Supporting Information

Synthesis of 6-Acyl Phenanthridines by Oxidative Radical Decarboxylation/Cyclization of α-Oxocarboxylates and Isocyanides

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Contents:

General Considerations

All manipulations were carried out using standard Schlenk techniques. Unless otherwise

stated, analytical grade solvents and commercially available reagents were used to conduct the reactions. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum ether (bp. 60-90 ^{o}C). Gradient flash chromatography was conducted eluting with a continuous gradient from petroleum ether to the ethyl acetate. All new compounds were characterized by ^{1}H NMR, ^{13}C NMR and HRMS. The known compounds were characterized by ^{1}H NMR and ^{13}C NMR. The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz NMR spectrometer. The chemical shifts (δ) were given in part per million relative to internal tetramethyl silane (TMS, 0 ppm for ^{1}H), $CDCl_3$ (77.3 ppm for ^{13}C). High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument and accurate masses were reported for the molecular ion + Hydrogen (M+H).

Experimental Procedures

1. Preparation of substituted α-oxocarboxylic acids:

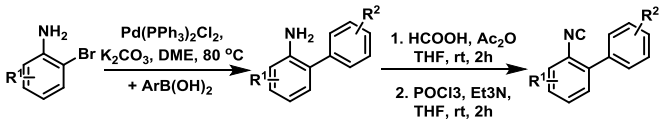
All kinds of substituted α-oxocarboxylic acids were prepared from oxidation of corresponding methyl ketones with SeO_2 according to the reported procedure.[1]

2. Preparation of substituted α-oxocarboxylates:

All the substituted α-oxocarboxylic acids were reacted with KOH (1:1) in *i*PrOH for 3h, and the desired α-oxocarboxylates was obtained by removing the *i*PrOH.[2]

3. General procedure for synthesis of 2-isocyanobiaryls:

All the 2-isocyanobiaryls were prepared according to the following procedure in Angew Chem Int Ed, 2013, 51, 11363.[3]



4. General procedure for synthesis of 6-Acyl Phenanthridines:

General procedure: A mixture of 2-isocyanobiphenyl **1a** (0.75 mmol) and potassium oxophenylacetate **2a** (0.5 mmol), Ag_2CO_3 (0.05 mmol) and $Na_2S_2O_8$ (1.0 mmol) under an N_2 atmosphere at 100 °C for 6 h. After completion of the reaction, it was quenched by water and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and evaporated under vacuum. The pure product was obtained by flash column chromatography on silica gel (eluent: petroleum ether/ethyl acetate= 50:1) to afford **3a** in 71% yield.

Radical trapping experiments

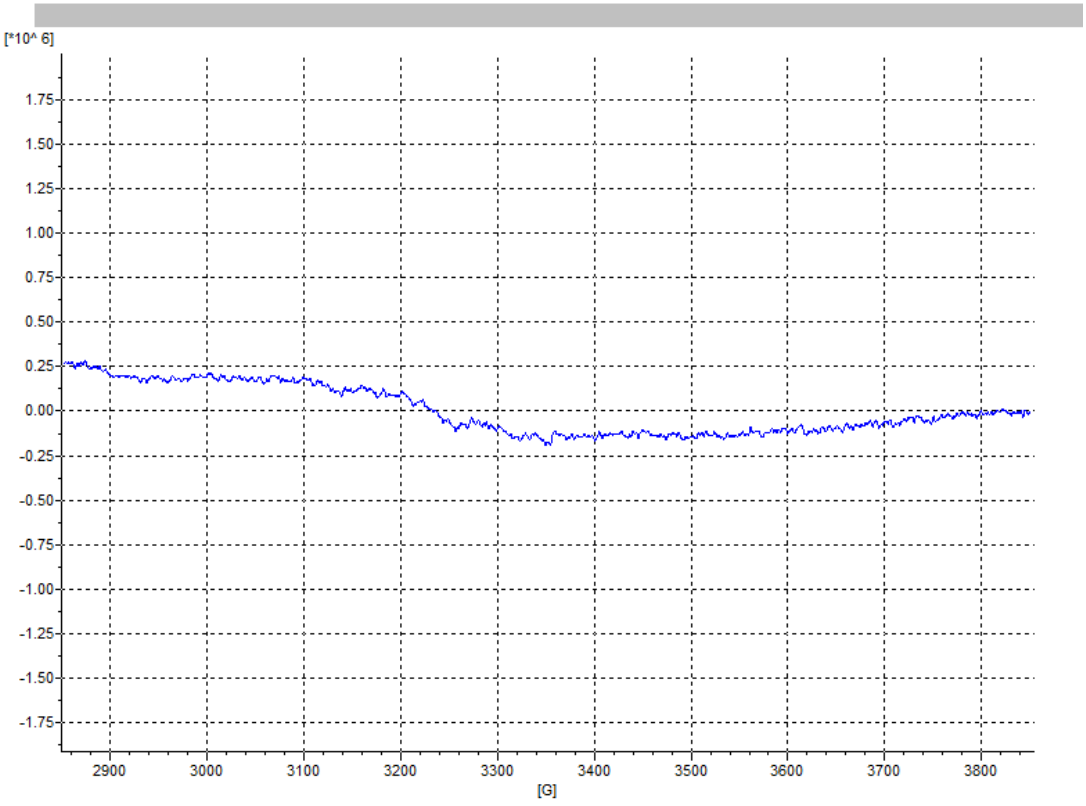
Procedure: to a 25 mL schlenk tube equipped with a stir bar, a mixture of potassium oxophenylacetate **2a** (0.25 mmol), Ag_2CO_3 (0.025 mmol), $Na_2S_2O_8$ (0.5 mmol) and radical trapping reagent (TEMPO or BHT 0.5 mmol) were under N_2 atmosphere, then 1.5 mL DMSO was injected to the tube. After 5 min, 2-isocyanobiphenyl **1a** (0.75 mmol) was added to the tube under N_2.

Then the reaction was conducted at 100 °C for 6 h. After completion of the reaction, it was analysis by GC using biphenyl as the internal standard.

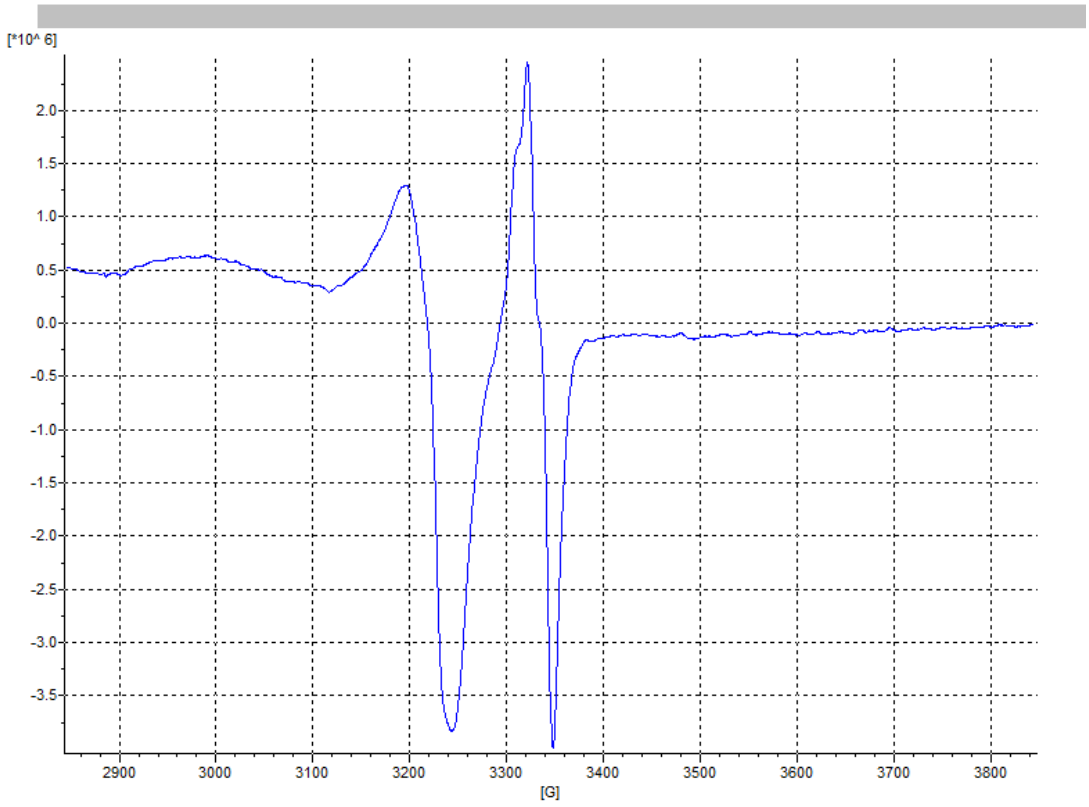
EPR experiments

Procedure: X band, 9.4 GHz, at 160 K

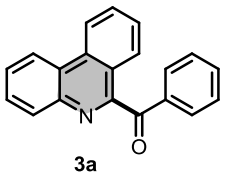
1. Blank experiment: to a 25 mL schlenk tube equipped with a stir bar, 0.025 mmol AgOTf was added under N2 atmosphere, then 1.5 mL DMSO was injected to the tube. The reaction was conducted at 80 °C for 2 h. Then sample 0.5 mL from it and preserved in liquid nitrogen for EPR exam.



2. Experiment: to a 25 mL schlenk tube equipped with a stir bar, a mixture of 0.025 mmol AgOTf and 0.5 mmol $Na_2S_2O_8$ was added under N_2 atmosphere, then 1.5 mL DMSO was injected to the tube. The reaction was conducted at 80 °C for 2 h. Then sample 0.5 mL from it and preserved in liquid nitrogen for EPR exam.



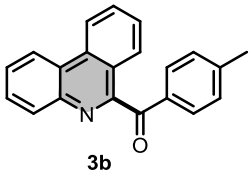
Characterization of Products



3a

phenanthridin-6-yl(phenyl)methanone

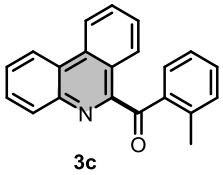
100.5 mg (0.5 mmol scale) for 71% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 Mhz, in $CDCl_3$): 8.73-8.71 (m, 1H), 8.67-8.65 (m, 1H), 8.23-8.21 (m, 1H), 8.15-8.13 (m, 1H), 8.05-8.03 (m, 2H), 7.92-7.88 (m, 1H), 7.81-7.75 (m, 2H), 7.69-7.61 (m, 2H), 7.50-7.46 (m, 2H); ^{13}C NMR (101 MHz, in $CDCl_3$): 195.09, 157.75, 142.91, 136.39, 134.28, 133.54, 131.55, 131.09, 130.90, 129.38, 128.86, 128.46, 128.08, 127.59, 124.74, 124.05, 122.59, 122.44 ppm. HRMS (ESI) calculated $[M+H]^+$: 284.1070; found $[M+H]^+$: 284.1071.



3b

phenanthridin-6-yl(p-tolyl)methanone

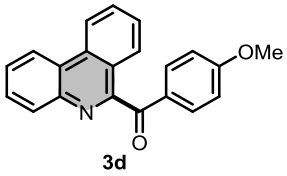
109.9 mg (0.5 mmol scale) for 74% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.74-8.72 (m, 1H), 8.68-8.66 (m, 1H), 8.26-8.24 (m, 1H), 8.16-8.14 (m, 1H), 7.97-7.95 (m, 2H), 7.93-7.89 (m, 1H), 7.83-7.76 (m, 2H), 7.70-7.65 (m, 1H), 7.31-7.29 (m, 2H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 194.80, 158.08, 145.37, 142.95, 133.93, 133.48, 131.47, 131.17, 130.84, 129.58, 129.31, 129.04, 128.32, 128.00, 127.62, 124.67, 124.04, 122.53, 122.40, 22.11. HRMS (ESI) calculated $[M+H]^+$: 298.1226; found $[M+H]^+$: 298.1230.



3c

phenanthridin-6-yl(o-tolyl)methanone

105.4 mg (0.5 mmol scale) for 71% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.70-8.67 (m, 1H), 8.62-8.60 (m, 1H), 8.26-8.24 (m, 1H), 8.20-8.18 (m, 1H), 7.89-7.85 (m, 1H), 7.77-7.70 (m, 2H), 7.69-7.65 (m, 1H), 7.56-7.54 (m, 1H), 7.47-7.43 (m, 1H), 7.37-7.35 (m, 1H), 7.20-7.16 (m, 1H), 2.72 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 197.56, 158.65, 142.92, 140.98, 136.14, 133.49, 133.28, 132.83, 132.31, 131.36, 130.82, 129.21, 128.35, 128.04, 127.51, 125.79, 124.64, 123.98, 122.50, 122.32, 22.19. HRMS (ESI) calculated $[M+H]^+$: 298.1226; found $[M+H]^+$: 298.1230.

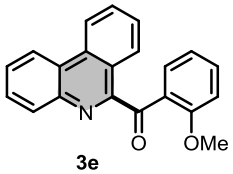


3d

(4-methoxyphenyl)(phenanthridin-6-yl)methanone

111.1 mg (0.5 mmol scale) for 71% isolated yield, white solid, PE:EA = 20:1. ^{1}H NMR (400 MHz, in

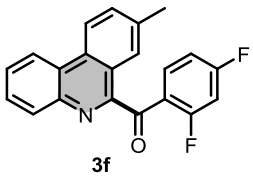
$CDCl_3$): 8.68 (d, *J* = 8.0 Hz, 1H), 8.63-8.61 (m, 1H), 8.23-8.21 (m, 1H), 8.12-8.10 (m, 1H), 8.01 (d, *J* = 9.2 Hz, 2H), 7.88-7.84 (m, 1H), 7.79-7.71 (m, 2H), 7.65-7.61 (m, 1H), 6.93 (d, *J* = 9.2 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 193.68, 164.56, 158.22, 142.90, 133.41, 131.42, 130.72, 129.38, 129.25, 128.22, 127.93, 127.61, 124.57, 123.99, 122.48, 122.37, 114.11, 55.76. HRMS (ESI) calculated $[M+H]^+$: 314.1176; found $[M+H]^+$: 314.1176.



3e

(2-methoxyphenyl)(phenanthridin-6-yl)methanone

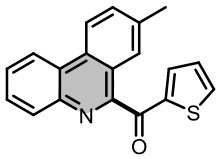
112.7 mg (0.5 mmol scale) for 72% isolated yield, white solid, PE:EA = 20:1. ^{1}H NMR (400 M, in $CDCl_3$): 8.66 (d, *J* = 8.4 Hz, 1H), 8.59 (d, *J* = 7.2 Hz, 1H), 8.22 (d, *J* = 8.0 Hz, 1H), 8.13 (d, *J* = 7.2 Hz, 1H), 8.03-8.02 (m, 1H), 7.87-7.83 (m, 1H), 7.73-7.63 (m, 3H), 7.56-7.51 (m, 1H), 7.13-7.09 (m, 1H), 6.88 (d, *J* = 8.4 Hz, 1H), 3.25 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 195.65, 160.11, 159.80, 143.03, 135.17, 133.28, 131.83, 130.99, 130.56, 128.94, 127.84, 127.75, 127.54, 127.45, 122.30, 121.13, 112.62, 55.91. HRMS (ESI) calculated $[M+H]^+$: 314.1176; found $[M+H]^+$: 314.1176.



3f

(2,4-difluorophenyl)(8-methylphenanthridin-6-yl)methanone

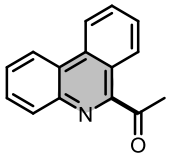
69.9 mg (0.5 mmol scale) for 42% isolated yield, yellow solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.56-8.54 (m, 2H), 8.08-8.02 (m, 3H), 7.70-7.67 (m, 3H), 7.05-7.00 (m, 1H), 6.82-6.77 (m, 1H), 2.53 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 191.80, 166.57 (dd, J_{CF1} = 258.56 Hz, J_{CF2} = 12.22 Hz), 163.32 (dd, J_{CF1} = 261.39 Hz, J_{CF2} = 12.73 Hz), 156.75, 142.59, 138.35, 134.07 (dd, J_{CF1} = 10.81 Hz, J_{CF2} = 3.23 Hz), 133.27, 131.65, 130.80, 129.94, 128.82, 128.60, 126.53, 125.14, 123.45, 122.46, 122.26, 112.36 (dd, J_{CF1} = 21.72 Hz, J_{CF2} = 3.64 Hz), 105.15 (t, J_{CF} = 25.86 Hz), 22.02. ^{19}F NMR (376 MHz, in $CDCl_3$): -100.48 (d, J_{FF} = 12.41 Hz), -102.79 (d, J_{FF} = 12.41 Hz) ppm. HRMS (ESI) calculated $[M+H]^+$: 334.1038; found $[M+H]^+$: 334.1033.



3g

(8-methylphenanthridin-6-yl)(thiophen-2-yl)methanone

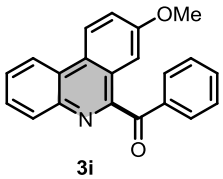
80.3 mg (0.5 mmol scale) for 53% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.58-8.54 (m, 2H), 8.28-8.24 (m, 2H), 7.93-7.92 (m, 1H), 7.80-7.79 (m, 1H), 7.76-7.73 (m, 2H), 7.70-7.68 (m, 1H), 7.17-7.15 (m, 1H), 2.55 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 186.58, 155.45, 142.88, 142.26, 138.32, 136.98, 136.48, 133.25, 131.61, 130.77, 128.85, 128.71, 128.41, 126.99, 125.17, 123.84, 122.30, 122.25, 22.00 ppm. HRMS (ESI) calculated $[M+H]^+$: 304.0791; found $[M+H]^+$: 304.0790.



3h

1-(phenanthridin-6-yl)ethan-1-one

40.9 mg (0.5 mmol scale) for 37% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.89 (d, *J* = 8.4 Hz, 1H), 8.59 (d, *J* = 8.4 Hz, 1H), 8.53 (d, *J* = 7.6 Hz, 1H), 8.22-8.20 (m, 1H), 7.84-7.80 (m, 1H), 7.78-7.68 (m, 3H), 2.95 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 202.99, 153.97, 142.61, 133.67, 131.18, 130.93, 129.08, 129.01, 128.26, 128.03, 125.50, 123.18, 122.26, 122.16, 28.82. HRMS (ESI) calculated $[M+H]^+$: 222.0913; found $[M+H]^+$: 222.0922.

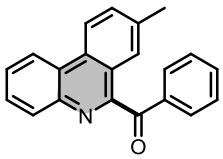


3i

(8-methoxyphenanthridin-6-yl)(phenyl)methanone

133.0 mg (0.5 mmol scale) for 85% isolated yield, white solid, PE:EA = 20:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.60 (d, J = 8.8 Hz, 1H), 8.55-8.53 (m, 1H), 8.20-8.17 (m, 1H), 8.07-8.04 (m, 2H), 7.73-7.70

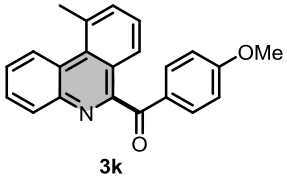
(m, 2H), 7.65-7.61 (m, 1H), 7.54-7.47 (m, 4H), 3.87 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 195.16, 159.18, 156.31, 141.98, 136.52, 134.16, 131.14, 130.79, 128.78, 128.57, 128.31, 128.06, 125.37, 124.93, 124.20, 122.73, 121.92, 106.79, 55.78 ppm. HRMS (ESI) calculated $[M+H]^+$: 314.1176; found $[M+H]^+$: 314.1182.



3j

(8-methylphenanthridin-6-yl)(phenyl)methanone

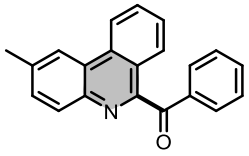
74.3 mg (0.5 mmol scale) for 50% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.60-8.57 (m, 2H), 8.21-8.19 (m, 1H), 8.07-8.04 (m, 2H), 7.91 (s, 1H), 7.76-7.68 (m, 3H), 7.65-7.60 (m, 1H), 7.50-7.46 (m, 2H), 2.51 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 195.18, 157.41, 142.53, 138.17, 136.39, 134.20, 133.32, 131.39, 131.05, 130.70, 128.83, 128.80, 128.29, 126.73, 124.76, 124.13, 122.42, 122.22, 21.89 ppm. HRMS (ESI) calculated $[M+H]^+$: 298.1226; found $[M+H]^+$: 298.1230.



3k

(4-methoxyphenyl)(10-methylphenanthridin-6-yl)methanone

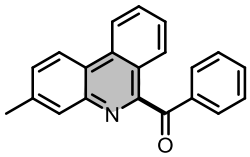
107.9 mg (0.5 mmol scale) for 66% isolated yield, white solid, PE:EA = 20:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.89-8.87 (m, 1H), 8.27-8.24 (m, 1H), 7.98-7.95 (m, 3H), 7.79-7.69 (m, 3H), 7.54-7.50 (m, 1H), 6.93-6.91 (m, 2H), 3.84 (s, 3H), 3.16 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 194.33, 164.58, 159.29, 144.24, 135.81, 135.62, 133.44, 133.31, 132.79, 131.02, 129.43, 128.48, 127.35, 126.85, 126.29, 126.01, 125.39, 114.15, 55.79, 27.09 ppm. HRMS (ESI) calculated $[M+H]^+$: 328.1332; found $[M+H]^+$: 328.1332.



3l

(2-methylphenanthridin-6-yl)(phenyl)methanone

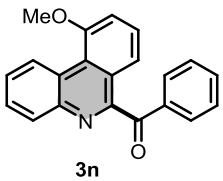
65.3 mg (0.5 mmol scale) for 44% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.68-8.65 (m, 1H), 8.40 (s, 1H), 8.15-8.10 (m, 2H), 8.06-8.04 (m, 2H), 7.86-7.82 (m, 1H), 7.64-7.58 (m, 3H), 7.49-7.45 (m, 2H), 2.64 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 195.08, 156.63, 141.15, 138.56, 136.57, 134.06, 133.19, 131.18, 131.02, 130.54, 128.74, 127.83, 127.42, 124.54, 124.11, 122.47, 121.98, 22.29 ppm. HRMS (ESI) calculated $[M+H]^+$: 298.1226; found $[M+H]^+$: 298.1232.



3m

(3-methylphenanthridin-6-yl)(phenyl)methanone

69.8 mg (0.5 mmol scale) for 47% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.65 (d, *J* = 8.4 Hz, 1H), 8.52-8.50 (m, 1H), 8.16-8.14 (m, 1H), 8.08-8.03 (m, 3H), 7.88-7.84 (m, 1H), 7.66-7.60 (m, 2H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.51-7.47 (m, 2H), 2.60 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 195.06, 157.57, 142.93, 139.52, 136.45, 134.11, 133.50, 131.34, 130.99, 130.25, 130.15, 128.75, 127.49, 127.41, 123.67, 122.31, 122.14, 21.71 ppm. HRMS (ESI) calculated $[M+H]^+$: 298.1226; found $[M+H]^+$: 298.1227.

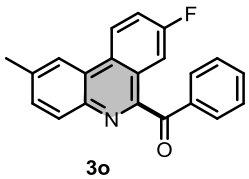


3n

(10-methoxyphenanthridin-6-yl)(phenyl)methanone

103.3 mg (0.5 mmol scale) for 66% isolated yield, white solid, PE:EA = 20:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.26-8.24 (m, 1H), 8.12-8.10 (m, 1H), 8.02-8.00 (m, 2H), 7.79-7.71 (m, 2H), 7.70-7.67 (m,

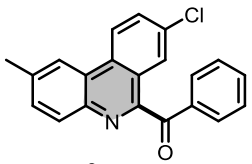
1H), 7.62-7.55 (m, 2H), 7.48-7.44 (m, 2H), 7.33-7.31 (m, 1H), 4.14 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 195.47, 158.39, 157.90, 143.44, 136.30, 134.25, 133.87, 130.89, 130.35, 128.82, 128.63, 128.62, 128.30, 128.25, 128.16, 125.89, 124.49, 123.81, 119.68, 112.35, 56.07 ppm. HRMS (ESI) calculated $[M+H]^+$: 314.1176; found $[M+H]^+$: 314.1176.



3o

(8-fluoro-2-methylphenanthridin-6-yl)(phenyl)methanone

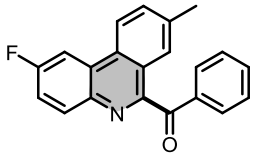
85.1 mg (0.5 mmol scale) for 54% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.69-8.65 (m, 1H), 8.34 (s, 1H), 8.10-8.05 (m, 3H), 7.89-7.86 (m, 1H), 7.65-7.58 (m, 3H), 7.51-7.47 (m, 2H), 2.66 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 194.52, 161.68 (d, J_{CF} = 250.08 Hz), 155.19 (d, J_{CF} = 4.14 Hz), 140.75, 140.74, 139.28, 136.38, 134.21, 131.19, 130.99, 130.77, 130.01, 129.99, 128.79, 125.28 (d, J_{CF} = 8.59 Hz), 125.10 (d, J_{CF} = 8.59 Hz), 124.29, 121.78, 120.59 (d, J_{CF} = 24.14 Hz), 112.04 (d, J_{CF} = 22.42 Hz), 22.40. ^{19}F NMR (376 MHz, in $CDCl_3$): -111.20 ppm. HRMS (ESI) calculated $[M+H]^+$: 316.1132; found $[M+H]^+$: 316.1133.



3p

(8-chloro-2-methylphenanthridin-6-yl)(phenyl)methanone

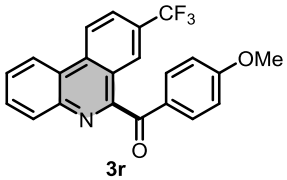
67.9 mg (0.5 mmol scale) for 41% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.61-8.57 (m, 2H), 8.24-8.22 (m, 2H), 7.81-7.71 (m, 5H), 7.40-7.39 (m, 1H), 6.63-6.62 (m, 1H), 2.57 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 181.83, 155.24, 152.31, 148.62, 142.39, 138.36, 133.31, 131.53, 130.85, 128.88, 128.71, 126.83, 125.18, 124.03, 123.88, 122.32, 122.27, 112.93, 22.00 ppm. HRMS (ESI) calculated $[M+H]^+$: 332.0837; found $[M+H]^+$: 332.0838.



3q

(2-fluoro-8-methylphenanthridin-6-yl)(phenyl)methanone

88.2 mg (0.5 mmol scale) for 56% isolated yield, white solid, PE:EA = 50:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.48 (d, *J* = 8.4 Hz, 1H), 8.22-8.18 (m, 2H), 8.07-8.05 (m, 2H), 7.95 (s, 1H), 7.75-7.73 (m, 1H), 7.68-7.64 (m, 1H), 7.53-7.47 (m, 3H), 2.55 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 194.98, 162.28 (d, J_{CF} = 249.67 Hz), 156.61 (d, J_{CF} = 2.83 Hz), 139.34, 139.03, 136.37, 134.29, 133.41, 133.05 (d, J_{CF} = 9.39 Hz), 131.07, 128.85, 126.31 (d, J_{CF} = 9.49 Hz), 126.88, 124.21, 122.62, 117.89 (d, J_{CF} = 24.54 Hz), 107.23 (d, J_{CF} = 23.53 Hz), 21.98; ^{19}F NMR (376 MHz, in $CDCl_3$): -110.77 ppm. HRMS (ESI) calculated $[M+H]^+$: 316.1132; found $[M+H]^+$: 316.1136.



3r

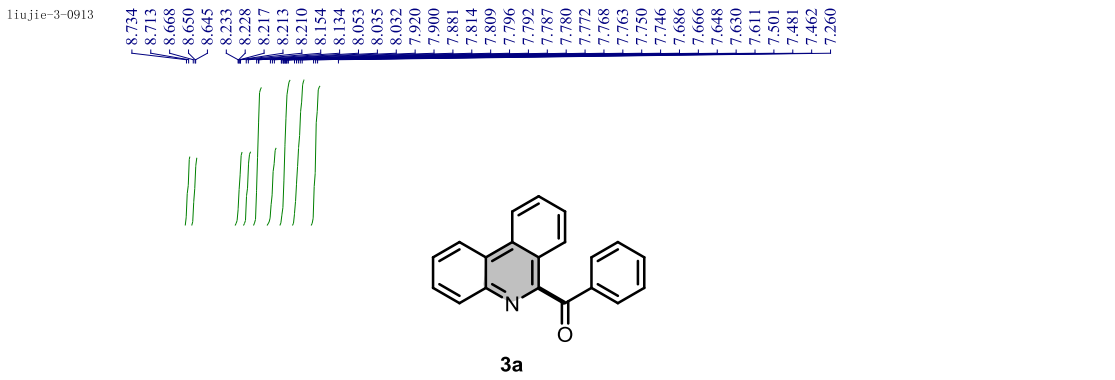
(4-methoxyphenyl)(8-(trifluoromethyl)phenanthridin-6-yl)methanone

75.1 mg (0.5 mmol scale) for 39% isolated yield, yellow solid, PE:EA = 20:1. ^{1}H NMR (400 MHz, in $CDCl_3$): 8.80 (d, J = 8.8 Hz, 1H), 8.65-8.63 (m, 1H), 8.48 (s, 1H), 8.25-8.23 (m, 1H), 8.07-8.05 (m, 3H), 7.87-7.78 (m, 2H), 6.98-6.96 (m, 2H), 3.88 (s, 3H); ^{13}C NMR (101 MHz, in $CDCl_3$): 192.72, 164.82, 157.50, 143.40, 135.67, 133.67, 131.06, 130.50, 129.79 (t, J_{CF} = 33.23 Hz), 129.11, 129.01, 127.25 (t, J_{CF} = 3.13 Hz), 125.36, 125.26 (t, J_{CF} = 4.24 Hz), 123.75, 123.68, 123.43, 122.77, 114.24, 55.86; ^{19}F NMR (376 MHz, $CDCl_3$): -62.26 ppm. HRMS (ESI) calculated $[M+H]^+$: 382.1049; found $[M+H]^+$: 382.1052.

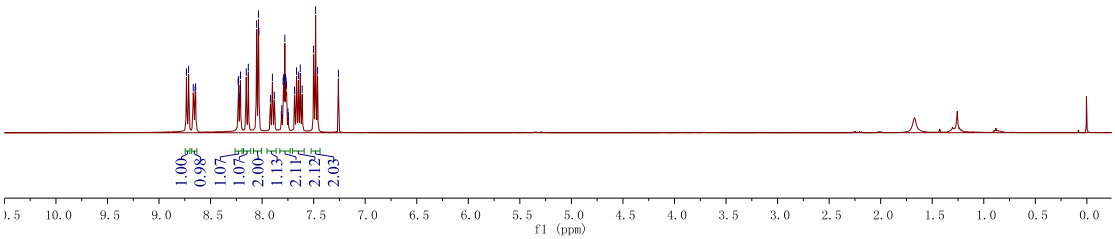
References

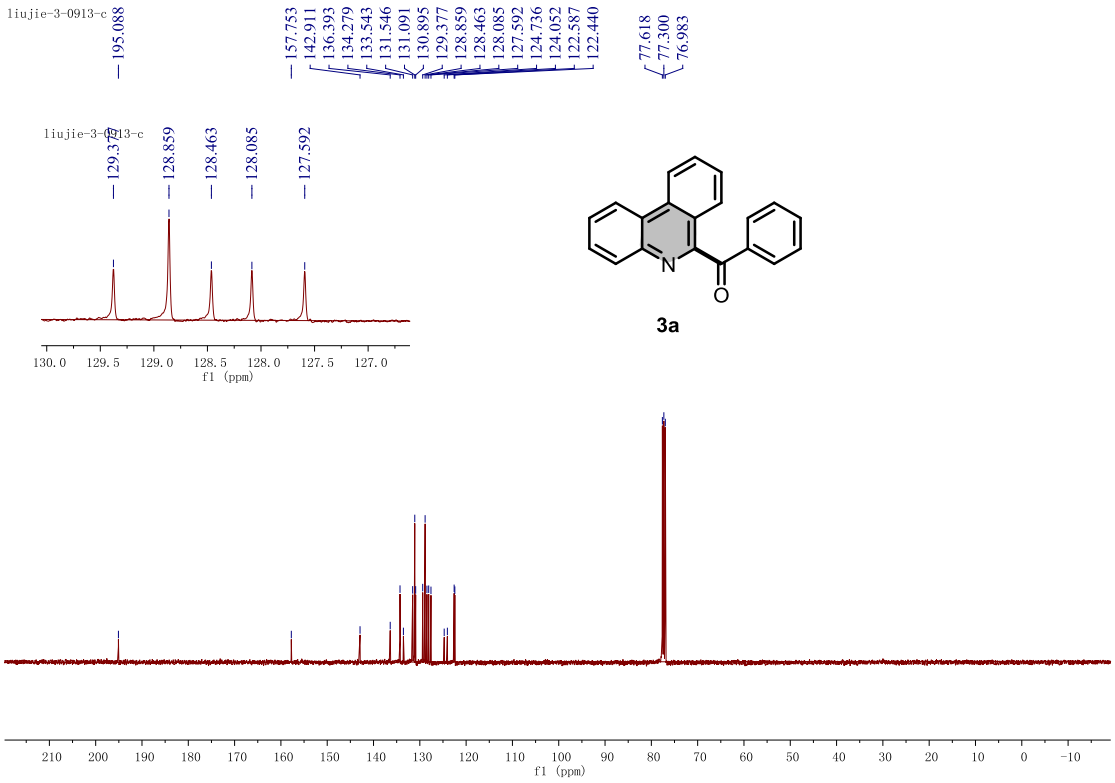
(1) Kuldeep, W.; Yang, C.; R. West, P.; Deming, K. C.; R., C. S.; E., R. R. *Synth. Commun.* **2008**, *38*, 4434.
(2) Gooßen, L. J.; Rudolphi, F.; Oppel, C.; Rodríguez, N. *Angewandte Chemie International Edition* **2008**, *47*, 3043.
(3) Tobisu, M.; Koh, K.; Furukawa, T.; Chatani, N. *Angew. Chem. Int. Ed.* **2012**, *51*, 11363.

NMR and HRMS Spectra of Products



3a





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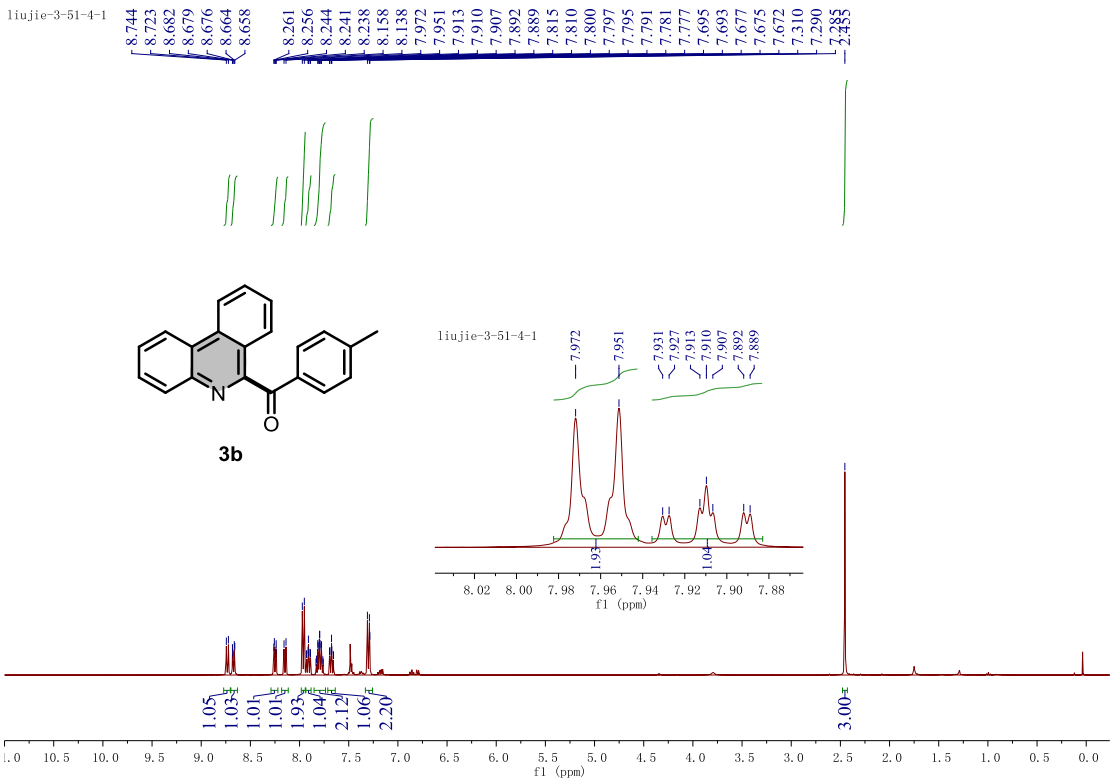
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8.679
8.676
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8.261
8.256
8.244
8.241
8.238
8.158
8.138
7.972
7.951
7.913
7.910
7.907
7.892
7.889
7.815
7.810
7.800
7.797
7.795
7.791
7.781
7.777
7.695
7.693
7.677
7.675
7.672
7.310
7.290
7.285
7.255
3b
liujie-3-51-4-1
7.972
7.951
7.931
7.927
7.913
7.910
7.907
7.892
7.889
1.93
1.04
8.02 8.00 7.98 7.96 7.94 7.92 7.90 7.88
f1 (ppm)
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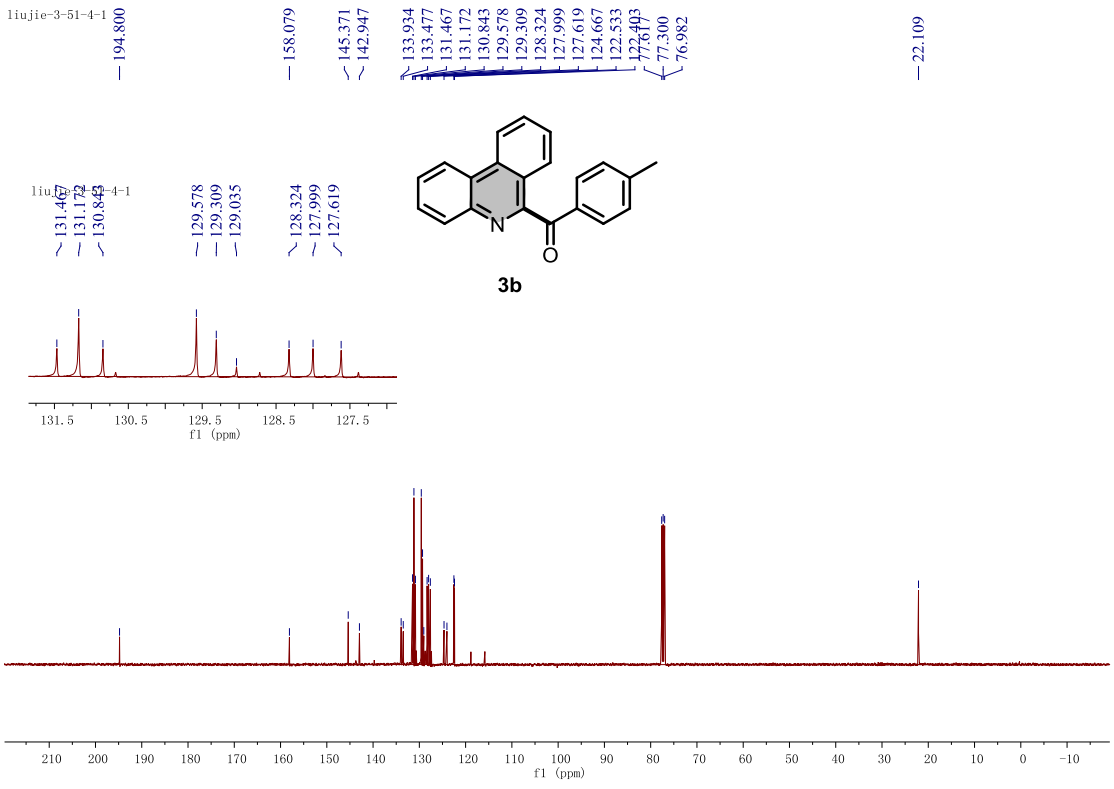
1.03
1.01
1.01
1.93
1.04
2.12
1.06
2.20
3.00
f1 (ppm)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145.371
142.947
133.934
133.477
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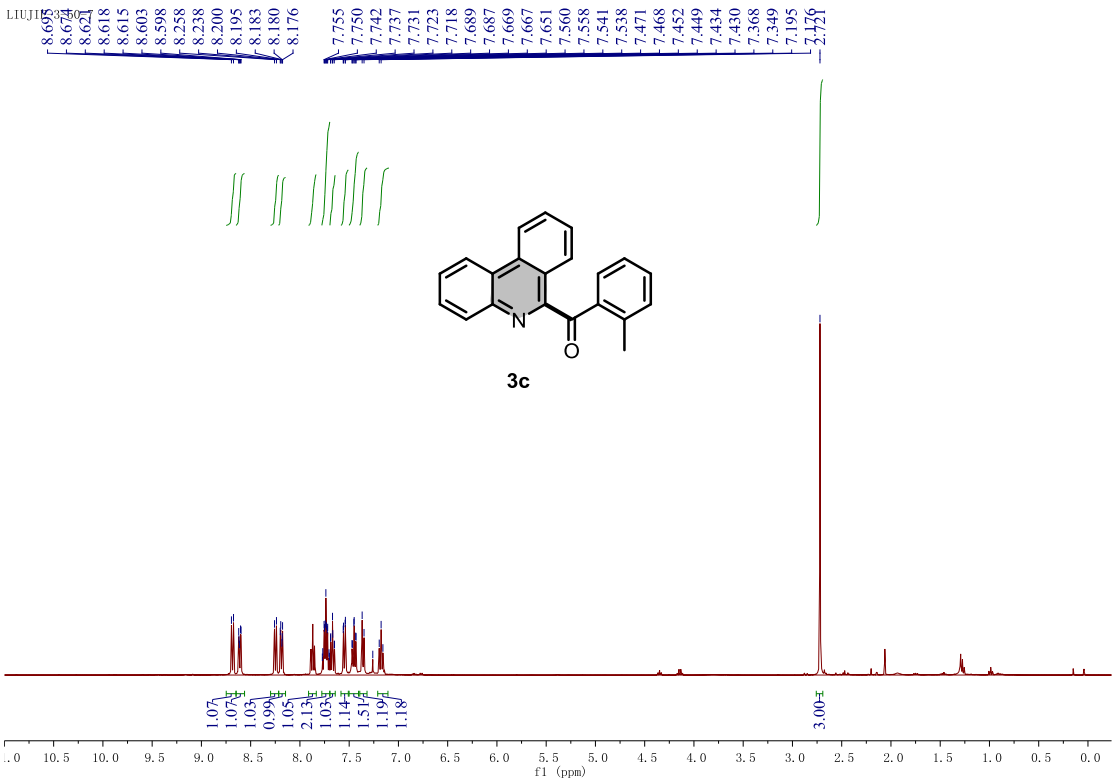
131.172
130.843
129.578
129.309
128.324
127.999
127.619
124.667
122.533
77.317
77.300
76.982
22.109
3b
131.467
131.172
130.843
129.578
129.309
129.035
128.324
127.999
127.619
131.5 130.5 129.5 128.5 127.5
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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8.603
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8.258
8.238
8.200
8.195
8.183
8.180
8.176
7.755
7.750
7.742
7.737
7.731
7.723
7.718
7.689
7.687
7.669
7.667
7.651
7.560
7.558
7.541
7.538
7.471
7.468
7.452
7.449
7.434
7.430
7.368
7.349
7.195
7.176
2.721
N
O
3c
1.07
1.07
1.03
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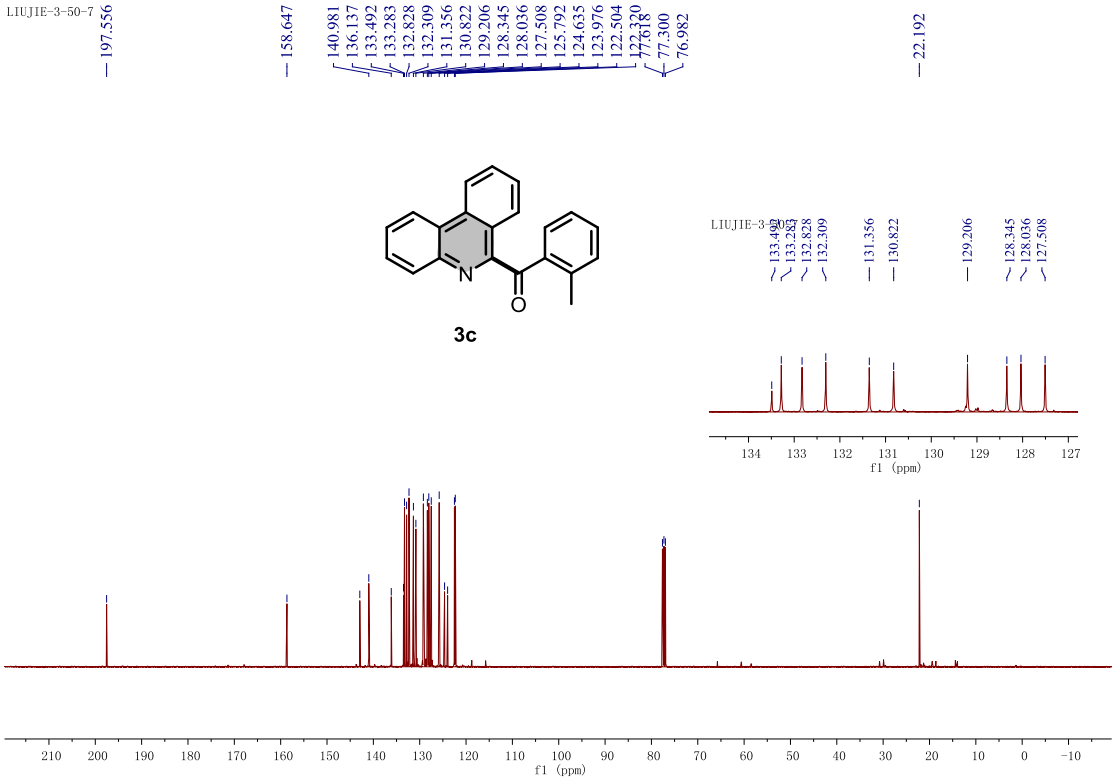
1.05
2.13
1.03
1.14
1.51
1.19
1.18
3.00
f1 (ppm)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128.345
128.036
127.508
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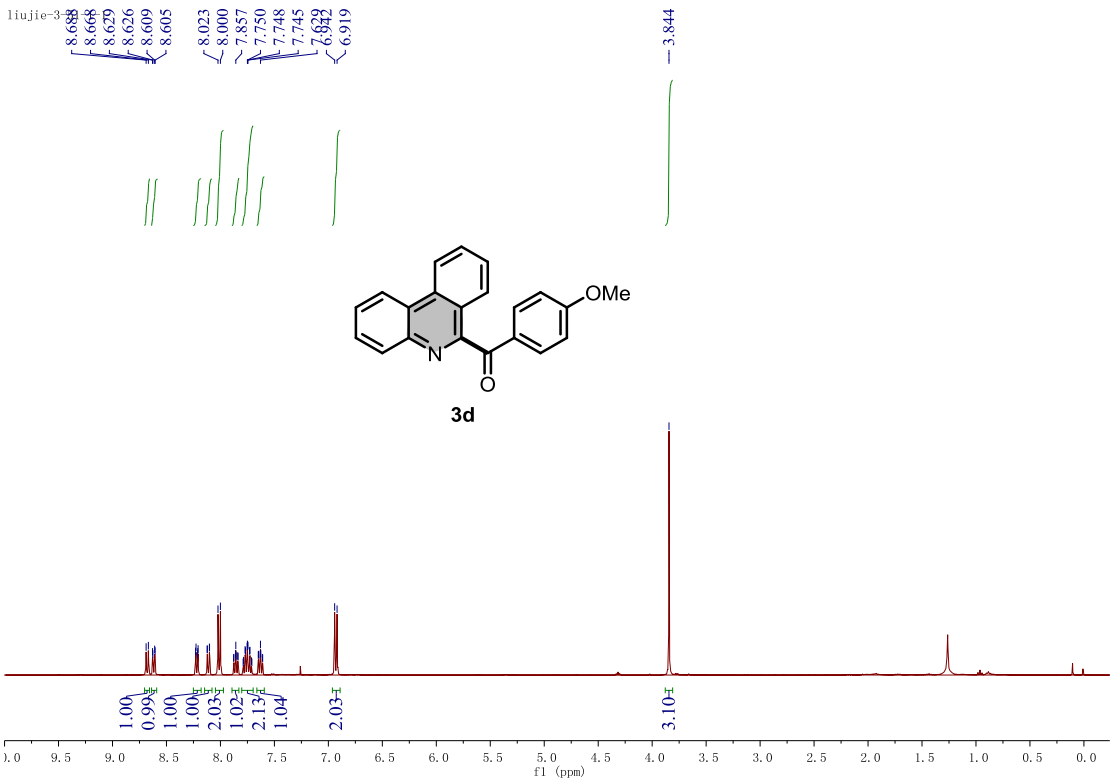
22.192
N
O
3c
f1 (ppm)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8.000
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7.750
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7.745
7.629
7.622
6.942
6.919
3.844
OMe
N
O
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1.00
1.00
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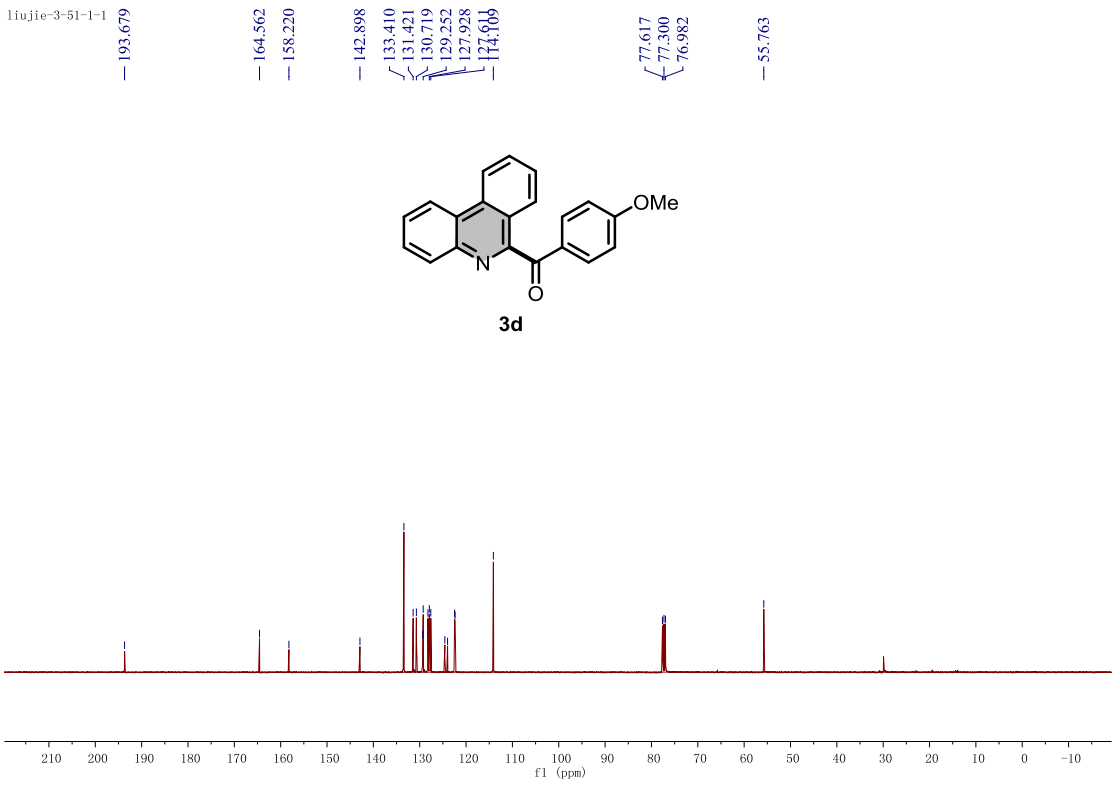
1.02
2.13
1.04
2.03
3.10
f1 (ppm)

3d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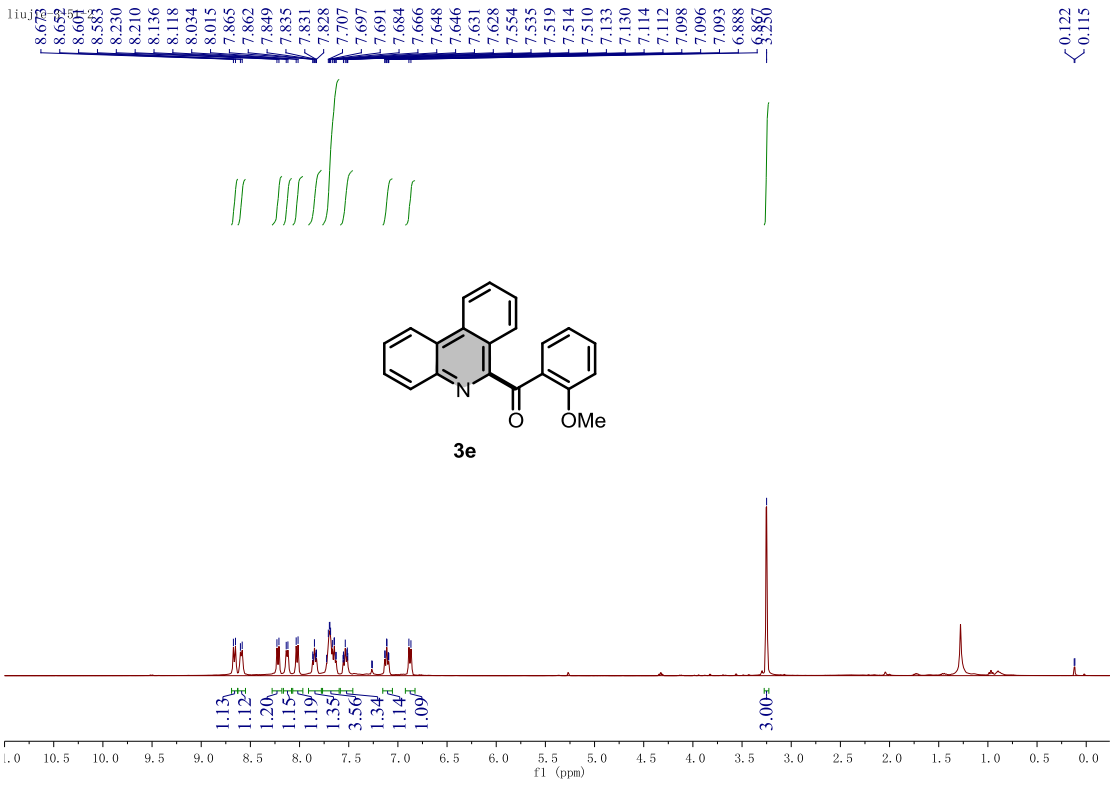
OMe
N
O
f1 (ppm)

3d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7.849
7.835
7.831
7.828
7.707
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7.691
7.684
7.666
7.648
7.646
7.631
7.628
7.554
7.535
7.519
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7.510
7.133
7.130
7.114
7.112
7.098
7.096
7.093
6.888
6.867
3.250
0.122
0.115
N
O
OMe
3e
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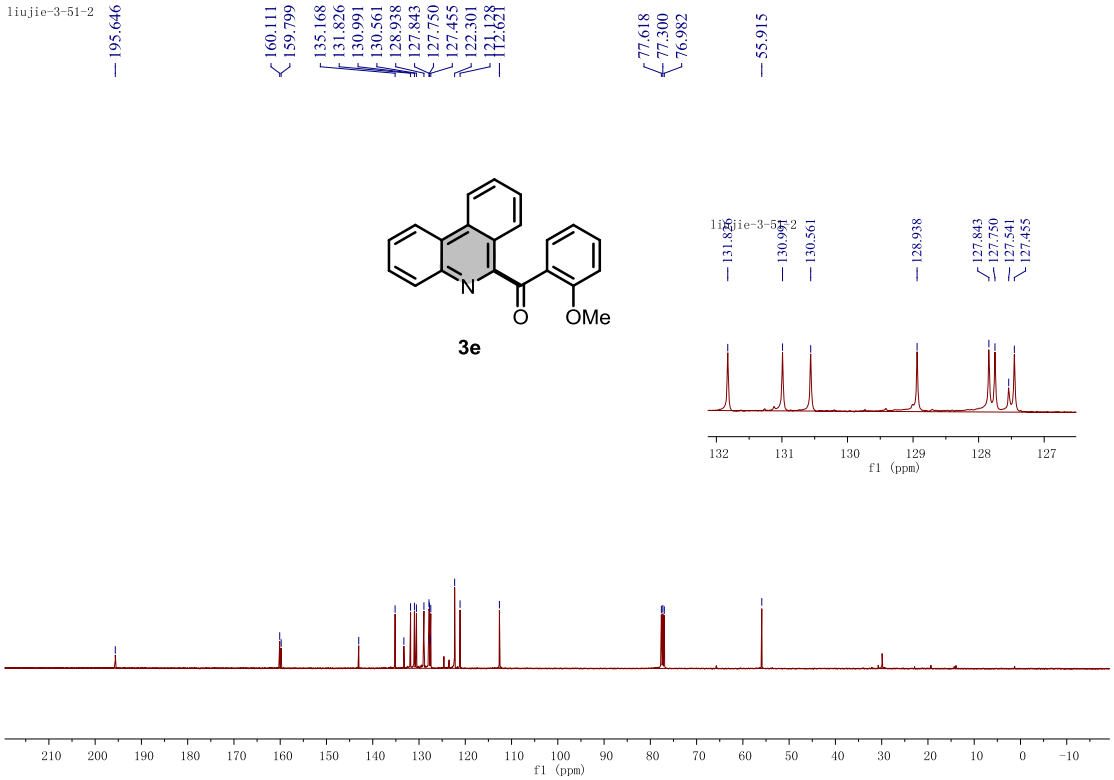
1.09
3.00
f1 (ppm)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127.750
127.455
122.301
121.128
112.621
77.618
77.300
76.982
55.915
N
O
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3e
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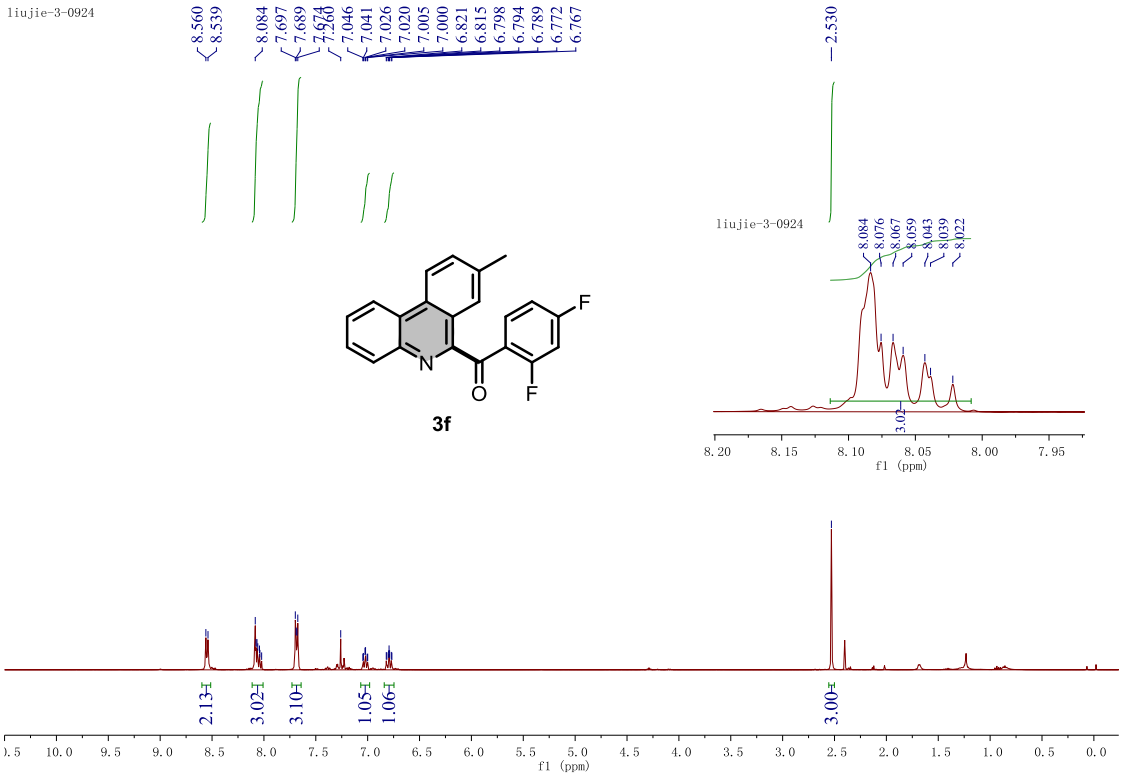
127.750
127.541
127.455
f1 (ppm)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7.026
7.020
7.005
7.000
6.821
6.815
6.798
6.794
6.789
6.772
6.767
2.530
F
N
O
F
3f
liujie-3-0924
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8.076
8.067
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8.039
8.022
3.02
8.20
8.15
8.10
8.05
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7.95
f1 (ppm)
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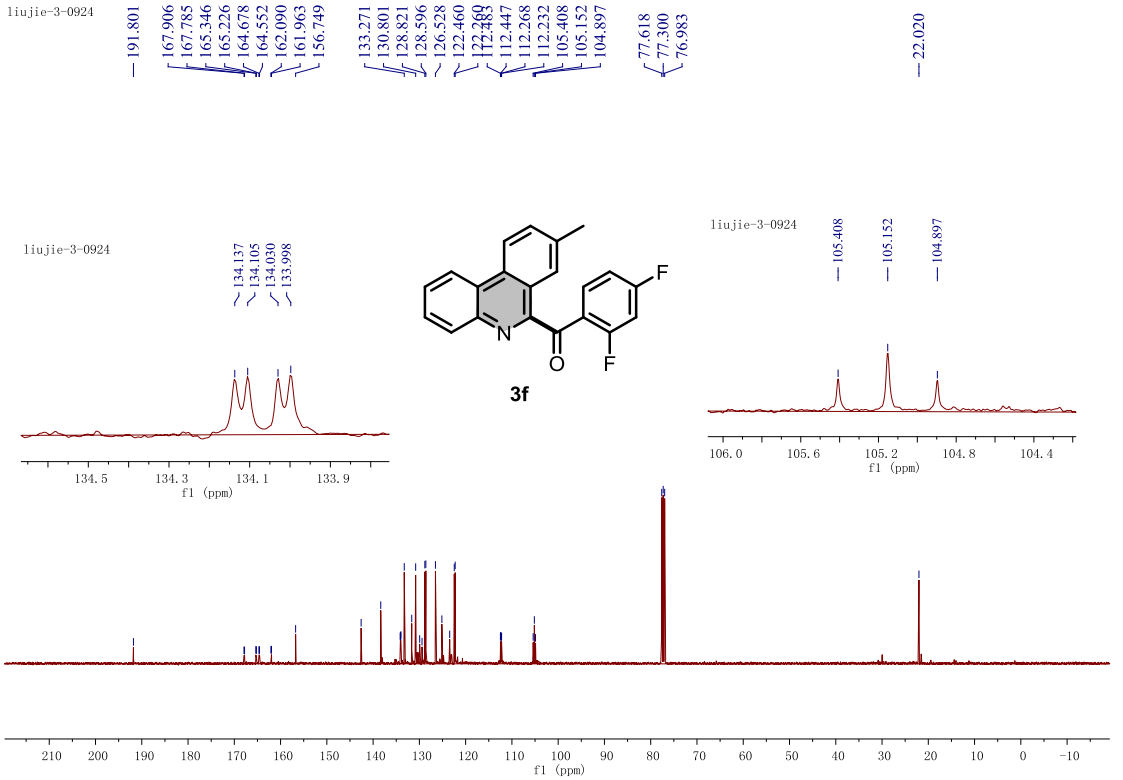
3.02
3.10
1.05
1.06
3.00
f1 (ppm)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133.271
130.801
128.821
128.596
126.528
122.460
122.260
112.483
112.447
112.268
112.232
105.408
105.152
104.897
77.618
77.300
76.983
22.020
liujie-3-0924
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134.105
134.030
133.998
134.5
134.3
134.1
133.9
f1 (ppm)
F
N
O
F
3f
liujie-3-0924
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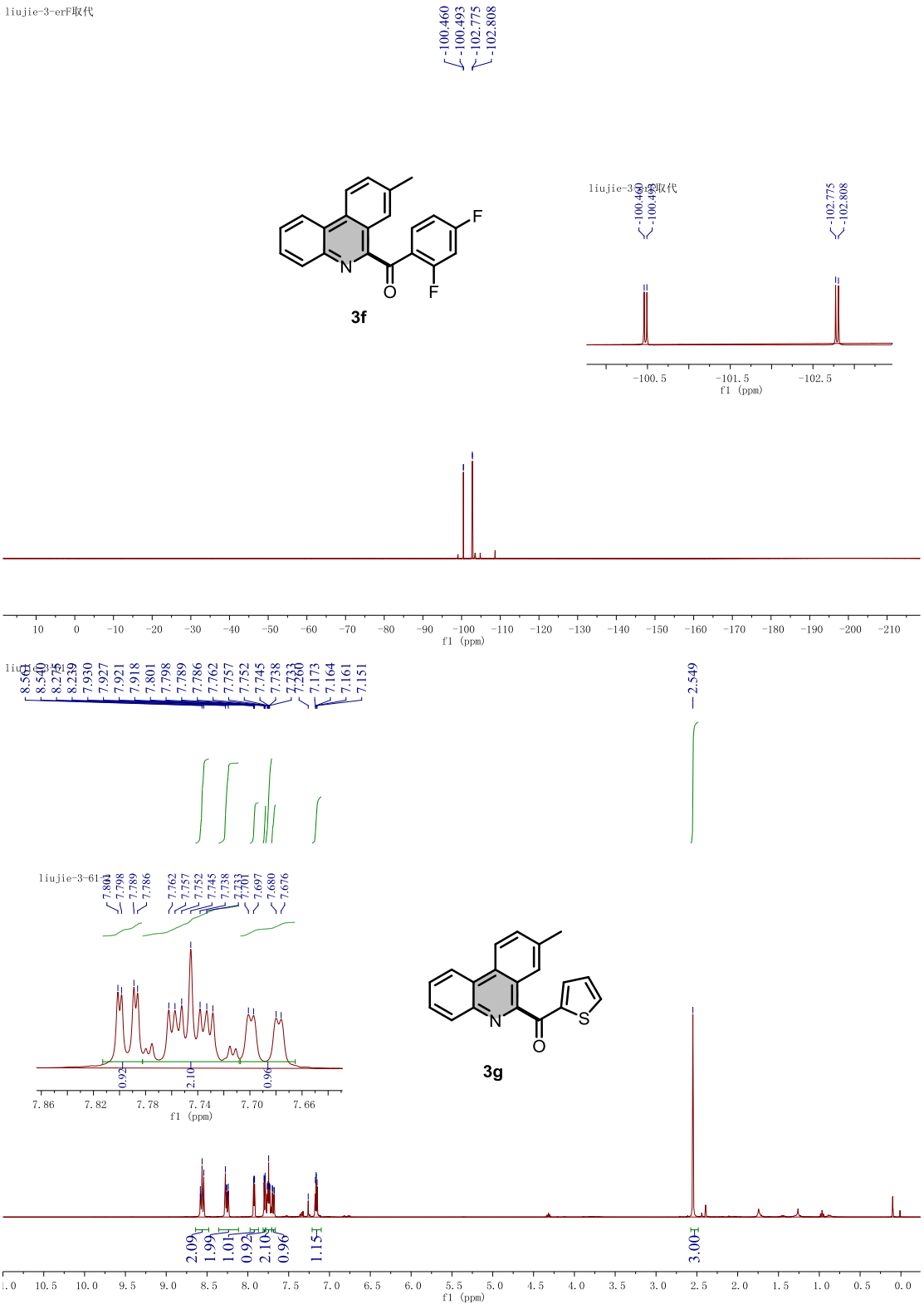
f1 (ppm)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F
N
O
F
3f
liujie-3-erF取代
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-100.493
-102.775
-102.808
-100.5
-101.5
-102.5
f1 (ppm)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
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8.540
8.275
8.239
7.930
7.927
7.921
7.918
7.801
7.798
7.789
7.786
7.762
7.757
7.752
7.745
7.738
7.733
7.697
7.680
7.676
7.173
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7.161
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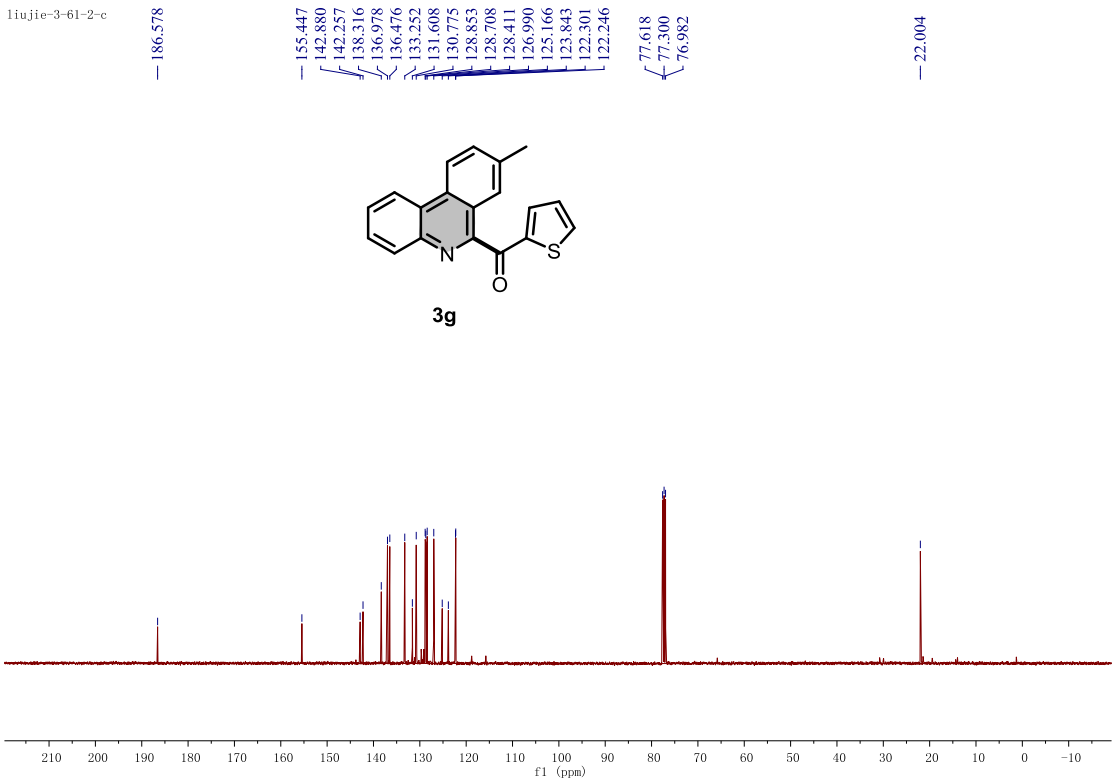
7.789
7.786
7.762
7.757
7.752
7.745
7.738
7.733
7.701
7.697
7.680
7.676
0.92
2.10
0.96
7.86 7.82 7.78 7.74 7.70 7.66
f1 (ppm)
N
S
O
3g
2.09
1.99
1.01
0.92
2.10
0.96
1.15
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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131.608
130.775
128.853
128.708
128.411
126.990
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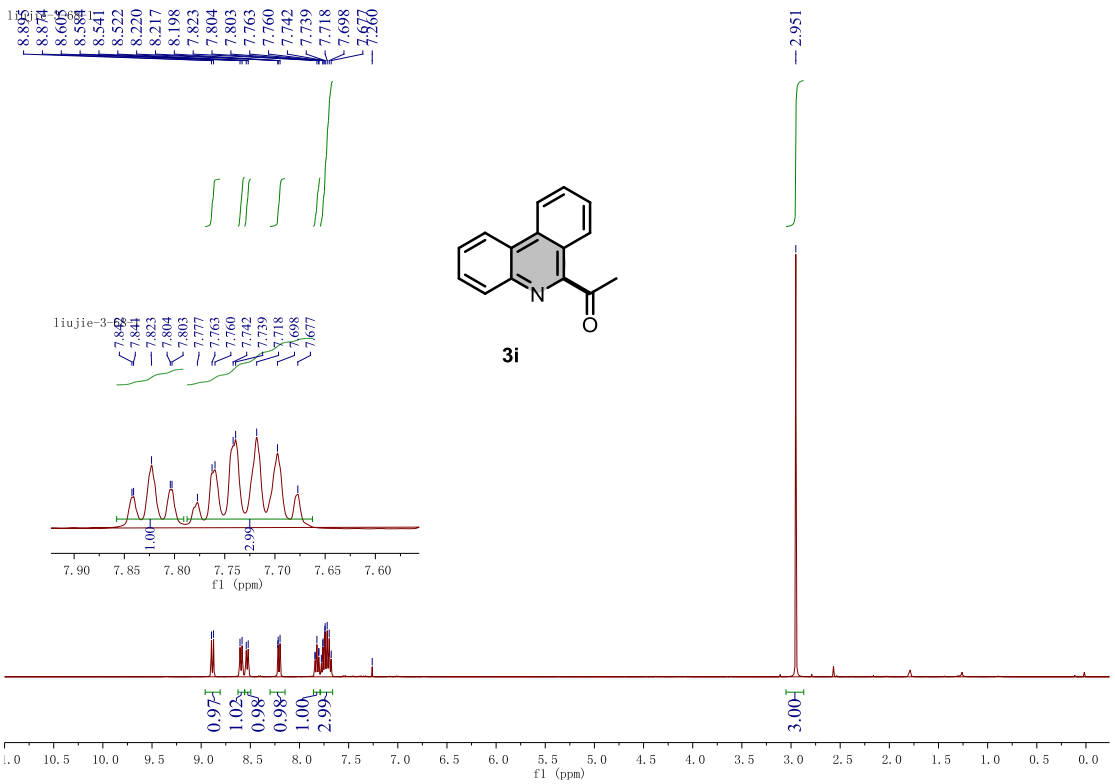
22.004
N
S
O
f1 (ppm)

3g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7.763
7.760
7.742
7.739
7.718
7.698
7.677
7.260
2.951
liujie-3-62
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7.841
7.823
7.804
7.803
7.777
7.763
7.760
7.742
7.739
7.718
7.698
7.677
1.00
2.99
N
O
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0.98
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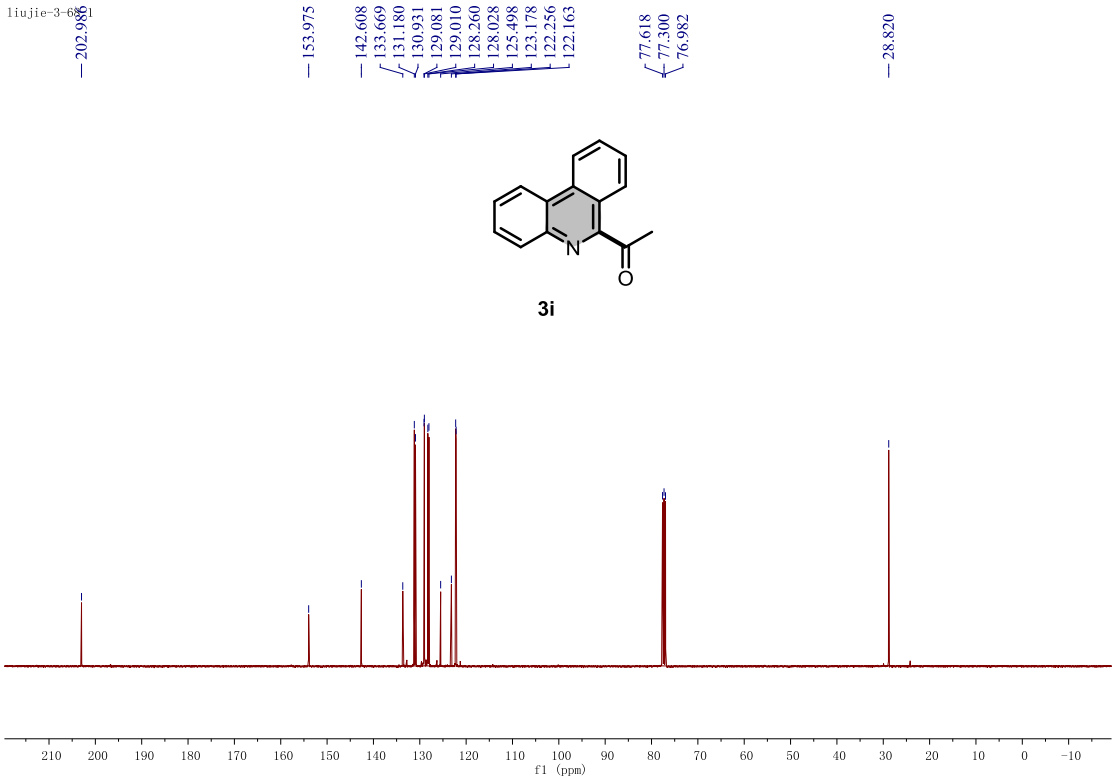
1.00
2.99
3.00
f1 (ppm)

3i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129.010
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122.256
122.163
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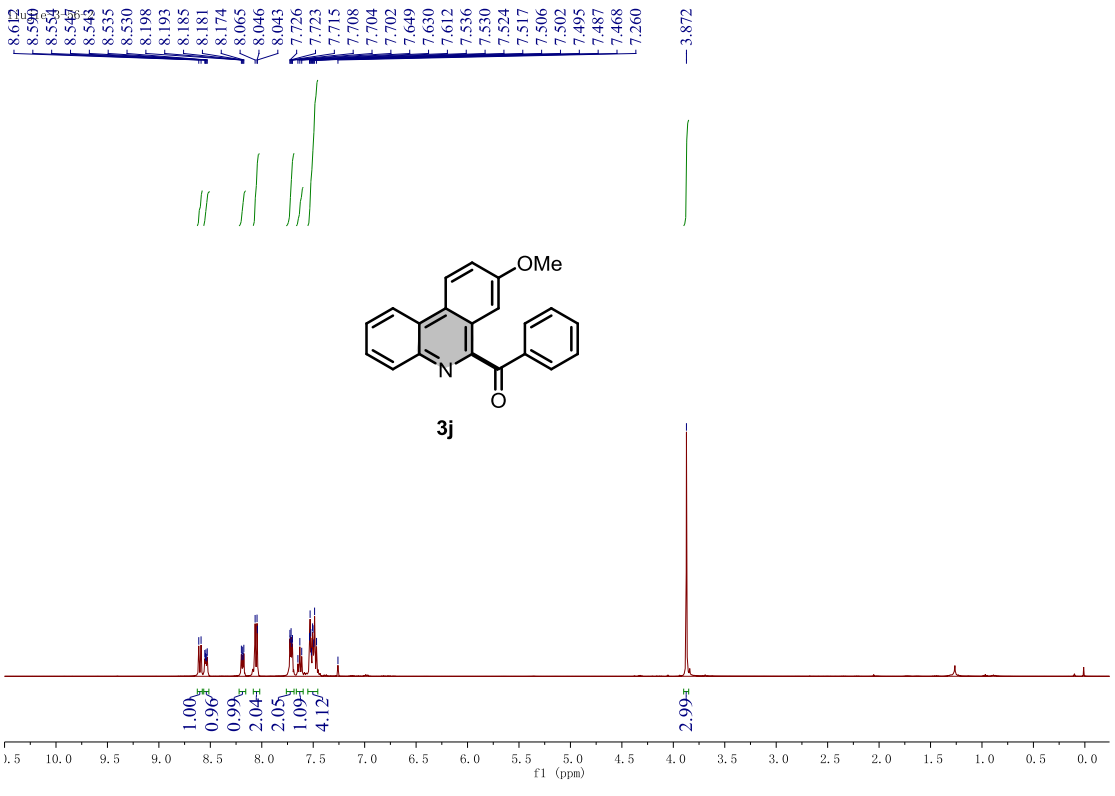
77.300
76.982
28.820
N
O
f1 (ppm)

3i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8.535
8.530
8.198
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8.181
8.174
8.065
8.046
8.043
7.726
7.723
7.715
7.708
7.704
7.702
7.649
7.630
7.612
7.536
7.530
7.524
7.517
7.506
7.502
7.495
7.487
7.468
7.260
3.872
OMe
N
O
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0.96
0.99
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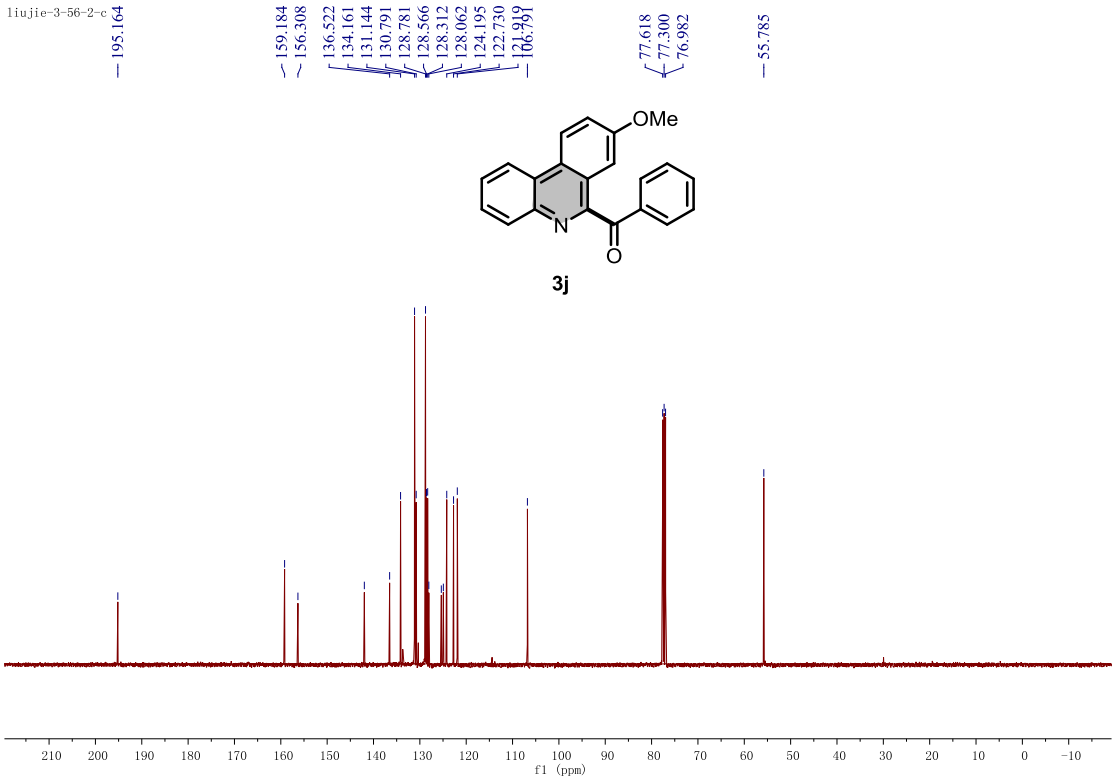
2.05
1.09
4.12
2.99
f1 (ppm)

3j


liujie-3-56-2-c
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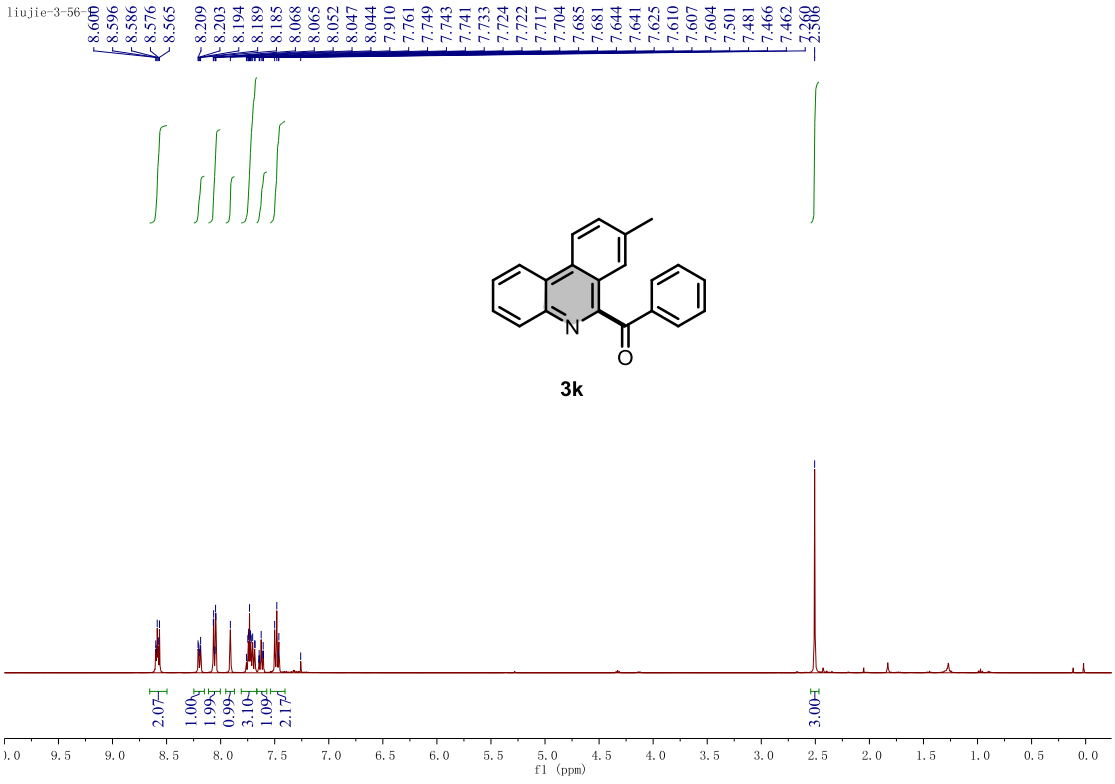
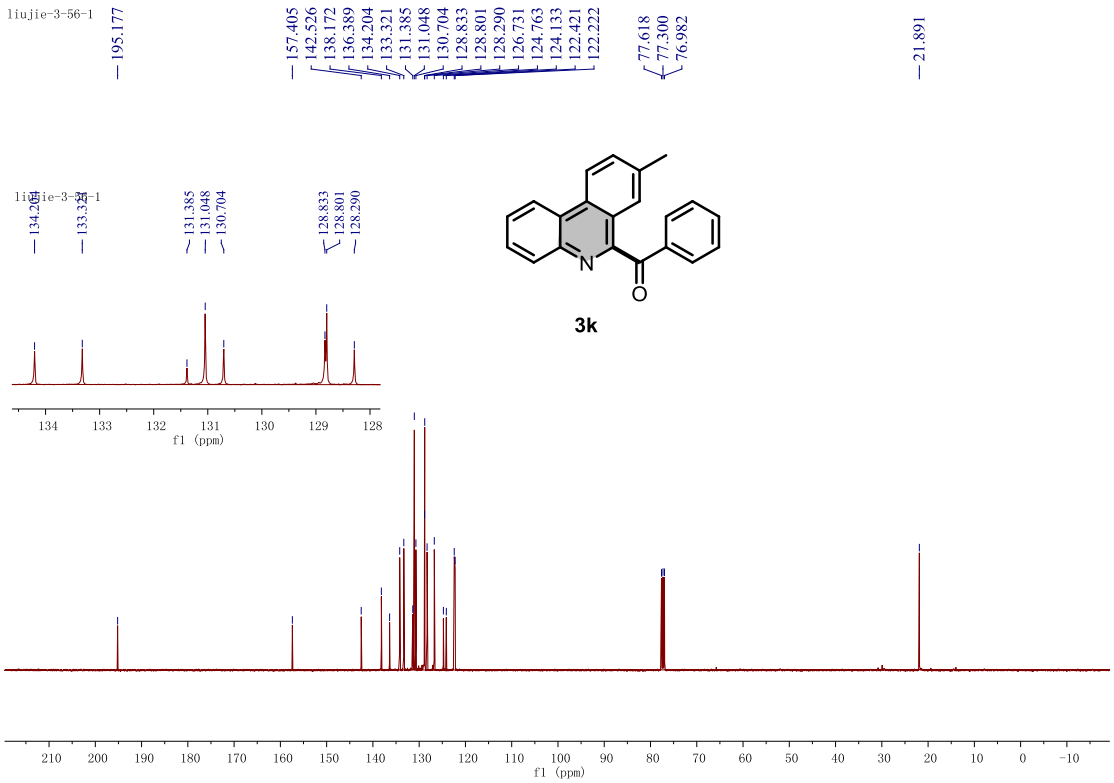
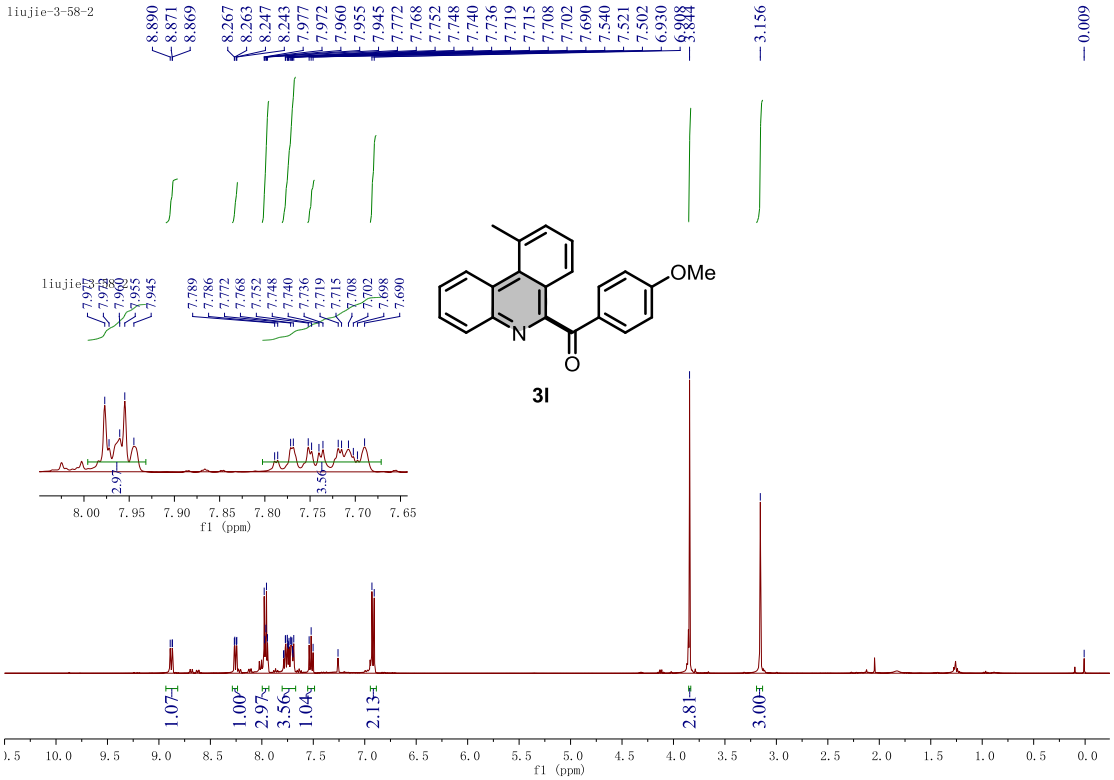
128.781
128.566
128.312
128.062
124.195
122.730
121.919
106.791
77.618
77.300
76.982
55.785
OMe
N
O
f1 (ppm)

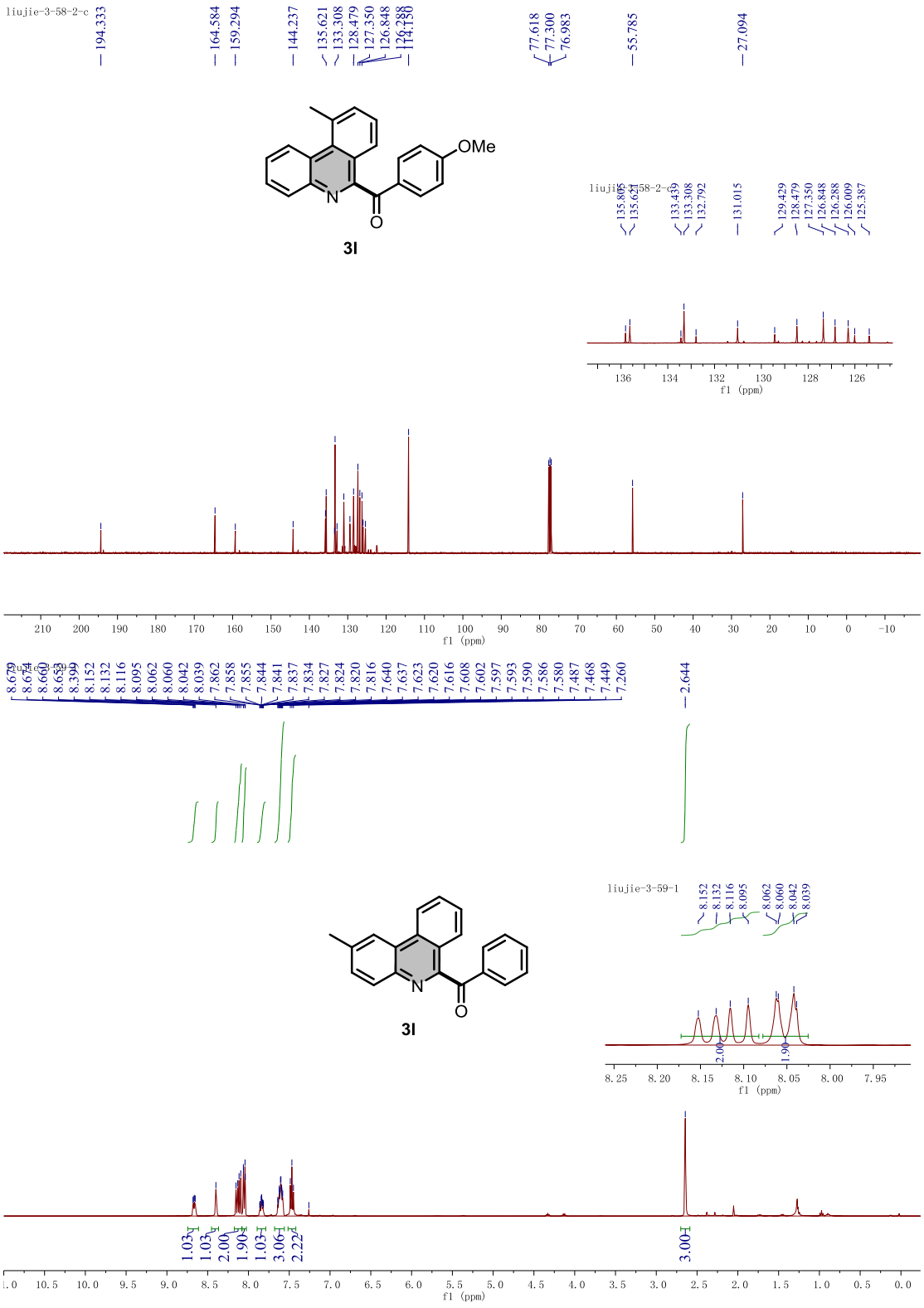
3j

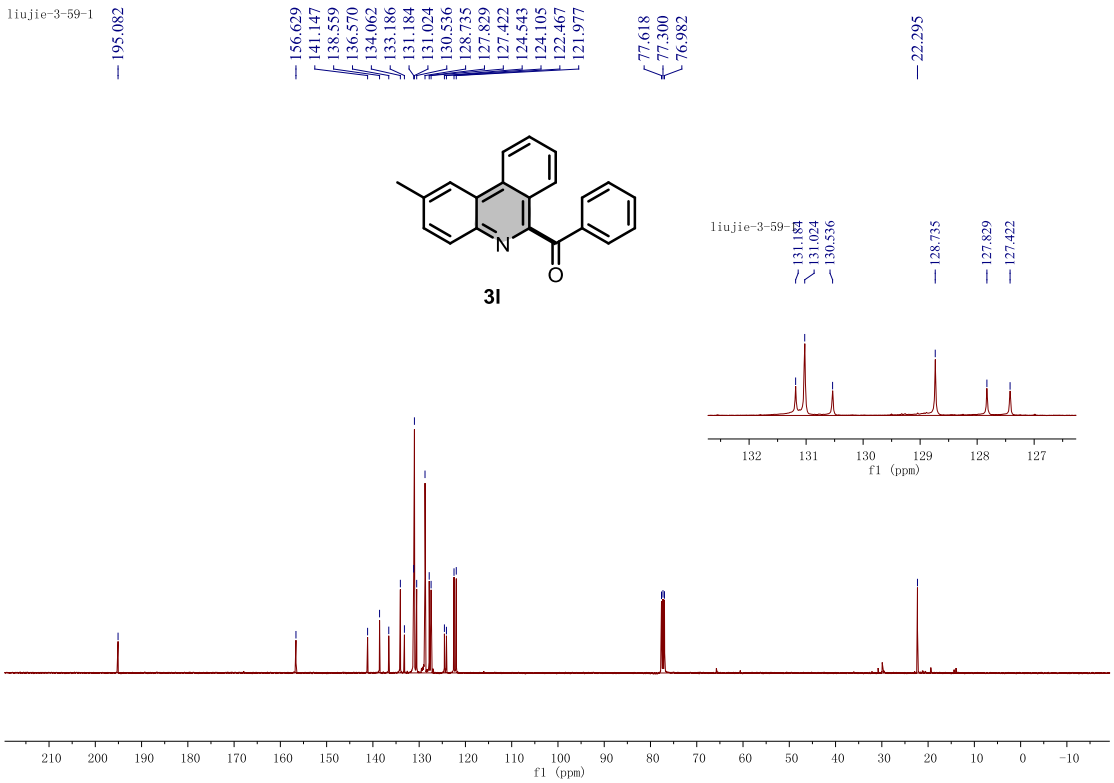

liujie-3-56-
8.600
8.596
8.586
8.576
8.565
8.209
8.203
8.194
8.189
8.185
8.068
8.065
8.052
8.047
8.044
7.910
7.761
7.749
7.743
7.741
7.733
7.724
7.722
7.717
7.704
7.685
7.681
7.644
7.641
7.625
7.610
7.607
7.604
7.501
7.481
7.466
7.462
2.506
N
O
2.07
1.00
1.99
0.99
3.10
1.09
2.17
3.00
f1 (ppm)

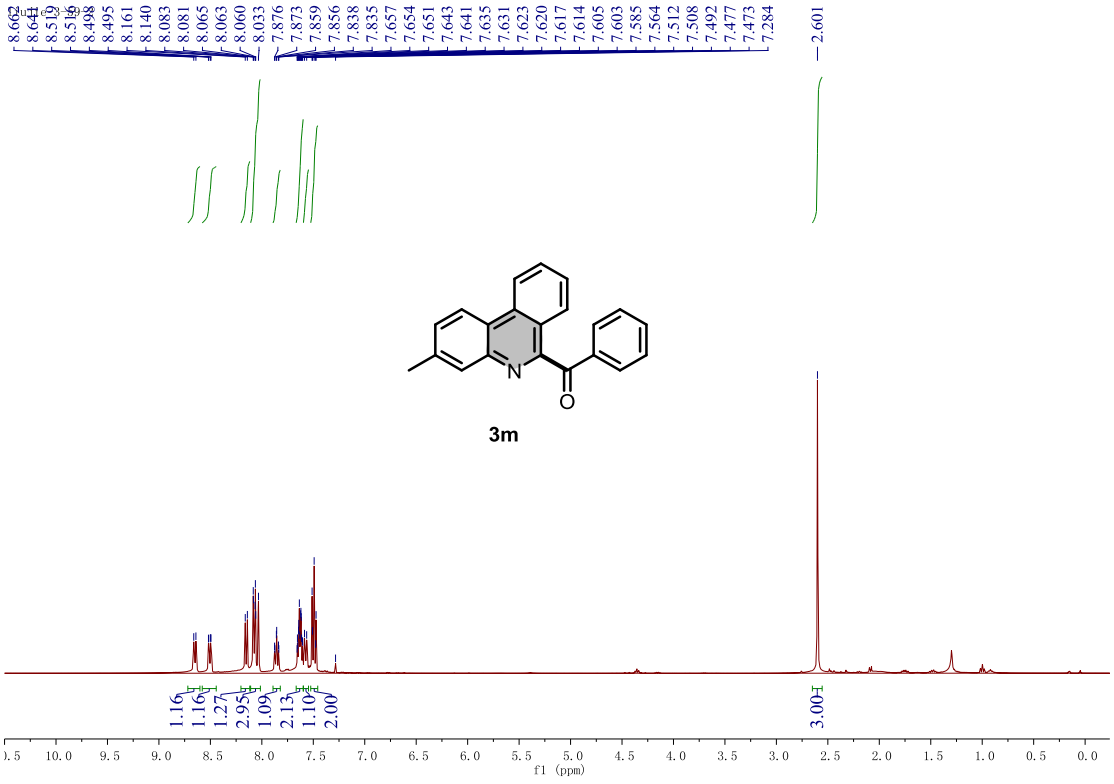
3k

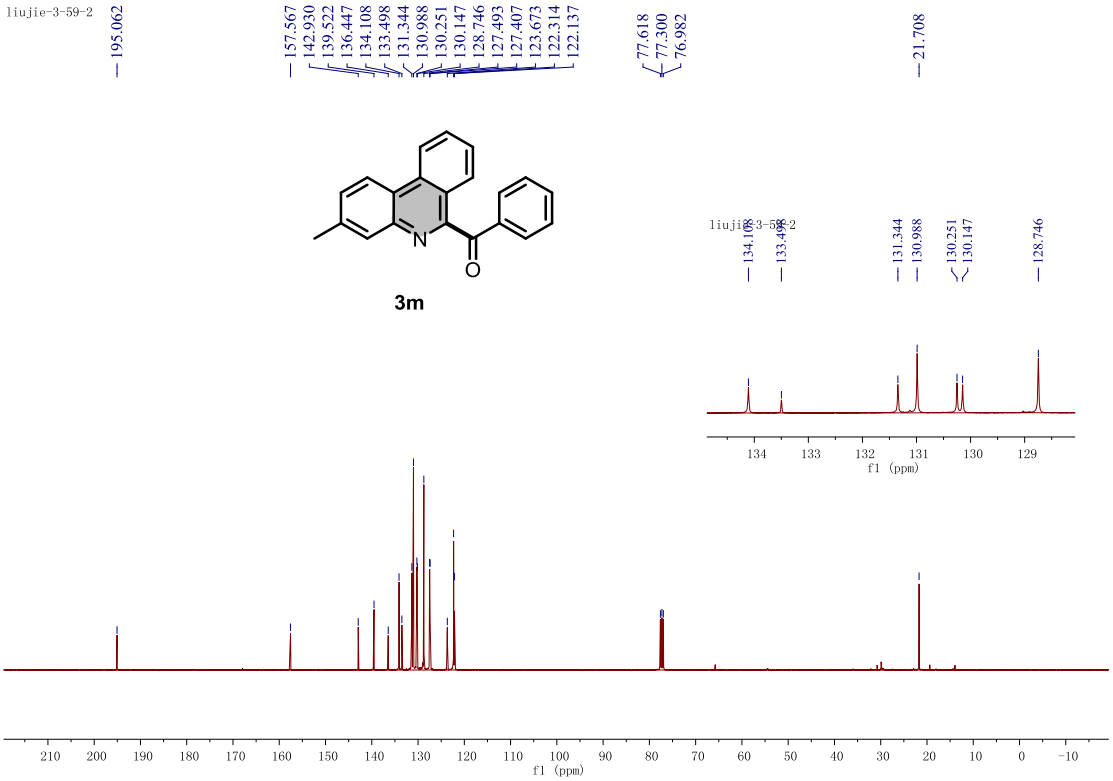

liujie-3-56-1
195.177
157.405
142.526
138.172
136.389
134.204
133.321
131.385
131.048
130.704
128.833
128.801
128.290
126.731
124.763
124.133
122.421
122.222
77.618
77.300
76.982
21.891
3k
f1 (ppm)

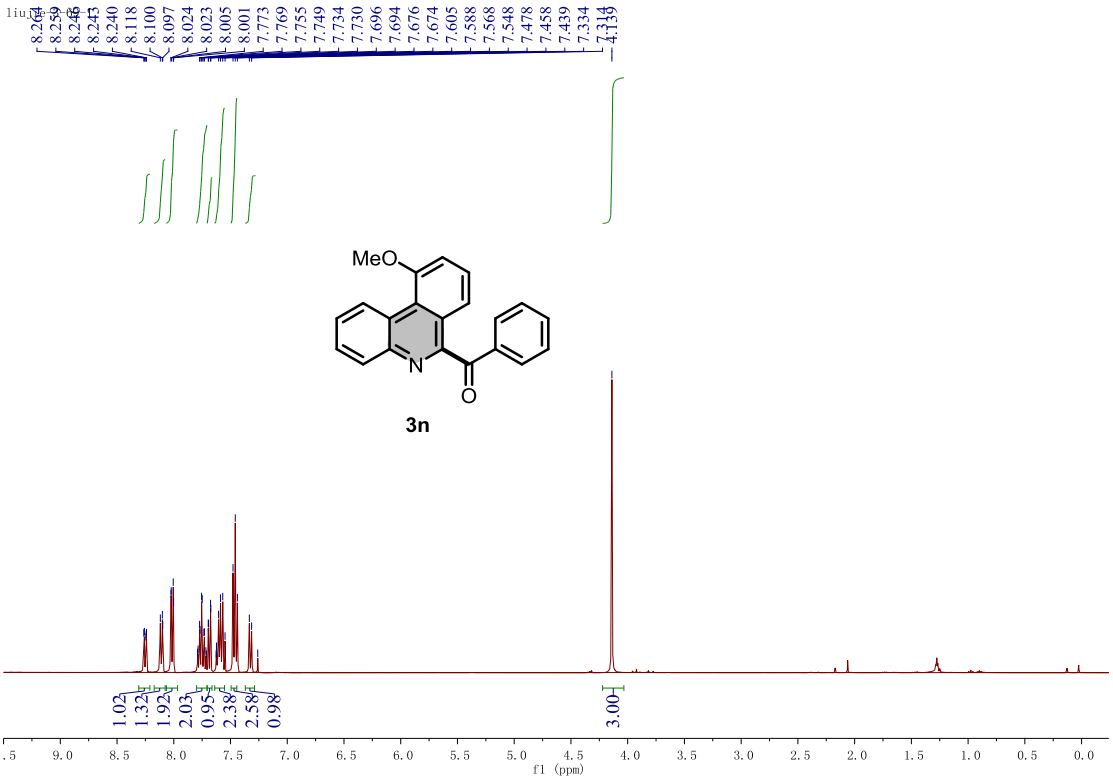

liujie-3-58-2
8.890
8.871
8.869
8.267
8.263
8.247
8.243
7.977
7.972
7.960
7.955
7.945
7.772
7.768
7.752
7.748
7.740
7.736
7.719
7.715
7.708
7.702
7.690
7.540
7.521
7.502
6.930
6.908
3.844
3.156
0.009
OMe
3l
1.07
1.00
2.97
3.56
1.04
2.13
2.81
3.00
f1 (ppm)

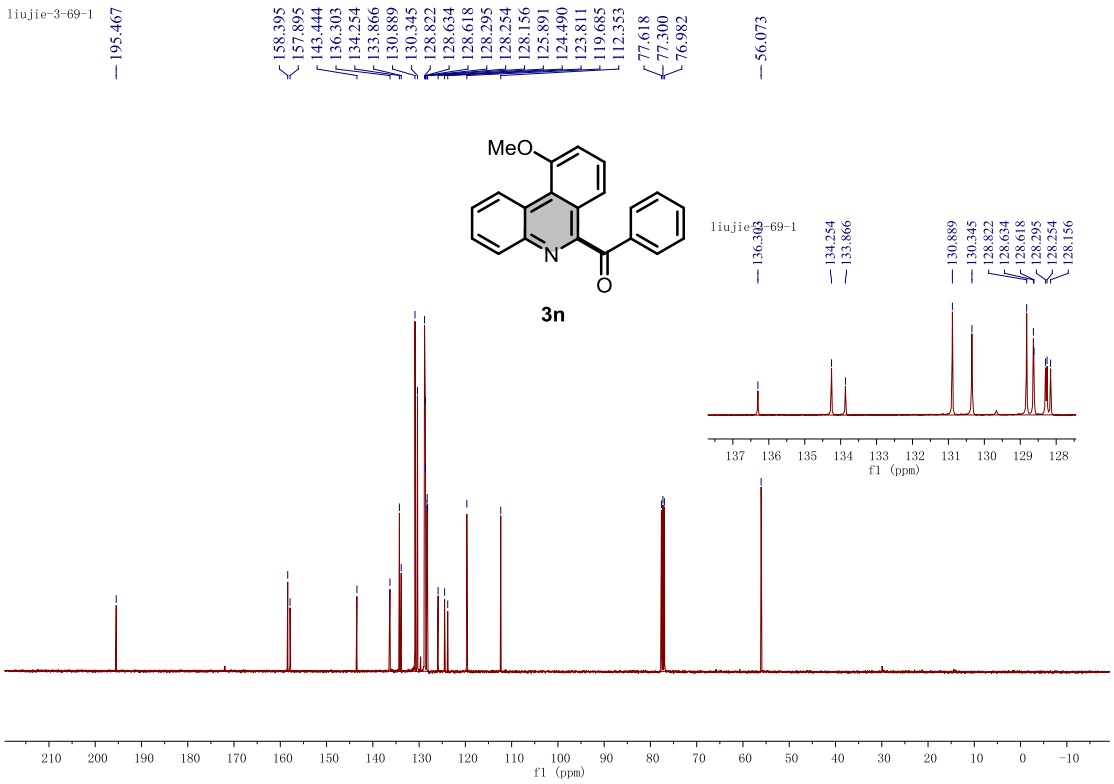

liujie-3-58-2-c
194.333
164.584
159.294
144.237
135.621
133.308
128.479
127.350
126.848
126.288
114.130
77.618
77.300
76.983
55.785
27.094
OMe
N
O
3l
liujie-3-58-2-c
135.805
135.621
133.439
133.308
132.792
131.015
129.429
128.479
127.350
126.848
126.288
126.009
125.387
f1 (ppm)
8.679
8.674
8.660
8.653
8.399
8.152
8.132
8.116
8.095
8.062
8.060
8.042
8.039
7.862
7.858
7.855
7.844
7.841
7.837
7.834
7.827
7.824
7.820
7.816
7.640
7.637
7.623
7.620
7.616
7.608
7.602
7.597
7.593
7.590
7.586
7.580
7.487
7.468
7.449
7.260
2.644
liujie-3-59-1
8.152
8.132
8.116
8.095
8.062
8.060
8.042
8.039
2.00
1.90
1.03
1.03
2.00
1.90
1.03
3.06
2.22
3.00
f1 (ppm)

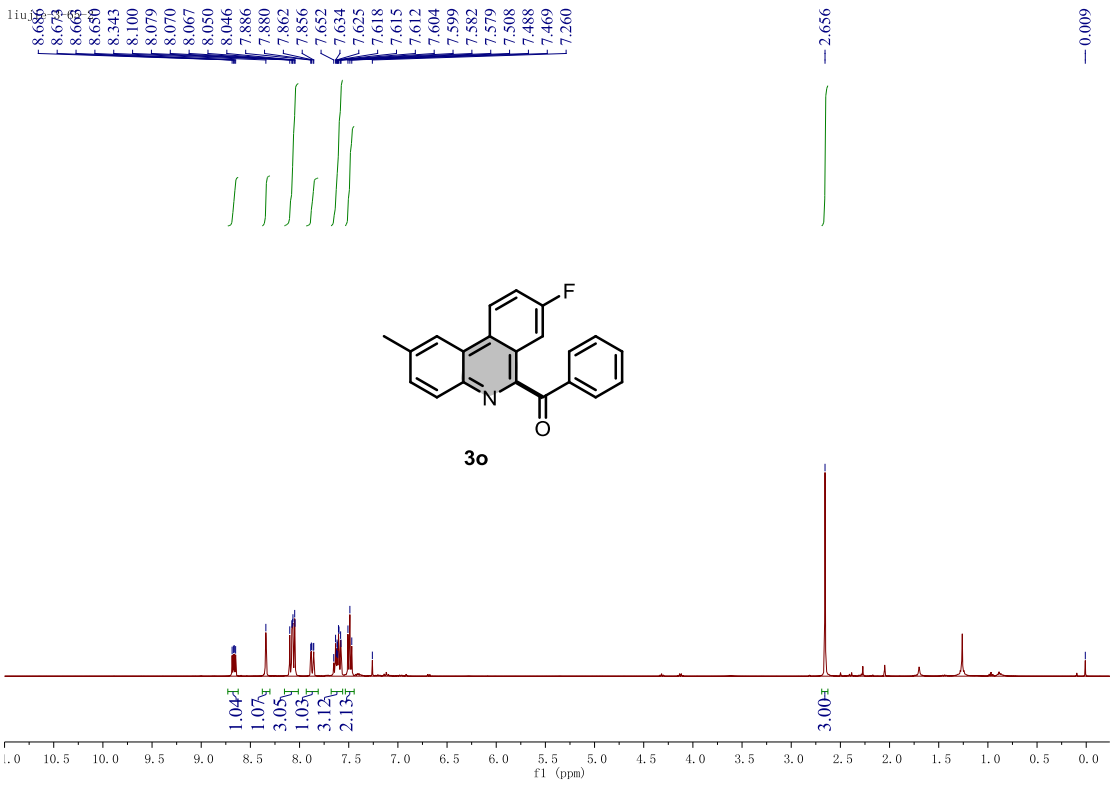

liujie-3-59-1
195.082
156.629
141.147
138.559
136.570
134.062
133.186
131.184
131.024
130.536
128.735
127.829
127.422
124.543
124.105
122.467
121.977
77.618
77.300
76.982
22.295
N
O
3l
liujie-3-59-
131.184
131.024
130.536
128.735
127.829
127.422
132
131
130
129
128
127
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

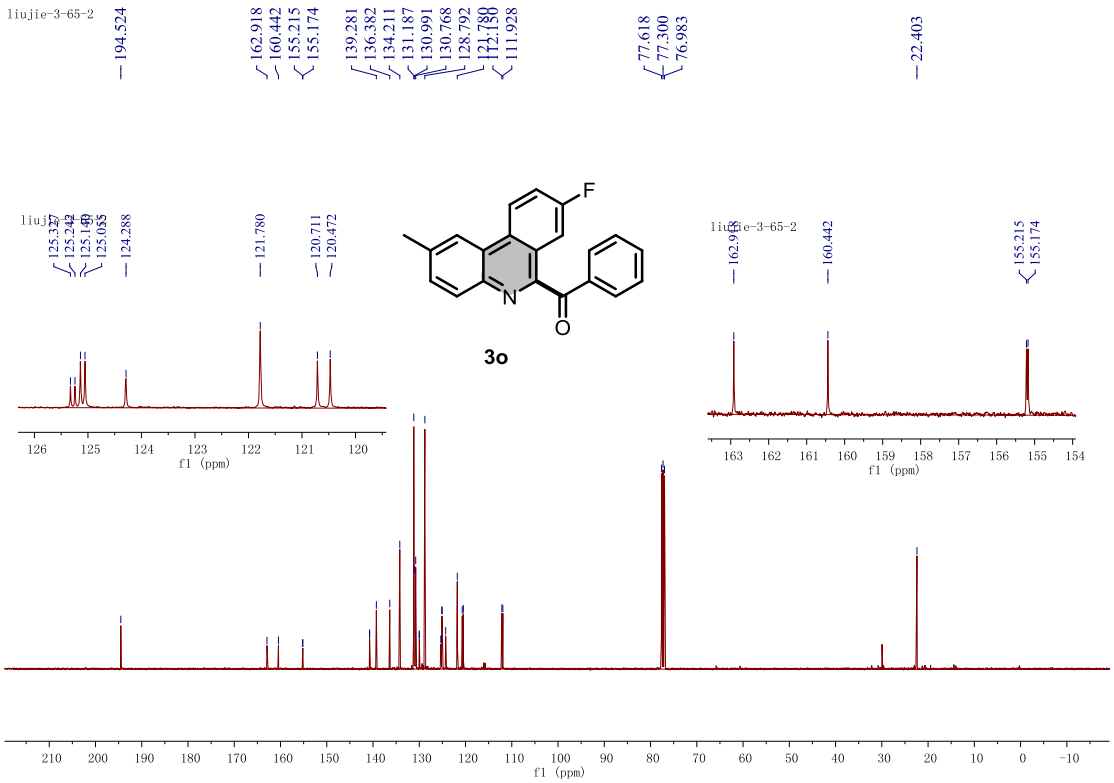

8.662
8.644
8.519
8.516
8.498
8.495
8.161
8.140
8.083
8.081
8.065
8.063
8.060
8.033
7.876
7.873
7.859
7.856
7.838
7.835
7.657
7.654
7.651
7.643
7.641
7.635
7.631
7.623
7.620
7.617
7.614
7.605
7.603
7.585
7.564
7.512
7.508
7.492
7.477
7.473
7.284
2.601
N
O
3m
1.16
1.16
1.27
2.95
1.09
2.13
1.10
2.00
3.00
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)

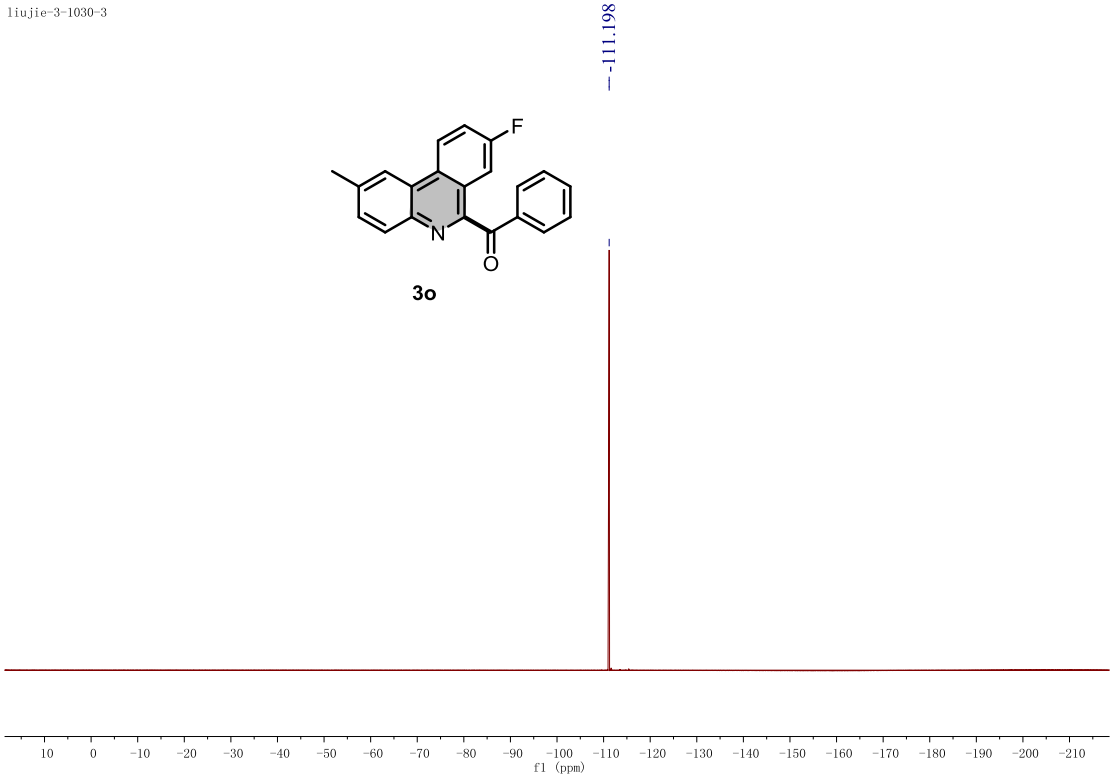

liujie-3-59-2
195.062
157.567
142.930
139.522
136.447
134.108
133.498
131.344
130.988
130.251
130.147
128.746
127.493
127.407
123.673
122.314
122.137
77.618
77.300
76.982
21.708
N
O
3m
liujie-3-59-2
134.108
133.498
131.344
130.988
130.251
130.147
128.746
134
133
132
131
130
129
f1 (ppm)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

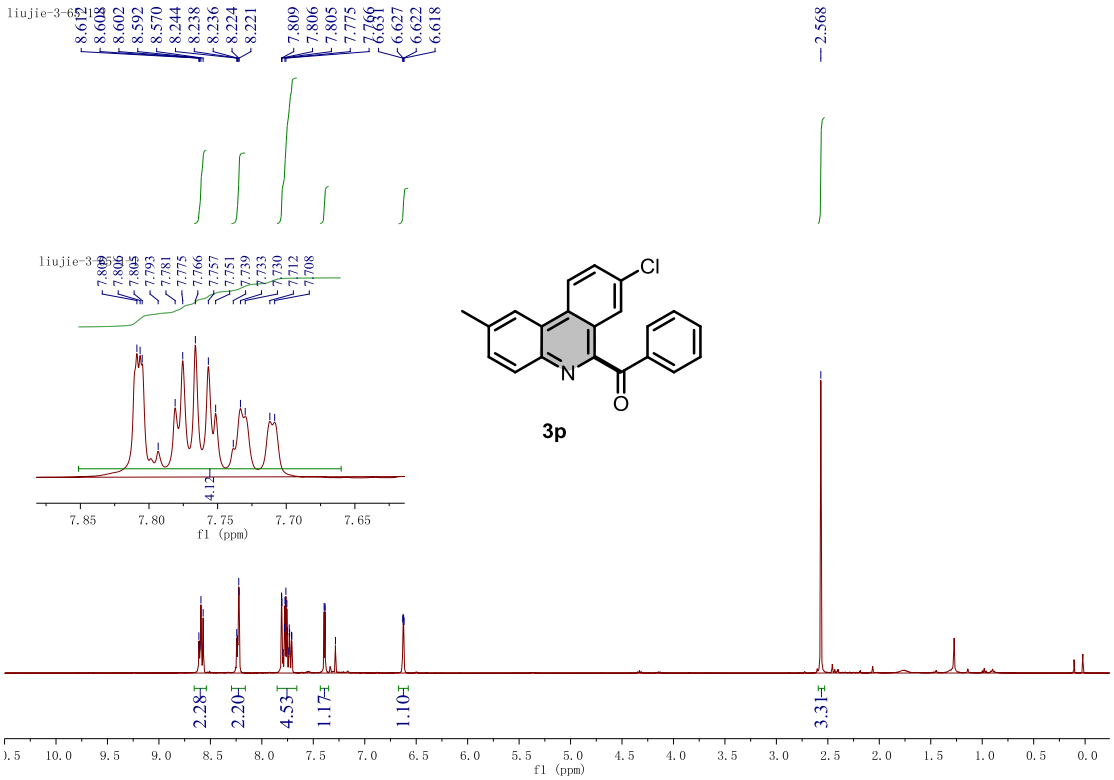

liujie-3-59-2
8.264
8.259
8.246
8.243
8.240
8.118
8.100
8.097
8.024
8.023
8.005
8.001
7.773
7.769
7.755
7.749
7.734
7.730
7.696
7.694
7.676
7.674
7.605
7.588
7.568
7.548
7.478
7.458
7.439
7.334
7.314
4.139
MeO
N
O
3n
1.02
1.32
1.92
2.03
0.95
2.38
2.58
0.98
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

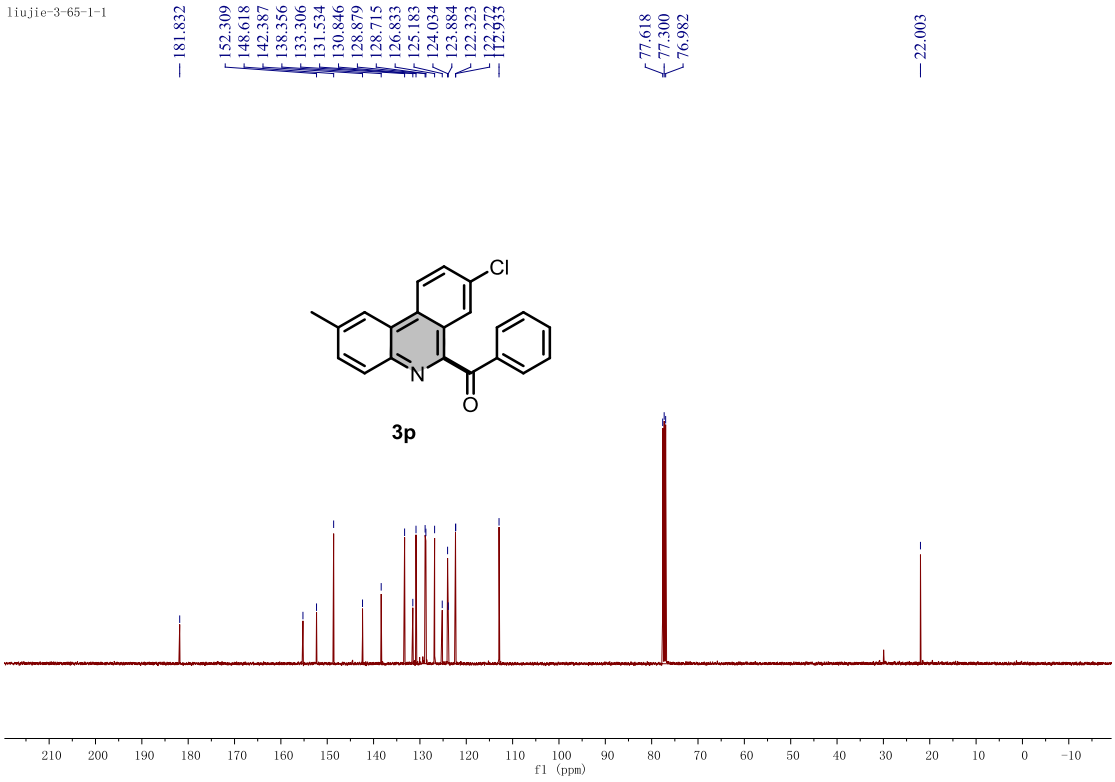

liujie-3-69-1
195.467
158.395
157.895
143.444
136.303
134.254
133.866
130.889
130.345
128.822
128.634
128.618
128.295
128.254
128.156
125.891
124.490
123.811
119.685
112.353
77.618
77.300
76.982
56.073
MeO
N
O
3n
f1 (ppm)

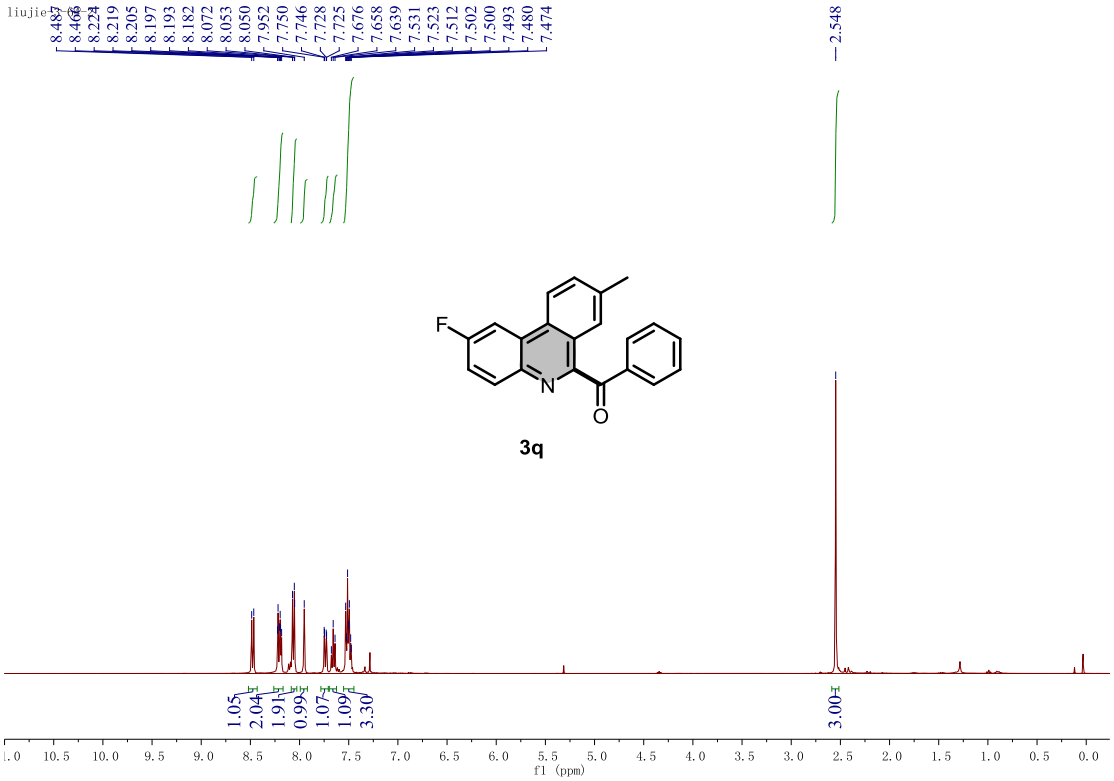

8.685
8.674
8.665
8.638
8.343
8.100
8.079
8.070
8.067
8.050
8.046
7.886
7.880
7.862
7.856
7.652
7.634
7.625
7.618
7.615
7.612
7.604
7.599
7.582
7.579
7.508
7.488
7.469
7.260
2.656
0.009
F
N
O
3o
1.04
1.07
3.05
1.03
3.12
2.13
3.00
f1 (ppm)

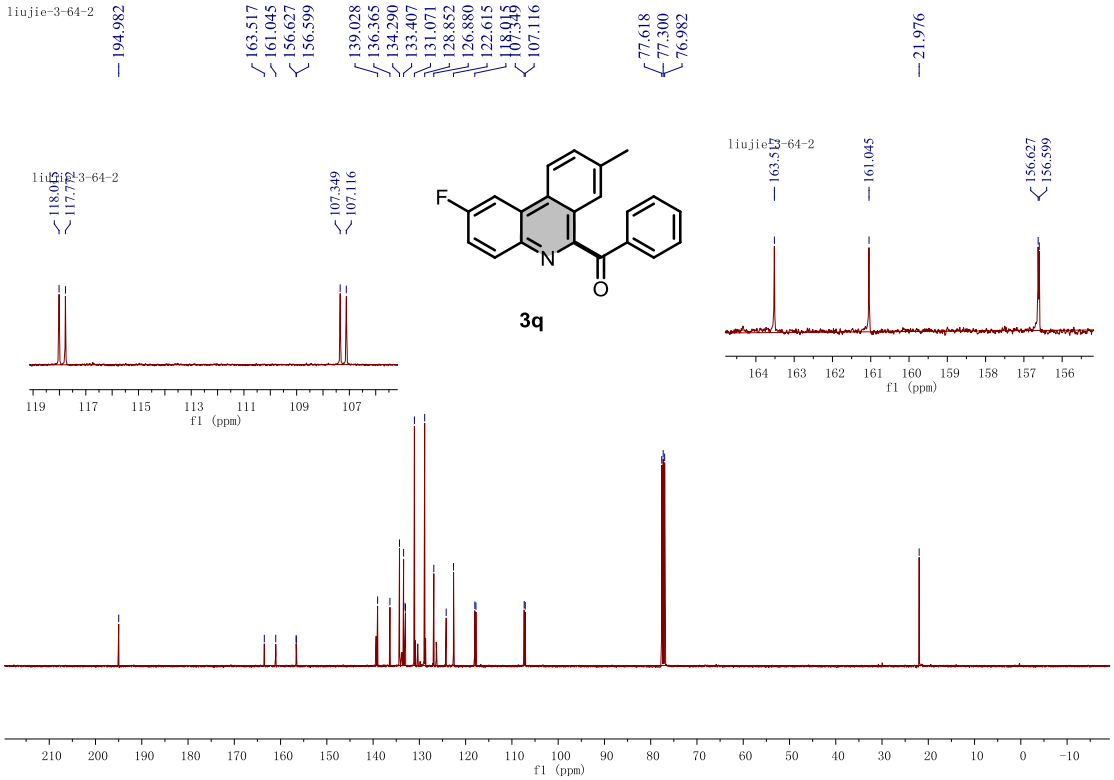

liujie-3-65-2
194.524
162.918
160.442
155.215
155.174
139.281
136.382
134.211
131.187
130.991
130.768
128.792
121.780
112.150
111.928
77.618
77.300
76.983
22.403
F
N
O
3o
f1 (ppm)

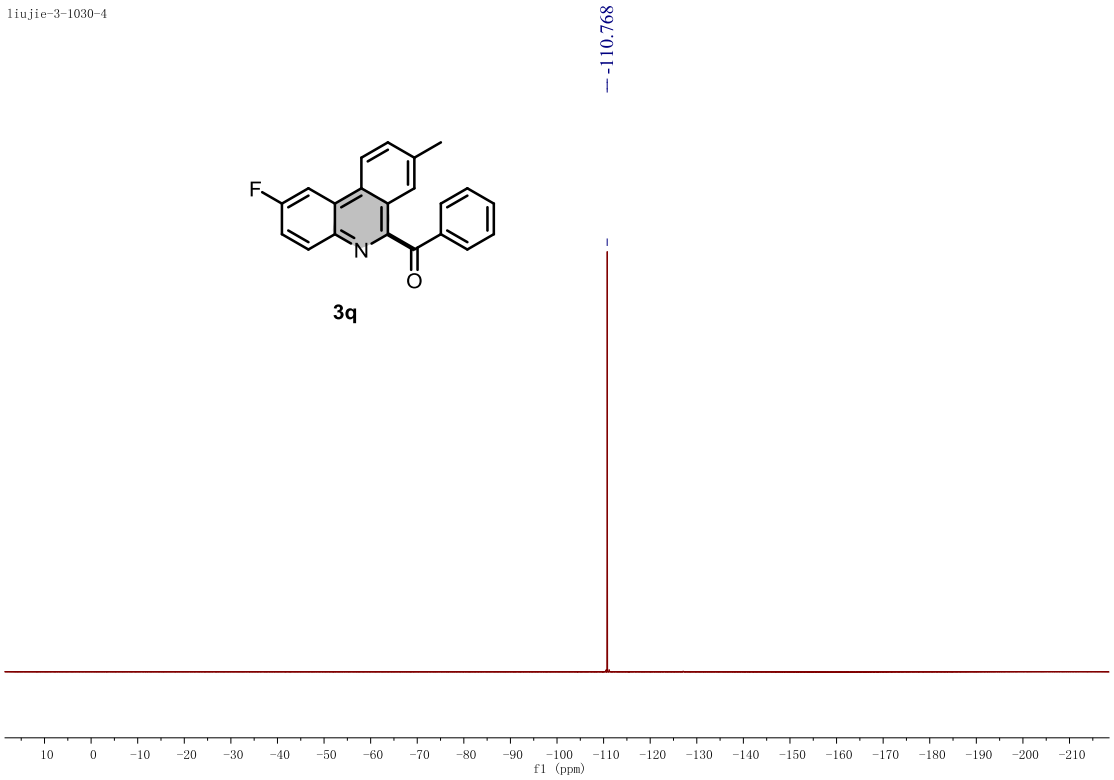

liujie-3-1030-3
-111.198
F
N
O
3o
f1 (ppm)


8.612
8.608
8.602
8.592
8.570
8.244
8.238
8.236
8.224
8.221
7.809
7.806
7.805
7.775
7.766
6.631
6.627
6.622
6.618
2.568
Cl
N
O
3p
2.28
2.20
4.53
1.17
1.10
3.31
f1 (ppm)

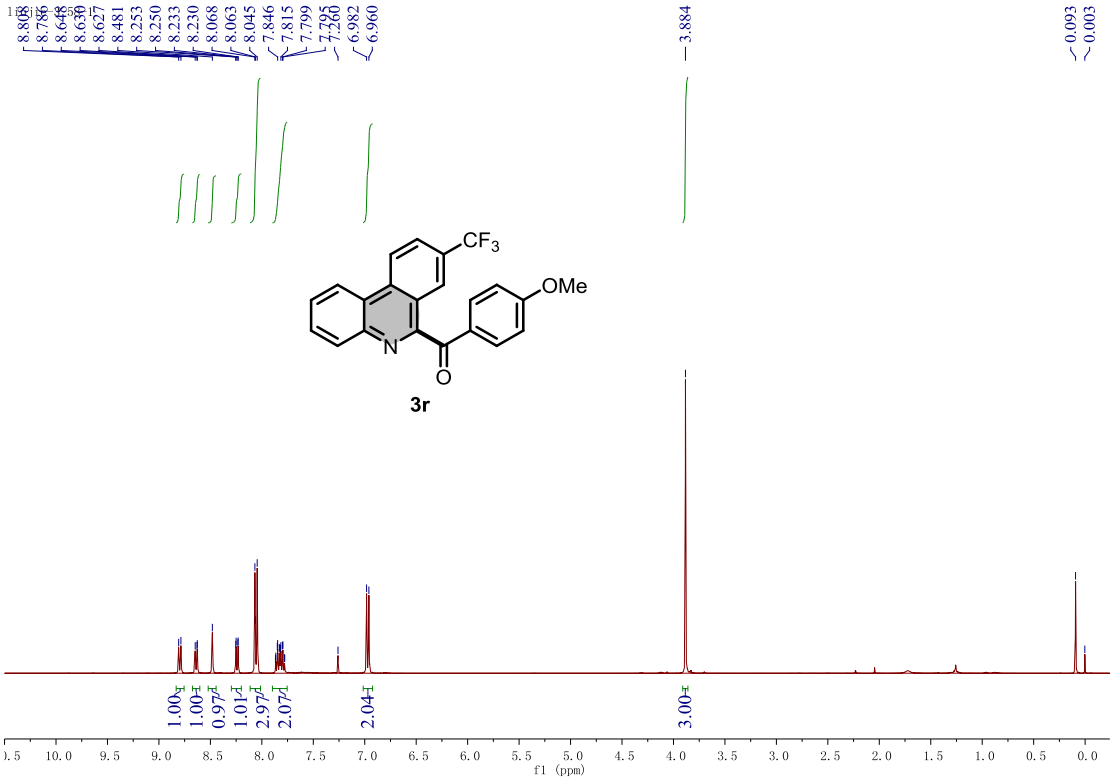

liujie-3-65-1-1
181.832
152.309
148.618
142.387
138.356
133.306
131.534
130.846
128.879
128.715
126.833
125.183
124.034
123.884
122.323
122.272
112.933
77.618
77.300
76.982
22.003
Cl
N
O
3p
f1 (ppm)


liujie-3-64
8.487
8.468
8.224
8.219
8.205
8.197
8.193
8.182
8.072
8.053
8.050
7.952
7.750
7.746
7.728
7.725
7.676
7.658
7.639
7.531
7.523
7.512
7.502
7.500
7.493
7.480
7.474
2.548
F
N
O
3q
1.05
2.04
1.91
0.99
1.07
1.09
3.30
3.00
f1 (ppm)

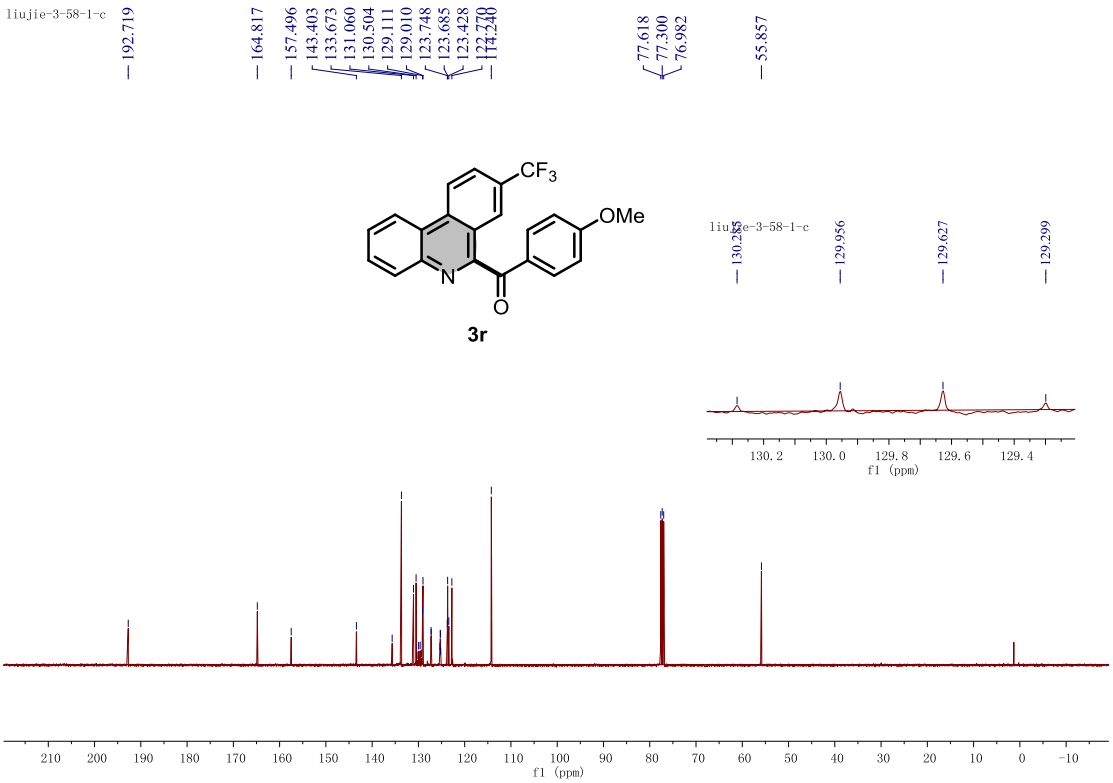

liujie-3-64-2
194.982
163.517
161.045
156.627
156.599
139.028
136.365
134.290
133.407
131.071
128.852
126.880
122.615
118.015
117.776
107.349
107.116
77.618
77.300
76.982
21.976
F
N
O
3q
f1 (ppm)

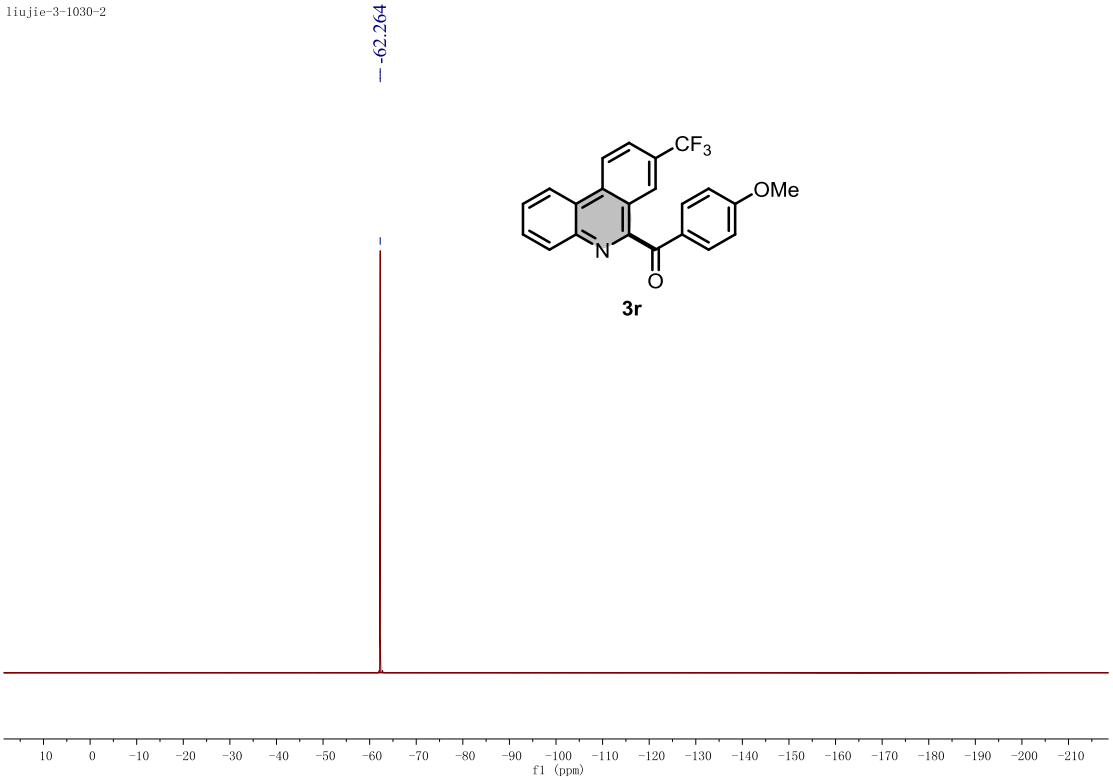

liujie-3-1030-4
-110.768
F
N
O
f1 (ppm)

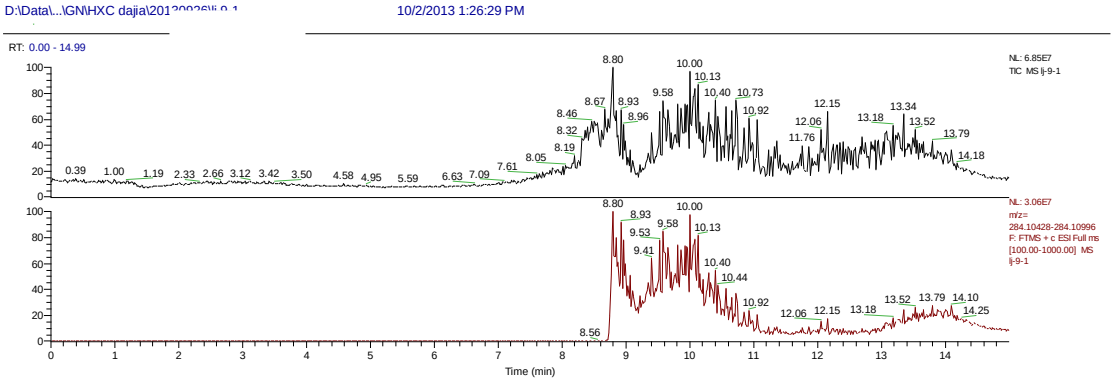
3q

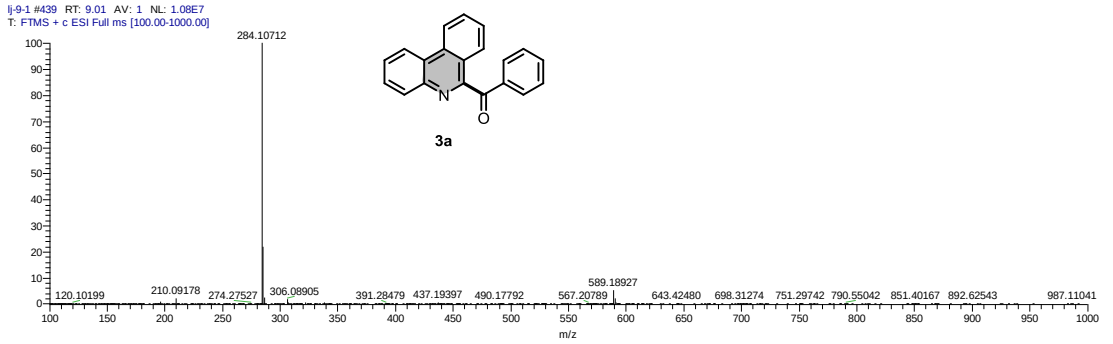

8.068
8.063
8.045
7.846
7.815
7.799
6.982
6.960
3.884
0.093
0.003
CF3
OMe
N
O
1.00
1.00
0.97
1.01
2.97
2.07
2.04
3.00
f1 (ppm)

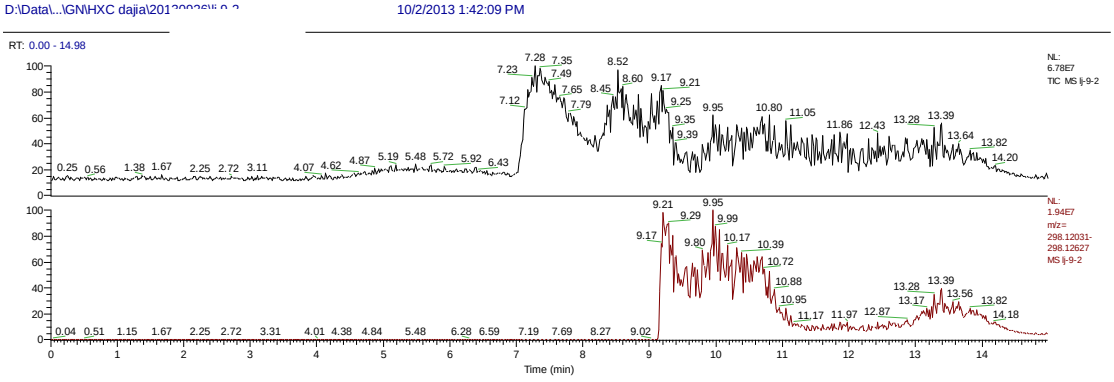
3r

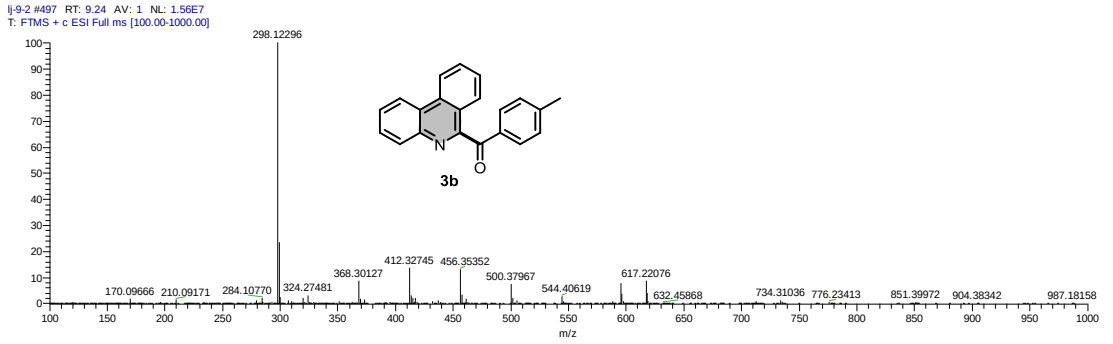

liujie-3-58-1-c
192.719
164.817
157.496
143.403
133.673
131.060
130.504
129.111
129.010
123.748
123.685
123.428
114.240
77.618
77.300
76.982
55.857
CF3
OMe
N
O
3r
liujie-3-58-1-c
130.285
129.956
129.627
129.299
130.2
130.0
129.8
129.6
129.4
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

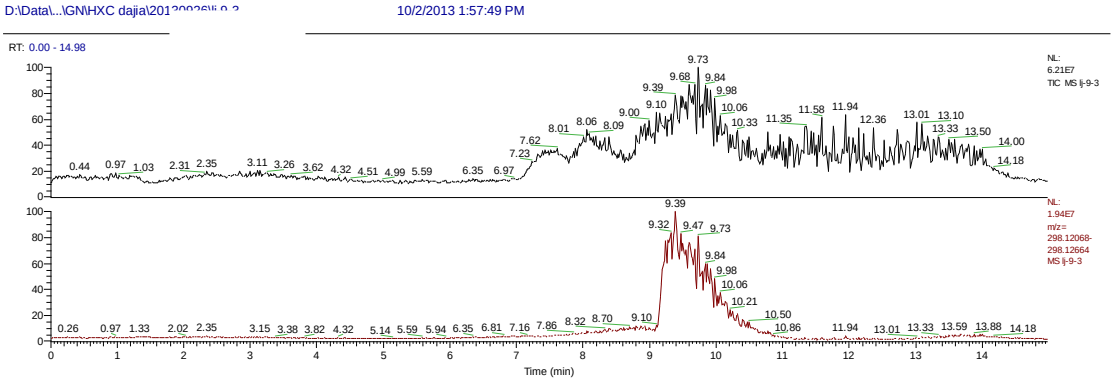

liujie-3-1030-2
-62.264
CF3
OMe
N
O
3r
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

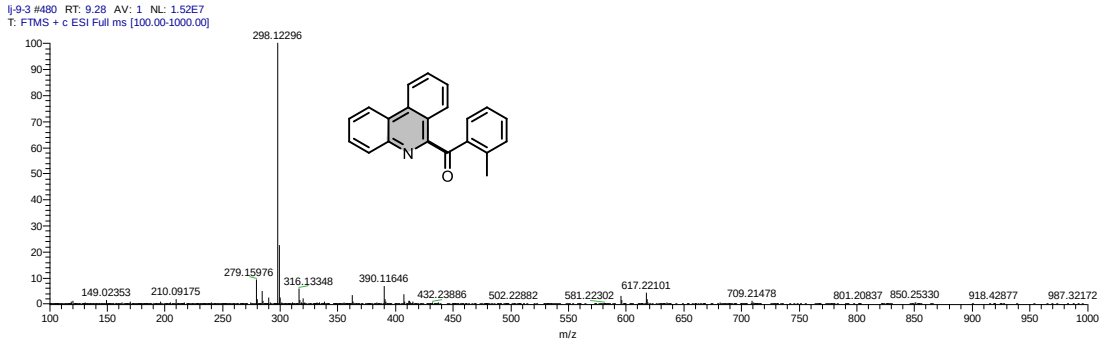

D:\Data\...\GNHXC dajia\2013
10/2/2013 1:26:29 PM
RT: 0.00 - 14.99
NL: 6.85E7
TIC MS lj-9-1
NL: 3.06E7
m/z= 284.10428-284.10996 F: FTMS + c ESI Full ms [100.00-1000.00] MS lj-9-1
Time (min)

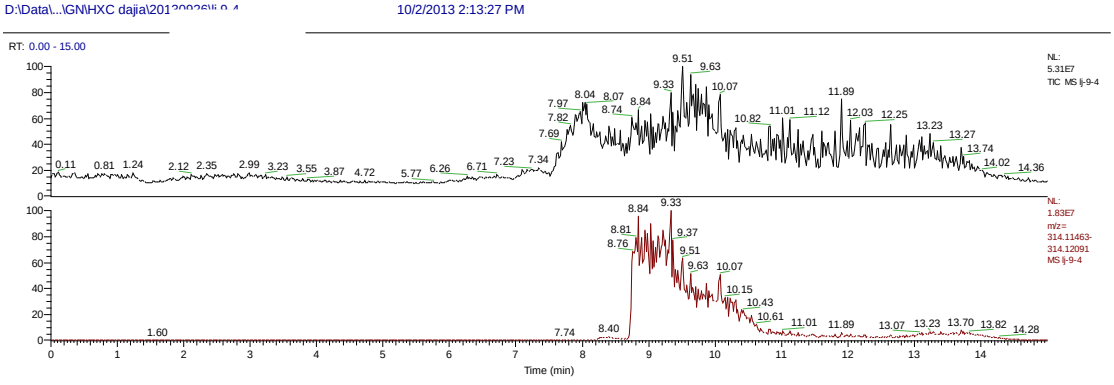

lj-9-1 #439 RT: 9.01 AV: 1 NL: 1.08E7
T: FTMS + c ESI Full ms [100.00-1000.00]
284.10712
3a
m/z

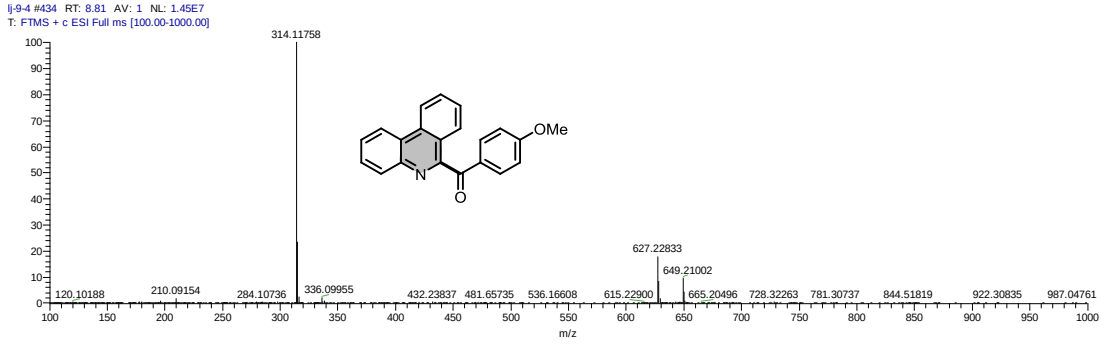

D:\Data\...\GNHXC dajia\2013
10/2/2013 1:42:09 PM
RT: 0.00 - 14.98
NL: 6.78E7
TIC MS lj-9-2
NL: 1.94E7
m/z= 298.12031-298.12627 MS lj-9-2
Time (min)

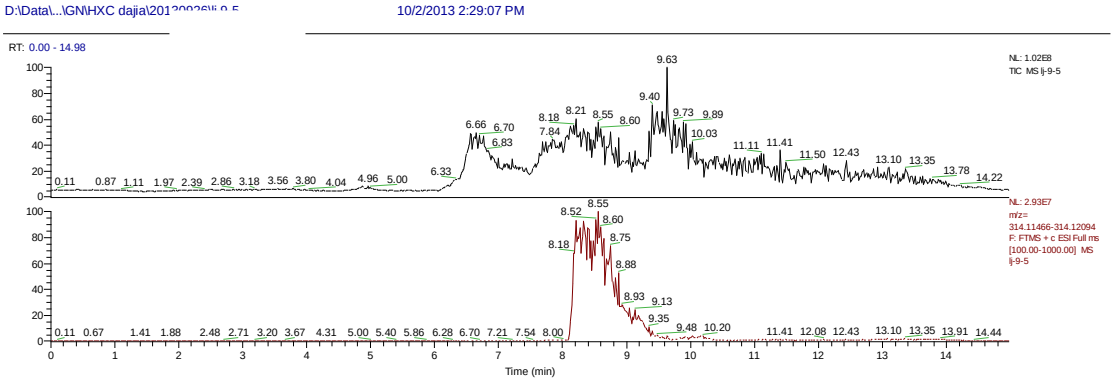

lj-9-2 #497 RT: 9.24 AV: 1 NL: 1.56E7
T: FTMS + c ESI Full ms [100.00-1000.00]
298.12296
3b
m/z

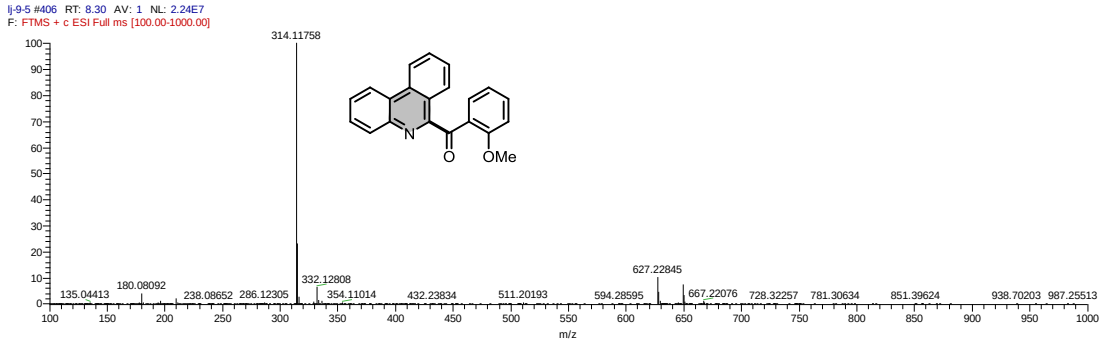

D:\Data\...\GN\HXC dajia\2013
10/2/2013 1:57:49 PM
RT: 0.00 - 14.98
NL: 6.21E7 TIC MS lj-9-3
NL: 1.94E7 m/z= 298.12068-298.12664 MS lj-9-3
Time (min)

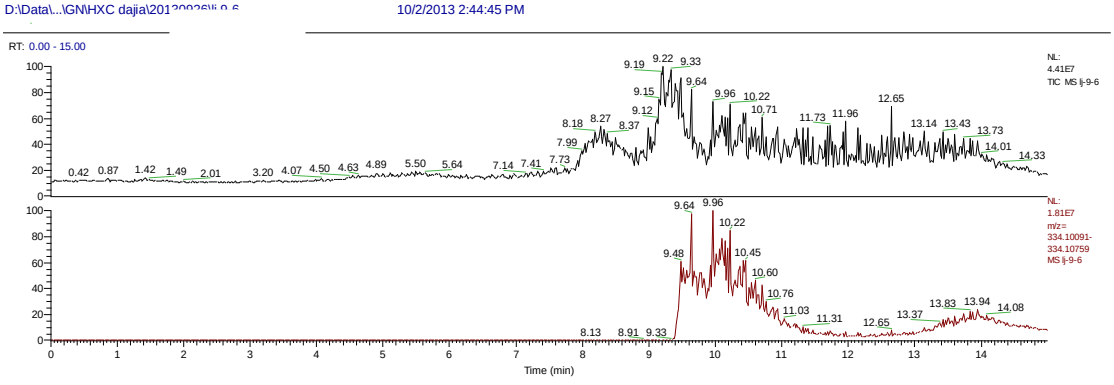

lj-9-3 #480 RT: 9.28 AV: 1 NL: 1.52E7
T: FTMS + c ESI Full ms [100.00-1000.00]
298.12296
279.15976
316.13348
390.11646
m/z

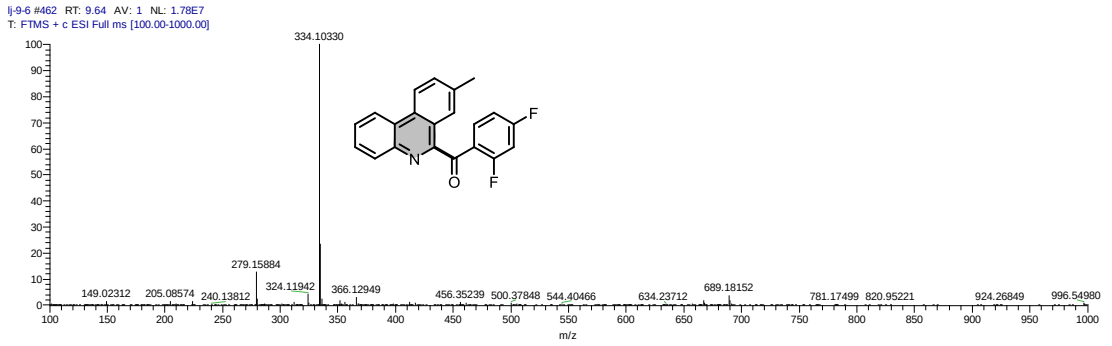

D:\Data\...\GN\HXC dajia\2013
10/2/2013 2:13:27 PM
RT: 0.00 - 15.00
NL: 5.31E7 TIC MS lj-9-4
NL: 1.83E7 m/z= 314.11463-314.12091 MS lj-9-4
Time (min)

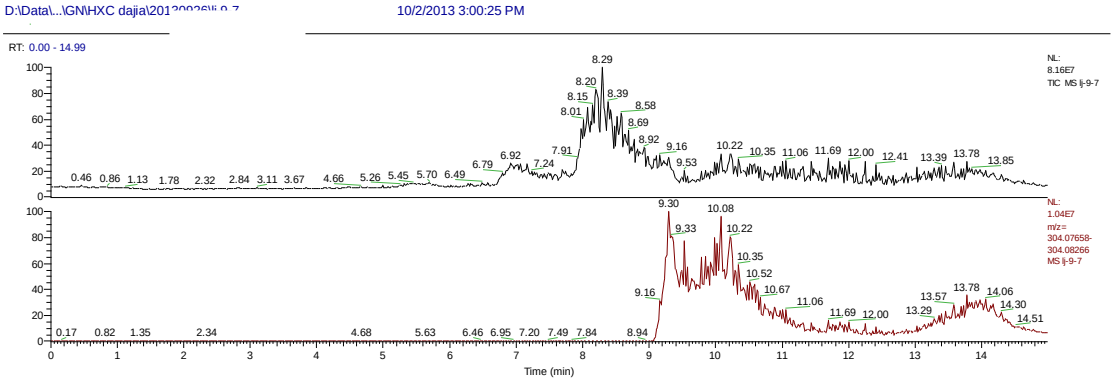

lj-9-4 #434 RT: 8.81 AV: 1 NL: 1.45E7
T: FTMS + c ESI Full ms [100.00-1000.00]
314.11758
627.22833
649.21002
m/z

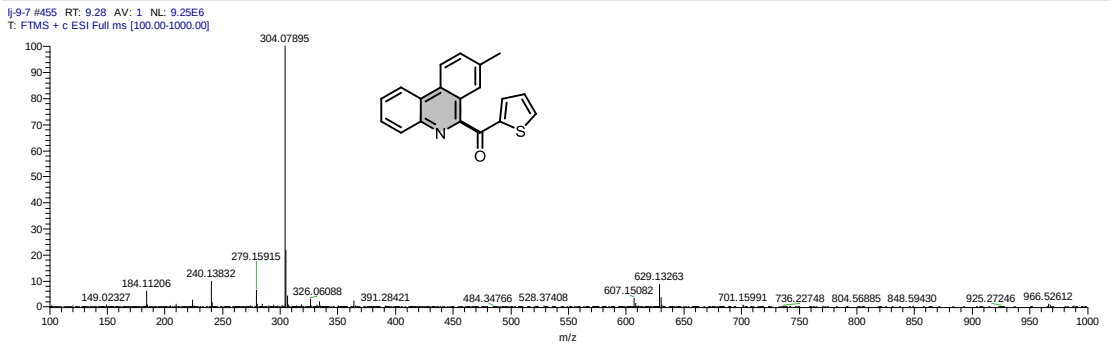

D:\Data\...\GN\HXC dajia\2013
10/2/2013 2:29:07 PM
RT: 0.00 - 14.98
NL: 1.02E8
TIC MS lj-9-5
NL: 2.93E7
m/z= 314.11466-314.12094 F: FTMS + c ESI Full ms [100.00-1000.00] MS lj-9-5
Time (min)

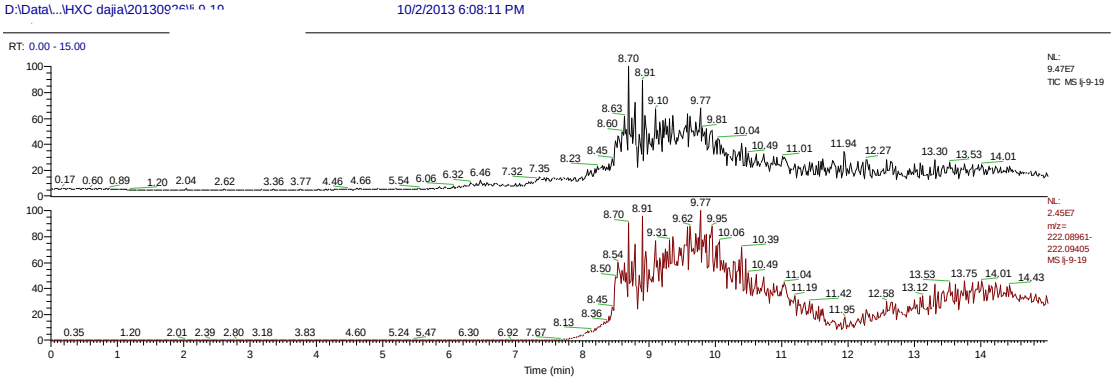

lj-9-5 #406 RT: 8.30 AV: 1 NL: 2.24E7
F: FTMS + c ESI Full ms [100.00-1000.00]
314.11758
O
OMe
m/z

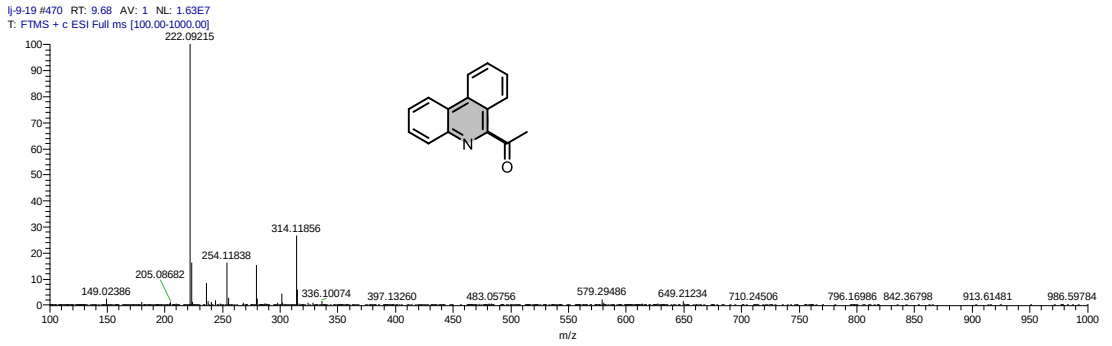

D:\Data\...\GN\HXC dajia\2013
10/2/2013 2:44:45 PM
RT: 0.00 - 15.00
NL: 4.41E7
TIC MS lj-9-6
NL: 1.81E7
m/z= 334.10091-334.10759 MS lj-9-6
Time (min)

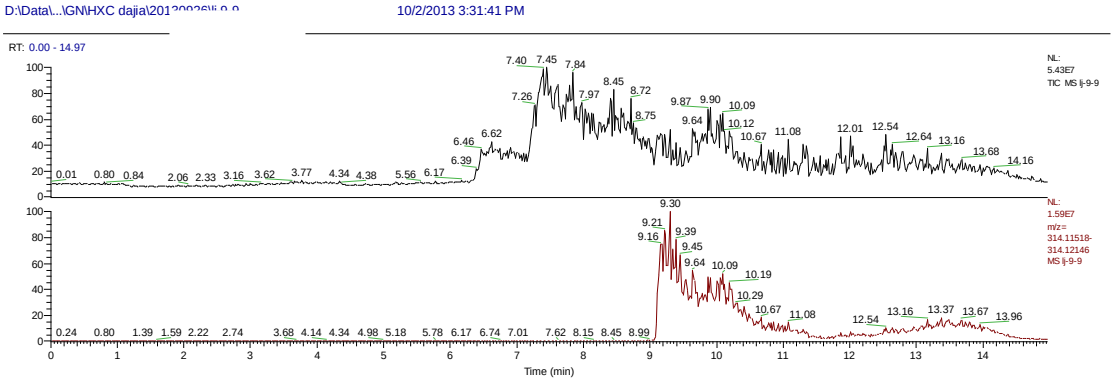

lj-9-6 #462 RT: 9.64 AV: 1 NL: 1.78E7
T: FTMS + c ESI Full ms [100.00-1000.00]
334.10330
F
O
F
m/z

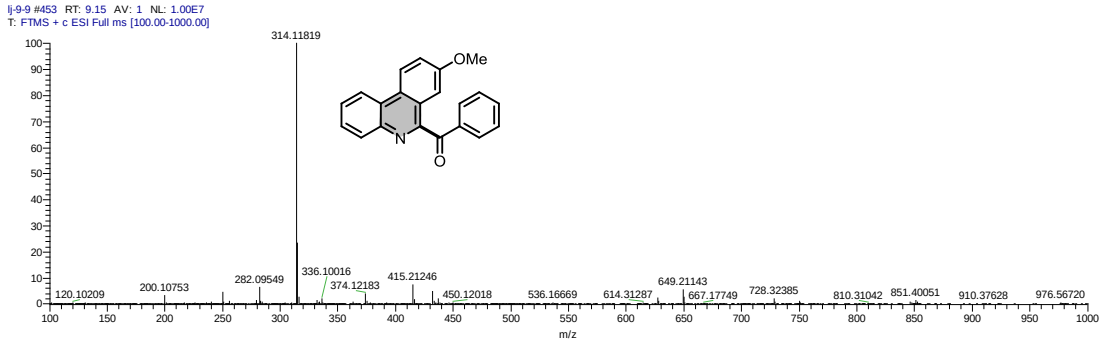

D:\Data\...\GN\HXC dajia\201
10/2/2013 3:00:25 PM
RT: 0.00 - 14.99
NL:
8.16E7
TIC MS lj-9-7
NL:
1.04E7
m/z=
304.07658-
304.08266
MS lj-9-7
Time (min)

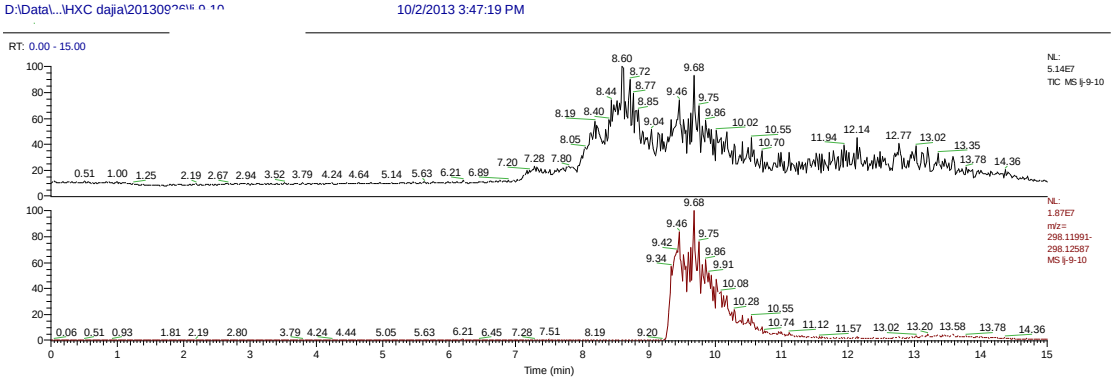

lj-9-7 #455 RT: 9.28 AV: 1 NL: 9.25E6
T: FTMS + c ESI Full ms [100.00-1000.00]
304.07895
279.15915
240.13832
184.11206
149.02327
326.06088
391.28421
484.34766
528.37408
607.15082
629.13263
m/z

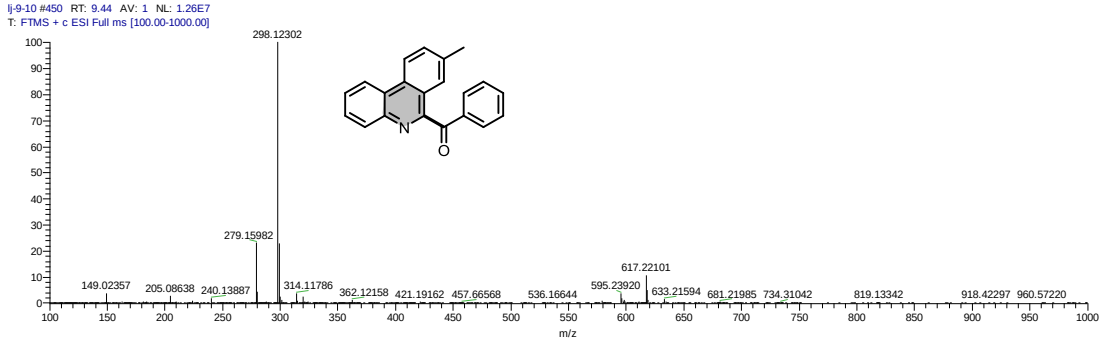

D:\Data\...\HXC dajia\201309
10/2/2013 6:08:11 PM
RT: 0.00 - 15.00
NL:
9.47E7
TIC MS lj-9-19
NL:
2.45E7
m/z=
222.08961-
222.09405
MS lj-9-19
Time (min)

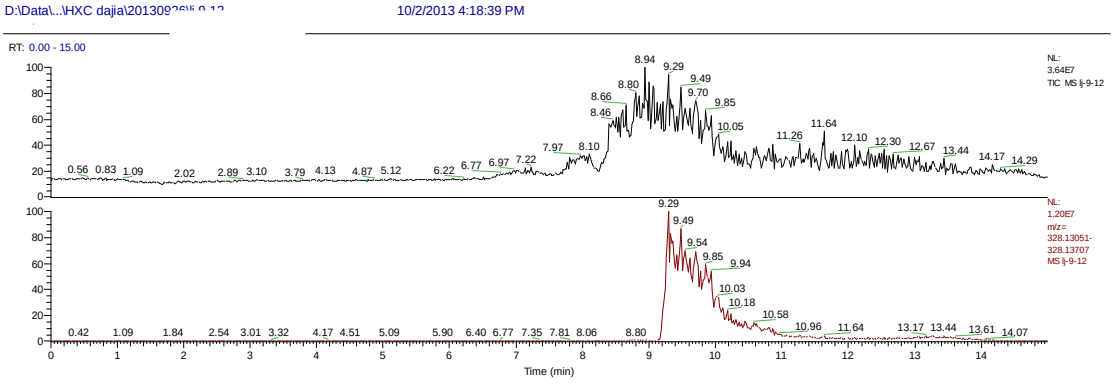

lj-9-19 #470 RT: 9.68 AV: 1 NL: 1.63E7
T: FTMS + c ESI Full ms [100.00-1000.00]
222.09215
314.11856
254.11838
205.08682
149.02386
336.10074
397.13260
483.05756
579.29486
649.21234
710.24506
796.16986
842.36798
913.61481
986.59784
m/z

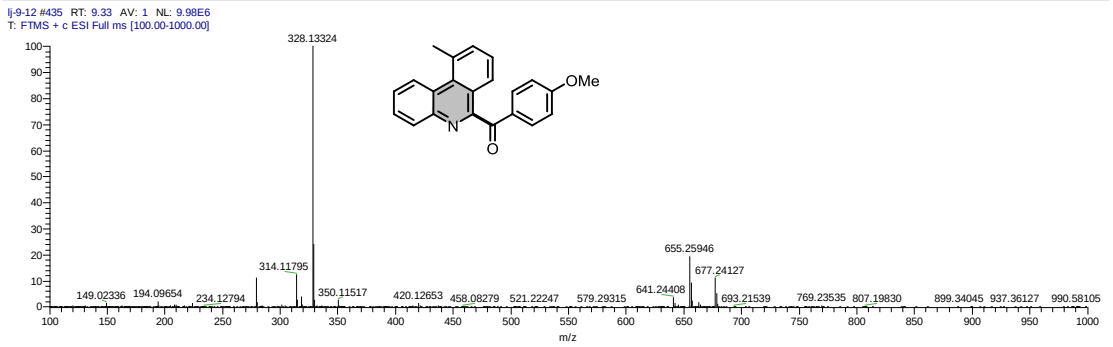

D:\Data\...\GN\HXC dajia\2013
10/2/2013 3:31:41 PM
RT: 0.00 - 14.97
NL: 5.43E7 TIC MS lj-9-9
NL: 1.59E7 m/z= 314.11518-314.12146 MS lj-9-9
Time (min)

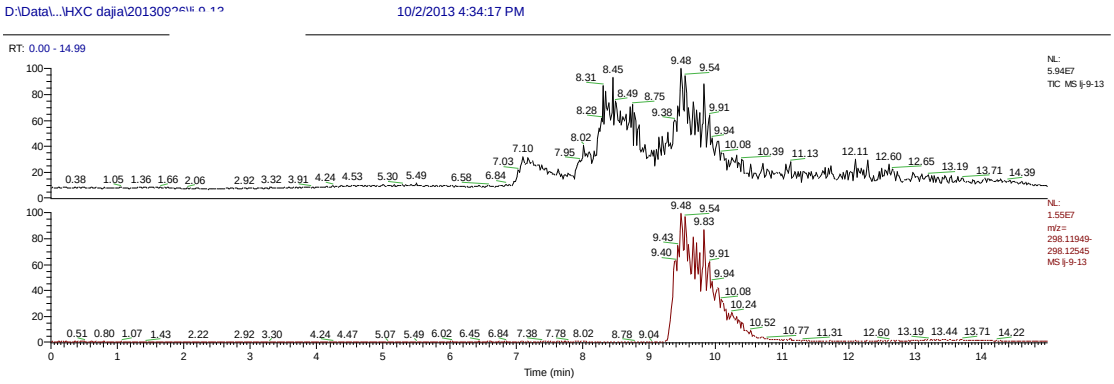

lj-9-9 #453 RT: 9.15 AV: 1 NL: 1.00E7
T: FTMS + c ESI Full ms [100.00-1000.00]
314.11819
OMe
N
O
m/z

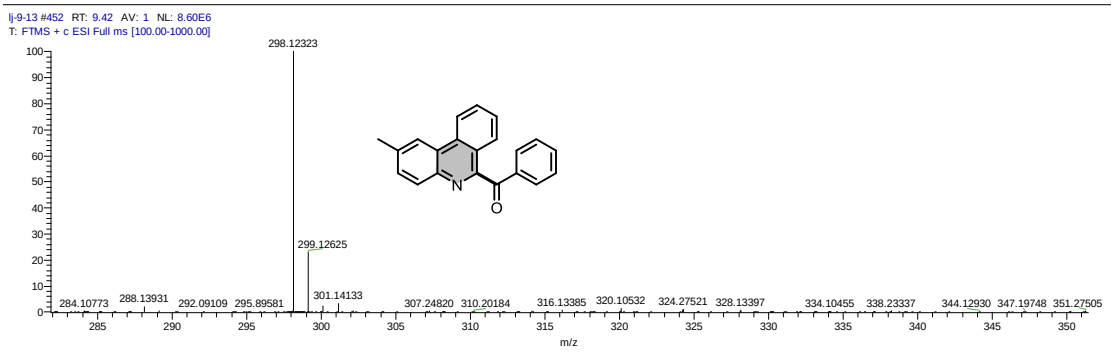

D:\Data\...\HXC dajia\2013
10/2/2013 3:47:19 PM
RT: 0.00 - 15.00
NL: 5.14E7 TIC MS lj-9-10
NL: 1.87E7 m/z= 298.11991-298.12587 MS lj-9-10
Time (min)

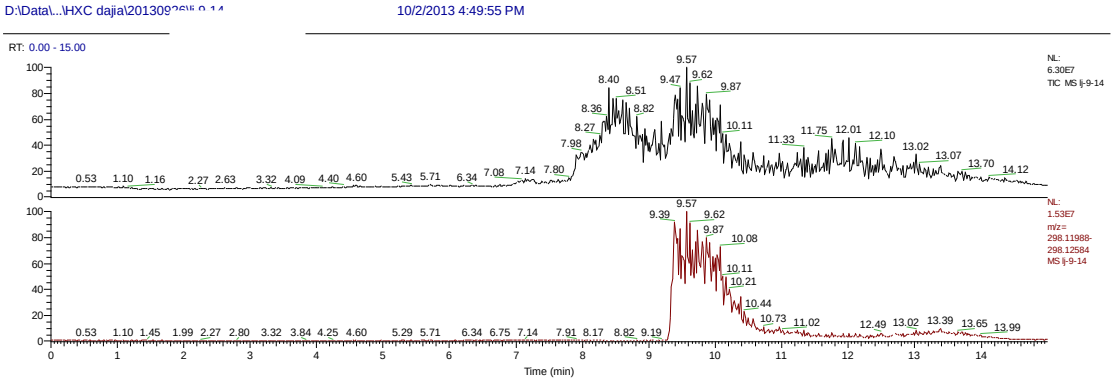

lj-9-10 #450 RT: 9.44 AV: 1 NL: 1.26E7
T: FTMS + c ESI Full ms [100.00-1000.00]
298.12302
N
O
m/z

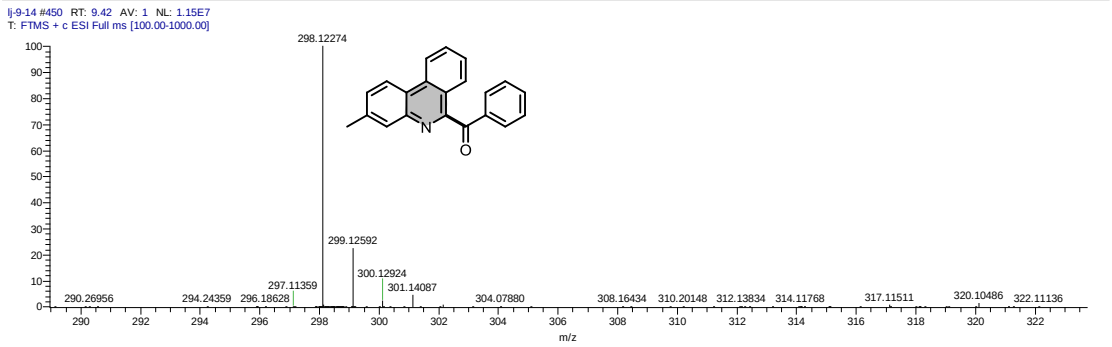

D:\Data\...\HXC dajia\20130926\lj-9-12
10/2/2013 4:18:39 PM
RT: 0.00 - 15.00
NL: 3.64E7 TIC MS lj-9-12
NL: 1.20E7 m/z= 328.13051-328.13707 MS lj-9-12
Time (min)

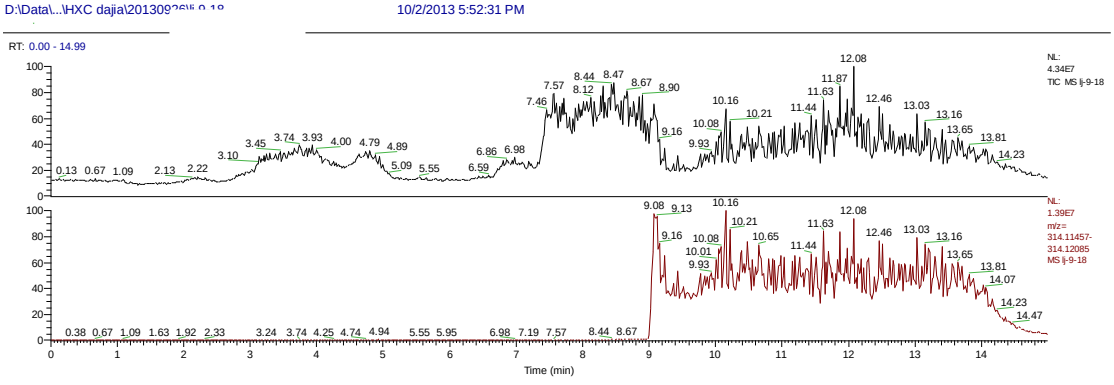

lj-9-12 #435 RT: 9.33 AV: 1 NL: 9.98E6
T: FTMS + c ESI Full ms [100.00-1000.00]
328.13324
OMe
N
O
m/z

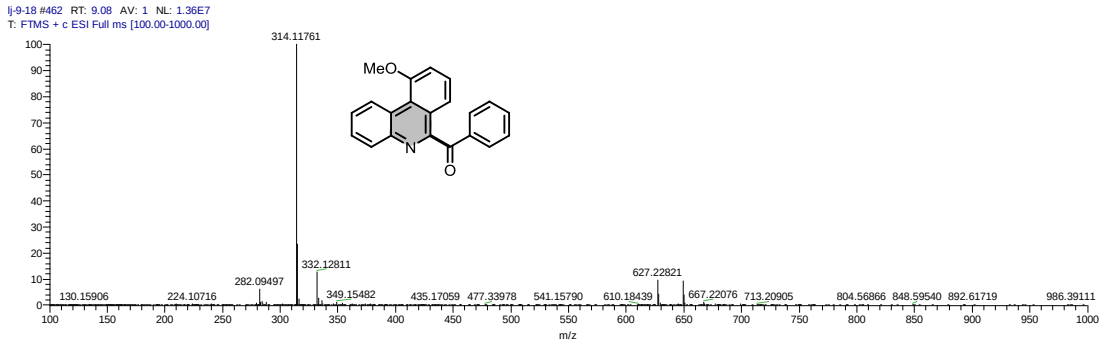

D:\Data\...\HXC dajia\20130926\lj-9-13
10/2/2013 4:34:17 PM
RT: 0.00 - 14.99
NL: 5.94E7 TIC MS lj-9-13
NL: 1.55E7 m/z= 298.11949-298.12545 MS lj-9-13
Time (min)

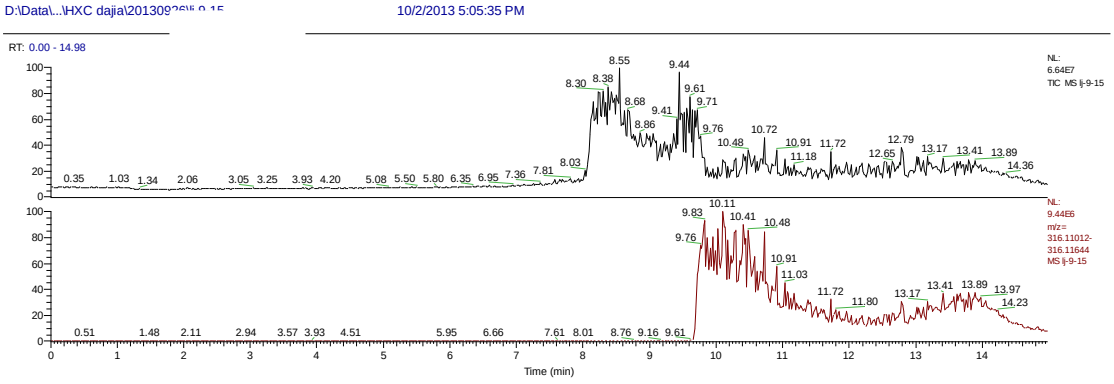

lj-9-13 #452 RT: 9.42 AV: 1 NL: 8.60E6
T: FTMS + c ESI Full ms [100.00-1000.00]
298.12323
N
O
m/z

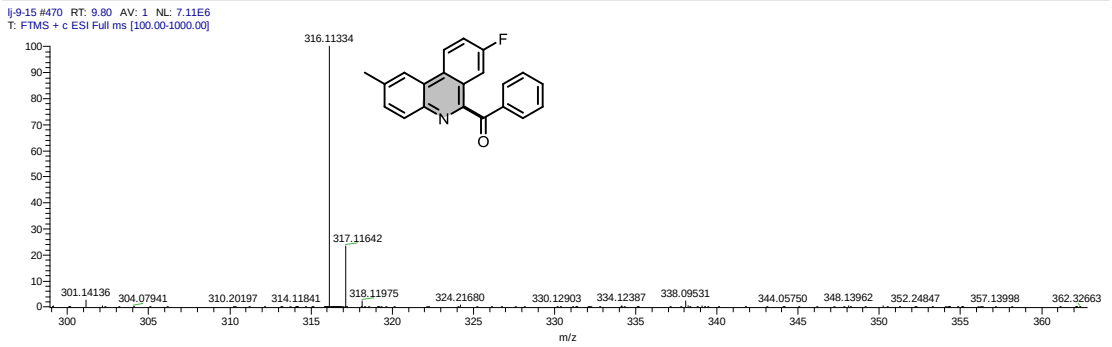

D:\Data\...\HXC dajia\20130926\lj-9-14
10/2/2013 4:49:55 PM
RT: 0.00 - 15.00
NL: 6.30E7 TIC MS lj-9-14
NL: 1.53E7 m/z= 298.11988-298.12584 MS lj-9-14
Time (min)

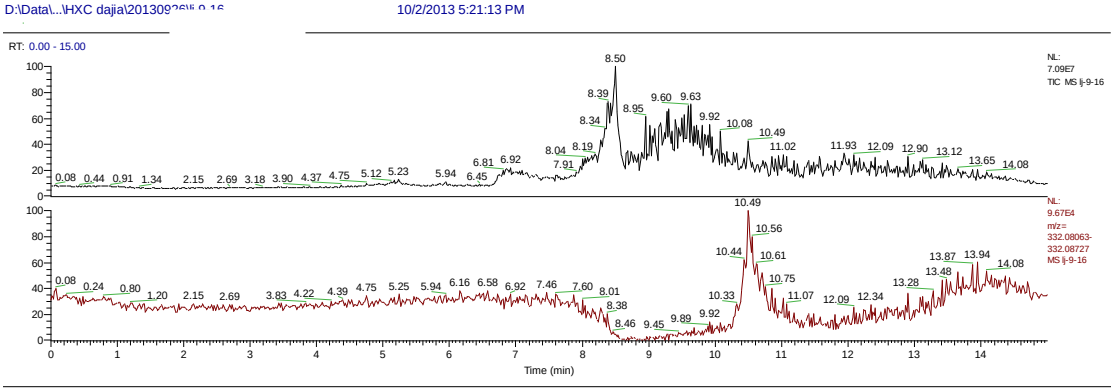

lj-9-14 #450 RT: 9.42 AV: 1 NL: 1.15E7
T: FTMS + c ESI Full ms [100.00-1000.00]
298.12274
299.12592
300.12924
301.14087
297.11359
m/z

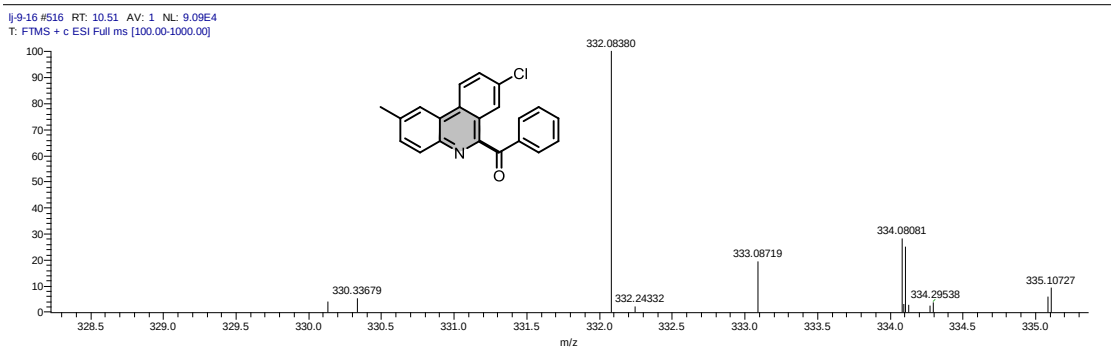

D:\Data\...\HXC dajia\20130926\lj-9-18
10/2/2013 5:52:31 PM
RT: 0.00 - 14.99
NL: 4.34E7 TIC MS lj-9-18
NL: 1.39E7 m/z= 314.11457-314.12085 MS lj-9-18
Time (min)

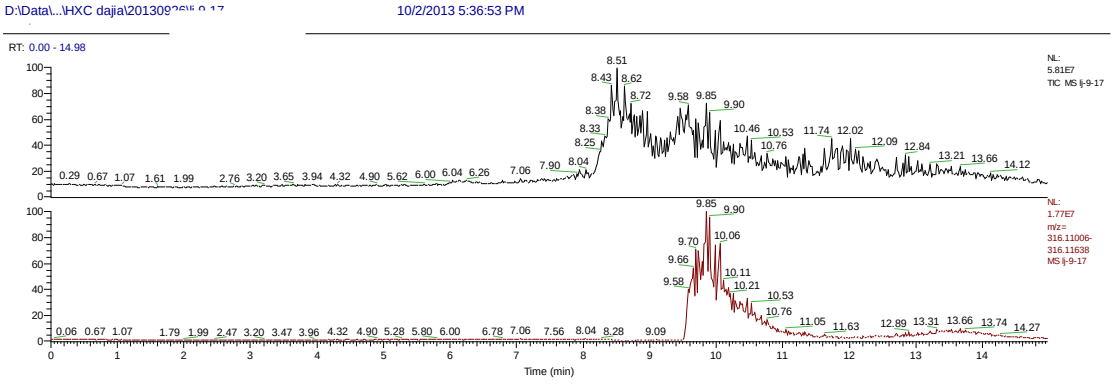

lj-9-18 #462 RT: 9.08 AV: 1 NL: 1.36E7
T: FTMS + c ESI Full ms [100.00-1000.00]
314.11761
332.12811
282.09497
627.22821
MeO
m/z

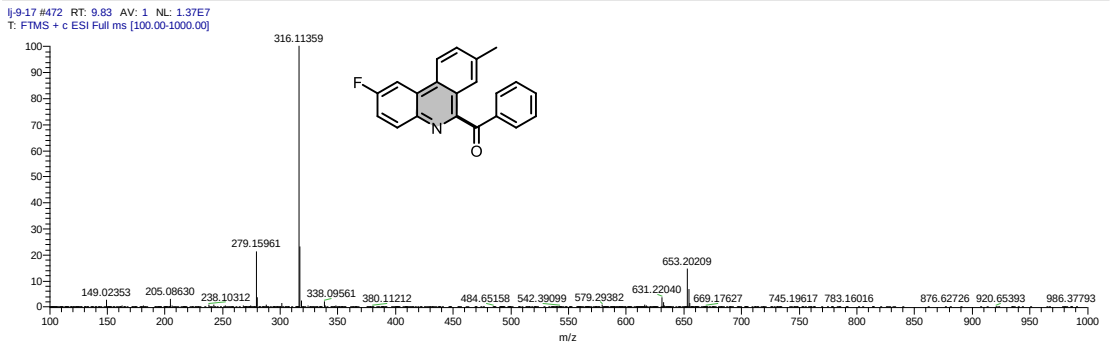

D:\Data\...\HXC dajia\20130926\5 9-15
10/2/2013 5:05:35 PM
RT: 0.00 - 14.98
NL: 6.64E7 TIC MS lj-9-15
NL: 9.44E6 m/z= 316.11012-316.11644 MS lj-9-15
Time (min)

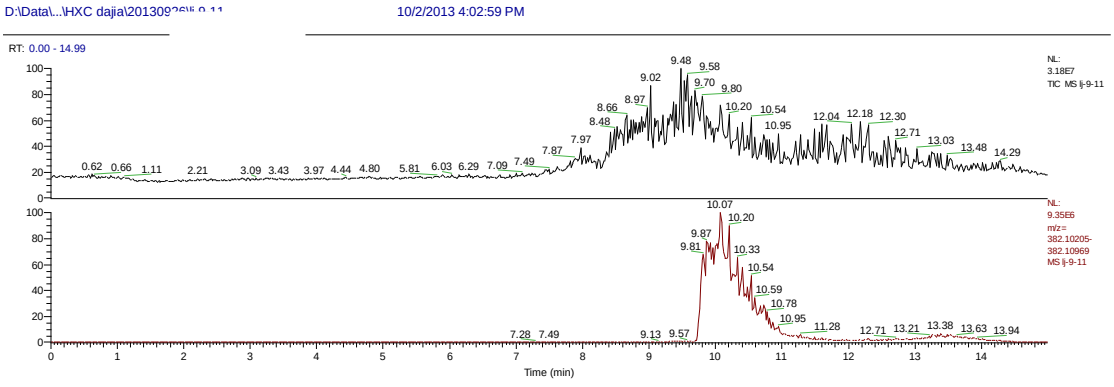

lj-9-15 #470 RT: 9.80 AV: 1 NL: 7.11E6
T: FTMS + c ESI Full ms [100.00-1000.00]
316.11334
317.11642
m/z

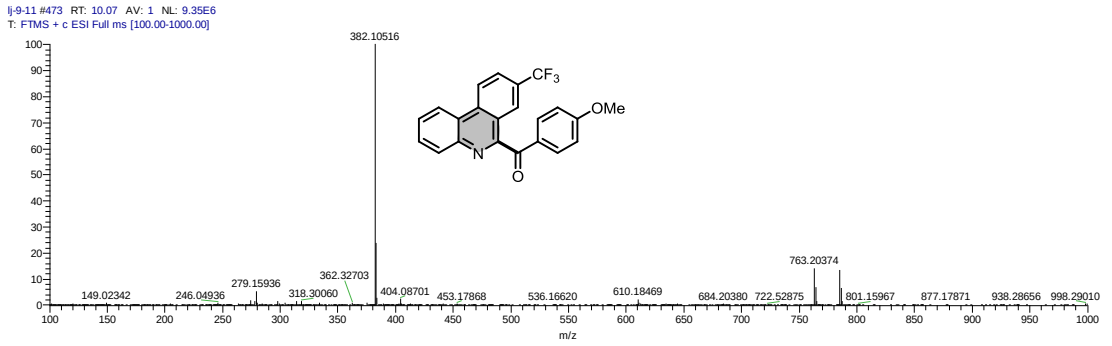

D:\Data\...\HXC dajia\20130926\5 9-16
10/2/2013 5:21:13 PM
RT: 0.00 - 15.00
NL: 7.09E7 TIC MS lj-9-16
NL: 9.67E4 m/z= 332.08063-332.08727 MS lj-9-16
Time (min)


lj-9-16 #516 RT: 10.51 AV: 1 NL: 9.09E4
T: FTMS + c ESI Full ms [100.00-1000.00]
332.08380
334.08081
333.08719
330.33679
332.24332
335.10727
334.29538
m/z


D:\Data\...\HXC dajia\20130926\5 9-17
10/2/2013 5:36:53 PM
RT: 0.00 - 14.98
NL: 5.81E7 TIC MS lj-9-17
NL: 1.77E7 m/z= 316.11006-316.11638 MS lj-9-17
Time (min)


lj-9-17 #472 RT: 9.83 AV: 1 NL: 1.37E7
T: FTMS + c ESI Full ms [100.00-1000.00]
316.11359
279.15961
653.20209
m/z


D:\Data\...\HXC dajia\20130926\5 9-11
10/2/2013 4:02:59 PM
RT: 0.00 - 14.99
NL: 3.18E7 TIC MS lj-9-11
NL: 9.35E6 m/z= 382.10205-382.10969 MS lj-9-11
Time (min)


lj-9-11 #473 RT: 10.07 AV: 1 NL: 9.35E6
T: FTMS + c ESI Full ms [100.00-1000.00]
382.10516
362.32703
763.20374
m/z