Supplementary Information

Green and Fast 2-Aryloxylation/Amination of Quinolines

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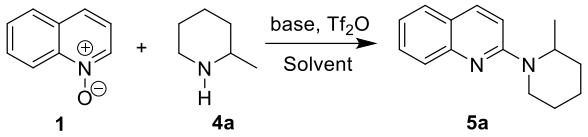
1. General Experimental

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. Nuclear magnetic resonance spectra (NMR) were recorded on Bruker AV-400 or 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 ThermoFisher Scientific Ultimate 3000/Q-Exactive mass spectrometer. Melting points were recorded on a Buchi Melting Point M-560. 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 Amination

Table S1 Optimization of the amination of quinoline *N*-oxide.



1 **4a** **5a**

entry	base	equiv of Tf_2O	solvent	C/mol·L^{-1}	yield, %
1	DIEA	1.2	EA/CH_3CN	0.25	71
2	DIEA	1.2	EA	0.25	60
3	DIEA	1.2	EA	0.5	68
4	DBU	1.2	EA	0.5	74
5	DBU	1.2	EA	0.25	71
6	DBU	1.2	EA	0.75	67
7	**DBU**	**1.5**	**EA**	**0.5**	**89**

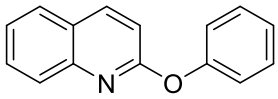
[a] Unless otherwise noted, all reactions were conducted with *N*-oxide (100 mg, 1.0 equiv), 2-methylpiperidine (1.2 equiv), Tf_2O and base (2.0 equiv).

3. General Procedure

General Procedure 1: Aryloxylation of Quinoline *N*-oxide. To a solution of a quinoline *N*-oxide derivative (1.0 eq.) in dry EA/CH_3CN (10/1, 0.25 M) is added ArOH (1.2 equiv) and DIEA (2.0 eq). The resulting solution is cooled to 0 °C, followed by the dropwise addition of Tf_2O (1.2 eq). The reaction mixture is then warmed to room temperature and stirred for 5 minutes to one hour until the reaction is complete as indicated by TLC. Finally, it is quenched with saturated sodium bicarbonate solution and extracted with CH_2Cl_2 three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash column chromatography furnishes the desired pure product.

General Procedure 2: Amination of Quinoline *N*-oxide. To a solution of a quinoline *N*-oxide derivative (1.0 eq.) in dry EA (0.5 M) is added amine (1.2 equiv) and DBU (2.0 eq). The resulting solution is cooled to 0 °C, followed by the dropwise addition of Tf_2O (1.5 eq). The reaction mixture is then warmed to room temperature and stirred for 5 minutes to one hour until the reaction is complete as indicated by TLC. Finally, it is quenched with saturated sodium bicarbonate solution and extracted with CH_2Cl_2 three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by flash column chromatography furnishes the desired pure product.

4. Preparation Procedure



3a

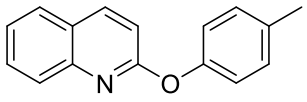
2-phenoxyquinoline (3a). Following **GP 1**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (125 mg, 82% yield) as a white solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.73 (PE:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.75 (dd, J = 1.2 Hz, 7.8 Hz, 1H), 7.60-7.62 (m, 1H), 7.41-7.43 (m, 3H), 7.22-7.26 (m, 3H), 7.07 (d, J = 8.4 Hz, 1H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{125}{152} \times 1 = 82\%$$

Gram scale synthesis:

In a 3-necked 100 ml round bottom flask equipped with a magnetic stir bar was added quinoline *N*-oxide (1.0 g, 6.9 mmol) and dry EA/CH_3CN (25 ml/2.5 ml), followed by PhOH (778 mg, 8.27 mmol) and DIEA (2.3 ml, 13.78 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of Tf_2O (1.4 ml, 8.27 mmol). The reaction mixture is then warmed to room temperature and stirred for one hour. The reaction is quenched with saturated sodium bicarbonate solution (30 ml) and extracted with CH_2Cl_2 (50 ml × 3). The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by chromatography (Hex:EA = 150:1-40:1) furnishes the desired pure product (1.1 g, 72%).

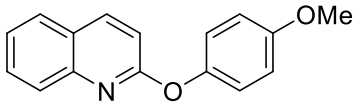
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{1.1}{1.53} \times 1 = 72\%$$



3b

2-(p-tolyloxy)quinoline (3b). Following **GP 1**, using quinoline *N*-oxide (96 mg, 0.66 mmol), the title compound was obtained (130 mg, 84% yield) as a white solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.3 (Hex:EA = 30:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 8.4 Hz, 1H), 7.75 (dd, *J* = 6.0 Hz, 7.8 Hz, 1H), 7.60-7.63 (m, 1H), 7.41-7.43 (m, 1H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 1H), 2.40 (s, 3H).

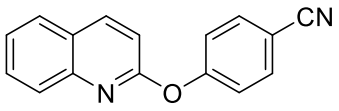
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{130}{155} \times 1 = 84\%$$



3c

2-(4-methoxyphenoxy)quinoline (3c). Following **GP 1**, using quinoline *N*-oxide (93 mg, 0.64 mmol), the title compound was obtained (134 mg, 83% yield) as a white solid. The spectroscopic data are consistent with previously reported.[2] TLC: R_f = 0.2 (PE:EA = 20:1). ^{1}H NMR (600 MHz, $CDCl_3$) *δ* 8.09 (d, *J* = 9.0 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.62 (dd, *J* = 6.0 Hz, 7.8 Hz, 1H), 7.59-7.62 (m, 1H), 7.39-7.42 (m, 1H), 7.18 (d, *J* = 9.0 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 1H), 6.95 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H).

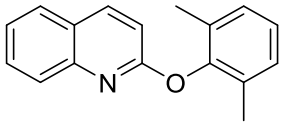
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{134}{161} \times 1 = 83\%$$



3d

4-(quinolin-2-yloxy)benzonitrile (3d). Following **GP 1**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (169 mg, 99% yield) as a white solid. TLC: R_f = 0.3 (Hex:EA = 50:1). Melting point: 124.8-125.0 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (d, J = 9.0 Hz, 1H), 7.79 (t, J = 8.4 Hz, 2H), 7.71 (d, J = 8.4 Hz, 2H), 7.64-7.67 (m, 1H), 7.46-7.49 (m, 1H), 7.39 (d, J = 8.4 Hz, 2H), 7.15 (d, J = 9.0 Hz, 1H). ^{13}C{^{1}H}NMR (150 MHz, $CDCl_3$) δ 160.4, 157.6, 146.1, 140.5, 133.9, 130.3, 128.0, 127.6, 126.2, 125.6, 122.1, 118.9, 113.1, 108.0. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{16}H_{11}N_2O$ 247.0866; found 247.0862.

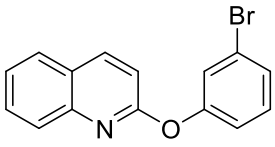
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{169}{170} \times 1 = 99\%$$



3e

2-(2,6-dimethylphenoxy)quinoline (3e). Following **GP 1**, using quinoline *N*-oxide (97 mg, 0.67 mmol), the title compound was obtained (150 mg, 89% yield) as a white solid. TLC: R_f = 0.69 (PE:EA = 20:1). Melting point: 85.4-85.8 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (d, J = 8.4 Hz, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.73 (dd, J = 0.6 Hz, 9.6 Hz, 1H), 7.56-7.59 (m, 1H), 7.37-7.39 (m, 1H), 7.09-7.14 (m, 3H), 6.99 (d, J = 8.4 Hz, 1H), 2.15 (s, 6H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.2, 150.6, 147.0, 140.0, 131.4, 129.8, 128.8, 128.0, 127.4, 125.5, 125.3, 124.6, 111.3, 16.8. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{16}NO$ 250.1226; found 250.1222.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{150}{167} \times 1 = 89\%$$

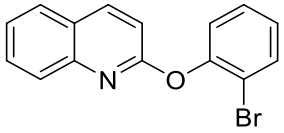


3f

2-(3-bromophenoxy)quinoline (3f). Following **GP 1**, using quinoline *N*-oxide (97 mg, 0.67 mmol), the title compound was obtained (150 mg, 75% yield) as a white solid. TLC: R_f = 0.32

(PE:EA = 50:1). Melting point: 57.9-58.3 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 9.0 Hz, 1H), 7.76 (dd, J = 1.2 Hz, 8.4 Hz, 1H), 7.61-7.64 (m, 1H), 7.42-7.45 (m, 2H), 7.35-7.36 (m, 1H), 7.28 (t, J = 7.8 Hz, 1H), 7.20-7.21 (m, 1H), 7.08 (d, J = 8.4 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.2, 154.6, 146.4, 140.2, 130.6, 130.1, 128.1, 127.9, 127.5, 126.0, 125.2, 124.9, 122.6, 120.4, 112.8. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{11}BrNO$ 300.0018; found 300.0015.

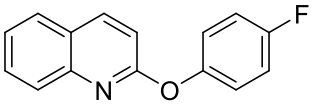
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{150}{201} \times 1 = 75\%$$



3g

2-(2-bromophenoxy)quinoline (3g). Following **GP 1**, using quinoline *N*-oxide (99 mg, 0.68 mmol), the title compound was obtained (170 mg, 83% yield) as a white solid. The spectroscopic data are consistent with previously reported.[3] TLC: R_f = 0.32 (PE:EA = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.15 (d, J = 9.0 Hz, 1H), 7.75-7.78 (m, 2H), 7.68 (dd, J = 1.8 Hz, 8.4 Hz, 1H), 7.59-7.62 (m, 1H), 7.42-7.44 (m, 1H), 7.38-7.41 (m, 1H), 7.33 (dd, J = 1.8 Hz, 8.4 Hz, 1H), 7.14-7.17 (m, 2H).

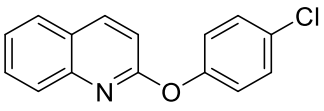
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{170}{205} \times 1 = 83\%$$



3h

2-(4-fluorophenoxy)quinoline (3h). Following **GP 1**, using quinoline *N*-oxide (92 mg, 0.63 mmol), the title compound was obtained (115 mg, 76% yield) as a white solid. TLC: R_f = 0.39 (PE:EA = 10:1). Melting point: 81.1-81.9 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, J = 9.0 Hz, 1H), 7.68 (d, J = 8.4 Hz, 1H), 7.66 (dd, J = 1.2 Hz, 8.4 Hz, 1H), 7.50-7.53 (m, 1H), 7.31-7.34 (m, 1H), 7.11-7.15 (m, 2H), 7.00-7.03 (m, 2H), 6.98 (d, J = 9.0 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.7, 160.5, 158.9, 149.7 (d, J = 3.0 Hz), 149.6, 146.4, 140.0, 130.0, 128.0, 127.5, 125.8, 125.0, 123.1 (d, J = 7.5 Hz), 123.0, 116.3, 116.1, 112.7. HRMS (+ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{15}H_{10}FNONa$ 262.0639; found 262.0636.

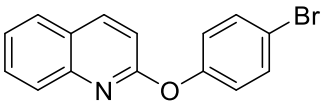
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{115}{152} \times 1 = 76\%$$



3i

2-(4-chlorophenoxy)quinoline (3i). Following **GP 1**, using quinoline *N*-oxide (99 mg, 0.68 mmol), the title compound was obtained (127 mg, 73% yield) as a yellow solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.23 (PE:EA = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.77 (dd, J = 6.0 Hz, 7.8 Hz, 1H), 7.61-7.64 (m, 1H), 7.42-7.45 (m, 1H), 7.39 (d, J = 9.0 Hz, 2H), 7.22 (d, J = 9.0 Hz, 2H), 7.09 (d, J = 8.4 Hz, 1H).

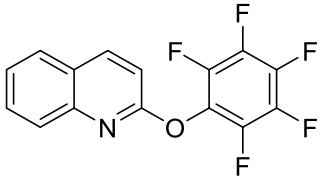
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{127}{174} \times 1 = 73\%$$



3j

2-(4-chlorophenoxy)quinoline (3j). Following **GP 1**, using quinoline *N*-oxide (93 mg, 0.64 mmol), the title compound was obtained (134 mg, 70% yield) as a white solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.32 (PE:EA = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (d, J = 9.0 Hz, 1H), 7.76-7.79 (m, 2H), 7.61-7.64 (m, 1H), 7.54 (d, J = 9.0 Hz, 2H), 7.43-7.45 (m, 1H), 7.17 (d, J = 9.0 Hz, 2H), 7.09 (d, J = 8.4 Hz, 1H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{134}{192} \times 1 = 70\%$$

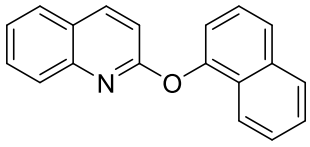


3k

2-(perfluorophenoxy)quinoline (3k). Following **GP 1**, using quinoline *N*-oxide (93 mg, 0.64 mmol), the title compound was obtained (190 mg, 95% yield) as a white solid. The spectroscopic data are consistent with previously reported.[4] TLC: R_f = 0.51 (Hex:EA = 100:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (d, J = 9.0 Hz, 1H), 7.79 (d, J = 7.8 Hz, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.63 (t,

J = 7.8 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 7.24 (d, J = 9.0 Hz, 1H).

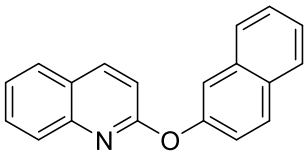
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{190}{199} \times 1 = 95\%$$



3l

2-(naphthalen-1-yloxy)quinoline (3l). Following **GP 1**, using quinoline *N*-oxide (103 mg, 0.71 mmol), the title compound was obtained (135 mg, 70% yield) as a white solid. TLC: R_f = 0.20 (PE:EA = 50:1). Melting point: 83.3-83.6 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (d, J = 9.0 Hz, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 7.8 Hz, 1H), 7.72-7.76 (m, 3H), 7.56-7.59 (m, 1H), 7.47-7.51 (m, 2H), 7.41-7.44 (m, 1H), 7.38-7.41 (m, 1H), 7.35 (d, J = 7.8 Hz, 1H), 7.08 (d, J = 9.0 Hz, 1H). ^{13}C NMR {^{1}H} (150 MHz, $CDCl_3$) δ 162.3, 150.0, 146.7, 140.1, 135.1, 130.0, 128.1, 128.1, 127.7, 127.5, 126.5, 126.3, 125.9, 125.8, 125.1, 125.0, 122.3, 117.5, 112.2. HRMS (+ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{13}NONa$ 294.0889; found 294.0884.

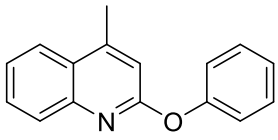
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{135}{193} \times 1 = 70\%$$



3m

2-(naphthalen-2-yloxy)quinoline (3m). Following **GP 1**, using quinoline *N*-oxide (98 mg, 0.67 mmol), the title compound was obtained (113 mg, 62% yield) as a white solid. TLC: R_f = 0.38 (Hex:EA = 50:1). Melting point: 70.3-70.9 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 9.0 Hz, 1H), 7.87 (d, J = 7.8 Hz, 1H), 7.75-7.81 (m, 3H), 7.68 (d, J = 2.4 Hz, 1H), 7.60-7.62 (m, 1H), 7.40-7.50 (m, 4H), 7.13 (d, J = 9.0 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.9, 151.8, 146.6, 140.0, 134.4, 131.2, 130.0, 129.5, 128.1, 127.9, 127.7, 127.5, 126.5, 125.9, 125.3, 125.1, 121.9, 117.8, 112.9. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{14}NO$ 272.1070; found 272.1065.

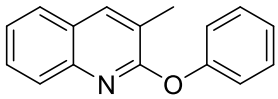
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{113}{183} \times 1 = 62\%$$



3n

4-methyl-2-phenoxyquinoline (3n). Following **GP 1**, using 4-methylquinoline *N*-oxide (98 mg, 0.62 mmol), the title compound was obtained (115 mg, 80% yield) as a white solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.38 (Hex:EA = 30:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (dd, J = 6.0 Hz, 7.8 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.56-7.59 (m, 1H), 7.38-7.41 (m, 3H), 7.23 (d, J = 7.2 Hz, 2H), 7.20 (d, J = 7.2 Hz, 1H), 6.89 (s, 1H), 2.61 (d, J = 6.0 Hz, 3H).

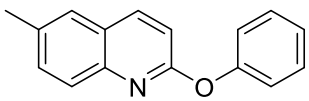
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{115}{144} \times 1 = 80\%$$



3o

3-methyl-2-phenoxyquinoline (3o). Following **GP 1**, using 3-methylquinoline *N*-oxide (100 mg, 0.63 mmol), the title compound was obtained (90 mg, 61% yield) as a white solid. Melting point: 50.7-51.2 ℃. TLC: R_f = 0.63 (PE:EA = 20:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.69 (dd, J = 1.2 Hz, 8.4 Hz, 1H), 7.50-7.53 (m, 1H), 7.41-7.44 (m, 2H), 7.36-7.39 (m, 1H), 7.24-7.26 (m, 2H), 7.20-7.23 (m, 1H), 2.50 (d, J = 6.0 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 160.8, 154.2, 145.2, 138.4, 129.5, 128.6, 127.7, 126.6, 126.5, 124.8, 124.5, 123.1, 121.6, 16.9. HRMS (+ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{16}H_{13}NONa$ 258.0889; found 258.0885.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{90}{148} \times 1 = 61\%$$

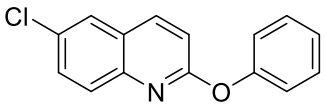


3p

6-methyl-2-phenoxyquinoline (3p). Following **GP 1**, using 6-methylquinoline *N*-oxide (101 mg, 0.63 mmol), the title compound was obtained (122 mg, 82% yield) as a white solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.37 (Hex:EA = 30:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, J = 8.4 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.52 (s, 1H), 7.45 (dd, J = 1.8 Hz, 6.6 Hz, 1H), 7.40-7.43 (m, 2H), 7.20-7.25 (m, 3H), 7.03 (d, J = 8.4 Hz, 1H), 2.49 (s,

3H).

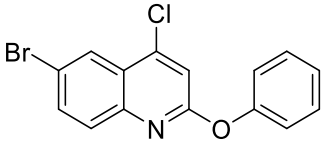
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{122}{149} \times 1 = 82\%$$



3q

6-chloro-2-phenoxyquinoline (3q). Following **GP 1**, using 6-chloroquinoline *N*-oxide (97 mg, 0.54 mmol), the title compound was obtained (100 mg, 72% yield) as a white solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.74 (PE:EA = 20:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02 (d, *J* = 9.0 Hz, 1H), 7.73 (d, *J* = 2.4 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.54 (dd, *J* = 1.8 Hz, 8.4 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.24-7.26 (m, 3H), 7.11 (d, *J* = 8.4 Hz, 1H).

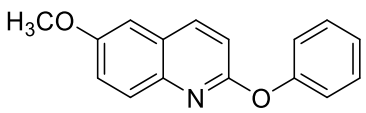
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{100}{138} \times 1 = 72\%$$



3r

6-bromo-4-chloro-2-phenoxyquinoline (3r). Following **GP 1**, using 6-bromo-4-chloroquinoline *N*-oxide (102 mg, 0.39 mmol), the title compound was obtained (90 mg, 68% yield) as a white solid. TLC: R_f = 0.50 (Hex:EA = 30:1). Melting point: 125.6-125.8 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.18 (d, *J* = 2.4 Hz, 1H), 7.61 (dd, *J* = 1.8 Hz, 9.0 Hz, 1H), 7.54 (d, *J* = 9.0 Hz, 1H), 7.32-7.36 (m, 2H), 7.15-7.18 (m, 1H), 7.12-7.14 (m, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 161.5, 153.3, 145.6, 143.8, 134.3, 130.1, 129.8, 126.5, 125.4, 125.3, 121.7, 119.5, 113.6. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{10}BrClNO$ 333.9629; found 333.9615.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{90}{132} \times 1 = 68\%$$

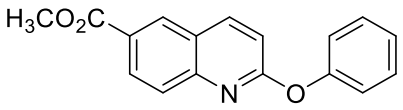


3s

6-methoxy-2-phenoxyquinoline (3s). To a solution of 6-methoxyquinoline *N*-oxide (100 mg, 0.57 mmol) in dry EA/CH_3CN (2/0.2 ml) is added PhOH (64 mg, 0.684 mmol) and DIEA (147 mg,

1.14 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of Tf_2O (193 mg, 0.684 mmol). The reaction mixture is then warmed to room temperature and stirred for 24 h. Extra Tf_2O (80 mg, 0.285 mmol) is added to the reaction mixture, and the reaction is complete after 6 h. The reaction is quenched with saturated sodium bicarbonate solution and extracted with CH_2Cl_2 three times. The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by column chromatography (Hex:EA = 200:1) furnishes the desired pure product (103 mg, 72% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.21 (Hex:EA = 200:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.00 (d, J = 9.0 Hz, 1H), 7.72 (d, J = 9.0 Hz, 1H), 7.40 (m, 2H), 7.27 (dd, J = 3.0 Hz, 9.6 Hz, 1H), 7.19-7.24 (m, 3H), 7.02-7.05 (m, 2H), 3.88 (s, 3H).

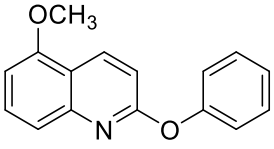
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{103}{143} \times 1 = 72\%$$



3t

Methyl-2-phenoxyquinoline-6-carboxylate (3t). Following **GP 1**, using 6-(methoxycarbonyl)-quinoline *N*-oxide (100 mg, 0.49 mmol), the title compound was obtained (77 mg, 56% yield) as a yellow solid. TLC: R_f = 0.23 (Hex:EA = 100:1). Melting point: 106.8-107.2 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.51 (d, J = 1.8 Hz, 1H), 8.20 (d, J = 7.2 Hz, 2H), 7.79 (d, J = 8.4 Hz, 1H), 7.43-7.46 (m, 2H), 7.25-7.28 (m, 3H), 7.14 (d, J = 9.0 Hz, 1H), 3.97 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 166.9, 163.3, 153.5, 149.1, 140.9, 130.5, 129.7, 129.6, 128.2, 126.5, 125.2, 124.9, 121.8, 113.8, 52.4. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{14}NO_3$ 280.0968; Found 280.0962.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{77}{136} \times 1 = 56\%$$

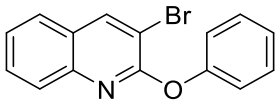


3u

5-Methoxy-2-phenoxyquinoline (3u). Following **GP 1**, using 5-methoxyquinoline *N*-oxide (100 mg, 0.57 mmol), the title compound was obtained (46 mg, 32% yield) as a white solid. This reaction is complete in 24 h. TLC: R_f = 0.21 (Hex:EA = 100:1). Melting point: 103.7-103.8 °C. ^{1}H NMR

(600 MHz, $CDCl_3$) δ 8.55 (d, J = 9.0 Hz, 1H), 7.54 (t, J = 8.4 Hz, 1H), 7.44 (t, J = 7.8 Hz, 3H), 7.24 - 7.28 (m, 3H), 7.04 (d, J = 9.0 Hz, 1H), 6.78 (d, J = 7.8 Hz, 1H), 4.01 (s, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 162.2, 155.5, 154.1, 147.7, 134.9, 130.1, 129.7, 124.7, 121.5, 120.3, 117.9, 111.3, 103.4, 55.8. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{16}H_{14}NO_2$ 252.1019; Found 252.1015.

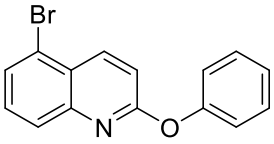
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{46}{143} \times 1 = 32\%$$



3v

3-bromo-2-phenoxyquinoline (3v). Following **GP 1**, using 3-bromoquinoline *N*-oxide (100 mg, 0.45 mmol), the title compound was obtained (85 mg, 63% yield) as a white solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.18 (Hex:EA = 100:1). ^1H NMR (600 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.69 (t, J = 8.4 Hz, 2H), 7.59 (td, J = 1.2 Hz, 7.2 Hz, 1H), 7.45-7.42 (m, 3H), 7.25-7.28 (m, 3H).

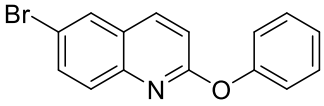
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{85}{134} \times 1 = 63\%$$



3w

5-bromo-2-phenoxyquinoline (3w). Following **GP 1**, using 5-bromoquinoline *N*-oxide (100 mg, 0.45 mmol), the title compound was obtained (98 mg, 73% yield) as a white solid. TLC: R_f = 0.15 (Hex:EA = 100:1). Melting point: 93.8-94.2 °C. ^1H NMR (600 MHz, $CDCl_3$) δ 8.50 (d, J = 9.0 Hz, 1H), 7.74 (d, J = 8.4 Hz, 1H), 7.68 (dd, J = 1.2 Hz, 7.8 Hz, 1H), 7.44 (t, J = 7.8 Hz, 3H), 7.25-7.27 (m, 3H), 7.17 (d, J = 9.0 Hz, 1H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 162.3, 153.7, 147.4, 139.4, 130.2, 129.7, 128.8, 127.9, 125.2, 125.1, 121.8, 121.6, 114.0. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{11}NOBr$ 300.0018; found 300.0015.

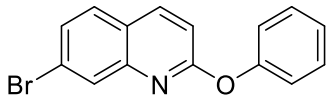
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{98}{134} \times 1 = 73\%$$



3x

6-bromo-2-phenoxyquinoline (3x). Following **GP 1**, using 6-bromoquinoline *N*-oxide (100 mg, 0.45 mmol), the title compound was obtained (105 mg, 78% yield) as a white solid. The spectroscopic data are consistent with previously reported.[1] TLC: R_f = 0.16 (Hex:EA = 100:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, J = 9.0 Hz, 1H), 7.89 (d, J = 1.8 Hz, 1H), 7.63-7.67 (m, 2H), 7.43 (t, J = 7.8 Hz, 2H), 7.25-7.23 (m, 3H), 7.09 (d, J = 9.0 Hz, 1H).

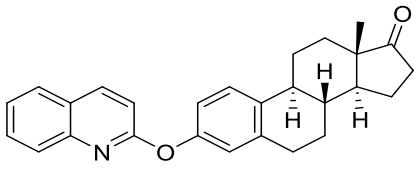
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{105}{134} \times 1 = 78\%$$



3y

7-bromo-2-phenoxyquinoline (3y). Following **GP 1**, using 7-bromoquinoline N-oxide (100 mg, 0.45 mmol), the title compound was obtained (85 mg, 63% yield) as a white solid. TLC: R_f = 0.25 (Hex:EA = 100:1). Melting point: 79.4-79.6 ℃. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, J = 9.0 Hz, 1H), 7.96 (s, 1H), 7.59 (d, J = 9.0 Hz, 1H), 7.49 (d, J = 7.2 Hz, 1H), 7.43 (t, J = 8.4 Hz, 2H), 7.25 (m, 3H), 7.09 (d, J = 9.0 Hz, 1H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 162.4, 153.6, 147.3, 139.6, 130.4, 129.7, 128.6, 128.4, 125.1, 124.4, 124.1, 121.7, 113.3. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{11}NOBr$ 300.0018; Found 300.0014.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{85}{134} \times 1 = 63\%$$

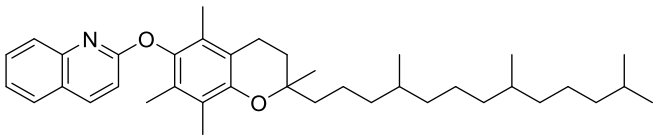


3z

(8R,9S,13S,14S)-13-methyl-3-(quinolin-2-yloxy)-6,7,8,9,11,12,13,14,15,16-decahydro-17H-cyclopenta[a]phenanthren-17-one (3z). Following **GP 1**, using quinoline *N*-oxide (97 mg, 0.68 mmol), the title compound was obtained (190 mg, 72% yield) as a white solid. TLC: R_f = 0.34 (Hex:EA = 5:1). Melting point: 192.5-192.7 ℃. ^{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 (dd, J = 1.2 Hz, 8.4 Hz, 1H), 7.59 -7.62 (m, 1H), 7.40 -7.43 (m, 1H), 7.32 (d, J = 8.4 Hz, 1H), 7.06 (d, J = 9.0 Hz, 1H), 7.04 (dd, J = 2.4 Hz, 8.4 Hz, 1H), 6.99 (d, J = 2.4 Hz, 1H), 2.92-2.95 (m, 2H), 2.51 (dd, J = 8.4 Hz, 19.2 Hz, 1H), 2.42-2.46 (m, 1H), 2.33 (td, J = 4.2 Hz, 10.8 Hz, 1H), 2.12-2.19 (m, 1H), 2.09-1.97 (m, 3H), 1.44-1.68 (m, 6H), 0.94

(s, 3H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$) δ 221.0, 161.9, 151.8, 146.6, 139.8, 138.2, 136.2, 129.8, 128.0, 127.5, 126.5, 125.8, 124.9, 121.3, 118.8, 112.8, 50.6, 48.1, 44.3, 38.3, 36.0, 31.7, 29.6, 26.6, 26.0, 21.7, 14.0. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{27}H_{28}NO_2$ 398.2115; Found 398.2110.

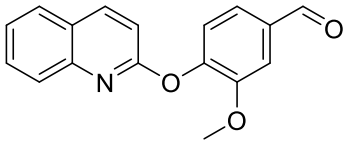
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{190}{264} \times 1 = 72\%$$



3aa

2-((2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)chroman-6-yl)oxy)quinoline (3aa). Following **GP 1**, using quinoline *N*-oxide (101 mg, 0.69 mmol), the title compound was obtained (290 mg, 75% yield) as a yellow oil. TLC: R_f = 0.47 (Hex:EA = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.59 (t, *J* = 8.4 Hz, 1H), 7.37 (t, *J* = 8.4 Hz, 1H), 6.85 (d, *J* = 9.0 Hz, 1H), 2.63 (t, *J* = 6.6 Hz, 2H), 2.14 (s, 3H), 2.04 (s, 3H), 2.00 (s, 3H), 1.84-1.88 (m, 1H), 1.77-1.82 (m, 1H), 1.50-1.67 (m, 4H), 1.26-1.28 (m, 12H), 1.07-1.56 (m, 7H), 0.85-0.88 (m, 13H). $^{13}C\{^{1}H\}$ NMR (150 MHz, $CDCl_3$) δ 162.3, 149.1, 147.2, 142.9, 139.8, 129.8, 128.1, 128.0, 127.4, 126.2, 125.4, 124.4, 123.2, 117.8, 110.8, 75.2, 39.5, 37.6, 37.6, 37.5, 37.4, 33.0, 32.9, 28.1, 24.97, 24.95, 24.6, 24.1, 22.9, 22.8, 21.2, 20.8, 19.9, 19.8, 13.3, 12.5, 12.1. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{38}H_{56}NO_2$ 558.4306; Found 558.4301.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{290}{388} \times 1 = 75\%$$

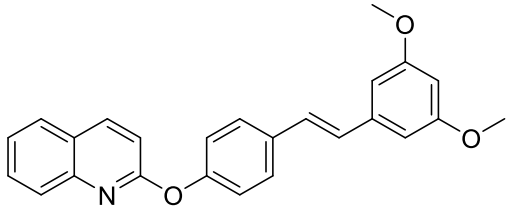


3ab

3-methoxy-4-(quinolin-2-yloxy)benzaldehyde (3ab). Following **GP 1**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (123 mg, 64% yield) as a white solid. TLC: R_f = 0.67 (PE:EA = 5:1). Melting point: 121.5-122.2 °C. ^{1}H NMR (600 MHz, $CDCl_3$) *δ* 9.99 (s, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.77 (dd, *J* = 1.2 Hz, 7.8 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.58-7.61 (m, 1H), 7.57 (d, *J* = 1.8 Hz, 1H), 7.54 (dd, *J* = 1.8 Hz, 8.4 Hz, 1H), 7.40-7.44 (m, 2H), 7.17 (d, *J* =

8.4 Hz, 1H), 3.81 (s, 3H). $^{13}C\{^{1}H\}$NMR (150 MHz, $CDCl_3$) δ 191.3, 161.0, 152.6, 148.3, 146.4, 140.0, 134.3, 129.9, 128.0, 127.5, 126.0, 125.3, 125.1, 123.4, 112.5, 111.3, 56.2. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{14}NO_3$ 280.0968; found 280.0967.

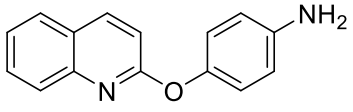
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{123}{193} \times 1 = 64\%$$



3ac

(E)-**2-(4-(3,5-dimethoxystyryl)phenoxy)quinoline (3ac)**. Following **GP 1**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (141 mg, 53% yield) as a white solid. TLC: R_f = 0.82 (PE:EA = 3:1). Melting point: 66.1-66.8 °C. ^1H NMR (600 MHz, $CDCl_3$) *δ* 8.12 (d, *J* = 9.0 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.2 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 2H), 7.42 (t, *J* = 15.0 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.10 (t, *J* = 15.6 Hz, 2H), 7.01 (d, *J* = 16.2 Hz, 1H), 6.68 (d, *J* = 1.8 Hz, 2H), 6.40 (s, 1H), 3.83 (s, 6H). $^{13}C\{^{1}H\}$NMR (150 MHz, $CDCl_3$) δ 161.6, 161.1, 153.6, 146.6, 140.0, 139.5, 133.9, 130.0, 128.7, 128.4, 128.0, 127.8, 127.5, 125.9, 125.0, 121.7, 112.9, 104.7, 100.1, 55.5. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{25}H_{22}NO_3$ 384.1594; found 384.1592.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{141}{264} \times 1 = 53\%$$



3ad

4-(quinolin-2-yloxy)aniline (3ad). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (123 mg, 75% yield) as a white solid. TLC: R_f = 0.51 (Hex:EA = 1:1). Melting point: 204.4-204.6 °C. ^1H NMR (600 MHz, DMSO-d_6) *δ* 9.09 (d, *J* = 27.6 Hz, 2H), 7.95 (d, *J* = 9.0 Hz, 1H), 7.73 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 7.8 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.52 (t, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.2 Hz, 1H), 6.97 (d, *J* = 9.0 Hz, 1H), 6.78 (d, *J* = 8.4 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (150 MHz, DMSO-d_6) δ 154.6, 152.2, 147.3, 136.6, 133.2, 129.4, 127.5 126.1, 123.4, 122.1, 120.7, 115.2, 113.9. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{13}N_2O$

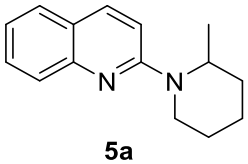
237.1022; found 237.1019.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{123}{163} \times 1 = 75\%$$

0.5 g scale synthesis:

In a 3-necked 25 ml round bottom flask equipped with a magnetic stir bar was added quinoline *N*-oxide (0.5 g, 3.4 mmol) and dry EA (6.9 ml), followed by 4-aminophenol (451 mg, 4.13 mmol) and DBU (1.0 ml, 6.9 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of Tf_2O (0.87 ml, 5.2 mmol). The reaction mixture is then warmed to room temperature and stirred for one hour. The reaction is quenched with saturated sodium bicarbonate solution (20 ml) and extracted with CH_2Cl_2 (30 ml × 3). The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by chromatography (Hex:EA = 10:1-1:1) furnishes the desired pure product (0.57 g, 70% yield).

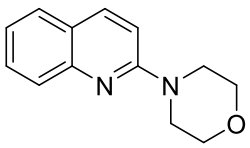
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{570}{803} \times 1 = 70\%$$



5a

N-benzyl-N-methylquinolin-2-amine (5a). Following **GP 2**, using quinoline *N*-oxide (94 mg, 0.65 mmol), the title compound was obtained (131 mg, 89% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[5] TLC: R_f = 0.43 (Hex:EA = 30:1). ^1H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 9.0 Hz, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.56 (dd, *J* = 1.2 Hz, 7.8 Hz, 1H), 7.48-7.51 (m, 1H), 7.16-7.18 (m, 1H), 6.96 (d, *J* = 9.0 Hz, 1H), 4.80 (quin, *J* = 6.6 Hz, 1H), 4.48 (d, *J* = 13.2 Hz, 1H), 3.02 (td, *J* = 3.0 Hz, 16.2 Hz, 1H), 1.78-1.83 (m, 2H), 1.64-1.73 (m, 3H), 1.54-1.57 (m, 1H), 1.20 (d, *J* = 6.6 Hz, 3H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{131}{147} \times 1 = 89\%$$

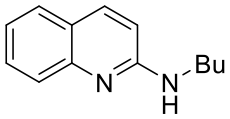


5b

4-(quinolin-2-yl)morpholine (5b). Following **GP 2**, using quinoline *N*-oxide (93 mg, 0.63 mmol), the title compound was obtained (100 mg, 73% yield) as a white solid. The spectroscopic

data are consistent with previously reported.[6] TLC: R_f = 0.22 (Hex:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, J = 9.0 Hz, 1H), 7.62 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 7.8 Hz, 1H), 7.43-7.45 (m, 1H), 7.12-7.15 (m, 1H), 6.82 (d, J = 9.6 Hz, 1H), 3.73 (t, J = 4.8 Hz, 4H), 3.58 (t, J = 4.8 Hz, 4H).

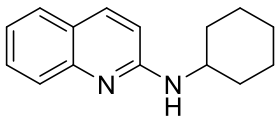
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{100}{137} \times 1 = 73\%$$



5c

N-butylquinolin-2-amine (5c). Following **GP 2**, using quinoline *N*-oxide (99 mg, 0.68 mmol), the title compound was obtained (132 mg, 97% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[7] TLC: R_f = 0.10 (Hex:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, J = 9.0 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.57 (dd, J = 1.2 Hz, 8.4 Hz, 1H), 7.51-7.54 (m, 1H), 7.18-7.21 (m, 1H), 6.61 (d, J = 9.0 Hz, 1H), 4.91 (s, 1H), 3.47 (dd, J = 1.2 Hz, 12.6 Hz, 2H), 1.60-1.65 (m, 2H), 1.41-1.47 (m, 2H), 0.96 (t, J = 7.2 Hz, 3H).

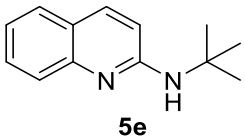
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{132}{136} \times 1 = 97\%$$



5d

N-cyclohexylquinolin-2-amine (5d). Following **GP 2**, using quinoline *N*-oxide (97 mg, 0.67 mmol), the title compound was obtained (119 mg, 78% yield) as a white solid. The spectroscopic data are consistent with previously reported.[8] TLC: R_f = 0.41 (Hex:EA = 5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, J = 9.0 Hz, 1H), 7.65 (d, J = 8.4 Hz, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.50-7.53 (m, 1H), 7.17-7.20 (m, 1H), 6.63 (d, J = 8.4 Hz, 1H), 4.87 (s, 1H), 3.81-3.86 (m, 1H), 2.09-2.12 (m, 2H), 1.78 (dt, J =3.6 Hz, 13.8 Hz, 2H), 1.66 (dt, J = 3.6 Hz, 13.2 Hz, 1H), 1.41-1.48 (m, 2H), 1.22-1.29 (m, 3H).

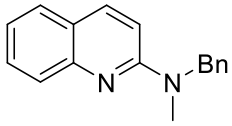
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{119}{152} \times 1 = 78\%$$



5e

N-(tert-butyl)quinolin-2-amine (5e). Following **GP 2**, using quinoline *N*-oxide (98 mg, 0.67 mmol), the title compound was obtained (128 mg, 95% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[7] TLC: R_f = 0.52 (Hex:EA = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (d, J = 9.0 Hz, 1H), 7.66 (d, J = 8.4 Hz, 1H), 7.53 (d, J = 7.8 Hz, 1H), 7.47-7.50 (m, 1H), 7.15-7.18 (m, 1H), 6.56 (d, J = 9.0 Hz, 1H), 4.61 (s, 1H), 1.52 (s, 9 H).

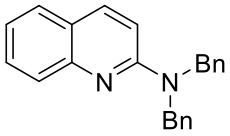
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{128}{135} \times 1 = 95\%$$



5f

N-benzyl-N-methylquinolin-2-amine (5f). Following **GP 2**, using quinoline *N*-oxide (96 mg, 0.66 mmol), the title compound was obtained (110 mg, 67% yield) as a white solid. The spectroscopic data are consistent with previously reported.[6] TLC: R_f = 0.59 (PE:EA = 20:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, J = 9.0 Hz, 1H), 7.68 (d, J = 8.4 Hz, 1H), 7.54 (dd, J = 0.6 Hz, 7.8 Hz, 1H), 7.47-7.50 (m, 1H), 7.23-7.27 (m, 4H), 7.19-7.21 (m, 1H), 7.13-7.16 (m, 1H), 6.82 (d, J = 9.0 Hz, 1H), 4.89 (s, 2H), 3.18 (s, 3H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{110}{164} \times 1 = 67\%$$



5g

N,N-dibenzylquinolin-2-amine (5g). Following **GP 2**, using quinoline *N*-oxide (98 mg, 0.67 mmol), the title compound was obtained (175 mg, 80% yield) as a white solid. The spectroscopic data are consistent with previously reported.[7] TLC: R_f = 0.31 (Hex:EA = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, J = 9.6 Hz, 1H), 7.69 (d, J = 8.4 Hz, 1H), 7.54 (dd, J = 1.2 Hz , 8.4 Hz, 1H), 7.49-7.51 (m, 1H), 7.25-7.27 (m, 8H), 7.21-7.23 (m, 2H), 7.15-7.18 (m, 1H), 6.78 (d, J = 9.0 Hz, 1H), 4.90 (s, 4H).

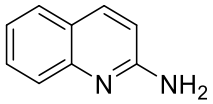
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{175}{219} \times 1 = 80\%$$

Gram scale synthesis:

In a 3-necked 50 ml round bottom flask equipped with a magnetic stir bar was added quinoline

N-oxide (1.0 g, 6.9 mmol) and dry EA (13.8 ml), followed by Bn_2NH (1.6 g, 8.3 mmol) and DBU (2.1 ml, 13.8 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of Tf_2O (1.7 ml, 10.3 mmol). The reaction mixture is then warmed to room temperature and stirred for one hour. The reaction is quenched with saturated sodium bicarbonate solution (30 ml) and extracted with CH_2Cl_2 (50 ml × 3). The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by chromatography (Hex:EA = 150:1-50:1) furnishes the desired pure product (1.64 g, 74%).

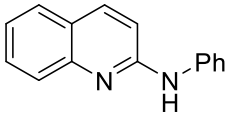
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{1.64}{2.23} \times 1 = 74\%$$



5h

Quinolin-2-amine (5h). In a 3-necked 10 ml round bottom flask equipped with a magnetic stir bar was added quinoline *N*-oxide (100 mg, 0.69 mmol) and dry EA (1.4 ml), followed by ammonia (120 μl, 7.0 M in MeOH, 0.83 mmol) and DBU (210 mg, 1.4 mmol). The resulting solution is cooled to -20 °C, followed by the dropwise addition of Tf_2O (155 mg, 1.03 mmol). The reaction mixture is stirred at -20 °C for 24 h. Extra ammonia (0.12 ml, 7.0 M in MeOH, 0.83 mmol) was added to the reaction mixture, and kept stirring at -20 °C for a further 12 h, then warmed to room temperature and stirred for 12 h. The reaction is complete as indicated by TLC. The reaction is quenched with saturated sodium bicarbonate solution (30 ml) and extracted with CH_2Cl_2 (50 ml × 3). The combined organic phases are dried over Na_2SO_4, and concentrated in vacuo to give the crude product. Purification by chromatography (Hex:EA = 1:4) furnishes the desired product (60 mg, 61% yield) as a white solid. The spectroscopic data are consistent with previously reported.[7] TLC: R_f = 0.23 (DCM:MeOH = 20:1). ^{1}H NMR (600 MHz, DMSO-d_6) δ 7.87 (d, J = 9.0 Hz, 1H), 7.61 (d, J = 7.8 Hz, 1H), 7.43-7.47 (m, 2H), 7.12-7.15 (m, 1H), 6.74 (d, J = 9.0 Hz, 1H), 6.40 (s, 2H).

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{60}{99} \times 1 = 61\%$$

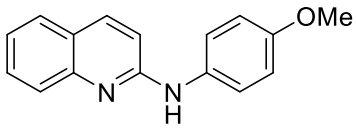


5i

N-phenylquinolin-2-amine (5i). Following **GP 2**, using quinoline *N*-oxide (94 mg, 0.65 mmol),

the title compound was obtained (84 mg, 59% yield) as a white solid. The spectroscopic data are consistent with previously reported.[7] TLC: R_f = 0.66 (PE:EA =5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (d, J = 9.0 Hz, 1H), 7.78 (d, J = 8.4 Hz, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.55-7.59 (m, 3H), 7.36 (t, J = 7.8 Hz, 2H), 7.27-7.30 (m, 1H), 7.08 (t, J = 7.8 Hz, 1H), 6.97 (d, J = 9.0 Hz, 1H), 6.93 (s, 1H).

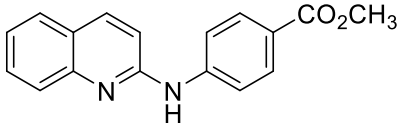
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{84}{143} \times 1 = 59\%$$



5j

N-(4-methoxyphenyl)quinolin-2-amine (5j). Following **GP 2**, using quinoline *N*-oxide (96 mg, 0.66 mmol), the title compound was obtained (128 mg, 77% yield) as a white solid. The spectroscopic data are consistent with previously reported.[7] TLC: R_f = 0.73 (PE:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, J = 9.0 Hz, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.62 (dd, J = 1.2 Hz, 8.4 Hz, 1H), 7.55-7.58 (m, 1H), 7.42 (dt, J = 3.0 Hz, 10.2 Hz, 2H), 7.25-7.27 (m, 1H), 6.93 (dt, J = 3.6 Hz, 10.2 Hz, 2H), 6.86 (d, J = 9.0 Hz, 1H), 6.75 (s, 1H), 3.82 (s, 3H).

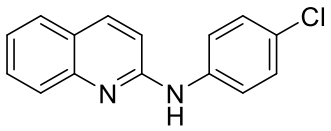
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{128}{166} \times 1 = 77\%$$



5k

Methyl 4-(quinolin-2-ylamino)benzoate (5k). Following **GP 2**, using quinoline *N*-oxide (100 mg, 0.69 mmol), the title compound was obtained (23 mg, 12% yield) as a yellow oil. TLC: R_f = 0.55 (Hex:EA = 5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.16 (d, J = 8.4 Hz, 1H), 8.11 (d, J = 9.0 Hz, 2H), 8.03 (d, J = 8.4 Hz, 1H), 7.80 (d, J = 8.4 Hz, 1H), 7.73-7.76 (m, 1H), 7.66 (d, J = 8.4 Hz, 2H), 7.57 (t, J = 7.2 Hz, 1H), 7.21 (d, J = 8.4 Hz, 1H), 3.92 (s, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 166.0, 150.9, 146.8, 141.9, 139.5, 131.03, 130.98, 130.7, 129.6, 129.3, 127.7, 127.6, 127.1, 118.1, 52.6. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{15}N_2O_2$ 279.1128; found 279.1127.

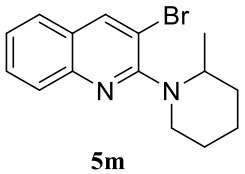
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{23}{192} \times 1 = 12\%$$



5l

N-(4-chlorophenyl)quinolin-2-amine (5l). Following **GP 2**, using quinoline *N*-oxide (92 mg, 0.63 mmol), the title compound was obtained (71 mg, 44% yield) as a white solid. The spectroscopic data are consistent with previously reported.[7] TLC: R_f = 0.51 (Hex:EA = 5:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (d, J = 9.0 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.65 (dd, J = 6.0 Hz, 7.8 Hz, 1H), 7.58-7.61 (m, 3H), 7.30-7.32 (m, 3H), 6.88 (d, J = 9.0 Hz, 1H), 6.77 (s, 1H).

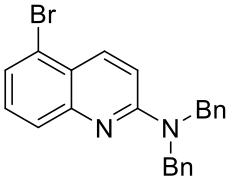
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{71}{161} \times 1 = 44\%$$



5m

3-Bromo-2-(2-methylpiperidin-1-yl)quinoline (5m). Following **GP 2**, using 3-bromoquinoline *N*-oxide (100 mg, 0.45 mmol), the title compound was obtained (64 mg, 47% yield) as a colorless oil. TLC: R_f = 0.41 (Hex:EA = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (s, 1H), 7.83 (d, J = 9.0 Hz, 1H), 7.59-7.61 (m, 2H), 7.36 (t, J = 7.8 Hz, 1H), 4.15 (m, 1H), 3.37-3.42 (m, 1H), 3.28-3.30 (m, 1H), 1.89-1.94 (m, 1H), 1.74-1.79 (m, 3H),1.52-1.62 (m, 2H), 1.16 (d, J = 6.6 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 158.6, 146.1, 141.2, 129.5, 127.8, 126.4, 126.3, 124.8, 114.5, 52.2, 47.0, 31.9, 26.0, 21.0, 16.7. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{18}N_2Br$ 305.0648; found 305.0644.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{64}{136} \times 1 = 47\%$$

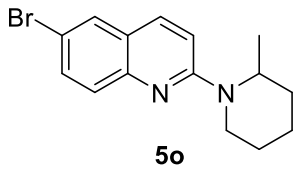


5n

N,N-dibenzyl-5-bromoquinolin-2-amine (5n). Following **GP 2**, using 5-bromoquinoline *N*-oxide (100 mg, 0.45 mmol), the title compound was obtained (165 mg, 92% yield) as a white solid. TLC: R_f = 0.63 (Hex:EA = 30:1). Melting point: 127.3-127.8 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ

8.17 (d, *J* = 9.6 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.43 (d, *J* = 7.2 Hz, 1H), 7.35 (t, *J* = 8.4 Hz, 1H), 7.23-7.31 (m, 10H), 6.86 (d, *J* = 9.0 Hz, 1H), 4.93 (s, 4H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 157.4, 149.2, 138.3, 137.0, 129.9, 128.8, 127.4, 127.3, 126.6, 125.7, 122.4, 121.8, 110.4, 50.9. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{20}BrN_2$ 403.0804; found 403.0814.

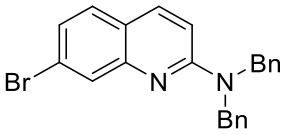
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{165}{180} \times 1 = 92\%$$



5o

6-Bromo-2-(2-methylpiperidin-1-yl)quinoline (5o). Following **GP 2**, using 6-bromoquinoline *N*-oxide (100 mg, 0.45 mmol), the title compound was obtained (90 mg, 66% yield) as a yellow oil. TLC: R_f = 0.69 (PE:EA = 20:1). ^1H NMR (600 MHz, $CDCl_3$) *δ* 7.73 (d, *J* = 9.6 Hz, 1H), 7.68 (s, 1H), 7.52-7.56 (m, 2H), 6.96 (d, *J* = 9.6 Hz, 1H), 4.78 (quin, *J* = 6.0 Hz, 1H), 4.46 (d, *J* = 12.6 Hz, 1H), 3.02 (td, *J* = 2.4 Hz, 13.2 Hz, 1H), 1.54-1.84, (m, 6H), 1.21 (d, *J* = 7.2 Hz, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 157.4, 136.3, 132.5, 129.2, 128.3, 124.0, 114.5, 114.4, 110.6, 47.1, 39.4, 30.7, 26.0, 19.1, 14.8. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{15}H_{18}BrN_2$ 305.0648; found 305.0644.

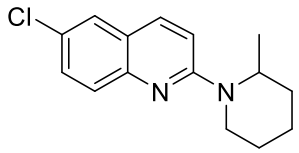
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{90}{136} \times 1 = 66\%$$



5p

N,N-dibenzyl-7-bromoquinolin-2-amine (5p). Following **GP 2**, using 7-bromoquinoline *N*-oxide (97 mg, 0.43 mmol), the title compound was obtained (155 mg, 89% yield) as a white solid. TLC: R_f = 0.63 (Hex:EA = 30:1). Melting point: 100.3-100.4 °C. ^1H NMR (600 MHz, $CDCl_3$) *δ* 7.90 (s, 1H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.23-7.32 (m, 11H), 6.79 (d, *J* = 9.0 Hz, 1H), 4.91 (s, 4H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 157.5, 149.1, 138.3, 137.5, 129.1, 128.8, 128.5, 127.4, 127.3, 125.3, 123.7, 121.7, 109.6, 50.9. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{20}BrN_2$ 403.0804; found 403.0812.

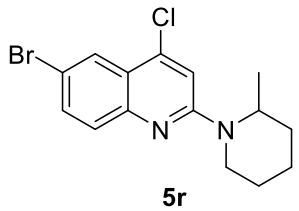
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{155}{175} \times 1 = 89\%$$



5q

6-Chloro-2-(2-methylpiperidin-1-yl)quinoline (5q). Following **GP 2**, using 6-chloroquinoline *N*-oxide (96 mg, 0.53 mmol), the title compound was obtained (99 mg, 71% yield) as a yellow oil. TLC: R_f = 0.67 (PE:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, J = 9.0 Hz, 1H), 7.58 (d, J = 9.0 Hz, 1H), 7.52 (d, J = 2.4 Hz, 1H), 7.42 (dd, J = 2.4 Hz, 9.0 Hz, 1H), 6.96 (d, J = 9.0 Hz, 1H), 4.78 (quin, J = 6.0 Hz, 1H), 4.45 (d, J = 13.2 Hz, 1H), 3.01 (td, J = 3.0 Hz, 13.2 Hz, 1H), 1.51-1.84 (m, 6H), 1.20 (d, J = 6.6 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 157.4, 146.8, 136.4, 130.0, 128.1, 126.8, 125.9 123.3, 110.6, 47.1, 39.4, 30.7, 26.0, 19.1, 14.8. HRMS (+ESI-TOF) *m/z*: [M + H]$^+$ calcd for $C_{15}H_{18}ClN_2$ 261.1153; found 261.1149.

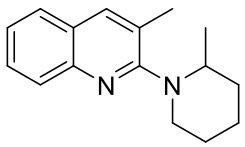
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{99}{139} \times 1 = 71\%$$



5r

6-Bromo-4-chloro-2-(2-methylpiperidin-1-yl)quinoline (5r). Following **GP 2**, using 6-bromo-4-chloroquinoline *N*-oxide (99 mg, 0.38 mmol), the title compound was obtained (114 mg, 88% yield) as a yellow oil. TLC: R_f = 0.67 (PE:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (d, J = 2.4 Hz, 1H), 7.58 (dd, J = 2.4 Hz, 9.0 Hz, 1H), 7.50 (d, J = 9.0 Hz, 1H), 7.06 (s, 1H), 4.73 (quin, J = 6.0 Hz, 1H), 4.39 (d, J = 13.2 Hz, 1H), 3.01 (td, J = 3.0 Hz, 13.2 Hz, 1H), 1.51-1.82 (m, 6H), 1.21 (d, J = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 157.0, 147.7, 142.0, 133.6, 128.6, 126.2, 122.2, 115.5, 110.3, 47.3, 39.6, 30.6, 25.9, 19.0, 14.9. HRMS (+ESI-TOF) *m/z*: [M + H]$^+$ calcd for $C_{15}H_{17}BrClN_2$ 339.0258; found 339.0266.

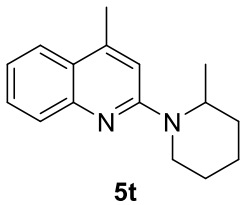
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{114}{130} \times 1 = 88\%$$



5s

3-Methyl-2-(2-methylpiperidin-1-yl)quinoline (5s). Following **GP 2**, using 3-methylquinoline *N*-oxide (95 mg, 0.60 mmol), the title compound was obtained (122 mg, 85% yield) as a yellow oil. TLC: R_f = 0.62 (PE:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, J = 8.4 Hz, 1H), 7.63 (s, 1H), 7.47 (d, J = 7.8 Hz, 1H), 7.39-7.41 (m, 1H), 7.18-7.21 (m, 1H), 3.63-3.68 (m, 1H), 3.10 (quin, J = 6.6 Hz, 1H), 2.91 (quin, J = 6.6 Hz, 1H), 2.28 (s, 3H), 1.36-1.77 (m, 6H), 0.94 (d, J = 6.6 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 162.4 146.2, 137.6, 128.1, 127.7, 127.4, 126.5, 125.9, 124.2, 52.1, 48.5, 32.9, 26.4, 22.1, 18.7, 17.7. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{16}H_{21}N_2$ 241.1699; found 241.1694.

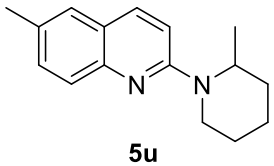
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{122}{143} \times 1 = 85\%$$



5t

4-Methyl-2-(2-methylpiperidin-1-yl)quinoline (5t). Following **GP 2**, using 4-methylquinoline *N*-oxide (95 mg, 0.60 mmol), the title compound was obtained (139 mg, 97% yield) as a yellow oil. TLC: R_f = 0.67 (PE:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.68 (d, J = 8.4 Hz, 2H), 7.47 (t, J = 6.6 Hz, 1H), 7.14-7.17 (m, 1H), 6.77 (s, 1H), 4.77 (quin, J = 4.8 Hz, 1H), 4.43 (d, J = 13.2 Hz, 1H), 2.96 (td, J = 3.0 Hz, 13.2 Hz, 1H), 2.51 (s, 3H), 1.49-1.80 (m, 6H), 1.14-1.16 (m, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 157.2, 148.2, 144.6, 129.0, 127.0, 123.3, 123.1, 121.5, 110.0, 46.8, 39.2, 30.6, 25.9, 19.3, 19.1, 14.5. HRMS (+ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{16}H_{20}N_2Na$ 263.1519; found 263.1511.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{139}{143} \times 1 = 97\%$$

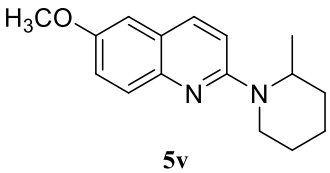


5u

6-Methyl-2-(2-methylpiperidin-1-yl)quinoline (5u). Following **GP 2**, using 6-methylquinoline *N*-oxide (99 mg, 0.62 mmol), the title compound was obtained (105 mg, 70% yield) as a yellow oil. TLC: R_f = 0.67 (PE:EA = 10:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, J = 9.6 Hz, 1H), 7.58 (d, J = 8.4 Hz, 1H), 7.31 (dd, J = 6.6 Hz, 8.4 Hz, 1H), 7.29 (s, 1H), 6.86 (d, J = 9.0 Hz, 1H), 4.72 (quin, J

= 6.0 Hz, 1H), 4.40 (d, *J* = 13.2 Hz, 1H), 2.97 (td, *J* = 3.0 Hz, 13.2 Hz, 1H), 2.39 (s, 3H), 1.48-1.79 (m, 6H), 1.15 (d, *J* = 6.6 Hz, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 157.1, 146.5, 136.6, 131.3, 131.1, 126.3, 126.2, 122.7, 109.8, 47.0, 39.4, 30.6, 25.9, 21.2, 19.1, 14.4. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{16}H_{21}N_2$ 241.1699; found 241.1694.

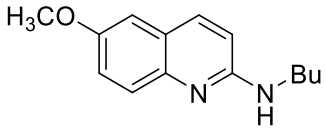
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{105}{150} \times 1 = 70\%$$



5v

6-Methoxy-2-(2-methylpiperidin-1-yl)quinoline (5v). Following **GP 2**, using 6-methoxy-quinoline *N*-oxide (100 mg, 0.57 mmol), the title compound was obtained (75 mg, 51% yield) as a yellow oil. This reaction is complete in 44 h. TLC: R_f = 0.23 (Hex:EA = 200:1). ^1H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, *J* = 9.6 Hz, 1H), 7.62 (d, *J* = 9.0 Hz, 1H), 7.20 (dd, *J* = 2.4 Hz, 9.0 Hz, 1H), 6.93-6.97 (m, 2H), 4.73 (t, *J* = 6.6 Hz, 1H), 4.39 (d, *J* = 13.2 Hz, 1H), 3.86 (s, 3H), 3.01 (td, *J* = 3.0 Hz, 13.2 Hz, 1H), 1.79-1.84 (m, 2H), 1.65-1.72 (m, 3H), 1.53-1.56 (m, 1H), 1.19 (d, *J* = 6.6 Hz, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 156.6, 154.8, 143.8, 136.4, 128.1, 123.1, 120.9, 110.3, 106.1, 55.6, 47.3, 39.6, 30.8, 26.0, 19.2, 14.4. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{16}H_{21}N_2O$ 257.1648; found 257.1644.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{75}{146} \times 1 = 51\%$$

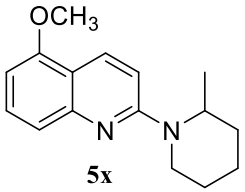


5w

N-butyl-6-methoxyquinolin-2-amine (5w). To a solution of 6-methoxyquinoline *N*-oxide (100 mg, 0.57 mmol) in dry EA (1 ml) is added butylamine (50 mg, 0.685 mmol) and DBU (174 mg, 1.14 mmol). The resulting solution is cooled to 0 °C, followed by the dropwise addition of Tf_2O (241 mg, 0.856 mmol). The reaction mixture is then warmed to room temperature and stirred for 24 h. Extra Tf_2O (80 mg, 0.285 mmol) is added to the reaction mixture, and the reaction is complete after 2 h. The reaction is quenched with saturated sodium bicarbonate solution and extracted with CH_2Cl_2 three times. The combined organic phases are dried over Na_2SO_4, and concentrated in

vacuo to give the crude product. Purification by flash column chromatography (Hex:EA = 100:1~50:1) furnishes the desired pure product (80 mg, 61% yield) as a yellow oil. The spectroscopic data are consistent with previously reported.[6] TLC: R_f = 0.21 (Hex:EA = 50:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (d, J = 9.0 Hz, 1H), 7.61 (d, J = 9.0 Hz, 1H), 7.20 (dd, J = 3.0 Hz, 9.0 Hz, 1H), 6.91 (d, J = 3.0 Hz, 1H), 6.59 (d, J = 9.0 Hz, 1H), 4.79 (s, 1H), 3.82 (s, 3H), 3.41 (q, J = 4.8 Hz, 7.2 Hz, 2H), 1.60 (quin, J = 7.2 Hz, 2H), 1.42 (sex, J = 7.8 Hz, 2H), 0.94 (t, J = 7.2 Hz, 3H).

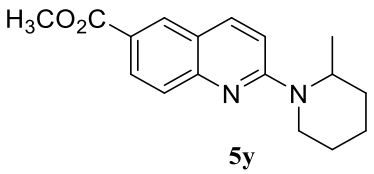
$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{80}{132} \times 1 = 61\%$$



5x

5-Methoxy-2-(2-methylpiperidin-1-yl)quinoline (5x). Following **GP 2**, using 5-methoxy-quinoline N-oxide (100 mg, 0.57 mmol), the title compound was obtained (59 mg, 40% yield) as a yellow oil. This reaction is complete in 44 h. TLC: R_f = 0.25 (Hex:EA = 100:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, J = 9.6 Hz, 1H), 7.43 (t, J = 8.4 Hz, 1H), 7.31 (d, J = 8.4 Hz, 1H), 6.92 (d, J = 9.6 Hz, 1H), 6.56 (d, J = 7.8 Hz, 1H), 4.81 (quin, J = 6.0 Hz, 1H), 4.49 (d, J = 13.2 Hz, 1H), 3.94 (s, 3H), 3.03 (td, J = 3.0 Hz, 13.2 Hz, 1H), 1.79-1.86 (m, 2H), 1.65-1.74 (m, 3H), 1.55-1.60 (m, 1H), 1.21 (d, J = 6.6 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$) δ 157.6, 155.4, 149.3, 131.8, 129.2, 119.3, 114.3, 108.4, 100.7, 55.5, 46.9, 39.3, 30.7, 25.9, 19.1, 14.5. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{16}H_{21}N_2O$ 257.1648; found 257.1642.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{59}{146} \times 1 = 40\%$$



5y

Methyl-2-(2-methylpiperidin-1-yl)quinoline-6-carboxylate (5y). Following **GP 2**, using 6-(methoxycarbonyl)quinoline *N*-oxide (100 mg, 0.49 mmol), the title compound was obtained (30 mg, 21% yield) as a colorless oil. TLC: R_f = 0.22 (Hex:EA = 100:1). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (d, J = 1.8 Hz, 1H), 8.09 (dd, J = 1.8 Hz, 8.4 Hz, 1H), 7.88 (d, J = 9.0 Hz, 1H), 7.63 (d, J = 9.0

Hz, 1H), 6.98 (d, J = 9.6 Hz, 1H), 4.85 (quin, J = 6.0 Hz, 1H), 4.55 (d, J = 13.2 Hz, 1H), 3.93 (s, 3H), 3.05 (td, J = 2.4 Hz, 13.2 Hz, 1H), 1.82-1.66 (m, 6H), 1.24 (d, J = 7.2 Hz, 3H). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 167.5, 158.2, 151.1, 138.3, 130.4, 129.5, 126.3, 123.0, 121.7, 110.3, 52.1, 47.1, 39.4, 30.7, 25.9, 19.1, 15.1. HRMS (+ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{17}H_{21}N_2O_2$ 285.1598; found 285.1595.

$$Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100\% = \frac{30}{139} \times 1 = 21\%$$

5. Green Chemistry Metrics Analysis

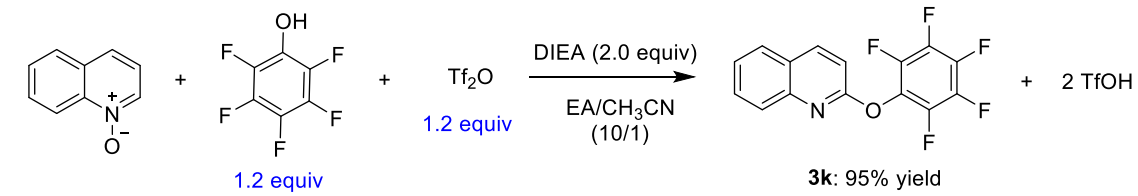
The following formula were used for calculating Atom Economy (AE), atom efficiency (AEf), carbon efficiency (CE).

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

$$\mathrm{AEf} = \mathrm{AE} \times \text{yield}\%$$

$$\mathrm{CE} = \frac{Amount\ of\ carbon\ in\ the\ product}{Total\ carbon\ present\ in\ reactants} \times 100$$

5.1 Process A (our developed method)



3k: 95% yield

1.53 g, 10.5 mmol 2.32 g, 12.6 mmol 3.56 g, 12.6 mmol 3.11 g, 10 mmol

$$\mathrm{AE} = \frac{311.21}{145.16 + 184.07 + 282.13} X\ 100 = 51$$

$$\mathrm{AEf} = 51\ \mathrm{X}\ 95\% = 48$$

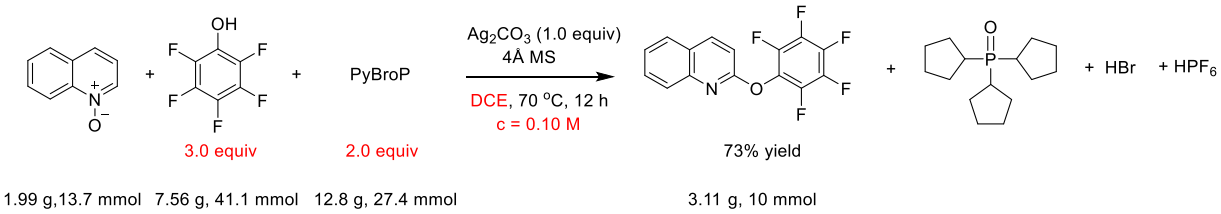
$$\mathrm{CE} = \frac{10 \times 15}{10.5 \times 9 + 12.6 \times 6 + 12.6 \times 2} X\ 100 = 77$$

Table S2 The penalty points of process A.

Parameters	Penalty
1. Yield: 95%	2.5
2. Price of reaction components (to obtain 10 mmol of end product)	

Quinoline *N*-O (1.53 g, 10.5 mmol)	0
Pentafluorophenol (2.32 g, 12.6 mmol)	0
Tf_2O (3.56 g, 12.6 mmol)	0
DIEA (2.71 g, 21 mmol)	0
3. Safety	
EtOAc (F)	5
4. Technical setup	
Common setup	0
5. Temperature/time	
Room temperature, < 1 h	0
6. Workup and purification	
Extraction with EtOAc	3
Classical chromatography	10
Penalty points total:	20.5

5.1 Process B[4]



$$AE = \frac{311.21}{145.16 + 184.07 + 466.19} X\ 100 = 39$$

$$AEf = 39\ X\ 73\% = 28$$

$$CE = \frac{10 \times 15}{13.7 \times 9 + 41.1 \times 6 + 27.4 \times 12} X\ 100 = 21$$

Table S3 The penalty points of process B.

Parameters	Penalty
1. Yield: 73%	13.5
2. Price of reaction components (to obtain 10 mmol of end product)	
Quinoline *N*-O (1.99 g, 13.7 mmol)	0
Pentafluorophenol (7.56 g, 41.1 mmol)	0
PyBroP (12.8 g, 27.4 mmol)	3
Ag_2CO_3 (3.78 g, 13.7 mmol)	0
Molecular sieves 4Å (13.7 g)	0
3. Safety	
DCE (T, F)	10
4. Technical setup	

Common setup	0
5. Temperature/time	
70 ℃, 12 h	3
6. Workup and purification	
Classical chromatography	10
Penalty points total:	39.5

6. References

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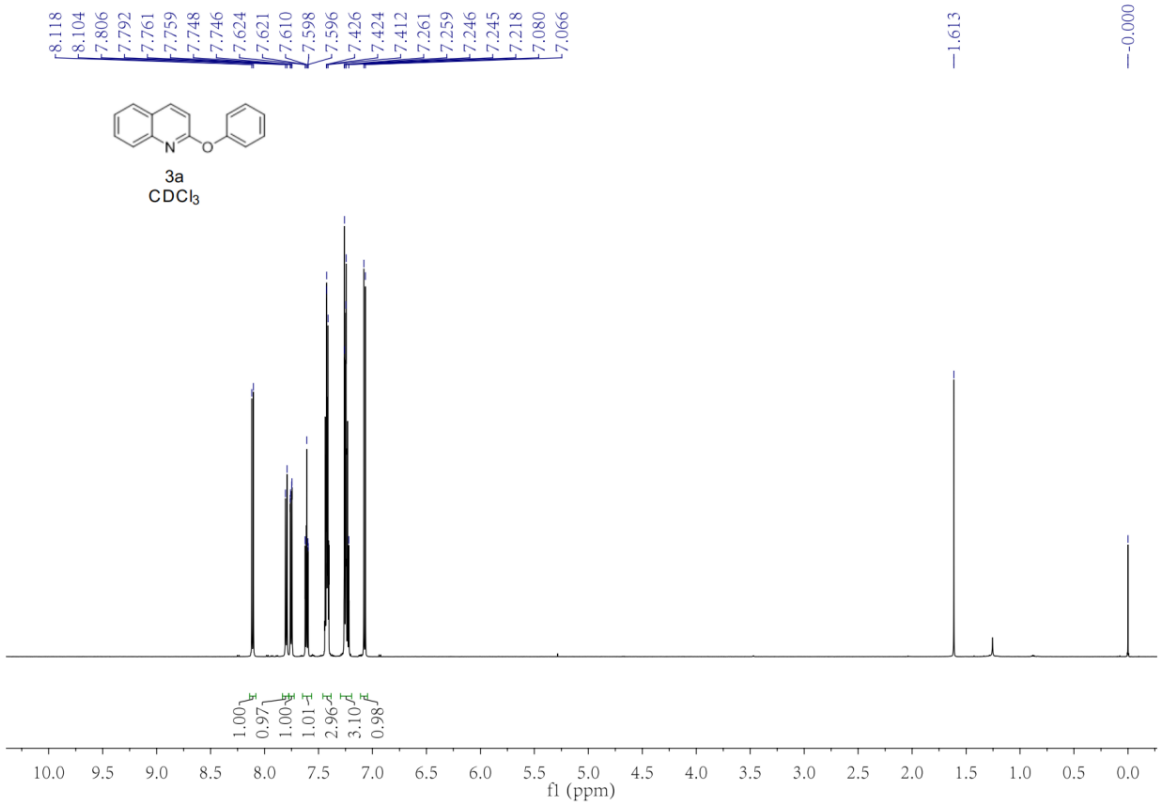
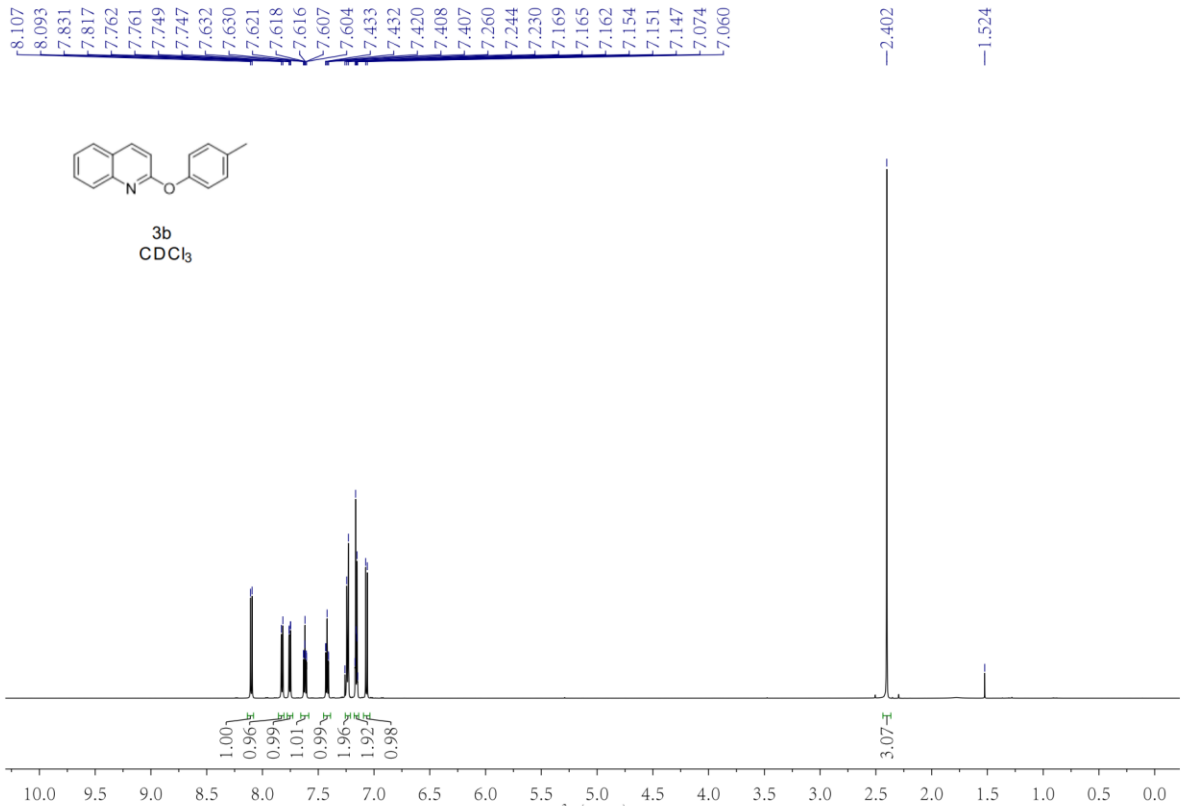
7. NMR Spectra

Spectra data are shown from the next page.


8.118
8.104
7.806
7.792
7.761
7.759
7.748
7.746
7.624
7.621
7.610
7.598
7.596
7.426
7.424
7.412
7.261
7.259
7.246
7.245
7.218
7.080
7.066
1.613
0.000
3a
CDCl3
1.00
0.97
1.00
1.01
2.96
3.10
0.98
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)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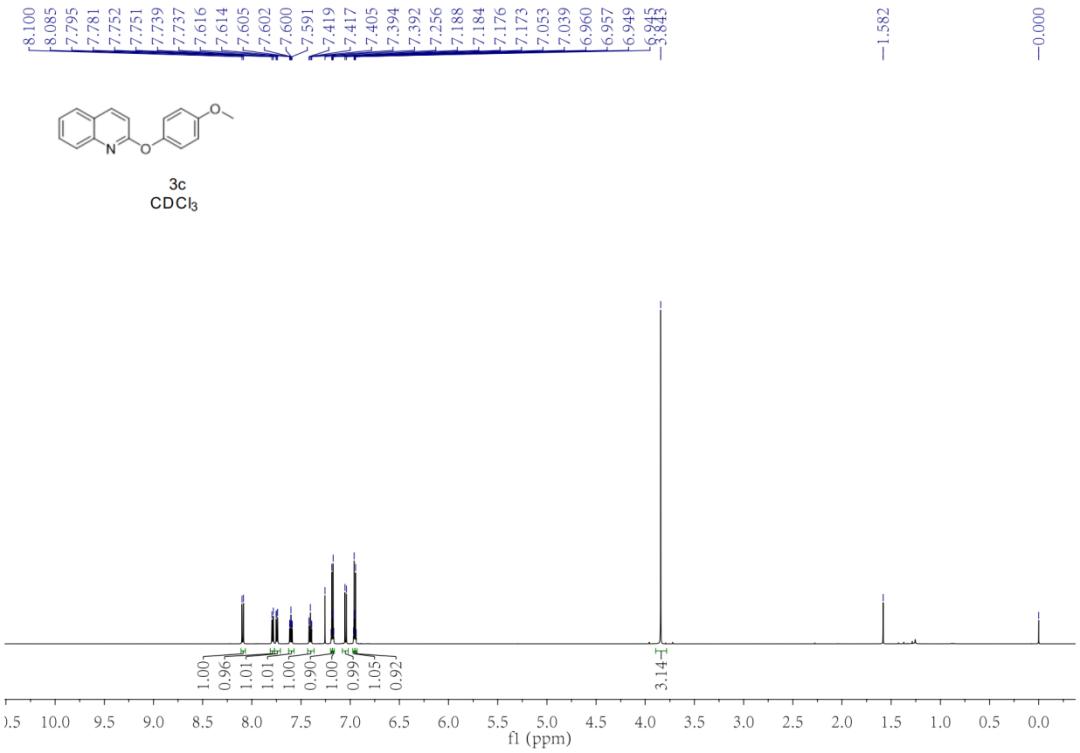
8.093
7.831
7.817
7.762
7.761
7.749
7.747
7.632
7.630
7.621
7.618
7.616
7.607
7.604
7.433
7.432
7.420
7.408
7.407
7.260
7.244
7.230
7.169
7.165
7.162
7.154
7.151
7.147
7.074
7.060
2.402
1.524
3b
CDCl3
1.00
0.96
0.99
1.01
0.99
1.96
1.92
0.98
3.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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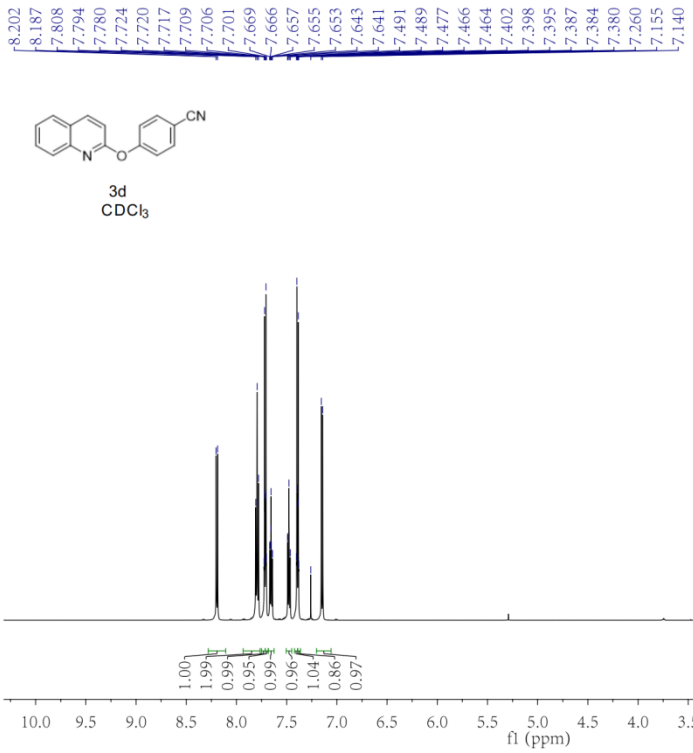
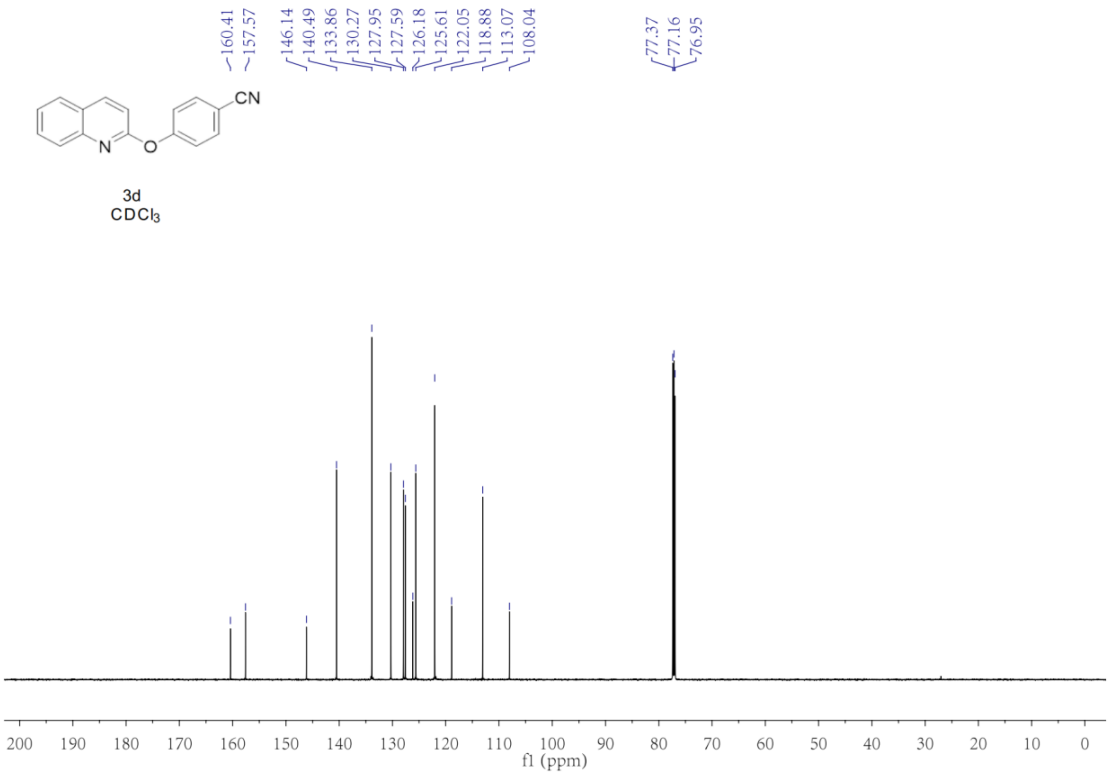
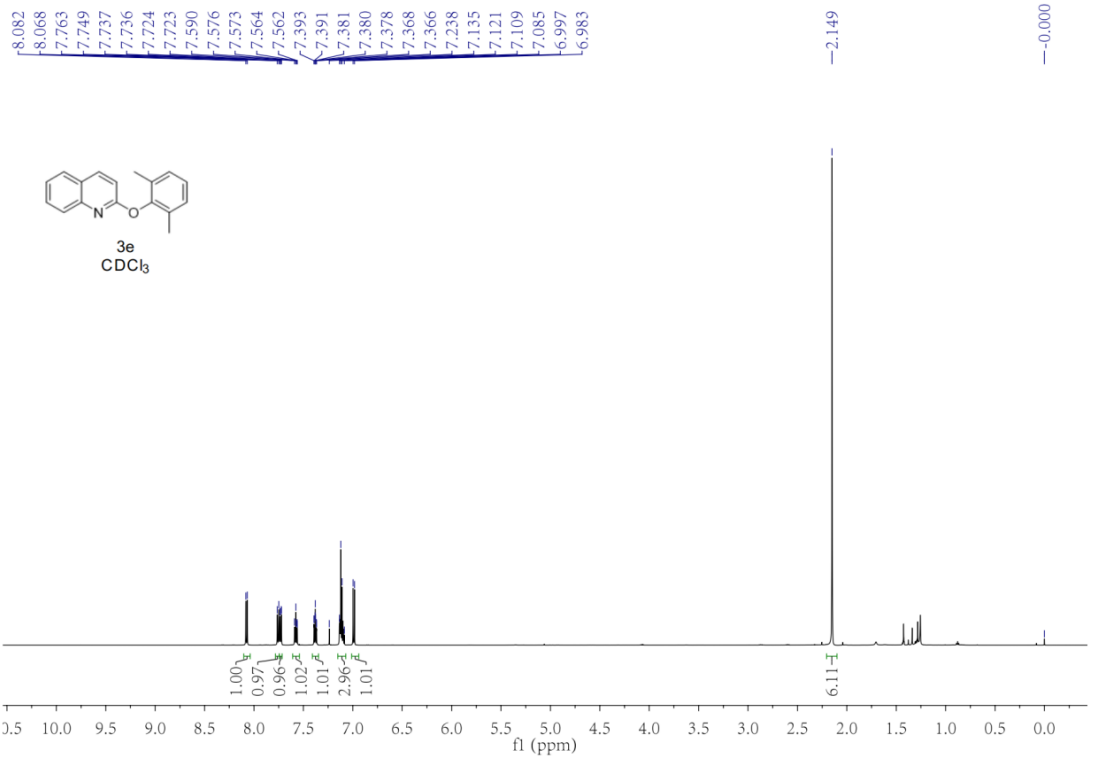
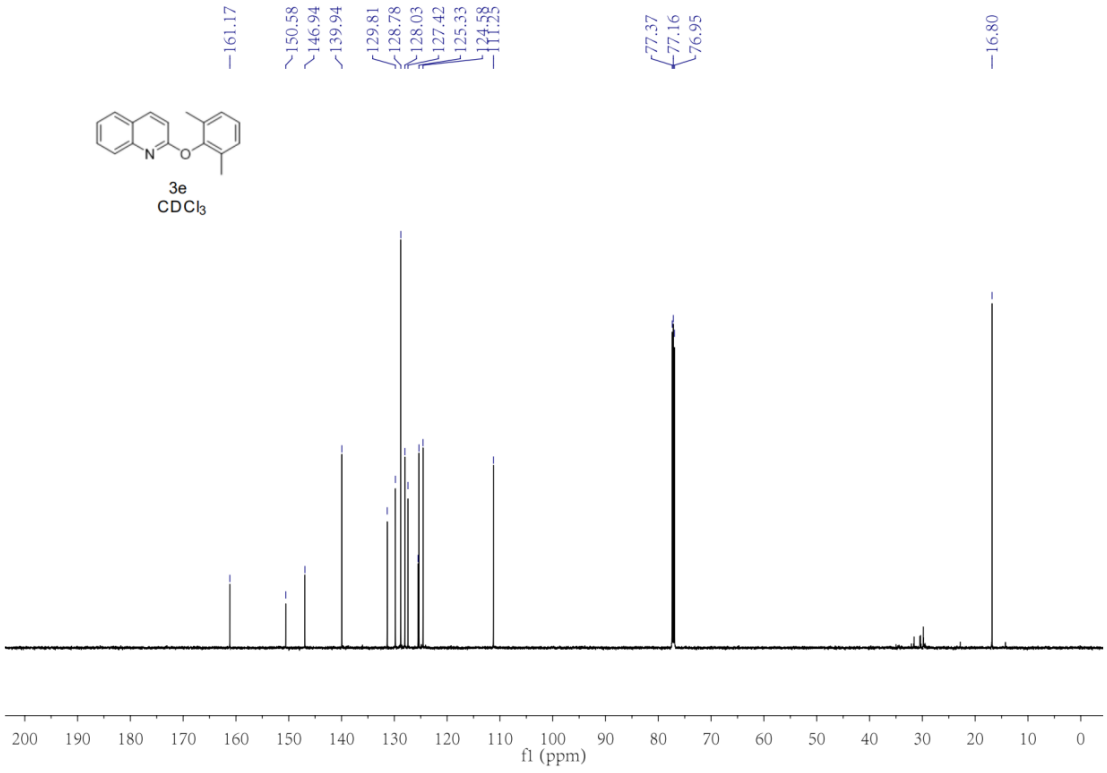
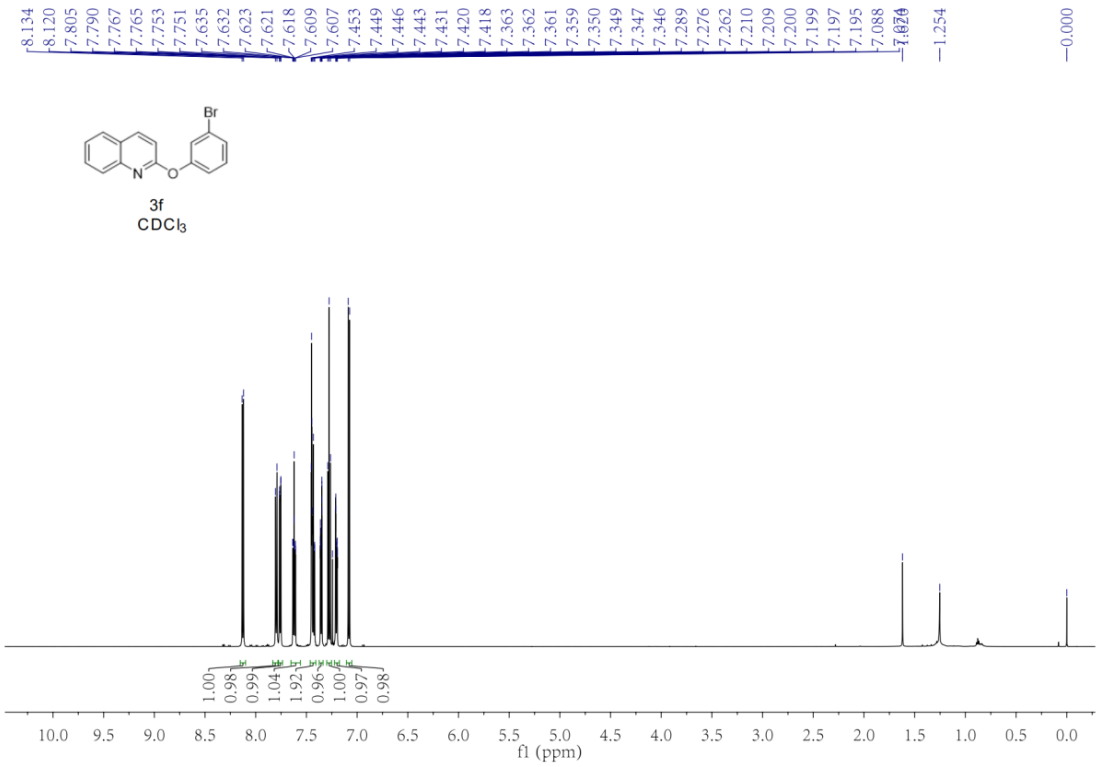
8.085
7.795
7.781
7.752
7.751
7.739
7.737
7.616
7.614
7.605
7.602
7.600
7.591
7.419
7.417
7.405
7.394
7.392
7.256
7.188
7.184
7.176
7.173
7.053
7.039
6.960
6.957
6.949
6.845
6.843
1.582
0.000
3c
CDCl3
1.00
0.96
1.01
1.01
1.00
0.90
1.00
0.99
1.05
0.92
3.14
f1 (ppm)


8.202
8.187
7.808
7.794
7.780
7.724
7.720
7.717
7.709
7.706
7.701
7.669
7.666
7.657
7.655
7.653
7.643
7.641
7.491
7.489
7.477
7.466
7.464
7.402
7.398
7.395
7.387
7.384
7.380
7.260
7.155
7.140
CN
N
O
3d
CDCl3
1.00
1.99
0.99
0.95
0.99
0.96
1.04
0.86
0.97
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)


160.41
157.57
146.14
140.49
133.86
130.27
127.95
127.59
126.18
125.61
122.05
118.88
113.07
108.04
77.37
77.16
76.95
CN
N
O
3d
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.082
8.068
7.763
7.749
7.737
7.736
7.724
7.723
7.590
7.576
7.573
7.564
7.562
7.393
7.391
7.381
7.380
7.378
7.368
7.366
7.238
7.135
7.121
7.109
7.085
6.997
6.983
2.149
-0.000
3e
CDCl3
1.00
0.97
0.96
1.02
1.01
2.96
1.01
6.11
f1 (ppm)


161.17
150.58
146.94
139.94
129.81
128.78
128.03
127.42
125.33
124.58
111.25
77.37
77.16
76.95
16.80
3e
CDCl3
f1 (ppm)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8.120
7.805
7.790
7.767
7.765
7.753
7.751
7.635
7.632
7.623
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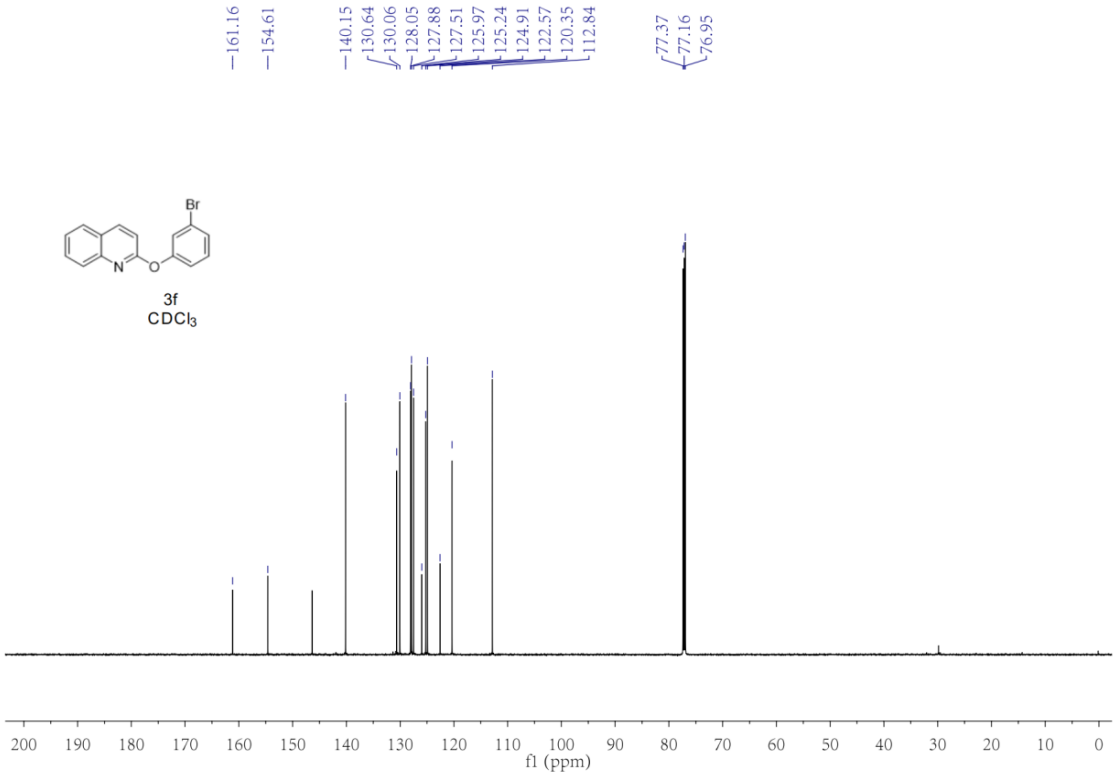
7.618
7.609
7.607
7.453
7.449
7.446
7.443
7.431
7.420
7.418
7.363
7.362
7.361
7.359
7.350
7.349
7.347
7.346
7.289
7.276
7.262
7.210
7.209
7.200
7.199
7.197
7.195
7.088
1.254
0.000
Br
N
O
3f
CDCl3
1.00
0.98
0.99
1.04
1.92
0.96
1.00
0.97
0.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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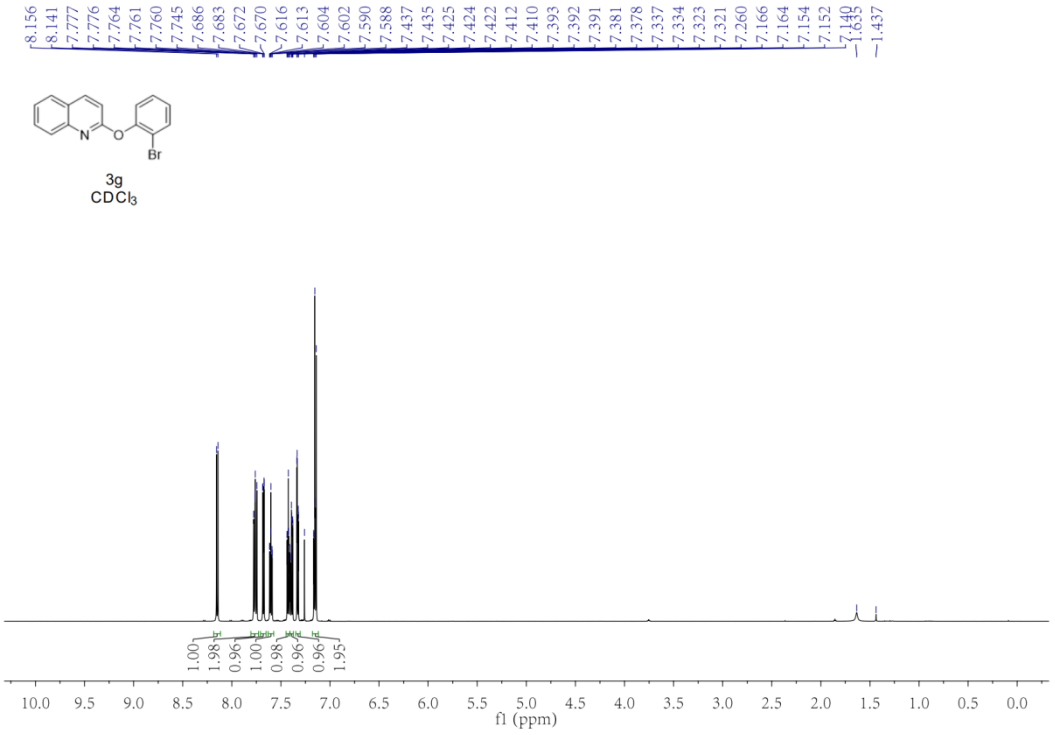
154.61
140.15
130.64
130.06
128.05
127.88
127.51
125.97
125.24
124.91
122.57
120.35
112.84
77.37
77.16
76.95
Br
N
O
3f
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.141
7.777
7.776
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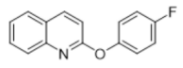
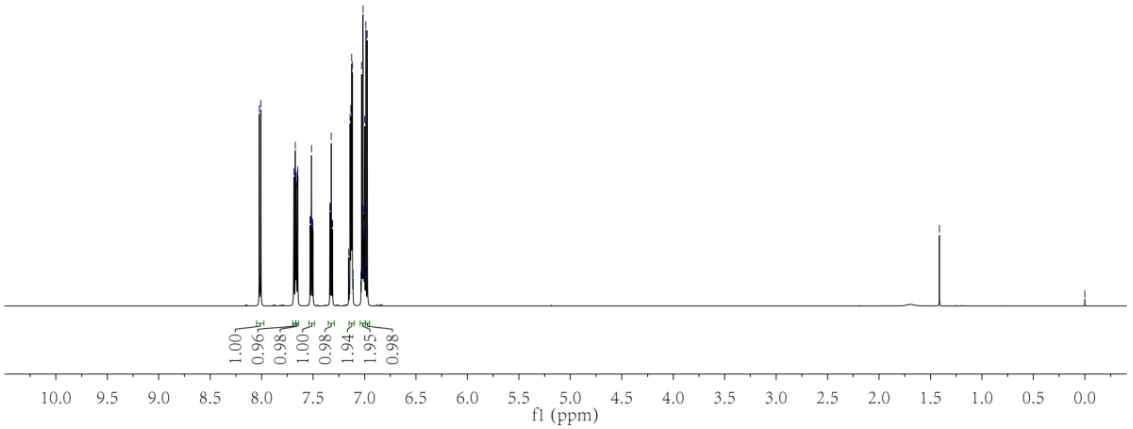
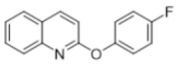
7.761
7.760
7.745
7.686
7.683
7.672
7.670
7.616
7.613
7.604
7.602
7.590
7.588
7.437
7.435
7.425
7.424
7.422
7.412
7.410
7.393
7.392
7.391
7.381
7.378
7.337
7.334
7.323
7.321
7.260
7.166
7.164
7.154
7.152
7.140
1.635
1.437
N
O
Br
3g
CDCl3
1.00
1.98
0.96
1.00
0.98
0.96
0.96
1.95
10.0
9.5
9.0
8.5
8.0
7.5
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)

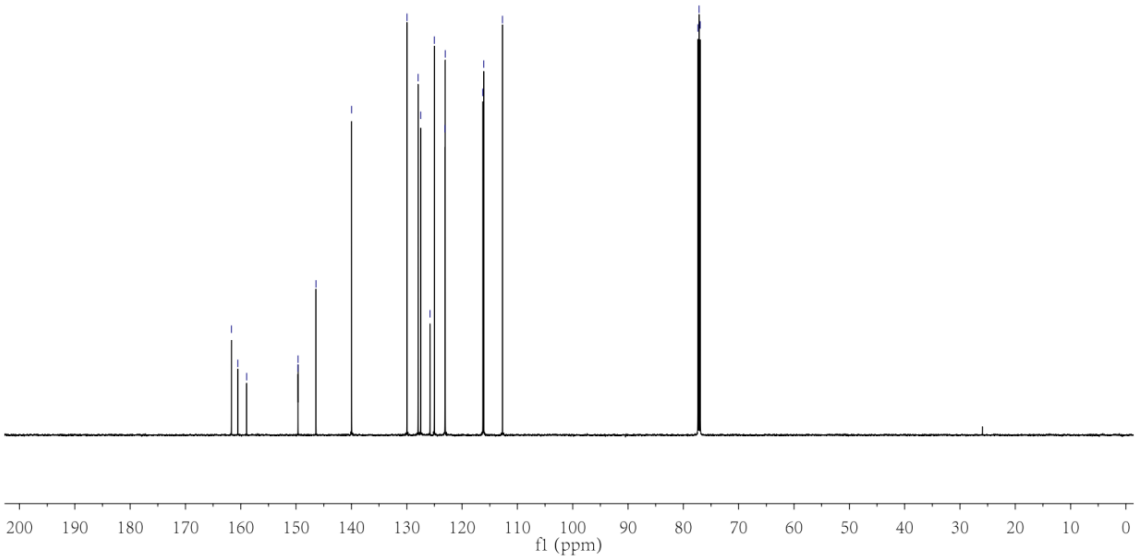


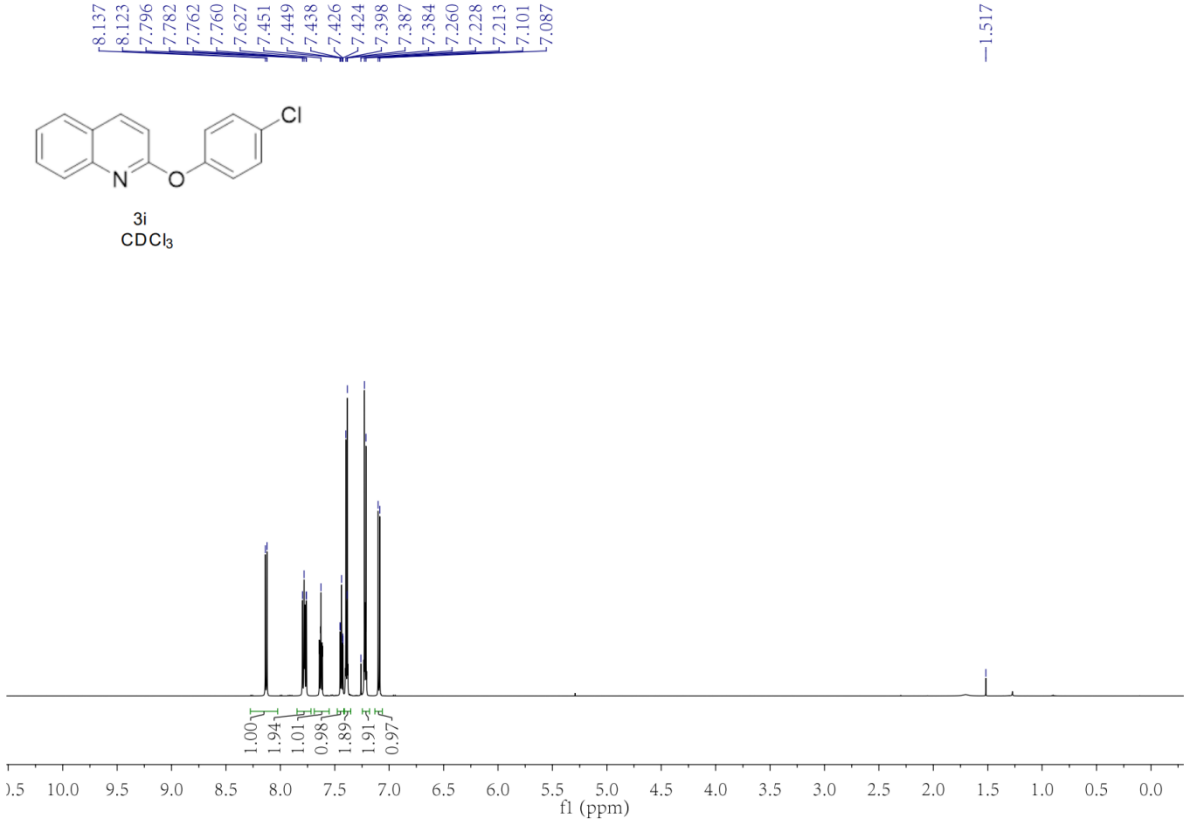
3h
$CDCl_3$





3h
$CDCl_3$

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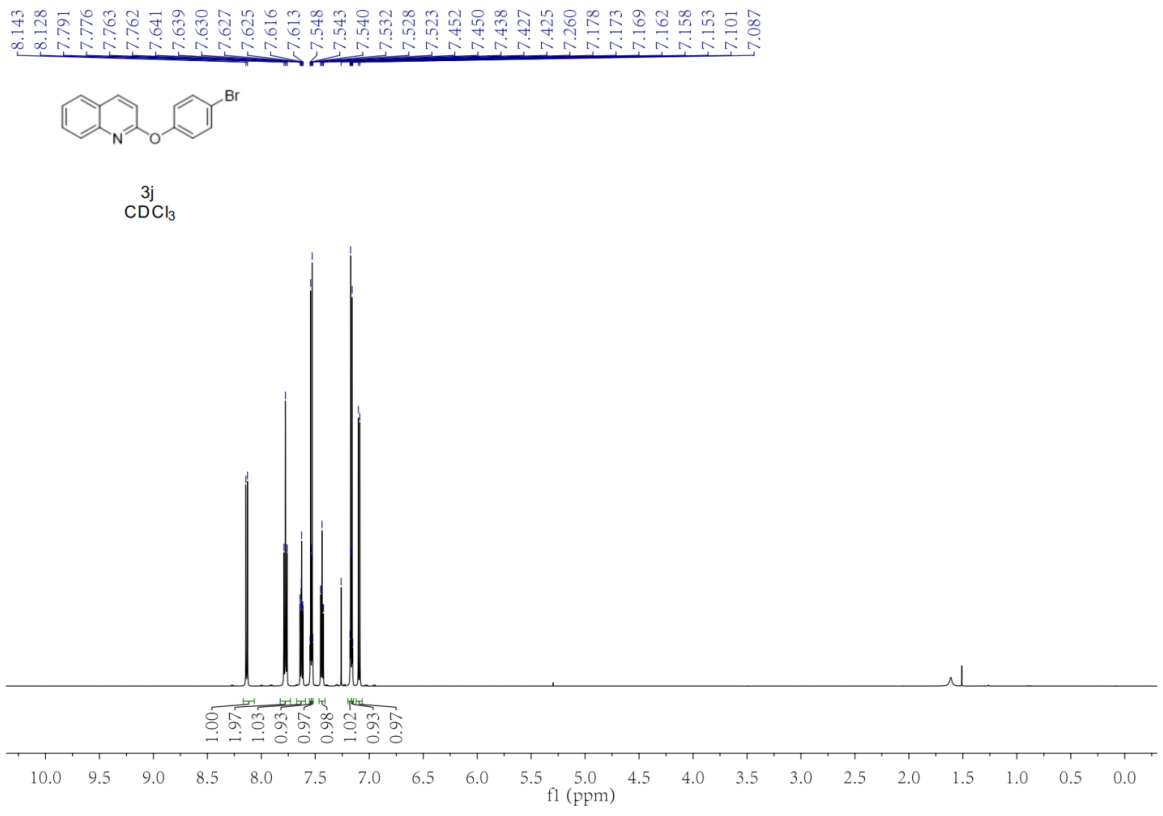
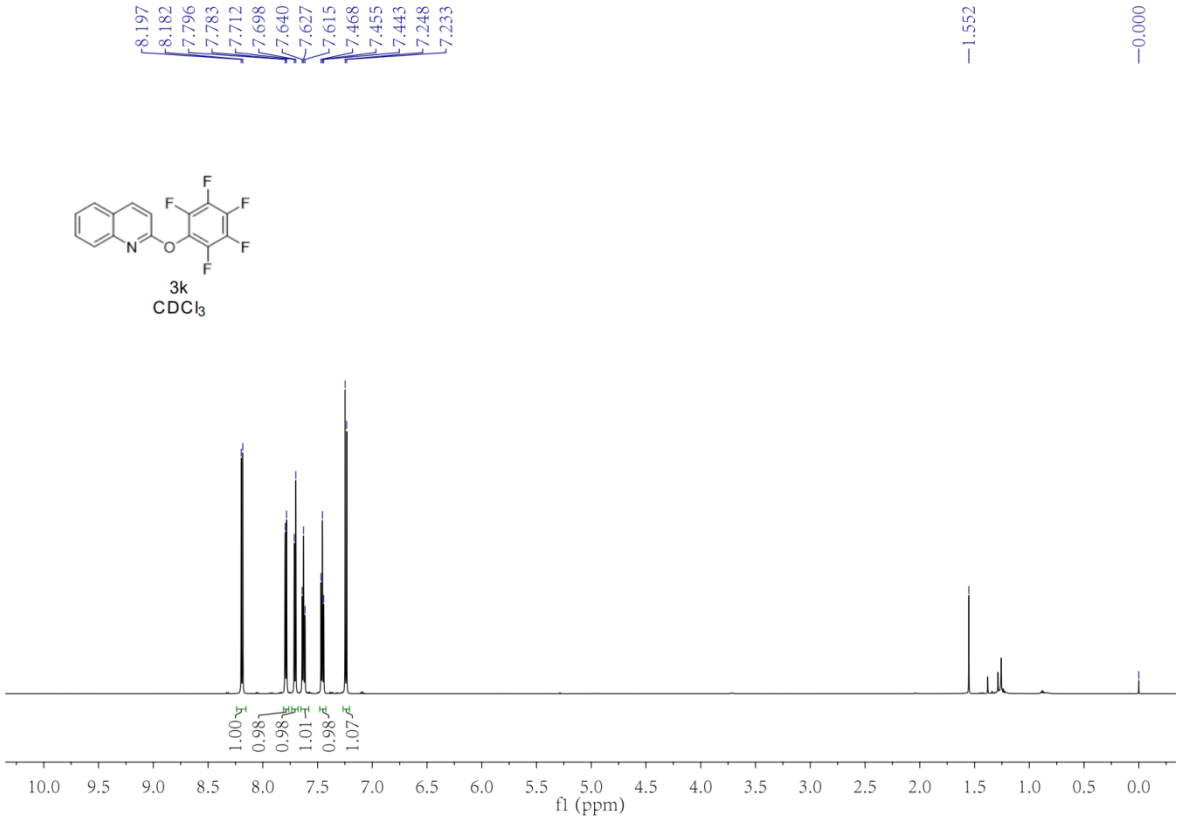
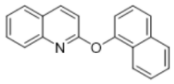
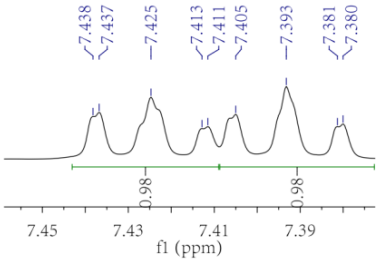
7.796
7.782
7.762
7.760
7.627
7.451
7.449
7.438
7.426
7.424
7.398
7.387
7.384
7.260
7.228
7.213
7.101
7.087
1.517
Cl
N
O
3i
CDCl3
1.00
1.94
1.01
0.98
1.89
1.91
0.97
f1 (ppm)

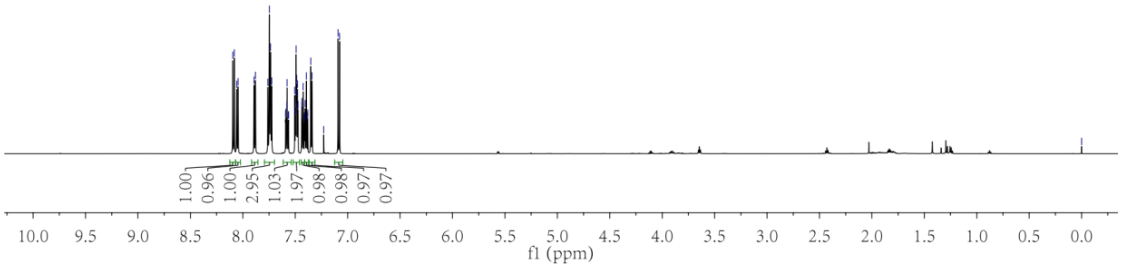

8.143
8.128
7.791
7.776
7.763
7.762
7.641
7.639
7.630
7.627
7.625
7.616
7.613
7.548
7.543
7.540
7.532
7.528
7.523
7.452
7.450
7.438
7.427
7.425
7.260
7.178
7.173
7.169
7.162
7.158
7.153
7.101
7.087
Br
N
O
3j
CDCl3
1.00
1.97
1.03
0.93
0.97
0.98
1.02
0.93
0.97
f1 (ppm)

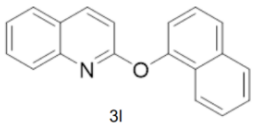

8.197
8.182
7.796
7.783
7.712
7.698
7.640
7.627
7.615
7.468
7.455
7.443
7.248
7.233
1.552
0.000
F
F
F
F
F
N
O
3k
CDCl3
1.00
0.98
0.98
1.01
0.98
1.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



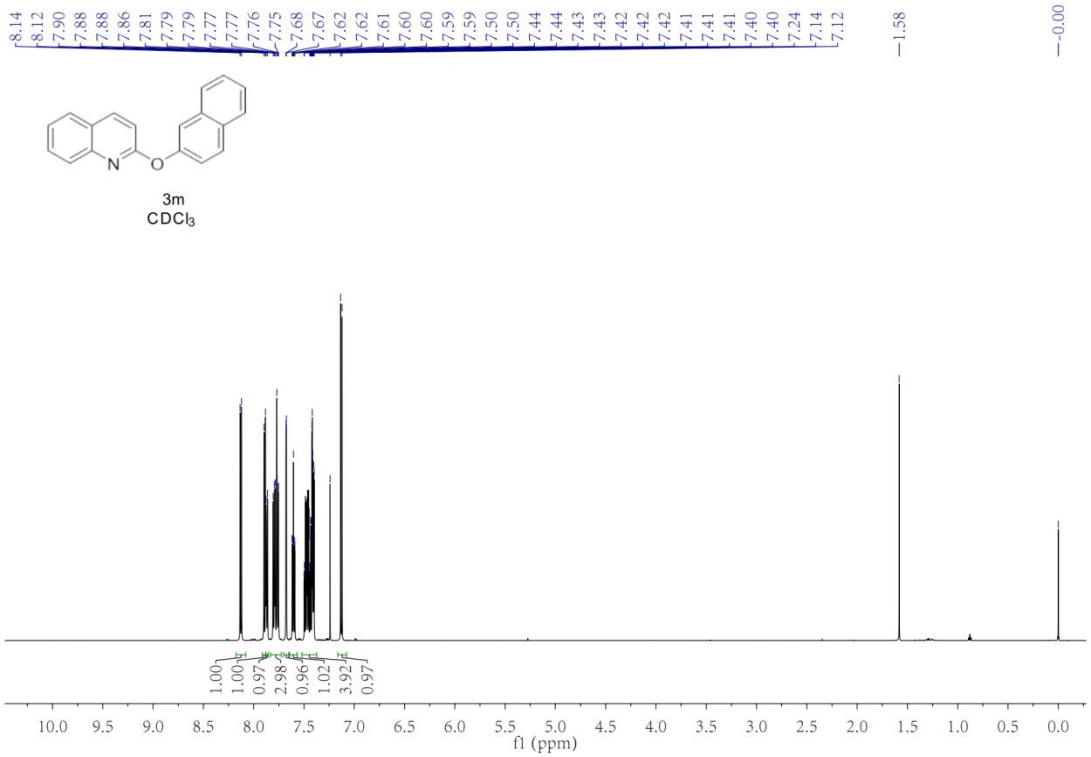
3l
$CDCl_3$







3l
$CDCl_3$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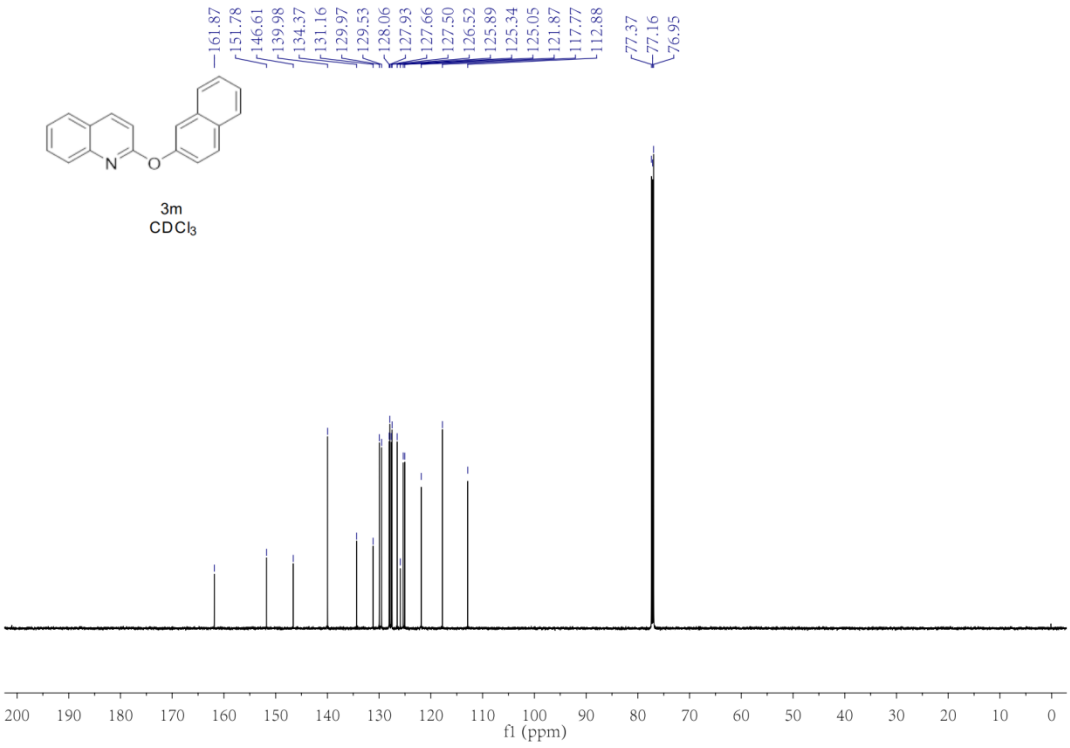
7.88
7.86
7.81
7.79
7.79
7.77
7.77
7.76
7.75
7.68
7.67
7.62
7.62
7.61
7.60
7.60
7.59
7.59
7.50
7.50
7.44
7.44
7.43
7.43
7.42
7.42
7.42
7.41
7.41
7.41
7.40
7.40
7.24
7.14
7.12
1.58
0.00
3m
CDCl3
1.00
1.00
0.97
2.98
0.96
1.02
3.92
0.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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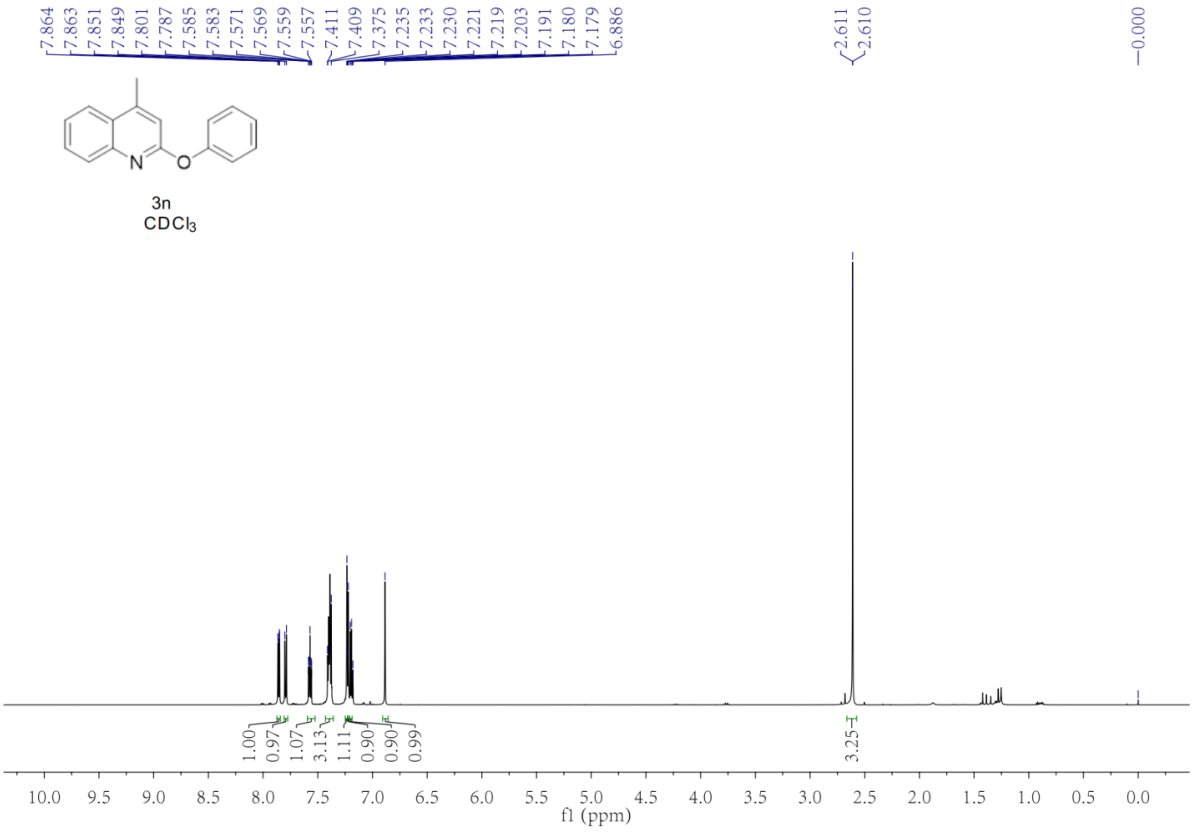
139.98
134.37
131.16
129.97
129.53
128.06
127.93
127.66
127.50
126.52
125.89
125.34
125.05
121.87
117.77
112.88
77.37
77.16
76.95
3m
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.849
7.801
7.787
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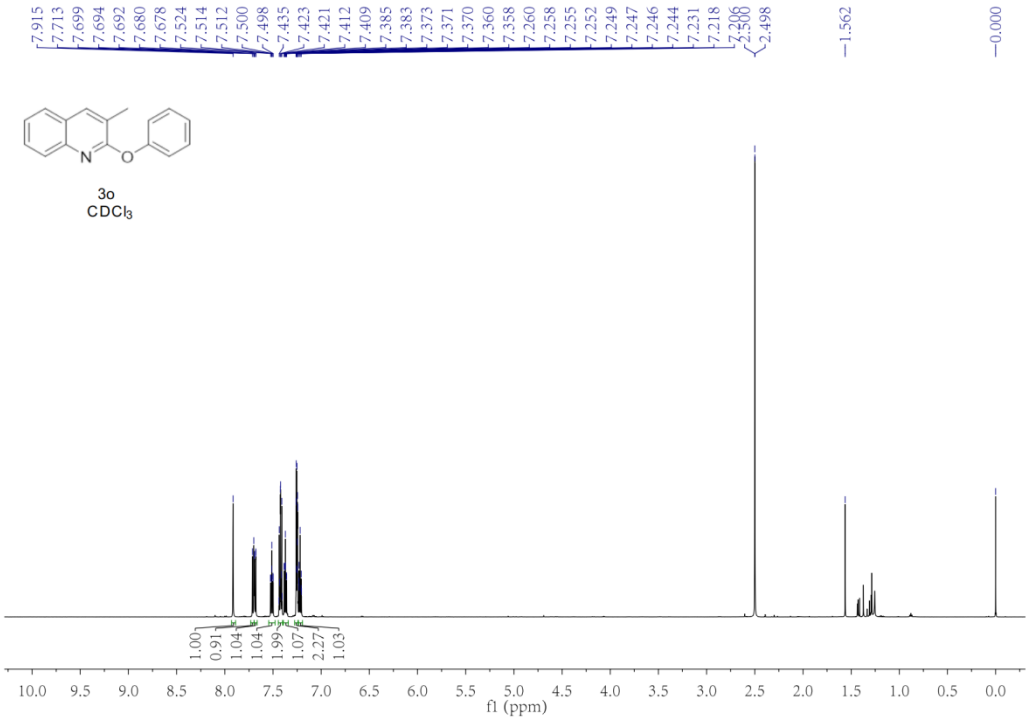
7.583
7.571
7.569
7.559
7.557
7.411
7.409
7.375
7.235
7.233
7.230
7.221
7.219
7.203
7.191
7.180
7.179
6.886
2.611
2.610
0.000
N
O
3n
CDCl3
1.00
0.97
1.07
3.13
1.11
0.90
0.90
0.99
3.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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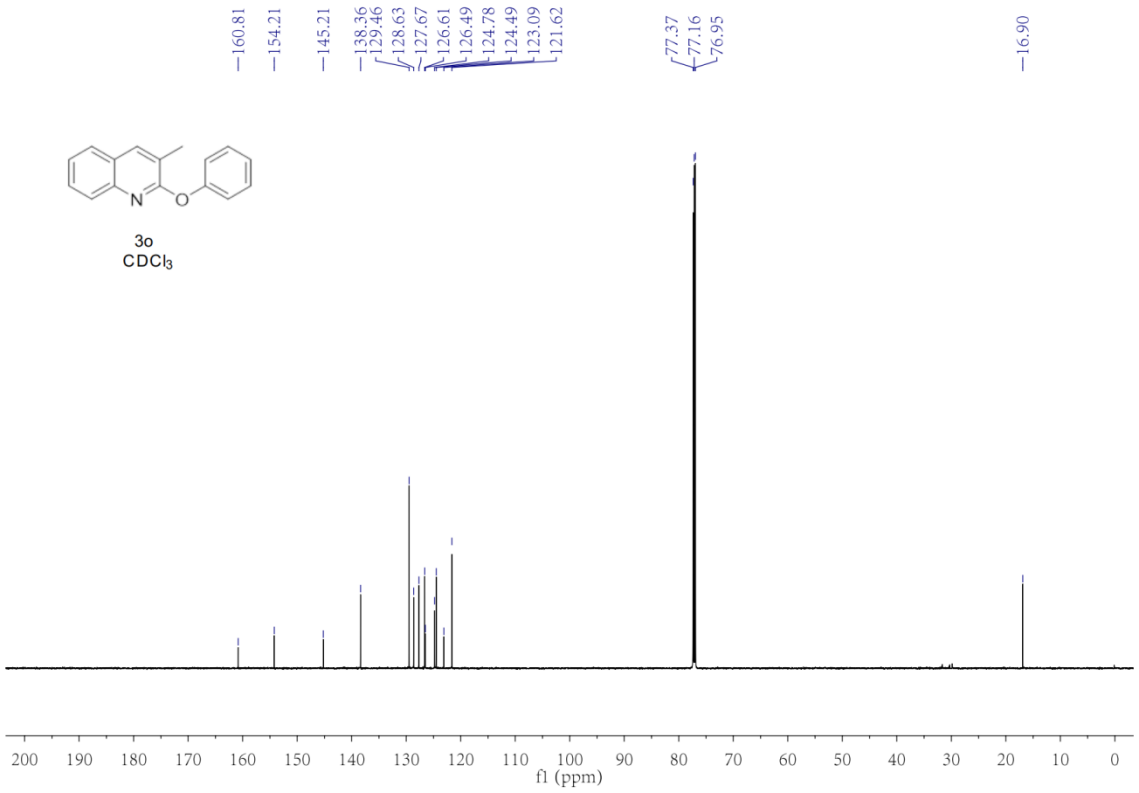
7.692
7.680
7.678
7.524
7.514
7.512
7.500
7.498
7.435
7.423
7.421
7.412
7.409
7.385
7.383
7.373
7.371
7.370
7.360
7.358
7.260
7.258
7.255
7.252
7.249
7.247
7.246
7.244
7.231
7.218
7.206
2.500
2.498
1.562
0.000
3o
CDCl3
1.00
0.91
1.04
1.04
1.99
1.07
2.27
1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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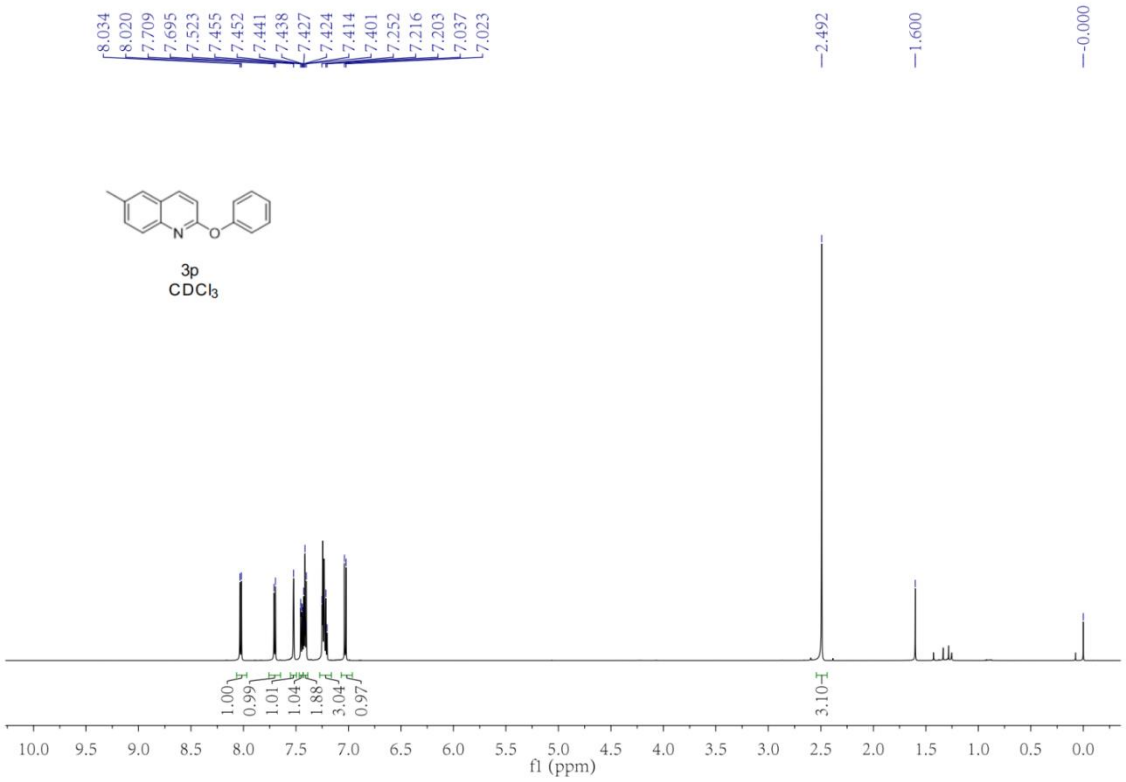
129.46
128.63
127.67
126.61
126.49
124.78
124.49
123.09
121.62
77.37
77.16
76.95
16.90
3o
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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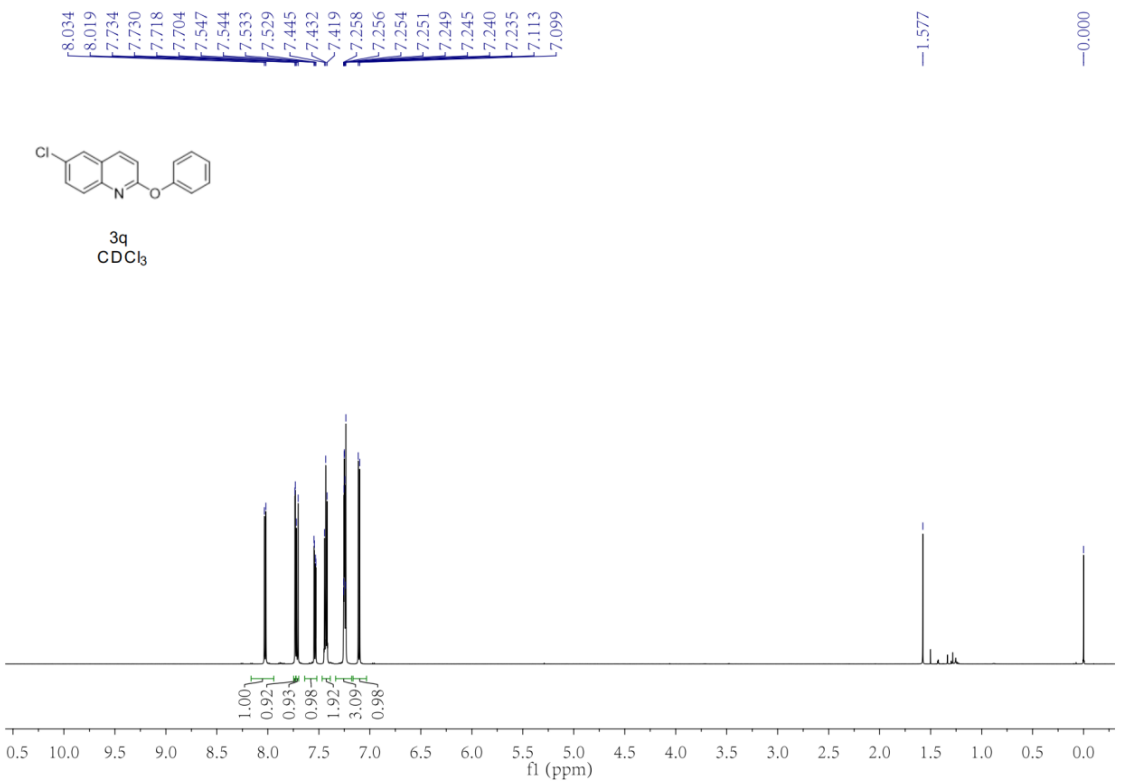
7.695
7.523
7.455
7.452
7.441
7.438
7.427
7.424
7.414
7.401
7.252
7.216
7.203
7.037
7.023
2.492
1.600
0.000
3p
CDCl3
1.00
0.99
1.01
1.04
1.88
3.04
0.97
3.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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8.019
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7.730
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7.704
7.547
7.544
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7.529
7.445
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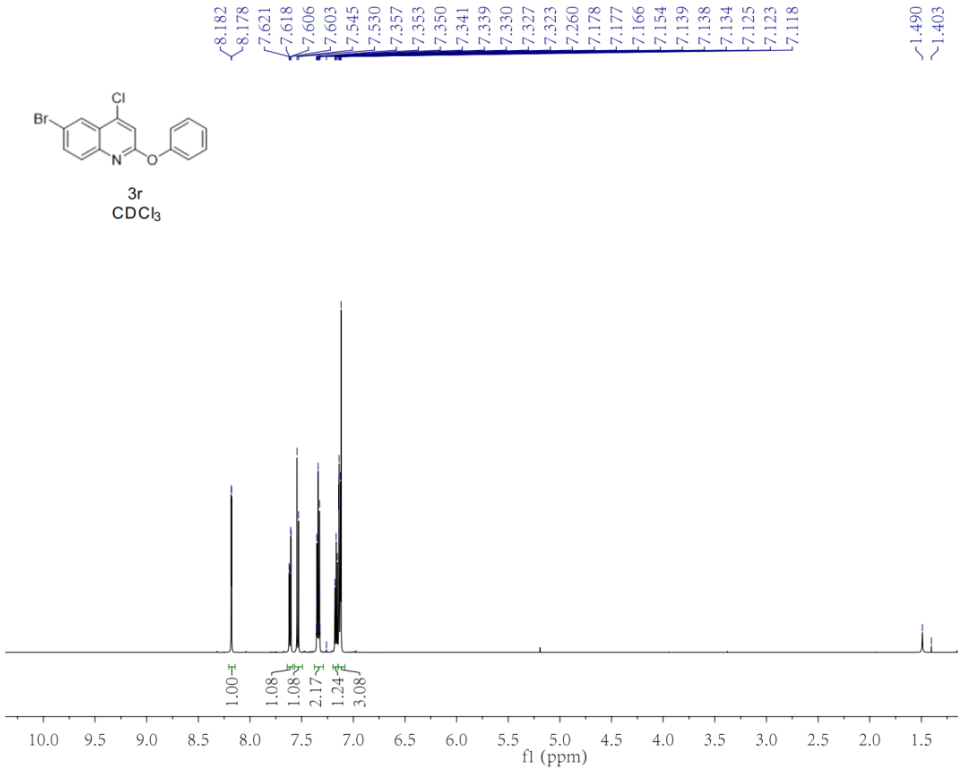
7.419
7.258
7.256
7.254
7.251
7.249
7.245
7.240
7.235
7.113
7.099
1.577
0.000
Cl
3q
CDCl3
1.00
0.92
0.93
0.98
1.92
3.09
0.98
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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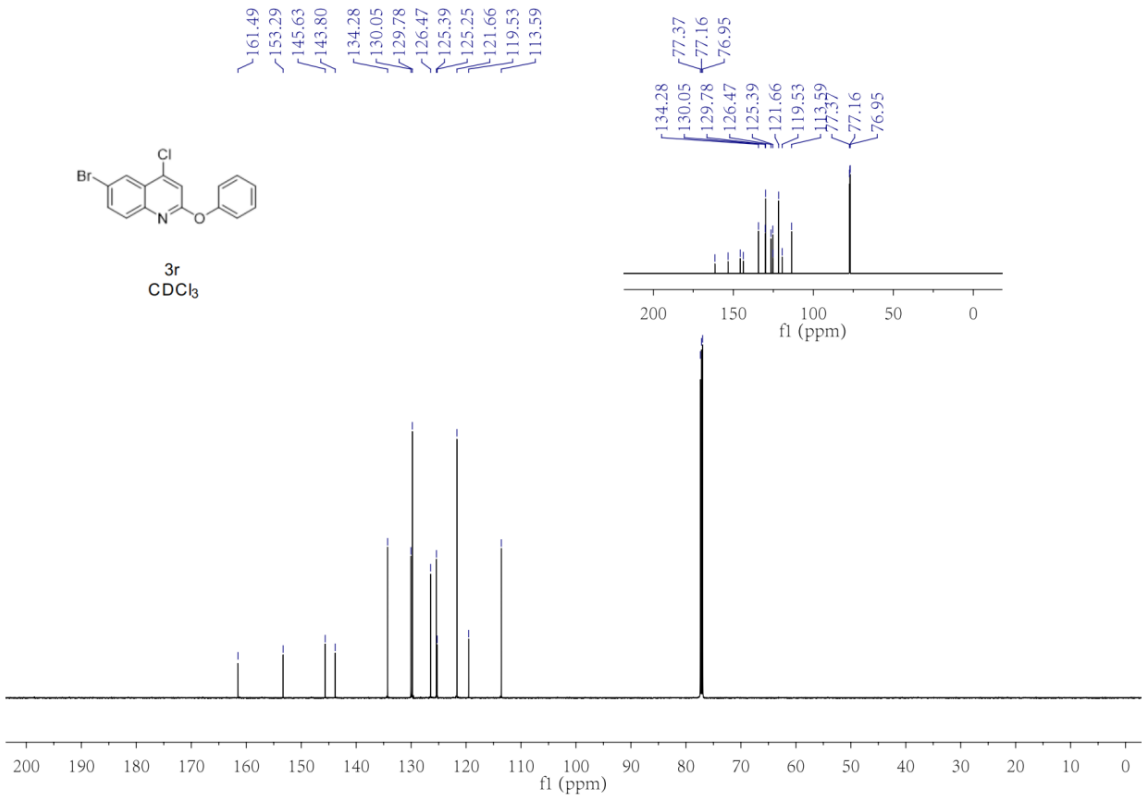
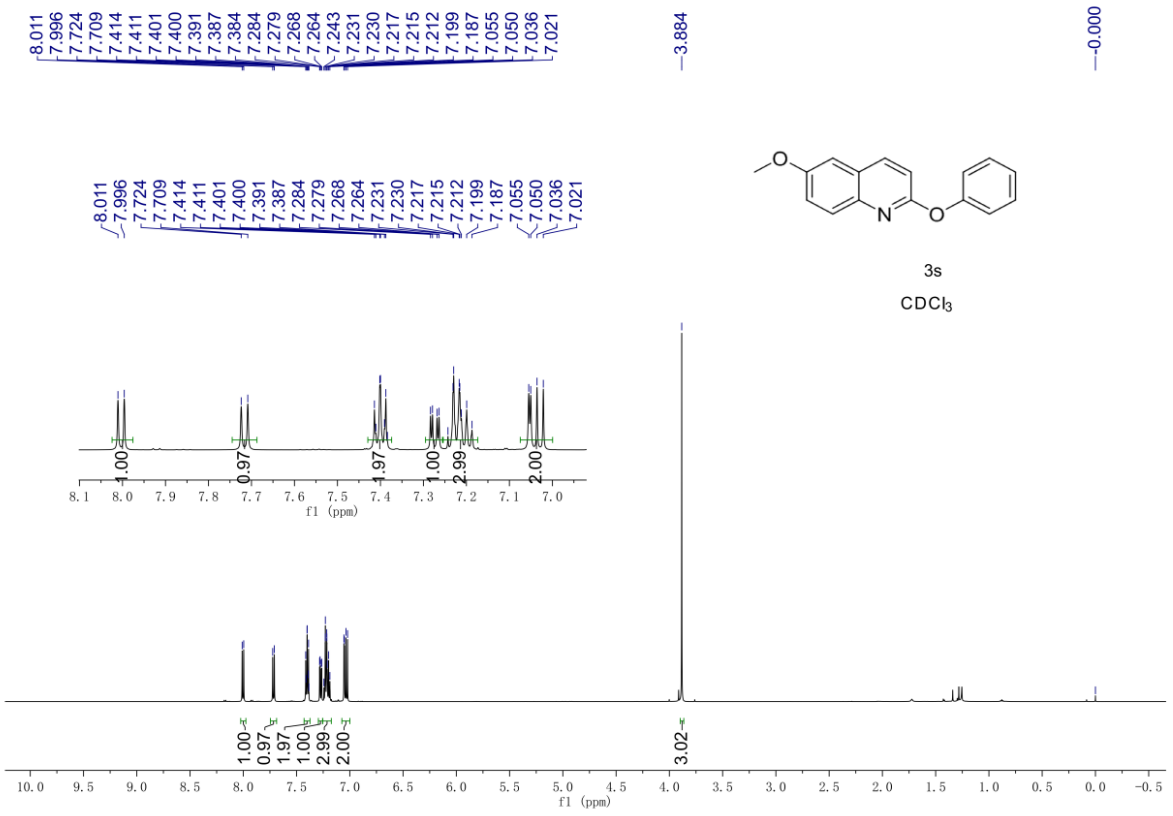
8.178
7.621
7.618
7.606
7.603
7.545
7.530
7.357
7.353
7.350
7.341
7.339
7.330
7.327
7.323
7.260
7.178
7.177
7.166
7.154
7.139
7.138
7.134
7.125
7.123
7.118
1.490
1.403
Cl
Br
N
O
3r
CDCl3
1.00
1.08
1.08
2.17
1.24
3.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.49
153.29
145.63
143.80
134.28
130.05
129.78
126.47
125.39
125.25
121.66
119.53
113.59
77.37
77.16
76.95
Cl
Br
N
O
3r
CDCl3
200 150 100 50 0
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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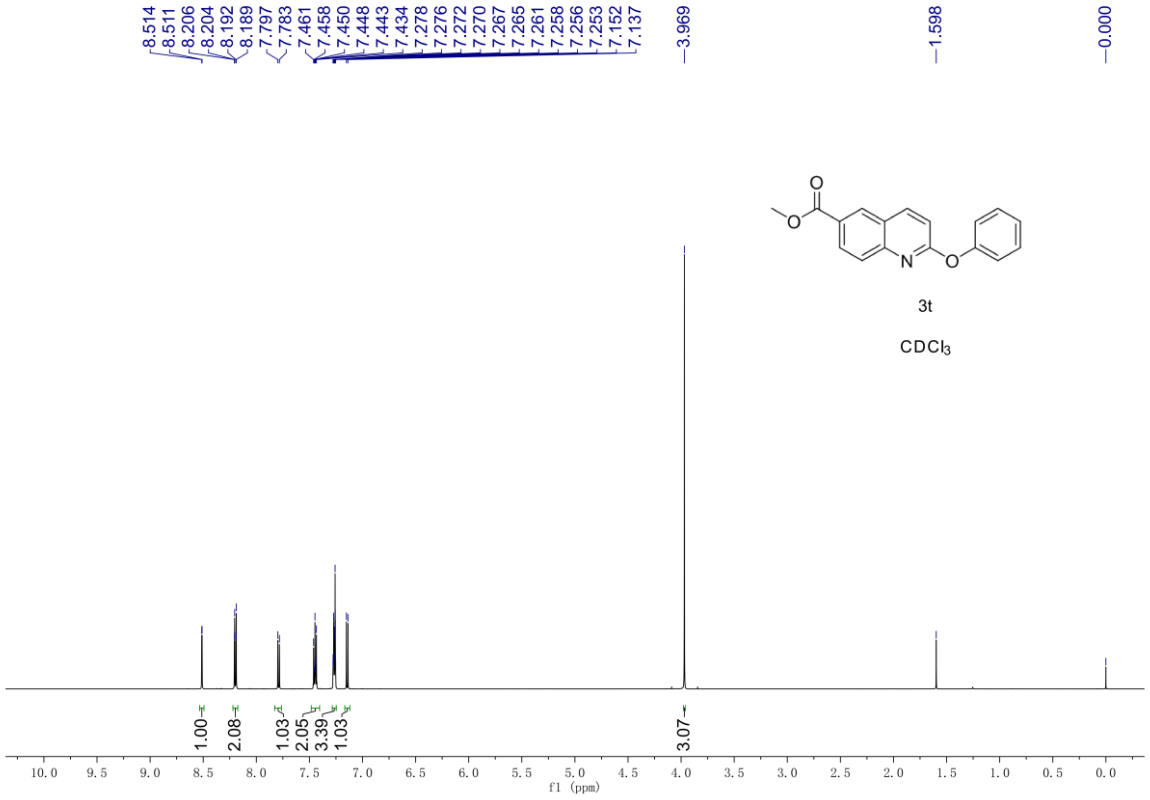
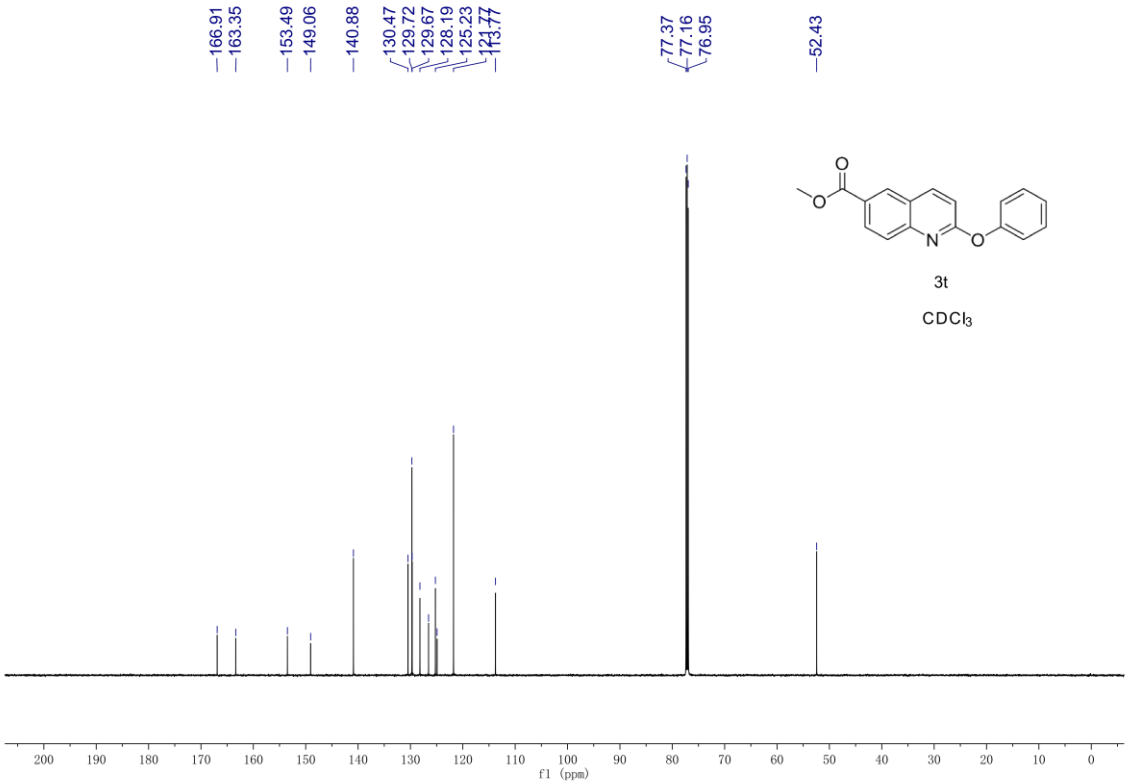
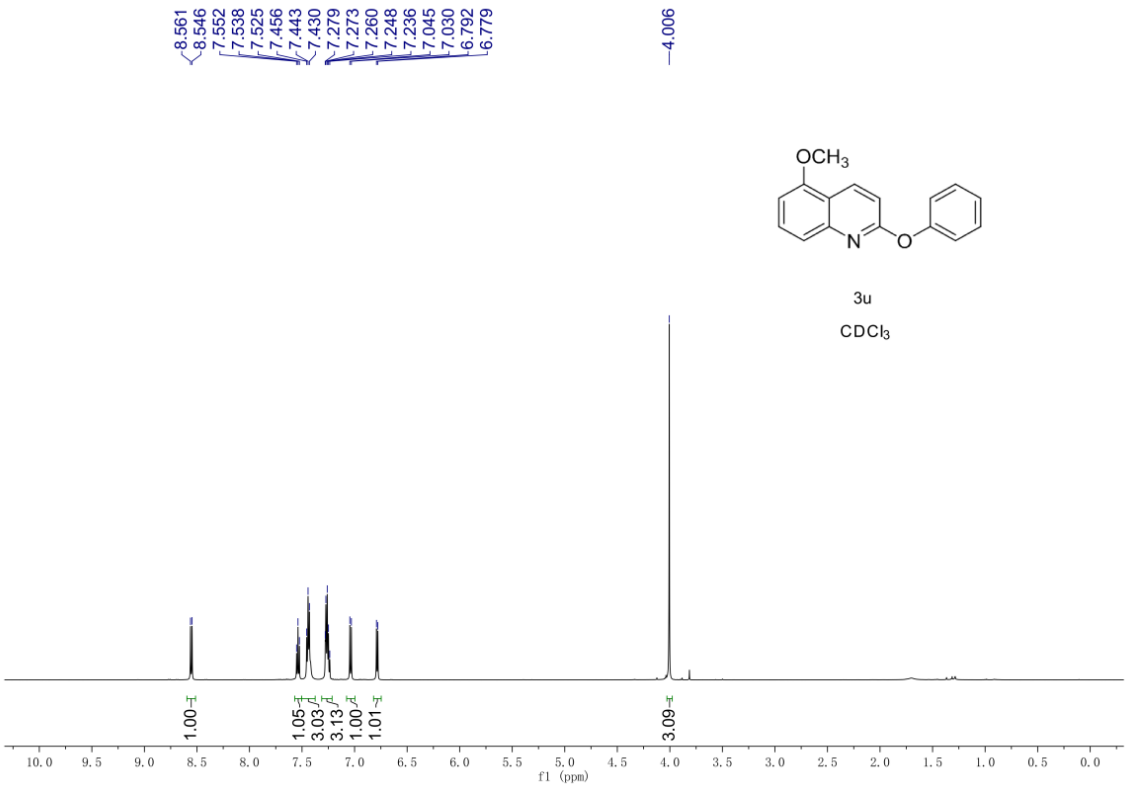
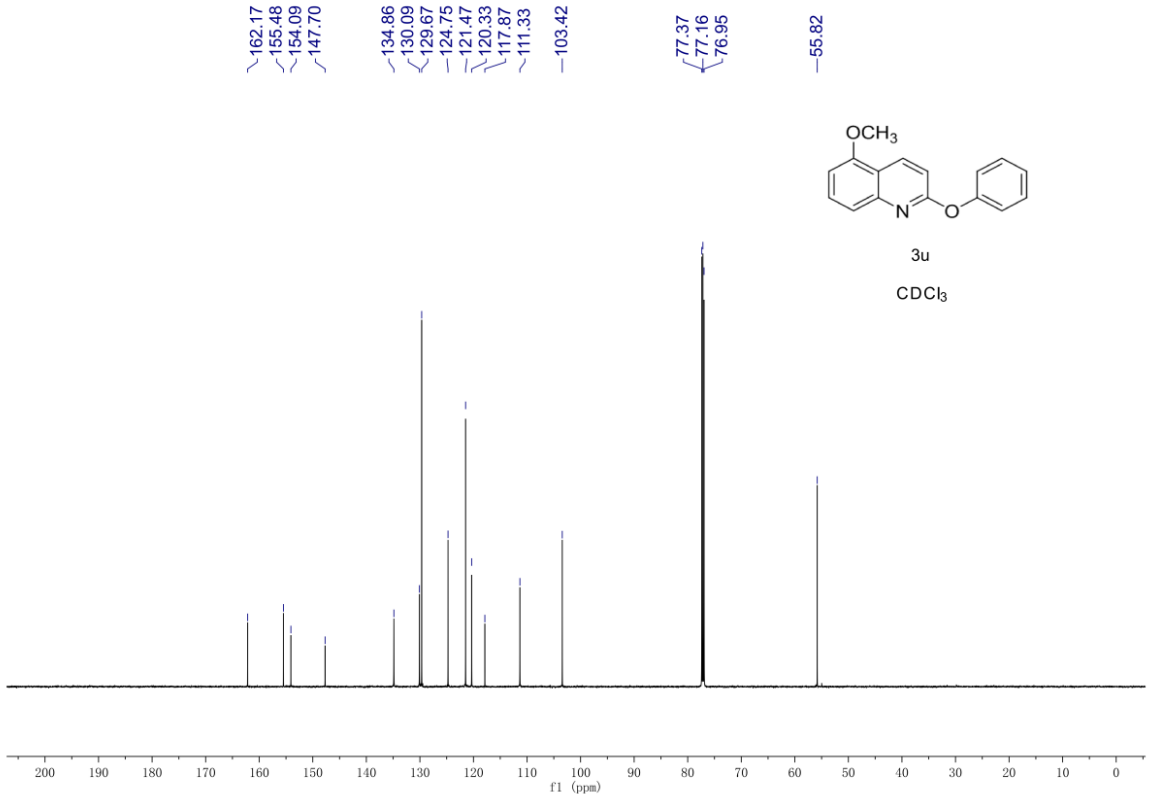
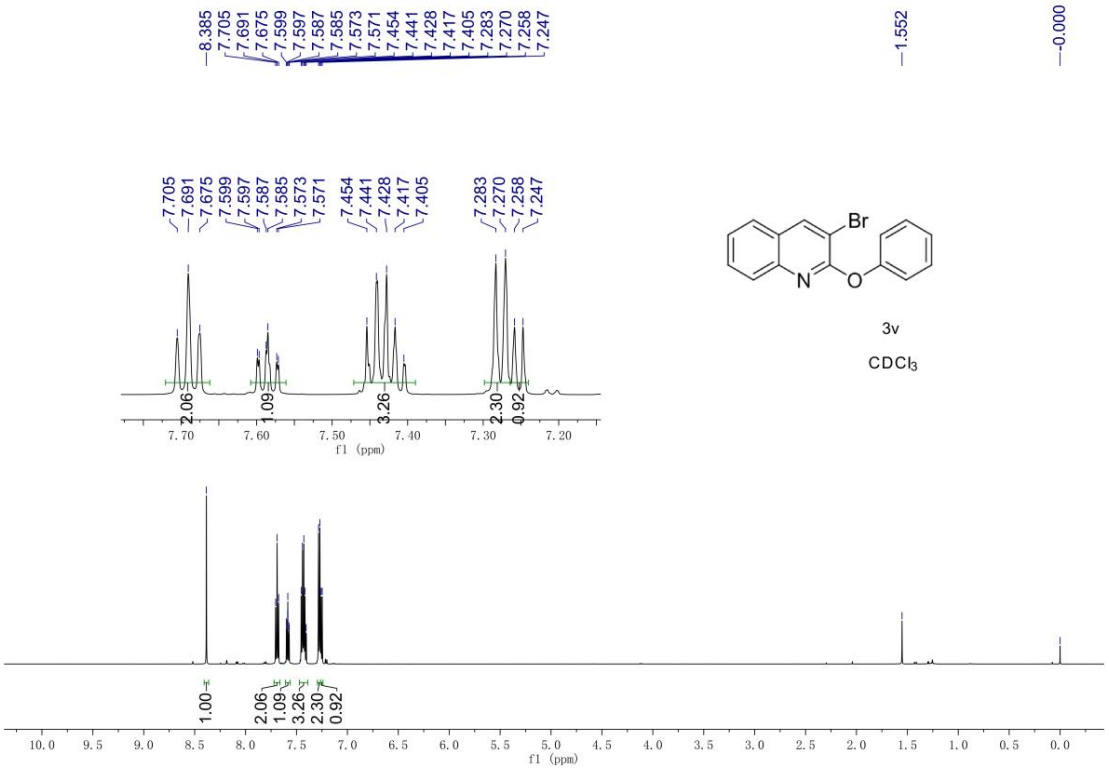
7.996
7.724
7.709
7.414
7.411
7.401
7.400
7.391
7.387
7.384
7.284
7.279
7.268
7.264
7.243
7.231
7.230
7.217
7.215
7.212
7.199
7.187
7.055
7.050
7.036
7.021
3.884
0.000
3s
CDCl3
1.00
0.97
1.97
1.00
2.99
2.00
3.02
f1 (ppm)

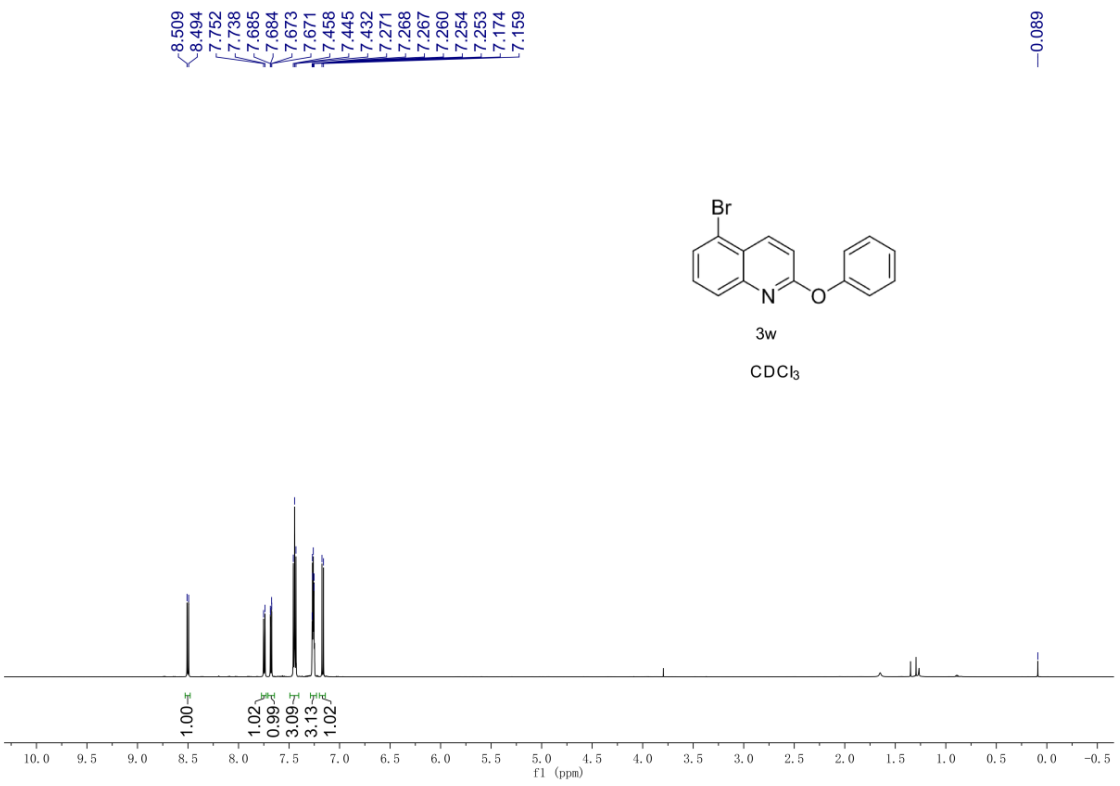

8.514
8.511
8.206
8.204
8.192
8.189
7.797
7.783
7.461
7.458
7.450
7.448
7.443
7.434
7.278
7.276
7.272
7.270
7.267
7.265
7.261
7.258
7.256
7.253
7.152
7.137
3.969
1.598
0.000
3t
CDCl3
1.00
2.08
1.03
2.05
3.39
1.03
3.07
f1 (ppm)

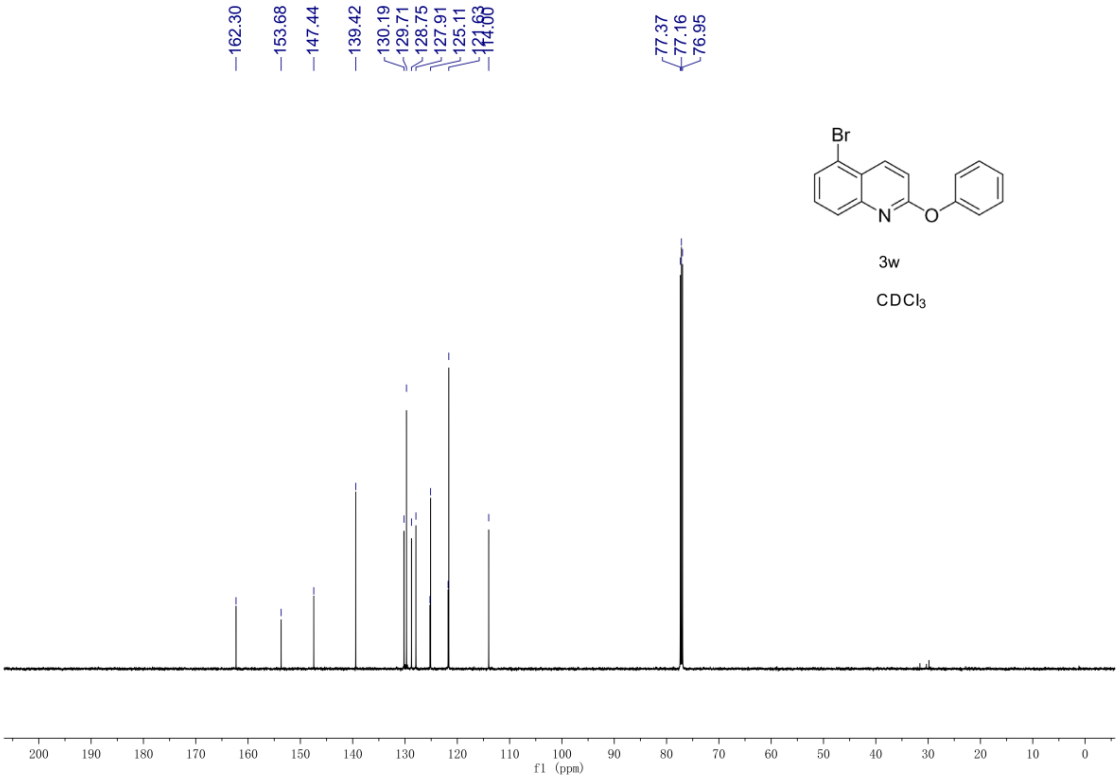

166.91
163.35
153.49
149.06
140.88
130.47
129.72
129.67
128.19
125.23
121.77
113.77
77.37
77.16
76.95
52.43
3t
CDCl3
f1 (ppm)

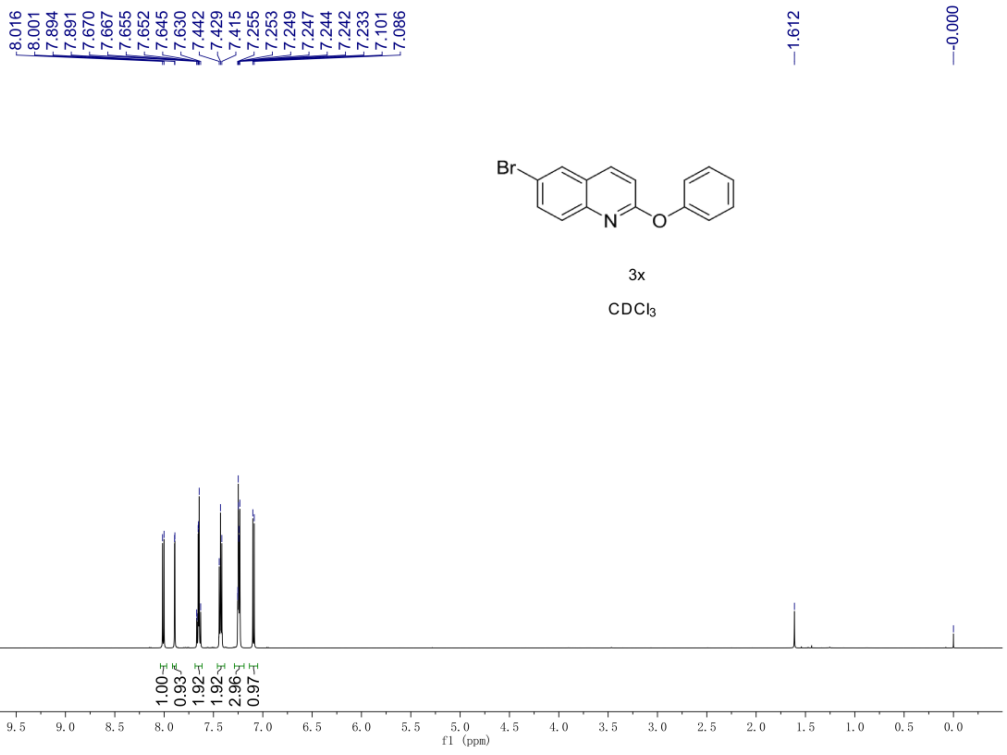

8.561
8.546
7.552
7.538
7.525
7.456
7.443
7.430
7.279
7.273
7.260
7.248
7.236
7.045
7.030
6.792
6.779
4.006
OCH3
N
O
3u
CDCl3
1.00
1.05
3.03
3.13
1.00
1.01
3.09
f1 (ppm)

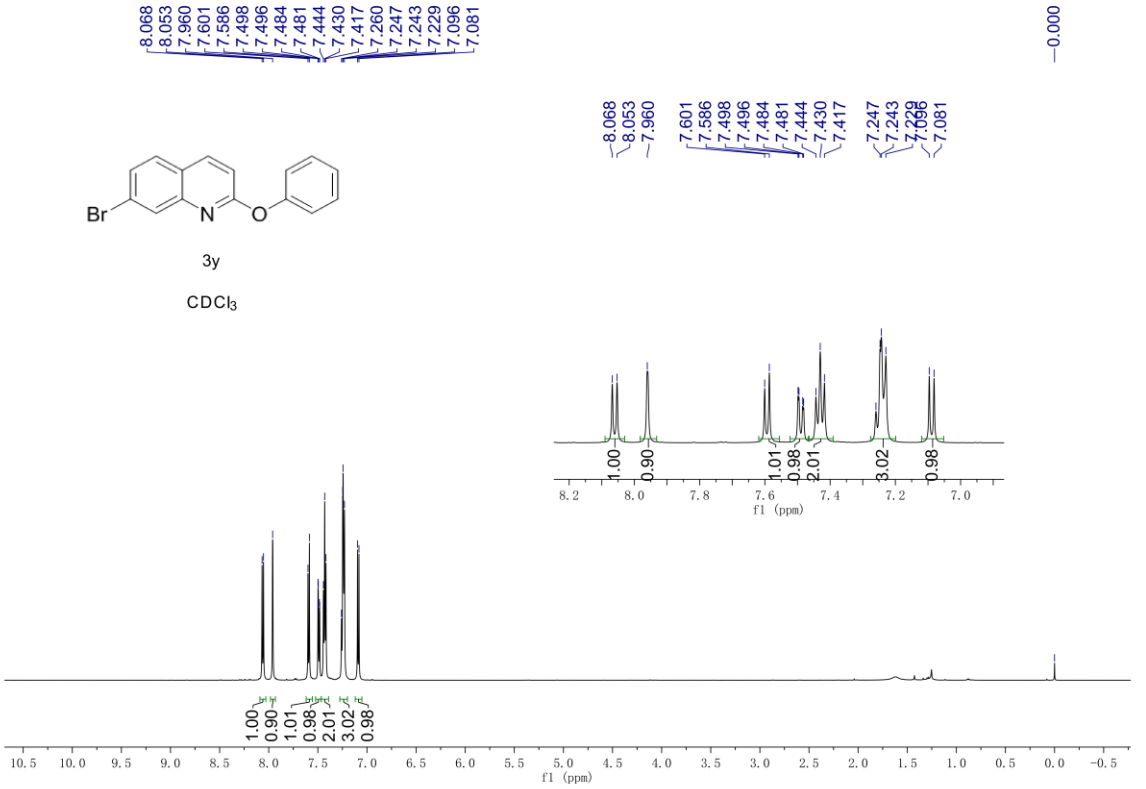

162.17
155.48
154.09
147.70
134.86
130.09
129.67
124.75
121.47
120.33
117.87
111.33
103.42
77.37
77.16
76.95
55.82
OCH3
N
O
3u
CDCl3
f1 (ppm)

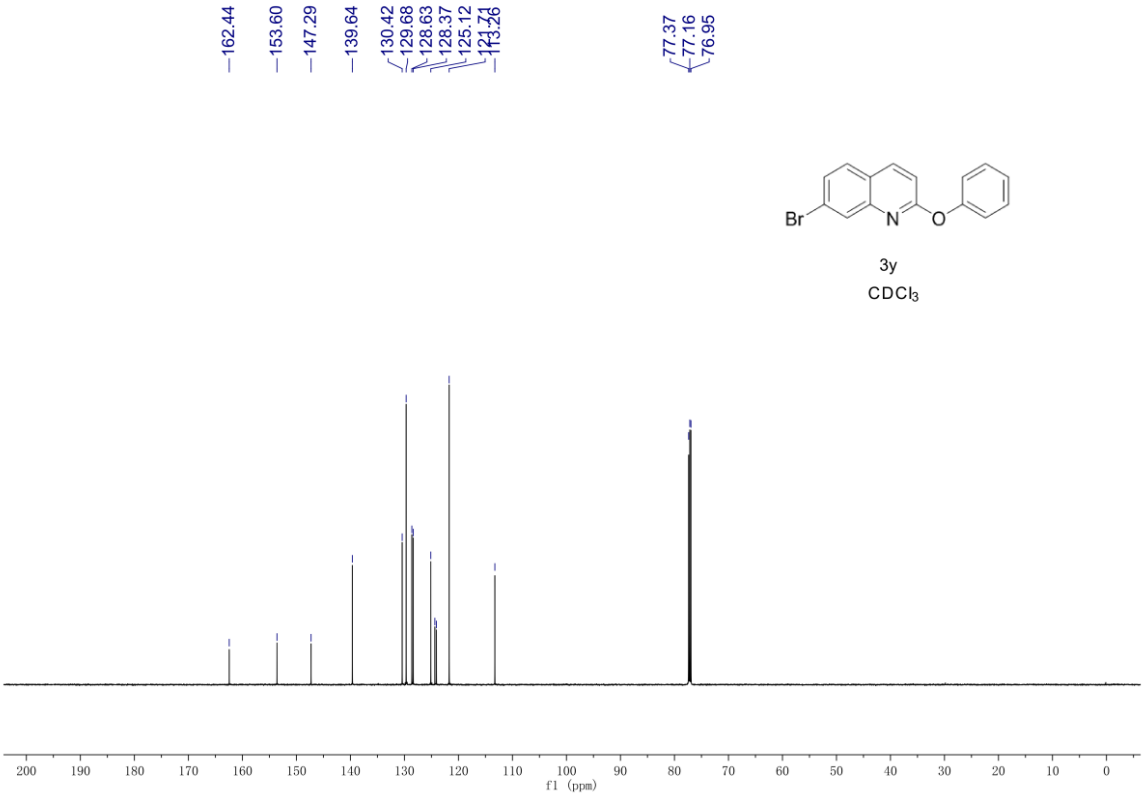

8.385
7.705
7.691
7.675
7.599
7.597
7.587
7.585
7.573
7.571
7.454
7.441
7.428
7.417
7.405
7.283
7.270
7.258
7.247
1.552
0.000
Br
N
O
3v
CDCl3
2.06
1.09
3.26
2.30
0.92
1.00
f1 (ppm)

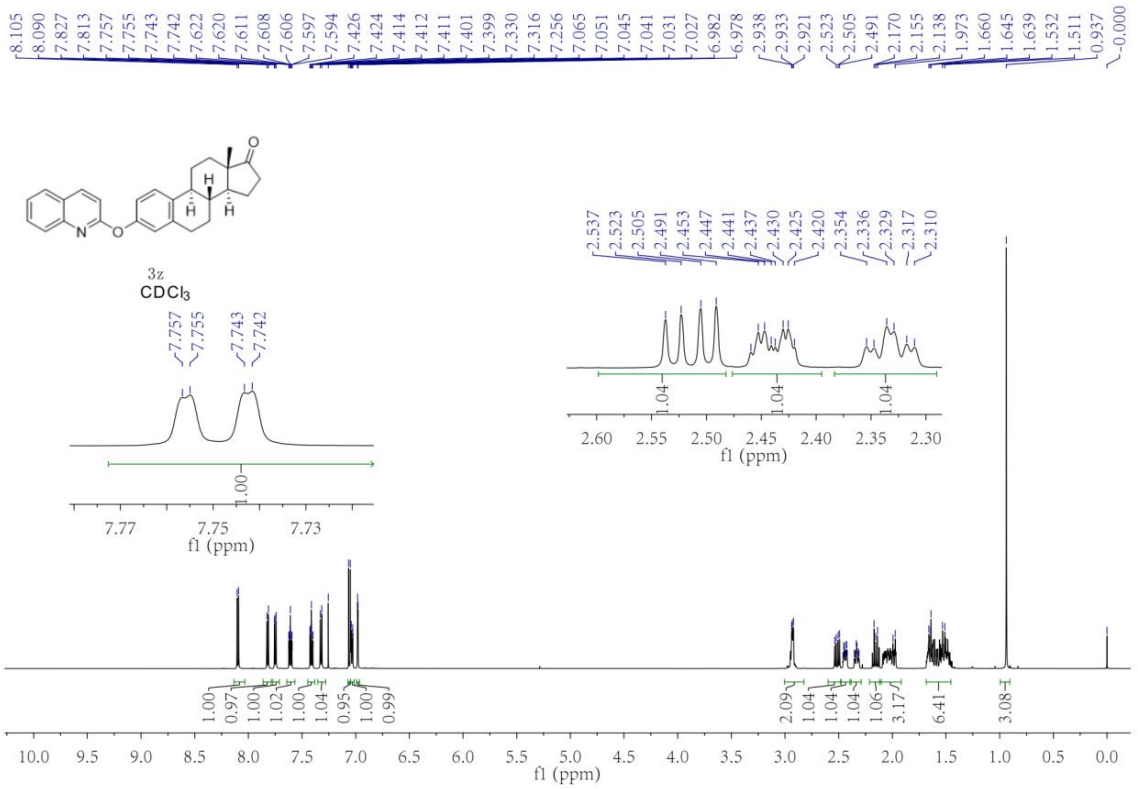

8.509
8.494
7.752
7.738
7.685
7.684
7.673
7.671
7.458
7.445
7.432
7.271
7.268
7.267
7.260
7.254
7.253
7.174
7.159
0.089
Br
N
O
3w
CDCl3
1.00
1.02
0.99
3.09
3.13
1.02
f1 (ppm)

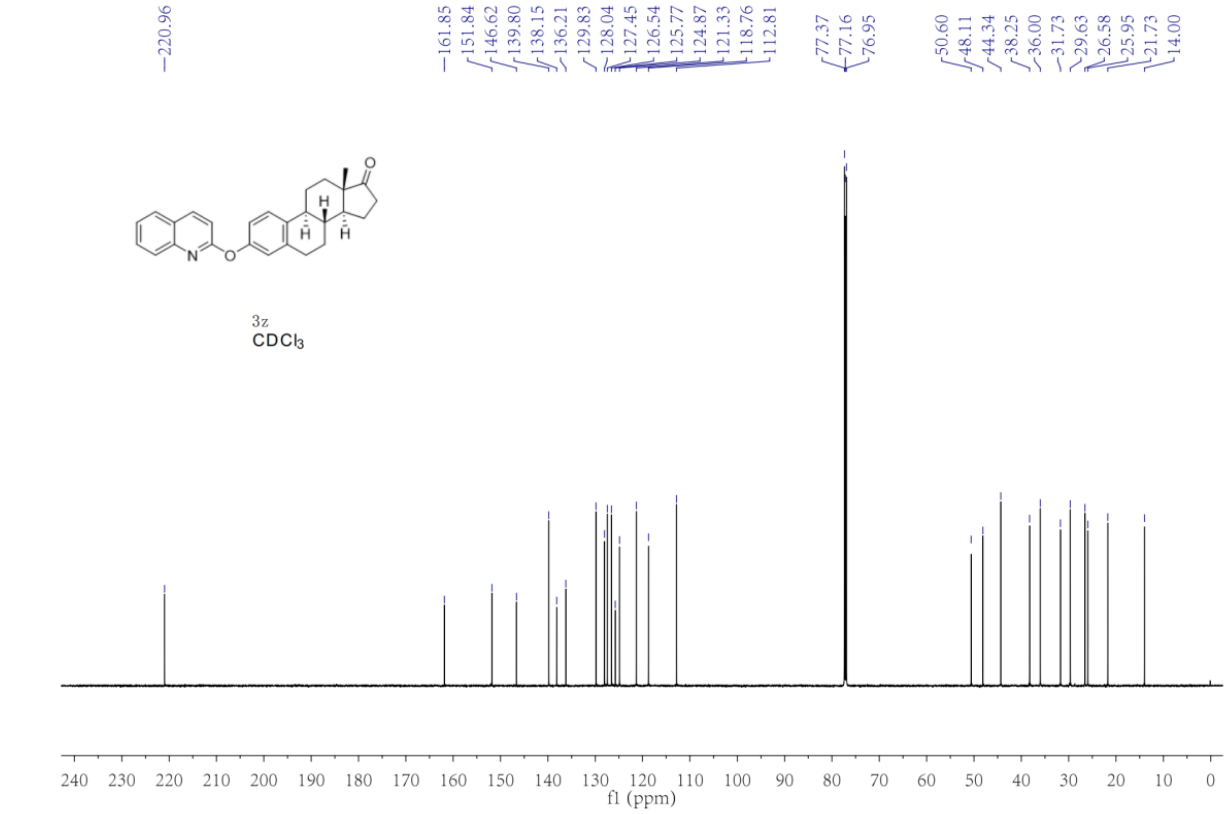

162.30
153.68
147.44
139.42
130.19
129.71
128.75
127.91
125.11
121.63
114.00
77.37
77.16
76.95
Br
N
O
3w
CDCl3
f1 (ppm)

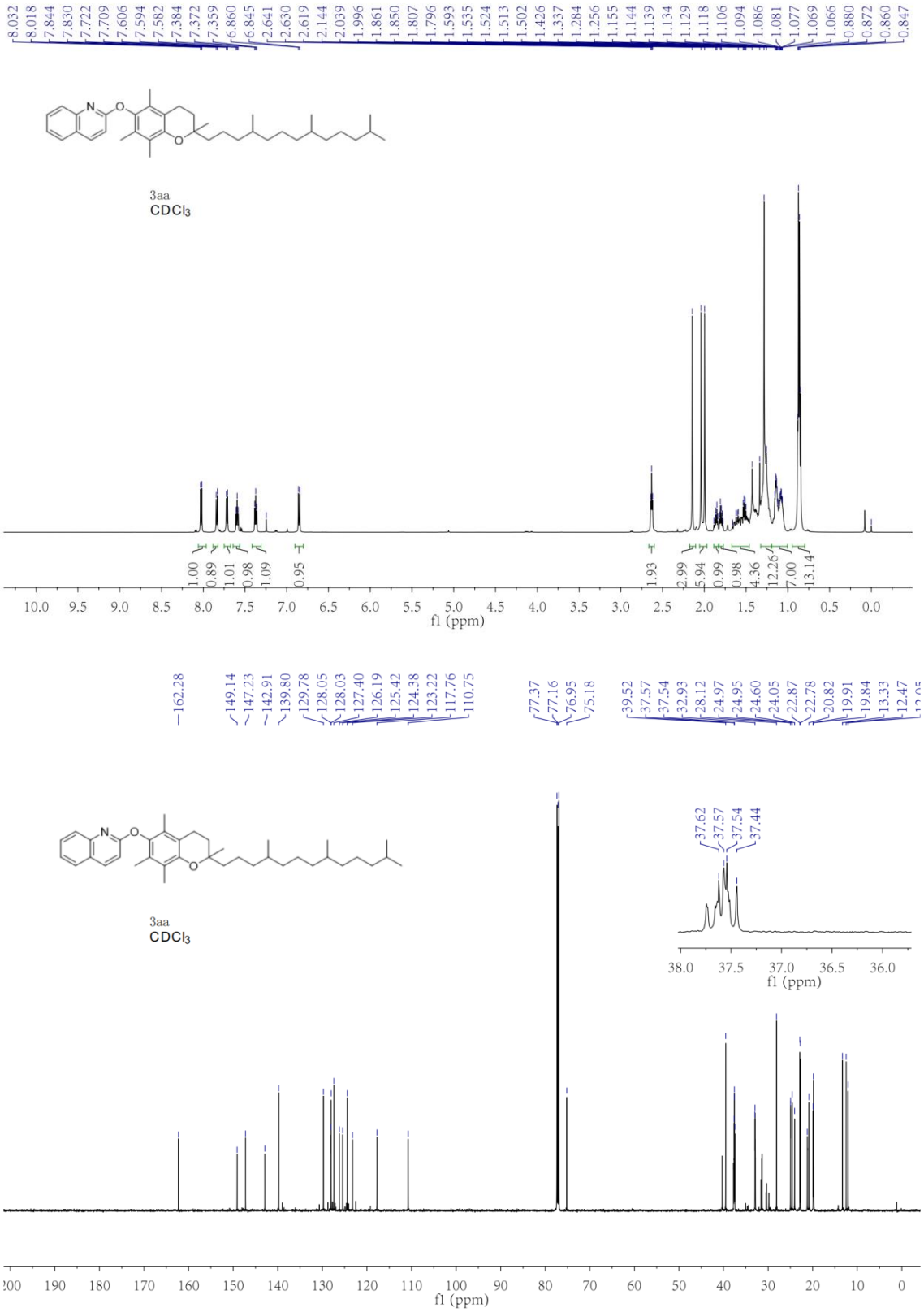

8.016
8.001
7.894
7.891
7.670
7.667
7.655
7.652
7.645
7.630
7.442
7.429
7.415
7.255
7.253
7.249
7.247
7.244
7.242
7.233
7.101
7.086
1.612
0.000
Br
N
O
3x
CDCl3
1.00
0.93
1.92
1.92
2.96
0.97
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

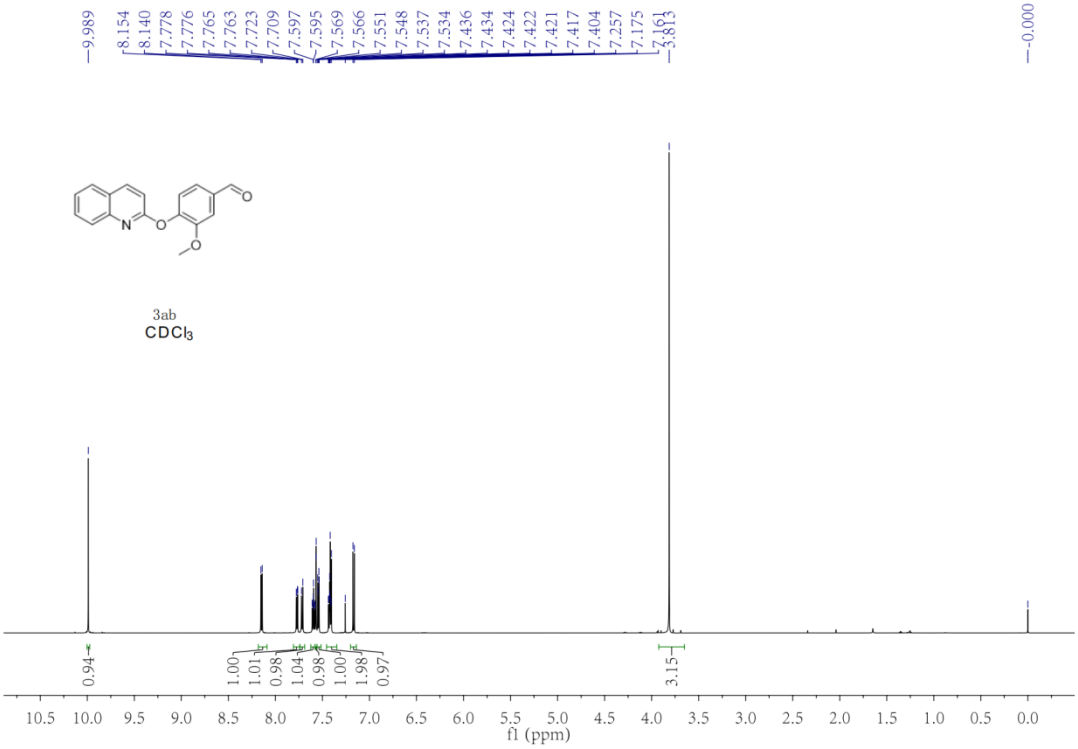

8.068
8.053
7.960
7.601
7.586
7.498
7.496
7.484
7.481
7.444
7.430
7.417
7.260
7.247
7.243
7.229
7.096
7.081
0.000
Br
N
O
3y
CDCl3
1.00
0.90
1.01
0.98
2.01
3.02
0.98
f1 (ppm)


162.44
153.60
147.29
139.64
130.42
129.68
128.63
128.37
125.12
121.74
113.26
77.37
77.16
76.95
Br
N
O
3y
CDCl3
f1 (ppm)


3z
CDCl3
fl (ppm)


3z
CDCl3
fl (ppm)


8.032
8.018
7.844
7.830
7.722
7.709
7.606
7.594
7.582
7.384
7.372
7.359
6.860
6.845
2.641
2.630
2.619
2.144
2.039
1.996
1.861
1.850
1.807
1.796
1.593
1.535
1.524
1.513
1.502
1.426
1.337
1.284
1.256
1.155
1.144
1.139
1.134
1.129
1.118
1.106
1.094
1.086
1.081
1.077
1.069
1.066
0.880
0.872
0.860
0.847
3aa
CDCl3
1.00
0.89
1.01
0.98
1.09
0.95
1.93
2.99
5.94
0.99
0.98
4.36
12.26
7.00
13.14
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)
162.28
149.14
147.23
142.91
139.80
129.78
128.05
128.03
127.40
126.19
125.42
124.38
123.22
117.76
110.75
77.37
77.16
76.95
75.18
39.52
37.57
37.54
32.93
28.12
24.97
24.95
24.60
24.05
22.87
22.78
20.82
19.91
19.84
13.33
12.47
3aa
CDCl3
37.62
37.57
37.54
37.44
38.0 37.5 37.0 36.5 36.0
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.989
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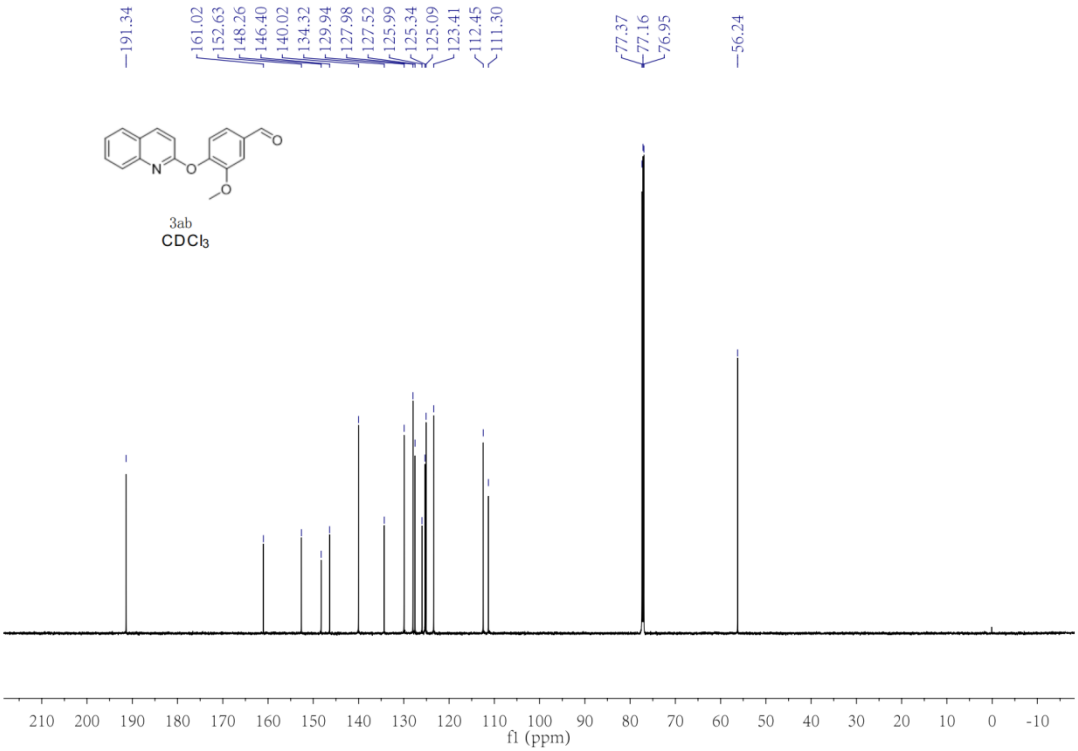
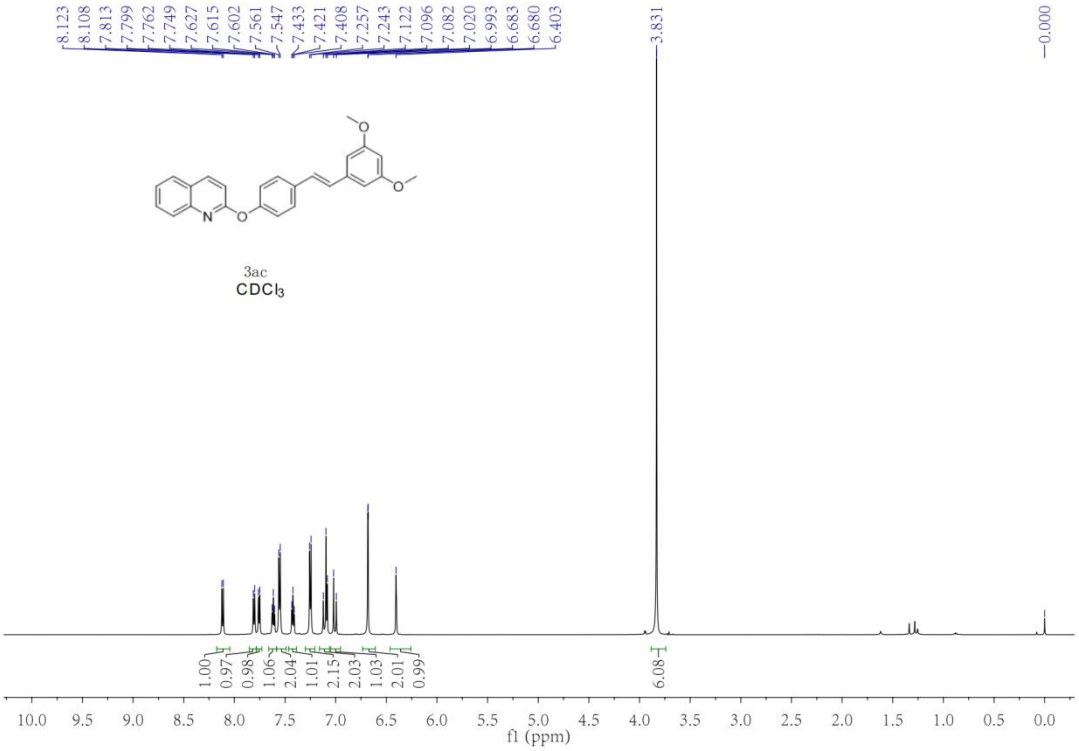
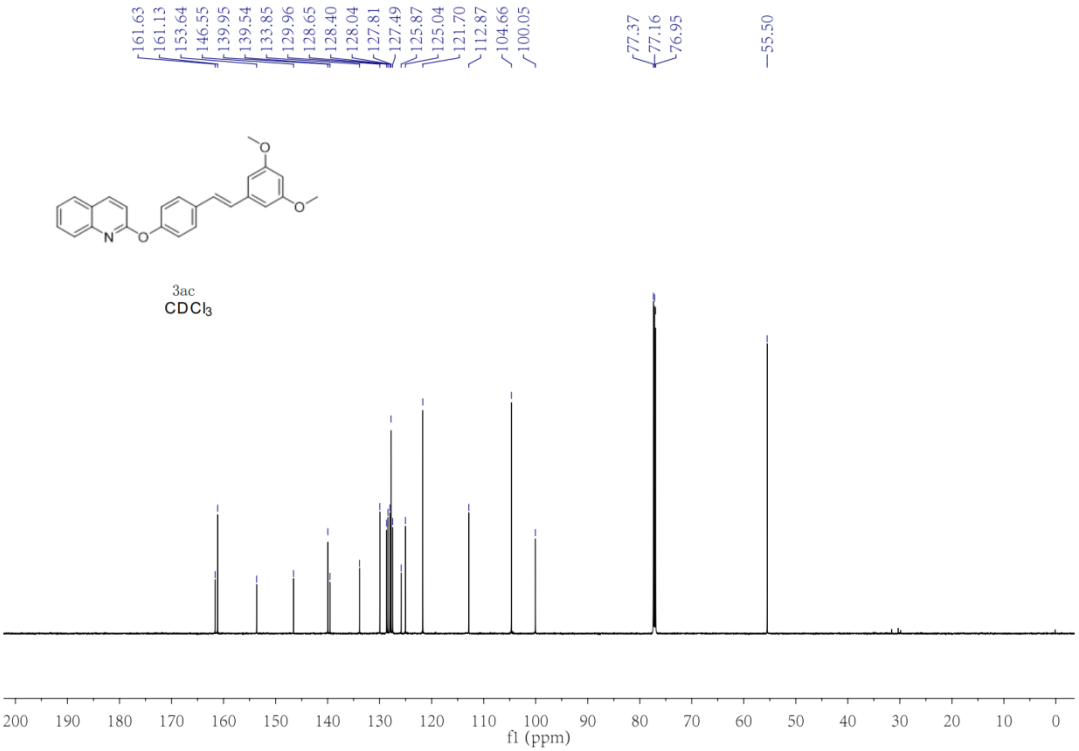
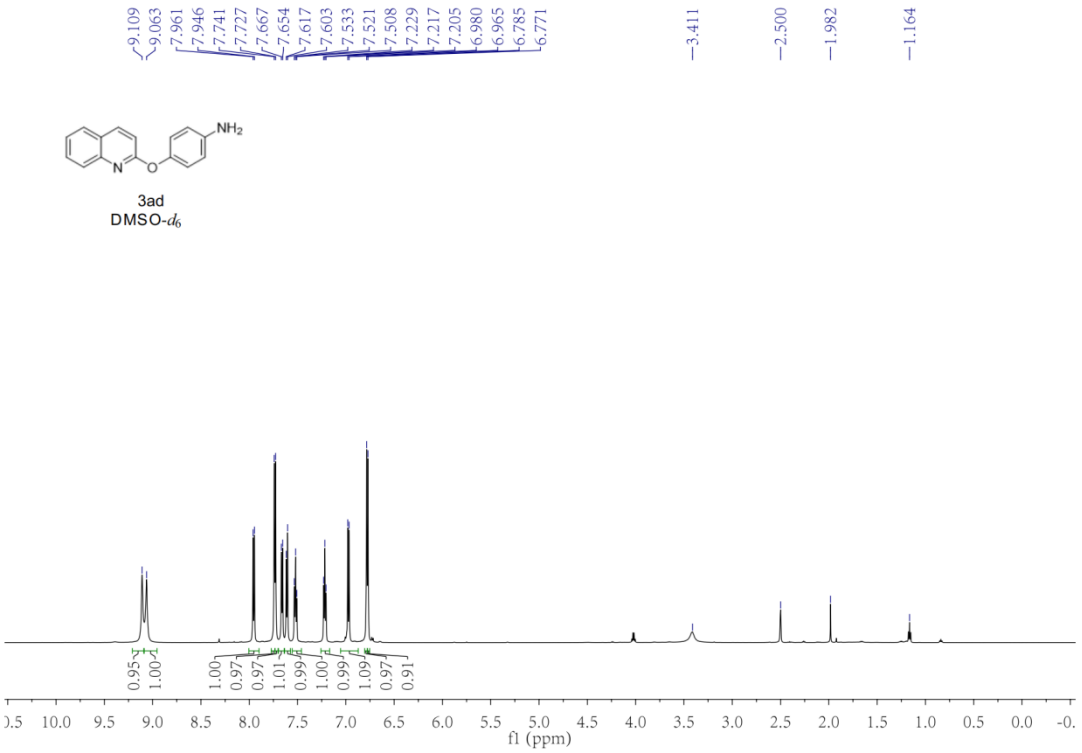
8.140
7.778
7.776
7.765
7.763
7.723
7.709
7.597
7.595
7.569
7.566
7.551
7.548
7.537
7.534
7.436
7.434
7.424
7.422
7.421
7.417
7.404
7.257
7.175
3.813
0.000
3ab
CDCl3
0.94
1.00
1.01
0.98
1.04
0.98
1.00
1.98
0.97
3.15
fl (ppm)


191.34
161.02
152.63
148.26
146.40
140.02
134.32
129.94
127.98
127.52
125.99
125.34
125.09
123.41
112.45
111.30
77.37
77.16
76.95
56.24
3ab
CDCl3
fl (ppm)


8.123
8.108
7.813
7.799
7.762
7.749
7.627
7.615
7.602
7.561
7.547
7.433
7.421
7.408
7.257
7.243
7.122
7.096
7.082
7.020
6.993
6.683
6.680
6.403
3.831
0.000
3ac
CDCl3
1.00
0.97
0.98
1.06
2.04
1.01
2.15
2.03
1.03
2.01
0.99
6.08
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)


161.63
161.13
153.64
146.55
139.95
139.54
133.85
129.96
128.65
128.40
128.04
127.81
127.49
125.87
125.04
121.70
112.87
104.66
100.05
77.37
77.16
76.95
55.50
3ac
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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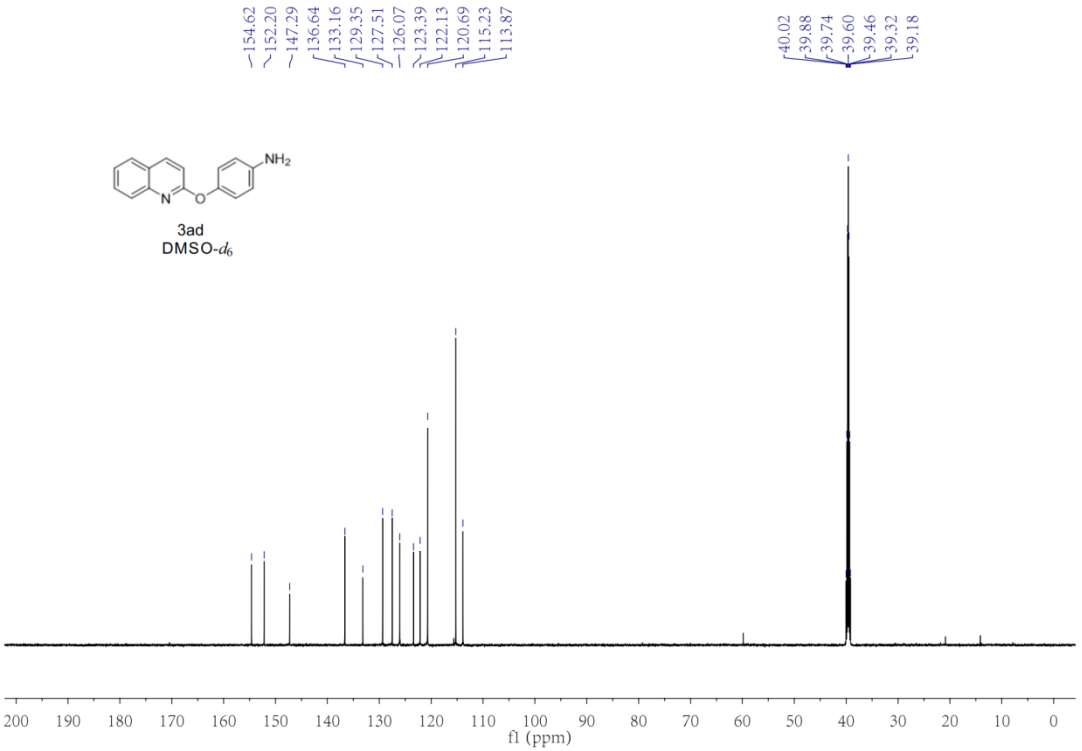
9.063
7.961
7.946
7.741
7.727
7.667
7.654
7.617
7.603
7.533
7.521
7.508
7.229
7.217
7.205
6.980
6.965
6.785
6.771
3.411
2.500
1.982
1.164
NH2
O
N
3ad
DMSO-d6
0.95
1.00
1.00
0.97
0.97
1.01
0.99
1.00
0.99
1.09
0.97
0.91
f1 (ppm)


154.62
152.20
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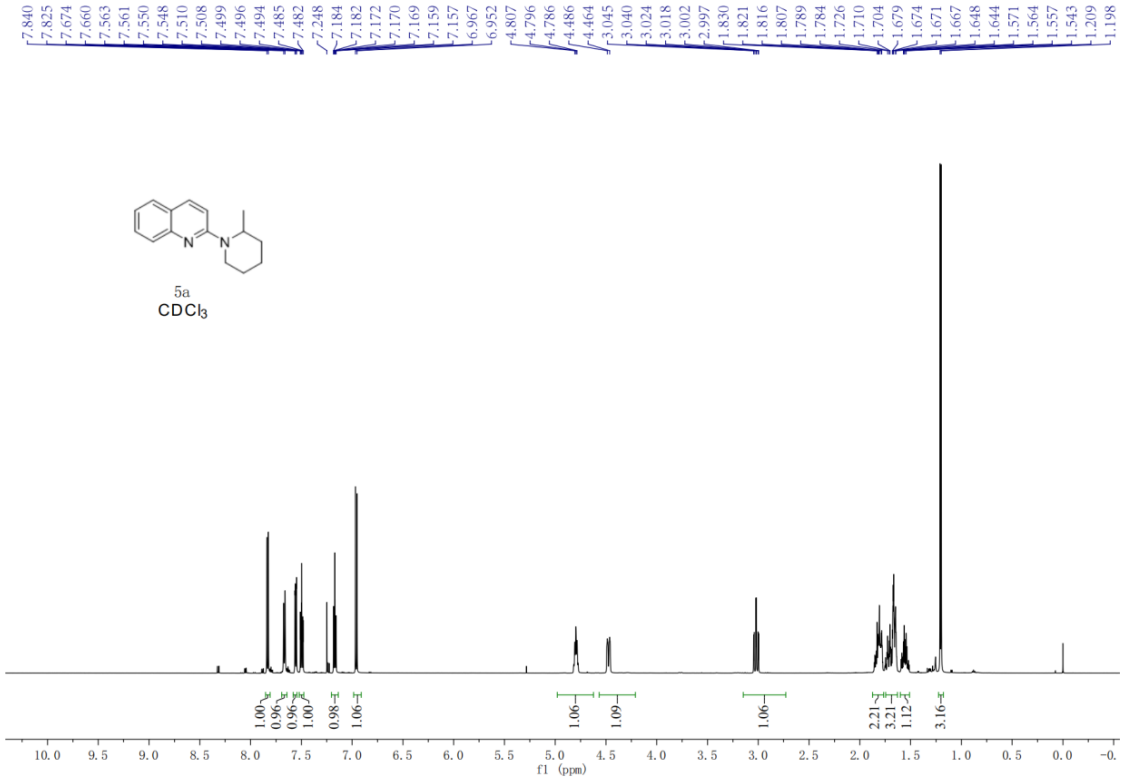
136.64
133.16
129.35
127.51
126.07
123.39
122.13
120.69
115.23
113.87
40.02
39.88
39.74
39.60
39.46
39.32
39.18
NH2
O
N
3ad
DMSO-d6
f1 (ppm)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7.674
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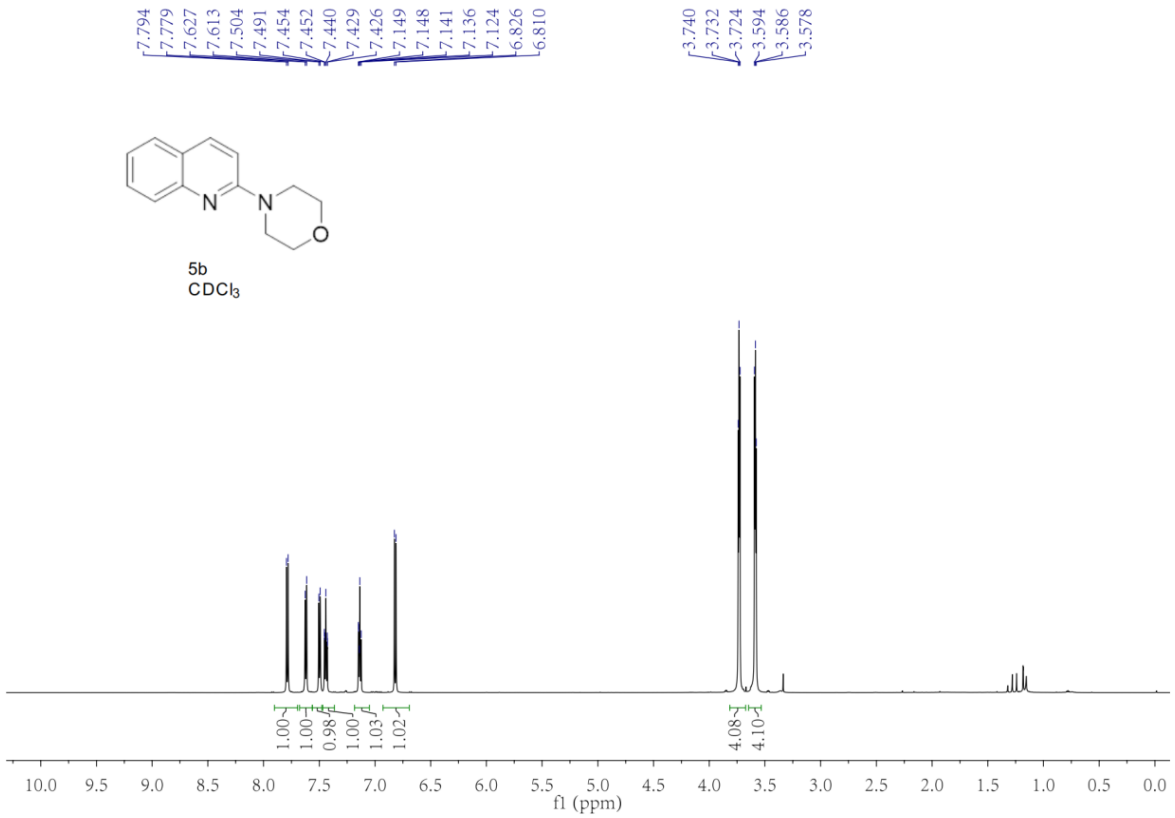
7.548
7.510
7.508
7.499
7.496
7.494
7.485
7.482
7.248
7.184
7.182
7.172
7.170
7.169
7.159
7.157
6.967
6.952
4.807
4.796
4.786
4.486
4.464
3.045
3.040
3.024
3.018
3.002
2.997
1.830
1.821
1.816
1.807
1.789
1.784
1.726
1.710
1.704
1.679
1.674
1.671
1.667
1.648
1.644
1.571
1.564
1.557
1.543
1.209
1.198
5a
CDCl3
1.00
0.96
0.96
1.00
0.98
1.06
1.06
1.09
1.06
2.21
3.21
1.12
3.16
f1 (ppm)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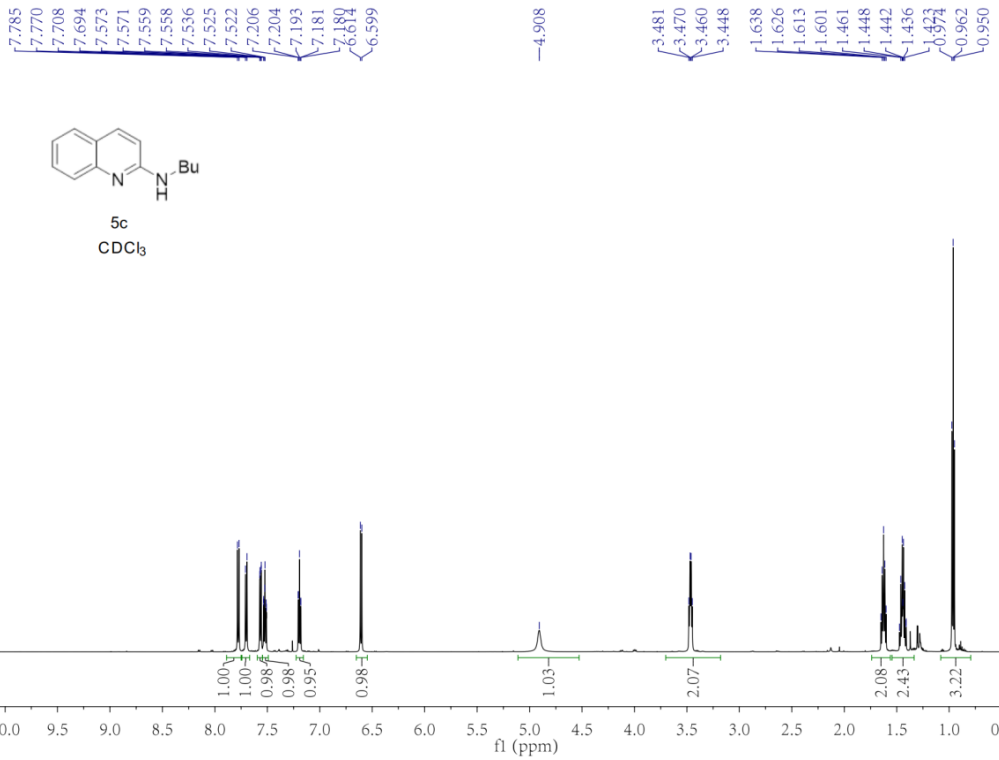
7.452
7.440
7.429
7.426
7.149
7.148
7.141
7.136
7.124
6.826
6.810
3.740
3.732
3.724
3.594
3.586
3.578
5b
CDCl3
1.00
1.00
0.98
1.00
1.03
1.02
4.08
4.10
f1 (ppm)


7.785
7.770
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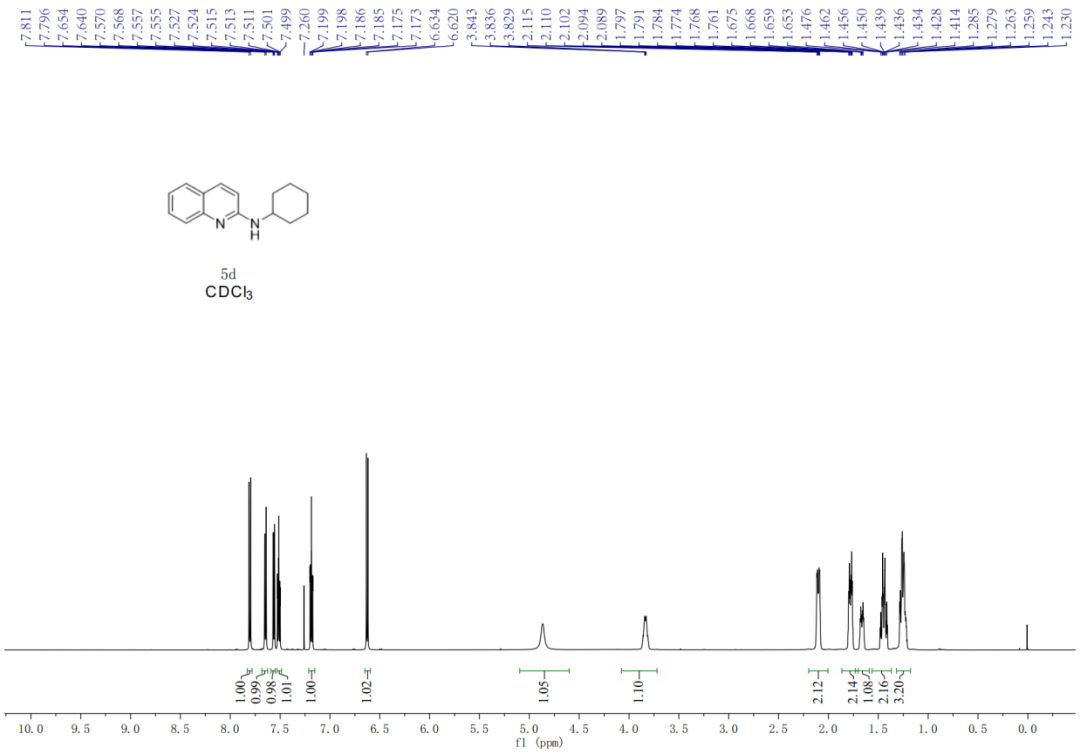
7.694
7.573
7.571
7.559
7.558
7.536
7.525
7.522
7.206
7.204
7.193
7.181
7.180
6.614
6.599
4.908
3.481
3.470
3.460
3.448
1.638
1.626
1.613
1.601
1.461
1.448
1.442
1.436
0.974
0.962
0.950
Bu
N
H
5c
CDCl3
1.00
1.00
0.98
0.98
0.95
0.98
1.03
2.07
2.08
2.43
3.22
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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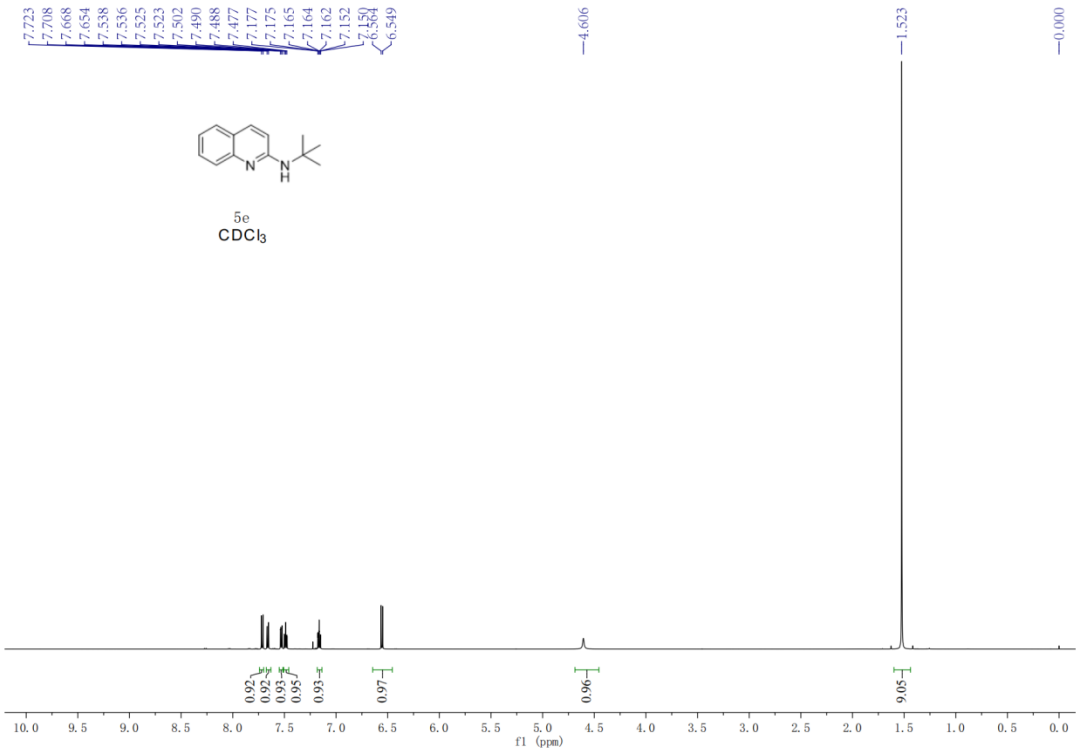
7.654
7.640
7.570
7.568
7.557
7.555
7.527
7.524
7.515
7.513
7.511
7.501
7.499
7.260
7.199
7.198
7.186
7.185
7.175
7.173
6.634
6.620
3.843
3.836
3.829
2.115
2.110
2.102
2.094
2.089
1.797
1.791
1.784
1.774
1.768
1.761
1.675
1.668
1.659
1.653
1.476
1.462
1.456
1.450
1.439
1.436
1.434
1.428
1.414
1.285
1.279
1.263
1.259
1.243
1.230
N
H
5d
CDCl3
1.00
0.99
0.98
1.01
1.00
1.02
1.05
1.10
2.12
2.14
1.08
2.16
3.20
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)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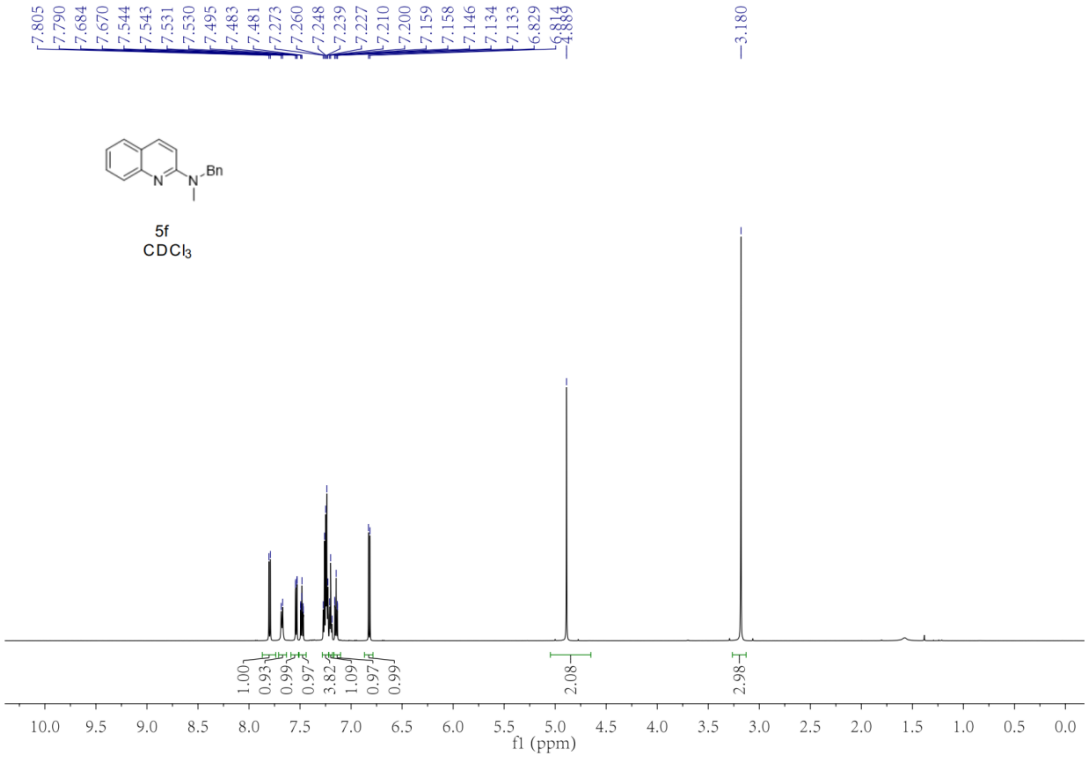
7.708
7.668
7.654
7.538
7.536
7.525
7.523
7.502
7.490
7.488
7.477
7.177
7.175
7.165
7.164
7.162
7.152
7.150
6.564
6.549
4.606
1.523
0.000
5e
CDCl3
0.92
0.92
0.93
0.95
0.93
0.97
0.96
9.05
f1 (ppm)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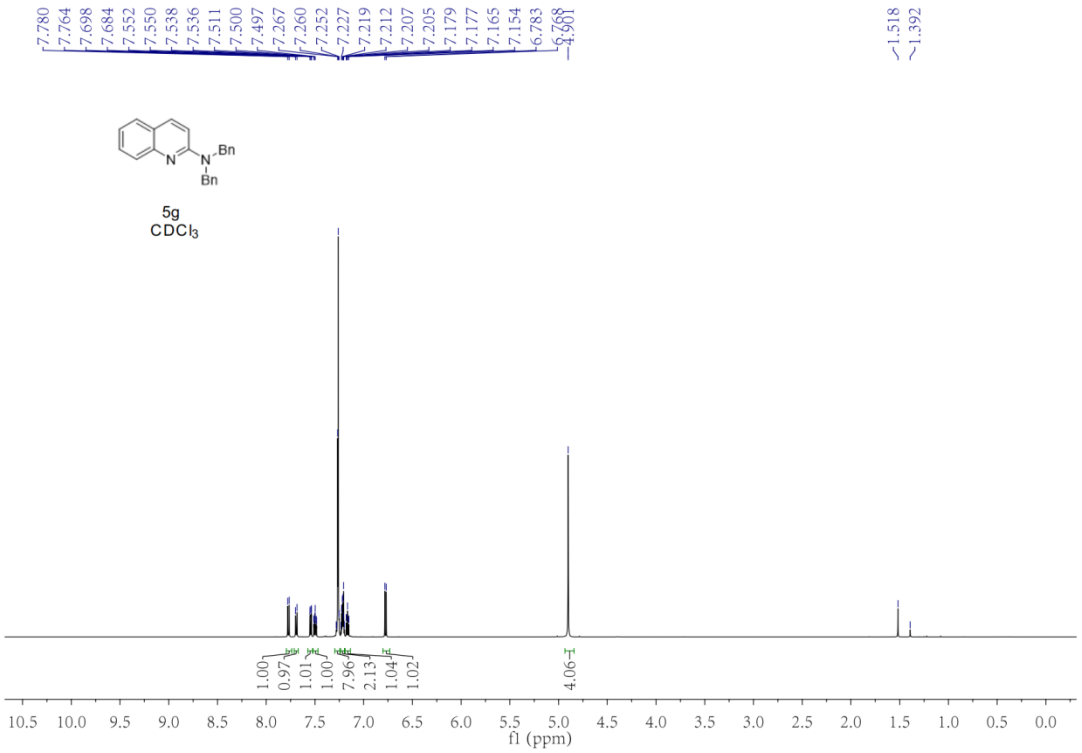
7.684
7.670
7.544
7.543
7.531
7.530
7.495
7.483
7.481
7.273
7.260
7.248
7.239
7.227
7.210
7.200
7.159
7.158
7.146
7.134
7.133
6.829
6.814
4.885
3.180
Bn
5f
CDCl3
1.00
0.93
0.99
0.97
3.82
1.09
0.97
0.99
2.08
2.98
f1 (ppm)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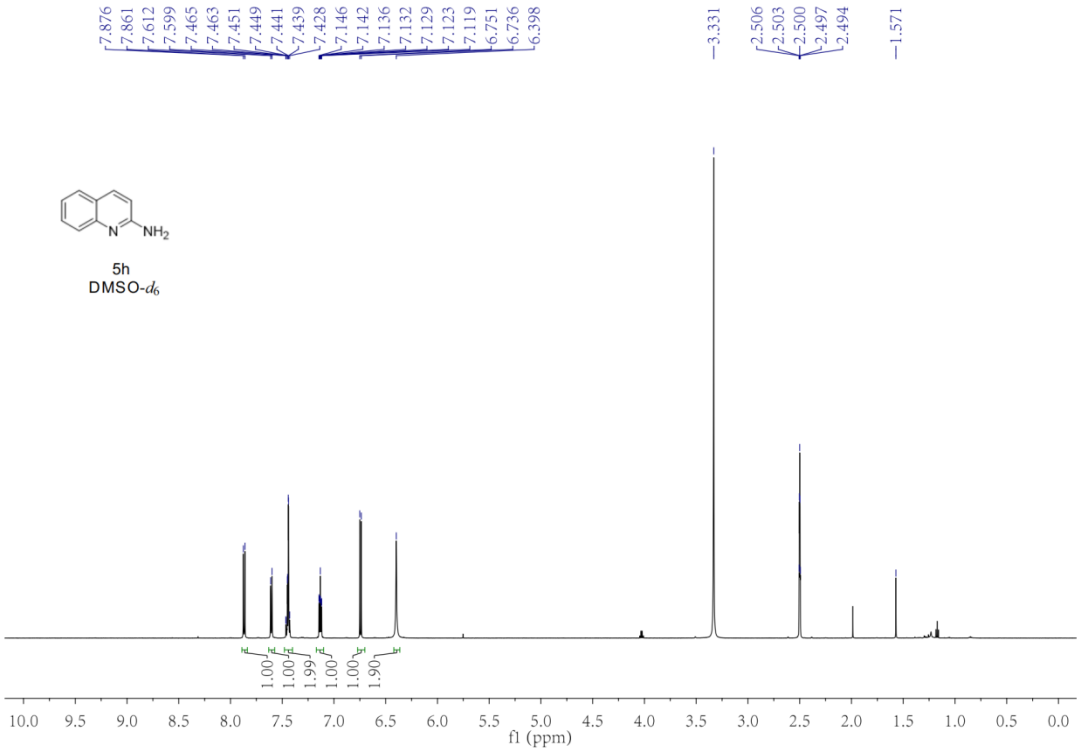
7.764
7.698
7.684
7.552
7.550
7.538
7.536
7.511
7.500
7.497
7.267
7.260
7.252
7.227
7.219
7.212
7.207
7.205
7.179
7.177
7.165
7.154
6.783
6.768
4.901
1.518
1.392
N
N
Bn
Bn
5g
CDCl3
1.00
0.97
1.01
1.00
7.96
2.13
1.04
1.02
4.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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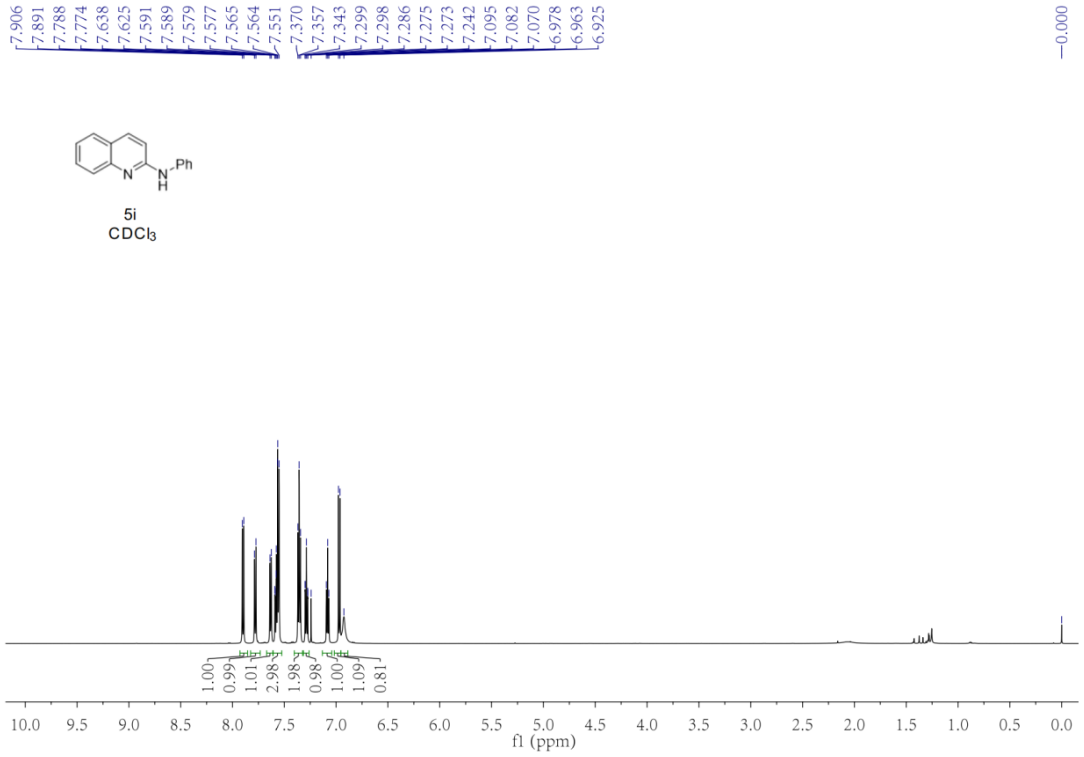
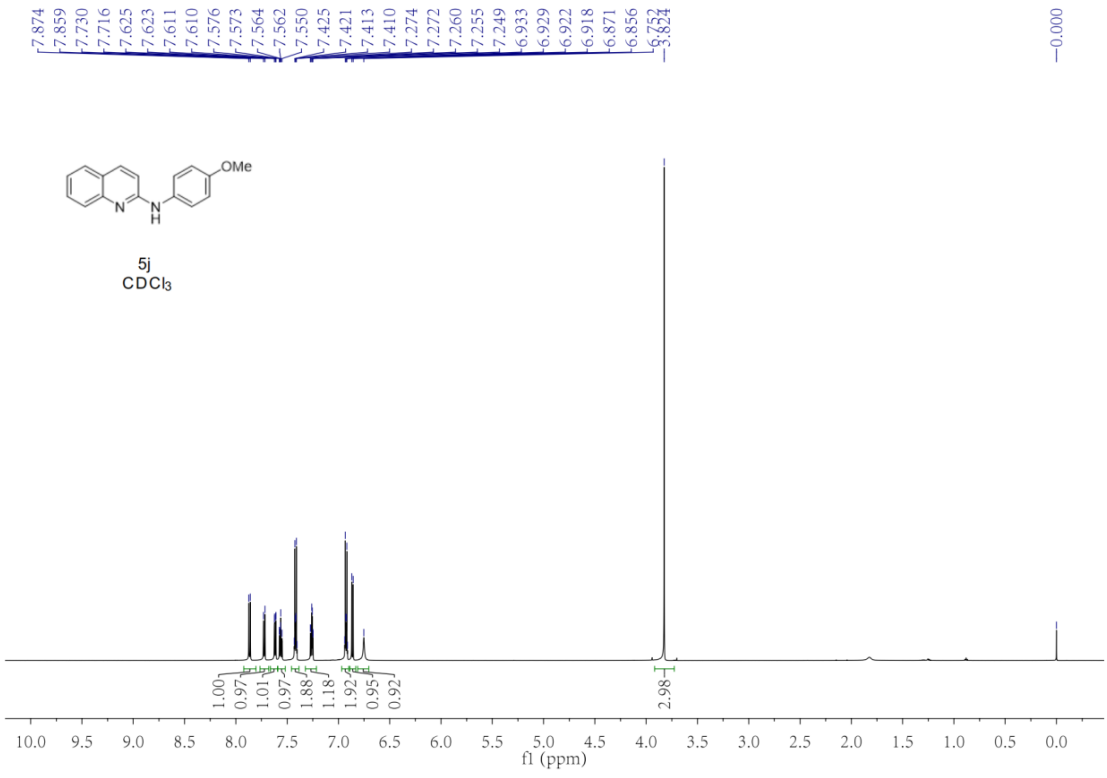
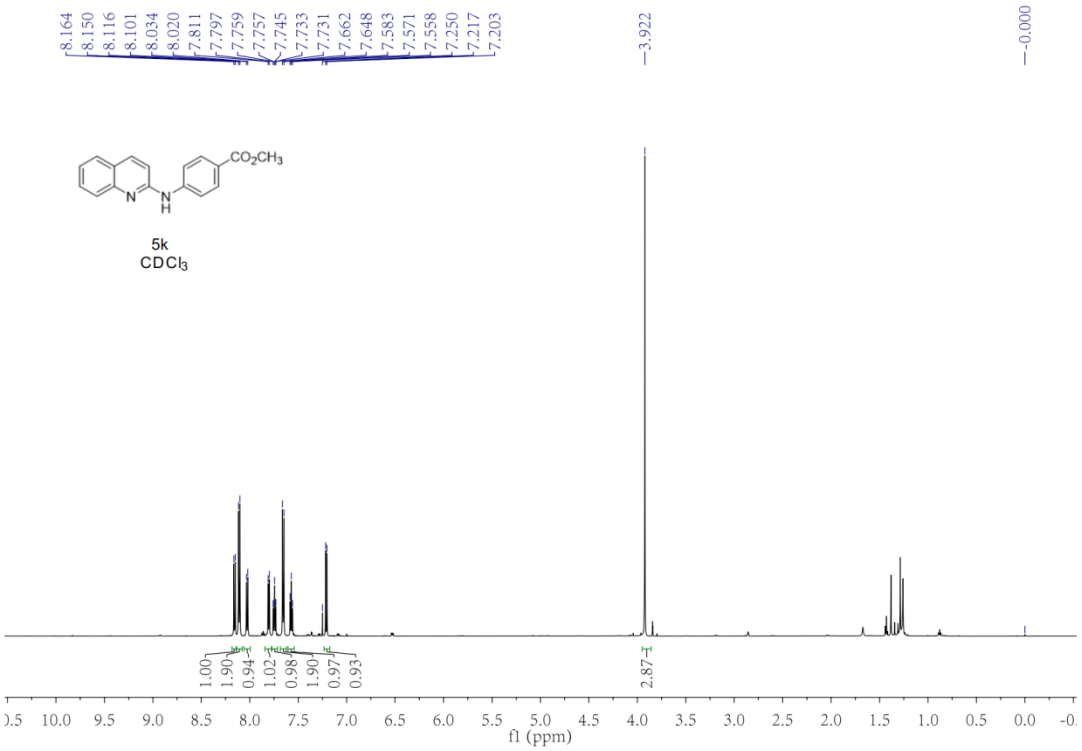
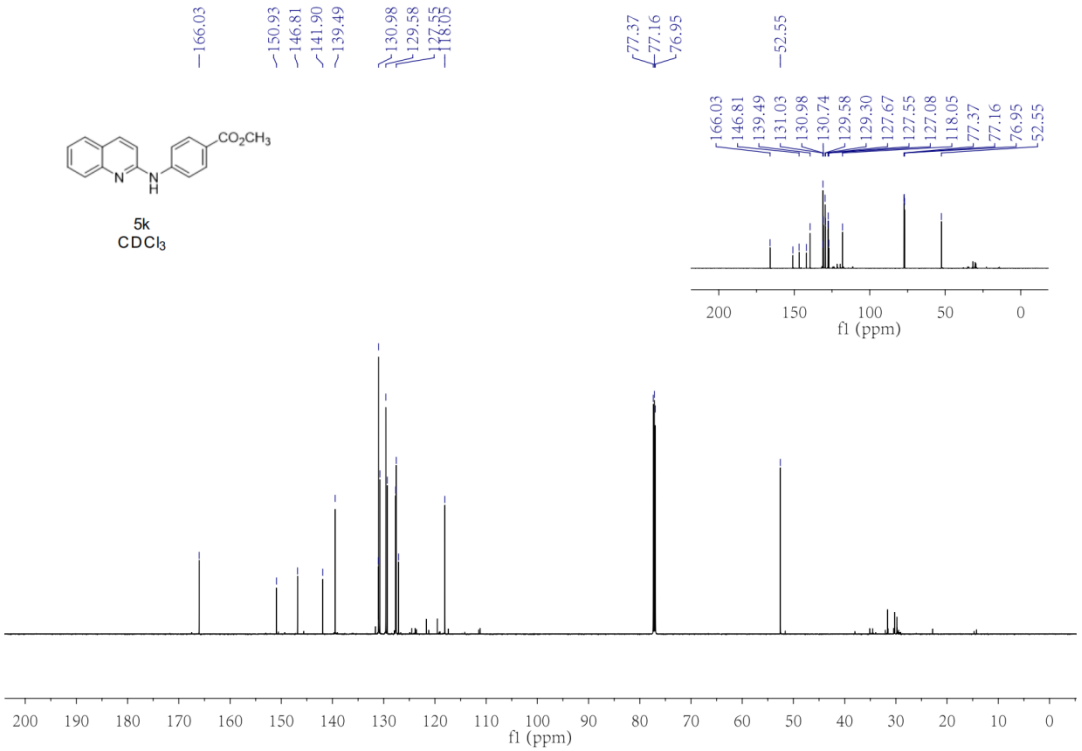
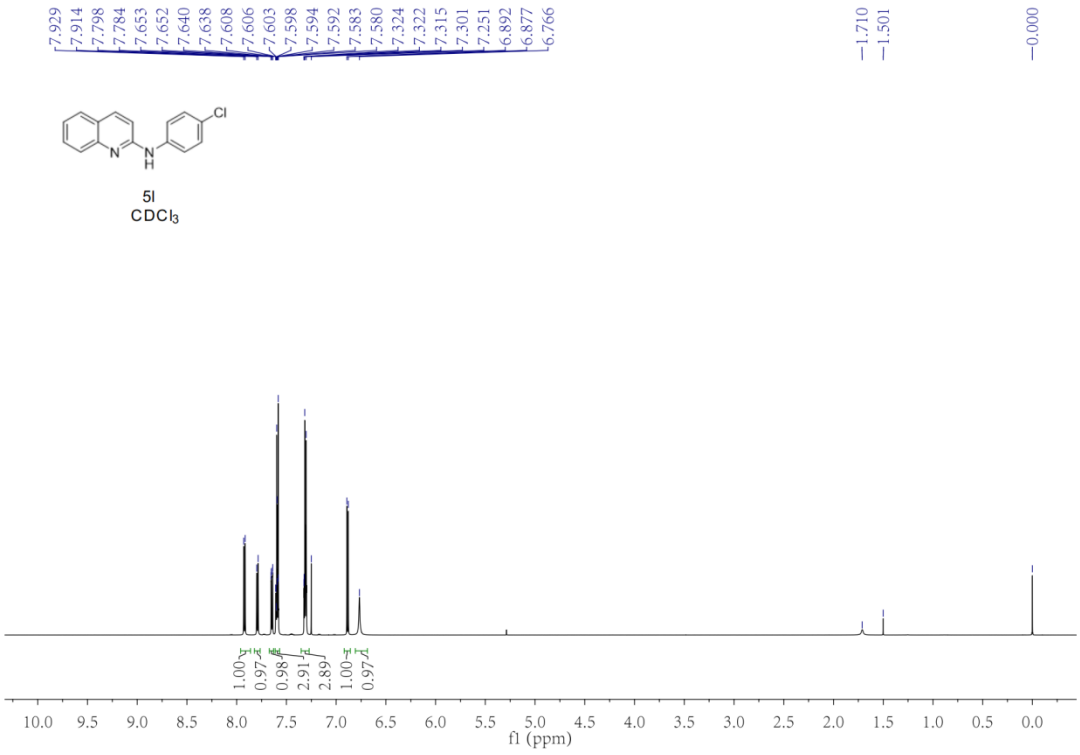
7.612
7.599
7.465
7.463
7.451
7.449
7.441
7.439
7.428
7.146
7.142
7.136
7.132
7.129
7.123
7.119
6.751
6.736
6.398
3.331
2.506
2.503
2.500
2.497
2.494
1.571
N
NH2
5h
DMSO-d6
1.00
1.00
1.99
1.00
1.00
1.90
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

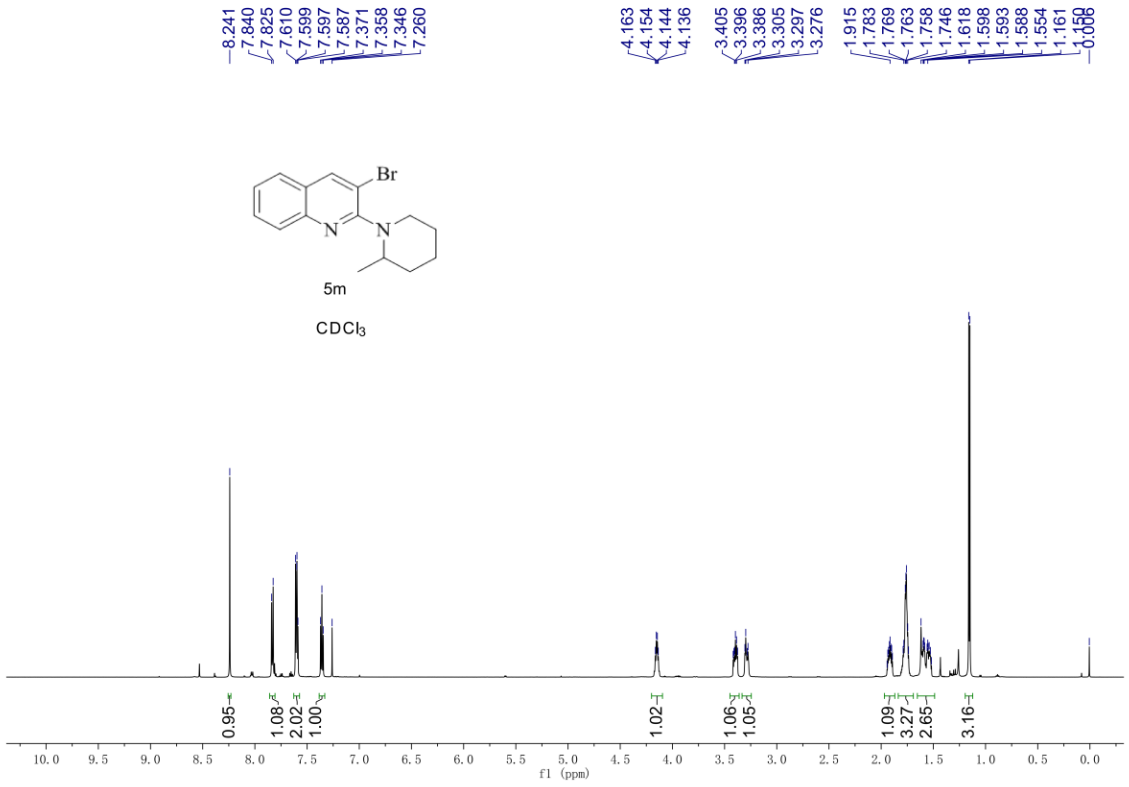

7.906
7.891
7.788
7.774
7.638
7.625
7.591
7.589
7.579
7.577
7.565
7.564
7.551
7.370
7.357
7.343
7.299
7.298
7.286
7.275
7.273
7.242
7.095
7.082
7.070
6.978
6.963
6.925
0.000
Ph
N
H
5i
CDCl3
1.00
0.99
1.01
2.98
1.98
0.98
1.00
1.09
0.81
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


7.874
7.859
7.730
7.716
7.625
7.623
7.611
7.610
7.576
7.573
7.564
7.562
7.550
7.425
7.421
7.413
7.410
7.274
7.272
7.260
7.255
7.249
6.933
6.929
6.922
6.918
6.871
6.856
6.752
3.824
0.000
OMe
N
H
5j
CDCl3
1.00
0.97
1.01
0.97
1.88
1.18
1.92
0.95
0.92
2.98
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)


8.164
8.150
8.116
8.101
8.034
8.020
7.811
7.797
7.759
7.757
7.745
7.733
7.731
7.662
7.648
7.583
7.571
7.558
7.250
7.217
7.203
3.922
0.000
CO2CH3
N
H
5k
CDCl3
1.00
1.90
0.94
1.02
0.98
1.90
0.97
0.93
2.87
f1 (ppm)


166.03
150.93
146.81
141.90
139.49
130.98
129.58
127.55
118.05
77.37
77.16
76.95
52.55
CO2CH3
N
H
5k
CDCl3
f1 (ppm)


7.929
7.914
7.798
7.784
7.653
7.652
7.640
7.638
7.608
7.606
7.603
7.598
7.594
7.592
7.583
7.580
7.324
7.322
7.315
7.301
7.251
6.892
6.877
6.766
1.710
1.501
0.000
Cl
N
H
5l
CDCl3
1.00
0.97
0.98
2.91
2.89
1.00
0.97
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)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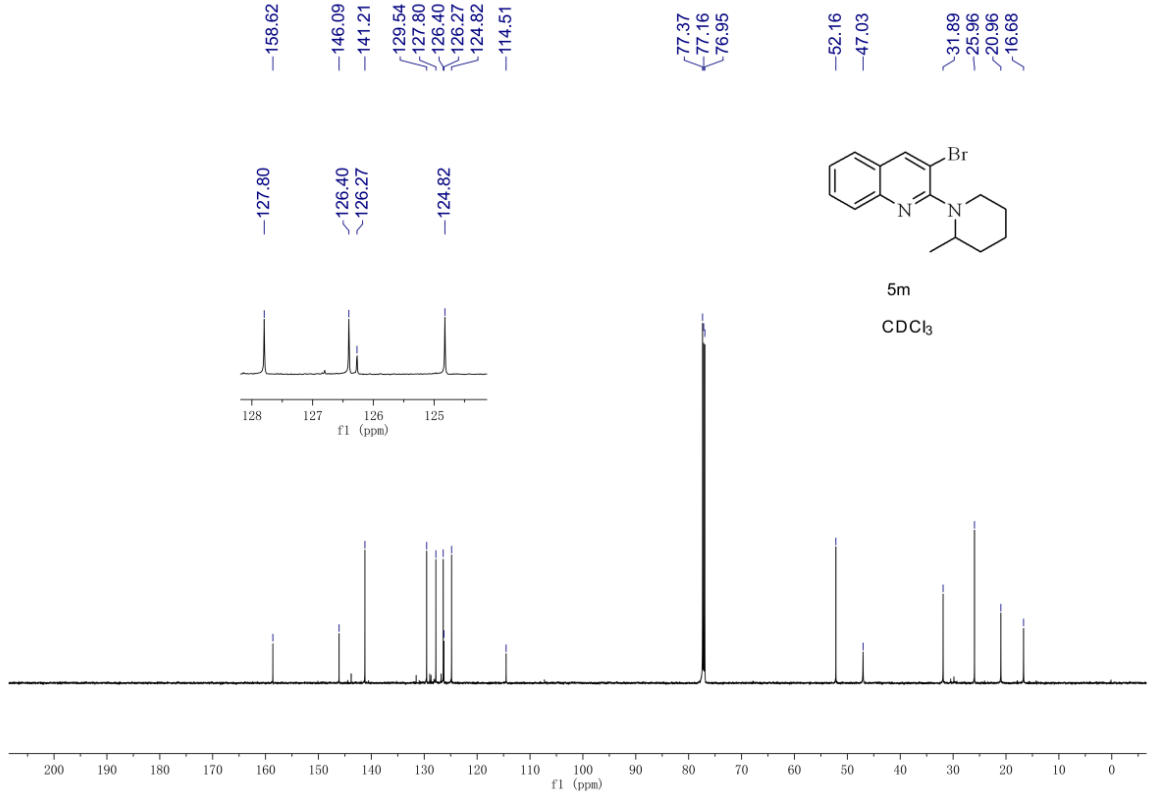
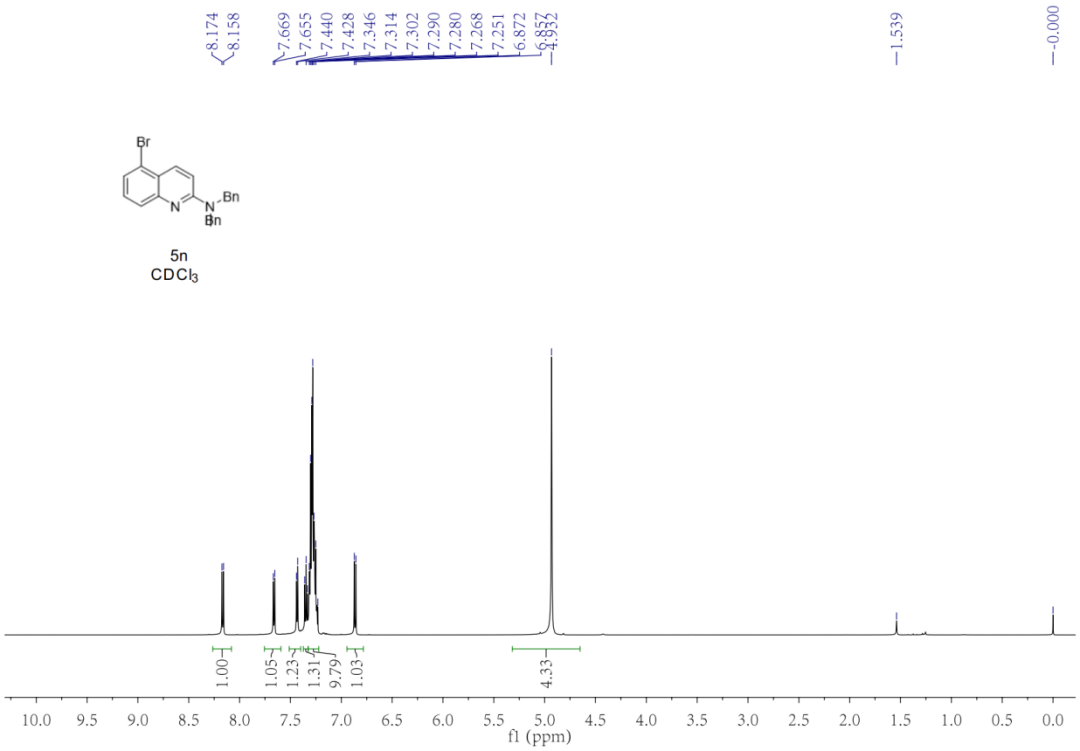
7.599
7.597
7.587
7.371
7.358
7.346
7.260
4.163
4.154
4.144
4.136
3.405
3.396
3.386
3.305
3.297
3.276
1.915
1.783
1.769
1.763
1.758
1.746
1.618
1.598
1.593
1.588
1.554
1.161
1.150
0.000
Br
N
N
5m
CDCl3
0.95
1.08
2.02
1.00
1.02
1.06
1.05
1.09
3.27
2.65
3.16
f1 (ppm)


158.62
146.09
141.21
129.54
127.80
126.40
126.27
124.82
114.51
77.37
77.16
76.95
52.16
47.03
31.89
25.96
20.96
16.68
127.80
126.40
126.27
124.82
Br
N
N
5m
CDCl3
f1 (ppm)
f1 (ppm)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8.158
7.669
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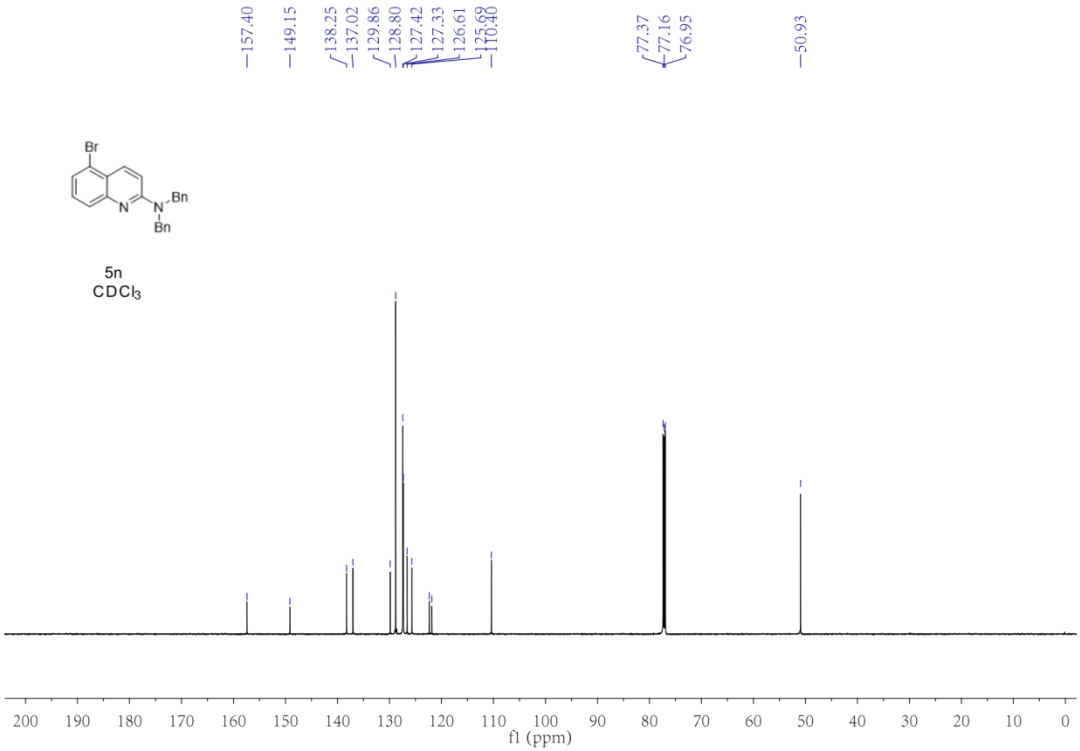
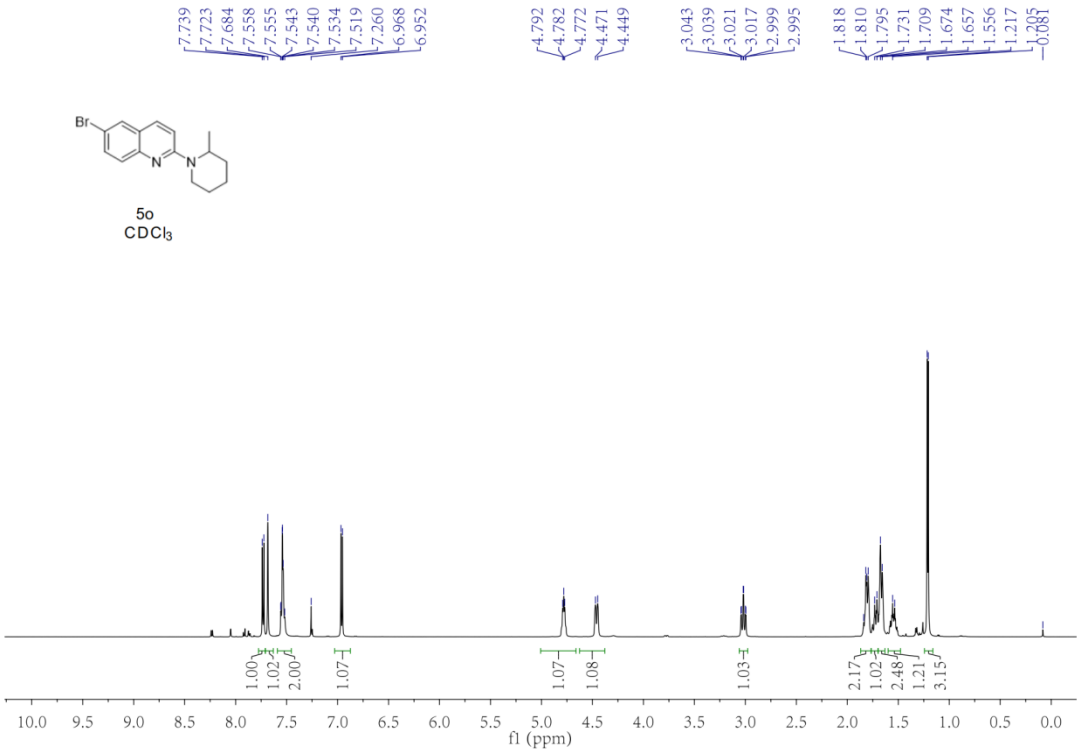
7.440
7.428
7.346
7.314
7.302
7.290
7.280
7.268
7.251
6.872
6.857
4.932
1.539
0.000
Br
N
Bn
Bn
5n
CDCl3
1.00
1.05
1.23
1.31
9.79
1.03
4.33
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


157.40
149.15
138.25
137.02
129.86
128.80
127.42
127.33
126.61
125.68
110.40
77.37
77.16
76.95
50.93
Br
N
Bn
Bn
5n
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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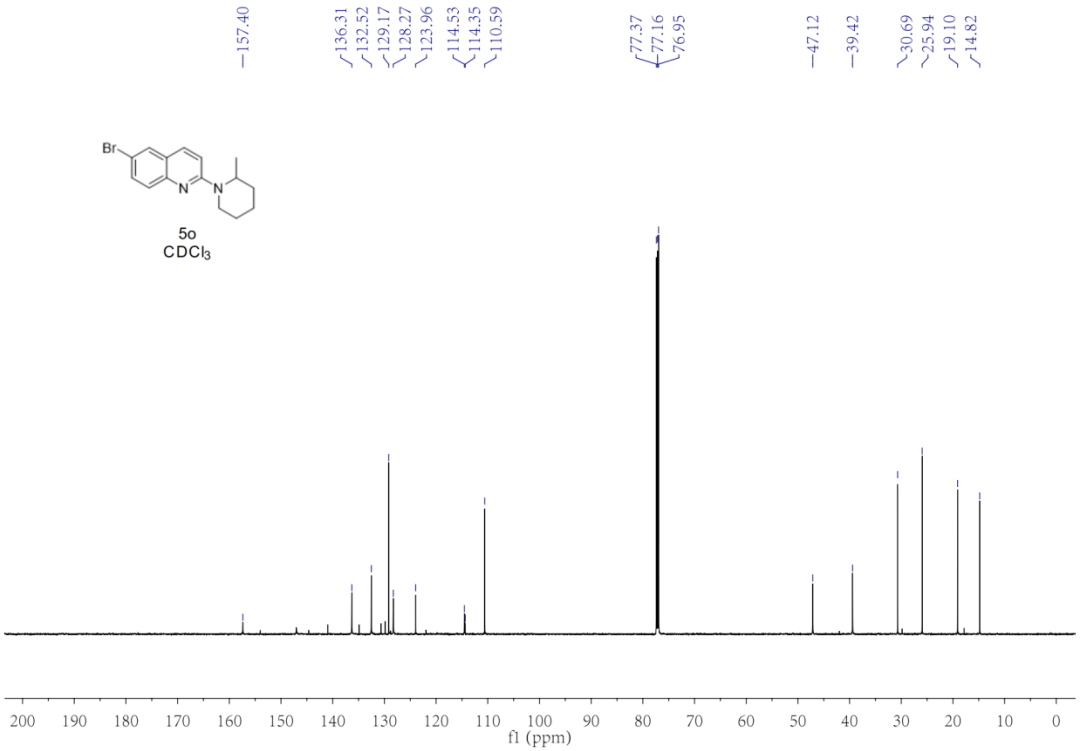
7.558
7.555
7.543
7.540
7.534
7.519
7.260
6.968
6.952
4.792
4.782
4.772
4.471
4.449
3.043
3.039
3.021
3.017
2.999
2.995
1.818
1.810
1.795
1.731
1.709
1.674
1.657
1.556
1.217
1.205
0.081
Br
N
N
5o
CDCl3
1.00
1.02
2.00
1.07
1.07
1.08
1.03
2.17
1.02
2.48
1.21
3.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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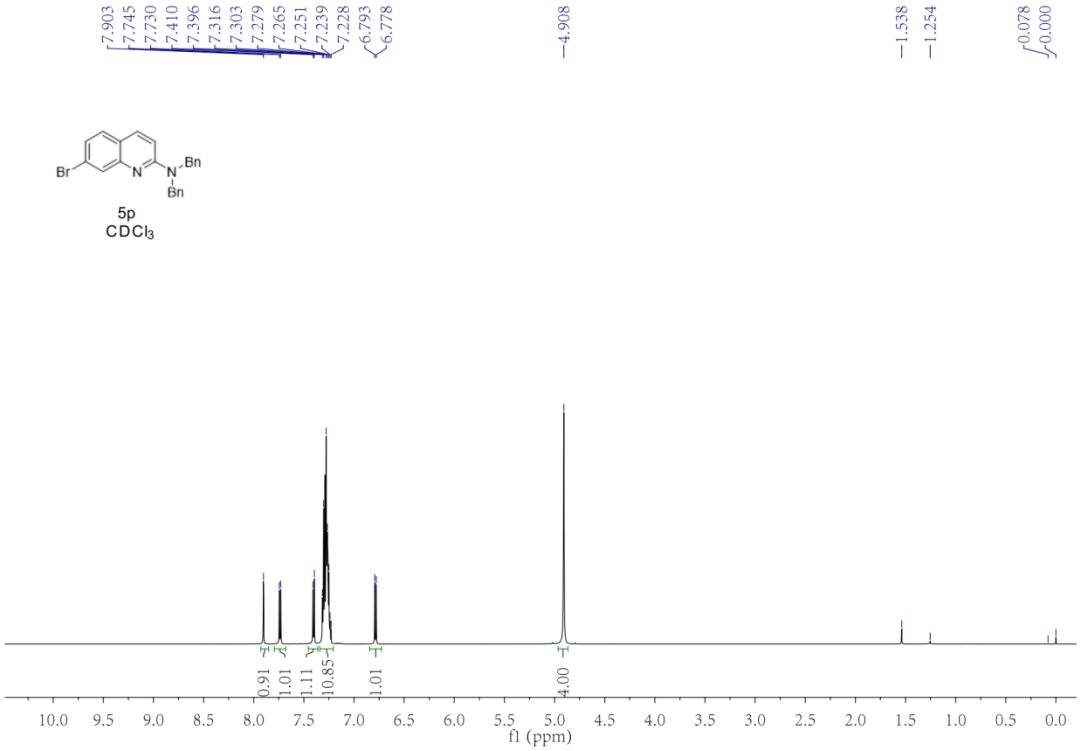
136.31
132.52
129.17
128.27
123.96
114.53
114.35
110.59
77.37
77.16
76.95
47.12
39.42
30.69
25.94
19.10
14.82
Br
N
N
5o
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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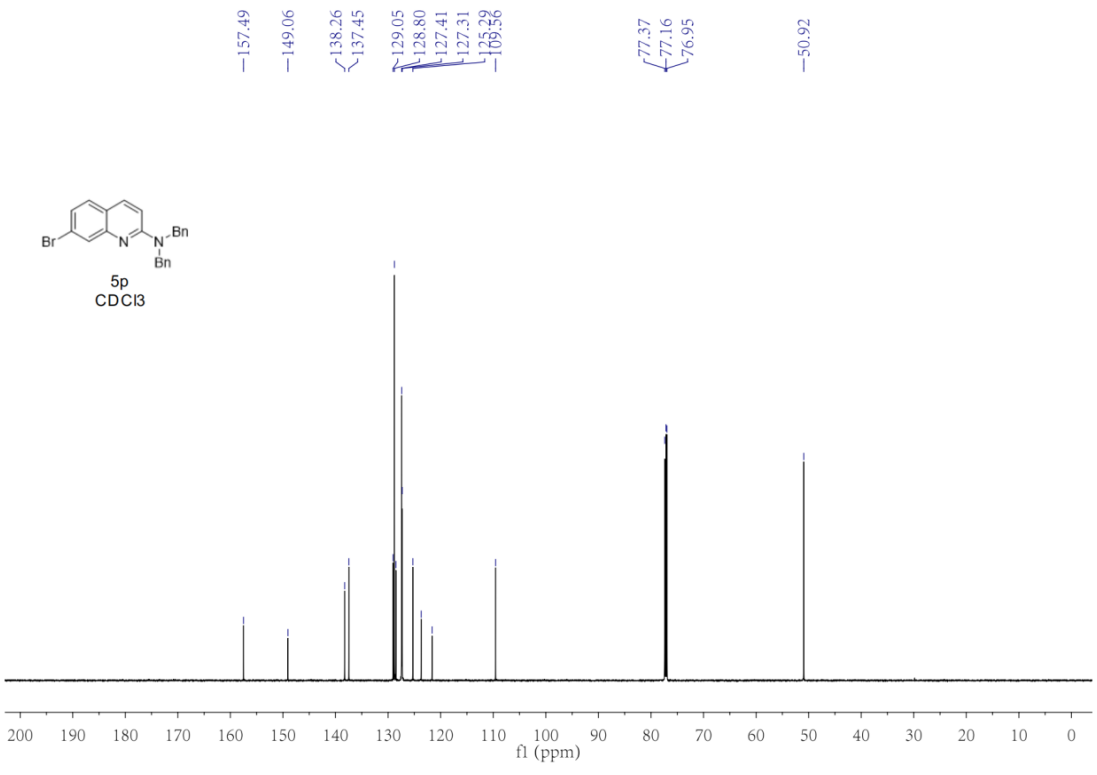
7.730
7.410
7.396
7.316
7.303
7.279
7.265
7.251
7.239
7.228
6.793
6.778
4.908
1.538
1.254
0.078
0.000
Br
N
N
Bn
Bn
5p
CDCl3
0.91
1.01
1.11
10.85
1.01
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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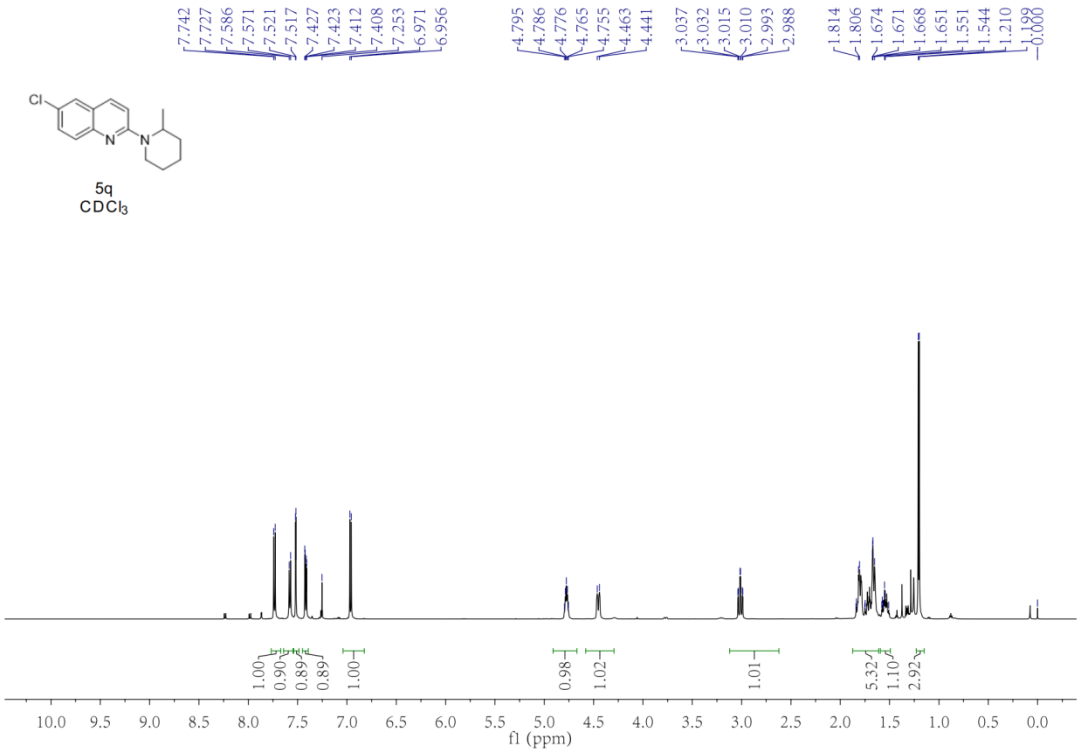
149.06
138.26
137.45
129.05
128.80
127.41
127.31
125.29
109.56
77.37
77.16
76.95
50.92
Br
N
N
Bn
Bn
5p
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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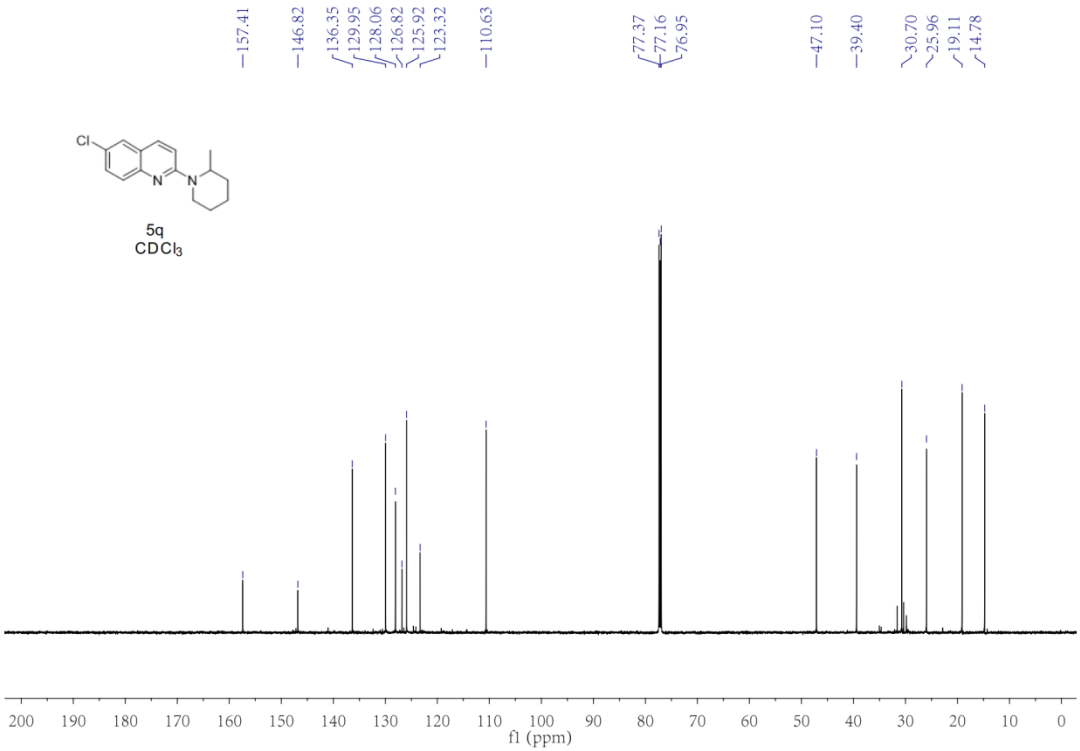
7.517
7.427
7.423
7.412
7.408
7.253
6.971
6.956
4.795
4.786
4.776
4.765
4.755
4.463
4.441
3.037
3.032
3.015
3.010
2.993
2.988
1.814
1.806
1.674
1.671
1.668
1.651
1.551
1.544
1.210
1.198
0.000
Cl
N
N
5q
CDCl3
1.00
0.90
0.89
0.89
1.00
0.98
1.02
1.01
5.32
1.10
2.92
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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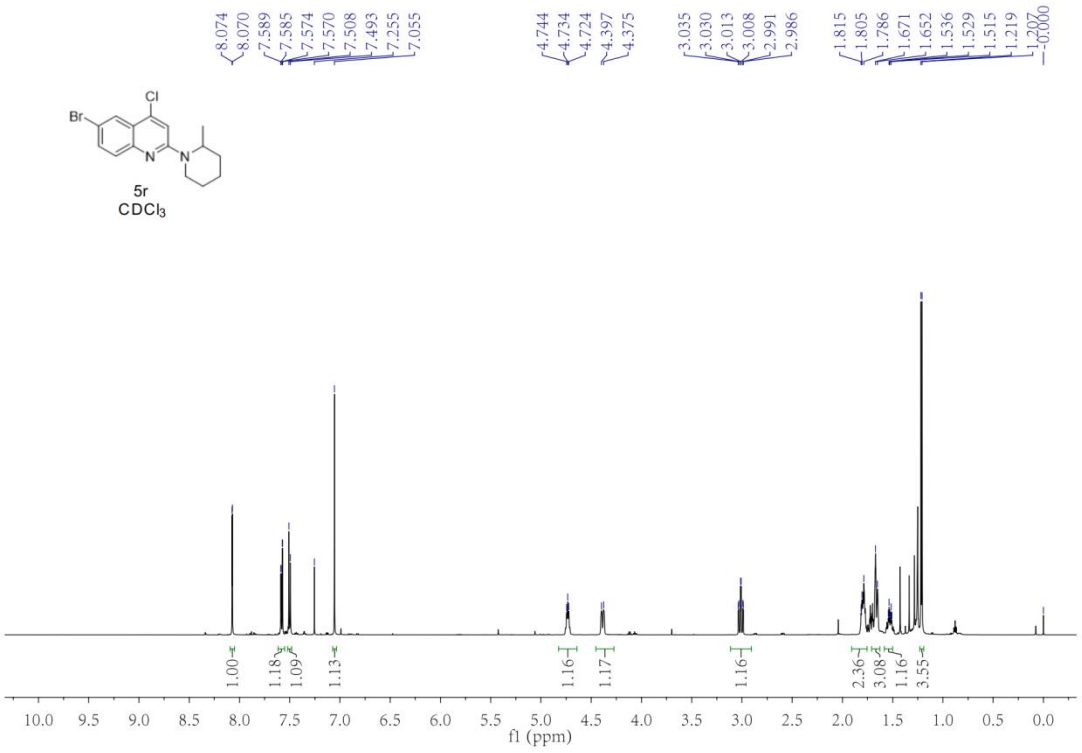
136.35
129.95
128.06
126.82
125.92
123.32
110.63
77.37
77.16
76.95
47.10
39.40
30.70
25.96
19.11
14.78
Cl
N
N
5q
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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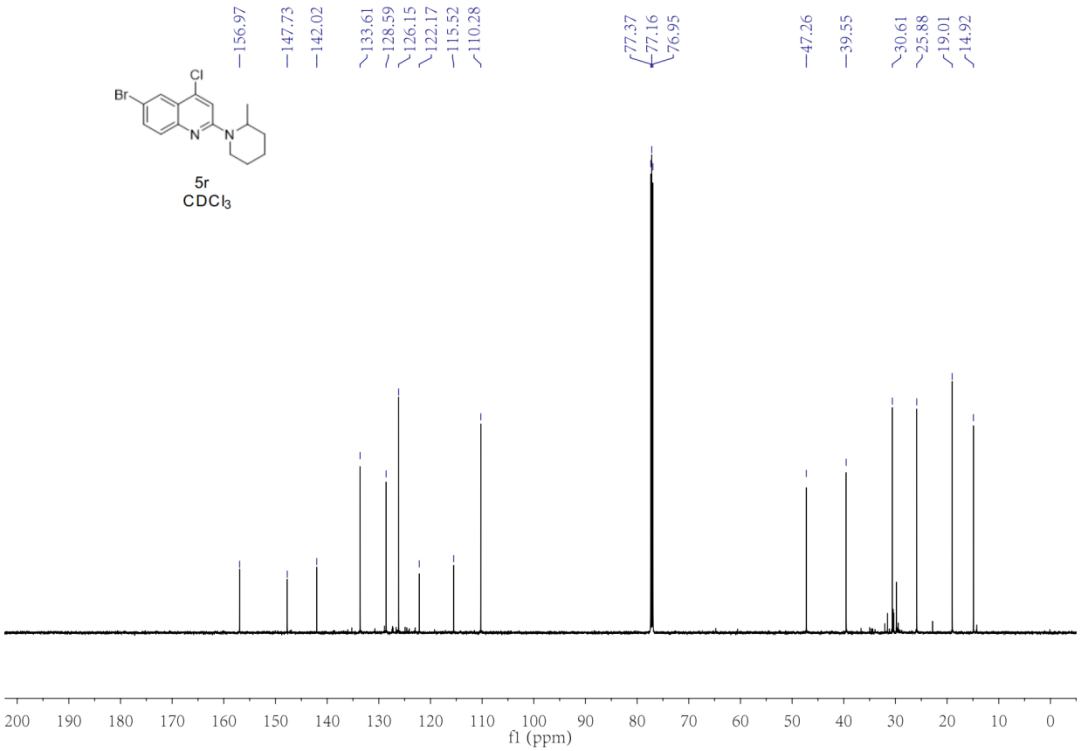
7.570
7.508
7.493
7.255
7.055
4.744
4.734
4.724
4.397
4.375
3.035
3.030
3.013
3.008
2.991
2.986
1.815
1.805
1.786
1.671
1.652
1.536
1.529
1.515
1.219
1.207
0.000
Br
Cl
N
N
5r
CDCl3
1.00
1.18
1.09
1.13
1.16
1.17
1.16
2.36
3.08
1.16
3.55
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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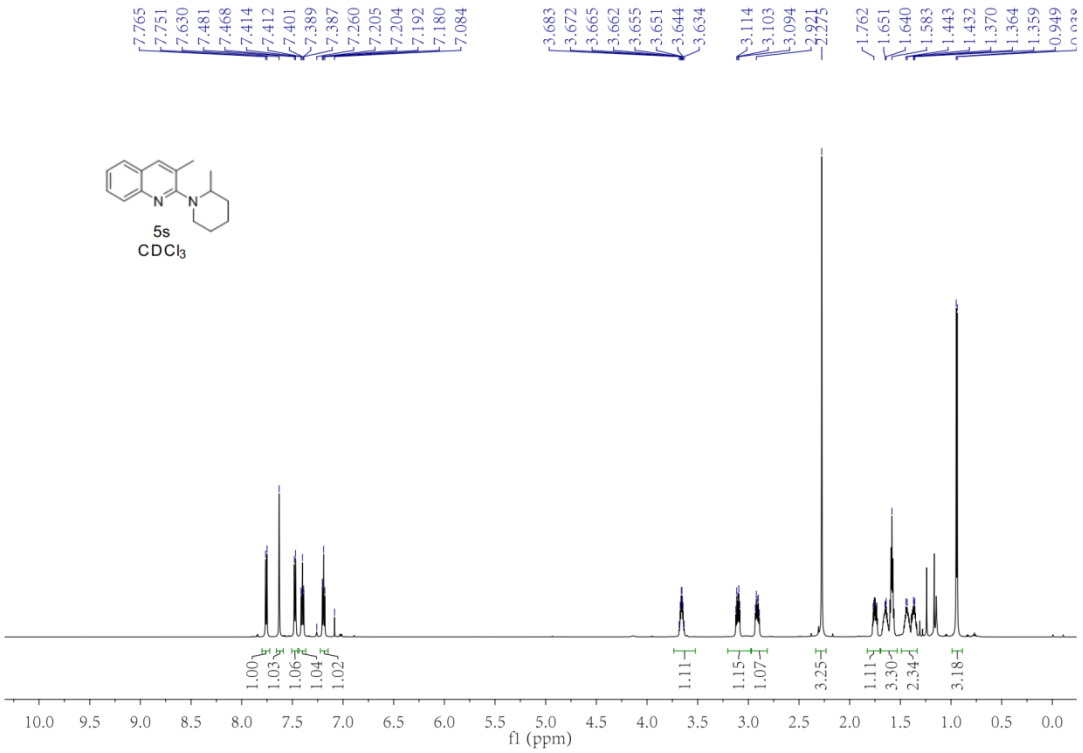
142.02
133.61
128.59
126.15
122.17
115.52
110.28
77.37
77.16
76.95
47.26
39.55
30.61
25.88
19.01
14.92
Br
Cl
N
N
5r
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.468
7.414
7.412
7.401
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7.387
7.260
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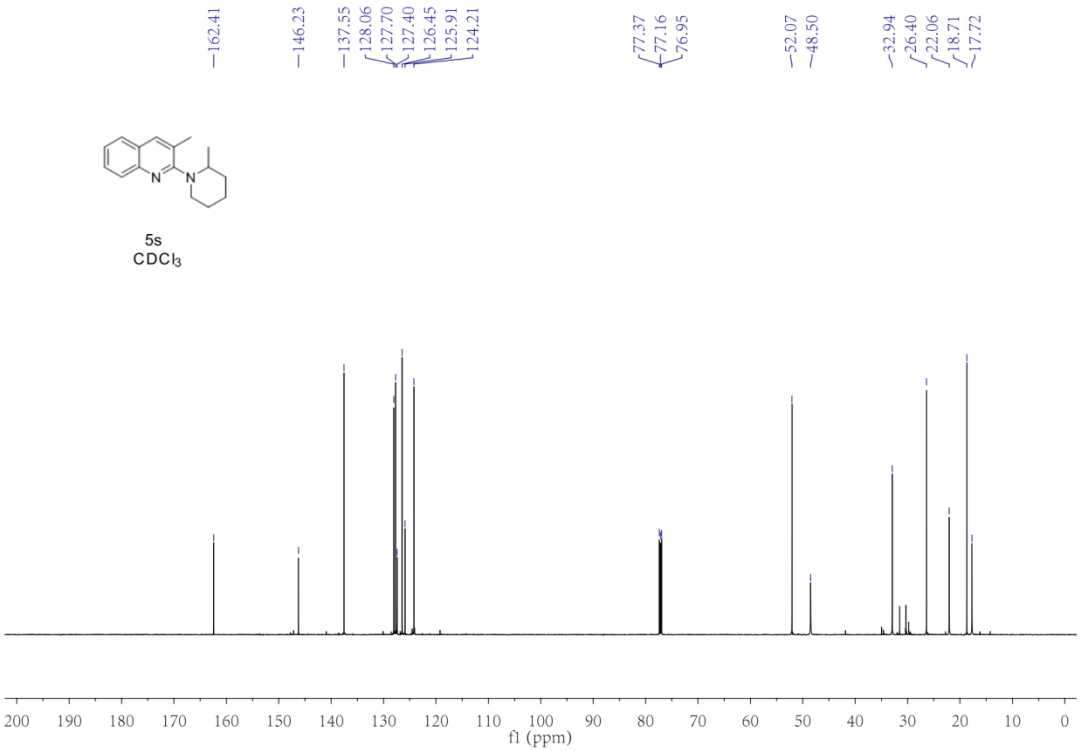
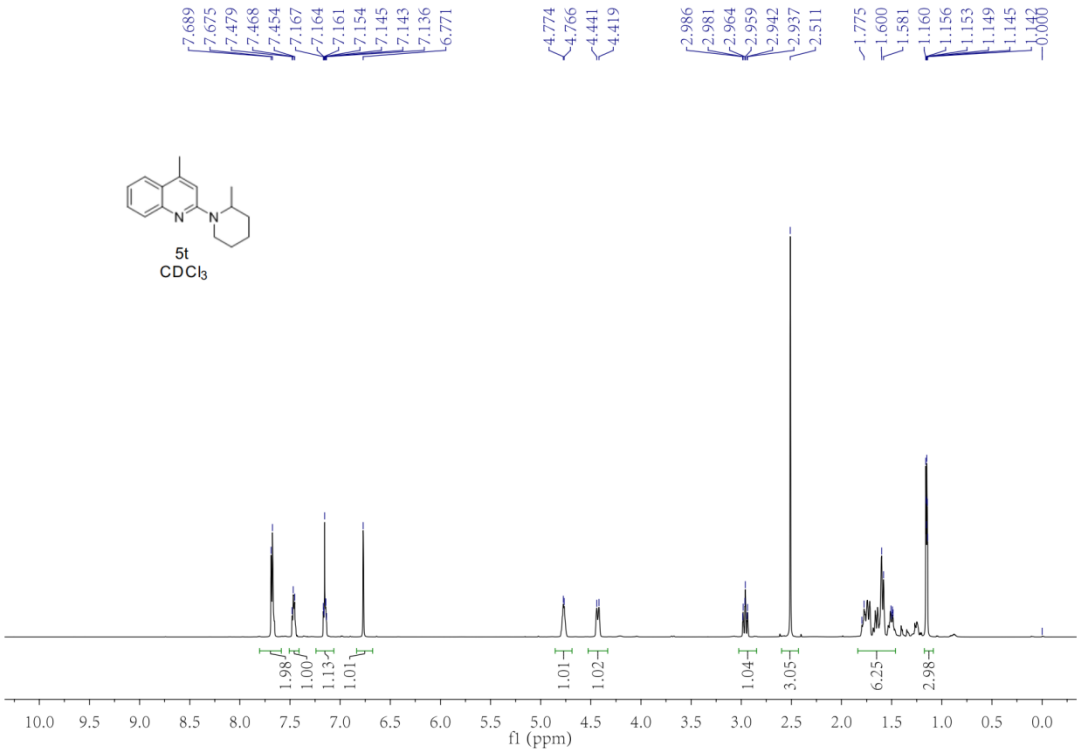
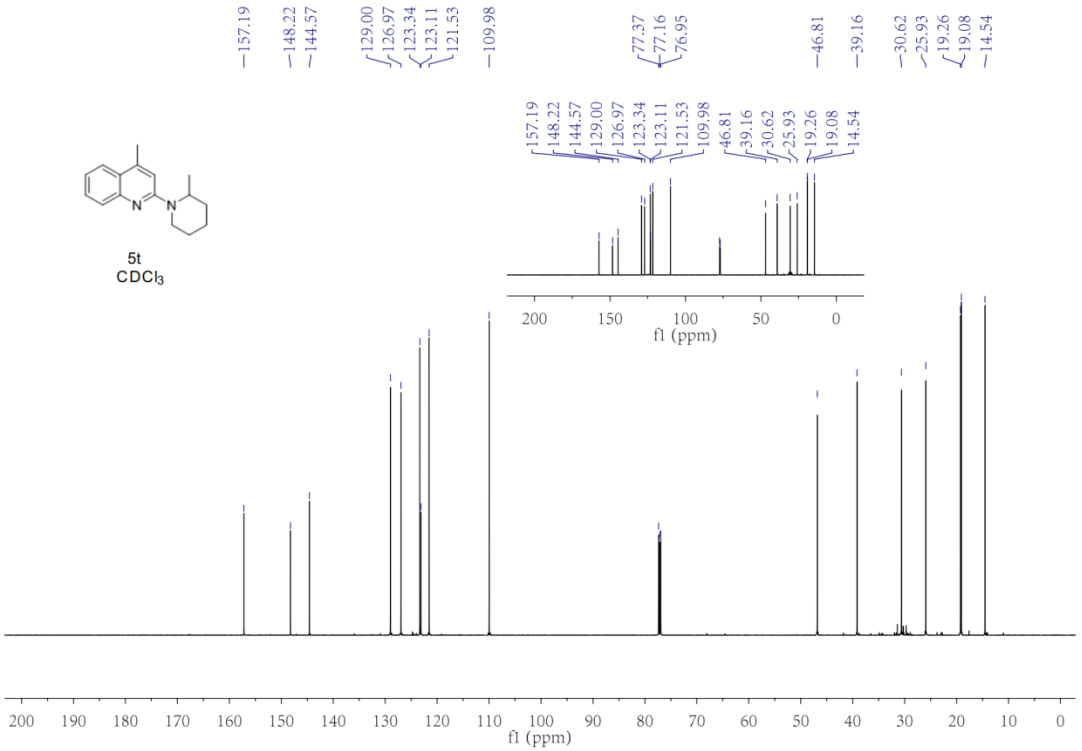
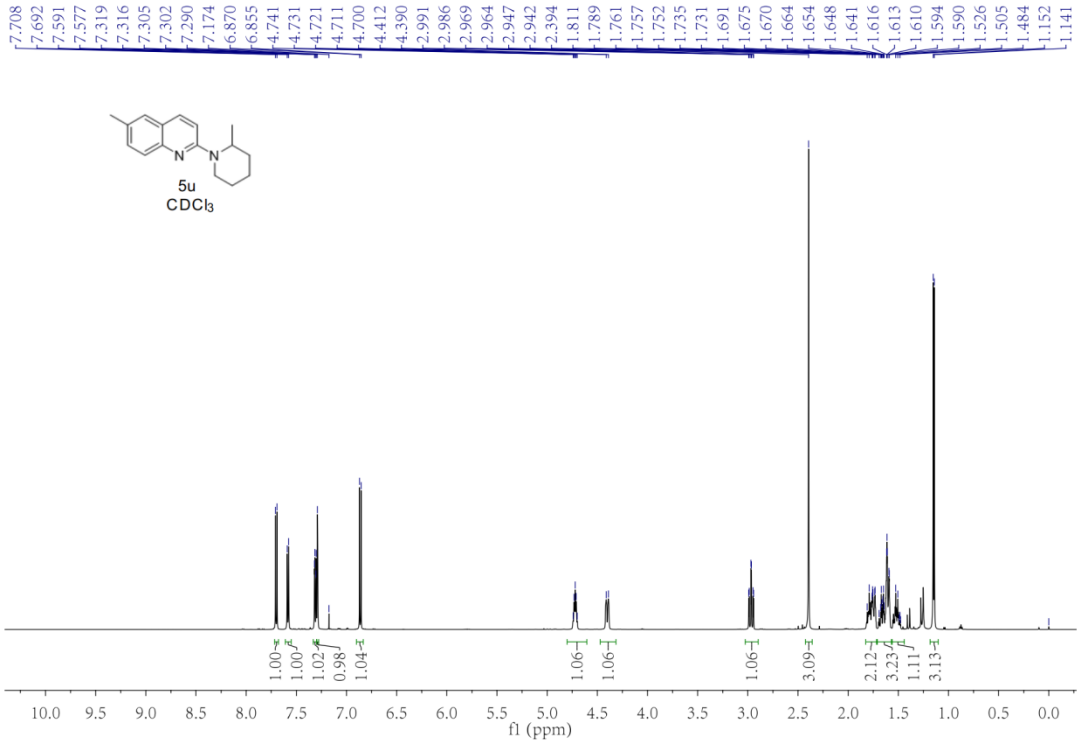
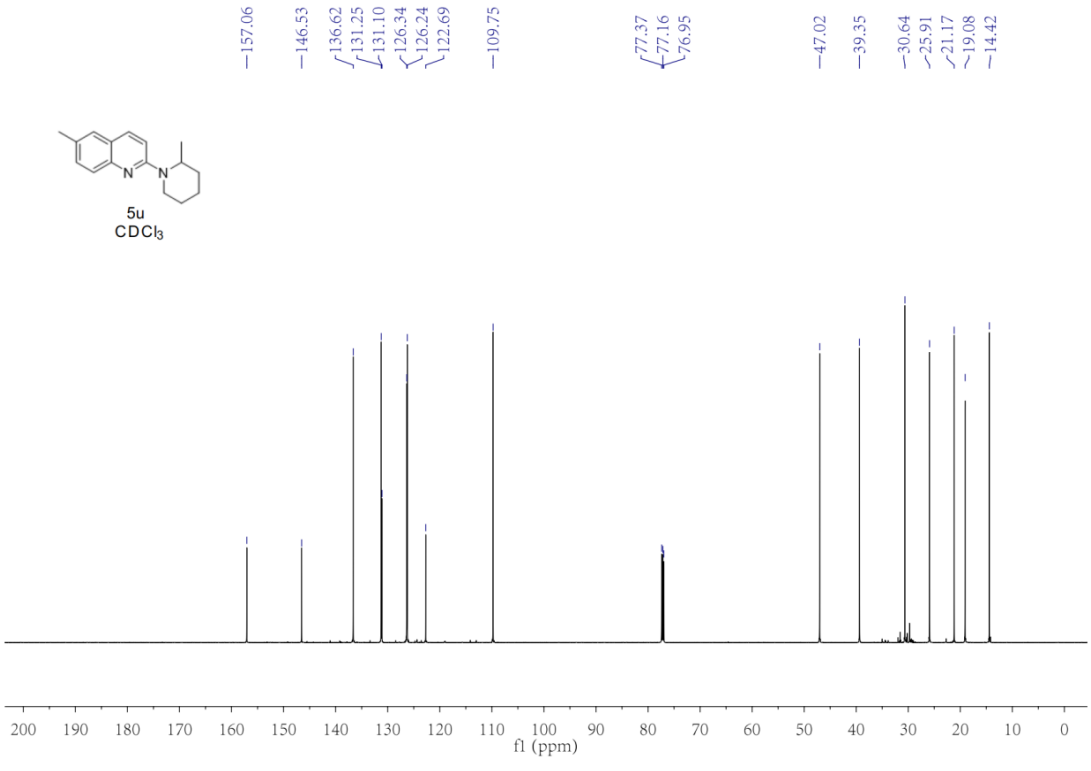
7.204
7.192
7.180
7.084
3.683
3.672
3.665
3.662
3.655
3.651
3.644
3.634
3.114
3.103
3.094
2.921
2.275
1.762
1.651
1.640
1.583
1.443
1.432
1.370
1.364
1.359
0.949
5s
CDCl3
1.00
1.03
1.06
1.04
1.02
1.11
1.15
1.07
3.25
1.11
3.30
2.34
3.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

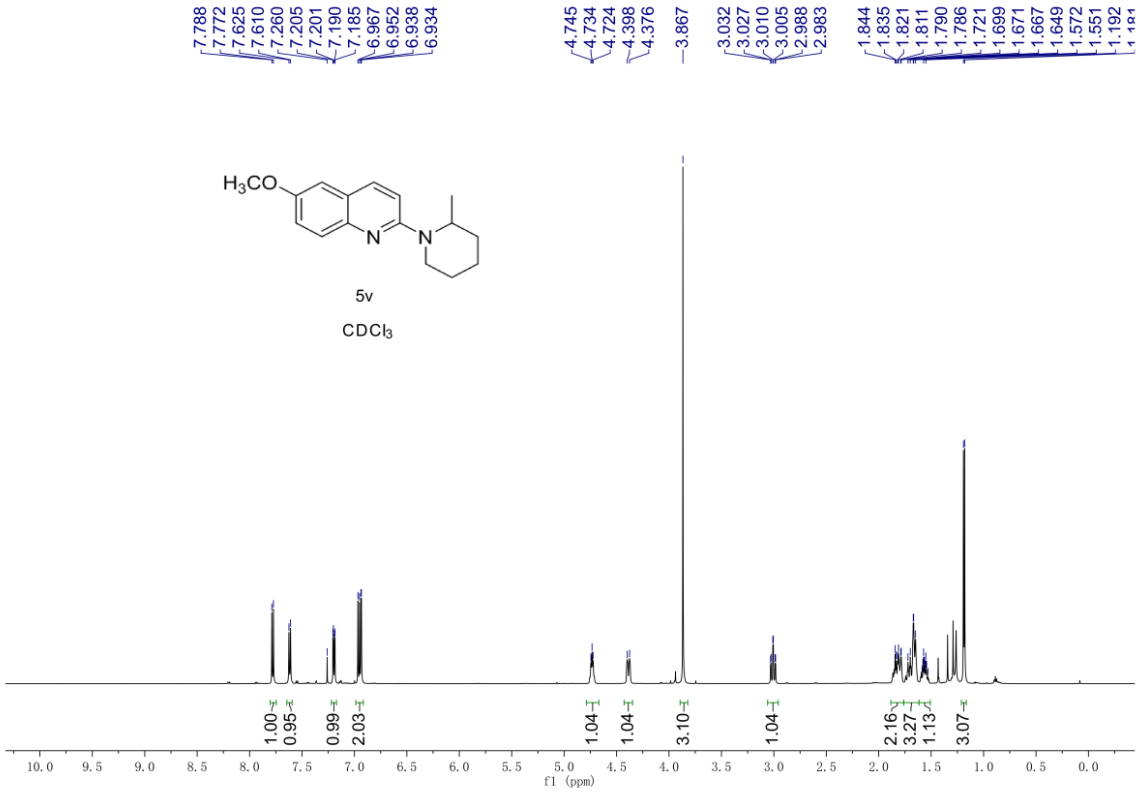

162.41
146.23
137.55
128.06
127.70
127.40
126.45
125.91
124.21
77.37
77.16
76.95
52.07
48.50
32.94
26.40
22.06
18.71
17.72
5s
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

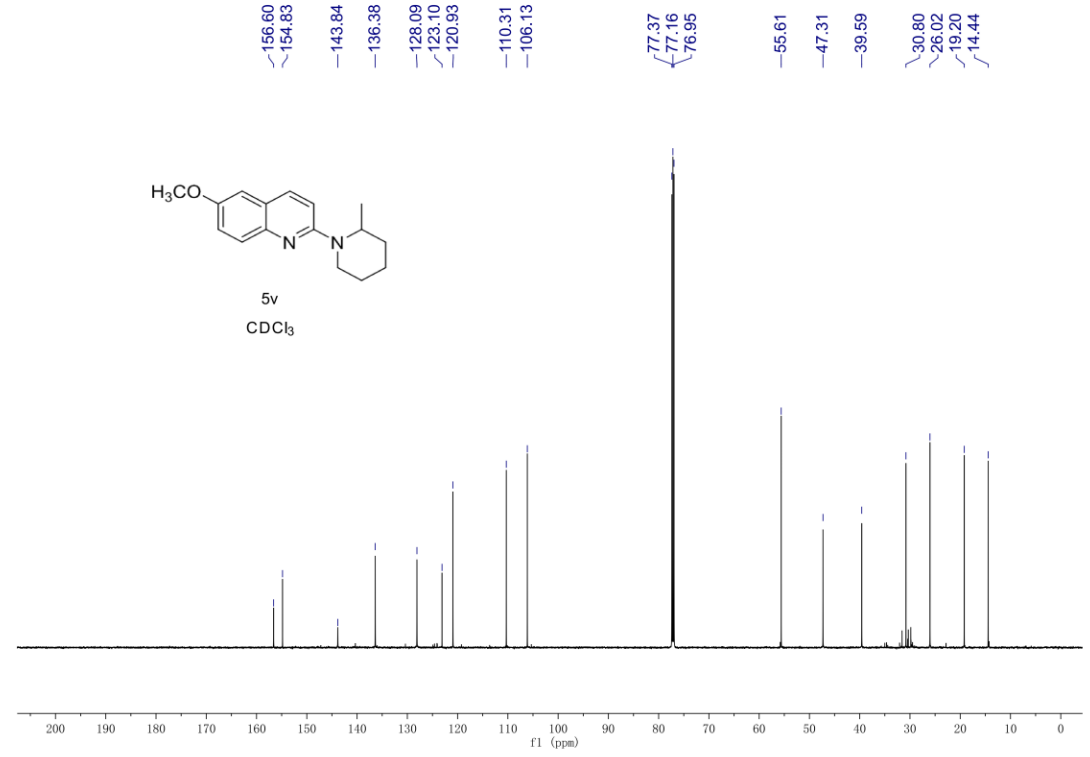

7.689
7.675
7.479
7.468
7.454
7.167
7.164
7.161
7.154
7.145
7.143
7.136
6.771
4.774
4.766
4.441
4.419
2.986
2.981
2.964
2.959
2.942
2.937
2.511
1.775
1.600
1.581
1.160
1.156
1.153
1.149
1.145
1.142
0.000
5t
CDCl3
1.98
1.00
1.13
1.01
1.01
1.02
1.04
3.05
6.25
2.98
fl (ppm)

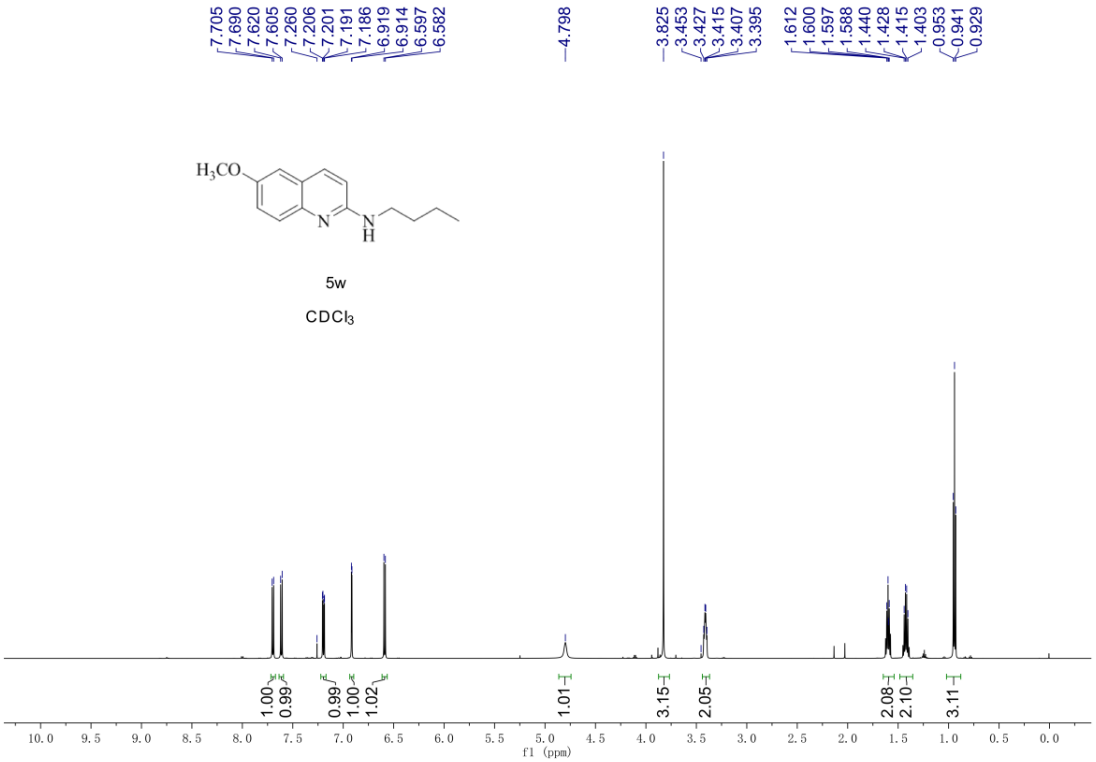

157.19
148.22
144.57
129.00
126.97
123.34
123.11
121.53
109.98
77.37
77.16
76.95
46.81
39.16
30.62
25.93
19.26
19.08
14.54
5t
CDCl3
fl (ppm)
fl (ppm)

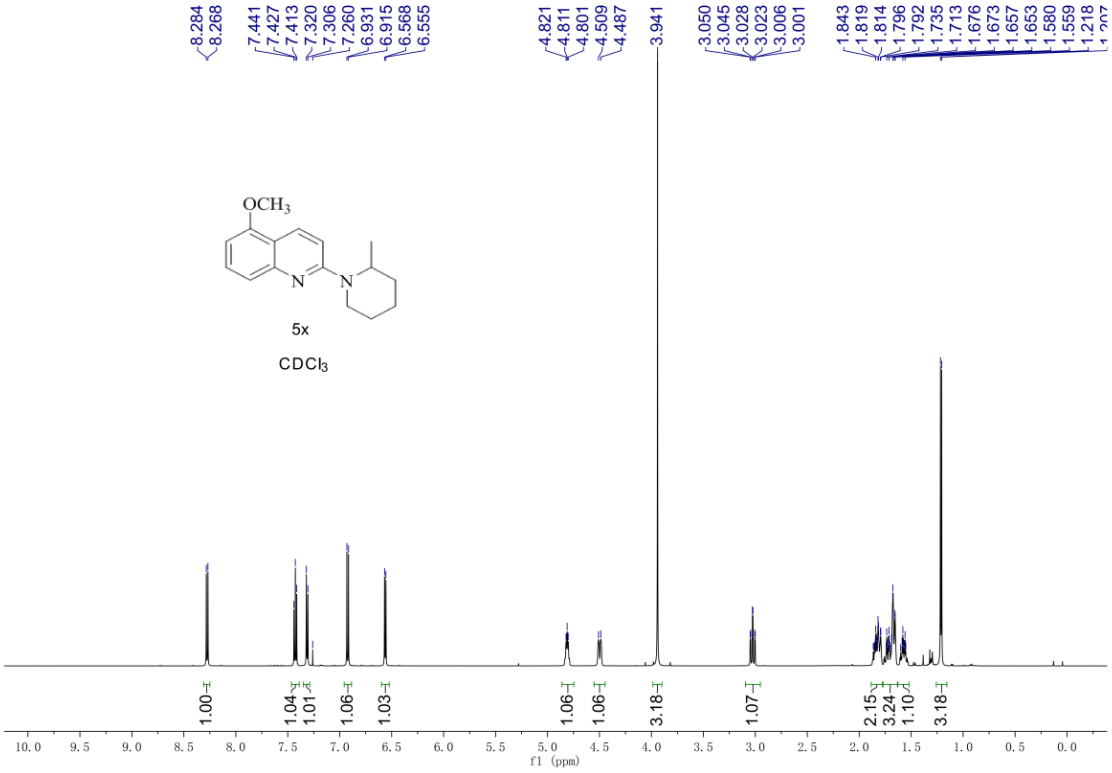

7.708
7.692
7.591
7.577
7.319
7.316
7.305
7.302
7.290
7.174
6.870
6.855
4.741
4.731
4.721
4.711
4.700
4.412
4.390
2.991
2.986
2.969
2.964
2.947
2.942
2.394
1.811
1.789
1.761
1.757
1.752
1.735
1.731
1.691
1.675
1.670
1.664
1.654
1.648
1.641
1.616
1.613
1.610
1.594
1.590
1.526
1.505
1.484
1.152
1.141
5u
CDCl3
1.00
1.00
1.02
0.98
1.04
1.06
1.06
1.06
3.09
2.12
3.23
1.11
3.13
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)

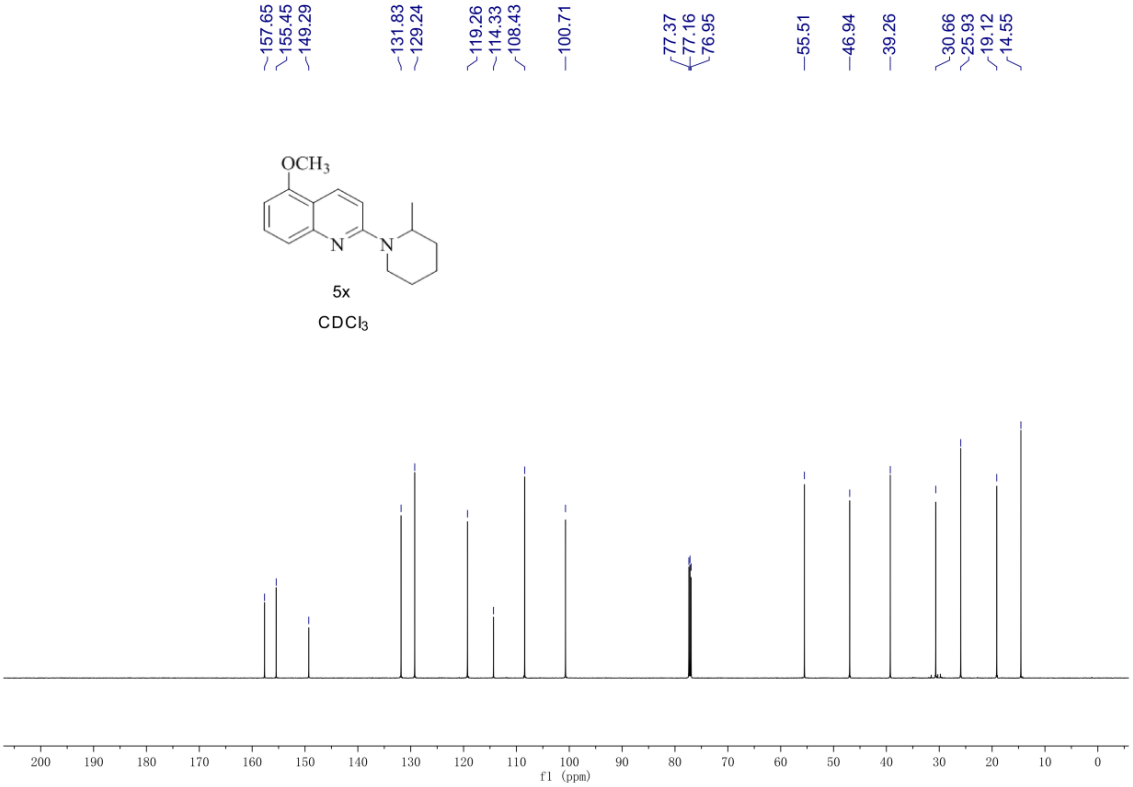

157.06
146.53
136.62
131.25
131.10
126.34
126.24
122.69
109.75
77.37
77.16
76.95
47.02
39.35
30.64
25.91
21.17
19.08
14.42
5u
CDCl3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

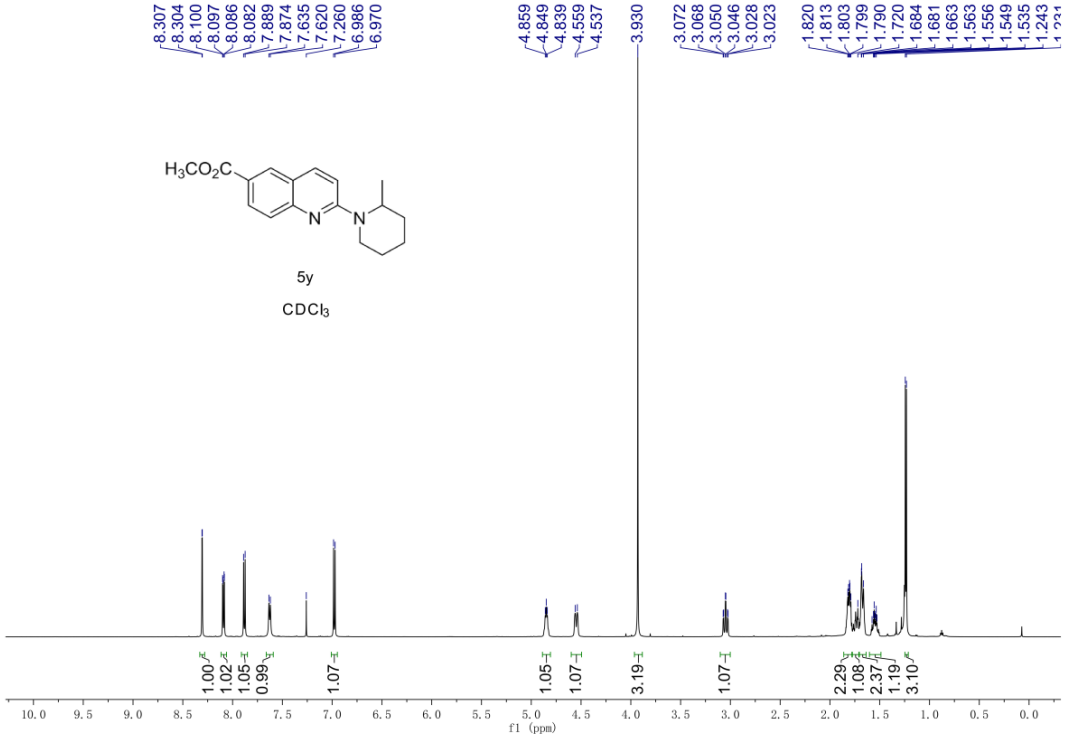

7.788
7.772
7.625
7.610
7.260
7.205
7.201
7.190
7.185
6.967
6.952
6.938
6.934
4.745
4.734
4.724
4.398
4.376
3.867
3.032
3.027
3.010
3.005
2.988
2.983
1.844
1.835
1.821
1.811
1.790
1.786
1.721
1.699
1.671
1.667
1.649
1.572
1.551
1.192
H3CO
N
N
5v
CDCl3
1.00
0.95
0.99
2.03
1.04
1.04
3.10
1.04
2.16
3.27
1.13
3.07
f1 (ppm)

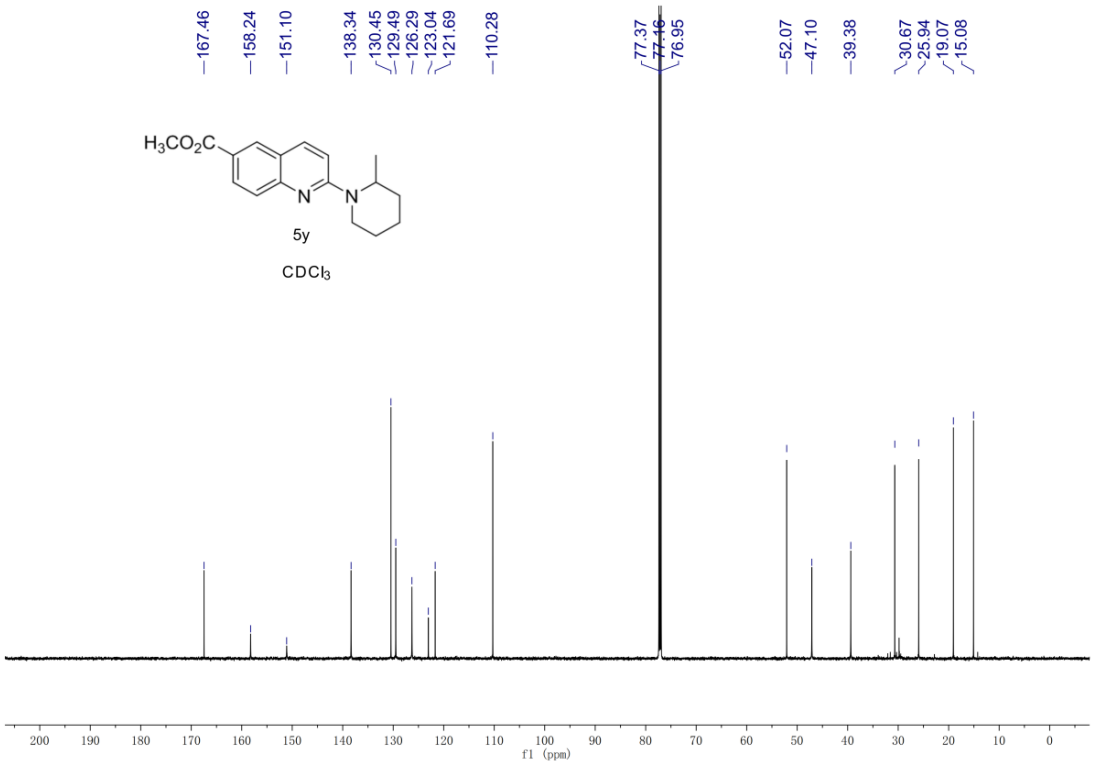

156.60
154.83
143.84
136.38
128.09
123.10
120.93
110.31
106.13
77.37
77.16
76.95
55.61
47.31
39.59
30.80
26.02
19.20
14.44
H3CO
N
N
5v
CDCl3
f1 (ppm)


7.705
7.690
7.620
7.605
7.260
7.206
7.201
7.191
7.186
6.919
6.914
6.597
6.582
4.798
3.825
3.453
3.427
3.415
3.407
3.395
1.612
1.600
1.597
1.588
1.440
1.428
1.415
1.403
0.953
0.941
0.929
H3CO
N
N
H
5w
CDCl3
1.00
0.99
0.99
1.00
1.02
1.01
3.15
2.05
2.08
2.10
3.11
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)


8.284
8.268
7.441
7.427
7.413
7.320
7.306
7.260
6.931
6.915
6.568
6.555
4.821
4.811
4.801
4.509
4.487
3.941
3.050
3.045
3.028
3.023
3.006
3.001
1.843
1.819
1.814
1.796
1.792
1.735
1.713
1.676
1.673
1.657
1.653
1.580
1.559
1.218
OCH3
N
N
5x
CDCl3
1.00
1.04
1.01
1.06
1.03
1.06
1.06
3.18
1.07
2.15
3.24
1.10
3.18
f1 (ppm)


157.65
155.45
149.29
131.83
129.24
119.26
114.33
108.43
100.71
77.37
77.16
76.95
55.51
46.94
39.26
30.66
25.93
19.12
14.55
OCH3
N
N
5x
CDCl3
f1 (ppm)

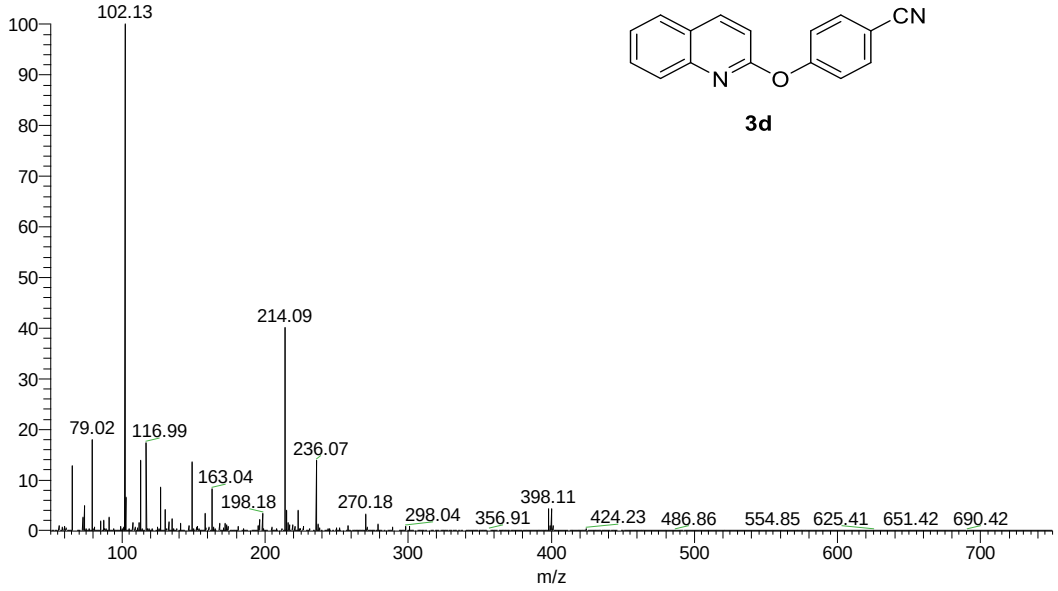




8. HRMS Spectra

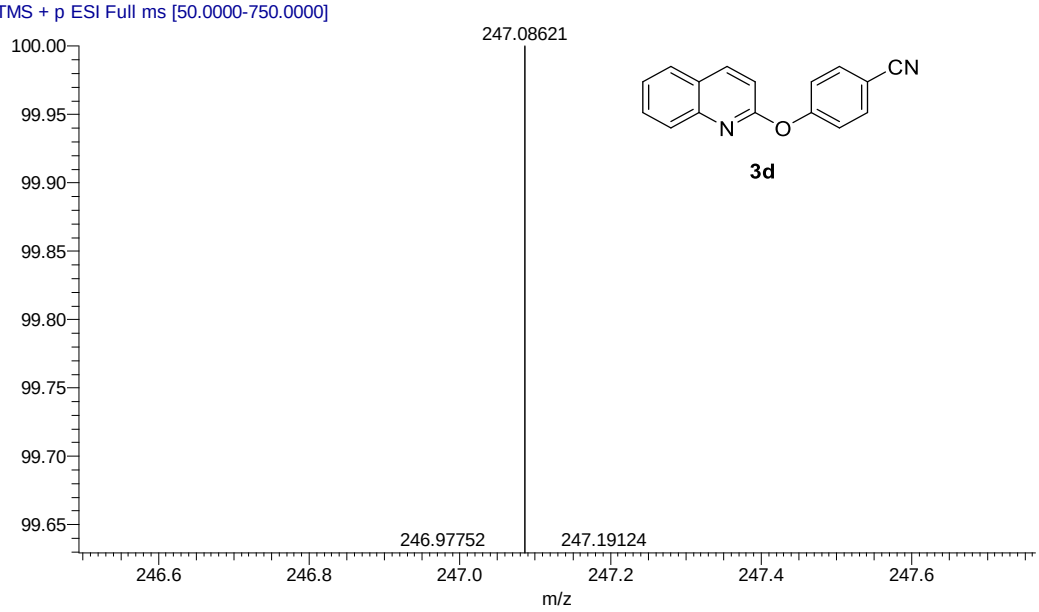
Spectra data are shown from the next page.

B-069 #1 RT: 0.00 AV: 1 NL: 1.28E8
T: FTMS + p ESI Full ms [50.0000-750.0000]



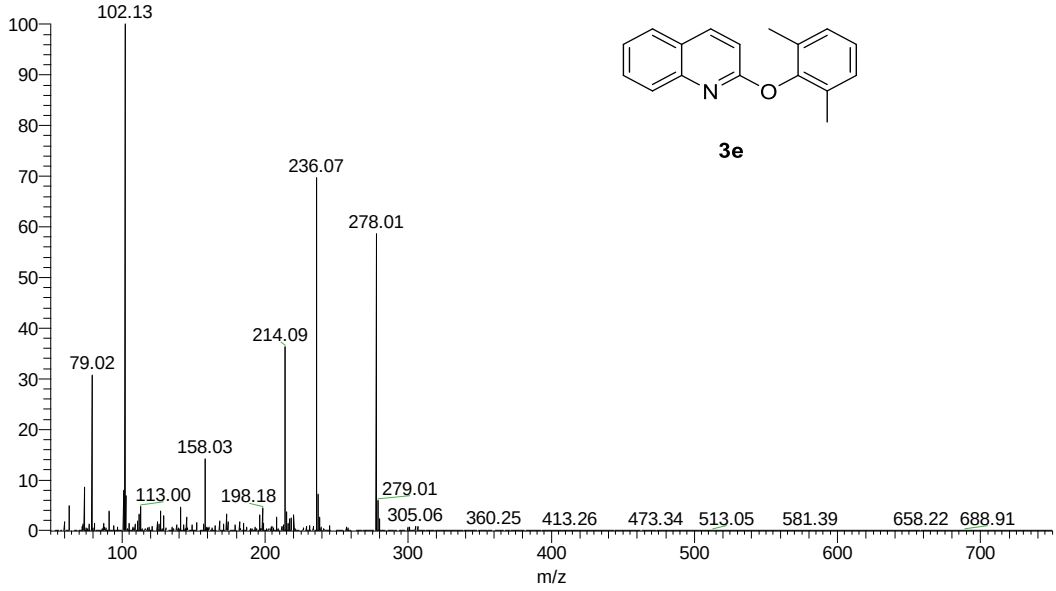
3d

B-069 #27 RT: 0.26 AV: 1 NL: 3.54E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



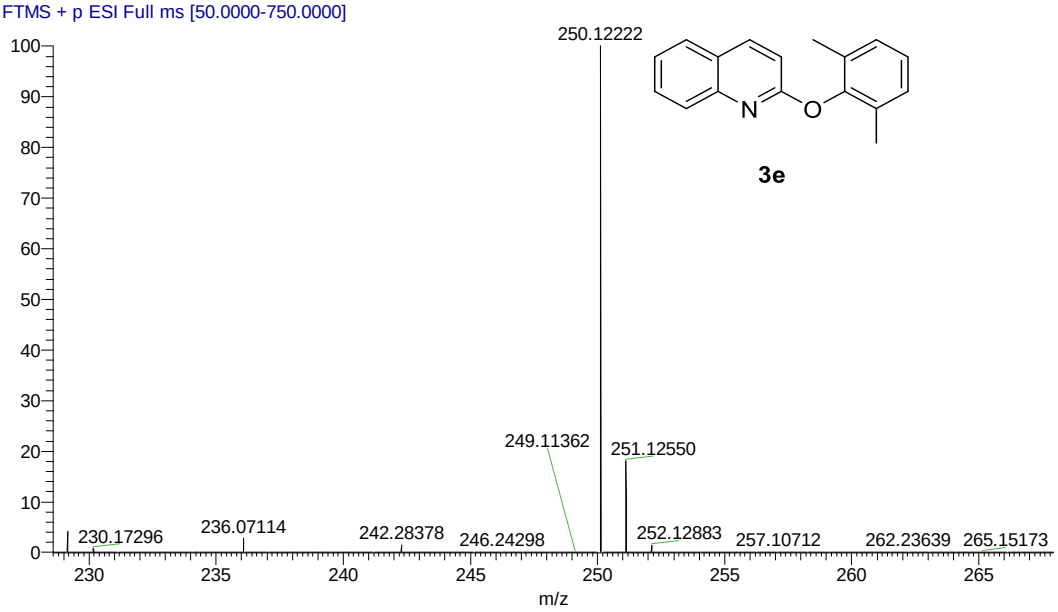
3d

B131 #1 RT: 0.00 AV: 1 NL: 3.47E7
T: FTMS + p ESI Full ms [50.0000-750.0000]



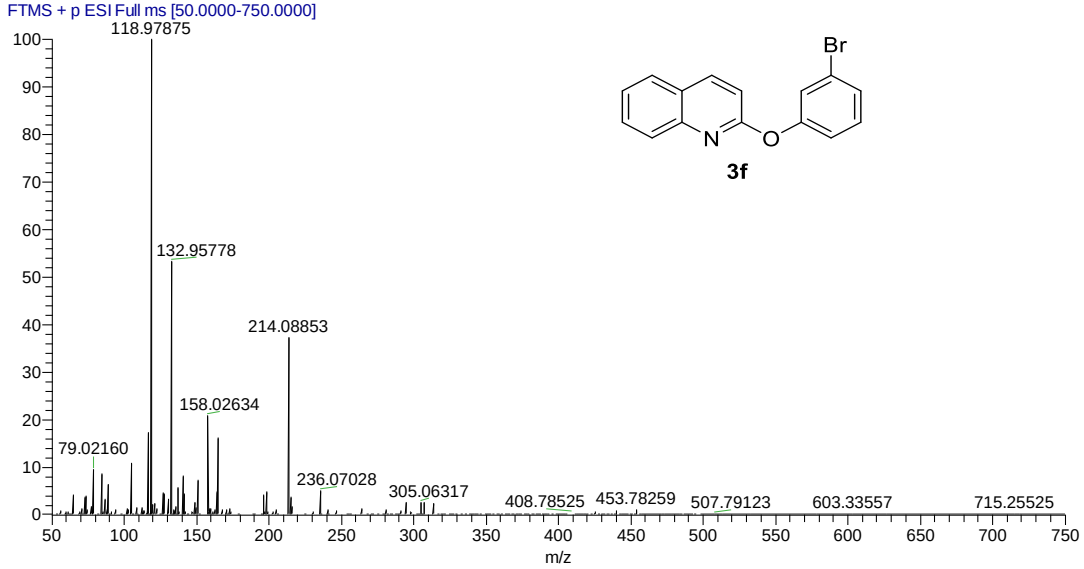
3e

B131 #27 RT: 0.26 AV: 1 NL: 2.38E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



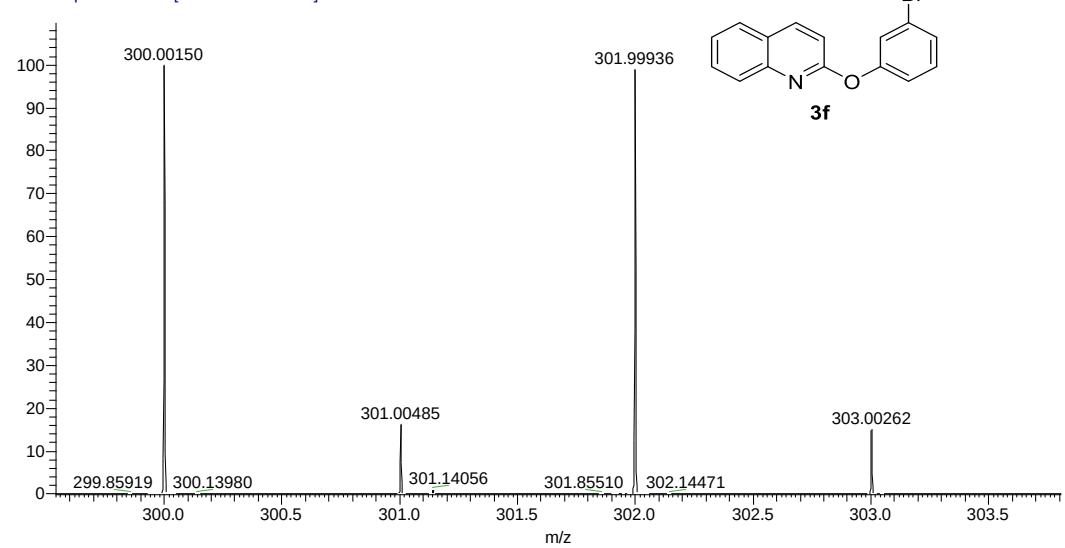
3e

B85 #1 RT: 0.00 AV: 1 NL: 7.80E7
T: FTMS + p ESI Full ms [50.0000-750.0000]

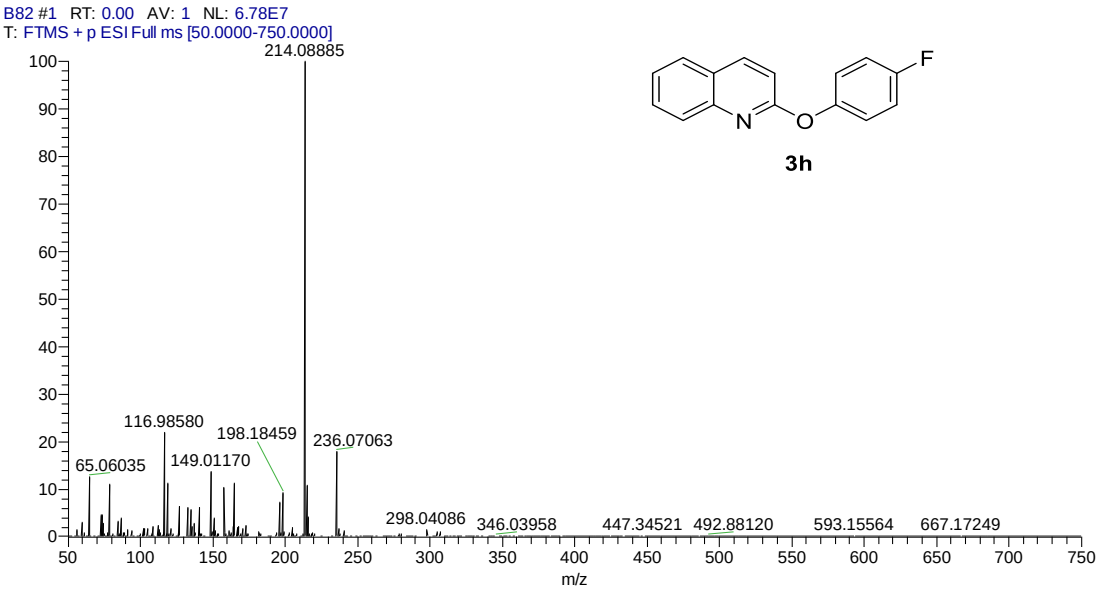


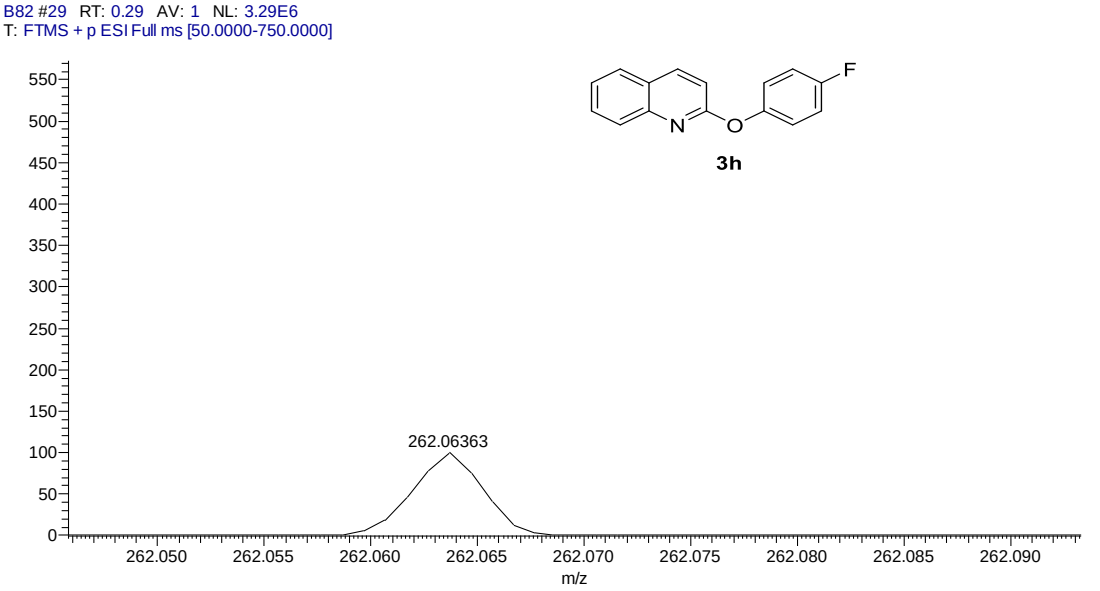
3f

B85 #35 RT: 0.35 AV: 1 NL: 3.09E8
T: FTMS + p ESI Full ms [50.0000-750.0000]

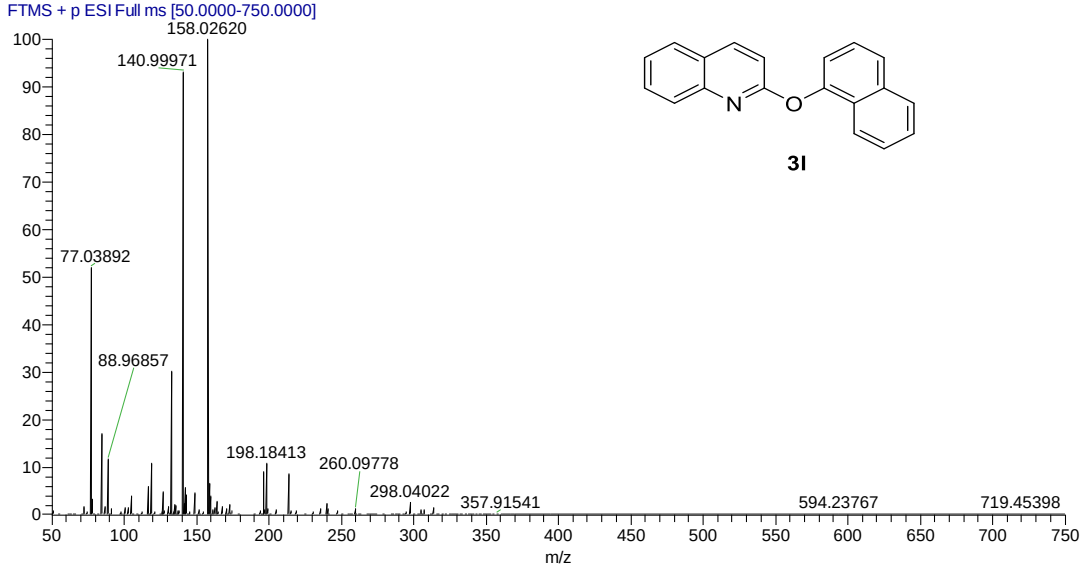


3f


B82 #1 RT: 0.00 AV: 1 NL: 6.78E7
T: FTMS + p ESI Full ms [50.0000-750.0000]
214.08885
116.98580
198.18459
236.07063
65.06035
149.01170
298.04086
346.03958
447.34521
492.88120
593.15564
667.17249
m/z
F
N
O
3h

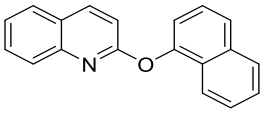

B82 #29 RT: 0.29 AV: 1 NL: 3.29E6
T: FTMS + p ESI Full ms [50.0000-750.0000]
262.06363
m/z
F
N
O
3h

B95 #1 RT: 0.00 AV: 1 NL: 2.00E7
T: FTMS + p ESI Full ms [50.0000-750.0000]



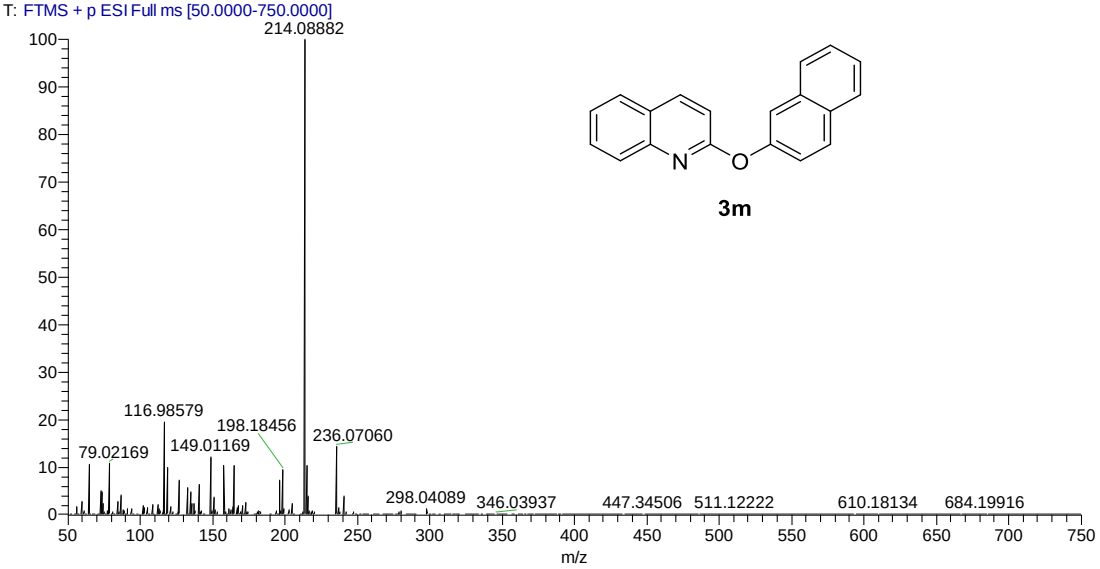
3l

B95 #27 RT: 0.27 AV: 1 NL: 2.56E5
T: FTMS + p ESI Full ms [50.0000-750.0000]



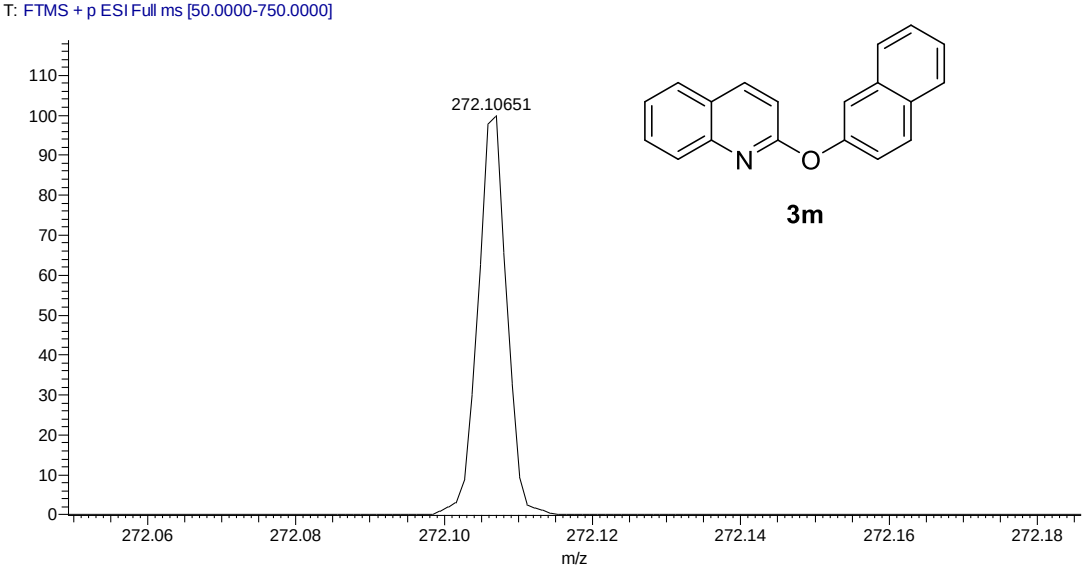
3l

B92 #1 RT: 0.00 AV: 1 NL: 7.05E7
T: FTMS + p ESI Full ms [50.0000-750.0000]

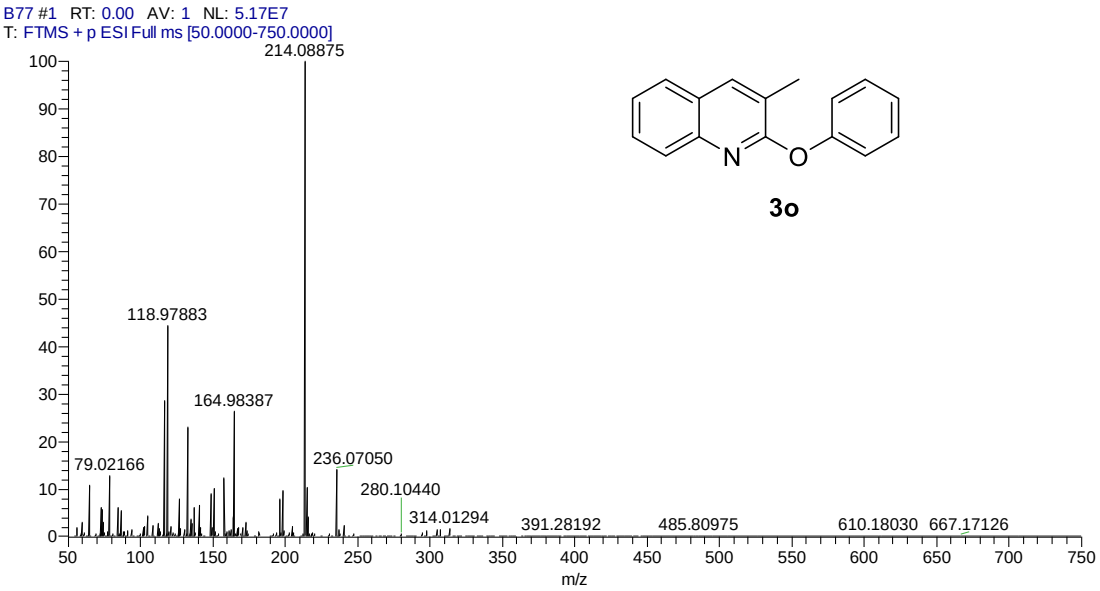


3m

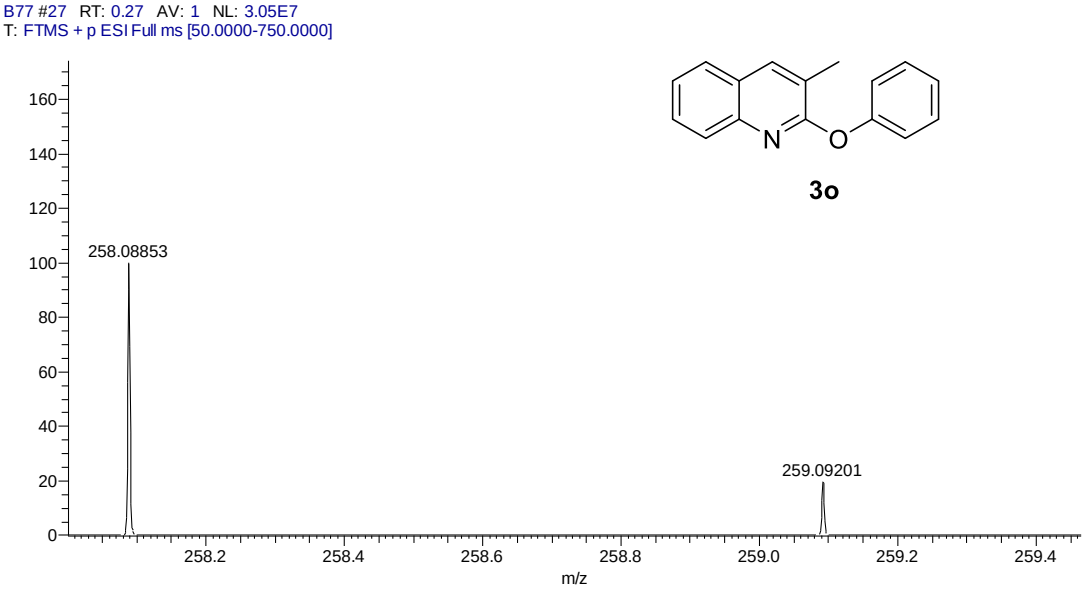
B92 #29 RT: 0.29 AV: 1 NL: 3.52E7
T: FTMS + p ESI Full ms [50.0000-750.0000]



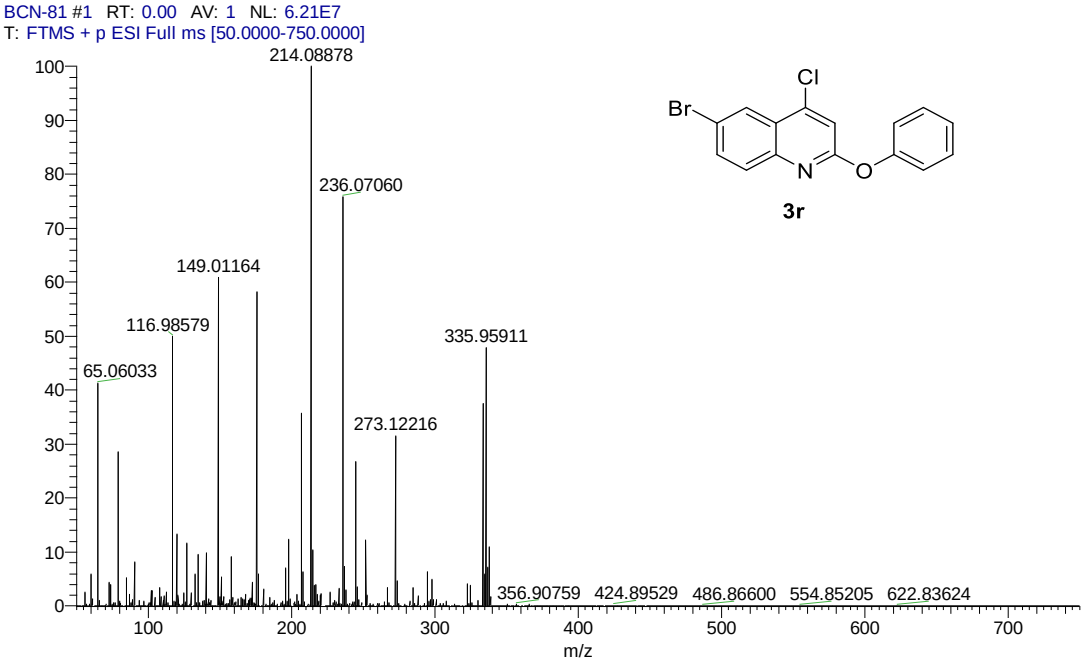
3m

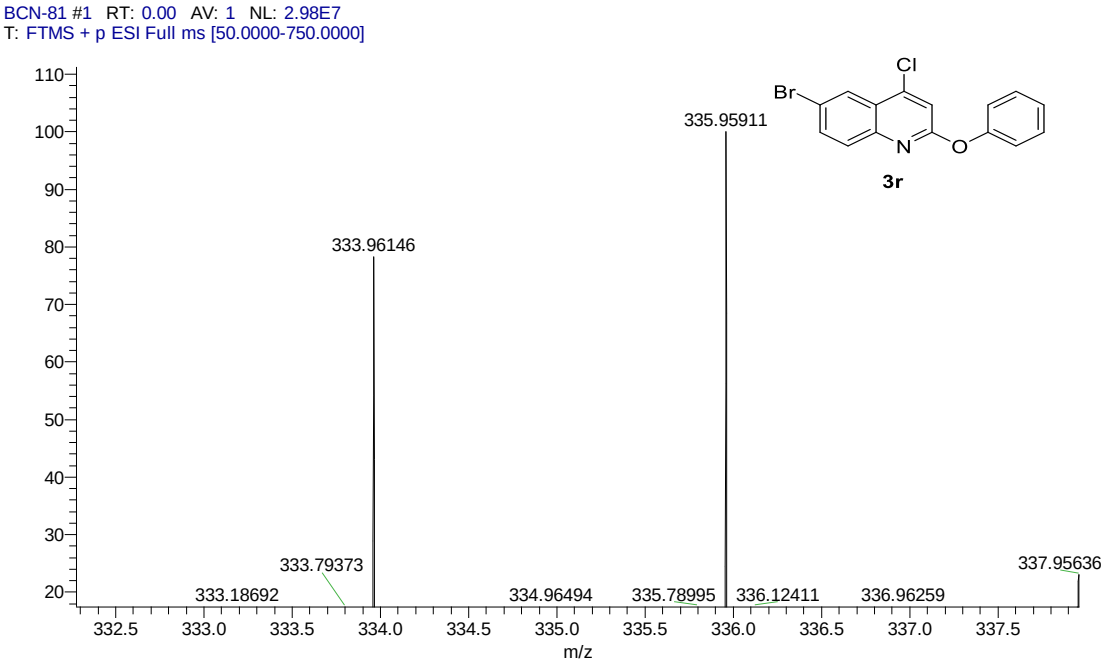

B77 #1 RT: 0.00 AV: 1 NL: 5.17E7
T: FTMS + p ESI Full ms [50.0000-750.0000]
214.08875
118.97883
164.98387
79.02166
236.07050
280.10440
314.01294
391.28192
485.80975
610.18030
667.17126
m/z

3o

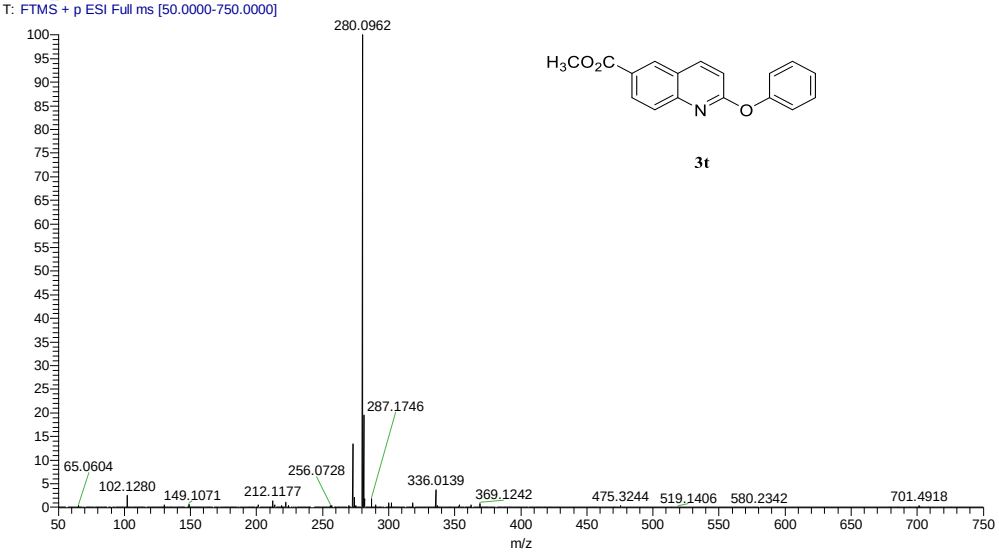

B77 #27 RT: 0.27 AV: 1 NL: 3.05E7
T: FTMS + p ESI Full ms [50.0000-750.0000]
258.08853
259.09201
m/z

3o


BCN-81 #1 RT: 0.00 AV: 1 NL: 6.21E7
T: FTMS + p ESI Full ms [50.0000-750.0000]
214.08878
236.07060
149.01164
116.98579
335.95911
65.06033
273.12216
356.90759
424.89529
486.86600
554.85205
622.83624
m/z
Cl
Br
N
O
3r

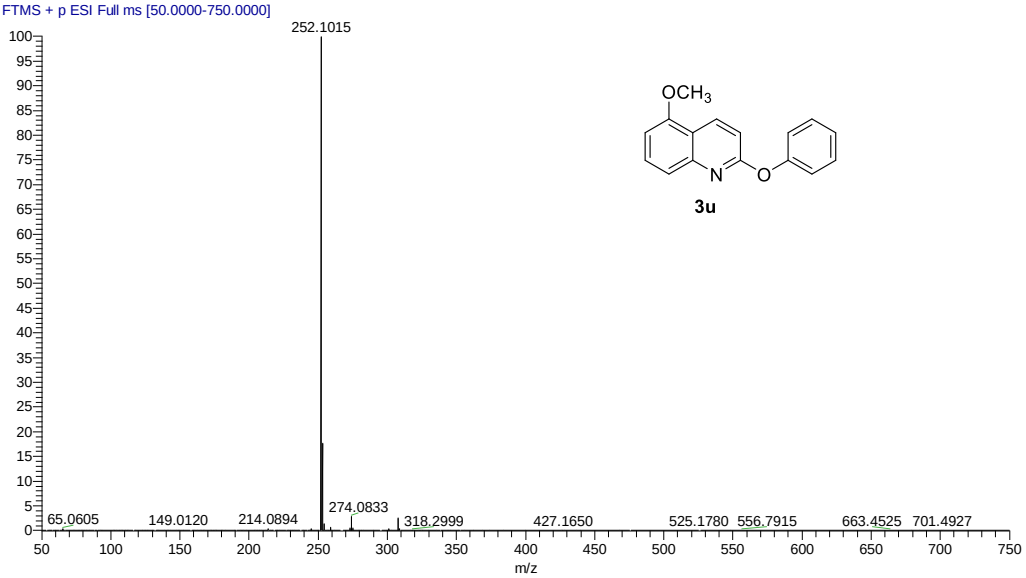

BCN-81 #1 RT: 0.00 AV: 1 NL: 2.98E7
T: FTMS + p ESI Full ms [50.0000-750.0000]
335.95911
333.96146
333.79373
333.18692
334.96494
335.78995
336.12411
336.96259
337.95636
m/z
Cl
Br
N
O
3r

WKJ-95 230829111336 #27 RT: 0.26 AV: 1 NL: 4.93E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



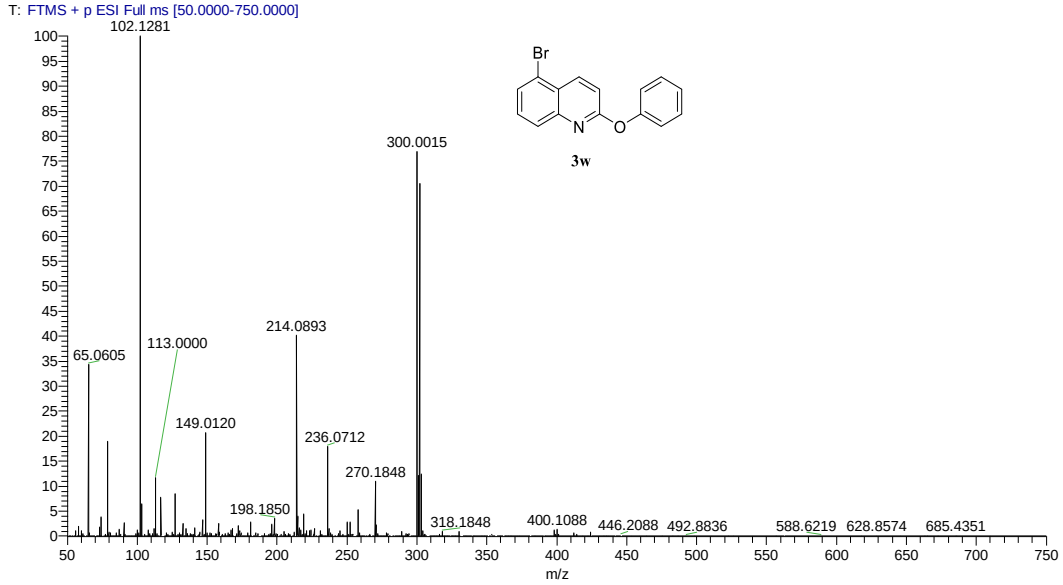
3t

WKJ-93 #31 RT: 0.30 AV: 1 NL: 7.68E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



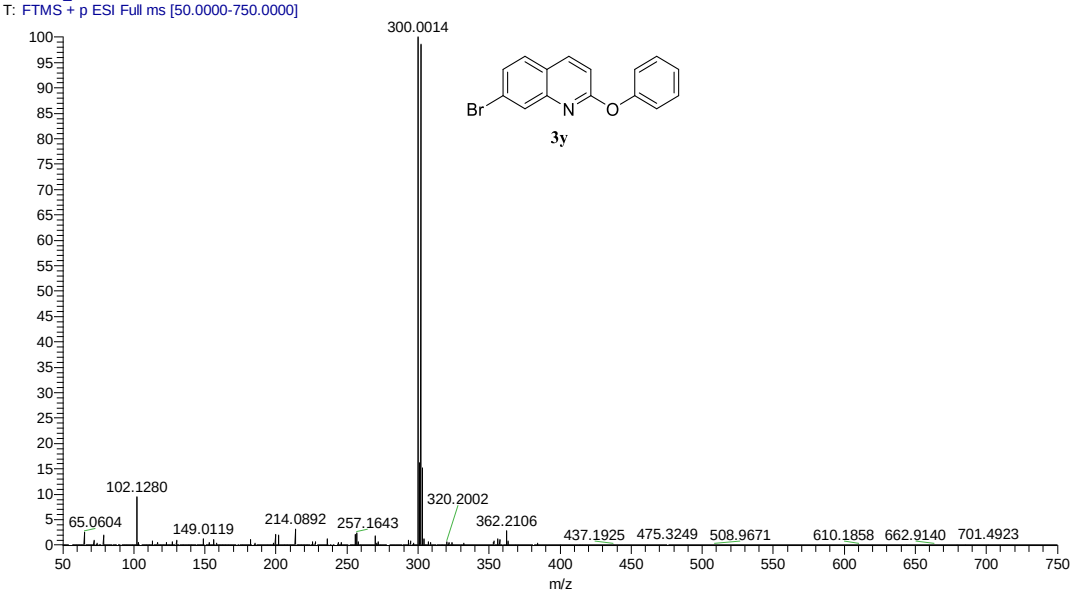
3u

WKJ-98 #27 RT: 0.26 AV: 1 NL: 1.50E8
T: FTMS + p ESI Full ms [50.0000-750.0000]

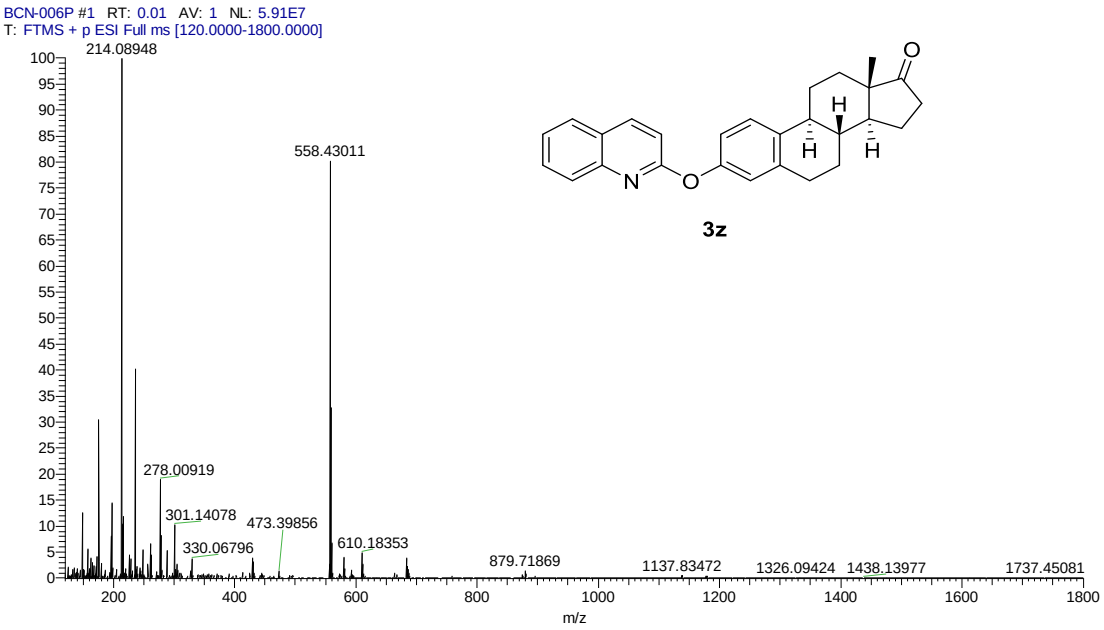


3w

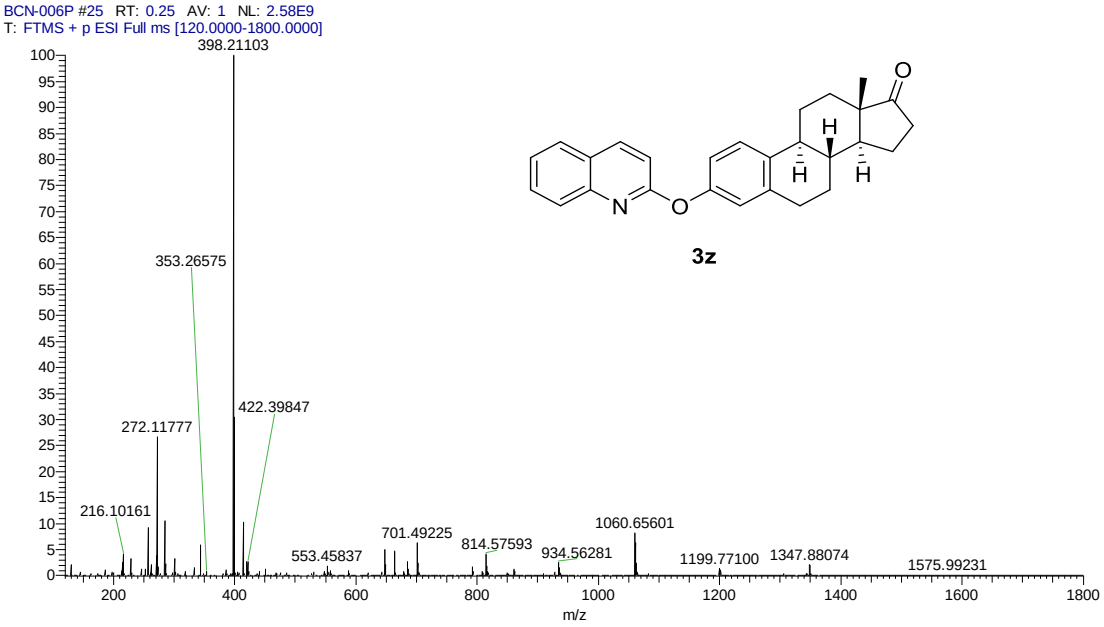
WKJ-100_230829111033 #45 RT: 0.43 AV: 1 NL: 1.60E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



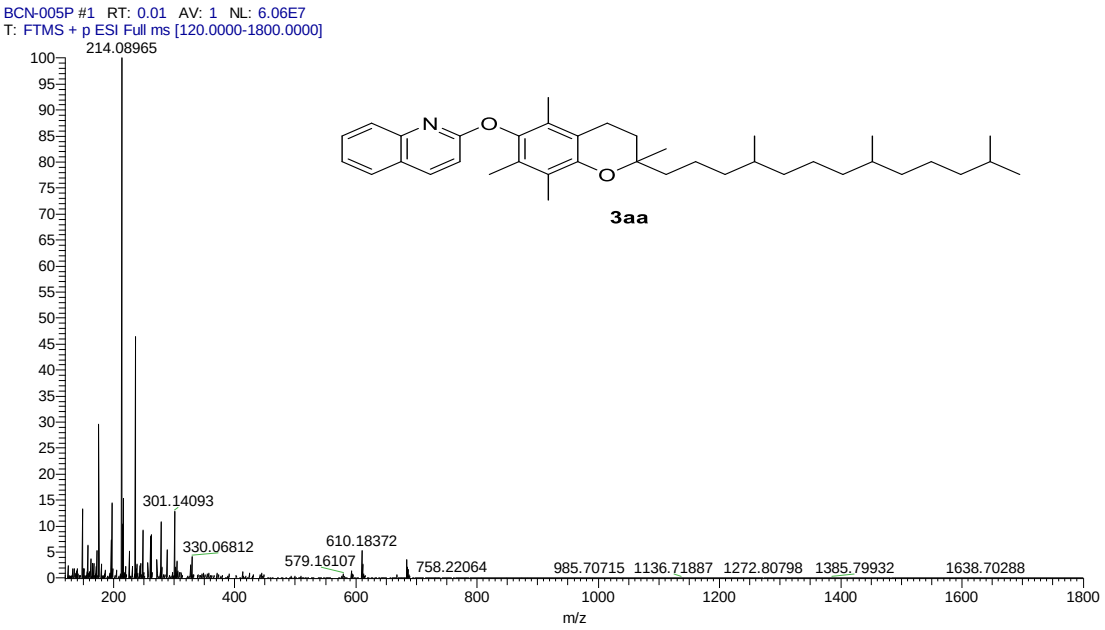
3y


BCN-006P #1 RT: 0.01 AV: 1 NL: 5.91E7
T: FTMS + p ESI Full ms [120.0000-1800.0000]
214.08948
558.43011
278.00919
301.14078
473.39856
330.06796
610.18353
879.71869
1137.83472
1326.09424
1438.13977
1737.45081
m/z

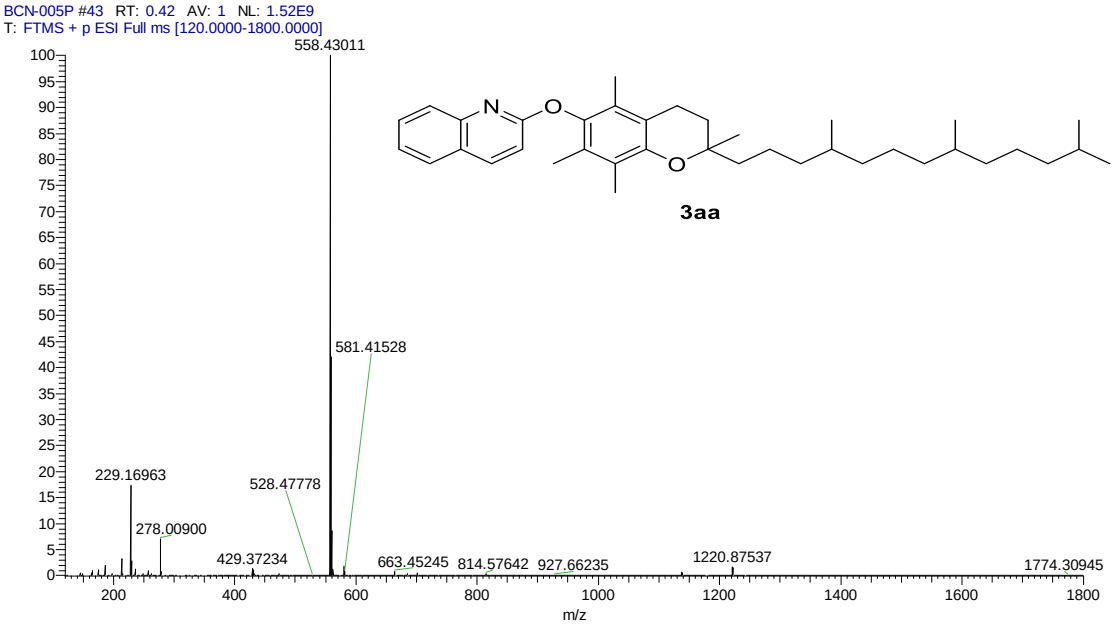
3z


BCN-006P #25 RT: 0.25 AV: 1 NL: 2.58E9
T: FTMS + p ESI Full ms [120.0000-1800.0000]
398.21103
353.26575
422.39847
272.11777
216.10161
701.49225
553.45837
814.57593
934.56281
1060.65601
1199.77100
1347.88074
1575.99231
m/z

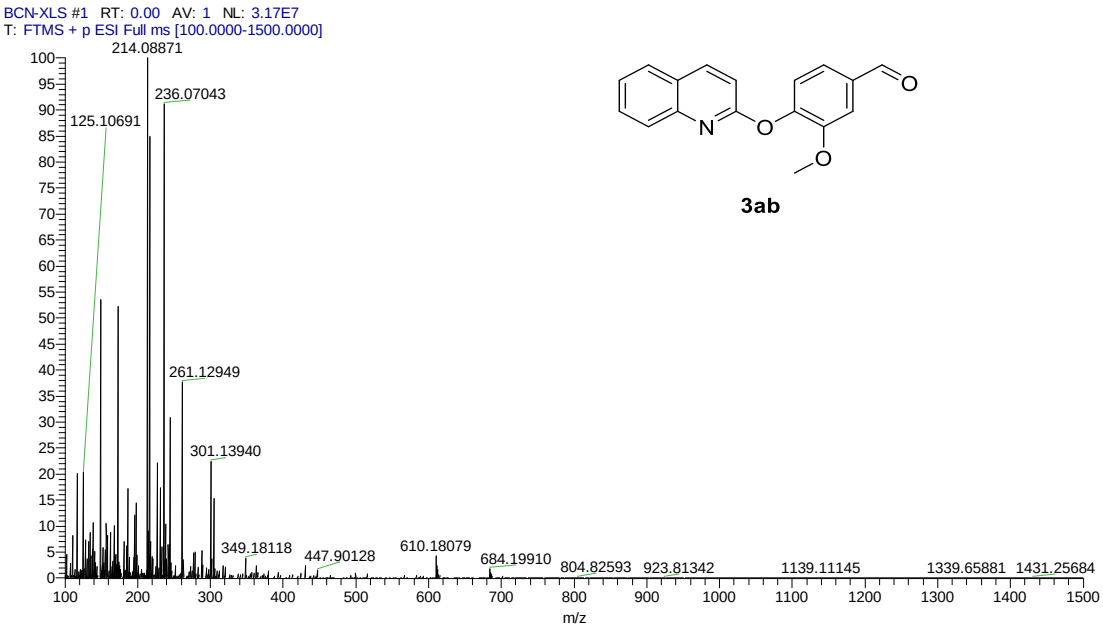
3z


BCN-005P #1 RT: 0.01 AV: 1 NL: 6.06E7
T: FTMS + p ESI Full ms [120.0000-1800.0000]
214.08965
301.14093
330.06812
579.16107
610.18372
758.22064
985.70715
1136.71887
1272.80798
1385.79932
1638.70288
m/z

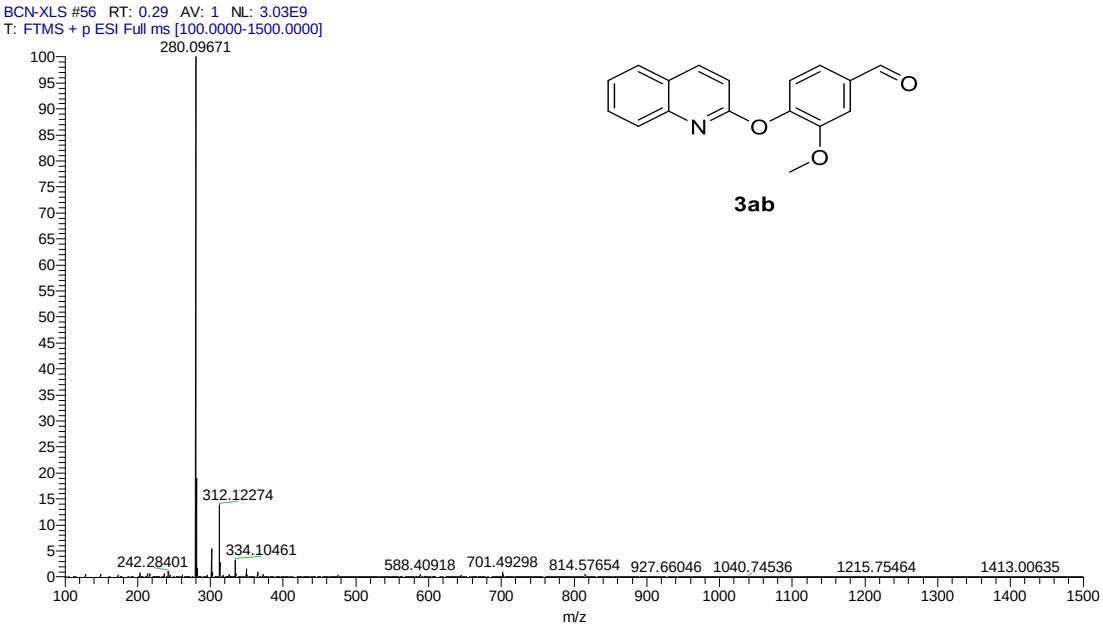
3aa


BCN-005P #43 RT: 0.42 AV: 1 NL: 1.52E9
T: FTMS + p ESI Full ms [120.0000-1800.0000]
558.43011
581.41528
229.16963
528.47778
278.00900
429.37234
663.45245
814.57642
927.66235
1220.87537
1774.30945
m/z

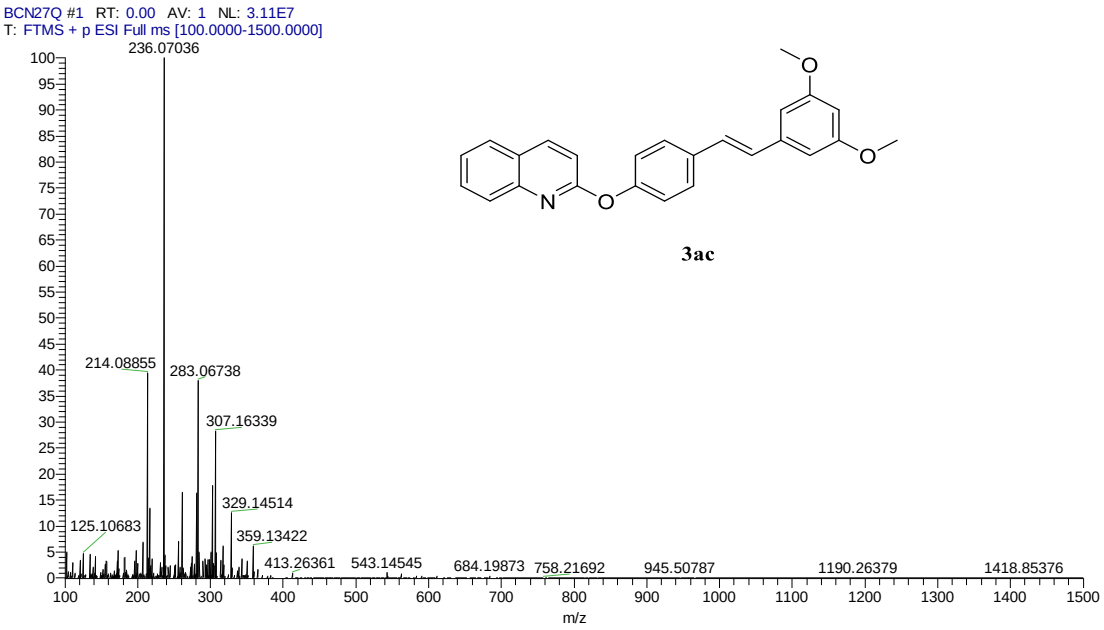
3aa


BCN-XLS #1 RT: 0.00 AV: 1 NL: 3.17E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]
214.08871
236.07043
125.10691
261.12949
301.13940
349.18118
447.90128
610.18079
684.19910
804.82593
923.81342
1139.11145
1339.65881
1431.25684
m/z

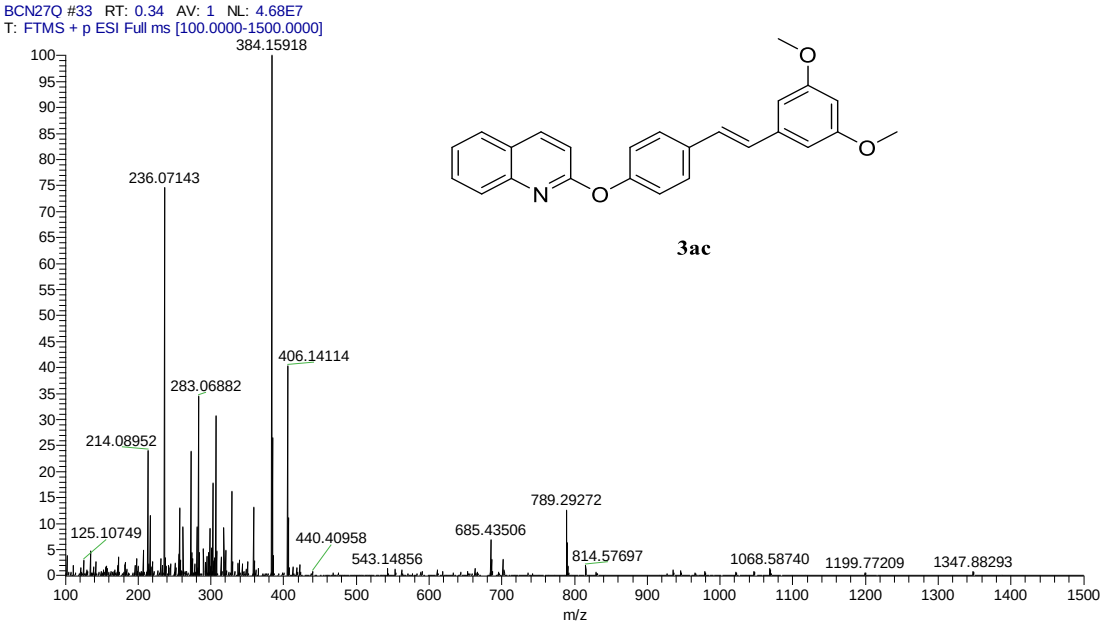
3ab


BCN-XLS #56 RT: 0.29 AV: 1 NL: 3.03E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]
280.09671
312.12274
334.10461
242.28401
588.40918
701.49298
814.57654
927.66046
1040.74536
1215.75464
1413.00635
m/z

3ab

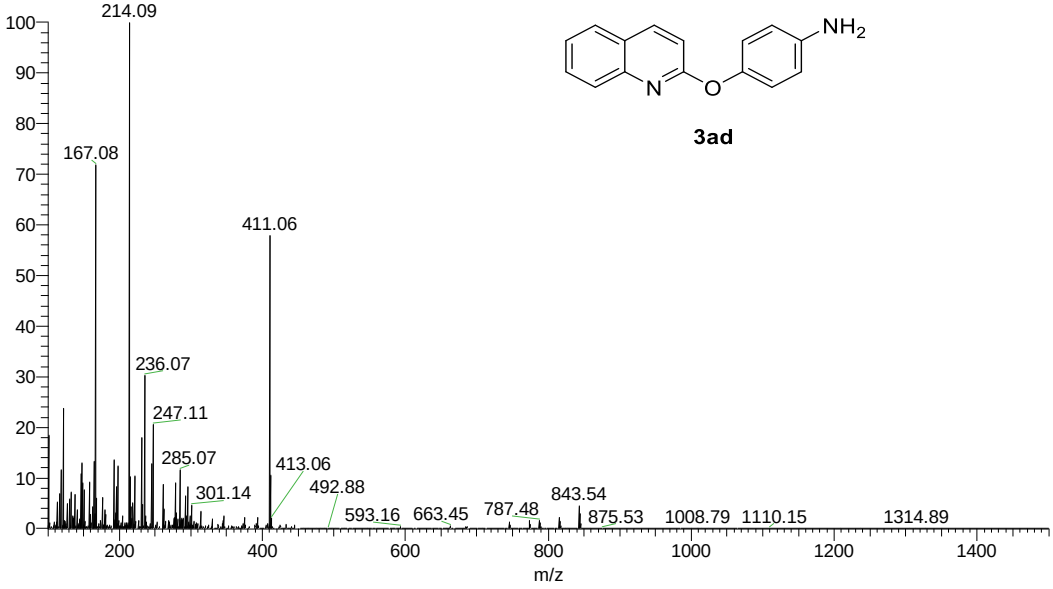

BCN27Q #1 RT: 0.00 AV: 1 NL: 3.11E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]
236.07036
214.08855
283.06738
307.16339
329.14514
125.10683
359.13422
413.26361
543.14545
684.19873
758.21692
945.50787
1190.26379
1418.85376
m/z
O
O
N
O

3ac


BCN27Q #33 RT: 0.34 AV: 1 NL: 4.68E7
T: FTMS + p ESI Full ms [100.0000-1500.0000]
384.15918
236.07143
406.14114
283.06882
214.08952
789.29272
125.10749
685.43506
440.40958
543.14856
814.57697
1068.58740
1199.77209
1347.88293
m/z
O
O
N
O

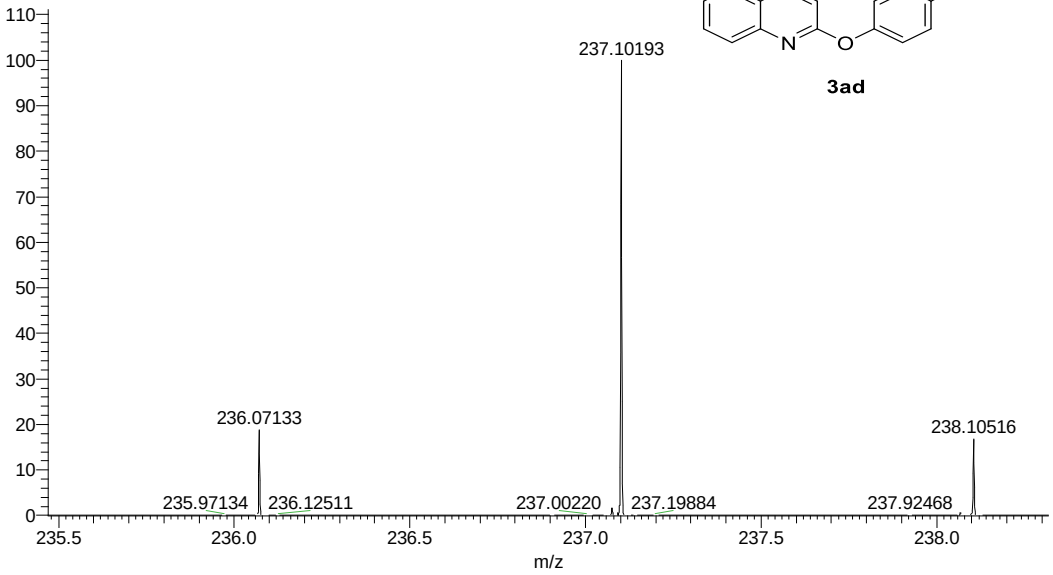
3ac

B-157-D #1 RT: 0.01 AV: 1 NL: 1.12E8
T: FTMS + p ESI Full ms [100.0000-1500.0000



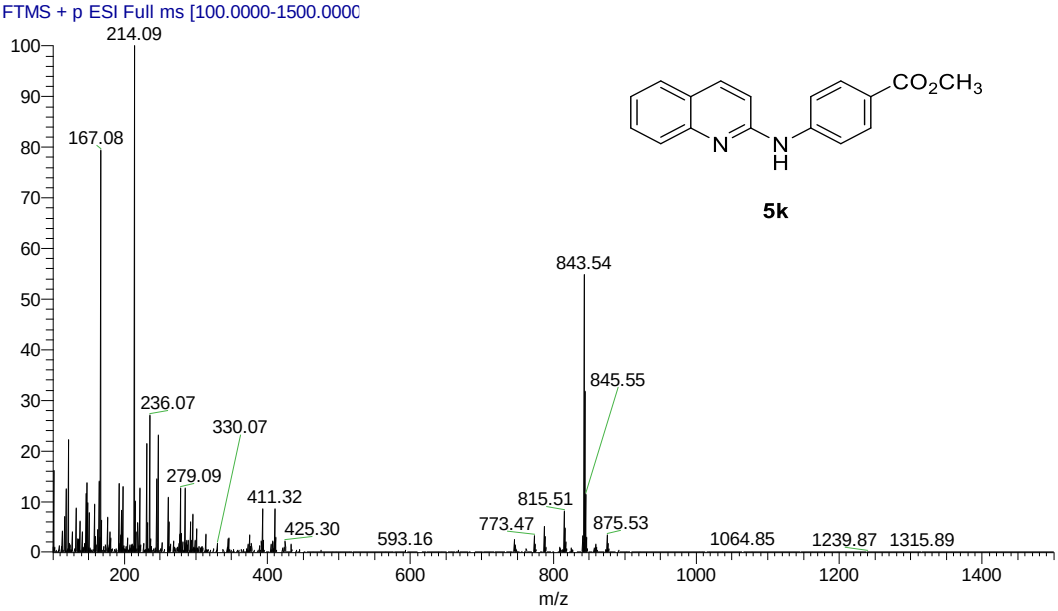
3ad

B-157-D #21 RT: 0.21 AV: 1 NL: 1.65E8
T: FTMS + p ESI Full ms [100.0000-1500.0000



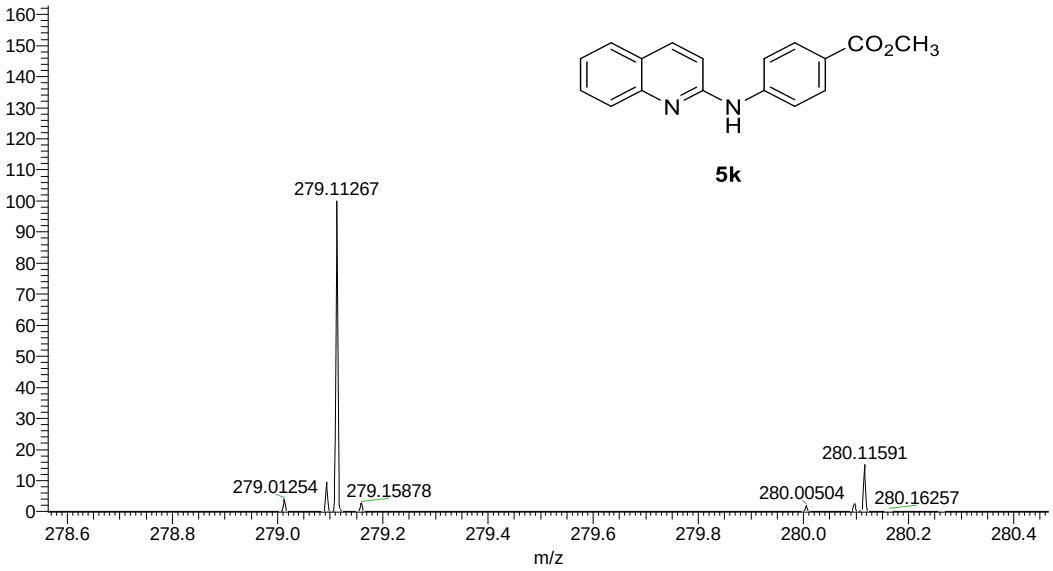
3ad

BCN-1626 #1 RT: 0.01 AV: 1 NL: 1.21E8
T: FTMS + p ESI Full ms [100.0000-1500.0000

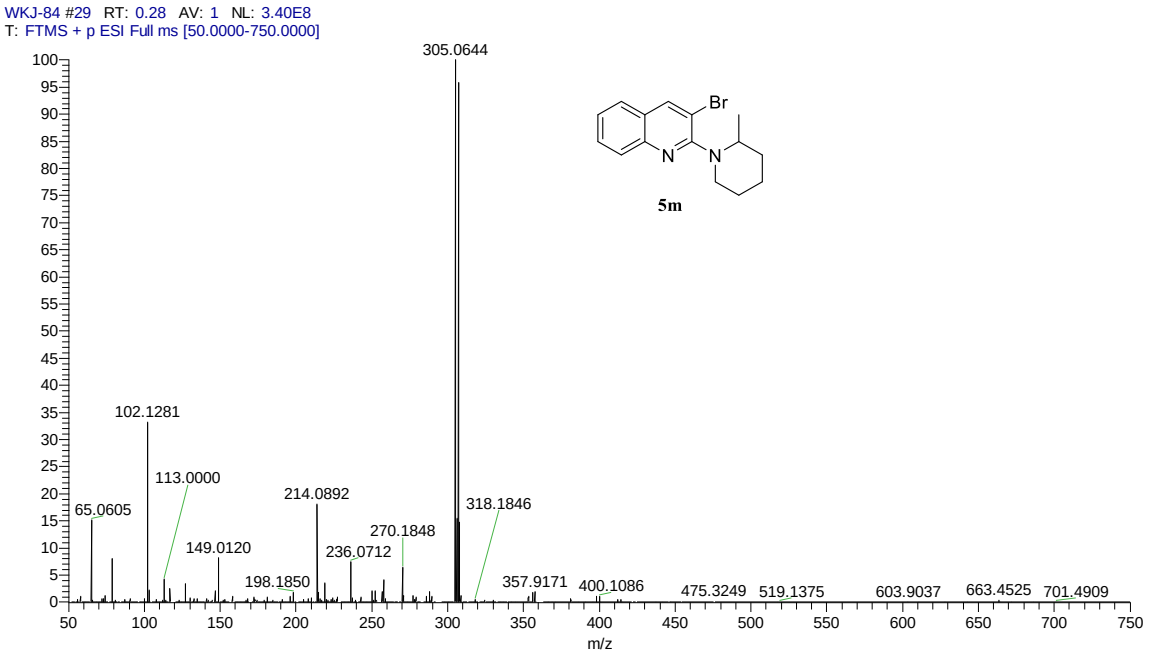


5k

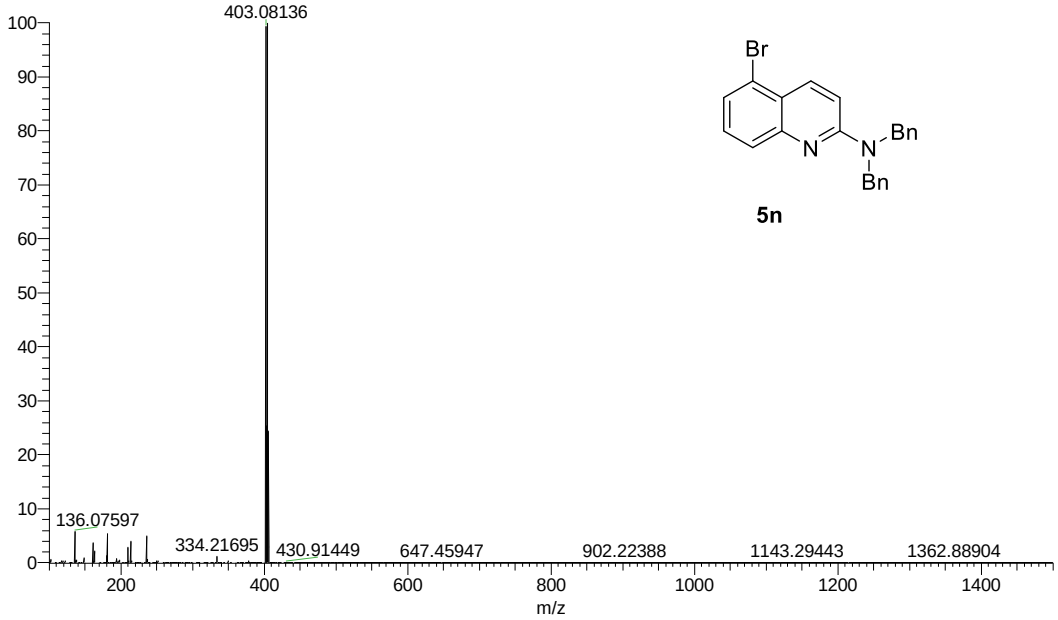
BCN-1626 #29 RT: 0.29 AV: 1 NL: 1.27E8
T: FTMS + p ESI Full ms [100.0000-1500.0000



5k

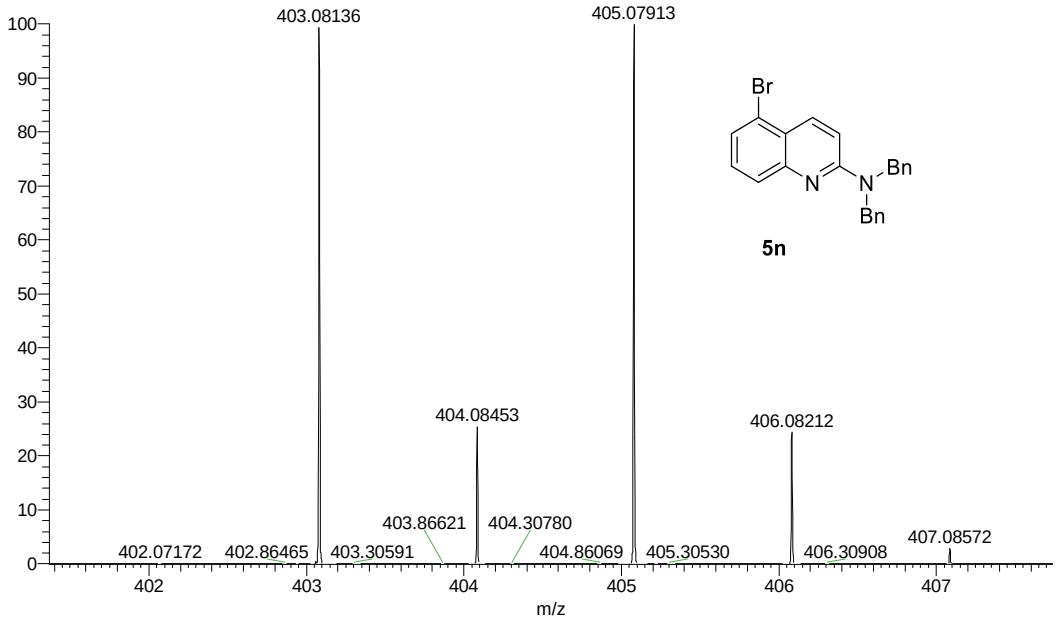

WKJ-84 #29 RT: 0.28 AV: 1 NL: 3.40E8
T: FTMS + p ESI Full ms [50.0000-750.0000]
305.0644
102.1281
113.0000
65.0605
214.0892
318.1846
270.1848
149.0120
236.0712
198.1850
357.9171
400.1086
475.3249
519.1375
603.9037
663.4525
701.4909
Br
N
N
5m
m/z

BCN5B2 #1 RT: 0.01 AV: 1 NL: 1.85E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



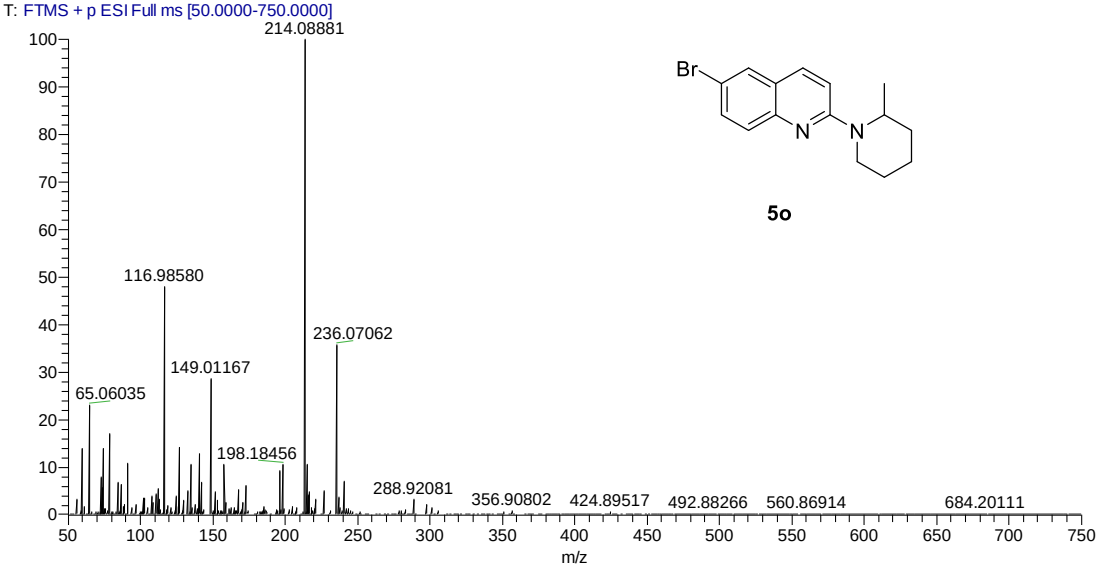
5n

BCN5B2 #1 RT: 0.01 AV: 1 NL: 1.85E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]



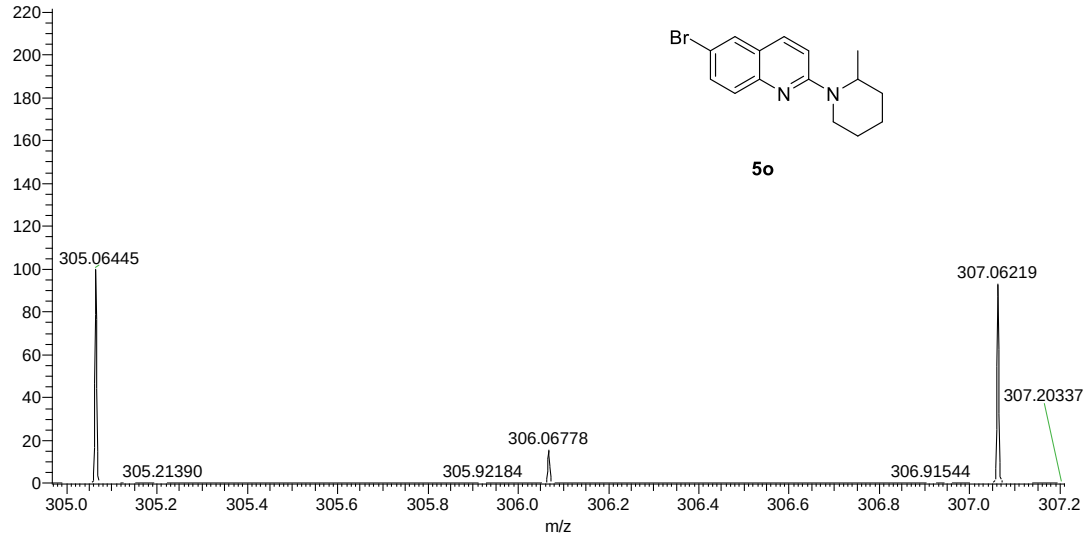
5n

B59 #1 RT: 0.00 AV: 1 NL: 4.04E7
T: FTMS + p ESI Full ms [50.0000-750.0000]

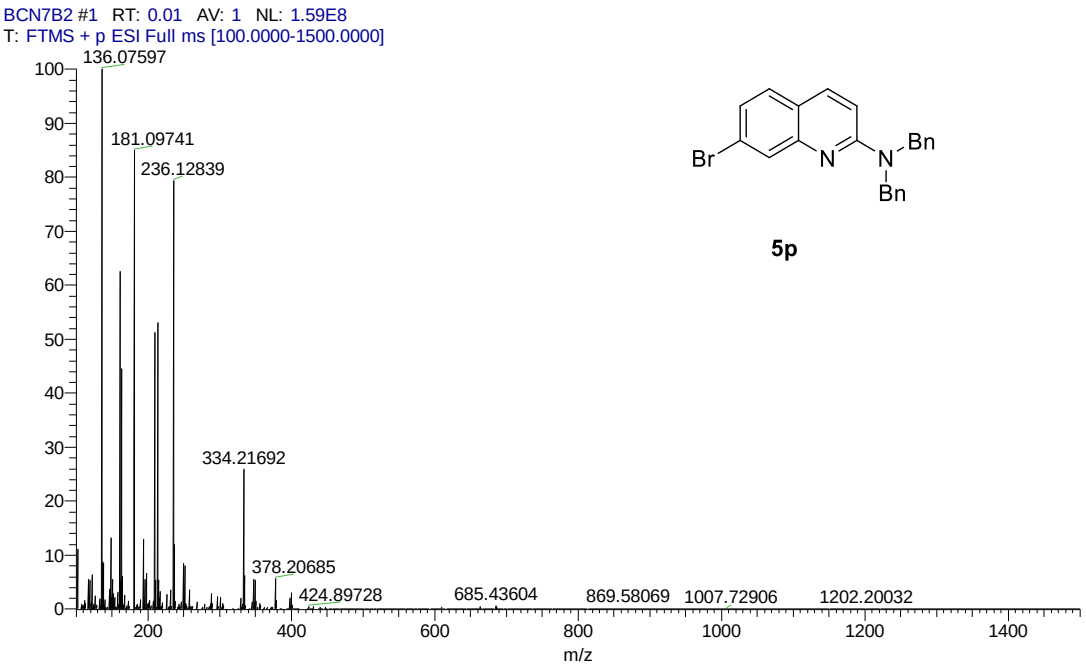


5o

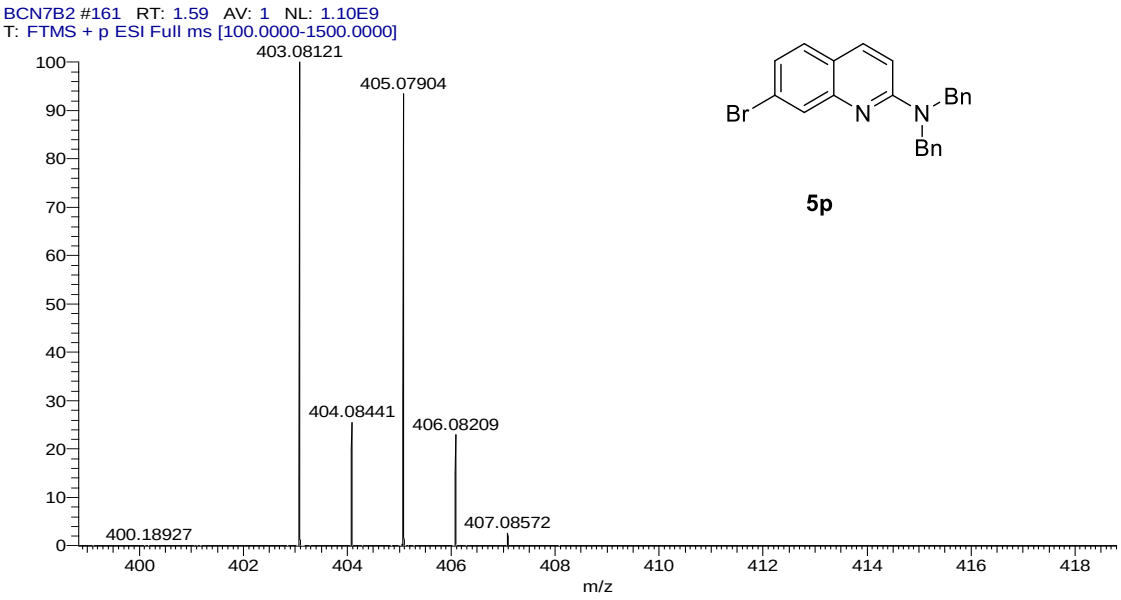
B59 #29 RT: 0.28 AV: 1 NL: 5.41E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



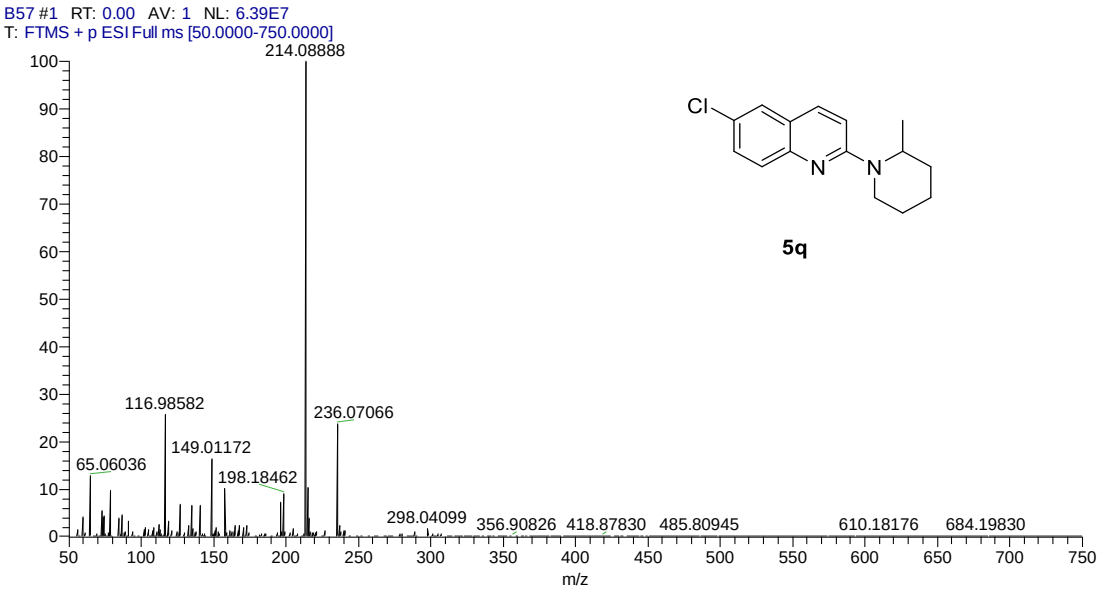
5o


BCN7B2 #1 RT: 0.01 AV: 1 NL: 1.59E8
T: FTMS + p ESI Full ms [100.0000-1500.0000]
136.07597
181.09741
236.12839
334.21692
378.20685
424.89728
685.43604
869.58069
1007.72906
1202.20032
m/z
Br
N
N
Bn
Bn

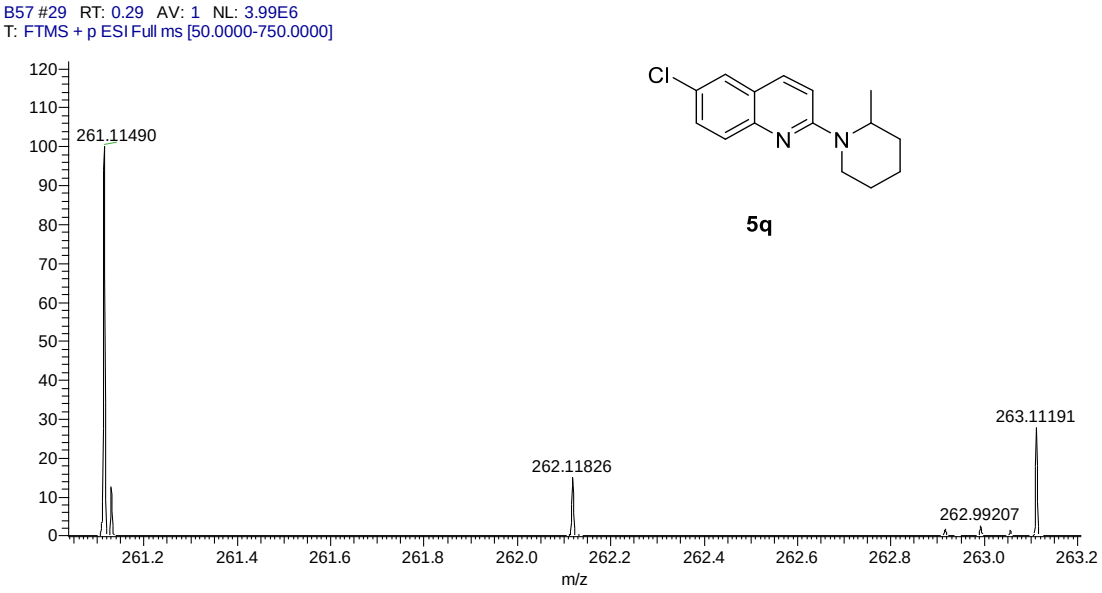
5p


BCN7B2 #161 RT: 1.59 AV: 1 NL: 1.10E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]
403.08121
405.07904
404.08441
406.08209
407.08572
400.18927
m/z
Br
N
N
Bn
Bn

5p

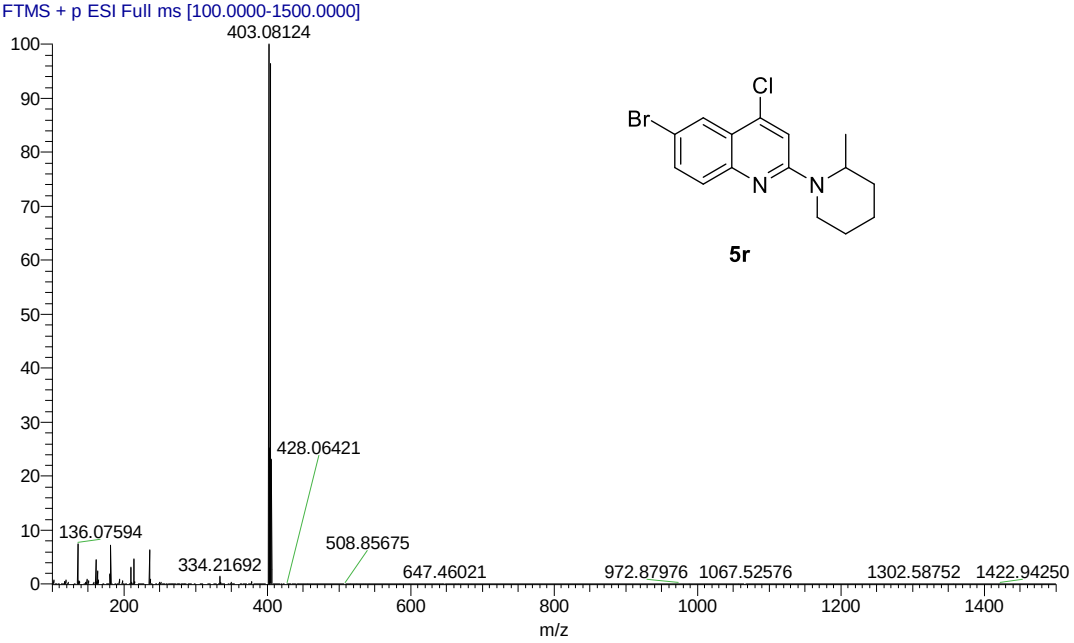

B57 #1 RT: 0.00 AV: 1 NL: 6.39E7
T: FTMS + p ESI Full ms [50.0000-750.0000]
214.08888
116.98582
236.07066
149.01172
65.06036
198.18462
298.04099
356.90826
418.87830
485.80945
610.18176
684.19830
m/z

5q


B57 #29 RT: 0.29 AV: 1 NL: 3.99E6
T: FTMS + p ESI Full ms [50.0000-750.0000]
261.11490
262.11826
263.11191
262.99207
m/z

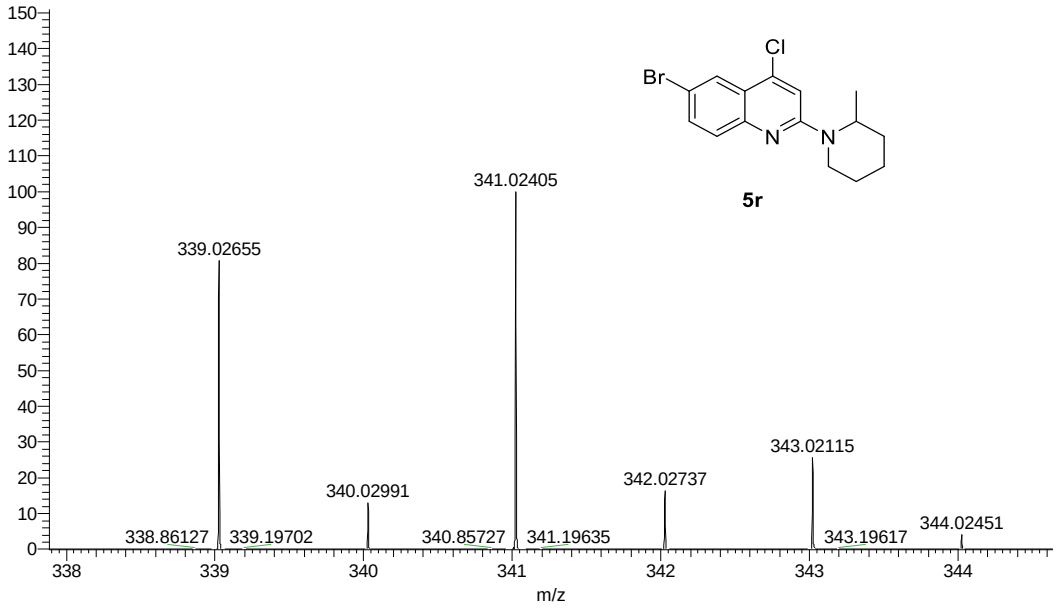
5q

BCN87 #1 RT: 0.01 AV: 1 NL: 1.50E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

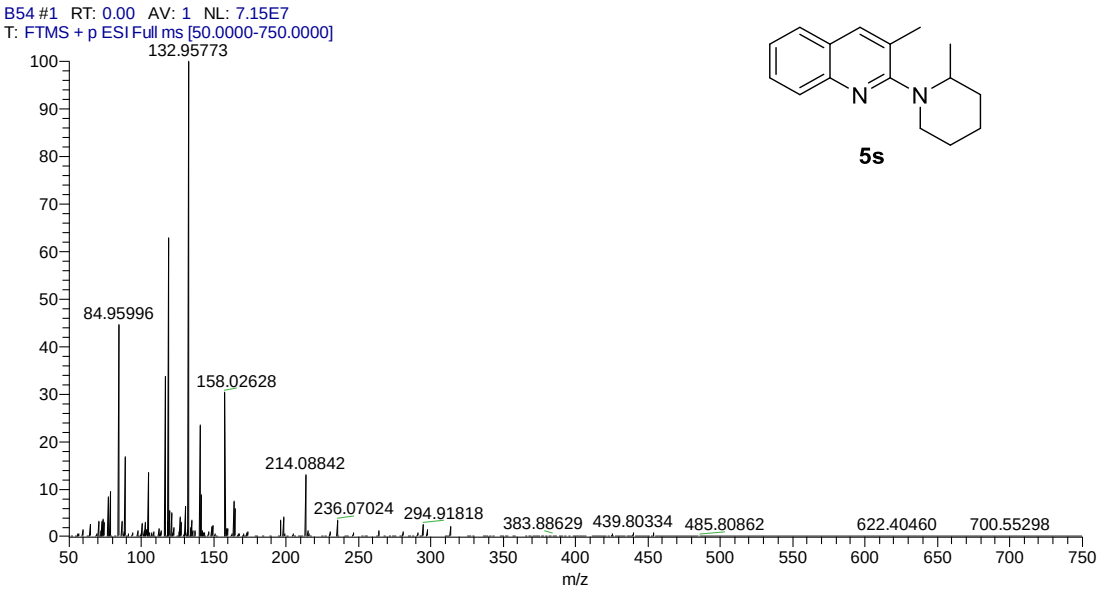


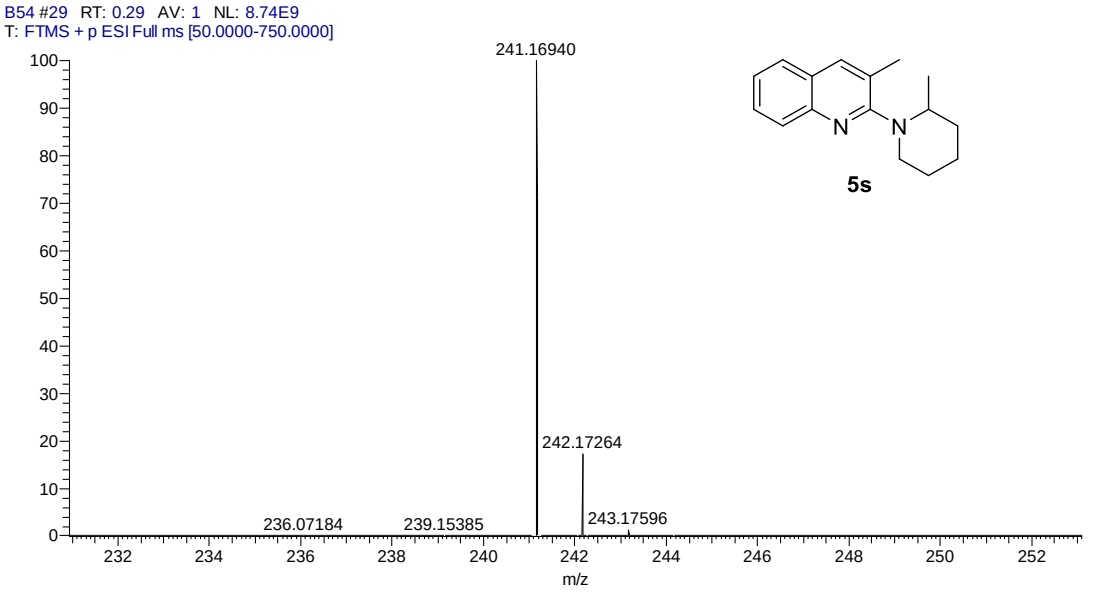
5r

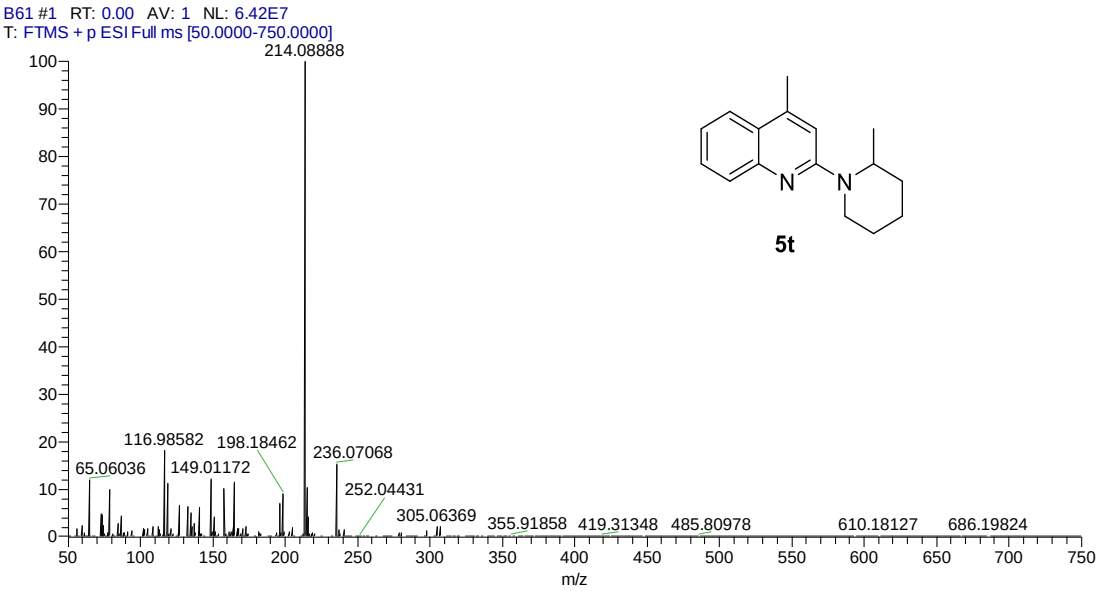
BCN87 #27 RT: 0.26 AV: 1 NL: 6.04E9
T: FTMS + p ESI Full ms [100.0000-1500.0000]

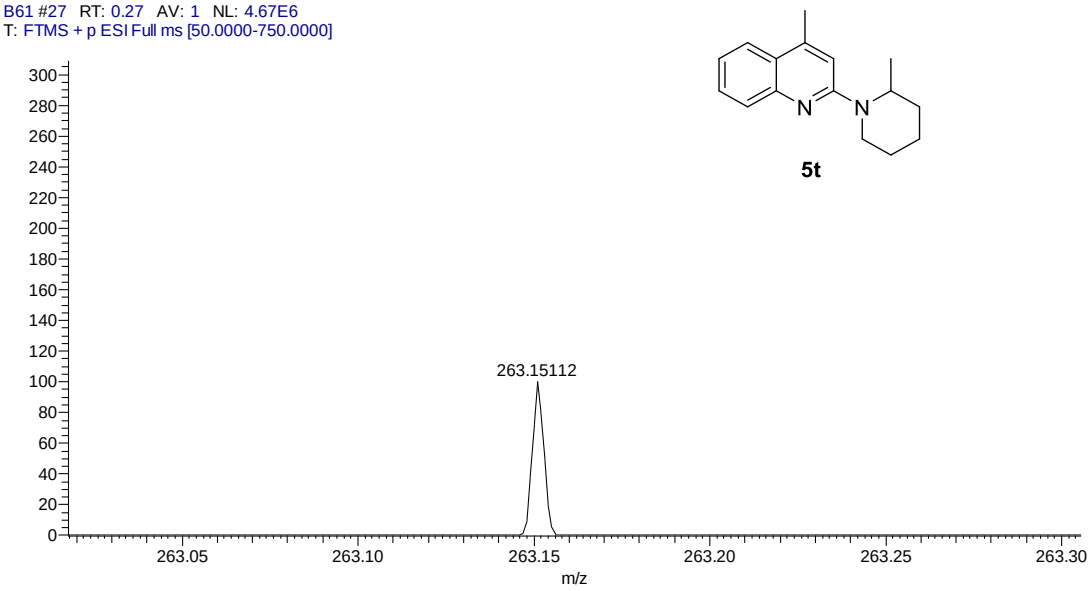


5r

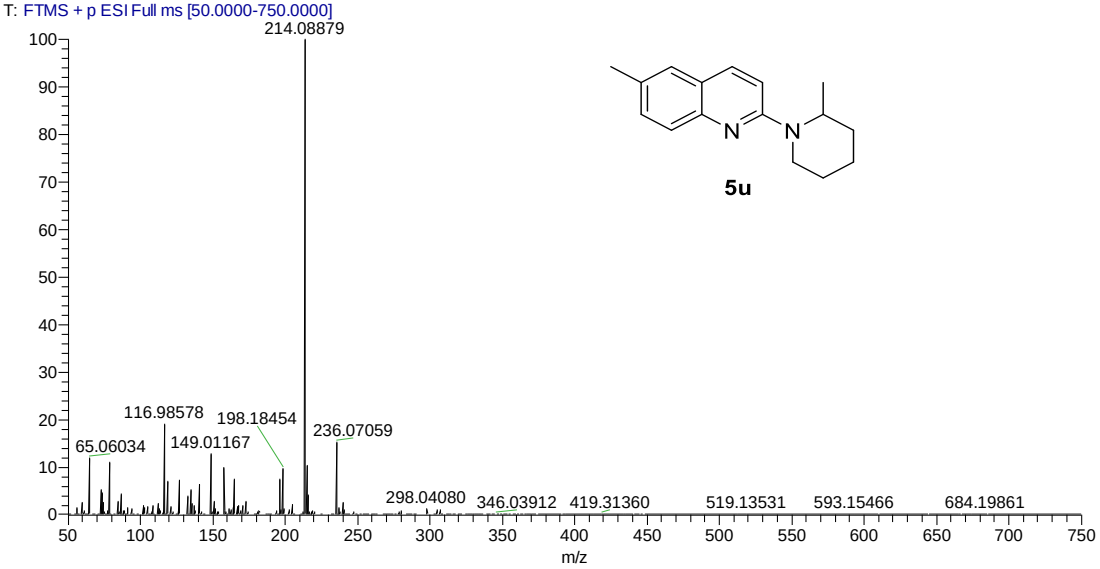

B54 #1 RT: 0.00 AV: 1 NL: 7.15E7
T: FTMS + p ESI Full ms [50.0000-750.0000]
132.95773
84.95996
158.02628
214.08842
236.07024
294.91818
383.88629
439.80334
485.80862
622.40460
700.55298
m/z
5s


B54 #29 RT: 0.29 AV: 1 NL: 8.74E9
T: FTMS + p ESI Full ms [50.0000-750.0000]
241.16940
242.17264
236.07184
239.15385
243.17596
m/z
5s


B61 #1 RT: 0.00 AV: 1 NL: 6.42E7
T: FTMS + p ESI Full ms [50.0000-750.0000]
214.08888
116.98582
198.18462
65.06036
149.01172
236.07068
252.04431
305.06369
355.91858
419.31348
485.80978
610.18127
686.19824
m/z
5t

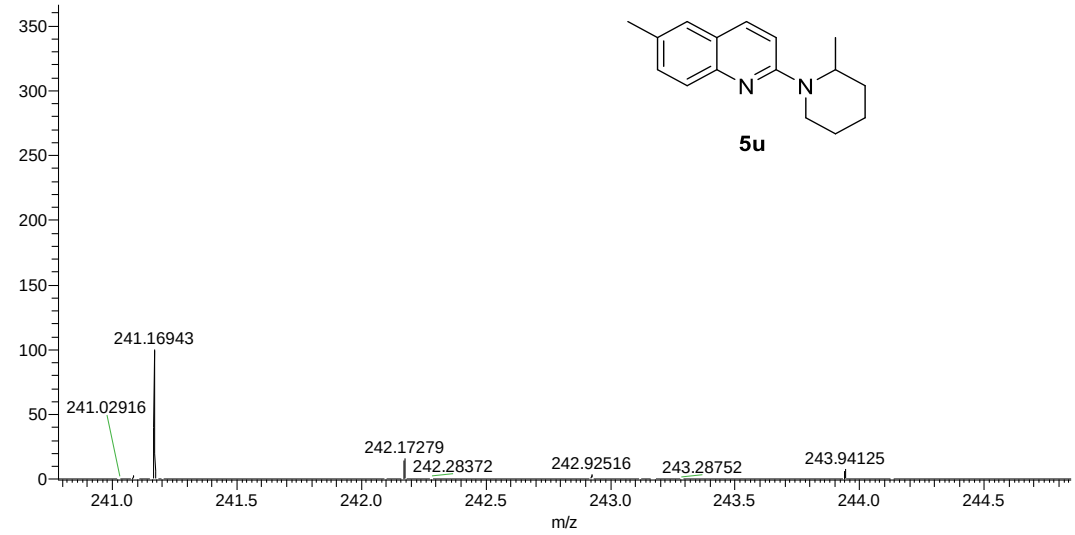

B61 #27 RT: 0.27 AV: 1 NL: 4.67E6
T: FTMS + p ESI Full ms [50.0000-750.0000]
263.15112
m/z
5t

B58 #1 RT: 0.00 AV: 1 NL: 6.17E7
T: FTMS + p ESI Full ms [50.0000-750.0000]



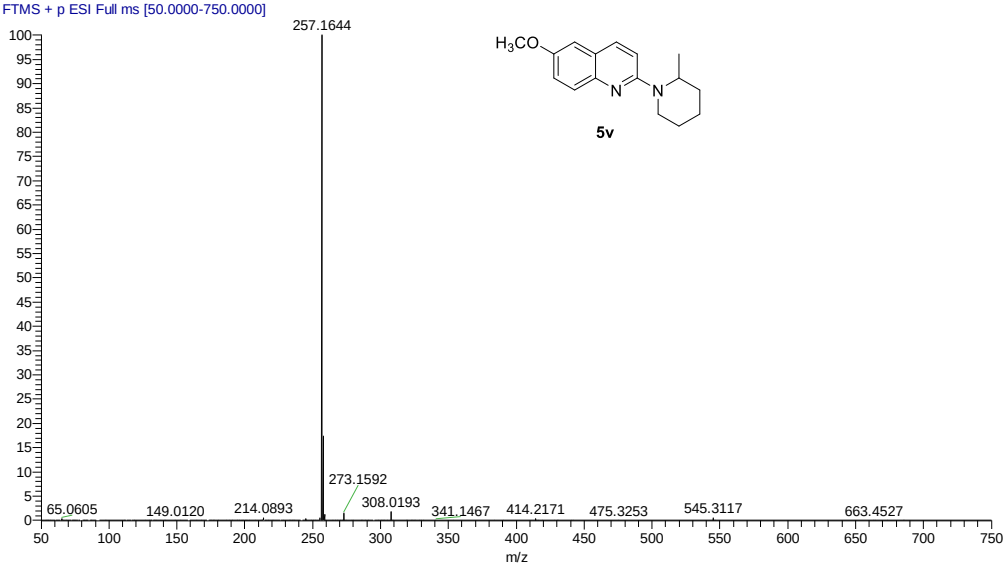
5u

B58 #35 RT: 0.35 AV: 1 NL: 1.15E7
T: FTMS + p ESI Full ms [50.0000-750.0000]



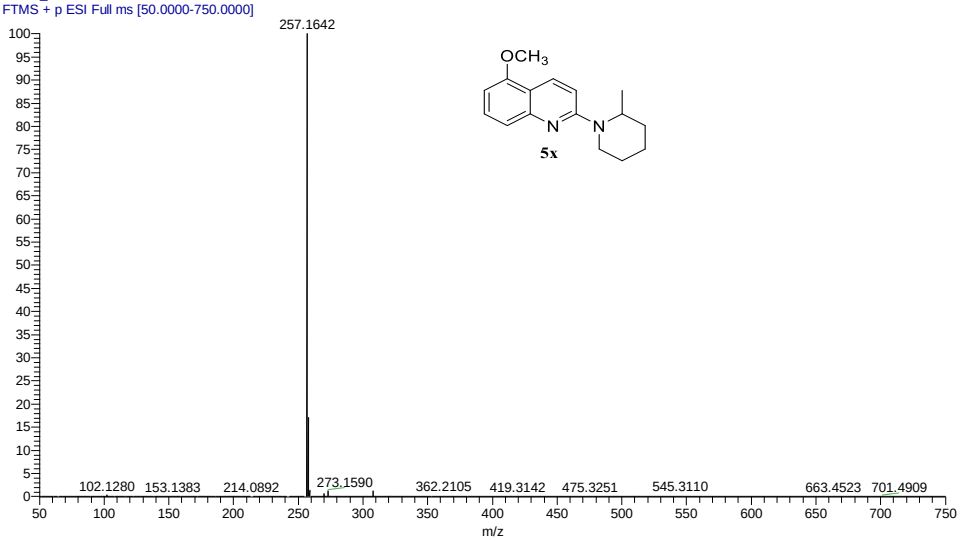
5u

WKJ-78 #25 RT: 0.24 AV: 1 NL: 7.21E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



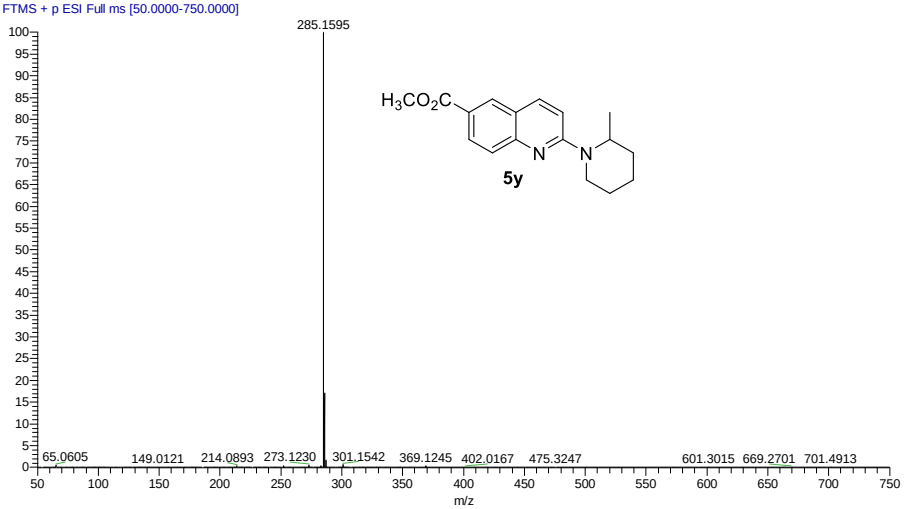
5v

WKJ-135_230829110130 #35 RT: 0.34 AV: 1 NL: 1.08E10
T: FTMS + p ESI Full ms [50.0000-750.0000]



5x

WKJ-83 #27 RT: 0.26 AV: 1 NL: 6.90E9
T: FTMS + p ESI Full ms [50.0000-750.0000]



5y