Supporting Information

for

Direct Use of Hydroxyl Ion as an Oxygen Source for Oxidation of Isoquinolinium Salts to Isoquinolinones in Water Solution

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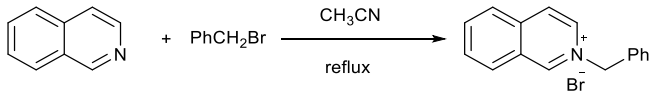
1. General Information

Commercially available materials purchased from *Energy Chemical* or TCI was used as received. All the solvents and reagents were obtained from commercial sources and used without purification unless stated otherwise. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance III 400 MHz spectrometer operating at 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR in deuterated solvent. The chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. ^{1}HNMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublets); m (multiplets), and etc. GC-MS was recorded by an Agilent 7890A/5975C. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. High resolution mass spectral analysis (HRMS) was performed on a Waters Q–TOF Permier Spectrometer. Column chromatography was generally performed on silica gel (300-400 mesh) and TLC inspections were on silica gel GF_{254} plates.

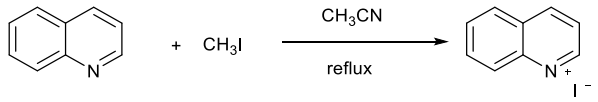
2. Preparation of N-alkyl iminium salts 1 & 3

a) General procedure for the preparation of isoquinolinium salts (1**a** as the example)



The oven-dried round-bottom flask were charged with CH_3CN (15 mL), isoquinoline (10 mmol, 1.0 equiv.), Benzyl bromide (12 mmol, 1.2 equiv.). The reaction mixture was refluxed for 12 hours, and then cooled to room temperature. When ethyl acetate was added to the system, the isoquinoline salt precipitated quickly as a solid, which was filtered and washed with ethyl acetate to give pure product 1**a**.

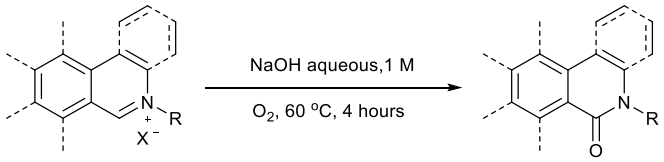
b) General procedure for the preparation of quinolinium salts (3**h** as the example)



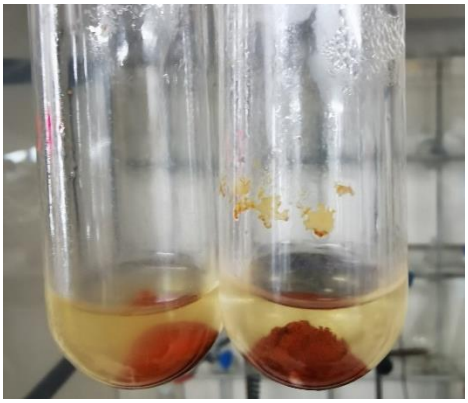
The oven-dried round-bottom flask were charged with CH_3CN (15 mL), quinoline (10 mmol, 1.0 equiv.), CH_3I (12 mmol, 1.2 equiv.). The reaction mixture was refluxed for 12 hours, and then cooled to room temperature. When ethyl acetate was added to the system, the quinoline salt precipitated quickly as a solid, which was filtered and w ethyl acetate to give pure product 3**h**.

3. Procedure and synthetic application

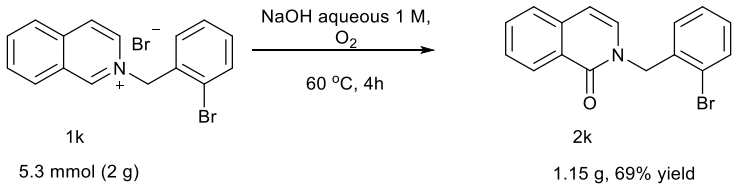
a) General procedure for the oxidation of N-alkyl iminium salts.



A 10 mL oven-dried screw-capped test tube with stir bar was charged with O_2, isoquinolinium salts 1 (0.3 mmol, 1.0 equiv.) and solution of sodium hydroxide (1 M in water) 3 mL, and the mixture was stirred at 60 °C for 4h. Stop the reaction and cool to room temperature, product 2 was deposited as a solid on the stirred magneton or separated from the solution as an oil. The mixture was extract with ethyl acetate (2×5 mL), organic phase was concentrated under vacuum after combine and dry with Na_2SO_4, and purified by column chromatography on silica gel (petroleum ether/ethyl acetate=5:1) to afford desired product 2, which was confirmed by ^1H NMR, ^{13}C NMR spectra and compare to already reported data.



b) Procedure for the scale-up synthesis of product 2**k**.



1k

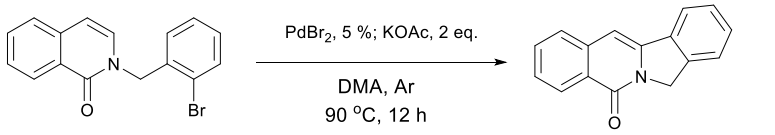
5.3 mmol (2 g)

2k

1.15 g, 69% yield

A 100 mL round bottom flask with stir bar was charged with O_2, isoquinolinium salts 1**k** (5.3 mmol, 2 g, 1.0 equiv.) and solution of sodium hydroxide (1 M in water) 30 mL, and the mixture was stirred at 60 °C for 4h. Stop the reaction and cool to room temperature, the mixture was extract with ethyl acetate (3×20 mL), organic phase was concentrated under vacuum after combine and dry with Na_2SO_4, and purified by column chromatography on silica gel (petroleum ether/ethyl acetate=5:1) to afford 2**k** with 69 % yield.

c) Synthetic application: Synthesis of topoisomerase I inhibitor 5. [1]



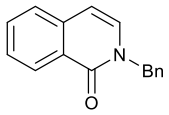
2k, 0.5 mmol

topoisomerase I inhibitor (5).
88 mg, 76 % yield

A dry 10 mL Schlenk tube with stir bar was charged with 2**k** (0.50 mmol, 1.0 equiv.), $PdBr_2$ (6.70 mg, 5 mol %), KOAc (98 mg, 2.0 equiv.). The tube was evacuated, and refilled with Argon. Then the mixture was dissolved with 3mL DMA. The mixture was stirred at 90 ℃ for 15 h when the substrate was consumed completely (monitored by TLC). The mixture was concentrated under vacuum and purified by column chromatography on silica gel (Ethyl acetate dichloromethane 1:1) to afford desired product **5** as a yellow solid (88 mg, 76 % yield)

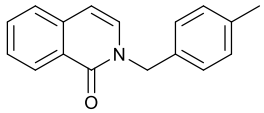
4. Spectra data of products

N-benzylisoquinolin-1(2H)-one (2**a**) [1]



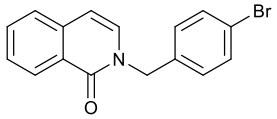
The reaction was performed according to procedure (a). white solid (51 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 7.6 Hz, 1H), 7.67 – 7.58 (m, 1H), 7.52 – 7.43 (m, 2H), 7.33 – 7.25 (m, 5H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.48 (d, *J* = 7.4 Hz, 1H), 5.22 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 137.0, 136.9, 132.2, 131.3, 128.8, 128. 1, 127.9, 127.8, 126.9, 126.3, 125.9, 106.4, 51.7.

N-(4-methylbenzyl)isoquinolin-1(2H)-one (2**b**) [3]



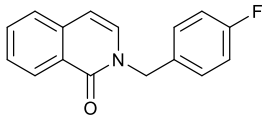
The reaction was performed according to procedure (a). white solid (55mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.37 (m, 1H), 7.71 – 7.55 (m, 1H), 7.50 – 7.38 (m, 2H), 7.32 – 7.17 (m, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 7.04 (d, *J* = 7.4 Hz, 1H), 6.43 (d, *J* = 7.4 Hz, 1H), 5.15 (s, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 137.6, 137.0, 133.9, 132.2, 131.3, 129.5, 128.0, 128.0, 126.8, 126.3, 125.9, 106.3, 51.4, 21.1.

N-(4-bromobenzyl)isoquinolin-1(2H)-one (2**c**) [2]



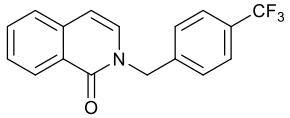
The reaction was performed according to procedure (a). white solid (63.8mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.7 Hz, 1H), 7.70 – 7.48 (m, 1H), 7.44 – 7.38 (m, 2H), 7.37 – 7.32 (m, 2H), 7.13 – 7.04 (m, 2H), 6.97 (d, *J* = 7.4 Hz, 1H), 6.40 (d, *J* = 7.4 Hz, 1H), 5.06 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 136.9, 135.9, 132.4, 131.9, 131.1, 129.6, 128.0, 127.0, 126.2, 126.04, 121.8, 106.7, 51.3.

N -(4-fluorobenzyl)isoquinolin-1(2H)-one (2**d**) [3]



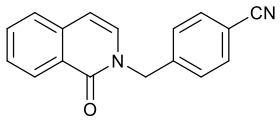
The reaction was performed according to procedure (a). White solid (49 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 7.8 Hz, 1H), 7.78 – 7.59 (m, 1H), 7.49 (dd, *J* = 11.3, 4.3 Hz, 2H), 7.39 – 7.28 (m, 2H), 7.08 (d, *J* = 7.4 Hz, 1H), 7.04 – 6.96 (m, 2H), 6.50 (d, *J* = 7.4 Hz, 1H), 5.18 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.6, 162.2, 161.1, 136.9, 132.7, 132.7, 132.3, 131.1, 129.8, 129.7, 128.0, 127.0, 126.3, 125.9, 115.8, 115.6, 106.6, 51.1.

N -(4-(trifluoromethyl)benzyl)isoquinolin-1(2H)-one (2**e**) [11]



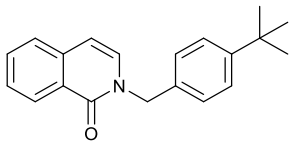
The reaction was performed according to procedure (a). White solid (57mg, 63%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 7.9 Hz, 1H), 7.73 – 7.62 (m, 1H), 7.59 (d, *J* = 8.1 Hz, 2H), 7.52 (t, *J* = 8.3 Hz, 2H), 7.43 (d, *J* = 8.1 Hz, 2H), 7.09 (d, *J* = 7.4 Hz, 1H), 6.54 (d, *J* = 7.4 Hz, 1H), 5.27 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 140.9, 137.0, 132.5, 131.1, 128.0, 128.0, 127.1, 126.2, 126.0, 125.8, 125.7, 106.8, 51.5.

N -((1-oxoisoquinolin-2(1H)-yl)methyl)benzonitrile (2**f**) [2]



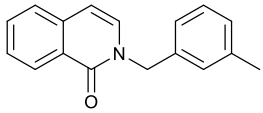
The reaction was performed according to procedure (a). Yellow solid (25 mg, 32%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.1 Hz, 1H), 7.60 – 7.53 (m, 1H), 7.53 – 7.48 (m, 2H), 7.46 – 7.37 (m, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 7.00 (d, *J* = 7.4 Hz, 1H), 6.45 (d, *J* = 7.4 Hz, 1H), 5.15 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 142.2, 137.0, 132.6, 132.5, 131.1, 128.3, 127.9, 127.2, 126.1, 126.1, 118.6, 111.6, 107.0, 51.7.

N -(4-(tert-butyl)benzyl)isoquinolin-1(2H)-one (2**g**) [8]



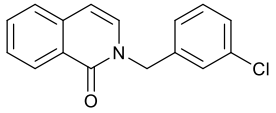
The reaction was performed according to procedure (a). White solid (63.5mg, 73%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 7.7 Hz, 1H), 7.59 – 7.47 (m, 1H), 7.39 (dd, *J* = 11.3, 4.3 Hz, 2H), 7.32 – 7.24 (m, 2H), 7.18 (d, *J* = 8.5 Hz, 2H), 7.02 (d, *J* = 7.4 Hz, 1H), 6.39 (d, *J* = 7.4 Hz, 1H), 5.11 (s, 2H), 1.20 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 150.8, 137.0, 133.8, 132.2, 131.4, 128.0, 127.7, 126.8, 126.3, 125.9, 125.7, 106.3, 51.4, 34.5, 31.3.

N -(3-methylbenzyl)isoquinolin-1(2H)-one (2**h**) [3]



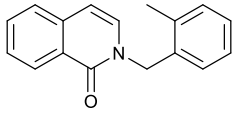
The reaction was performed according to procedure (a). yellow solid (45mg, 61%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 – 8.34 (m, 1H), 7.62 (td, *J* = 7.3, 1.3 Hz, 1H), 7.53 – 7.38 (m, 2H), 7.22 (dd, *J* = 15.4, 7.9 Hz, 1H), 7.15 – 7.00 (m, 4H), 6.47 (d, *J* = 7.4 Hz, 1H), 5.18 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 138.5, 137.0, 136.8, 132.2, 131.3, 128.7, 128.6, 128.6, 128.1, 126.8, 126.3, 125.9, 125.0, 106.4, 51.6, 21.4.

N -(3-chlorobenzyl)isoquinolin-1(2H)-one (2**i**) [10]



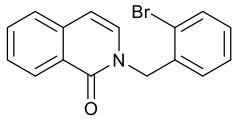
The reaction was performed according to procedure (a). yellow solid (43.5mg, 54%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.8 Hz, 1H), 7.55 (ddd, *J* = 8.1, 7.1, 1.3 Hz, 1H), 7.46 – 7.34 (m, 2H), 7.21-7.15 (m, 3H), 7.13 – 7.09 (m, 1H), 6.97 (d, *J* = 7.4 Hz, 1H), 6.41 (d, *J* = 7.4 Hz, 1H), 5.08 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 138.9, 137.0, 134.6, 132.4, 131.1, 130.2, 128.0, 127.9, 127.0, 126.2, 126.0, 106.7, 51.2.

N -(2-methylbenzyl)isoquinolin-1(2H)-one (2**j**) [3]



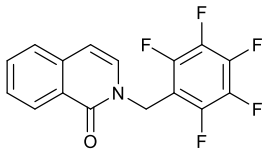
The reaction was performed according to procedure (a). yellow solid (46.2mg, 62%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 7.8 Hz, 1H), 7.73 – 7.55 (m, 1H), 7.49 (dd, *J* = 11.4, 4.4 Hz, 2H), 7.22 – 7.11 (m, 3H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.94 (d, *J* = 7.4 Hz, 1H), 6.47 (d, *J* = 7.4 Hz, 1H), 5.22 (s, 2H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 136.9, 136.5, 134.4, 132.2, 130.8, 130.7, 128.3, 128.1, 128.0, 126.9, 126.3, 126.1, 125.9, 106.3, 49.3, 19.2.

N -(2-bromobenzyl)isoquinolin-1(2H)-one (2**k**) [1]



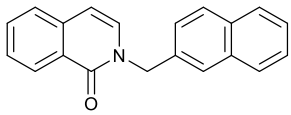
The reaction was performed according to procedure (a). White solid (62mg, 67%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.0 Hz, 1H), 7.69 – 7.62 (m, 1H), 7.59 (dd, *J* = 5.9, 3.4 Hz, 1H), 7.54 – 7.45 (m, 2H), 7.25 – 7.20 (m, 1H), 7.16-7.12 (m, 2H), 7.10 (d, *J* = 7.4 Hz, 1H), 5.32 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3, 137.0, 135.9, 132.9, 132.4, 131.5, 129.4, 129.3, 128.1, 127.9, 127.0, 126.2, 126.0, 123.3, 106.5, 51.7.

N -((perfluorophenyl)methyl)isoquinolin-1(2H)-one (2**l**)



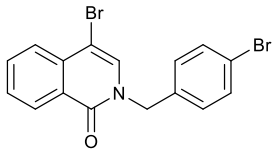
The reaction was performed according to procedure (a). White solid (66mg, 68%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.74 – 7.52 (m, 1H), 7.49 – 7.31 (m, 2H), 7.12 (d, *J* = 7.4 Hz, 1H), 6.46 (d, *J* = 7.4 Hz, 1H), 5.13 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 136.9, 132.6, 131.3, 127.7, 127.2, 126.0, 125.9, 106.7, 41.4. Calcd for $C_{16}H_9F_5NO$ $[M+H]^+$: 326.0599, found: 326.1602.

N -(naphthalen-2-ylmethyl)isoquinolin-1(2H)-one (2**m**)[8]



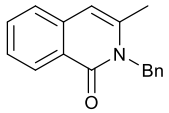
The reaction was performed according to procedure (a). White solid (57.3mg, 74%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.9 Hz, 1H), 7.88 – 7.70 (m, 4H), 7.67 – 7.57 (m, 1H), 7.53 – 7.37 (m, 5H), 7.09 (d, *J* = 7.4 Hz, 1H), 6.45 (d, *J* = 7.4 Hz, 1H), 5.36 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 137.0, 134.4, 133.3, 132.9, 132.3, 131.2, 128.8, 128.1, 127.8, 127.7, 126.9, 126.9, 126.3, 126.3, 126.1, 126.0, 125.8, 106.6, 51.7.

N -bromo-2-(4-bromobenzyl)isoquinolin-1(2H)-one (2**n**)



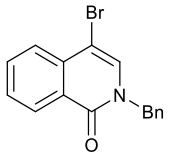
The reaction was performed according to procedure (a). White solid (79mg, 68%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.0 Hz, 1H), 7.93 – 7.68 (m, 2H), 7.64 – 7.50 (m, 1H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.33 (s, 1H), 7.21 (d, *J* = 8.3 Hz, 2H), 5.12 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.3, 135.4, 135.3, 133.2, 132.0, 131.5, 129.7, 128.4, 128.0, 126.4, 125.9, 122.2, 100.4, 51.3. Calcd for $C_{16}H_{12}Br_2NO$ $[M+H]^+$:391.9280, found: 391.9284.

N -benzyl-3-methylisoquinolin-1(2H)-one (2**o**) [9]



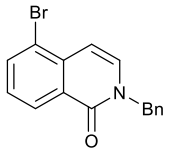
The reaction was performed according to procedure (a). White solid (47mg, 63%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.39 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.30 – 7.21 (m, 1H), 7.20-7.16 (m, 2H), 7.16 – 7.08 (m, 4H), 7.05 (t, *J* = 7.5 Hz, 1H), 5.47 (s, 2H), 2.23 (d, *J* = 1.1 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 138.6, 136.6, 136.3, 130.0, 129.3, 128.7, 127.9, 127.2, 126.6, 122.1, 121.0, 114.7, 46.2, 17.8.

N -benzyl-4-bromoisoquinolin-1(2H)-one (2**p**) [8]



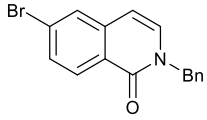
The reaction was performed according to procedure (a). White solid (61 mg, 65%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 8.0, 0.7 Hz, 1H), 7.87 – 7.77 (m, 1H), 7.73 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.59 – 7.51 (m, 1H), 7.41 – 7.29 (m, 6H), 5.20 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4, 136.2, 135.4, 133.0, 131.8, 128.9, 128.5, 128.1, 128.1, 127.9, 126.5, 125.9, 100.2, 51.7.

N -benzyl-5-bromoisoquinolin-1(2H)-one (2**q**) [3]



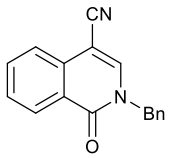
The reaction was performed according to procedure (a). White solid (63mg, 67%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.6 Hz, 1H), 7.49 (s, 1H), 7.42 (d, *J* = 8.6 Hz, 1H), 7.33 – 7.09 (m, 5H), 6.96 (d, *J* = 7.4 Hz, 1H), 6.21 (d, *J* = 7.4 Hz, 1H), 5.05 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.7, 138.4, 136.6, 132.7, 130.1, 129.9, 128.9, 128.3, 128.0, 128.0, 127.3, 124.9, 105.2, 51.8.

N -benzyl-6-bromoisoquinolin-1(2H)-one (2**r**) [3]



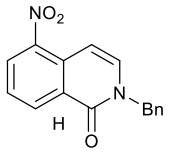
The reaction was performed according to procedure (a). White solid (62mg, 66%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 8.1 Hz, 1H), 7.76 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.31 – 7.17 (m, 6H), 7.07 (d, *J* = 7.7 Hz, 1H), 6.71 (d, *J* = 7.7 Hz, 1H), 5.11 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.4, 136.4, 136.3, 136.0, 132.5, 128.9, 128.0, 128.0, 127.8, 127.7, 127.4, 120.6, 105.0, 51.9.

N-benzyl-1-oxo-1,2-dihydroisoquinoline-4-carbonitrile (2**s**)



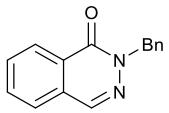
The reaction was performed according to procedure (a). yellow solid (51mg, 66%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.1 Hz, 1H), 7.69 (d, *J* = 3.9 Hz, 2H), 7.63 (s, 1H), 7.51 (dt, *J* = 8.2, 4.1 Hz, 1H), 7.38 – 7.20 (m, 5H), 5.14 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2, 140.1, 135.3, 133.7, 133.3, 129.2, 128.7, 128.6, 128.5, 128.3, 125.2, 124.1, 115.7, 91.3, 52.3. Calcd for $C_{17}H_{13}N_2O$ $[M+H]^+$: 261.1028, found: 261.1022.

N-benzyl-5-nitroisoquinolin-1(2H)-one (2**t**)



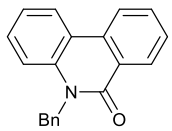
The reaction was performed according to procedure (a). White solid (27 mg, 32%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 8.0 Hz, 1H), 8.30 (d, *J* = 7.9 Hz, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.37 – 7.12 (m, 7H), 5.14 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.7, 144.6, 135.9, 135.0, 134.5, 130.8, 129.4, 129.0, 128.2, 128.2, 128.1, 125.8, 100.9, 52.0. Calcd for $C_{16}H_{13}N_2O_3$ $[M+H]^+$: 281.0926, found: 281.0929.

N -benzylphthalazin-1(2H)-one (2**u**) [3]



The reaction was performed according to procedure (a). White solid (49mg, 70%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.2 Hz, 1H), 8.06 (s, 1H), 7.77 – 7.59 (m, 2H), 7.58 – 7.51 (m, 1H), 7.38 (d, *J* = 7.0 Hz, 2H), 7.29 – 7.05 (m, 4H), 5.32 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 138.0, 137.0, 133.1, 131.6, 129.7, 128.6, 128.5, 128.0, 127.7, 126.8, 126.0, 54.6.

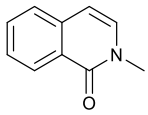
5-benzylphenanthridin-6(5H)-one (2**v**) [4]



The reaction was performed according to procedure (a). White solid (65mg, 77%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 7.9 Hz, 1H), 8.18 (t, *J* = 8.9 Hz, 2H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H),

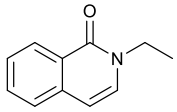
7.45 – 7.23 (m, 7H), 7.19 (t, *J* = 7.5 Hz, 1H), 5.65 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.8, 137.2, 136.7, 133.8, 132.7, 129.5, 129.1, 128.8, 128.0, 127.2, 126.6, 125.4, 123.3, 122.5, 121.7, 119.4, 115.9, 46.4.

N -methylisoquinolin-1(2H)-one (2**w**) [2]



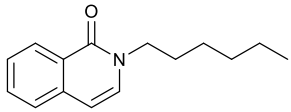
The reaction was performed according to procedure (a). Yellow oil (27.2mg, 57%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 8.1 Hz, 1H), 7.63 – 7.53 (m, 1H), 7.51 – 7.41 (m, 2H), 7.02 (dd, *J* = 7.3, 1.2 Hz, 1H), 6.44 (d, *J* = 7.3 Hz, 1H), 3.56 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5, 137.1, 132.4, 131.9, 127.5, 126.7, 126.0, 125.8, 105.8, 36.9

N-ethylisoquinolin-1(2H)-one (2**x**) [5]



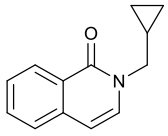
The reaction was performed according to procedure (a).Colorless oil (31.5 mg, 61%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.0 Hz, 1H), 7.66 – 7.46 (m, 1H), 7.39 (dd, *J* = 14.2, 7.3 Hz, 2H), 6.98 (d, *J* = 7.3 Hz, 1H), 6.41 (d, *J* = 7.3 Hz, 1H), 3.96 (q, *J* = 7.2 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.0, 131.9, 131.1, 127.7, 126.7, 126.3, 125.8, 106.2, 44.2, 14.6.

N-hexylisoquinolin-1(2H)-one (2**y**)



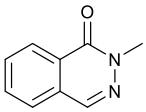
The reaction was performed according to procedure (a). White solid (45mg, 66%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.1 Hz, 1H), 7.70 – 7.48 (m, 1H), 7.43 – 7.31 (m, 2H), 6.97 (d, *J* = 7.3 Hz, 1H), 6.40 (d, *J* = 7.3 Hz, 1H), 4.11 – 3.70 (m, 2H), 1.88 – 1.54 (m, 2H), 1.52 – 1.13 (m, 6H), 0.79 (dd, *J* = 9.4, 4.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.0, 137.0, 131.9, 131.7, 127.8, 126.7, 126.3, 125.8, 105.8, 49.4, 31.4, 29.2, 26.4, 22.5, 14.0. Calcd for $C_{15}H_{20}NO$ $[M+H]^+$: 230.1539, found: 230.1537.

N -(cyclopropylmethyl)isoquinolin-1(2H)-one (2**z**) [1]



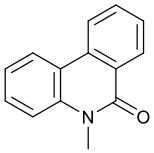
The reaction was performed according to procedure (a). White solid (38.4mg, 64%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.1 Hz, 1H), 7.76 – 7.57 (m, 1H), 7.51 – 7.43 (m, 2H), 7.16 (d, *J* = 7.4 Hz, 1H), 6.50 (d, *J* = 7.4 Hz, 1H), 3.88 (d, *J* = 7.1 Hz, 2H), 1.36 – 1.15 (m, 1H), 0.67 – 0.51 (m, 2H), 0.41 (q, *J* = 4.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 137.0, 132.0, 131.4, 127.8, 126.6, 126.3, 125.8, 105.9, 53.1, 10.7, 3.8.

2-methylphthalazin-1(2H)-one (2**aa**) [4]



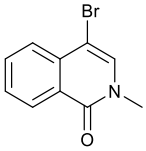
The reaction was performed according to procedure (a). yellow solid (29.5mg, 62%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.6 Hz, 1H), 7.99 (s, 1H), 7.74 – 7.57 (m, 2H), 7.54 (d, *J* = 7.2 Hz, 1H), 3.71 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 137.4, 132.8, 131.4, 129.6, 127.5, 126.3, 125.8, 39.3.

5-methylphenanthridin-6(5H)-one (2**ab**) [2]



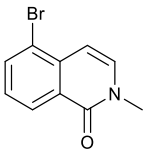
The reaction was performed according to procedure (a). White solid (47mg, 75%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.9 Hz, 1H), 7.79 (t, *J* = 6.9 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.29 (t, *J* = 7.5 Hz, 1H), 7.17 (dd, *J* = 9.5, 5.7 Hz, 1H), 7.03 – 6.85 (m, 2H), 3.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.2, 137.6, 133.2, 132.0, 129.2, 128.5, 127.6, 125.2, 122.8, 122.1, 121.40, 118.8, 114.7, 29.7.

4-bromo-2-methylisoquinolin-1(2H)-one (2**ac**) **[1]**



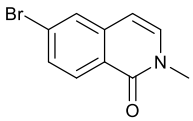
The reaction was performed according to procedure (a). White solid (46 mg, 65%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 – 8.37 (m, 1H), 7.94 – 7.65 (m, 2H), 7.61 – 7.48 (m, 1H), 7.36 (s, 1H), 3.60 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.6, 135.4, 132.9, 132.8, 128.0, 127.8, 126.2, 125.7, 99.5, 36.9.

5-bromo-2-methylisoquinolin-1(2H)-one (2**ad**) [1]



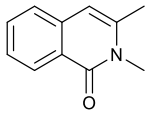
The reaction was performed according to procedure (a). White solid (48mg, 68%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.1 Hz, 1H), 7.73 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 6.65 (d, *J* = 7.6 Hz, 1H), 3.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.7, 136.3, 135.7, 133.5, 127.4, 127.2, 120.4, 104.4, 37.1.

6-bromo-2-methylisoquinolin-1(2H)-one (2**ae**) [1]



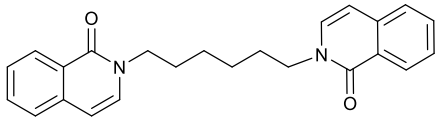
The reaction was performed according to procedure (a). White solid (47mg, 66%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.6 Hz, 1H), 7.49 (d, *J* = 1.8 Hz, 1H), 7.41 (dd, *J* = 8.6, 1.9 Hz, 1H), 6.96 (d, *J* = 7.3 Hz, 1H), 6.22 (d, *J* = 7.3 Hz, 1H), 3.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 138.4, 133.7, 129.8, 129.4, 128.1, 127.0, 124.6, 104.6, 37.0.

2,3-dimethylisoquinolin-1(2H)-one (2**af**) [6]



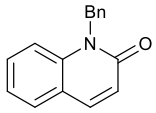
The reaction was performed according to procedure (a). White solid (31mg, 60%) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.50 (t, *J* = 7.3 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 3.74 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.9, 139.0, 135.6, 130.0, 129.2, 127.8, 121.9, 120.7, 113.9, 29.7, 17.7.

2,2'-(hexane-1,6-diyl)bis(isoquinolin-1(2H)-one) (2**ag**) [2]



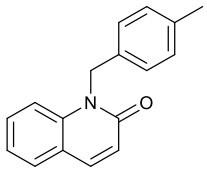
The reaction was performed according to procedure (a). White solid (36mg, 65%) ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.42 (dd, *J* = 8.0, 1.3 Hz, 2H), 7.65 – 7.55 (m, 2H), 7.53 – 7.38 (m, 4H), 7.01 (d, *J* = 7.3 Hz, 2H), 6.45 (d, *J* = 7.3 Hz, 2H), 3.96 (t, *J* = 7.4 Hz, 4H), 1.76 (t, *J* = 7.3 Hz, 4H), 1.47 – 1.35 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 162.0, 137.0, 132.0, 131.6, 127.7, 126.7, 126.2, 125.8, 105.9, 49.1, 29.1, 26.3. Calcd for $C_{24}H_{25}N_2O2$ $[M+H]^+$: 373.1911, found: 373.1915.

N-benzylquinolin-2(1H)-one (4**a**) [4]



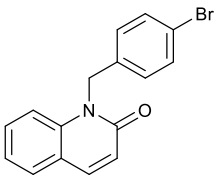
The reaction was performed according to procedure (a). White solid (37 mg, 52 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 9.5 Hz, 1H), 7.47 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.32 (ddd, *J* = 8.7, 7.3, 1.5 Hz, 1H), 7.26 – 7.02 (m, 7H), 6.72 (d, *J* = 9.5 Hz, 1H), 5.47 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5, 139.6, 139.4, 136.3, 130.6, 128.8, 128.8, 127.2, 126.6, 122.2, 121.6, 120.9, 115.0, 45.9.

N-(4-methylbenzyl)quinolin-2(1H)-one (4**b**) [4]



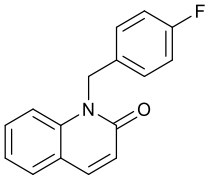
The reaction was performed according to procedure (a). White solid (42 mg, 56 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 9.5 Hz, 1H), 7.54 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.40 (ddd, *J* = 8.6, 7.3, 1.5 Hz, 1H), 7.30 – 7.24 (m, 1H), 7.20 – 7.03 (m, 5H), 6.79 (d, *J* = 9.5 Hz, 1H), 5.51 (s, 2H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.5, 139.5, 136.9, 133.3, 130.6, 129.4, 128.8, 126.6, 122.1, 121.7, 120.9, 115.0, 45.7, 21.0.

N-(4-bromobenzyl)quinolin-2(1H)-one (4**c**) [7]



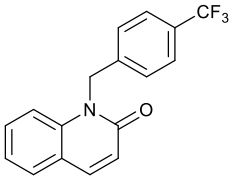
The reaction was performed according to procedure (a). White solid (47 mg, 50 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 9.5 Hz, 1H), 7.57 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.49 – 7.33 (m, 3H), 7.20 (dd, *J* = 7.9, 4.5 Hz, 2H), 7.10 (d, *J* = 8.4 Hz, 2H), 6.79 (d, *J* = 9.5 Hz, 1H), 5.49 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 139.7, 139.2, 135.4, 131.9, 130.7, 129.0, 128.4, 122.4, 121.6, 121.17, 120.9, 114.7, 45.3.

N-(4-fluorobenzyl)quinolin-2(1H)-one (4**d**) [7]



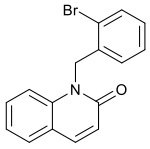
The reaction was performed according to procedure (a). White solid (42mg, 55 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 9.5, 2.1 Hz, 1H), 7.54 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.42 (ddd, *J* = 8.8, 7.3, 1.7 Hz, 1H), 7.27 – 7.11 (m, 4H), 6.96 (td, *J* = 8.6, 1.9 Hz, 2H), 6.85 – 6.71 (m, 1H), 5.50 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.2, 162.4, 160.7, 139.7, 139.3, 132.1, 132.0, 130.7, 128.9, 128.4, 128.3, 122.3, 121.5, 120.9, 115.8, 115.5, 114.8, 45.2.

N-(4-(trifluoromethyl)benzyl)quinolin-2(1H)-one (4**e**) [7]



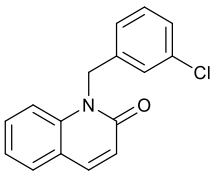
The reaction was performed according to procedure (a). White solid (61 mg, 58 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 9.5 Hz, 1H), 7.71 – 7.50 (m, 3H), 7.49 – 7.38 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.09 (m, 2H), 6.81 (d, *J* = 9.5 Hz, 1H), 5.61 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 140.5, 139.8, 139.2, 130.8, 129.1, 126.9, 125.8, 125.8, 125.8, 125.7, 122.5, 121.5, 120.9, 114.6, 45.5.

N-(2-bromobenzyl)quinolin-2(1H)-one (4**f**) [4]



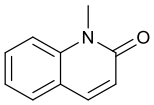
The reaction was performed according to procedure (a). White solid (42 mg, 45 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 9.5 Hz, 1H), 7.60 (ddd, *J* = 9.5, 6.3, 1.9 Hz, 2H), 7.42 (ddd, *J* = 8.7, 7.3, 1.5 Hz, 1H), 7.24 – 7.16 (m, 1H), 7.12 – 7.06 (m, 2H), 7.02 (d, *J* = 8.5 Hz, 1H), 6.81 (d, *J* = 9.5 Hz, 1H), 6.75 – 6.62 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 139.8, 139.2, 134.75, 132.9, 130.9, 128.9, 128.8, 127.8, 126.9, 122.5, 122.5, 121.5, 120.9, 114.9, 46.4.

N-(3-chlorobenzyl)quinolin-2(1H)-one (4**g**)



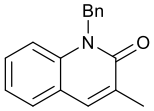
The reaction was performed according to procedure (a). The reaction was performed according to procedure (a). White solid (41 mg, 51 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 9.5 Hz, 1H), 7.63 – 7.52 (m, 1H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.22 – 7.16 (m, 5H), 7.12 – 7.04 (m, 1H), 6.79 (d, *J* = 9.5 Hz, 1H), 5.43 (d, *J* = 60.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.4, 139.8, 139.2, 138.5, 134.7, 130.8, 130.1, 129.0, 127.6, 126.7, 124.8, 122.4, 121.5, 120.9, 114.7, 45.4. Calcd for $C_{16}H_{13}ClNO$ $[M+H]^+$: 270.0680, found: 270.1682.

1-methylquinolin-2(1H)-one (4**h**) [2]



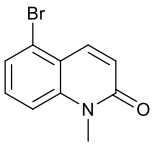
The reaction was performed according to procedure (a). Yellow solide (27 mg, 58 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 9.5 Hz, 1H), 7.58 (dd, *J* = 12.7, 4.4 Hz, 2H), 7.37 (d, *J* = 8.4 Hz, 1H), 7.26 – 7.18 (m, 1H), 6.71 (d, *J* = 9.5 Hz, 1H), 3.72 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.3, 140.0, 138.9, 130.6, 128.7, 122.1, 121.7, 120.6, 114.1, 29.4.

1-benzyl-3-methylquinolin-2(1H)-one (4**i**) [6]



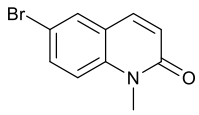
The reaction was performed according to procedure (a). White solid (40 mg, 54 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (s, 1H), 7.50 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.36 (ddd, *J* = 8.6, 7.3, 1.5 Hz, 1H), 7.32 – 7.19 (m, 7H), 7.19 – 7.12 (m, 1H), 5.58 (s, 2H), 2.32 (d, *J* = 1.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 138.6, 136.6, 136.3, 130.0, 129.3, 128.7, 127.9, 127.2, 126.6, 122.1, 121.1, 114.7, 46.2, 17.8.

5-bromo-1-methylquinolin-2(1H)-one (4**j**) [2]



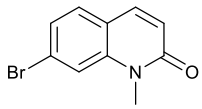
The reaction was performed according to procedure (a). White solid (37 mg, 53 %) ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, *J* = 9.8 Hz, 1H), 7.45 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.30 (d, *J* = 8.2 Hz, 1H), 6.74 (dd, *J* = 9.8, 1.0 Hz, 1H), 3.69 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.7, 141.1, 137.4, 130.9, 126.3, 123.7, 122.7, 119.6, 113.8, 29.8.

6-bromo-1-methylquinolin-2(1H)-one (4**k**) [2]



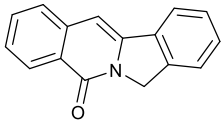
The reaction was performed according to procedure (a). White solid (35 mg, 50 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 9.5 Hz, 1H), 7.52 (d, *J* = 1.0 Hz, 1H), 7.41 (d, *J* = 8.3 Hz, 1H), 7.34 (dd, *J* = 8.3, 1.6 Hz, 1H), 6.71 (d, *J* = 9.5 Hz, 1H), 3.68 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 140.9, 138.4, 129.8, 125.3, 125.1, 122.1, 119.4, 117.2, 29.5.

7-bromo-1-methylquinolin-2(1H)-one (4**l**)



The reaction was performed according to procedure (a). White solid (32 mg, 46 %) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 2.1 Hz, 1H), 7.64 (dd, *J* = 9.0, 2.2 Hz, 1H), 7.59 (d, *J* = 9.5 Hz, 1H), 7.24 (d, *J* = 9.0 Hz, 1H), 6.74 (d, *J* = 9.5 Hz, 1H), 3.70 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.9, 139.0, 137.7, 133.3, 130.8, 123.0, 122.1, 115.8, 114.9, 29.5. Calcd for $C_{10}H_9BrNO$ $[M+H]^+$: 237.9862, found: 237.9860.

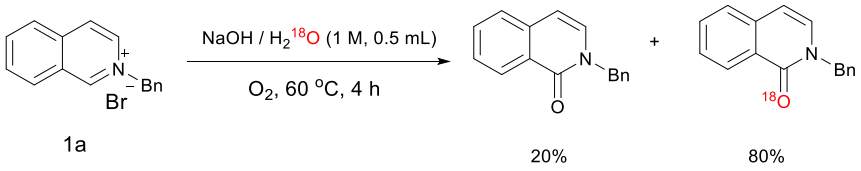
topoisomerase I inhibitor 5 [2, 4]



The reaction was performed according to procedure (c). White solid (88 mg, 76 % yield) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.1 Hz, 1H), 7.73 (dt, *J* = 7.6, 3.9 Hz, 1H), 7.61 – 7.54 (m, 2H), 7.51 (dt, *J* = 6.3, 3.4 Hz, 1H), 7.46 – 7.39 (m, 3H), 6.95 (s, 1H), 5.12 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.0, 142.1, 137.9, 137.6, 134.0, 132.1, 129.7, 128.3, 127.3, 126.3, 126.13, 124.7, 123.4, 120.9, 97.9, 52.0.

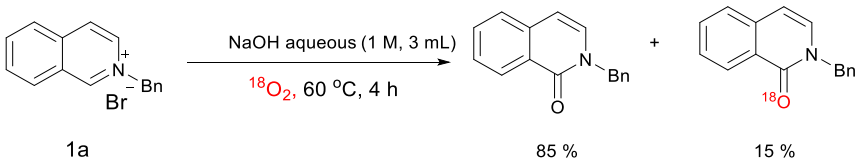
5. Isotope labeling experiment and control experiment

a) procedure for the oxidation of N-alkyl iminium salts in $H_2{}^{18}O$ with O_2 as oxidant.



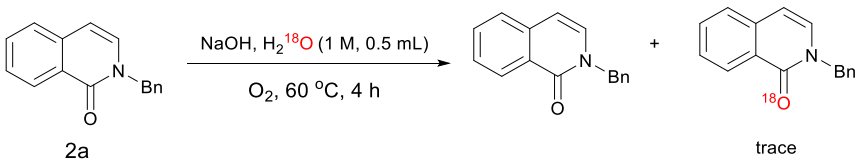
A 10 mL oven-dried screw-capped test tube with stir bar was charged with O_2, isoquinolinium salts 1**a** (0.1 mmol, 1.0 equiv.) and solution of sodium hydroxide (1 M in $H_2{}^{18}O$) 0.5 mL, and the mixture was stirred at 60 °C for 4h. Stop the reaction and cool to room temperature, the mixture was extract with ethyl acetate (2×5 mL), organic phase was concentrated under vacuum after combine and dry with Na_2SO_4. And ^{18}O labeling product was detected by GC-MS with high deuterium substitution rate (up to 80 %).

b) procedure for the oxidation of N-alkyl iminium salts in H_2O with $^{18}O_2$ as oxidant.

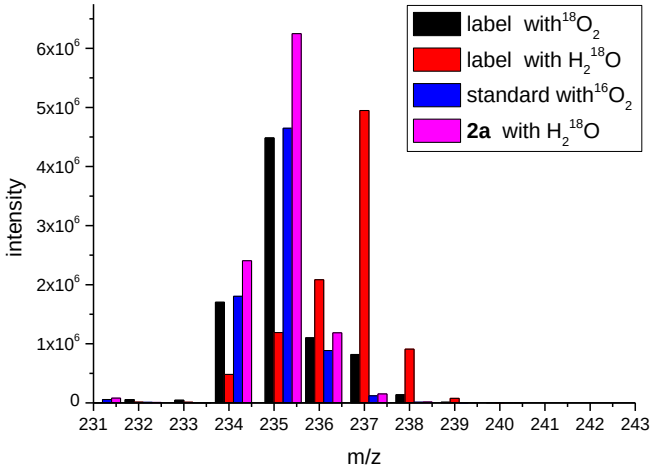


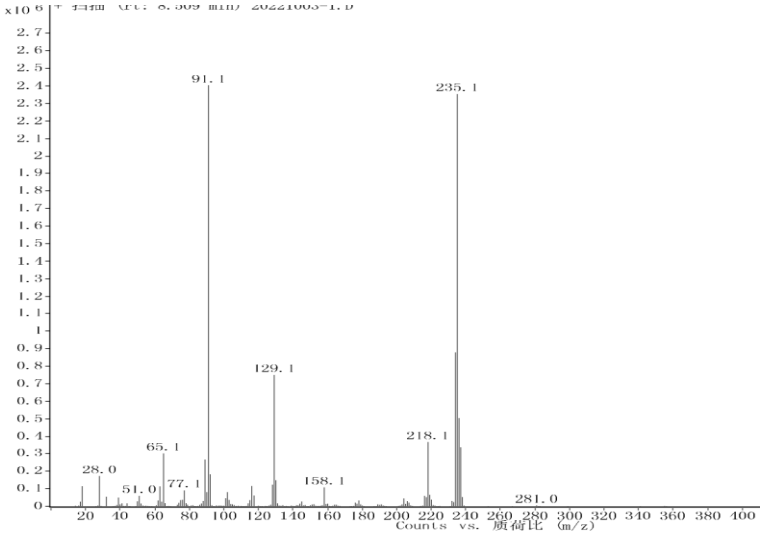
A 10 mL oven-dried screw-capped test tube with stir bar was charged with $^{18}O_2$, isoquinolinium salts 1**a** (0.3 mmol, 1.0 equiv.) and solution of sodium hydroxide (1 M in H_2O) 3 mL, and the mixture was stirred at 60 °C for 4h. Stop the reaction and cool to room temperature, the mixture was extract with ethyl acetate (2×5 mL), organic phase was concentrated under vacuum after combine and dry with Na_2SO_4. And ^{18}O labeling product was detected by GC-MS with only 13 % deuterium substitution rate.

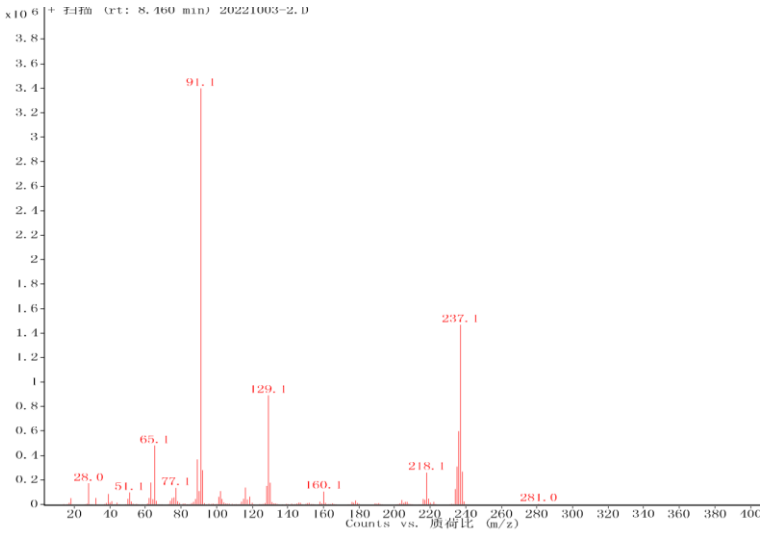
c) procedure for the ^{18}O exchange of 2a with $H_2{}^{18}O$ in standard condition.

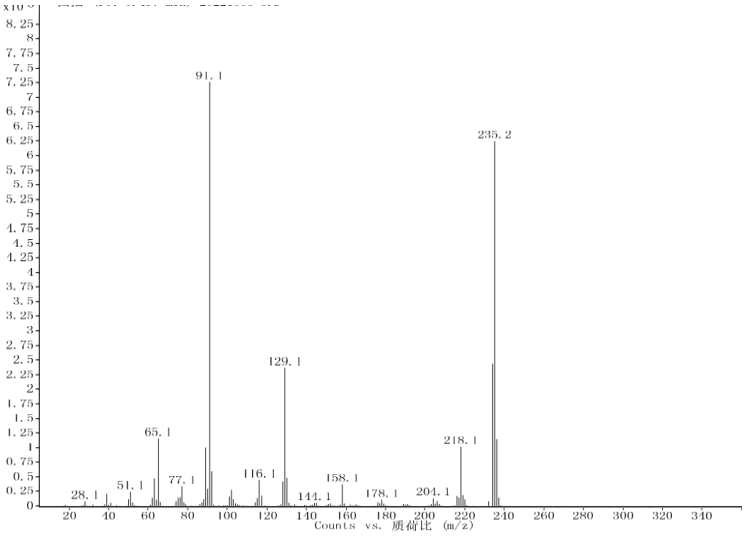


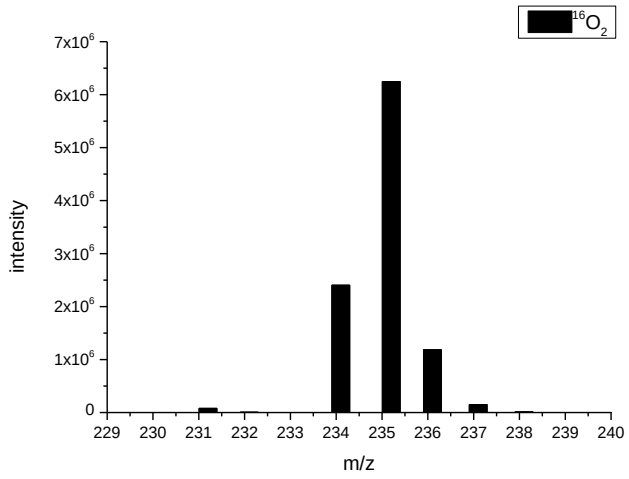
A 10 mL oven-dried screw-capped test tube with stir bar was charged with O_2, 2**a** (0.1 mmol, 1.0 equiv.) and solution of sodium hydroxide (1 M in $H_2{}^{18}O$) 0.5 mL, and the mixture was stirred at 60 °C for 4h. Stop the reaction and cool to room temperature, the mixture was extract with ethyl acetate (2×5 mL), organic phase was dry with Na_2SO_4. And ^{18}O labeling product was detected by GC-MS with only trace deuterium substitution rate.

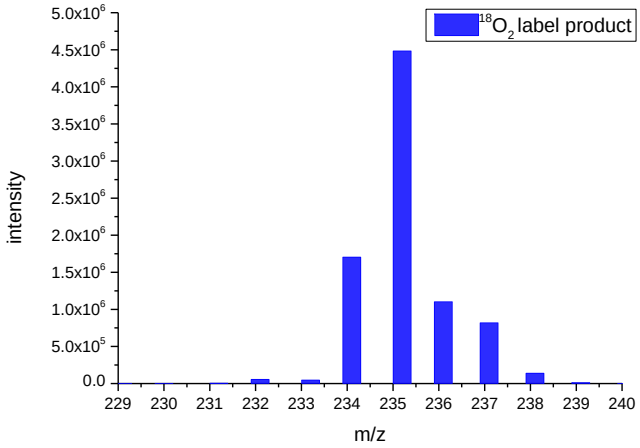

label with $^{18}O_2$
label with $H_2{}^{18}O$
standard with $^{16}O_2$
2a with $H_2{}^{18}O$
intensity
m/z

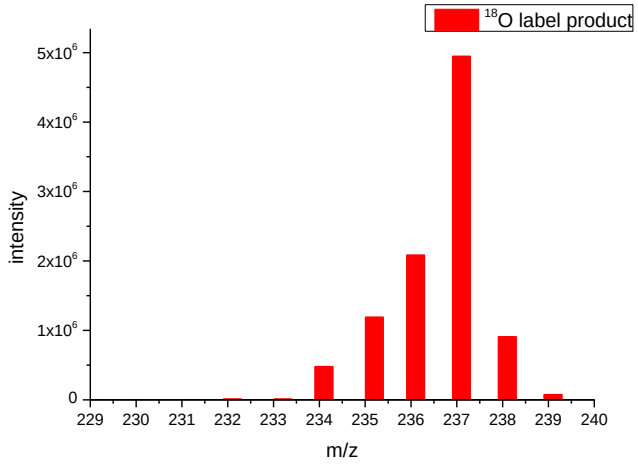

91.1
235.1
129.1
218.1
65.1
28.0
51.0
77.1
158.1
281.0
Counts vs. 质荷比 (m/z)

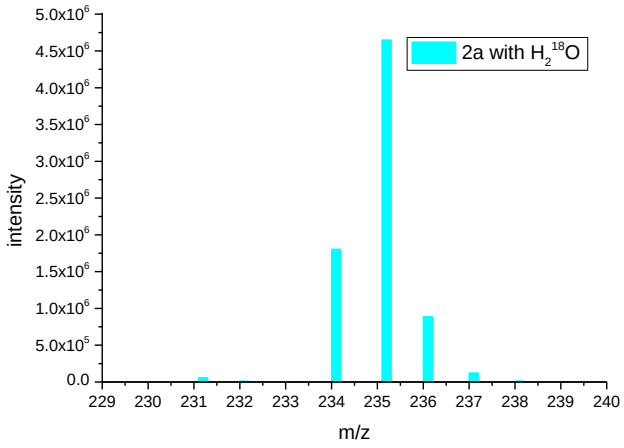

91.1
237.1
129.1
65.1
28.0
51.1
77.1
160.1
218.1
281.0
Counts vs. 质荷比 (m/z)


91.1
235.2
129.1
65.1
218.1
116.1
77.1
158.1
51.1
28.1
144.1
178.1
204.1
Counts vs. 质荷比 (m/z)


16O2
intensity
m/z


18O2 label product
intensity
m/z


^{18}O label product
intensity
5x10^6
4x10^6
3x10^6
2x10^6
1x10^6
0
229 230 231 232 233 234 235 236 237 238 239 240
m/z


2a with $H_2{}^{18}O$
intensity
5.0x10^6
4.5x10^6
4.0x10^6
3.5x10^6
3.0x10^6
2.5x10^6
2.0x10^6
1.5x10^6
1.0x10^6
5.0x10^5
0.0
229 230 231 232 233 234 235 236 237 238 239 240
m/z

6. References

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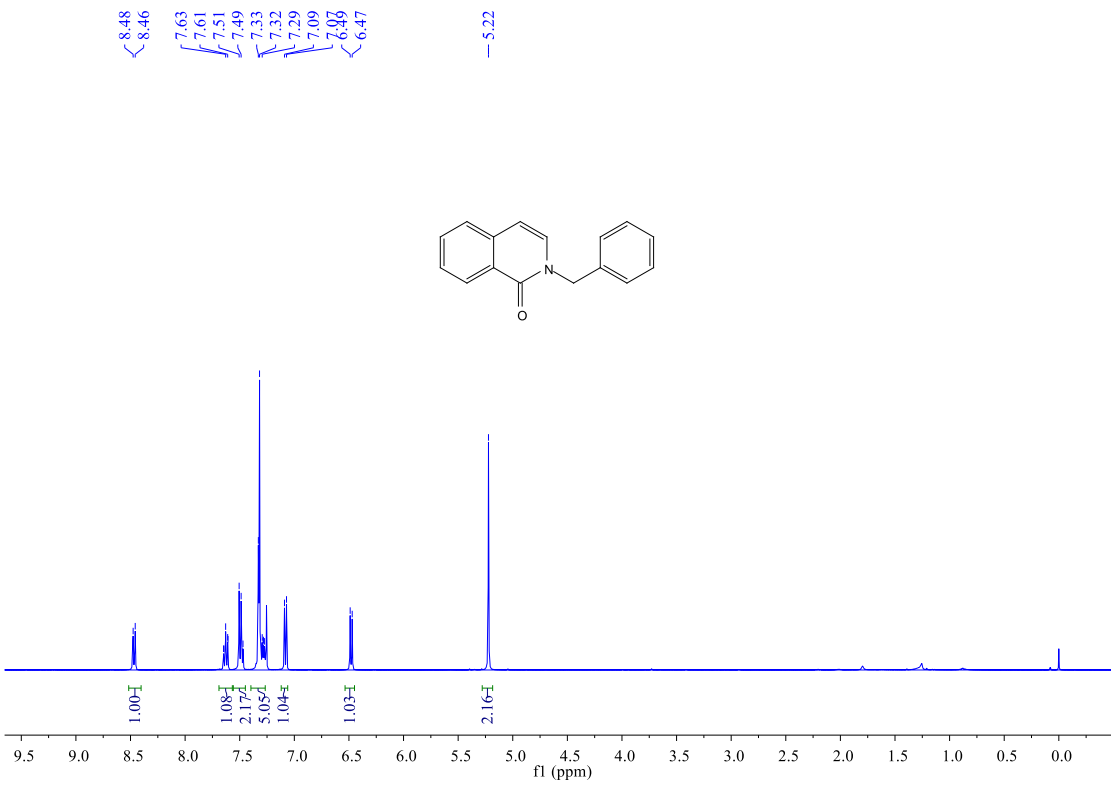
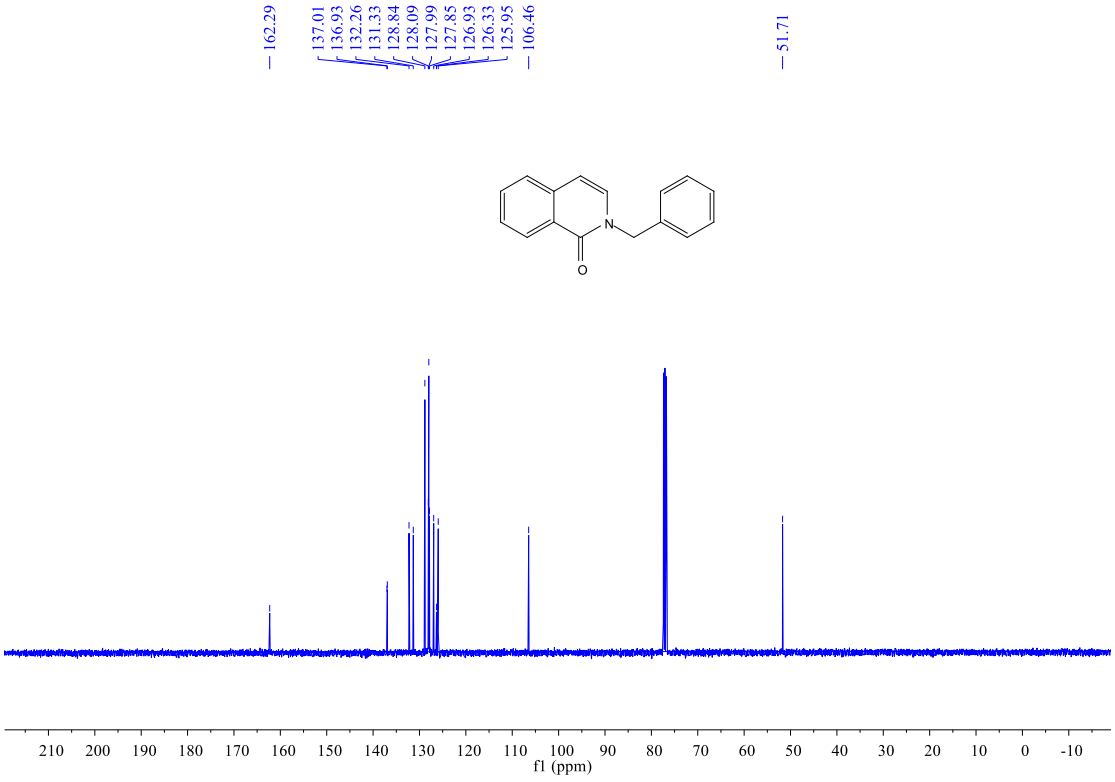
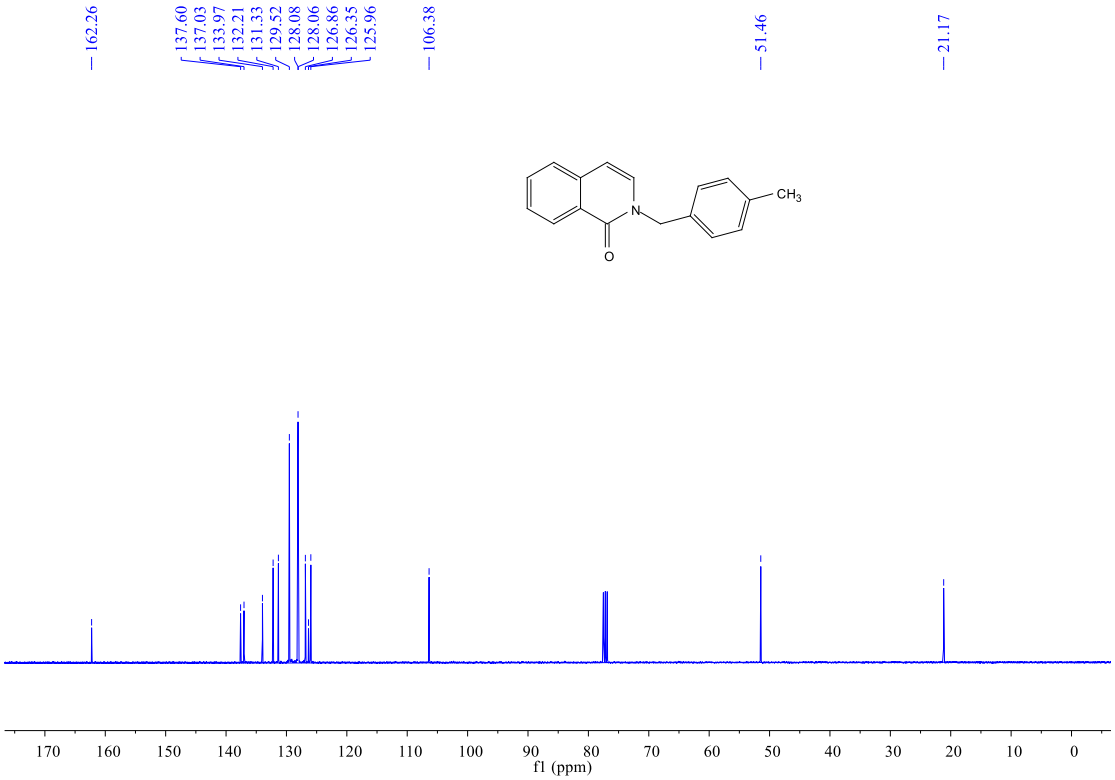
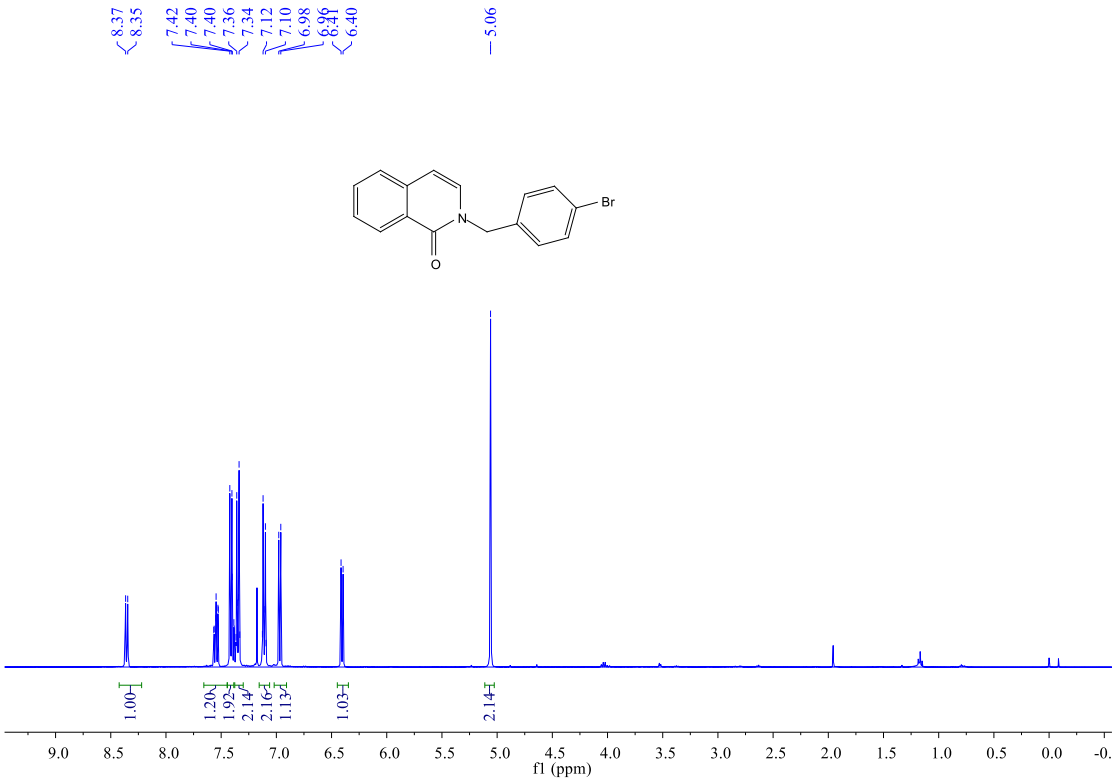
7.Copies of NMR for 2a-2k and 3a-3g

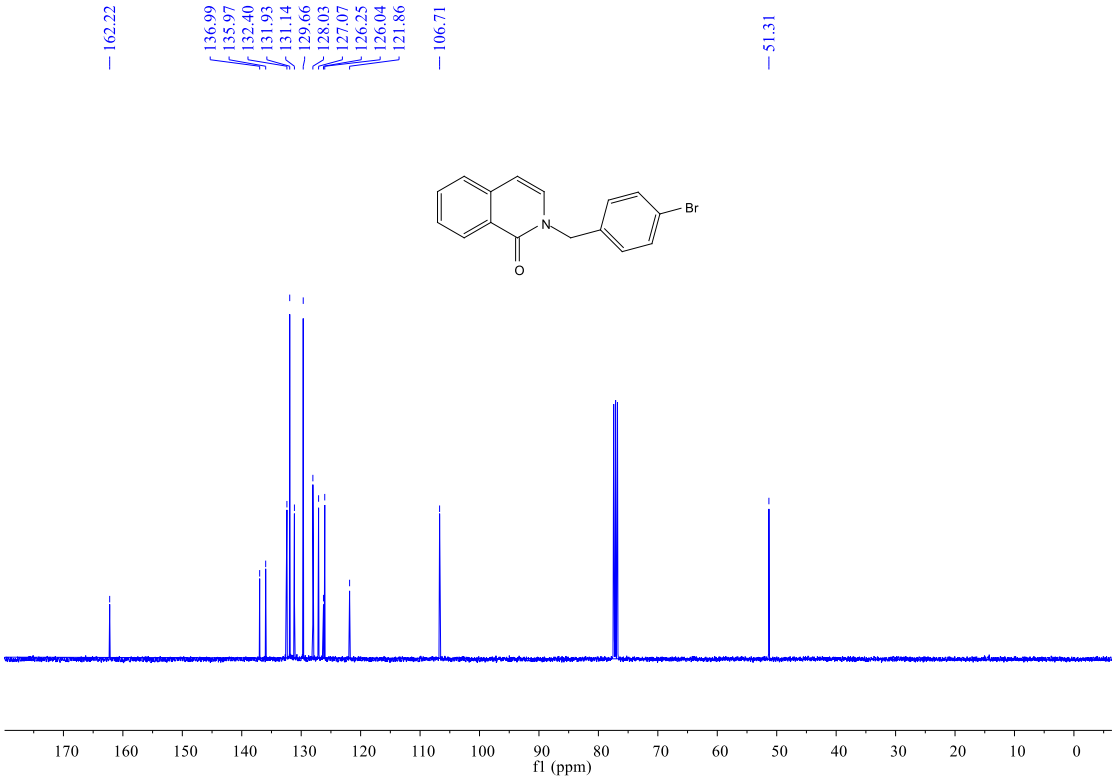





8.47
8.47
8.45
7.46
7.46
7.45
7.22
7.20
7.12
7.10
7.05
6.44
6.42
5.15
2.29
CH3
N
O
1.00
1.07
2.11
2.31
2.13
1.16
1.05
2.15
3.43
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


162.26
137.60
137.03
133.97
132.21
131.33
129.52
128.08
128.06
126.86
126.35
125.96
106.38
51.46
21.17
CH3
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.37
8.35
7.42
7.40
7.40
7.36
7.34
7.12
7.10
6.98
6.96
6.41
6.40
5.06
Br
N
O
1.00
1.20
1.92
2.14
2.16
1.13
1.03
2.14
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
-0.
f1 (ppm)


162.22
136.99
135.97
132.40
131.93
131.14
129.66
128.03
127.07
126.25
126.04
121.86
106.71
51.31
Br
N
O
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130
120
110
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90
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50
40
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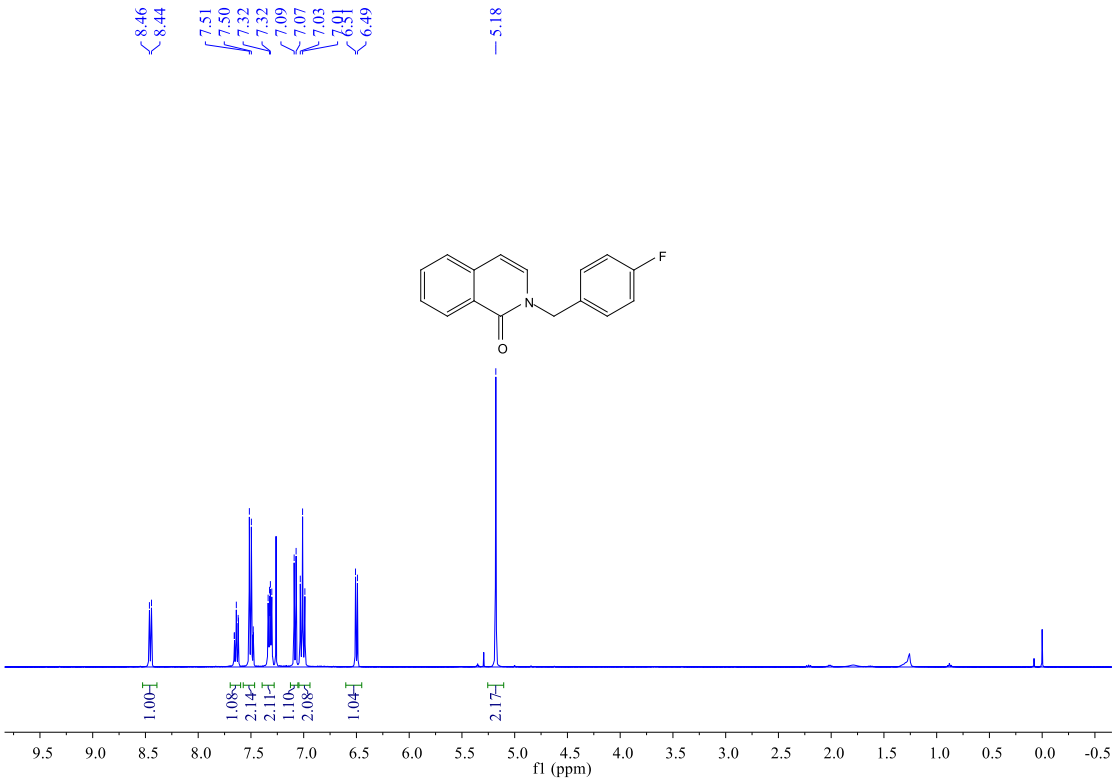
10
0
f1 (ppm)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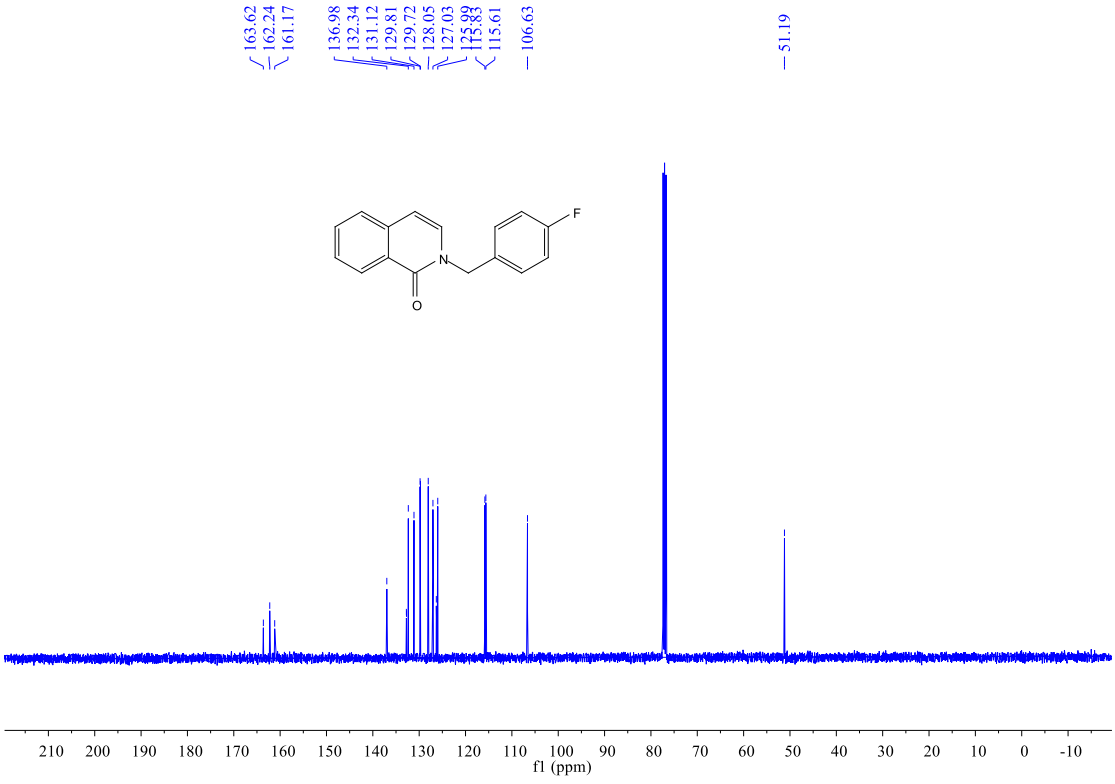
7.51
7.50
7.32
7.09
7.07
7.03
7.01
6.49
5.18
F
N
O
1.00
1.08
2.14
2.11
1.10
2.08
1.04
2.17
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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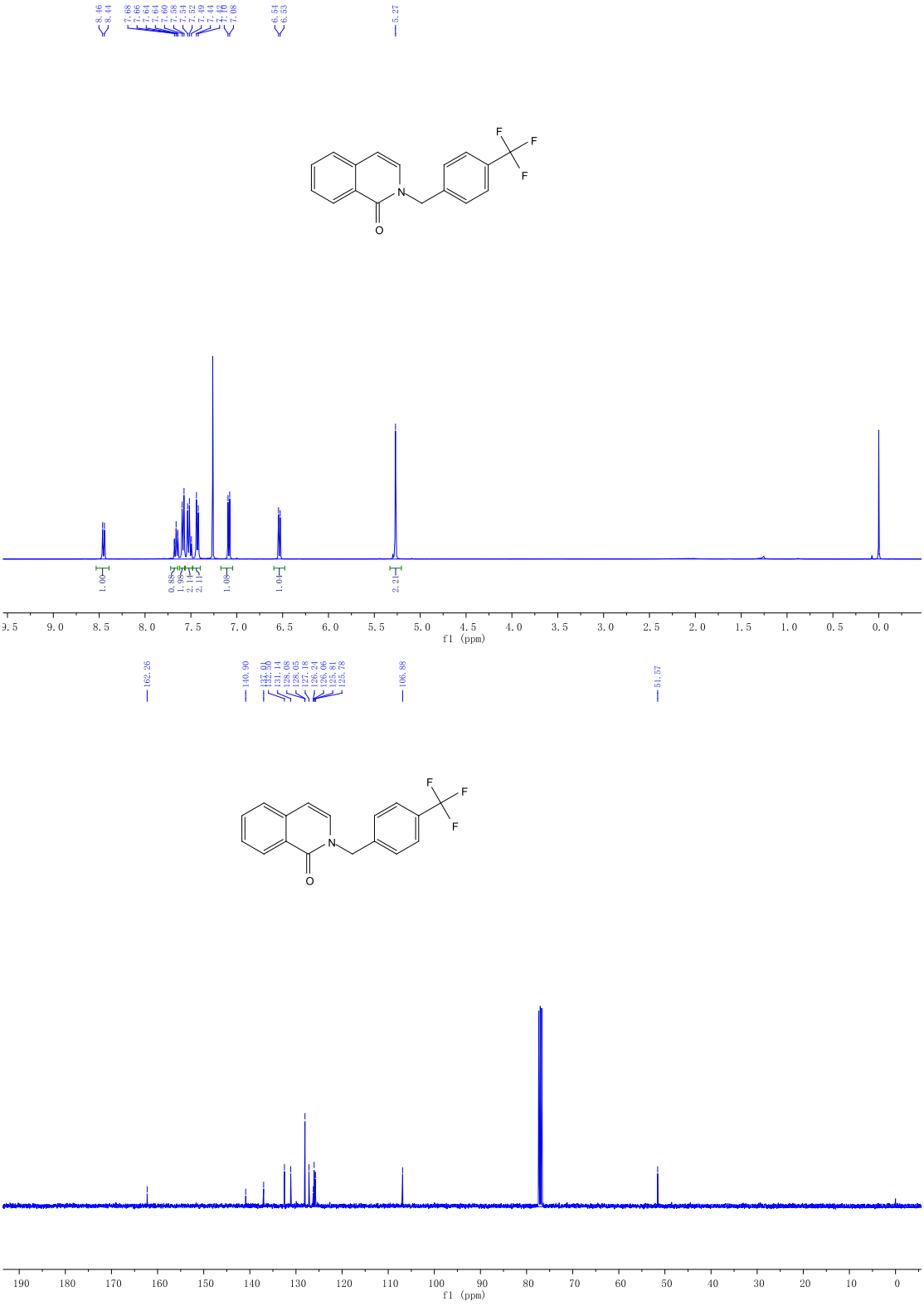
132.34
131.12
129.81
129.72
128.05
127.03
115.85
115.61
106.63
51.19
F
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.44
7.68
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7.64
7.60
7.58
7.54
7.52
7.49
7.44
7.42
7.10
7.08
6.54
6.53
5.27
F
F
F
N
O
1.00
0.88
1.96
2.17
2.14
1.08
1.04
2.21
f1 (ppm)
162.26
140.90
137.01
135.58
131.14
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128.05
127.18
126.74
126.06
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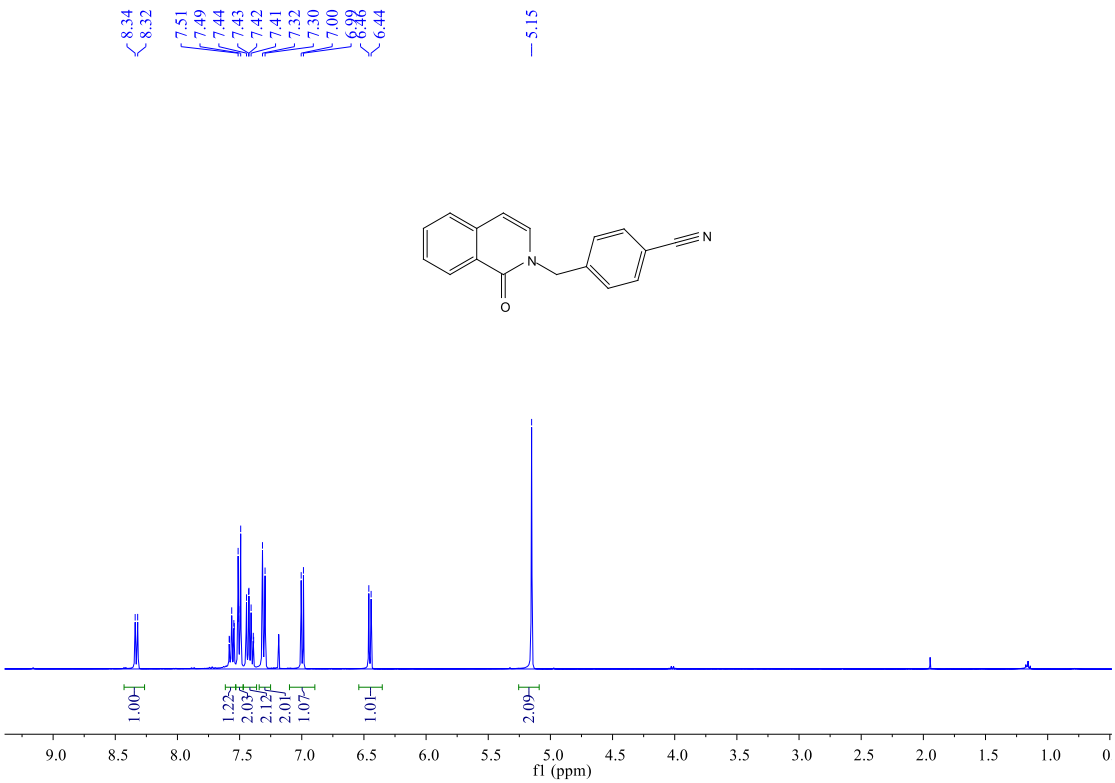
125.78
106.88
51.57
f1 (ppm)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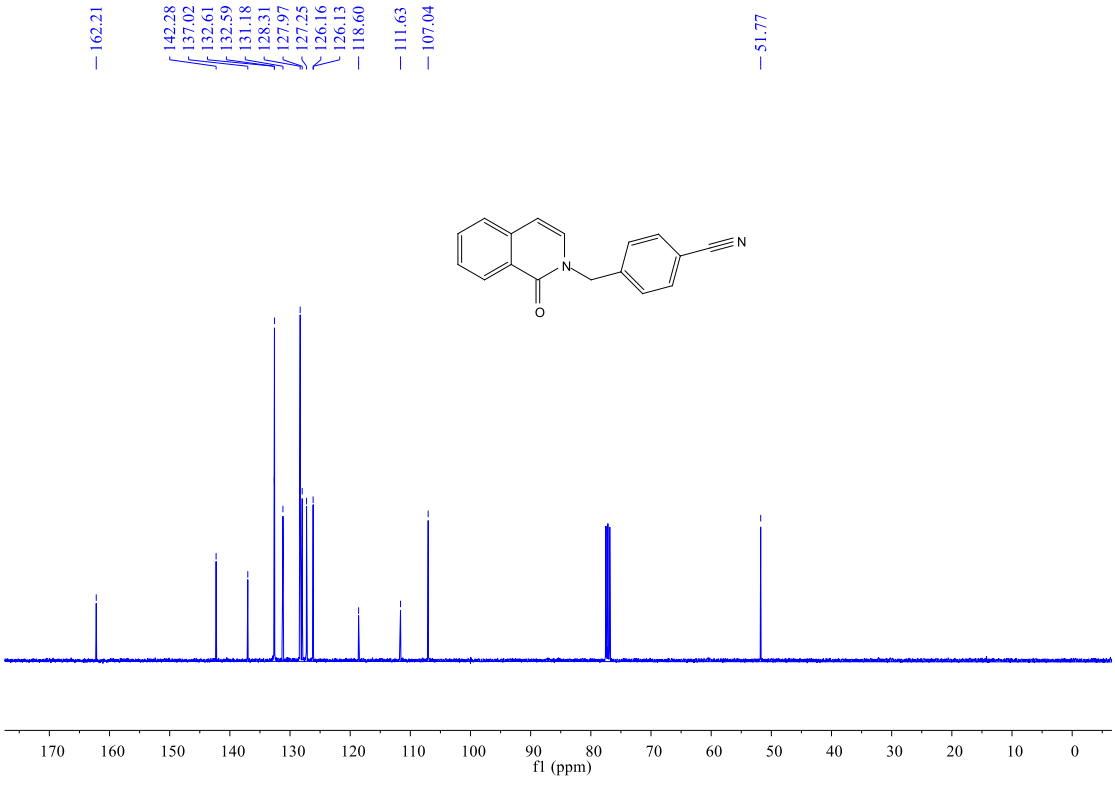
7.42
7.41
7.32
7.30
7.00
6.99
6.46
6.44
5.15
N
O
1.00
1.22
2.03
2.12
2.01
1.07
1.01
2.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0
f1 (ppm)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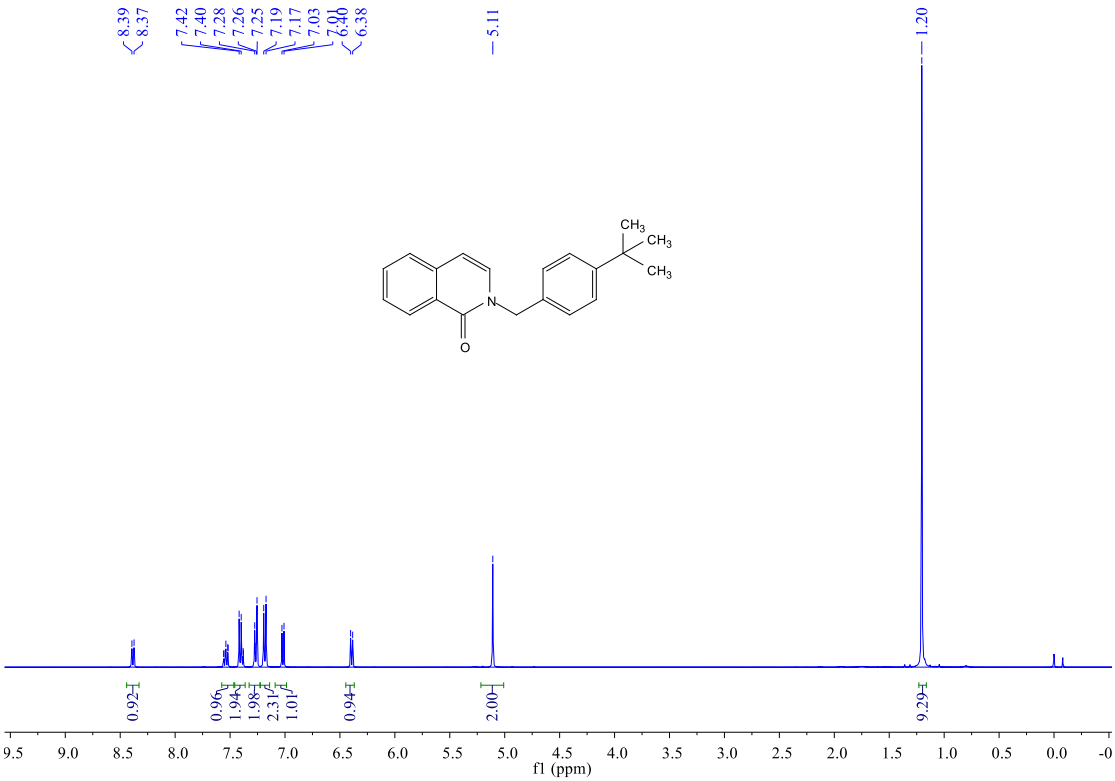
132.61
132.59
131.18
128.31
127.97
127.25
126.16
126.13
118.60
111.63
107.04
51.77
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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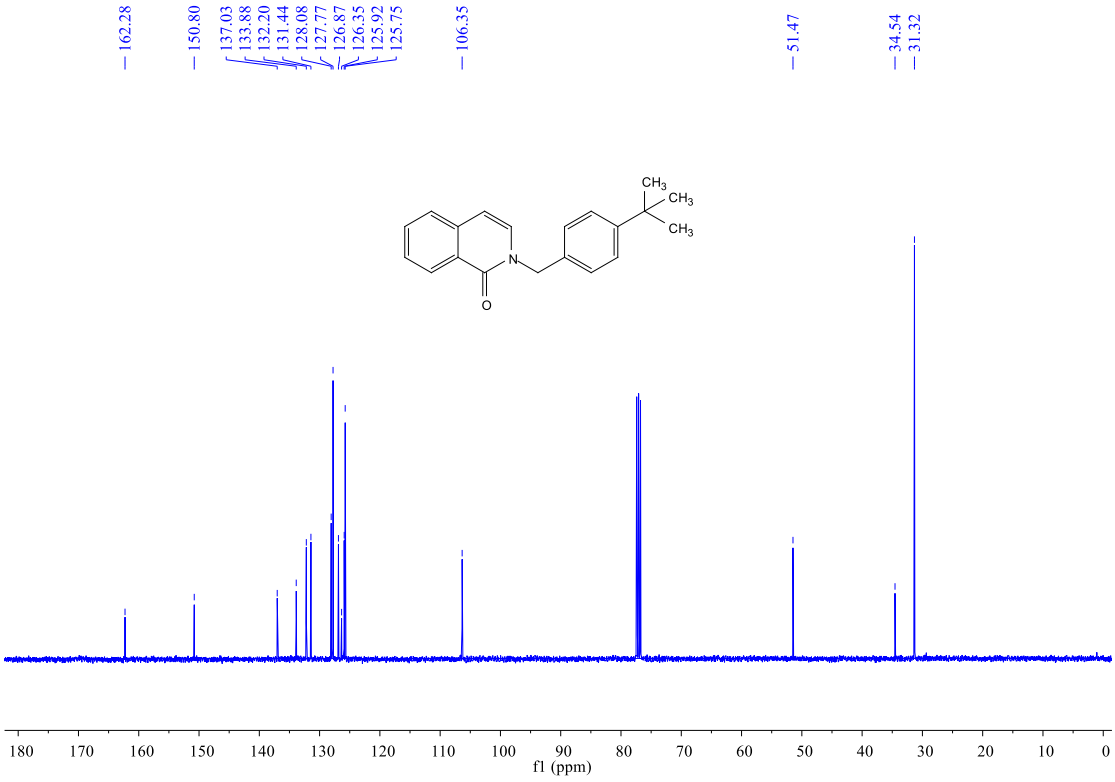
8.37
7.42
7.40
7.28
7.26
7.25
7.19
7.17
7.03
7.01
6.40
6.38
5.11
1.20
CH3
CH3
CH3
N
O
0.92
0.96
1.94
1.98
2.31
1.01
0.94
2.00
9.29
f1 (ppm)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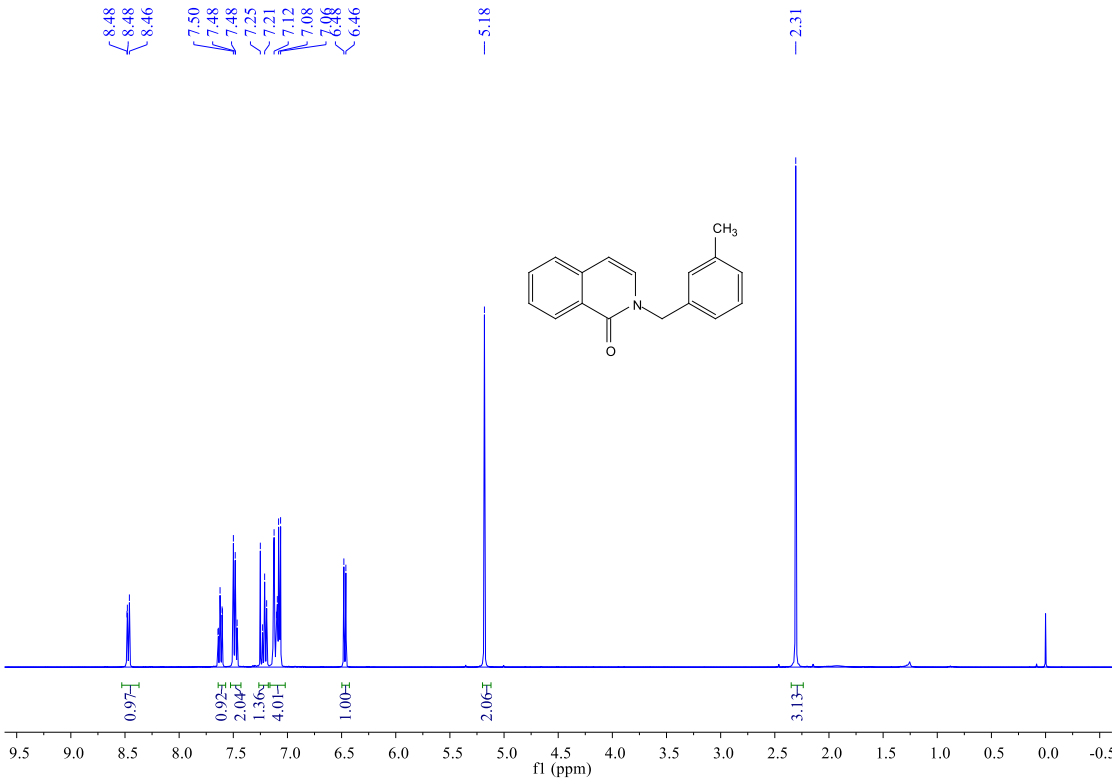
132.20
131.44
128.08
127.77
126.87
126.35
125.92
125.75
106.35
51.47
34.54
31.32
CH3
CH3
CH3
N
O
f1 (ppm)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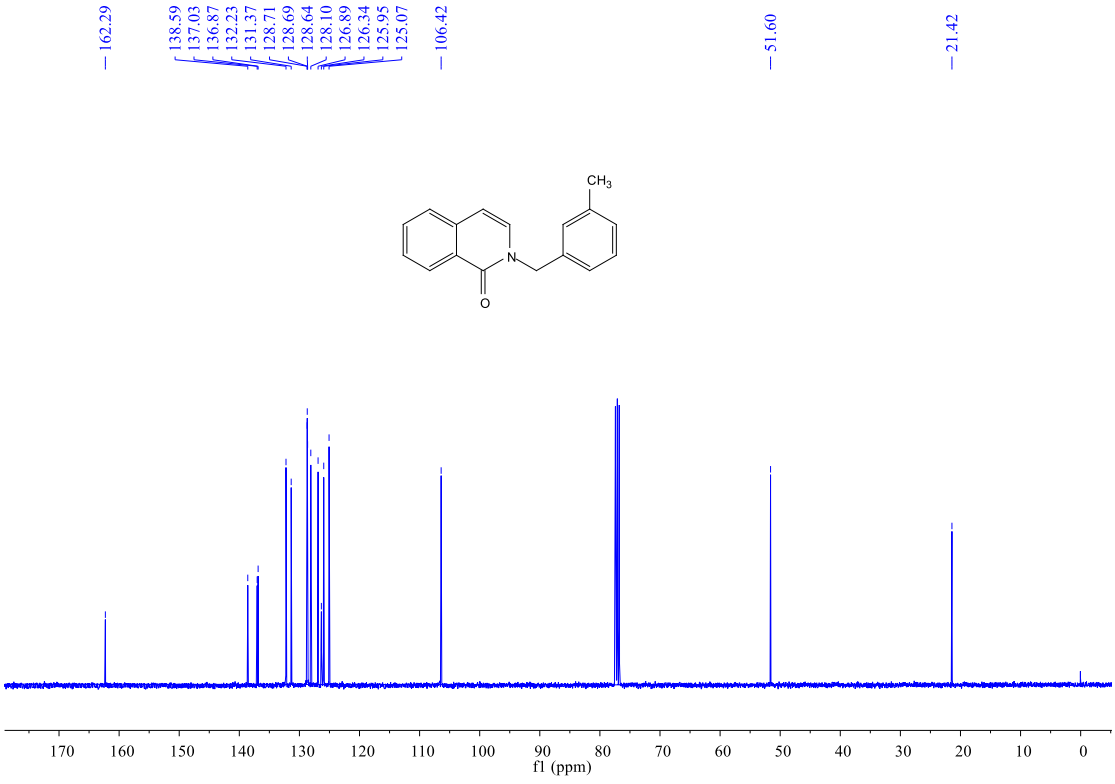
8.48
8.46
7.50
7.48
7.48
7.25
7.21
7.12
7.08
6.48
6.46
5.18
2.31
CH3
N
O
0.97
0.92
2.04
1.36
4.01
1.00
2.06
3.13
f1 (ppm)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138.59
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132.23
131.37
128.71
128.69
128.64
128.10
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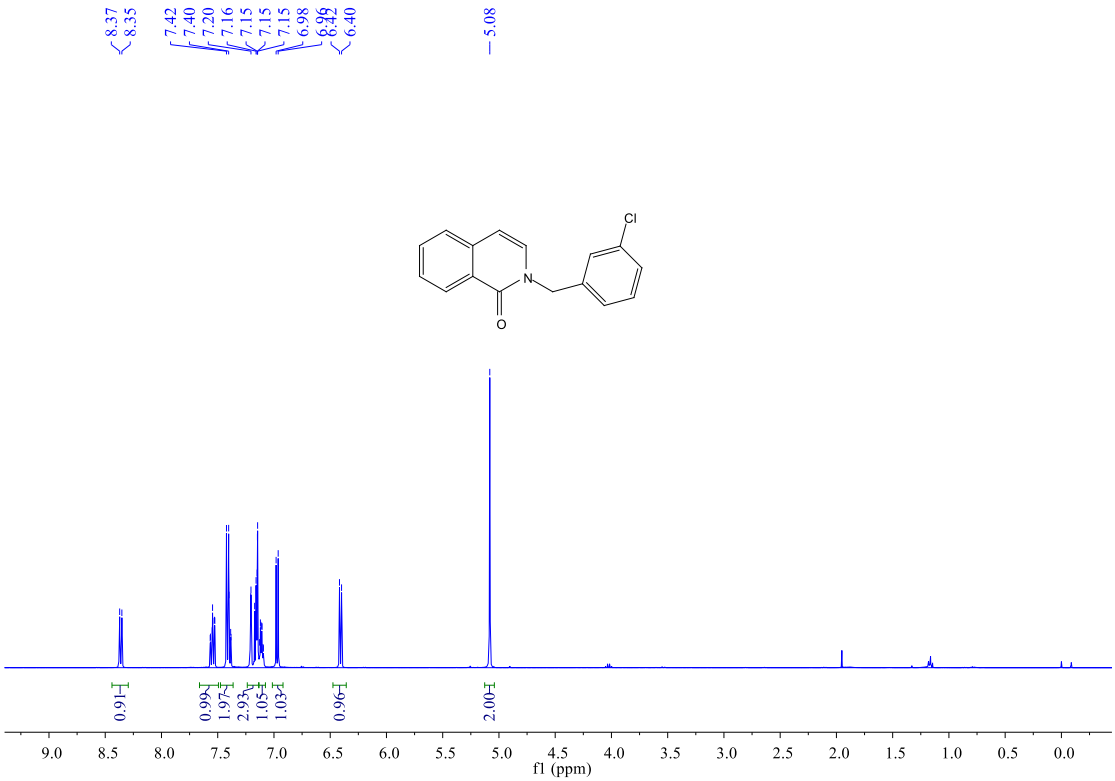
126.34
125.95
125.07
106.42
51.60
21.42
CH3
N
O
f1 (ppm)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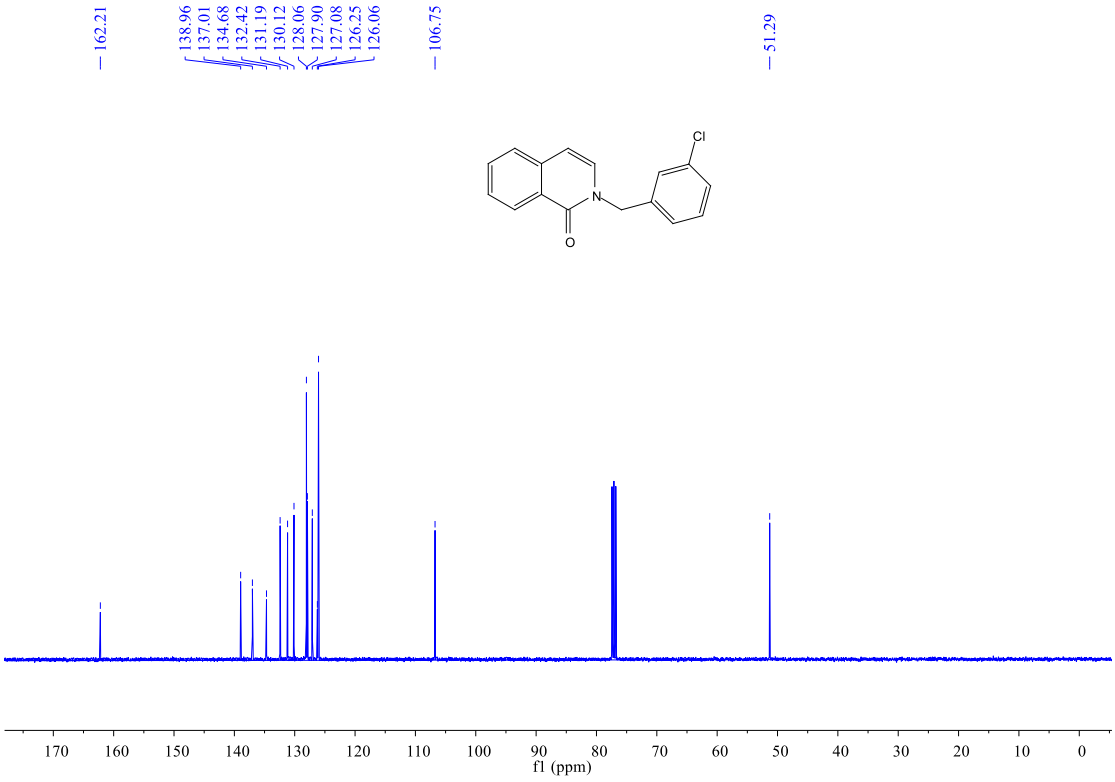
8.35
7.42
7.40
7.20
7.16
7.15
7.15
7.15
6.98
6.96
6.42
6.40
5.08
Cl
N
O
0.91
0.99
1.97
2.93
1.05
1.03
0.96
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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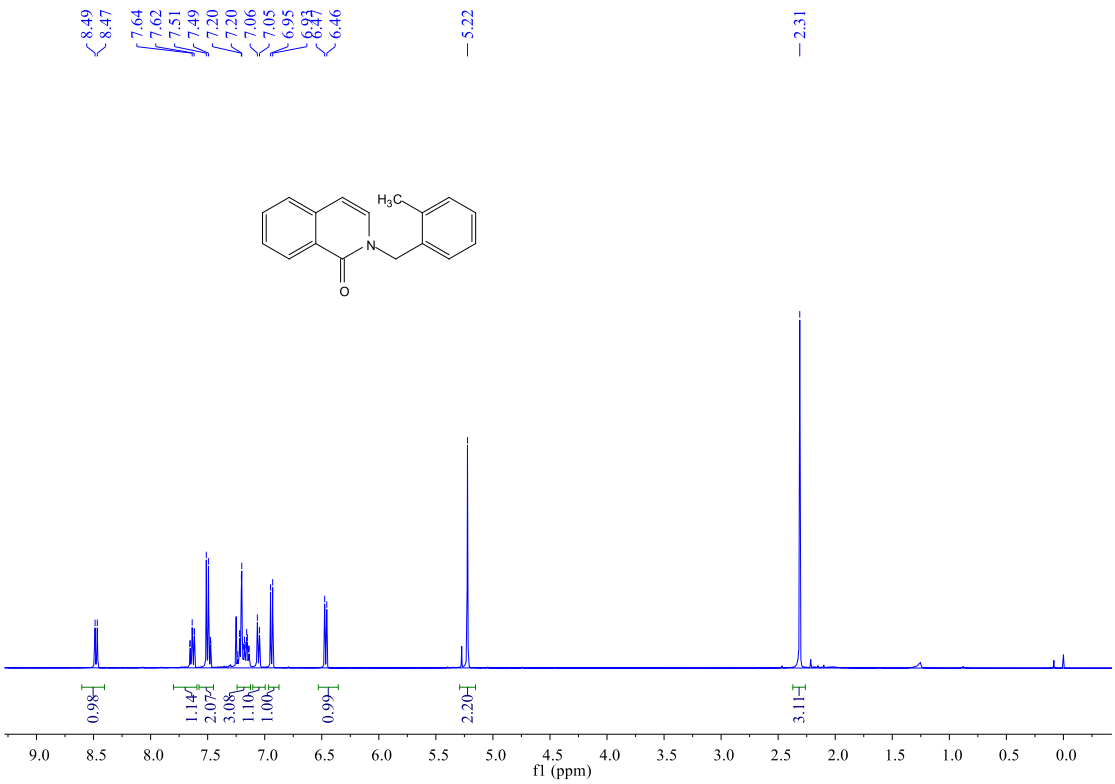
138.96
137.01
134.68
132.42
131.19
130.12
128.06
127.90
127.08
126.25
126.06
106.75
51.29
Cl
N
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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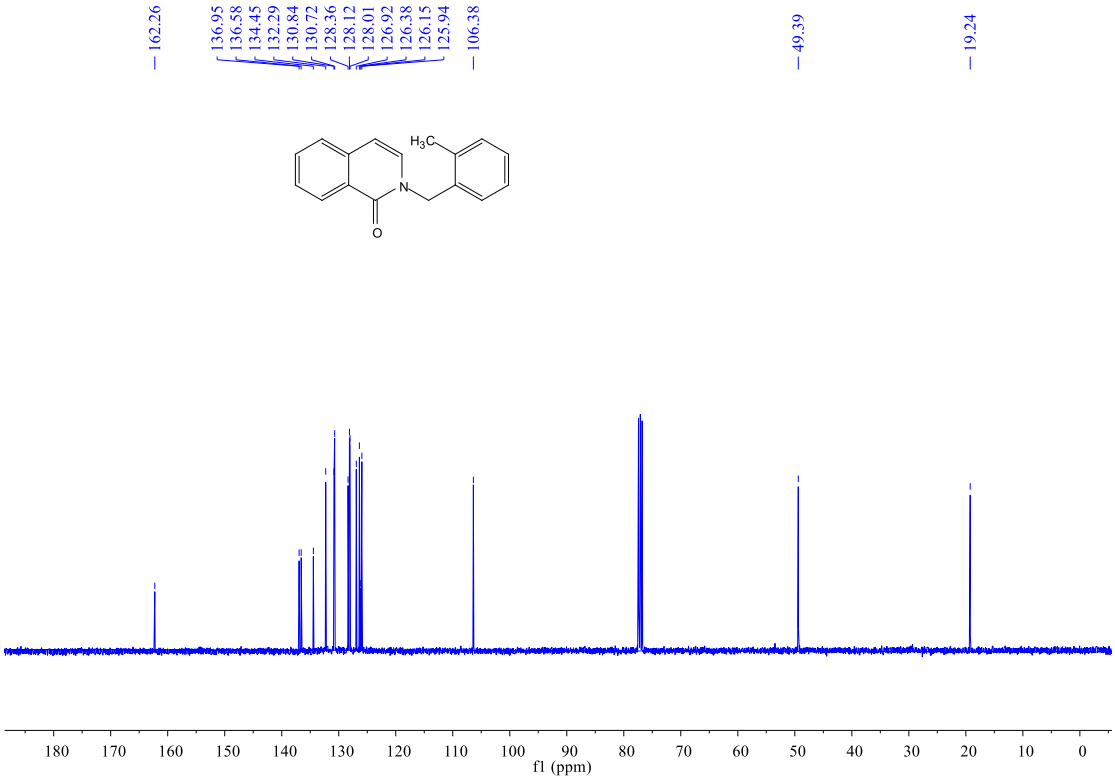
8.47
7.64
7.62
7.51
7.49
7.20
7.20
7.06
7.05
6.95
6.93
6.47
6.46
5.22
2.31
H3C
N
O
0.98
1.14
2.07
3.08
1.10
1.00
0.99
2.20
3.11
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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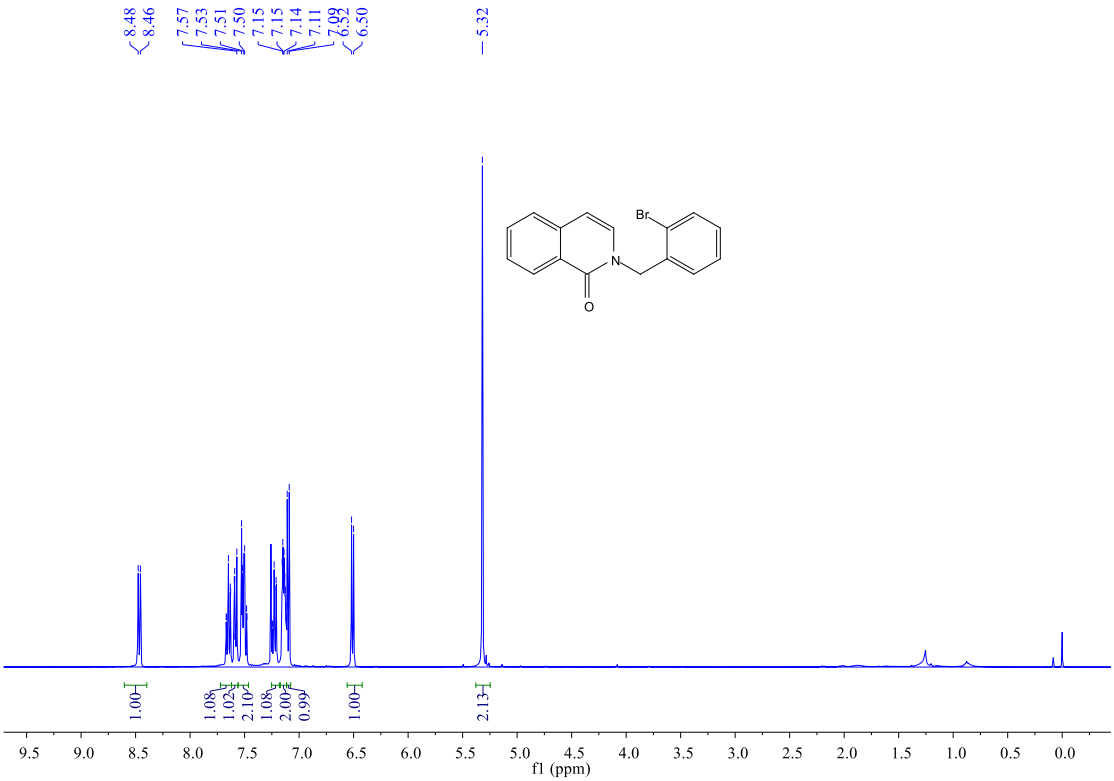
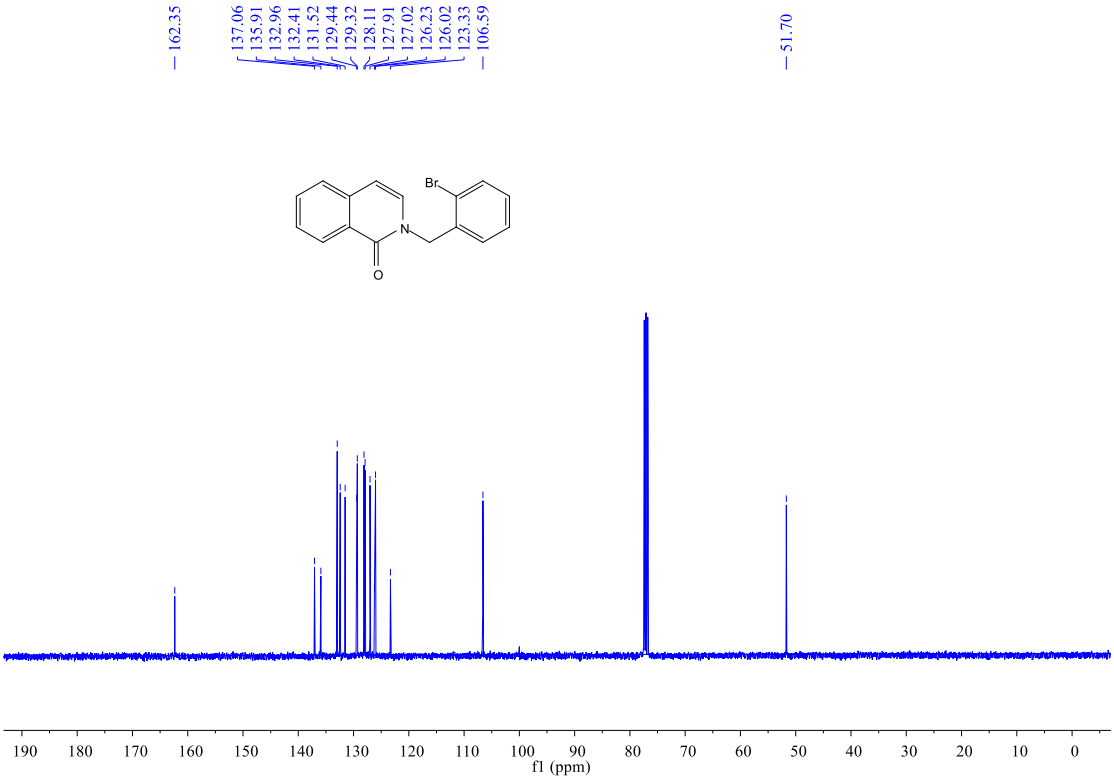
132.29
130.84
130.72
128.36
128.12
128.01
126.92
126.38
126.15
125.94
106.38
49.39
19.24
H3C
N
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.48
8.46
7.57
7.53
7.51
7.50
7.15
7.15
7.14
7.11
7.09
6.52
6.50
5.32
Br
N
O
1.00
1.08
1.02
2.10
1.08
2.00
0.99
1.00
2.13
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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137.06
135.91
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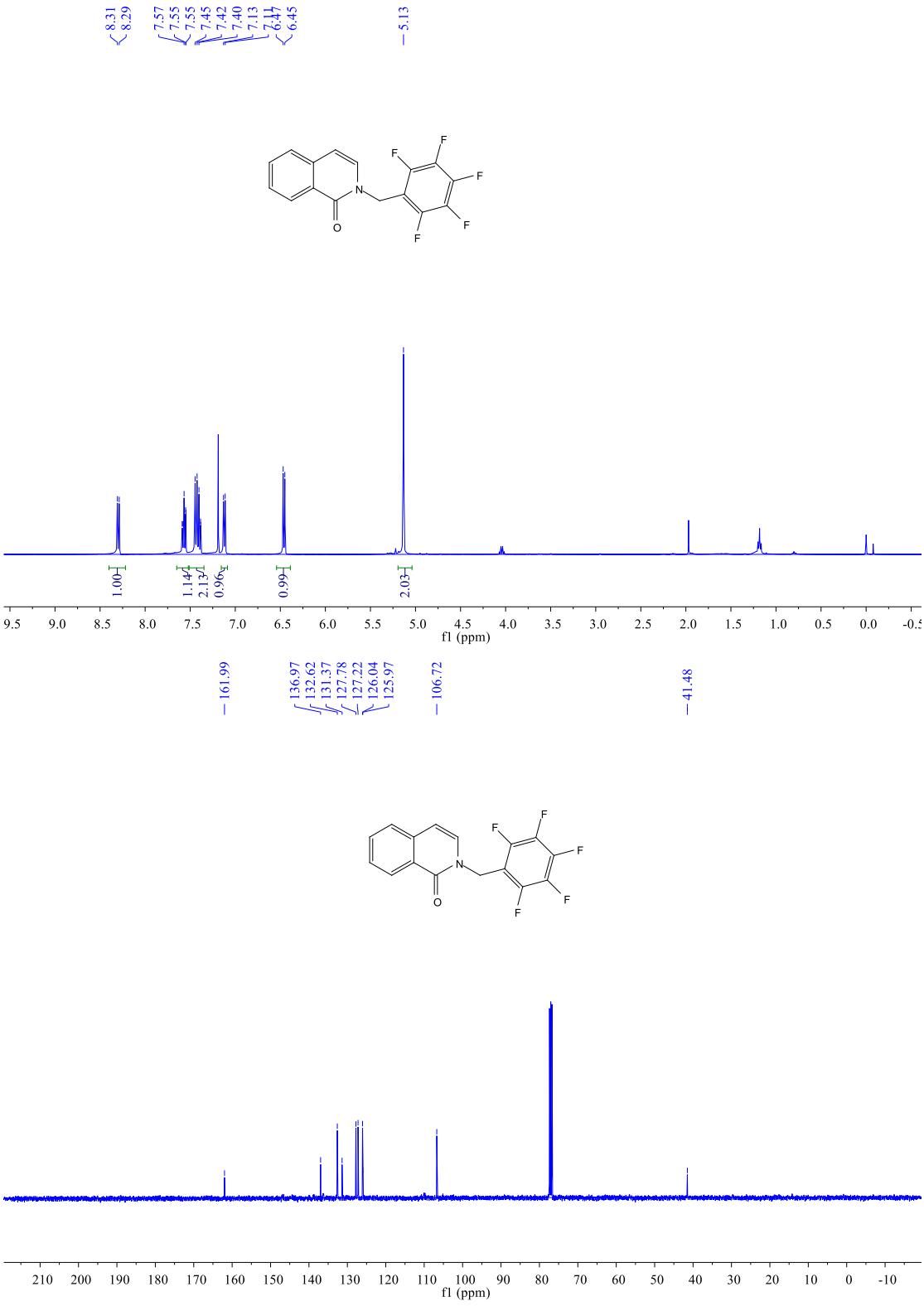
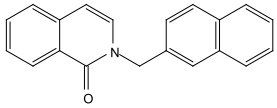
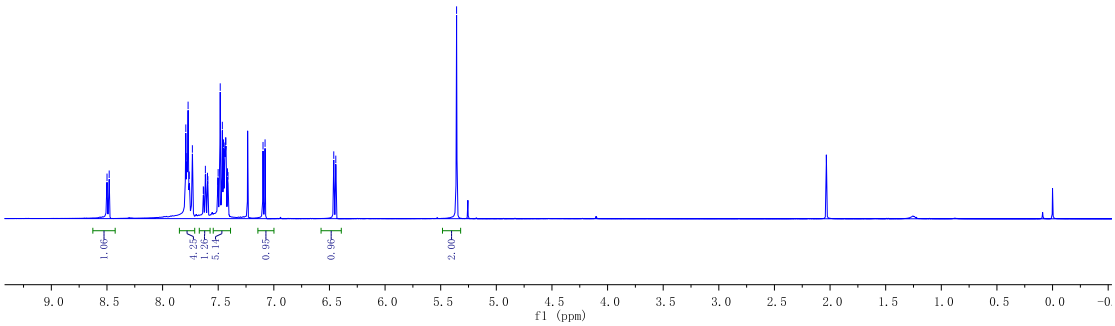
132.41
131.52
129.44
129.32
128.11
127.91
127.02
126.23
126.02
123.33
106.59
51.70
Br
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.31
8.29
7.57
7.55
7.55
7.45
7.42
7.40
7.13
7.11
6.47
6.45
5.13
F
F
F
F
F
N
O
1.00
1.14
2.13
0.96
0.99
2.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
161.99
136.97
132.62
131.37
127.78
127.22
126.04
125.97
106.72
41.48
F
F
F
F
F
N
O
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)


8.50
8.48
7.79
7.77
7.73
7.48
7.46
7.45
7.45
7.44
7.44
7.44
7.43
7.43
7.10
7.08
6.46
6.44
5.36


N
O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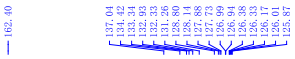
4.24
1.26
5.14
0.95
0.96
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)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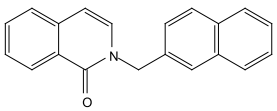
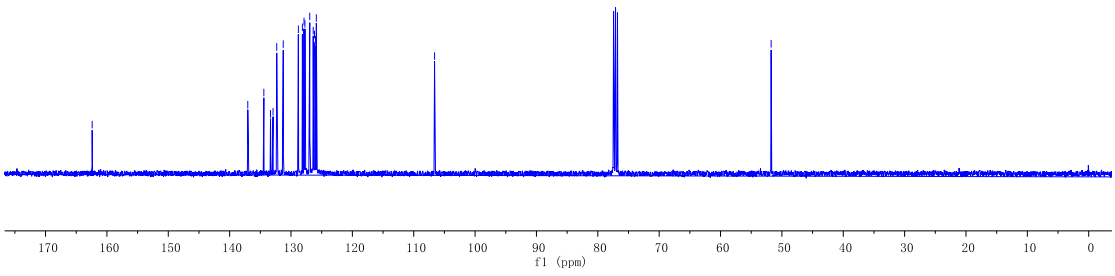
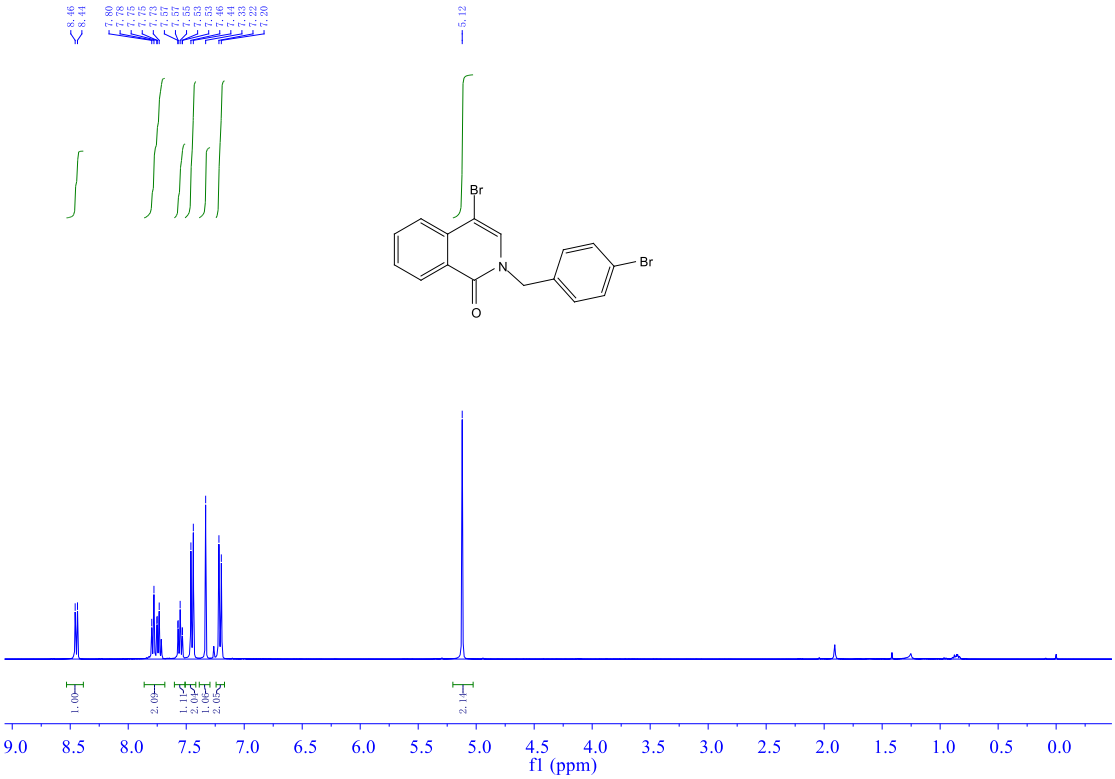
132.33
131.26
128.80
128.14
127.88
127.73
126.99
126.94
126.38
126.33
126.17
126.01
125.87

106.60

51.75


N
O


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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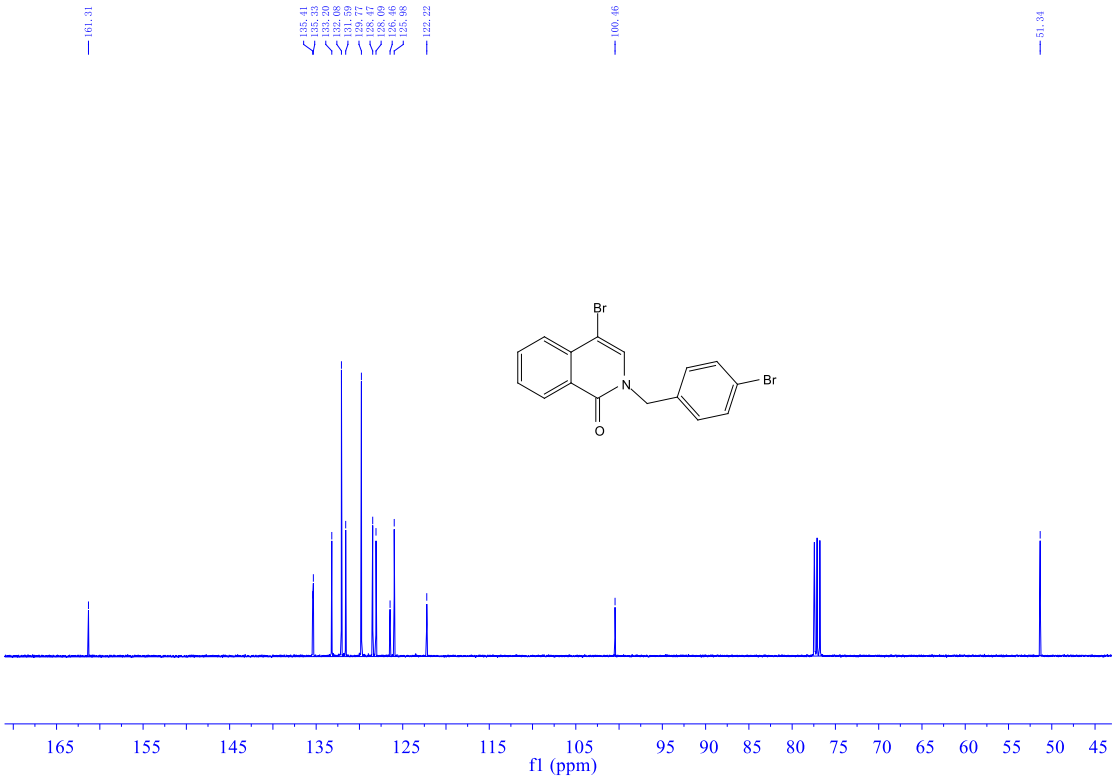
8.44
7.80
7.78
7.75
7.75
7.73
7.73
7.57
7.57
7.55
7.55
7.53
7.53
7.46
7.44
7.33
7.22
7.20
5.12
Br
Br
N
O
1.00
2.09
1.12
2.04
1.06
2.05
2.14
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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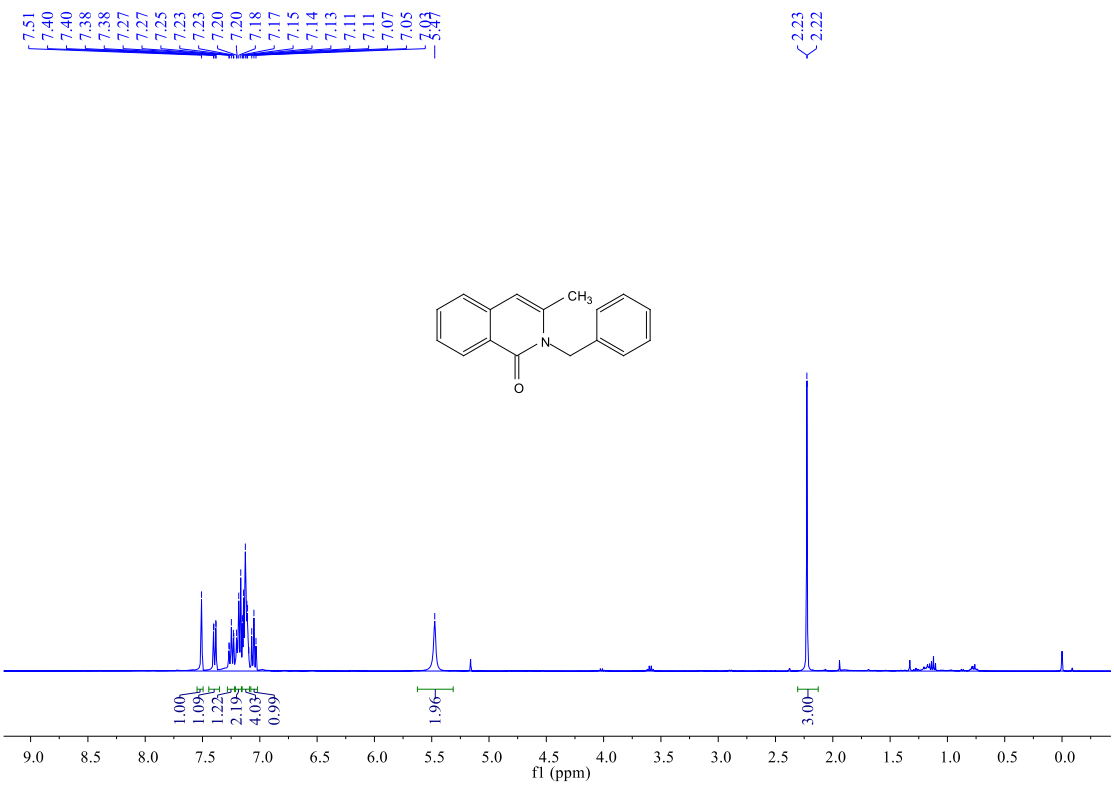
132.98
131.59
129.77
128.47
128.09
126.46
125.98
122.22
100.46
51.34
Br
Br
N
O
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
f1 (ppm)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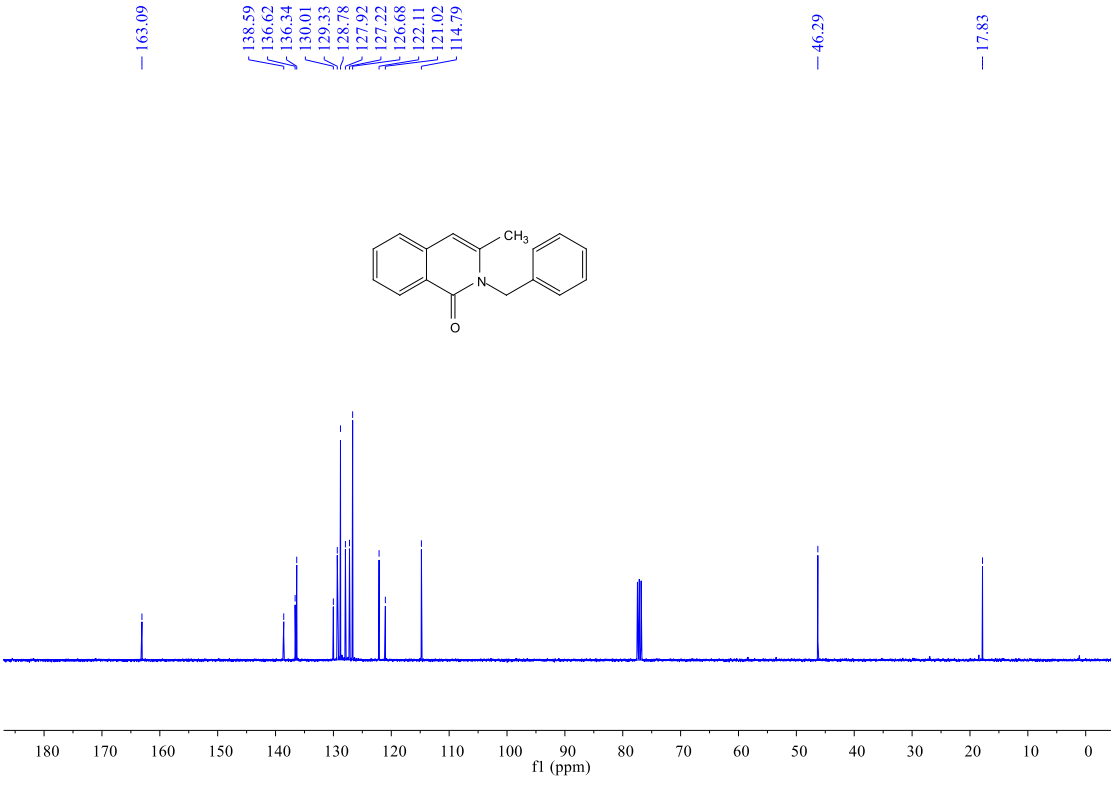
7.27
7.25
7.23
7.23
7.20
7.20
7.18
7.17
7.15
7.14
7.13
7.11
7.11
7.07
7.05
5.47
2.23
2.22
CH3
N
O
1.00
1.09
1.22
2.19
4.03
0.99
1.96
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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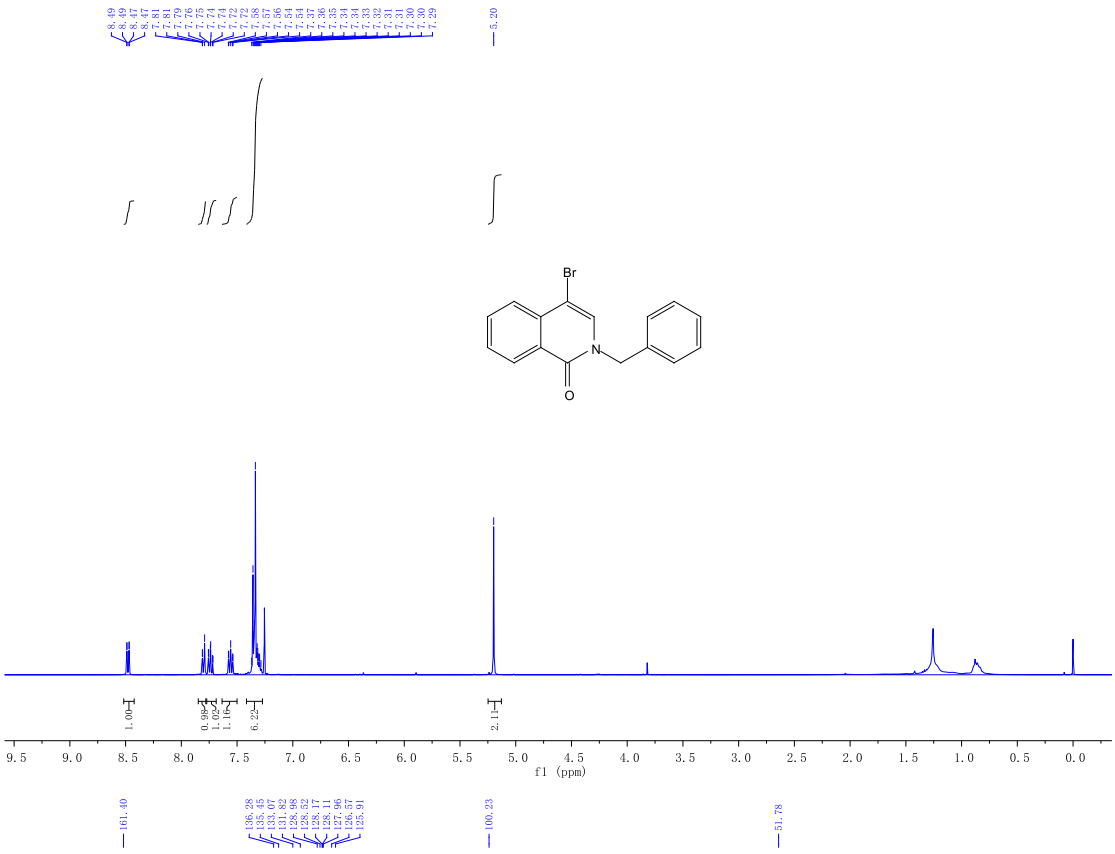
136.34
130.01
129.33
128.78
127.92
127.22
126.68
122.11
121.02
114.79
46.29
17.83
CH3
N
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.49
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8.47
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7.76
7.75
7.74
7.74
7.72
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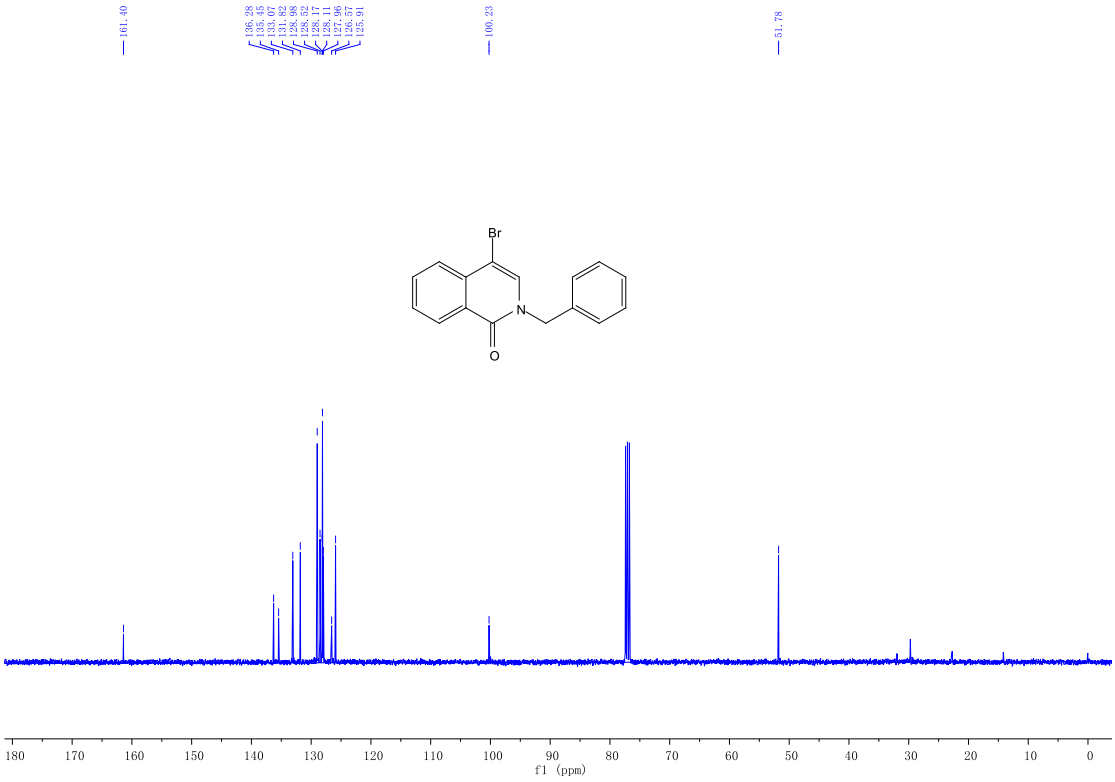
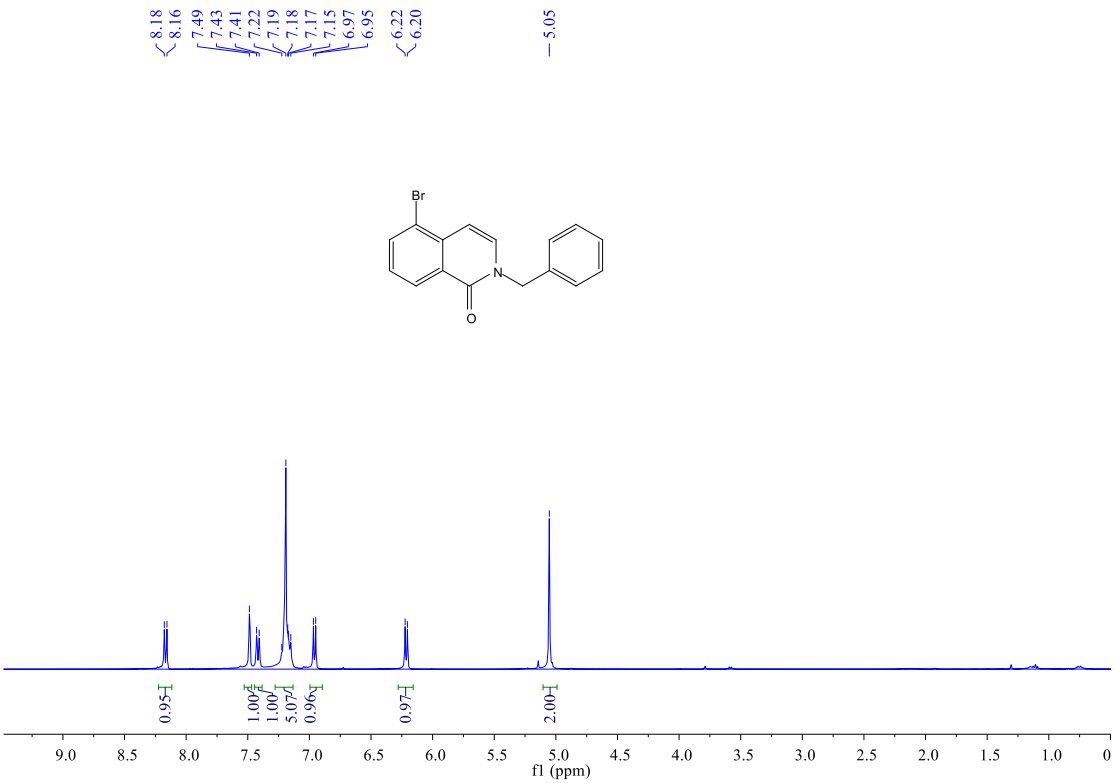
7.36
7.35
7.34
7.34
7.33
7.33
7.31
7.31
7.30
7.30
7.29
7.29
5.20
Br
N
O
1.00
0.98
1.02
1.10
6.22
2.11
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.40
136.28
135.45
133.07
131.82
131.36
128.52
128.17
128.11
127.86
126.57
125.91
100.23
51.78
Br
N
O
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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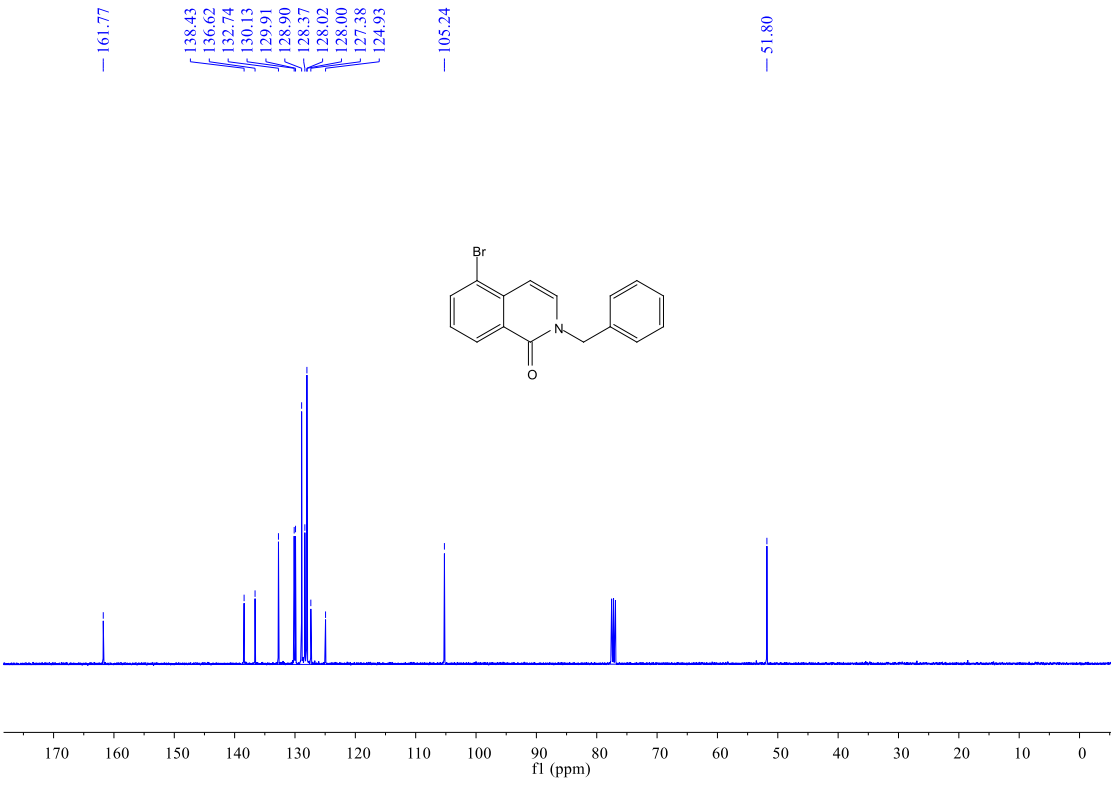
7.41
7.22
7.19
7.18
7.17
7.15
6.97
6.95
6.22
6.20
5.05
Br
N
O
0.95
1.00
1.00
5.07
0.96
0.97
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0
f1 (ppm)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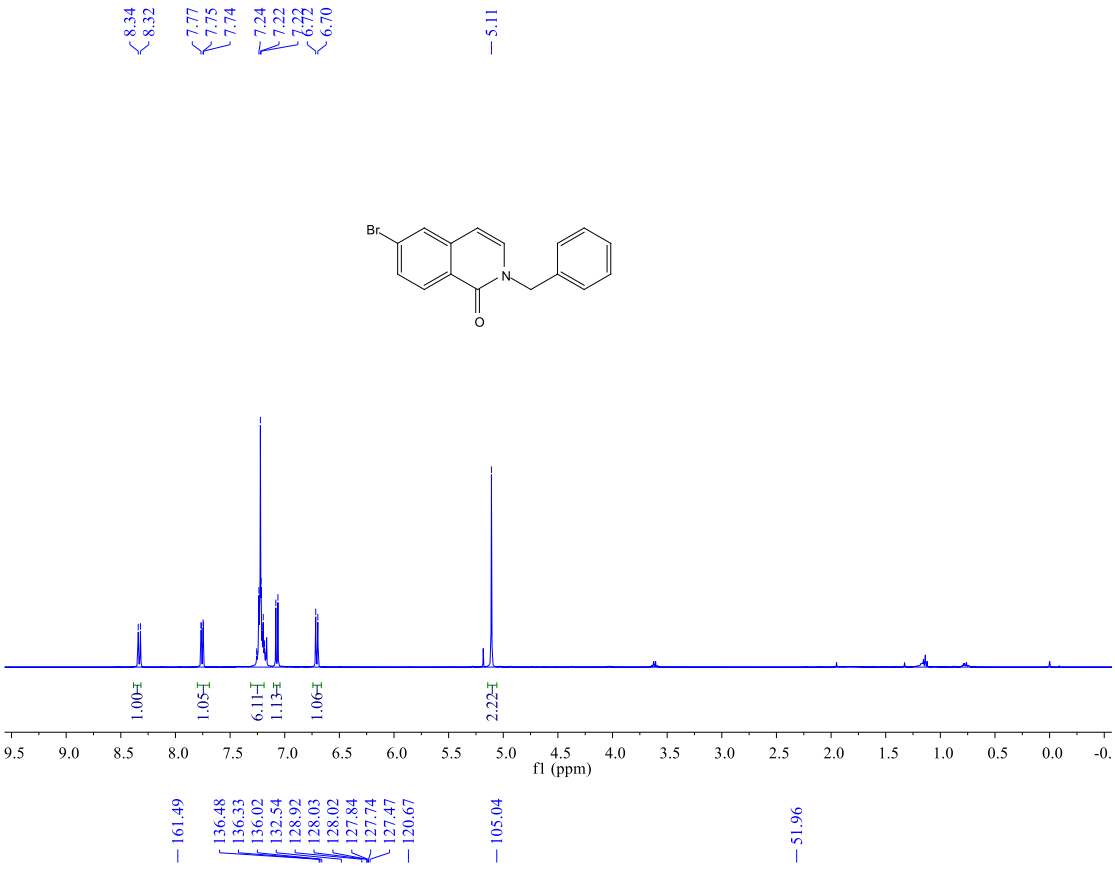
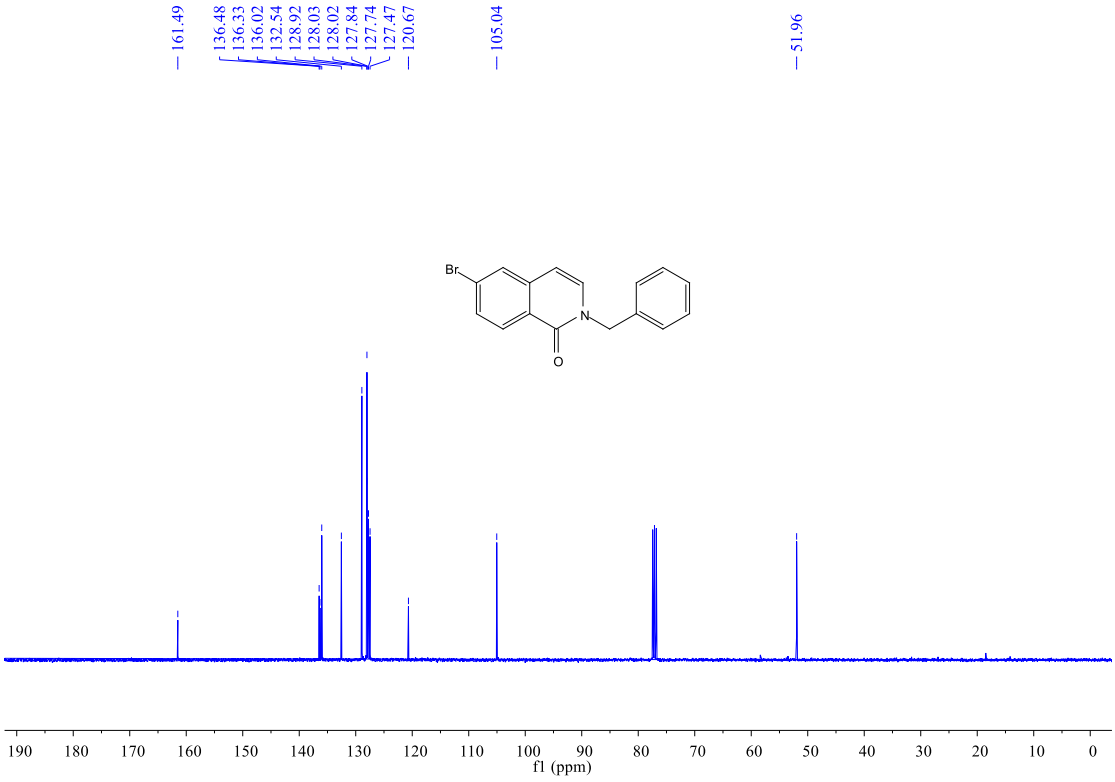
138.43
136.62
132.74
130.13
129.91
128.90
128.37
128.02
128.00
127.38
124.93
105.24
51.80
Br
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.34
8.32
7.77
7.75
7.74
7.24
7.22
7.22
6.72
6.70
5.11
Br
N
O
1.00
1.05
6.11
1.13
1.06
2.22
fl (ppm)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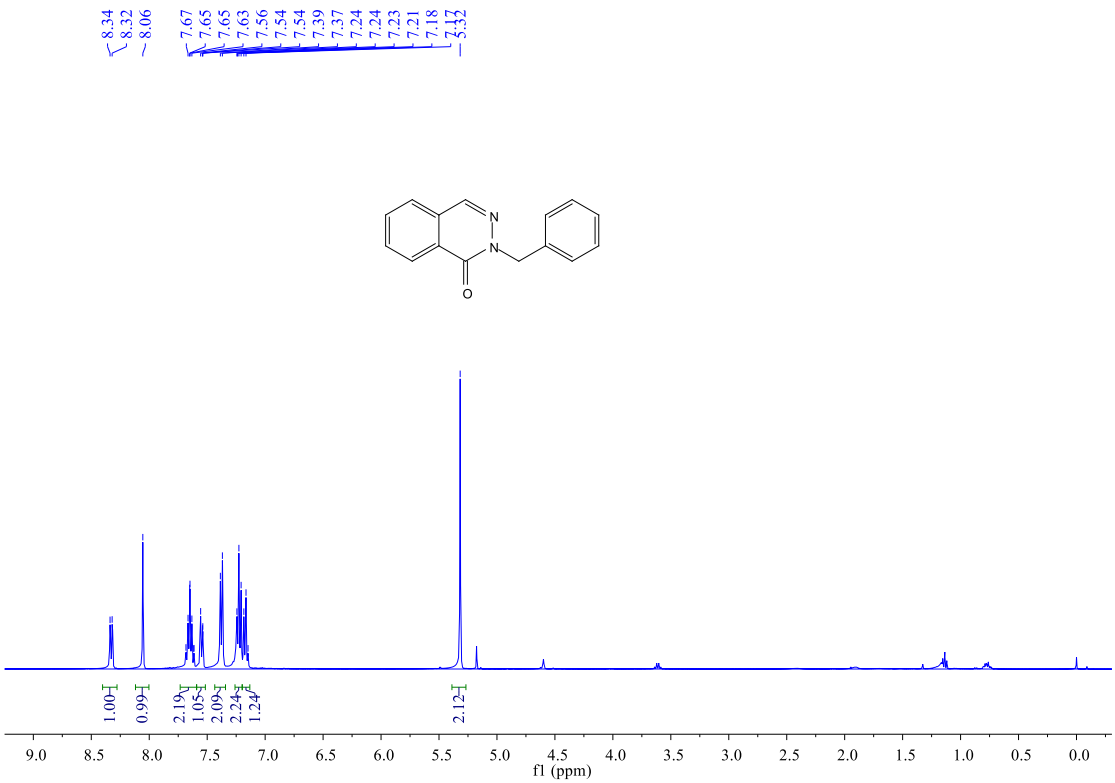
136.48
136.33
136.02
132.54
128.92
128.03
128.02
127.84
127.74
127.47
120.67
105.04
51.96
Br
N
O
fl (ppm)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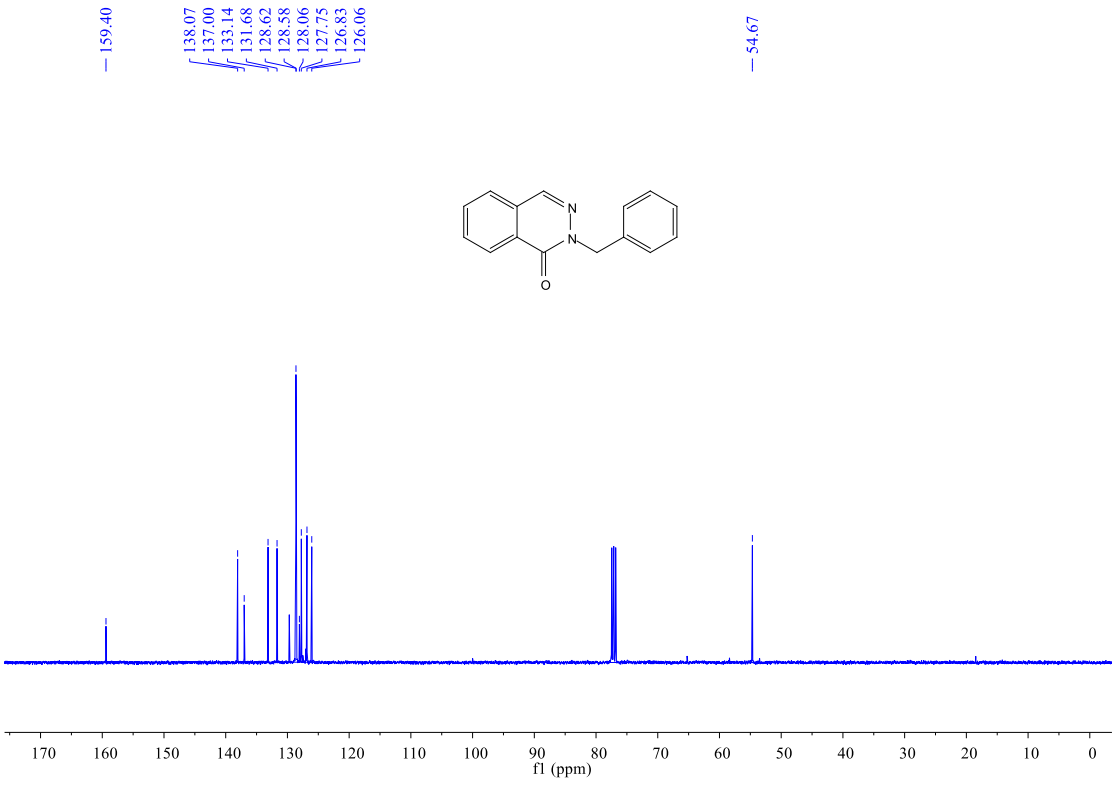
8.32
8.06
7.67
7.65
7.65
7.63
7.56
7.54
7.54
7.39
7.37
7.24
7.24
7.23
7.21
7.18
5.32
N
N
O
1.00
0.99
2.19
1.05
2.09
2.24
1.24
2.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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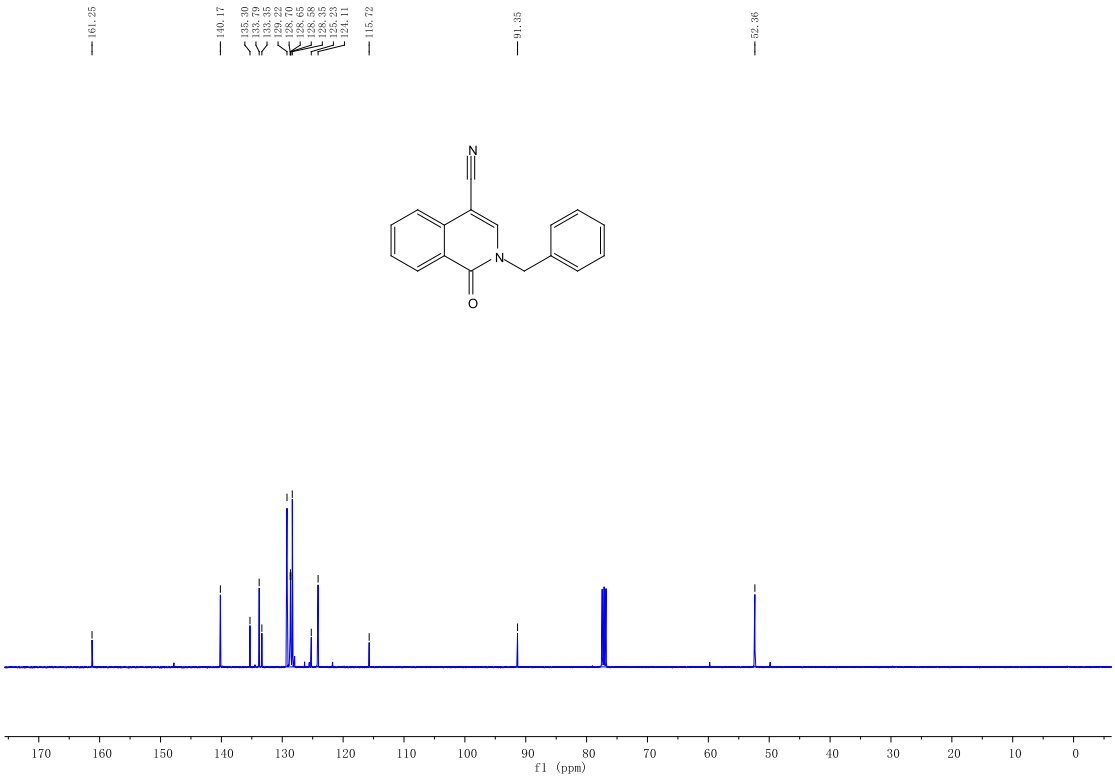
138.07
137.00
133.14
131.68
128.62
128.58
128.06
127.75
126.83
126.06
54.67
N
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.36
8.34
7.70
7.69
7.63
7.53
7.52
7.51
7.50
7.49
7.30
7.28
7.27
7.26
7.25
7.24
7.23
5.14
N
N
O
1.00
2.15
1.04
1.14
5.39
2.14
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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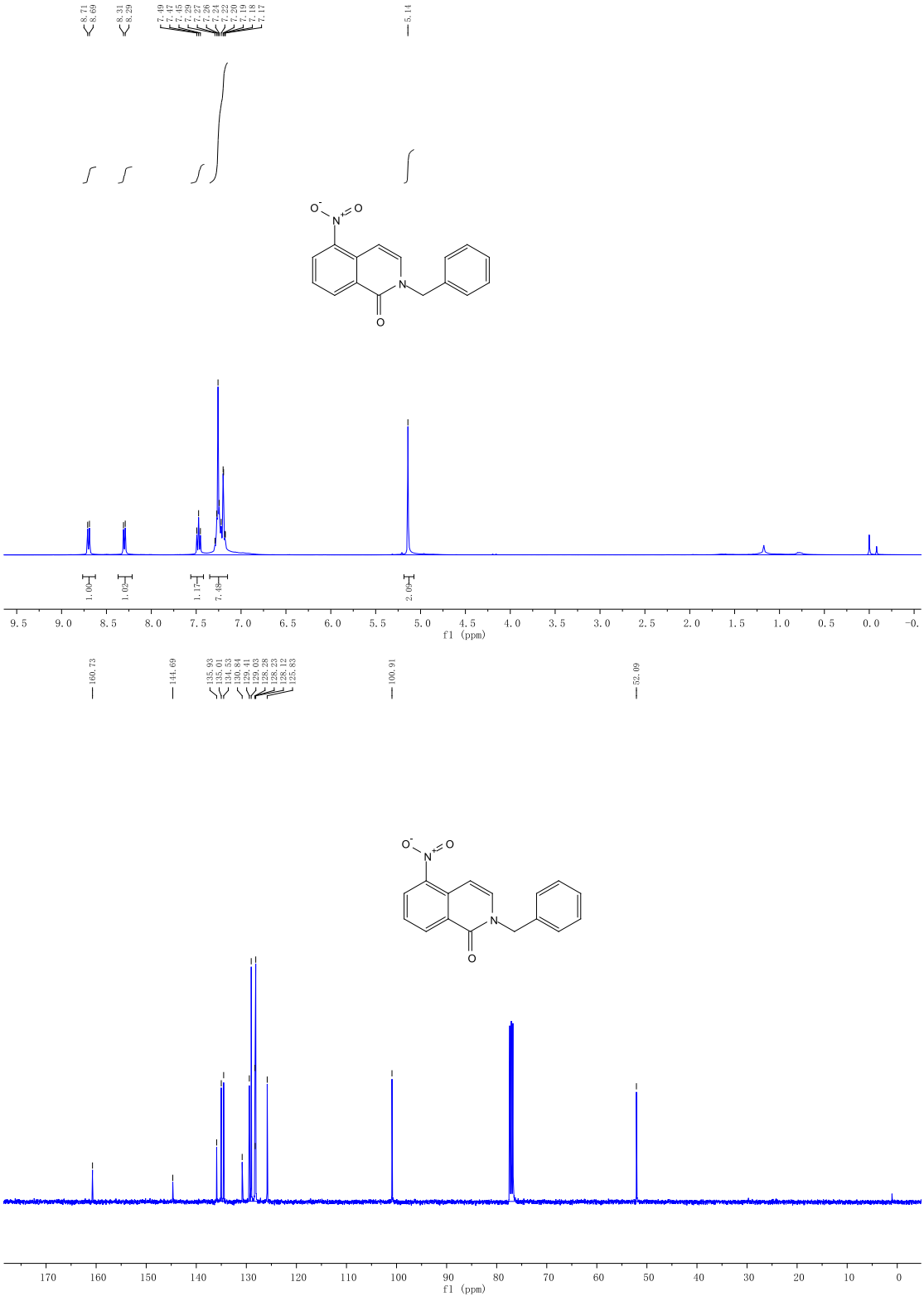
140.17
135.30
133.79
133.15
129.22
128.70
128.65
128.38
128.35
125.23
124.11
115.72
91.35
52.36
N
N
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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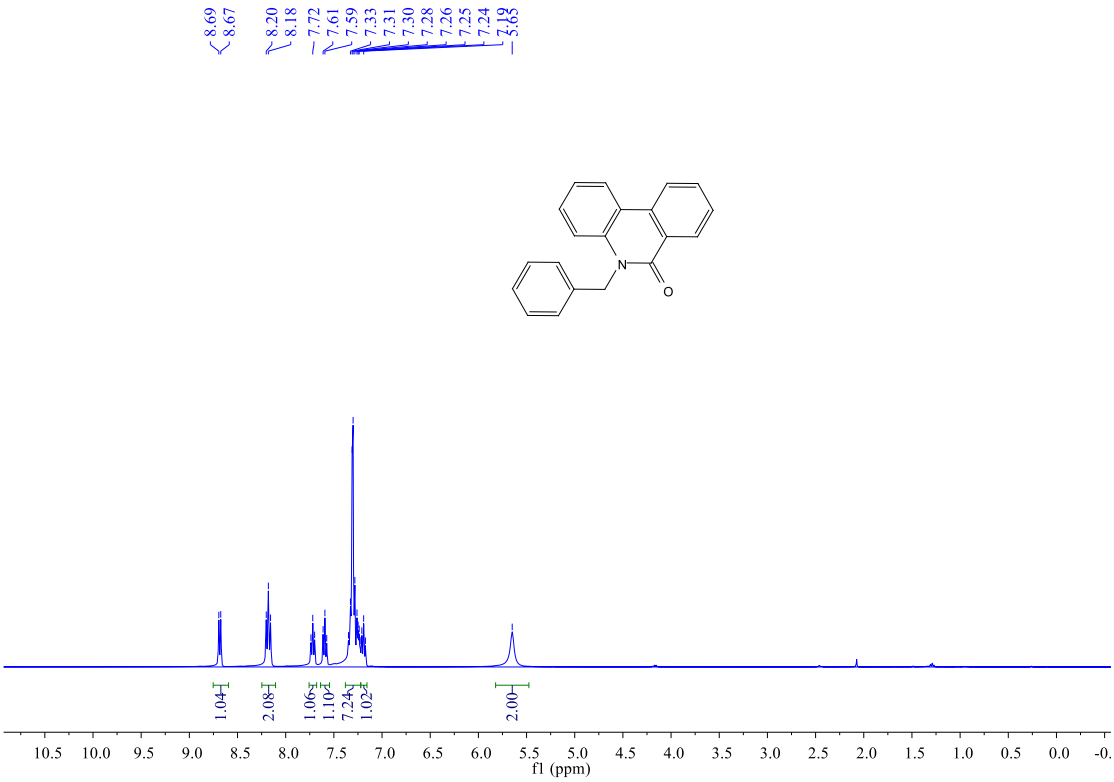
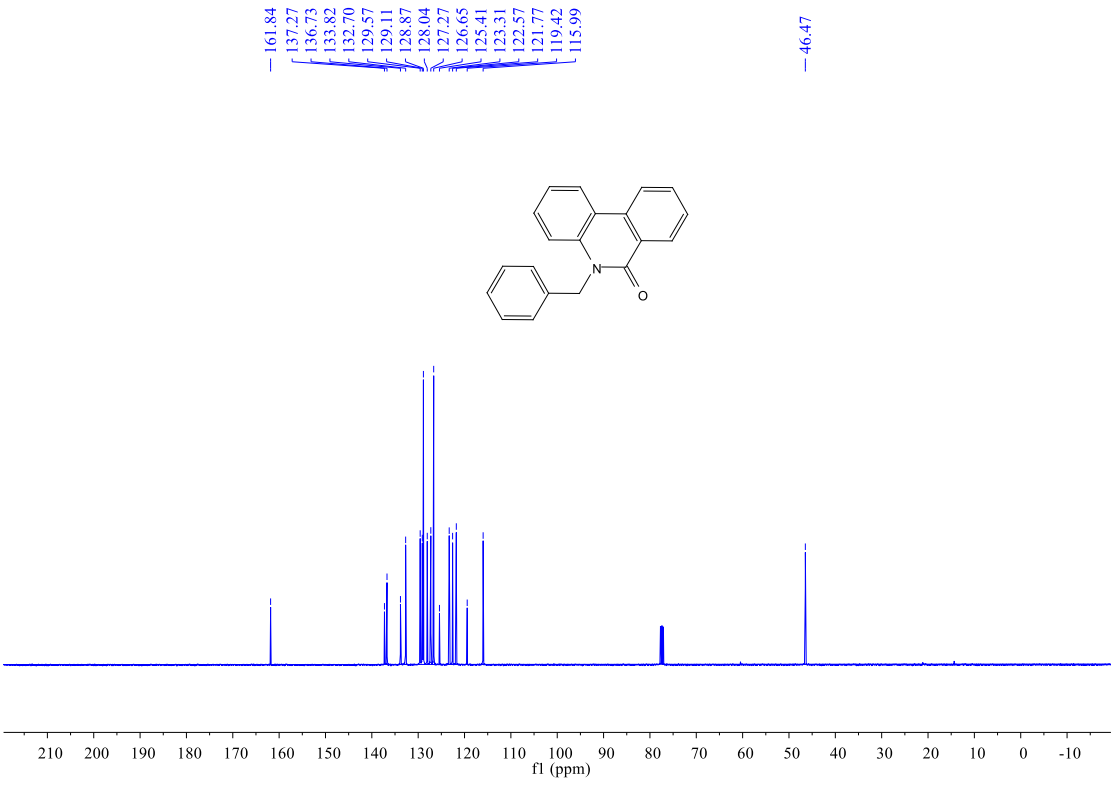
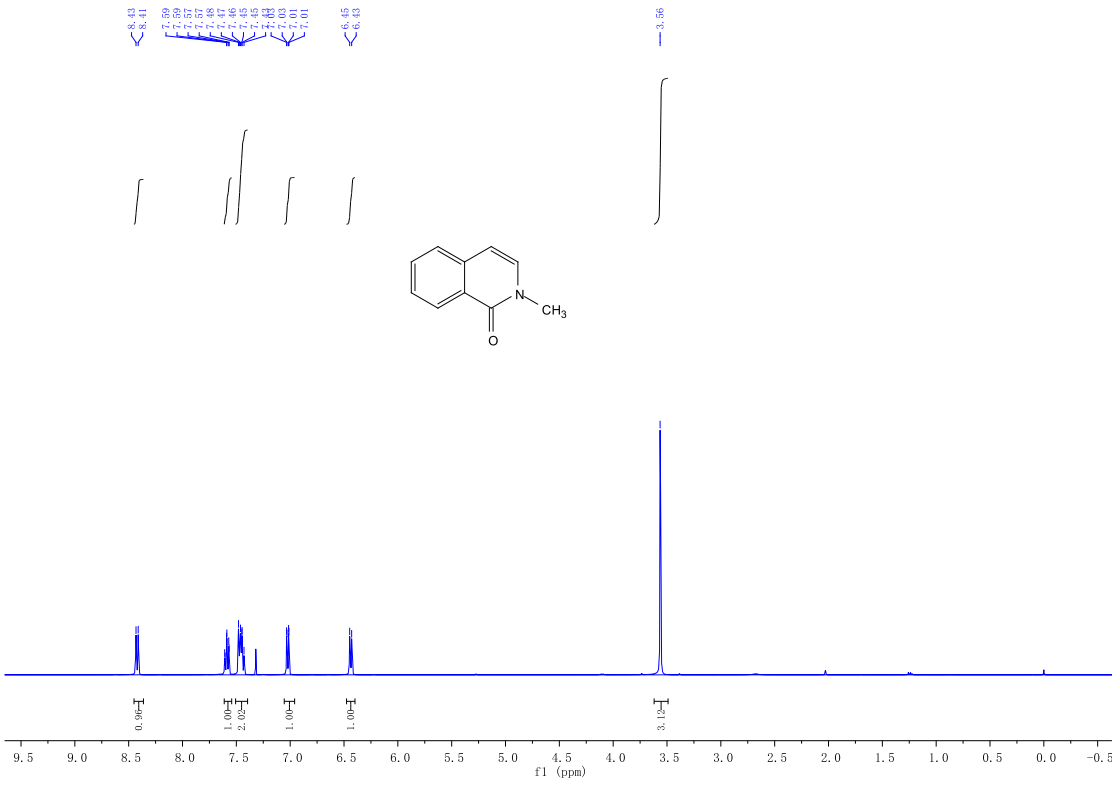
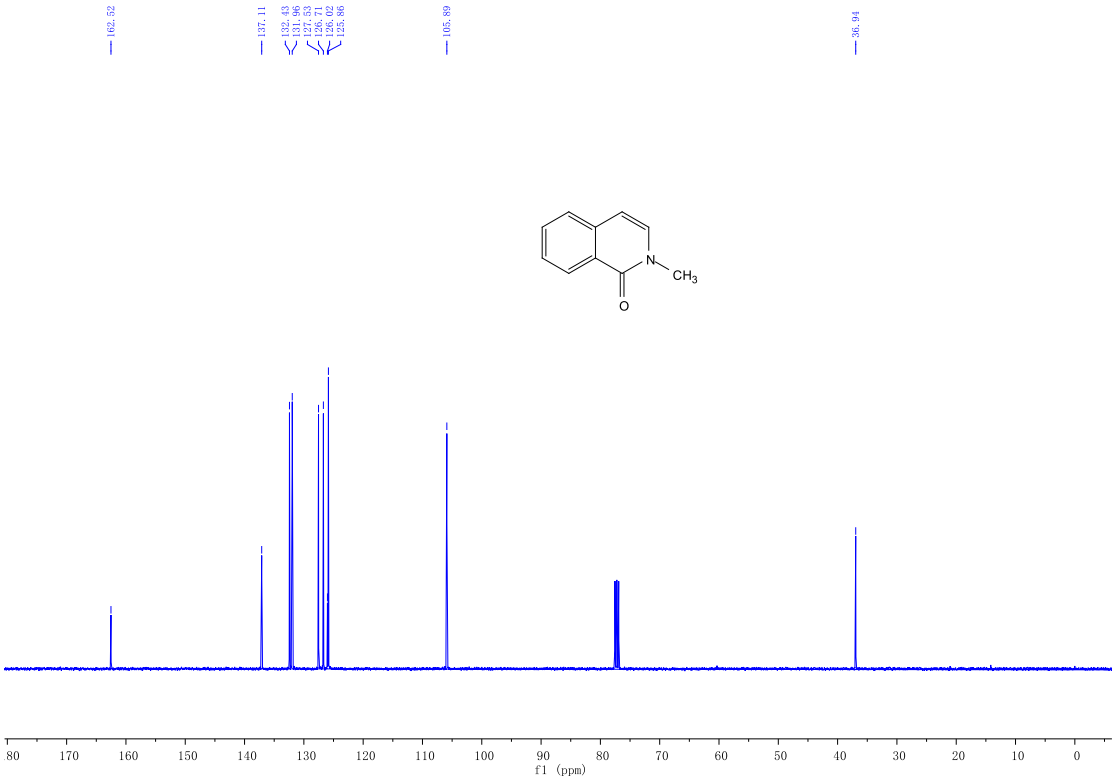
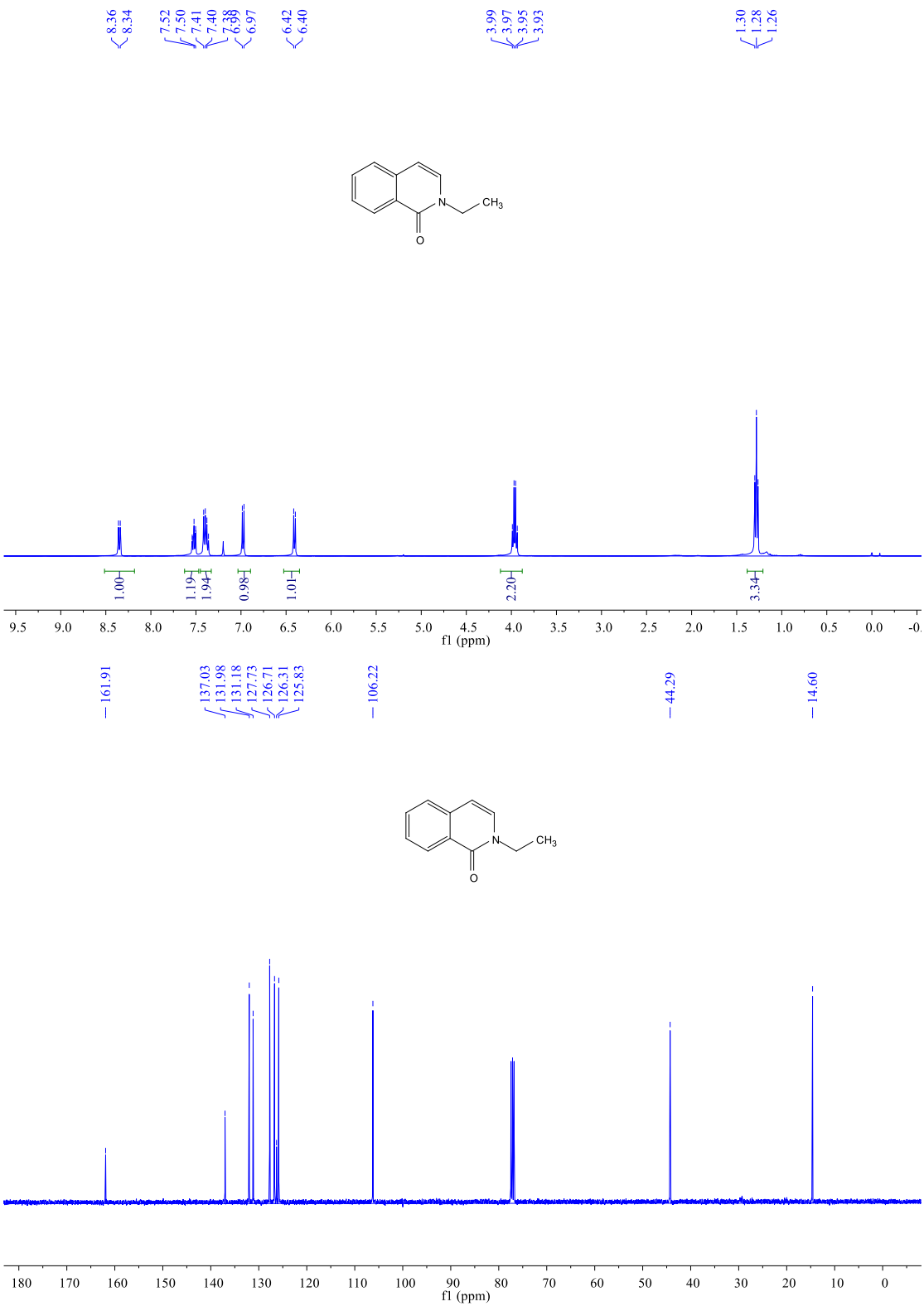
8.69
8.31
8.29
7.49
7.47
7.45
7.29
7.27
7.26
7.24
7.22
7.20
7.19
7.18
7.17
5.14
O
N
O
O
N
1.00
1.02
1.17
7.48
2.09
f1 (ppm)
160.73
144.69
135.93
135.01
134.53
130.84
129.41
129.05
128.28
128.23
128.12
125.83
100.91
52.09
f1 (ppm)

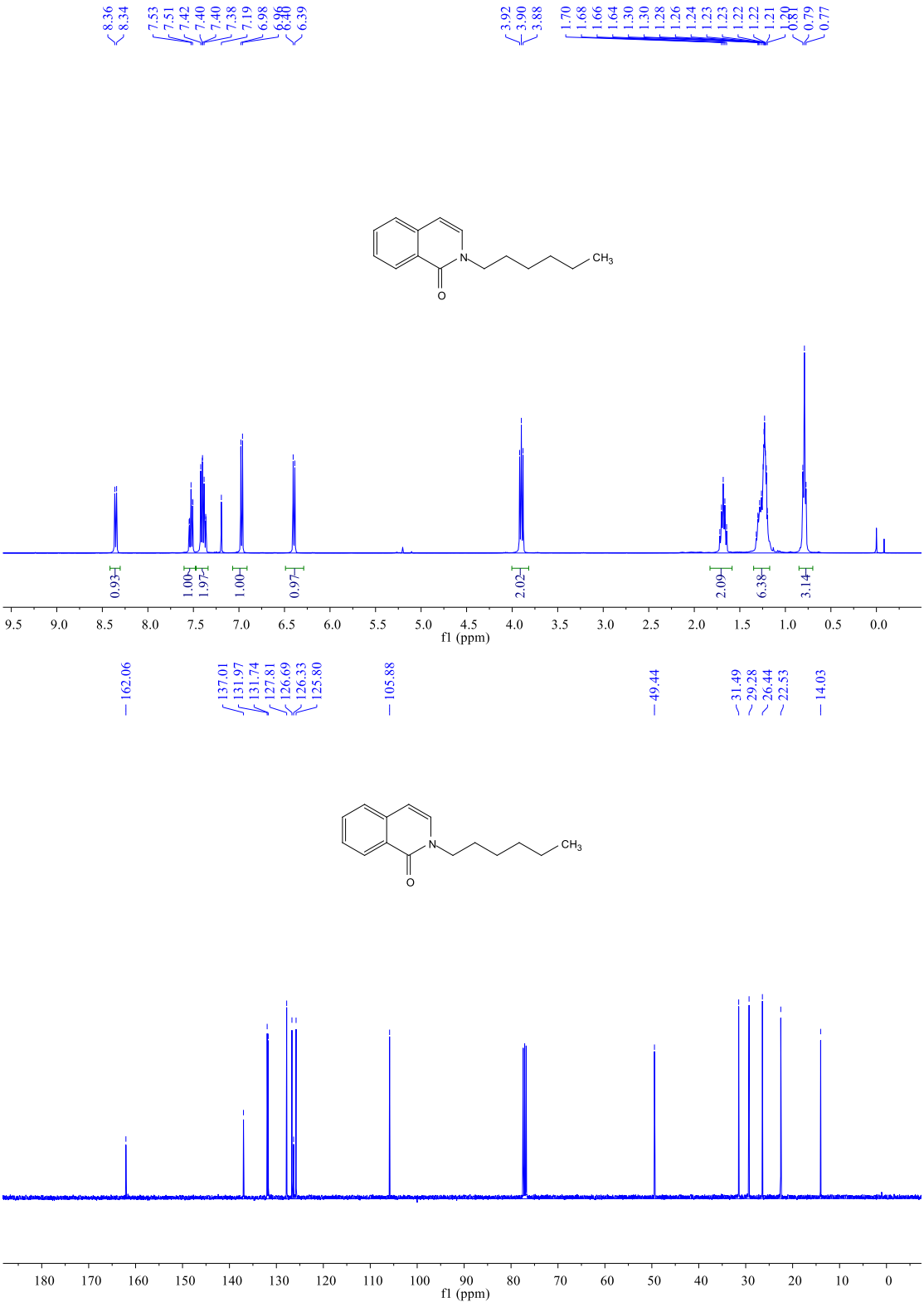

8.69
8.67
8.20
8.18
7.72
7.61
7.59
7.33
7.31
7.30
7.28
7.26
7.25
7.24
7.19
5.65
N
O
1.04
2.08
1.06
1.10
7.24
1.02
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)

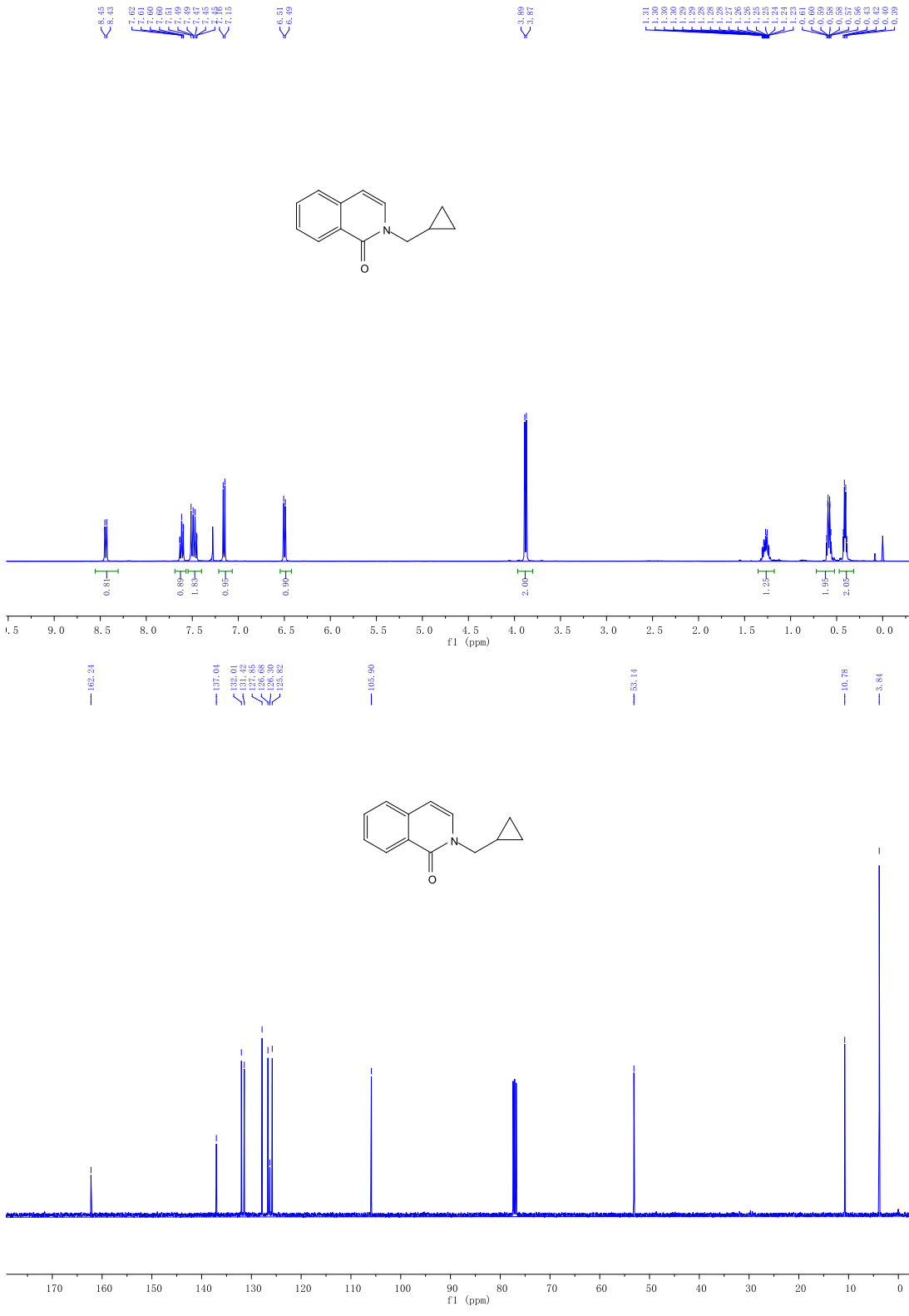

161.84
137.27
136.73
133.82
132.70
129.57
129.11
128.87
128.04
127.27
126.65
125.41
123.31
122.57
121.77
119.42
115.99
46.47
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

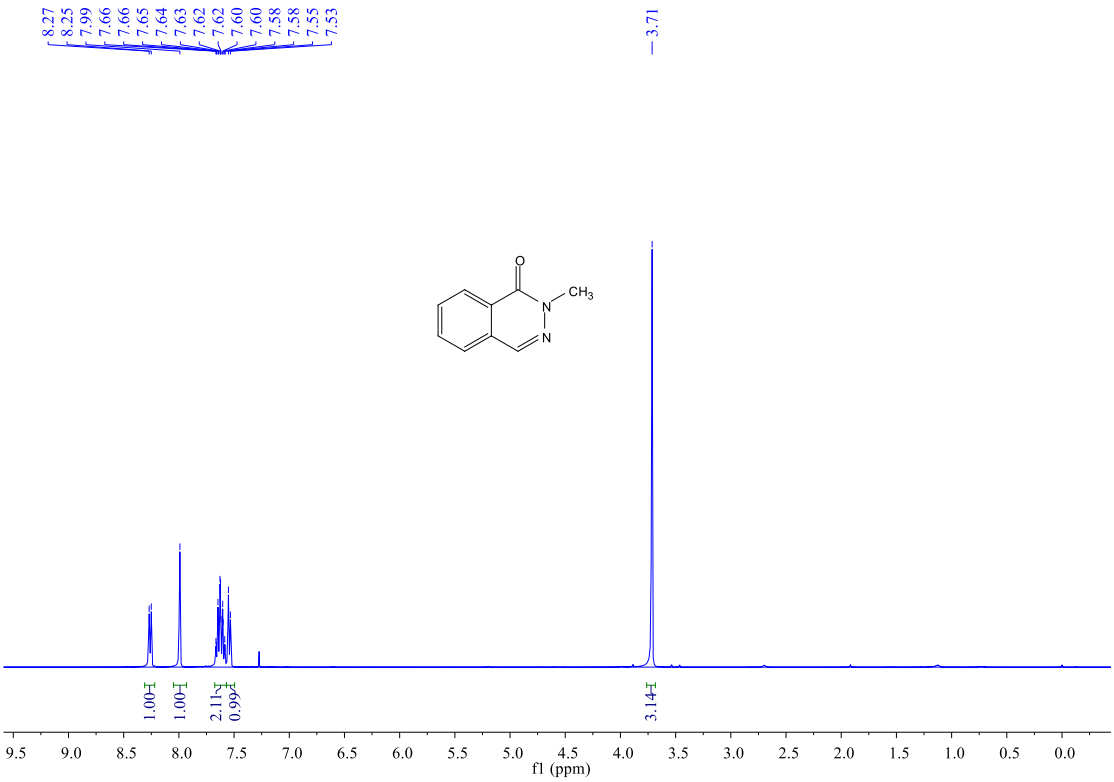

8.43
8.41
7.59
7.59
7.57
7.57
7.48
7.47
7.46
7.45
7.45
7.03
7.03
7.01
7.01
6.45
6.43
3.56
N
CH3
O
0.96
1.00
2.02
1.00
1.00
3.12
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.52
137.11
132.43
131.96
127.53
126.71
126.02
125.86
105.89
36.94
N
CH3
O
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.36
8.34
7.52
7.50
7.41
7.40
7.38
6.99
6.97
6.42
6.40
3.99
3.97
3.95
3.93
1.30
1.28
1.26
N
CH3
O
1.00
1.19
1.94
0.98
1.01
2.20
3.34
f1 (ppm)
161.91
137.03
131.98
131.18
127.73
126.71
126.31
125.83
106.22
44.29
14.60
N
CH3
O
f1 (ppm)


8.36
8.34
7.53
7.51
7.42
7.40
7.40
7.38
7.19
6.98
6.96
6.40
6.39
3.92
3.90
3.88
1.70
1.68
1.66
1.64
1.30
1.30
1.28
1.26
1.24
1.23
1.23
1.22
1.22
1.21
1.20
0.81
0.79
0.77
N
CH3
O
0.93
1.00
1.97
1.00
0.97
2.02
2.09
6.38
3.14
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
162.06
137.01
131.97
131.74
127.81
126.69
126.33
125.80
105.88
49.44
31.49
29.28
26.44
22.53
14.03
N
CH3
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.45
8.43
7.62
7.61
7.60
7.60
7.51
7.49
7.49
7.47
7.45
7.45
7.16
7.15
6.51
6.49
3.89
3.87
1.31
1.30
1.30
1.29
1.29
1.28
1.28
1.28
1.27
1.26
1.26
1.25
1.25
1.24
1.24
1.23
0.61
0.60
0.59
0.58
0.58
0.57
0.56
0.43
0.42
0.40
0.39
N
O
0.81
0.89
1.89
0.95
0.96
2.00
1.25
1.95
2.05
f1 (ppm)
162.24
137.04
132.01
131.42
127.85
126.68
126.30
125.82
105.90
53.14
10.78
3.84
f1 (ppm)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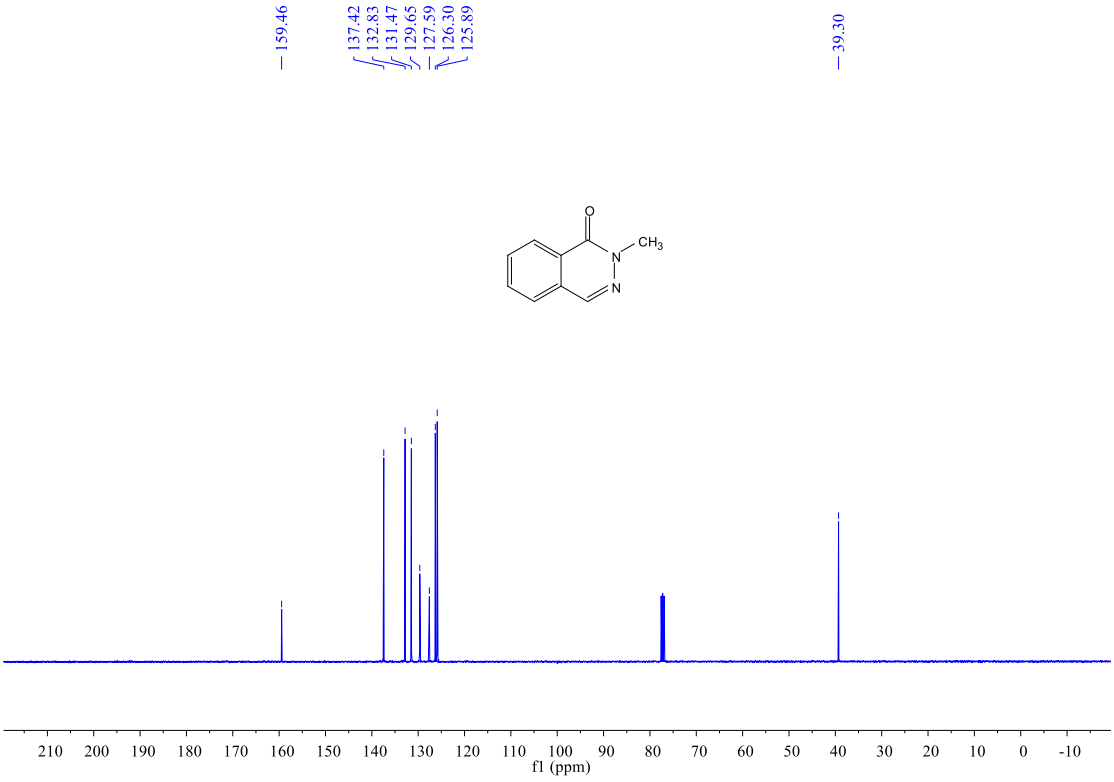
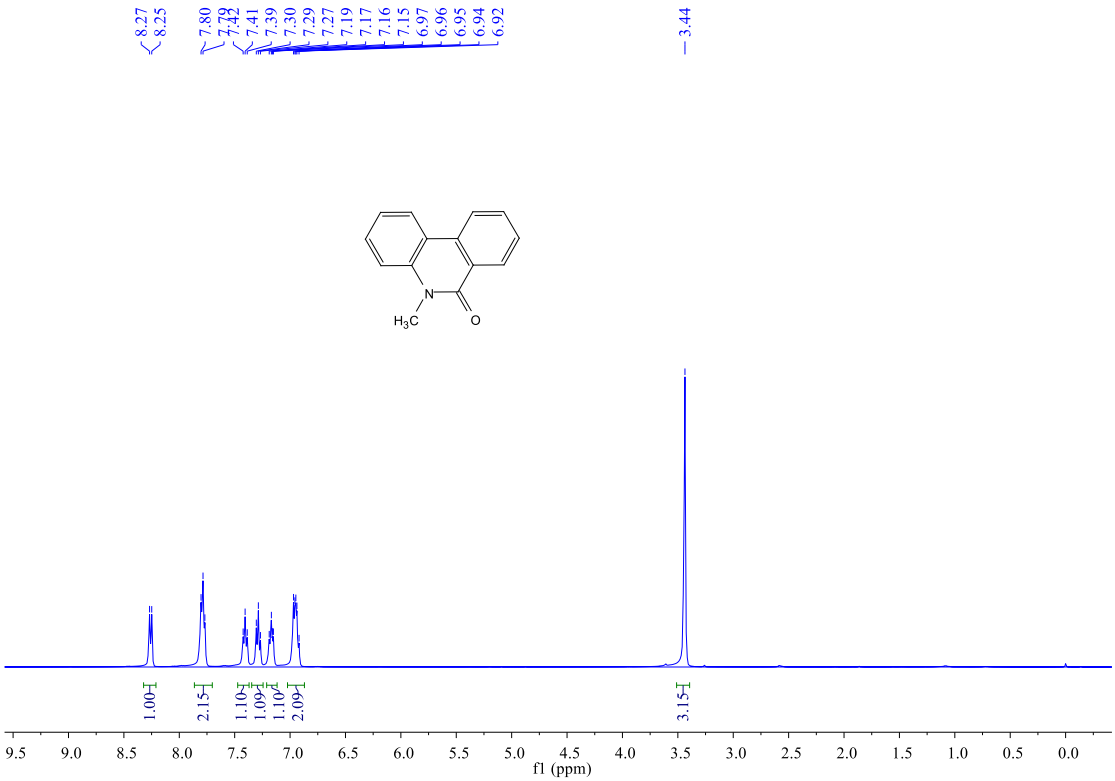
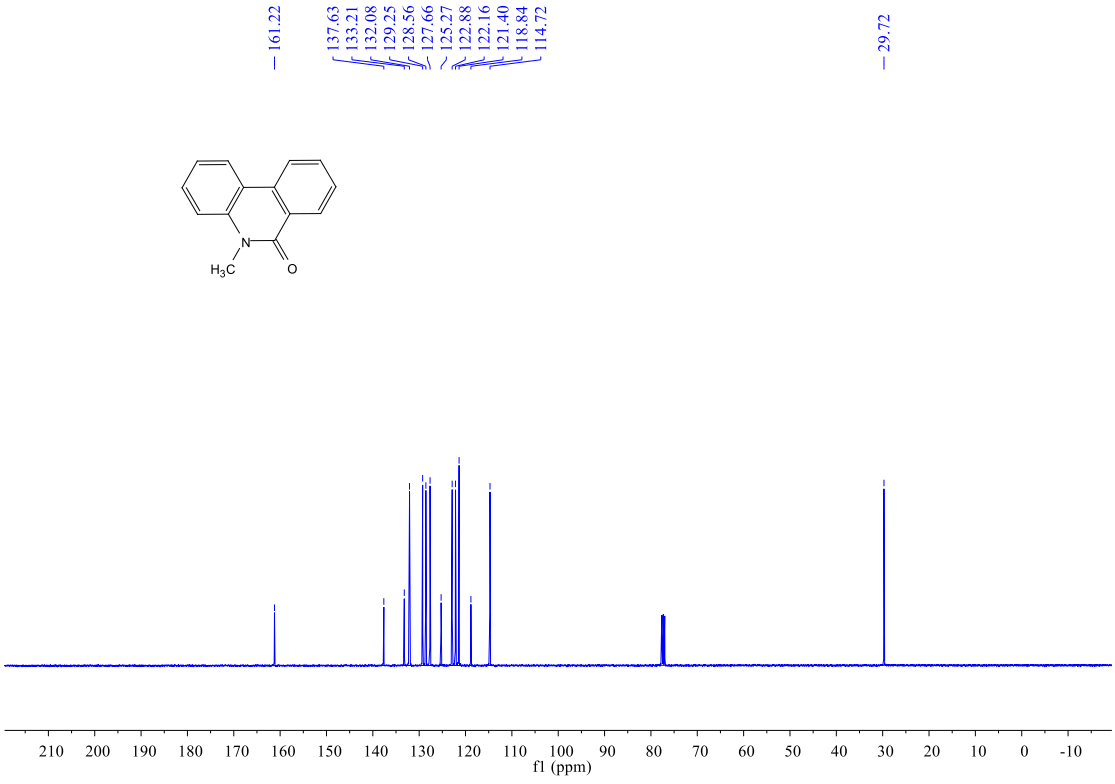
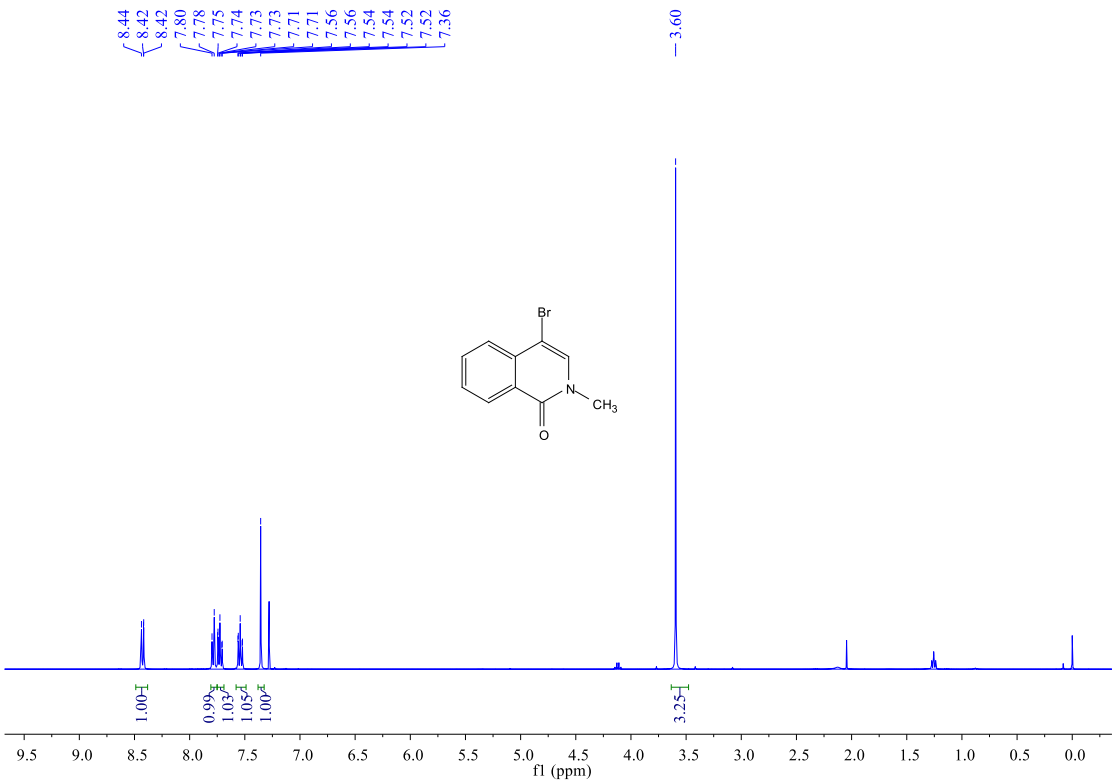
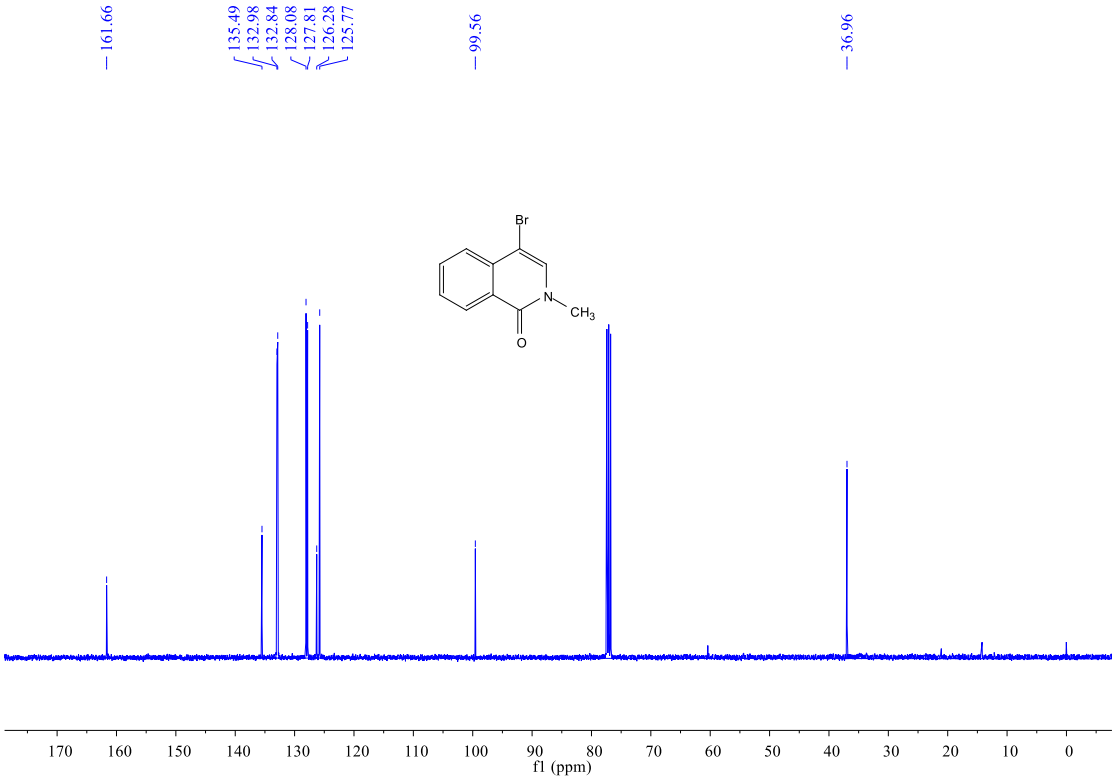
7.99
7.66
7.66
7.65
7.64
7.63
7.62
7.62
7.60
7.60
7.58
7.58
7.55
7.53
3.71
O
N
CH3
N
1.00
1.00
2.11
0.99
3.14
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


159.46
137.42
132.83
131.47
129.65
127.59
126.30
125.89
39.30
O
N
CH3
N
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)


8.27
8.25
7.80
7.79
7.42
7.41
7.39
7.30
7.29
7.27
7.19
7.17
7.16
7.15
6.97
6.96
6.95
6.94
6.92
3.44
N
H3C
O
1.00
2.15
1.10
1.09
1.10
2.09
3.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.22
137.63
133.21
132.08
129.25
128.56
127.66
125.27
122.88
122.16
121.40
118.84
114.72
29.72
N
H3C
O
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)


8.44
8.42
8.42
7.80
7.78
7.75
7.74
7.73
7.73
7.71
7.71
7.56
7.56
7.54
7.54
7.52
7.52
7.36
3.60
Br
N
CH3
O
1.00
0.99
1.03
1.05
1.00
3.25
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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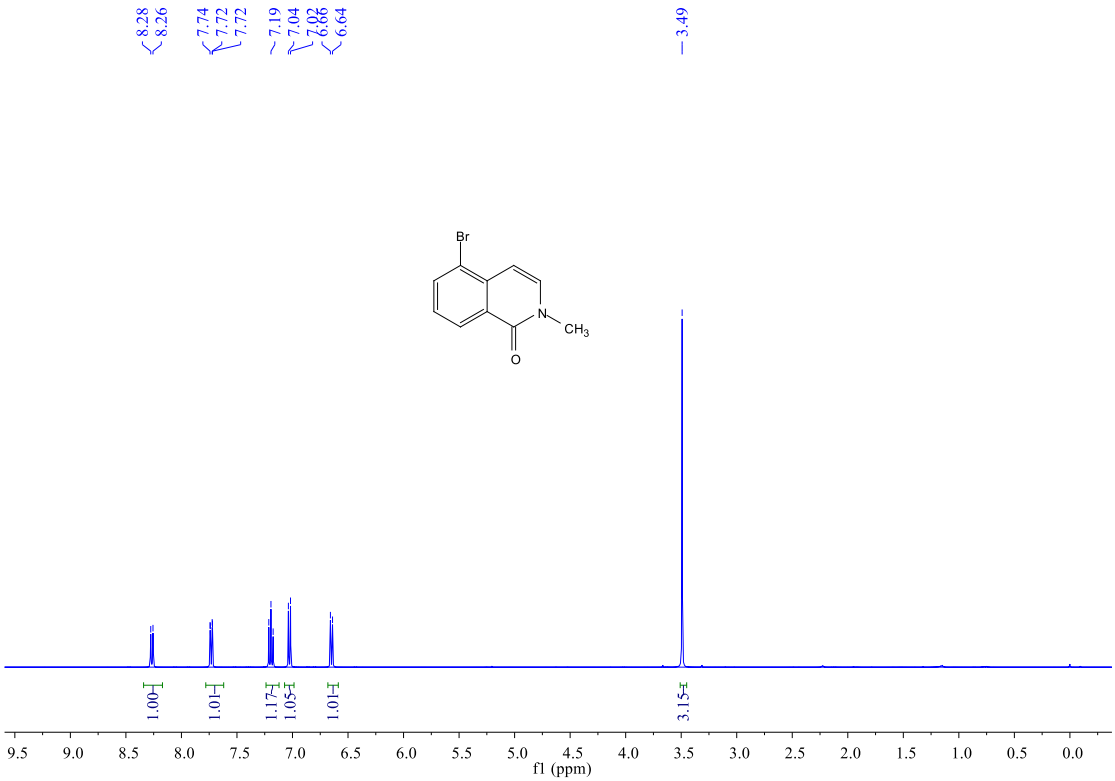
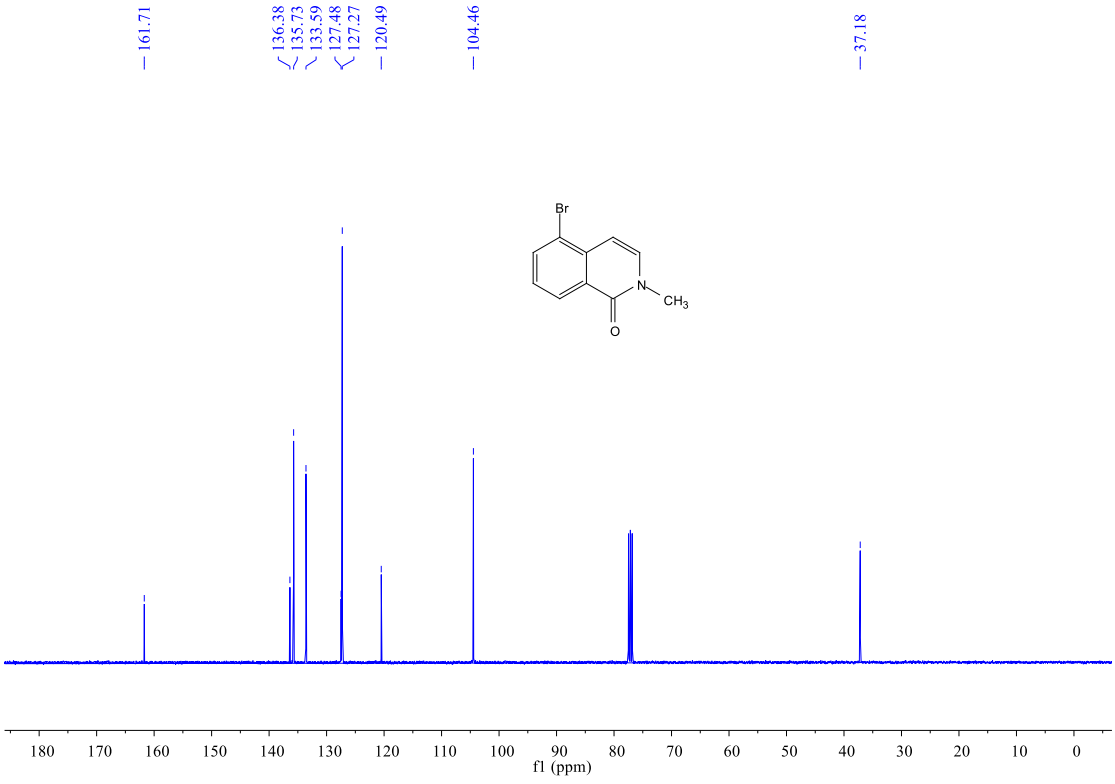
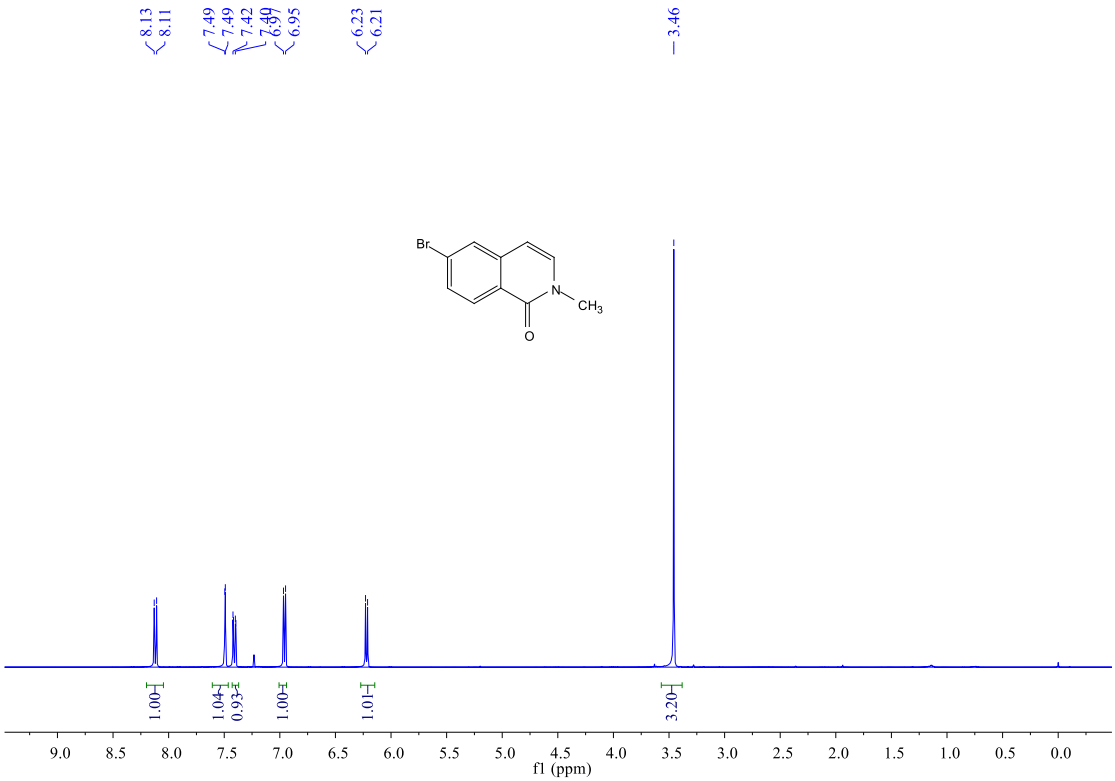
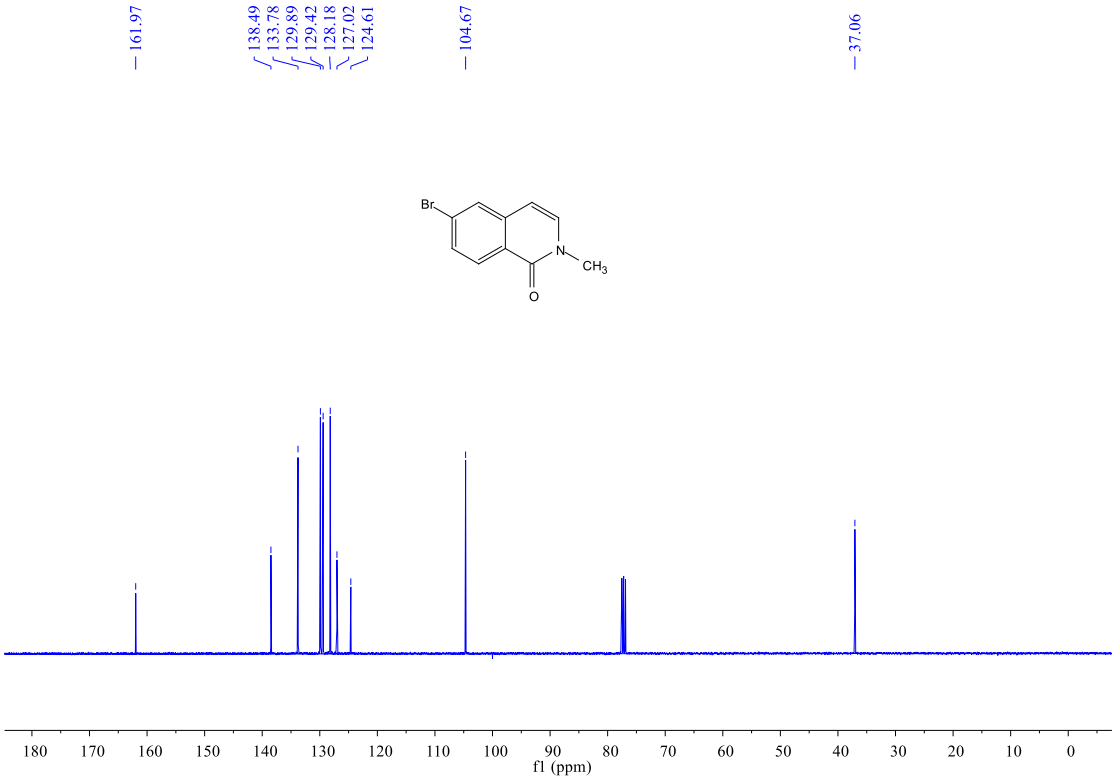
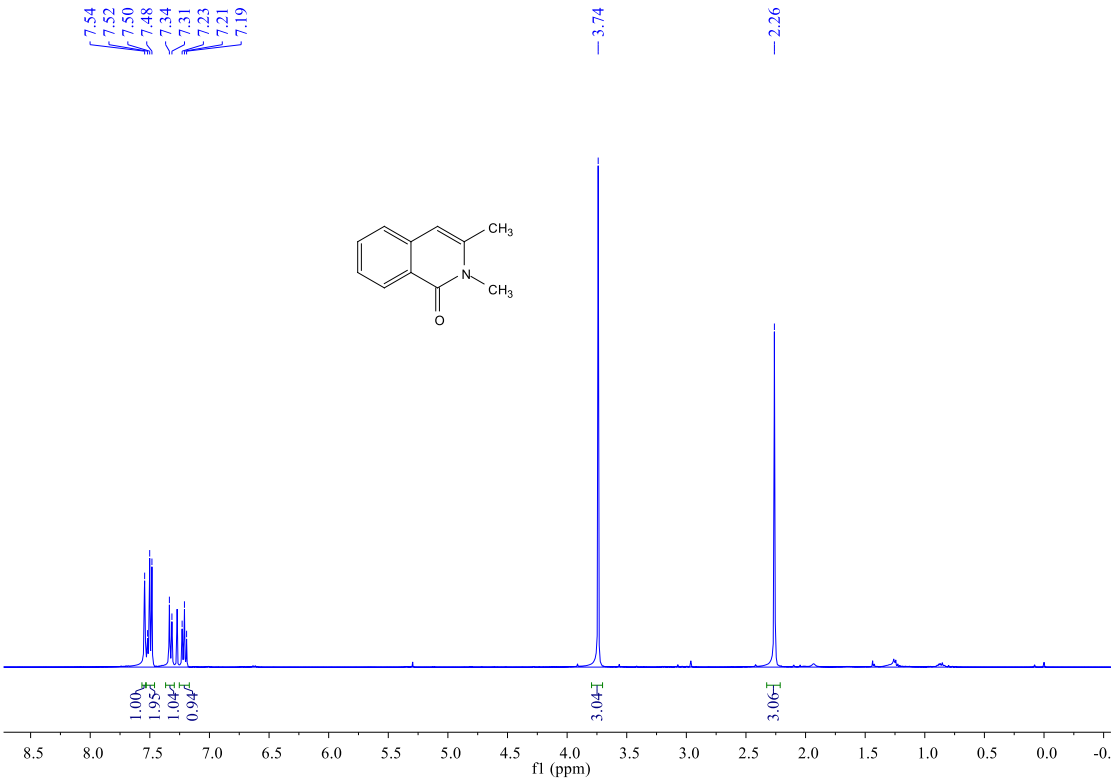
135.49
132.98
132.84
128.08
127.81
126.28
125.77
99.56
36.96
Br
N
CH3
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

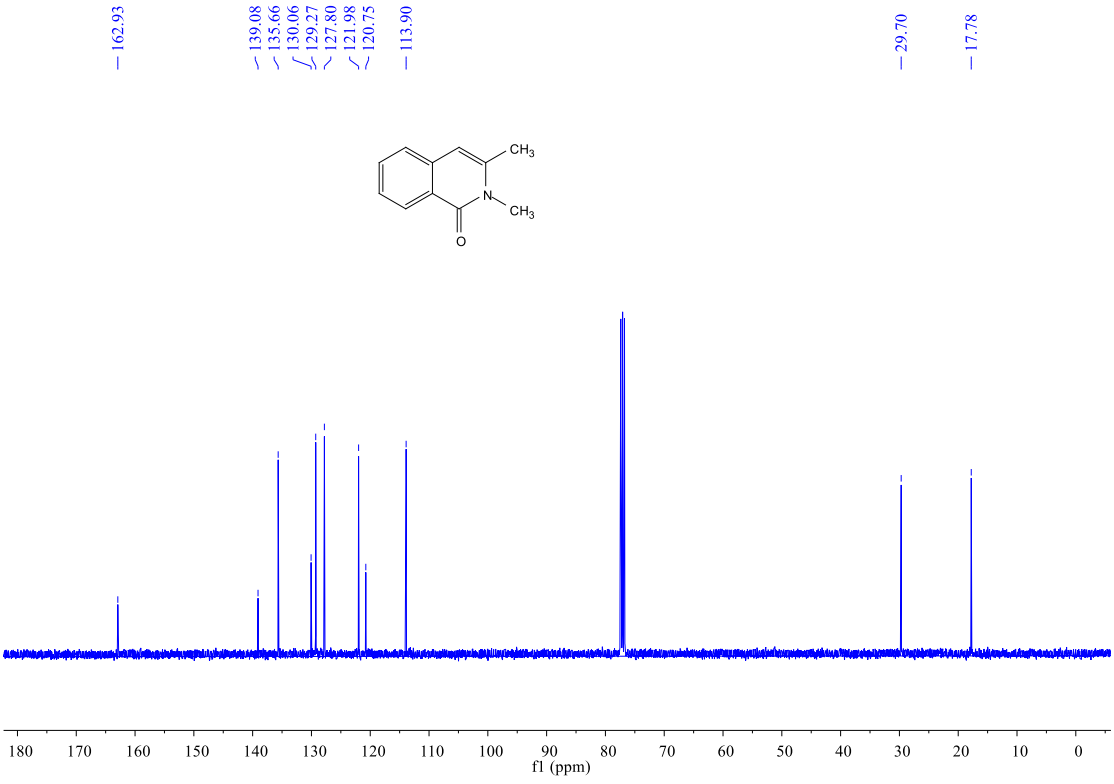

8.28
8.26
7.74
7.72
7.72
7.19
7.04
7.02
6.66
6.64
3.49
Br
N
CH3
O
1.00
1.01
1.17
1.05
1.01
3.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

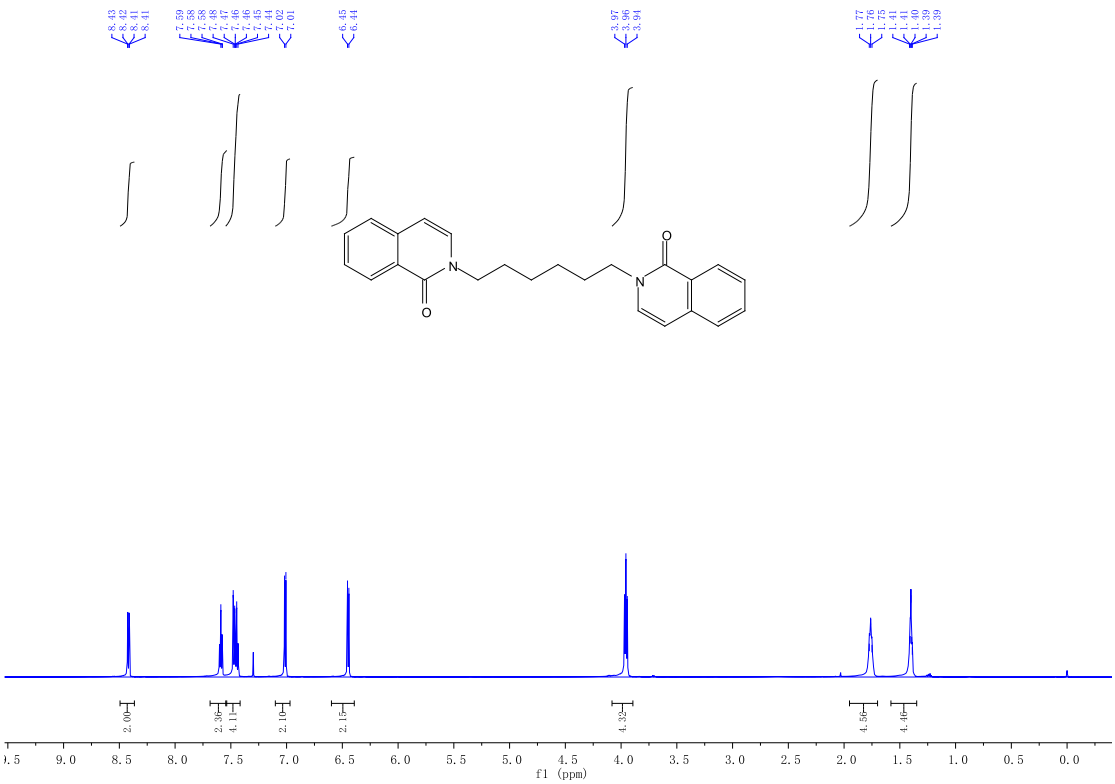

161.71
136.38
135.73
133.59
127.48
127.27
120.49
104.46
37.18
Br
N
CH3
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.13
8.11
7.49
7.49
7.42
7.40
6.97
6.95
6.23
6.21
3.46
Br
N
CH3
O
1.00
1.04
0.93
1.00
1.01
3.20
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


161.97
138.49
133.78
129.89
129.42
128.18
127.02
124.61
104.67
37.06
Br
N
CH3
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.54
7.52
7.50
7.48
7.34
7.31
7.23
7.21
7.19
3.74
2.26
CH3
N
CH3
O
1.00
1.95
1.04
0.94
3.04
3.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


162.93
139.08
135.66
130.06
129.27
127.80
121.98
120.75
113.90
29.70
17.78
CH3
N
CH3
O
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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7.58
7.58
7.48
7.47
7.46
7.45
7.44
7.02
7.01
6.45
6.44
3.97
3.96
3.94
1.77
1.76
1.75
1.41
1.41
1.40
1.39
1.39
O
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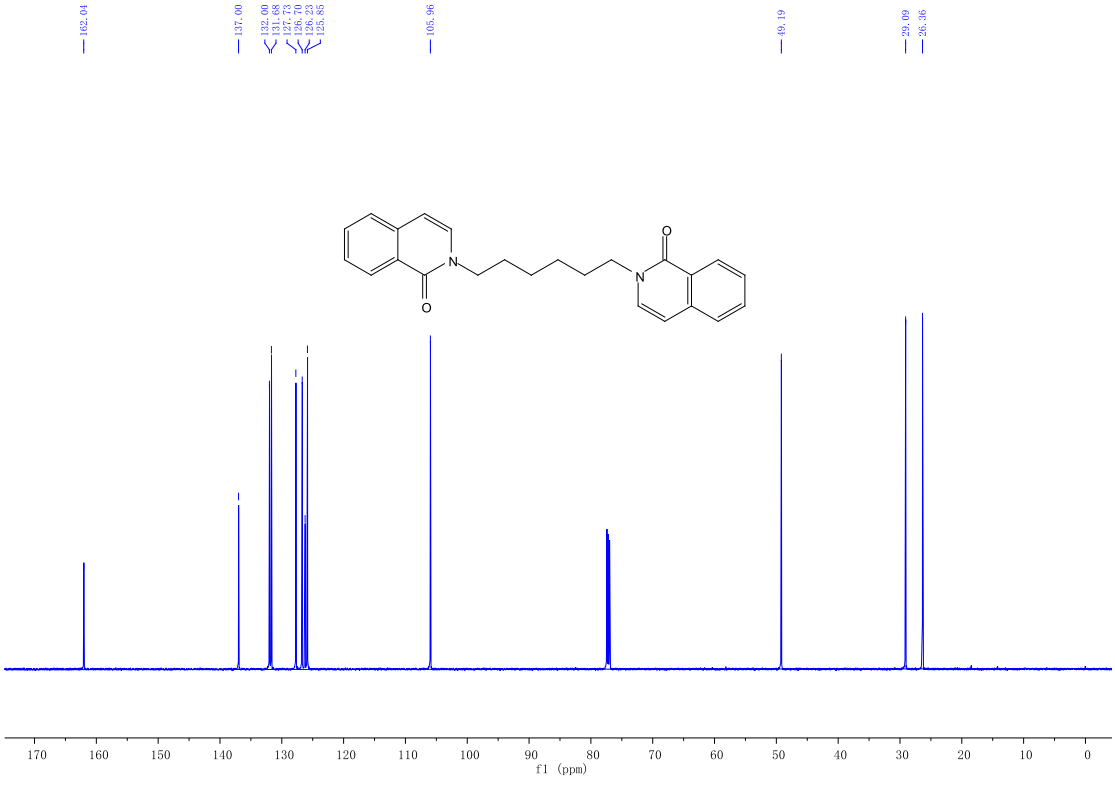
O
N
O
2.00
2.36
4.11
2.10
2.15
4.32
4.56
4.40
f1 (ppm)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132.00
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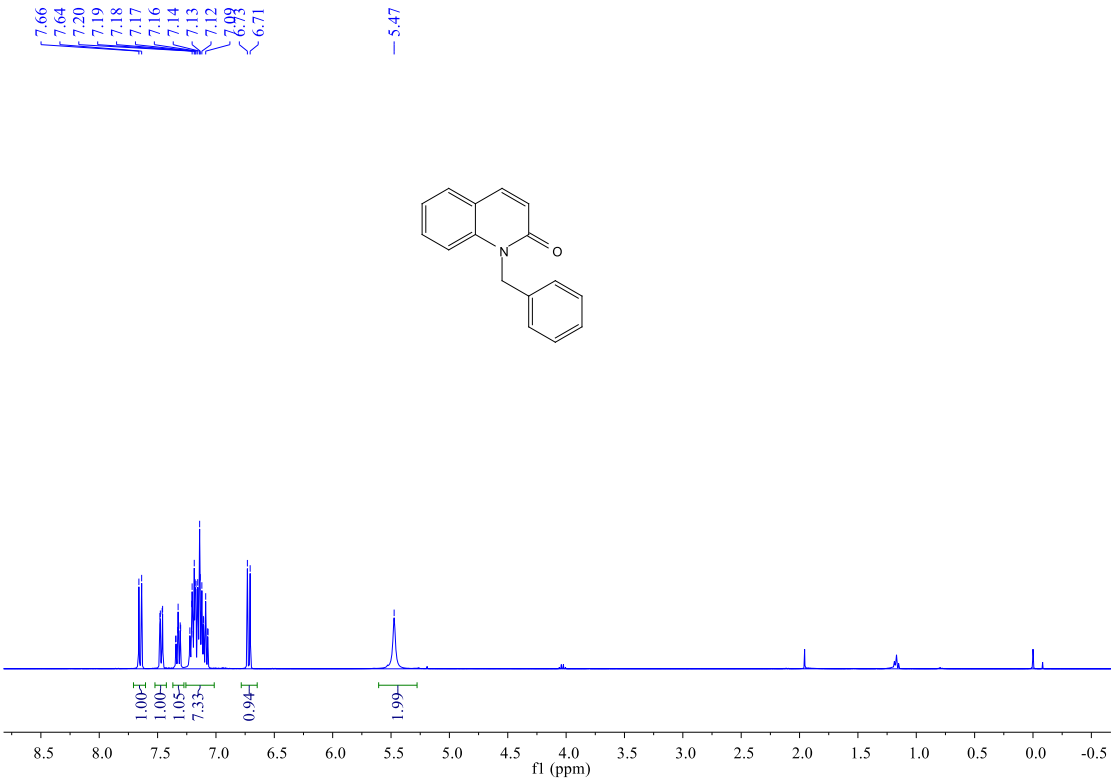
125.85
105.96
49.19
29.09
26.36
O
N
O
N
O
f1 (ppm)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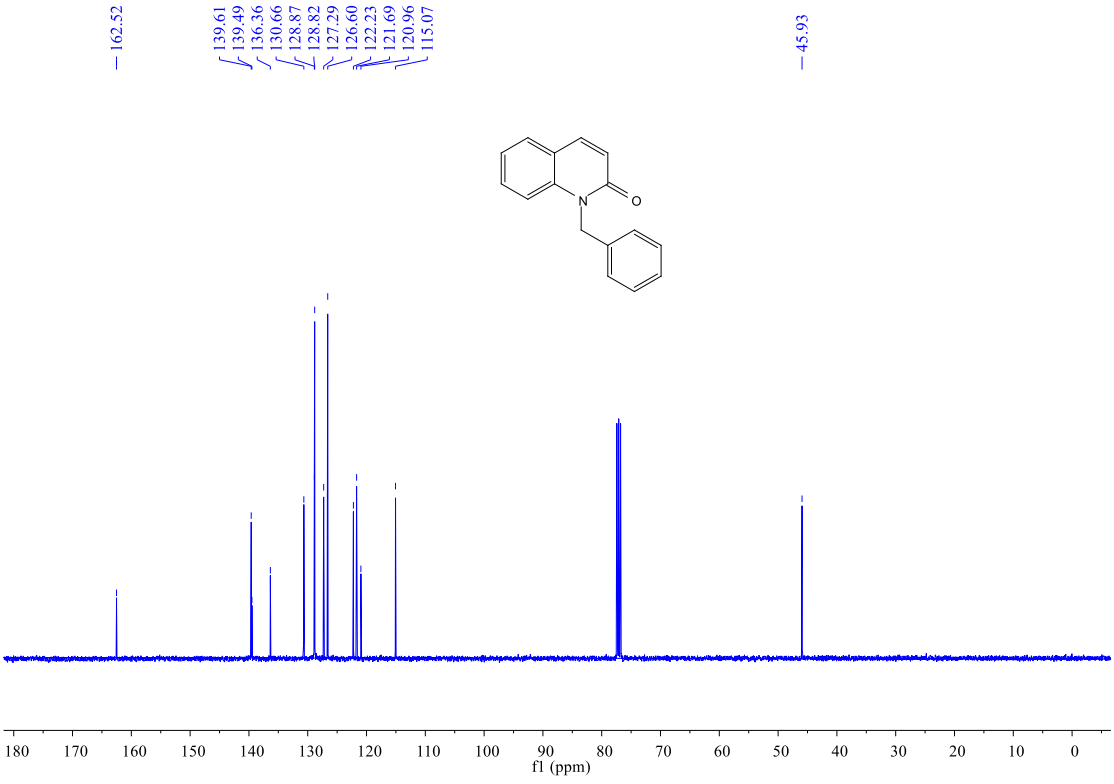
7.16
7.14
7.13
7.12
7.09
6.73
6.71
5.47
O
N
1.00
1.00
1.05
7.33
0.94
1.99
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.29
126.60
122.23
121.69
120.96
115.07
45.93
O
N
180
170
160
150
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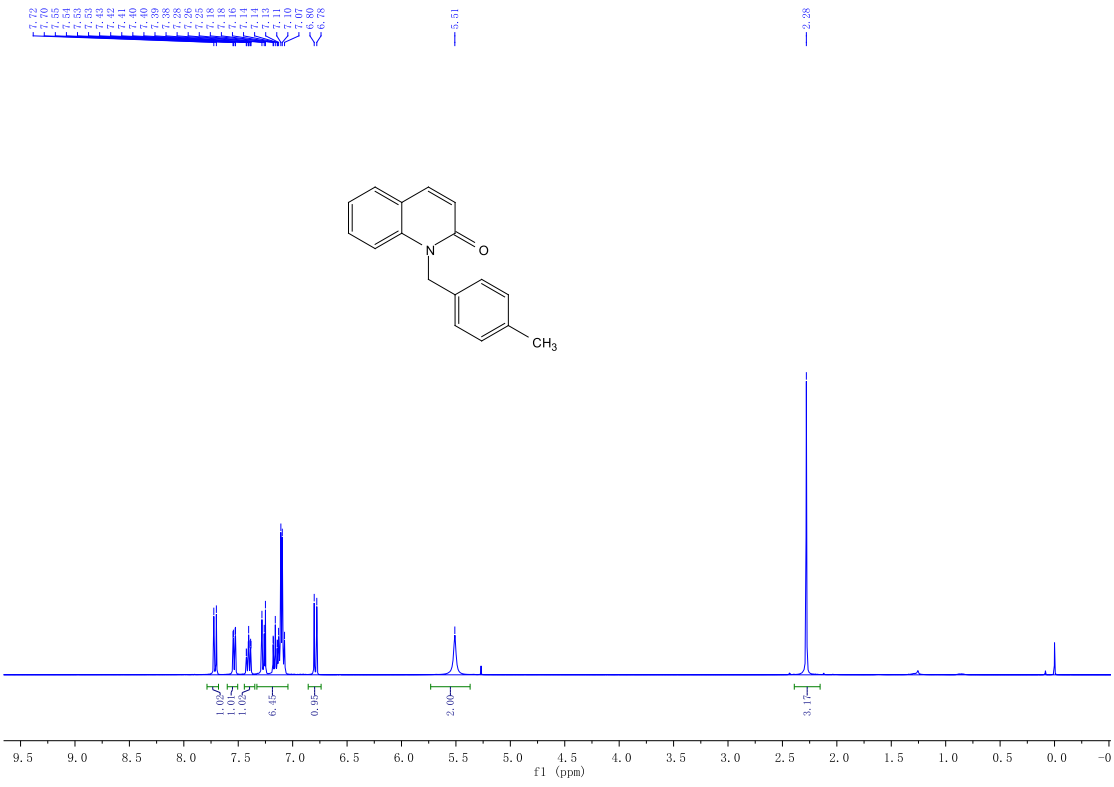
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.54
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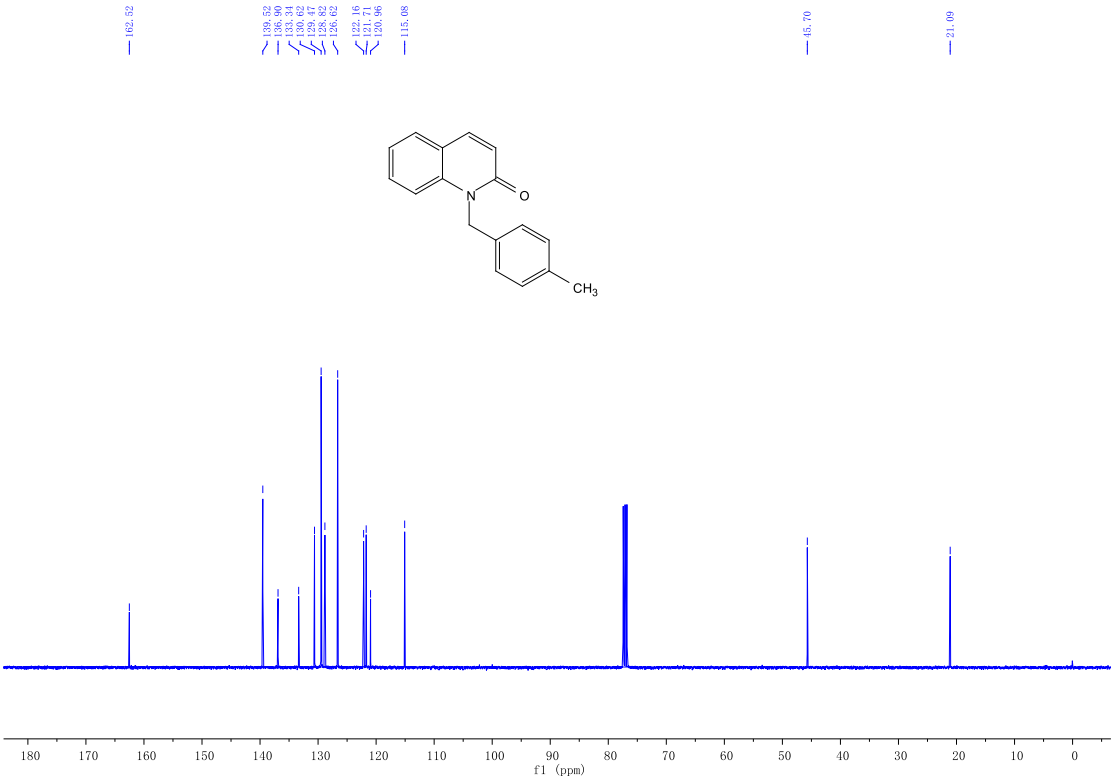
7.41
7.40
7.39
7.38
7.28
7.26
7.25
7.18
7.16
7.14
7.13
7.11
7.10
7.07
6.80
6.78
5.51
2.28
O
N
CH3
1.02
1.01
1.05
6.45
0.95
2.00
3.17
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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126.62
122.16
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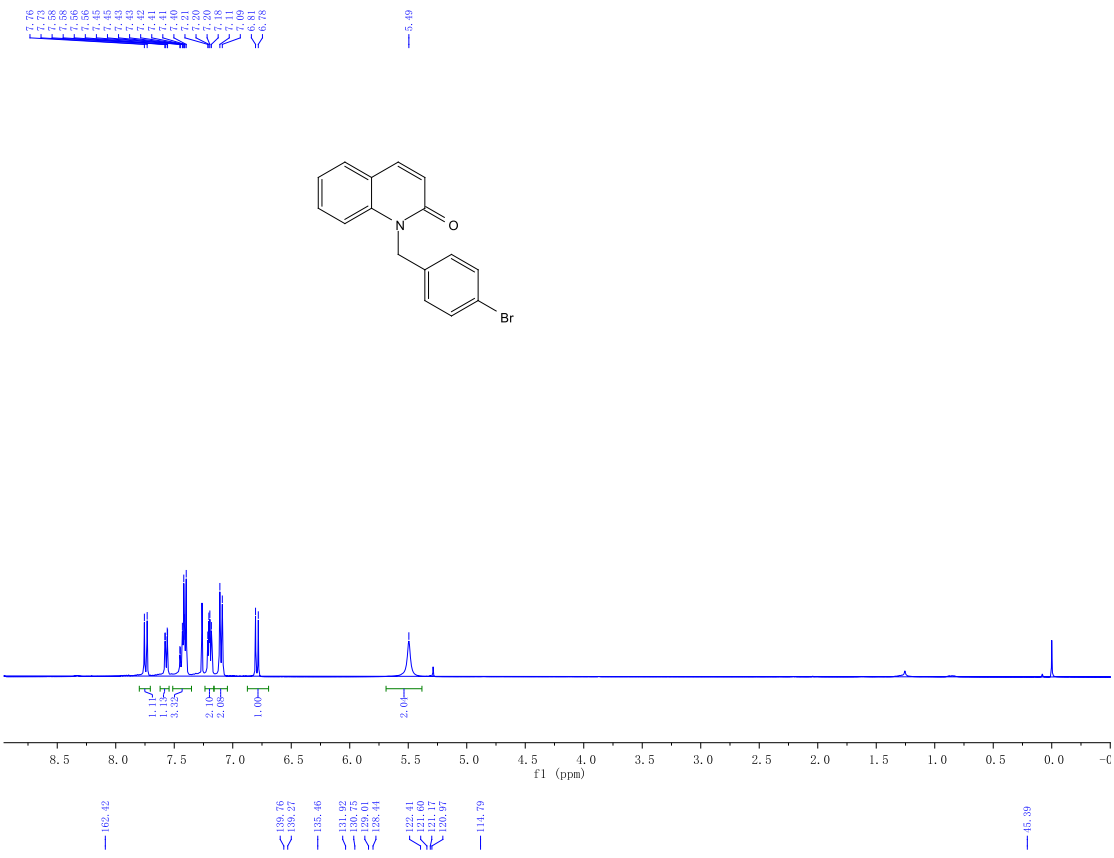
45.70
21.09
O
N
CH3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.73
7.58
7.58
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7.56
7.46
7.45
7.43
7.43
7.42
7.41
7.41
7.40
7.21
7.20
7.20
7.18
7.11
7.09
6.81
6.78
5.49
O
N
Br
1.14
1.15
3.32
2.10
2.08
1.00
2.04
f1 (ppm)
162.42
139.76
139.27
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130.01
128.44
122.41
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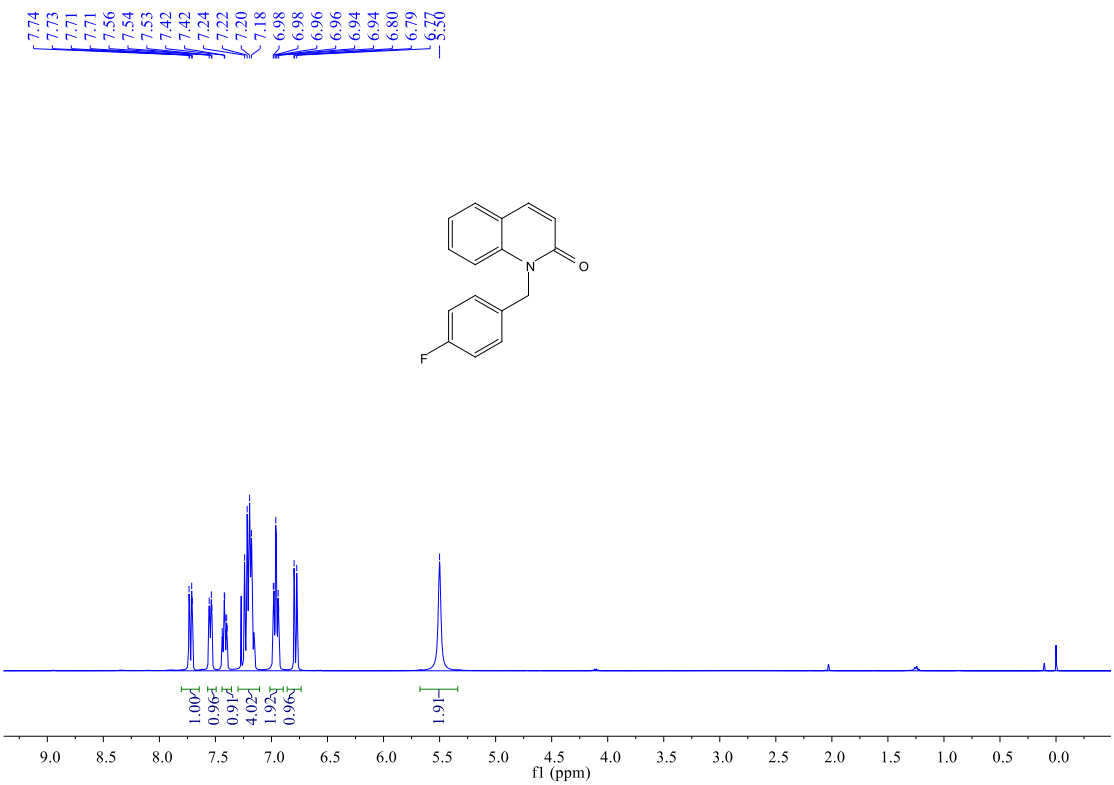
120.97
114.79
45.39
f1 (ppm)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7.71
7.71
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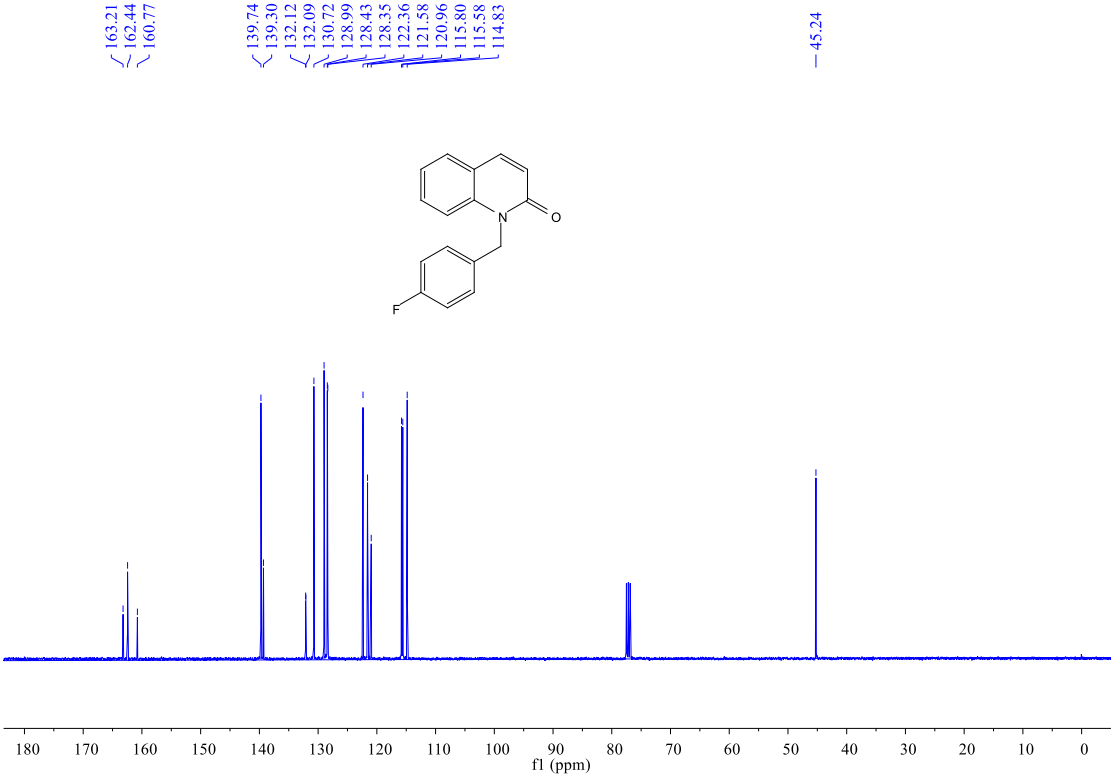
7.54
7.53
7.42
7.42
7.24
7.22
7.20
7.18
6.98
6.98
6.96
6.96
6.94
6.94
6.80
6.79
5.50
O
N
F
1.00
0.96
0.91
4.02
1.92
0.96
1.91
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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139.74
139.30
132.12
132.09
130.72
128.99
128.43
128.35
122.36
121.58
120.96
115.80
115.58
114.83
45.24
O
N
F
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.78
7.76
7.60
7.60
7.58
7.58
7.56
7.54
7.46
7.46
7.44
7.42
7.42
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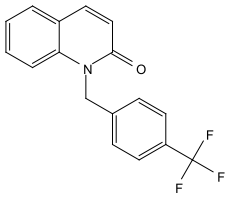
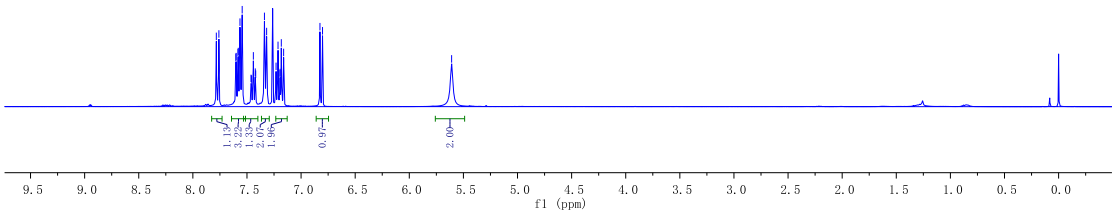
7.23
7.21
7.20
7.19
7.18
7.16
6.83
6.80
5.61


N
O
F
F
F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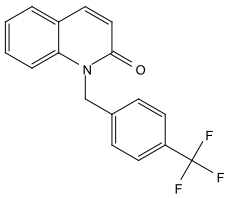
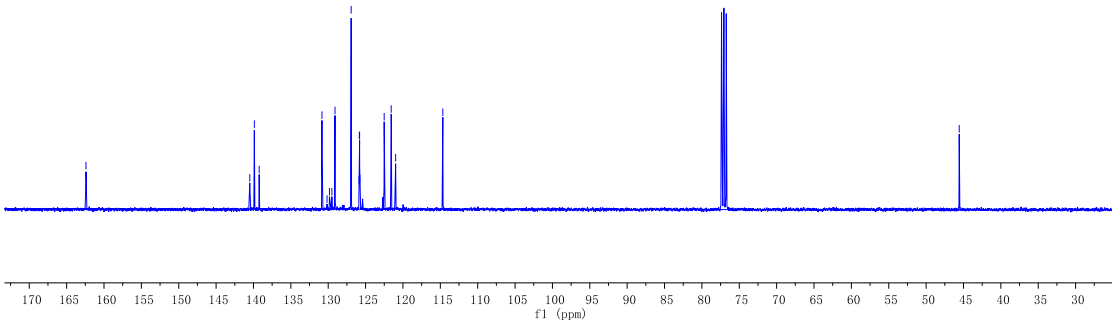
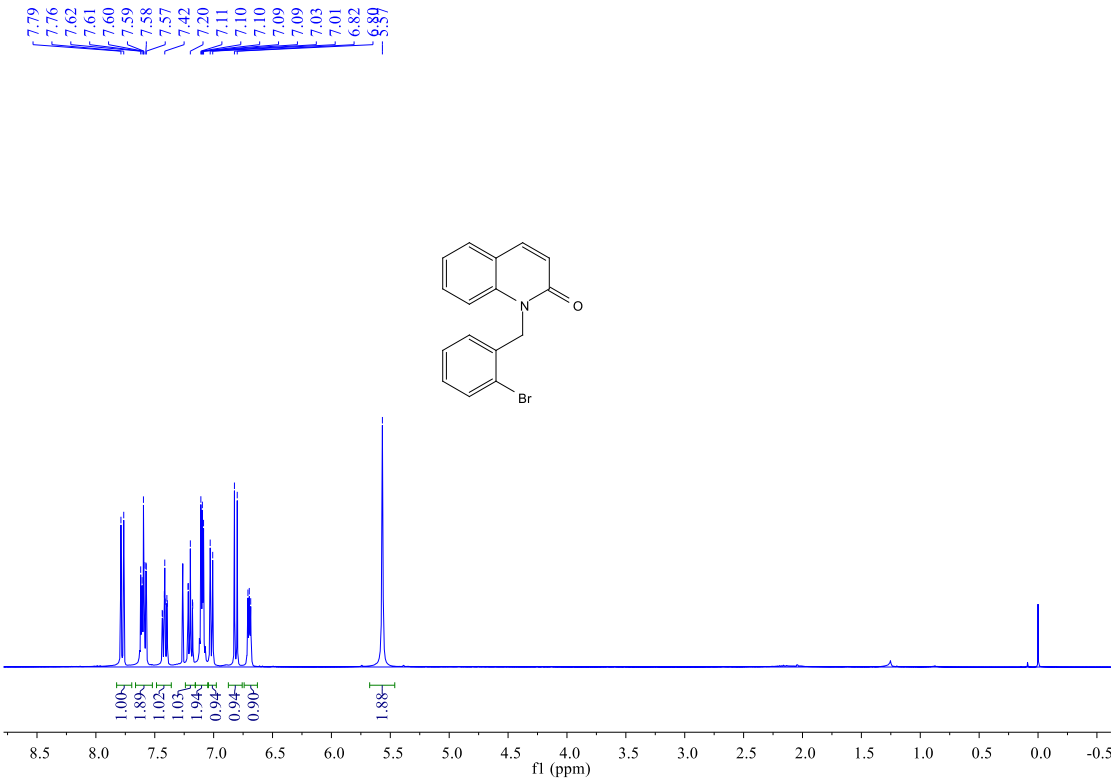
3.44
3.22
1.38
2.05
1.96
0.97
2.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


162.41
140.50
139.98
139.24
130.84
129.83
129.51
129.09
126.93
125.87
125.84
125.80
122.57
121.57
120.98
114.66
45.57


N
O
F
F
F


170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30
f1 (ppm)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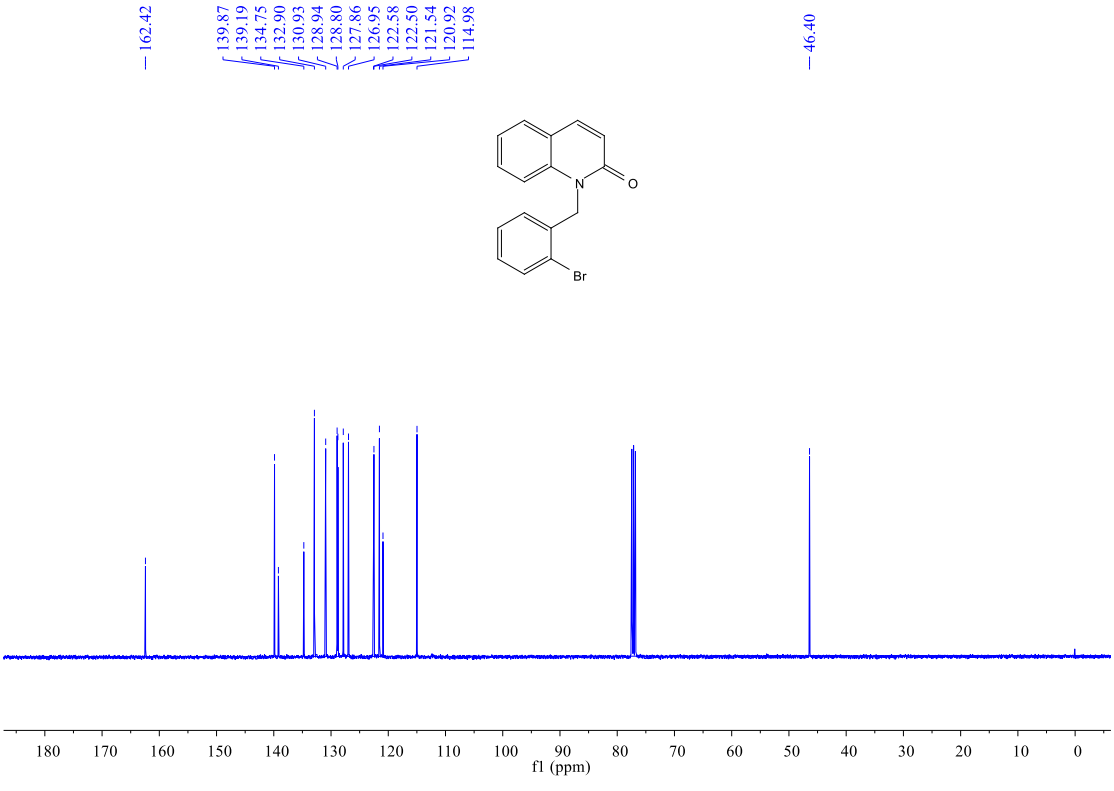
7.60
7.59
7.58
7.57
7.42
7.20
7.11
7.10
7.10
7.09
7.09
7.03
7.01
6.82
6.80
5.37
O
N
Br
1.00
1.89
1.02
1.03
1.94
0.94
0.94
0.90
1.88
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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139.87
139.19
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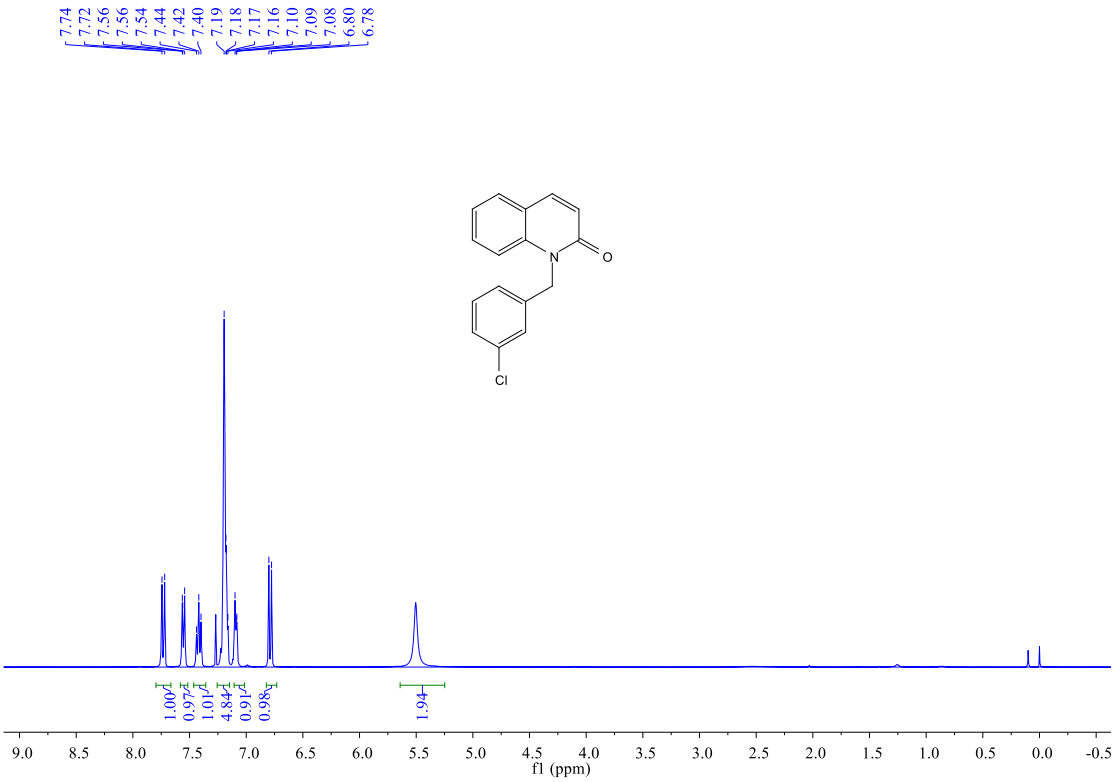
132.90
130.93
128.94
128.80
127.86
126.95
122.58
122.50
121.54
120.92
114.98
46.40
O
N
Br
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

.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7.72
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7.56
7.54
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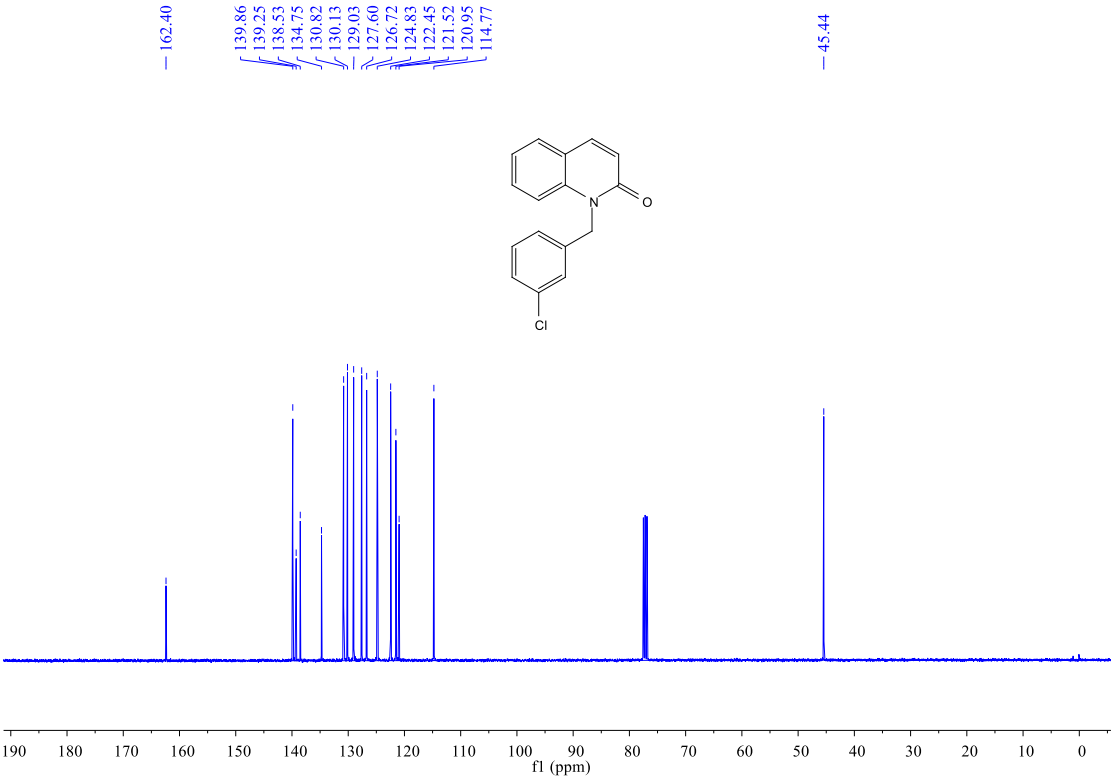
7.42
7.40
7.19
7.18
7.17
7.16
7.10
7.09
7.08
6.80
6.78
O
N
Cl
1.00
0.97
1.01
4.84
0.91
0.98
1.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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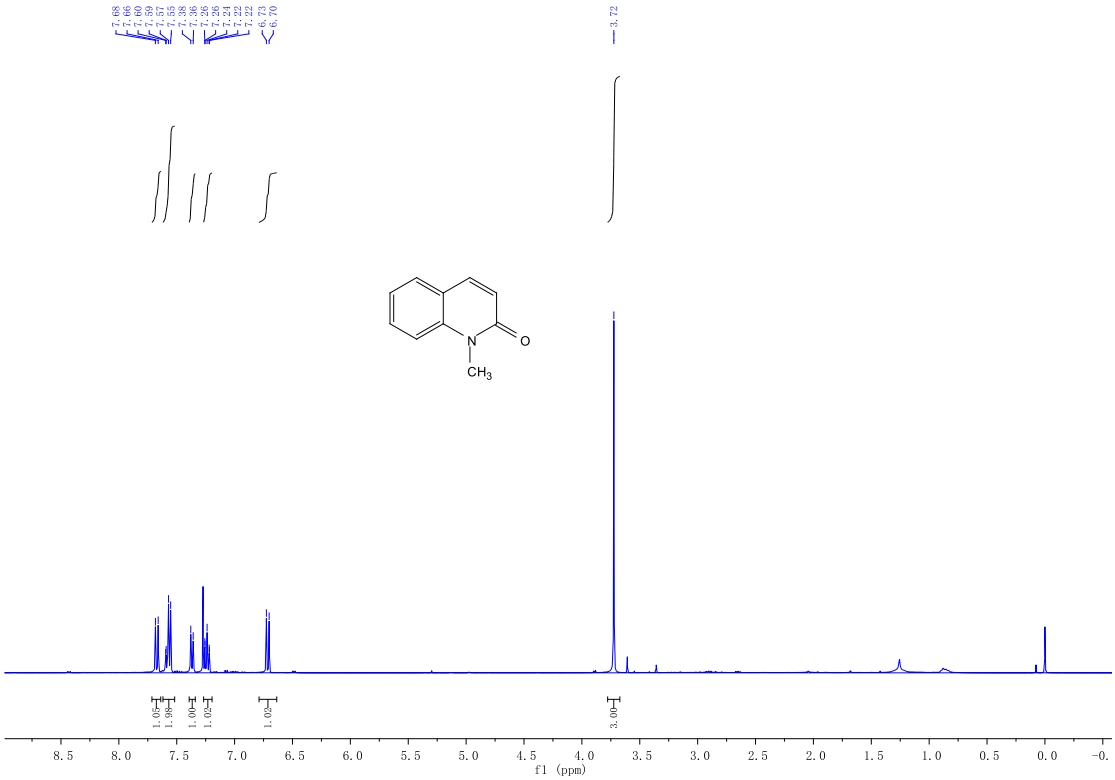
130.82
130.13
129.03
127.60
126.72
124.83
122.45
121.52
120.95
114.77
45.44
O
N
Cl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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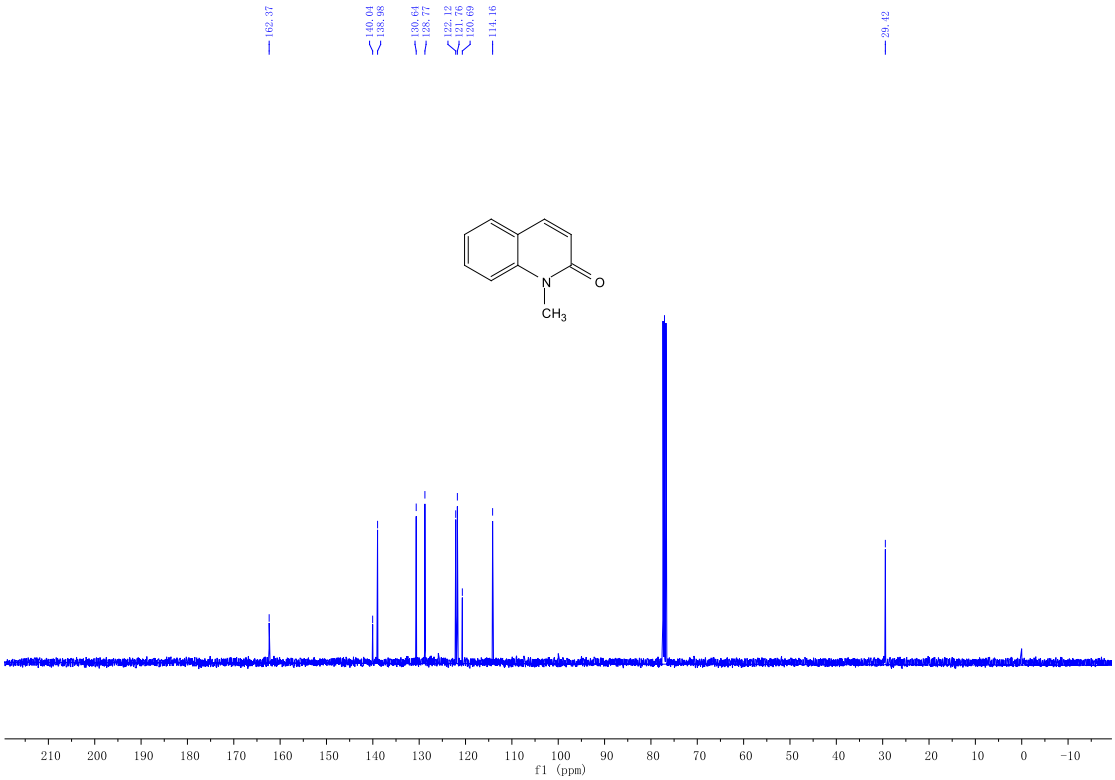
7.26
7.24
7.24
7.22
7.22
6.73
6.70
3.72
1.05
1.96
1.00
1.02
1.02
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)
O
N
CH3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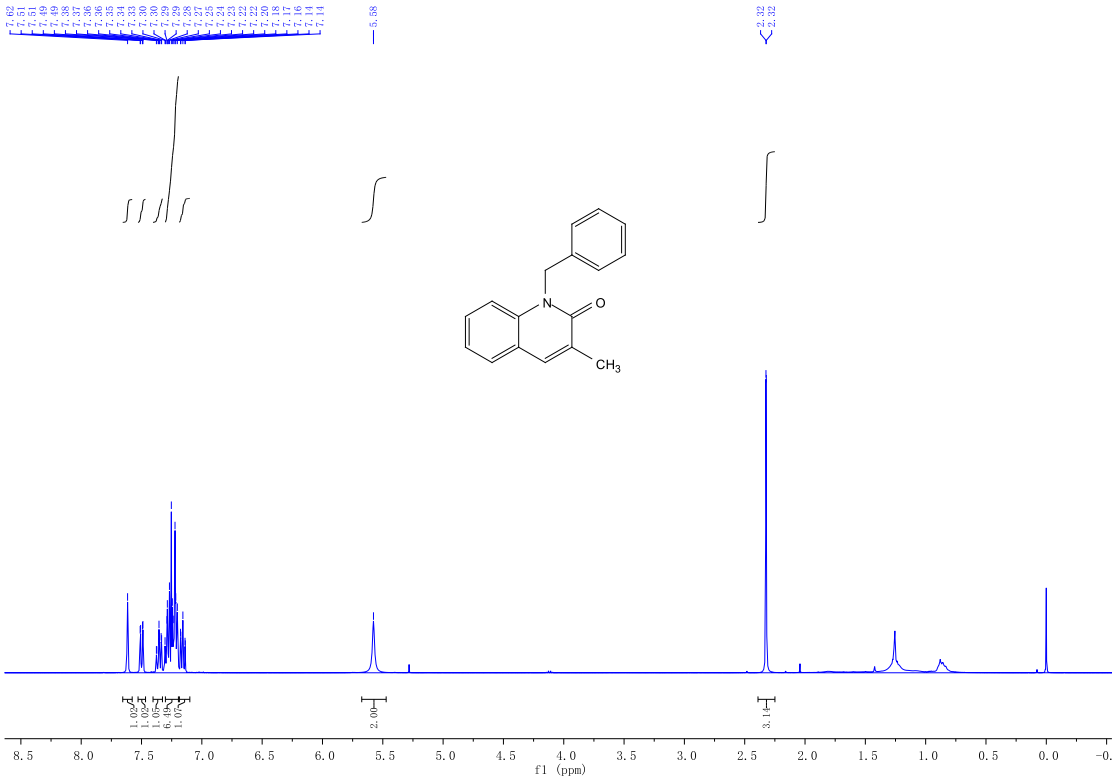
120.69
114.16
29.42
O
N
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.38
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7.36
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7.33
7.30
7.30
7.29
7.29
7.28
7.27
7.25
7.24
7.23
7.22
7.22
7.20
7.18
7.17
7.16
7.14
7.14
5.58
3.32
2.32
N
O
CH3
1.02
2.27
1.05
6.49
1.07
2.00
3.14
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
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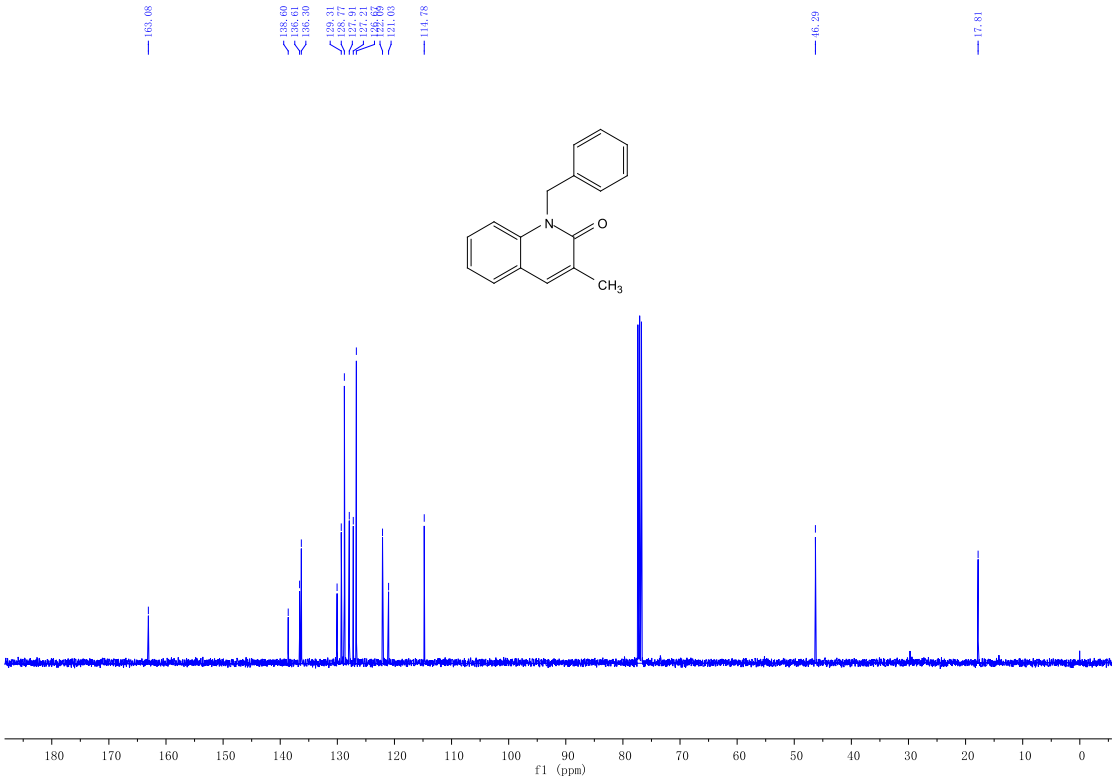
-0.
f1 (ppm)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136.30
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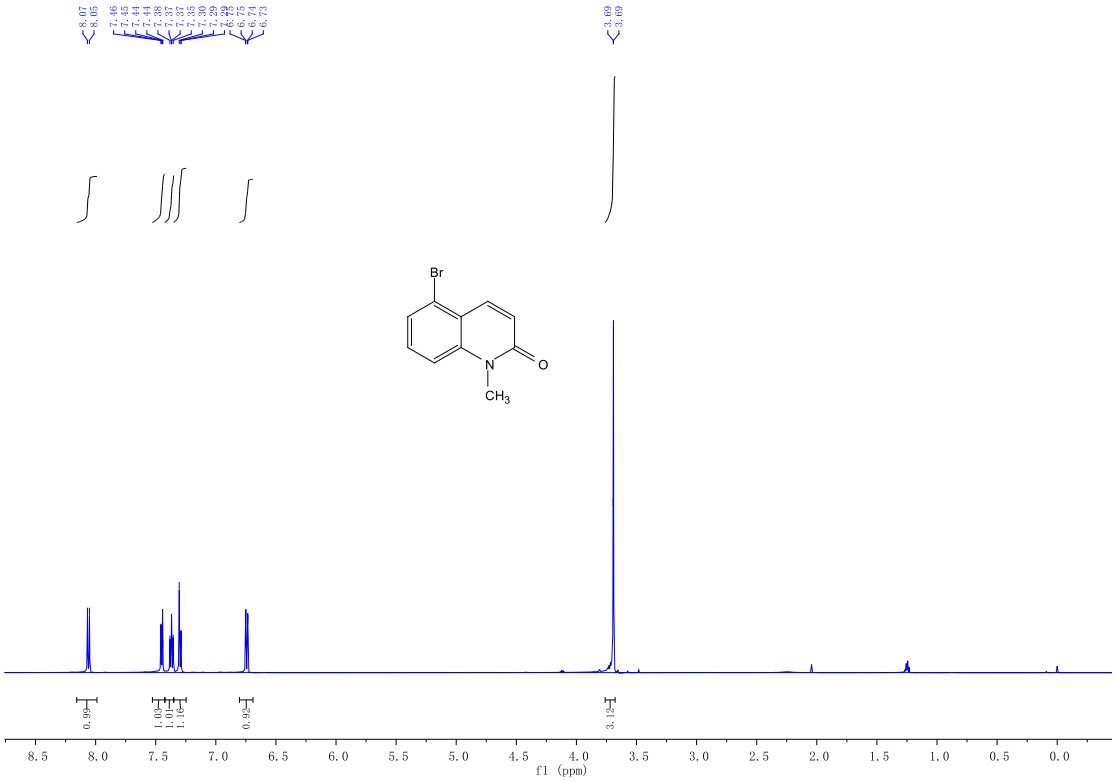
128.77
128.54
127.91
127.31
126.65
126.58
121.03
114.78
46.29
17.81
N
O
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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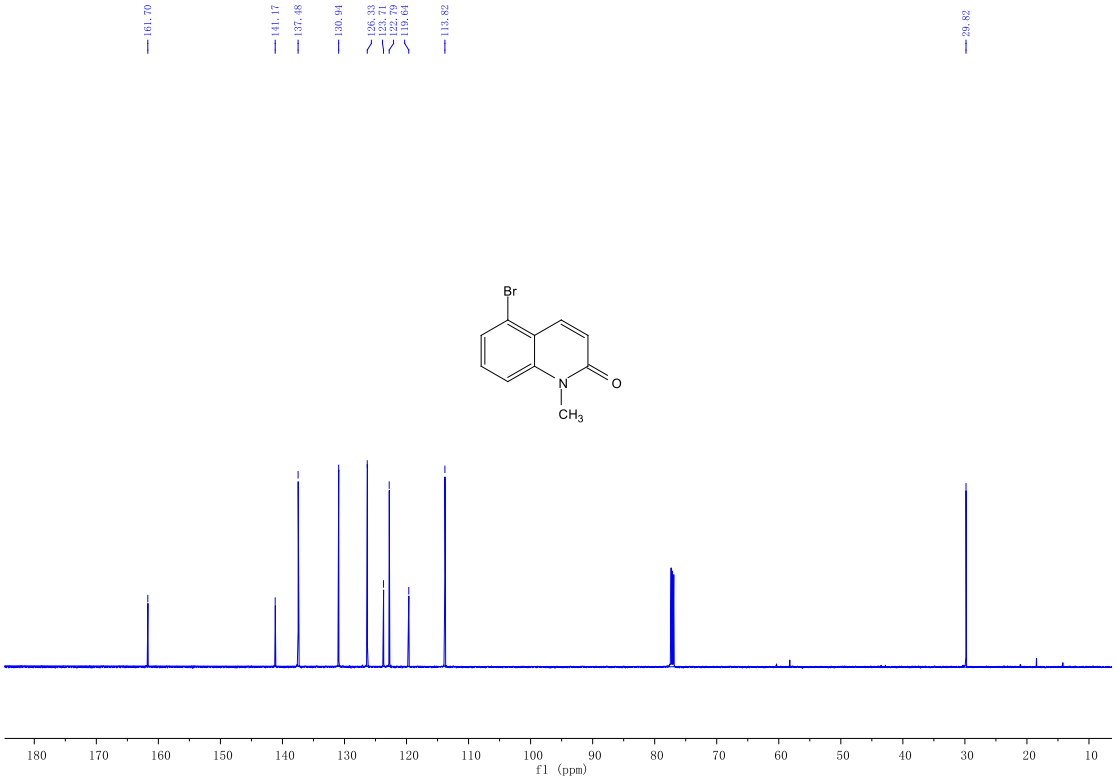
7.44
7.38
7.37
7.37
7.35
7.30
7.29
7.29
6.75
6.74
6.73
3.69
3.69
Br
N
O
CH3
0.99
1.02
1.01
1.16
0.99
3.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.70
141.17
137.48
130.94
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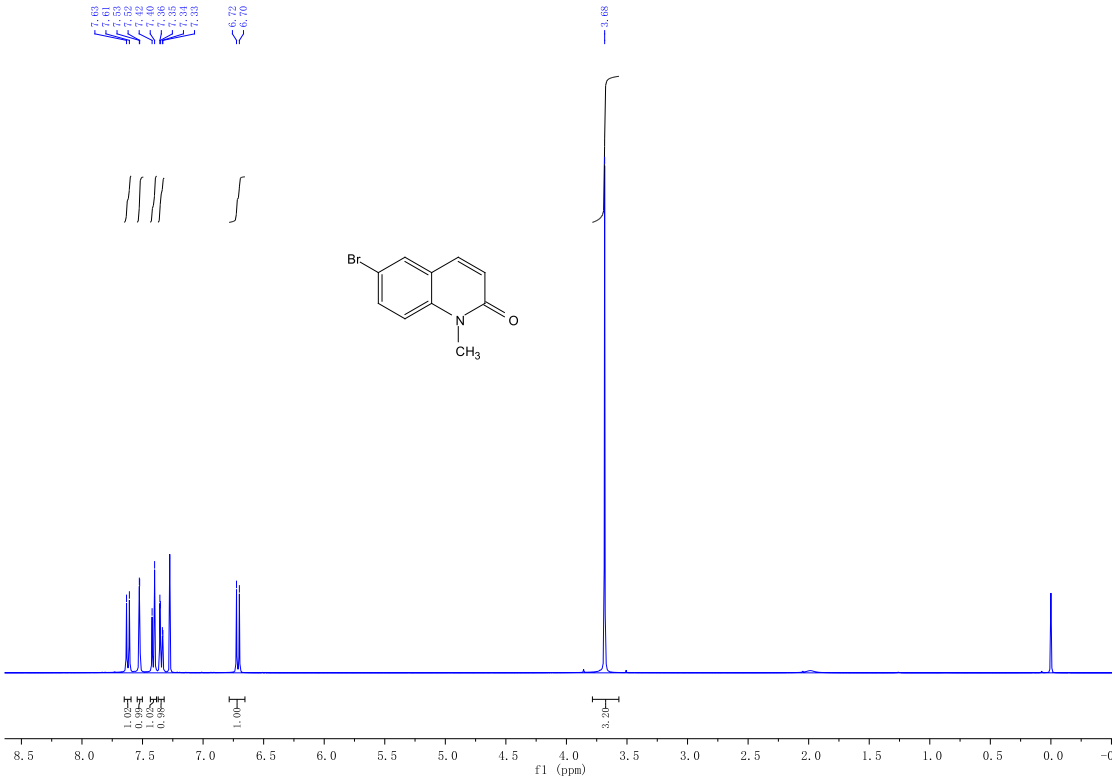
123.71
122.79
119.64
113.82
29.82
Br
N
O
CH3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.53
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7.40
7.36
7.35
7.34
7.33
6.72
6.70
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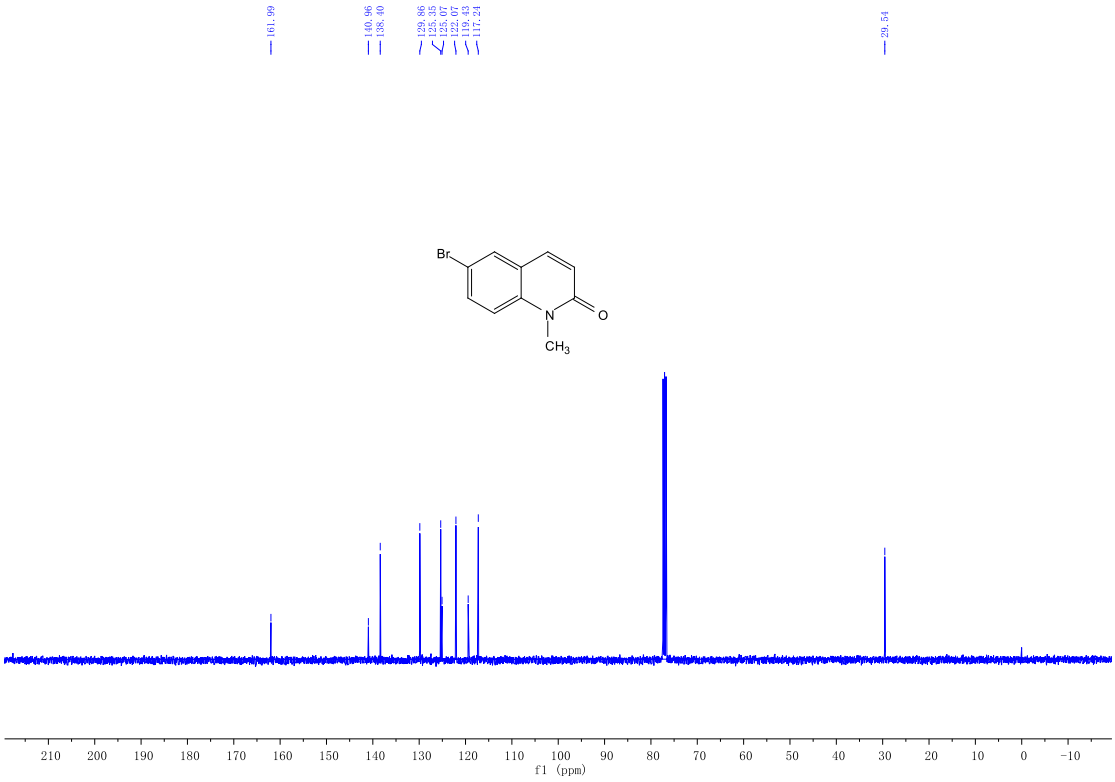
Br
N
O
CH3
1.02
0.99
1.02
0.98
1.00
3.20
f1 (ppm)


161.99
140.96
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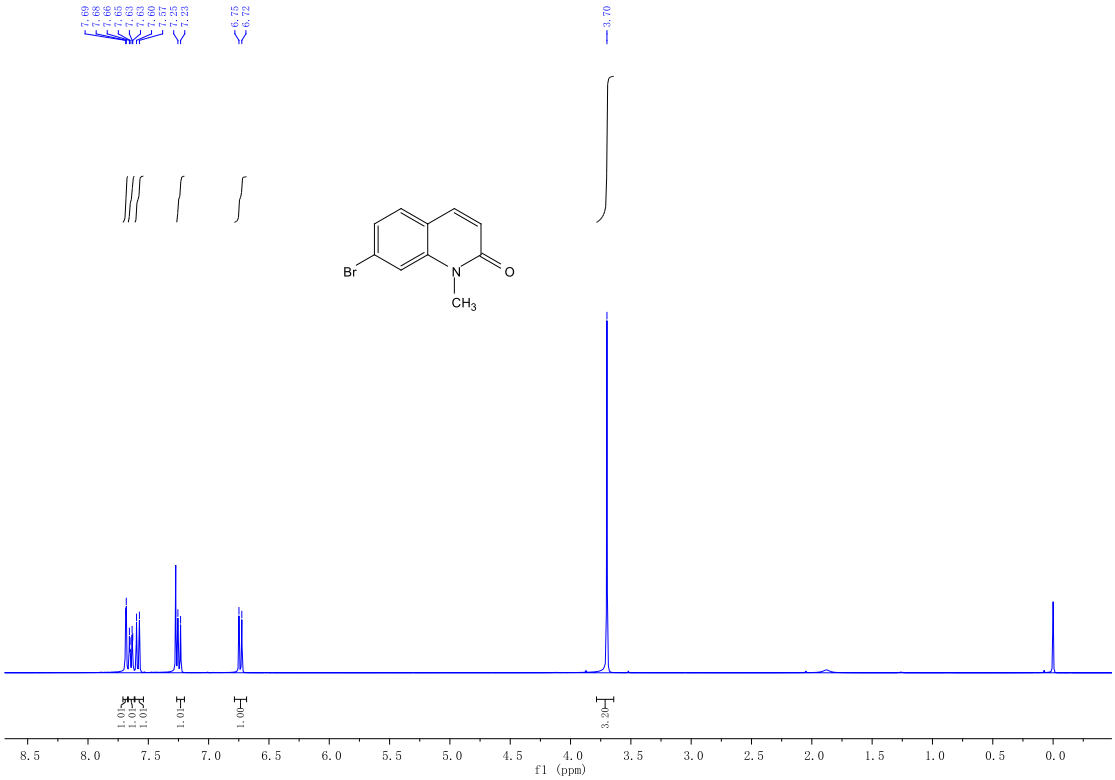
129.86
125.35
125.07
122.07
119.43
117.24
29.54
Br
N
O
CH3
f1 (ppm)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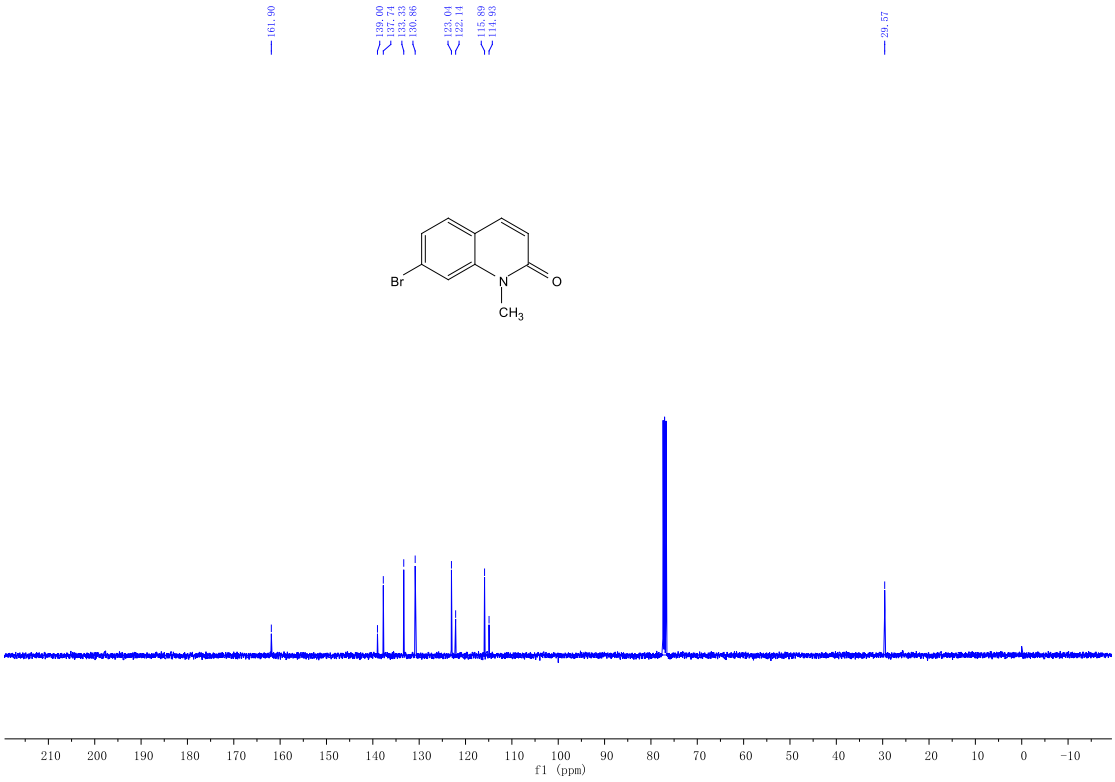
7.68
7.66
7.65
7.63
7.63
7.60
7.57
7.25
7.23
6.75
6.72
3.70
Br
N
O
CH3
1.01
1.01
1.02
1.01
1.00
3.20
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.90
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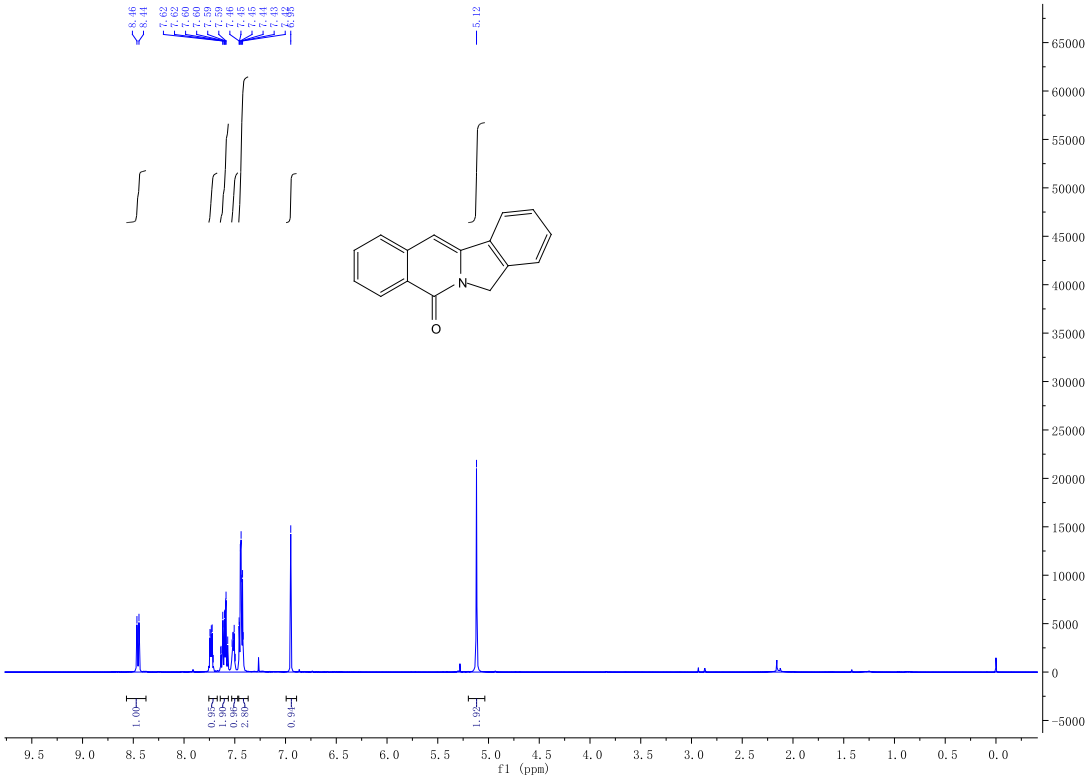
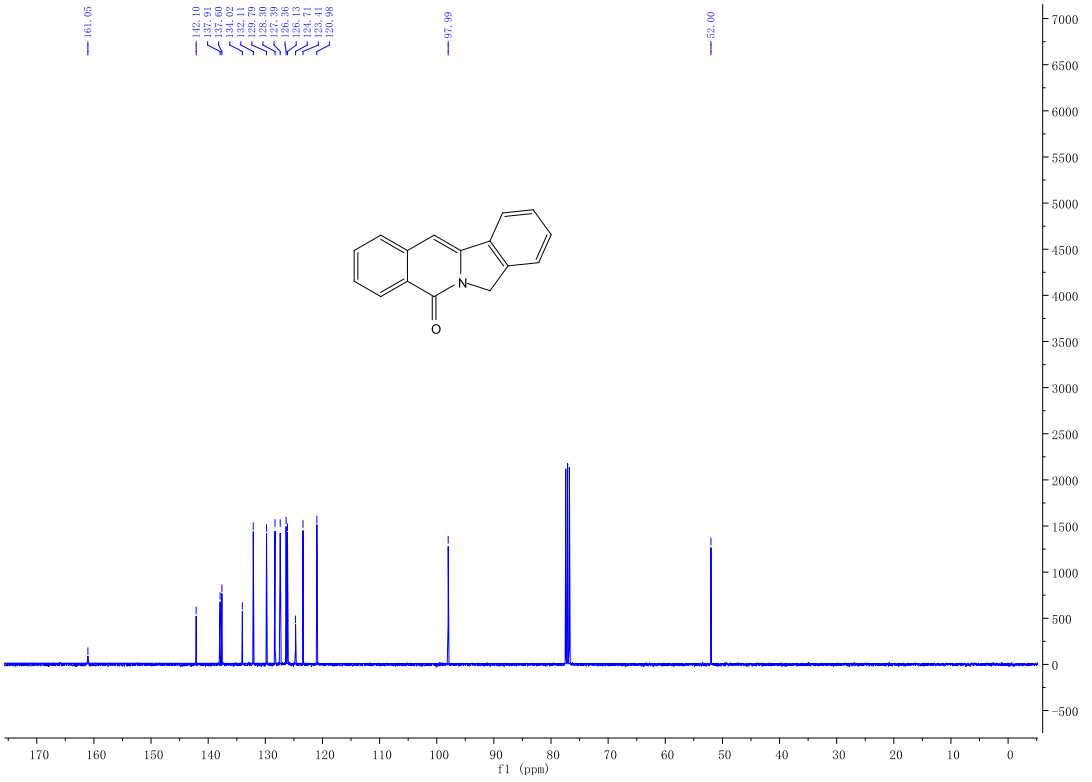
133.33
130.86
123.04
122.14
115.89
114.93
29.57
Br
N
O
CH3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


8.46
8.44
7.62
7.62
7.60
7.60
7.59
7.59
7.46
7.45
7.45
7.44
7.43
6.98
6.98
5.12
1.00
0.95
1.96
0.96
2.80
0.94
1.95
f1 (ppm)


161.65
142.10
137.91
137.60
134.02
132.11
129.79
128.30
127.39
126.36
126.13
124.71
123.41
120.98
97.99
52.00
f1 (ppm)