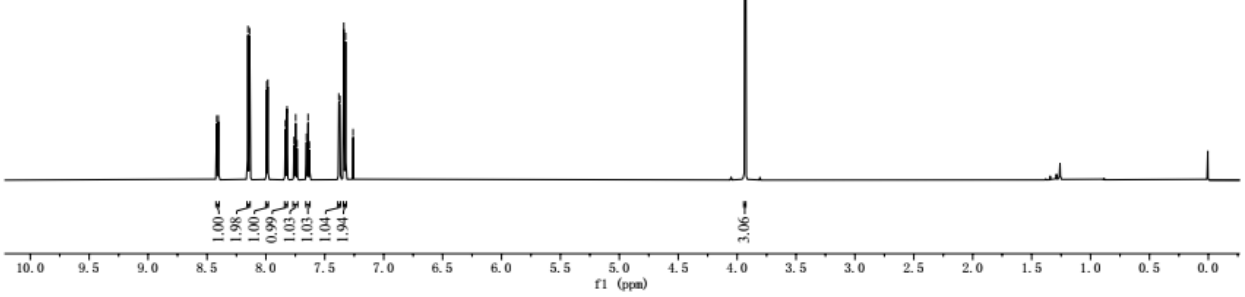

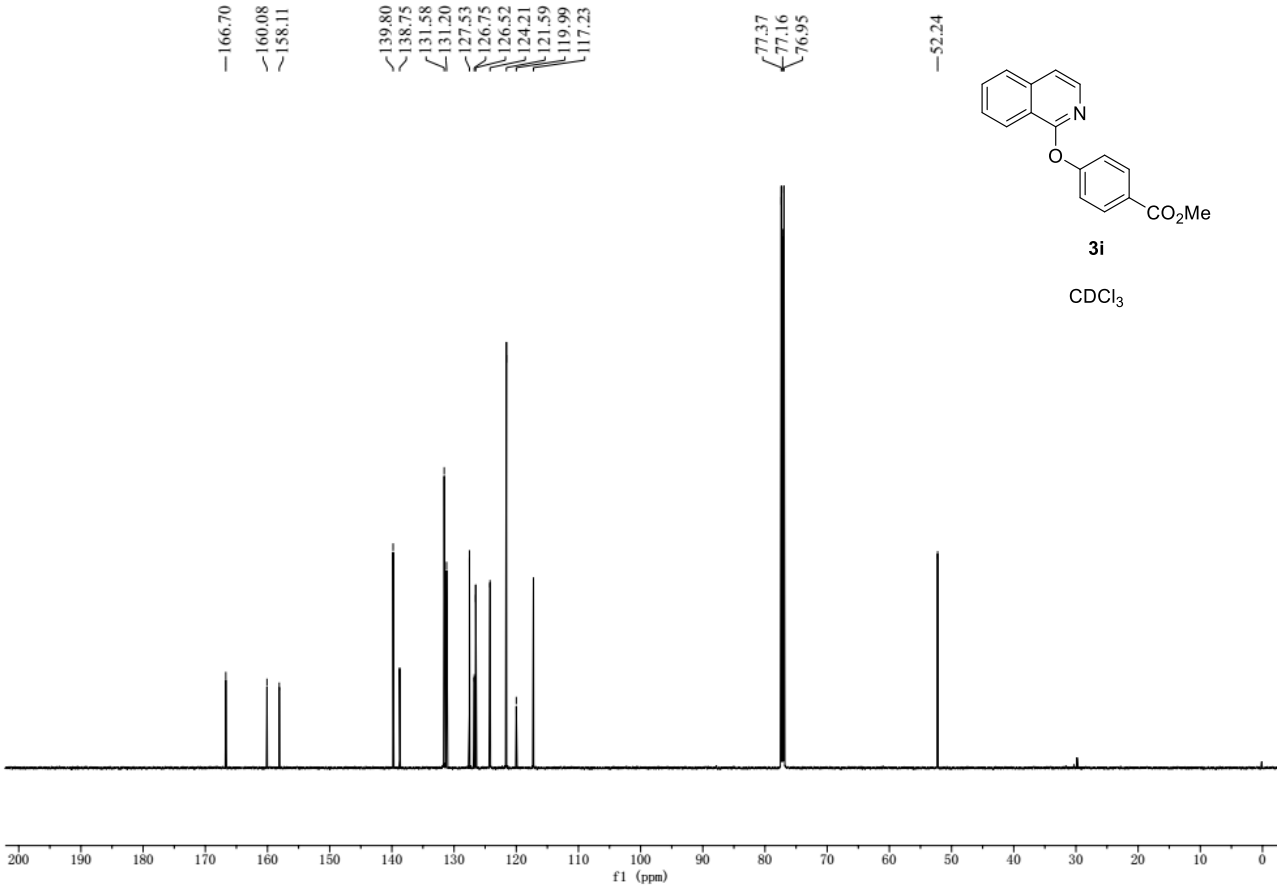

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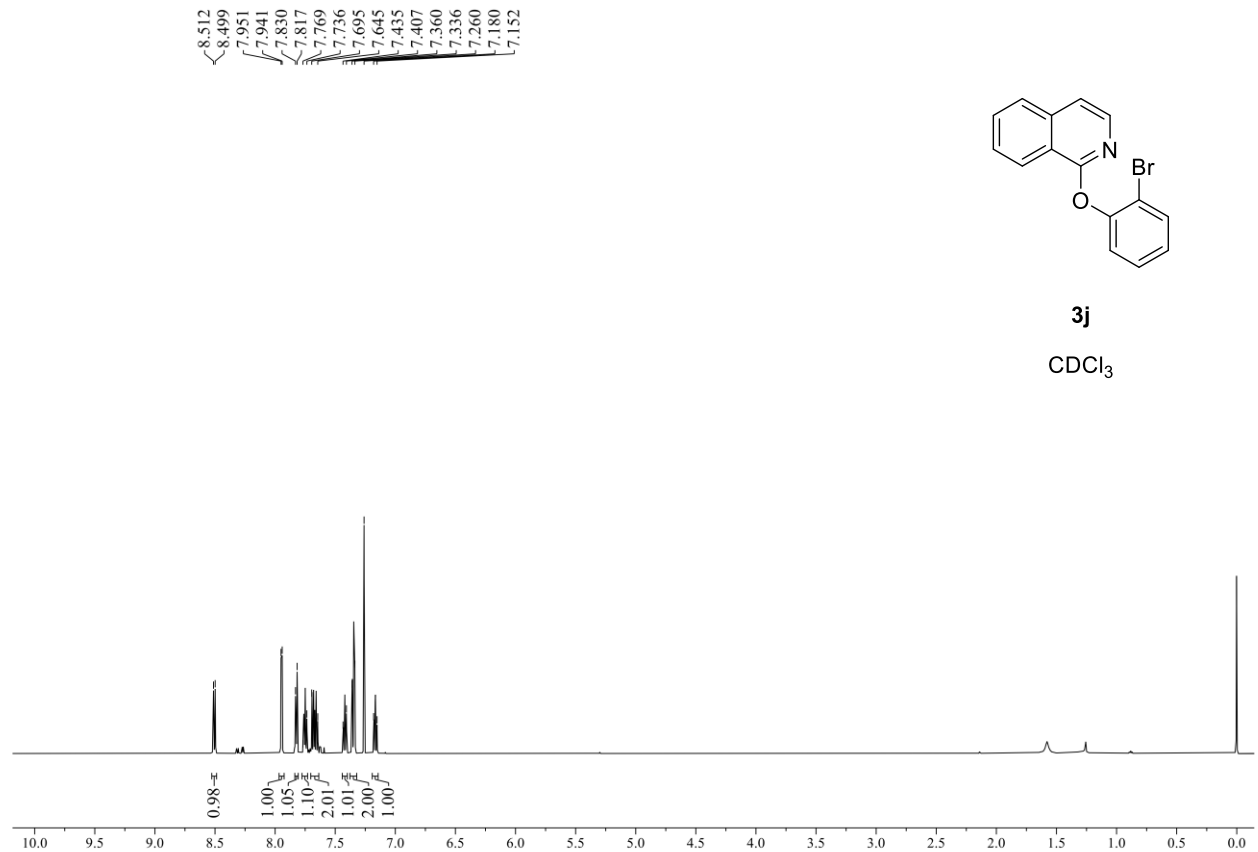

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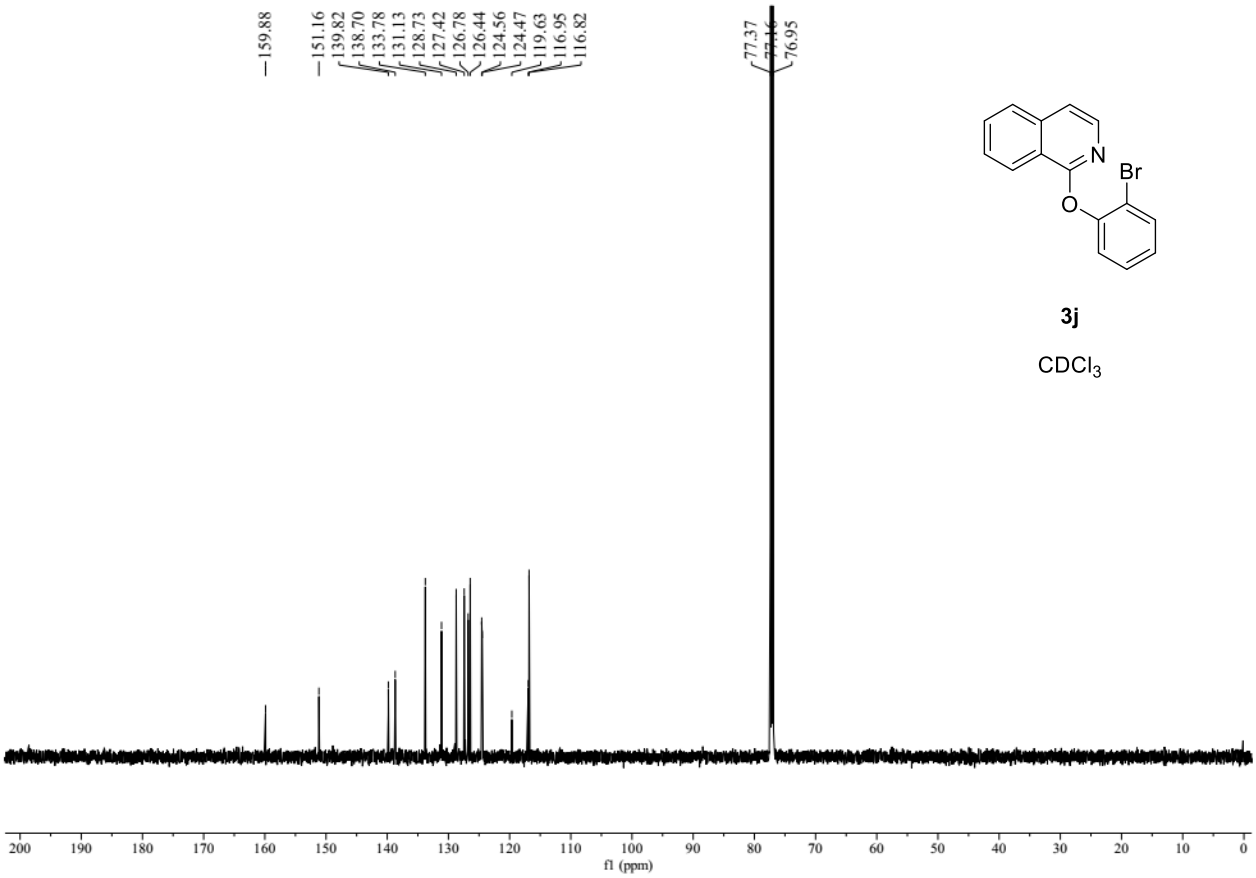

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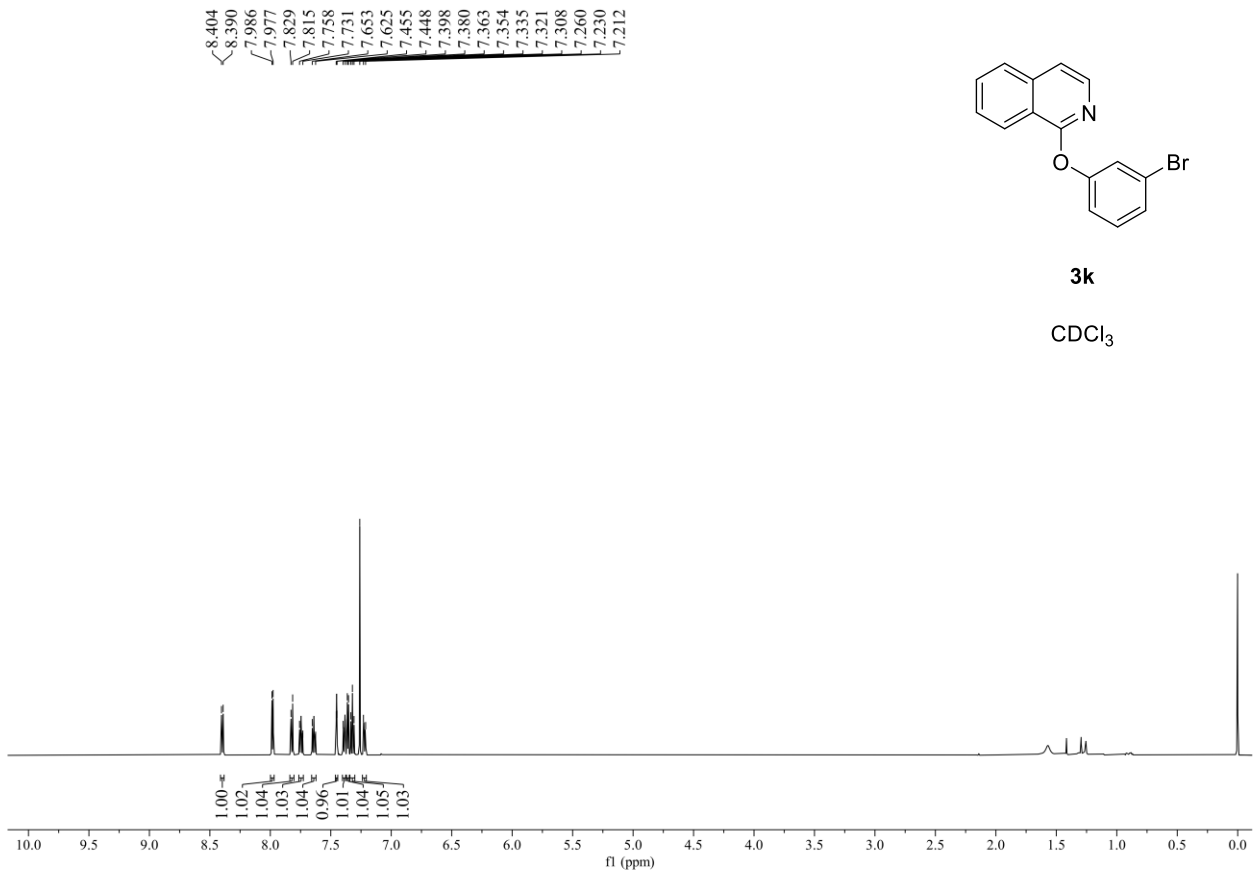

3k

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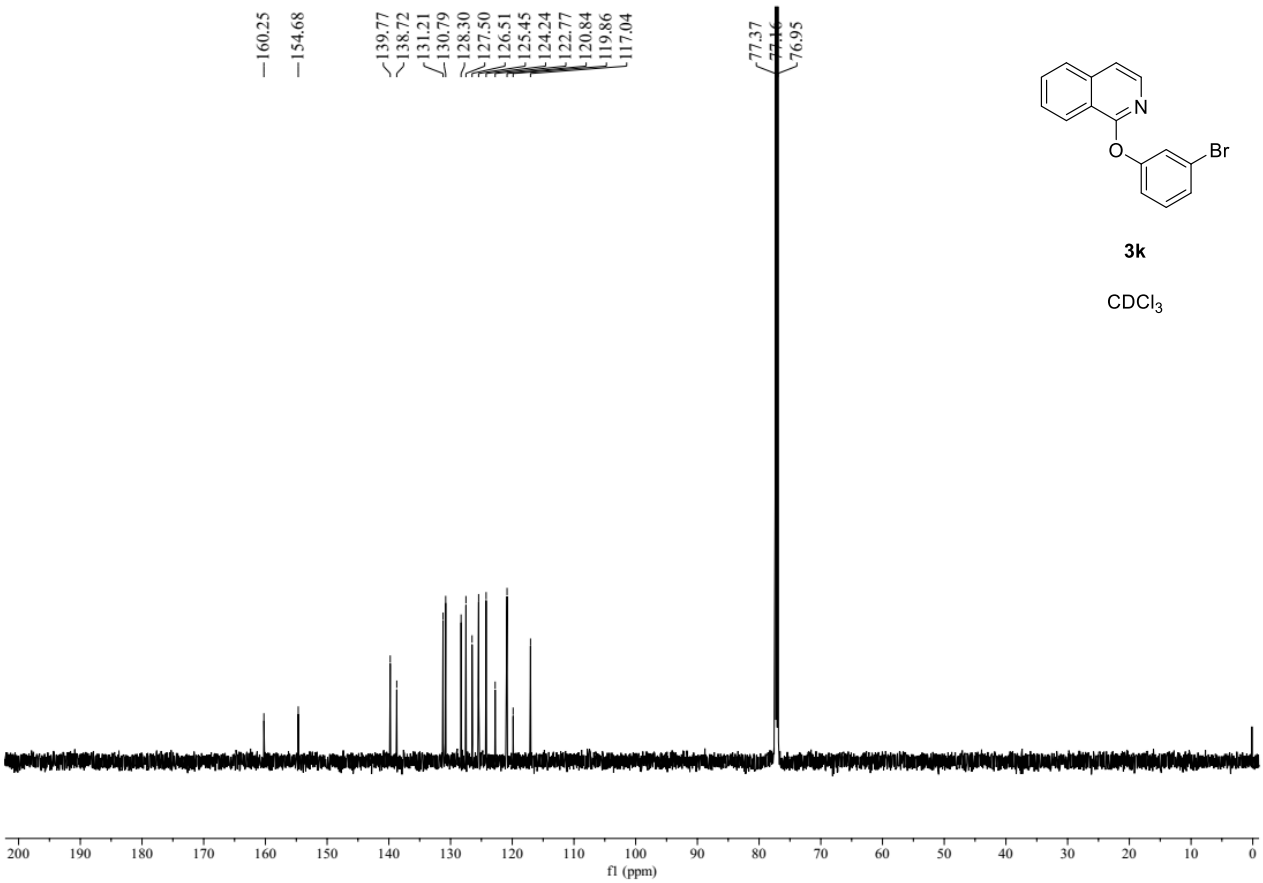

3k

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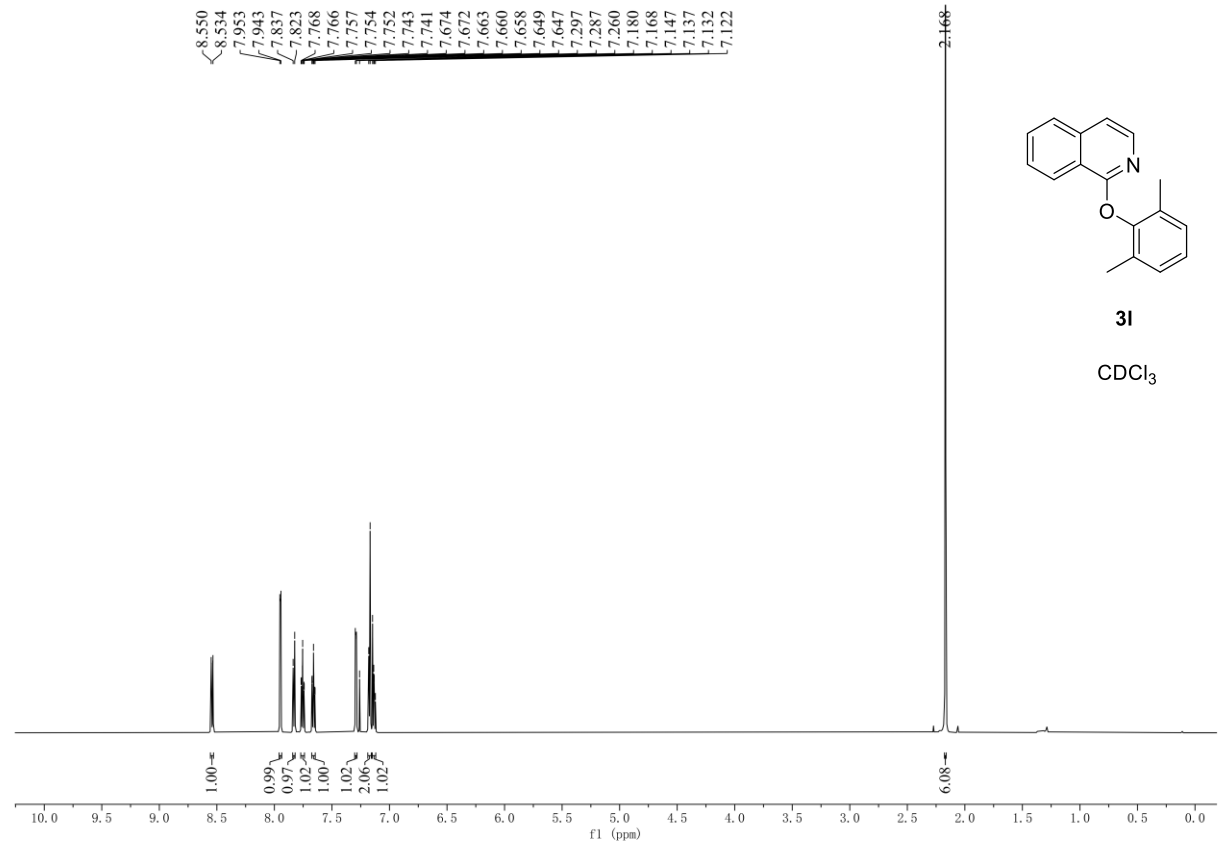

3l

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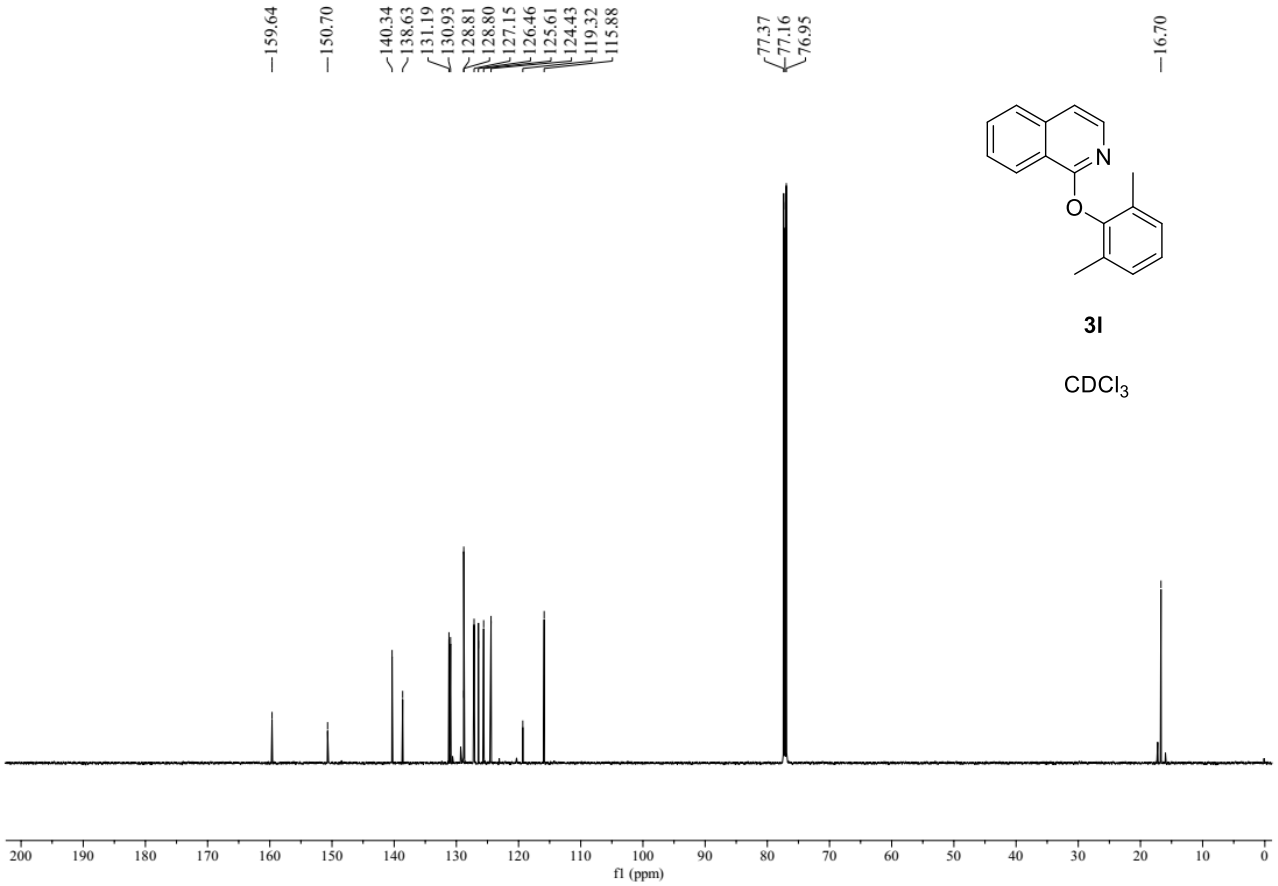

3l

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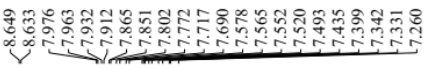
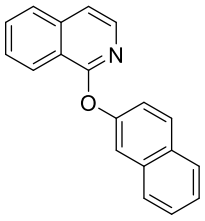
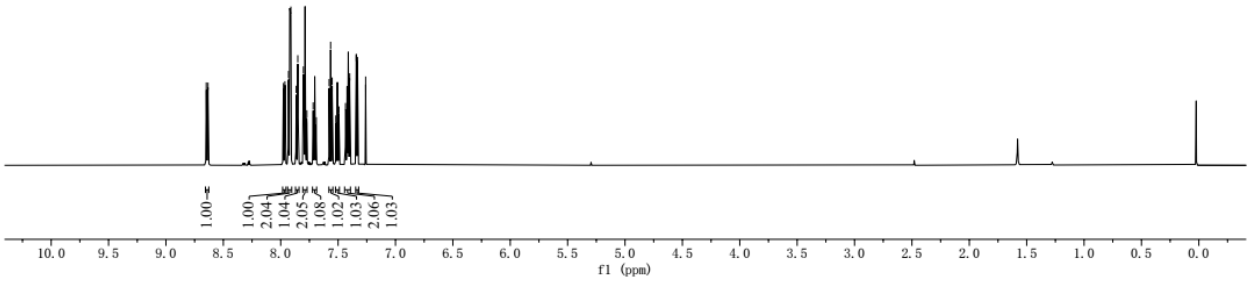
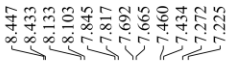


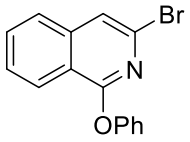


3m

$CDCl_3$







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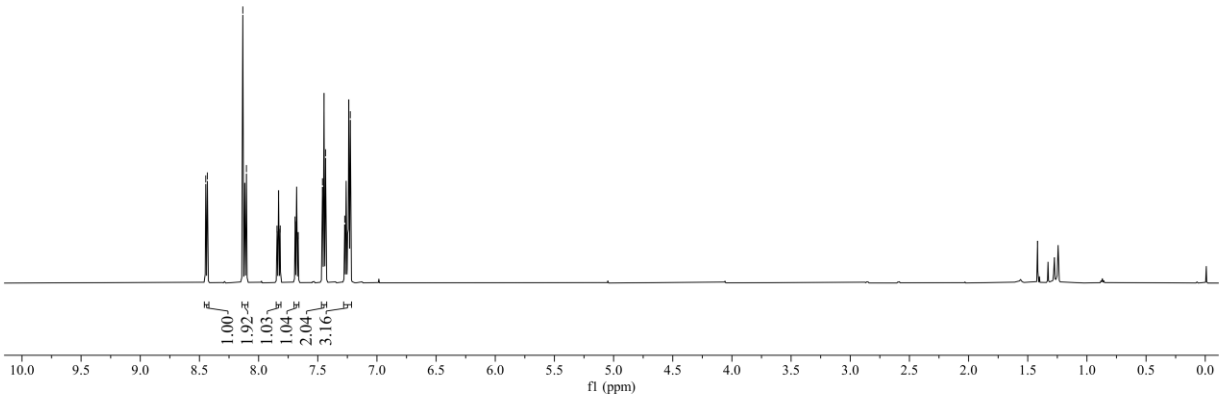
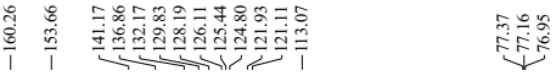
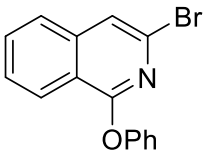
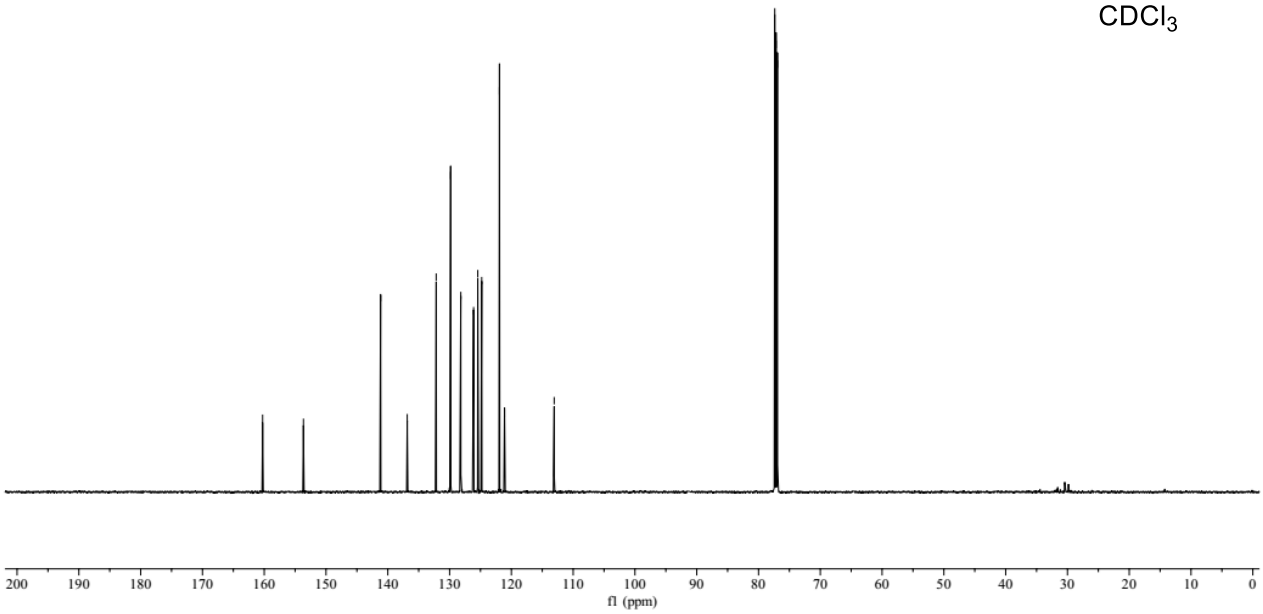


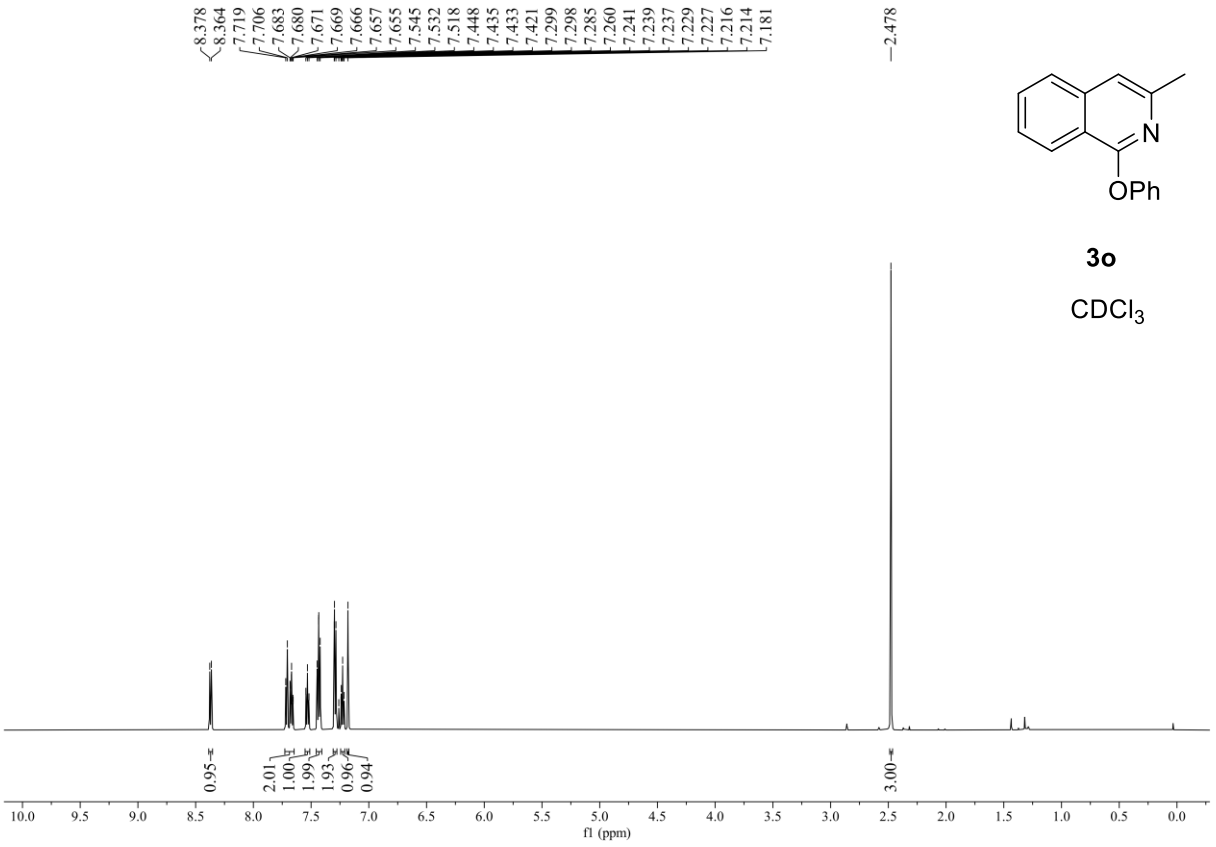




3n

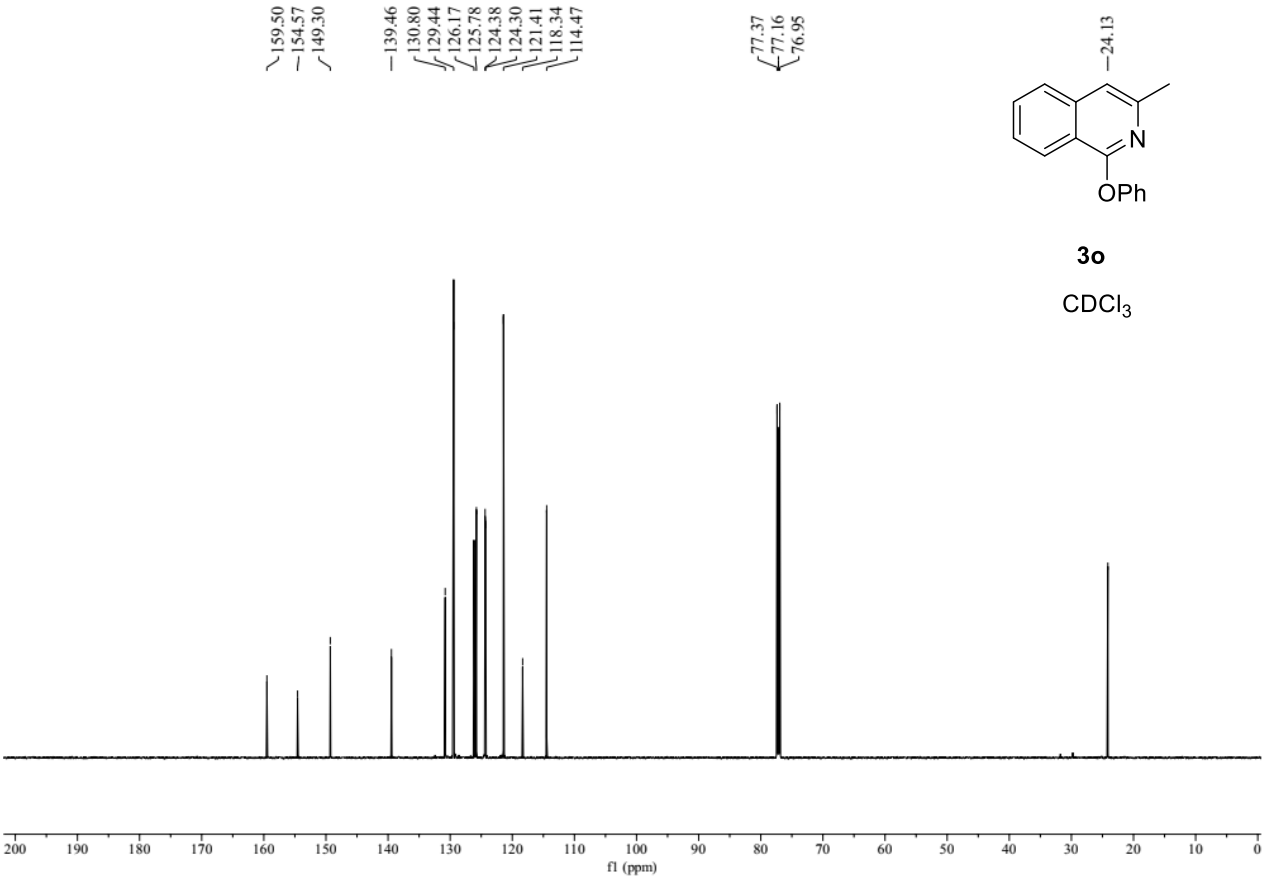
$CDCl_3$





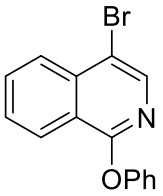
3o

$CDCl_3$



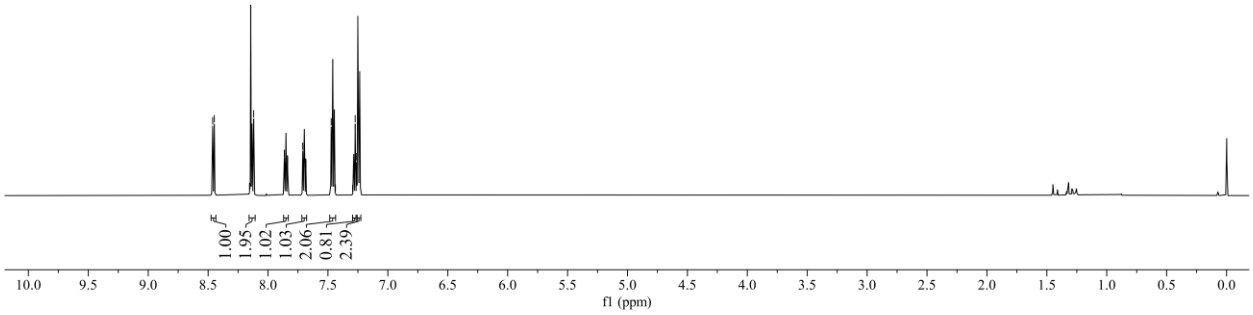
3o

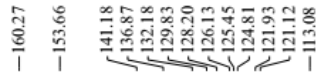
$CDCl_3$

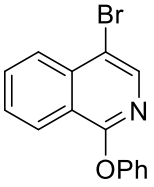


3p

$CDCl_3$

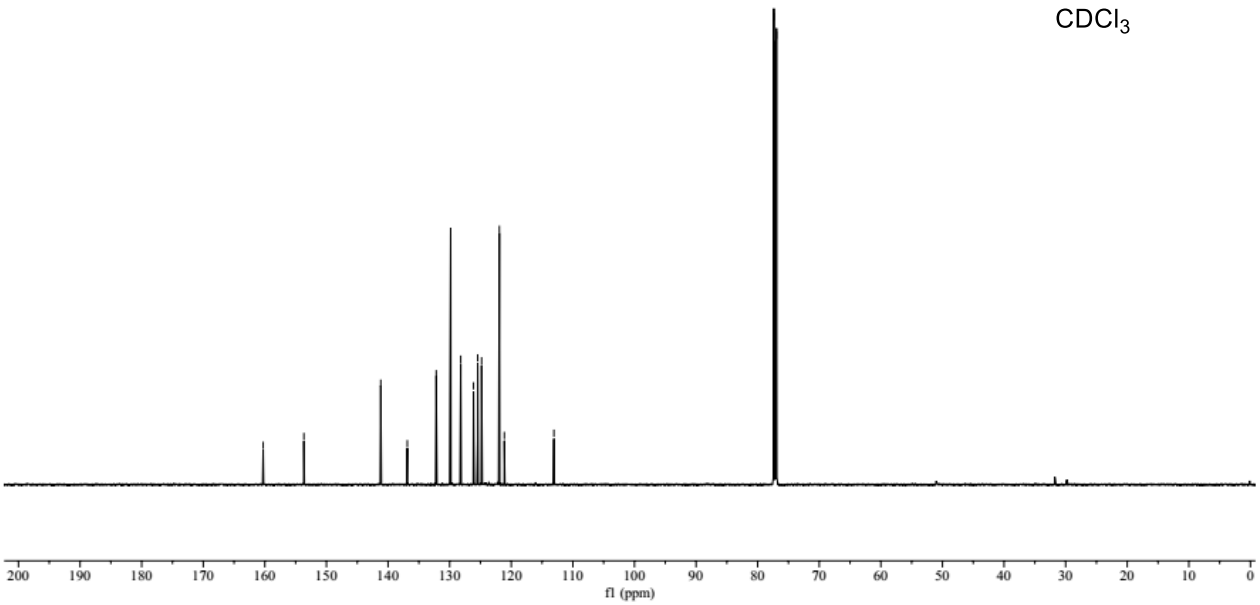


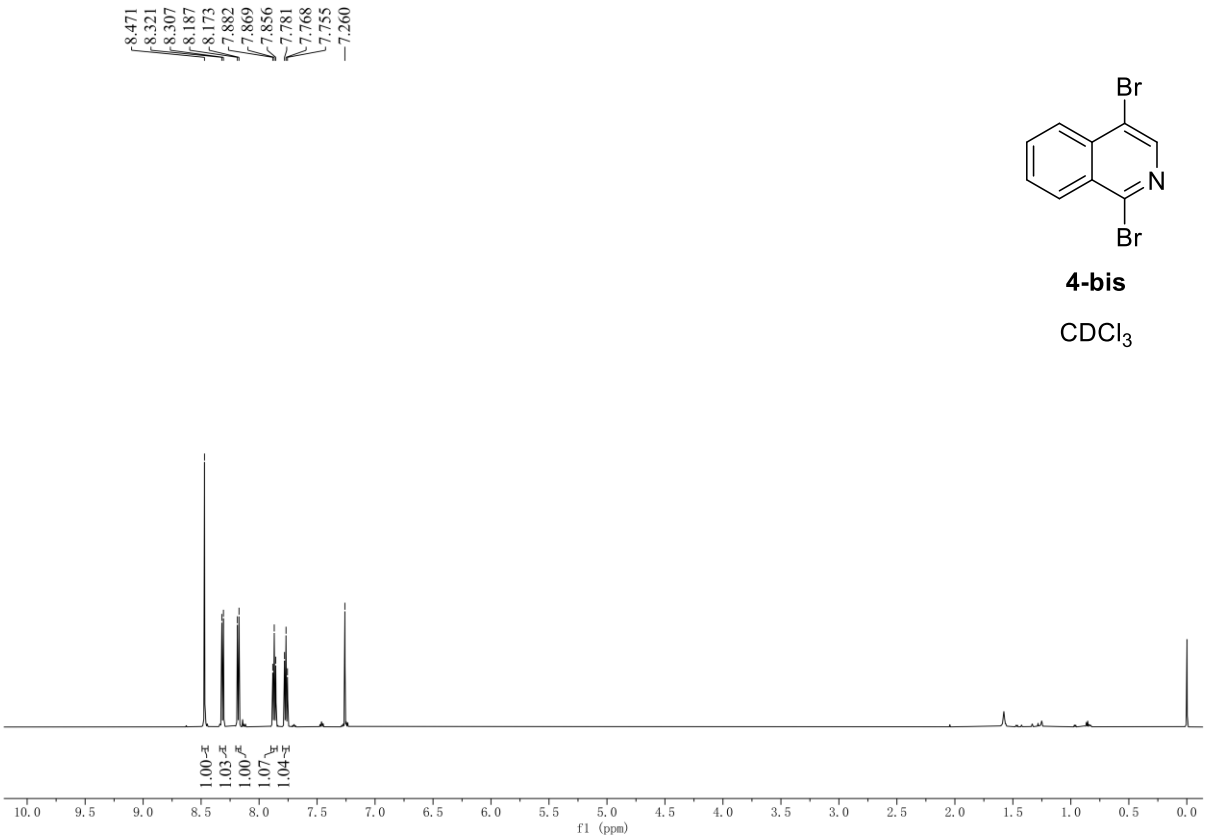


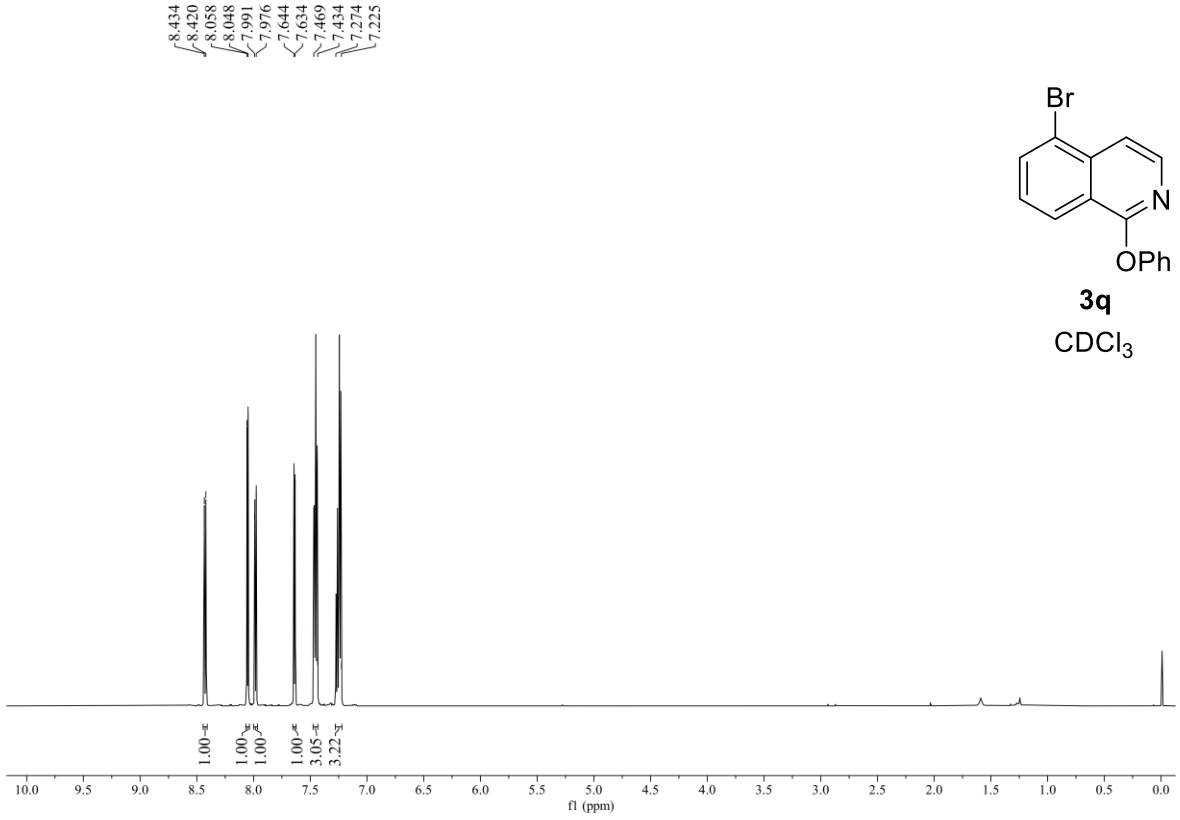


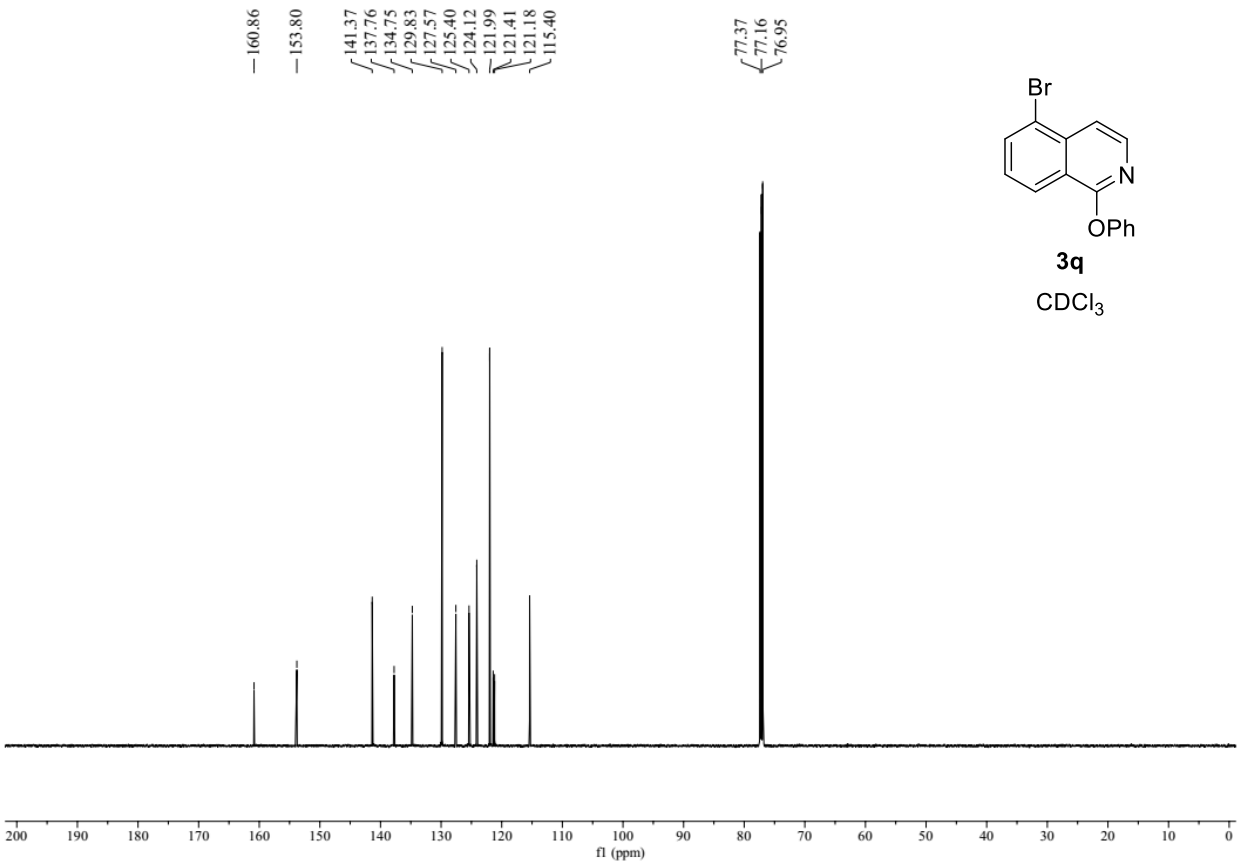
3p

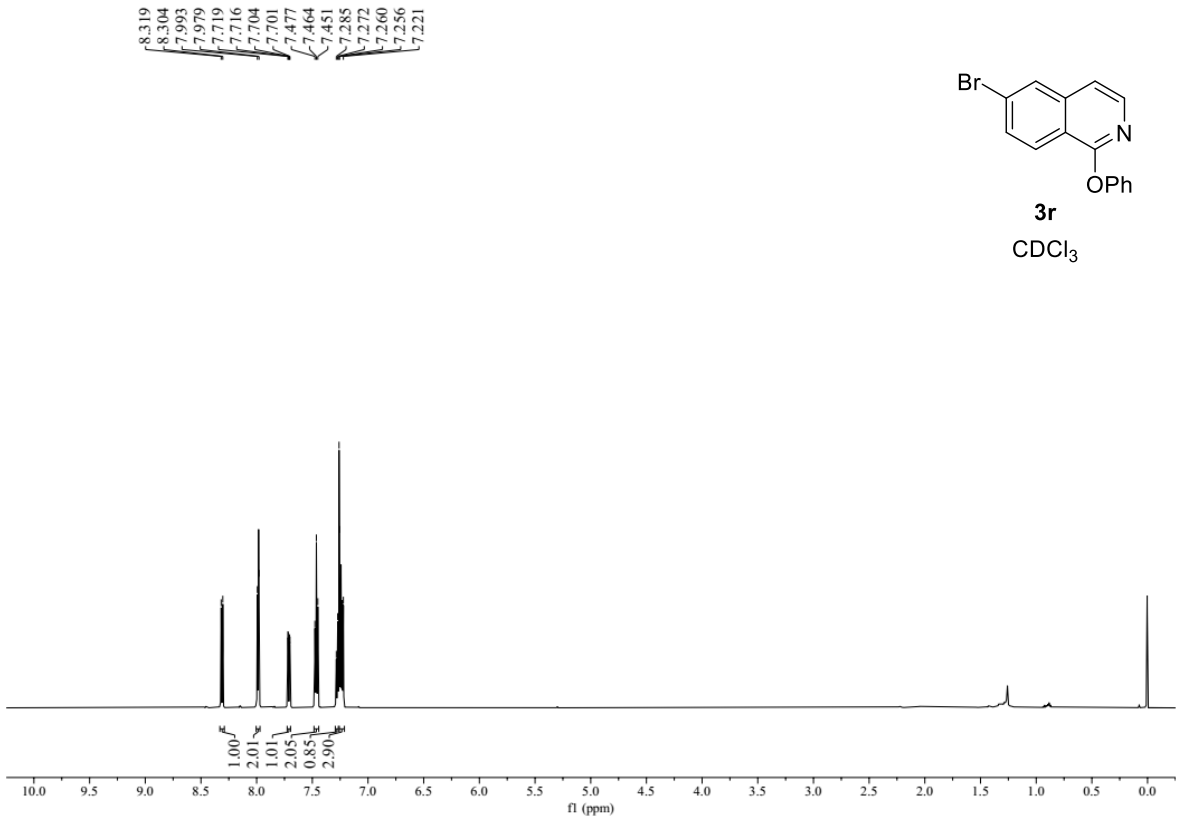
$CDCl_3$

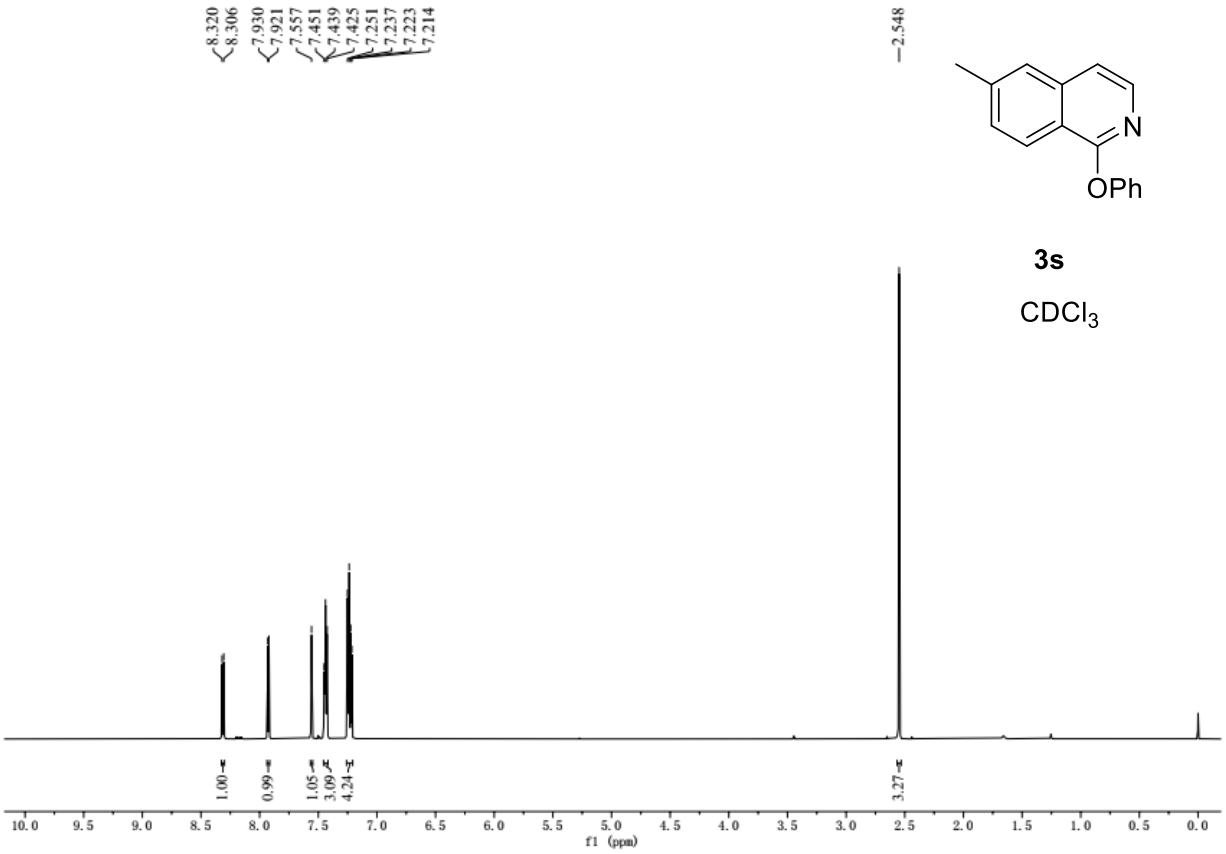



8.471
8.321
8.307
8.187
8.173
7.882
7.869
7.856
7.781
7.768
7.755
7.260
Br
N
Br
4-bis
CDCl3
1.00
1.03
1.00
1.07
1.04
f1 (ppm)


8.434
8.420
8.058
8.048
7.991
7.976
7.644
7.634
7.469
7.434
7.274
7.225
Br
N
OPh
3q
CDCl3
1.00
1.00
1.00
1.00
3.05
3.22
f1 (ppm)

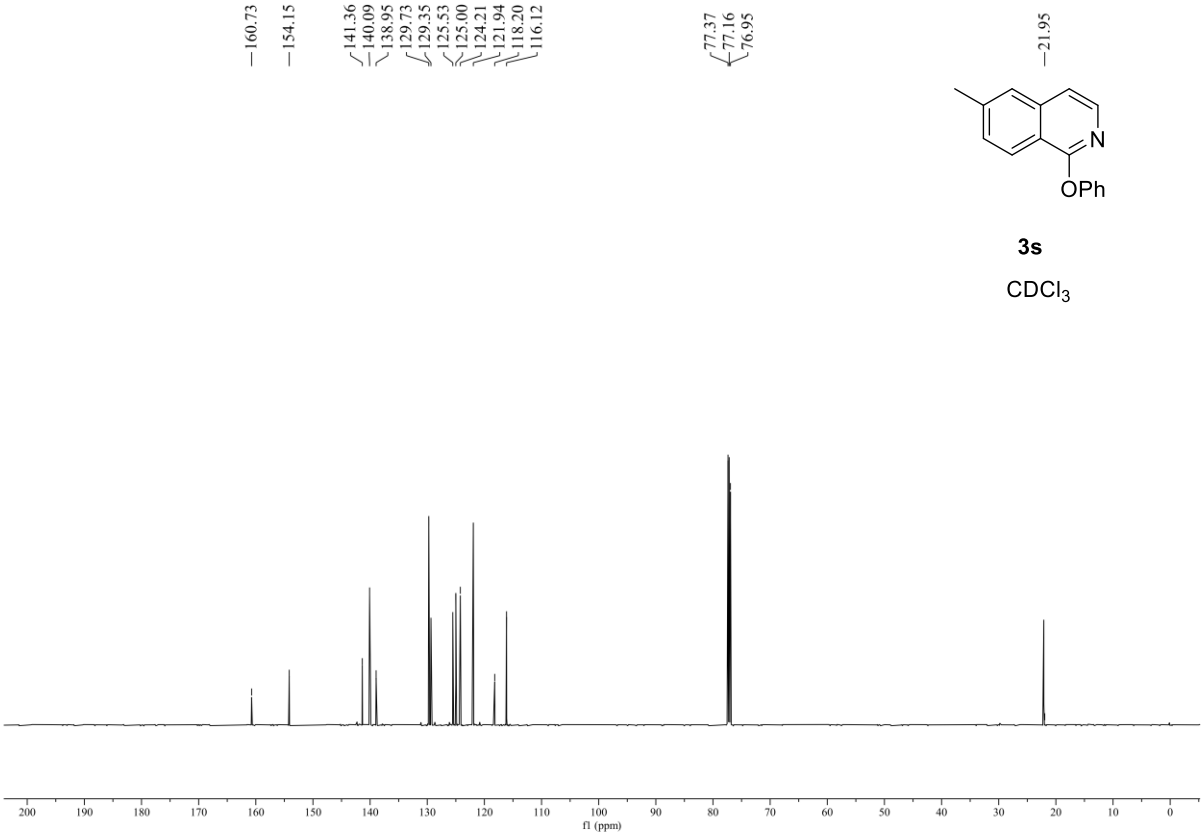

160.86
153.80
141.37
137.76
134.75
129.83
127.57
125.40
124.12
121.99
121.41
121.18
115.40
77.37
77.16
76.95
Br
N
OPh
3q
CDCl3
f1 (ppm)


8.319
8.304
7.993
7.979
7.719
7.716
7.704
7.701
7.477
7.464
7.451
7.285
7.272
7.260
7.256
7.221
Br
N
OPh
3r
CDCl3
1.00
2.01
1.01
2.05
0.85
2.90
f1 (ppm)



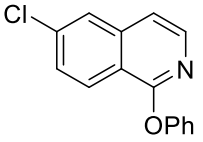
3s

$CDCl_3$



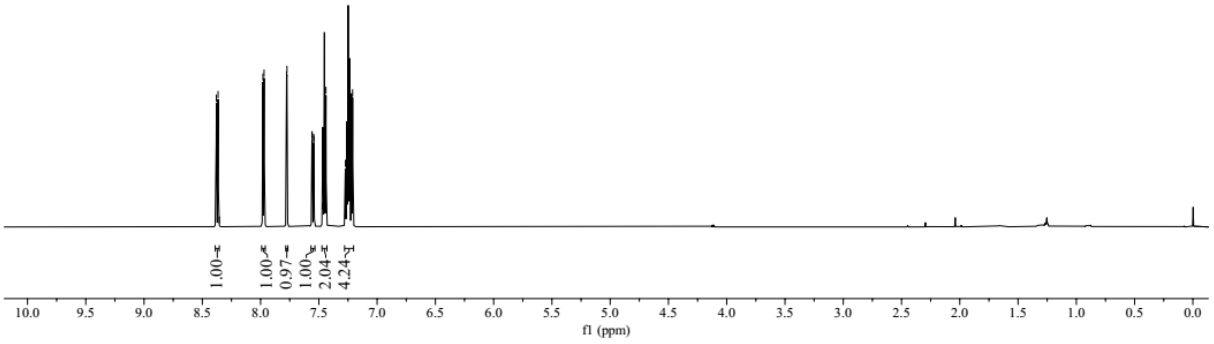
3s

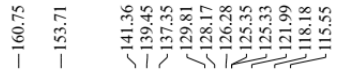
$CDCl_3$

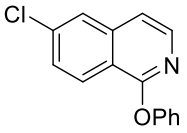


3t

$CDCl_3$

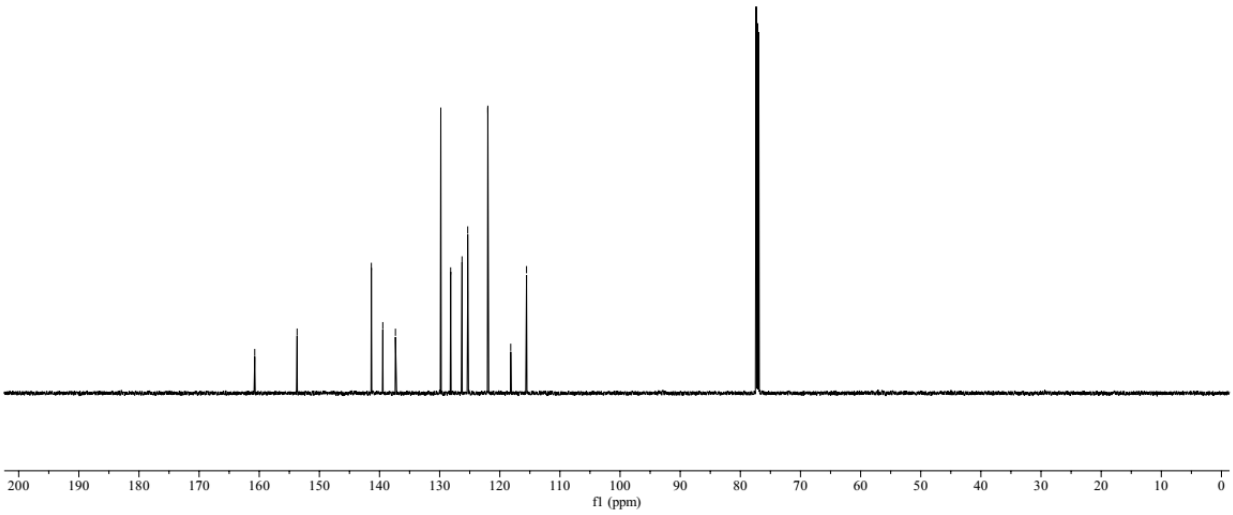




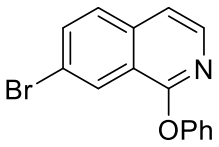


3t

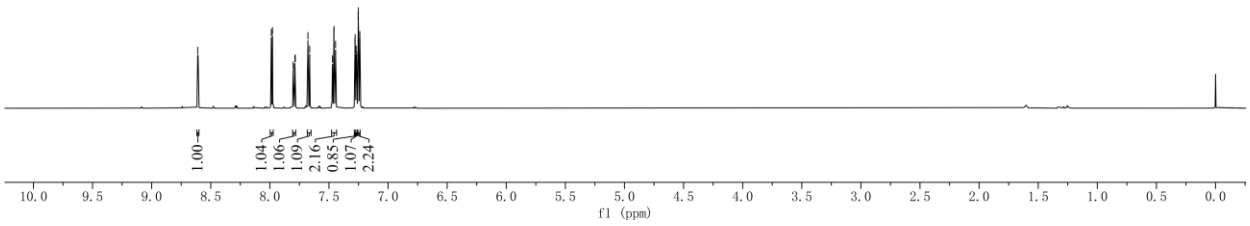
$CDCl_3$




8.611
7.988
7.978
7.803
7.800
7.788
7.785
7.678
7.663
7.471
7.458
7.457
7.444
7.280
7.279
7.270
7.266
7.253
7.251
7.239

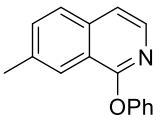

Br
N
OPh

3u


1.00
1.04
1.06
1.09
2.16
0.85
1.07
2.24
10.0 9.5 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)

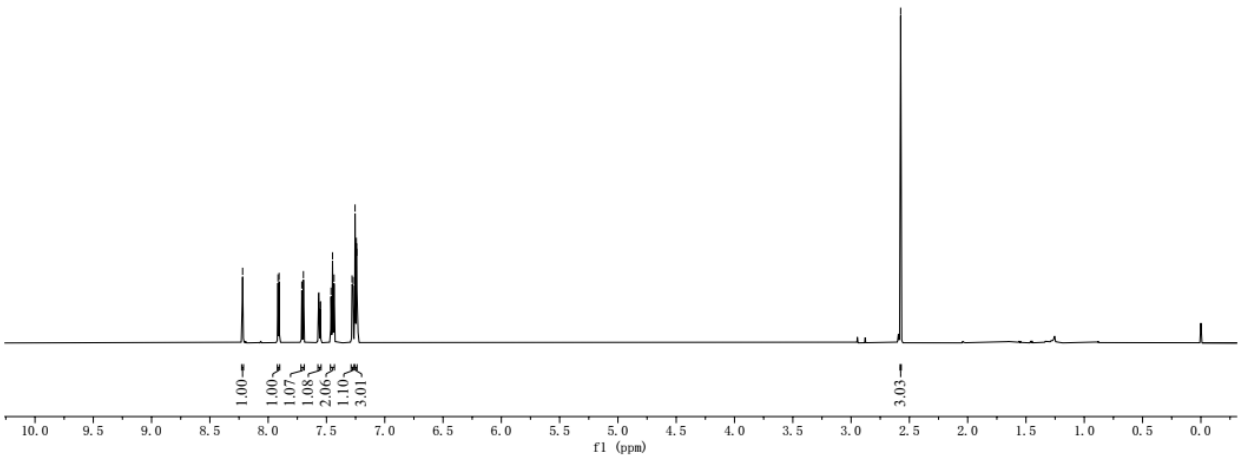

8.219
7.916
7.906
7.712
7.698
7.568
7.565
7.554
7.551
7.461
7.448
7.435
7.281
7.271
7.255
7.251
7.243
7.240

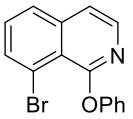

2.575


N
OPh

3v

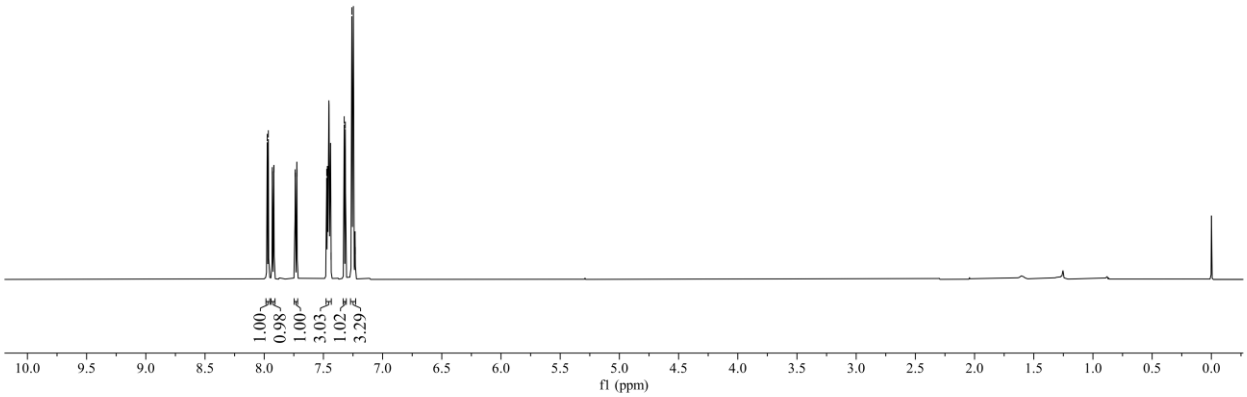
$CDCl_3$

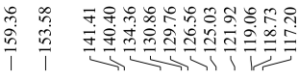

1.00
1.00
1.07
1.08
2.06
1.10
3.01
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

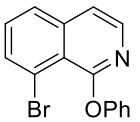


3w

$CDCl_3$

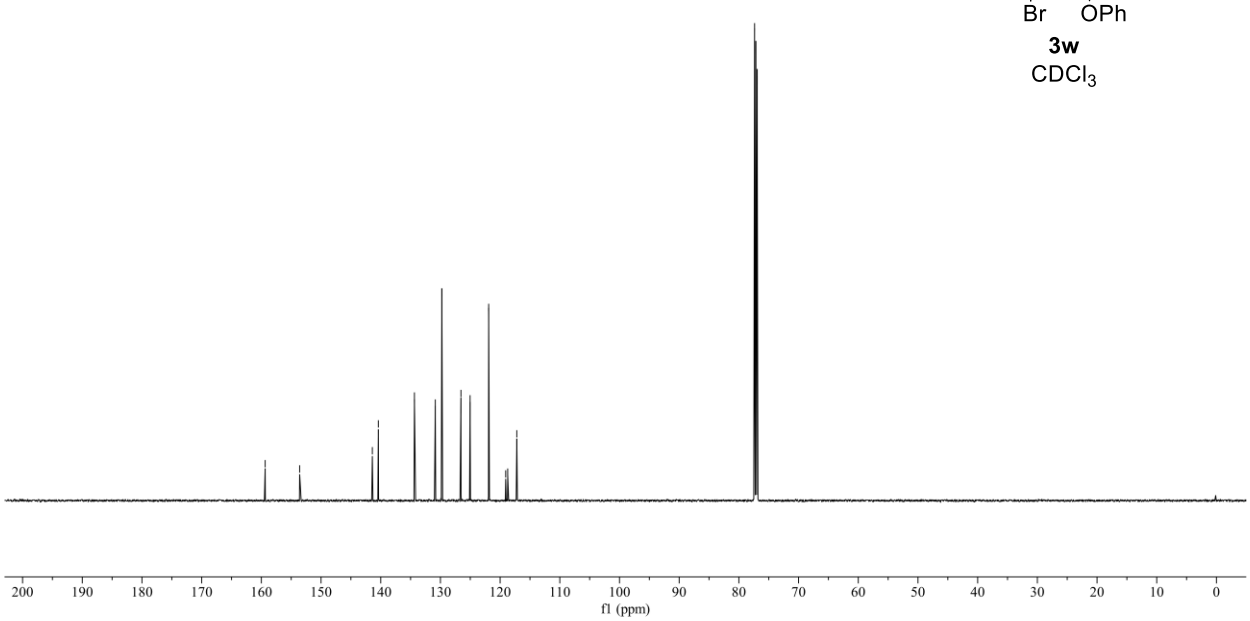


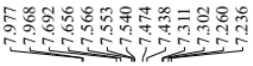


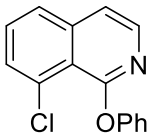


3w

$CDCl_3$

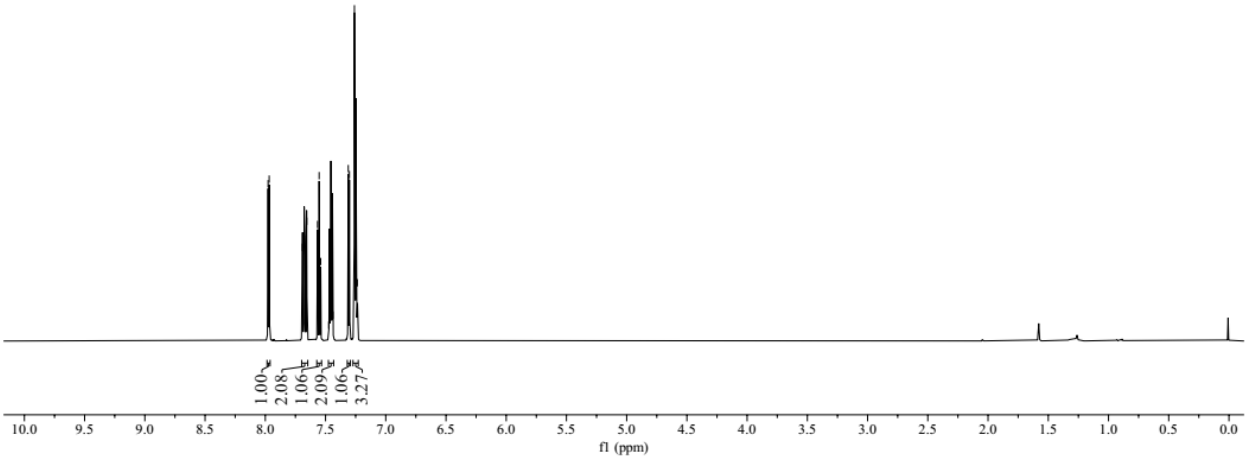


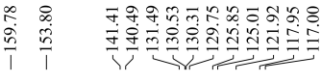


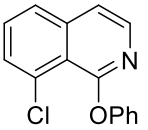


3x

$CDCl_3$

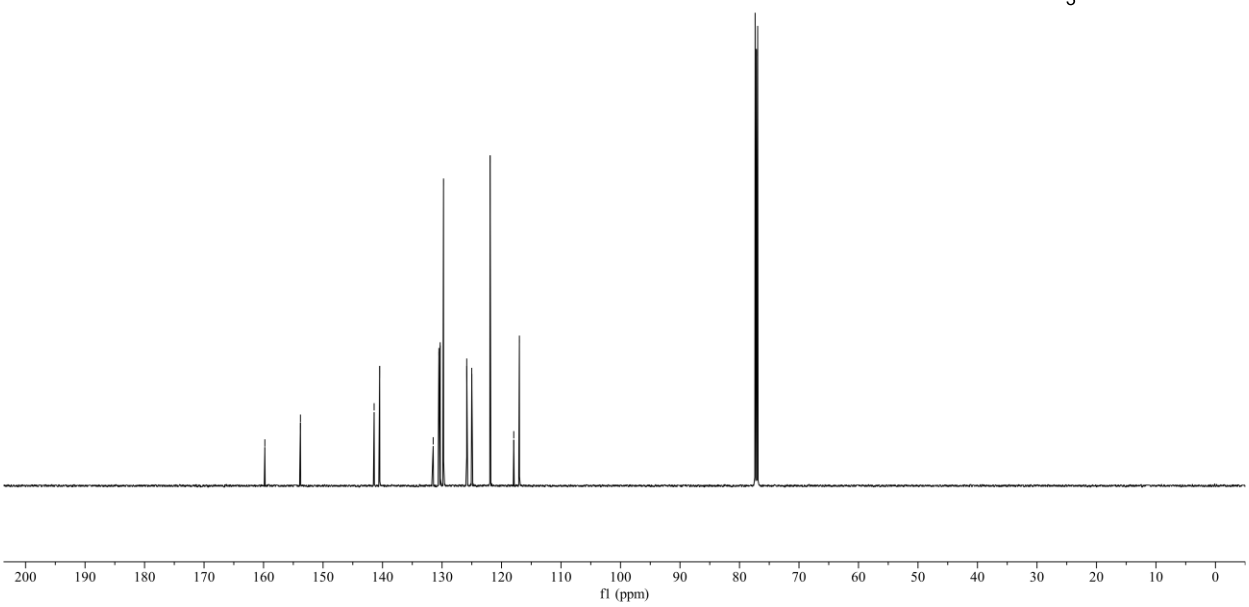


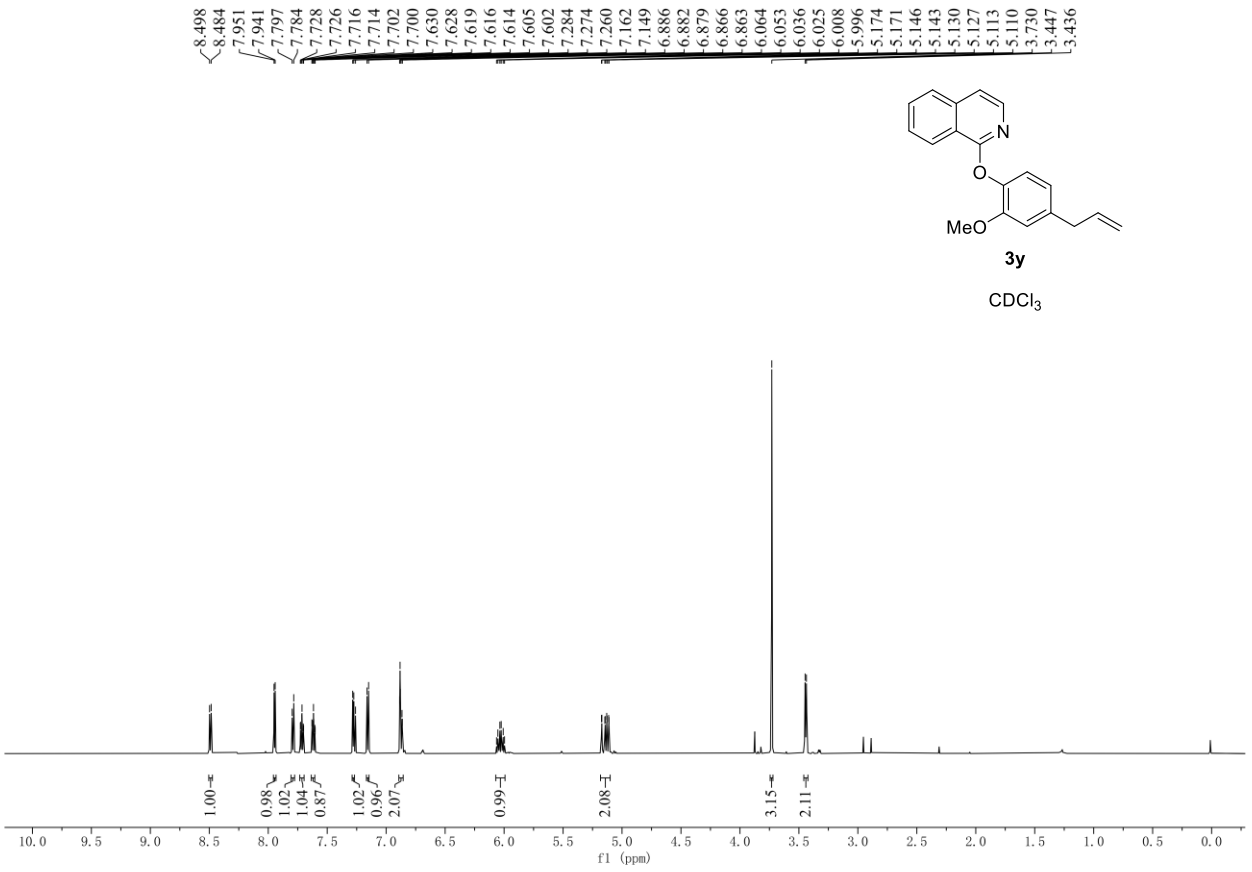




3x

$CDCl_3$

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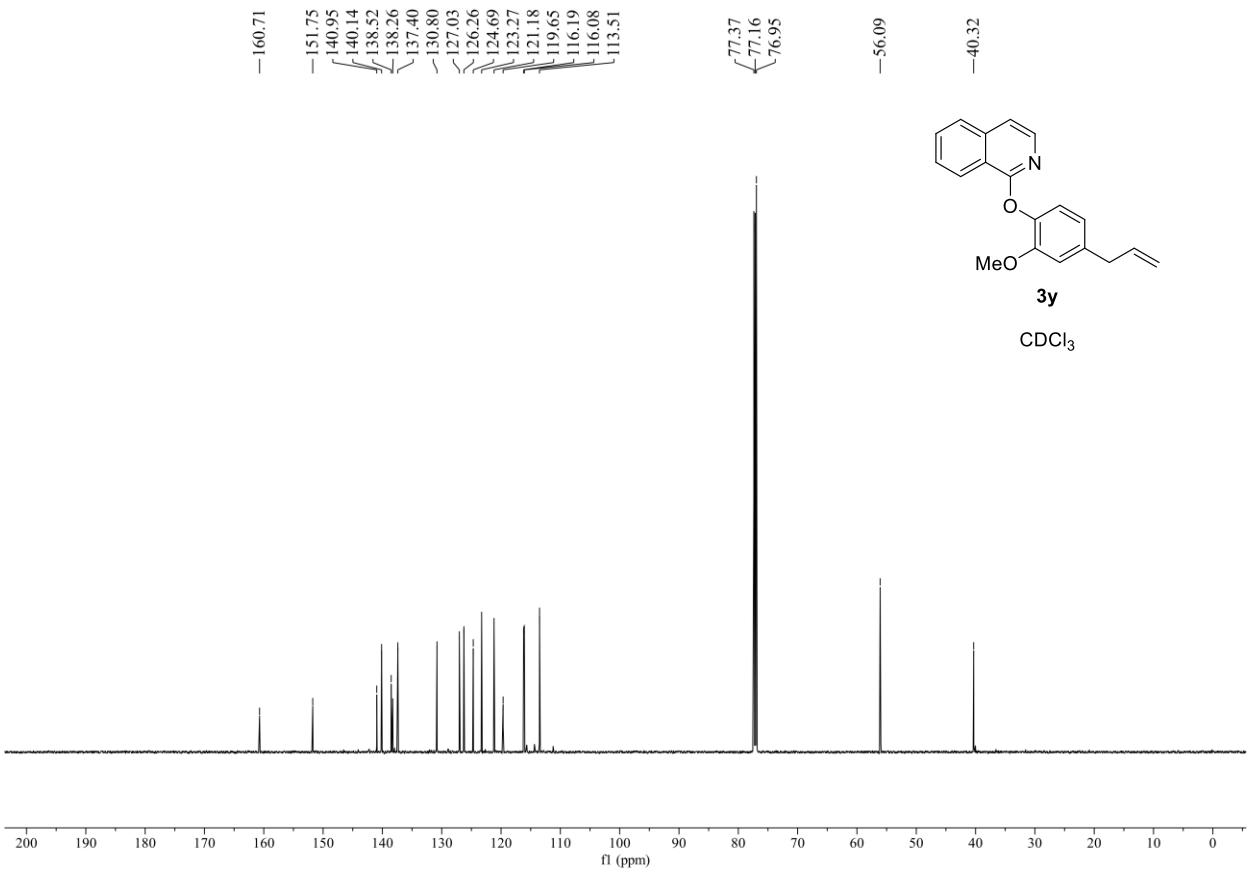
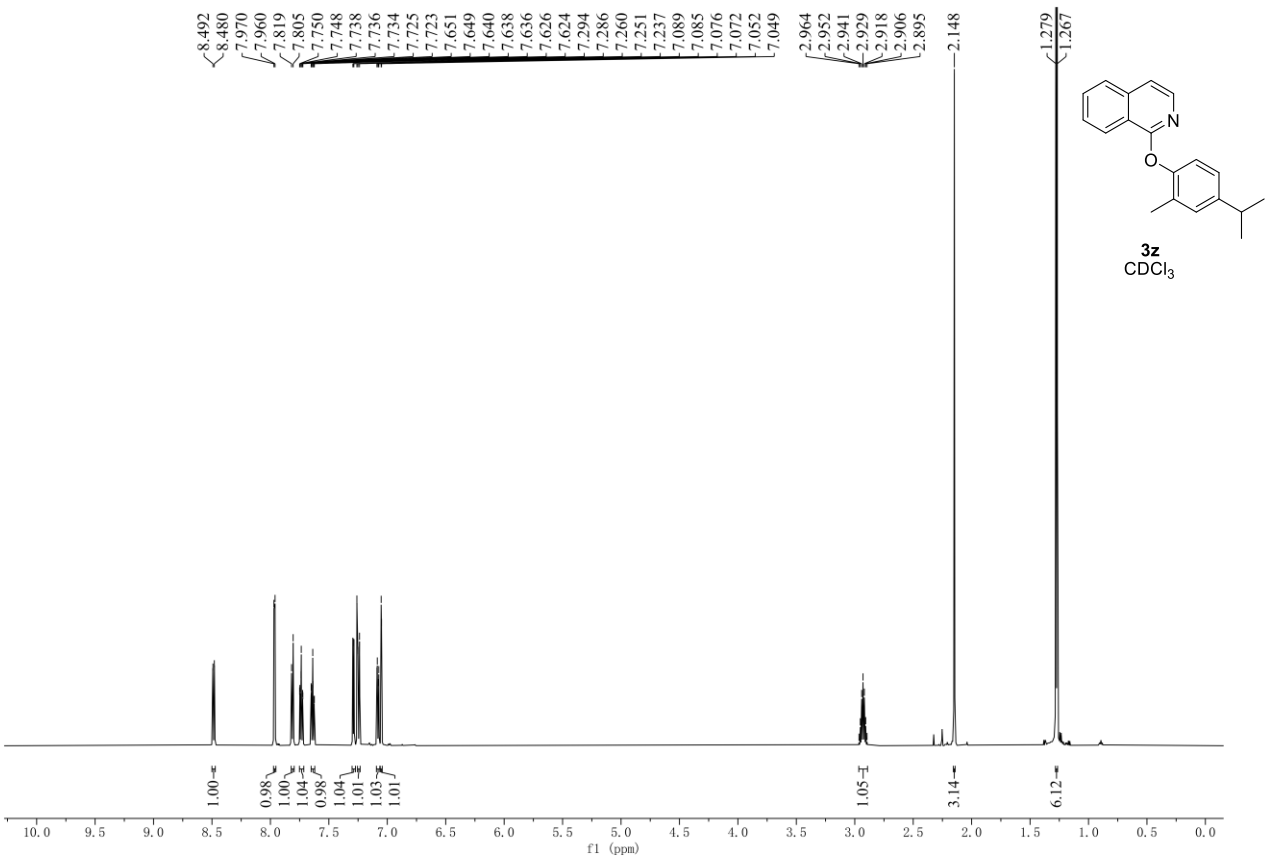
8.484
7.951
7.941
7.797
7.784
7.728
7.726
7.716
7.714
7.702
7.700
7.630
7.628
7.619
7.616
7.614
7.605
7.602
7.284
7.274
7.260
7.162
7.149
6.886
6.882
6.879
6.866
6.863
6.064
6.053
6.036
6.025
6.008
5.996
5.174
5.171
5.146
5.143
5.130
5.127
5.113
5.110
3.730
3.447
3.436
N
O
MeO
3y
CDCl3
1.00
0.98
1.02
1.04
0.87
1.02
0.96
2.07
0.99
2.08
3.15
2.11
f1 (ppm)


160.71
151.75
140.95
140.14
138.52
138.26
137.40
130.80
127.03
126.26
124.69
123.27
121.18
119.65
116.19
116.08
113.51
77.37
77.16
76.95
56.09
40.32
N
O
MeO
3y
CDCl3
f1 (ppm)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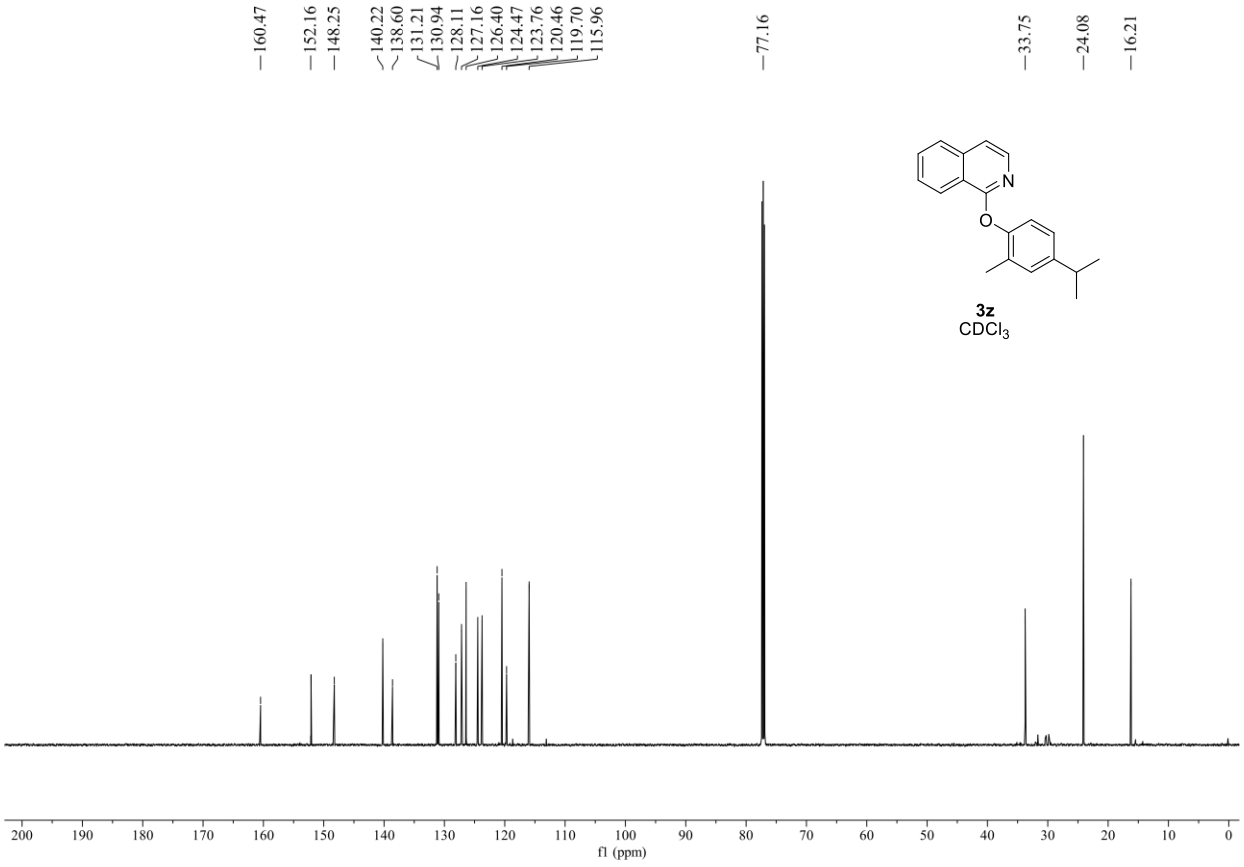
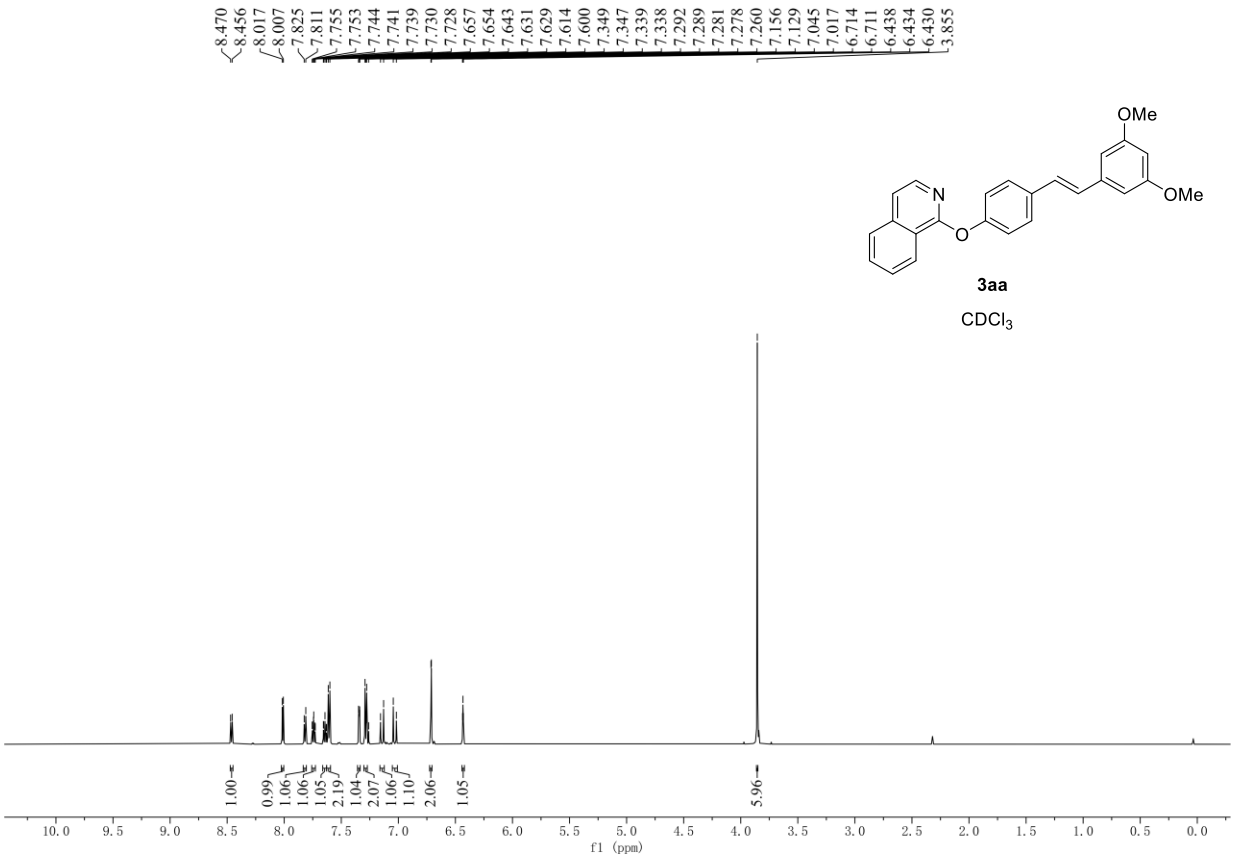
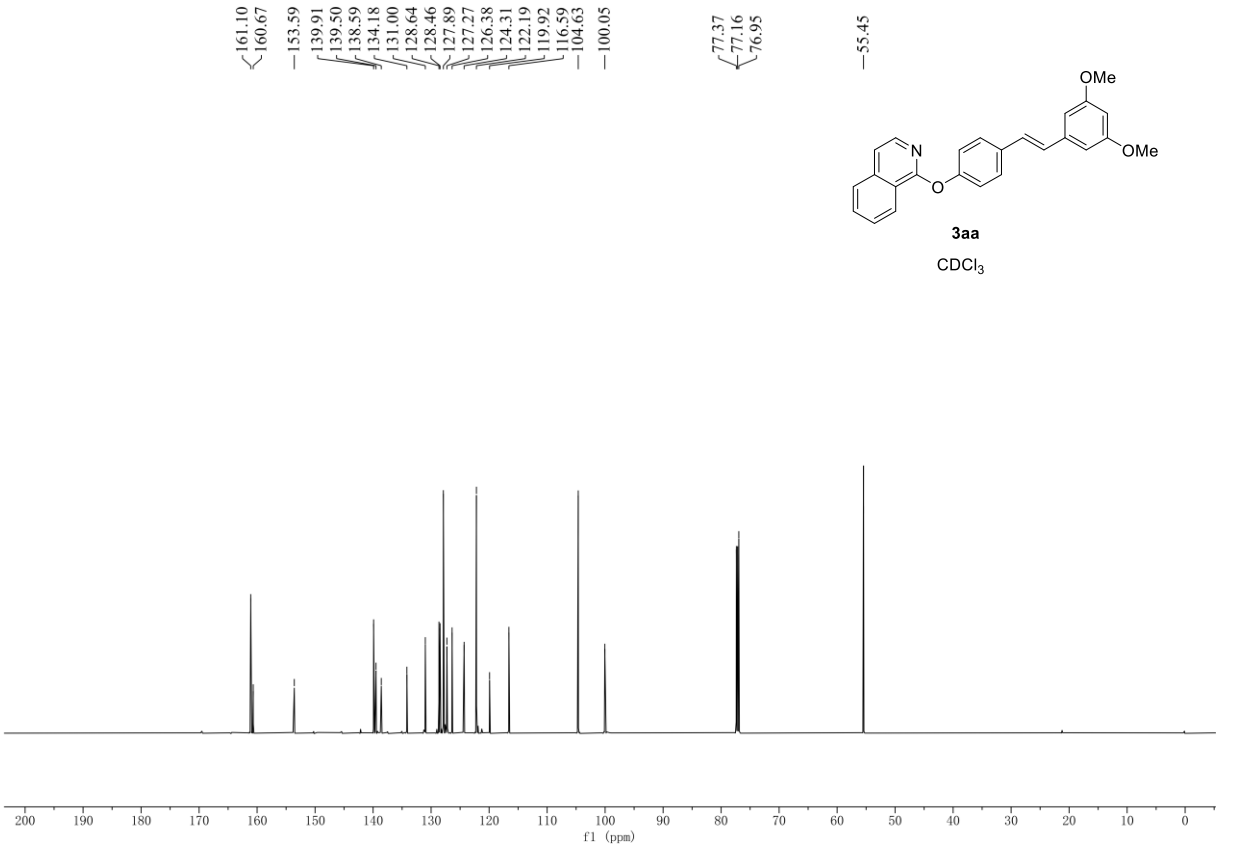
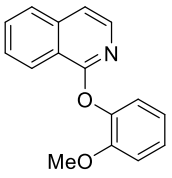
8.480
7.970
7.960
7.819
7.805
7.750
7.748
7.738
7.736
7.734
7.725
7.723
7.651
7.649
7.640
7.638
7.636
7.626
7.624
7.294
7.286
7.260
7.251
7.237
7.089
7.085
7.076
7.072
7.052
7.049
2.964
2.952
2.941
2.929
2.918
2.906
2.895
2.148
1.279
1.267
1.00
0.98
1.00
1.04
0.98
1.04
1.01
1.03
1.01
1.05
3.14
6.12
f1 (ppm)
3z
CDCl3


160.47
152.16
148.25
140.22
138.60
131.21
130.94
128.11
127.16
126.40
124.47
123.76
120.46
119.70
115.96
77.16
33.75
24.08
16.21
f1 (ppm)
3z
CDCl3

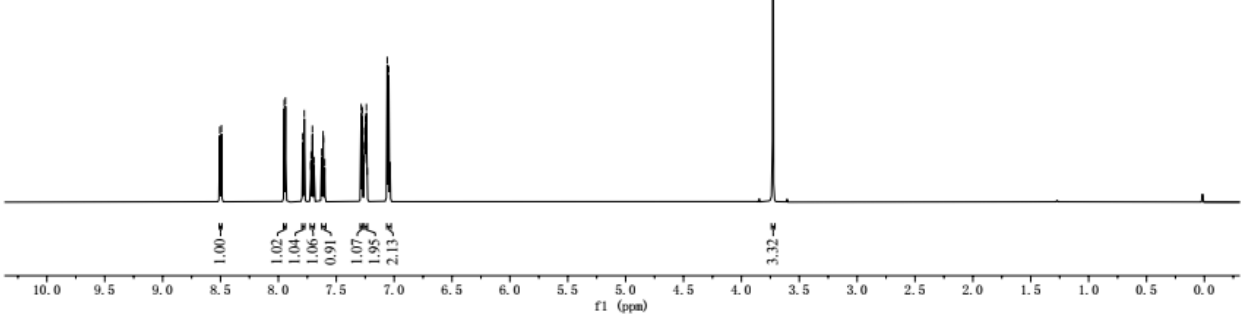

8.470
8.456
8.017
8.007
7.825
7.811
7.755
7.753
7.744
7.741
7.739
7.730
7.728
7.657
7.654
7.643
7.631
7.629
7.614
7.600
7.349
7.347
7.339
7.338
7.292
7.289
7.281
7.278
7.260
7.156
7.129
7.045
7.017
6.714
6.711
6.438
6.434
6.430
3.855
OMe
OMe
N
O
3aa
CDCl3
1.00
0.99
1.06
1.06
1.05
2.19
1.04
2.07
1.06
1.10
2.06
1.05
5.96
f1 (ppm)

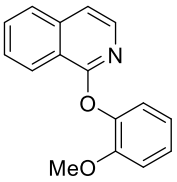

161.10
160.67
153.59
139.91
139.50
138.59
134.18
131.00
128.64
128.46
127.89
127.27
126.38
124.31
122.19
119.92
116.59
104.63
100.05
77.37
77.16
76.95
55.45
OMe
OMe
N
O
3aa
CDCl3
f1 (ppm)



3ab

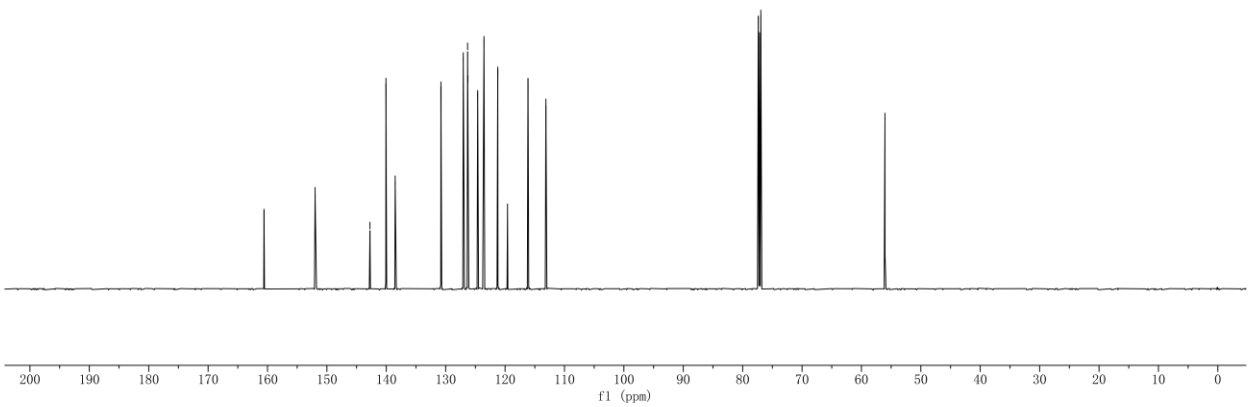
$CDCl_3$

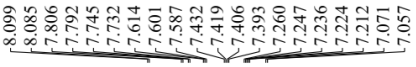


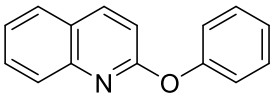


3ab

$CDCl_3$

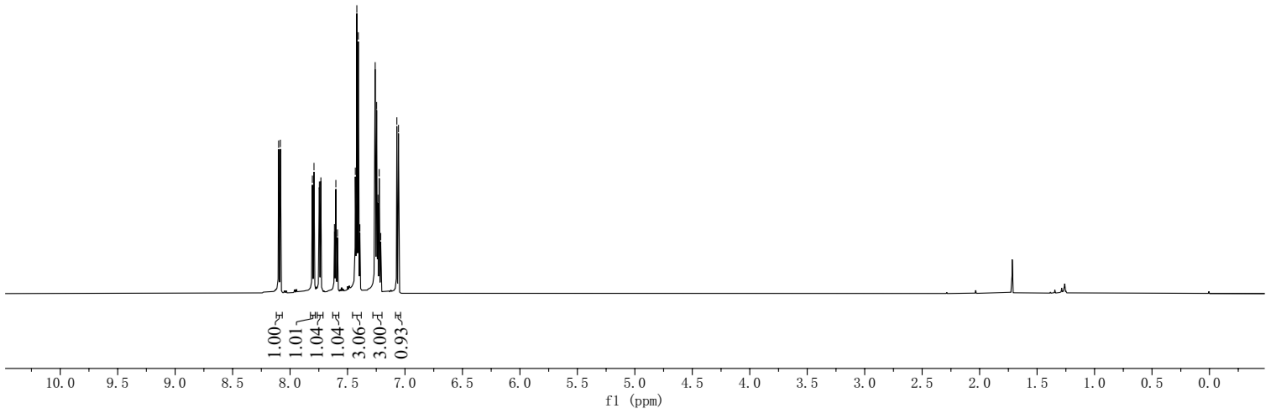


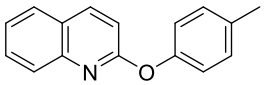




6a

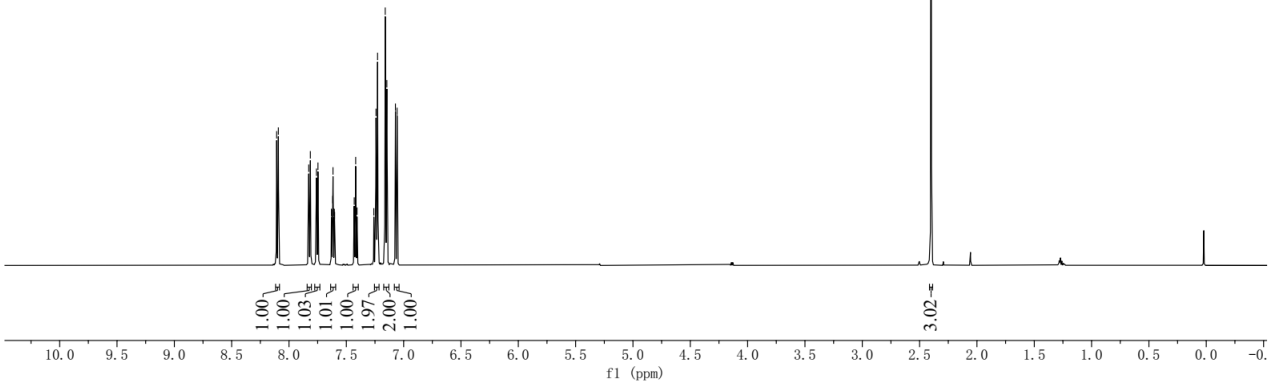
$CDCl_3$

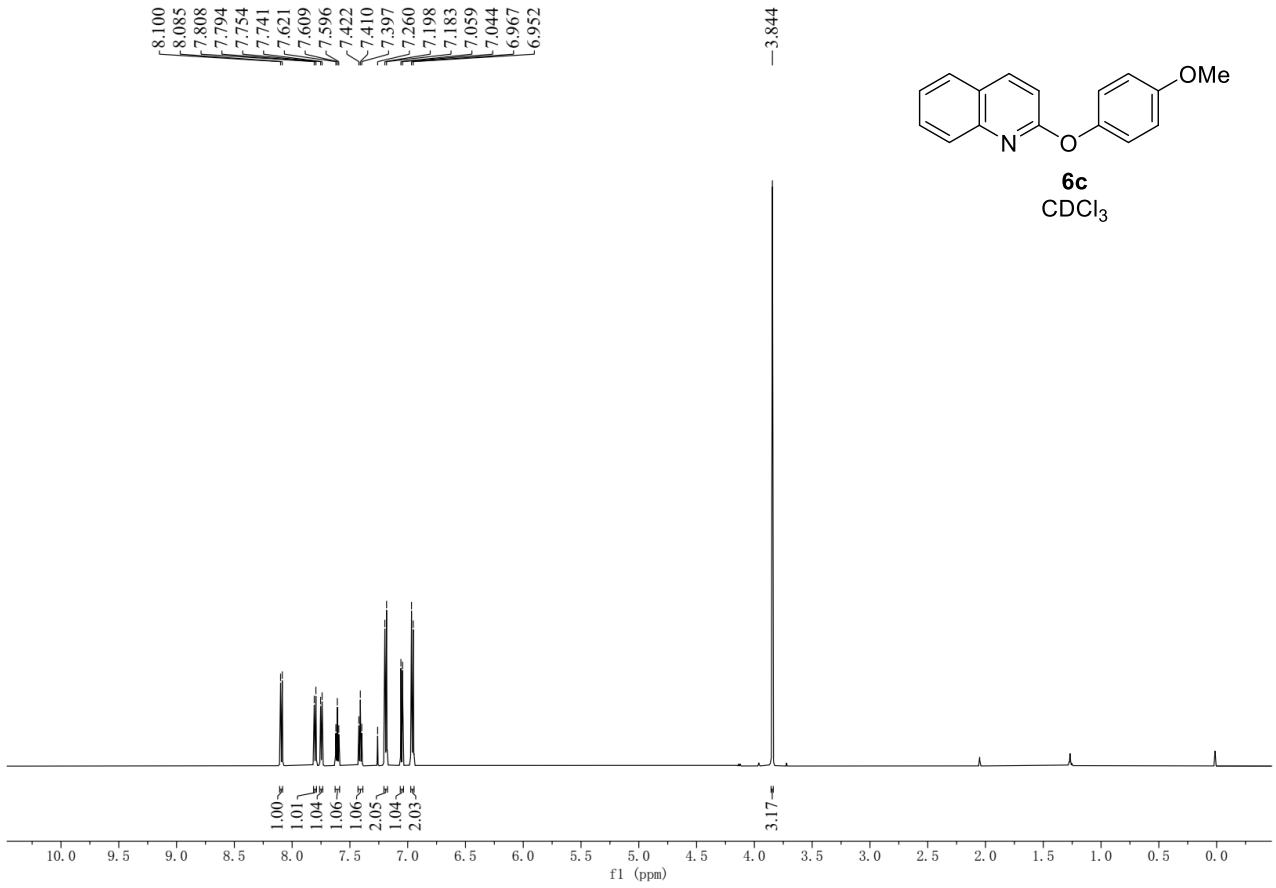


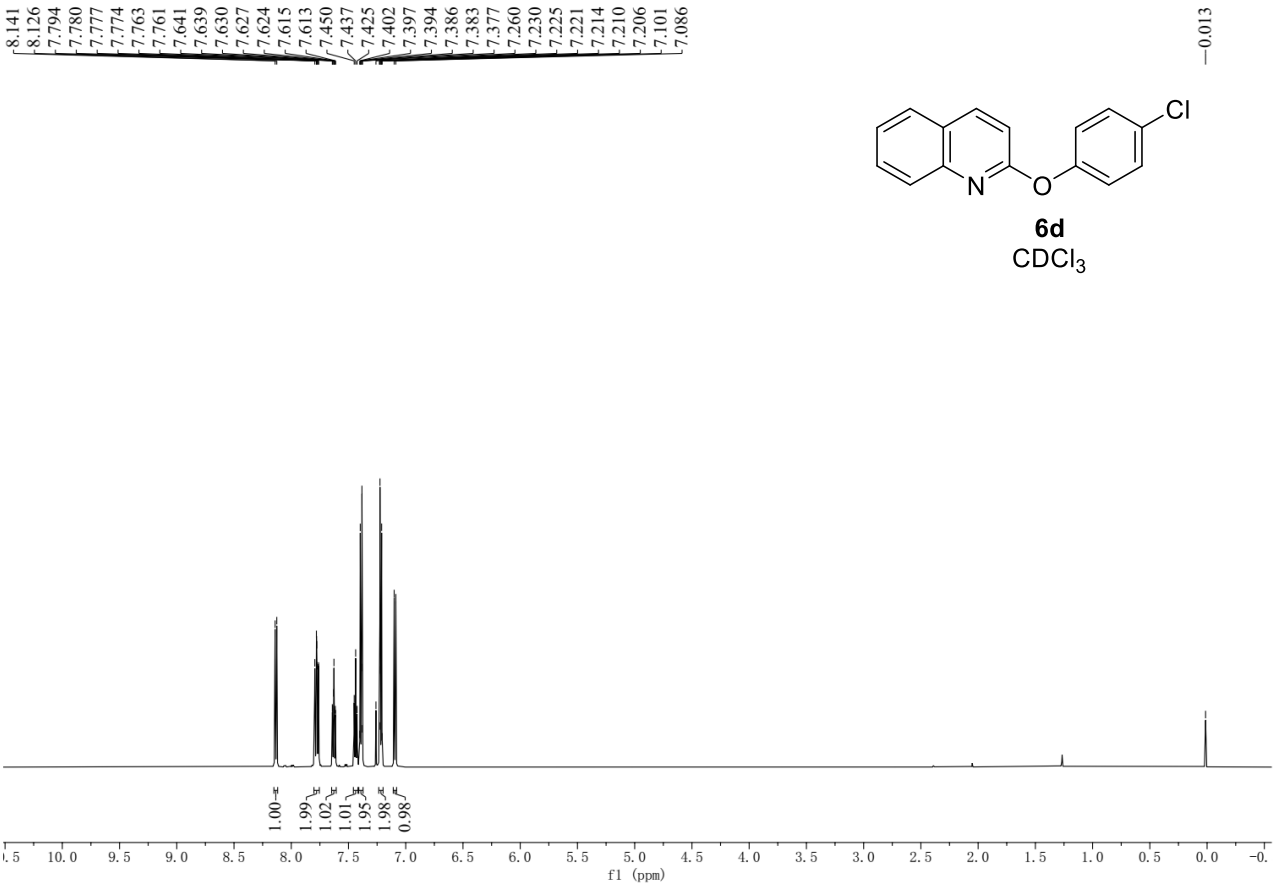


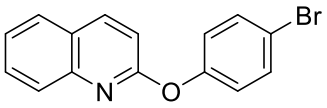
6b

$CDCl_3$



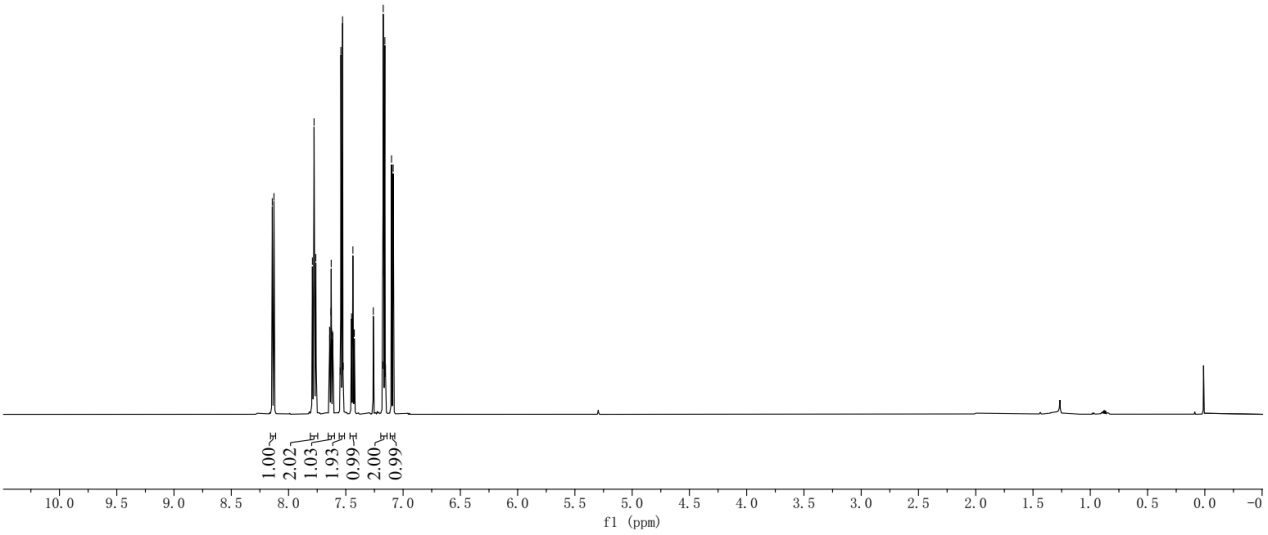

8.100
8.085
7.808
7.794
7.754
7.741
7.621
7.609
7.596
7.422
7.410
7.397
7.260
7.198
7.183
7.059
7.044
6.967
6.952
3.844
OMe
N
O
6c
CDCl3
1.00
1.01
1.04
1.06
1.06
2.05
1.04
2.03
3.17
f1 (ppm)

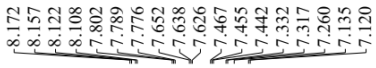

8.141
8.126
7.794
7.780
7.777
7.774
7.763
7.761
7.641
7.639
7.630
7.627
7.624
7.615
7.613
7.450
7.437
7.425
7.402
7.397
7.394
7.386
7.383
7.377
7.260
7.230
7.225
7.221
7.214
7.210
7.206
7.101
7.086
0.013
Cl
N
O
6d
CDCl3
1.00
1.99
1.02
1.01
1.95
1.98
0.98
f1 (ppm)

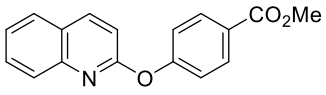


6e

$CDCl_3$

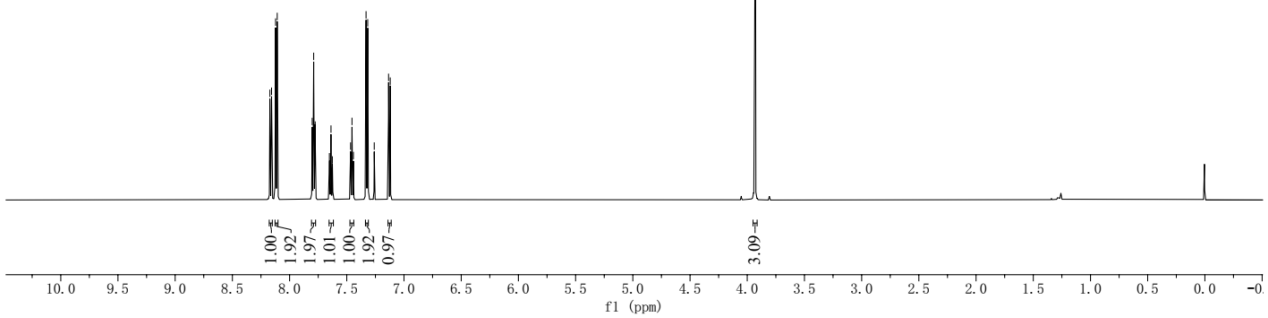


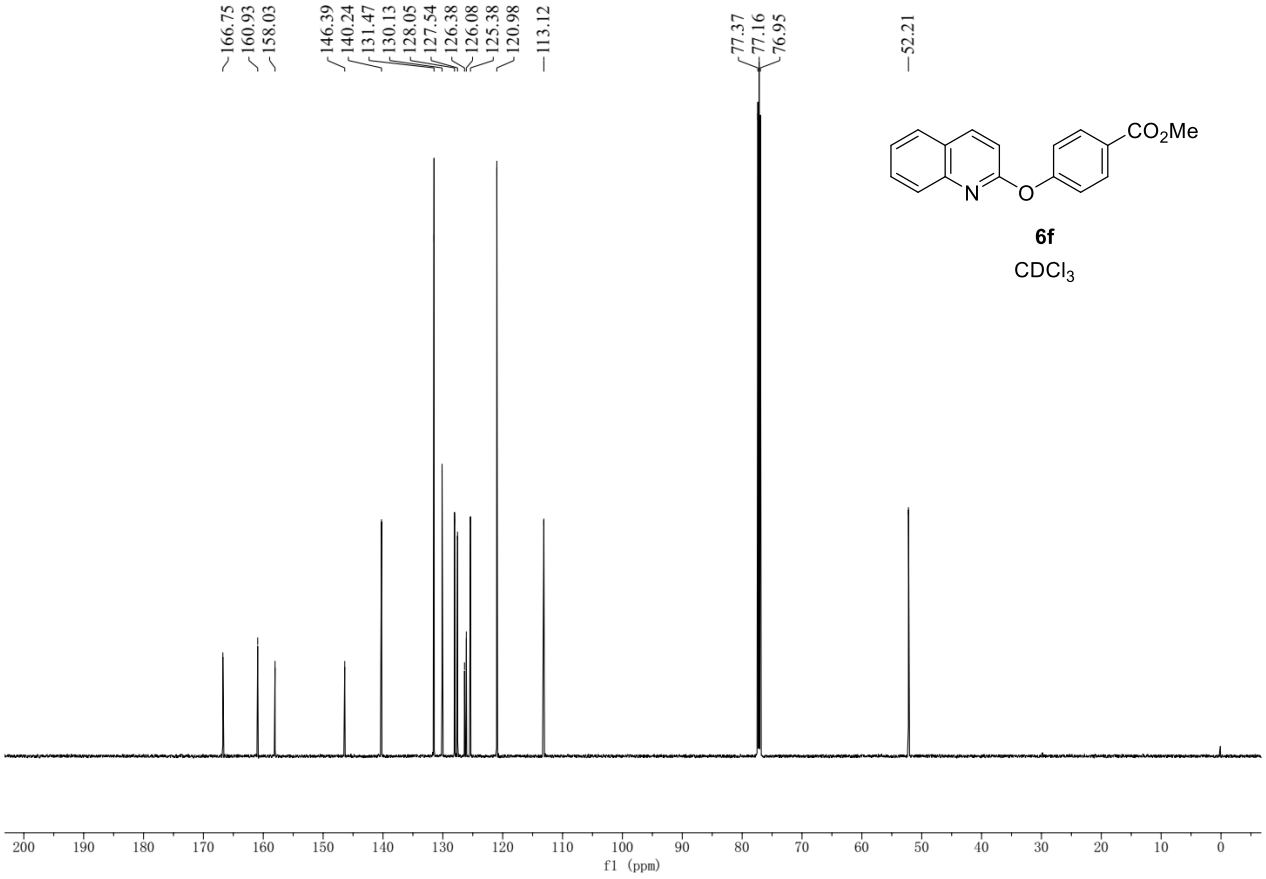


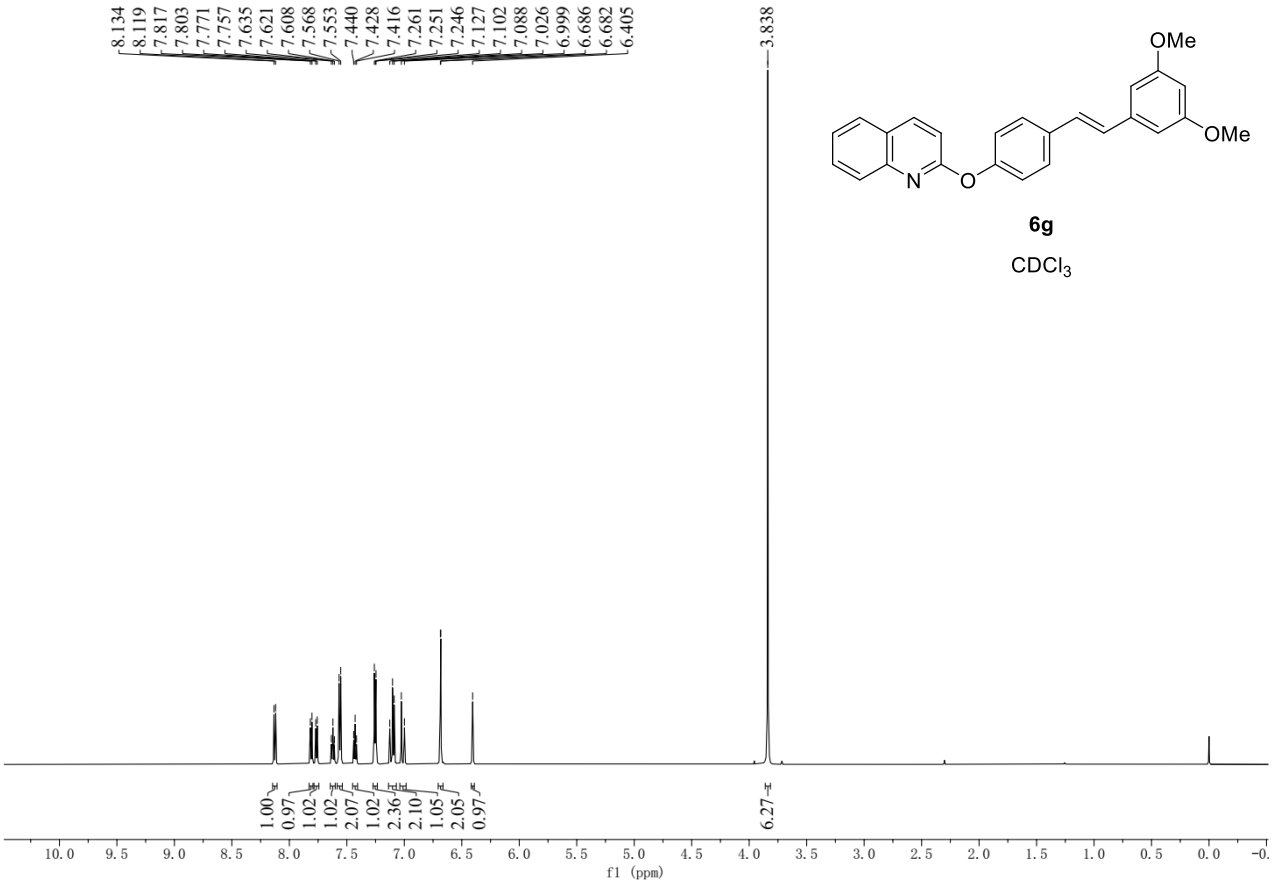


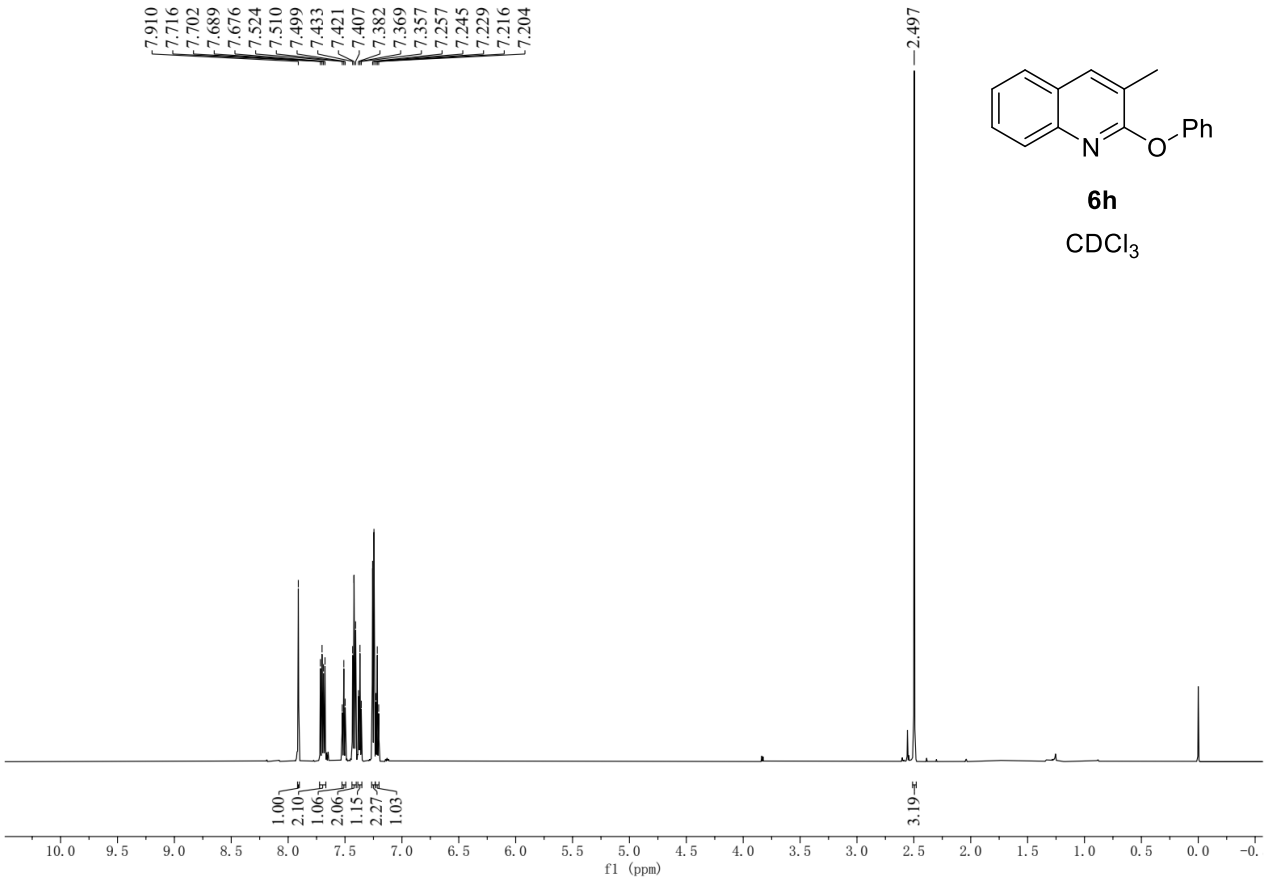
6f

$CDCl_3$



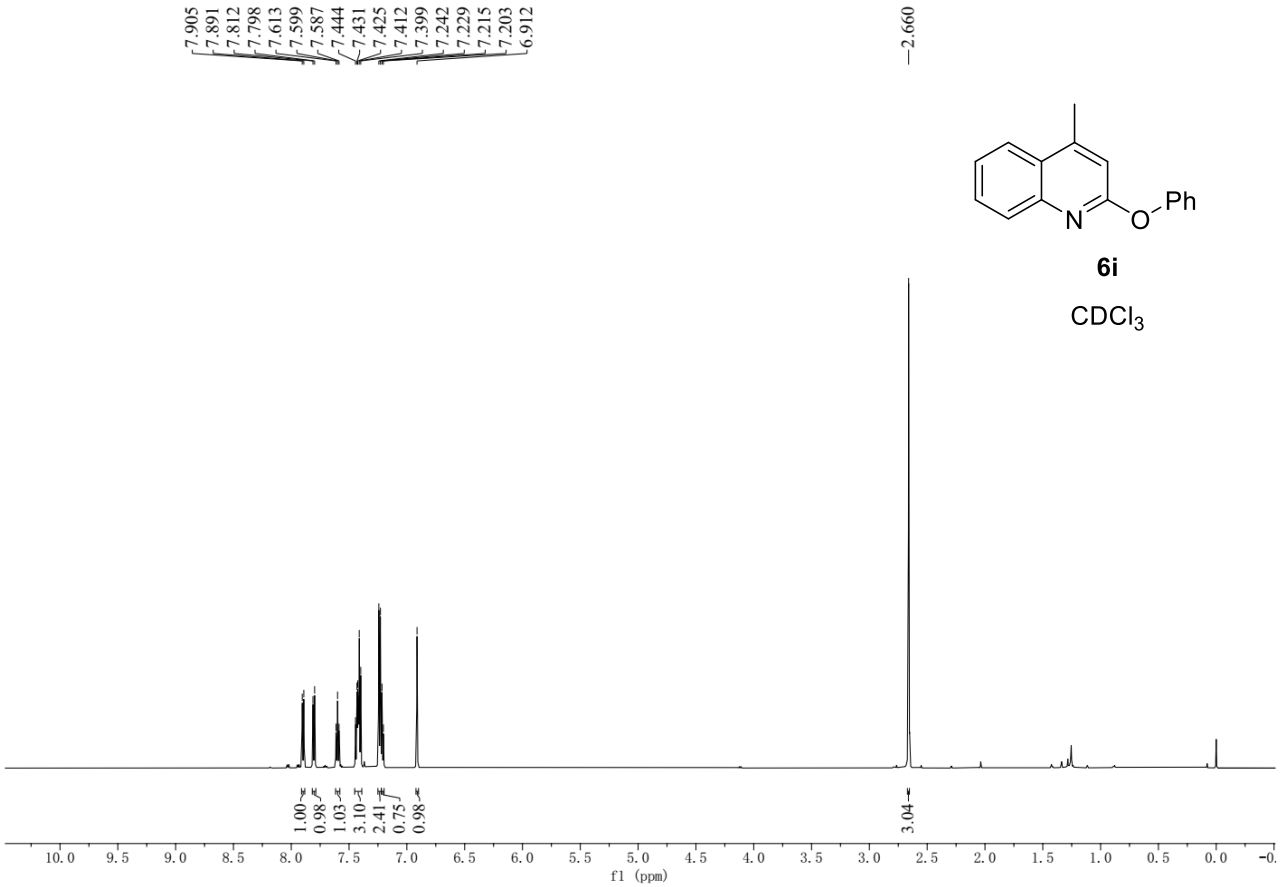

166.75
160.93
158.03
146.39
140.24
131.47
130.13
128.05
127.54
126.38
126.08
125.38
120.98
113.12
77.37
77.16
76.95
52.21
CO2Me
N
O
6f
CDCl3
f1 (ppm)


8.134
8.119
7.817
7.803
7.771
7.757
7.635
7.621
7.608
7.568
7.553
7.440
7.428
7.416
7.261
7.251
7.246
7.127
7.102
7.088
7.026
6.999
6.686
6.682
6.405
3.838
OMe
OMe
N
O
6g
CDCl3
1.00
0.97
1.02
1.02
2.07
1.02
2.36
2.10
1.05
2.05
0.97
6.27
f1 (ppm)



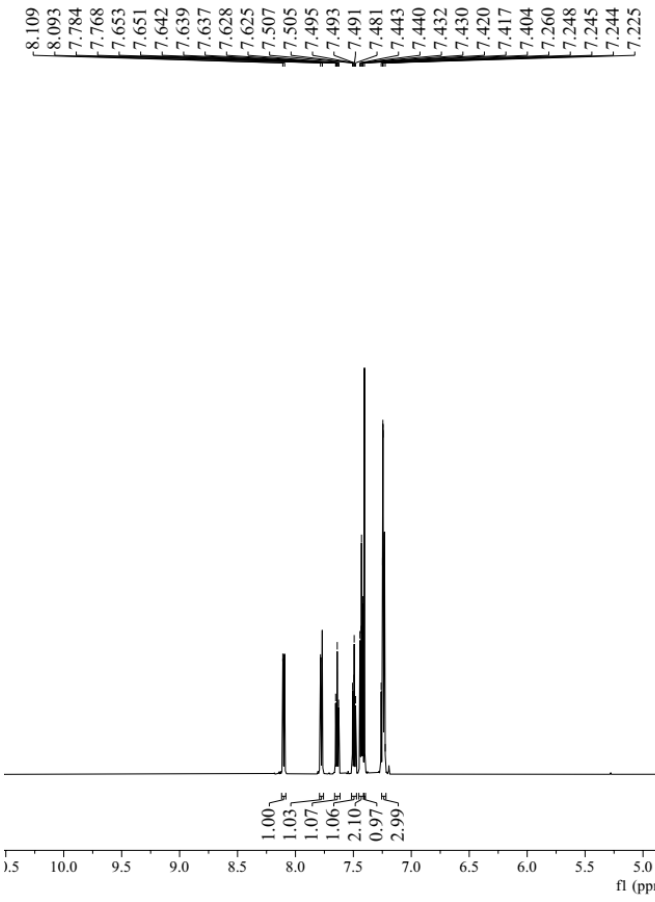
6h

$CDCl_3$



6i

$CDCl_3$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8.093
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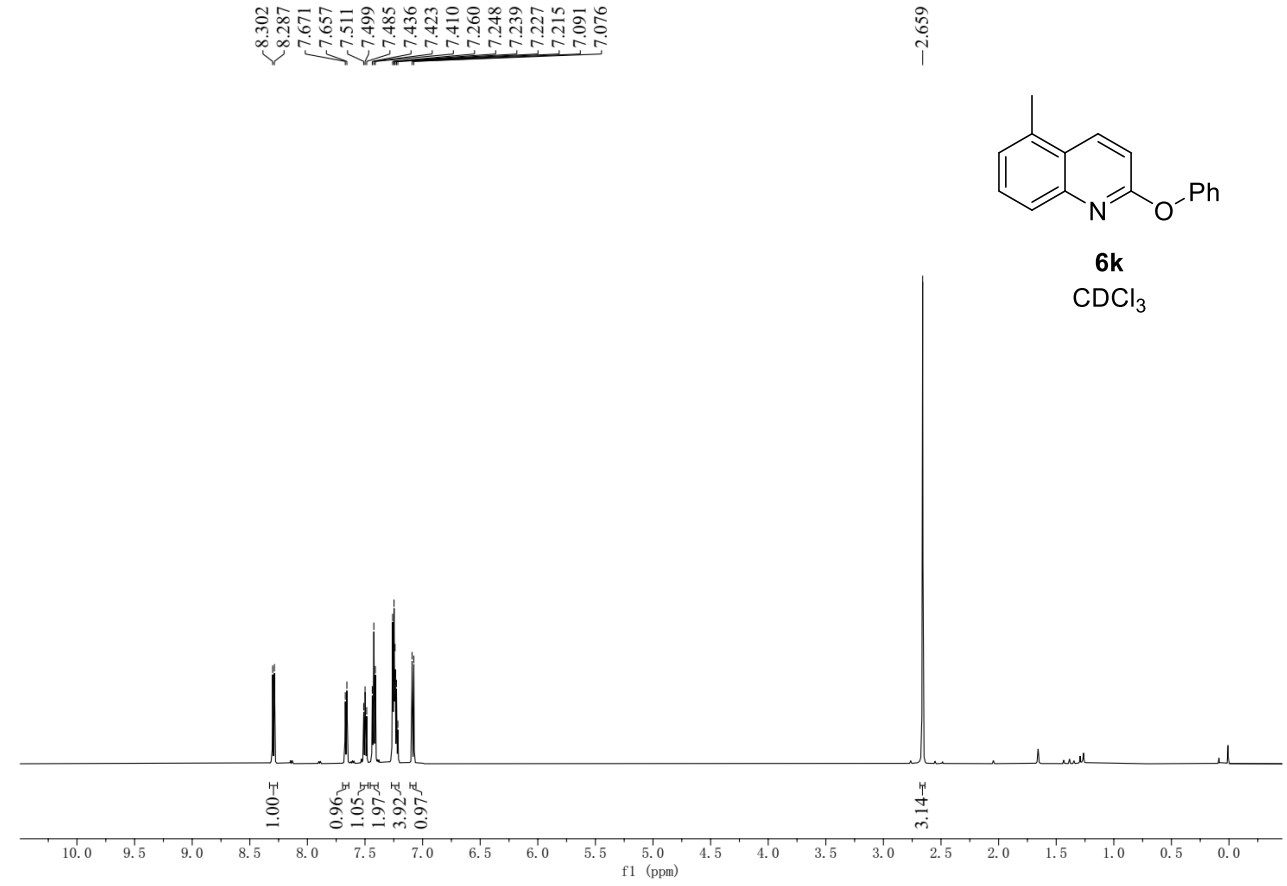
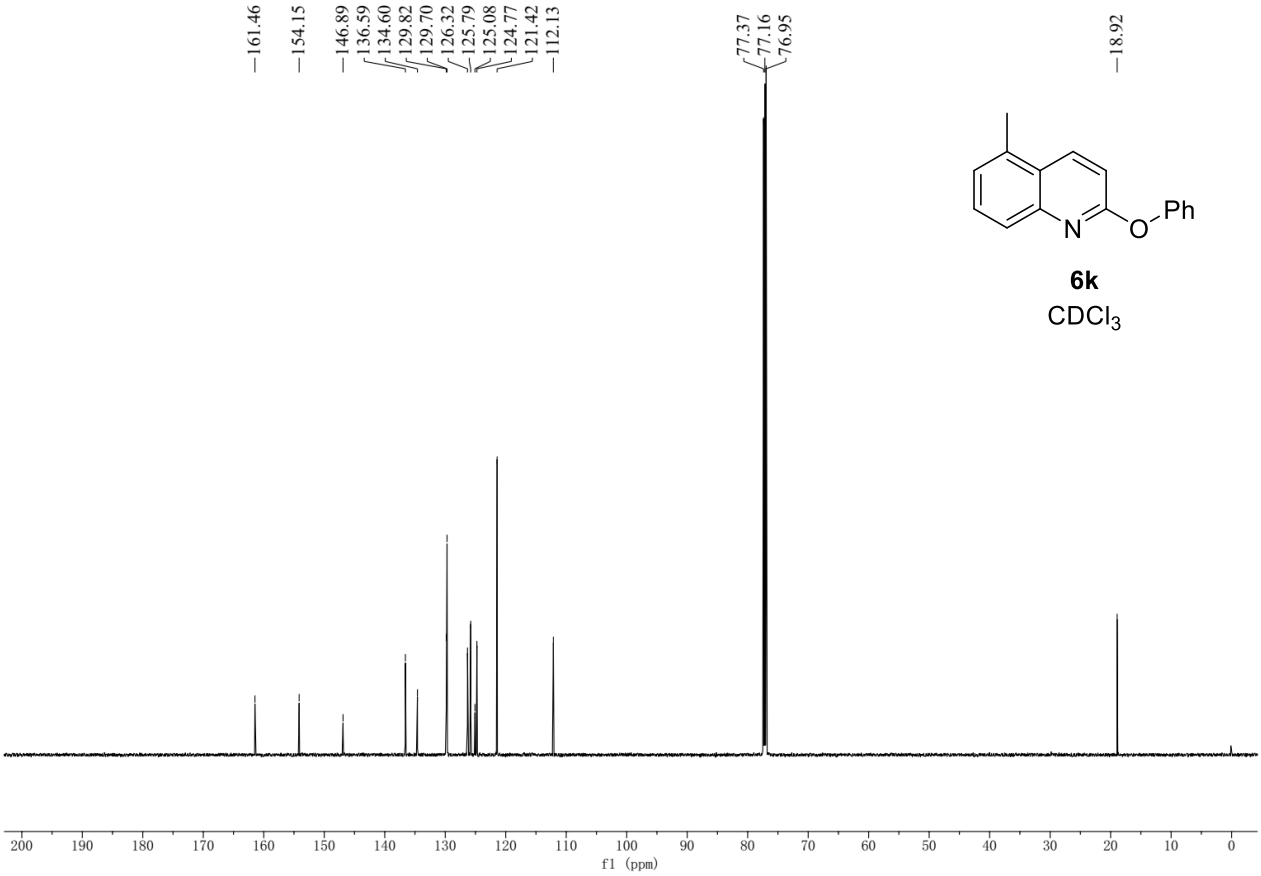
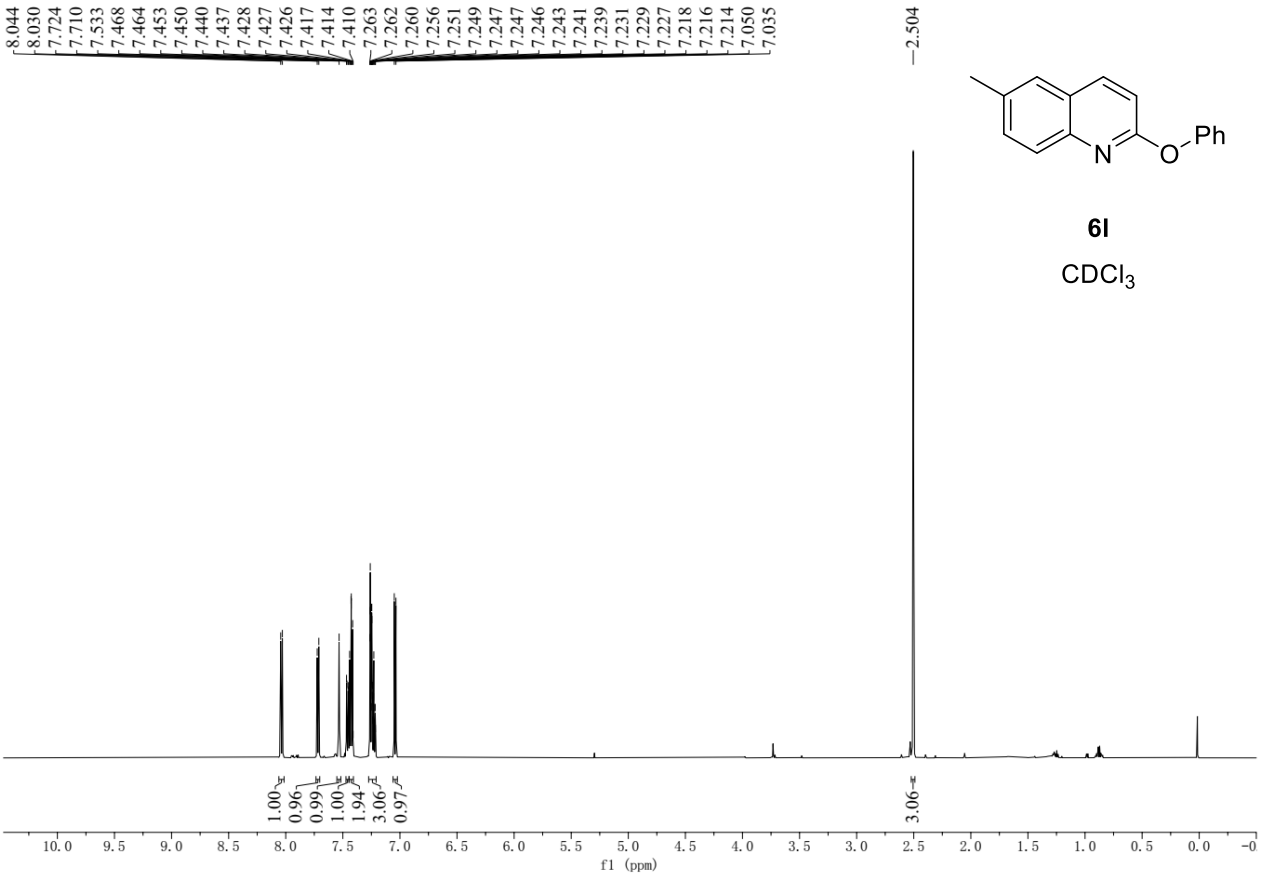
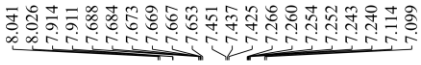
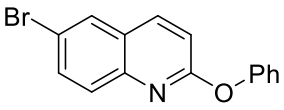
7.768
7.653
7.651
7.642
7.639
7.637
7.628
7.625
7.507
7.505
7.495
7.493
7.491
7.481
7.443
7.440
7.432
7.430
7.420
7.417
7.404
7.260
7.248
7.245
7.244
7.225
Br
N
O
Ph
6j
CDCl3
1.00
1.03
1.07
1.06
2.10
0.97
2.99
f1 (ppm)


8.302
8.287
7.671
7.657
7.511
7.499
7.485
7.436
7.423
7.410
7.260
7.248
7.239
7.227
7.215
7.091
7.076
2.659
N
O
Ph
6k
CDCl3
1.00
0.96
1.05
1.97
3.92
0.97
3.14
f1 (ppm)


161.46
154.15
146.89
136.59
134.60
129.82
129.70
126.32
125.79
125.08
124.77
121.42
112.13
77.37
77.16
76.95
18.92
Ph
N
O
6k
CDCl3
f1 (ppm)

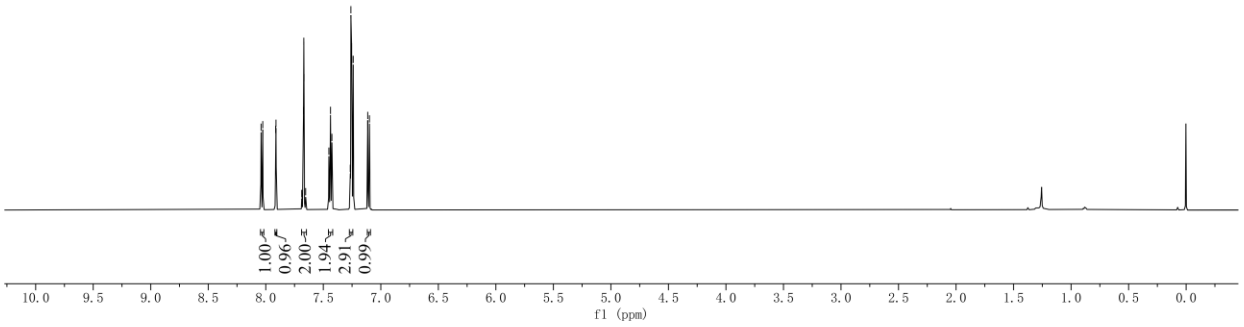

8.044
8.030
7.724
7.710
7.533
7.468
7.464
7.453
7.450
7.440
7.437
7.428
7.427
7.426
7.417
7.414
7.410
7.263
7.262
7.260
7.256
7.251
7.249
7.247
7.247
7.246
7.243
7.241
7.239
7.231
7.229
7.227
7.218
7.216
7.214
7.050
7.035
2.504
Ph
N
O
6l
CDCl3
1.00
0.96
0.99
1.00
1.94
3.06
0.97
3.06
f1 (ppm)

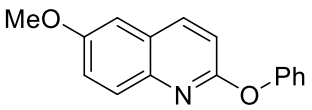




6m

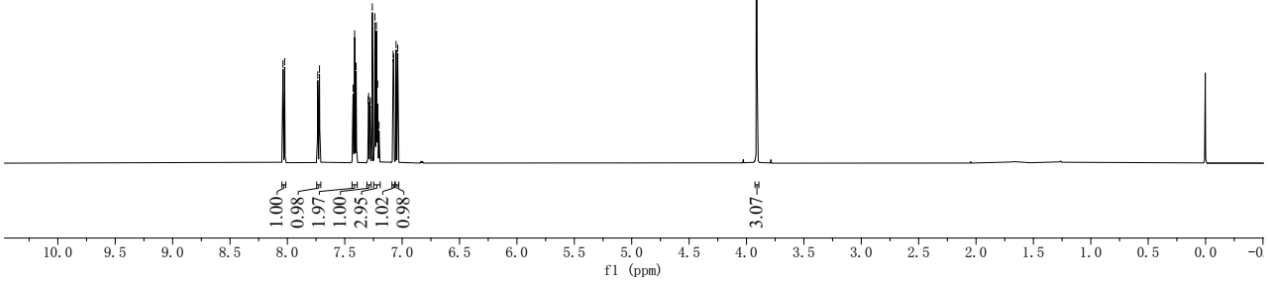
$CDCl_3$

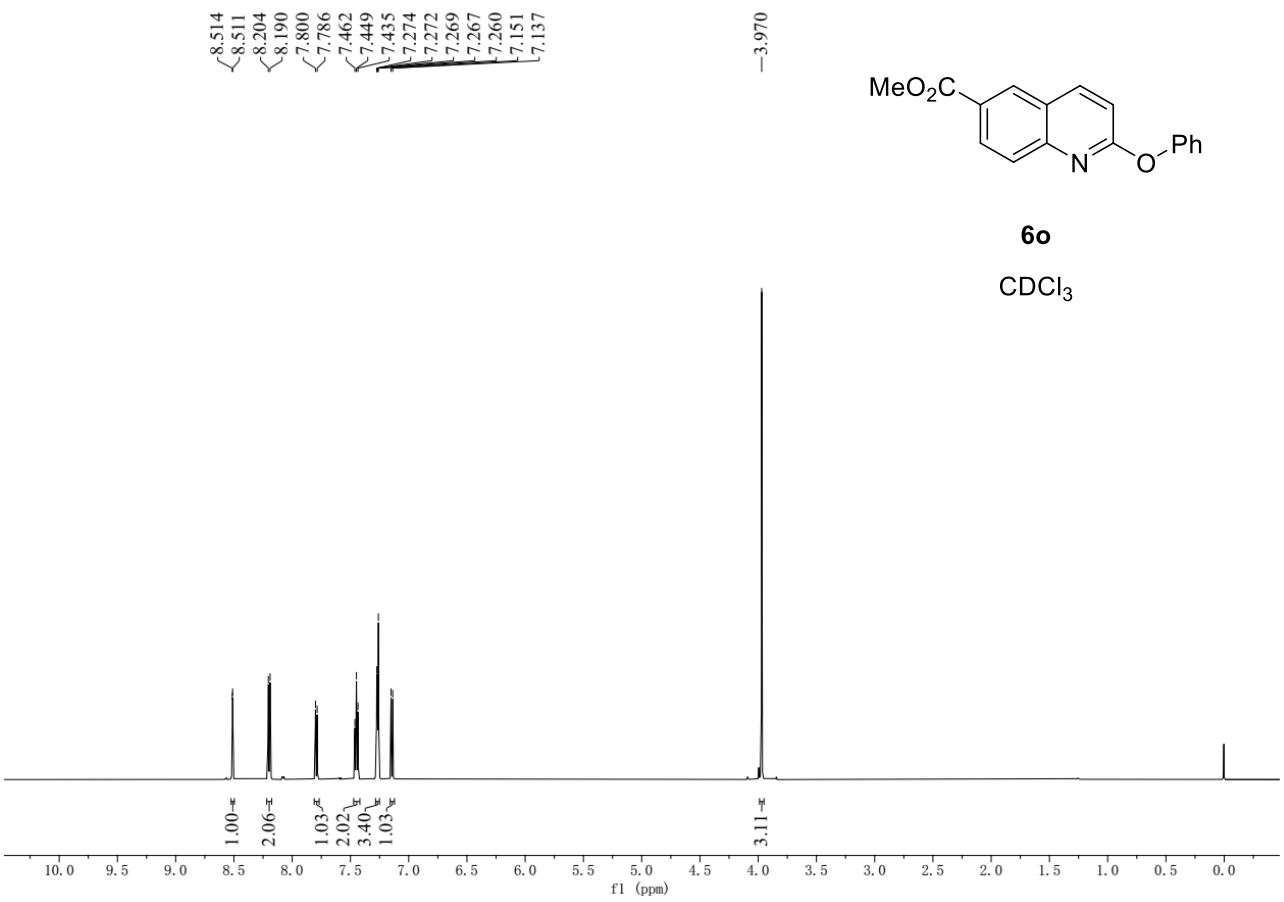




6n

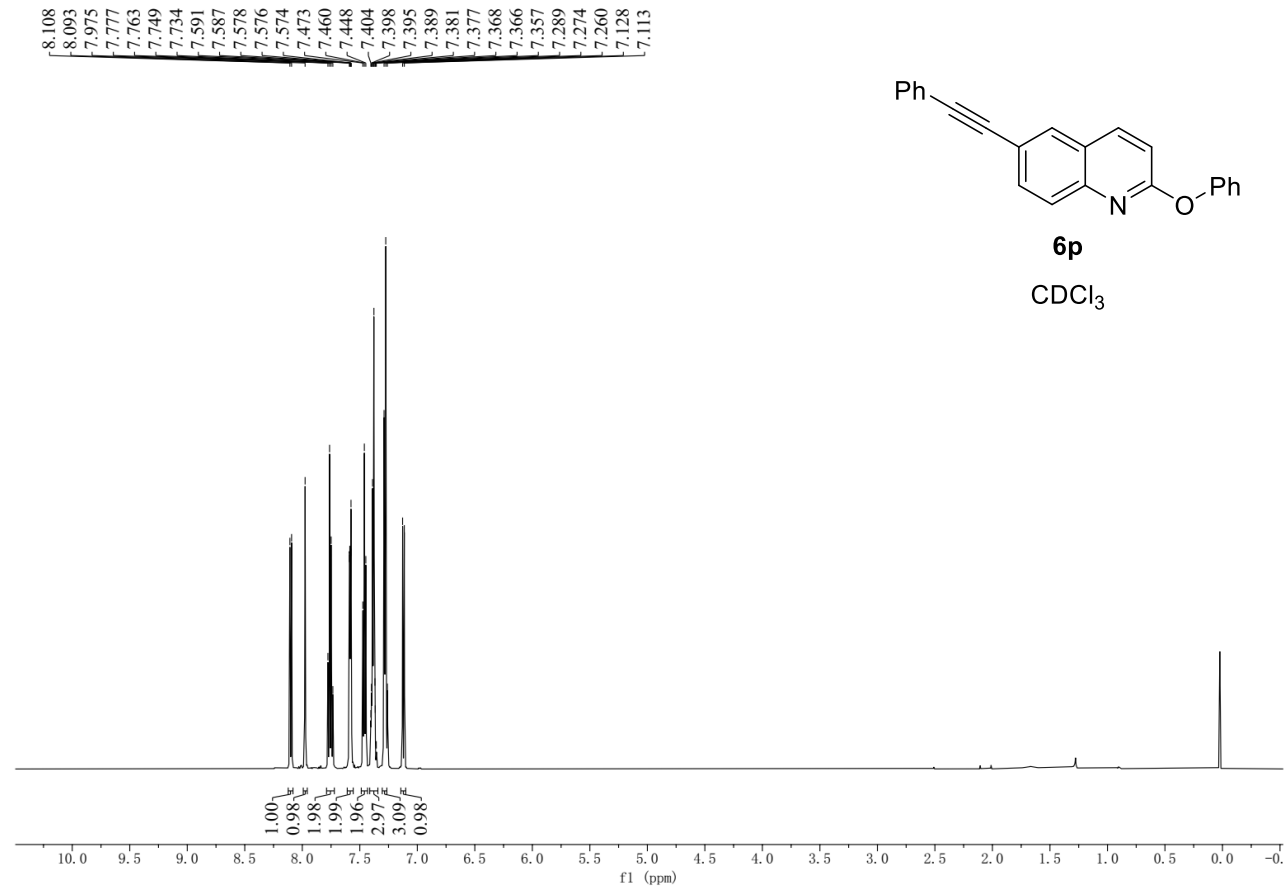
$CDCl_3$





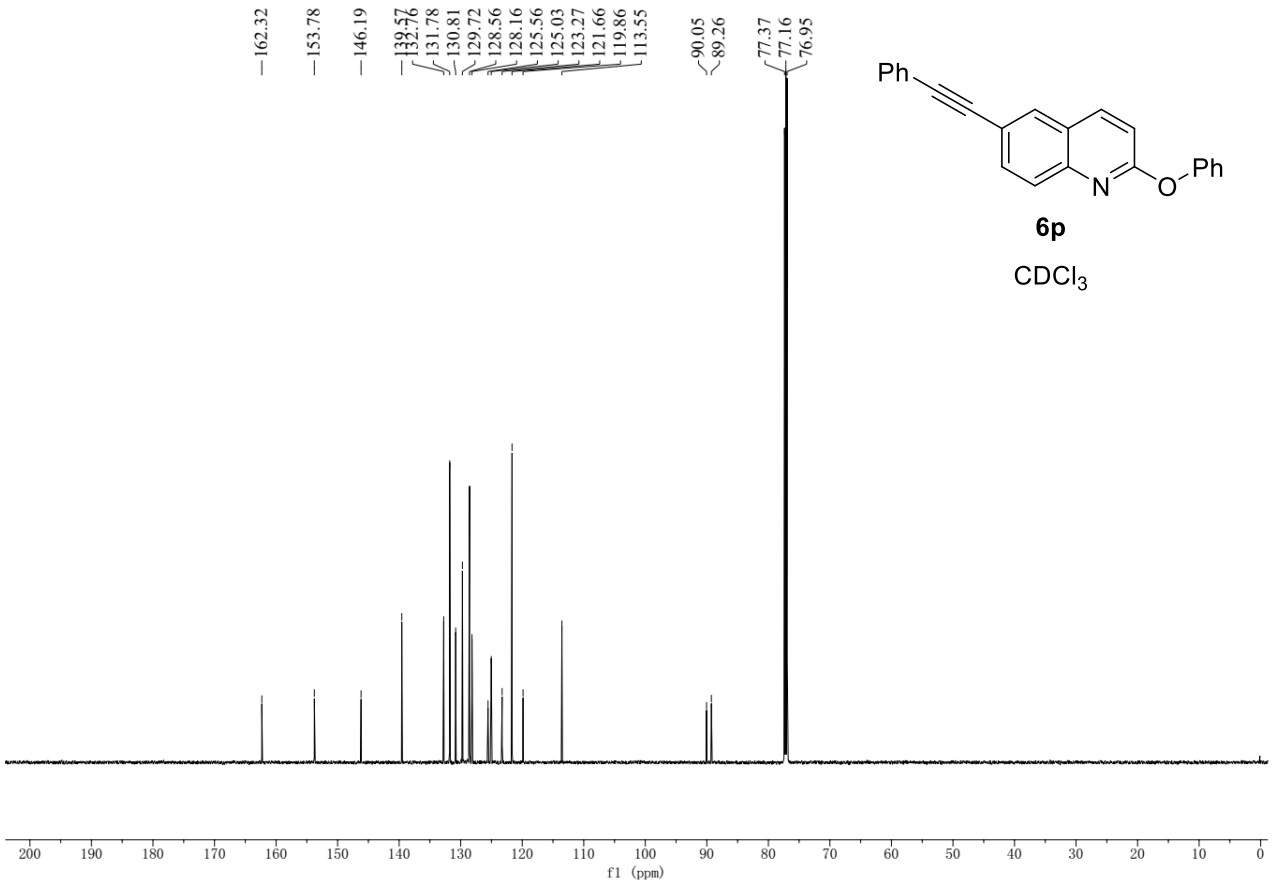
6o

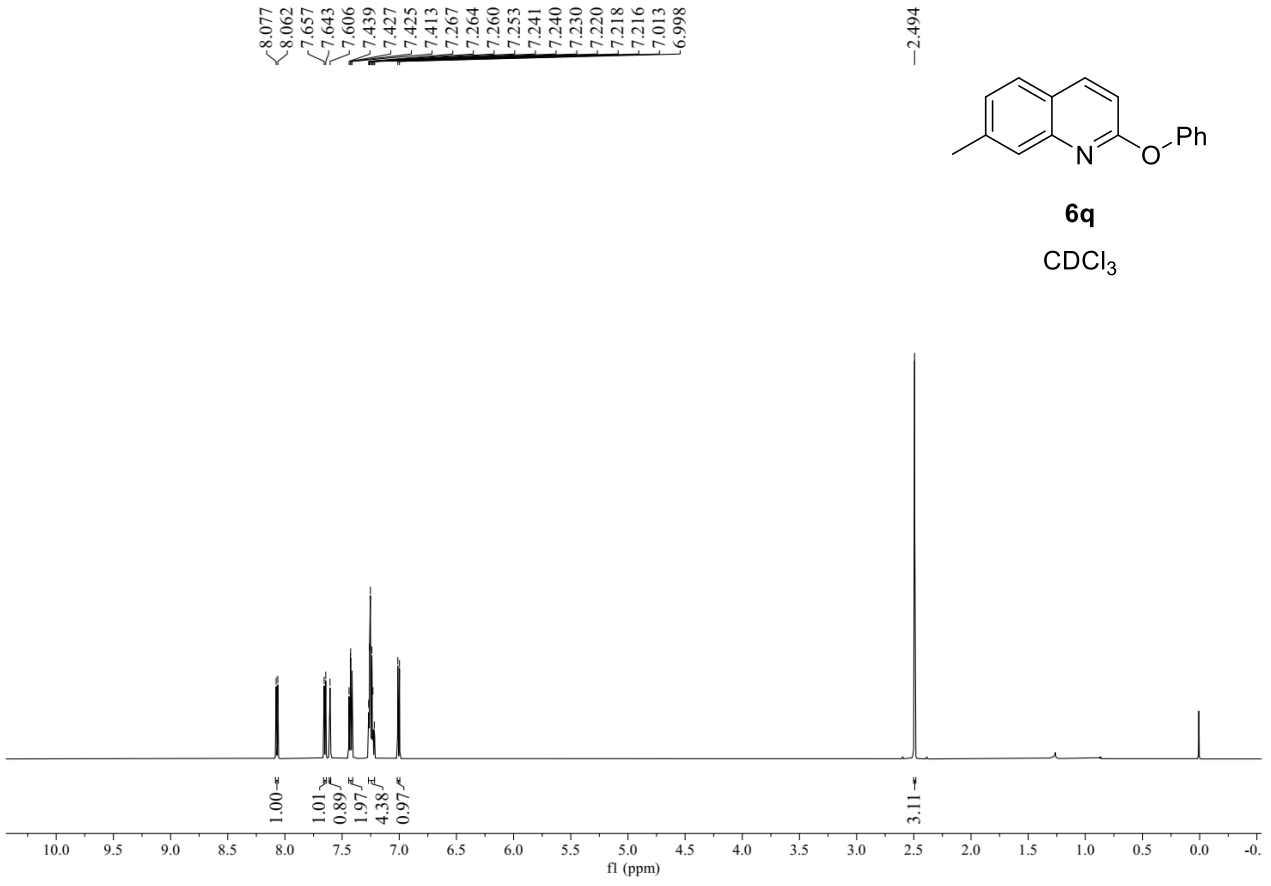
$CDCl_3$

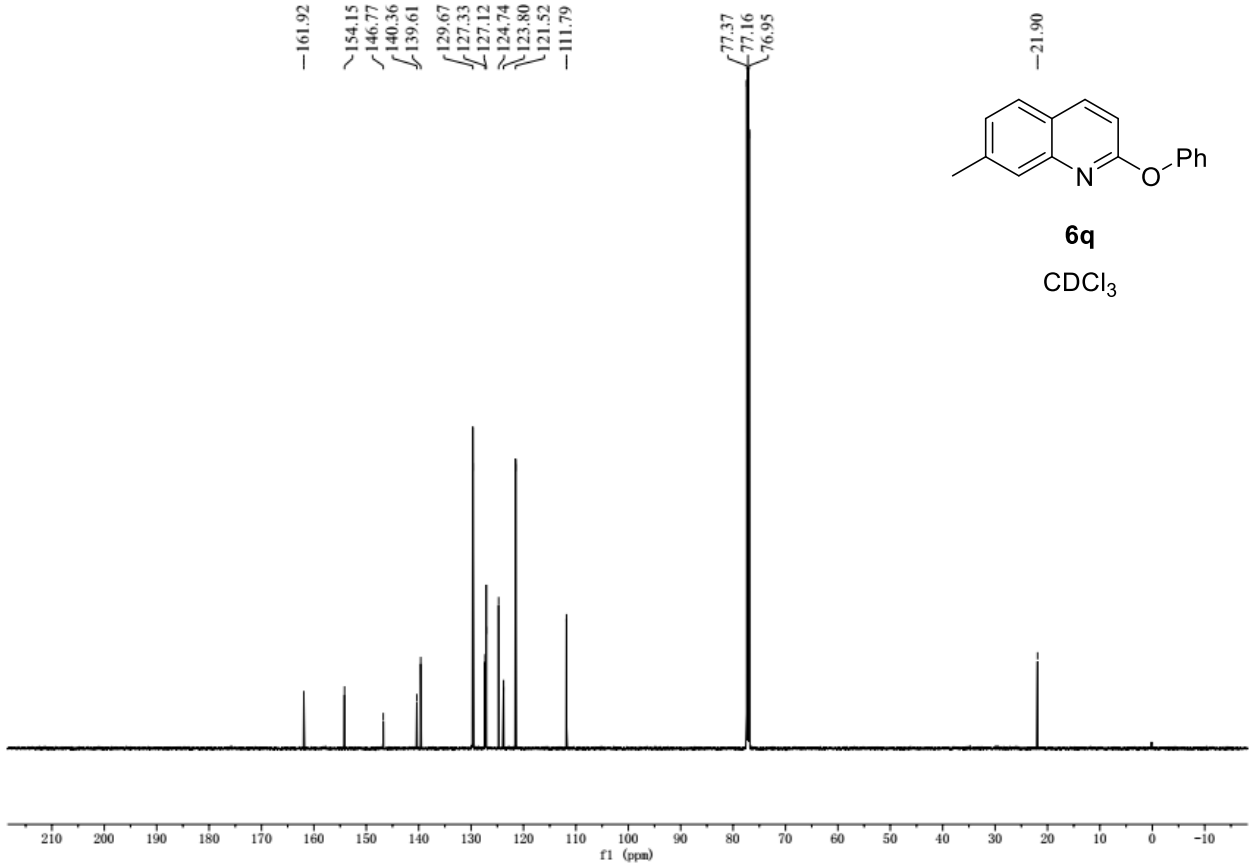


6p

$CDCl_3$

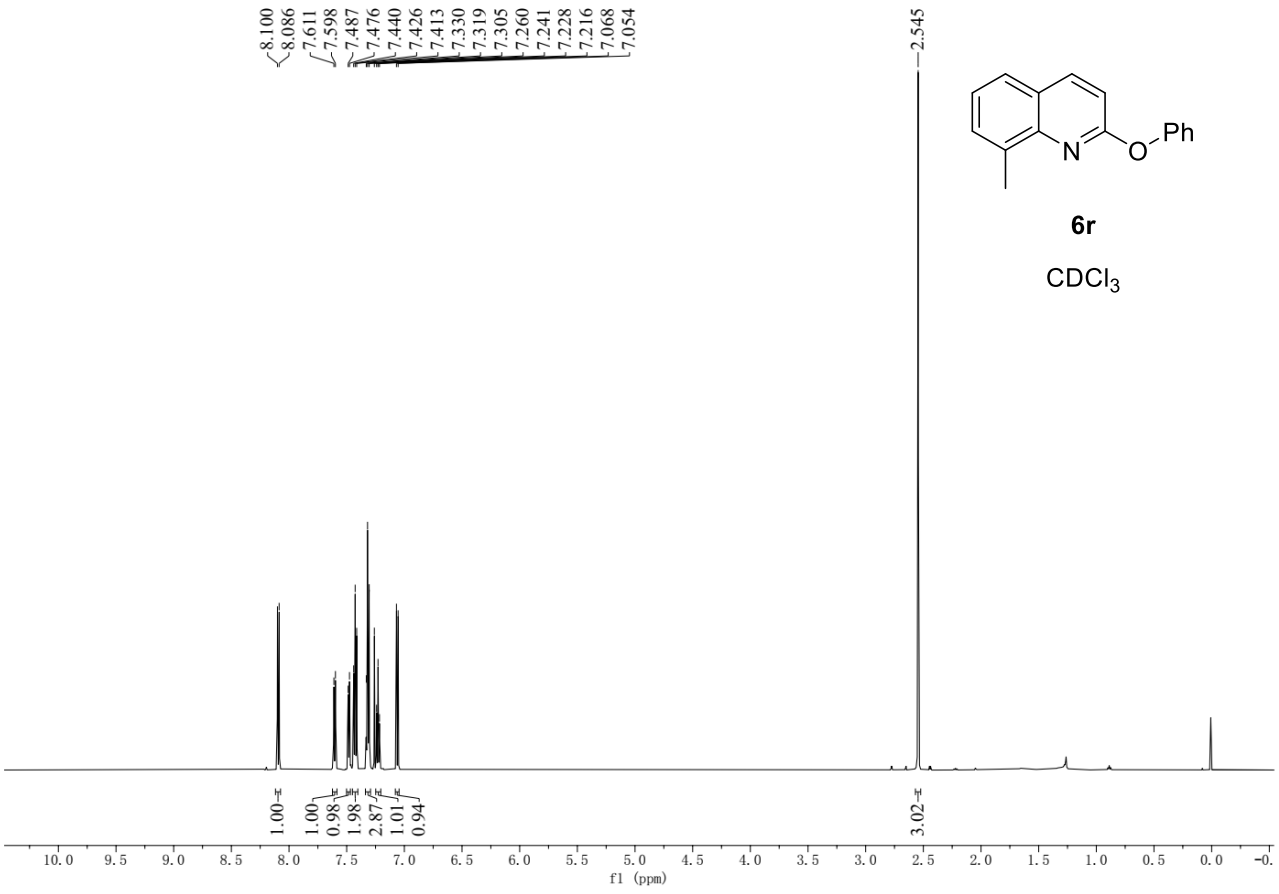

162.32
153.78
146.19
139.57
132.76
131.78
130.81
129.72
128.56
128.16
125.56
125.03
123.27
121.66
119.86
113.55
90.05
89.26
77.37
77.16
76.95
Ph
N
O
Ph
6p
CDCl3
f1 (ppm)


8.077
8.062
7.657
7.643
7.606
7.439
7.427
7.425
7.413
7.267
7.264
7.260
7.253
7.241
7.240
7.230
7.220
7.218
7.216
7.013
6.998
2.494
N
O
Ph
6q
CDCl3
1.00
1.01
0.89
1.97
4.38
0.97
3.11
f1 (ppm)



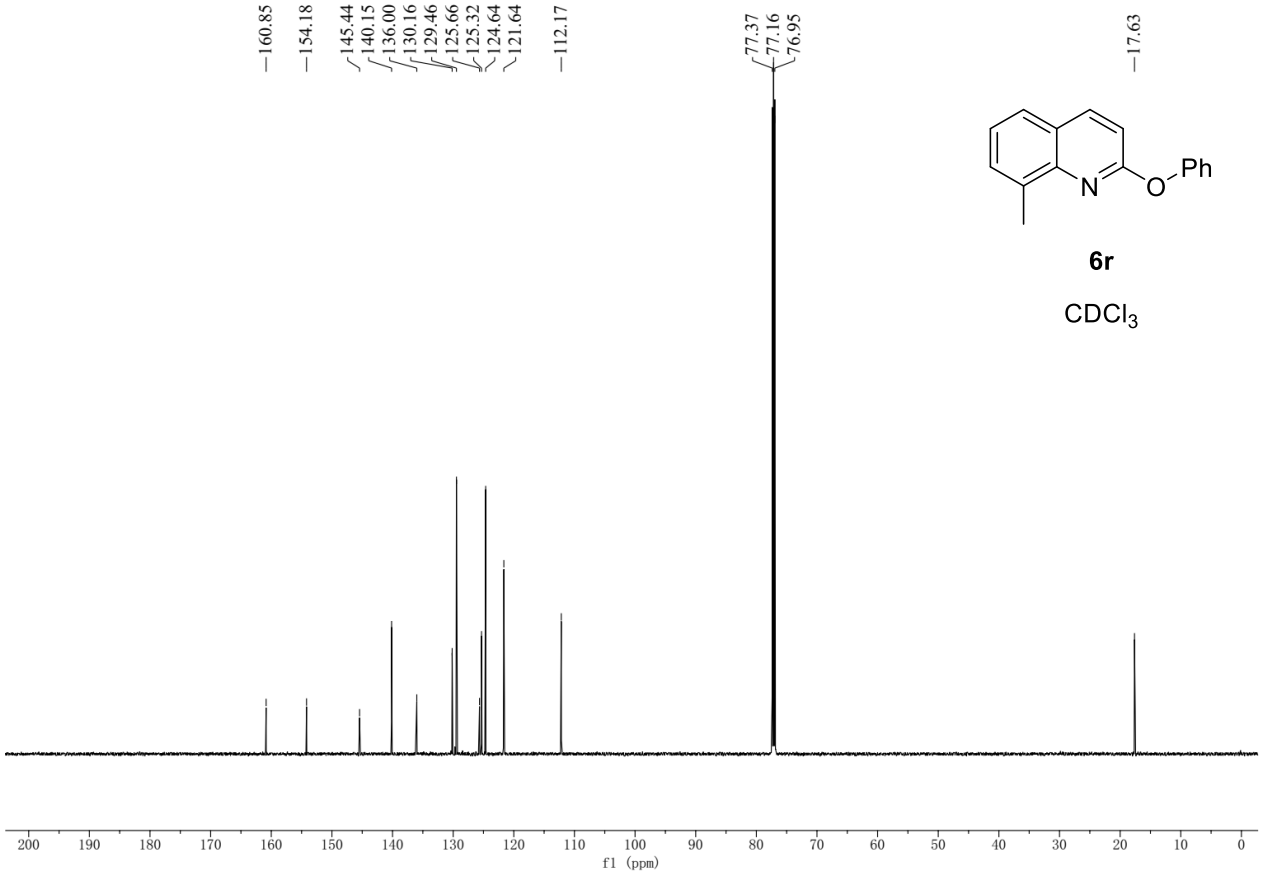
6q

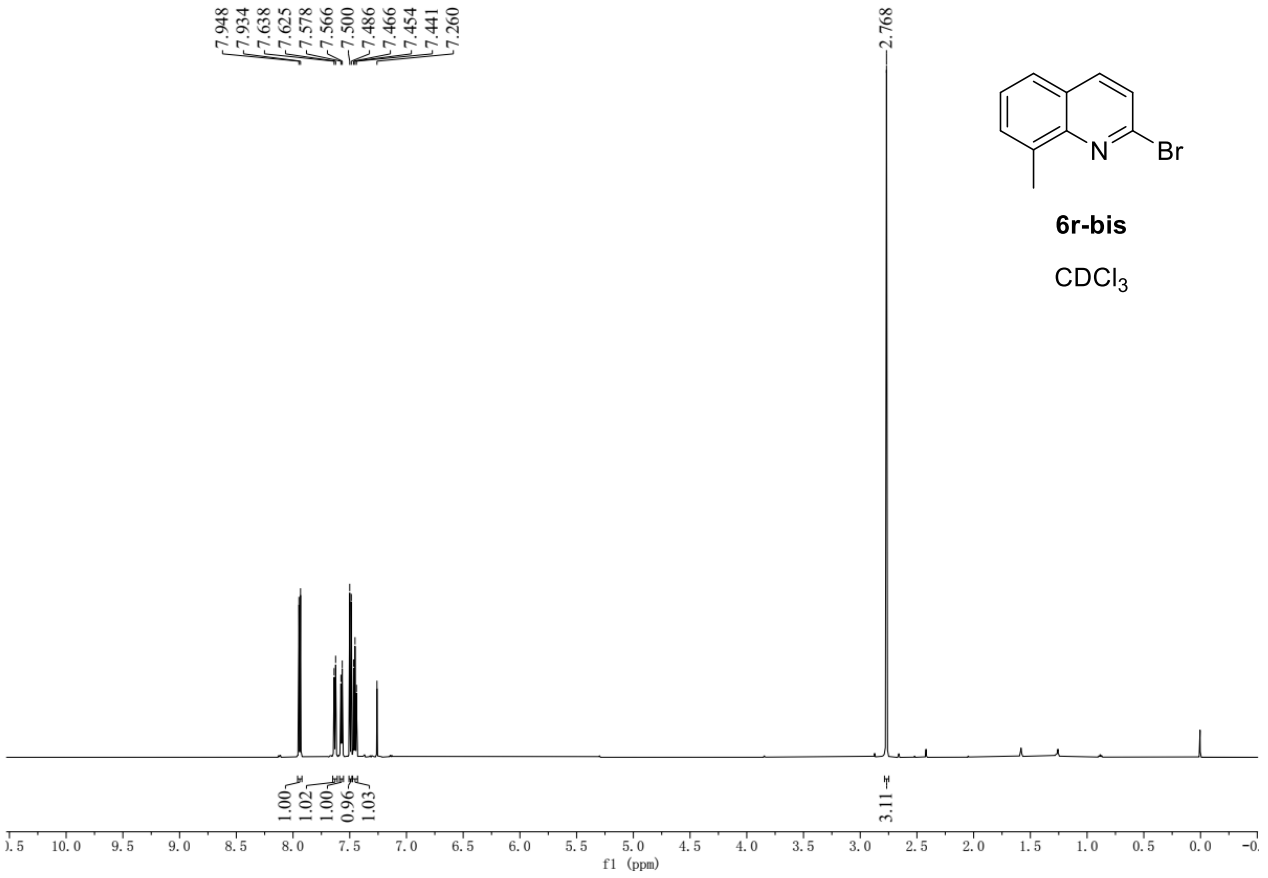
$CDCl_3$

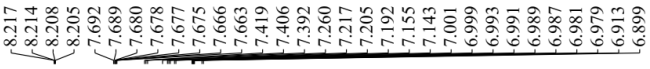


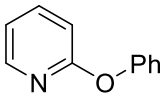
6r

$CDCl_3$


160.85
154.18
145.44
140.15
136.00
130.16
129.46
125.66
125.32
124.64
121.64
112.17
77.37
77.16
76.95
17.63
N
O
Ph
6r
CDCl3
f1 (ppm)

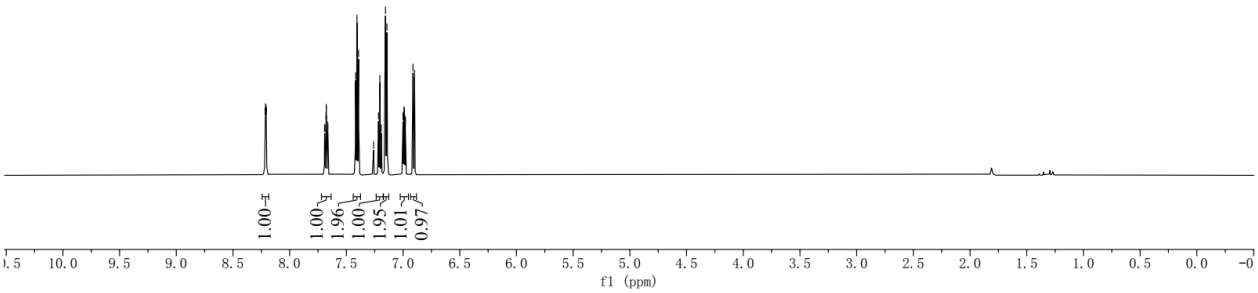

7.948
7.934
7.638
7.625
7.578
7.566
7.500
7.486
7.466
7.454
7.441
7.260
2.768
N
Br
6r-bis
CDCl3
1.00
1.02
1.00
0.96
1.03
3.11
f1 (ppm)

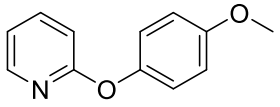




7a

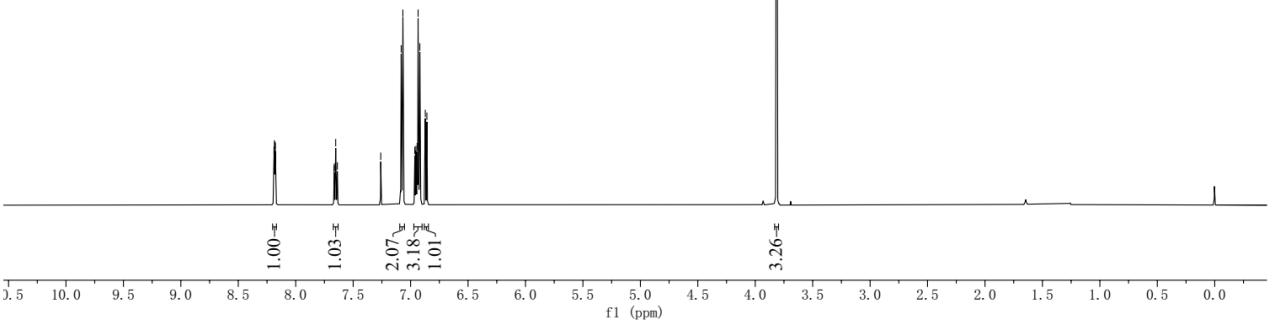
$CDCl_3$

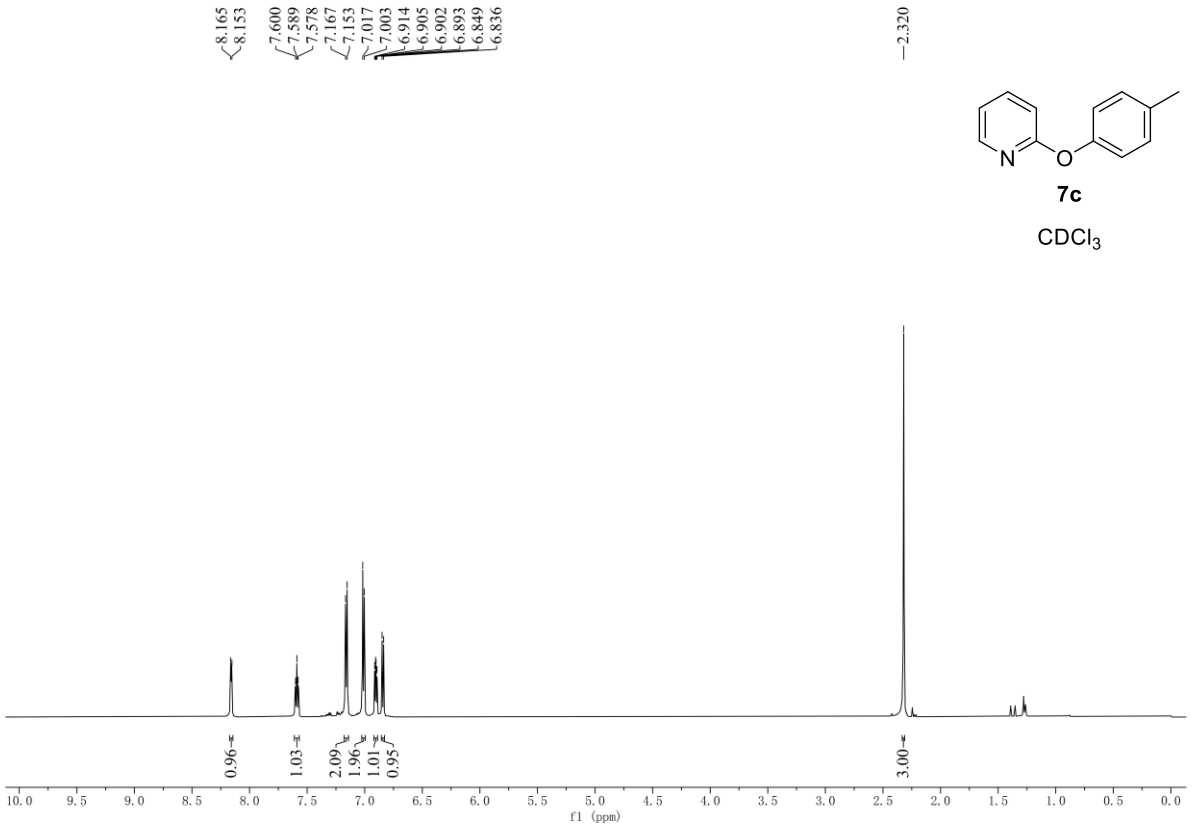


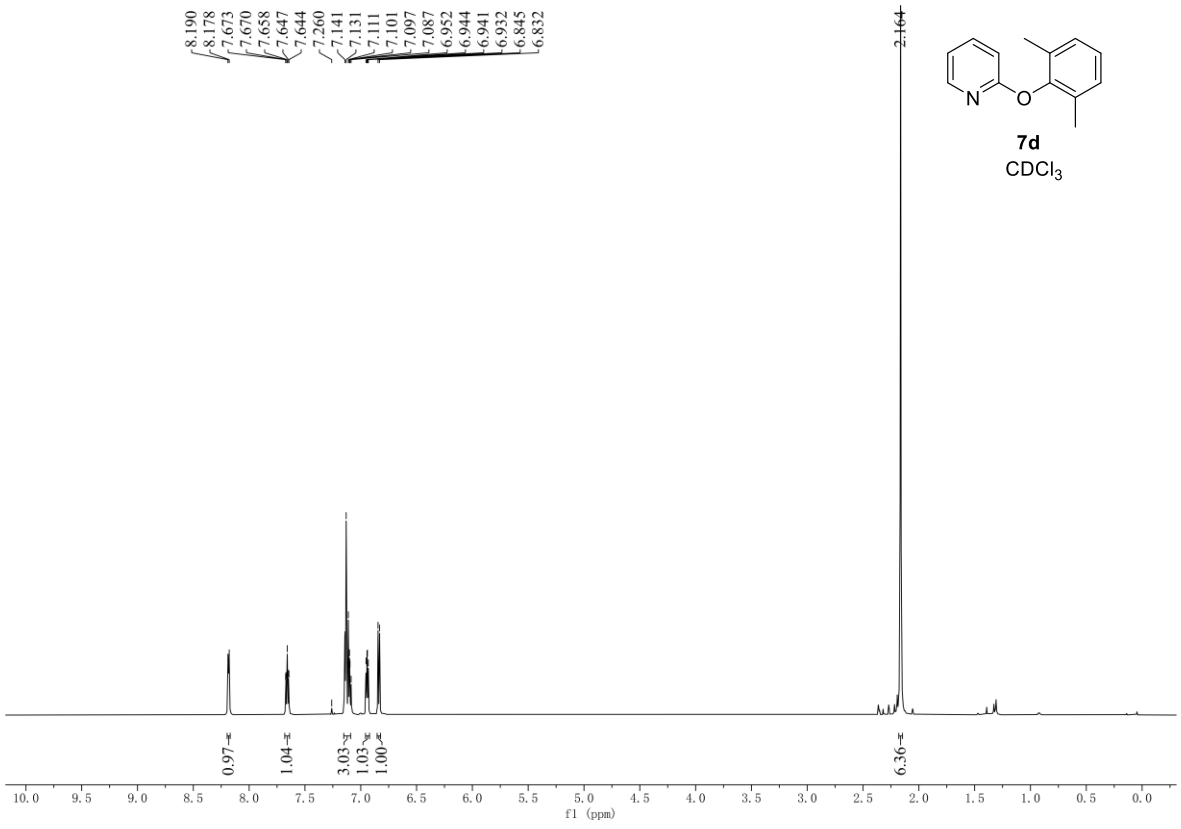


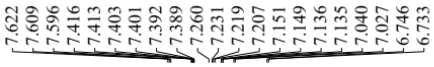
7b

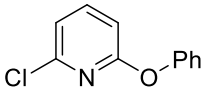
$CDCl_3$




8.165
8.153
7.600
7.589
7.578
7.167
7.153
7.017
7.003
6.914
6.905
6.902
6.893
6.849
6.836
2.320
N
O
7c
CDCl3
0.96
1.03
2.09
1.96
1.01
0.95
3.00
f1 (ppm)

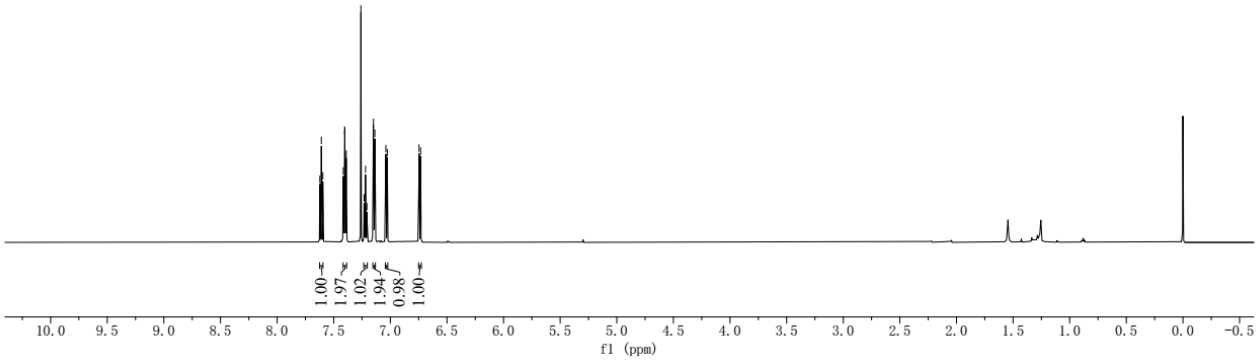

8.190
8.178
7.673
7.670
7.658
7.647
7.644
7.260
7.141
7.131
7.111
7.101
7.097
7.087
6.952
6.944
6.941
6.932
6.845
6.832
2.164
N
O
7d
CDCl3
0.97
1.04
3.03
1.03
1.00
6.36
f1 (ppm)

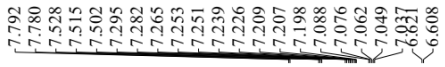


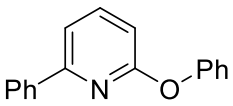


7e

$CDCl_3$

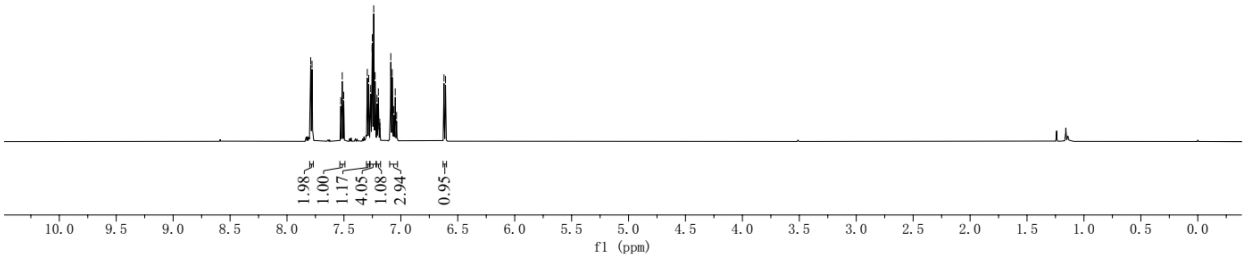


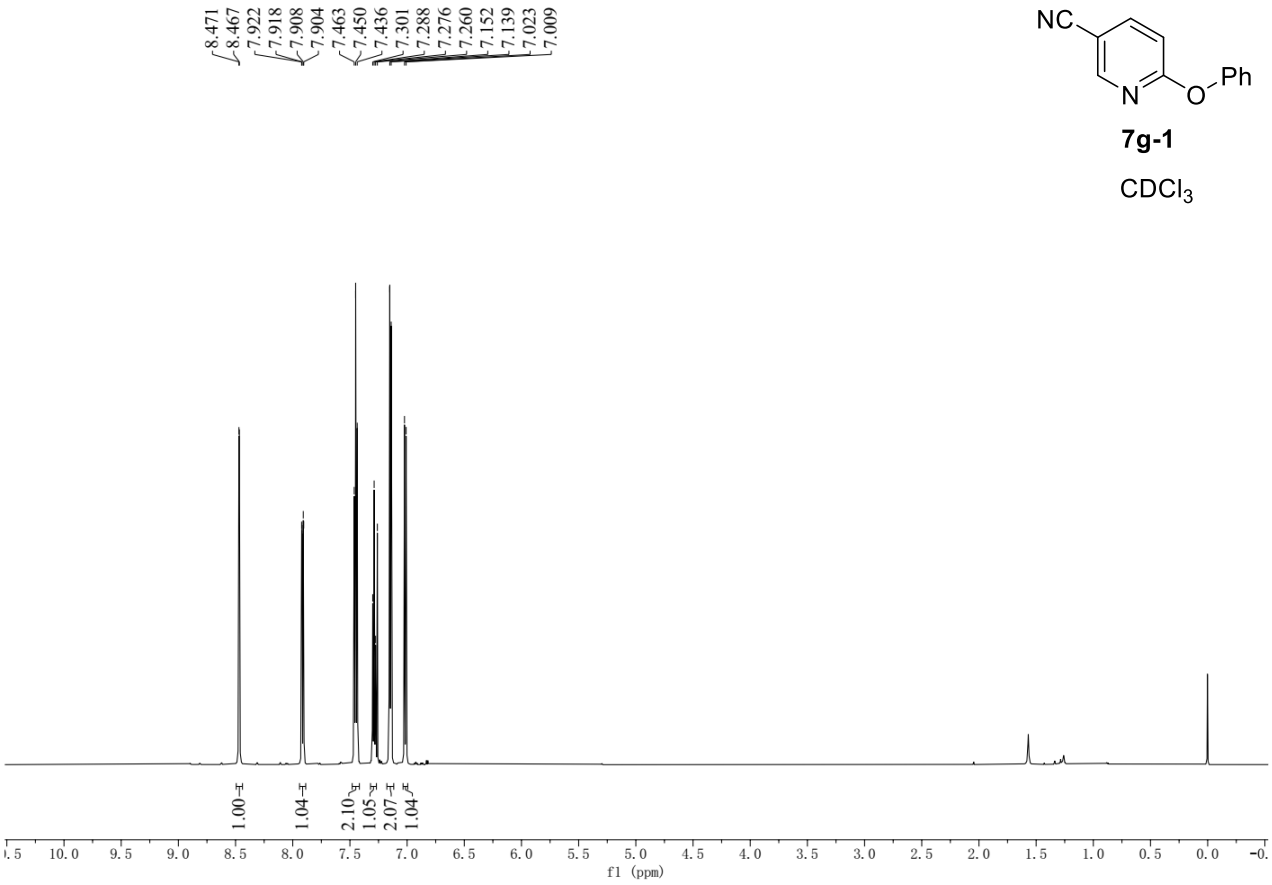




7f

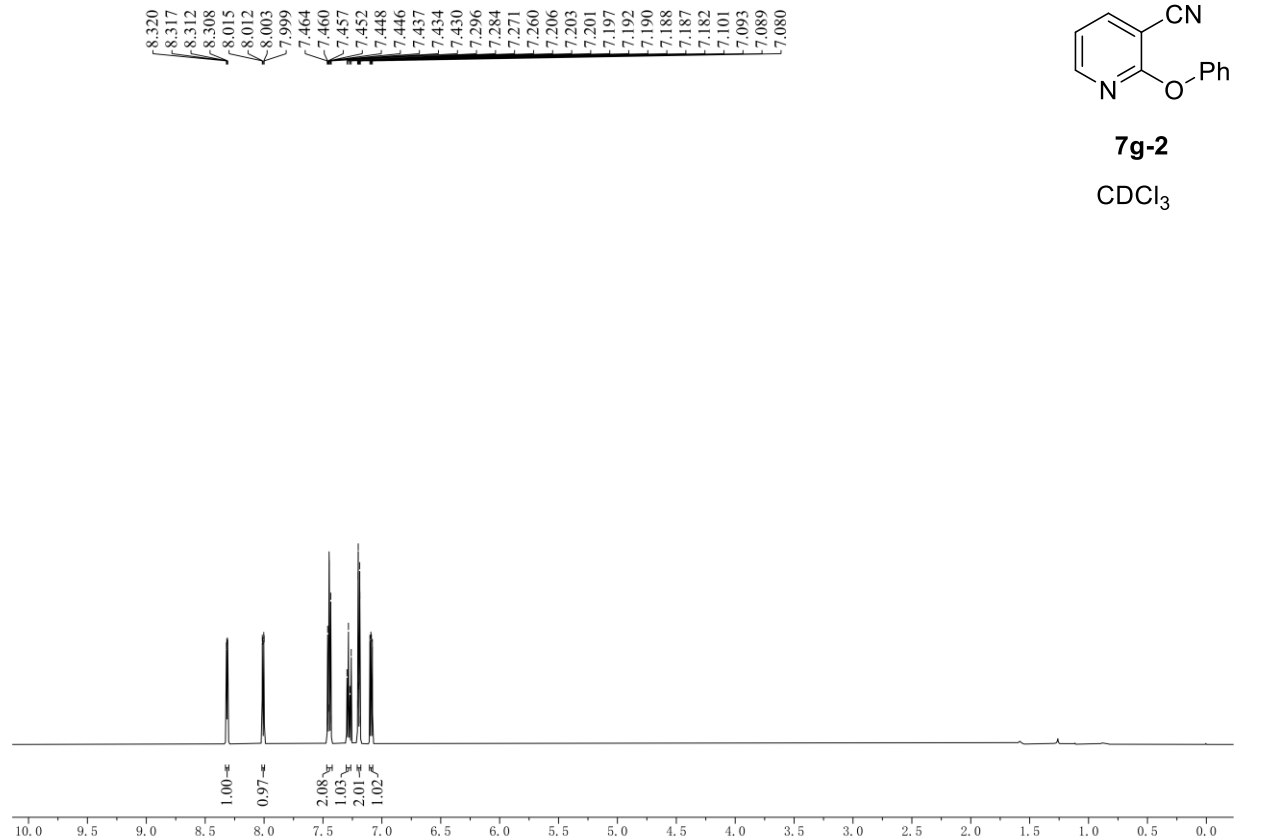
$CDCl_3$





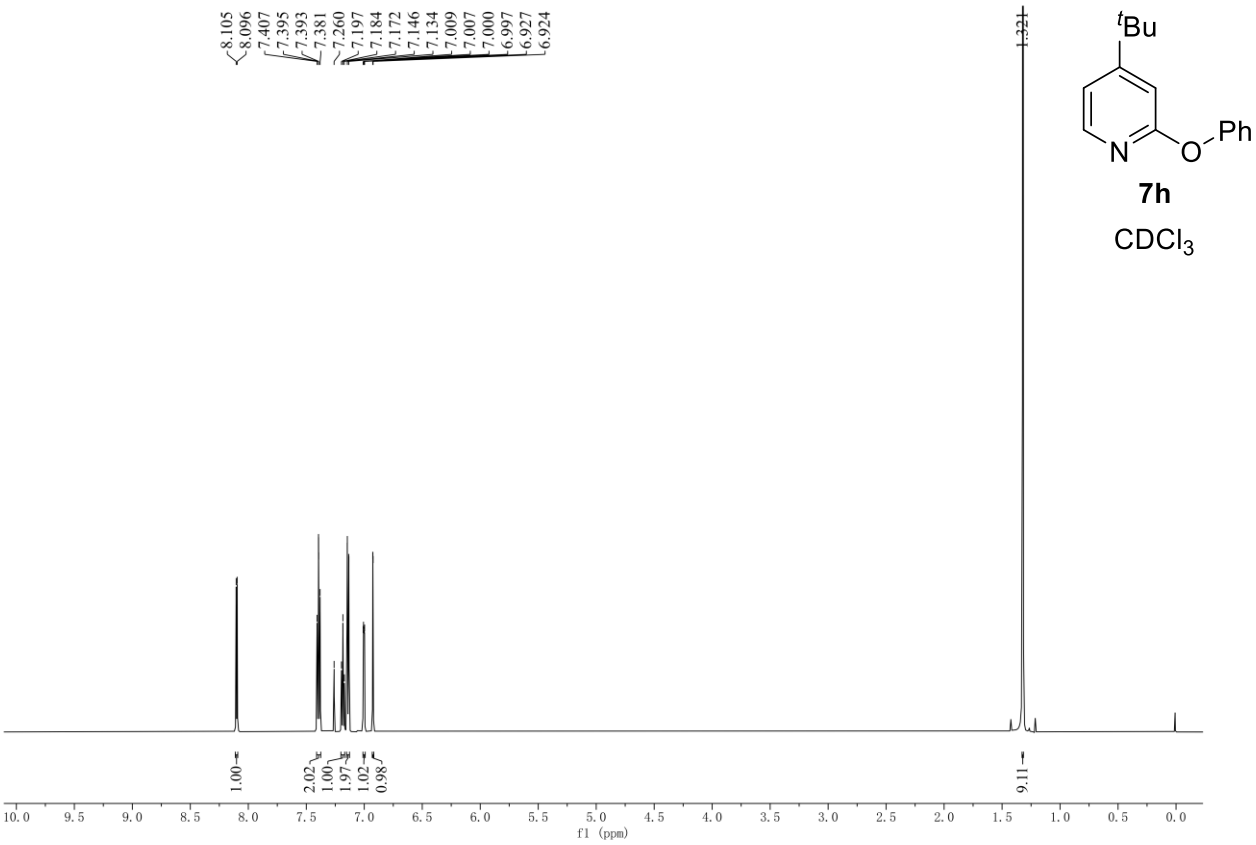
7g-1

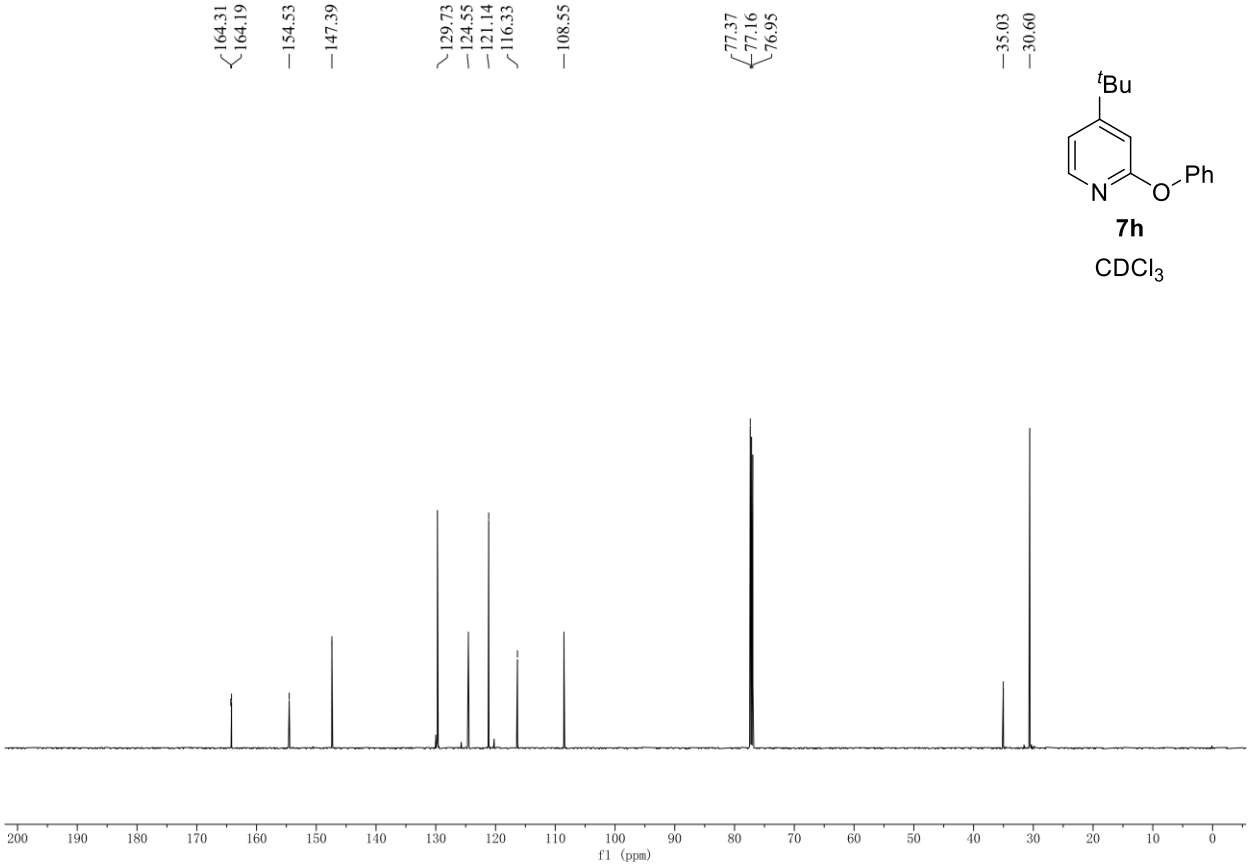
$CDCl_3$

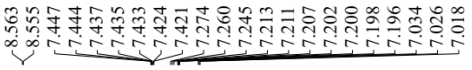


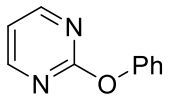
7g-2

$CDCl_3$


8.105
8.096
7.407
7.395
7.393
7.381
7.260
7.197
7.184
7.172
7.146
7.134
7.009
7.007
7.000
6.997
6.927
6.924
1.321
1.00
2.02
1.00
1.97
1.02
0.98
9.11
f1 (ppm)
tBu
Ph
N
O
7h
CDCl3

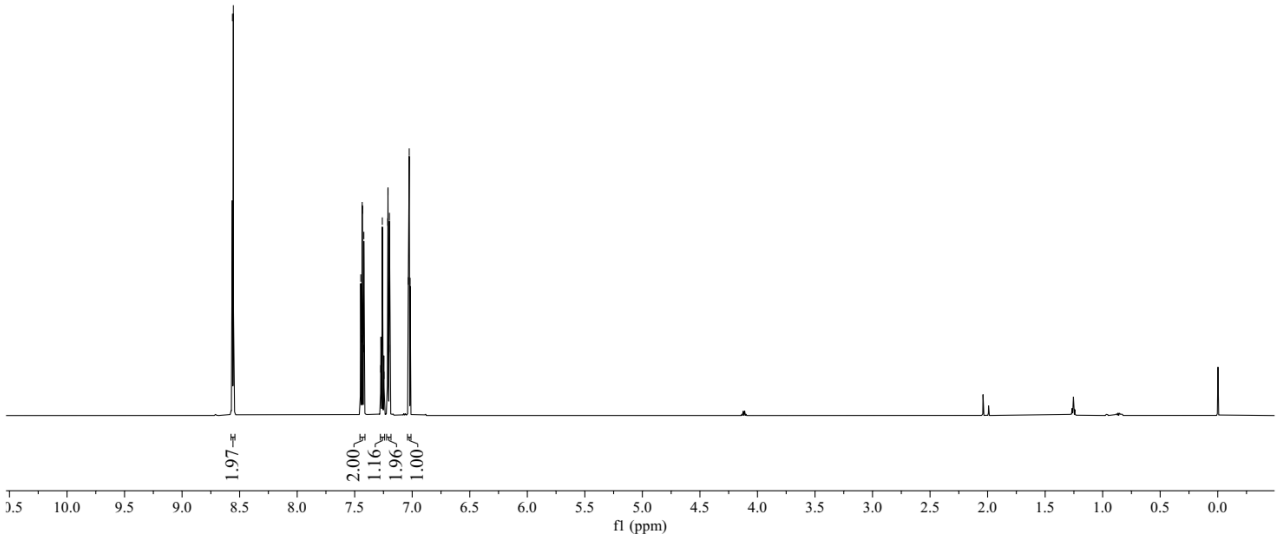

164.31
164.19
154.53
147.39
129.73
124.55
121.14
116.33
108.55
77.37
77.16
76.95
35.03
30.60
f1 (ppm)
tBu
Ph
N
O
7h
CDCl3

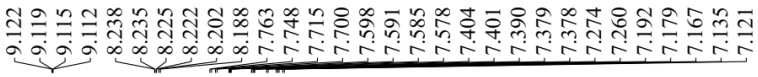


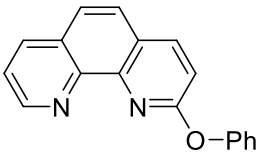


8

$CDCl_3$

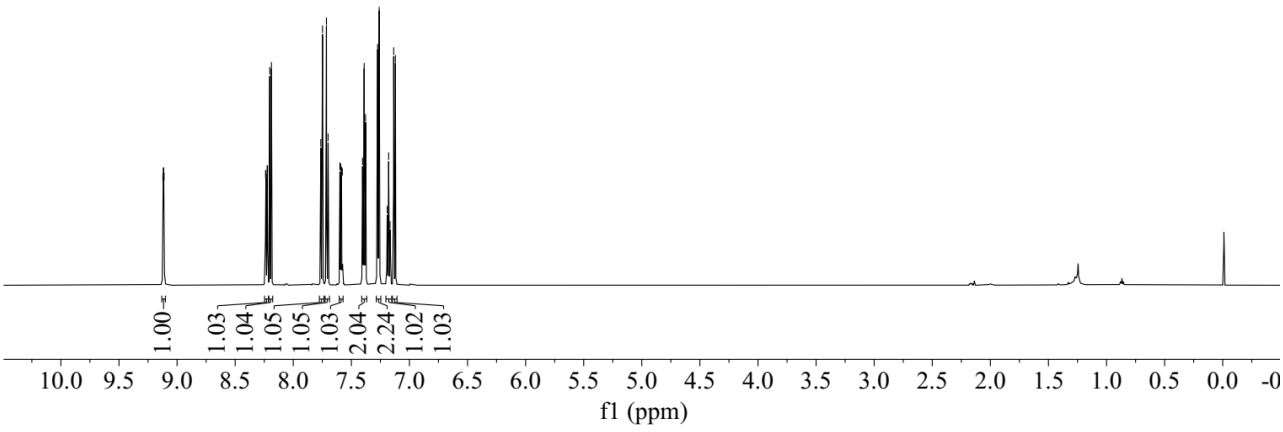


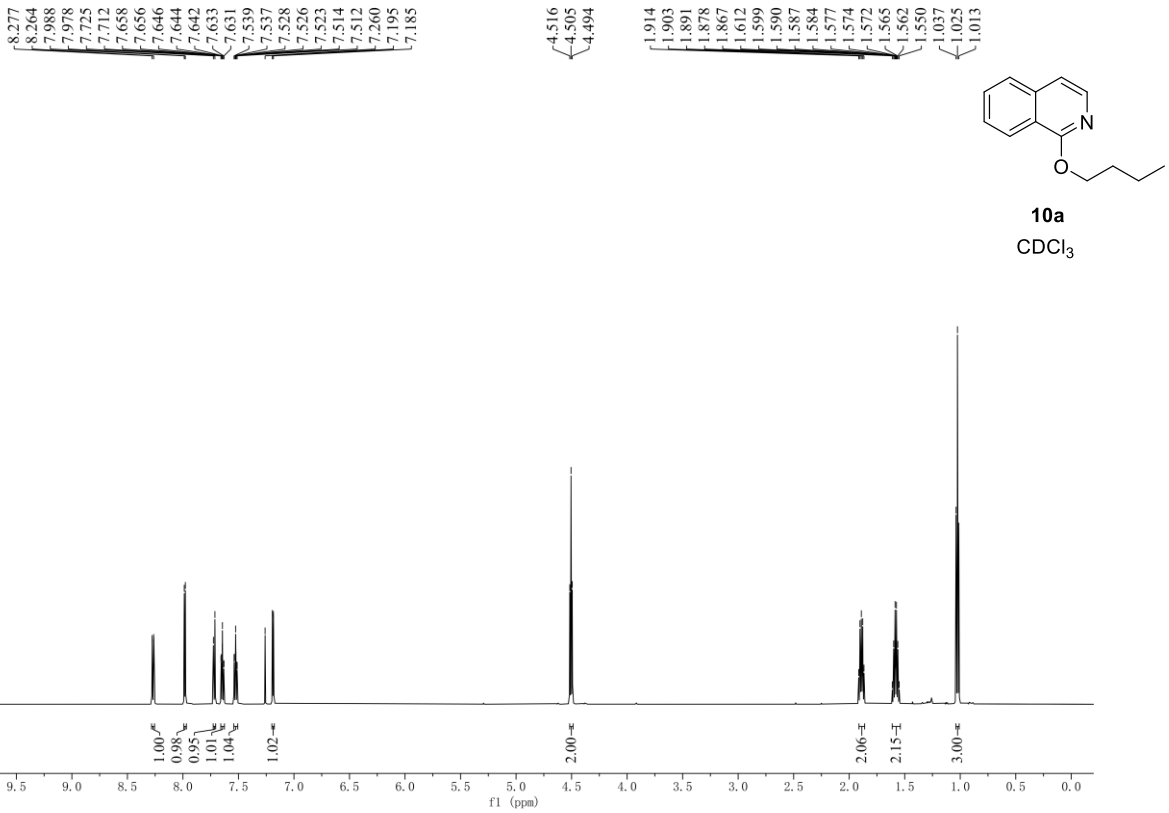


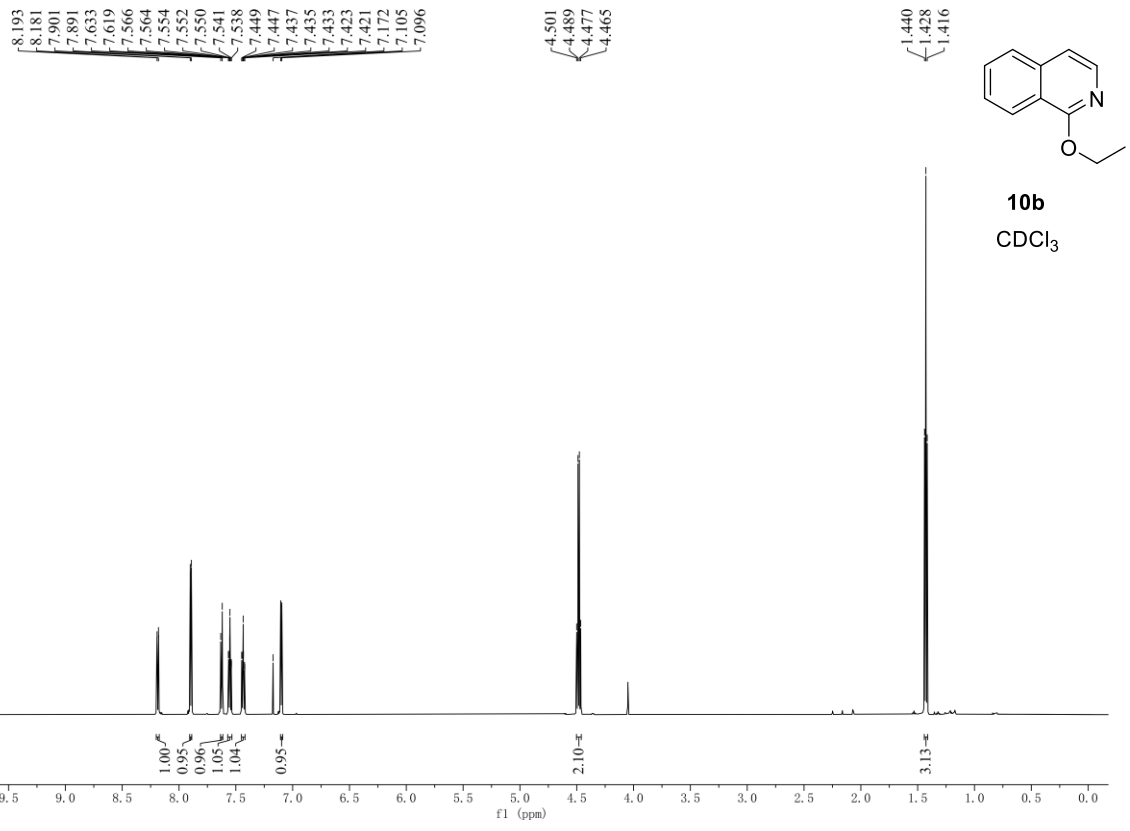


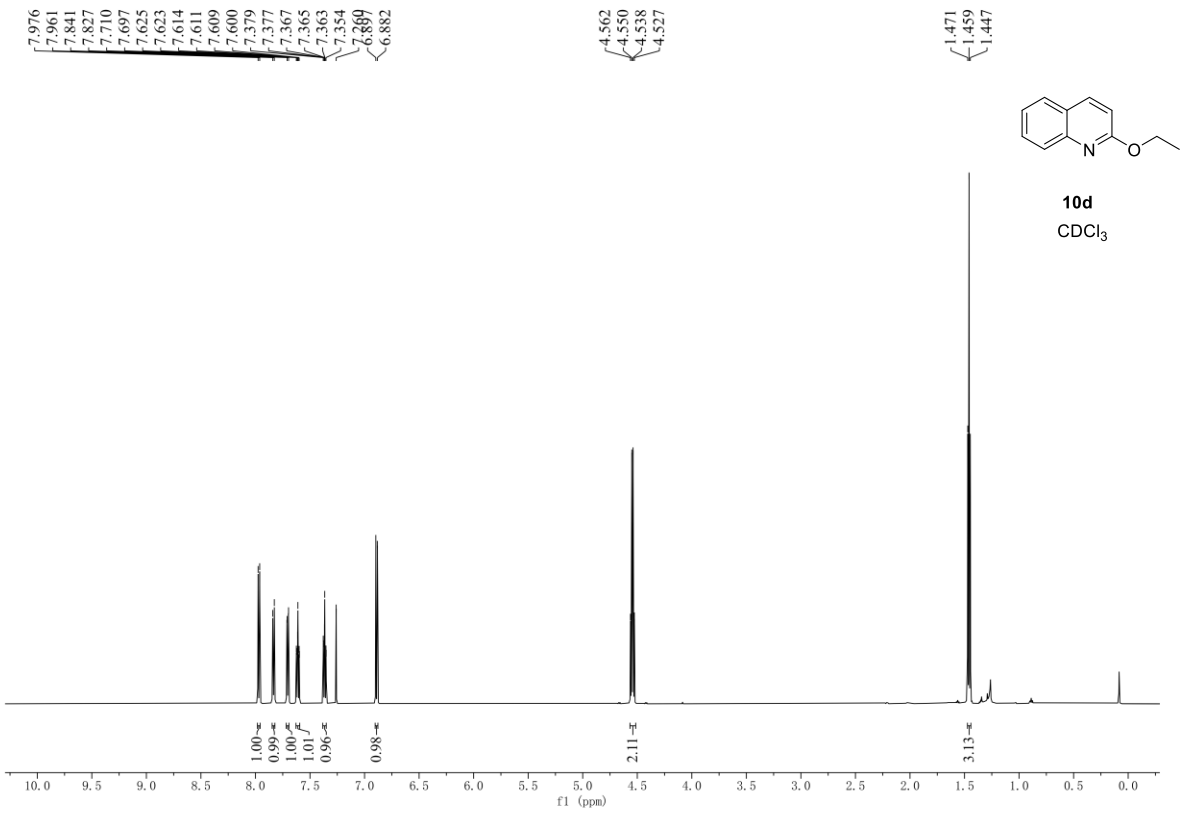
9

$CDCl_3$




8.277
8.264
7.988
7.978
7.725
7.712
7.658
7.656
7.646
7.644
7.642
7.633
7.631
7.539
7.537
7.528
7.526
7.523
7.514
7.512
7.260
7.195
7.185
4.516
4.505
4.494
1.914
1.903
1.891
1.878
1.867
1.612
1.599
1.590
1.587
1.584
1.577
1.574
1.572
1.565
1.562
1.550
1.037
1.025
1.013
N
O
10a
CDCl3
1.00
0.98
0.95
1.01
1.04
1.02
2.00
2.06
2.15
3.00
f1 (ppm)

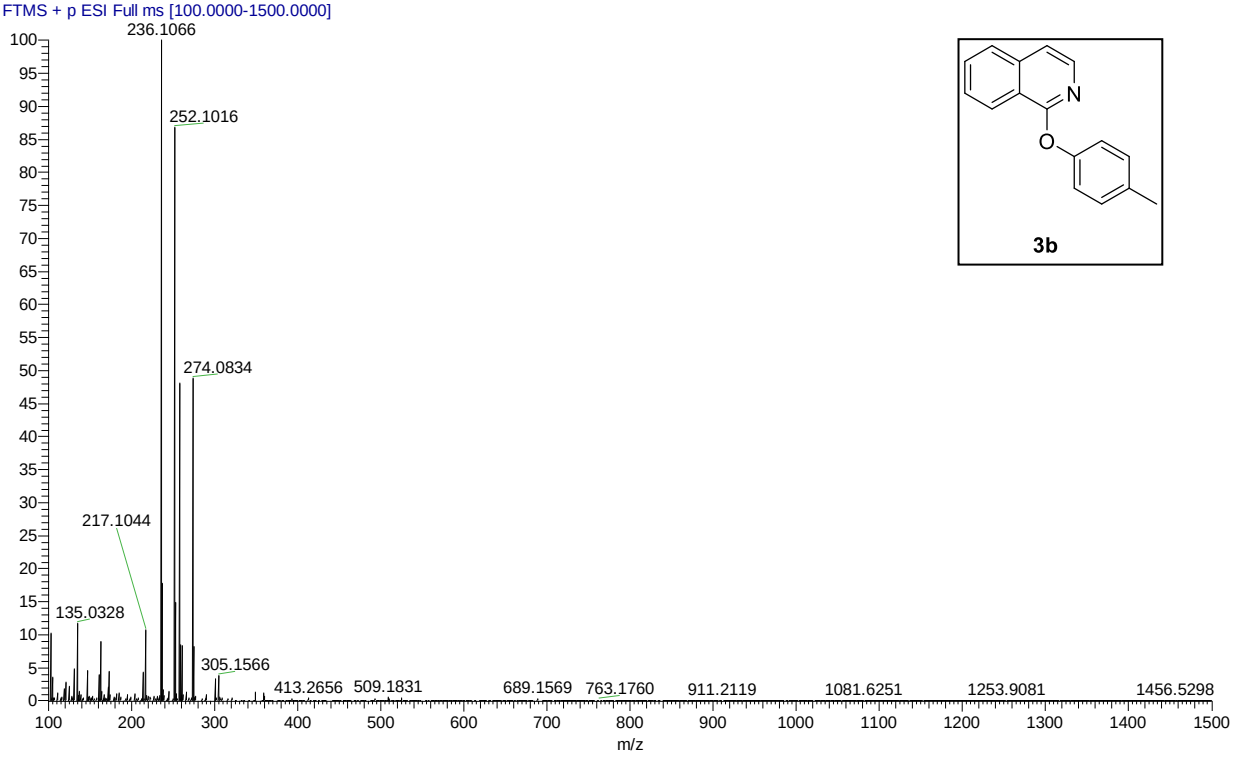

8.193
8.181
7.901
7.891
7.633
7.619
7.566
7.564
7.554
7.552
7.550
7.541
7.538
7.449
7.447
7.437
7.435
7.433
7.423
7.421
7.172
7.105
7.096
4.501
4.489
4.477
4.465
1.440
1.428
1.416
N
O
10b
CDCl3
1.00
0.95
0.96
1.05
1.04
0.95
2.10
3.13
f1 (ppm)



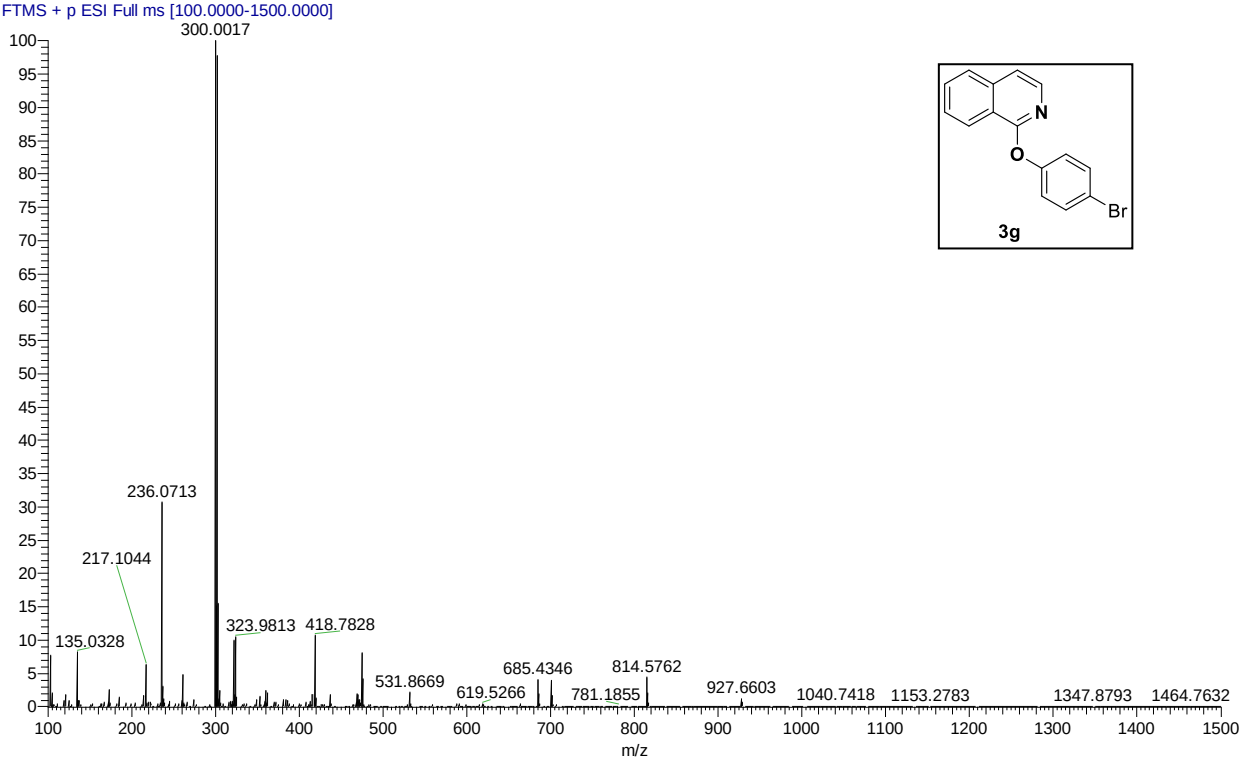
9. HRMS Spectra

Spectra data are shown from the next page.

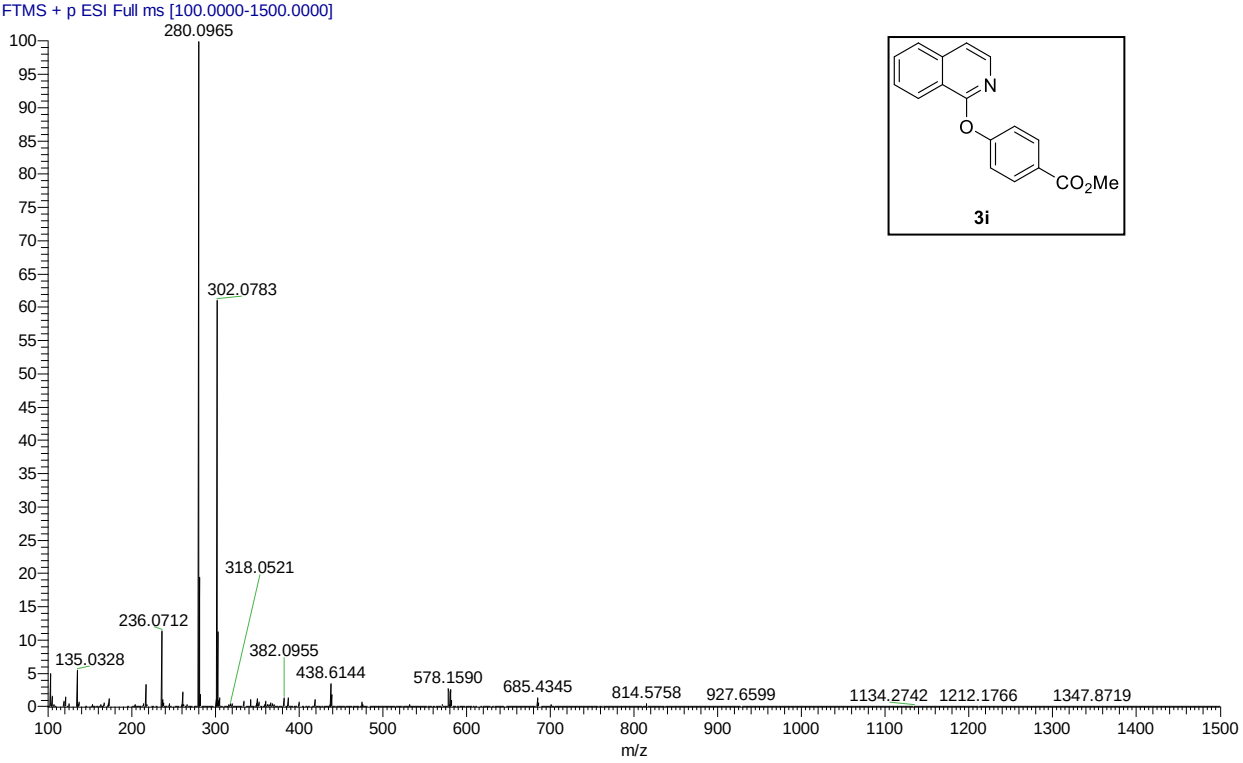
3B #23 RT: 0.23 AV: 1 NL: 1.35E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3G #23 RT: 0.23 AV: 1 NL: 3.06E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

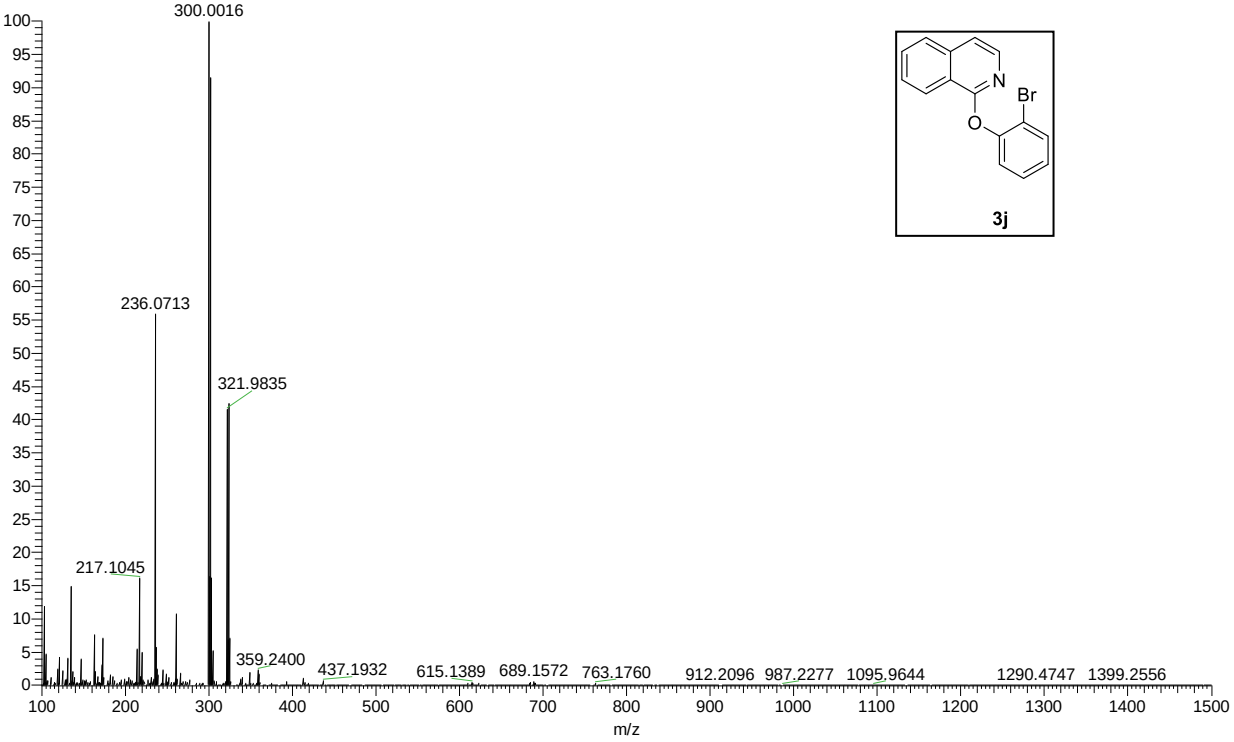


3I #21 RT: 0.21 AV: 1 NL: 4.61E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



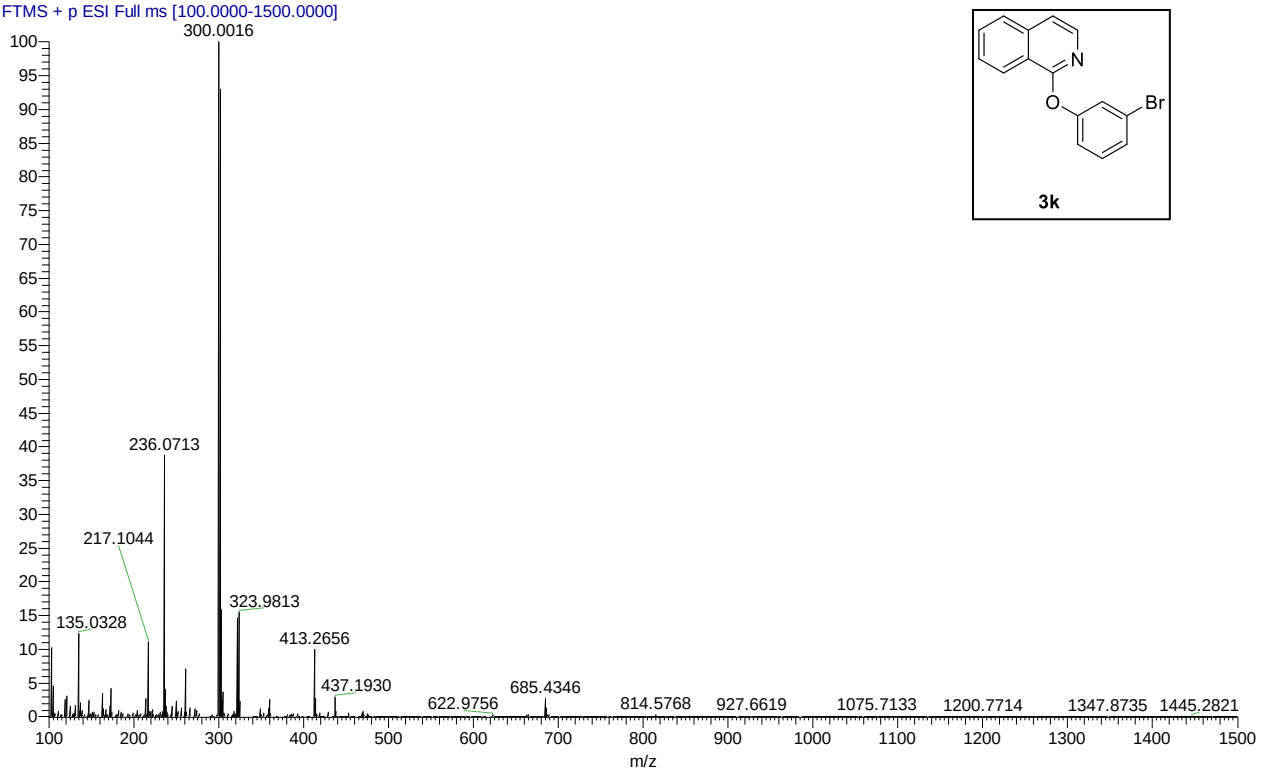
3i

3J #23 RT: 0.23 AV: 1 NL: 6.04E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



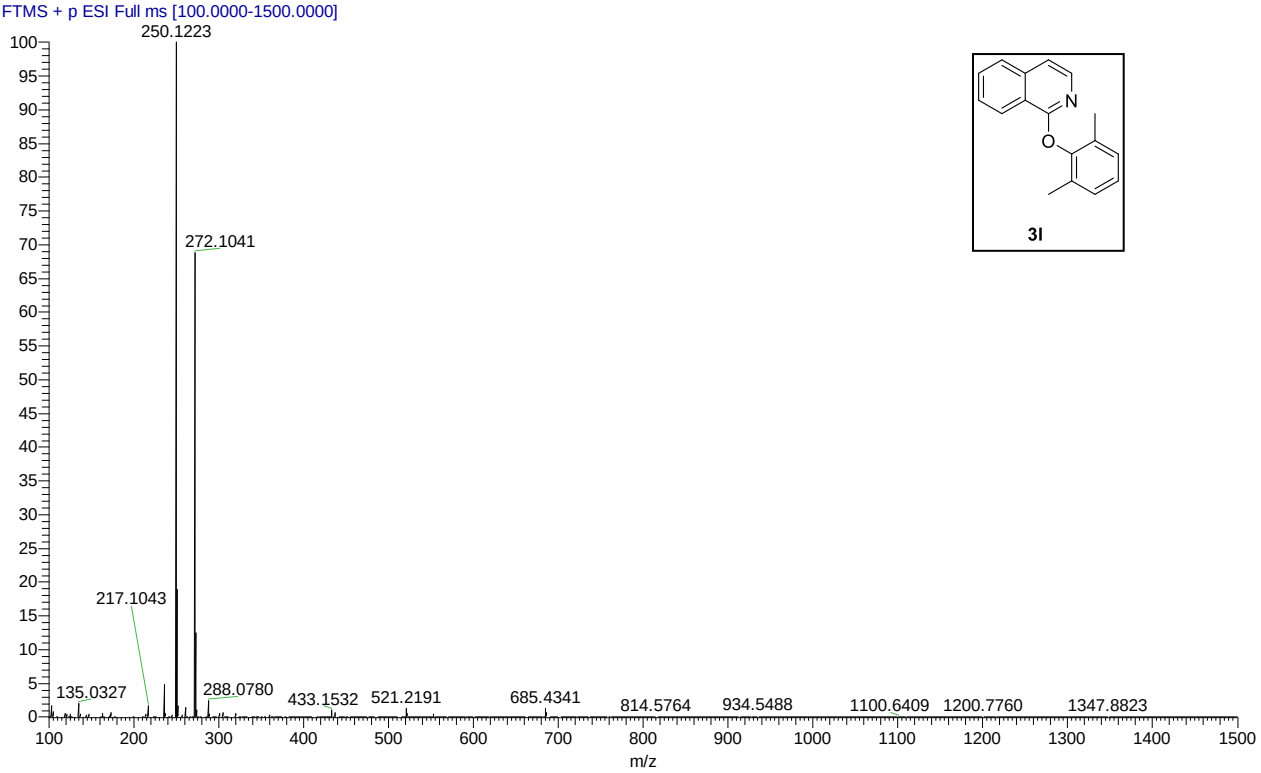
3j

3K #23 RT: 0.23 AV: 1 NL: 1.39E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



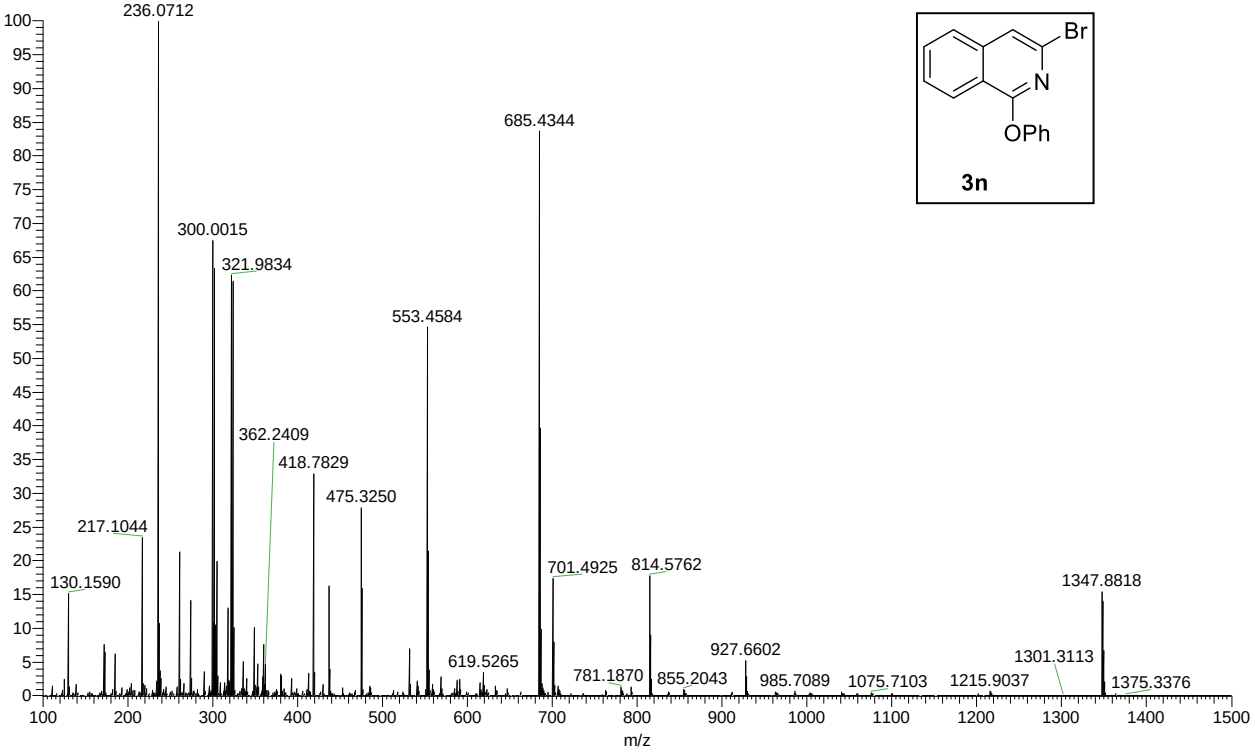
3k

3L #27 RT: 0.27 AV: 1 NL: 7.71E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

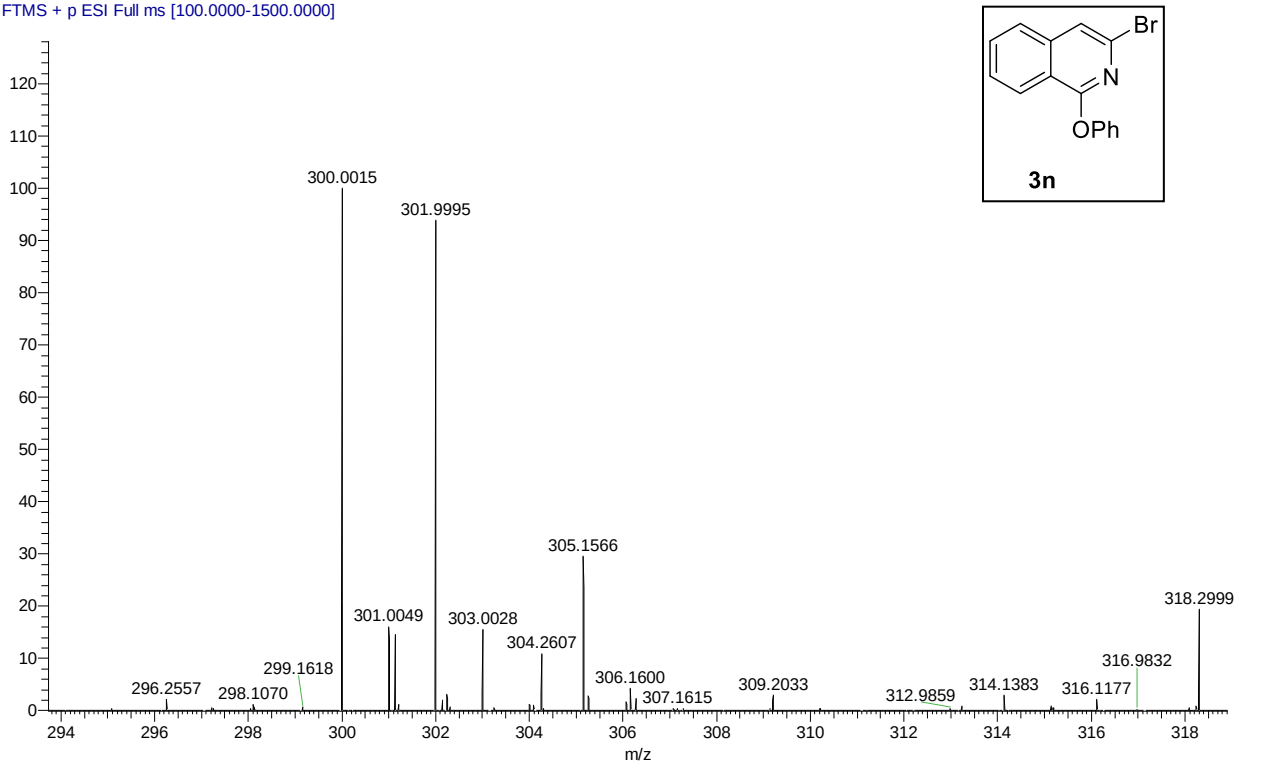


3l

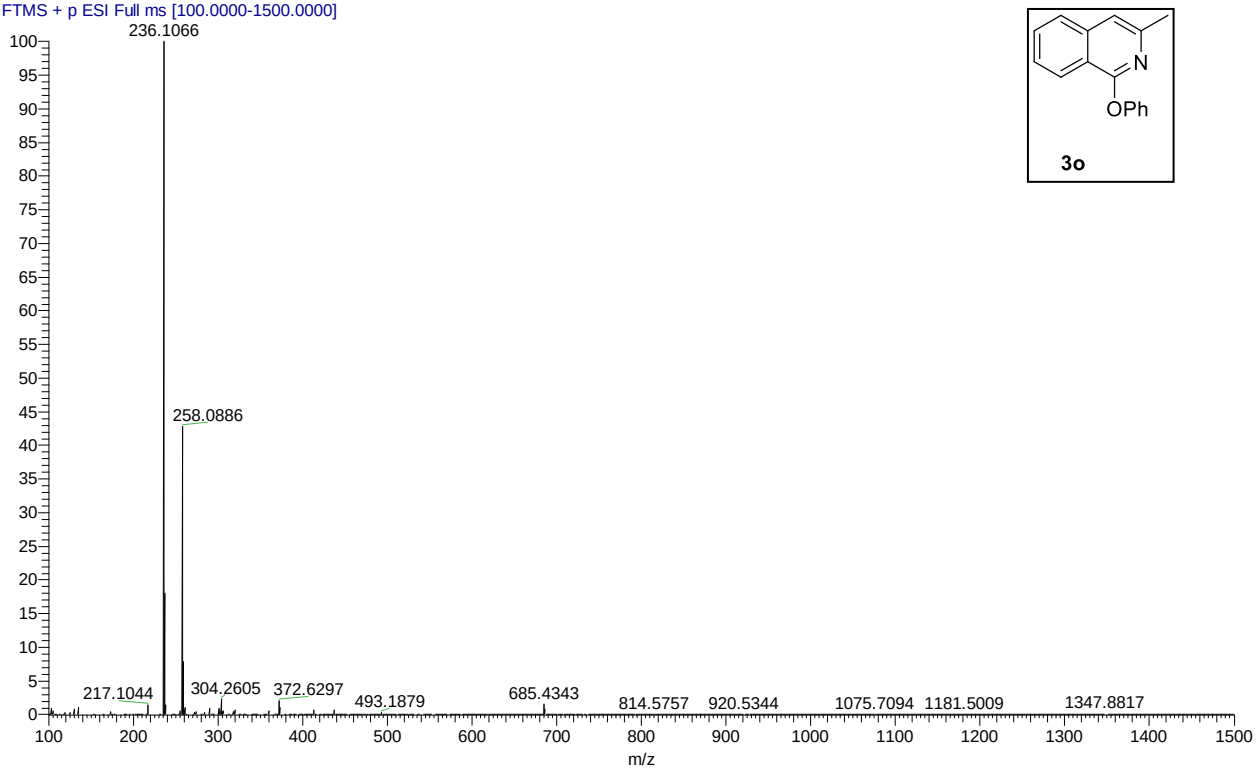
3N #27 RT: 0.26 AV: 1 NL: 3.01E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



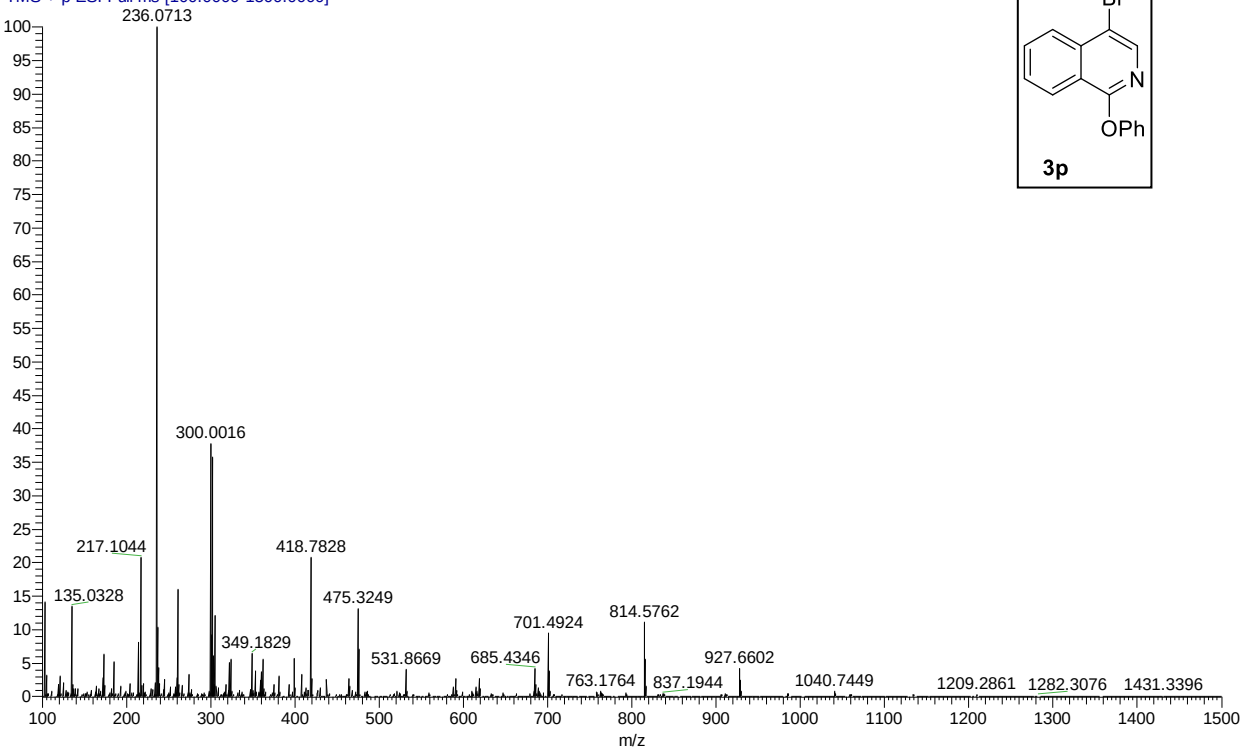
3N #27 RT: 0.26 AV: 1 NL: 2.03E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



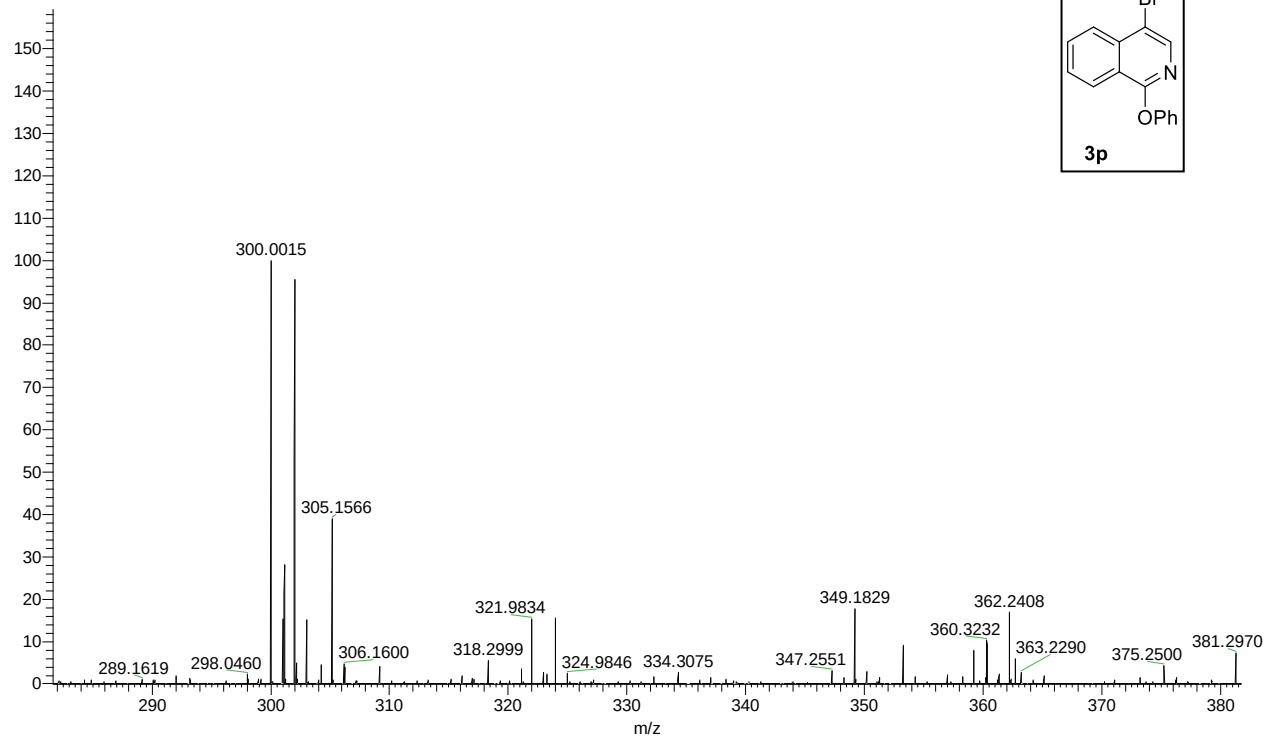
3O #25 RT: 0.25 AV: 1 NL: 1.55E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



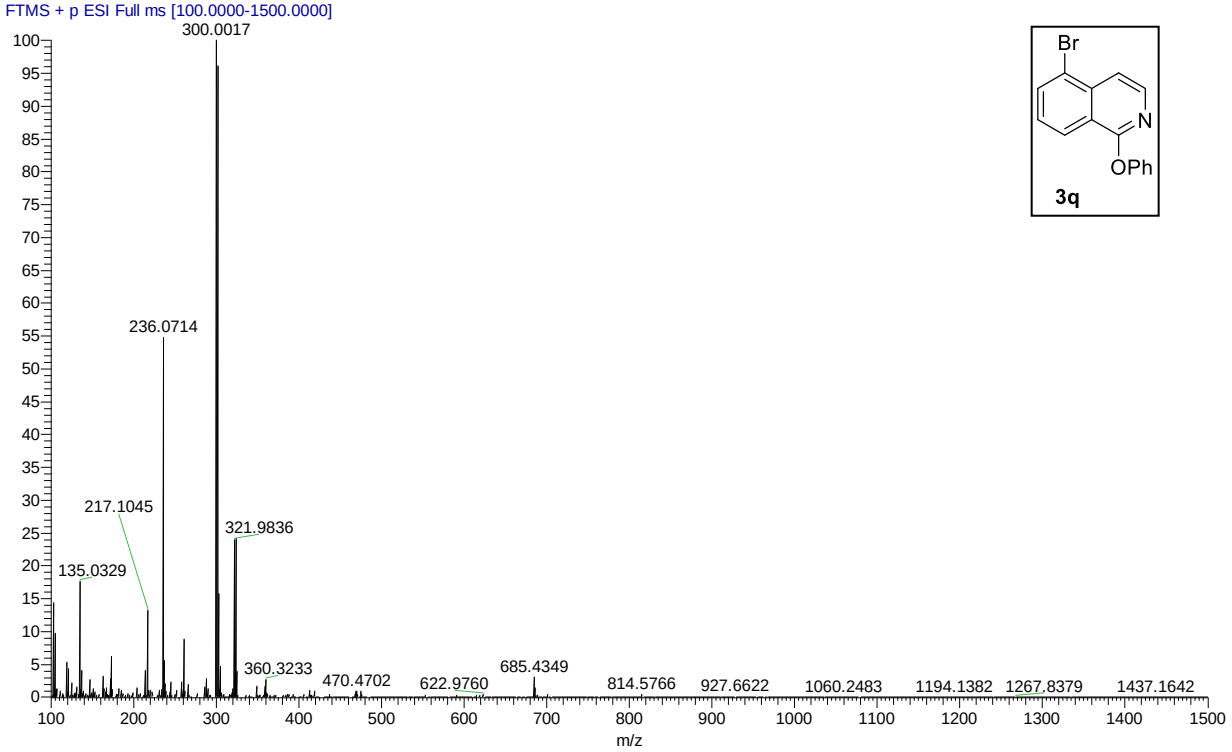
3P #25 RT: 0.26 AV: 1 NL: 8.34E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



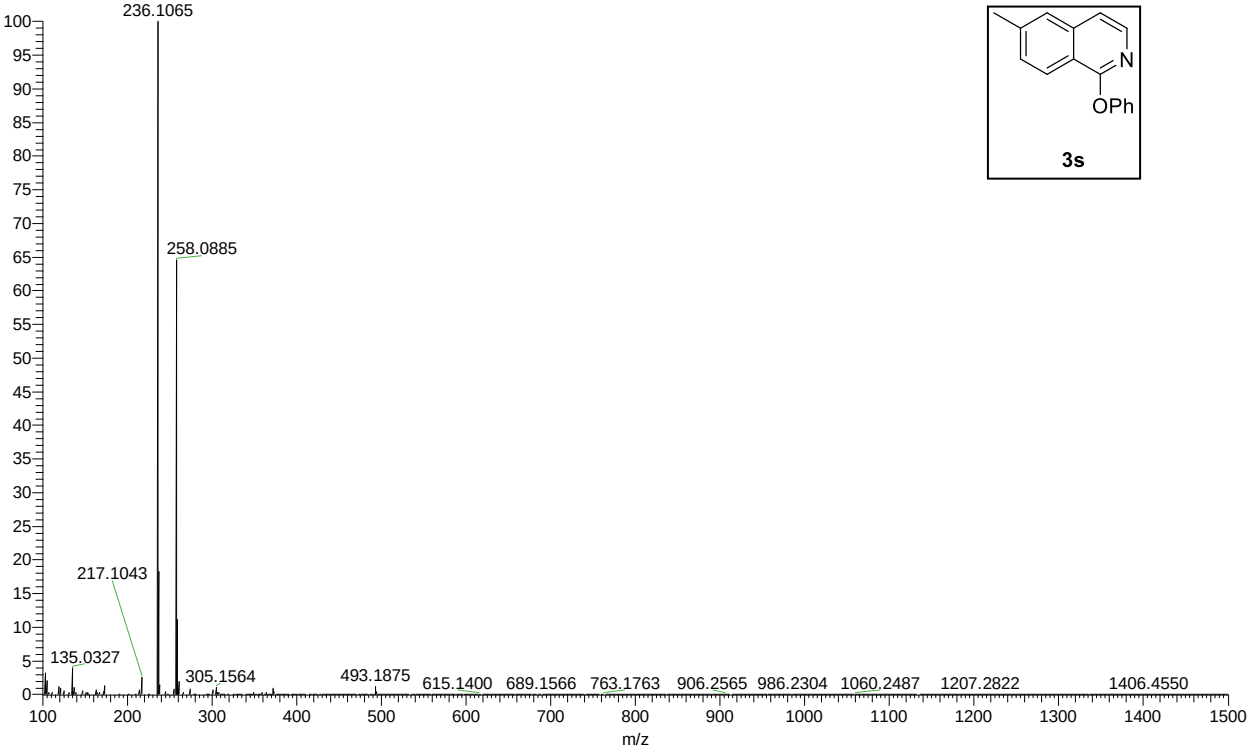
3P #27 RT: 0.28 AV: 1 NL: 2.57E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3Q #25 RT: 0.25 AV: 1 NL: 9.52E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]

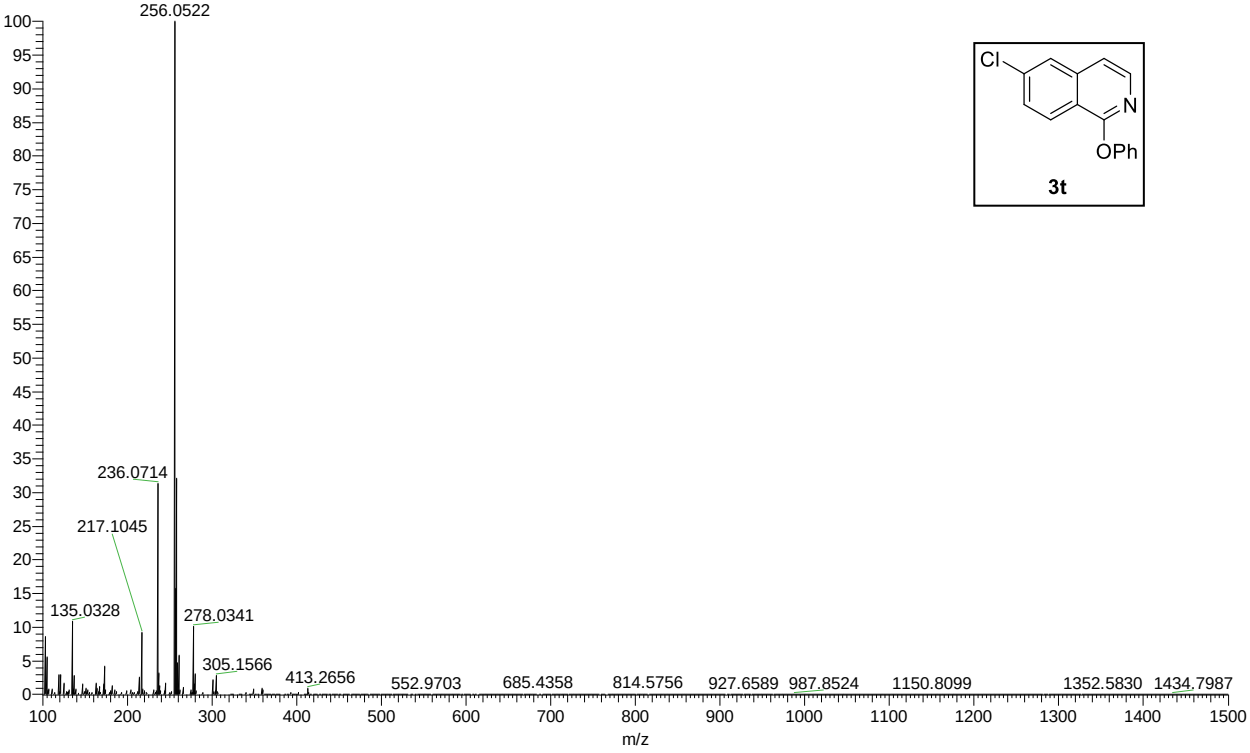


3S #25 RT: 0.25 AV: 1 NL: 5.20E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



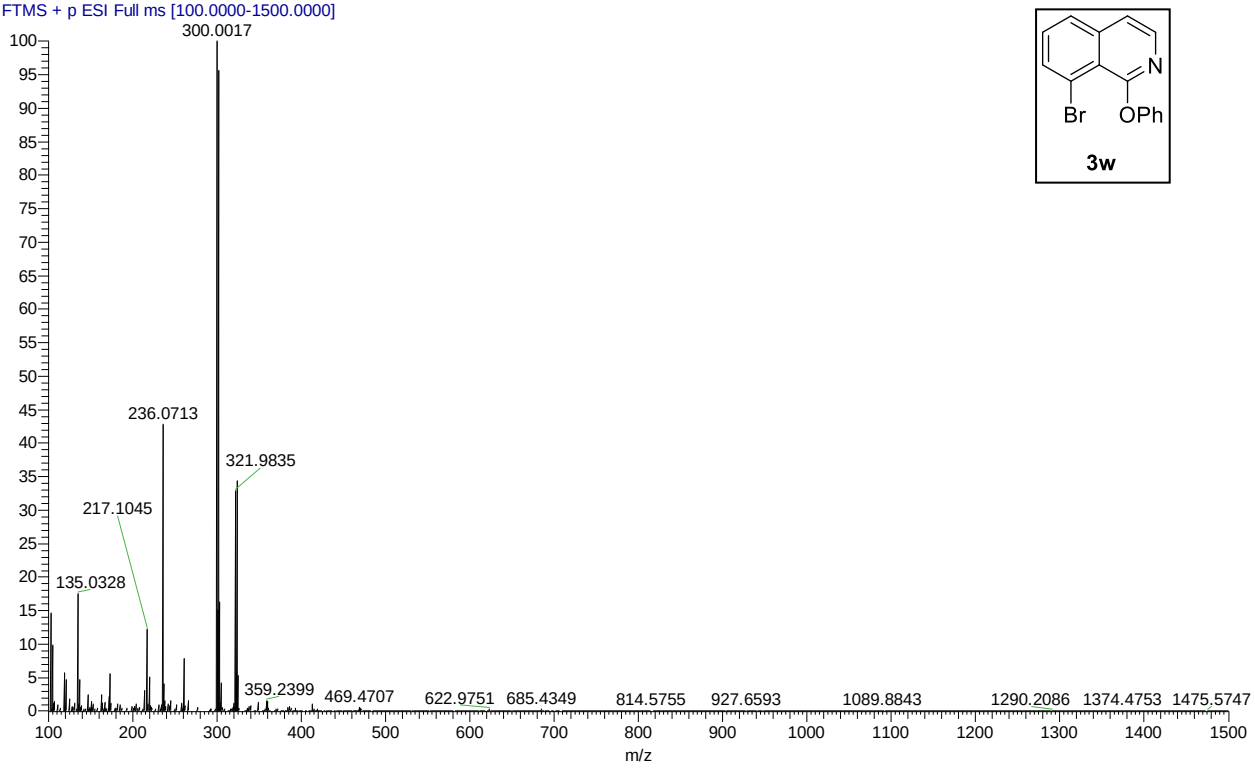
3s

3t #29 RT: 0.29 AV: 1 NL: 2.03E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

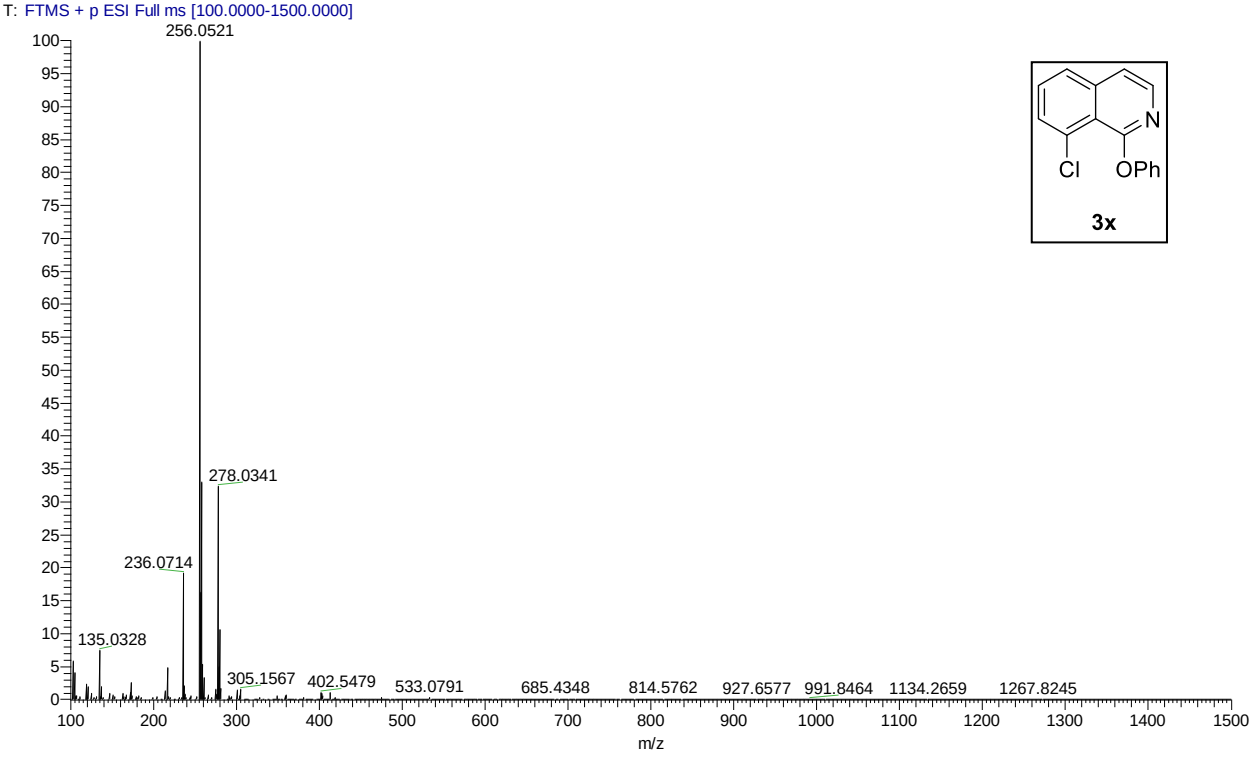


3t

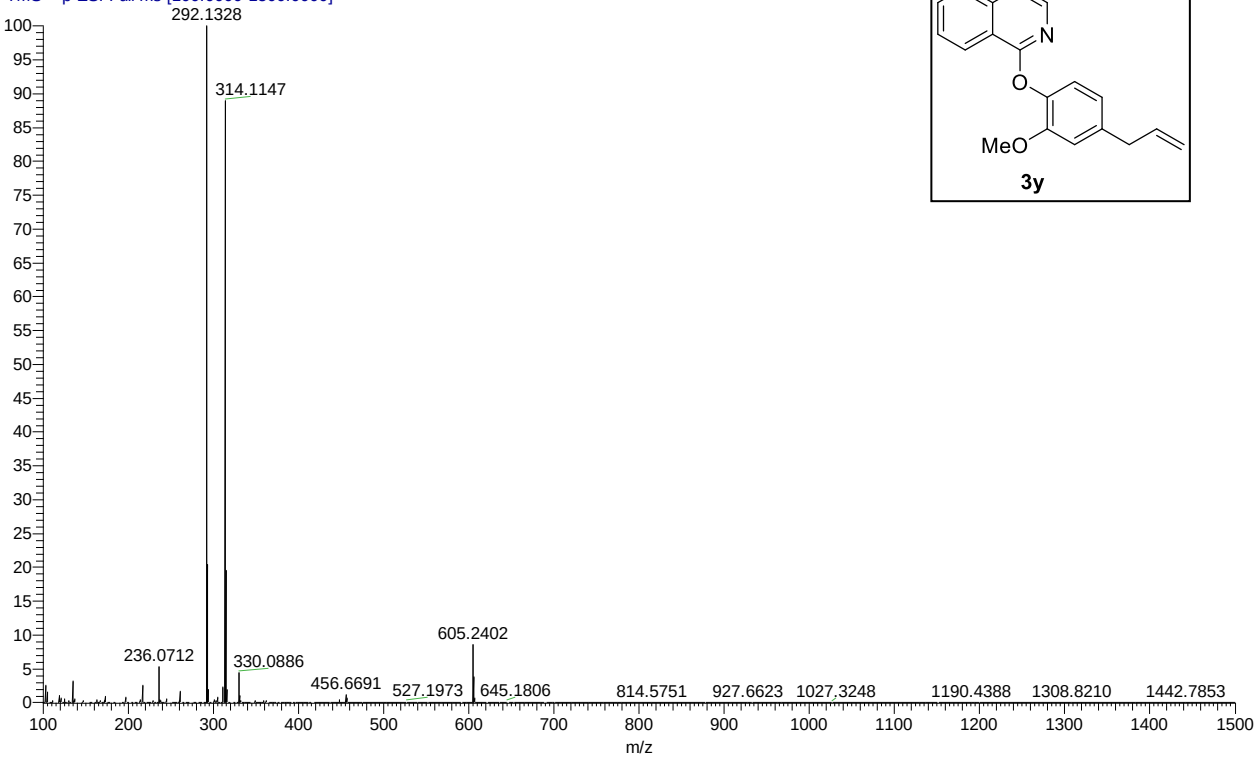
3W #25 RT: 0.26 AV: 1 NL: 9.68E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



3X #21 RT: 0.21 AV: 1 NL: 2.92E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

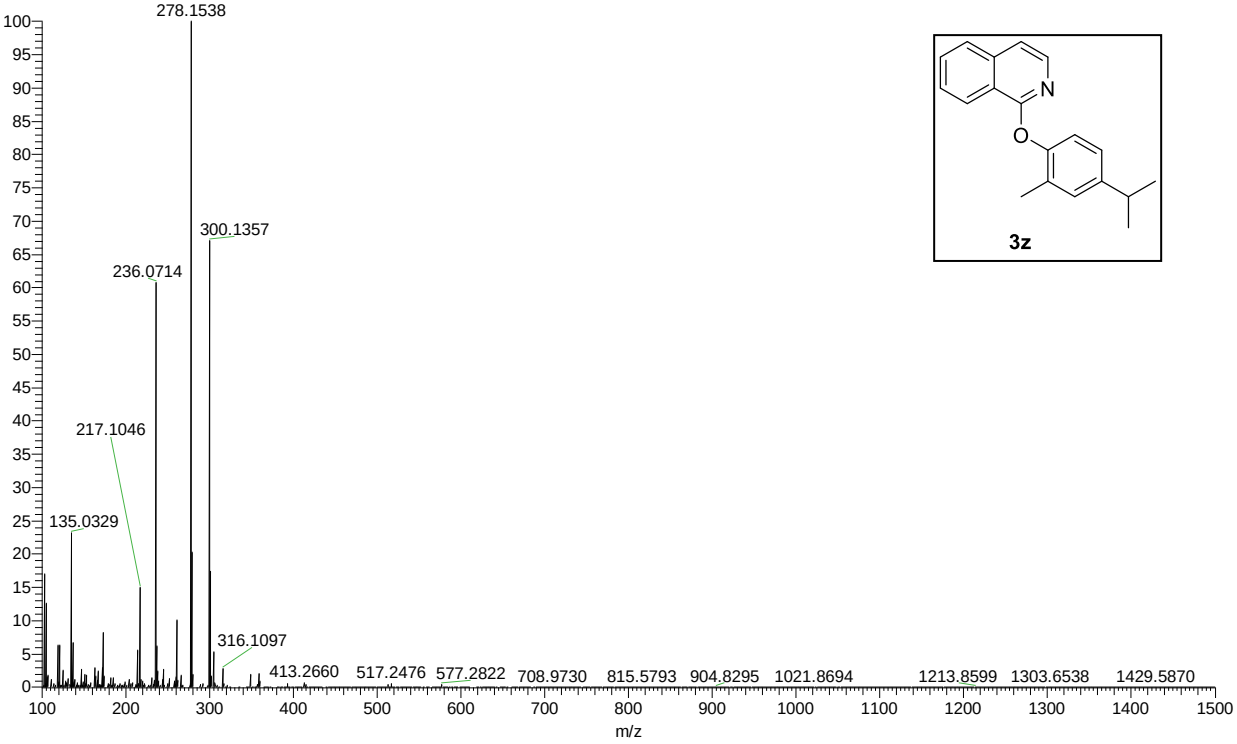


3Y #27 RT: 0.27 AV: 1 NL: 4.09E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



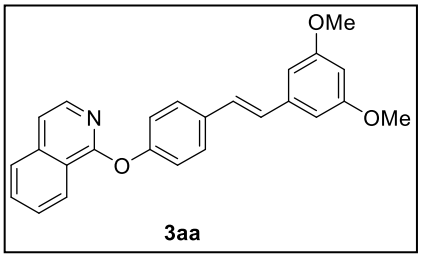
3y

3Z #41 RT: 0.42 AV: 1 NL: 5.62E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



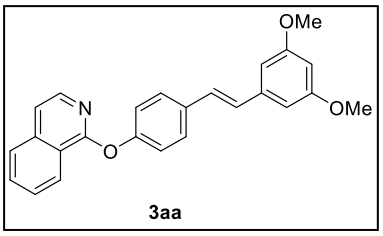
3z

3AA #37 RT: 0.37 AV: 1 NL: 7.13E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



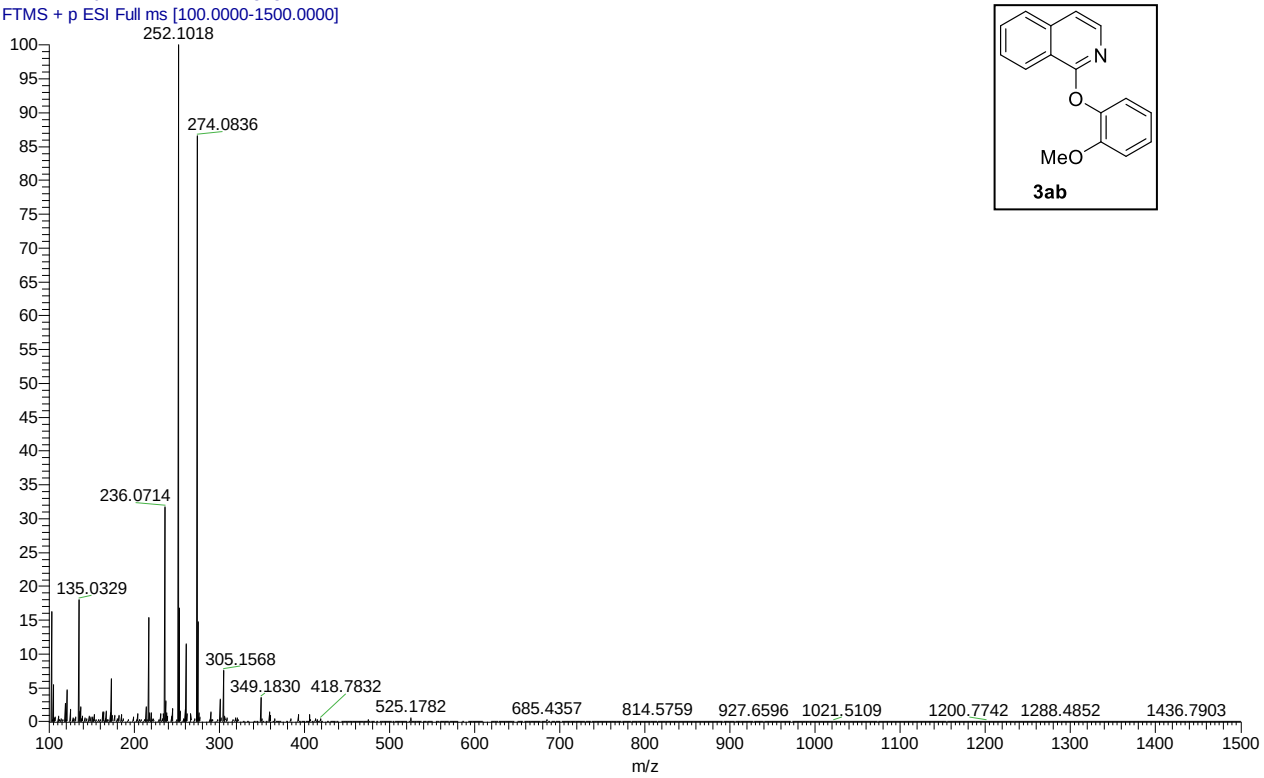
3aa

3AA #37 RT: 0.37 AV: 1 NL: 6.06E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



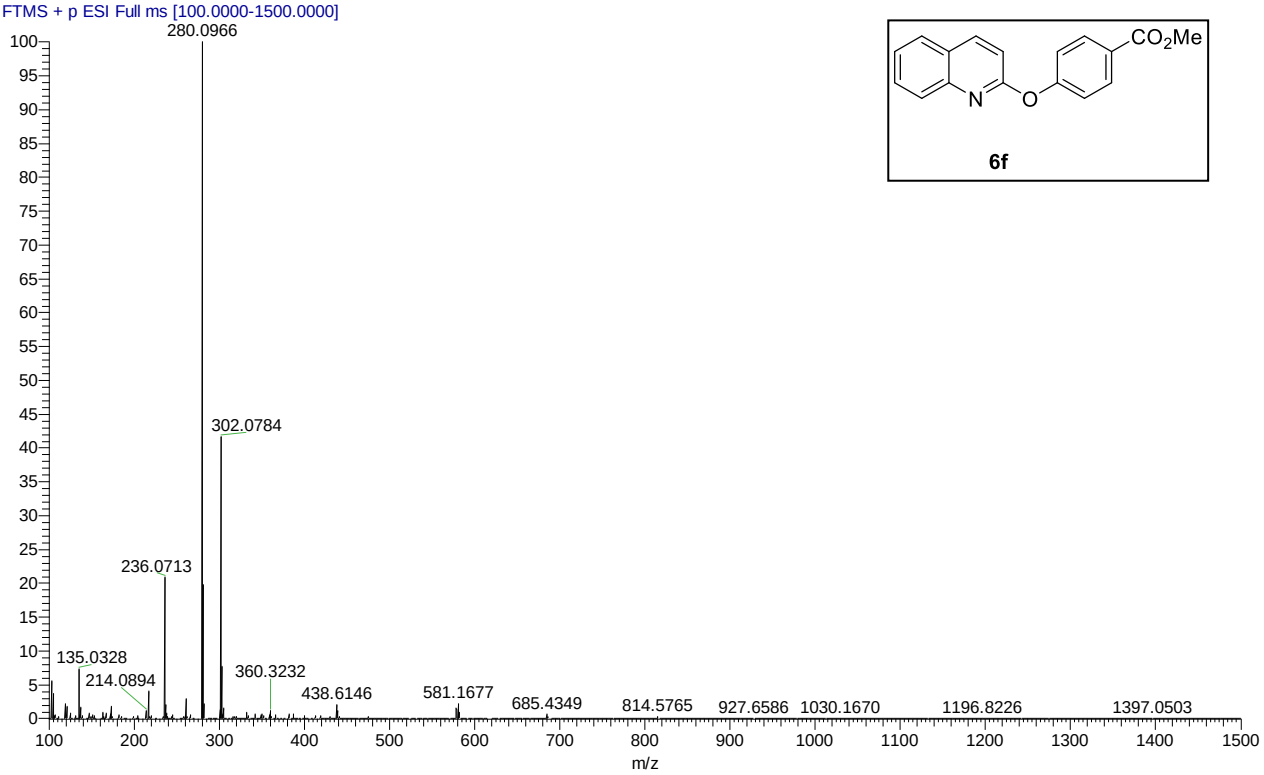
3aa

3AB #47 RT: 0.47 AV: 1 NL: 1.13E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



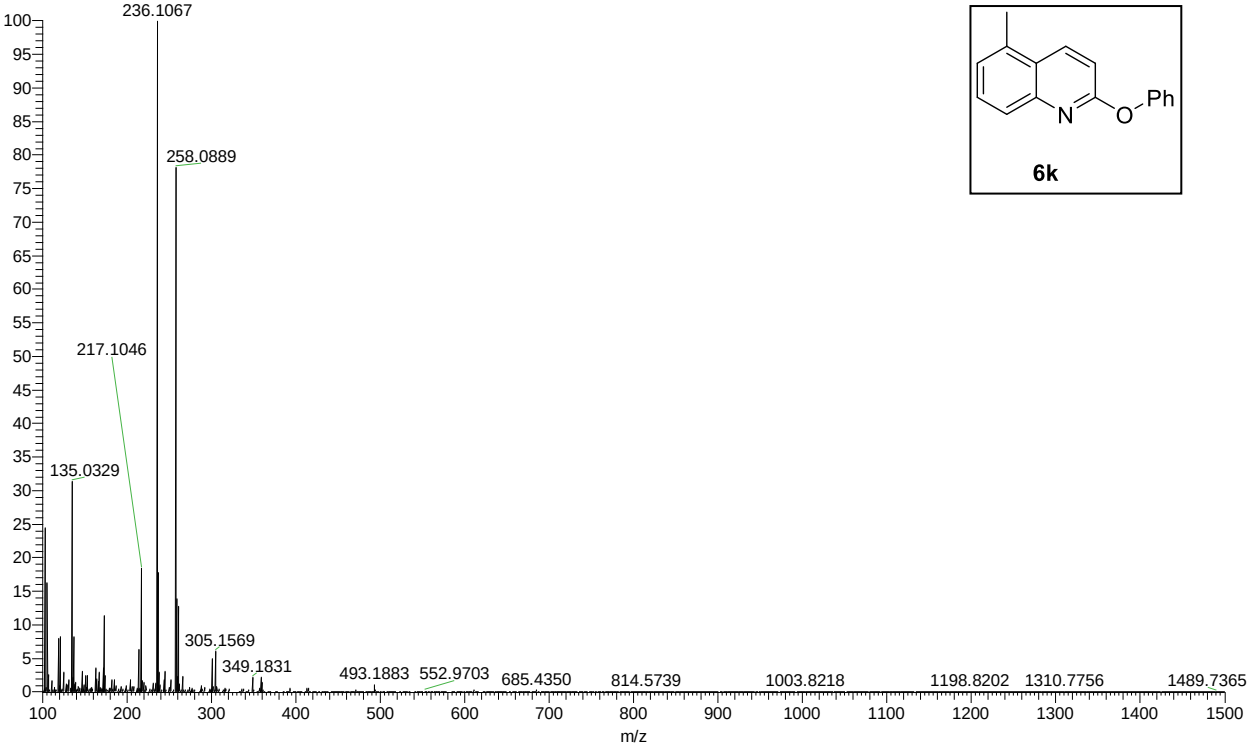
3ab

6F #29 RT: 0.29 AV: 1 NL: 1.63E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



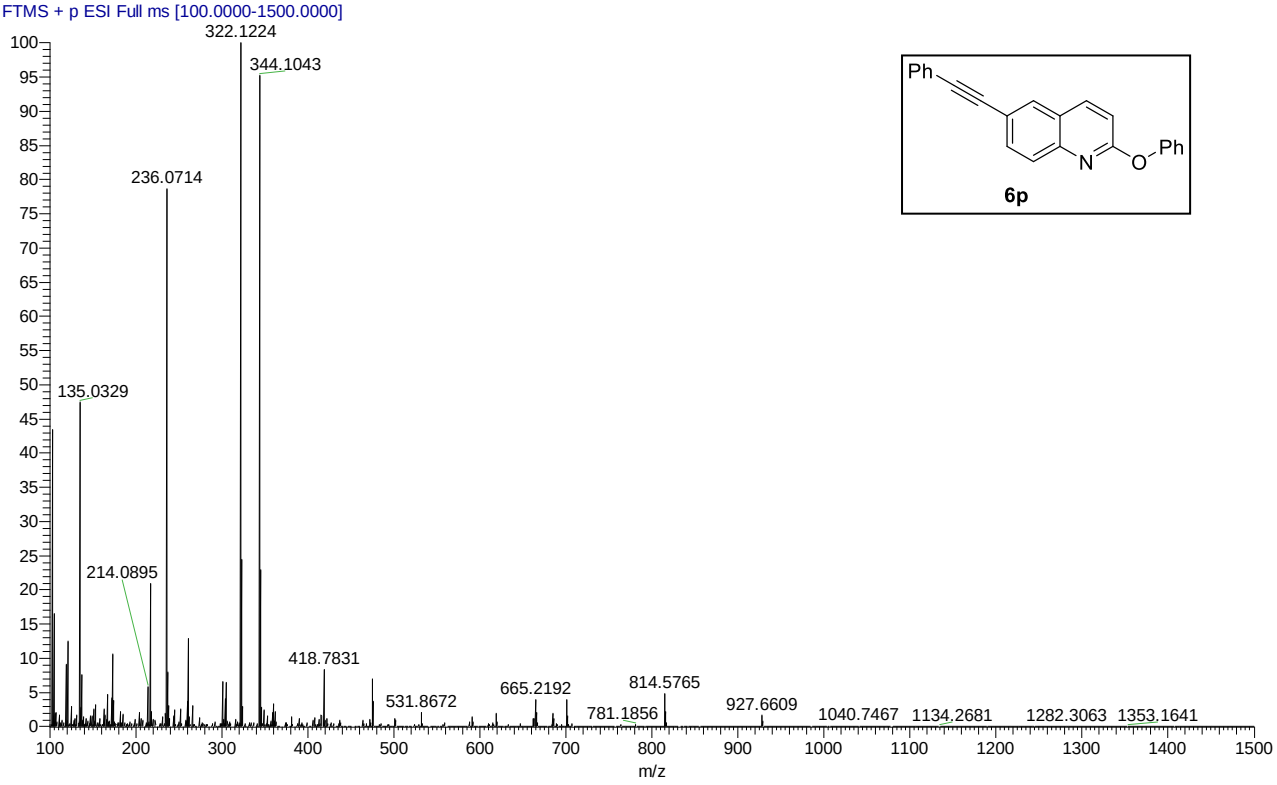
6f

6K #39 RT: 0.40 AV: 1 NL: 5.21E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



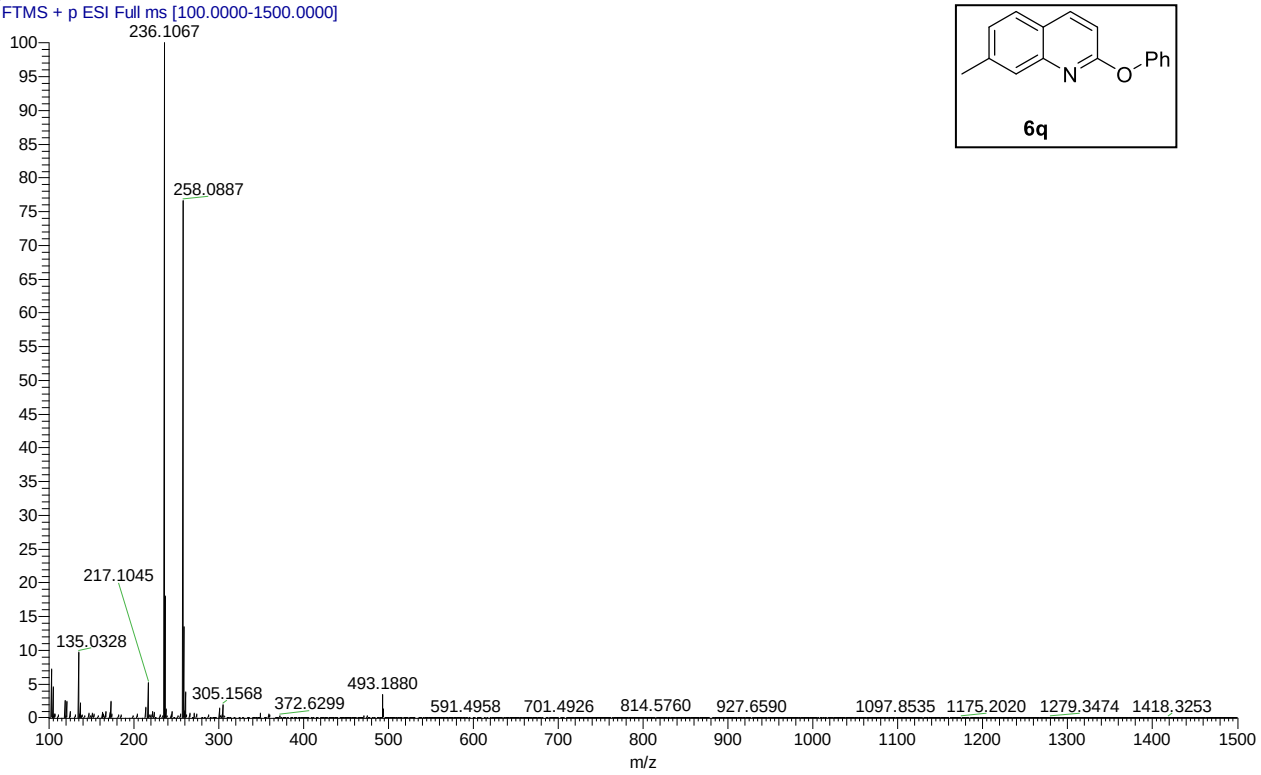
6k

6P #27 RT: 0.27 AV: 1 NL: 4.89E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]



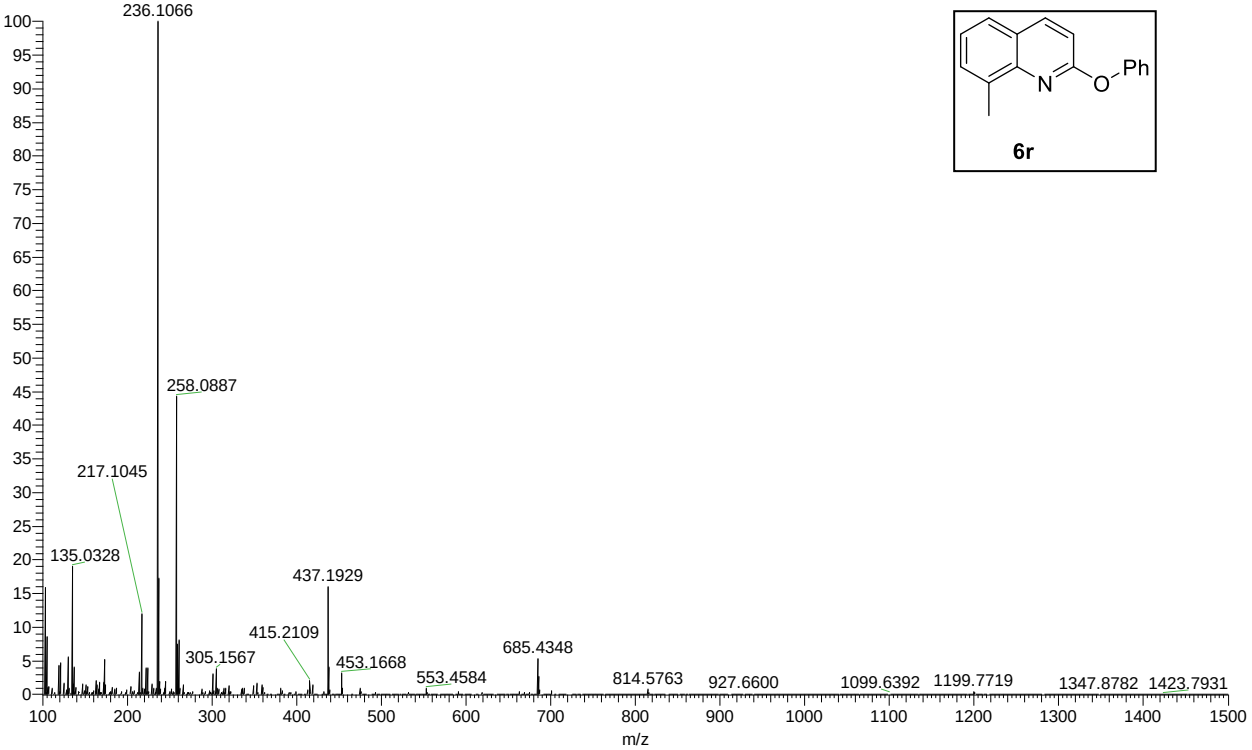
6p

6Q #31 RT: 0.31 AV: 1 NL: 2.54E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]

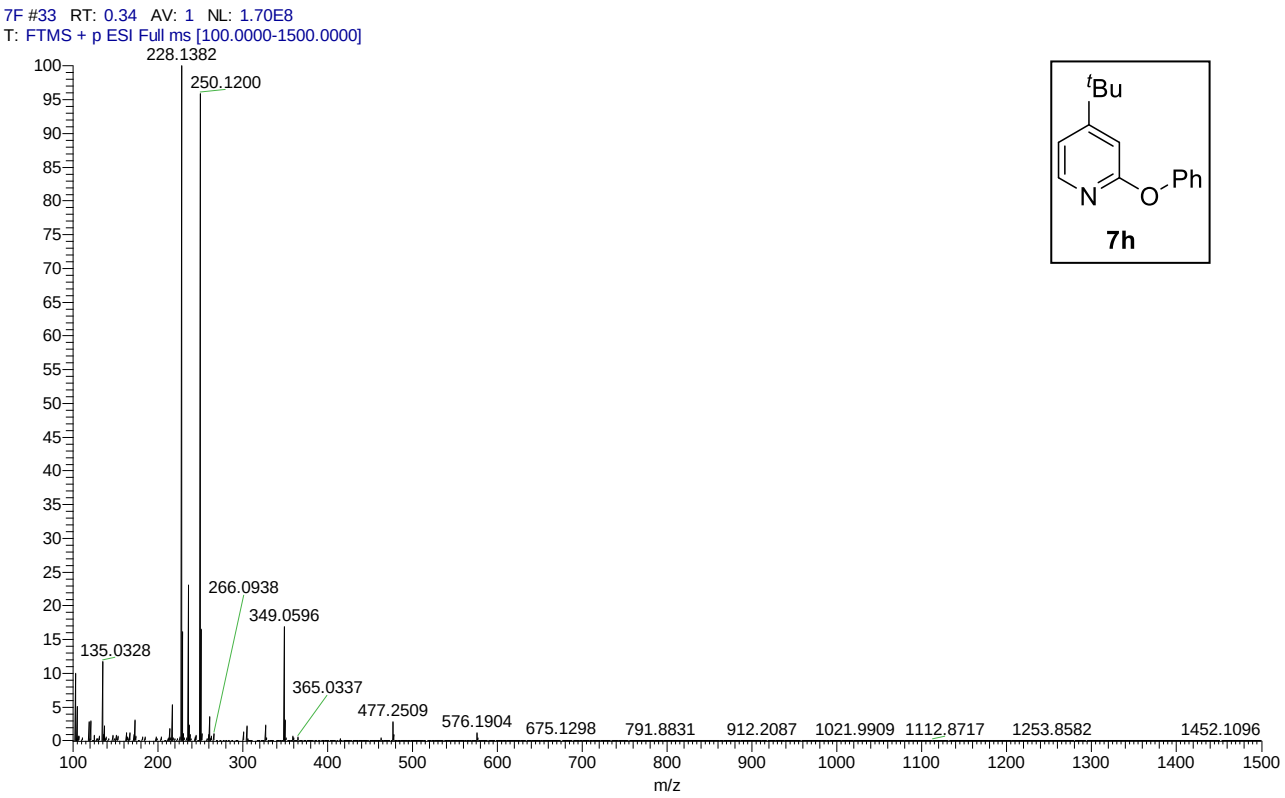


6q

6R #25 RT: 0.25 AV: 1 NL: 1.27E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]



6r


7F #33 RT: 0.34 AV: 1 NL: 1.70E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]
228.1382
250.1200
266.0938
349.0596
135.0328
365.0337
477.2509
576.1904
675.1298
791.8831
912.2087
1021.9909
1112.8717
1253.8582
1452.1096
m/z
tBu
Ph
N
O
7h