Supporting Information

Ir(III)-Catalyzed Synthesis of Isoquinolines from Benzimidates and α-Diazocarbonyl Compounds

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General experimental procedures

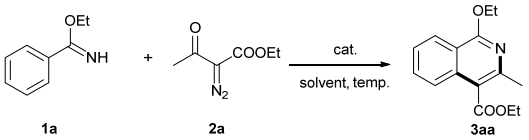
All reactions were carried out under nitrogen atmosphere. Proton and carbon magnetic resonance spectra (^{1}H NMR and ^{13}C NMR) were recorded using tetramethylsilane (TMS) in the solvent of $CDCl_3$ as the internal standard (^{1}H NMR: TMS at 0.00 ppm, $CDCl_3$ at 7.26 ppm; ^{13}C NMR: $CDCl_3$ at 77.16 ppm).

General procedure for synthesis of compounds 3aa-3kb.

Substituted ethyl benzimidate (0.25 mmol), ethyl 2-diazo-3-oxobutanoate (0.3 mmol), $[Cp^*IrCl_2]_2$ (0.0125 mmol, 10 mg), $AgNTf_2$ (0.05 mmol, 20 mg), MeOH (2 mL) were added to a 25 mL Schlenk tube with a magnetic stirrer under nitrogen atmosphere. The mixture was allowed to stir under nitrogen atmosphere at 50℃ for 12 h. After cooled to room temperature, the resulting solution was concentrated via rotary evaporation, and the residue was purified by column chromatography on silica gel to provide the desired product (**3aa-3kb**).

Comparison of the reaction performance of Cp*M(III).

Table S1 Comparison of the catalytic performance of Cp*M(III) in the synthesis of ethyl 1-ethoxy-3-methylisoquinoline-4-carboxylate (**3aa**) via cascade reaction of ethyl benzimidate (**1a**) and ethyl 2-diazo-3-oxobutanoate (**2a**)

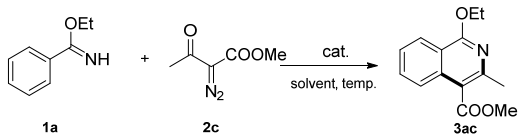


1a 2a 3aa

entry	catalyst system	solvent	temp (°C)	yield (%)[b]
1	$[Cp^*IrCl_2]_2/AgNTf_2$	MeOH	50	73%
2	$[Cp^*RhCl_2]_2$/Ag SbF_6	MeOH	50	79%
3	$Cp^*Co(CO)I_2/AgSbF_6$	MeOH	50	trace
4	$Cp^*Co(CO)I_2/AgSbF_6$	MeOH	120	trace

[a] Reaction conditions: ethyl benzimidate (**1a**) (0.25 mmol), ethyl 2-diazo-3-oxobutanoate (**2b**) (0.3 mmol), cat. (5 mol%, 20 mol%), 12 h, solvent (2 mL) under nitrogen atmosphere. [b] Isolated yield.

Table S2 Comparison of the catalytic performance of Cp*M(III) in the synthesis of methyl 1-ethoxy-3-methylisoquinoline-4-carboxylate(**3ac**) via cascade reaction of ethyl benzimidate (**1a**) and methyl 2-diazo-3-oxobutanoate (**2c**)

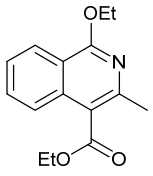


1a 2c 3ac

entry	catalyst system	solvent	temp (°C)	yield (%)[b]
1	$[Cp^*IrCl_2]_2/AgNTf_2$	MeOH	50	79%
2	$[Cp^*RhCl_2]_2$/Ag SbF_6	MeOH	50	74%
3	$Cp^*Co(CO)I_2/AgSbF_6$	MeOH	50	trace
4	$Cp^*Co(CO)I_2/AgSbF_6$	MeOH	120	trace

[a] Reaction conditions: ethyl benzimidate (**1a**) (0.25 mmol), ethyl 2-diazo-3-oxobutanoate (**2b**) (0.3 mmol), cat. (5 mol%, 20 mol%), 12 h, solvent (2 mL) under nitrogen atmosphere. [b] Isolated yield.

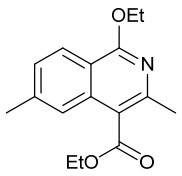
Characterization data of compounds 3aa-3kb



3aa

ethyl 1-ethoxy-3-methylisoquinoline-4-carboxylate (3aa).

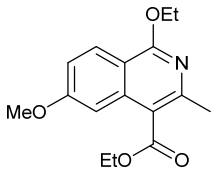
Eluent: petroleum ether/ethyl acetate (15:1). Yield 47 mg (73%). Yellow liquid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.24 (*d*, *J* = 8.2 Hz, 1H), 7.88 (*d*, *J* = 8.5 Hz, 1H), 7.64 (*t*, *J* = 8.3 Hz, 1H), 7.46 (*t*, *J* = 7.6 Hz, 1H), 4.58 (*q*, *J* = 7.1 Hz, 2H), 4.49 (*q*, *J* = 7.1 Hz, 2H), 2.61 (*s*, 3H), 1.48 (*t*, *J* = 7.1 Hz, 3H), 1.44 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.3, 165.5, 149.1, 135.9, 131.3, 126.1, 124.4, 123.8, 117.7, 117.2, 62.4, 61.4, 23.5, 14.7, 14.6. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{15}H_{17}NO_3$ 260.1281, found 260.1281.



3ba

ethyl 1-ethoxy-3,6-dimethylisoquinoline-4-carboxylate (3ba).

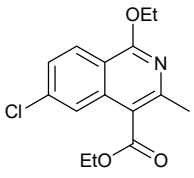
Eluent: petroleum ether/ethyl acetate (15:1). Yield 51 mg (74%). Light white solid, M.P. 63-65℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.12 (*d*, *J* = 8.4 Hz, 1H), 7.63 (*s*, 1H), 7.29 (*d*, *J* = 9.4 Hz, 1H), 4.56 (*q*, *J* = 7.1 Hz, 2H), 4.49 (*q*, *J* = 7.1 Hz, 2H), 2.58 (*s*, 3H), 2.49 (*s*, 3H), 1.46 (*m*, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.5, 160.5, 149.0, 141.7, 136.2, 123.1, 124.3, 123.0, 116.9, 115.9, 62.3, 61.3, 23.5, 22.5, 14.8, 14.6. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{16}H_{19}NO_3$ 274.1438, found 274.1438.



3ca

ethyl 1-ethoxy-6-methoxy-3-methylisoquinoline-4-carboxylate (3ca).

Eluent: petroleum ether/ethyl acetate (15:1). Yield 57 mg (79%). Light white solid, M.P. 65-67℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.13 (*d*, *J* = 9.1 Hz, 1H), 7.26 (*m*, 1H), 7.08 (*d*, *J* = 9.1 Hz, 1H), 4.55 (*q*, *J* = 7.1 Hz, 2H), 4.49 (*q*, *J* = 7.1 Hz, 2H), 3.90 (*s*, 3H), 2.59 (*s*, 3H), 1.46 (*m*, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.4, 161.9, 160.5, 150.6, 138.2, 126.3, 117.8, 116.4, 112.6, 103.0, 62.3, 61.2, 55.5, 23.9, 14.8, 14.6. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{16}H_{19}NO_4$ 290.1387, found 290.1386.

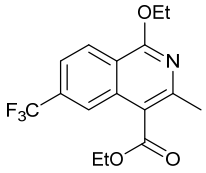


3da

ethyl 6-chloro-1-ethoxy-3-methylisoquinoline-4-carboxylate (3da).

Eluent: petroleum ether/ethyl acetate (15:1). Yield 59 mg (81%). Light white solid, M.P. 64-66℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.15 (*d*, *J* = 8.8 Hz, 1H), 7.93 (*s*, 1H), 7.39 (*d*, *J* = 8.8 Hz, 1H), 4.57 (*q*, *J* = 7.1 Hz, 2H), 4.49 (*q*, *J* = 7.1 Hz, 2H), 2.60 (*s*, 3H), 1.46

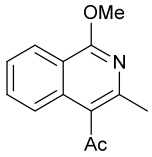
(*m*, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 168.6, 160.5, 151.2, 137.9, 137.0, 126.9, 126.2, 123.2, 116.2, 116.0, 62.7, 61.6, 23.8, 14.7, 14.6. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{15}H_{16}ClNO_3$ 294.0891, found 294.0876.



3ea

ethyl 1-ethoxy-3-methyl-6- (trifluoromethyl) isoquinoline-4-carboxylate (3ea).

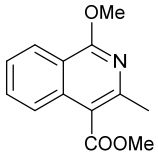
Eluent: petroleum ether/ethyl acetate (15:1). Yield 50 mg (62 %). Light white solid, M.P. 73-75℃. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.32 (*d*, *J* = 8.6 Hz, 1H), 8.27 (*s*, 1H), 7.63 (*d*, *J* = 8.5 Hz, 1H), 4.56 (*m*, 4H), 2.65 (*s*, 3H), 1.48 (*m*, 6H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 168.4, 160.3, 151.6, 135.5, 132.8 (*q*, *J* = 32.3 Hz), 125.7, 124.1 (*q*, *J* = 272.9 Hz), 121.8 (*q*, *J* = 4.0 Hz), 119.0, 117.1, 77.5, 63.0, 61.7, 23.8, 14.6, 14.5. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{16}H_{16}F_3NO_3$ 328.1155, found 328.1154.



3fb

1- (1-methoxy-3-methylisoquinolin-4-yl) ethan-1-one (3fb).

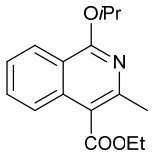
Eluent: petroleum ether/ethyl acetate (20:1). Yield 29 mg (54%). Yellow liquid. ^{1}H NMR ($CDCl_3$, 400 NMR) δ 8.23 (*d*, *J* = 8.3 Hz, 1H), 7.64 (*q*, *J* = 8.2 Hz, 1H), 7.56 (*q*, *J* = 8.2 Hz, 1H), 7.48 (*q*, *J* = 7.5 Hz, 1H), 4.12 (*s*, 3H), 2.62 (*s*, 3H), 2.51 (*s*, 3H). ^{13}C NMR ($CDCl_3$, 100 NMR) δ 206.4, 160.3, 144.7, 134.8, 131.2, 126.2, 126.1, 124.5, 123.0, 117.7, 53.9, 33.1, 22.6. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{13}H_{13}NO_2$ 216.1019, found 216.1015.



3fc

methyl 1-methoxy-3-methylisoquinoline-4-carboxylate (3fc).

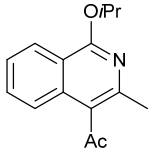
Eluent: petroleum ether/ethyl acetate (20:1). Yield 25 mg (44%). White solid, M.P. 68-70℃. ^{1}H NMR ($CDCl_3$, 400 NMR) δ 8.22 (*d*, *J* = 8.2 Hz, 1H), 7.87 (*d*, *J* = 8.5 Hz, 1H), 7.66 (*t*, *J* = 8.3 Hz, 1H), 7.48 (*t*, *J* = 8.0 Hz, 1H), 4.13 (*s*, 3H), 4.01 (*s*, 3H), 2.61 (*s*, 3H). ^{13}C NMR ($CDCl_3$, 100 NMR) δ 169.6, 160.8, 149.3, 136.9, 131.3, 126.2, 124.3, 123.8, 117.6, 117.0, 54.0, 52.3, 23.5. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{13}H_{13}NO_3$ 232.0968, found 232.0968.



3ga

ethyl 1-isopropoxy-3-methylisoquinoline-4-carboxylate (3ga).

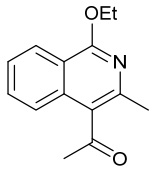
Eluent: petroleum ether/ethyl acetate (40:1). Yield 45 mg (63%). Yellow liquid. ^{1}H NMR ($CDCl_3$, 400 NMR) δ 8.24 (*d*, *J* = 8.2 Hz, 1H), 7.89 (*d*, *J* = 8.4 Hz, 1H), 7.65 (*t*, *J* = 8.0 Hz, 1H), 7.47 (*t*, *J* = 7.6 Hz, 1H), 5.64 (*hept*, *J* = 6.2 Hz, 1H), 4.50 (*q*, *J* = 7.2 Hz, 2H), 2.62 (*s*, 3H), 1.47 (*s*, 3H), 1.46 (*s*, 3H), 1.44 (*s*, 3H). ^{13}C NMR ($CDCl_3$, 100 NMR) δ 169.2, 160.0, 149.1, 135.9, 131.1, 125.9, 124.5, 123.7, 118.0, 116.7, 68.9, 6.3, 23.5, 22.1, 14.5. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{16}H_{19}NO_3$ 274.1438, found 274.1432.



3gb

1-(1-isopropoxy-3-methylisoquinolin-4-yl)ethan-1-one (3gb).

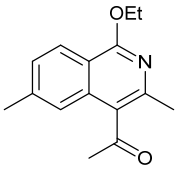
Eluent: petroleum ether/ethyl acetate (40:1). Yield 53 mg (88%). Yellow liquid. ^{1}H NMR ($CDCl_3$, 400 NMR) δ 8.25 (*d*, *J* = 8.3 Hz, 1H), 7.62 (*t*, *J* = 7.6 Hz, 1H), 7.55 (*d*, *J* = 8.3 Hz, 1H), 7.46 (*t*, *J* = 7.9 Hz, 1H), 5.62 (*hept*, *J* = 6.1 Hz, 1H), 2.62 (*s*, 3H), 2.50 (*s*, 3H), 1.45 (*s*, 3H), 1.44 (*s*, 3H). ^{13}C NMR ($CDCl_3$, 100 NMR) δ 206.5, 159.6, 144.9, 134.9, 131.1, 125.9, 125.5, 124.7, 122.9, 118.0, 68.8, 33.1, 22.8, 22.1. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{15}H_{17}NO_2$ 244.1332, found 244.1329.



3ab

1- (1-ethoxy-3-methylisoquinolin-4-yl) ethan-1-one (3ab).

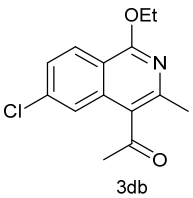
Eluent: petroleum ether/ethyl acetate (15:1). Yield 51 mg (89%). Yellow liquid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.28 (*d*, *J* = 8.2 Hz, 1H), 7.65 (*m*, 1H), 7.58 (*m*, 1H), 7.50 (*t*, *J* = 7.5 Hz, 1H), 4.60 (*q*, *J* = 7.1 Hz, 2H), 2.64 (*s*, 3H), 2.52 (*s*, 3H), 1.51 (*t*, *J* = 7.1 Hz, 3H).^{13}C NMR ($CDCl_3$, 100 MHz) δ 206.6, 160.2, 144.9, 134.9, 131.3, 126.2, 125.9, 124.7, 123.1, 117.8, 62.4, 33.2, 22.8, 14.8. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{14}H_{15}NO_2$ 230.1176, found 230.1174.



3bb

1- (1-ethoxy-3,6-dimethylisoquinolin-4-yl) ethan-1-one (3bb).

Eluent: petroleum ether/ethyl acetate (15:1). Yield 53 mg (86%). Light white solid, M.P. 59-61℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.13 (*d*, *J* = 8.3 Hz, 1H), 7.30 (*m*, 2H), 4.56 (*q*, *J* = 7.1 Hz, 2H), 2.62 (*s*, 3H), 2.48 (*s*, 6H), 1.48 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 206.9, 160.1, 144.8, 141.7, 135.2, 123.2, 125.6, 124.5, 122.3, 116.0, 62.3, 33.2, 22.8, 22.4, 14.8. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{15}H_{17}NO_2$ 244.1332, found 244.1331.

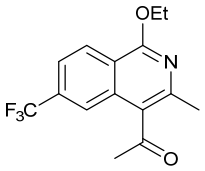


3db

1- (6-chloro-1-ethoxy-3-methylisoquinolin-4-yl) ethan-1-one (3db).

Eluent: petroleum ether/ethyl acetate (15:1). Yield 55 mg (84%). Light white solid, M.P. 61-63℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.19 (*d*, *J* = 8.8 Hz, 1H), 7.57 (*s*, 1H), 7.42 (*d*, *J* = 8.8 Hz, 1H), 4.57 (*q*, *J* = 7.1 Hz, 2H), 2.62 (*s*, 3H), 2.51 (*s*, 3H), 1.49 (*t*, *J* = 7.1 Hz,

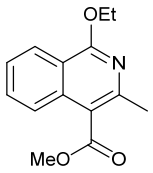
3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 205.8, 160.1, 146.8, 137.9, 135.9, 127.1, 126.5, 125.1, 122.4, 116.1, 62.7, 33.2, 23.1, 14.7. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{14}H_{14}ClNO_2$ 264.0786, found 264.0789.



3eb

1- (1-ethoxy-3-methyl-6- (trifluoromethyl) isoquinolin-4-yl) ethan-1-one (3eb).

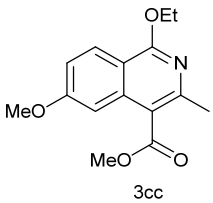
Eluent: petroleum ether/ethyl acetate (15:1). Yield 36 mg (49%). Light white solid, M.P. 68-70℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.37 (*d*, *J* = 8.6 Hz, 1H), 7.87 (*s*, 1H), 7.66 (*m*, 1H), 4.60 (*q*, *J* = 7.1 Hz, 2H), 2.65 (*s*, 3H), 2.55 (*s*, 3H), 1.51 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 205.5, 160.0, 147.0, 134.4, 133.0 (*q*, *J* = 32.4 Hz), 126.1, 124.0 (*q*, *J* = 272.9 Hz), 122.1, 120.8 (*q*, *J* = 4.1 Hz), 119.1, 77.5, 62.9, 33.2, 23.1, 14.7. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{15}H_{14}F_3NO_2$ 298.1049, found 298.1048.



3ac

methyl 1-ethoxy-3-methylisoquinoline-4-carboxylate (3ac).

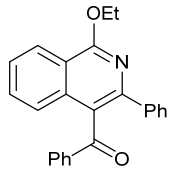
Eluent: petroleum ether/ethyl acetate (15:1). Yield 48 mg (79%). Light white solid, M.P. 59-61℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.24 (*d*, *J* = 8.2 Hz, 1H), 7.86 (*d*, *J* = 8.5 Hz, 1H), 7.65 (*t*, *J* = 8.3 Hz, 1H), 7.47 (*t*, *J* = 7.6 Hz, 1H), 4.58 (*q*, *J* = 7.1 Hz, 2H), 4.00 (*s*, 3H), 2.59 (*s*, 3H), 1.49 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.8, 160.7, 149.5, 136.0, 131.3, 126.1, 124.5, 123.9, 117.7, 116.8, 62.5, 52.4, 23.7, 14.7. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{14}H_{15}NO_3$ 246.1125, found 246.1125.



3cc

methyl 1-ethoxy-6-methoxy-3-methylisoquinoline-4-carboxylate (3cc).

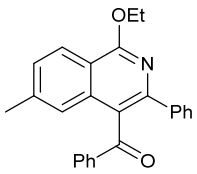
Eluent: petroleum ether/ethyl acetate (15:1). Yield 60 mg (87%). Light white solid, M.P. 60-62℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.14 (*d*, *J* = 9.1 Hz, 1H), 7.24 (*m*, 1H), 7.08 (*m*, 1H), 4.56 (*q*, *J* = 7.1 Hz, 2H), 4.00 (*s*, 3H), 3.90 (*s*, 3H), 2.58 (*s*, 3H), 1.47 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 169.9, 162.0, 160.6, 150.9, 138.2, 126.3, 117.8, 116.1, 112.6, 103.1, 62.3, 55.5, 52.2, 24.0, 14.8. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{15}H_{17}NO_4$ 276.1230, found 276.1229.



3ad

(1-ethoxy-3-phenylisoquinolin-4-yl) (phenyl) methanone (3ad).

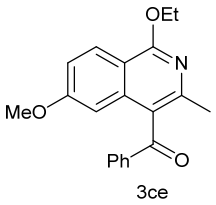
Eluent: petroleum ether/ethyl acetate (15:1). Yield 63 mg (72%). Light yellow solid, M.P. 151-153℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.38 (*d*, *J* = 8.6 Hz, 1H), 7.69 (*m*, 3H), 7.60 (*m*, 4H), 7.37 (*t*, *J* = 7.4 Hz, 1H), 7.21 (*m*, 5H), 4.72 (*q*, *J* = 7.1 Hz, 2H), 1.56 (*t*, *J* = 7.1 Hz, 3H).^{13}C NMR ($CDCl_3$, 100 MHz) δ 199.0, 160.6, 148.1, 140.1, 138.3, 136.8, 133.4, 131.5, 129.8, 129.7, 128.9, 128.5, 128.3, 127.4, 127.0, 124.6, 123.1, 118.4, 62.7, 14.9. HR-MS (ESI) $[M+Na]^+$ m/z calcd for $C_{24}H_{19}NO_2$ 376.1308, found 376.1307.



3bd

(1-ethoxy-6-methyl-3-phenylisoquinolin-4-yl) (phenyl) methanone (3bd).

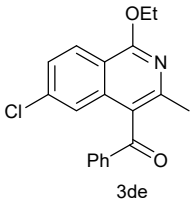
Eluent: petroleum ether/ethyl acetate (15:1). Yield 64 mg (70%). Light yellow solid, M.P. 152-154℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.26 (*d*, *J* = 8.4 Hz, 1H), 7.67 (*d*, *J* = 7.3 Hz, 2H), 7.62 (*d*, *J* = 7.7 Hz, 2H), 7.48 (*s*, 1H), 7.37 (*t*, *J* = 8.8 Hz, 2H), 7.21 (*m*, 5H), 4.71 (*q*, *J* = 7.1 Hz, 2H), 2.43 (*s*, 3H), 1.55 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 199.3, 160.7, 143.2, 142.0, 140.2, 138.4, 137.1, 133.3, 129.8, 129.8, 129.1, 128.5, 128.3, 127.4, 124.4, 123.7, 122.7, 116.5, 62.5, 22.4, 14.9. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{25}H_{21}NO_2$ 368.1645, found 368.1647.



3ce

(1-ethoxy-6-methoxy-3-methylisoquinolin-4-yl) (phenyl) methanone (3ce).

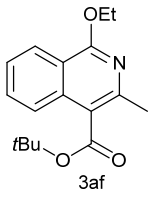
Eluent: petroleum ether/ethyl acetate (15:1). Yield 60 mg (75%). Light yellow solid, M.P. 107-109℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.19 (*d*, *J* = 9.1 Hz, 1H), 7.87 (*d*, *J* = 7.4 Hz, 2H), 7.58 (*t*, *J* = 7.4 Hz, 1H), 7.45 (*t*, *J* = 7.7 Hz, 2H), 7.07 (*m*, 1H), 6.69 (*m*, 1H), 4.59 (*q*, *J* = 7.1 Hz, 2H), 3.69 (*s*, 3H), 2.32 (*s*, 3H), 1.50 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 199.4, 161.7, 160.4, 147.6, 138.5, 138.4, 133.9, 129.9, 129.1, 126.4, 122.5, 117.9, 112.7, 103.0, 62.3, 55.5, 23.3, 14.8. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{20}H_{19}NO_3$ 322.1438, found 322.1440.



3de

(6-chloro-1-ethoxy-3-methylisoquinolin-4-yl) (phenyl) methanone (3de).

Eluent: petroleum ether/ethyl acetate (15:1). Yield 59 mg (73%). Light yellow solid, M.P. 108-110℃. ^{1}H NMR ($CDCl_3$, 600 MHz) δ 8.22 (*d*, *J* = 9.2 Hz, 1H), 7.86 (*d*, *J* = 7.4 Hz, 2H), 7.61 (*t*, *J* = 7.4 Hz, 1H), 7.46 (*t*, *J* = 7.8 Hz, 2H), 7.41 (*s*, 1H), 7.39 (*s*, 1H), 4.61 (*q*, *J* = 7.1 Hz, 2H), 2.33 (*s*, 3H), 1.52 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz) δ 198.3, 160.4, 143.1, 138.0, 137.7, 137.4, 134.2, 129.9, 129.2, 127.1, 126.4, 123.1, 122.2, 116.1, 62.7, 23.3, 14.8. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{19}H_{16}ClNO_2$ 326.0942, found 326.0945.

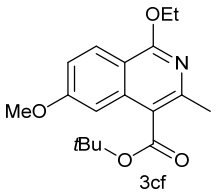


3af

tert-butyl 1-ethoxy-3-methylisoquinoline-4-carboxylate (3af).

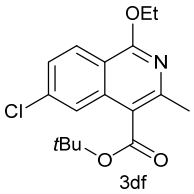
Eluent: petroleum ether/ethyl acetate (15:1). Yield 46 mg (65%). Yellow liquid. ^{1}H

NMR ($CDCl_3$, 600 MHz) δ 8.23 (*d*, *J* = 8.0 Hz, 1H), 7.86 (*d*, *J* = 8.4 Hz, 1H), 7.64 (*t*, *J* = 8.3 Hz, 1H), 7.45 (*t*, *J* = 8.0 Hz, 1H), 4.57 (*q*, *J* = 7.1 Hz, 2H), 2.60 (*s*, 3H), 1.67 (*s*, 9H), 1.48 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz) δ 163.6, 160.2, 147.8, 135.9, 131.1, 126.0, 124.4, 123.6, 118.8, 117.8, 82.2, 62.3, 28.6, 23.2, 14.8. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{17}H_{21}NO_3$ 288.1594, found 288.1595.



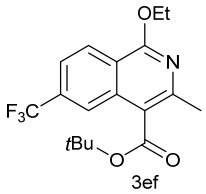
tert-butyl 1-ethoxy-6-methoxy-3-methylisoquinoline-4-carboxylate (3cf).

Eluent: petroleum ether/ethyl acetate (15:1). Yield 59 mg (75%). Yellow liquid. ^1H NMR ($CDCl_3$, 600 MHz) δ 8.12 (*d*, *J* = 9.0 Hz, 1H), 7.20 (*d*, *J* = 2.3 Hz, 1H), 7.07 (*m*, 1H), 4.54 (*q*, *J* = 7.1 Hz, 2H), 3.90 (*s*, 3H), 2.58 (*s*, 3H), 1.67 (*s*, 9H), 1.46 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz) δ 168.8, 161.8, 160.2, 149.1, 138.0, 126.3, 118.3, 117.7, 112.7, 102.8, 81.9, 62.2, 55.4, 28.6, 23.4, 14.8. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{18}H_{23}NO_4$ 318.1700, found 318.1695.



tert-butyl 6-chloro-1-ethoxy-3-methylisoquinoline-4-carboxylate (3n).

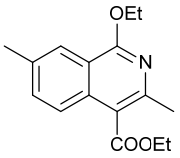
Eluent: petroleum ether/ethyl acetate (15:1). Yield 58 mg (72%). Yellow liquid. ^1H NMR ($CDCl_3$, 600 MHz) δ 8.15 (*d*, *J* = 8.8 Hz, 1H), 7.89 (*m*, 1H), 7.39 (*d*, *J* = 8.8 Hz, 1H), 4.56 (*q*, *J* = 7.1 Hz, 2H), 2.60 (*s*, 3H), 1.67 (*s*, 9H), 1.47 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 150 MHz) δ 168.0, 160.1, 149.9, 137.7, 137.0, 126.8, 126.2, 123.1, 117.8, 116.0, 82.6, 62.6, 28.6, 23.5, 14.7. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{17}H_{20}ClNO_3$ 322.1204, found 322.1205.



3ef

tert-butyl 1-ethoxy-3-methyl-6- (trifluoromethyl) isoquinoline-4-carboxylate (3ef).

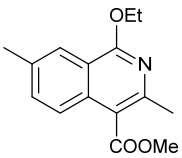
Eluent: petroleum ether/ethyl acetate (15:1). Yield 55 mg (62%). Yellow liquid. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.34 (*d*, *J* = 8.6 Hz, 1H), 8.24 (*s*, 1H), 7.63 (*m*, 1H), 4.60 (*q*, *J* = 7.0 Hz, 2H), 2.64 (*s*, 3H), 1.68 (*s*, 9H), 1.49 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 167.8, 160.0, 150.3, 135.4, 132.69 (*q*, *J* = 32.3 Hz), 125.8, 124.16 (*q*, *J* = 272.5 Hz), 121.68 (*q*, *J* = 3.8 Hz), 119.0, 118.8, 82.8, 77.5, 62.9, 28.5, 23.5, 14.7. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{18}H_{20}F_3NO_3$ 356.1468, found 356.1471.



3ha

ethyl 1-ethoxy-3,7-dimethylisoquinoline-4-carboxylate (3ha).

Eluent: petroleum ether/ethyl acetate (40:1). Yield 45 mg (66%). Yellow liquid. ^{1}H NMR ($CDCl_3$,400 MHz) δ 8.01 (*s*, 1H), 7.79 (*d*, *J* = 8.6 Hz, 1H), 7.48 (*d*, *J* = 8.6 Hz, 1H), 4.58 (*q*, *J* = 7.2 Hz, 2H), 4.49 (*q*, *J* = 7.1 Hz, 2H), 2.60 (*s*, 3H), 2.50 (*s*, 3H), 1.49 (*t*, *J* = 7.0 Hz, 3H), 1.44 (*t*, *J* = 7.0 Hz, 3H).^{13}C NMR ($CDCl_3$, 100 NMR) δ 169.3, 160.1, 148.0, 135.9, 134.0, 133.2, 123.6, 123.3, 117.8, 116.9, 62.3, 61.2, 23.3, 21.7, 14.7, 14.5. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{16}H_{19}NO_3$ 274.1438, found 274.1434.

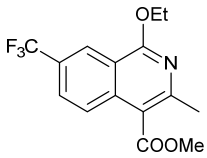


3hc

methyl 1-ethoxy-3,7-dimethylisoquinoline-4-carboxylate (3hc).

Eluent: petroleum ether/ethyl acetate (40:1). Yield 58 mg (90%). Yellow solid, M.P. 63-65℃. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.01 (s, 1H), 7.77 (*d*, *J* = 8.6 Hz, 1H), 7.48 (*d*, *J* = 8.8 Hz, 1H), 4.58 (*q*, *J* = 7.1 Hz, 2H), 3.99 (*s*, 3H), 2.58 (*s*, 3H), 2.50 (*s*, 3H), 1.49 (*t*, *J*

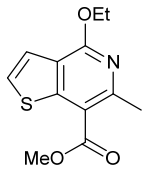
= 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 NMR) δ 169.7, 160.2, 148.4, 136.0, 134.1, 133.3, 123.7, 123.3, 117.8, 116.6, 62.3, 52.2, 23.5, 21.7, 14.7. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{15}H_{17}NO_3$ 260.1281, found 260.1281.



3ic

methyl 1-ethoxy-3-methyl-7-(trifluoromethyl) isoquinoline-4-carboxylate (3ic).

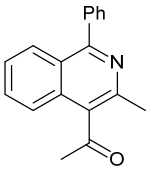
Eluent: petroleum ether/ethyl acetate (40:1). Yield 58 mg (74%). White solid, M.P. 108-110℃. ^{1}H NMR ($CDCl_3$, 400 NMR) δ 8.53 (*s*, 1H), 8.02 (*d*, *J* = 8.9 Hz, 1H), 7.81 (*d*, *J* = 8.9 Hz, 1H), 4.62 (*q*, *J* = 7.1 Hz, 2H), 4.02 (*s*, 3H), 2.63 (*s*, 3H), 1.51 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 NMR) δ 168.9, 160.8, 152.5, 137.6, 127.89 (*q*, *J* = 33.3 Hz), 126.9, 125.1, 124.11 (*d*, *J* = 272.1 Hz), 122.41 (*d*, *J* = 4.5 Hz), 116.8, 116.5, 63.0, 52.4, 23.9, 14.6. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{15}H_{14}F_3NO_3$ 314.0999, found 314.0995.



3jc

methyl 4-ethoxy-6-methylthieno[3,2-c]pyridine-7-carboxylate (3jc).

Eluent: petroleum ether/ethyl acetate (100:1). Yield 42 mg (71%). White solid, M.P. 80-82℃ .^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.44 (*d*, *J* = 5.6 Hz, 1H), 7.37 (*d*, *J* = 5.6 Hz, 1H), 4.60 (*q*, *J* = 7.2 Hz, 2H), 3.99 (*s*, 3H), 2.85 (*s*, 3H), 1.46 (*t*, *J* = 7.1 Hz, 3H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ 167.3, 159.1, 155.9, 150.9, 127.5, 123.1, 120.6, 112.9, 62.4, 52.0, 25.5, 14.8. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{12}H_{13}NO_3S$ 252.0689, found 252.0689.

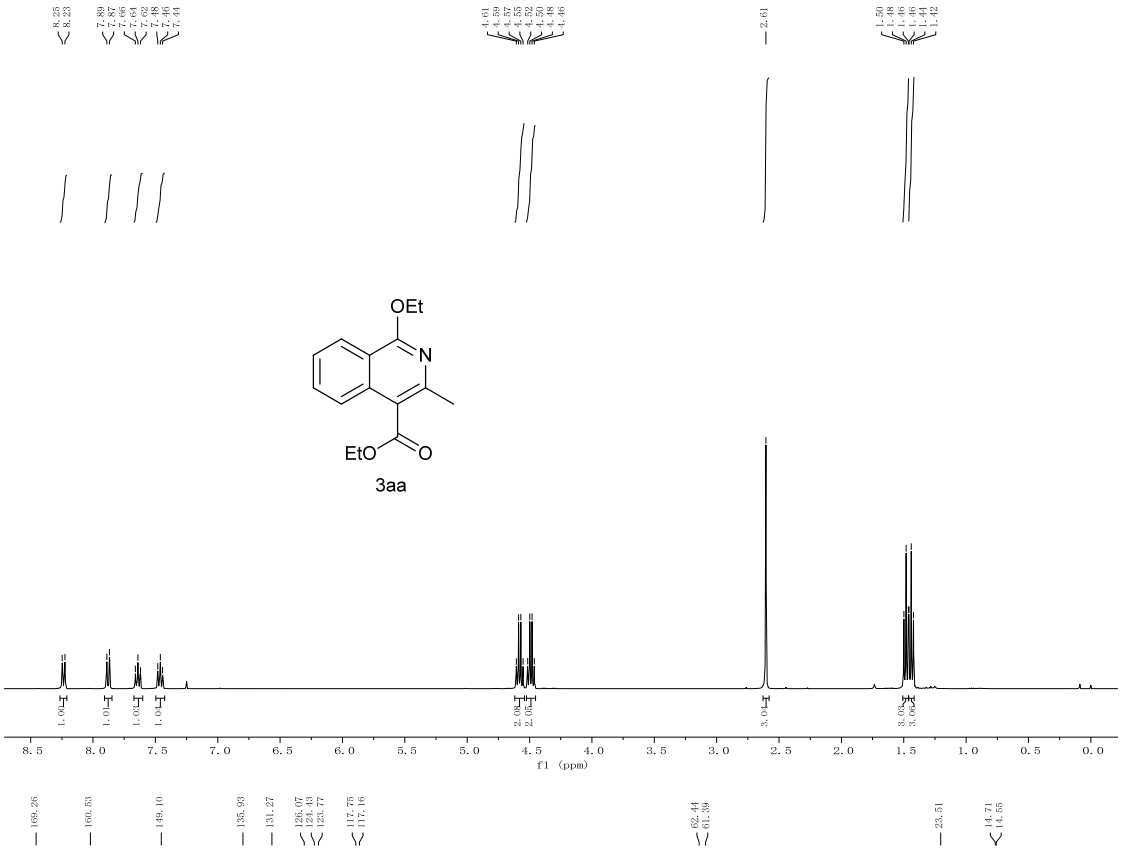


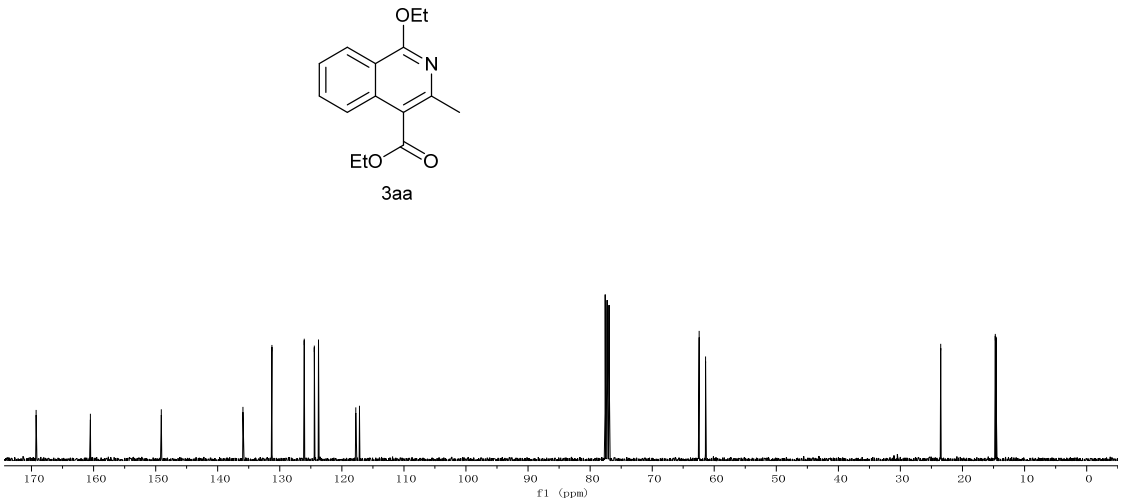
3kb

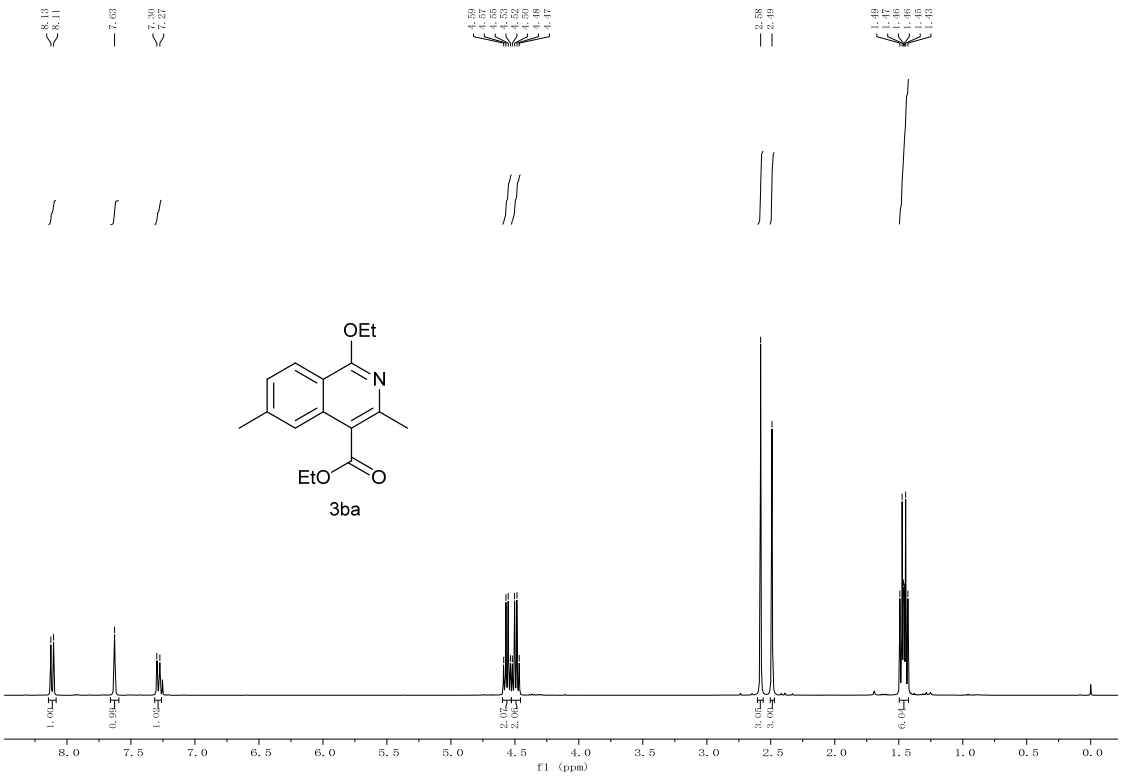
1- (3-methyl-1-phenylisoquinolin-4-yl) ethan-1-one (3kb).

Eluent: petroleum ether/ethyl acetate (20:1). Yield 58 mg (89%). Yellow solid, M.P. 109- 111℃. ^{1}H NMR ($CDCl_3$, 400 NMR) δ 8.06 (*d*, *J* = 8.5 Hz, 1H), 7.67 (*m*, 4H), 7.51 (*m*, 4H), 2.71 (*s*, 3H), 2.70 (*s*, 3H). ^{13}C NMR ($CDCl_3$, 100 NMR) δ 206.5, 161.3, 145.1, 139.2, 133.2, 131.0, 130.7, 129.9, 128.9, 128.5, 128.2, 126.7, 124.7, 123.3, 33.0, 22.6. HR-MS (ESI) $[M+H]^+$ m/z calcd for $C_{18}H_{15}NO$ 262.1226, found 262.1230.

The ^{1}H and ^{13}C NMR spectra of compounds 3aa-3kb.



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1.47
1.47
1.46
1.46
1.45
1.43
OEt
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EtO
O
3ba
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0.90
1.02
2.07
2.06
3.06
3.00
6.04
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7.0
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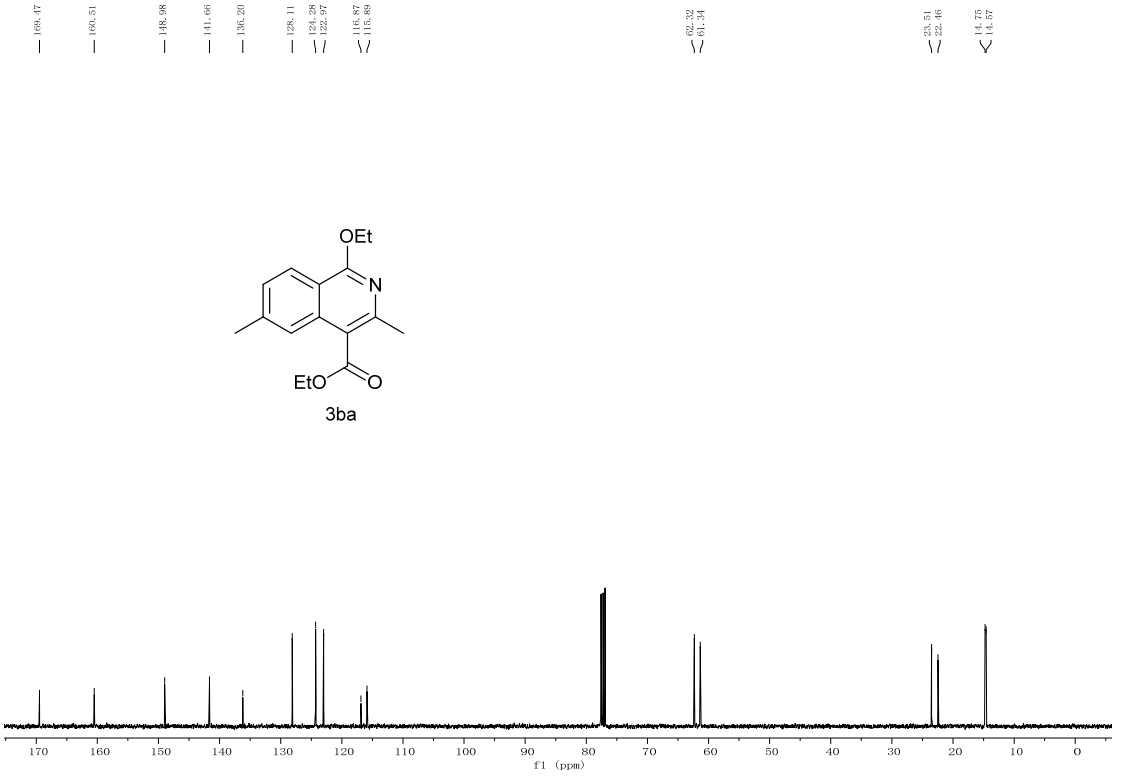
f1 (ppm)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N
EtO
O
3ba
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100
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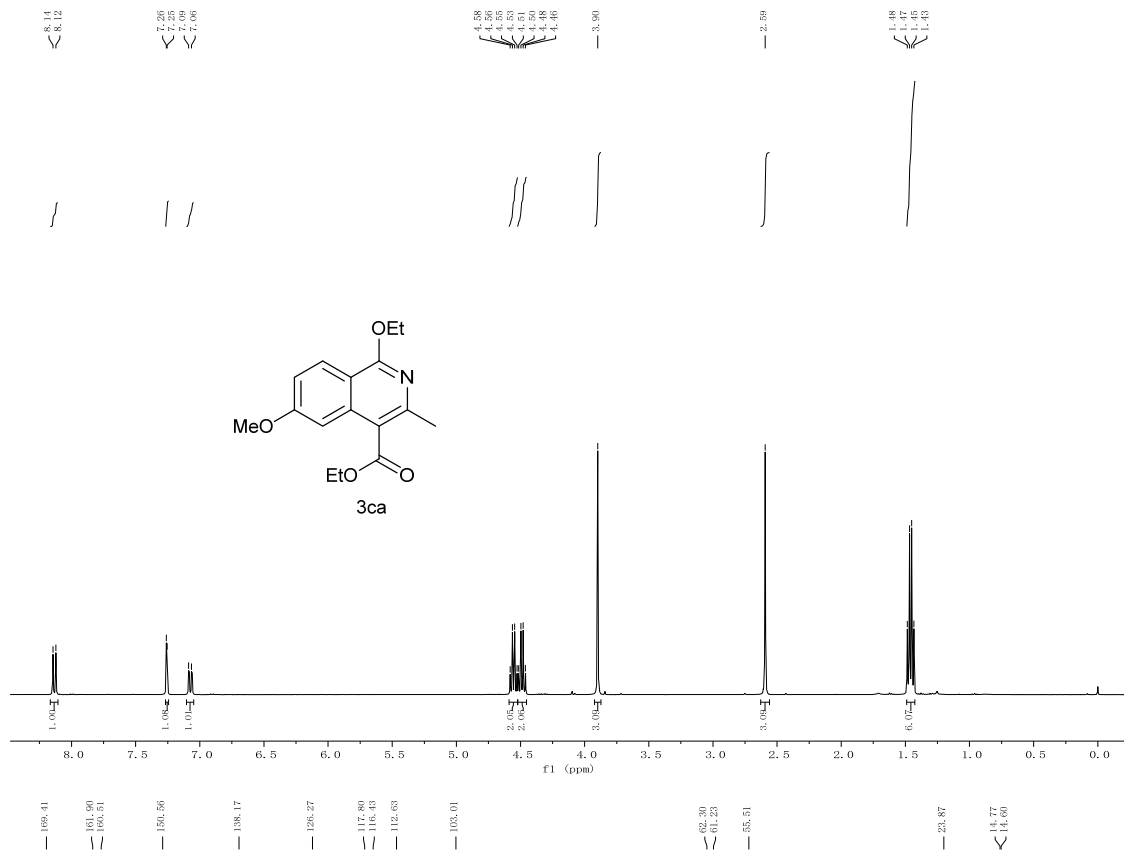
f1 (ppm)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EtO
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3.00
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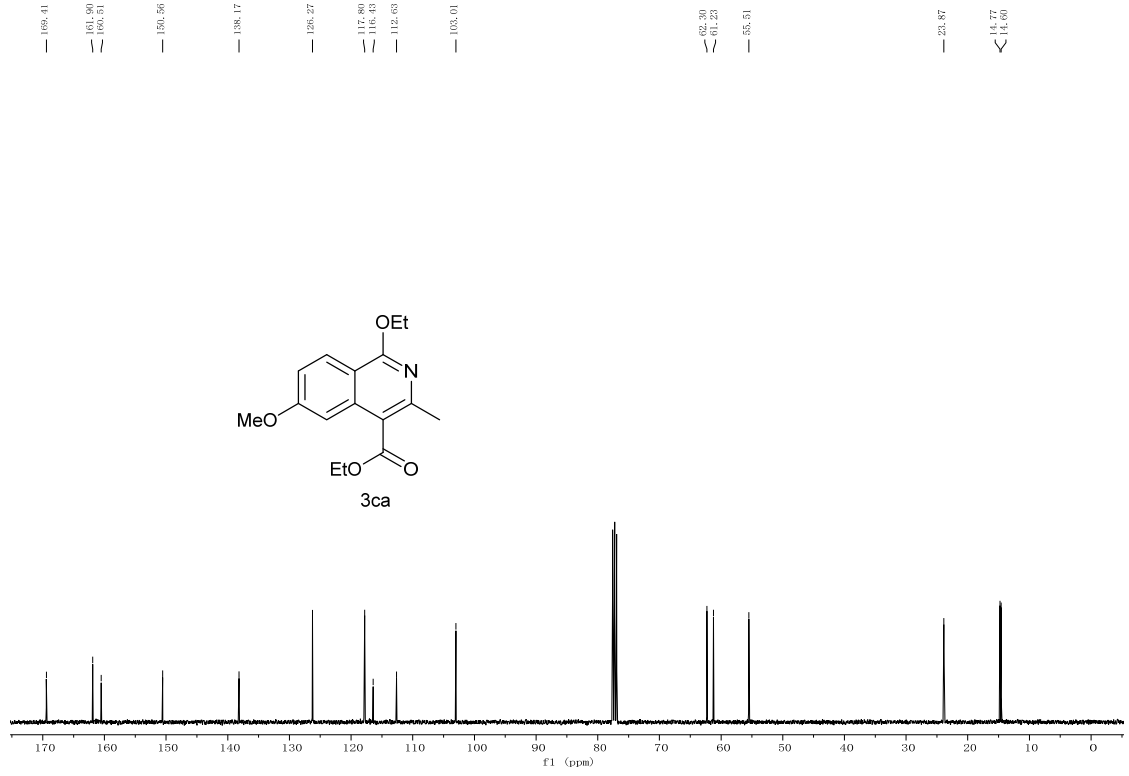
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14.60
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EtO
O
3ca
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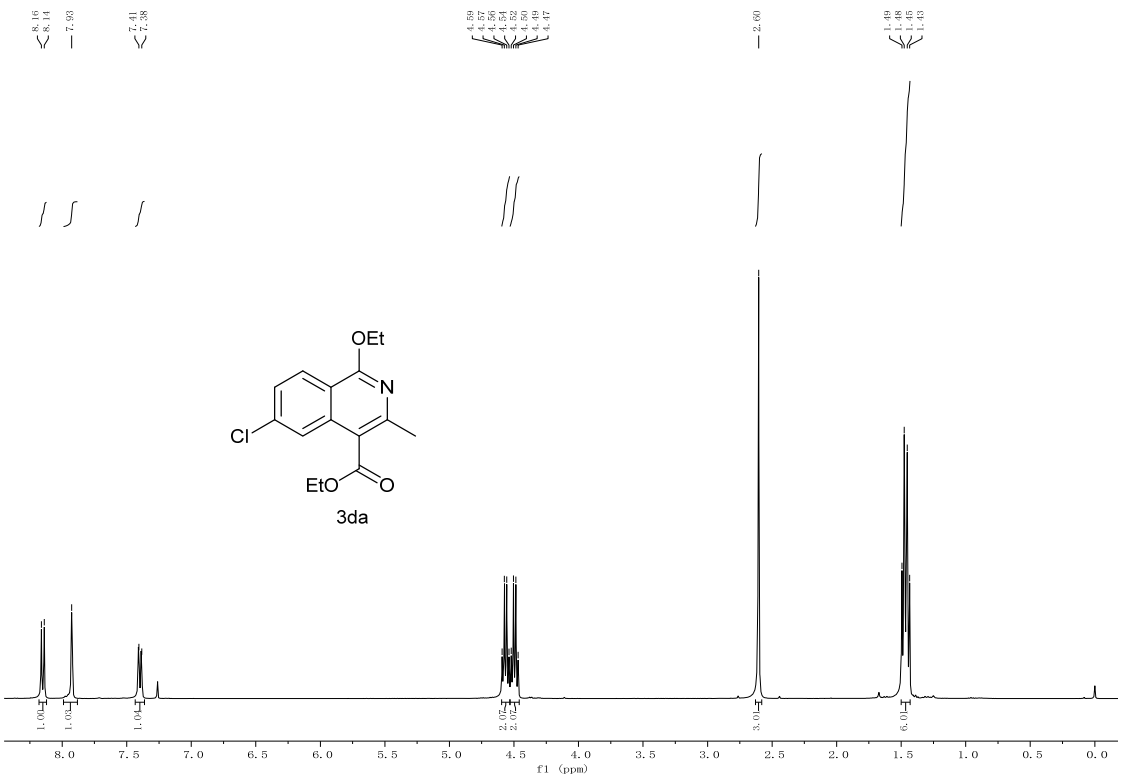
f1 (ppm)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1.45
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OEt
N
Cl
EtO
O
3da
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1.00
1.04
2.07
2.07
3.01
6.01
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


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160.45
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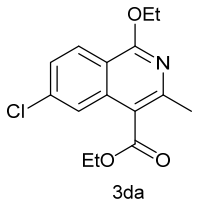
14.65


OEt
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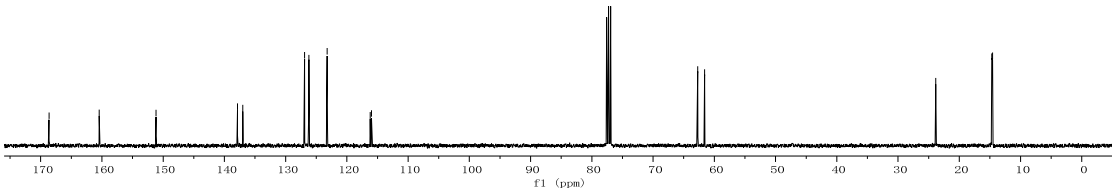
Cl
EtO
O
3da


170
160
150
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110
100
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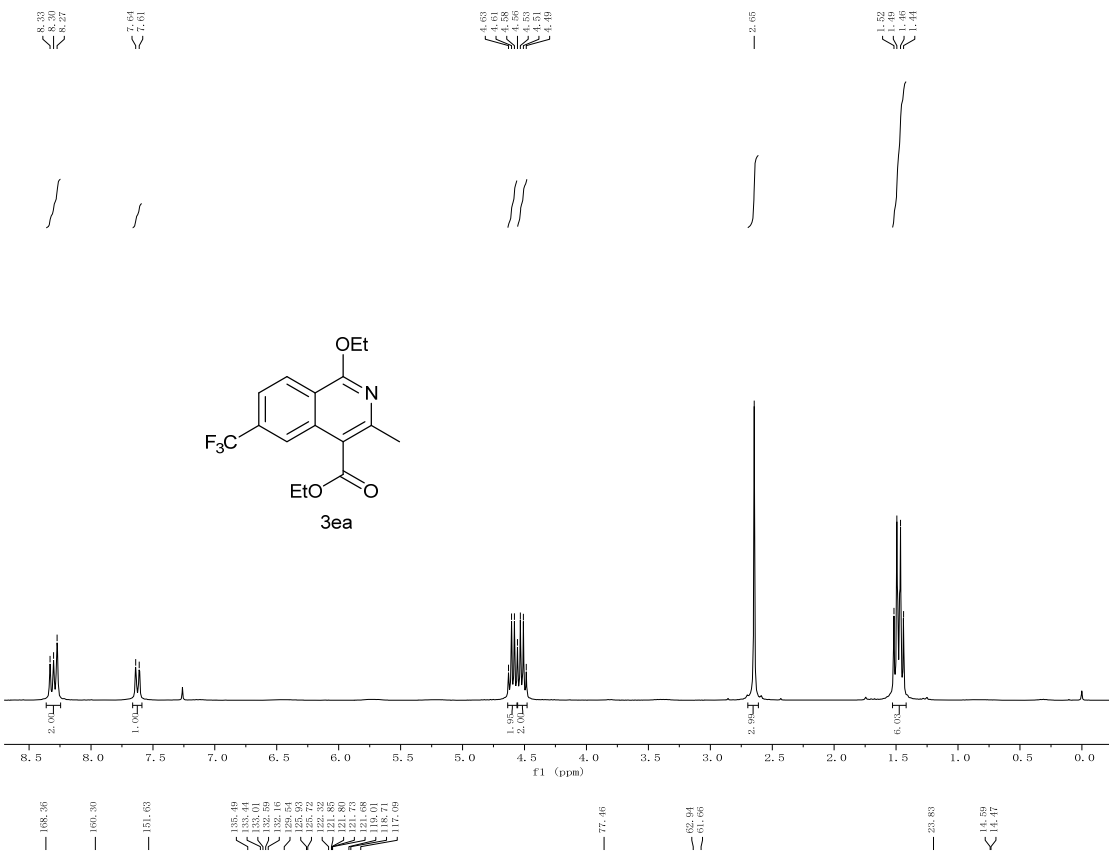
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.30
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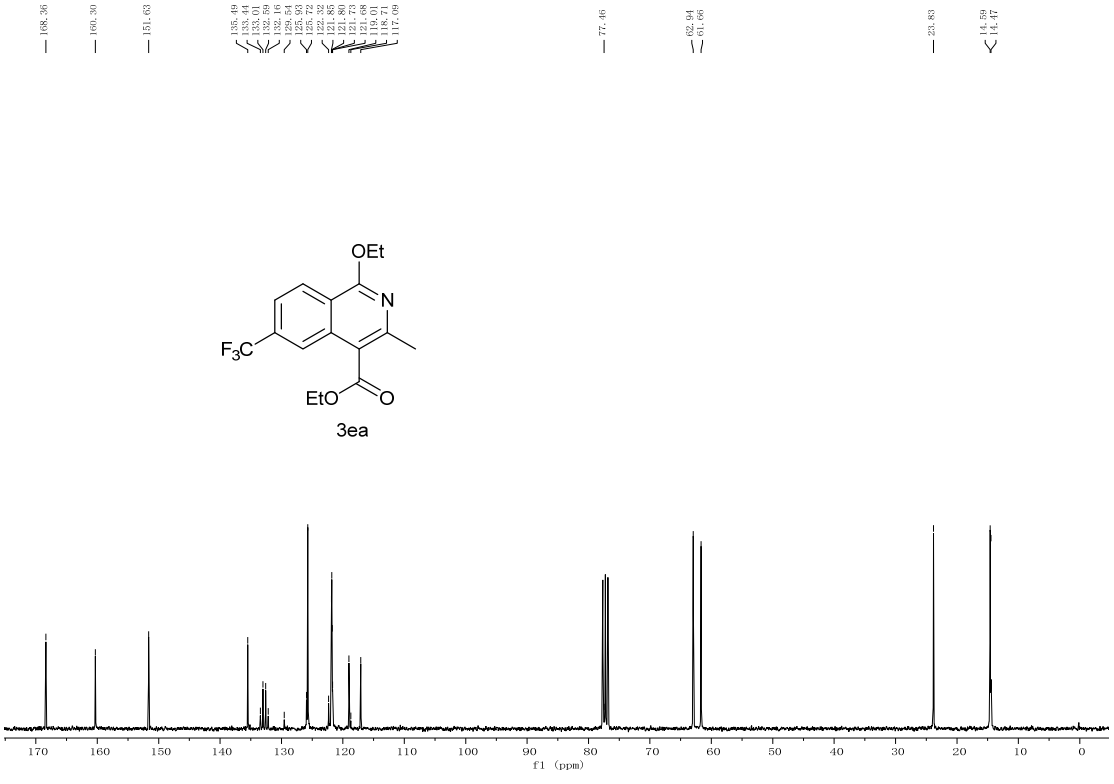
4.63
4.61
4.58
4.56
4.53
4.51
4.49
2.65
1.52
1.49
1.46
1.44
OEt
N
F3C
EtO
O
3ea
2.00
1.00
1.95
2.00
2.99
6.03
f1 (ppm)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135.49
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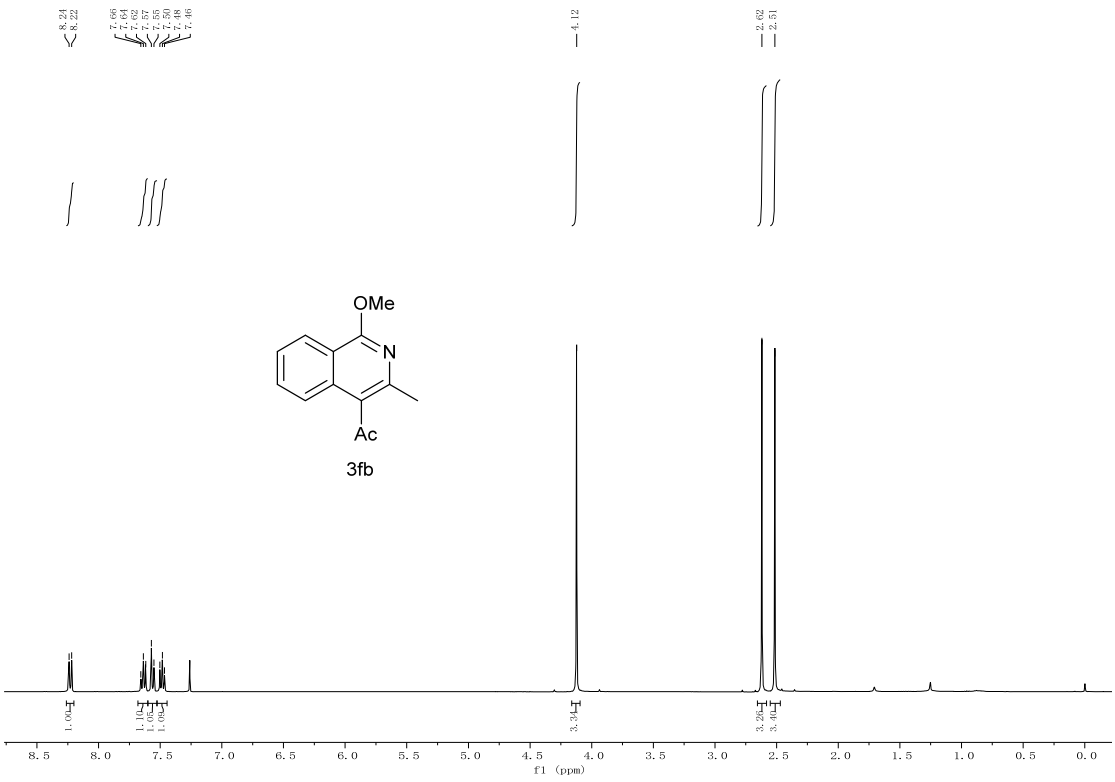
133.01
132.58
132.16
129.54
125.93
125.72
122.32
121.85
121.80
121.73
121.68
119.01
118.71
117.09
77.46
62.64
61.66
23.83
14.59
14.47
OEt
N
F3C
EtO
O
3ea
f1 (ppm)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8.22
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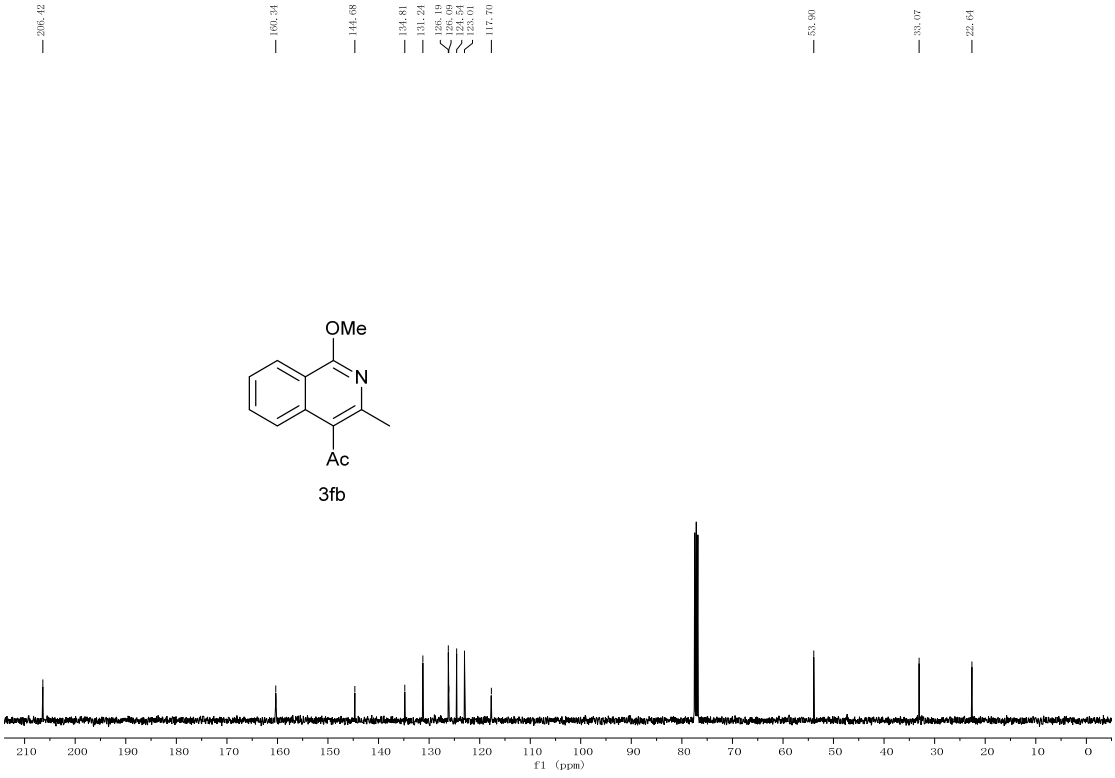
7.50
7.48
7.46
4.12
2.62
2.51
OMe
N
Ac
1.04
1.10
1.05
1.04
3.34
3.20
3.40
f1 (ppm)

3fb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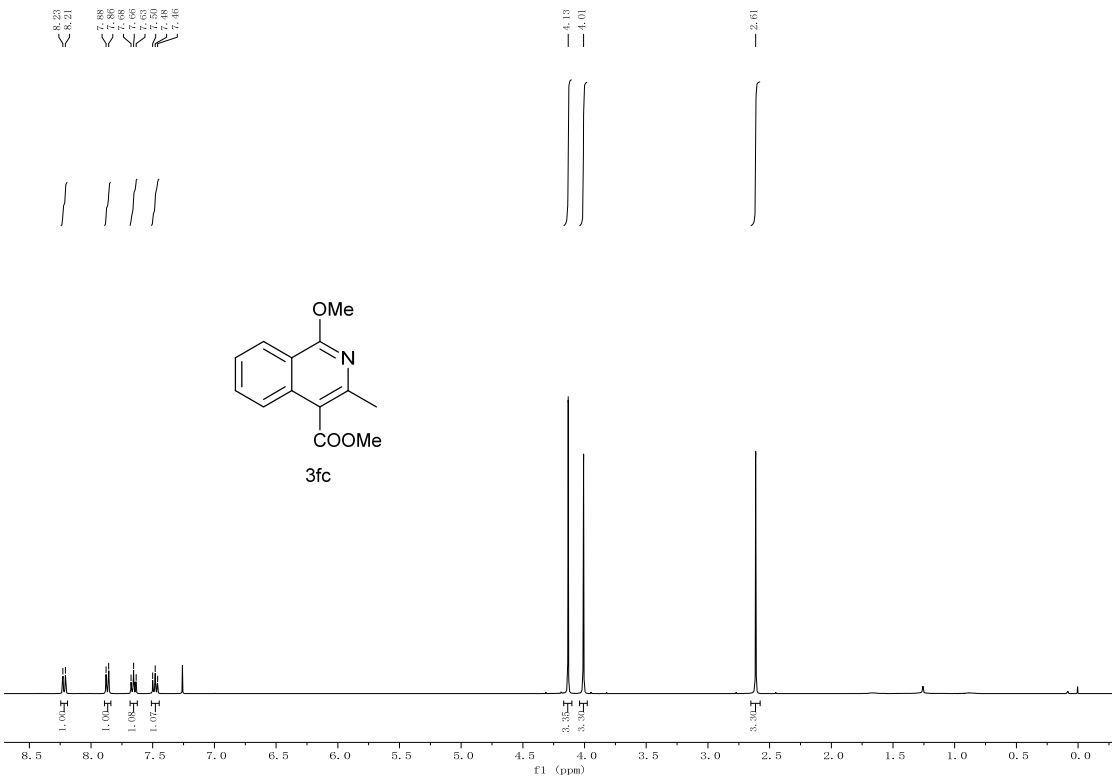
53.90
33.07
22.64
OMe
N
Ac
f1 (ppm)

3fb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8.21
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7.66
7.50
7.48
7.46
4.13
4.01
2.61
OMe
N
COOMe
3fc
1.04
1.00
1.08
1.07
3.33
3.30
3.30
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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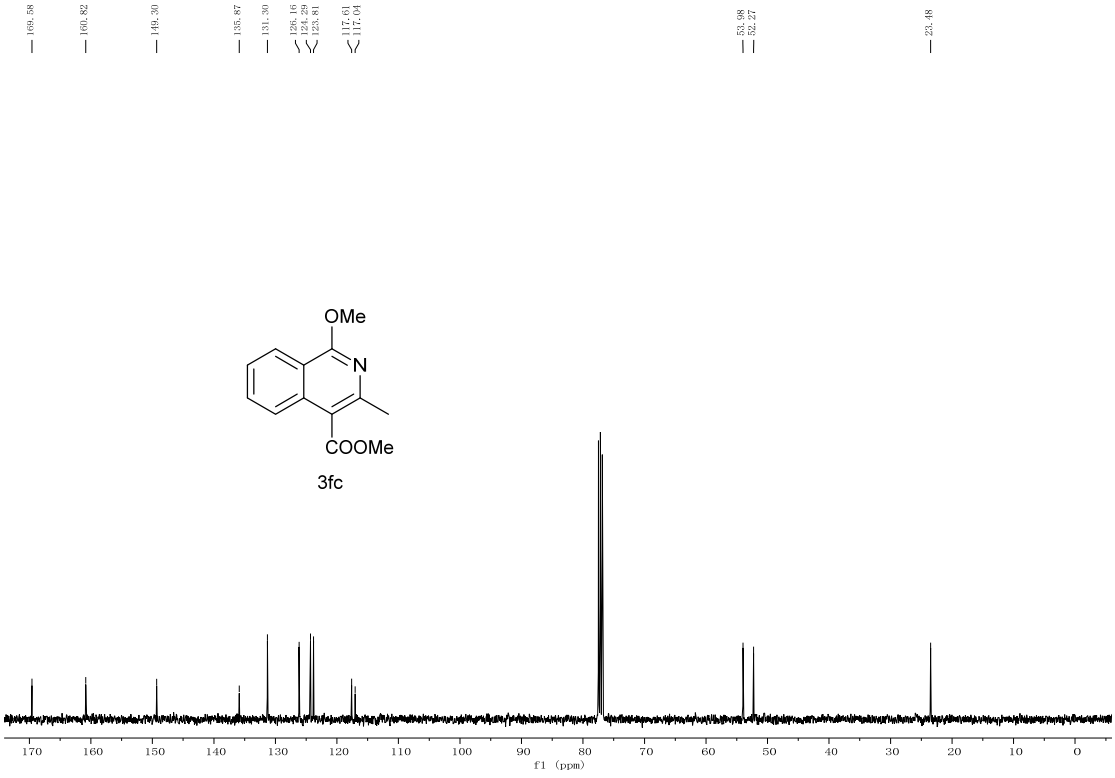
0.0
f1 (ppm)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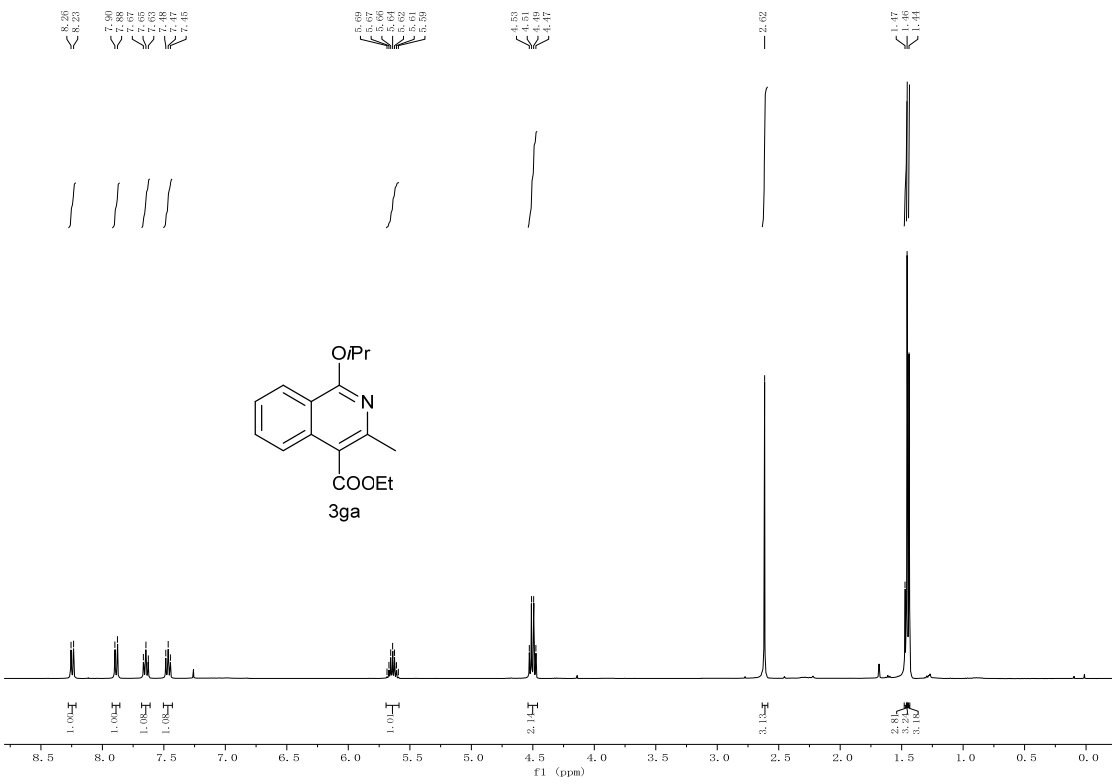
126.16
124.29
123.81
117.61
117.04
53.98
52.27
23.48
OMe
N
COOMe
3fc
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.48
7.47
7.45
5.69
5.67
5.66
5.64
5.62
5.61
5.59
4.53
4.51
4.49
4.47
2.62
1.47
1.46
1.44
OiPr
N
COOEt
3ga
1.00
1.00
1.00
1.09
1.04
2.14
3.13
2.81
3.24
3.10
f1 (ppm)


169.24
160.02
149.11
135.93
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124.46
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68.89
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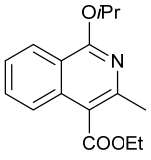
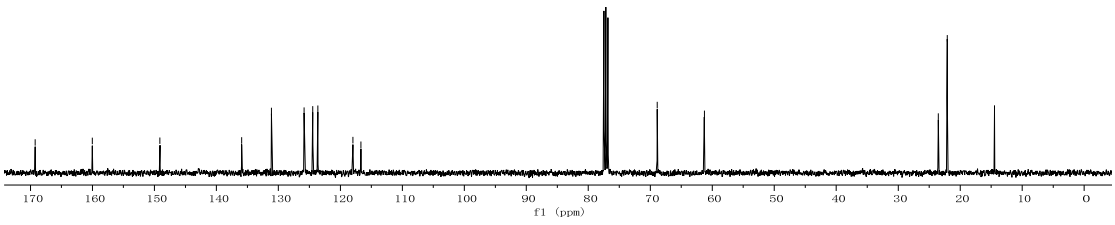
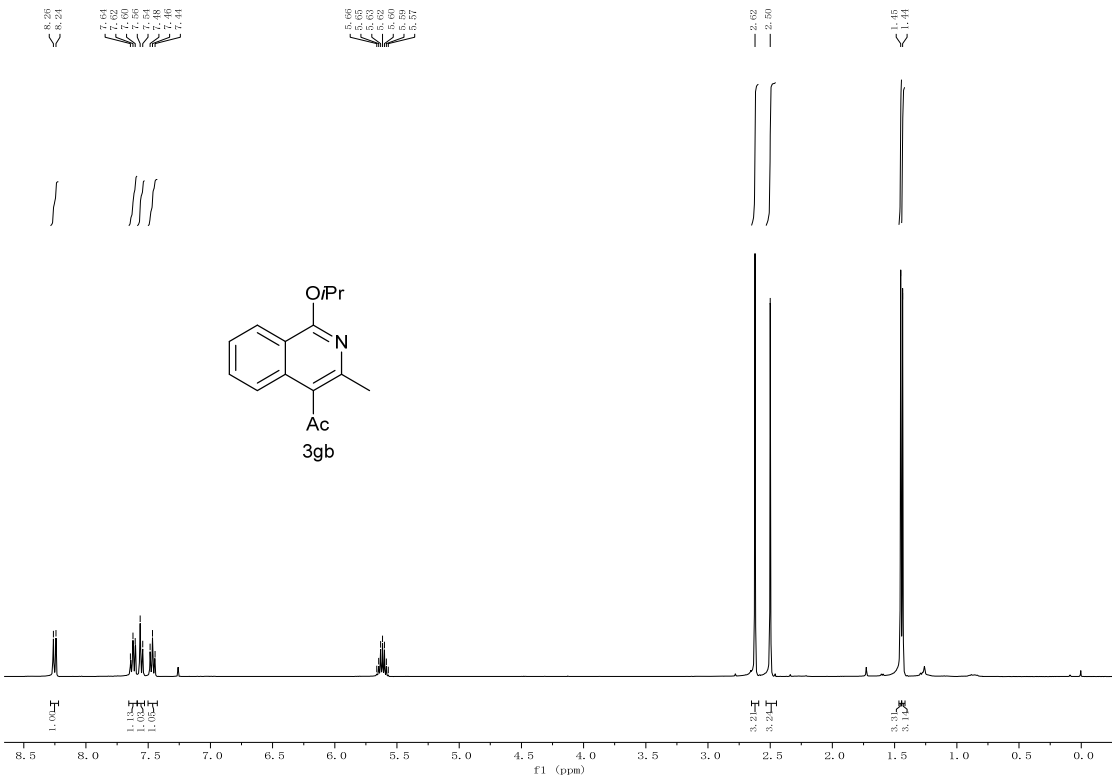
23.52
22.09
14.48


OiPr
N
COOEt
3ga


f1 (ppm)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8.24
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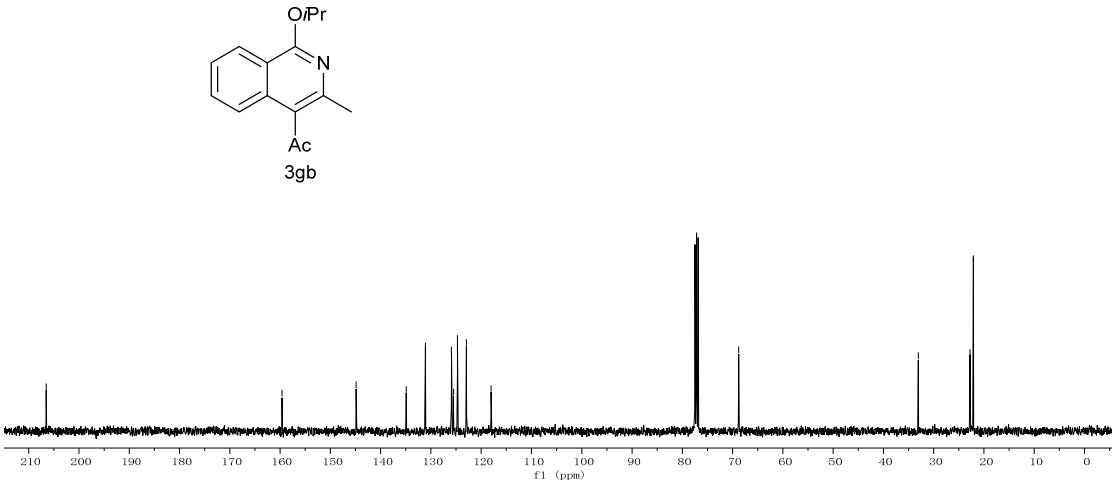
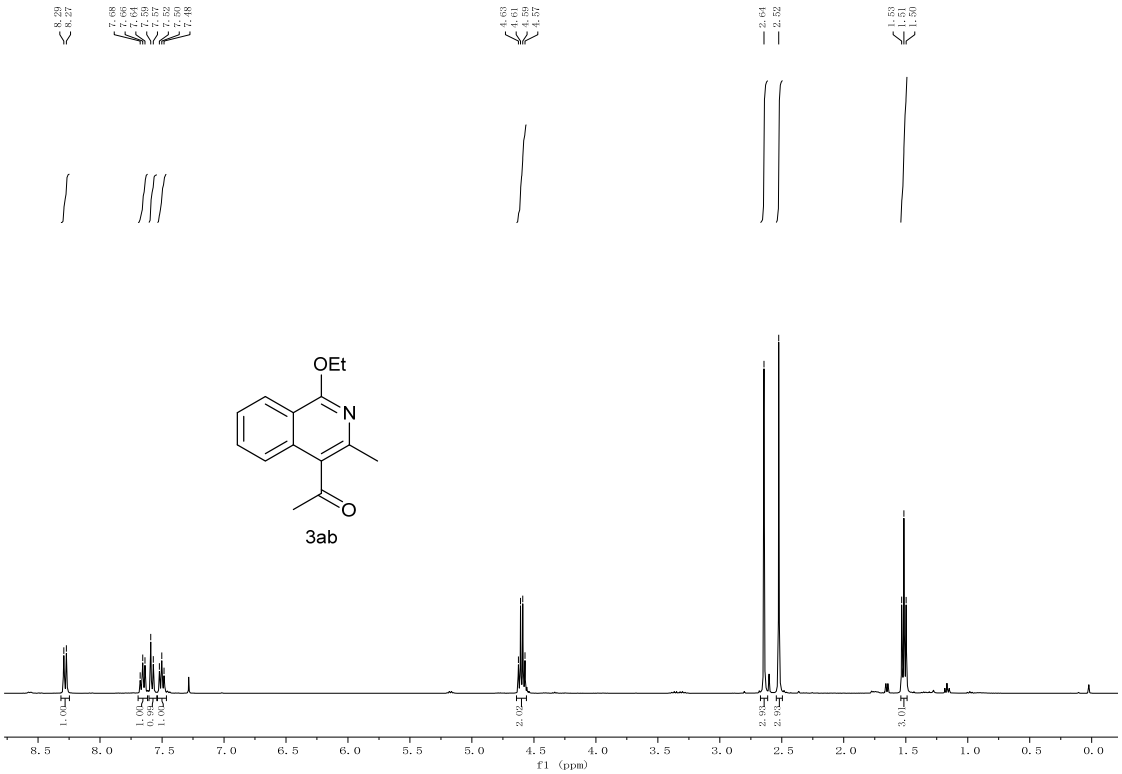
7.62
7.60
7.56
7.54
7.48
7.46
7.44
5.66
5.65
5.63
5.62
5.60
5.59
5.57
2.62
2.50
1.45
1.44
O*i*Pr
N
Ac
3gb
1.00
1.13
1.03
1.05
3.24
3.24
3.31
3.14
f1 (ppm)


206.52
159.61
144.87
134.91
131.09
125.92
125.80
124.72
122.93
118.04
68.78
33.07
22.78
22.11


O*i*Pr
N
Ac
3gb
f1 (ppm)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7.64
7.59
7.57
7.52
7.50
7.48
4.63
4.61
4.59
4.57
2.64
2.52
1.53
1.51
1.50
OEt
N
O
3ab
1.00
1.00
0.99
1.04
2.00
2.93
2.99
3.04
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)


206.62
169.16
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134.91
131.28
128.16
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124.72
123.06
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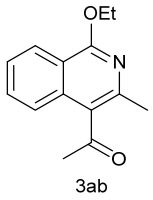
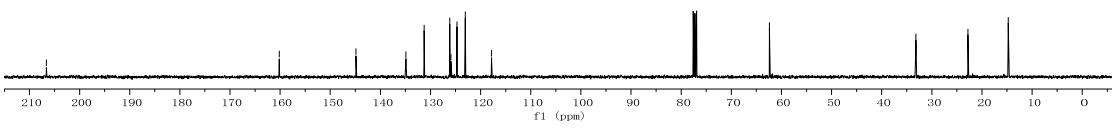
33.18
22.80
14.75


OEt
N
O
3ab


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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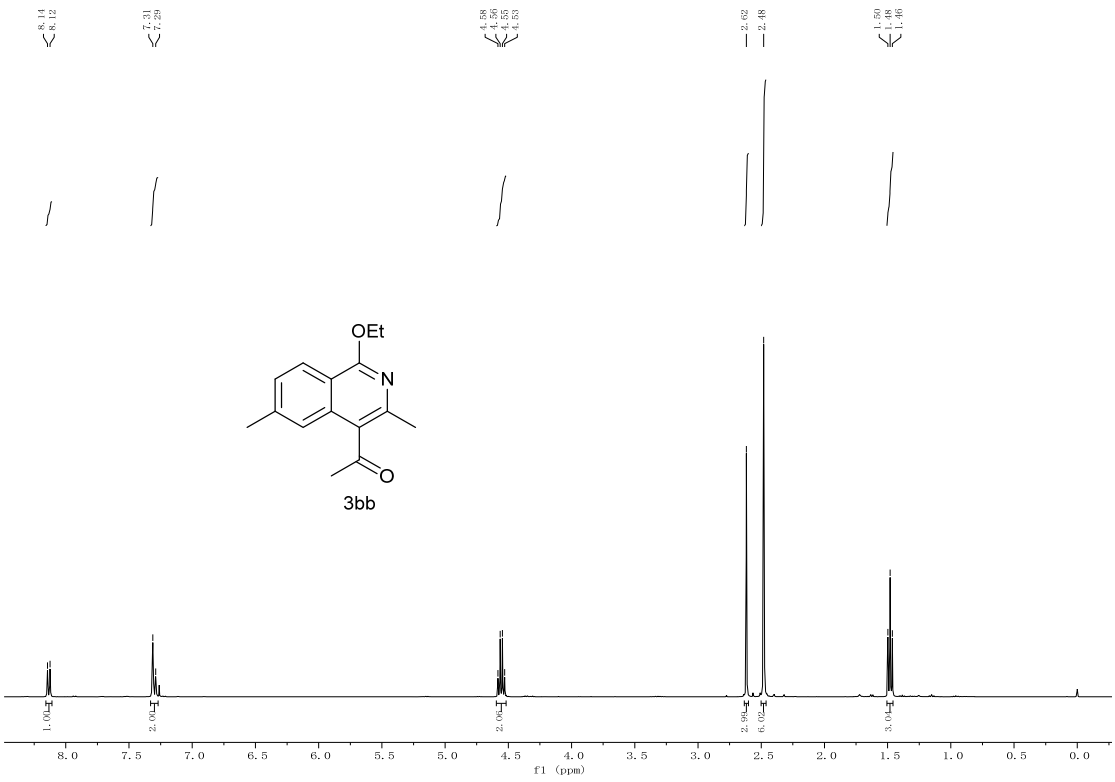
50
40
30
20
10
0
f1 (ppm)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8.12
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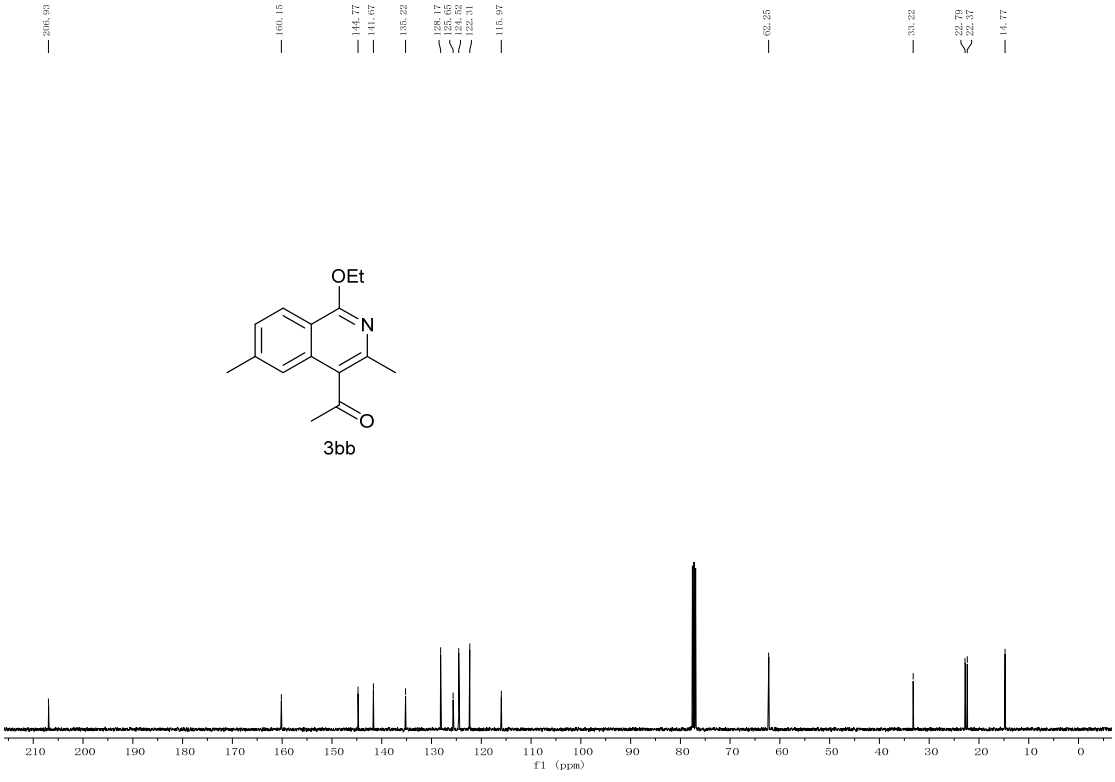
7.29
4.58
4.56
4.55
4.53
2.62
2.48
1.50
1.48
1.46
OEt
N
O
3bb
1.00
2.00
2.00
2.99
6.02
3.04
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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160.16
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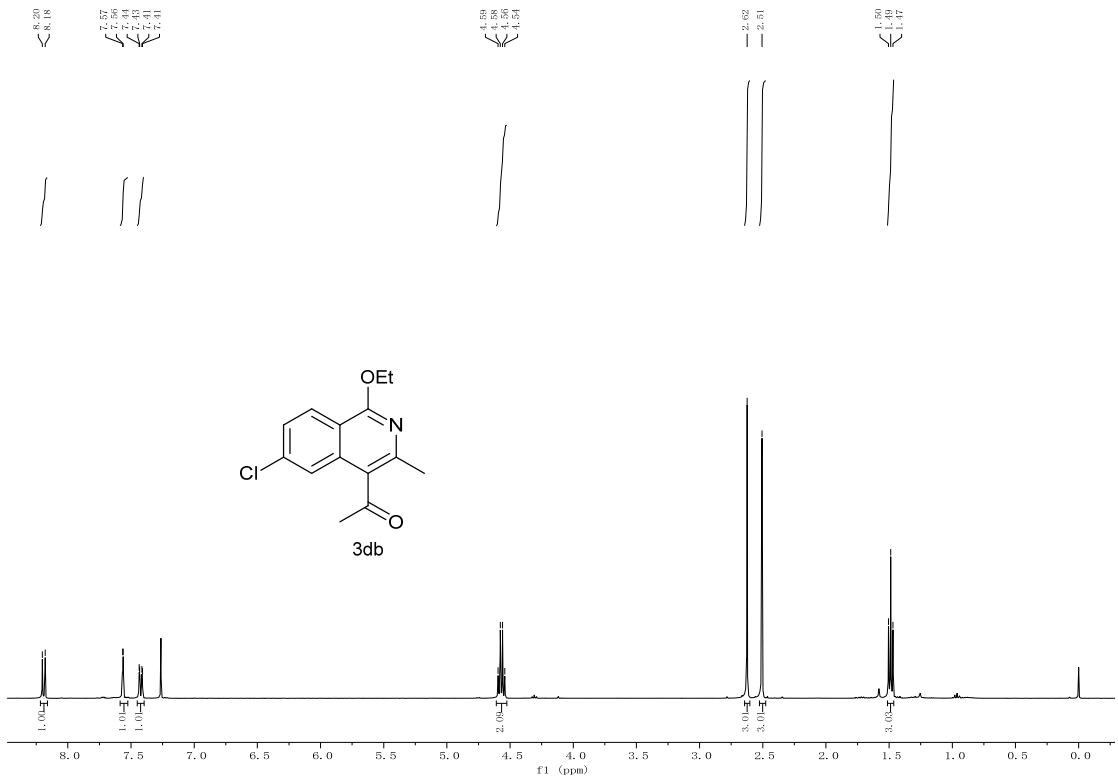
135.22
128.17
125.65
124.52
122.31
115.97
62.25
33.22
22.79
22.57
14.77
OEt
N
O
3bb
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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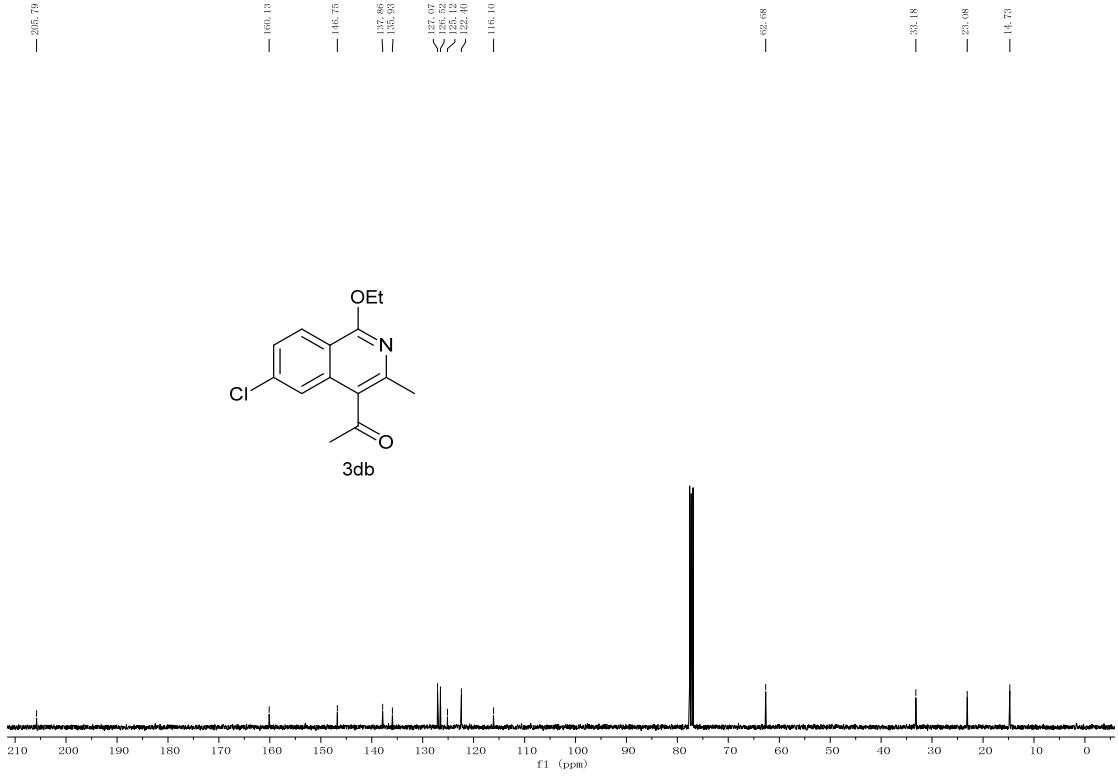
7.43
7.41
7.41
4.59
4.58
4.56
4.54
2.62
2.51
1.50
1.49
1.47
OEt
N
Cl
O
3db
1.00
1.01
1.01
2.04
3.01
3.00
f1 (ppm)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137.86
135.93
127.07
126.52
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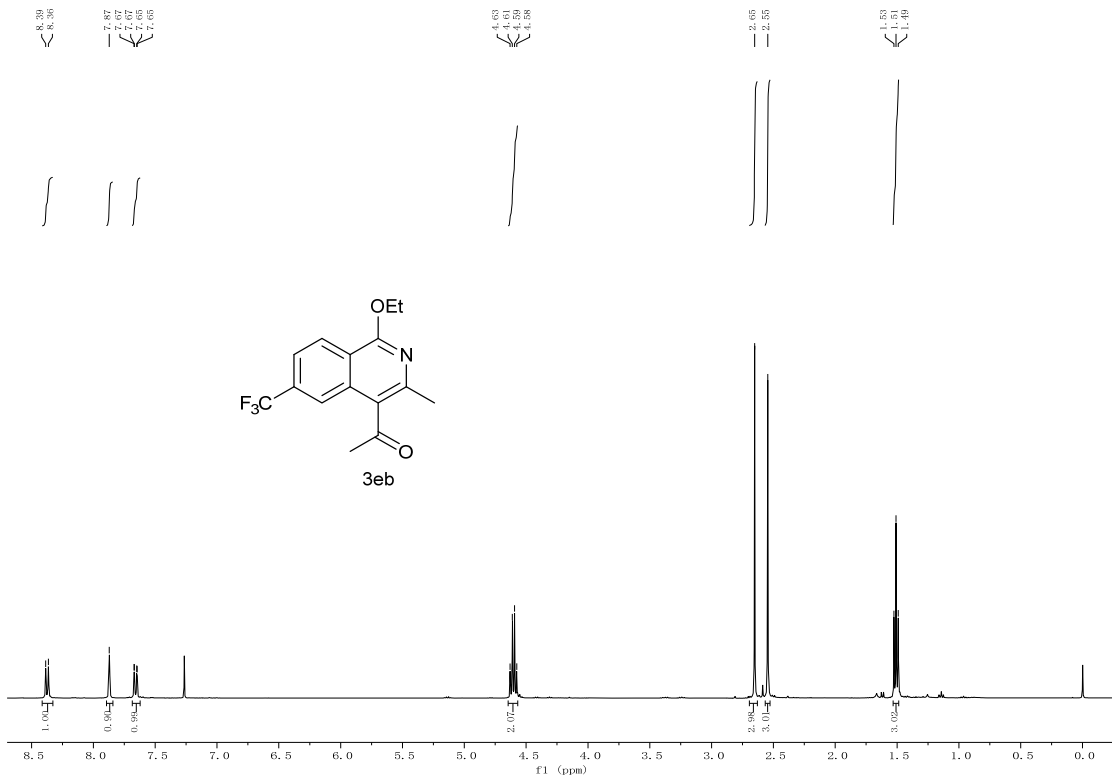
116.10
62.68
33.18
23.08
14.73
OEt
N
Cl
O
3db
f1 (ppm)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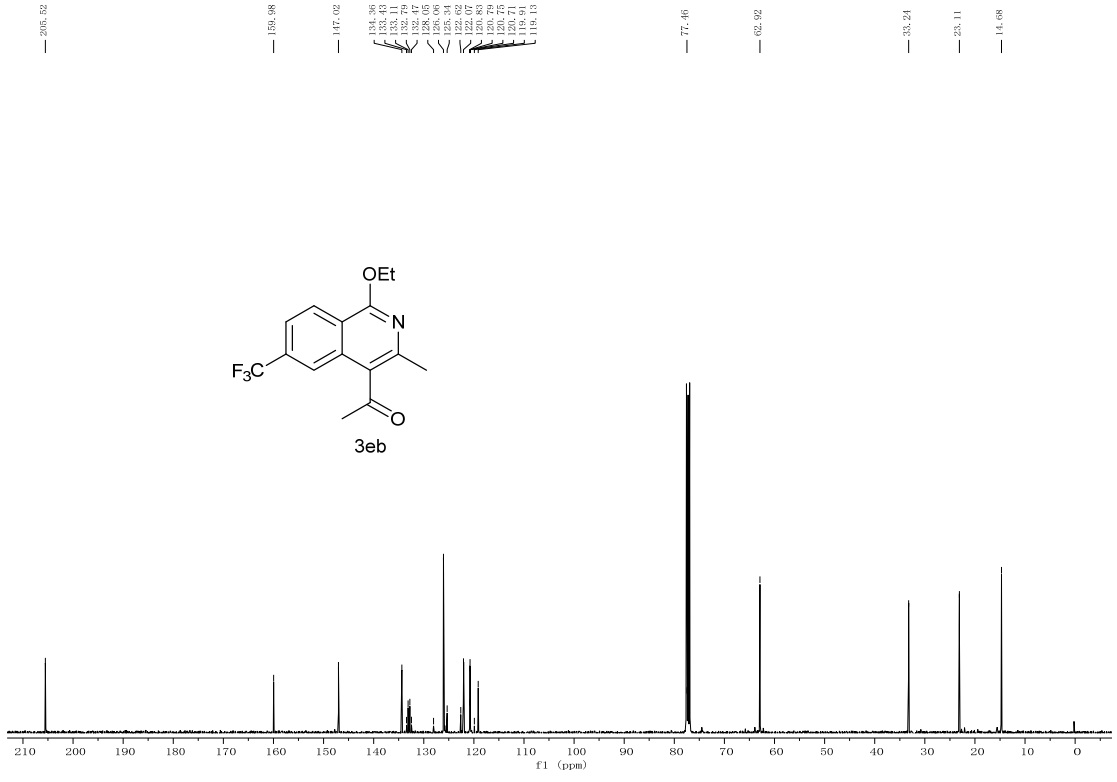
7.67
7.65
7.65
4.63
4.61
4.59
4.58
2.65
2.55
1.53
1.51
1.49
OEt
N
F3C
O
3eb
1.00
0.96
0.96
2.07
2.96
3.01
3.02
f1 (ppm)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133.11
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132.47
128.65
128.06
125.34
122.62
122.47
120.83
120.79
120.75
120.71
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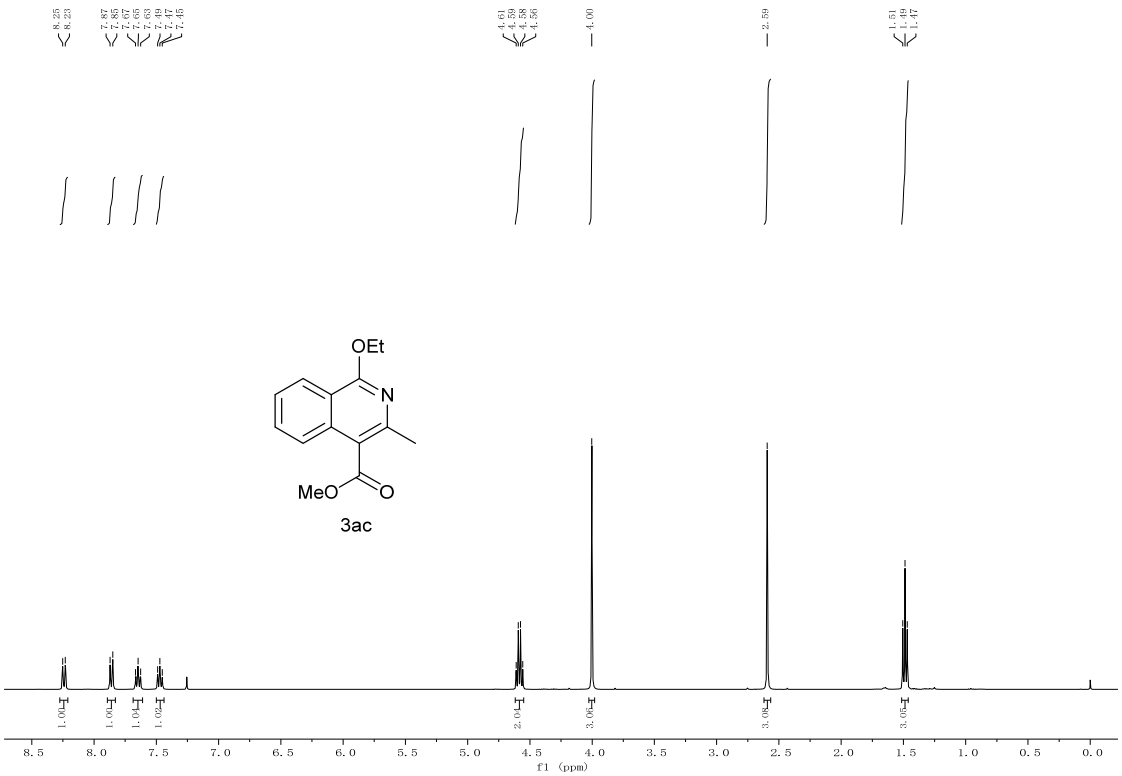
119.13
77.46
62.92
33.24
23.11
14.68
OEt
N
F3C
O
3eb
f1 (ppm)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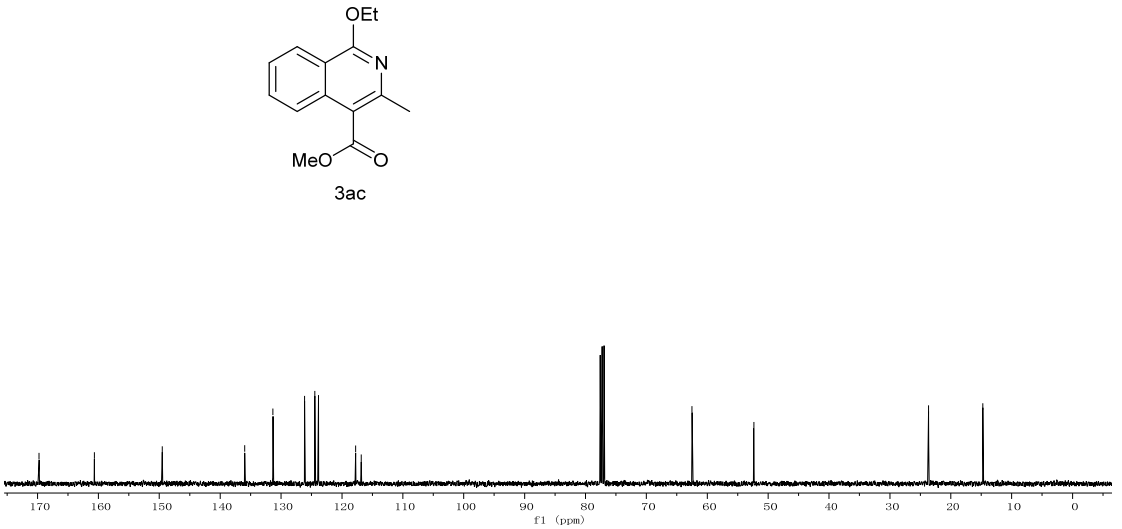
7.47
7.45
4.61
4.59
4.58
4.56
4.00
2.59
1.51
1.49
1.47
OEt
N
MeO
O
3ac
1.00
1.00
1.04
1.08
2.04
3.00
3.00
3.05
f1 (ppm)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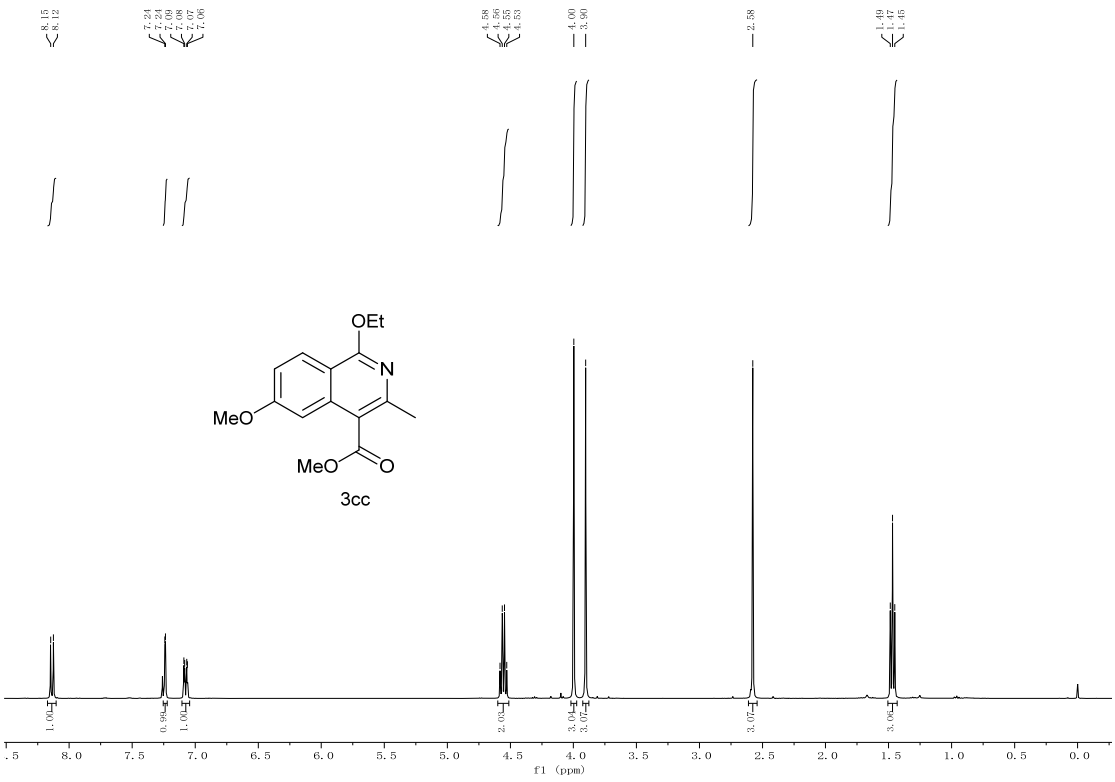
62.50
52.35
23.64
14.74
OEt
N
MeO
O
3ac
f1 (ppm)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7.08
7.07
7.06
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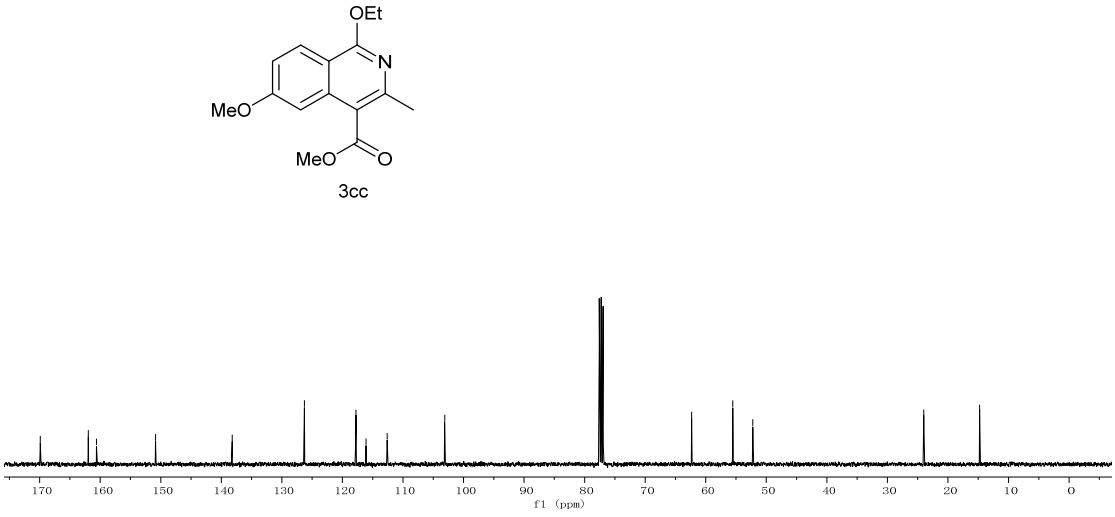
4.56
4.55
4.53
4.00
3.90
2.58
1.49
1.47
1.45
OEt
N
MeO
MeO
O
3cc
1.04
0.99
1.00
2.03
3.04
3.07
3.07
3.04
f1 (ppm)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116.11
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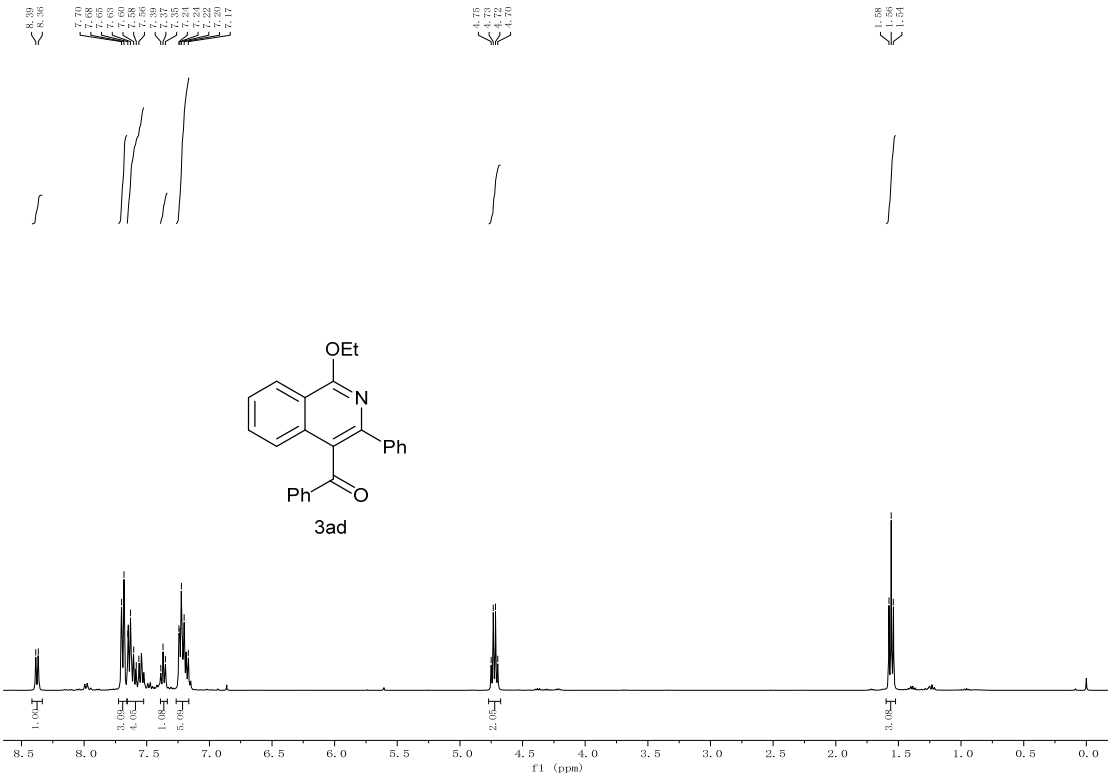
55.54
52.22
24.00
14.78
OEt
N
MeO
MeO
O
3cc
f1 (ppm)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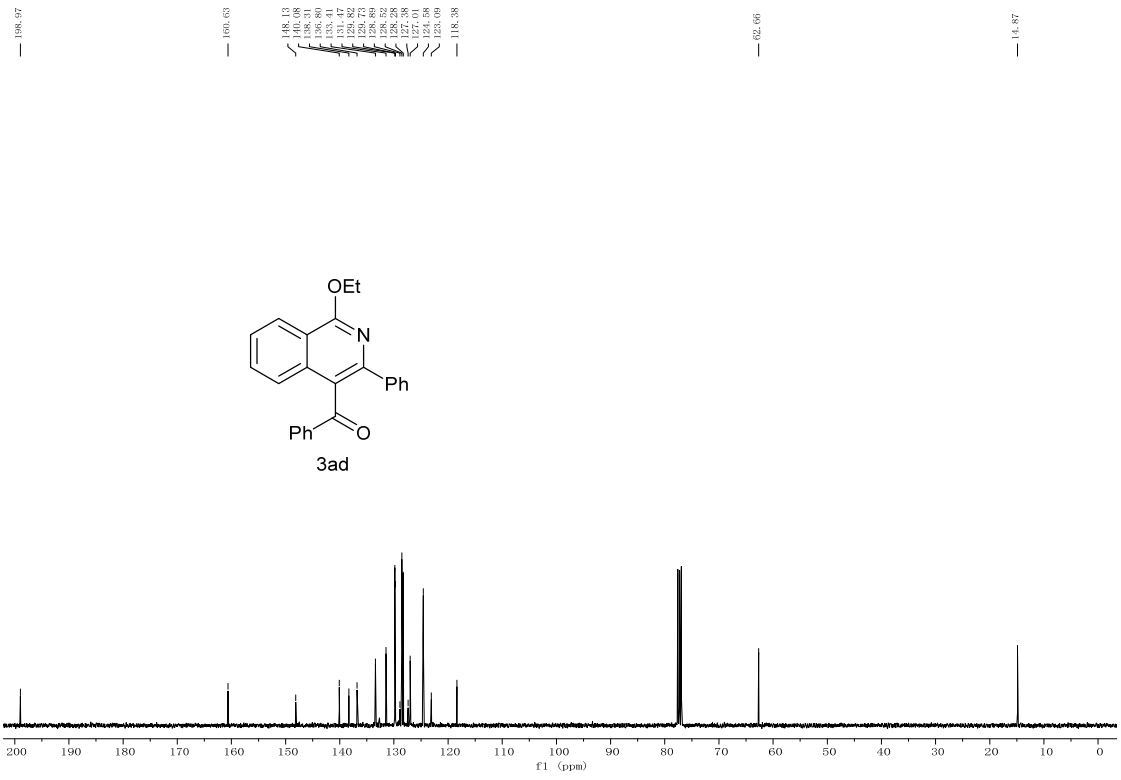
7.63
7.60
7.58
7.39
7.37
7.35
7.24
7.24
7.22
7.20
7.17
4.75
4.73
4.72
4.70
1.58
1.56
1.54
OEt
N
Ph
Ph
O
3ad
1.00
3.09
4.03
1.08
5.09
2.05
3.08
f1 (ppm)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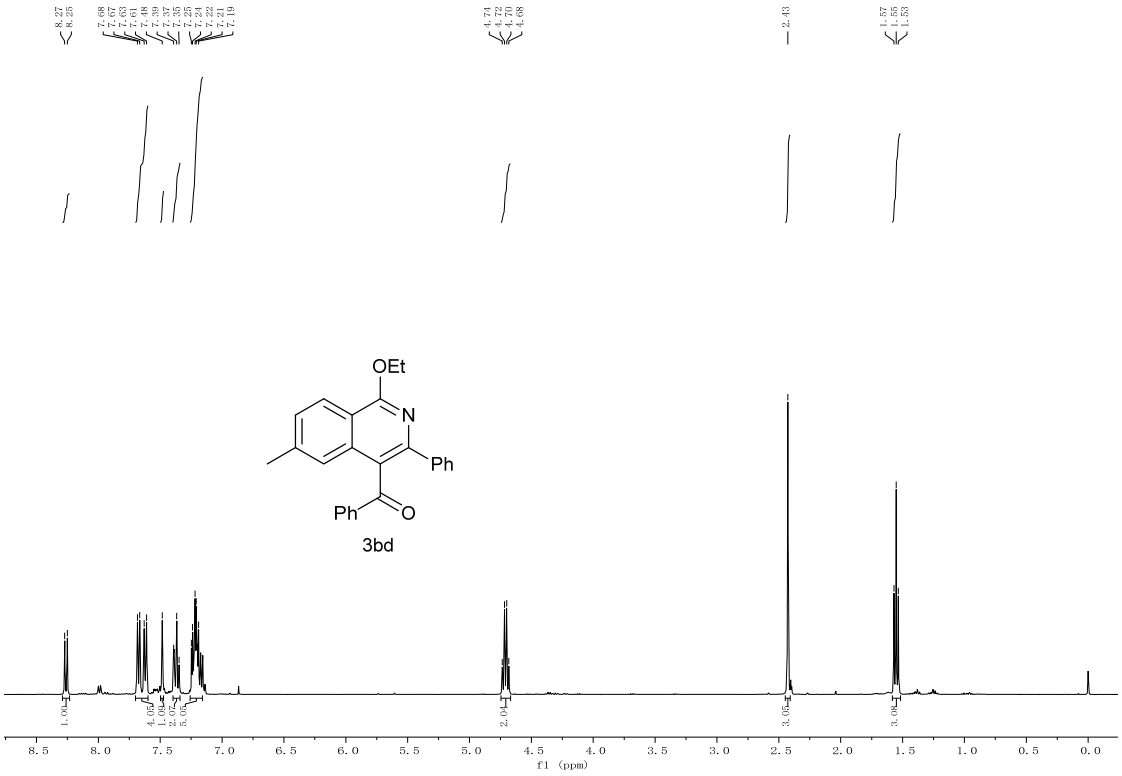
131.47
130.82
129.73
128.89
128.52
128.38
127.38
127.01
124.58
123.09
118.38
62.66
14.87
OEt
N
Ph
Ph
O
3ad
f1 (ppm)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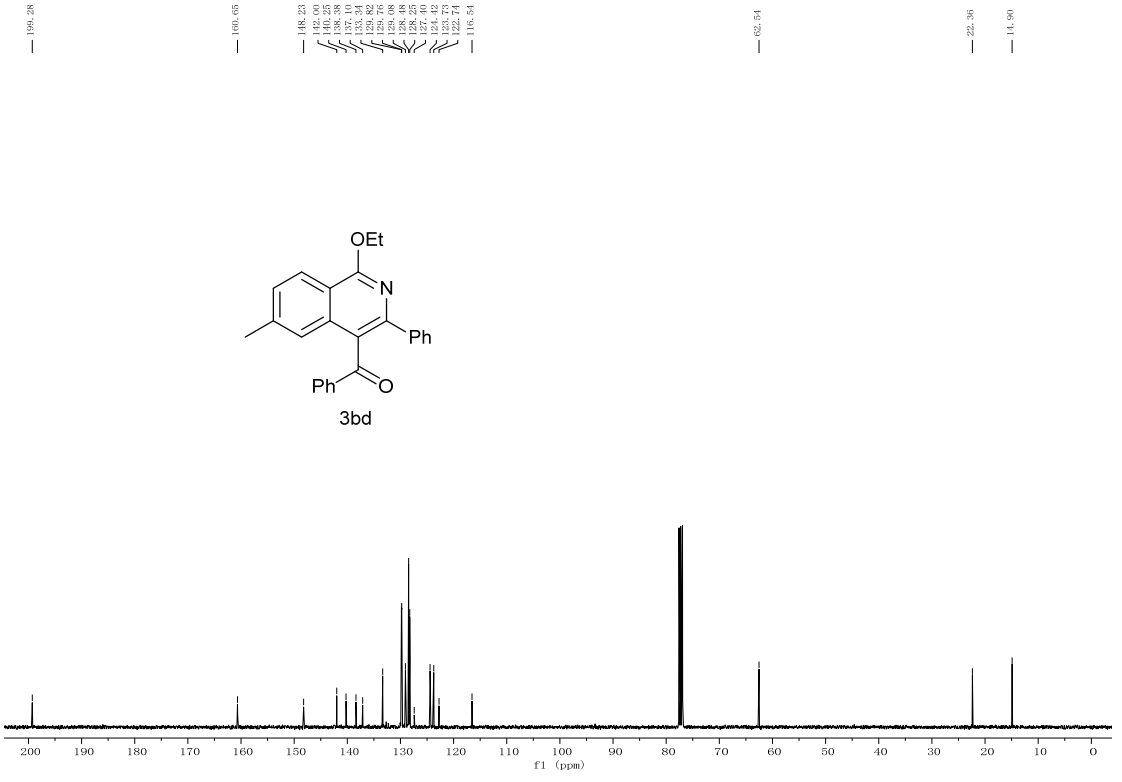
7.37
7.35
7.25
7.24
7.22
7.21
7.19
4.74
4.72
4.70
4.68
2.43
1.57
1.55
1.53
OEt
N
Ph
Ph
O
3bd
1.00
4.03
1.08
2.07
5.06
2.04
3.05
3.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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142.00
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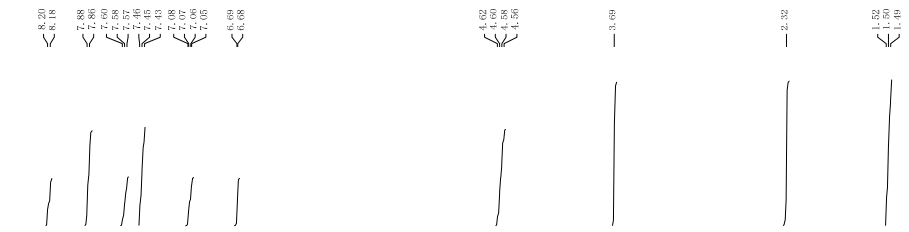
138.98
137.10
133.34
129.82
129.76
128.68
128.48
128.25
127.40
124.42
123.73
122.74
116.54
62.54
22.36
14.80
OEt
N
Ph
Ph
O
3bd
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.43
7.08
7.07
7.06
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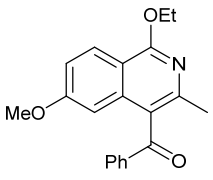
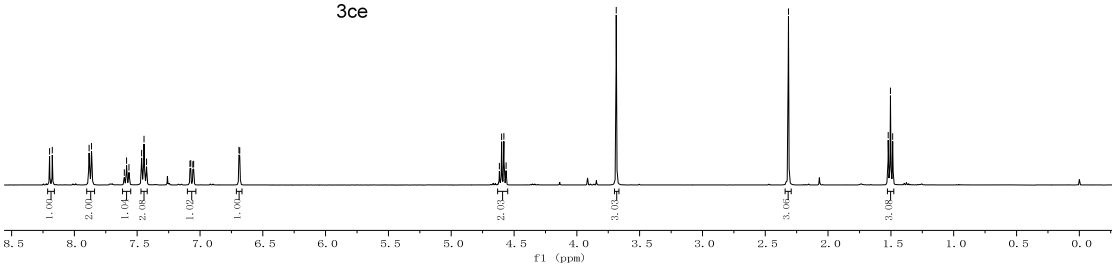
4.56
3.69
2.32
1.52
1.50
1.49


OEt
N
MeO
Ph
O

3ce


1.00
2.00
1.04
2.06
1.02
1.04
2.03
3.02
3.06
3.08
f1 (ppm)


199.38
161.65
160.42
147.63
138.50
138.36
133.89
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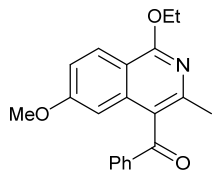
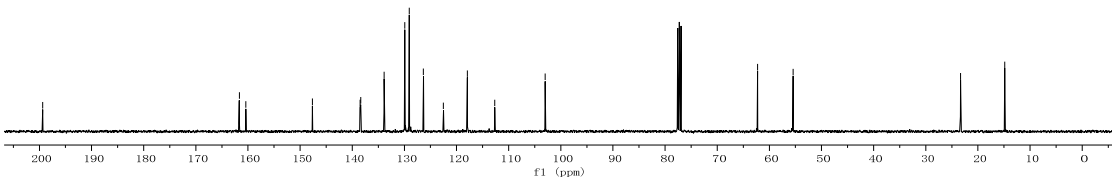
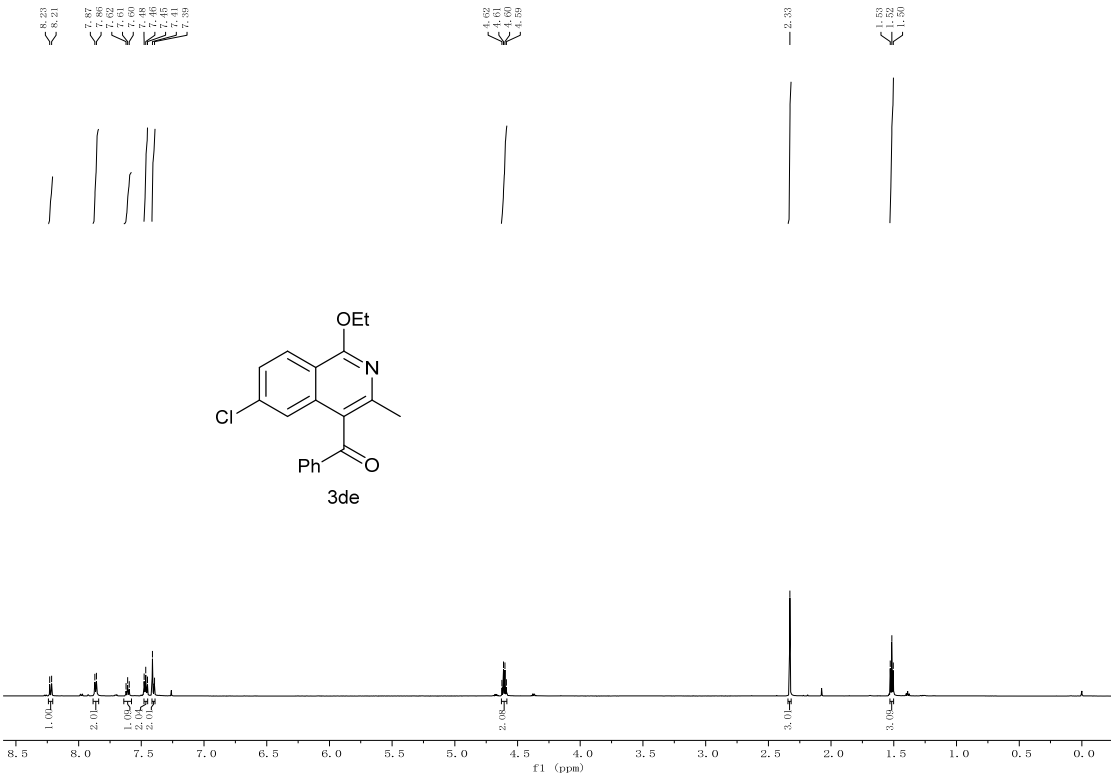
129.06
126.35
122.51
117.91
112.67
103.01
62.26
55.46
23.34
14.84


OEt
N
MeO
Ph
O

3ce


f1 (ppm)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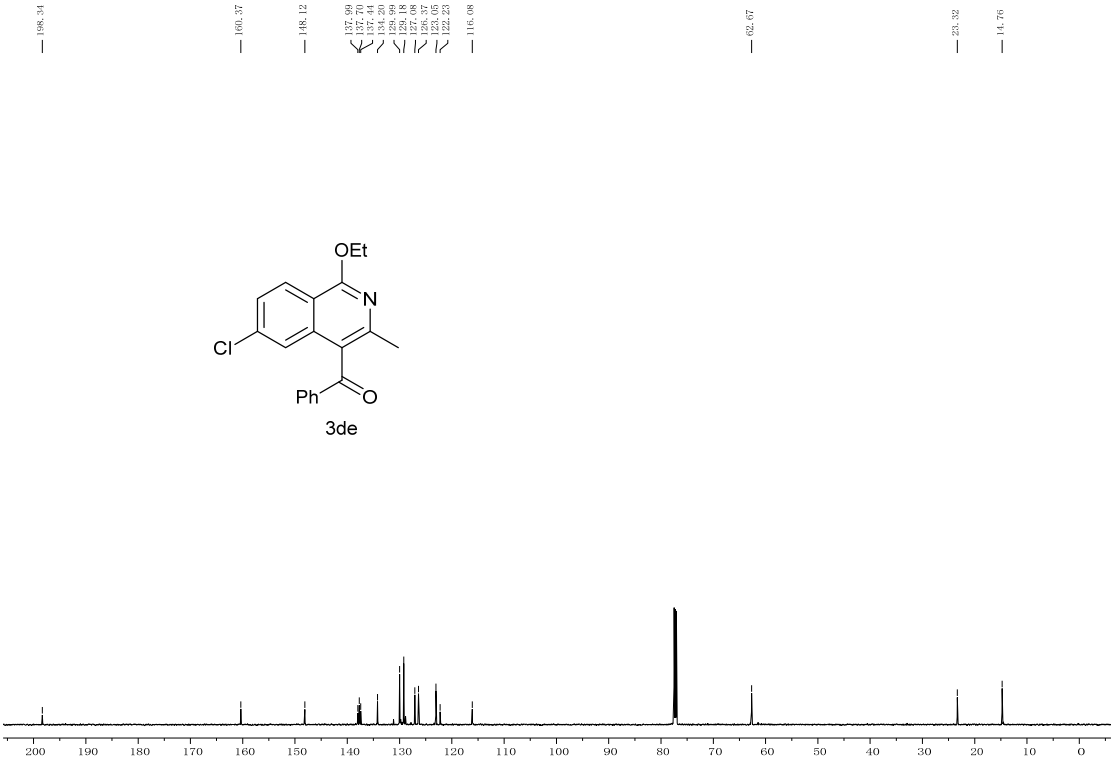
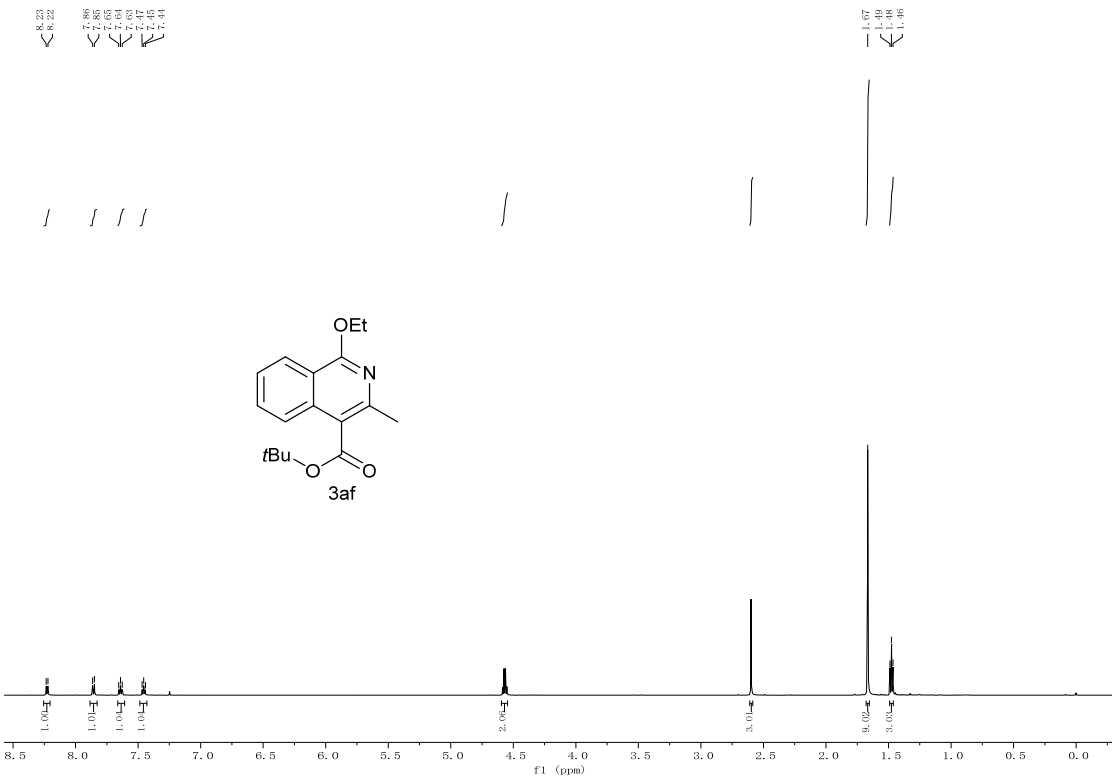
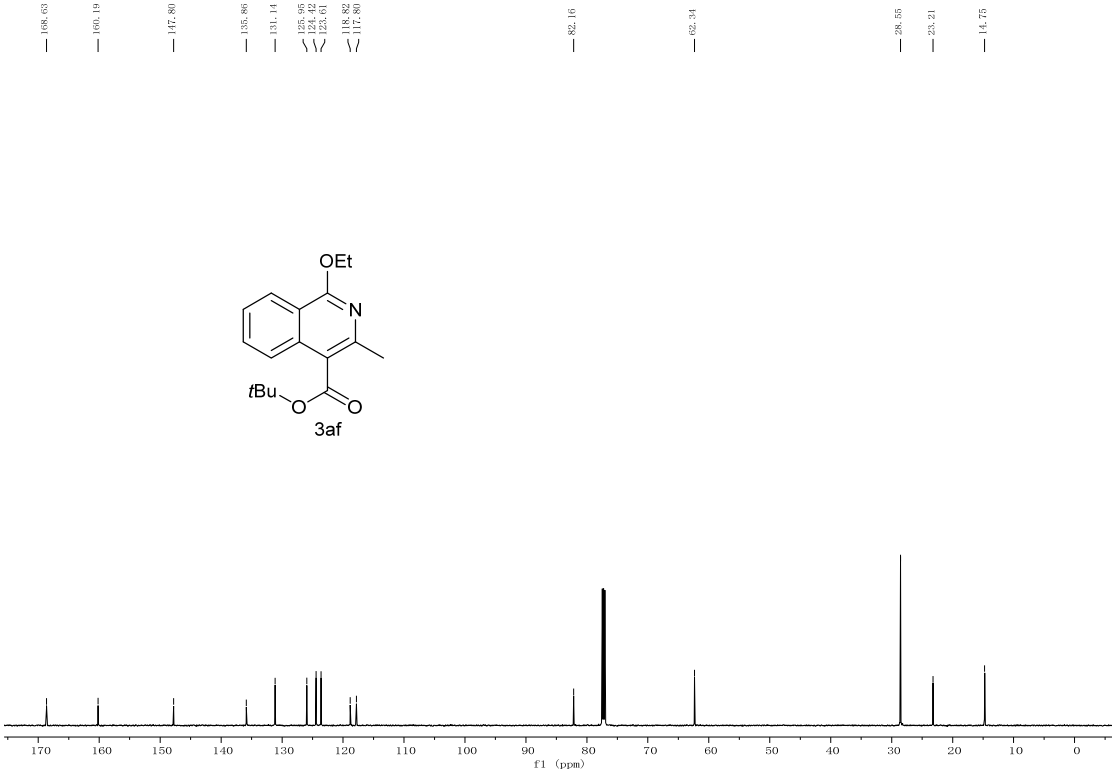
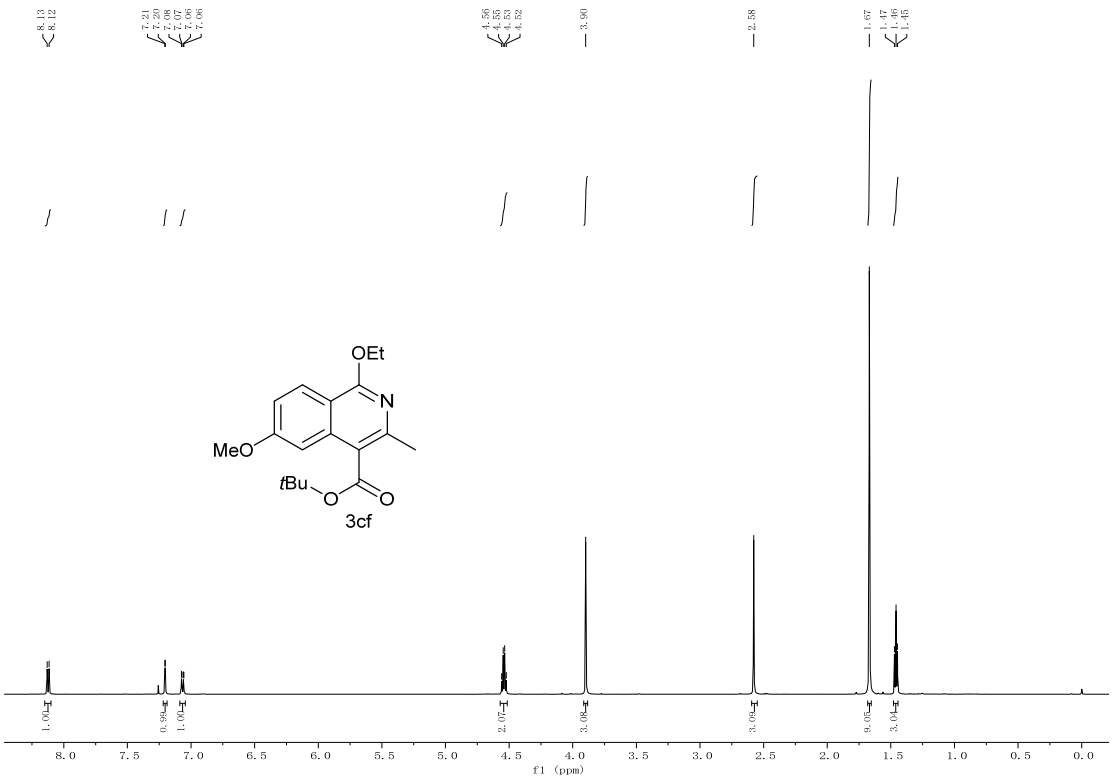
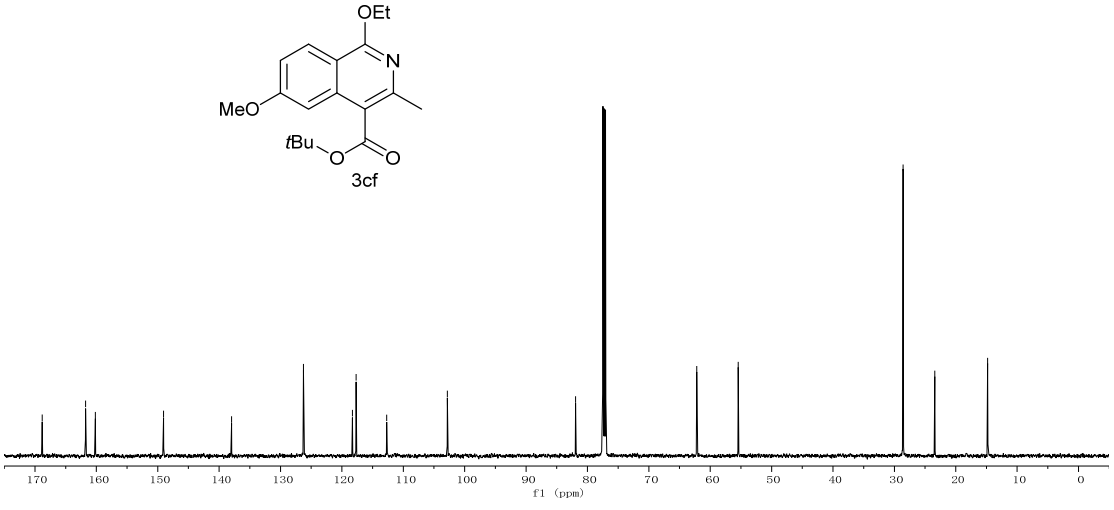
8.21
7.87
7.85
7.62
7.61
7.60
7.48
7.46
7.45
7.41
7.39
4.62
4.61
4.60
4.59
2.33
1.53
1.52
1.50
OEt
N
Cl
Ph
O
3de
1.00
2.01
1.00
2.04
2.01
2.08
3.01
3.08
f1 (ppm)


198.34
160.37
148.12
137.99
137.70
137.44
134.20
129.66
129.18
127.08
126.37
123.65
122.23
116.08
62.67
23.32
14.76
OEt
N
Cl
Ph
O
3de
f1 (ppm)


8.23
8.22
7.86
7.85
7.65
7.64
7.47
7.45
7.44
1.67
1.49
1.48
1.46
OEt
N
tBu
O
O
3af
1.00
1.01
1.04
1.04
2.04
3.01
9.02
3.03
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)


168.63
160.19
147.80
135.86
131.14
125.95
124.42
123.61
118.82
117.80
82.16
62.34
28.55
23.21
14.75
OEt
N
tBu
O
O
3af
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.13
8.12
7.21
7.20
7.08
7.07
7.06
4.56
4.55
4.53
4.52
3.90
2.58
1.47
1.46
1.45
OEt
N
MeO
tBu
O
O
3cf
1.00
0.99
1.04
2.07
3.08
3.09
9.05
3.04
f1 (ppm)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161.76
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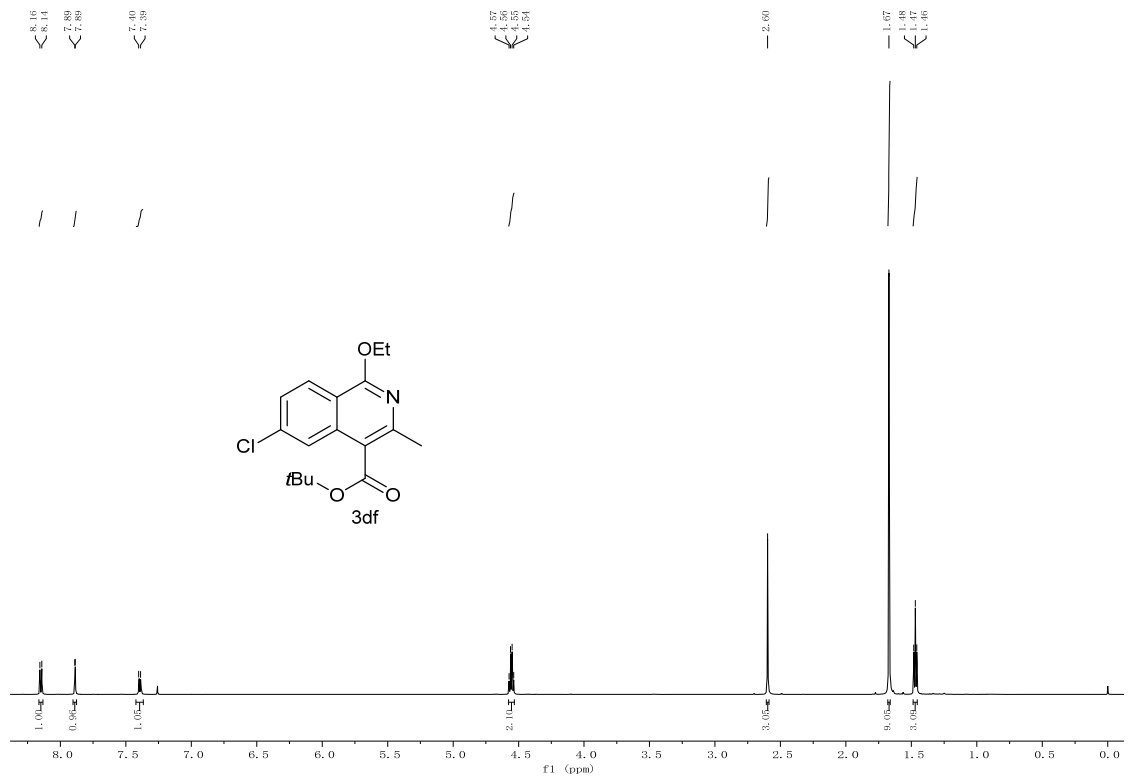
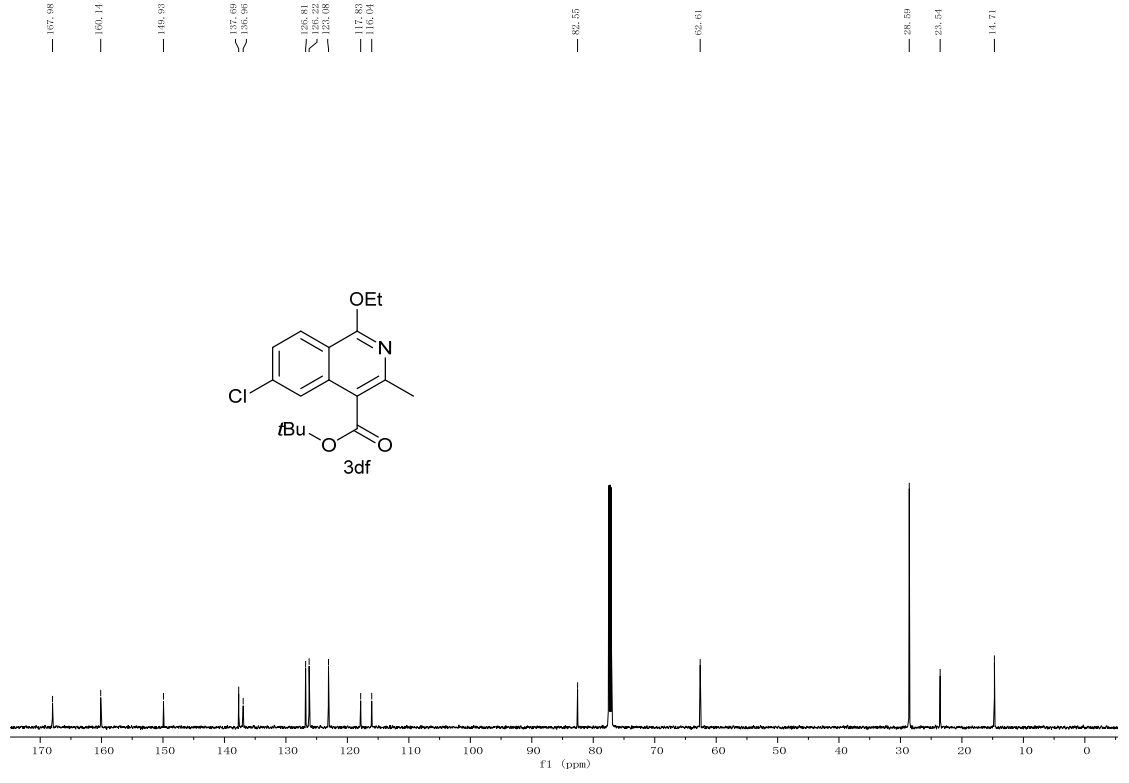
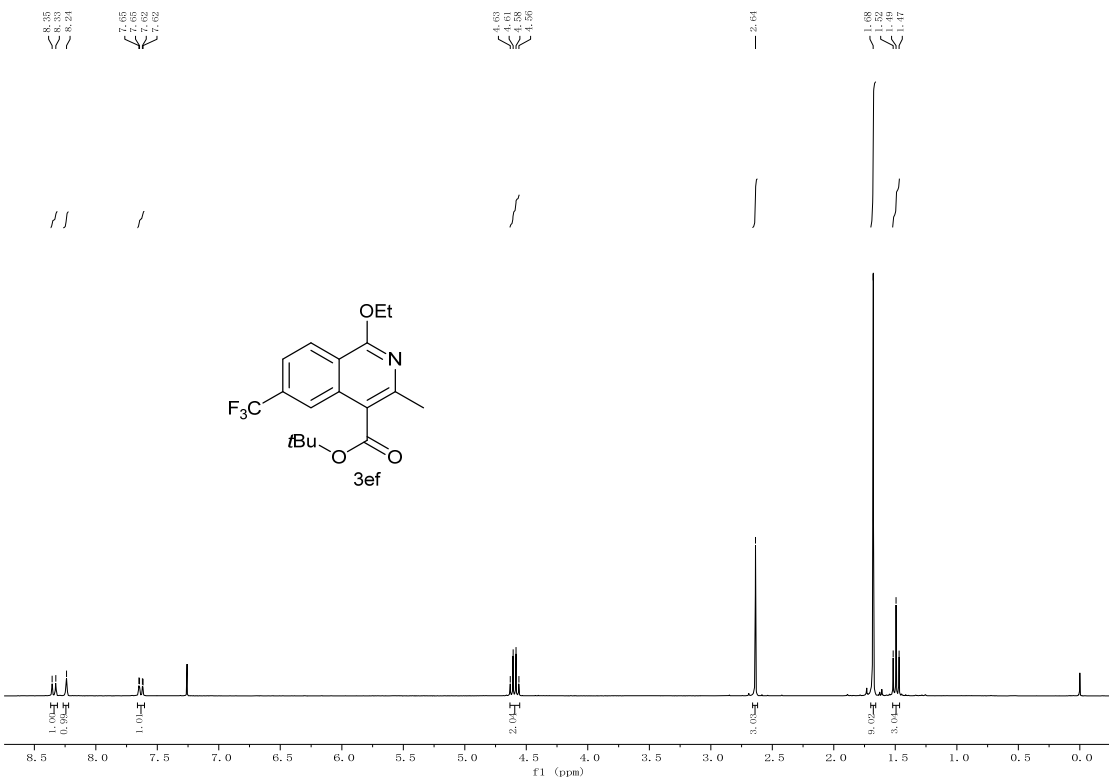
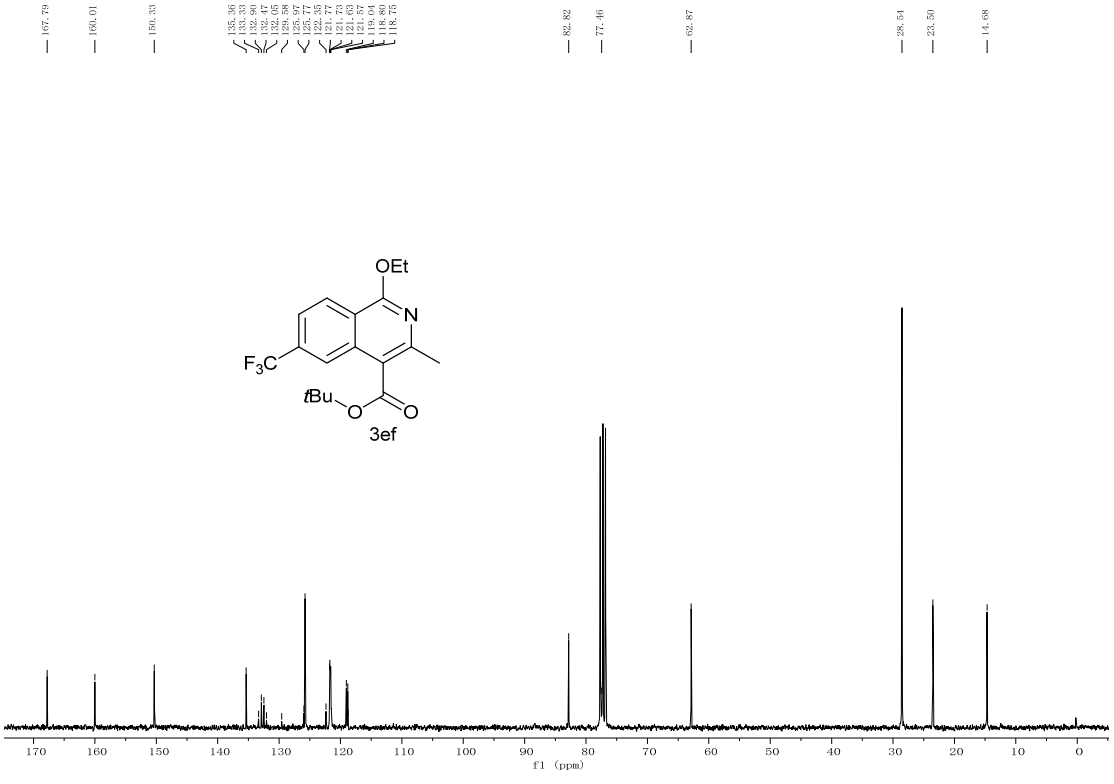
149.06
137.98
126.26
118.27
117.69
112.71
102.82
81.92
62.20
55.44
28.59
23.43
14.80
OEt
N
MeO
tBu
O
O
3cf
f1 (ppm)


8.16
8.14
7.89
7.89
7.40
7.39
4.57
4.56
4.55
4.54
2.60
1.67
1.48
1.47
1.46
OEt
N
Cl
tBu
O
O
3df
1.00
0.98
1.05
2.10
3.05
9.05
3.00
f1 (ppm)


167.98
160.14
149.93
137.69
136.96
126.81
126.22
123.08
117.83
116.04
82.55
62.61
28.59
23.54
14.71
OEt
N
Cl
tBu
O
O
3df
f1 (ppm)


8.35
8.33
8.24
7.65
7.62
7.62
7.62
4.63
4.61
4.58
4.56
2.64
1.68
1.52
1.49
1.47
OEt
N
F3C
tBu
O
O
3ef
1.00
0.99
1.01
2.04
3.03
9.02
3.04
f1 (ppm)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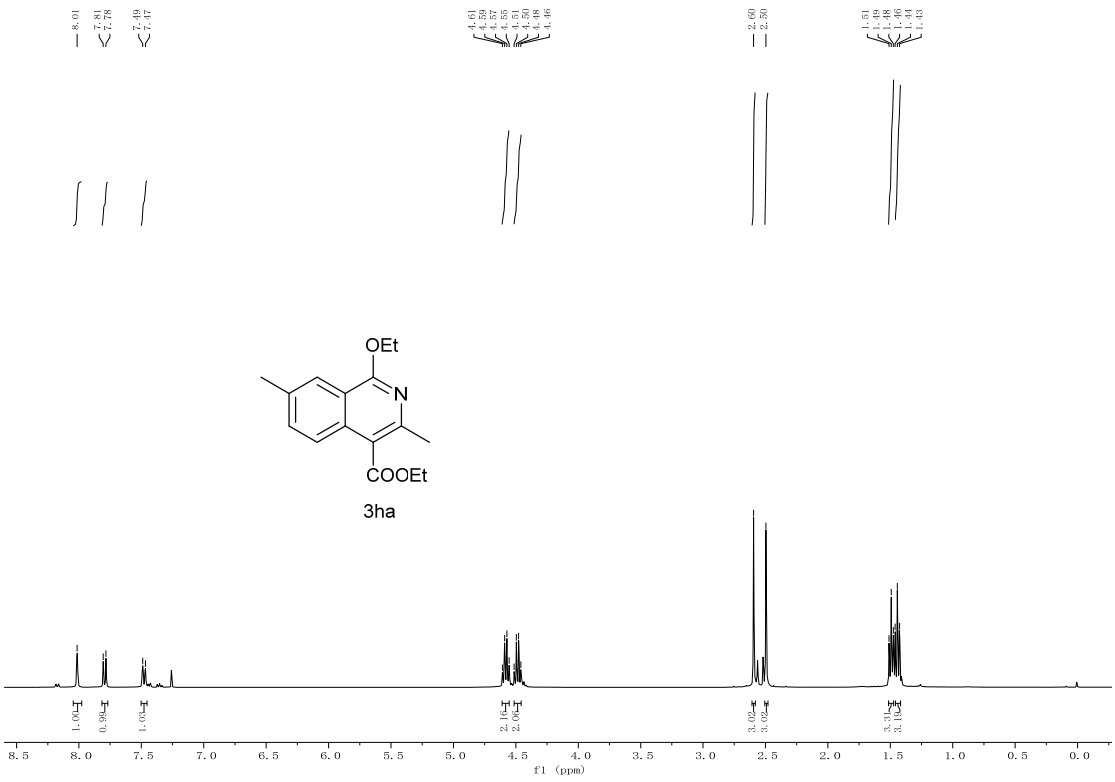
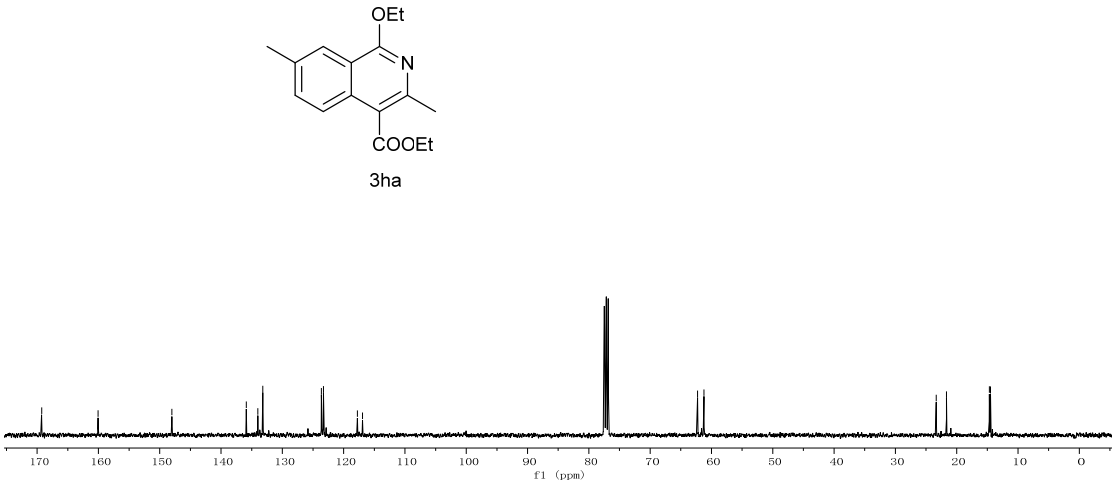
160.01
150.33
135.36
133.33
132.86
132.47
132.05
129.58
125.97
125.77
122.35
121.77
121.73
121.62
121.57
119.04
118.80
118.76
82.82
77.46
62.87
28.54
23.50
14.68
OEt
N
F3C
tBu
O
O
3ef
f1 (ppm)

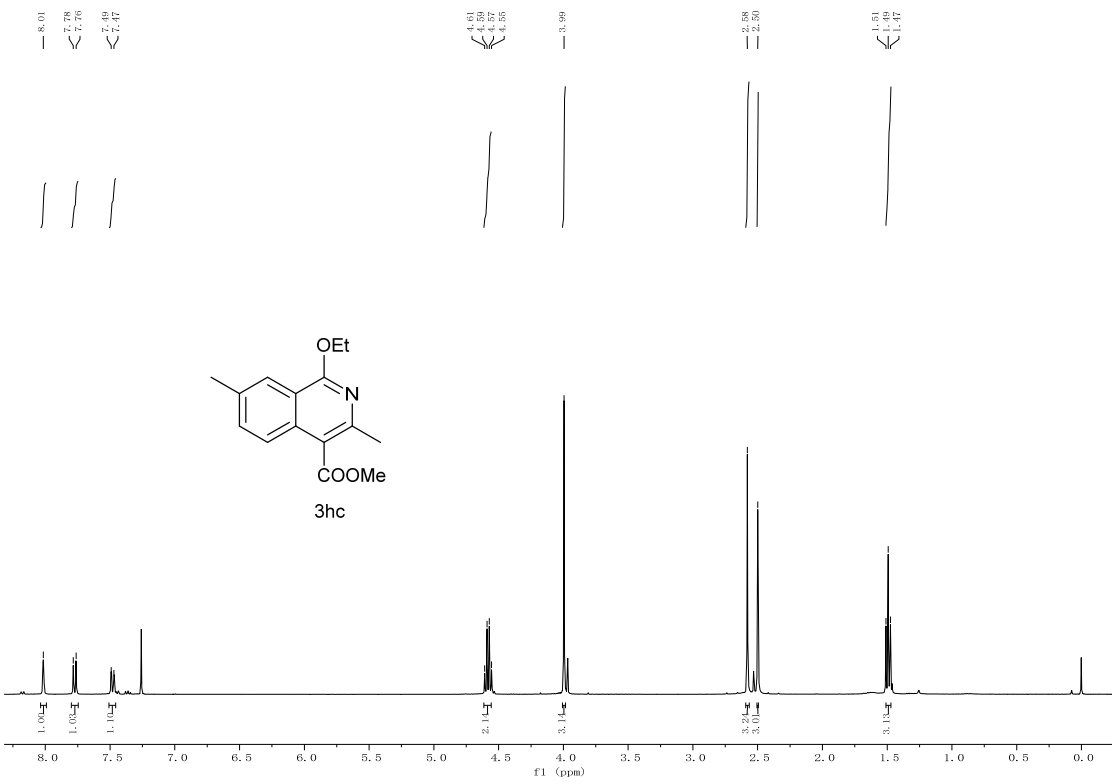

8.01
7.81
7.78
7.49
7.47
4.61
4.59
4.57
4.55
4.51
4.50
4.48
4.46
2.60
2.50
1.51
1.49
1.48
1.46
1.44
1.43
OEt
N
COOEt
1.00
0.99
1.03
2.16
2.00
3.02
3.02
3.31
3.10
f1 (ppm)

3ha


169.27
160.06
148.04
135.87
134.10
133.18
123.63
123.30
117.76
116.92
62.27
61.23
23.33
21.65
14.47
14.47
f1 (ppm)

OEt
N
COOEt

3ha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7.78
7.76
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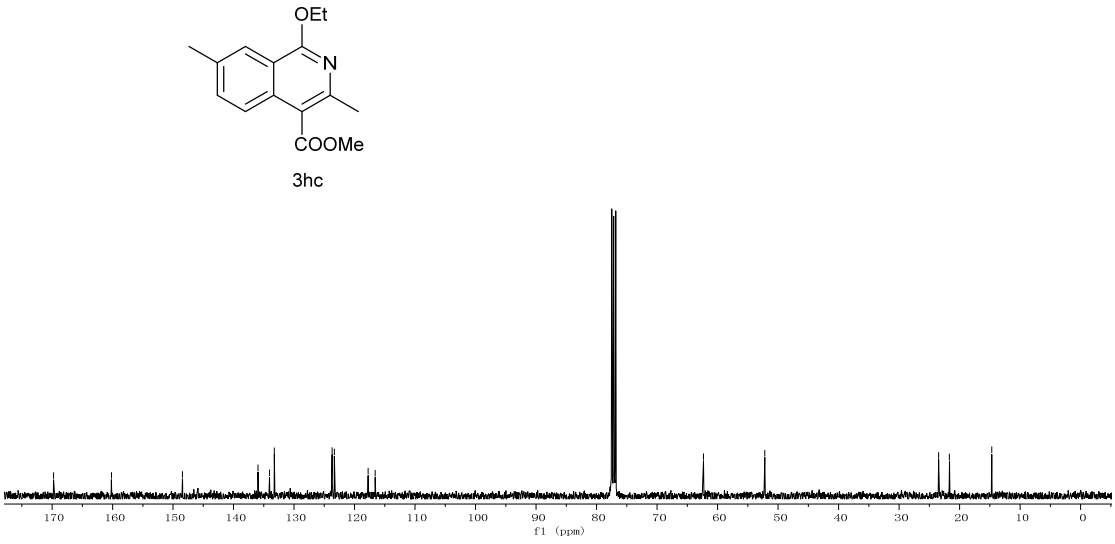
7.47
4.61
4.59
4.57
4.55
3.99
2.58
2.50
1.51
1.49
1.47
OEt
N
COOMe
1.04
1.03
1.10
2.14
3.14
3.24
3.04
3.12
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3hc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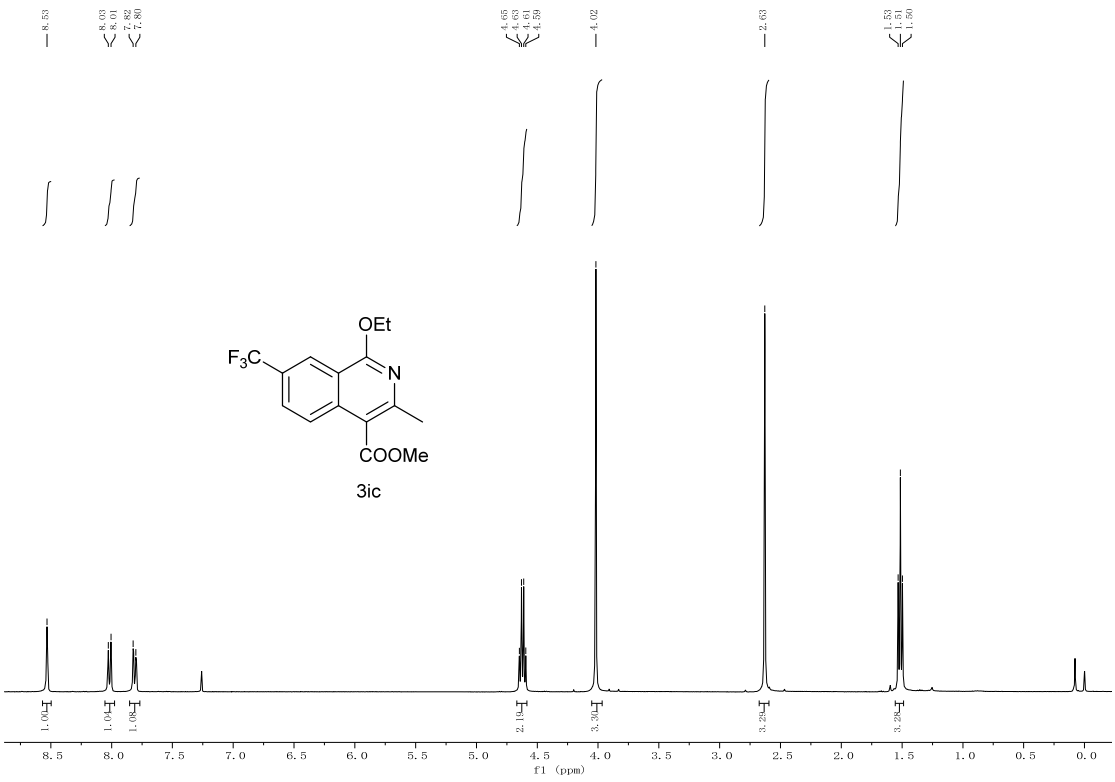
134.05
133.25
123.71
123.34
117.77
116.61
62.33
52.20
23.45
21.68
14.69
OEt
N
COOMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3hc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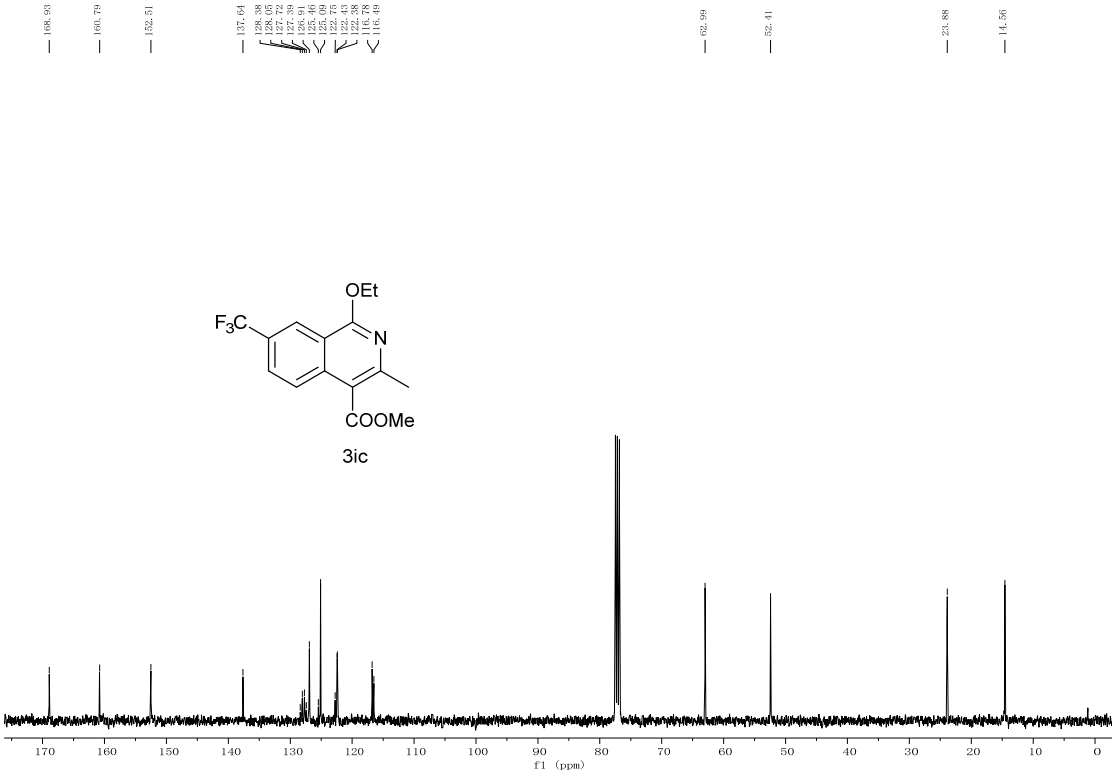
8.03
8.01
7.82
7.80
4.65
4.63
4.61
4.59
4.02
2.63
1.53
1.51
1.50
OEt
F3C
N
COOMe
3ic
1.00
1.04
1.08
2.14
3.30
3.28
3.28
f1 (ppm)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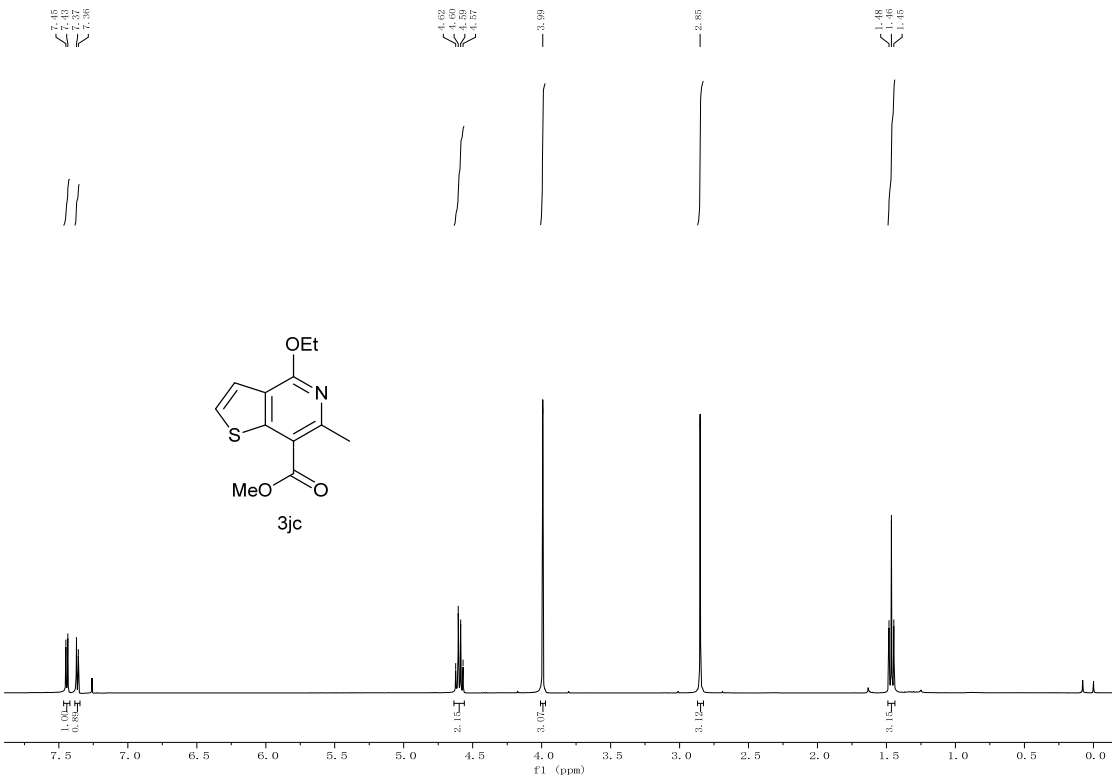
128.05
127.72
127.39
126.91
125.46
125.09
122.75
122.43
122.38
114.78
110.49
62.99
52.41
23.88
14.56
OEt
F3C
N
COOMe
3ic
f1 (ppm)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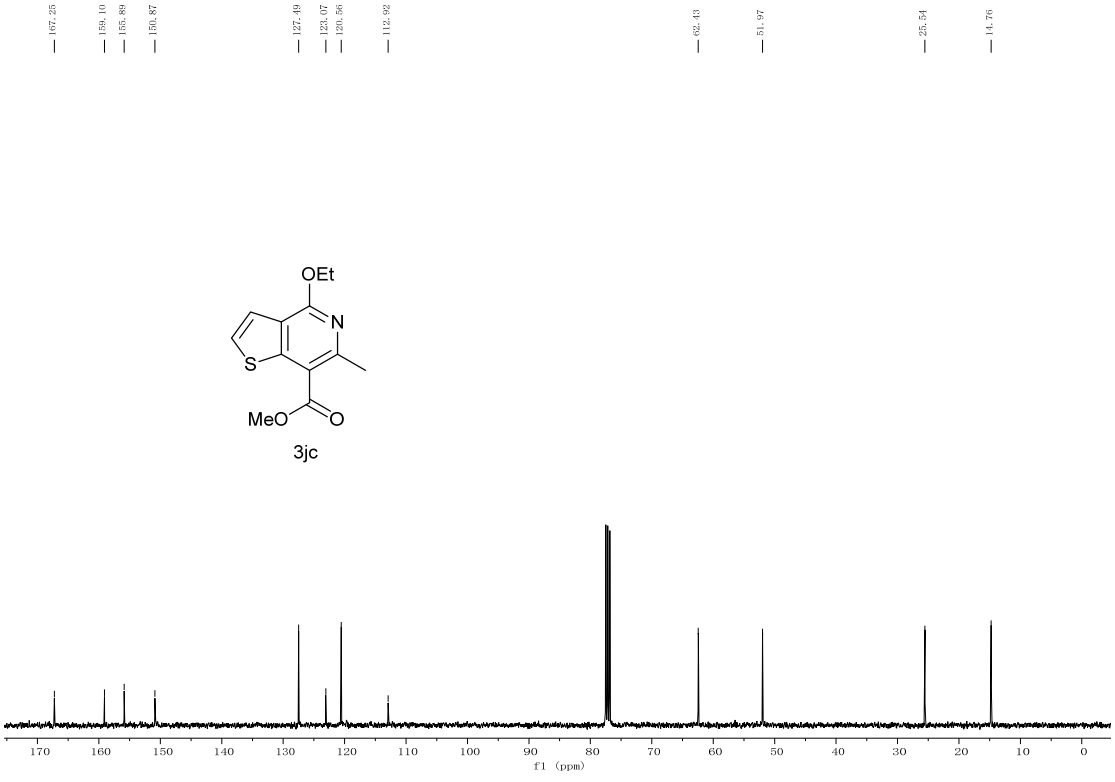
4.60
4.59
4.57
3.99
2.85
1.48
1.46
1.45
OEt
N
S
MeO
O
3jc
1.00
0.88
2.15
3.07
3.12
3.15
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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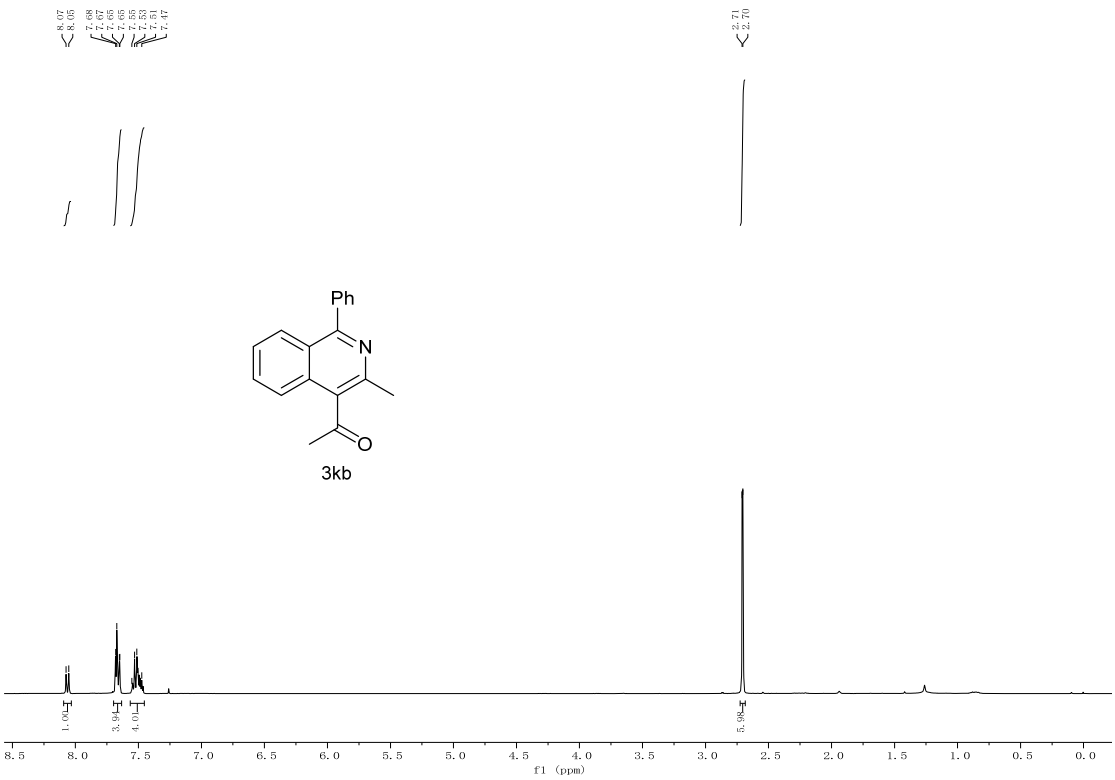
150.87
127.49
123.07
120.56
112.92
62.43
51.97
25.54
14.76
OEt
N
S
MeO
O
3jc
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.05
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7.65
7.55
7.53
7.51
7.47
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2.70
Ph
N
O
3kb
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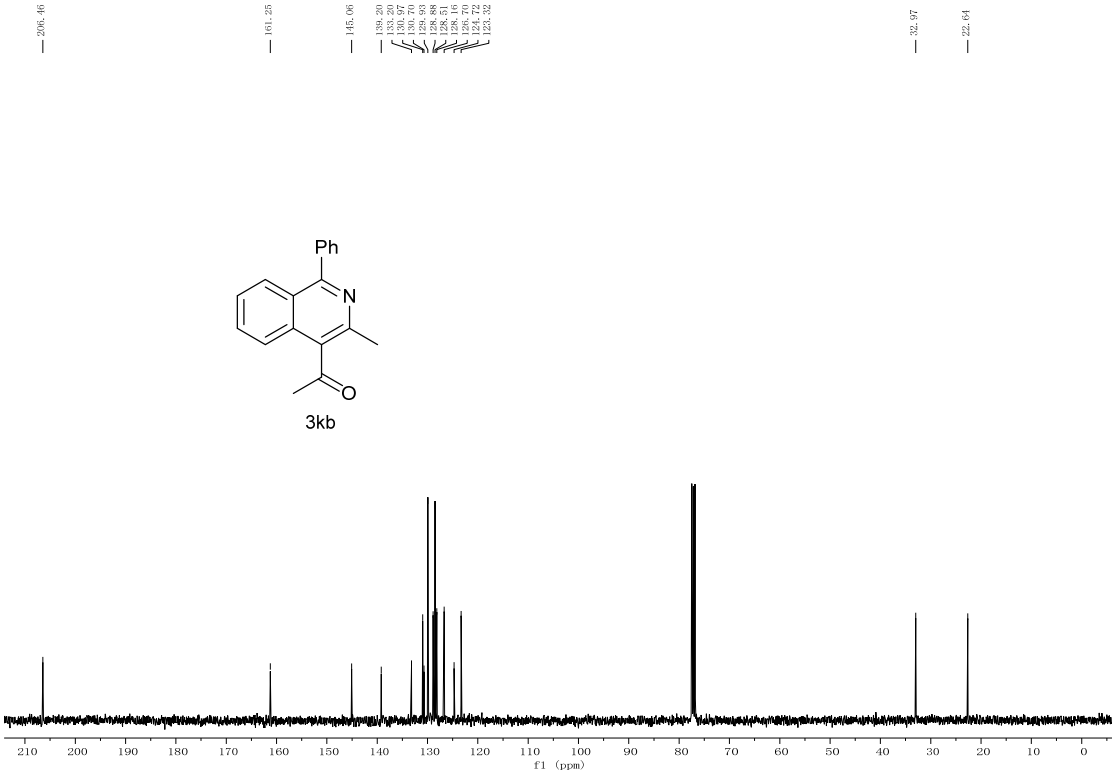
3.94
4.04
5.98
f1 (ppm)


206.46
161.25
145.06
139.20
133.20
130.70
130.48
128.88
128.51
128.16
126.70
124.72
123.32
32.97
22.64
Ph
N
O
3kb
f1 (ppm)