Supporting Information

Facile Synthesis of Isoquinolines and Isoquinoline *N*-Oxides *via* a Copper-Catalyzed Intramolecular Cyclization in Water

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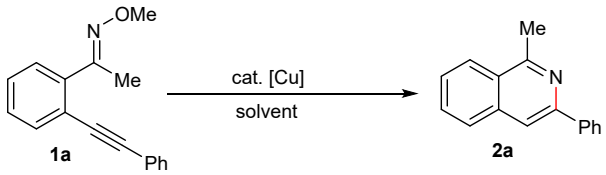
List of Contents

A. General methods

^{1}H, ^{13}C and ^{19}F NMR spectra were recorded at 400 MHz NMR spectrometer using $CDCl_3$ or DMSO-*d*6 as solvent and TMS as an internal standard. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). Coupling constants were reported in Hertz (Hz). IR spectra were obtained with an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets. HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). Melting points were measured using a melting point instrument and were uncorrected. TLC was performed using commercially available 100−400 mesh silica gel plates (GF254). X-ray structural analyses were conducted on an X-ray analysis instrument. Unless otherwise stated, all reagents and solvents were purchased from commercial suppliers and used without further purification.

B. Optimization of Reaction Conditions

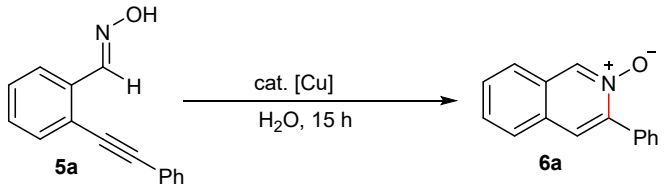
Table S1. Optimization of the Reaction Conditions for the Synthesis of Isoquinolines. [a]



Entry	[Cu]	Solvent	Time (h)	Yield[b] (%)
1	CuI (10 mol%)	H_2O	12	91
2	CuI (10 mol%)	H_2O	15	95
3	CuI (5 mol%)	H_2O	15	88
4	CuI (2.5 mol%)	H_2O	15	76
5	—	H_2O	15	NR
6	CuBr (10 mol%)	H_2O	15	73
7	CuCl (10 mol%)	H_2O	15	46
8	$CuBr_2$ (10 mol%)	H_2O	15	43
9	$Cu(OAc)_2$ (10 mol%)	H_2O	15	NR
10[c]	CuI (10 mol%)	H_2O	15	48
11[d]	CuI (10 mol%)	H_2O	7	92
12[e]	CuI (10 mol%)	H_2O	15	95
13	CuI (10 mol%)	1,4-dioxane	12	87
14	CuI (10 mol%)	toluene	12	28
15	CuI (10 mol%)	EtOH	12	65
16	CuI (10 mol%)	AcOH	12	Trace

[a]Reaction condition: **1a** (0.5 mmol), [Cu] (10 mol%), and solvent (2 mL) at 80 ℃ in a sealed tube, and reaction time as specified. [b]Isolated yields. [c]70 ℃. [d]90 ℃. [e]Under the nitrogen atmosphere.

Table S2. Optimization of the Reaction Conditionsa for the Synthesis of Isoquinoline N-Oxides. [a]

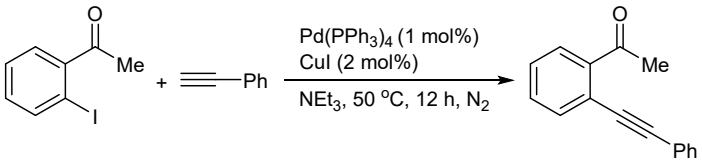


Entry	[Cu]	Temperature (℃℃)	Time (h)	Yield[b] (%)
1	CuI	50	15	NR
2	CuI	70	15	85
3		70	15	NR
4	CuBr	70	15	51
5	CuCl	70	15	35
6	$CuBr_2$	70	15	70
7[c]	CuI	70	15	84

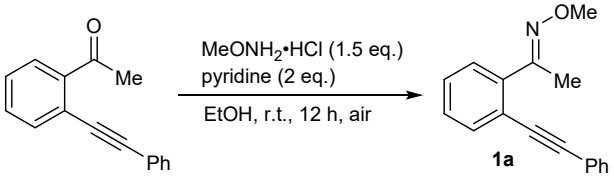
[a]Reaction condition: **1a** (0.5 mmol), [Cu] (10 mol%), and solvent (2 mL) at 70 ℃ in a sealed tube, and reaction time as specified. [b]Isolated yields. [c]Under the nitrogen atmosphere.

C. General Procedure for the Synthesis of Starting Materials

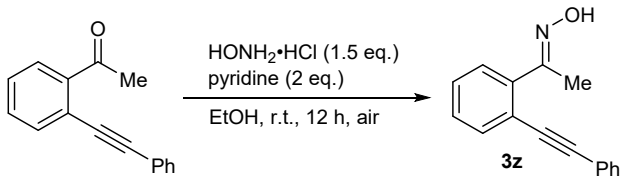
Unless otherwise specified, (*E*)-2-alkynylaryl oxime derivatives (**1a**、**1v** and **5z** were selected as examples) were synthesized *via* the following step:



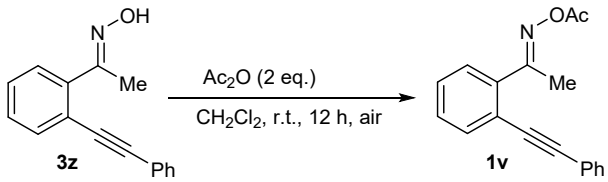
Under the nitrogen atmosphere, 2′-iodoacetophenone (2.46 g, 10 mmol), phenylacetylene (1.12 g, 11 mmol), $Pd(PPh_3)_4$ (116 mg, 0.1 mmol), CuI (38 mg, 0.2 mmol), and triethylamine (20 mL) were added in sequence, and then stirred at 50 ℃ for 12 h. Subsequently, the reaction mixture was quenched with an aqueous solution of saturated NH_4Cl and extracted with ethyl acetate. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was further purified through column chromatography to obtain a yellow liquid (2.06 g, 93%).



1-[2-(2-Phenylethynyl)phenyl]ethanone (1.10 g, 5 mmol) was first dissolved in ethanol (10 mL). Then, pyridine (791 mg, 10 mmol) and methoxyammonium chloride (626 mg, 7.5 mmol) were added to the resulting solution subsequently and the mixture was stirred at room temperature for 12 h. Subsequently, the reaction mixture was extracted with ethyl acetate. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was further purified through column chromatography to obtain a yellow liquid **1a** (935 mg, 75%).

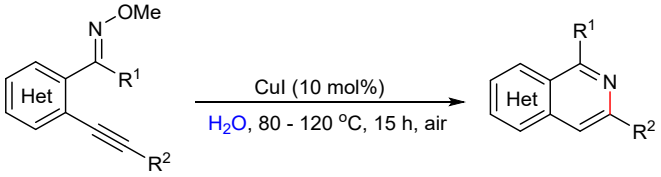


1-[2-(2-Phenylethynyl)phenyl]ethanone (881 mg, 4 mmol) was first dissolved in ethanol (8 mL). Then, pyridine (633 mg, 8 mmol) and hydroxylamine hydrochloride (417 mg, 6 mmol) were added to the resulting solution subsequently and the mixture was stirred at room temperature for 12 h. Subsequently, the reaction mixture was extracted with ethyl acetate. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was further purified through column chromatography to obtain a white solid **5z** (894 mg, 95%).



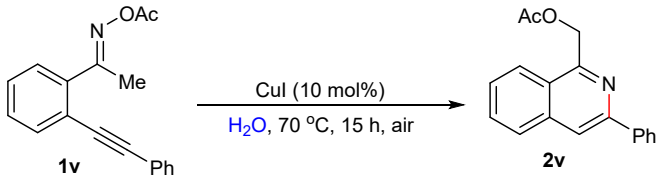
Compound **5z** (471 mg, 2 mmol) was first dissolved in dichloromethane (5 mL). Then, acetic anhydride (408 mg, 4 mmol) was added to the resulting solution and the mixture was stirred at room temperature for 12 h. Subsequently, water (5 mL) was added to the reaction mixture. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was further purified through column chromatography to obtain a white solid **5z** (521 mg, 94%).

D. General Procedure for the Synthesis of Isoquinolines and Isoquinoline *N*-Oxides

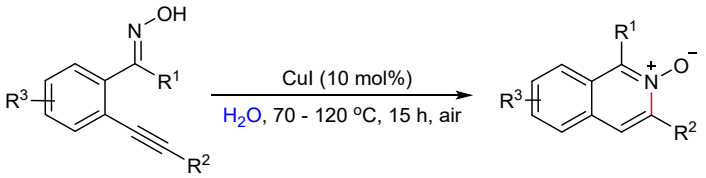


The (*E*)-2-alkynylaryl ketone *O*-methyl oximes **1a-1u** (0.5 mmol) or (*E*)-2-alkynylaryl aldehyde *O*-

methyl oximes **1aa-1ah** (0.5 mmol), CuI (9.5 mg, 0.05 mmol), and H_2O (2 mL) were added to a tube equipped with a stir bar and stirred at 80-100 °C for 15 h. Then the reaction mixture was extracted with ethyl acetate, dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to afford the desired products **2a-2u** and **2aa-2ah**.

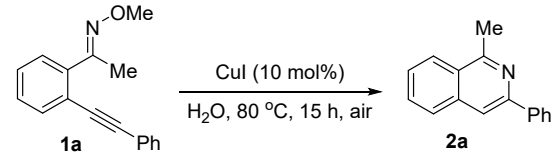


The *N*-Acetoxyl imine **1v** (139 mg, 0.5 mmol), CuI (9.5 mg, 0.05 mmol), and H_2O (2 mL) were added to a tube equipped with a stir bar and stirred at 70 °C for 15 h. Then the reaction mixture was extracted with ethyl acetate, dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to afford the desired product **2v**.



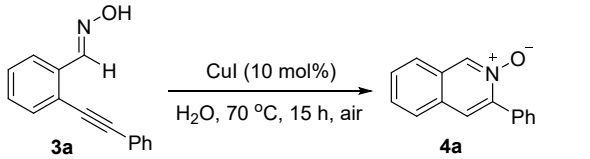
The (*E*)-2-alkynylaryl oximes **3a-3z** (0.5 mmol), CuI (9.5 mg, 0.05 mmol), and H_2O (2 mL) were added to a tube equipped with a stir bar and stirred at 70-120 °C for 15 h. Then the reaction mixture was extracted with ethyl acetate, dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel with ethyl acetate as eluent to afford the desired products **4a-4z**.

E. Gram Scale Experiments



The (*E*)-2-alkynylaryl ketone *O*-methyl oxime\ **1a** (2.49 g, 10 mmol), CuI (190 mg, 1 mmol), and H_2O (20 mL) were added to a tube equipped with a stir bar and stirred at 80 °C for 15 h. Then the reaction mixture was extracted with ethyl acetate, dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as

eluent to afford the desired products **2a** (2.06 g, 94%).

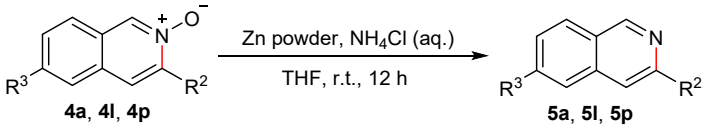


3a
2.21 g (10.0 mmol)

4a
85%, 1.88 g (8.5 mmol)

The (*E*)-2-alkynylaryl oxime **3a** (2.21 g, 10 mmol), CuI (190 mg, 1 mmol), and H_2O (20 mL) were added to a tube equipped with a stir bar and stirred at 70 °C for 15 h. Then the reaction mixture was extracted with ethyl acetate, dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel with ethyl acetate as eluent to afford the desired products **4a** (1.88 g, 85%).

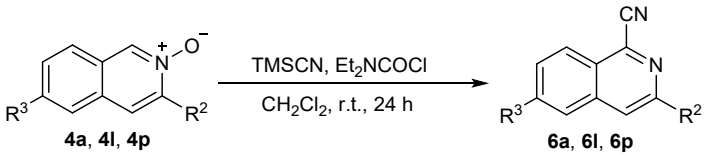
F. Synthetic Procedure for 5a, 5l, and 5p



4a, **4l**, **4p** **5a**, **5l**, **5p**

Isoquinoline *N*-oxides (0.2 mmol) was first dissolved in THF (2 mL). Then, Zn powder (131 mg, 2 mmol) and an aqueous solution of saturated NH_4Cl (2 mL) were added to the resulting solution subsequently and the mixture was stirred at room temperature for 12 h. Subsequently, the reaction mixture was extracted with ethyl acetate. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was further purified through column chromatography to obtain isoquinolines **5a**, **5l**, and **5p.**

G. Synthetic Procedure for 6a, 6l, and 6p

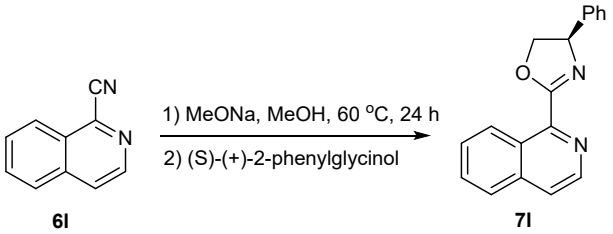


4a, **4l**, **4p** **6a**, **6l**, **6p**

The **4a, 4l** and **4p** were prepared according to the reported procedure [Org. Chem. Front., 2015, 2, 819–822.]. To a solution of isoquinoline *N*-oxides (0.5 mmol) in CH_2Cl_2 (5 mL) was added trimethylsilyl cyanide (248 mg, 2.5 mmol). Then a solution of diethylcarbamoyl chloride (339 mg, 2.5 mmol) in CH_2Cl_2 (10 mL) was slowly added in 10 min, and the reaction mixture was stirred at room temperature for 24 h. After K_2CO_3 (10 mL, 10 % aq.) was added, the mixture was extracted several times with CH_2Cl_2. The combined organic phases were washed with water and then dried over Na_2SO_4. The organic phase was concentrated and

purified by silica gel chromatography to afford the products **6a, 6l** and **6p**.

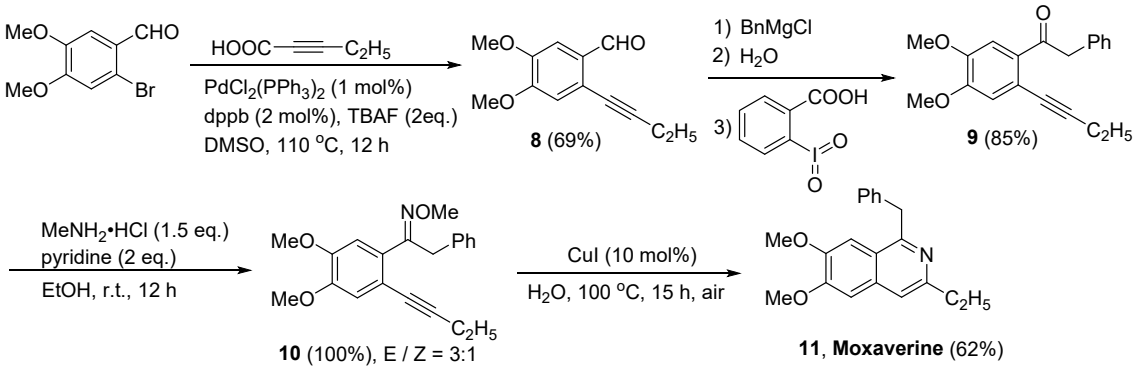
H. Synthetic Procedure for 7l



6l **7l**

The **6l** was prepared according to the reported procedure [Org. Chem. Front., 2015, 2, 819–822.]. To a stirred solution of **6l** (154 mg, 1 mmol) in MeOH (5 mL), NaOMe (18 mg, 0.3 mmol) was added under nitrogen. The mixture was stirred at 60 ℃ for 24 h. The solvent was removed under vacuum, and the residue was then dissolved in 10 mL of ethyl acetate and then washed with water and brine. The organic phase was separated and dried over Na_2SO_4. After removal of the solvent, the crude product was dissolved in dry THF (5 mL). (S)-(+)-2-Phenylglycinol (137 mg, 1 mmol) and HCl (1 drop, 33% aq.) were added, and the mixture was refluxed under nitrogen atmosphere. After 12 h, the mixture was diluted with water (20 mL) and extracted with ethyl acetate. The combined organic phases were washed with water and then dried over Na_2SO_4. After the removal of solvent under reduced pressure, the residue was purified by silica gel chromatography to afford product **7l** as a pale-yellow oil (82 mg, 30%).

I. Synthetic Procedure for Moxaverine



The alkyne **8** was prepared according to the reported procedure [Angew. Chem. 2015, 127, 13115–13119.]. To a 50 mL Schlenk tube, 6-bromoveratraldehyde (2.45 g, 10.0 mmol), 2-pentynoic acid (1.03 g, 10.5 mmol), $PdCl_2(PPh_3)_2$ (70 mg, 0.1 mmol), 1,4-bis(diphenylphosphino)butane (dppb) (85 mg, 0.2 mmol), TBAF (1 M in THF, 20 mL, 20 mmol), and DMSO (15 mL) were added. The resulting mixture was stirred under nitrogen at 110 ℃ for 12 h. After cooling to room temperature, the reaction mixture was quenched with an aqueous

solution of saturated NH_4Cl and extracted with ethyl acetate. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was further purified through column chromatography to obtain alkyne **8** as a yellow liquid (1.51 g, 69%).

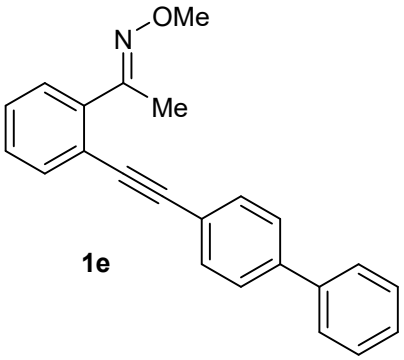
Under the nitrogen atmosphere, benzylmagnesium chloride (1.0 M in THF, 6.0 mL, 6.0 mmol) was added dropwise to a stirred solution of alkyne **8** (1.09 g, 5 mmol) in THF (10 mL) at -40 ℃. After 30 min, the reaction was warmed to room temperature and stirred for 12 h. The reaction mixture was quenched with an aqueous solution of saturated NH_4Cl and extracted with ethyl acetate. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was then dissolved in DMSO (15 mL). 2-Iodoxybenzoic acid (1.40 g, 5 mmol) was added, and the reaction mixture was stirred at room temperature for 12 h. Then the reaction mixture was diluted with an aqueous solution of saturated NH_4Cl and extracted with ethyl acetate. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was further purified through column chromatography to obtain a white solid **9** (1.31 g, 85 %).

The intermediate product **9** (1.23 g, 4 mmol) was first dissolved in ethanol (10 mL). Then, pyridine (633 mg, 8 mmol) and methoxyammonium chloride (501 mg, 6 mmol) were added to the resulting solution subsequently and the mixture was stirred at room temperature for 12 h. Subsequently, the reaction mixture was extracted with ethyl acetate. The organic layer was washed with water and brine, then dried over Na_2SO_4, filtered and concentrated under reduced pressure. The crude product was further purified through column chromatography to obtain a yellow liquid **10** (1.35 g, 100%, *E*/*Z*=3:1).

The 2-alkynylaryl ketone *O*-methyl oxime **10** (169 mg, 0.5 mmol), CuI (9.5 mg, 0.05 mmol), and H_2O (2 mL) were added to a tube equipped with a stir bar and stirred at 100 °C for 15 h. Then the reaction mixture was extracted with ethyl acetate, dried over anhydrous Na_2SO_4, filtered, and evaporated under vacuum. The crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to afford the moxaverine as a pale-yellow oil (72 mg, 62%).

J. Crystal structure determination

I. ORTEP representation with 50% probability thermal ellipsoids. Crystal data have been deposited to CCDC, number 2097802.



1e

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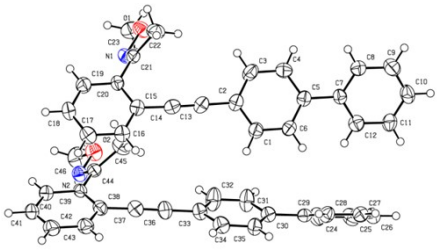
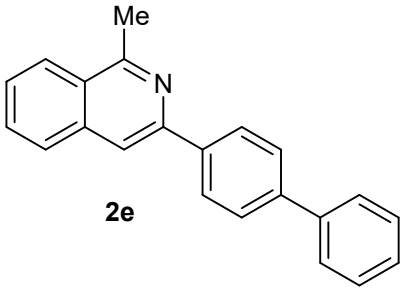


X-ray of **1e**
CCDC 2097802

Empirical formula	$C_{23}H_{19}NO$
Formula weight	325.39
Temperature/K	170.0
Crystal system	triclinic
Space group	P-1
a/Å	10.4869(10)
b/Å	10.7023(11)
c/Å	16.7778(18)
α/°	85.624(3)
β/°	82.721(3)
γ/°	72.345(3)
Volume/Å^3	1778.5(3)
Z	4
ρ_{calc}g/cm^3	1.215
μ/mm^{-1}	0.074
F(000)	688.0
Crystal size/mm^3	0.11 × 0.04 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.998 to 50.052
Index ranges	-11 ≤ h ≤ 12, -12 ≤ k ≤ 12, -19 ≤ l ≤ 19
Reflections collected	18380
Independent reflections	6253 [R_{int} = 0.1167, R_{sigma} = 0.1498]
Data/restraints/parameters	6253/0/455
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0766, wR_2 = 0.1380
Final R indexes [all data]	R_1 = 0.2061, wR_2 = 0.1993
Largest diff. peak/hole / e Å^{-3}	0.24/-0.25

II. ORTEP representation with 50% probability thermal ellipsoids. Crystal data have been deposited to CCDC, number 2095902.



2e

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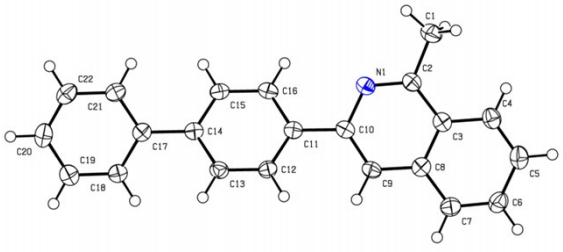
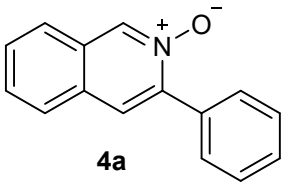


X-ray of **2e**
CCDC 2095902

Empirical formula	$C_{22}H_{17}N$
Formula weight	295.36
Temperature/K	140.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.0452(9)
b/Å	9.2637(12)
c/Å	23.462(4)
α/°	90
β/°	90.102(2)
γ/°	90
Volume/Å^3	1531.2(4)
Z	4
ρ_{calc}g/cm^3	1.281
μ/mm^{-1}	0.074
F(000)	624.0
Crystal size/mm^3	0.15 × 0.08 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.728 to 52.962
Index ranges	$-8 \le h \le 8$, $-10 \le k \le 11$, $-29 \le l \le 27$
Reflections collected	11289
Independent reflections	3117 [R_{int} = 0.0581, R_{sigma} = 0.0586]
Data/restraints/parameters	3117/0/209
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0506, wR_2 = 0.1114
Final R indexes [all data]	R_1 = 0.0822, wR_2 = 0.1330
Largest diff. peak/hole / e Å^{-3}	0.21/-0.20

I. ORTEP representation with 50% probability thermal ellipsoids. Crystal data have been deposited to CCDC, number 2128901.



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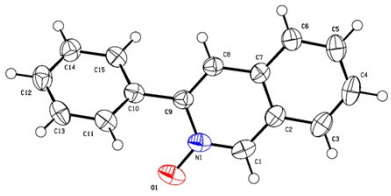
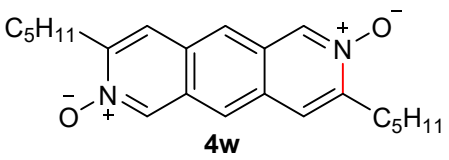


X-ray of **4a**
CCDC 2128901

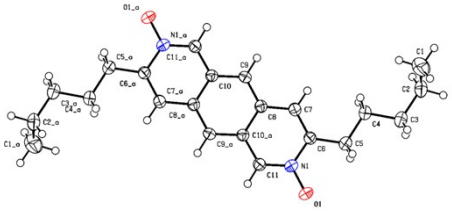
Empirical formula	$C_{15}H_{11}NO$
Formula weight	221.25
Temperature/K	170.0
Crystal system	monoclinic
Space group	C2/c
a/Å	18.473(2)
b/Å	6.0831(6)
c/Å	19.451(2)
α/°	90
β/°	100.583(6)
γ/°	90
Volume/Å^3	2148.5(4)
Z	8
ρ_{calc}g/cm^3	1.368
μ/mm^{-1}	0.086
F(000)	928.0
Crystal size/mm^3	0.12 × 0.08 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.26 to 53.03
Index ranges	-22 ≤ h ≤ 22, -7 ≤ k ≤ 6, -24 ≤ l ≤ 23
Reflections collected	9320
Independent reflections	2200 [R_{int} = 0.0738, R_{sigma} = 0.0702]
Data/restraints/parameters	2200/0/154
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0617, wR_2 = 0.1386
Final R indexes [all data]	R_1 = 0.1303, wR_2 = 0.1769
Largest diff. peak/hole / e Å^{-3}	0.18/-0.20

II. ORTEP representation with 50% probability thermal ellipsoids. Crystal data have been deposited to CCDC, number 2142641.



4w

≡

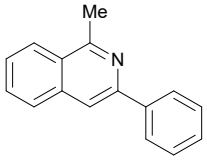


X-ray of **4w**
CCDC 2142641

Empirical formula	$C_{22}H_{28}N_2O_2$
Formula weight	352.46
Temperature/K	150.0
Crystal system	trigonal
Space group	R-3
a/Å	22.8147(12)
b/Å	22.8147(12)
c/Å	10.5217(7)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	4742.9(6)
Z	9
ρ_{calc}g/cm^3	1.111
μ/mm^{-1}	0.071
F(000)	1710.0
Crystal size/mm^3	0.15 × 0.06 × 0.04
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.386 to 52.918
Index ranges	-26 ≤ h ≤ 28, -28 ≤ k ≤ 26, -13 ≤ l ≤ 13
Reflections collected	13322
Independent reflections	2167 [R_{int} = 0.0801, R_{sigma} = 0.0566]
Data/restraints/parameters	2167/0/119
Goodness-of-fit on F^2	1.020
Final R indexes [I>=2σ (I)]	R_1 = 0.0565, wR_2 = 0.1309
Final R indexes [all data]	R_1 = 0.1042, wR_2 = 0.1559
Largest diff. peak/hole / e Å^{-3}	0.26/-0.24

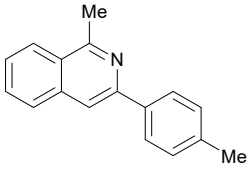
K. Analytical Date

1-methyl-3-phenylisoquinoline (2a)



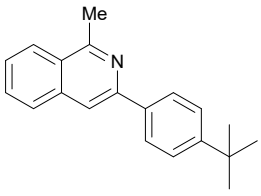
Reaction temperature was 80 ℃. Pale yellow solid (104 mg, 95 % yield, known product), mp 46 - 48 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.17 - 8.19 (m, 2H), 8.13 - 8.16 (m, 1H), 7.95 (s, 1H), 7.86 - 7.89 (m, 1H), 7.67 - 7.71 (m, 1H), 7.57 - 7.61 (m, 1H), 7.52 - 7.56 (m, 2H), 7.42 - 7.46 (m, 1H), 3.08 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) : δ 158.6, 150.0, 139.9, 136.8, 130.0, 128.8, 128.3, 127.7, 127.0, 126.8, 126.6, 125.7, 115.3, 22.7 ppm; IR (KBr): 3058, 2922, 1567, 1387, 1278, 745, 690 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}N$ $[M+H]^+$ 220.1121; found 220.1119.

1-methyl-3-(p-tolyl)isoquinoline (2b)



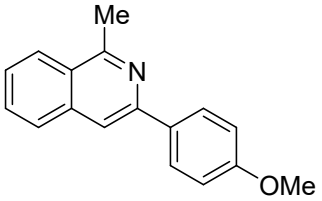
Reaction temperature was 80 ℃. Pale yellow oil (114 mg, 98 % yield, known product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 - 8.15 (m, 1H), 8.05 - 8.09 (m, 2H), 7.92 (s, 1H), 7.85 - 7.87 (m, 1H), 7.66 - 7.70 (m, 1H), 7.55 - 7.59 (m, 1H), 7.32 - 7.35 (m, 2H), 3.06 (s, 3H), 2.46 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.5, 150.1, 138.2, 137.1, 136.8, 130.0, 129.5, 127.6, 126.9, 126.6, 126.5, 125.6, 114.7, 22.7, 21.3 ppm; IR (KBr): 3058, 2921, 1567, 1441, 821, 749 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{17}H_{16}N$ $[M+H]^+$ 234.1277; found 234.1276.

3-(4-(*t*-butyl)phenyl)-1-methylisoquinoline (2c)



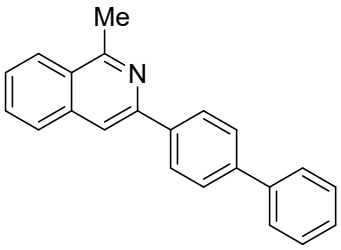
Reaction temperature was 80 ℃. Pale yellow oil (125 mg, 91 % yield, known product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 - 8.16 (m, 1H), 8.06 - 8.10 (m, 2H), 7.92 (s, 1H), 7.86 - 7.89 (m, 1H), 7.66 - 7.70 (m, 1H), 7.53 - 7.60 (m, 3H), 3.06 (s, 3H), 1.41 (s, 9H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.5, 151.4, 150.2, 137.1, 136.8, 129.9, 127.6, 126.7, 126.6, 126.5, 125.69, 125.66, 114.9, 34.7, 31.4, 22.7 ppm; IR (KBr): 3059, 2957, 1566, 1267, 835, 747 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{20}H_{22}N$ $[M+H]^+$ 276.1747; found 276.1744.

3-(4-methoxyphenyl)-1-methylisoquinoline (2d)



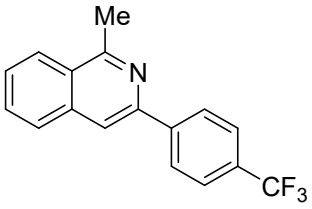
Reaction temperature was 80 ℃. Pale yellow solid (116 mg, 93 % yield, known product), mp 58 - 60 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 - 8.14 (m, 3H), 7.83 - 7.86 (m, 2H), 7.65 - 7.69 (m, 1H), 7.53 - 7.58 (m, 1H), 7.04 - 7.07 (m, 2H), 3.90 (s, 3H), 3.05 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.0, 158.4, 149.8, 136.9, 132.6, 130.0, 128.2, 127.5, 126.4, 126.3, 125.7, 114.1, 55.4, 22.7 ppm; IR (KBr): 3060, 2953, 1511, 1246, 831, 750 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{17}H_{16}NO$ $[M+H]^+$ 250.1226; found 250.1225.

3-([1,1'-biphenyl]-4-yl)-1-methylisoquinoline (2e)



Reaction temperature was 120 ℃. Pale yellow solid (126 mg, 85 % yield, known product), mp 145 - 147 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 - 8.27 (m, 2H), 8.15 - 8.18 (m, 1H), 8.00 (s, 1H), 7.89 - 7.91 (s, 1H), 7.75 - 7.78 (m, 2H), 7.69 - 7.73 (m, 3H), 7.58 - 7.63 (m, 1H), 7.48 - 7.52 (m, 2H), 7.38 - 7.42 (m, 1H), 3.09 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.7, 149.6, 141.1, 140.9, 138.8, 136.8, 130.1, 128.8, 127.7, 127.5, 127.38, 127.36, 127.1, 126.8, 126.7, 125.7, 115.1, 22.7 ppm; IR (KBr): 3058, 2921, 1567, 1440, 840, 730 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{18}N$ $[M+H]^+$ 296.1434; found 296.1432.

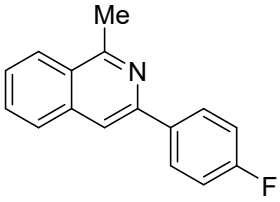
1-methyl-3-(4-(trifluoromethyl)phenyl)isoquinoline (2f)



Reaction temperature was 90 ℃. Pale yellow oil (89 mg, 62 % yield, known product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.26 - 8.28 (m, 2H), 8.14 - 8.17 (m, 1H), 7.97 (s, 1H), 7.87 - 7.90 (m, 1H), 7.75 - 7.78 (m, 2H), 7.70 - 7.74 (m, 1H), 7.61 - 7.65 (m, 1H), 3.06 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.0, 148.3, 143.2 (q, J = 1.8 Hz), 136.6, 130.3, 130.1 (q, J = 32.1 Hz), 127.8, 127.4, 127.2, 127.0, 125.7, 125.6 (q, J = 3.7 Hz), 124.4 (q, J = 270.3 Hz), 116.0, 22.6 ppm; ^{19}F NMR ($CDCl_3$): δ -62.4 ppm; IR (KBr): 3065, 2925,

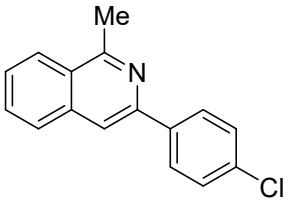
2854, 1619, 1571, 1324, 1121, 842, 747 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{17}H_{13}F_3N$ $[M+H]^+$ 288.0995; found 288.0992.

3-(4-fluorophenyl)-1-methylisoquinoline (2g)



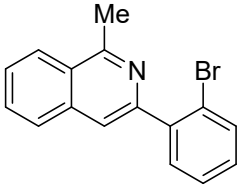
Reaction temperature was 90 ℃. Pale yellow solid (106 mg, 89 % yield, known product), mp 75 – 77 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 8.12 - 8.16 (m, 3H), 7.85 - 7.88 (m, 2H), 7.67 - 7.71 (m, 1H), 7.57 - 7.61 (m, 1H), 7.17 - 7.23 (m, 2H), 3.05 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.2 (d, J = 245.8 Hz), 158.7, 149.0, 136.8, 136.0 (d, J = 3.0Hz), 130.1, 128.7 (m, J = 8.1 Hz) 127.6, 126.9, 126.5, 125.7, 115.6 (d, J = 21.4 Hz), 114.9, 22.7 ppm; ^{19}F NMR ($CDCl_3$): δ -114.2 ppm; IR (KBr): 3051, 2924, 1510, 1228, 835, 723 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{13}FN$ $[M+H]^+$ 238.1027; found 238.1024.

3-(4-chlorophenyl)-1-methylisoquinoline (2h)



Reaction temperature was 90 ℃. Pale yellow solid (94 mg, 74 % yield, known product), mp 50 - 52 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 8.09 - 8.14 (m, 3H), 7.89 (s, 1H), 7.84 - 7.87 (m, 1H), 7.67 - 7.71 (m, 1H), 7.57 - 7.62 (m, 1H), 7.46 - 7.50 (m, 2H), 3.05 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.7, 148.7, 138.3, 136.7, 134.3, 130.2, 128.9, 128.2, 127.6, 127.0, 126.7, 125.7, 115.1, 22.7 ppm; IR (KBr): 3063, 2921, 1568, 1281, 838, 749 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{13}ClN$ $[M+H]^+$ 254.0731; found 254.0728.

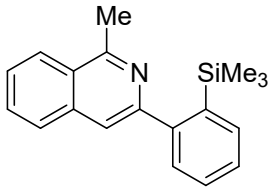
3-(2-bromophenyl)-1-methylisoquinoline (2i)



Reaction temperature was 90 ℃. Pale yellow oil (112 mg, 75 % yield, new product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.19 - 8.21 (m, 1H), 7.88 - 7.90 (m, 1H), 7.81 (s, 1H), 7.71 - 7.75 (m, 2H), 7.63 - 7.67 (m, 2H), 7.45 (td, J = 1.2, 7.6 Hz, 1H), 7.25 - 7.29 (m, 1H), 3.06 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.4, 150.7, 141.6, 135.9, 133.3, 131.8, 130.2, 129.3, 127.7, 127.5, 127.3, 126.5, 125.7, 122.4, 119.8, 22.5 ppm; IR

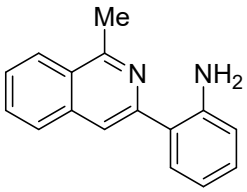
(KBr): 3060, 2922, 1566, 1437, 1389, 1261, 754 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{13}BrN$ $[M+H]^+$ 298.0226; found 298.0223.

1-methyl-3-(2-(trimethylsilyl)phenyl)isoquinoline (2j)



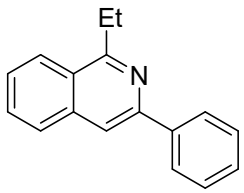
Reaction temperature was 90 ℃. Yellow oil (118 mg, 81 % yield, new product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.18 - 8.21 (m, 1H), 7.86 - 7.89 (m, 1H), 7.70 - 7.78 (m, 3H), 7.61 - 7.65 (m, 1H), 7.56 - 7.59 (m, 1H), 7.41 - 7.50 (m, 2H), 3.06 (s, 3H), 0.11 (s, 9H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.6, 154.4, 147.7, 139.3, 136.5, 135.4, 130.1, 129.4, 128.8, 127.5, 127.1, 126.8, 126.3, 125.6, 118.0, 22.0, 0.9 ppm; IR (KBr): 3052, 2952, 1566, 1245, 841, 730 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{19}H_{22}NSi$ $[M+H]^+$ 292.1516; found 292.1513.

2-(1-methylisoquinolin-3-yl)aniline (2k)



Reaction temperature was 80 ℃. Pale yellow oil (55 mg, 47 % yield, new product). ^1H NMR (400 MHz, DMSO-d6): δ 8.20 - 8.23 (m, 1H), 7.98 - 8.01 (m, 2H), 7.74 - 7.78 (m, 1H), 7.62 - 7.66 (m, 1H), 7.55 - 7.58 (m, 1H), 7.08 - 7.12 (m, 1H), 6.79 (d, J = 8.0 Hz, 1H), 6.65 - 6.89 (m, 1H), 6.37 (s, 2H, NH_2), 2.95 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO-d6): δ 157.3, 152.1, 147.9, 137.1, 130.8, 129.8, 129.7, 128.0, 127.4, 126.1, 125.5, 122.1, 116.94, 116.87, 1116.7, 22.7 ppm; IR (KBr): 3449, 3310, 3059, 2924, 2857, 1612, 1585, 1461, 1283, 883, 748 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{15}N_2$ $[M+H]^+$ 235.1230; found 235.1227.

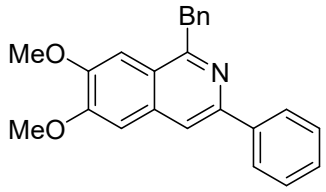
1-ethyl-3-phenylisoquinoline (2l)



Reaction temperature was 120 ℃. Pale yellow oil (73 mg, 63 % yield, known product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.19 - 8.24 (m, 3H), 7.96 (s, 1H), 7.88 - 7.91 (m, 1H), 7.67 - 7.71 (m, 1H), 7.57 - 7.61 (m, 1H), 7.52 - 7.56 (m, 2H), 7.42 - 7.46 (m, 1H), 3.45 (q, J = 7.6 Hz, 2H), 1.57 (t, J = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.9, 147.8, 137.9, 135.2, 128.0, 126.8, 126.4, 125.9, 125.1, 124.8, 124.0, 123.3,

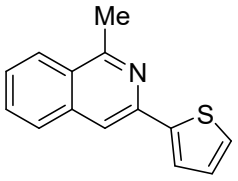
113.1, 26.5, 11.5 ppm; IR (KBr): 3059, 2970, 2928, 2853, 1569, 882, 769, 747, 693 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{17}H_{16}N$ $[M+H]^+$ 234.1277; found 234.1276.

1-benzyl-6,7-dimethoxy-3-phenylisoquinoline (2m)



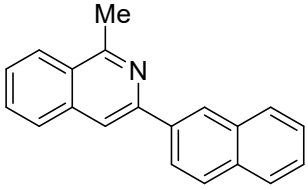
Reaction temperature was 120 ℃. Pale yellow solid (50 mg, 28 % yield, new product), mp 119 - 121 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 8.19 - 8.21 (m, 2H), 7.89 (s, 1H), 7.52 - 7.56 (m, 2H), 7.38 - 7.45 (m, 3H), 7.28 - 7.32 (m, 3H), 7.19 - 7.23 (m, 1H), 7.11 (s, 1H), 4.72 (s, 2H), 4.02 (s, 3H), 3.91 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.6, 152.5, 149.7, 149.0, 140.0, 139.8, 134.3, 128.7, 128.5, 128.1, 126.8, 126.2, 122.0, 114.8, 105.7, 104.3, 56.0, 55.9, 42.9 ppm; IR (KBr): 3060, 3025, 2927, 2836, 1505, 1422, 1245, 750, 697 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{24}H_{22}NO_2$ $[M+H]^+$ 356.1645; found 356.1642.

1-methyl-3-(thiophen-2-yl)isoquinoline (2n)



Reaction temperature was 80 ℃. Pale yellow oil (80 mg, 71 % yield, known product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.08 - 8.12 (s, 1H), 7.85 (s, 1H), 7.80 - 7.83 (m, 1H), 7.71 (dd, J = 1.2, 3.6 Hz, 1H), 7.64 - 7.69 (m, 1H), 7.53 - 7.57 (m, 1H), 7.40 - 7.41 (m, 1H), 7.17 (dd, J = 3.6, 5.2 Hz, 1H), 3.02 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.8, 145.5, 145.4, 136.6, 130.2, 128.1, 127.4, 126.7, 126.6, 125.8, 123.8, 113.1, 22.5 ppm; IR (KBr): 3067, 2921, 1568, 1447, 1278, 823, 710 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{14}H_{12}NS$ $[M+H]^+$ 226.0685; found 226.0683.

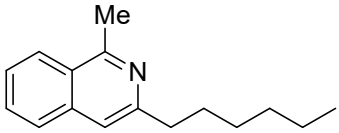
1-methyl-3-(naphthalen-2-yl)isoquinoline (2o)



Reaction temperature was 80 ℃. Pale yellow solid (122 mg, 90 % yield, known product), mp 131 - 133 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 8.71 - 8.72 (m, 1H), 8.29 - 8.32 (m, 1H), 8.15 - 8.18 (m, 1H), 8.08 (s, 1H), 7.99 - 8.04 (m, 2H), 7.88 - 7.93 (m, 2H), 7.68 - 7.72 (m, 1H), 7.51 - 7.63 (m, 3H), 3.12 (s, 3H) ppm; ^{13}C

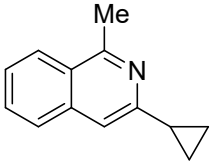
NMR (100 MHz, $CDCl_3$): δ 158.7, 149.8, 137.1, 136.8, 133.8, 133.5, 130.1, 128.8, 128.4, 127.7, 126.9, 126.7, 126.22, 126.20, 125.7, 124.8, 115.6, 22.8 ppm; IR (KBr): 3056, 2921, 1568, 1267, 816, 746 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{20}H_{16}N$ $[M+H]^+$ 270.1277; found 270.1274.

3-hexyl-1-methylisoquinoline (2p)



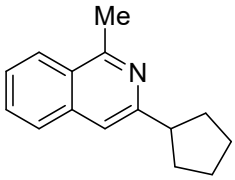
Reaction temperature was 80 ℃. Pale yellow oil (88 mg, 77 % yield, known product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.06 - 8.09 (m, 1H), 7.72 - 7.74 (m, 1H), 7.60 - 7.64 (m, 1H), 7.49 - 7.53 (m, 1H), 7.33 (s, 1H), 2.96 (s, 3H), 2.89 - 2.93 (m, 2H), 1.79 - 1.86 (m, 2H), 1.39 - 1.43 (m, 4H), 0.91 - 0.95 (m, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.0, 154.6, 136.7, 129.7, 126.8, 126.0, 125.8, 125.5, 116.5, 38.2, 31.7, 29.7, 22.6, 22.4, 14.1 ppm; IR (KBr): 3061, 2925, 2857, 1624, 1568, 877, 748 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{20}N$ $[M+H]^+$ 214.1590; found 214.1588.

3-cyclopropyl-1-methylisoquinoline (2q)



Reaction temperature was 80 ℃. Pale yellow solid (74 mg, 81 % yield, new product), mp 49 - 51 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 8.03 - 8.06 (s, 1H), 7.69 - 7.71 (m, 1H), 7.58 - 7.62 (m, 1H), 7.45 - 7.50 (m, 1H), 7.28 (s, 1H), 2.93 (s, 3H), 2.16 - 2.22 (m, 1H), 1.00 - 1.11 (m, 4H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.1, 154.9, 136.6, 129.7, 126.5, 125.9, 125.59, 125.55, 114.3, 22.4, 17.1, 8.9 ppm; IR (KBr): 3004, 2919, 1622, 1570, 1269, 949, 745 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{13}H_{14}N$ $[M+H]^+$ 184.1121; found 184.1120.

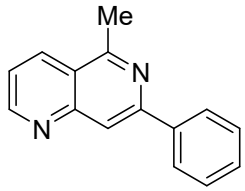
3-cyclopentyl-1-methylisoquinoline (2r)



Reaction temperature was 90 ℃. Pale yellow oil (90 mg, 85 % yield, known product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.00 - 8.03 (m, 1H), 7.67 - 7.70 (m, 1H), 7.54 - 7.58 (m, 1H), 7.43 - 7.48 (m, 1H), 7.32 (s, 1H), 3.24 - 3.32 (m, 1H), 2.92 (m, 3H), 2.10 - 2.17 (m, 2H), 1.70 - 1.89 (m, 6H) ppm; ^{13}C NMR (100 MHz,

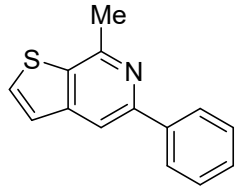
$CDCl_3$): δ 157.9, 157.8, 136.7, 129.6, 126.9, 126.0, 125.9, 125.5, 114.9, 47.9, 33.6, 25.7, 22.4 ppm; IR (KBr): 3059, 2952, 2866, 1624, 1569, 1446, 878, 748 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{18}N$ $[M+H]^+$ 212.1434; found 212.1432.

5-methyl-7-phenyl-1,6-naphthyridine (2s)



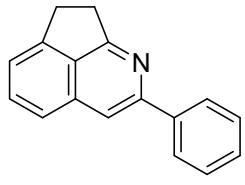
Reaction temperature was 120 ℃. Pale yellow solid (60 mg, 54 % yield, new product), mp 102 - 104 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 9.05 - 9.07 (m, 1H), 8.41 - 8.44 (m, 1H), 8.19 - 8.21 (m, 3H), 7.51 - 7.55 (m, 2H), 7.43 - 7.49 (m, 2H), 3.04 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.4, 154.4, 153.8, 151.7, 139.1, 133.9, 129.0, 128.8, 127.2, 121.7, 121.6, 116.3, 22.1 ppm; IR (KBr): 3057, 2921, 2857, 1603, 1578, 1440, 1332, 773, 697 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{13}N_2$ $[M+H]^+$ 221.1073; found 221.1072.

7-methyl-5-phenylthieno[2,3-c]pyridine (2t)



Reaction temperature was 100 ℃. Colorless oil (98 mg, 87 % yield, known product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.08 - 8.11 (m, 2H), 7.98 (s, 1H), 7.67 (d, J = 5.2 Hz, 1H), 7.50 - 7.55 (m, 2H), 7.41 - 7.45 (m, 2H), 2.91 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 151.9, 146.0, 140.1, 134.3, 131.3, 128.8, 128.3, 127.1, 124.1, 112.5, 23.8 ppm; IR (KBr): 3061, 2922, 2852, 1578, 1547, 1388, 1261, 765, 694 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{14}H_{12}NS$ $[M+H]^+$ 226.0685; found 226.0683.

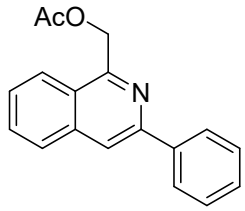
2-phenyl-7,8-dihydrocyclopenta[ij]isoquinoline (2u)



Reaction temperature was 80 ℃. Pale yellow oil (90 mg, 78 % yield, new product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.09 - 8.11 (m, 2H), 7.82 (s, 1H), 7.68 - 7.71 (m, 1H), 7.61 - 7.63 (m, 1H), 7.50 - 7.54 (m, 2H), 7.40 - 7.45 (m, 2H), 3.55 - 3.58 (m, 2H), 3.46 - 3.50 (m, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.4, 154.2, 147.5, 140.8, 134.5, 132.9, 131.9, 128.7, 128.2, 127.4, 121.4, 121.3, 112.5, 32.9, 28.7 ppm; IR (KBr):

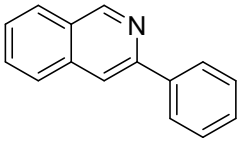
3050, 2923, 2856, 1616, 1579, 1436, 865, 779, 693 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{17}H_{14}N$ $[M+H]^+$ 232.1121; found 232.1119.

(3-phenylisoquinolin-1-yl)methyl acetate (2v)



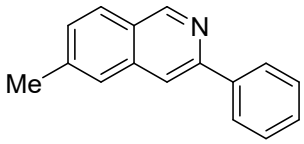
Reaction temperature was 80 ℃. Yellow oil (46 mg, 33 % yield, known product). ^1H NMR (400 MHz, $CDCl_3$): δ 8.17 - 8.19 (m, 2H), 8.13 (d, J = 8.4 Hz, 1H), 8.09 (s, 1H), 7.94 (d, J = 8.4 Hz, 1H), 7.71 - 7.75 (m, 1H), 7.61 - 7.65 (m, 1H), 7.51 - 7.55 (m, 2H), 7.42 - 7.46 (m, 1H), 5.82 (s, 2H), 2.22 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 170.8, 154.3, 150.0, 139.2, 137.4, 130.4, 128.8, 128.6, 127.9, 127.5, 127.0, 125.8, 124.6, 117.1, 66.0, 21.0 ppm; IR (KBr): 3060, 2925, 1739, 1572, 1232, 755, 694 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{18}H_{16}NO_2$ $[M+H]^+$ 278.1176; found 278.1174.

3-phenylisoquinoline (2aa)



Reaction temperature was 100 ℃. Pale yellow solid (92 mg, 90 % yield, known product), mp 104 - 106 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 9.37 (s, 1H), 8.15 - 8.18 (m, 2H), 8.09 (s, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.69 -7.73 (m, 1H), 7.53 - 7.63 (m, 3H), 7.43 - 7.47 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 151.3, 139.6, 136.7, 130.5, 128.8, 128.5, 127.8, 127.6, 127.1, 127.0, 126.9, 116.5 ppm; IR (KBr): 3035, 2922, 2852, 1452, 883, 761, 685 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{12}N$ $[M+H]^+$ 206.0964; found 206.0963.

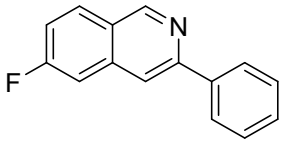
6-methyl-3-phenylisoquinoline (2ab)



Reaction temperature was 100 ℃. Pale yellow solid (104 mg, 95 % yield, known product), mp 176 - 178 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 9.30 (s, 1H), 8.13 - 8.16 (m, 2H), 8.00 (s, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.65 (s, 1H), 7.52 - 7.56 (m, 2H), 7.42 - 7.46 (m, 2H), 2.58 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0,

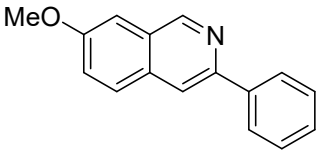
151.3, 140.9, 139.8, 137.0, 129.4, 128.8, 128.4, 127.3, 127.0, 126.3, 125.8, 116.1, 22.1 ppm; IR (KBr): 3052, 3025, 2977, 2921, 2851, 1454, 900, 700 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}N$ $[M+H]^+$ 220.1121; found 220.1119.

6-fluoro-3-phenylisoquinoline (2ac)



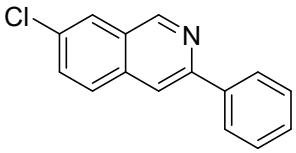
Reaction temperature was 120 ℃. Pale yellow solid (106 mg, 95 % yield, known product), mp 134 - 136 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 9.34 (s, 1H), 8.13 - 8.16 (m, 2H), 8.01 - 8.05 (m, 2H), 7.44 - 7.57 (m, 4H), 7.35 - 7.40 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.5 (d, J = 51.1 Hz), 152.1, 152.0, 139.1, 138.2 (d, J = 10.5 Hz), 130.6 (d, J = 9.5 Hz), 128.9, 127.1, 124.9, 117.7 (d, J = 26.0 Hz), 116.2, 116.1, 110.3 (d, J = 20.9 Hz) ppm; ^{19}F NMR ($CDCl_3$): δ -106.8 ppm; IR (KBr): 2921, 2854, 1215, 892, 755, 685 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{11}FN$ $[M+H]^+$ 224.0870; found 224.0869.

7-methoxy-3-phenylisoquinoline (2ad)



Reaction temperature was 100 ℃. Pale yellow solid (91 mg, 77 % yield, known product), mp 162 - 164 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 9.26 (s, 1H), 8.11 - 8.13 (m, 2H), 8.03 (s, 1H), 7.80 (dd, J = 2.0, 8.8 Hz, 1H), 7.53 (t, J = 7.2 Hz, 2H), 7.36 - 7.44 (m, 2H), 7.26 - 7.28 (m, 1H), 3.99 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.4, 150.9, 149.7, 139.7, 132.3, 128.9, 128.8, 128.5, 128.2, 126.8, 123.8, 116.5, 104.7, 55.5 ppm; IR (KBr): 2924, 1270, 754, 695 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}NO$ $[M+H]^+$ 236.1070; found 236.1069.

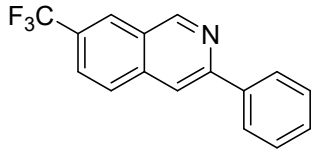
7-chloro-3-phenylisoquinoline (2ae)



Reaction temperature was 120 ℃. Pale yellow solid (115 mg, 96 % yield, known product), mp 157 - 159 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 9.29 (s, 1H), 8.12 - 8.15 (m, 2H), 8.06 (s, 1H), 7.99 (d, J = 2.0 Hz, 1H), 7.84 (d, J = 8.4 Hz, 1H), 7.65 (dd, J = 2.4, 8.8 Hz, 1H), 7.52 - 7.56 (m, 2H), 7.43 - 7.48 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.7, 151.4, 139.2, 134.9, 132.6, 131.6, 128.9, 128.8, 128.6, 128.1, 127.0, 126.4,

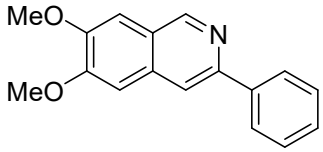
116.2 ppm; IR (KBr): 3060, 2999, 1271, 880, 756, 688 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{11}ClN$ $[M+H]^+$ 240.0575; found 240.0573.

3-phenyl-7-(trifluoromethyl)isoquinoline (2af)



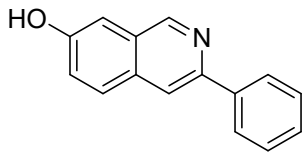
Reaction temperature was 120 ℃. Pale yellow solid (116 mg, 85 % yield, known product), mp 168 - 170 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 9.45 (s, 1H), 8.32 (s, 1H), 8.14 - 8.18 (m, 3H), 8.00 - 8.02 (m, 1H), 7.86 - 7.89 (m, 1H), 7.53 - 7.58 (m, 2H), 7.46 - 7.50 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.4, 153.1, 138.9, 138.0, 129.2, 128.9, 128.8 (d, J = 32.5 Hz), 128.2, 127.2, 126.4, 126.1 (q, J = 3.2 Hz), 125.5 (q, J = 4.5 Hz), 123.9 (q, J = 270.4 Hz), 116.1 ppm; ^{19}F NMR ($CDCl_3$): δ -62.6 ppm; IR (KBr): 2923, 2850, 1109, 886, 761, 688 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{11}F_3N$ $[M+H]^+$ 274.0838; found 274.0836.

6,7-dimethoxy-3-phenylisoquinoline (2ag)



Reaction temperature was 100 ℃. Pale yellow solid (103 mg, 78 % yield, known product), mp 128 - 130 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 9.14 (s, 1H), 8.09 - 8.11 (m, 2H), 7.95 (s, 1H), 7.50 - 7.53 (m, 2H), 7.40 - 7.44 (m, 1H), 7.23 (s, 1H), 7.13 (s, 1H), 4.06 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.2, 150.3, 150.27, 149.8, 139.9, 133.4, 128.8, 128.2, 126.8, 123.8, 115.6, 105.3, 105.0, 56.1, 56.09 ppm; IR (KBr): 3060, 3003, 2962, 2837, 1503, 1241, 1151, 751, 693 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{17}H_{16}NO_2$ $[M+H]^+$ 266.1176; found 266.1174.

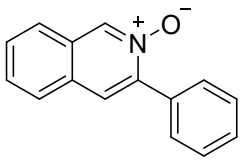
3-phenylisoquinolin-7-ol (2ah)



Reaction temperature was 100 ℃. Pale yellow solid (81 mg, 73 % yield, new product), mp 258 - 260 ℃. ^1H NMR (400 MHz, DMSO-d6): δ 11.36 (br, 1H, OH), 9.99 (s, 1H), 7.75 - 7.77 (m, 2H), 7.59 (d, J = 8.8 Hz, 1H), 7.55 (d, J = 2.8 Hz, 1H), 7.40 - 7.50 (m, 3H), 7.21 (dd, J = 2.8, 8.8 Hz, 1H), 6.85 (s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d6): δ 162.9, 156.8, 137.1, 134.6, 131.0, 129.2, 129.1, 129.0, 126.83, 126.77, 122.9, 110.6,

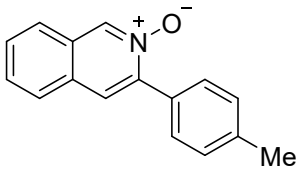
103.8 ppm; IR (KBr): 3453, 2924, 2852, 1631, 1269, 751 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{12}NO$ $[M+H]^+$ 222.0913; found 222.0910.

3-phenylisoquinoline *N*-oxide (4a)



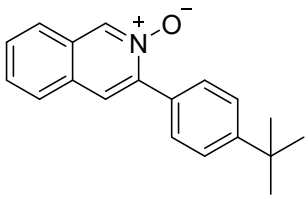
Reaction temperature was 70 ℃. White solid (94 mg, 85 % yield, known product), mp 157 - 159 ℃. ^1H NMR (400 MHz, DMSO-d6): δ 9.10 (s, 1H), 8.14 (s, 1H), 7.96 - 7.98 (m, 1H), 7.90 -7.92 (m, 1H), 7.80 - 7.82 (m, 2H), 7.60 - 7.68 (m, 2H), 7.48 - 7.54 (m, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 146.4, 136.6, 133.5, 130.2, 129.6, 129.5, 129.4, 128.9, 128.8, 128.3, 127.3, 125.4, 124.8 ppm; IR (KBr): 3056, 2924, 2850, 1750, 1374, 1233, 752, 694 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{12}NO$ $[M+H]^+$ 222.0913; found 222.0911.

3-(*p*-tolyl)isoquinoline *N*-oxide (4b)



Reaction temperature was 90 ℃. White solid (100 mg, 85 % yield, known product), mp 167 - 169 ℃. ^1H NMR (400 MHz, DMSO-d6): δ 9.06 (s, 1H), 8.09 (s, 1H), 7.87 - 7.96 (m, 2H), 7.58 - 7.73 (m, 4H), 7.29 - 7.31 (m, 2H), 2.38 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 146.5, 139.1, 136.5, 130.6, 130.0, 129.4, 129.3, 128.9, 128.8, 128.7, 127.2, 125.0, 124.7, 21.4 ppm; IR (KBr): 3058, 3022, 2922, 2854, 1630, 1436, 1312, 1178, 748 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}NO$ $[M+H]^+$ 236.1070; found 236.1069.

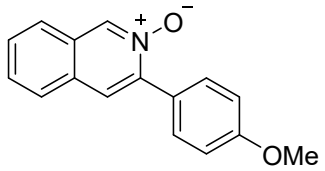
3-(4-(*tert*-butyl)phenyl)isoquinoline *N*-oxide (4c)



Reaction temperature was 120 ℃. White solid (111 mg, 80 % yield, known product), mp 203 - 205 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 9.07 (s, 1H), 8.10 (s, 1H), 7.94 (d, J =7.2 Hz, 1H), 7.89 (d, J =7.6 Hz, 1H), 7.75 (d, J =8.0 Hz, 2H), 7.58 - 7.66 (m, 2H), 7.51 (d, J =8.0 Hz, 2H), 1.33 (s, 9H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 152.1, 146.4, 136.5, 130.7, 129.9, 129.4, 129.3, 128.9, 128.8, 127.2, 125.1, 125.0, 124.8, 35.0,

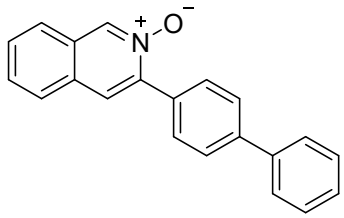
31.5 ppm; IR (KBr): 3055, 2959, 2866, 1312, 1178, 752 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{19}H_{20}NO$ $[M+H]^+$ 278.1539; found 278.1538.

3-(4-methoxyphenyl)isoquinoline *N*-oxide (4d)



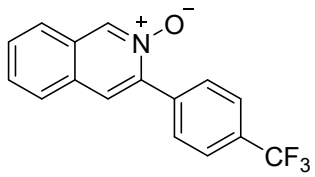
Reaction temperature was 90 ℃. White solid (107 mg, 85 % yield, known product), mp 194 - 196 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 9.05 (s, 1H), 8.08 (s, 1H), 7.86 - 7.95 (m, 2H), 7.78 - 7.82 (m, 2H), 7.56 - 7.64 (m, 2H), 7.03 - 7.06 (m, 2H), 3.83 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 160.3, 146.2, 136.6, 131.6, 129.2, 129.1, 128.9, 128.8, 127.1, 125.6, 124.7, 124.6, 113.7, 55.7 ppm; IR (KBr): 3061, 3016, 1606, 1310, 1248, 1178, 751 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}NO_2$ $[M+H]^+$ 252.1019; found 252.1017.

3-([1,1'-biphenyl]-4-yl)isoquinoline *N*-oxide (4e)



Reaction temperature was 120 ℃. White solid (113 mg, 76 % yield, known product), mp 245 - 247 ℃. ^1H NMR (400 MHz, $CDCl_3$): δ 8.95 (s, 1H), 7.84 - 7.95 (m, 4H), 7.74 - 7.76 (m, 3H), 7.59 - 7.69 (m, 4H), 7.48 - 7.52(m, 2H), 7.38 - 7.43 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.8, 142.3, 140.5, 137.5, 131.6, 130.2, 129.6, 129.2, 128.9, 128.8, 128.6, 127.7, 127.2, 127.0, 126.5, 124.7, 124.5 ppm; IR (KBr): 1315, 1179, 752 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{21}H_{16}NO$ $[M+H]^+$ 298.1226; found 298.1224.

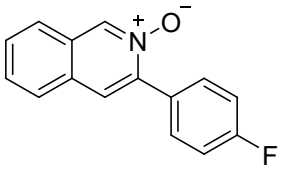
3-(4-(trifluoromethyl)phenyl)isoquinoline *N*-oxide (4f)



Reaction temperature was 90 ℃. White solid (101 mg, 70 % yield, known product), mp 210 - 212 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 9.12 (s, 1H), 8.21 (s, 1H), 8.03 - 8.05 (m, 2H), 7.90 - 7.99 (m, 2H), 7.84 - 7.87 (m, 2H), 7.61 - 7.70 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 144.9, 137.5, 136.7, 131.1, 130.0, 129.7, 129.6, 129.1, 128.7, 127.4, 125.9, 125.2 (q, J = 3.7 Hz), 124.9, 124.6 (d, J = 270.6 Hz) ppm; ^9F

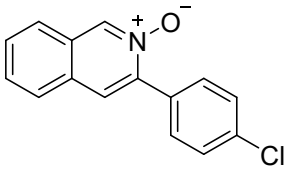
NMR (DMSO-d6) : δ -61.2 ppm; IR (KBr): 3030, 1632, 1405, 1177, 1116, 845, 750 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{11}F_3NO$ $[M+H]^+$ 290.0787; found 290.0784.

3-(4-fluorophenyl)isoquinoline *N*-oxide (4g)



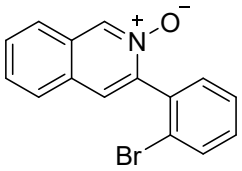
Reaction temperature was 90 ℃. White solid (96 mg, 80 % yield, known product), mp 190 - 192 ℃. ^1H NMR (400 MHz, DMSO-d^6) : δ 9.09 (s, 1H), 8.14 (s, 1H), 7.94 - 7.96 (m, 1H), 7.86 - 7.91 (m, 3H), 7.59 - 7.67 (m, 2H), 7.30 - 7.36 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO-d^6) : δ 162.9 (d, J = 245.0 Hz), 145.4, 136.6, 132.5 (d, J = 8.3 Hz), 129.8 (d, J = 3.2 Hz), 129.6, 129.4, 129.0, 128.7, 127.3, 125.3, 124.8, 115.3 (d, J = 21.4 Hz) ppm; ^9F NMR (DMSO-d^6) : δ -112.0 ppm; IR (KBr): 3028, 1603, 1514, 1314, 1179, 833, 749 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{11}FNO$ $[M+H]^+$ 240.0819; found 240.0817.

3-(4-chlorophenyl)isoquinoline *N*-oxide (4h)



Reaction temperature was 90 ℃. White solid (106 mg, 83 % yield, known product), mp 198 - 200 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 9.10 (s, 1H), 8.17 (s, 1H), 7.89 - 7.98 (m, 2H), 7.84 - 7.91 (m, 2H), 7.60 - 7.69 (m, 2H), 7.55 - 7.58 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 145.2, 136.6, 134.3, 132.3, 132.0, 129.7, 129.5, 129.0, 128.7, 128.4, 127.3, 125.5, 124.9 ppm; IR (KBr): 3020, 1632, 1601, 1314, 1177, 746 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{11}ClNO$ $[M+H]^+$ 256.0524; found 256.0523.

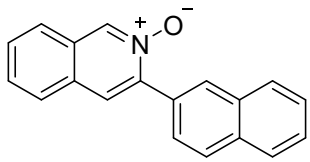
3-(2-bromophenyl)isoquinoline *N*-oxide (4i)



Reaction temperature was 90 ℃. White solid (92 mg, 61 % yield, new product), mp 178 - 180 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 9.09 (s, 1H), 8.06 (s, 1H), 7.95 (dd, J = 8, 16.8 Hz, 2H), 7.77 (d, J = 8 Hz, 1H), 7.62 - 7.72 (m, 2H), 7.51 - 7.55 (m, 2H), 7.42 - 7.47 (m, 1H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 146.6, 136.0, 135.5, 132.6, 132.5, 131.3, 129.9, 129.8, 129.0, 128.2, 128.0, 127.3, 125.8, 125.0, 124.3 ppm; IR

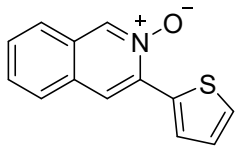
(KBr): 1635, 1432, 1316, 1180, 748 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{11}BrNO$ $[M+H]^+$ 300.0019; found 300.0017.

3-(naphthalen-2-yl)isoquinoline *N*-oxide (4j)



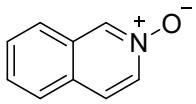
Reaction temperature was 90 ℃. White solid (117 mg, 86 % yield, known product), mp 218 - 220 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 9.14 (s, 1H), 8.34 (s, 1H), 8.27 (s, 1H), 7.92 - 8.04 (m, 6H), 7.56 - 7.69 (m, 4H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 146.4, 136.6, 133.4, 133.0, 131.4, 129.6, 129.54, 129.5, 129.0, 128.9, 128.8, 128.0, 127.7, 127.4, 127.3, 127.2, 126.8, 125.7, 124.9 ppm; IR (KBr): 1632, 1313, 1179, 1126, 748 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{19}H_{14}NO$ $[M+H]^+$ 272.1070; found 272.1067.

3-(thiophen-2-yl)isoquinoline *N*-oxide (4k)



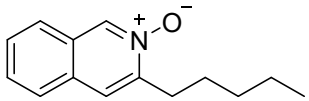
Reaction temperature was 90 ℃. White solid (101 mg, 89 % yield, known product), mp 178 - 180 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 9.19 (s, 1H), 8.84 (d, J = 6.0 Hz, 1H), 8.18 - 8.20 (m, 1H), 7.89 - 7.98 (m, 2H), 7.74 (d, J = 5.2 Hz, 1H), 7.59 - 7.64 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 140.2, 136.2, 131.7, 131.5, 129.3, 129.1, 129.0, 128.0, 127.9, 127.1, 126.6, 125.1, 120.1 ppm; IR (KBr): 3065, 1595, 1313, 1180, 749, 699 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{13}H_{10}NOS$ $[M+H]^+$ 228.0475; found 228.0478.

isoquinoline *N*-oxide (4l)



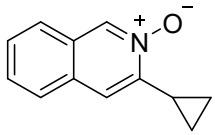
Reaction temperature was 70 ℃. Pale green solid (71 mg, 98 % yield, known product), mp 56 - 58 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 8.96 (s, 1H), 8.15 - 8.17 (m, 1H), 7.88 - 7.97 (m, 3H), 7.59 - 7.69 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 137.5, 135.5, 130.0, 129.8, 128.8, 128.3, 127.2, 125.2, 125.0 ppm; IR (KBr): 3062, 1326, 1177, 1124, 736 cm^{-1}. HRMS (ESI) m/z: calcd for C_9H_8NO $[M+H]^+$ 146.0600; found 146.0599.

3-pentylisoquinoline *N*-oxide (4m)



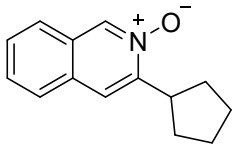
Reaction temperature was 90 ℃. Pale yellow oil (97 mg, 90 % yield, new product). ^{1}H NMR (400 MHz, DMSO- d6): δ 8.99 (s, 1H), 7.83 - 7.89 (m, 3H), 7.54 - 7.60 (m, 2H), 2.87 (t, J = 7.6 Hz, 2H), 1.66 - 1.73 (m, 2H), 1.31 - 1.36 (m, 4H), 0.85 - 0.89 (m, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 149.1, 135.9, 128.6, 128.5, 126.5, 124.8, 122.7, 31.5, 30.1, 26.5, 22.4, 14.3 ppm; IR (KBr): 2954, 2923, 2860, 1633, 1317, 1178, 1111, 748 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{14}H_{18}NO$ $[M+H]^+$ 216.1383; found 216.1382.

3-cyclopropylisoquinoline *N*-oxide (4n)



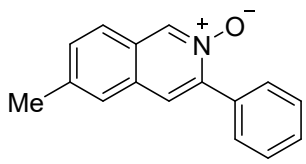
Reaction temperature was 90 ℃. White solid (81 mg, 87 % yield, known product), mp 95 - 97 ℃. ^{1}H NMR (400 MHz, DMSO- d6): δ 9.00 (s, 1H), 7.80 - 7.83 (m, 2H), 7.64 (s, 1H), 7.51 - 7.57 (s, 2H), 2.59 - 2.66 (m, 1H), 1.06 - 1.11 (m, 2H), 0.83 - 0.87 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 150.6, 135.7, 128.63, 128.60, 128.5, 128.1, 126.5, 124.7, 118.9, 10.7, 8.5 ppm; IR (KBr): 3056, 3008, 1318, 1174, 751 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{12}H_{12}NO$ $[M+H]^+$ 186.0913; found 186.0912.

3-cyclopentylisoquinoline *N*-oxide (4o)



Reaction temperature was 90 ℃. Pale yellow solid (79 mg, 74 % yield, new product), mp 80 - 82 ℃. ^{1}H NMR (400 MHz, DMSO- d6): δ 9.00 (s, 1H), 7.91 - 7.94 (m, 2H), 7.83 - 7.85 (m, 1H), 7.55 - 7.61 (m, 2H), 3.65 - 3.73 (m, 1H), 2.11 - 2.18 (m, 2H), 1.60 - 1.82 (m, 6H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 152.7, 136.0, 128.6, 128.5, 128.3, 126.7, 124.6, 120.4, 39.2, 31.3, 25.2 ppm; IR (KBr): 3056, 2951, 2867, 1319, 1176, 1133, 752 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{14}H_{16}NO$ $[M+H]^+$ 214.1226; found 214.1225.

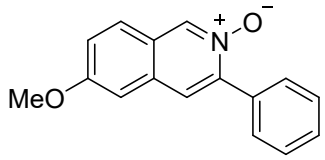
6-methyl-3-phenylisoquinoline *N*-oxide (4p)



Reaction temperature was 90 ℃. White solid (92 mg, 78 % yield, known product), mp 164 -166 ℃. ^{1}H NMR (400 MHz, DMSO- d6): δ 9.04 (s, 1H), 8.03 (s, 1H), 7.75 - 7.83 (m, 4H), 7.48 (m, 4H), 2.48 (s, 3H) ppm; ^{13}C

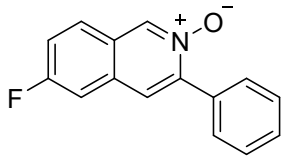
NMR (100 MHz, DMSO- d6): δ 146.4, 138.9, 136.4, 133.6, 131.7, 130.2, 129.4, 129.0, 128.3, 127.7, 126.1, 124.8, 124.7, 21.9 ppm; IR (KBr): 2925, 1753, 1273, 752 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}NO$ $[M+H]^+$ 236.1070; found 236.1068.

6-methoxy-3-phenylisoquinoline *N*-oxide (4q)



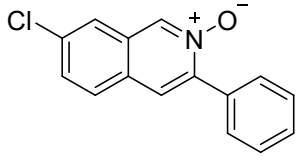
Reaction temperature was 90 ℃. White solid (96 mg, 76 % yield, known product), mp 198 -200 ℃. ^{1}H NMR (400 MHz, DMSO- d6): δ 8.91 (s, 1H), 8.06 (s, 1H), 7.87 - 7.90 (m, 1H), 7.79 - 7.80 (m, 2H), 7.44 - 7.51 (m, 3H), 7.21 - 7.32 (m, 2H), 3.90 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 159.8, 144.4, 135.8, 133.7, 130.9, 130.1, 129.2, 128.9, 128.3, 125.0, 124.5, 121.6, 103.0, 56.0 ppm; IR (KBr): 2927, 2854, 1754, 1271, 753, 697 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}NO_2$ $[M+H]^+$ 252.1019; found 252.1017.

6-fluoro-3-phenylisoquinoline *N*-oxide (4r)



Reaction temperature was 120 ℃. White solid (105 mg, 88 % yield, known product), mp 214 - 216 ℃. ^{1}H NMR (400 MHz, DMSO- d6) : δ 9.12 (s, 1H), 8.11 (s, 1H), 7.99 (dd, J = 5.6, 9.2 Hz, 1H), 7.75 - 7.82 (m, 3H), 7.56 - 7.61 (m, 1H), 7.48 - 7.52 (m, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 161.7 (d, J = 246.6 Hz), 147.2, 136.6, 133.3, 130.1, 129.8 (d, J = 10.3 Hz), 129.7, 128.4, 128.2 (d, J = 9.3 Hz), 126.8, 124.8 (d, J = 5.5 Hz), 119.9 (d, J = 25.9 Hz), 111.0 (d, J = 22.1 Hz) ppm; ^{9}F NMR (DMSO-d6): δ -110.2 ppm; IR (KBr): 2926, 2853, 1270, 1212, 754 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{11}FNO$ $[M+H]^+$ 240.0819; found 240.0817.

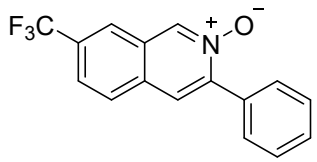
7-chloro-3-phenylisoquinoline *N*-oxide (4s)



Reaction temperature was 120 ℃. White solid (106 mg, 83 % yield, known product), mp 194 - 196 ℃. ^{1}H NMR (400 MHz, DMSO- d6) : δ 9.05 (s, 1H), 8.17 (s, 1H), 7.98 - 8.02 (m, 2H), 7.78 - 7.80 (m, 2H), 7.59 - 7.63 (m, 1H), 7.48 - 7.52 (m, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 146.9, 135.9, 134.0, 133.2,

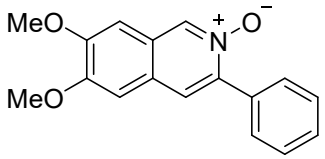
130.3, 130.1, 129.7, 129.6, 129.2, 128.4, 127.1, 125.2, 123.4 ppm; IR (KBr): 1274, 751 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{11}ClNO$ $[M+H]^+$ 256.0524; found 256.0522.

3-phenyl-7-(trifluoromethyl)isoquinoline *N*-oxide (4t)



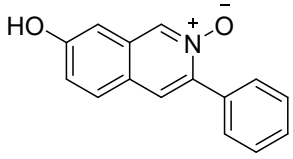
Reaction temperature was 120 ℃. White solid (132 mg, 91 % yield, known product), mp 213 - 215 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 9.25 (s, 1H), 8.39 (s, 1H), 8.28 (s, 1H), 8.17 (d, J = 8.4 Hz, 1H), 7.80 - 7.86 (m, 3H), 7.50 - 7.54 (m, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 148.6, 137.4, 133.0, 130.2, 130.0, 129.9, 129.3 (d, J = 31.7 Hz), 129.1, 128.7, 128.4, 125.3, 124.3 (d, J = 270.9 Hz), 123.8 (q, J = 3.2 Hz), 122.9 (q, J = 4.7 Hz) ppm; ^9F NMR (DMSO-d6): δ -61.5 ppm; IR (KBr): 3041, 1192, 1128, 749, 695 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{11}F_3NO$ $[M+H]^+$ 290.0787; found 290.0784.

6,7-dimethoxy-3-phenylisoquinoline *N*-oxide (4u)



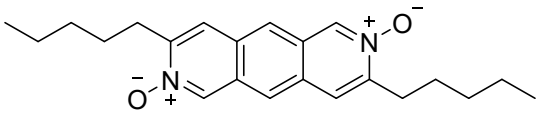
Reaction temperature was 90 ℃. White solid (100 mg, 71 % yield, known product), mp 215 - 217 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 8.83 (s, 1H), 7.92 (s, 1H), 7.79 - 7.81 (m, 2H), 7.43 - 7.51 (m, 3H), 7.39 (s, 1H), 7.32 (s, 1H), 3.91 (s, 3H), 3.90 (s, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6) : δ 152.0, 151.7, 144.1, 135.3, 133.9, 130.1, 129.2, 128.3, 125.6, 125.4, 123.7, 106.0, 103.4, 56.2 ppm; IR (KBr): 1273, 752 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{17}H_{16}NO_3$ $[M+H]^+$ 282.1125; found 282.1122.

7-hydroxy-3-phenylisoquinoline *N*-oxide (4v)



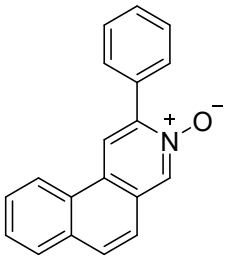
Reaction temperature was 120 ℃. White solid (80 mg, 67 % yield, new product), mp 232 - 234 ℃. ^1H NMR (400 MHz, DMSO- d6): δ 10.35 (s, 1H), 8.89 (s, 1H), 7.99 (s, 1H), 7.77 - 7.84 (m, 3H), 7.46 - 7.50 (m, 3H), 7.10 - 7.17 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 158.2, 143.4, 135.1, 133.8, 131.2, 130.1, 129.2, 129.1, 128.2, 125.0, 123.6, 121.6, 105.6 ppm; IR (KBr): 3708, 2924, 2852, 1753, 1272, 752 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{12}NO_2$ $[M+H]^+$ 238.0863; found 238.0861.

3,8-dipentylpyrido[3,4-g]isoquinoline *N*,*N*-dioxide (4w)



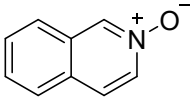
Reaction temperature was 90 ℃. Light yellow solid (169 mg, 96 % yield, new product), mp 242 - 244 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.88 (s, 2H), 8.09 (s, 2H), 7.72 (s, 2H), 3.05 - 3.08 (m, 4H), 1.82 - 1.85 (m, 4H), 1.40 - 1.50 (m, 8H), 0.95 (t, J = 6.8 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 150.6, 135.9, 127.5, 121.3, 31.5, 30.2, 26.7, 22.5, 14.0 ppm; IR (KBr): 3053, 2952, 2925, 2852, 1641, 1410, 1299, 1179, 1140, 749 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{22}H_{29}N_2O_2$ $[M+H]^+$ 353.2224; found 353.2221.

2-phenylbenzo[f]isoquinoline *N*-oxide (4x)



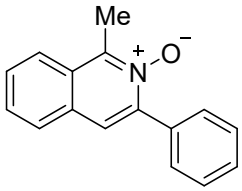
Reaction temperature was 120 ℃. White solid (81 mg, 60 % yield, new product), mp 167 -169 ℃. ^{1}H NMR (400 MHz, DMSO- d6): δ 9.12 (s, 1H), 8.89 - 8.91 (m, 2H), 7.94 - 8.03 (m, 4H), 7.71 - 7.81 (m, 3H), 7.51 - 7.57 (m, 3H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 146.9, 137.5, 133.6, 132.5, 130.7, 130.4, 129.6, 129.3, 128.7, 128.5, 128.4, 128.3, 126.5, 124.3, 122.7, 121.4 ppm; IR (KBr): 1263, 751 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{19}H_{14}NO$ $[M+H]^+$ 272.1070; found 272.1068.

isoquinoline *N*-oxide (4y)



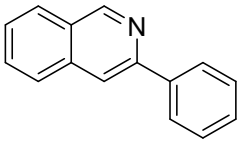
Reaction temperature was 90 ℃. Pale green solid (64 mg, 88 % yield, known product), mp 56 - 58 ℃. ^{1}H NMR (400 MHz, DMSO- d6): δ 8.96 (s, 1H), 8.15 - 8.17 (m, 1H), 7.88 - 7.97 (m, 3H), 7.59 - 7.69 (m, 2H) ppm; ^{13}C NMR (100 MHz, DMSO- d6): δ 137.5, 135.5, 130.0, 129.8, 128.8, 128.3, 127.2, 125.2, 125.0 ppm; IR (KBr): 3062, 1326, 1177, 1124, 736 cm^{-1}. HRMS (ESI) m/z: calcd for C_9H_8NO $[M+H]^+$ 146.0600; found 146.0599.

1-methyl-3-phenylisoquinoline *N*-oxide (4z)



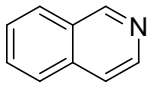
Reaction temperature was 50 ℃. Yellow oil (41 mg, 35 % yield, known product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 - 7.99 (m, 1H), 7.82 - 7.85 (m, 1H), 7.76 - 7.79 (m, 2H), 7.73 (s, 1H), 7.60 - 7. 69 (m, 2H), 7.43 - 7.48 (m, 3H), 2.94 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 146.6, 133.5, 129.8, 129.1, 128.8, 128.6, 128.2, 128.1, 127.5, 124.1, 122.8, 13.7 ppm; IR (KBr): 3057, 2955, 2924, 2853, 1713, 1222, 760, 698 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}NO$ $[M+H]^+$ 236.1070; found 236.1068.

3-phenylisoquinoline (5a)



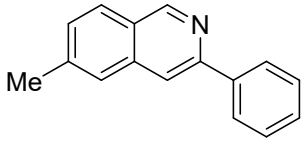
Pale yellow solid (41 mg, 98 % yield, known product), mp 104 - 106 ℃. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.37 (s, 1H), 8.15 - 8.18 (m, 2H), 8.09 (s, 1H), 8.01 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.69 -7.73 (m, 1H), 7.53 - 7.63 (m, 3H), 7.43 - 7.47 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.4, 151.3, 139.6, 136.7, 130.5, 128.8, 128.5, 127.8, 127.6, 127.1, 127.0, 126.9, 116.5 ppm; IR (KBr): 3035, 2922, 2852, 1452, 883, 761, 685 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{15}H_{12}N$ $[M+H]^+$ 206.0964; found 206.0963.

isoquinoline (5l)



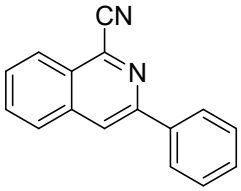
Pale yellow oil (25 mg, 97% yield, known product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.42 (s, 1H), 7.59 (d, J = 5.6 Hz, 1H), 8.03 (d, J = 8.4 Hz, 1H), 7.87 (d, J = 8.4 Hz, 1H), 7.76 - 7.81 (m, 2H), 7.65 - 7.69 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 141.3, 136.3, 131.9, 128.8, 128.3, 128.2, 126.6, 121.8 ppm; IR (KBr): 3057, 2924, 1630, 1454, 1384, 829, 748 cm^{-1}. HRMS (ESI) m/z: calcd for C_9H_8N $[M+H]^+$ 130.0651; found 130.0651.

6-methyl-3-phenylisoquinoline (5p)



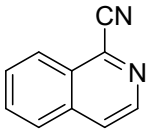
Pale yellow solid (43 mg, 98 % yield, known product), mp 176 - 178 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.30 (s, 1H), 8.13 - 8.16 (m, 2H), 8.00 (s, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.65 (s, 1H), 7.52 - 7.56 (m, 2H), 7.42 - 7.46 (m, 2H), 2.58 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.0, 151.3, 140.9, 139.8, 137.0, 129.4, 128.8, 128.4, 127.3, 127.0, 126.3, 125.8, 116.1, 22.1 ppm; IR (KBr): 3052, 3025, 2977, 2921, 2851, 1454, 900, 700 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{14}N$ $[M+H]^+$ 220.1121; found 220.1119.

3-phenylisoquinoline-1-carbonitrile (6a)



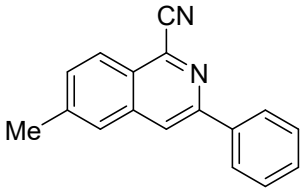
White solid (113 mg, 98 % yield, known product), mp 142 - 144 °C. ^{1}H NMR (400 MHz, $CDCl_3$) : δ 8.35 (d, *J* = 8.4 Hz, 1H), 8.30 (s, 1H), 8.15 - 8.18 (m, 2H), 8.00 (d, *J* = 8 Hz, 1H),7.75 - 7.85 (m, 2H), 7.53 - 7.58 (m, 2H), 7.47 - 7.51 (m, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) : δ 151.8, 137.6, 136.9, 134.6, 131.8, 129.49, 129.48, 129.0, 128.4, 127.7, 127.0, 125.3, 120.1, 116.0 ppm; IR (KBr): 3060, 2921, 2851, 2228, 1621, 1571, 1332, 1285, 897, 756, 681 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{16}H_{11}N_2$ $[M+H]^+$ 231.0917; found 231.0915.

isoquinoline-1-carbonitrile (6l)



White solid (66 mg, 86 % yield, known product), mp 89 – 91 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (dd, *J* = 1.6, 5.6 Hz, 1H), 8.33 - 8.37 (m, 1H), 7.96 - 7.98 (m, 1H), 7.91 - 7.93 (m, 1H), 7.79 - 7.87 (m, 2H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) : δ 143.3, 135.9, 134.8, 131.8, 129.9, 129.3, 127.3, 125.3, 124.5, 115.8 ppm; IR (KBr): 3058, 2921, 2850, 2227, 1621, 1576, 1386, 1340, 837, 747, 659 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{10}H_7N_2$ $[M+H]^+$ 155.0604; found 155.0601.

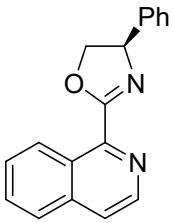
6-methyl-3-phenylisoquinoline-1-carbonitrile (6p)



White solid (116 mg, 95 % yield, new product), mp 155 - 157 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 - 8.21 (m, 4H), 7.72 (s, 1H), 7.46 - 7.59 (m, 4H), 2.61 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.8, 142.6,

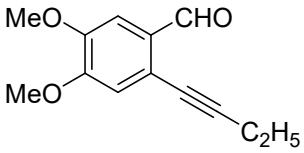
137.7, 137.2, 134.1, 131.9, 129.4, 129.0, 127.0, 126.9, 126.4, 125.0, 119.5, 116.1, 22.1 ppm; IR (KBr): 3057, 2919, 2847, 2232, 1624, 1574, 1378, 815, 767, 694 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{17}H_{13}N_2$ $[M+H]^+$ 245.1073; found 245.1070.

(R)-2-(isoquinolin-1-yl)-4-phenyl-4,5-dihydrooxazole (7l)



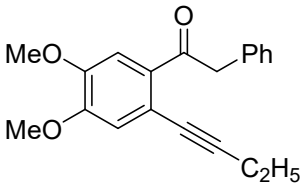
Pale yellow oil (82 mg, 30 % yield, known product). $[\alpha]^{25}_D$ = +90.1 (c 0.091, CH_2Cl_2); ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.37 - 9.40 (m, 1H), 8.70 (d, J = 5.6 Hz, 1H), 7.88 - 7.91 (m, 1H), 7.82 (d, J = 5.6 Hz, 1H), 7.67 - 7.76 (m, 2H), 7.40 - 7.46 (m, 4H), 7.32 - 7.36 (m, 1H), 5.67 (dd, J = 8.8, 10.4 Hz, 1H), 4.95 (dd, J = 8.8, 10.4 Hz, 1H), 4.42 (t, J = 8.4 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.2, 146.1, 142.0, 141.8, 136.8, 130.5, 128.9, 128.7, 127.8, 127.54, 127.52, 127.1, 126.9, 123.6, 74.2, 71.4 ppm; IR (KBr): 3054, 2922, 1633, 1130, 998, 831, 752, 698 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{18}H_{15}N_2O$ $[M+H]^+$ 275.1175; found 275.1176.

2-(but-1-yn-1-yl)-4,5-dimethoxybenzaldehyde (8)



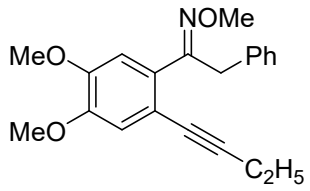
Pale yellow solid (1.51 g, 69 % yield, known product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.39 (s, 1H), 7.38 (s, 1H), 6.94 (s. 1H), 3.97 (s, 3H), 3.95 (s, 3H), 2.47 - 2.53 (q, J = 7.6 Hz, 2H), 1.29 (t, J = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.9, 153.6, 149.2, 130.2, 122.7, 114.4, 108.0, 97.7, 75.4, 56.2, 56.1, 13.7, 13.3 ppm.

1-(2-(but-1-yn-1-yl)-4,5-dimethoxyphenyl)-2-phenylethan-1-one (9)



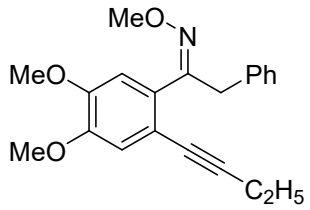
White solid (1.31 g, 85 % yield, new product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32 - 7.36 (m, 2H), 7.25 - 7.29 (m, 4H), 6.96 (s, 1H), 4.58 (s, 2H), 3.94 (s, 3H), 3.89 (s, 3H), 2.51 (q, J = 7.6 Hz, 2H), 1.28 (t, J = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) : δ 199.4, 151.3, 148.6, 135.2, 133.4, 129.7, 129.6, 128.5, 126.7, 116.3, 115.7, 111.6, 97.3, 79.6, 56.1, 55.9, 48.3, 13.6, 13.5 ppm.

1-(2-(but-1-yn-1-yl)-4,5-dimethoxyphenyl)-2-phenylethan-1-one *O*-methyl oxime (10)



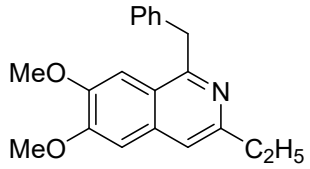
Pale yellow oil (*E* / *Z* = 3:1, 1.35 g, 100 % yield, new product). ^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.14 - 7.26 (m, 5H), 6.91 (s, 1H), 6.61 (s, 0.75 H), 6.10 (s, 0.25H), 4.27 (s, 1.5H), 4.03 (s, 2.25H), 3.90 (s, 0.75H), 3.88(s, 0.5H), 3.87 (s, 2.25H), 3.85 (s, 0.75H), 3.77 (s, 2.25H), 3.60 (s, 0.75H), 2.38 - 2.47 (m, 2H), 1.23 - 1.29 (m, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.6, 157.1, 148.7, 148.4, 148.1, 147.9, 136.8, 136.6, 131.7, 130.0, 129.5, 129.2, 126.5, 126.1, 115.1, 115.0, 114.3, 113.8, 112.3, 110.8, 94.7, 93.4, 78.6, 78.1, 61.9, 61.8, 55.9, 55.8, 55.7, 55.6, 41.5, 35.0, 13.9, 13.7, 13.3, 13.2 ppm.

(*Z*)-1-(2-(but-1-yn-1-yl)-4,5-dimethoxyphenyl)-2-phenylethan-1-one *O*-methyl oxime



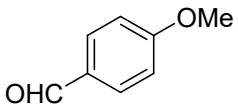
Pale yellow oil (*Z*-isomer, new product). ^{1}H NMR (400 MHz, $CDCl_3$) : δ 7.12 - 7.24 (m, 5H), 6.88 (s, 1H), 6.07 (s, 1H), 3.87 (s, 3H), 3.85 (s, 2H), 3.82 (s, 3H), 3.57 (s, 3H), 2.41 (q, *J* = 7.6 Hz, 2H), 1.24 (t, *J* = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.1, 148.1, 147.9, 136.6, 130.0, 129.5, 128.2, 126.5, 114.3, 113.8, 110.8, 93.4, 78.1, 61.9, 55.7, 55.6, 41.5, 13.9, 13.2 ppm.

1-benzyl-3-ethyl-6,7-dimethoxyisoquinoline (11)



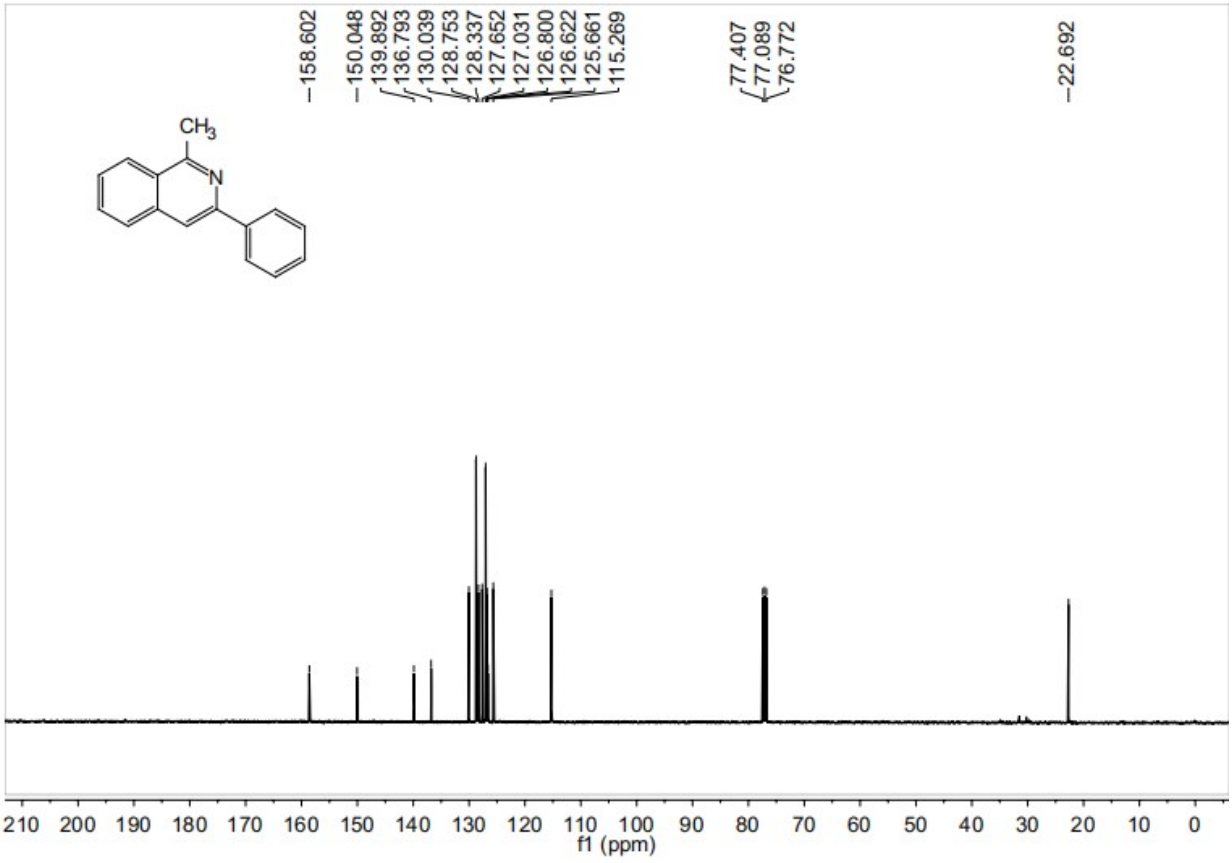
Pale yellow oil (72 mg, 62 % yield, known product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 - 7.28 (m, 6H), 7.13 - 7.17 (m, 1H), 6.99 (s, 1H), 4.60 (s, 2H), 3.98 (s, 3H), 3.83 (s, 3H), 2.94 - 3.00 (m, 2H), 1.40 (t, *J* = 7.6 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.0, 154.7, 149.1, 139.8, 134.3, 128.5, 128.4, 121.1, 115.5, 104.9, 104.3, 55.9, 55.8, 42.8, 31.0, 14.3 ppm; IR (KBr): 2961, 2930, 1571, 1505, 1463, 1425, 1243, 1216, 1159, 703 cm^{-1}. HRMS (ESI) m/z: calcd for $C_{20}H_{22}NO_2$ $[M+H]^+$ 308.1645; found 308.1643.

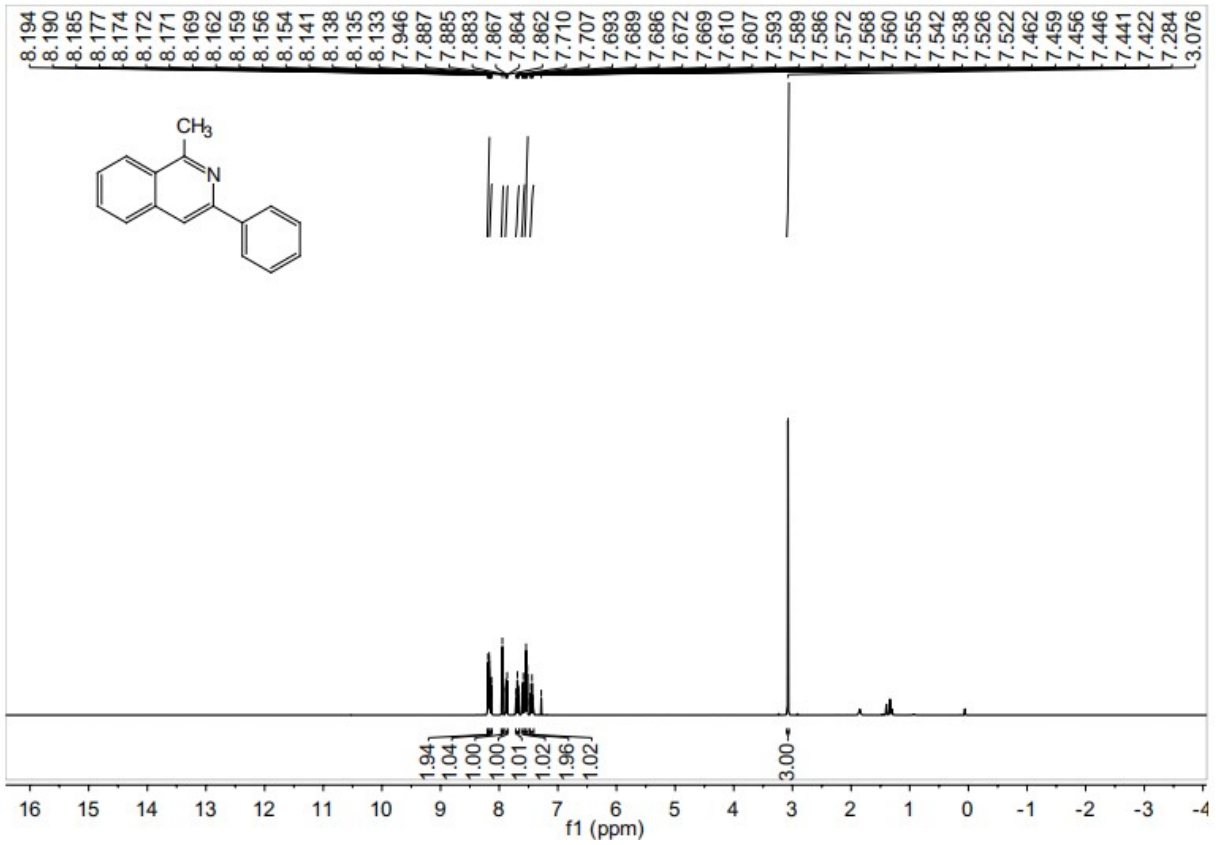
***p*-anisaldehyde (12)**



Pale yellow oil (51 mg, 75 % yield, known product). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.87 (s, 1H), 7.81 – 7.85 (m, 2H), 6.98 – 7.01 (m, 2H), 3.88 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.8, 164.5, 131.9, 129.9, 114.2, 55.5 ppm. HRMS (ESI) m/z: calcd for $C_8H_9O_2$ $[M+H]^+$ 137.0597; found 137.0596.

L. NMR Spectra




8.194
8.190
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8.172
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8.169
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8.159
8.156
8.154
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8.138
8.135
8.133
7.946
7.887
7.885
7.883
7.867
7.864
7.862
7.710
7.707
7.693
7.689
7.686
7.672
7.669
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7.607
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7.542
7.538
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7.522
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7.459
7.456
7.446
7.441
7.422
7.284
3.076
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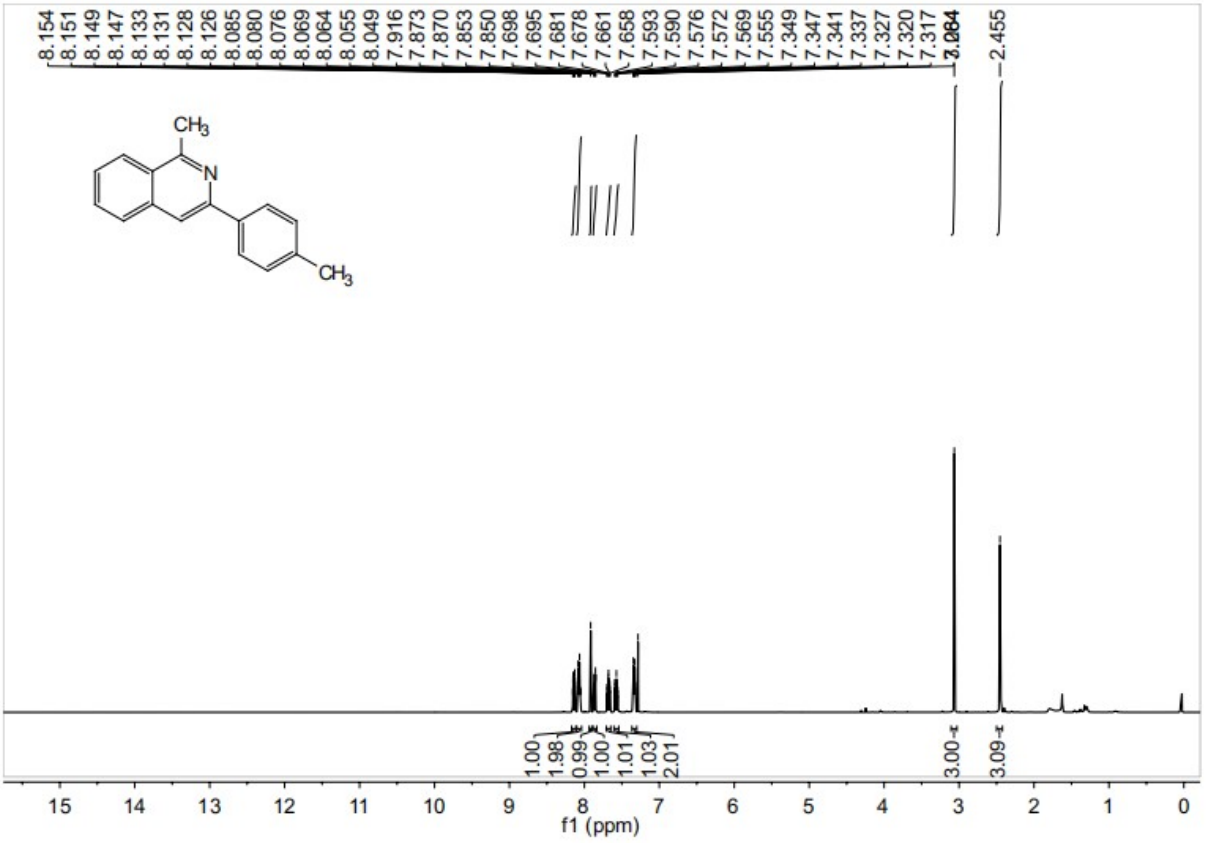
1.00
1.01
1.02
1.96
1.02
3.00
f1 (ppm)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7.347
7.341
7.337
7.327
7.320
7.317
2.455
CH3
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CH3
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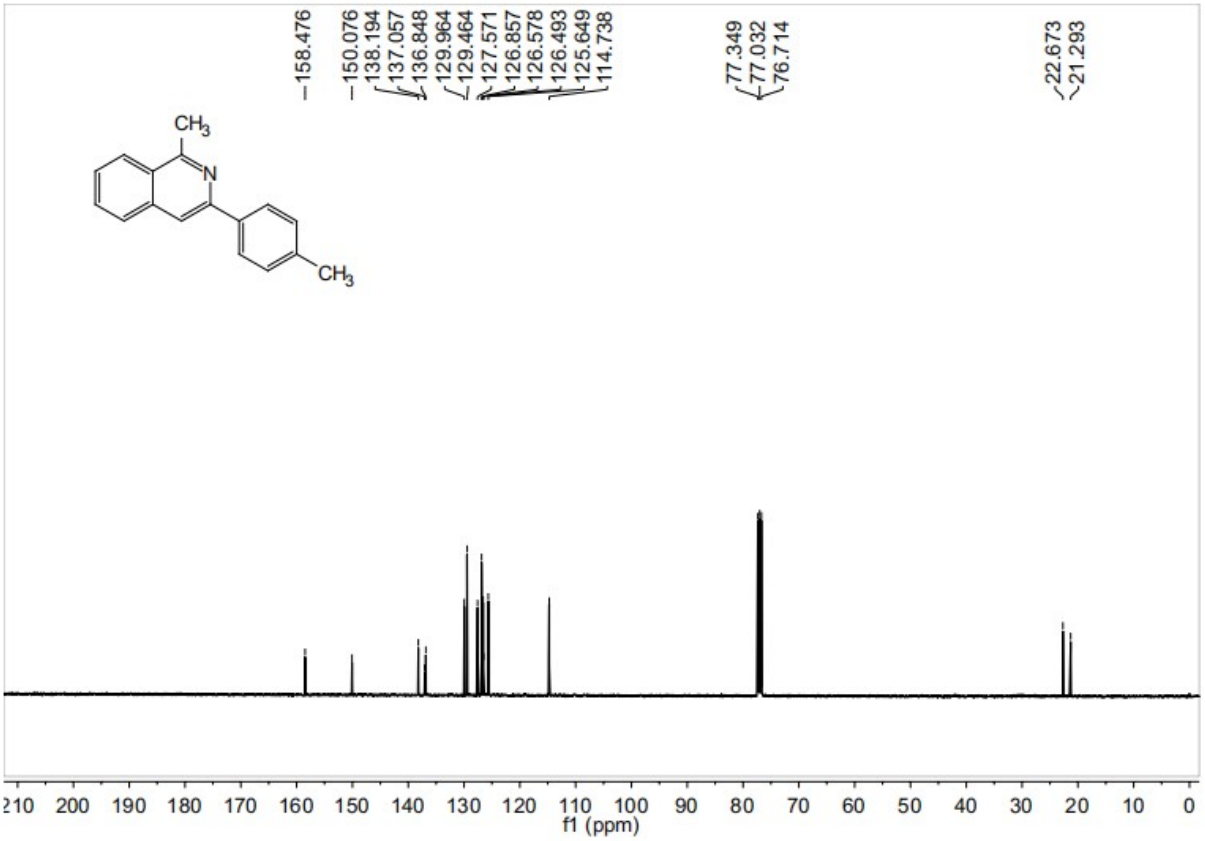
0.99
1.00
1.01
1.03
2.01
3.00
3.09
f1 (ppm)


158.476
150.076
138.194
137.057
136.848
129.964
129.464
127.571
126.857
126.578
126.493
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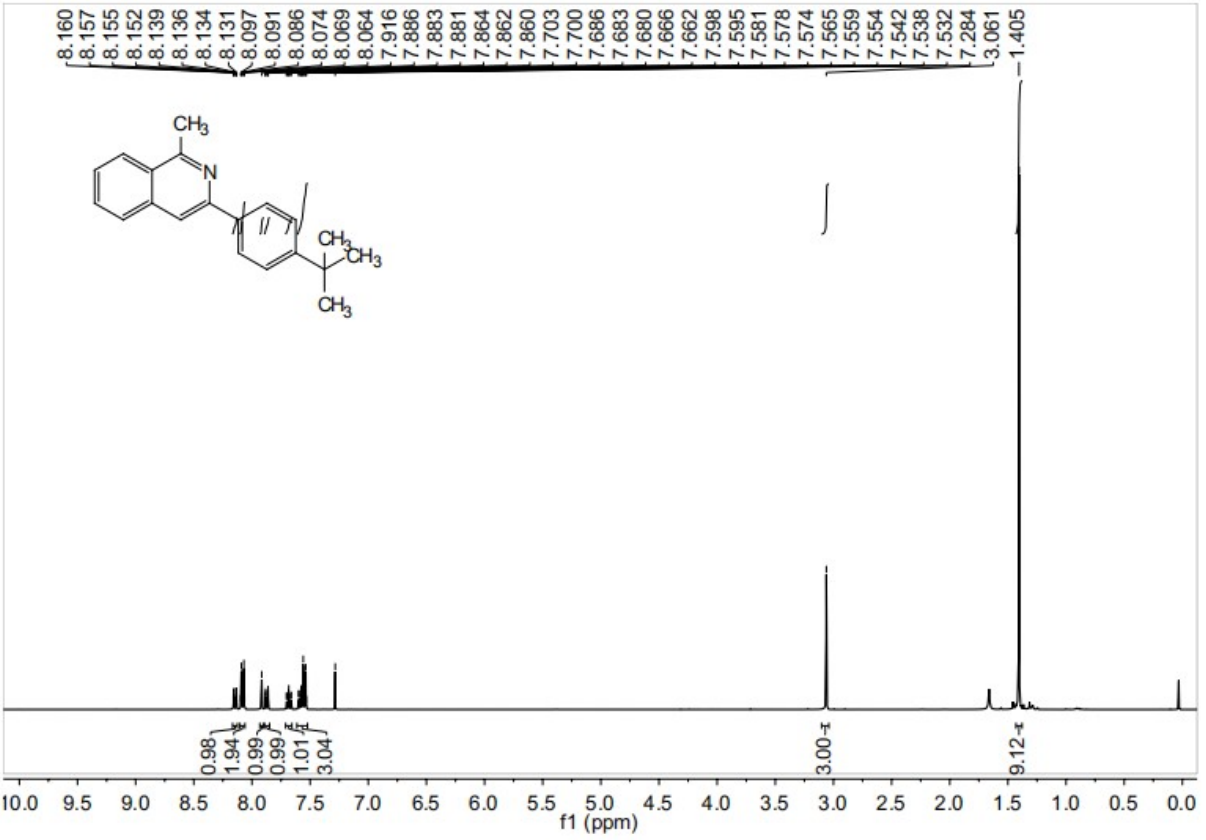
77.349
77.032
76.714
22.673
21.293
CH3
N
CH3
f1 (ppm)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8.131
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8.091
8.086
8.074
8.069
8.064
7.916
7.886
7.883
7.881
7.864
7.862
7.860
7.703
7.700
7.686
7.683
7.680
7.666
7.662
7.598
7.595
7.581
7.578
7.574
7.565
7.559
7.554
7.542
7.538
7.532
7.284
3.061
1.405
CH3
N
CH3
CH3
CH3
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0.99
0.99
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3.00
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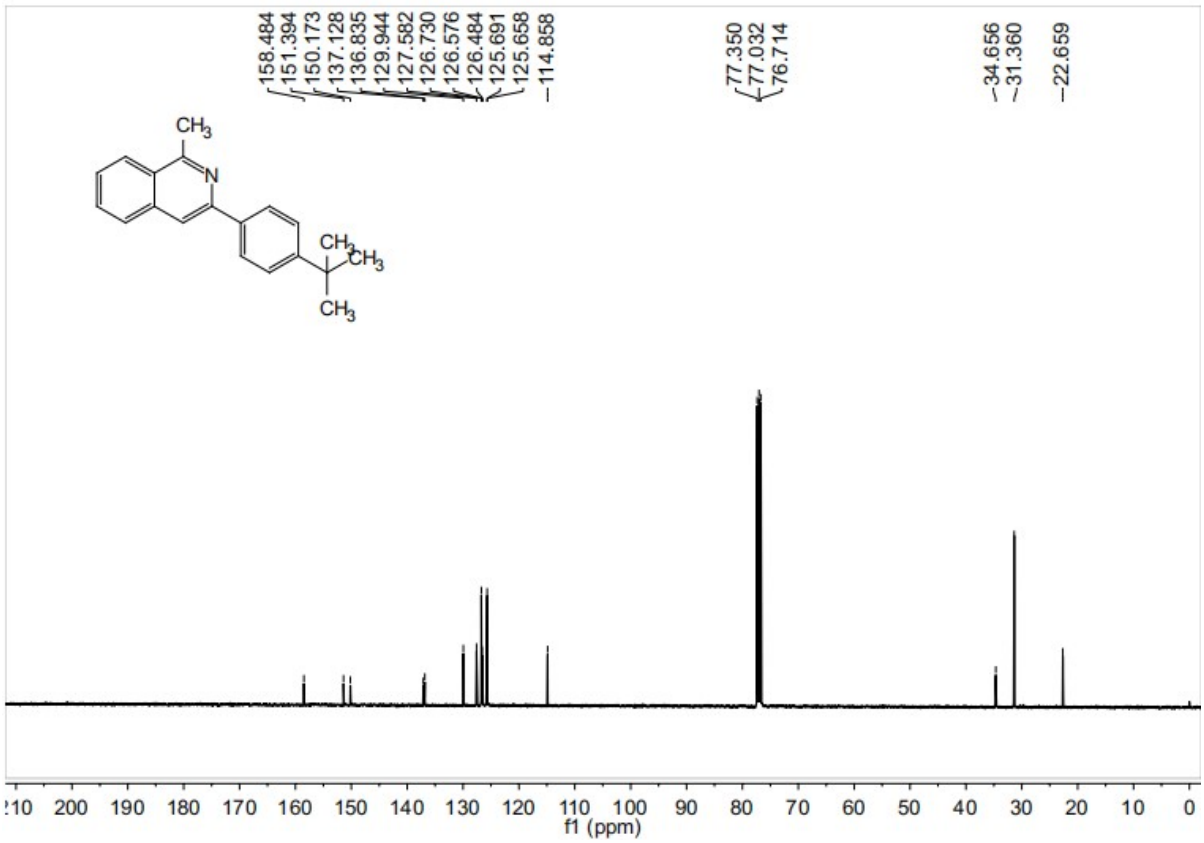
f1 (ppm)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150.173
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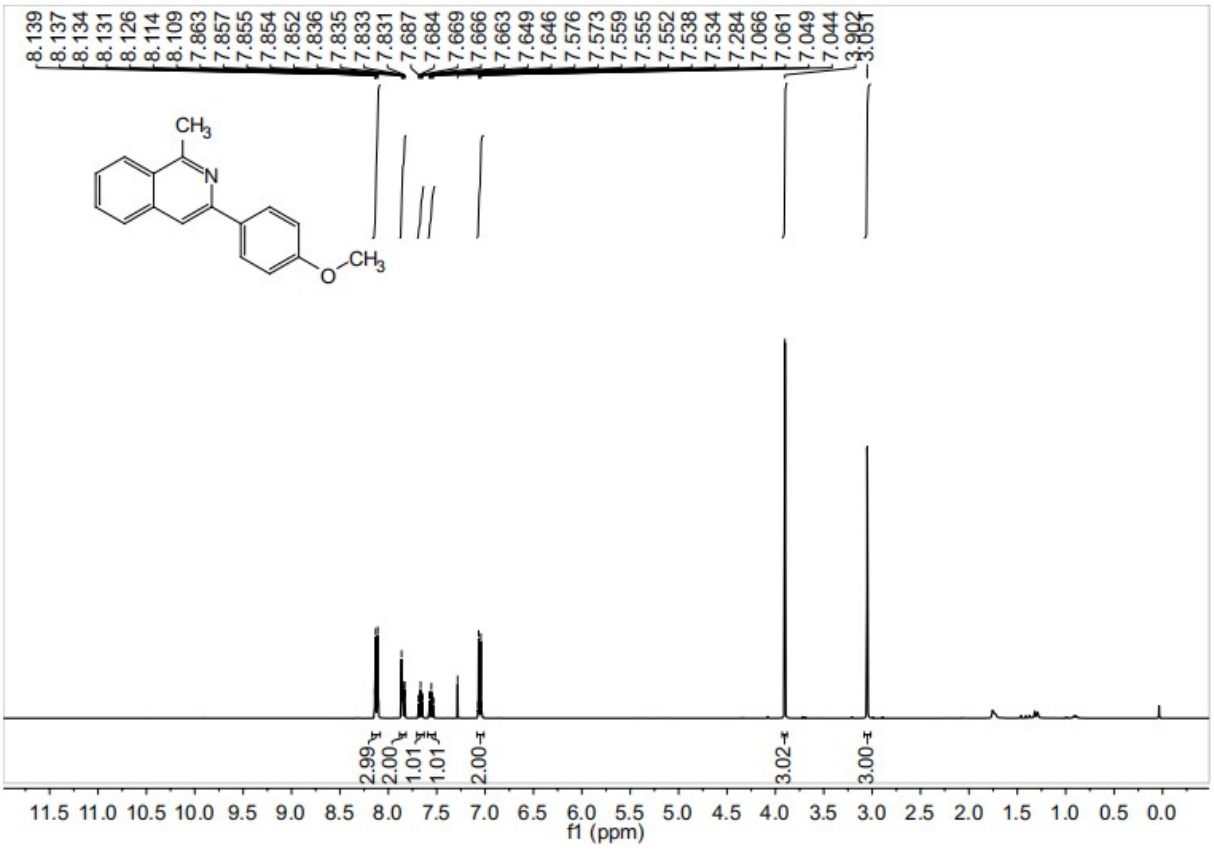
136.835
129.944
127.582
126.730
126.576
126.484
125.691
125.658
114.858
77.350
77.032
76.714
34.656
31.360
22.659
CH3
N
CH3
CH3
CH3
f1 (ppm)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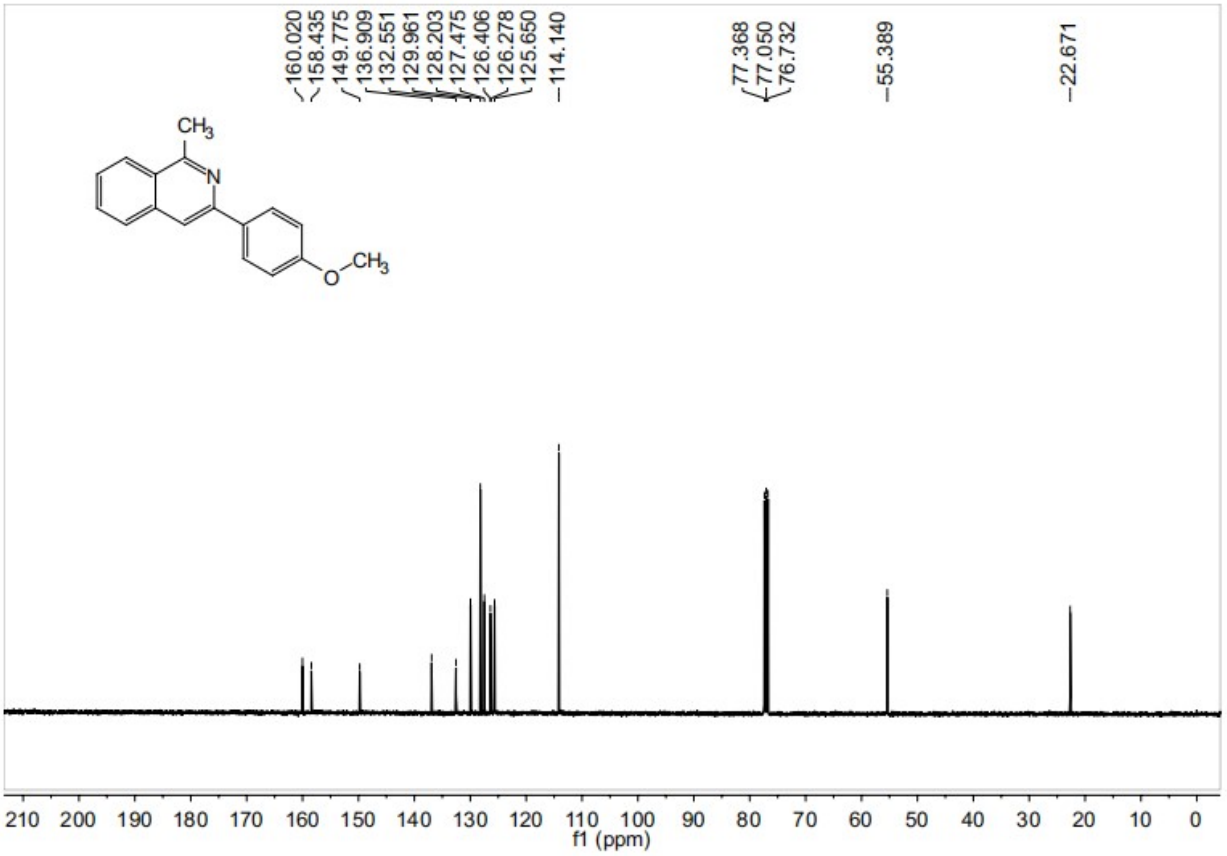
8.109
7.863
7.857
7.855
7.854
7.852
7.836
7.835
7.833
7.831
7.687
7.684
7.669
7.666
7.663
7.649
7.646
7.576
7.573
7.559
7.555
7.552
7.538
7.534
7.284
7.066
7.061
7.049
7.044
3.902
3.051
CH3
N
O
CH3
2.99
2.00
1.01
1.01
2.00
3.02
3.00
f1 (ppm)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114.140
77.368
77.050
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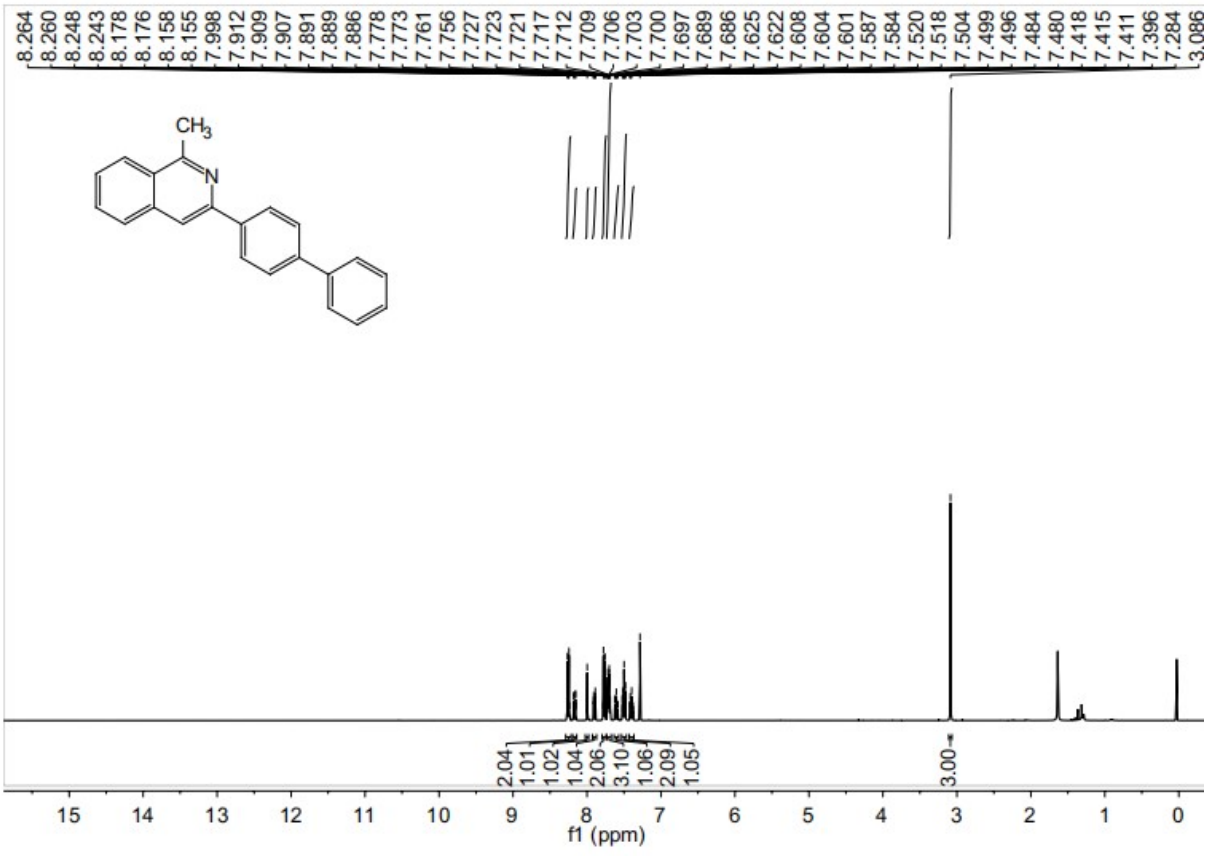
22.671
CH3
N
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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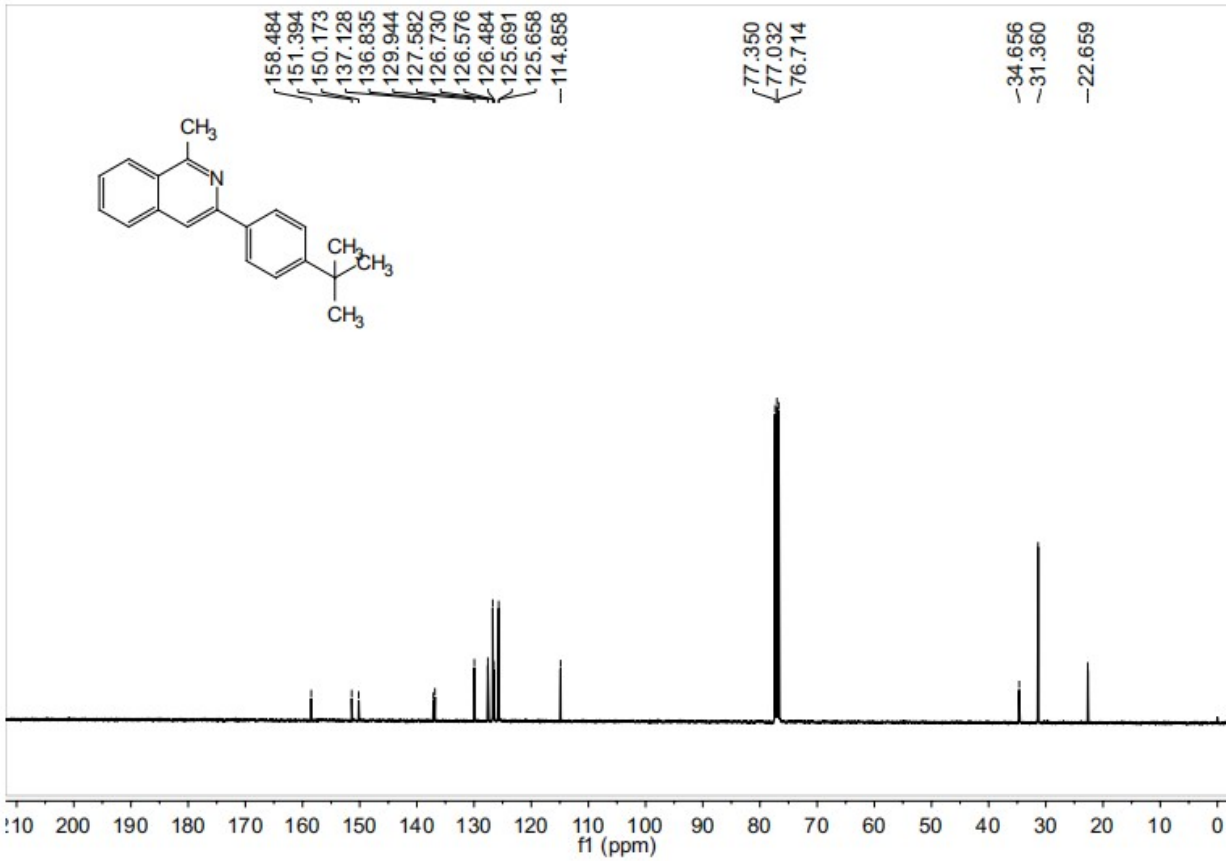
7.909
7.907
7.891
7.889
7.886
7.778
7.773
7.761
7.756
7.727
7.723
7.721
7.717
7.712
7.709
7.706
7.703
7.700
7.697
7.689
7.686
7.625
7.622
7.608
7.604
7.601
7.587
7.584
7.520
7.518
7.504
7.499
7.496
7.484
7.480
7.418
7.415
7.411
7.396
7.284
3.086
CH3
N
2.04
1.01
1.02
1.04
2.06
3.10
1.06
2.09
1.05
3.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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150.173
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136.835
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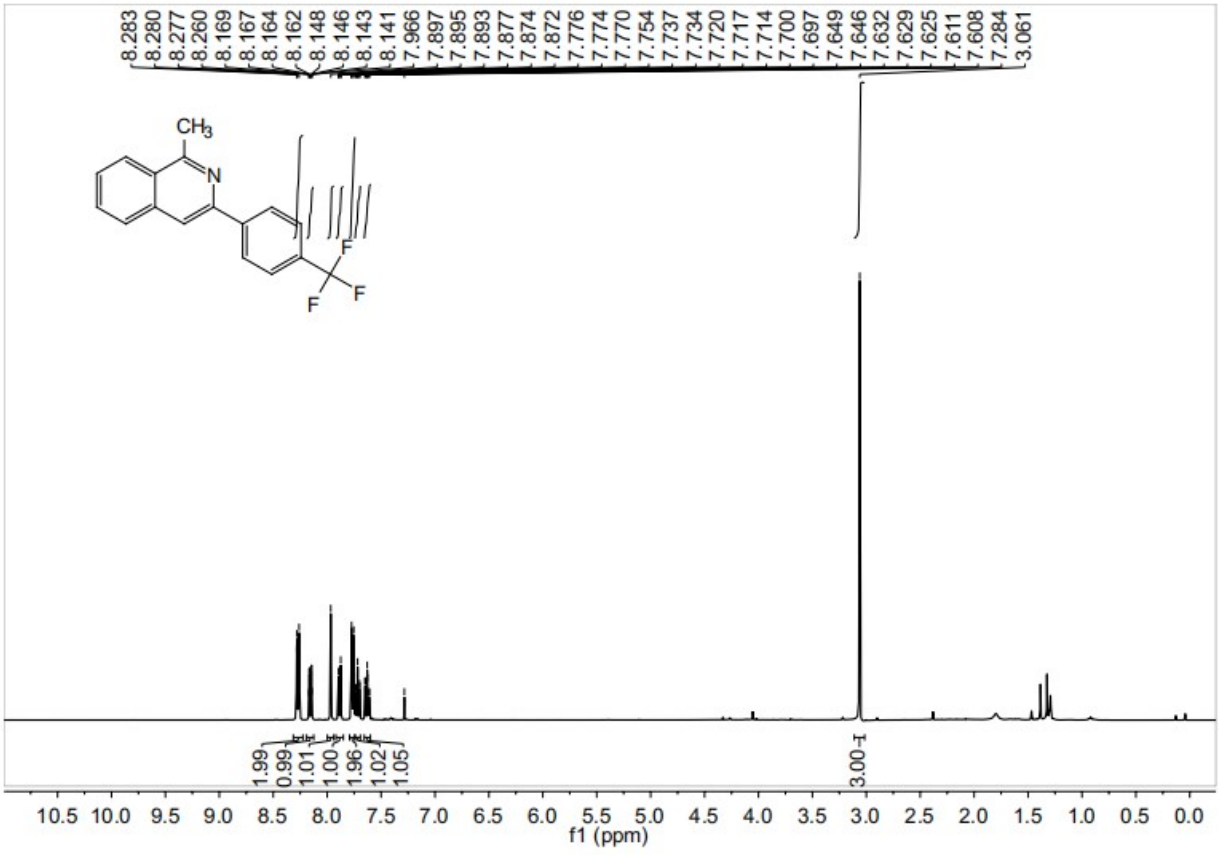
126.576
126.484
125.691
125.658
114.858
77.350
77.032
76.714
34.656
31.360
22.659
CH3
N
CH3
CH3
CH3
f1 (ppm)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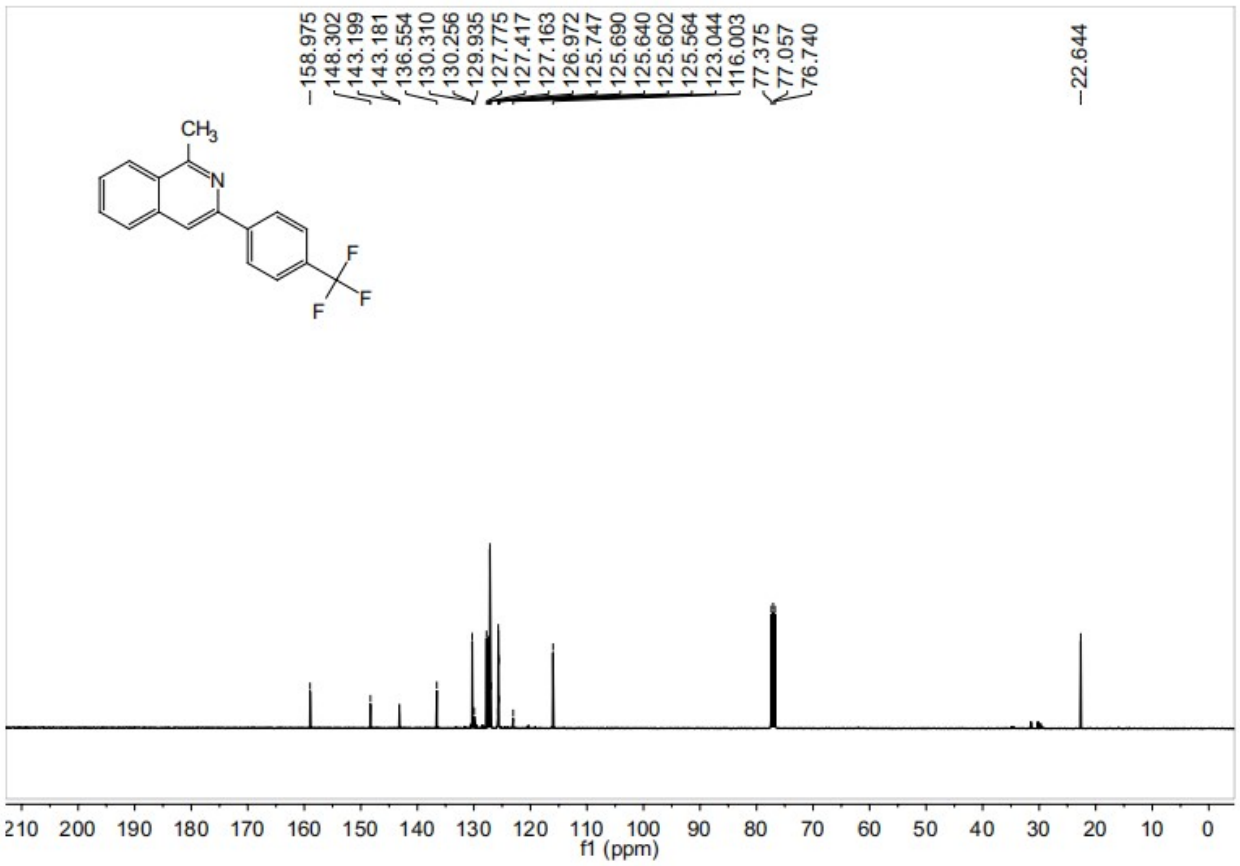
8.167
8.164
8.162
8.148
8.146
8.143
8.141
7.966
7.897
7.895
7.893
7.877
7.874
7.872
7.776
7.774
7.770
7.754
7.737
7.734
7.720
7.717
7.714
7.700
7.697
7.649
7.646
7.632
7.629
7.625
7.611
7.608
7.284
3.061
CH3
N
F
F
F
1.99
0.99
1.01
1.00
1.96
1.02
1.05
3.00
f1 (ppm)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143.181
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130.310
130.256
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127.775
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127.163
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125.747
125.690
125.640
125.602
125.564
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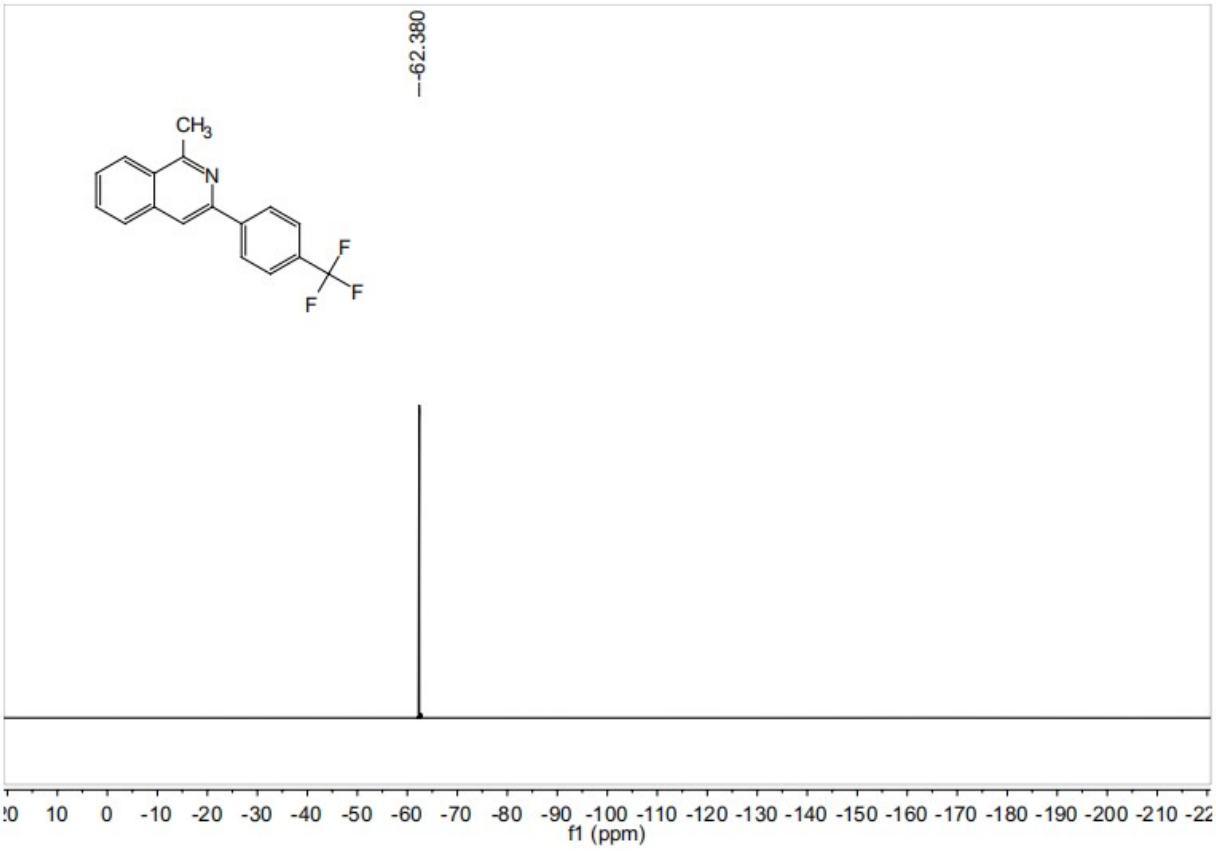
116.003
77.375
77.057
76.740
22.644
CH3
N
F
F
F
f1 (ppm)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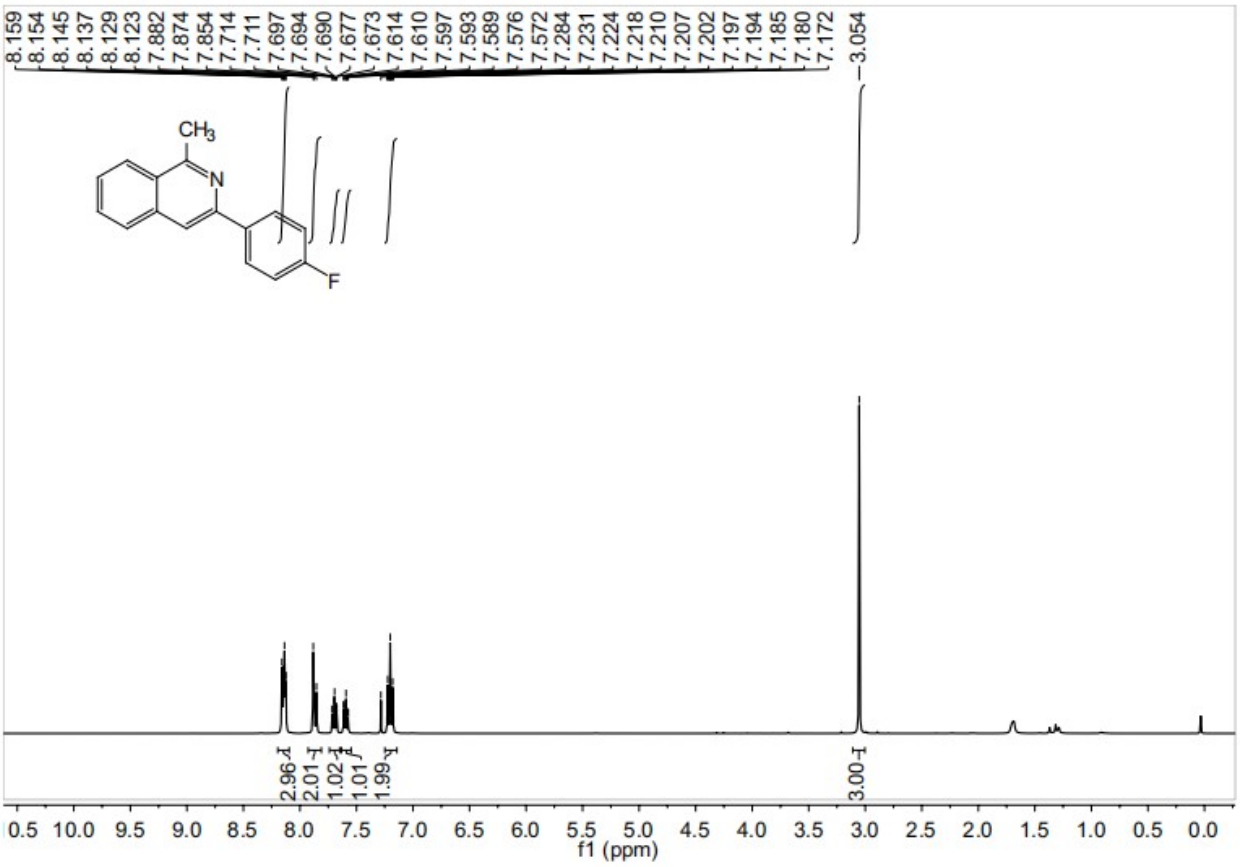
CH3
N
F
F
F
f1 (ppm)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8.154
8.145
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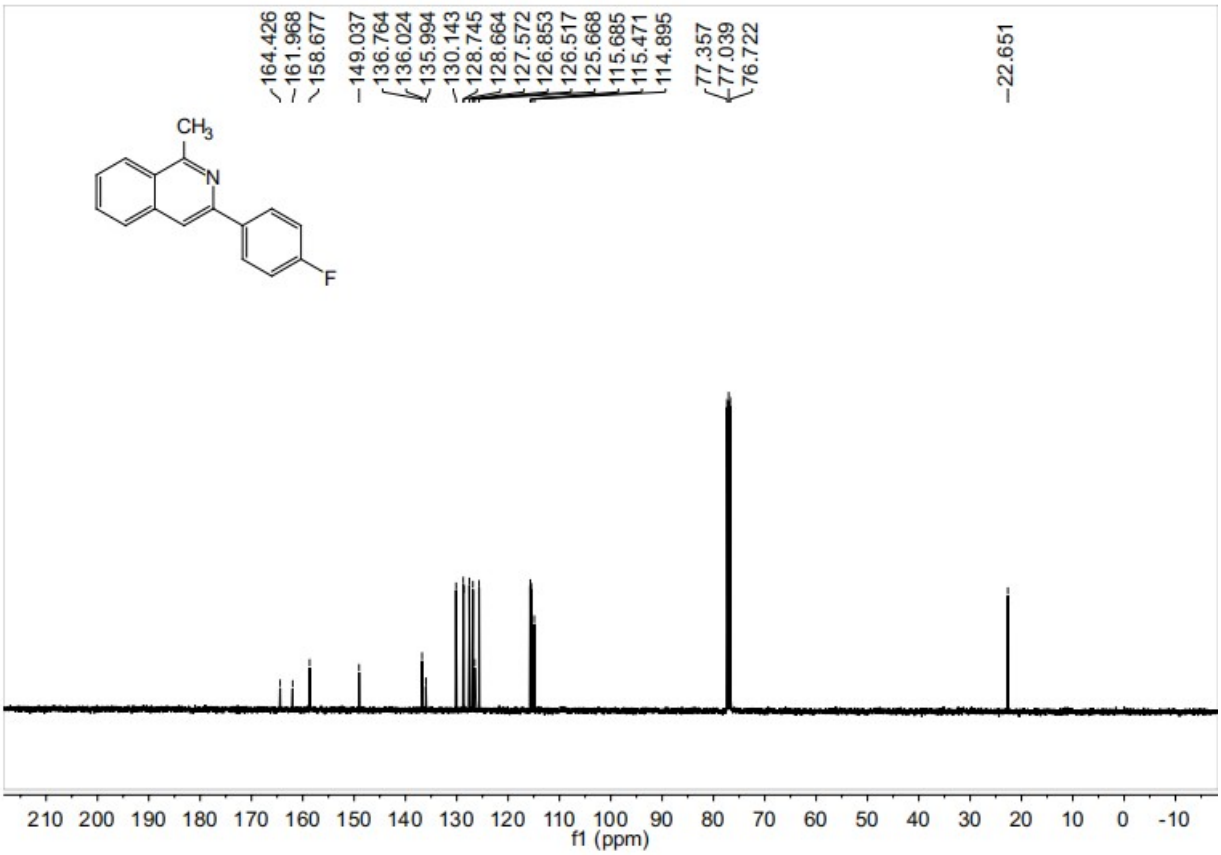
8.129
8.123
7.882
7.874
7.854
7.714
7.711
7.697
7.694
7.690
7.677
7.673
7.614
7.610
7.597
7.593
7.589
7.576
7.572
7.284
7.231
7.224
7.218
7.210
7.207
7.202
7.197
7.194
7.185
7.180
7.172
3.054
CH3
N
F
2.96
2.01
1.02
1.01
1.99
3.00
f1 (ppm)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115.471
114.895
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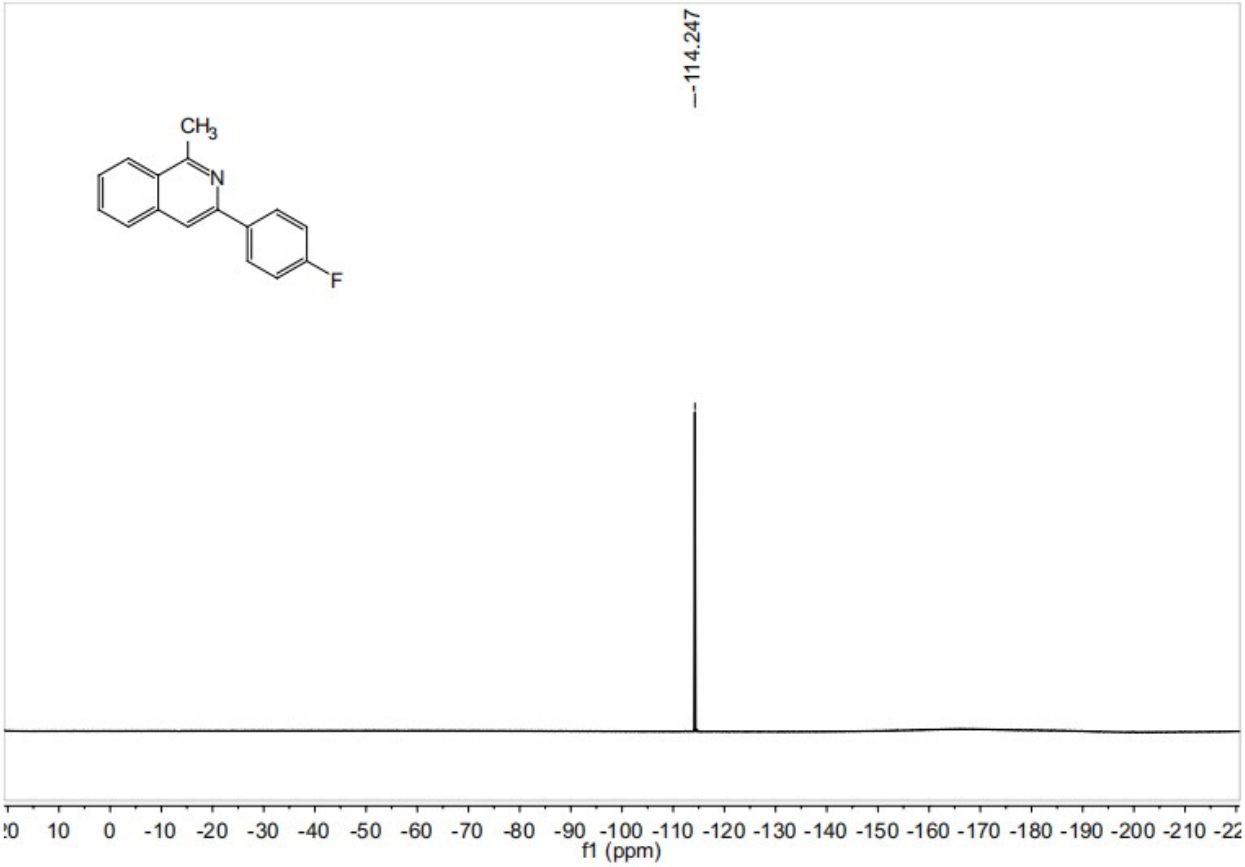
76.722
22.651
CH3
N
F
f1 (ppm)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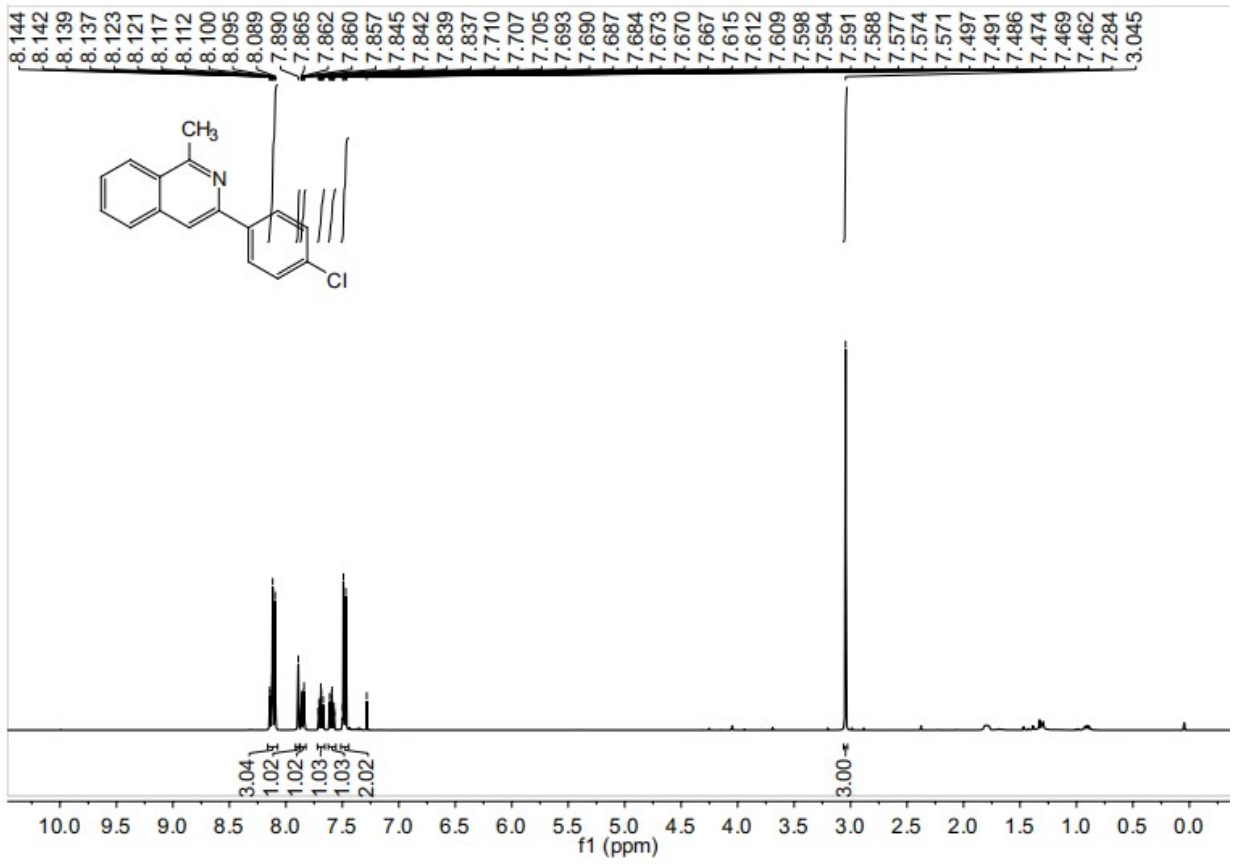
N
F
f1 (ppm)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7.865
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7.860
7.857
7.845
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7.710
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7.687
7.684
7.673
7.670
7.667
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7.612
7.609
7.598
7.594
7.591
7.588
7.577
7.574
7.571
7.497
7.491
7.486
7.474
7.469
7.462
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N
Cl
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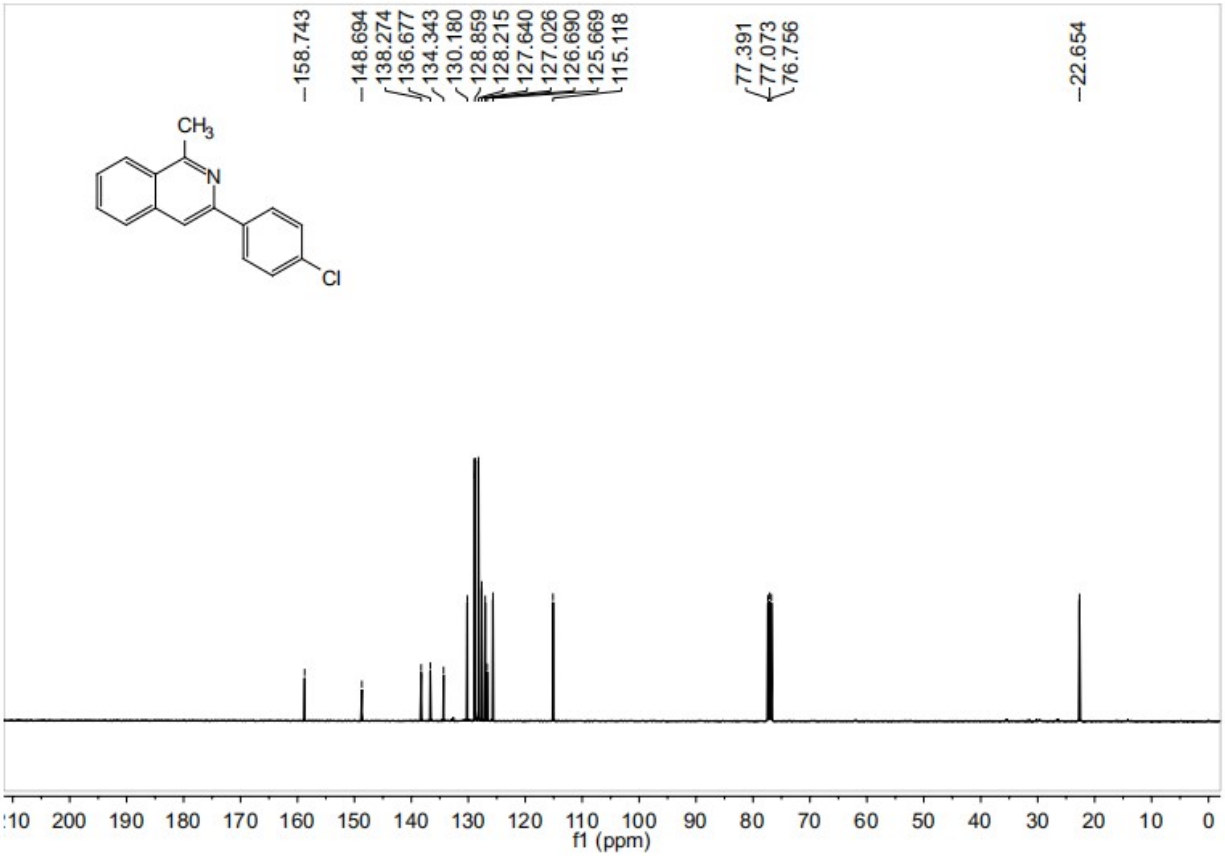
1.02
1.03
1.03
2.02
3.00
f1 (ppm)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128.215
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125.669
115.118
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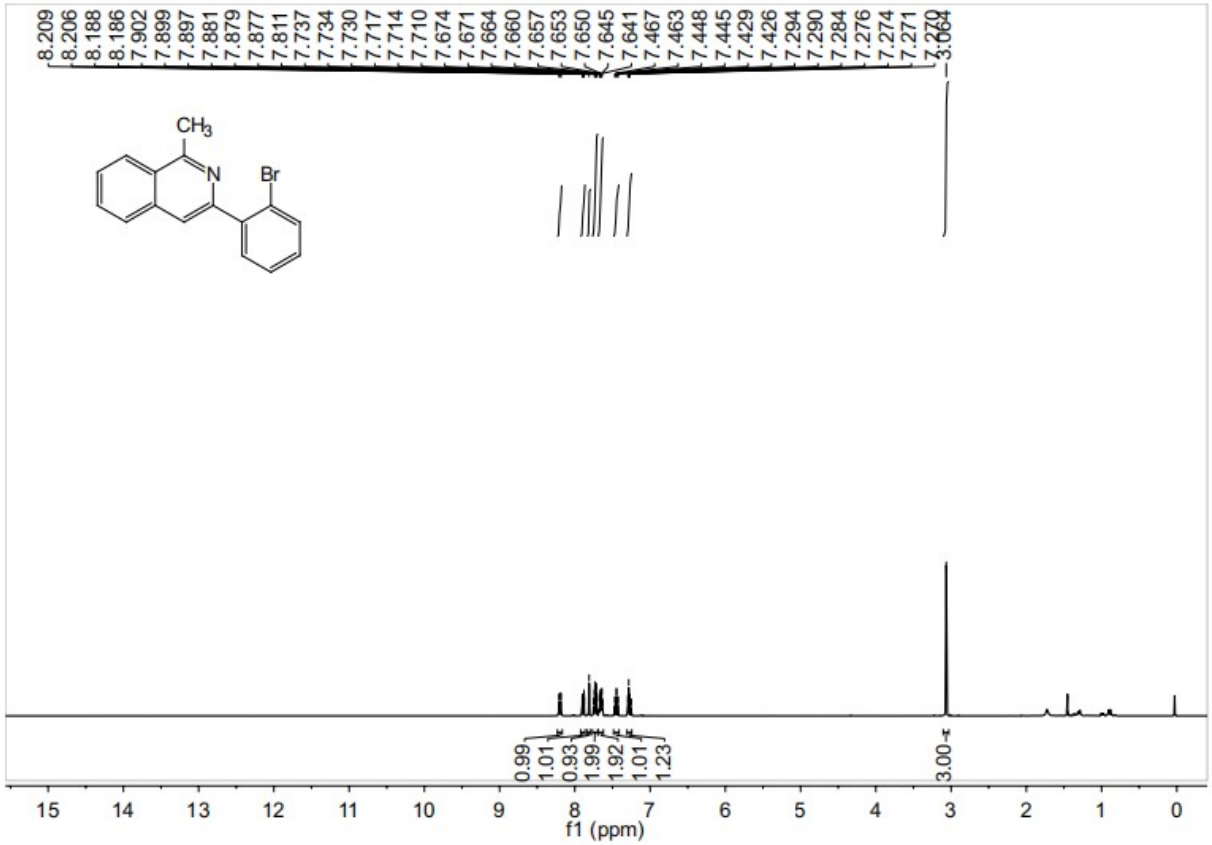
77.073
76.756
22.654
CH3
N
Cl
f1 (ppm)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7.897
7.881
7.879
7.877
7.811
7.737
7.734
7.730
7.717
7.714
7.710
7.674
7.671
7.664
7.660
7.657
7.653
7.650
7.645
7.641
7.467
7.463
7.448
7.445
7.429
7.426
7.294
7.290
7.284
7.276
7.274
7.271
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Br
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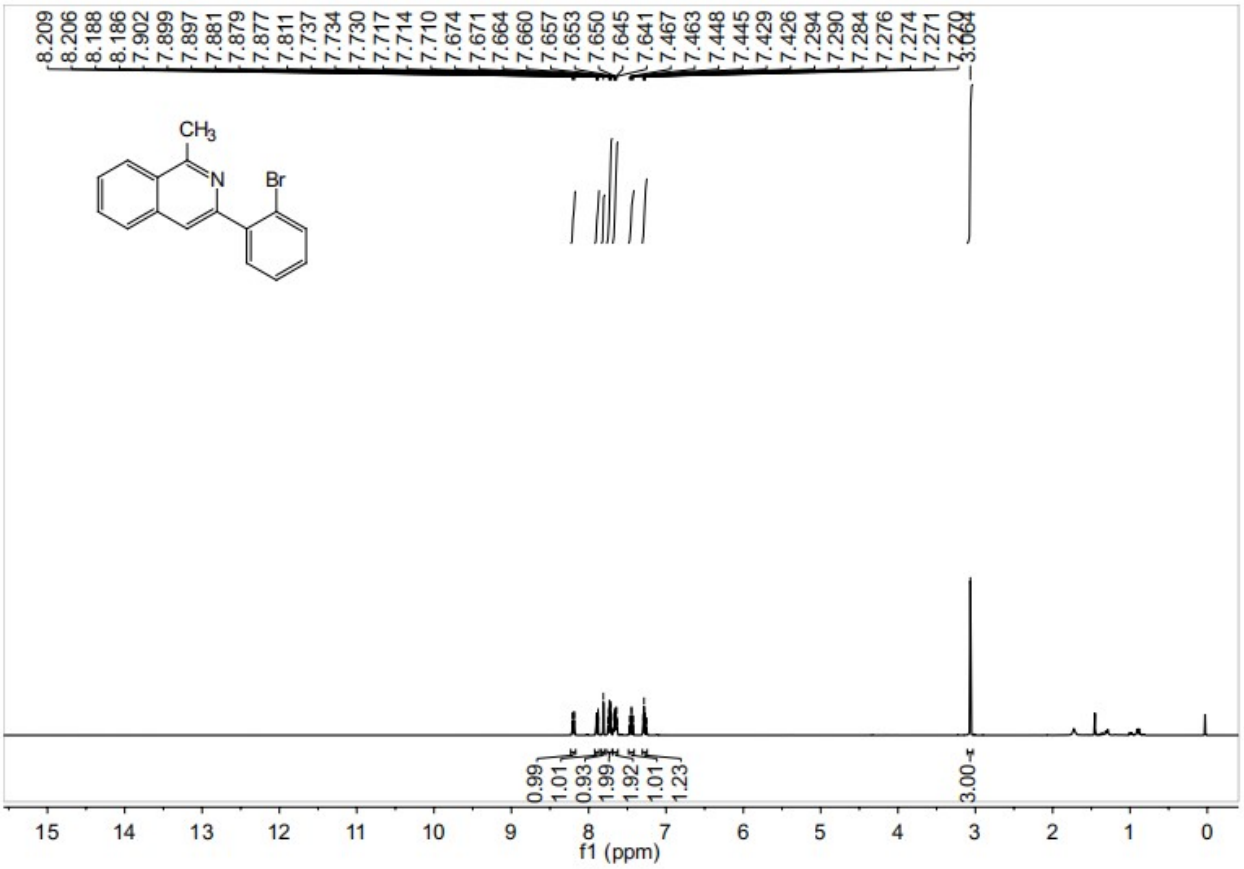
0.93
1.99
1.92
1.01
1.23
3.00
f1 (ppm)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7.717
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7.710
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7.671
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7.660
7.657
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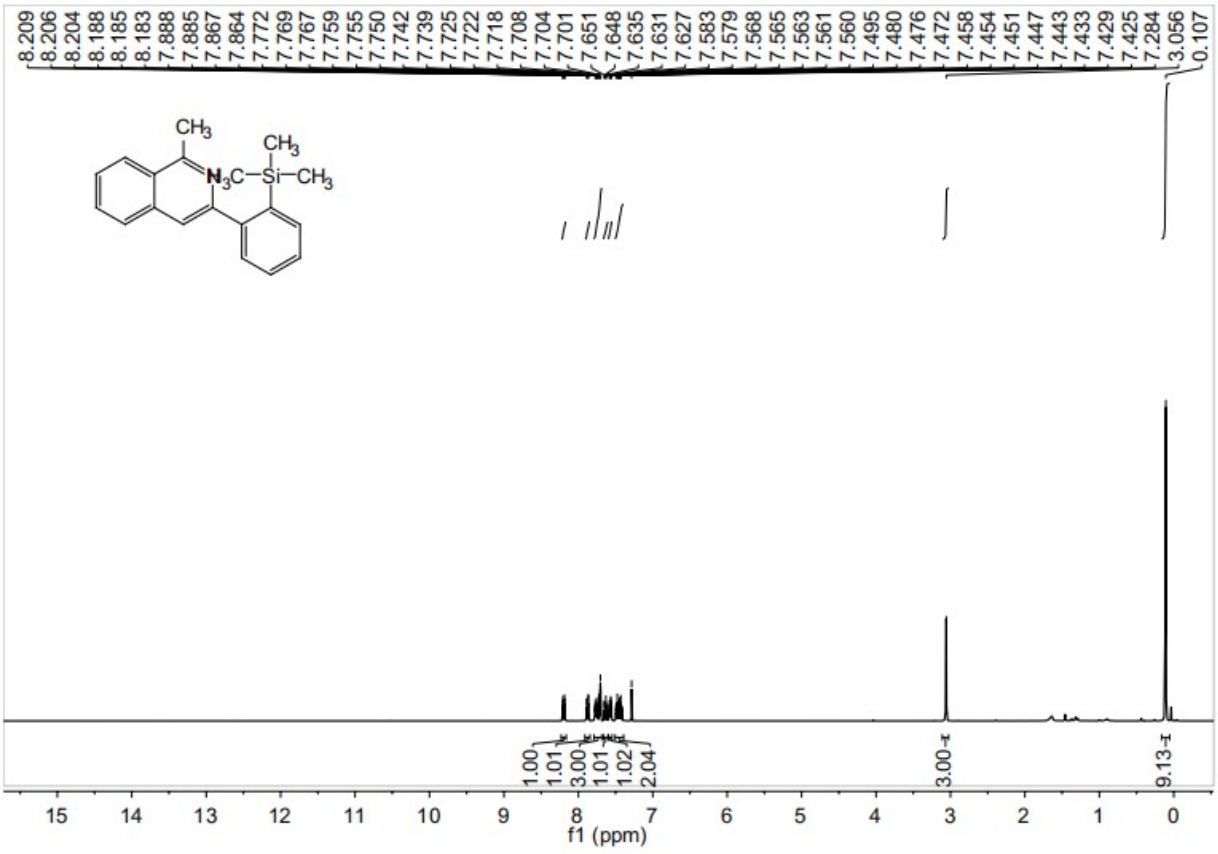
7.650
7.645
7.641
7.467
7.463
7.448
7.445
7.429
7.426
7.294
7.290
7.284
7.276
7.274
7.271
3.064
CH3
N
Br
0.99
1.01
0.93
1.99
1.92
1.01
1.23
3.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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7.755
7.750
7.742
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7.725
7.722
7.718
7.708
7.704
7.701
7.651
7.648
7.635
7.631
7.627
7.583
7.579
7.568
7.565
7.563
7.561
7.560
7.495
7.480
7.476
7.472
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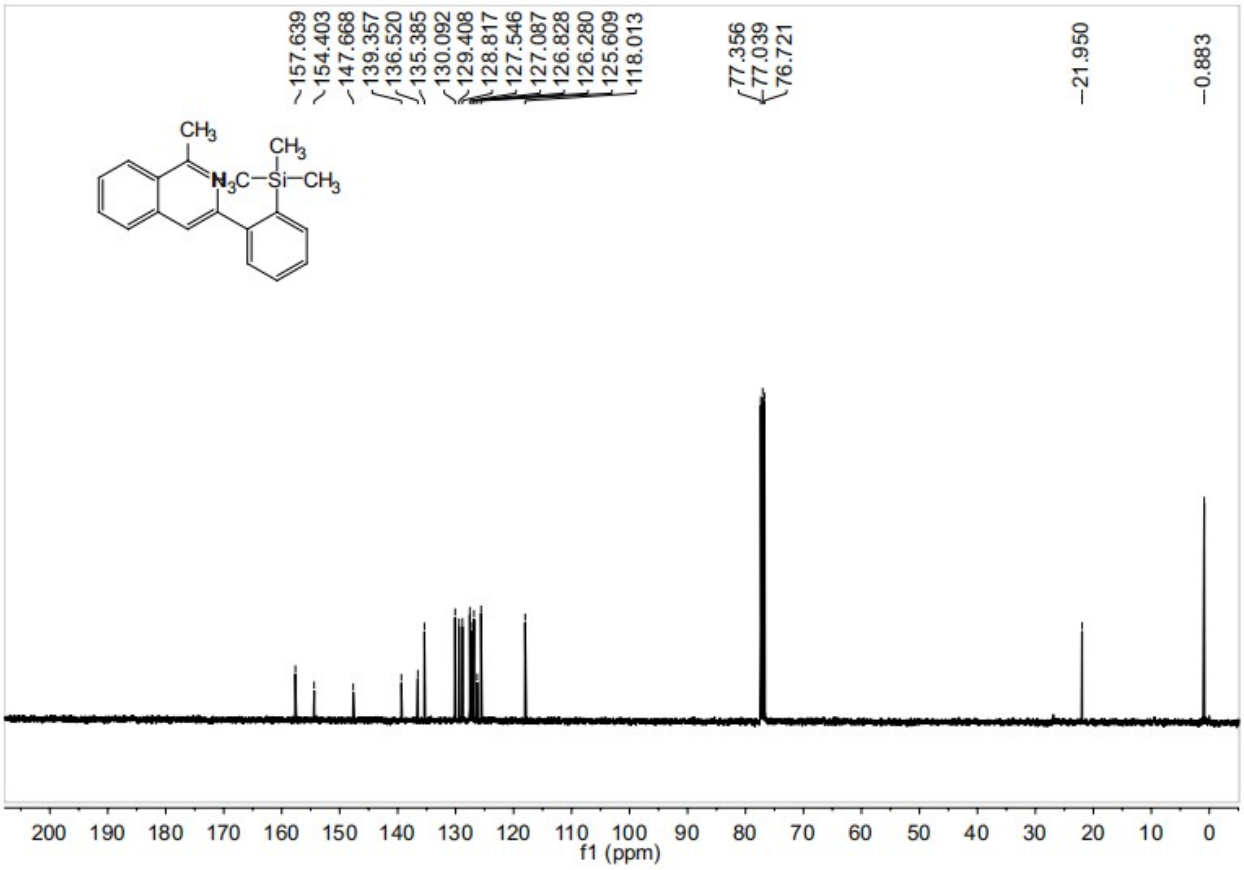
7.454
7.451
7.447
7.443
7.433
7.429
7.425
7.284
3.056
0.107
CH3
CH3
N3C–Si–CH3
1.00
1.01
3.00
1.01
1.02
2.04
3.00
9.13
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)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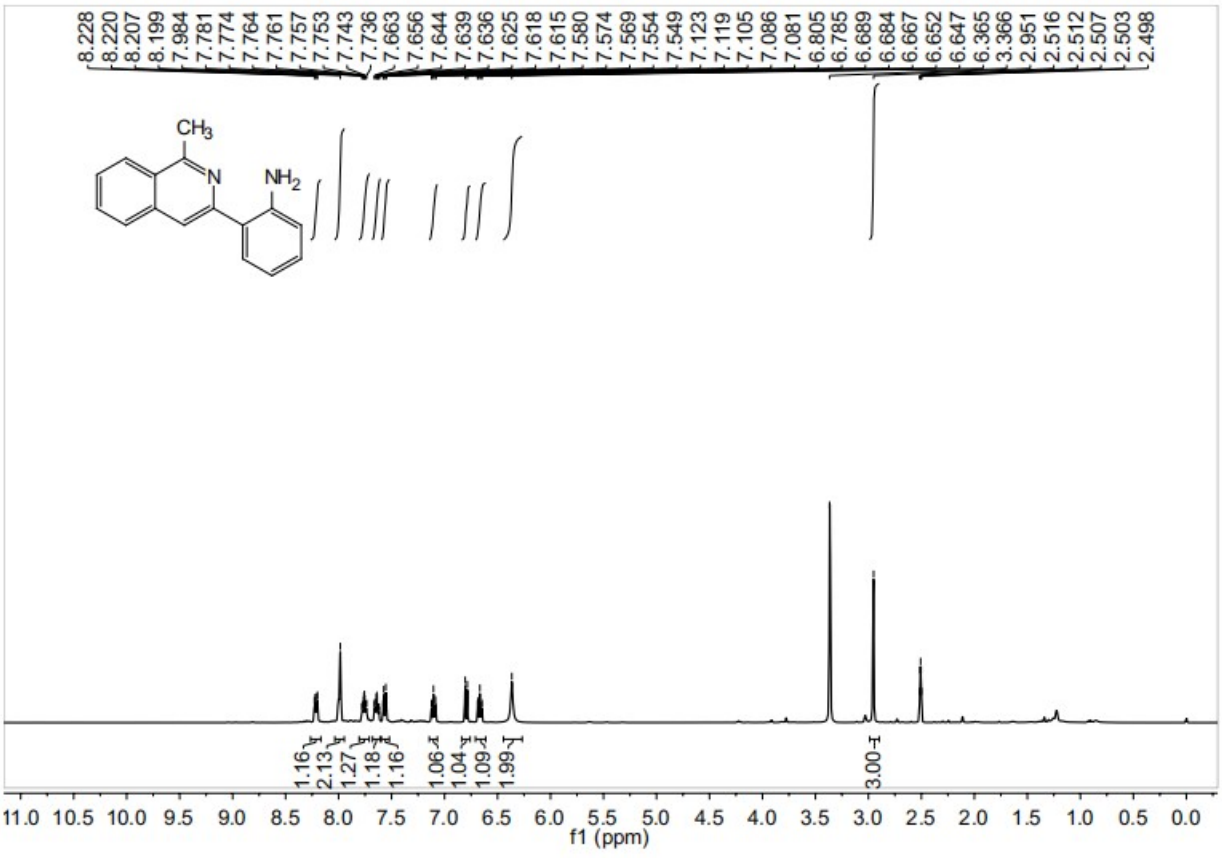
127.546
127.087
126.828
126.280
125.609
118.013
77.356
77.039
76.721
21.950
0.883
CH3
CH3
N3C–Si–CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.615
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7.105
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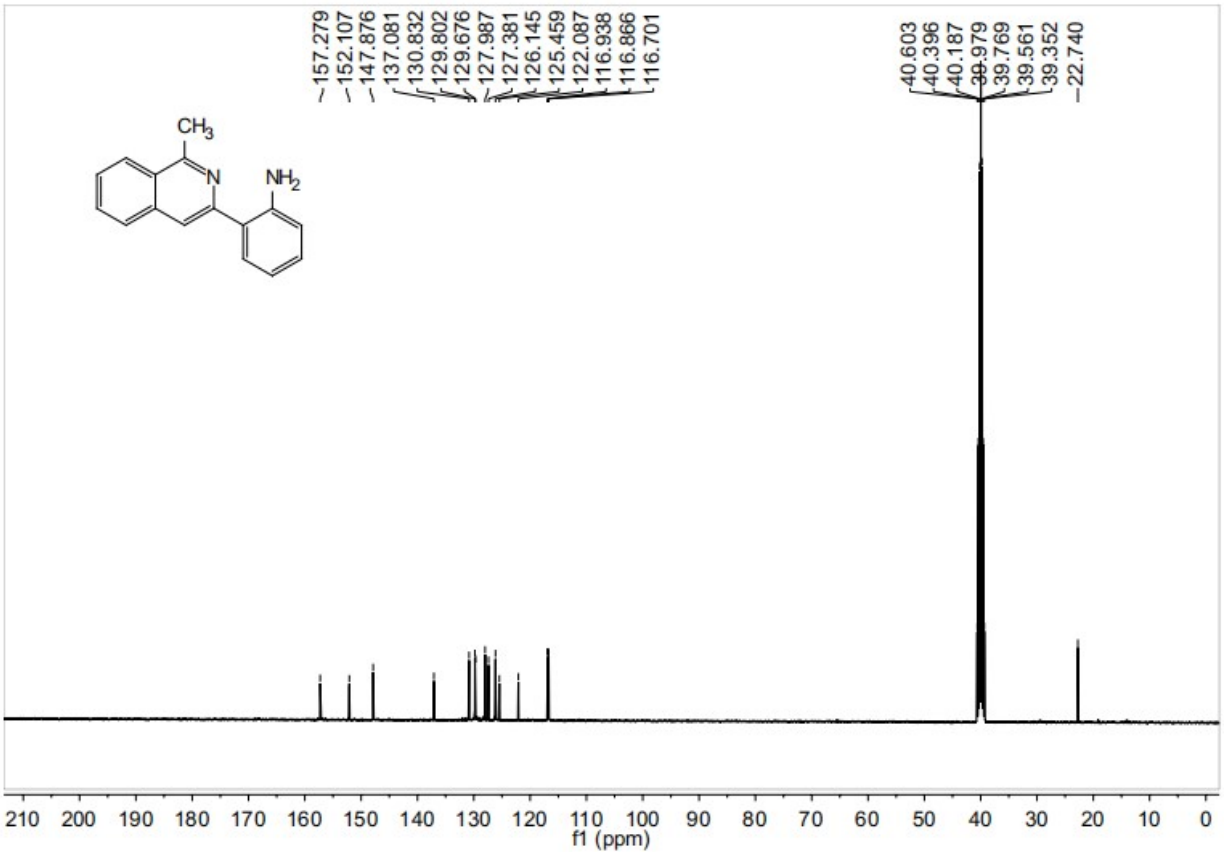
6.667
6.652
6.647
6.365
3.366
2.951
2.516
2.512
2.507
2.503
2.498
CH3
N
NH2
1.16
2.13
1.27
1.18
1.16
1.06
1.04
1.09
1.99
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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126.145
125.459
122.087
116.938
116.866
116.701
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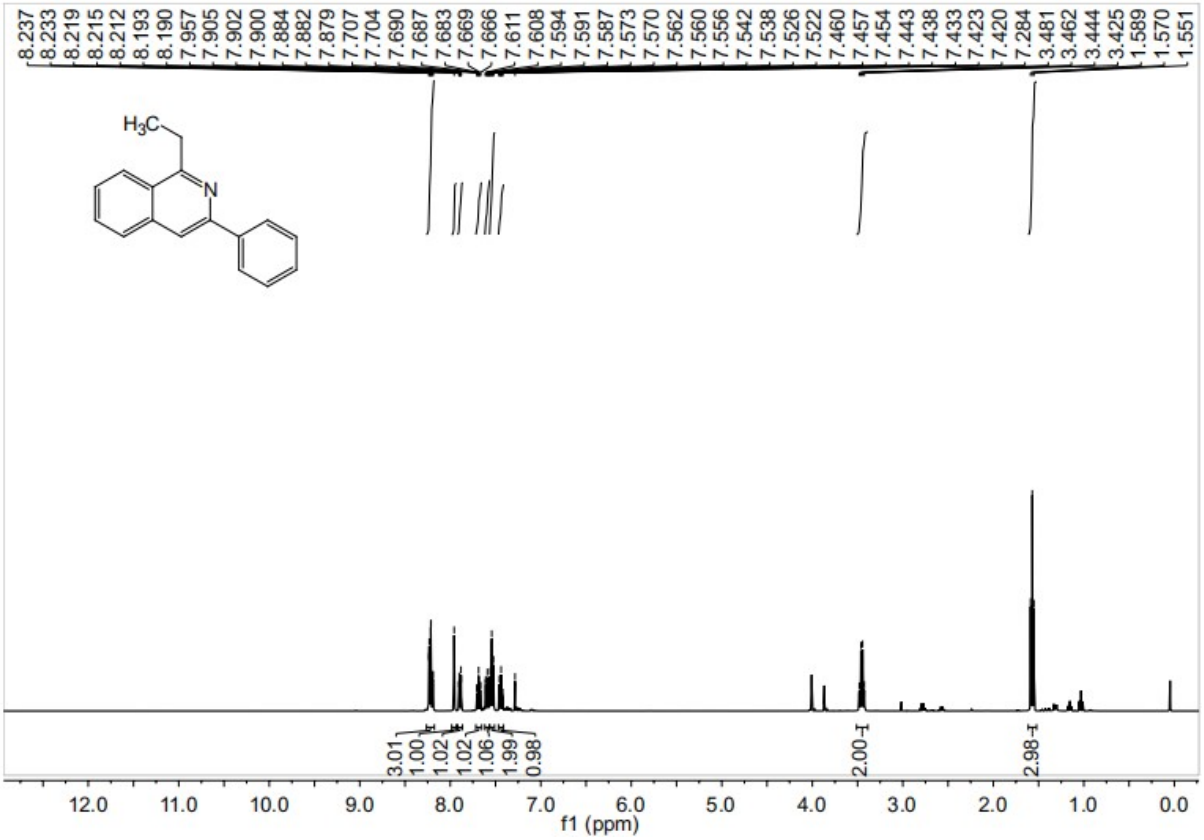
22.740
CH3
N
NH2
f1 (ppm)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7.879
7.707
7.704
7.690
7.687
7.683
7.669
7.666
7.611
7.608
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7.591
7.587
7.573
7.570
7.562
7.560
7.556
7.542
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7.460
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7.454
7.443
7.438
7.433
7.423
7.420
7.284
3.481
3.462
3.444
3.425
1.589
1.570
1.551
H3C
N
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1.02
1.02
1.06
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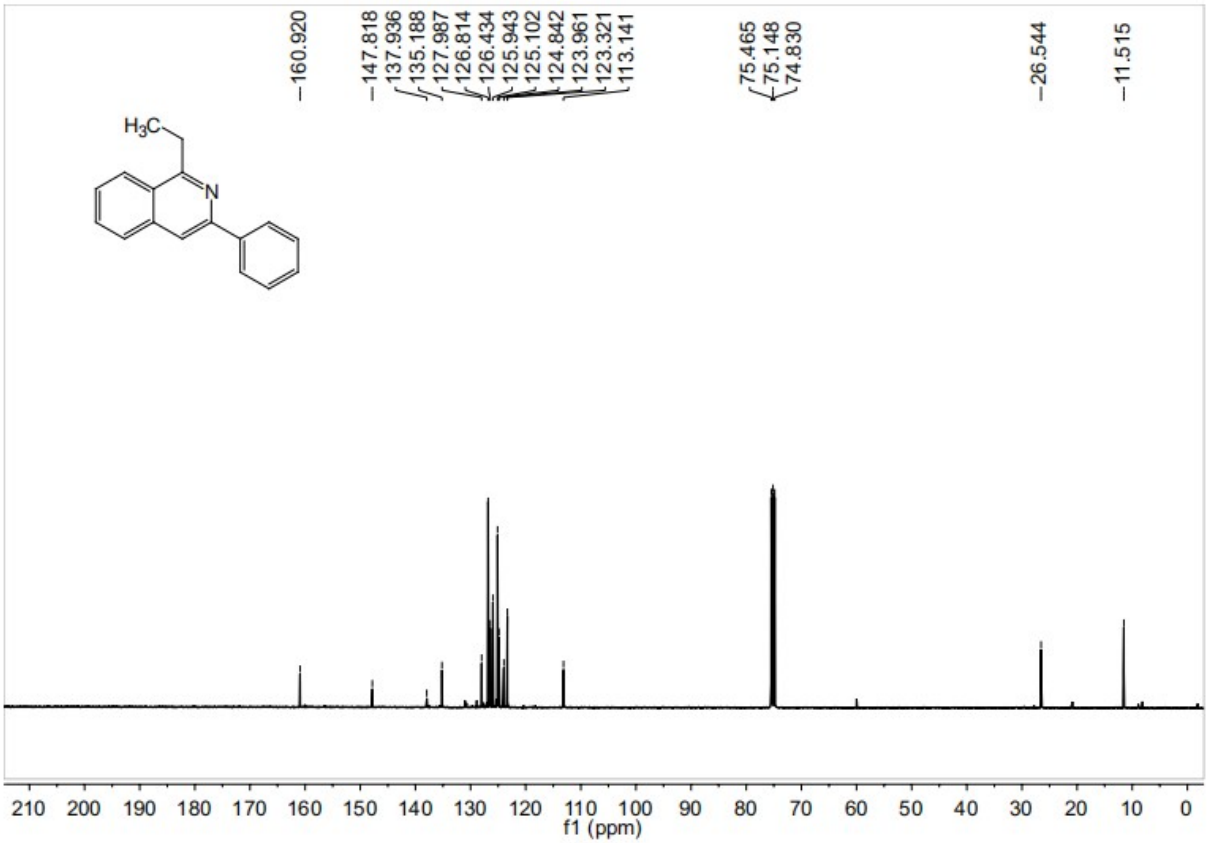
2.98
f1 (ppm)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26.544
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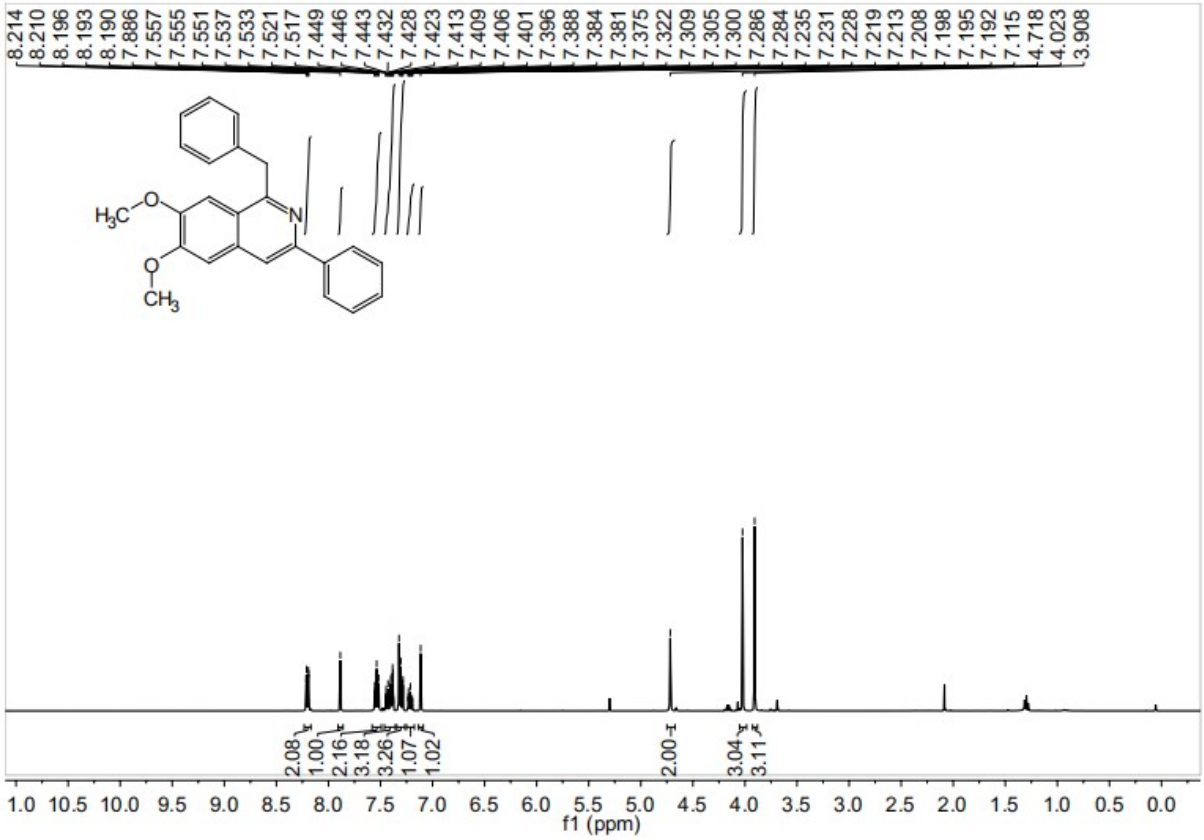
H3C
N
f1 (ppm)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7.443
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7.413
7.409
7.406
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7.396
7.388
7.384
7.381
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7.322
7.309
7.305
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7.235
7.231
7.228
7.219
7.213
7.208
7.198
7.195
7.192
7.115
4.718
4.023
3.908
H3C
O
N
O
CH3
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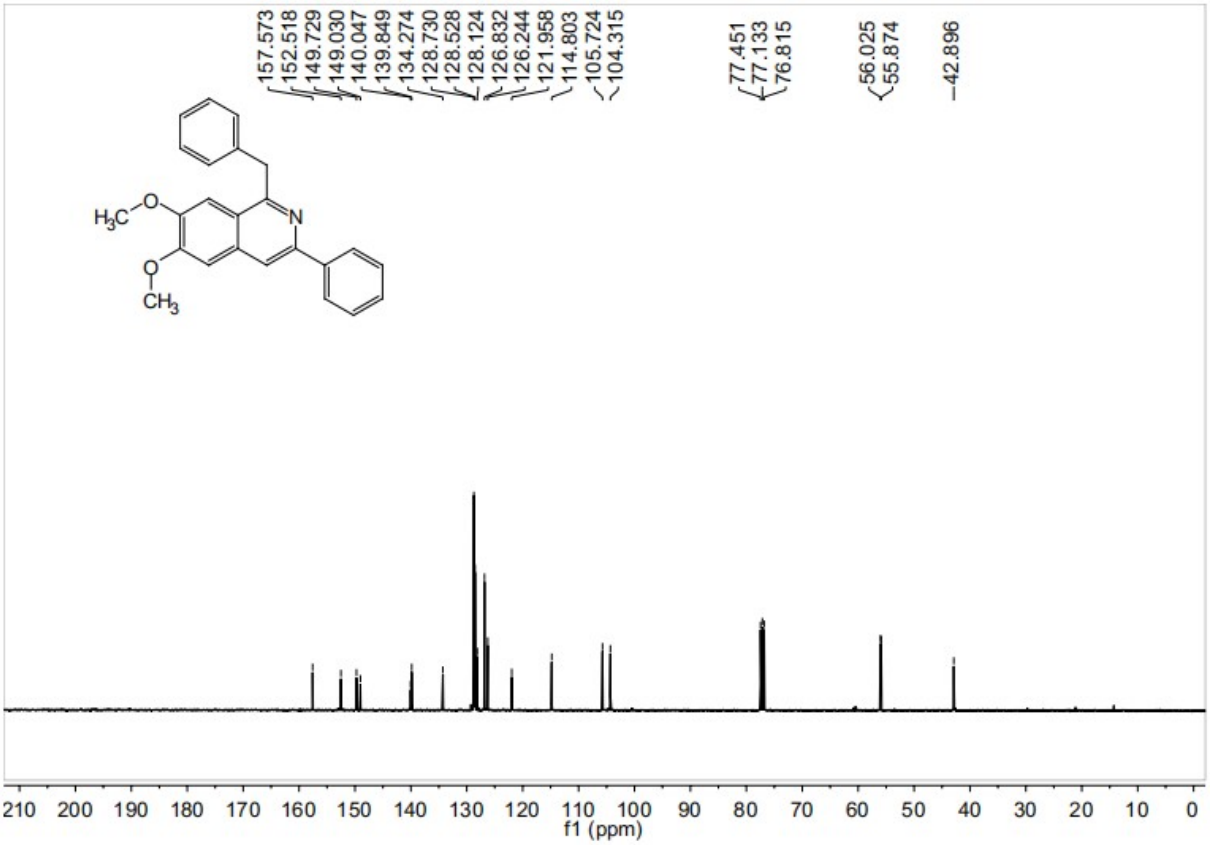
1.02
2.00
3.04
3.11
f1 (ppm)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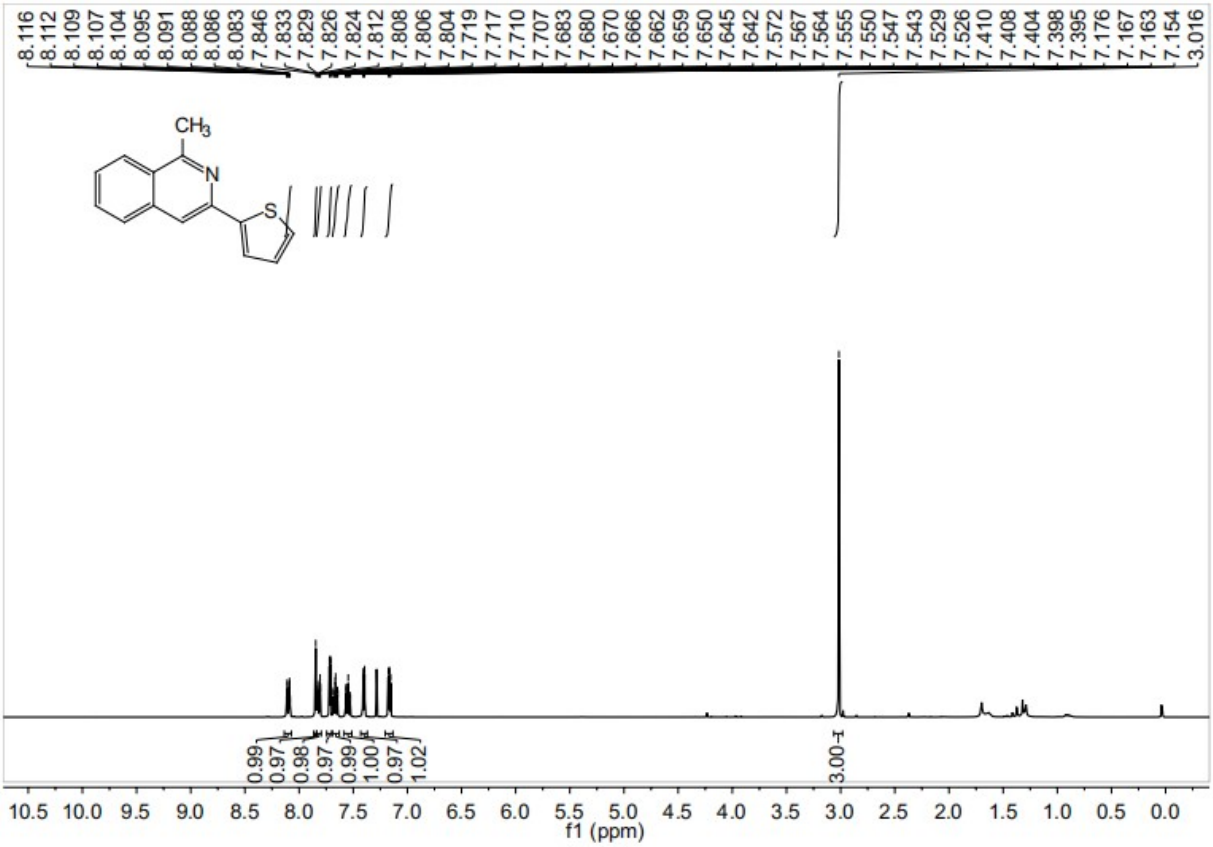
114.803
105.724
104.315
77.451
77.133
76.815
56.025
55.874
42.896
H3C
O
N
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.109
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8.104
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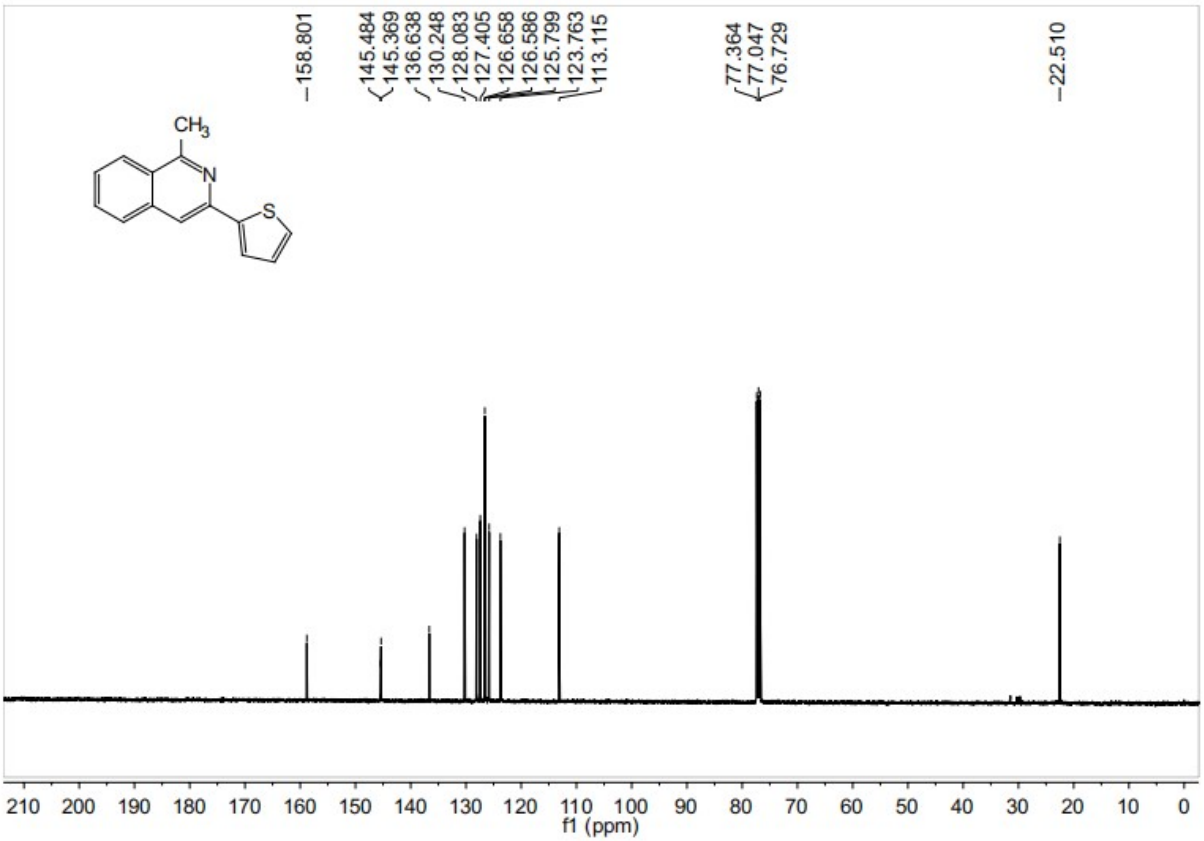
8.091
8.088
8.086
8.083
7.846
7.833
7.829
7.826
7.824
7.812
7.808
7.806
7.804
7.719
7.717
7.710
7.707
7.683
7.680
7.670
7.666
7.662
7.659
7.650
7.645
7.642
7.572
7.567
7.564
7.555
7.550
7.547
7.543
7.529
7.526
7.410
7.408
7.404
7.398
7.395
7.176
7.167
7.163
7.154
3.016
CH3
N
S
0.99
0.97
0.98
0.97
0.99
1.00
0.97
1.02
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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145.369
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128.083
127.405
126.658
126.586
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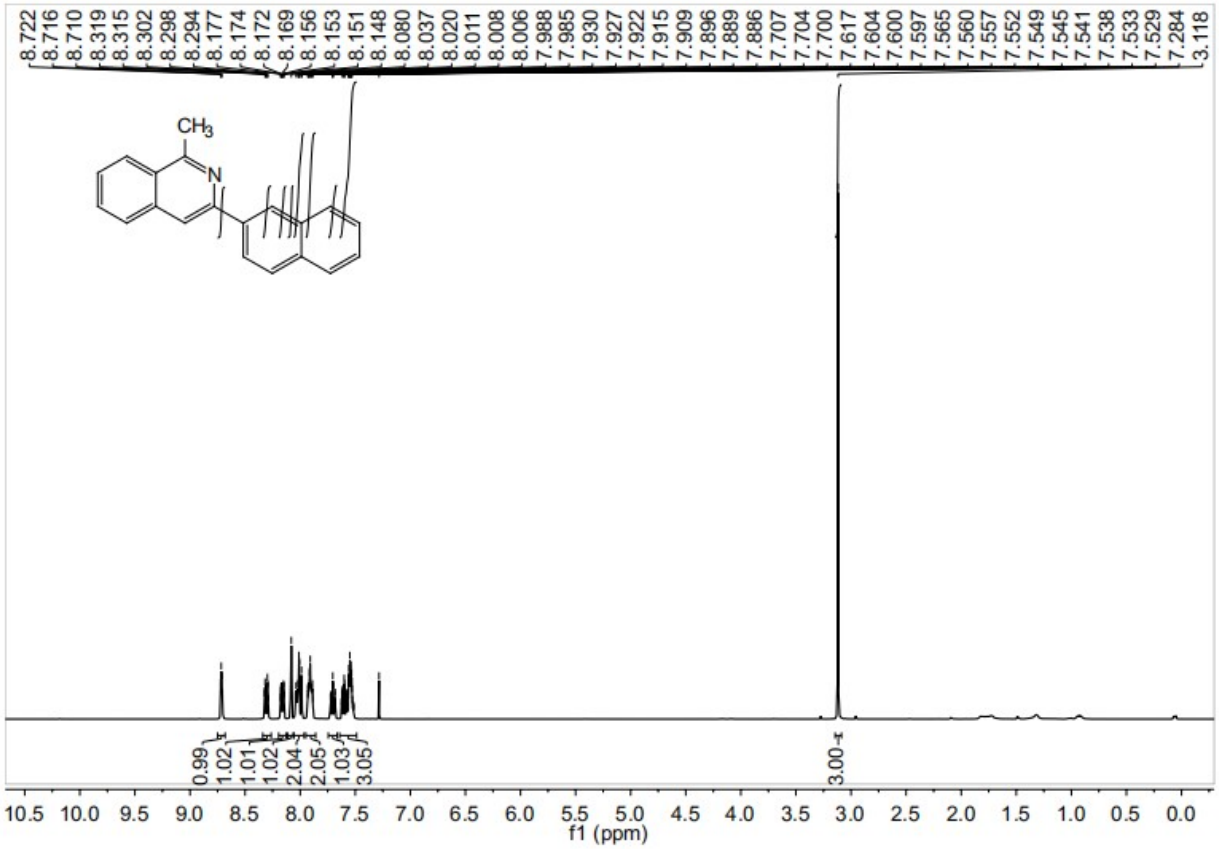
123.763
113.115
77.364
77.047
76.729
22.510
CH3
N
S
f1 (ppm)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8.710
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8.294
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8.174
8.172
8.169
8.156
8.153
8.151
8.148
8.080
8.037
8.020
8.011
8.008
8.006
7.988
7.985
7.930
7.927
7.922
7.915
7.909
7.896
7.889
7.886
7.707
7.704
7.700
7.617
7.604
7.600
7.597
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7.560
7.557
7.552
7.549
7.545
7.541
7.538
7.533
7.529
7.284
3.118
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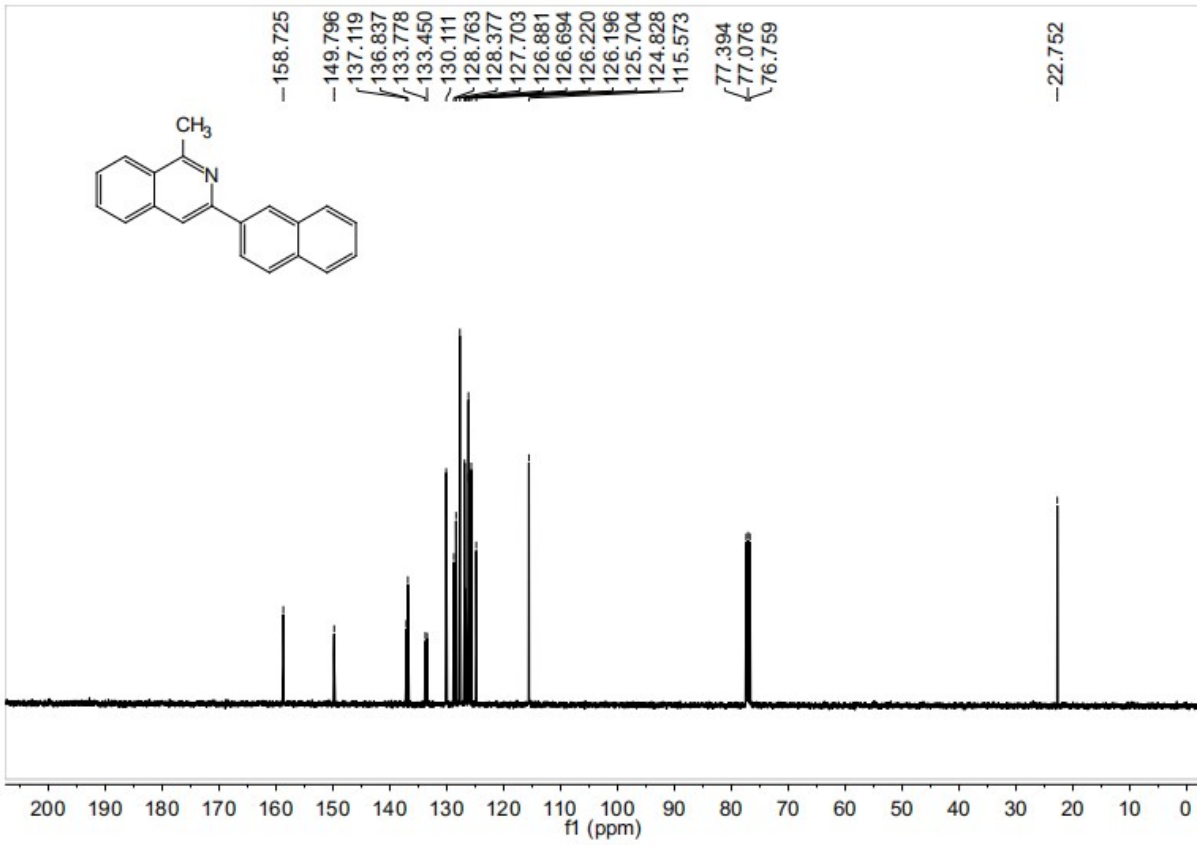
1.02
1.01
1.02
2.04
2.05
1.03
3.05
3.00
f1 (ppm)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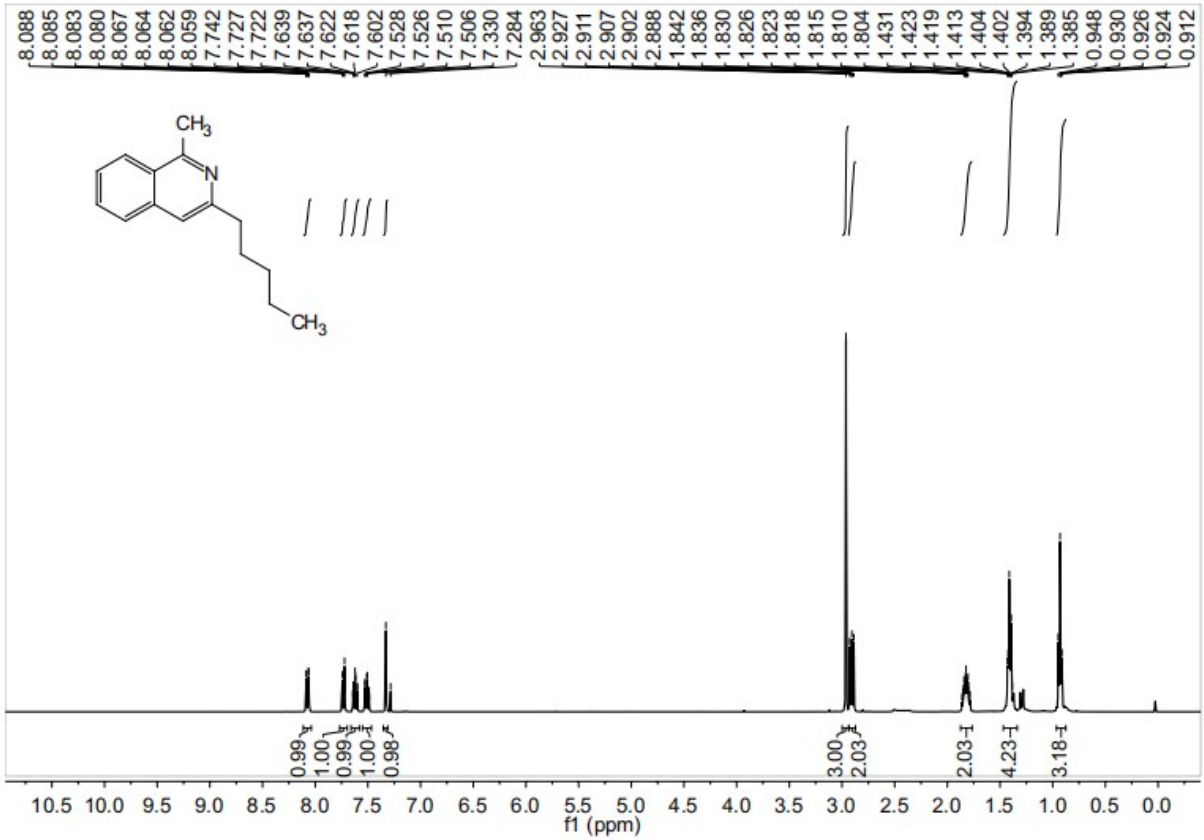
149.796
137.119
136.837
133.778
133.450
130.111
128.763
128.377
127.703
126.881
126.694
126.220
126.196
125.704
124.828
115.573
77.394
77.076
76.759
22.752
CH3
N
f1 (ppm)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8.083
8.080
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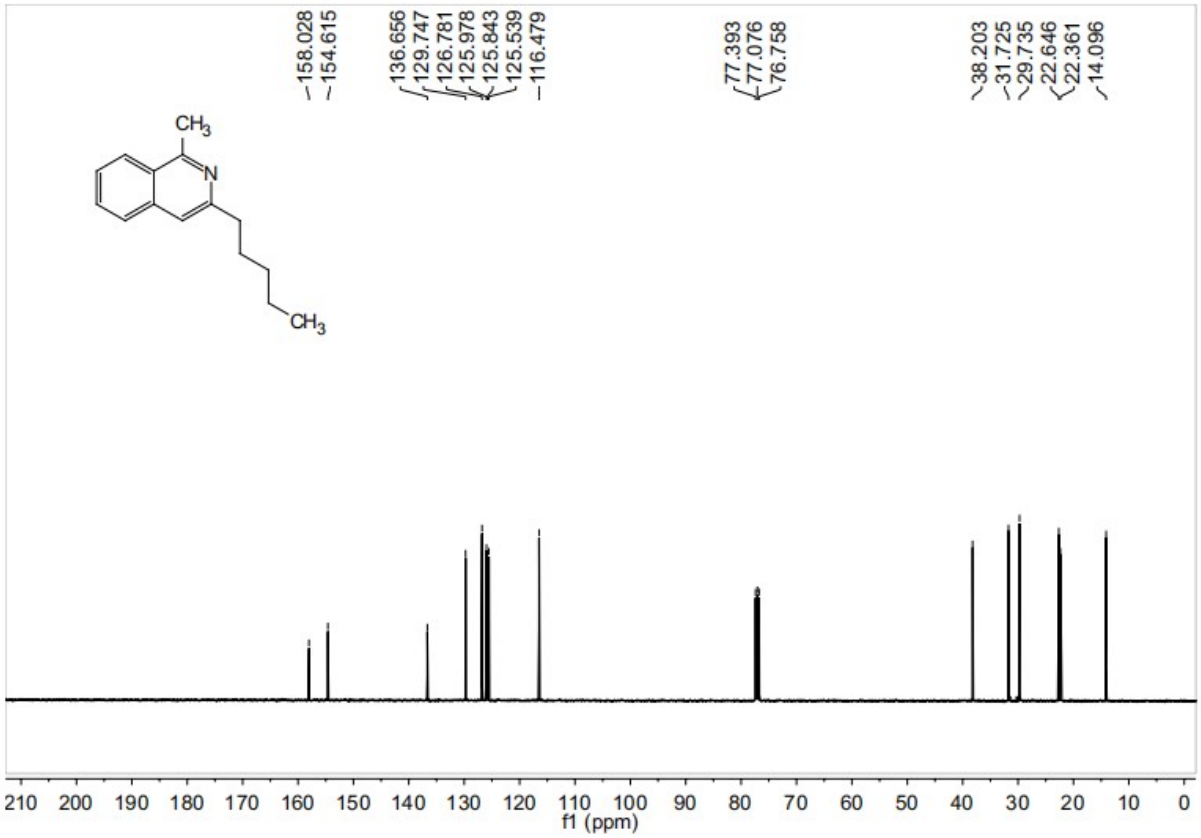
8.064
8.062
8.059
7.742
7.727
7.722
7.639
7.637
7.622
7.618
7.602
7.528
7.526
7.510
7.506
7.330
7.284
2.963
2.927
2.911
2.907
2.902
2.888
1.842
1.836
1.830
1.826
1.823
1.818
1.815
1.810
1.804
1.431
1.423
1.419
1.413
1.404
1.402
1.394
1.389
1.385
0.948
0.930
0.926
0.924
0.912
CH3
N
CH3
0.99
1.00
0.99
1.00
0.98
3.00
2.03
2.03
4.23
3.18
f1 (ppm)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136.656
129.747
126.781
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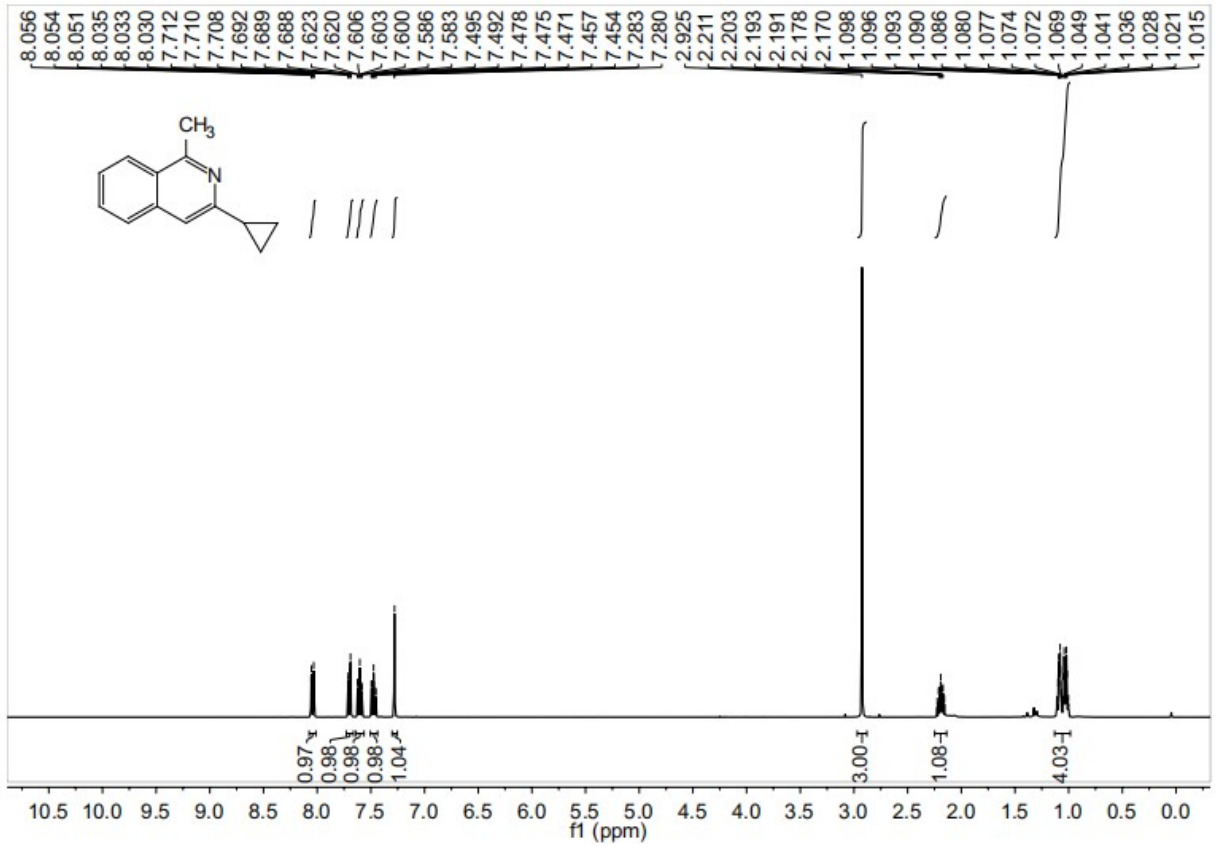
125.843
125.539
116.479
77.393
77.076
76.758
38.203
31.725
29.735
22.646
22.361
14.096
CH3
N
CH3
f1 (ppm)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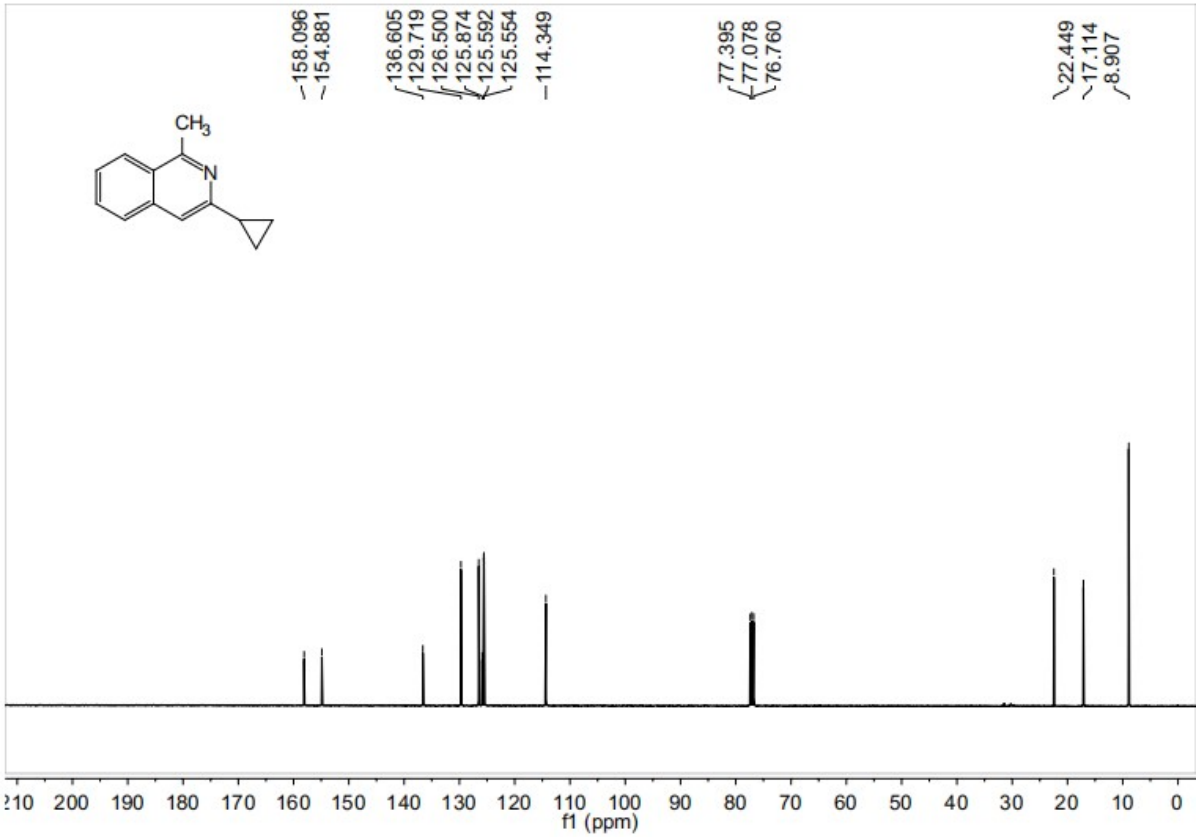
8.054
8.051
8.035
8.033
8.030
7.712
7.710
7.708
7.692
7.689
7.688
7.623
7.620
7.606
7.603
7.600
7.586
7.583
7.495
7.492
7.478
7.475
7.471
7.457
7.454
7.283
7.280
2.925
2.211
2.203
2.193
2.191
2.178
2.170
1.098
1.096
1.093
1.090
1.086
1.080
1.077
1.074
1.072
1.069
1.049
1.041
1.036
1.028
1.021
1.015
CH3
N
0.97
0.98
0.98
0.98
1.04
3.00
1.08
4.03
f1 (ppm)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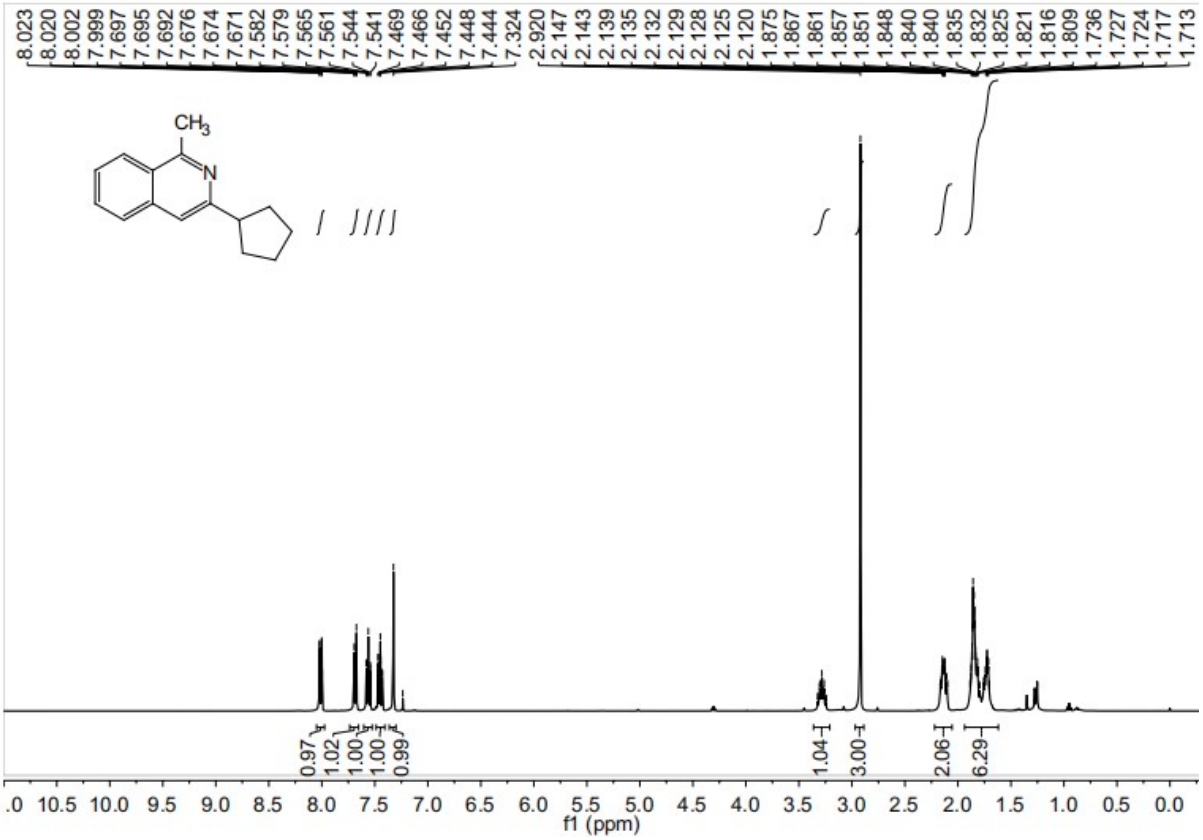
129.719
126.500
125.874
125.592
125.554
114.349
77.395
77.078
76.760
22.449
17.114
8.907
CH3
N
f1 (ppm)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8.020
8.002
7.999
7.697
7.695
7.692
7.676
7.674
7.671
7.582
7.579
7.565
7.561
7.544
7.541
7.469
7.466
7.452
7.448
7.444
7.324
2.920
2.147
2.143
2.139
2.135
2.132
2.129
2.128
2.125
2.120
1.875
1.867
1.861
1.857
1.851
1.848
1.840
1.840
1.835
1.832
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1.821
1.816
1.809
1.736
1.727
1.724
1.717
1.713
CH3
N
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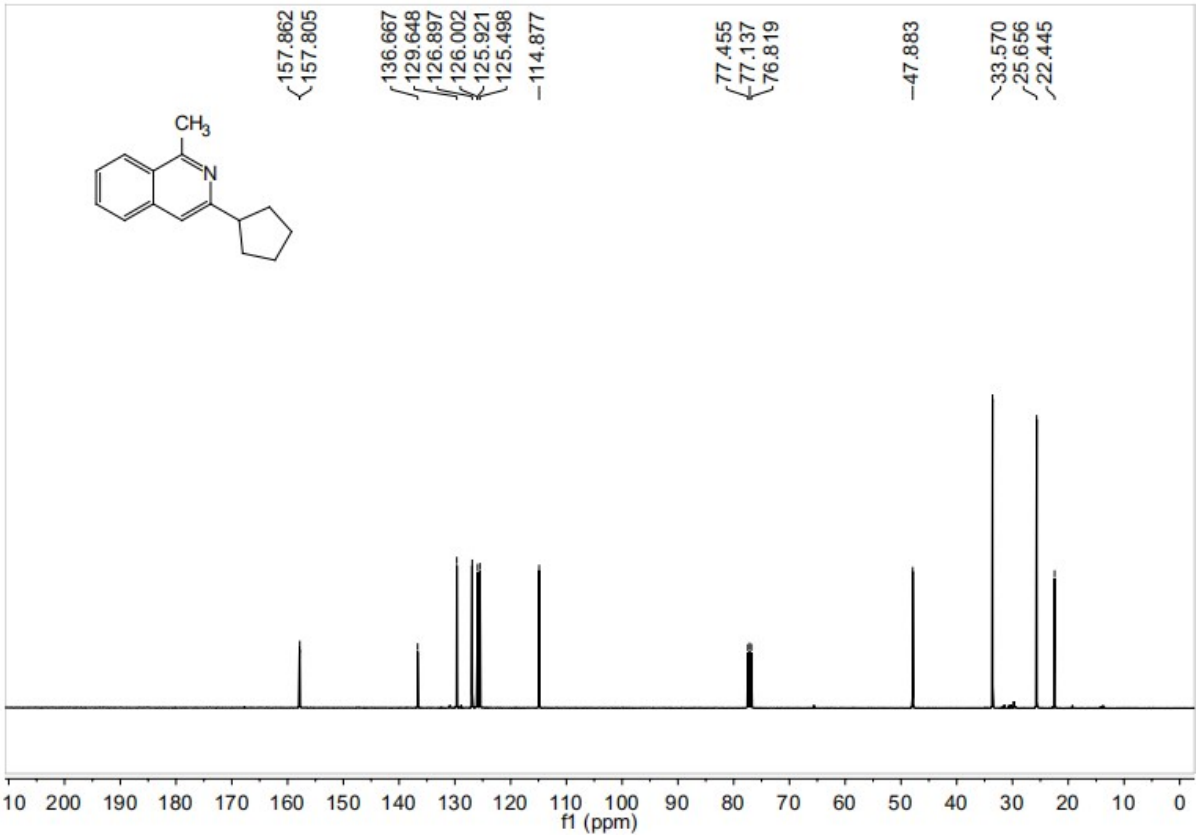
1.02
1.00
1.00
0.99
1.04
3.00
2.06
6.29
f1 (ppm)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126.002
125.921
125.498
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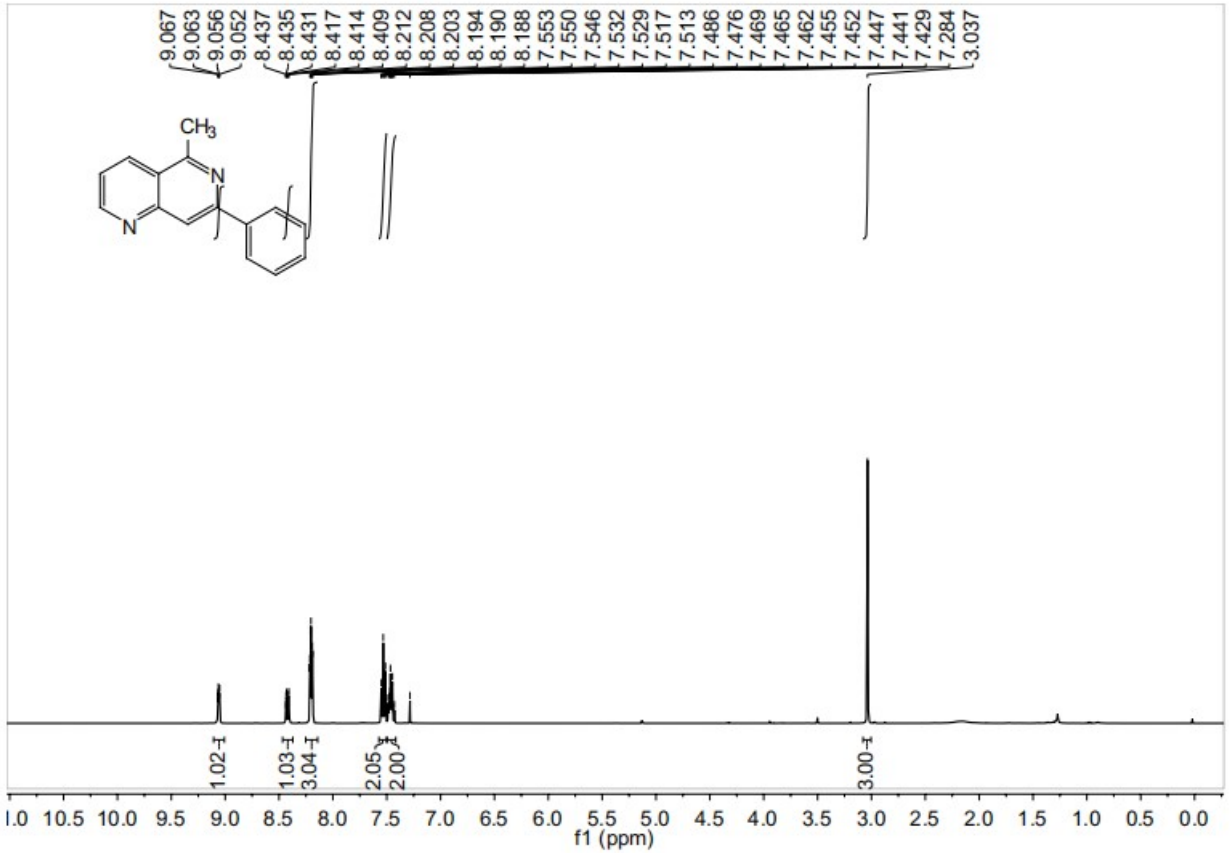
77.137
76.819
47.883
33.570
25.656
22.445
CH3
N
f1 (ppm)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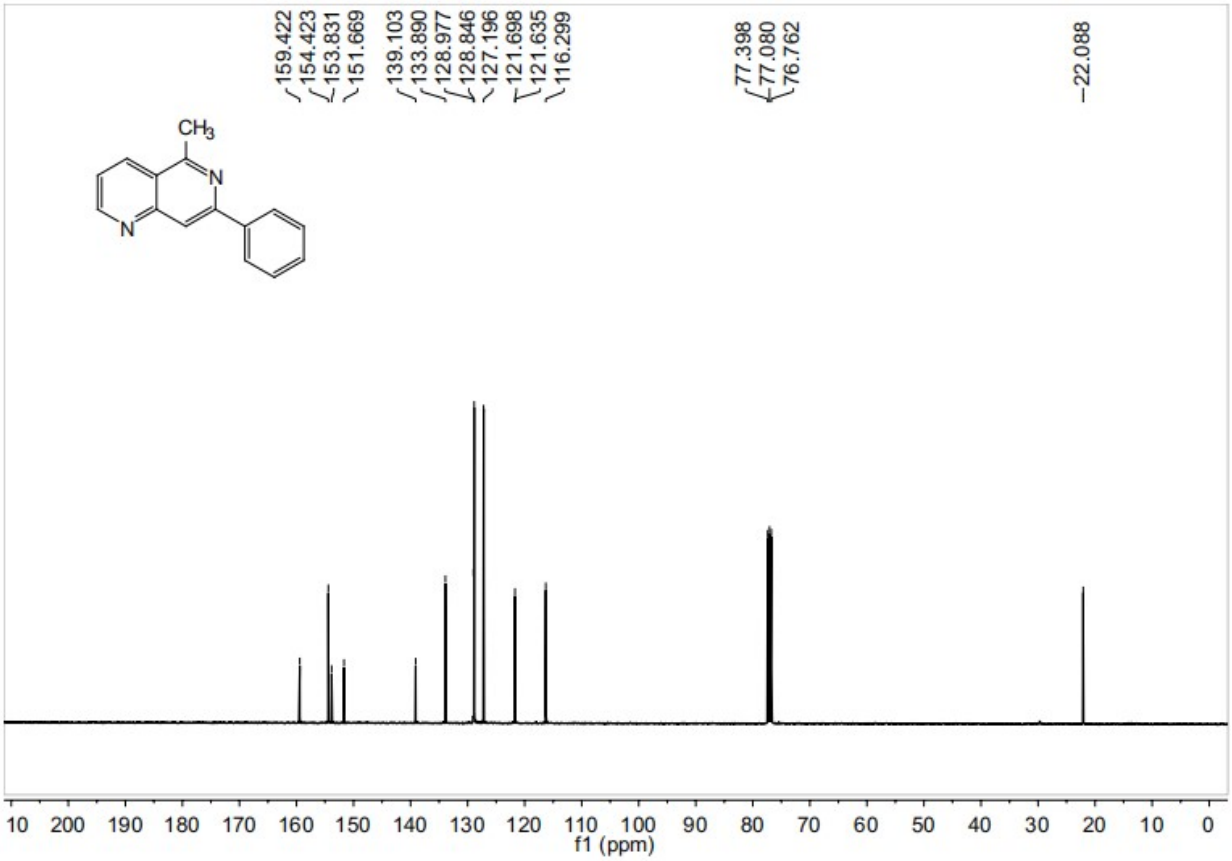
9.056
9.052
8.437
8.435
8.431
8.417
8.414
8.409
8.212
8.208
8.203
8.194
8.190
8.188
7.553
7.550
7.546
7.532
7.529
7.517
7.513
7.486
7.476
7.469
7.465
7.462
7.455
7.452
7.447
7.441
7.429
7.284
3.037
CH3
N
N
1.02
1.03
3.04
2.05
2.00
3.00
f1 (ppm)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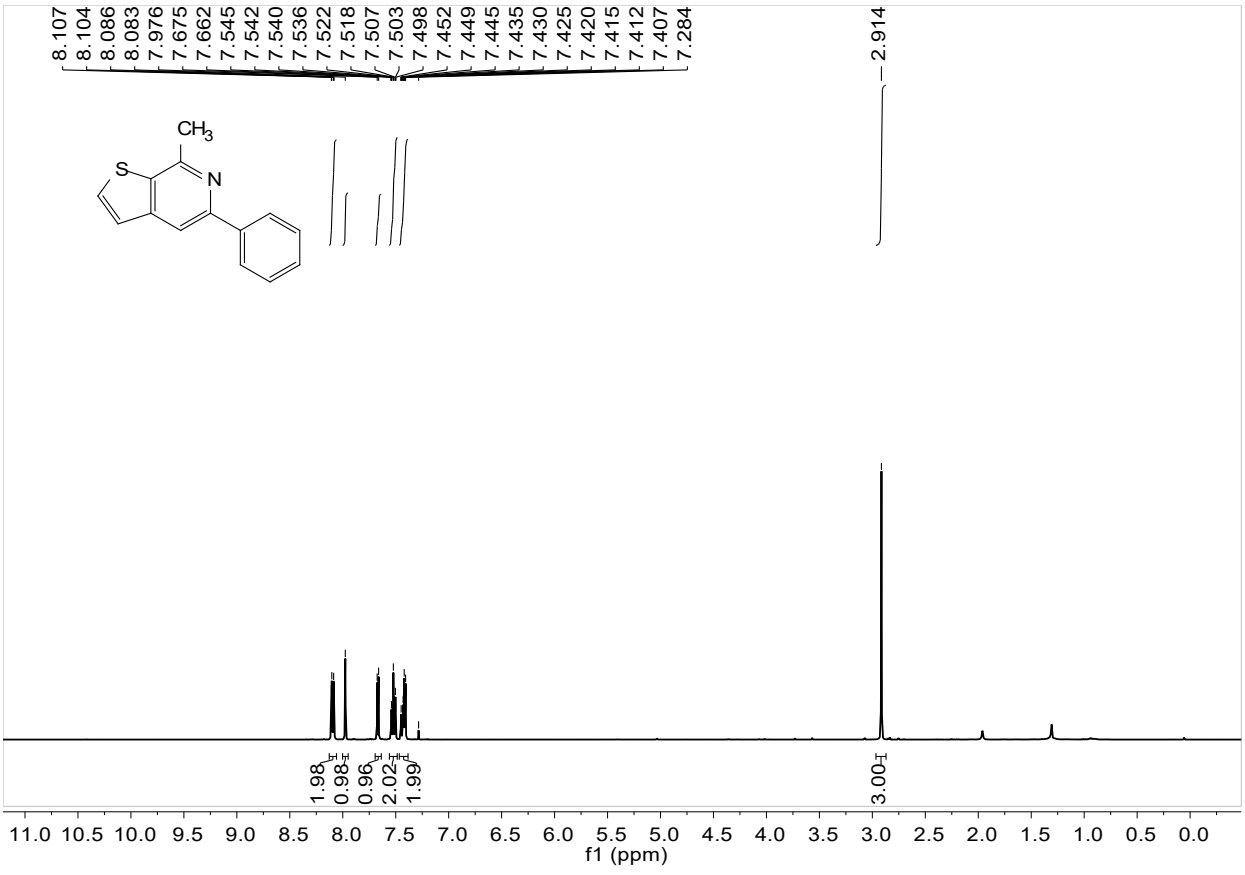
133.890
128.977
128.846
127.196
121.698
121.635
116.299
77.398
77.080
76.762
22.088
CH3
N
N
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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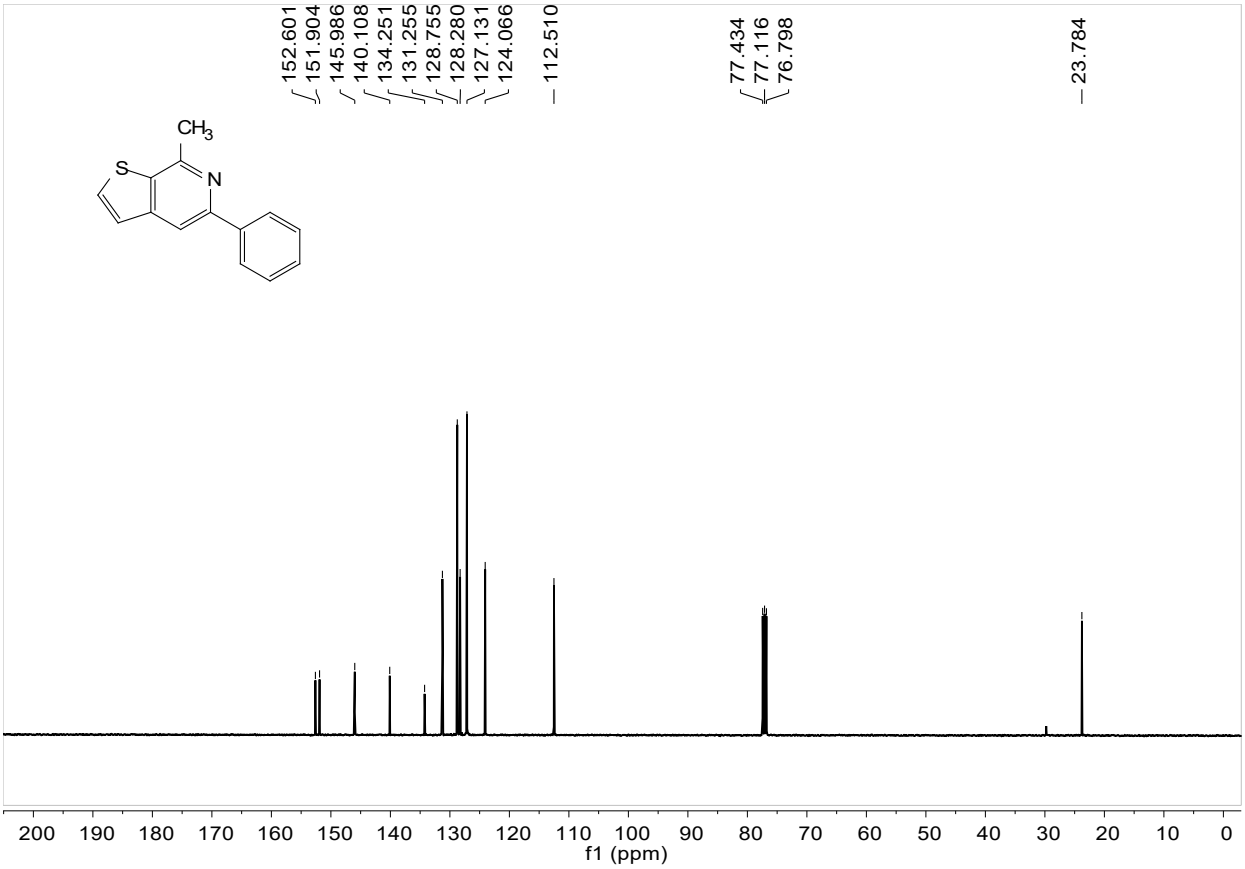
8.083
7.976
7.675
7.662
7.545
7.542
7.540
7.536
7.522
7.518
7.507
7.503
7.498
7.452
7.449
7.445
7.435
7.430
7.425
7.420
7.415
7.412
7.407
7.284
2.914
CH3
S
N
1.98
0.98
0.96
2.02
1.99
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.131
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112.510
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23.784
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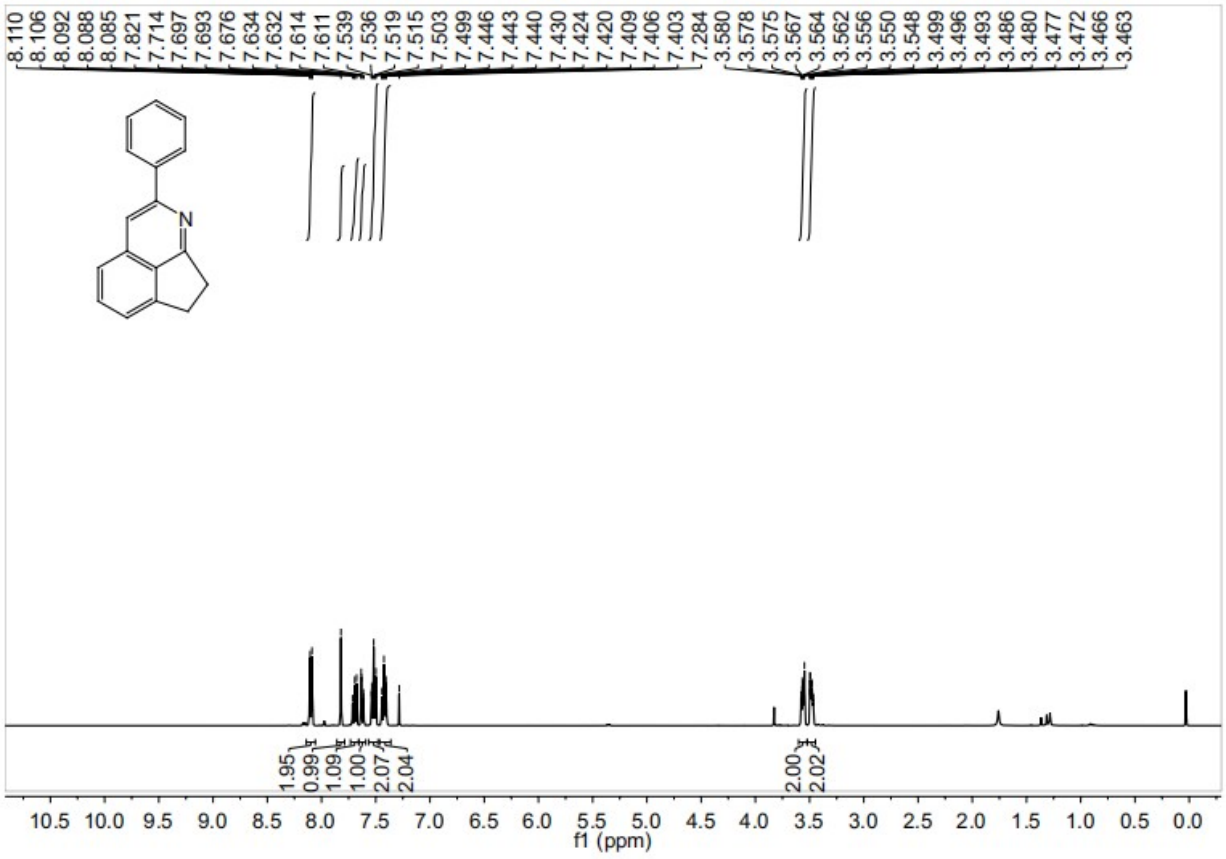
S
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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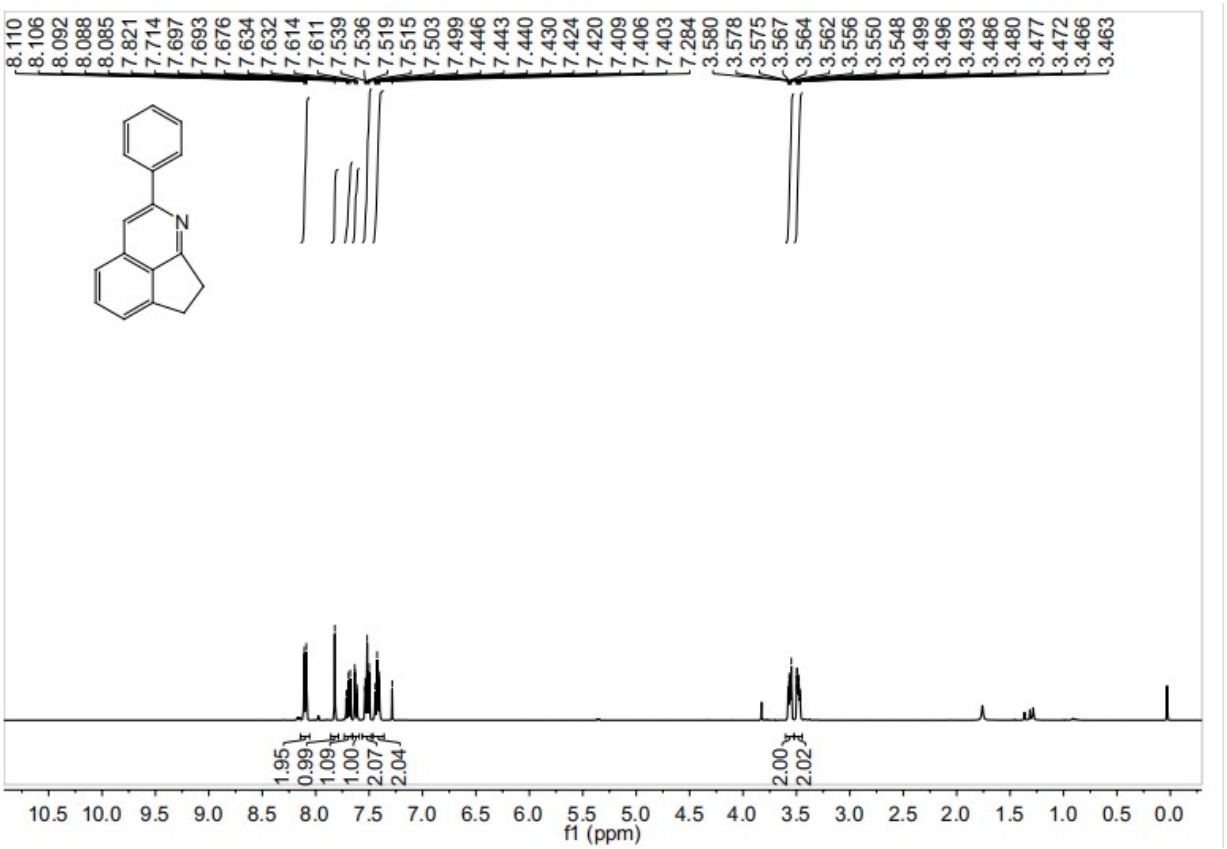
8.092
8.088
8.085
7.821
7.714
7.697
7.693
7.676
7.634
7.632
7.614
7.611
7.539
7.536
7.519
7.515
7.503
7.499
7.446
7.443
7.440
7.430
7.424
7.420
7.409
7.406
7.403
7.284
3.580
3.578
3.575
3.567
3.564
3.562
3.556
3.550
3.548
3.499
3.496
3.493
3.486
3.480
3.477
3.472
3.466
3.463
N
1.95
0.99
1.09
1.00
2.07
2.04
2.00
2.02
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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8.106
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8.088
8.085
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7.614
7.611
7.539
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7.515
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7.499
7.446
7.443
7.440
7.430
7.424
7.420
7.409
7.406
7.403
7.284
3.580
3.578
3.575
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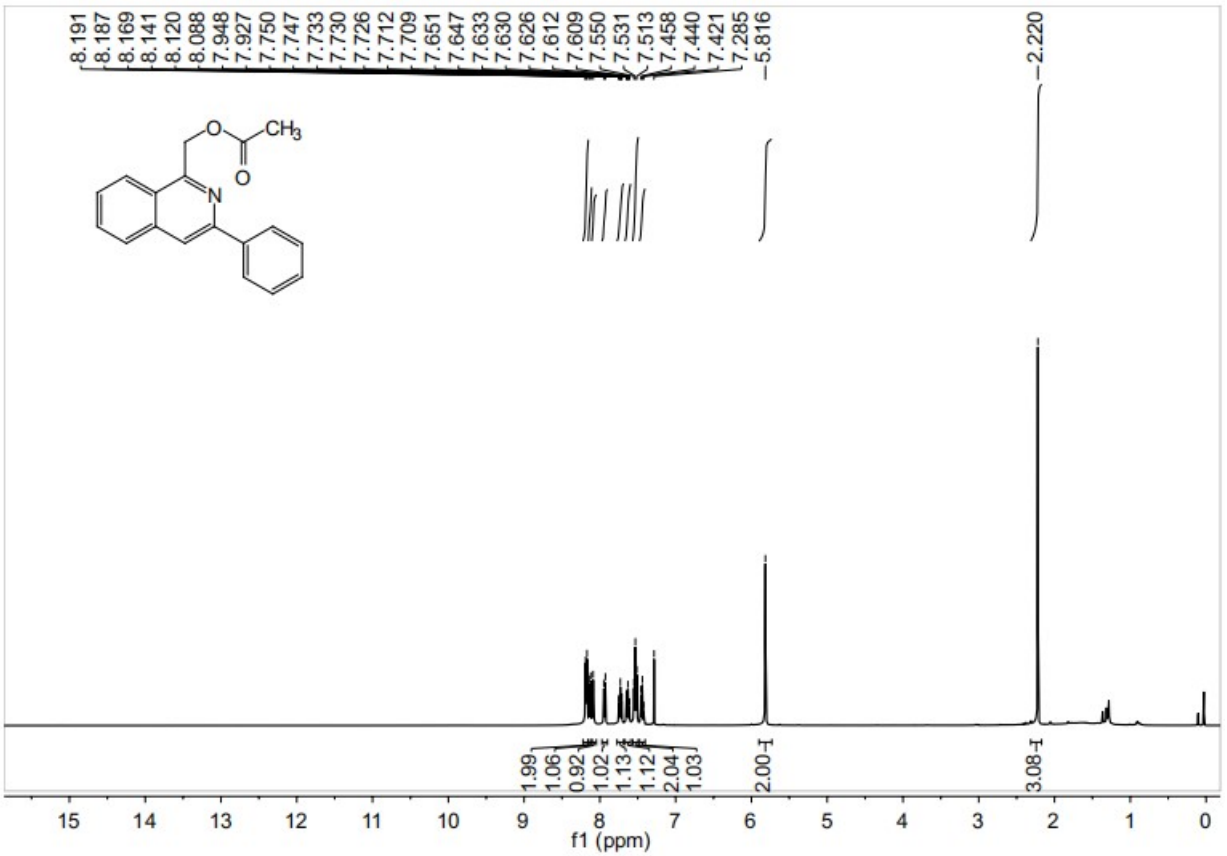
3.562
3.556
3.550
3.548
3.499
3.496
3.493
3.486
3.480
3.477
3.472
3.466
3.463
N
1.95
0.99
1.09
1.00
2.07
2.04
2.00
2.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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7.927
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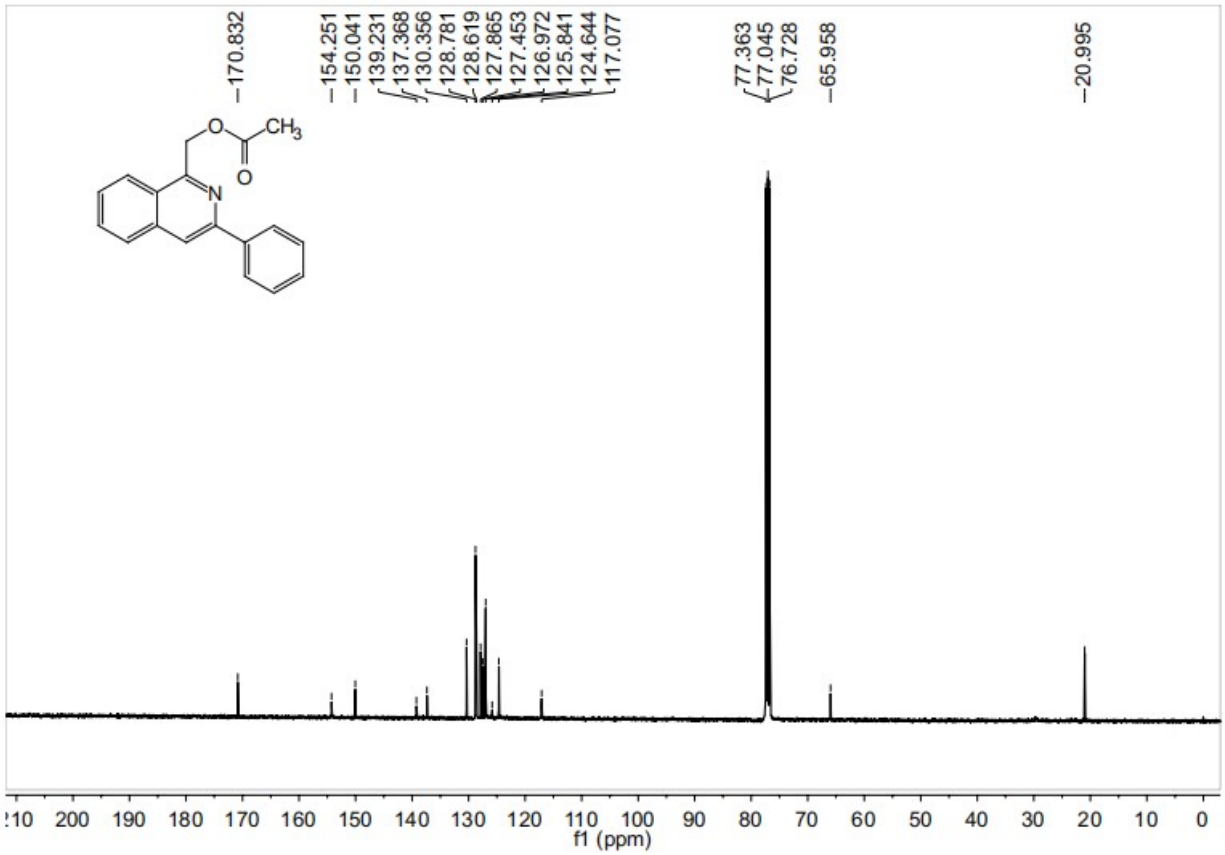
7.726
7.712
7.709
7.651
7.647
7.633
7.630
7.626
7.612
7.609
7.550
7.531
7.513
7.458
7.440
7.421
7.285
5.816
2.220
O
CH3
O
N
1.99
1.06
0.92
1.02
1.13
1.12
2.04
1.03
2.00
3.08
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)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130.356
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124.644
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77.363
77.045
76.728
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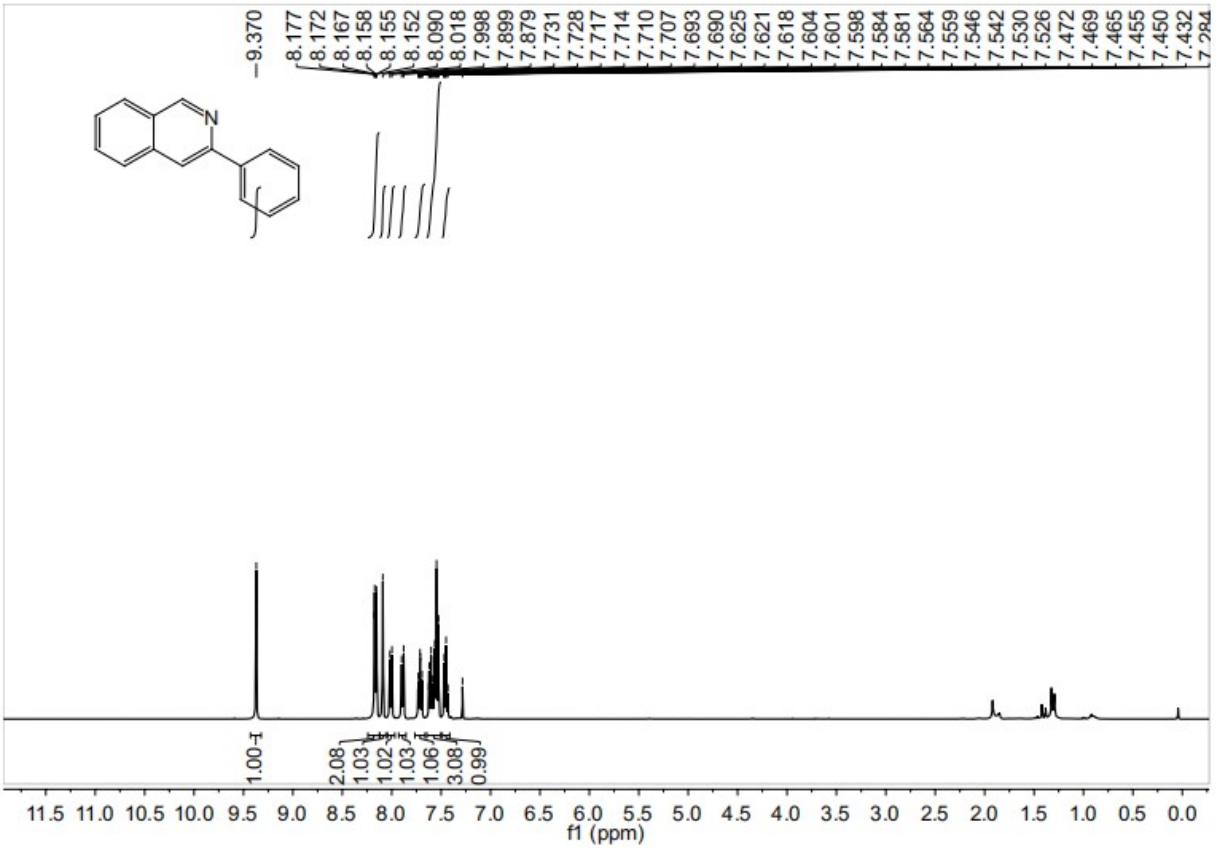
20.995
O
CH3
O
N
f1 (ppm)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8.090
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7.731
7.728
7.717
7.714
7.710
7.707
7.693
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7.625
7.621
7.618
7.604
7.601
7.598
7.584
7.581
7.564
7.559
7.546
7.542
7.530
7.526
7.472
7.469
7.465
7.455
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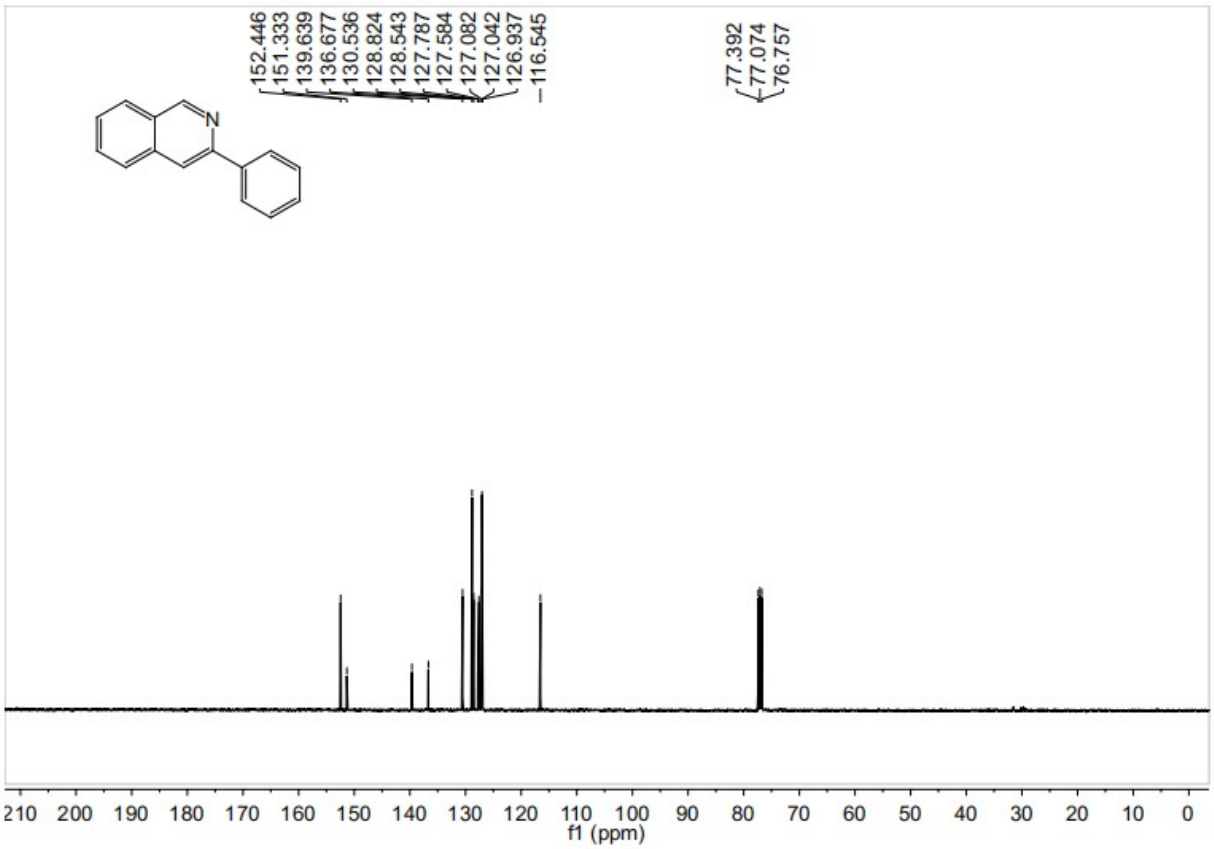
1.03
1.02
1.03
1.06
3.08
0.99
f1 (ppm)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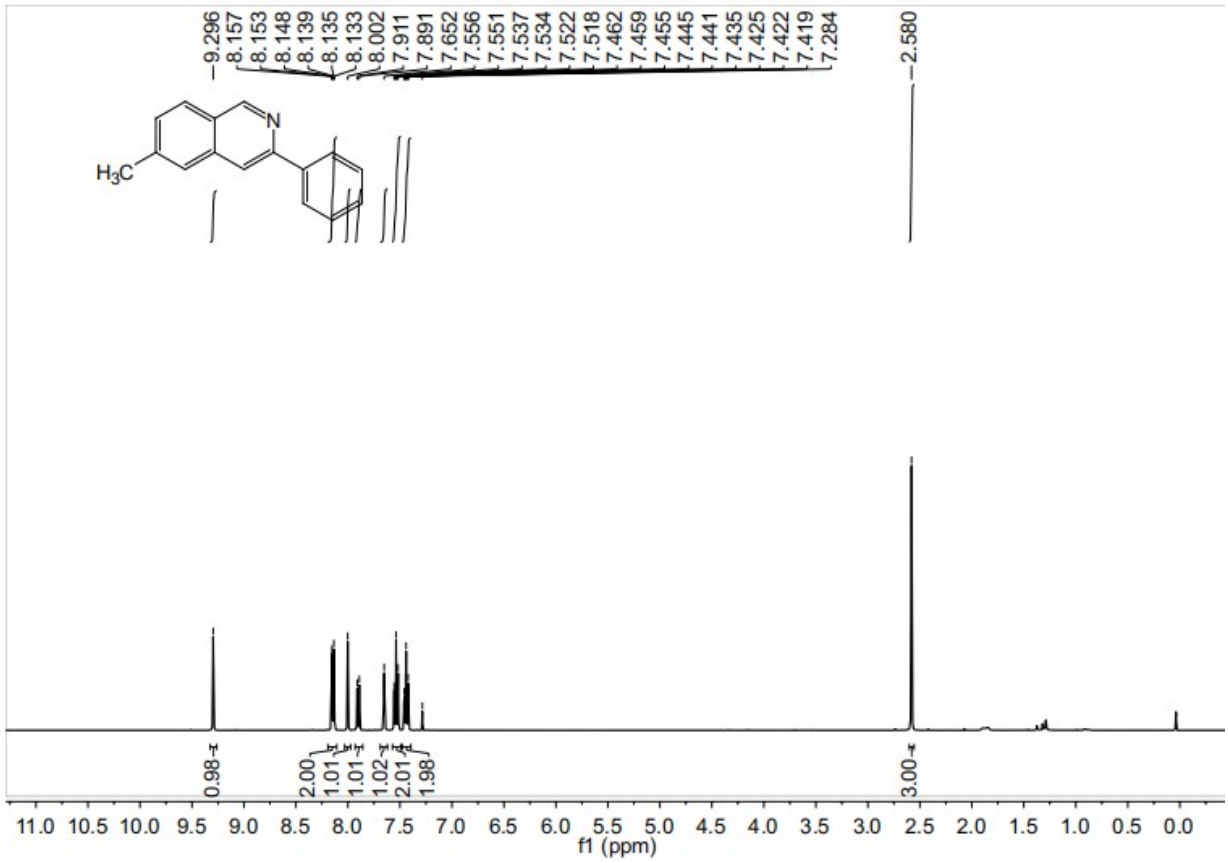
77.392
77.074
76.757
N
f1 (ppm)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7.891
7.652
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7.537
7.534
7.522
7.518
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7.459
7.455
7.445
7.441
7.435
7.425
7.422
7.419
7.284
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N
H3C
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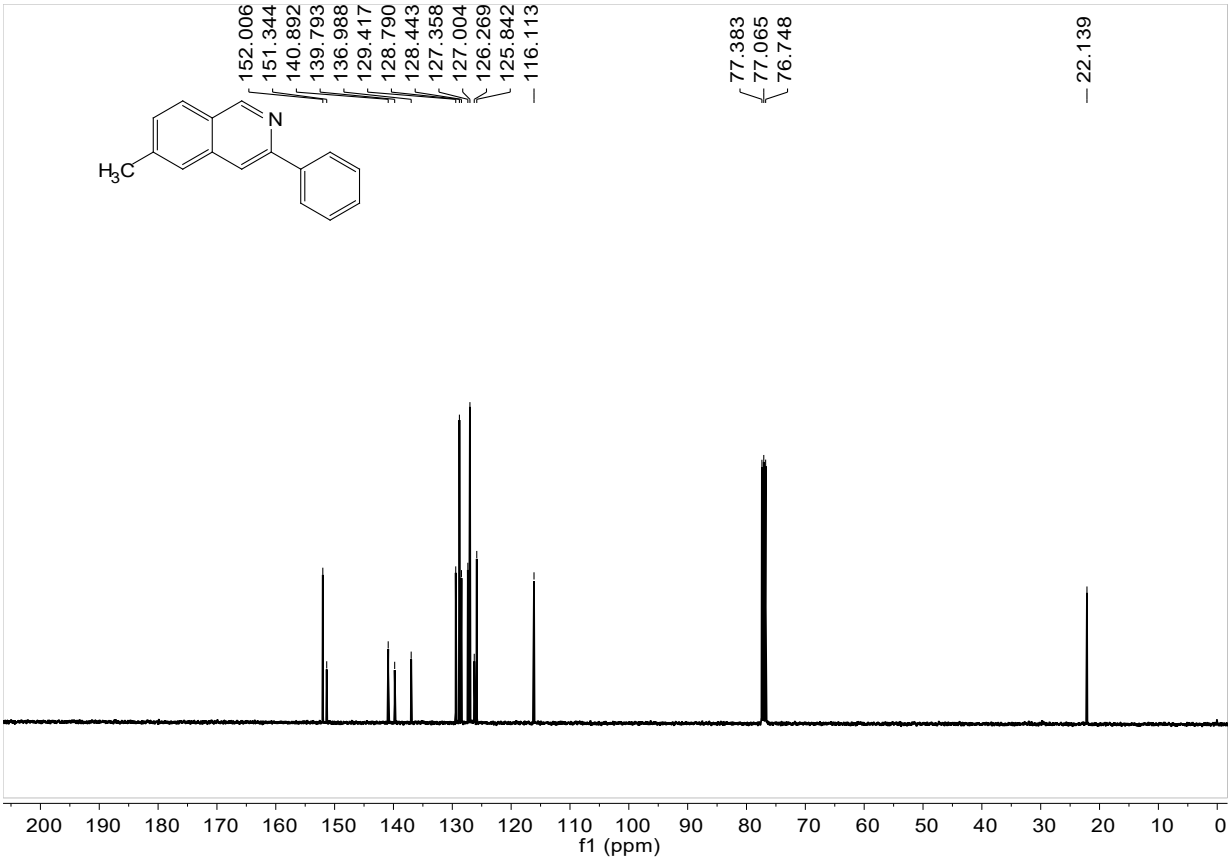
1.01
1.01
1.02
2.01
1.98
3.00
f1 (ppm)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127.358
127.004
126.269
125.842
116.113
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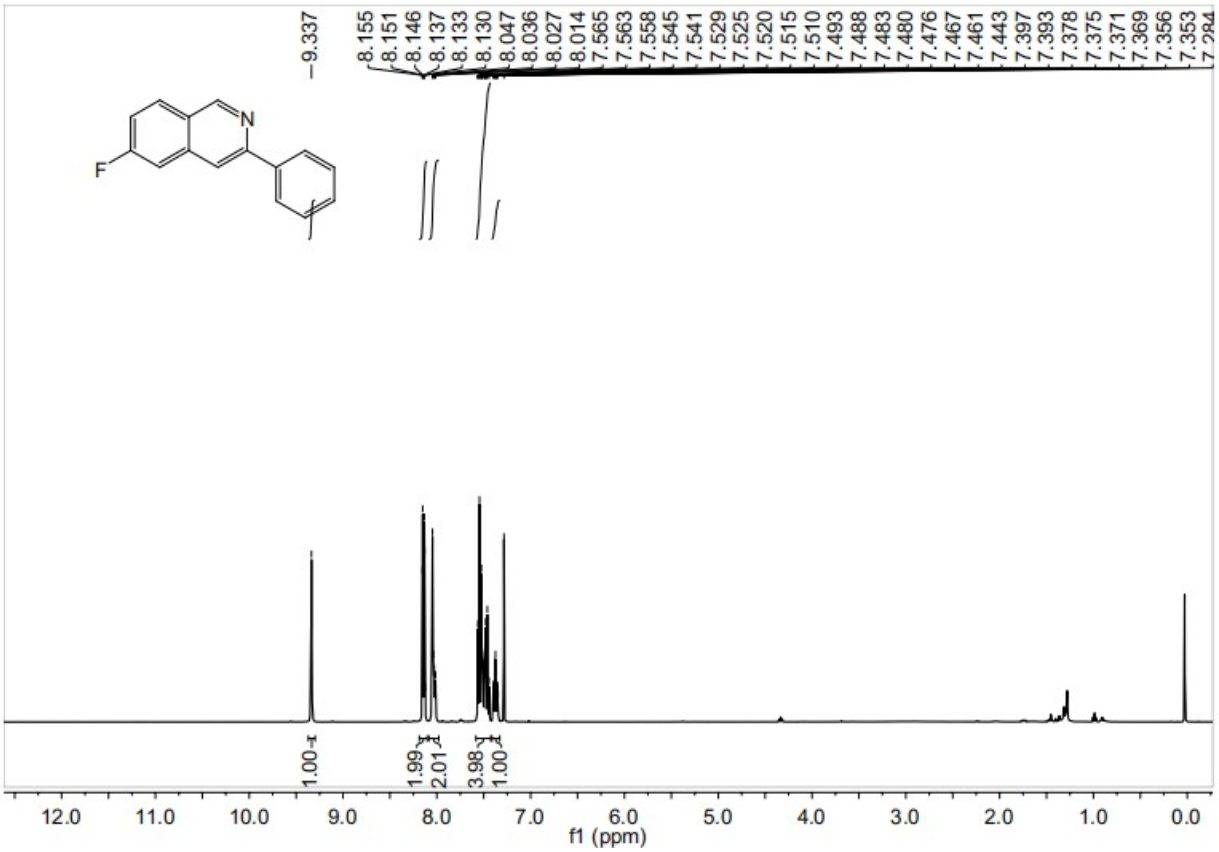
77.065
76.748
22.139
N
H3C
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.563
7.558
7.545
7.541
7.529
7.525
7.520
7.515
7.510
7.493
7.488
7.483
7.480
7.476
7.467
7.461
7.443
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7.393
7.378
7.375
7.371
7.369
7.356
7.353
N
F
1.00
1.99
2.01
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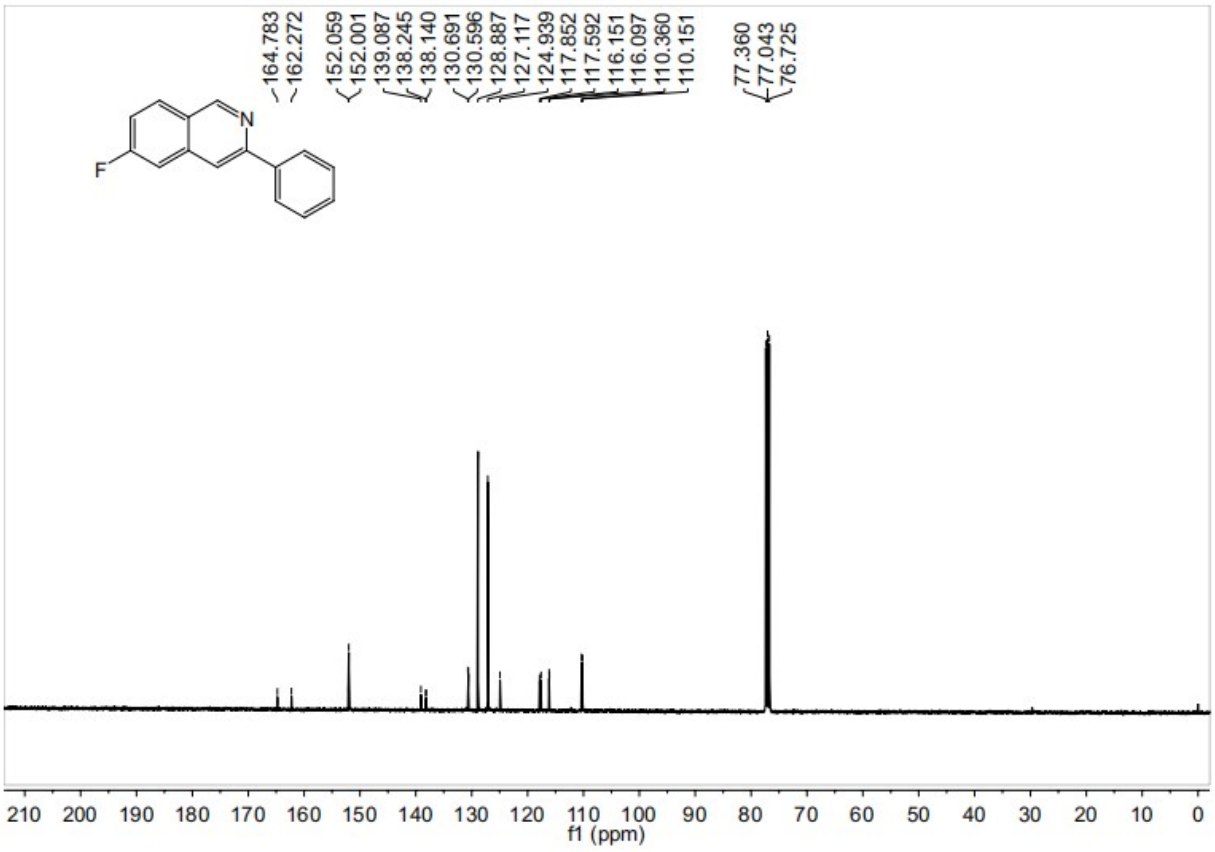
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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152.001
139.087
138.245
138.140
130.691
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128.887
127.117
124.939
117.852
117.592
116.151
116.097
110.360
110.151
77.360
77.043
76.725
N
F
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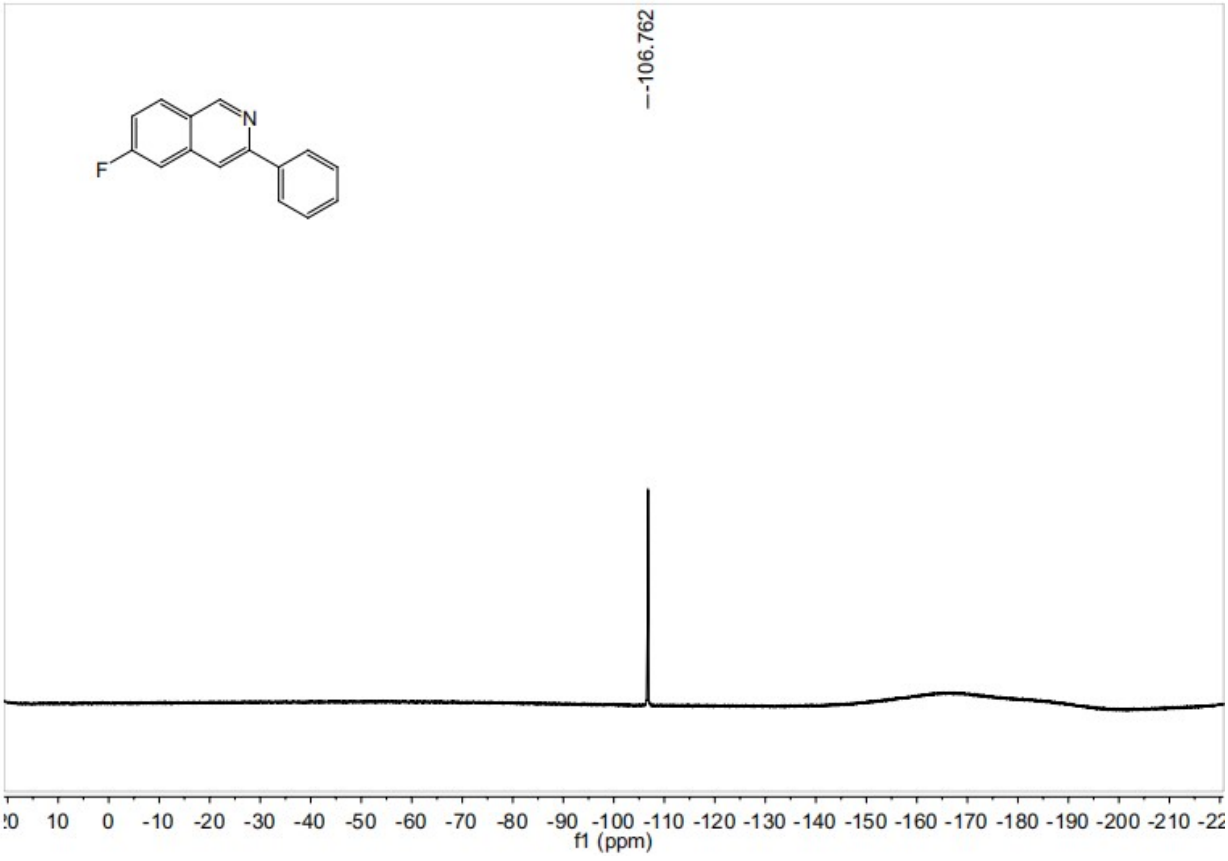
f1 (ppm)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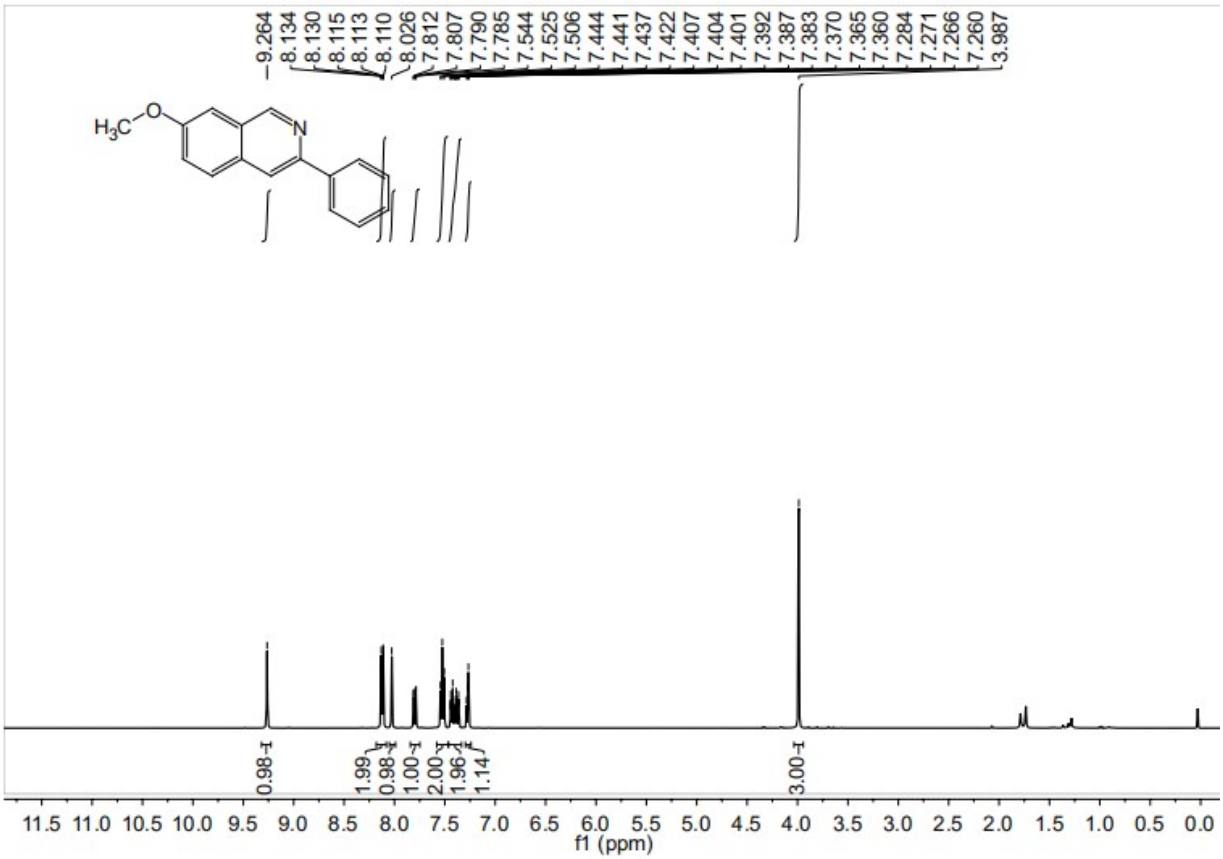
f1 (ppm)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8.134
8.130
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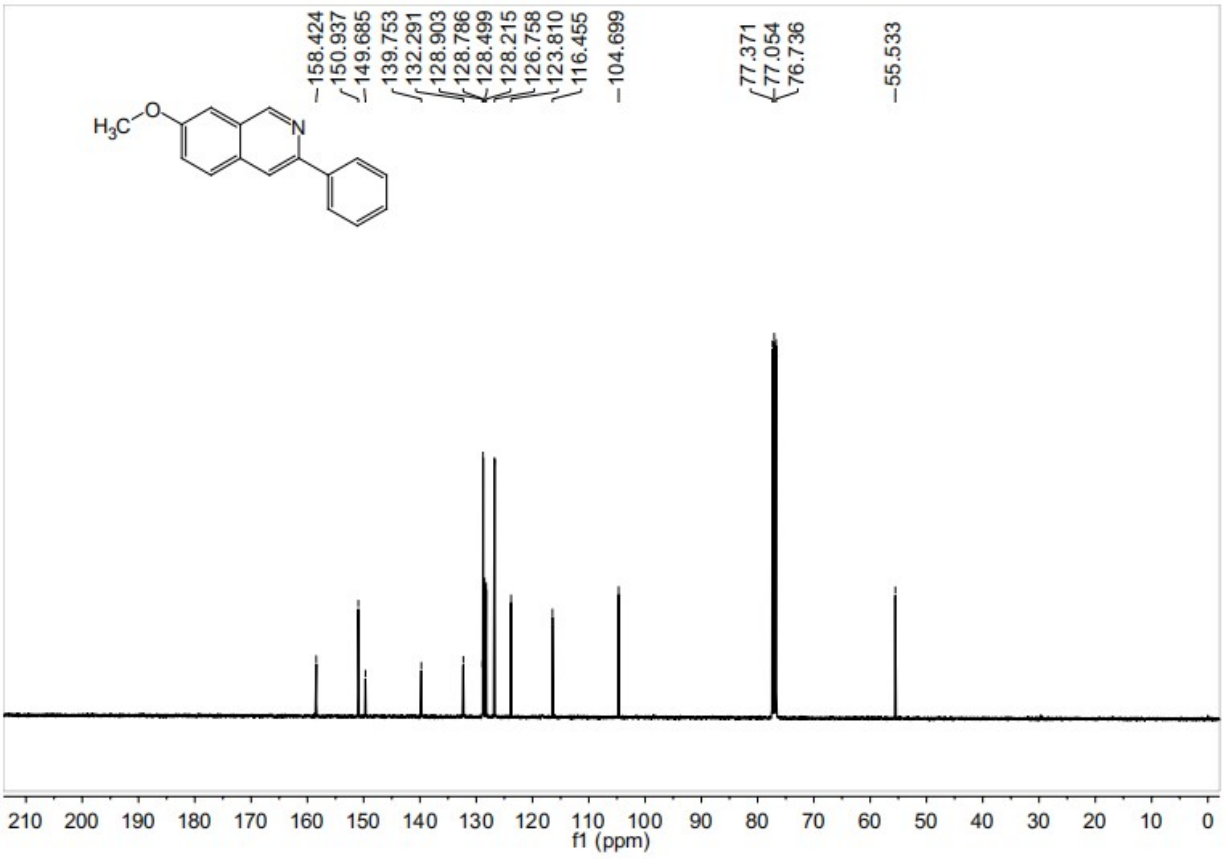
8.110
8.026
7.812
7.807
7.790
7.785
7.544
7.525
7.506
7.444
7.441
7.437
7.422
7.407
7.404
7.401
7.392
7.387
7.383
7.370
7.365
7.360
7.284
7.271
7.266
7.260
3.987
H3C
O
N
0.98
1.99
0.98
1.00
2.00
1.96
1.14
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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150.937
149.685
139.753
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128.786
128.499
128.215
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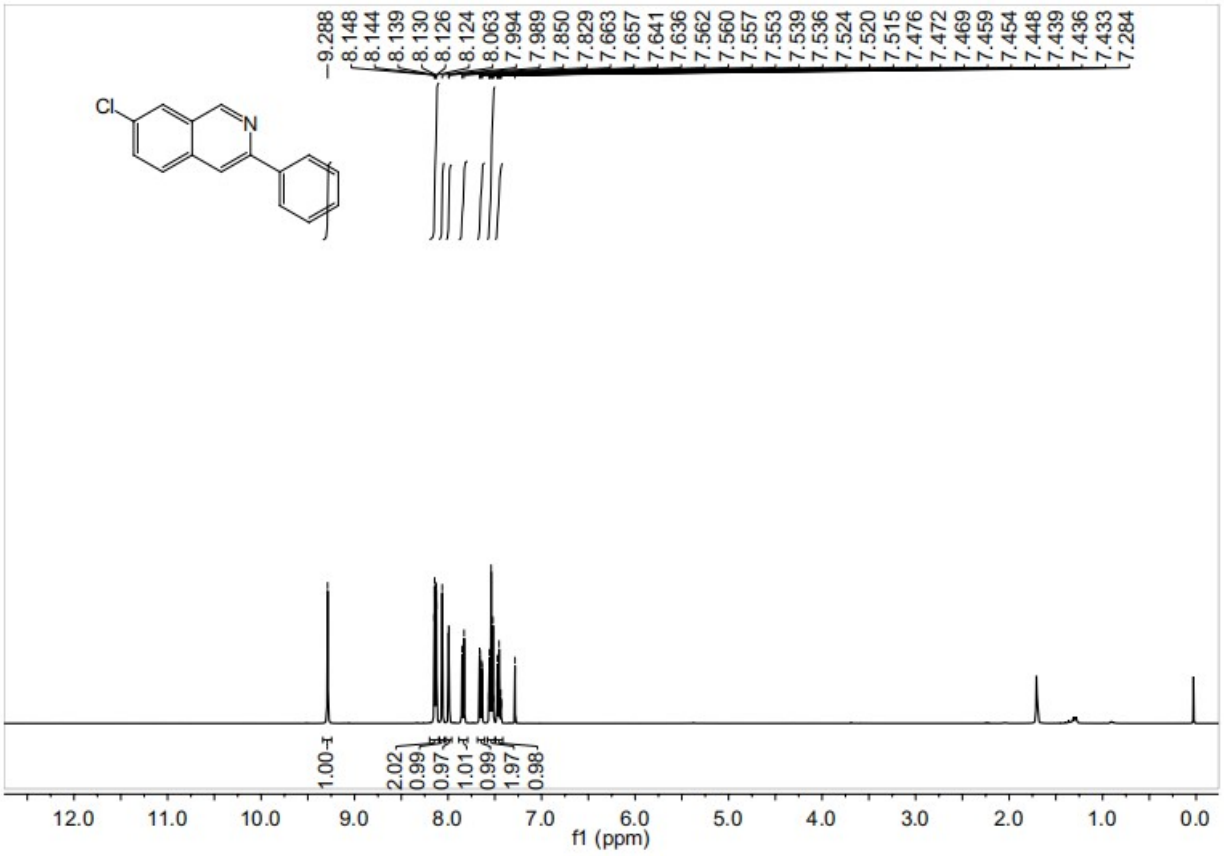
123.810
116.455
104.699
77.371
77.054
76.736
55.533
H3C
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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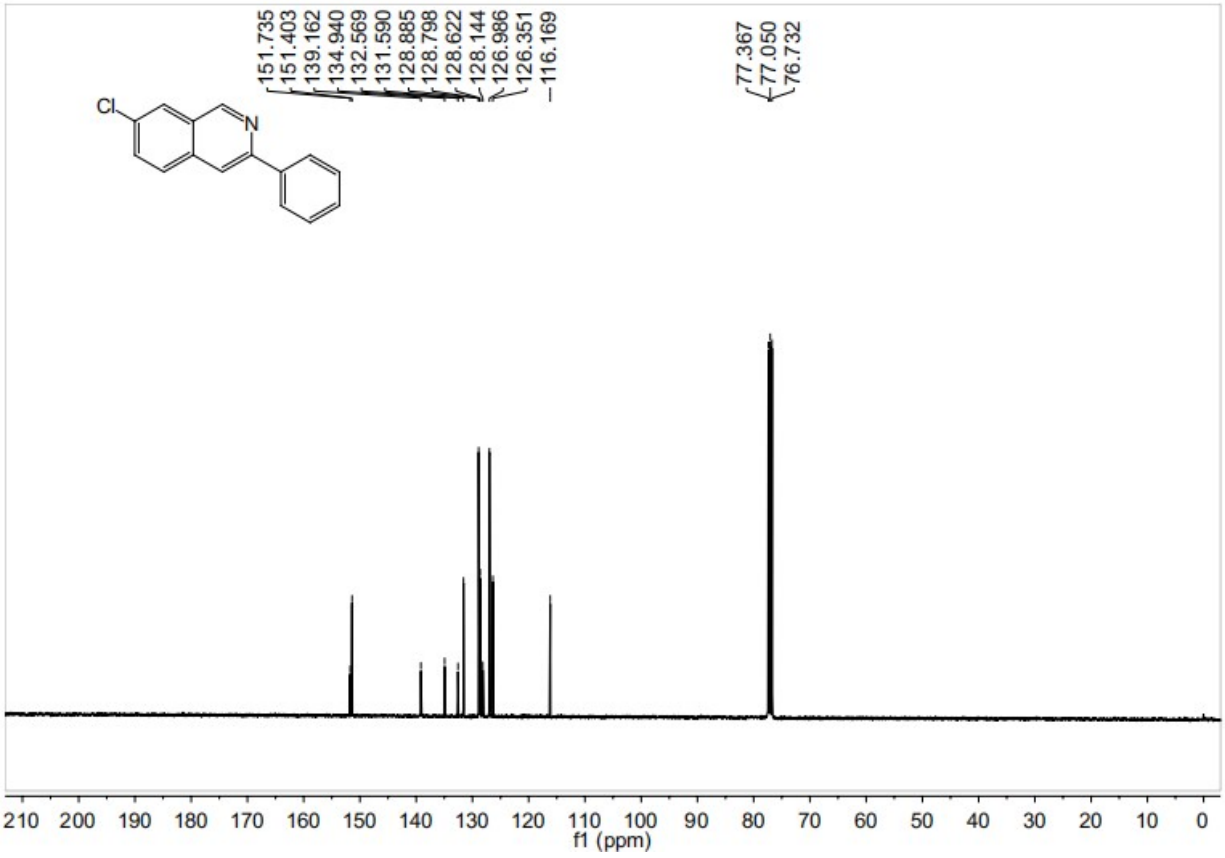
8.144
8.139
8.130
8.126
8.124
8.063
7.994
7.989
7.850
7.829
7.663
7.657
7.641
7.636
7.562
7.560
7.557
7.553
7.539
7.536
7.524
7.520
7.515
7.476
7.472
7.469
7.459
7.454
7.448
7.439
7.436
7.433
7.284
Cl
N
1.00
2.02
0.99
0.97
1.01
0.99
1.97
0.98
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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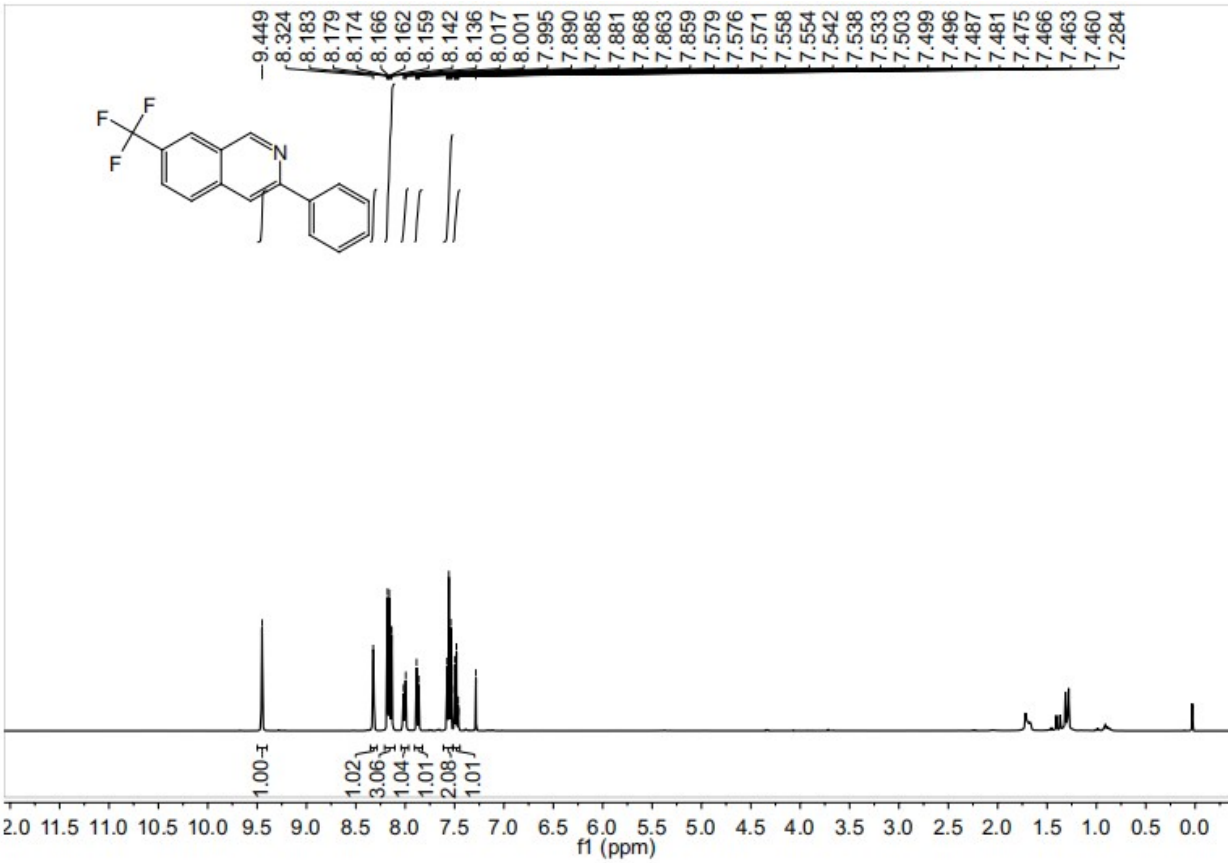
151.403
139.162
134.940
132.569
131.590
128.885
128.798
128.622
128.144
126.986
126.351
116.169
77.367
77.050
76.732
Cl
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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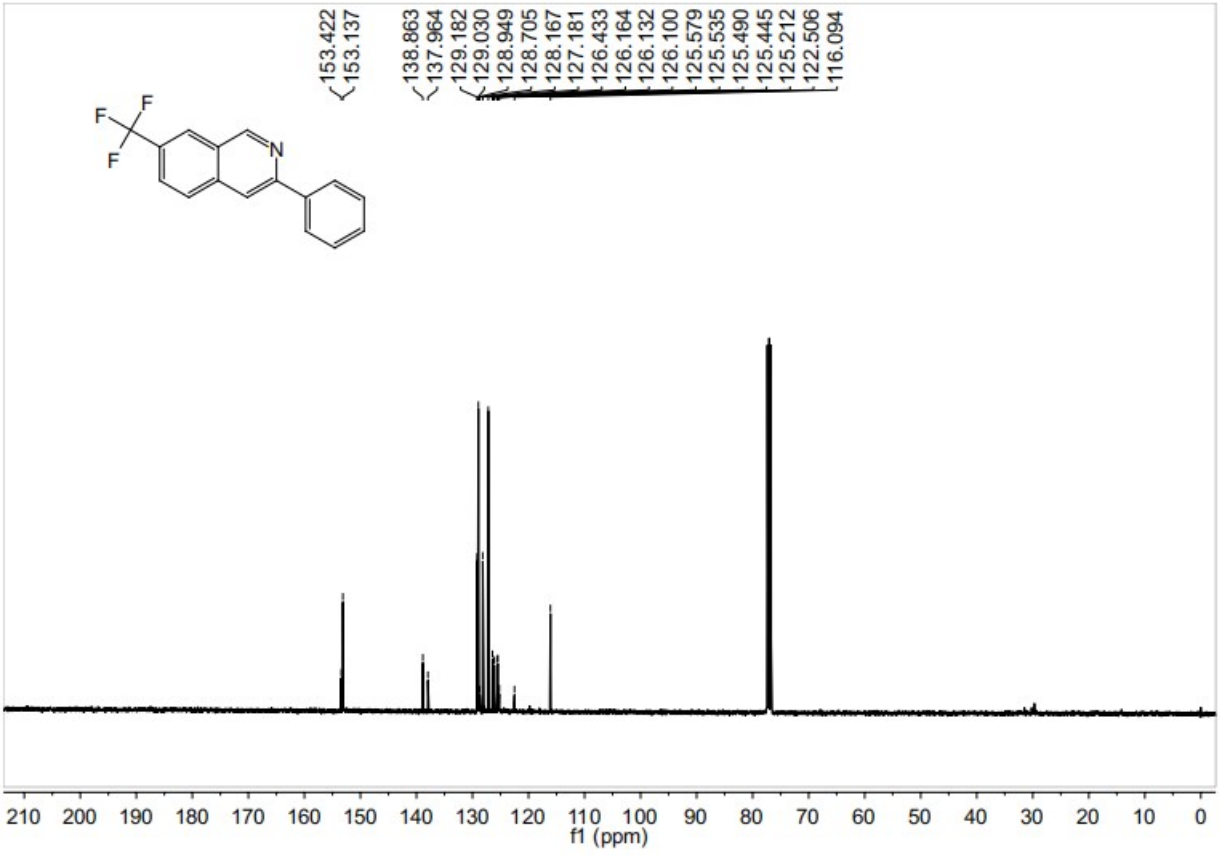
8.183
8.179
8.174
8.166
8.162
8.159
8.142
8.136
8.017
8.001
7.995
7.890
7.885
7.881
7.868
7.863
7.859
7.579
7.576
7.571
7.558
7.554
7.542
7.538
7.533
7.503
7.499
7.496
7.487
7.481
7.475
7.466
7.463
7.460
7.284
F
F
F
N
1.00
1.02
3.06
1.04
1.01
2.08
1.01
f1 (ppm)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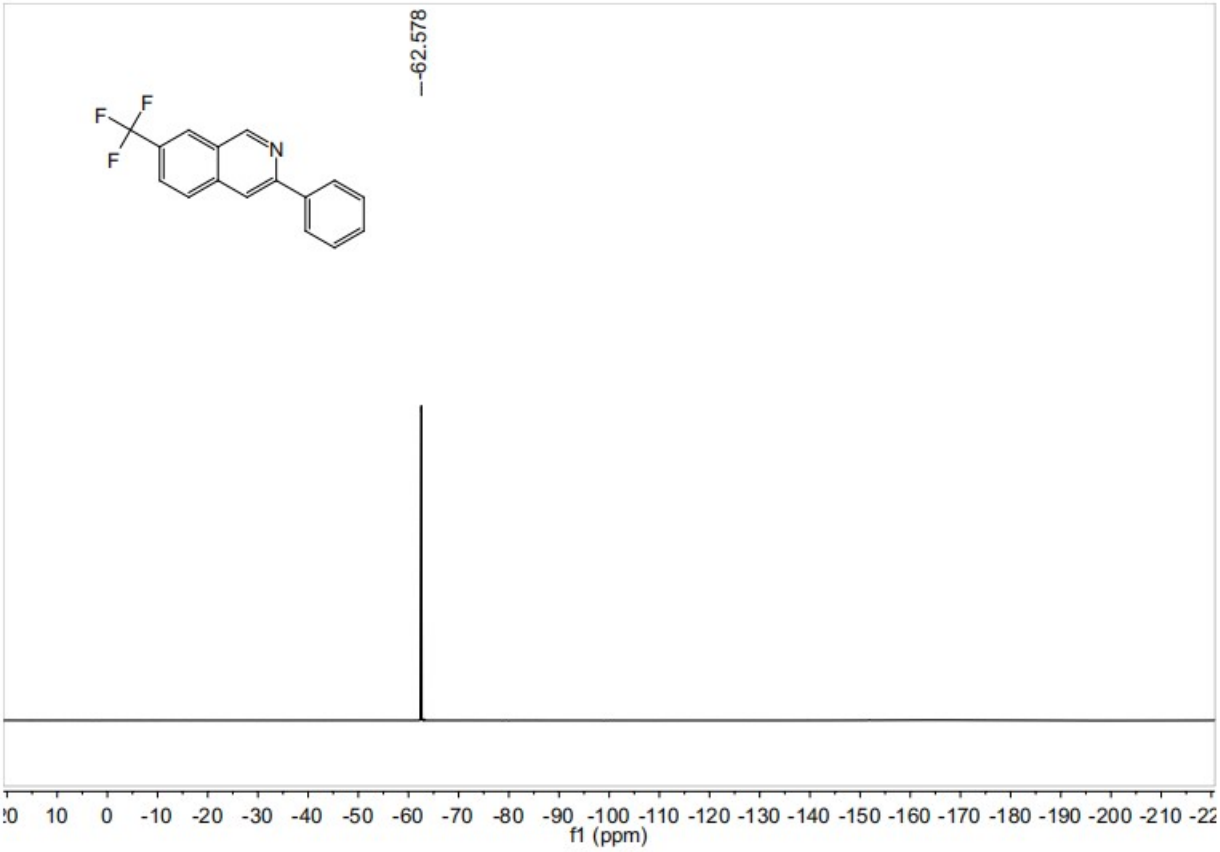
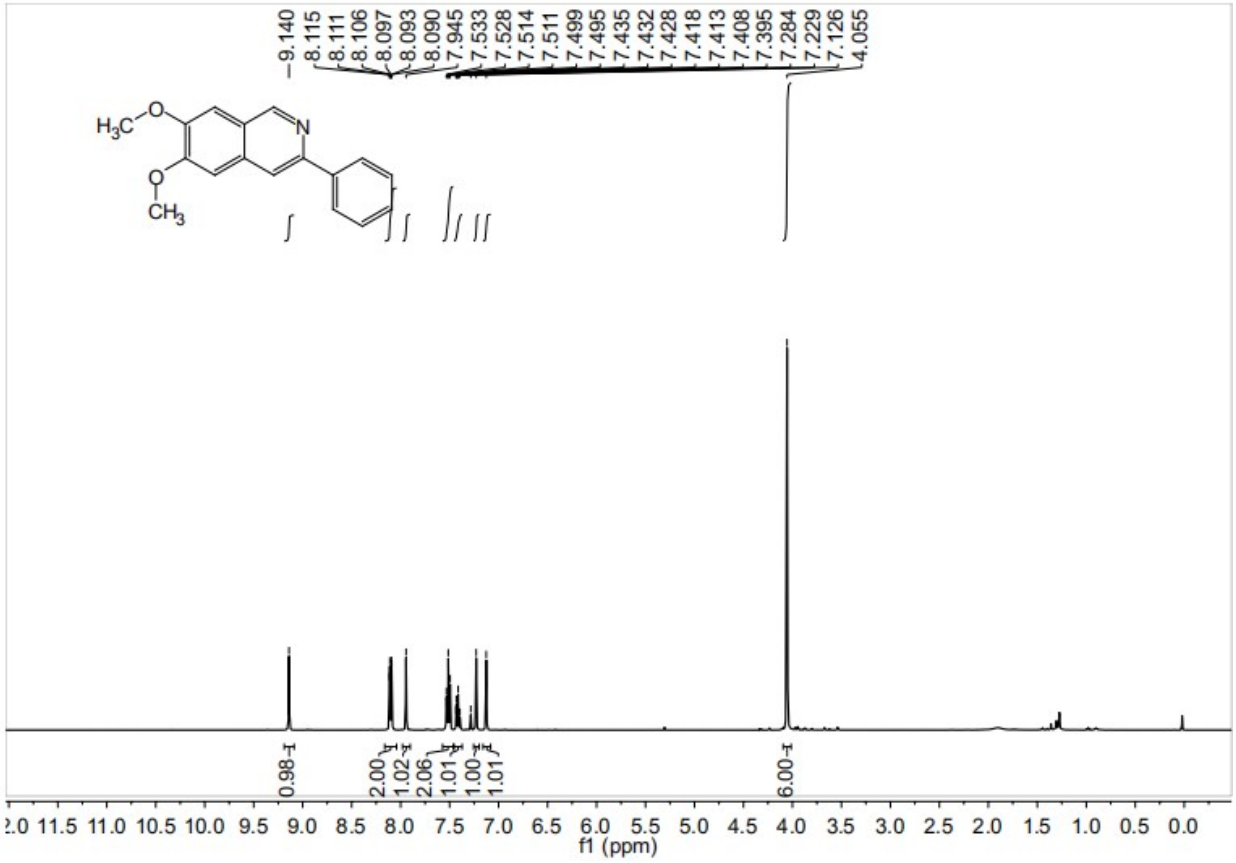
153.137
138.863
137.964
129.182
129.030
128.949
128.705
128.167
127.181
126.433
126.164
126.132
126.100
125.579
125.535
125.490
125.445
125.212
122.506
116.094
F
F
F
N
f1 (ppm)


-62.578
F
F
F
N
f1 (ppm)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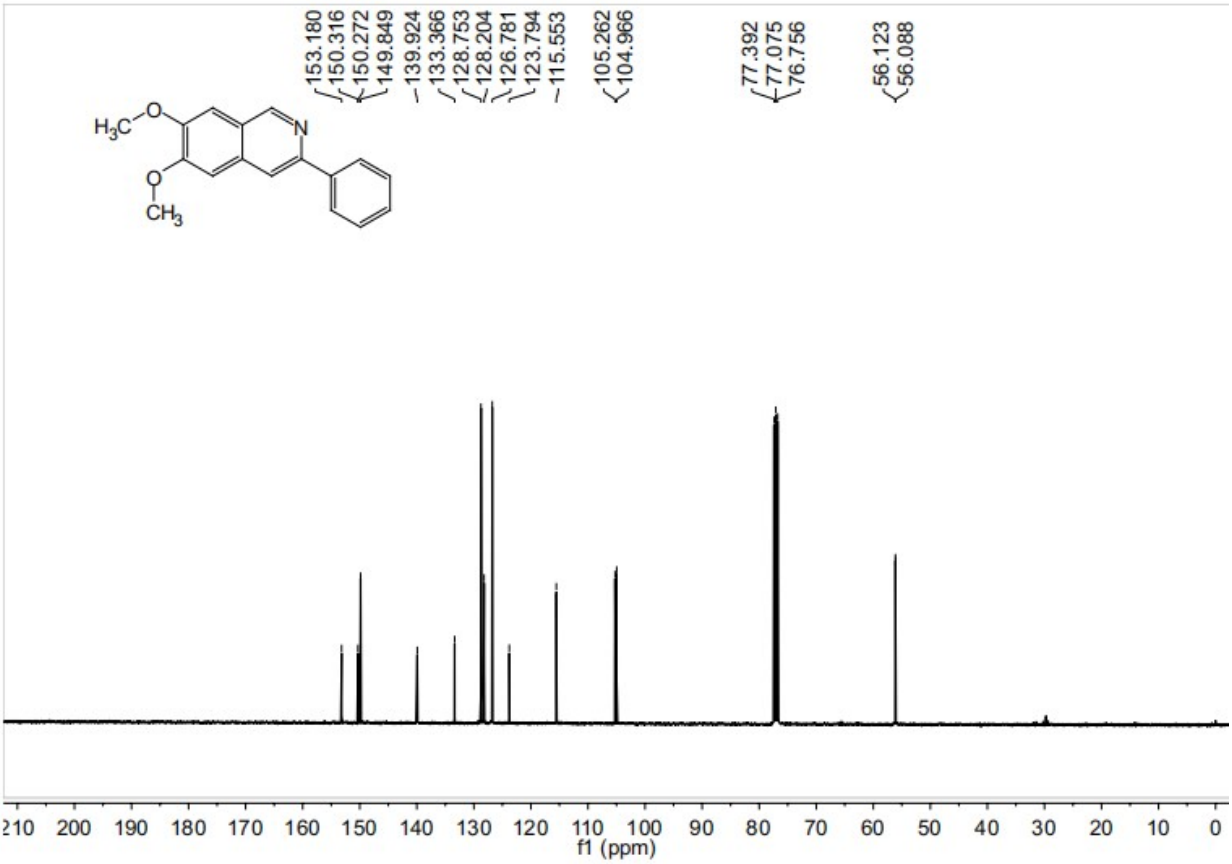
8.115
8.111
8.106
8.097
8.093
8.090
7.945
7.533
7.528
7.514
7.511
7.499
7.495
7.435
7.432
7.428
7.418
7.413
7.408
7.395
7.284
7.229
7.126
4.055
H3C
O
N
O
CH3
0.98
2.00
1.02
2.06
1.01
1.00
1.01
6.00
f1 (ppm)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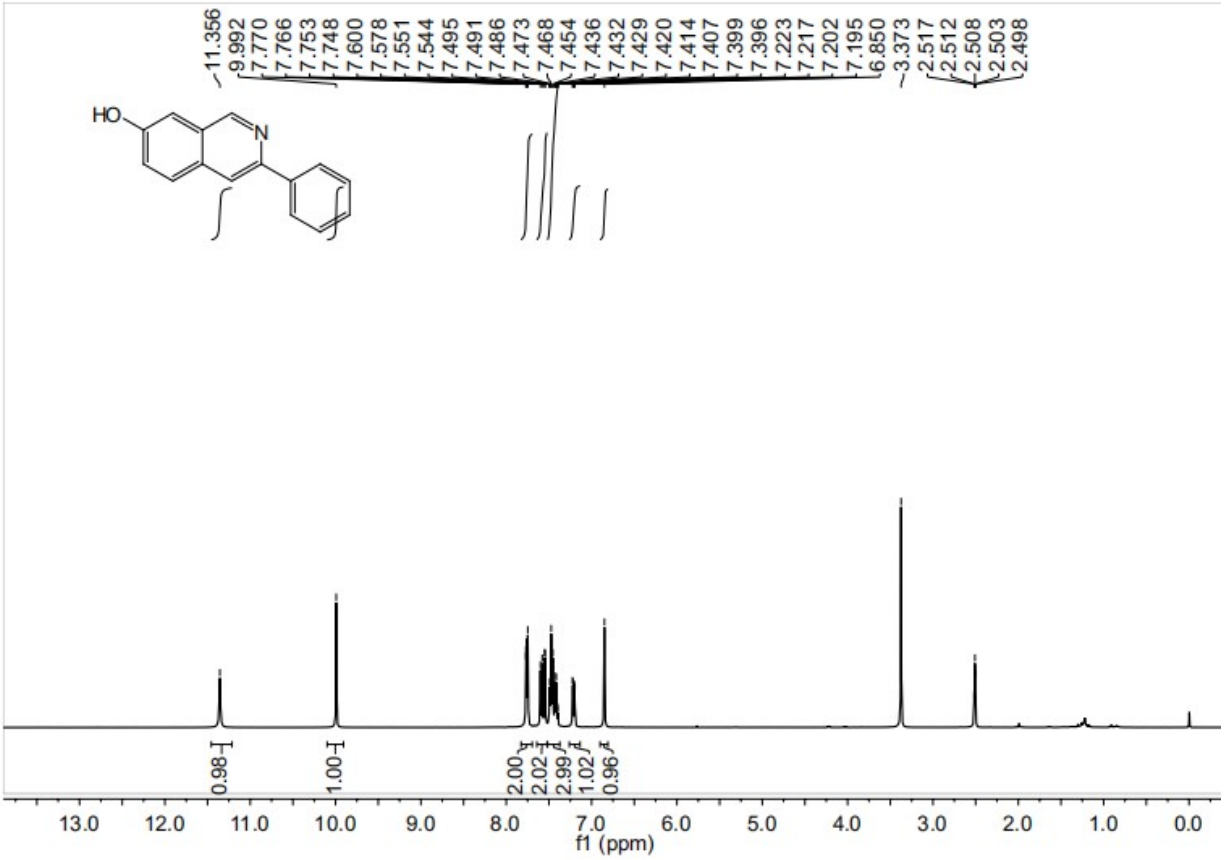
150.316
150.272
149.849
139.924
133.366
128.753
128.204
126.781
123.794
115.553
105.262
104.966
77.392
77.075
76.756
56.123
56.088
H3C
O
N
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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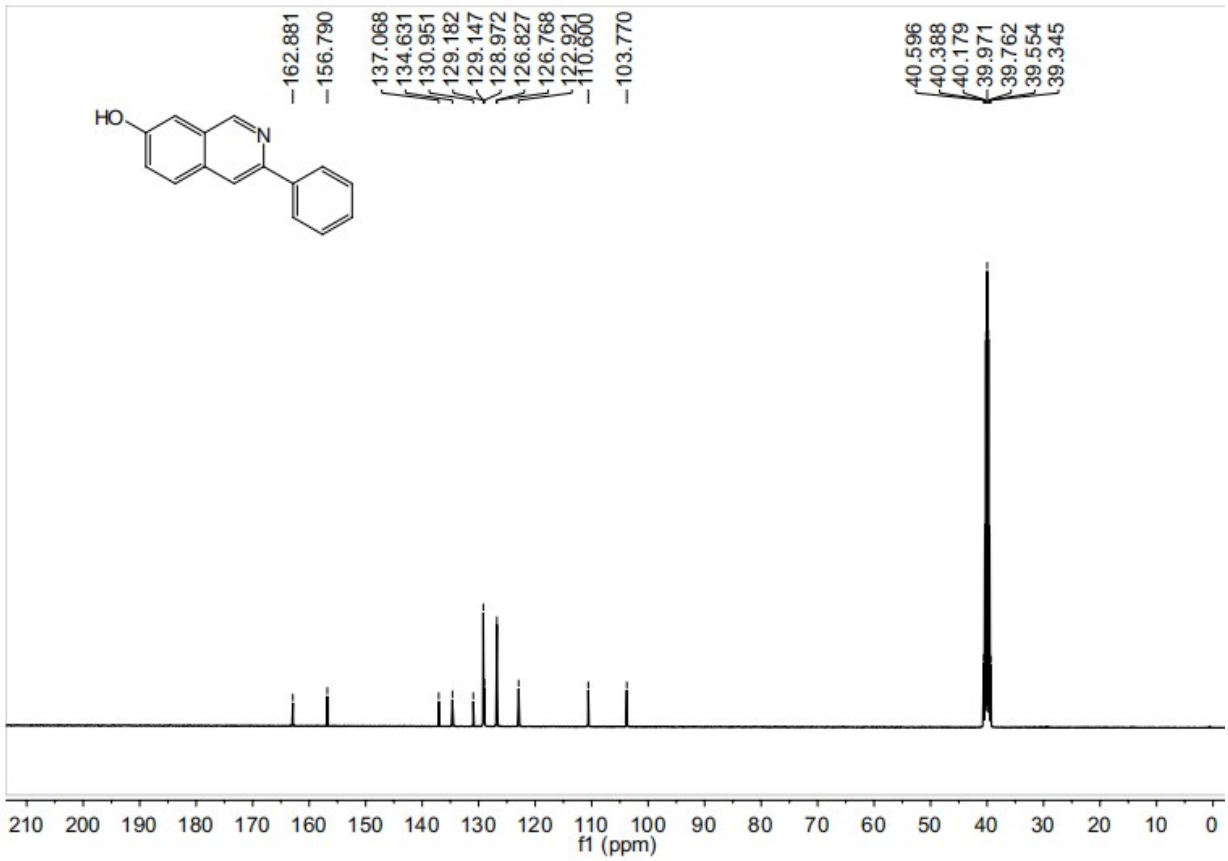
9.992
7.770
7.766
7.753
7.748
7.600
7.578
7.551
7.544
7.495
7.491
7.486
7.473
7.468
7.454
7.436
7.432
7.429
7.420
7.414
7.407
7.399
7.396
7.223
7.217
7.202
7.195
6.850
3.373
2.517
2.512
2.508
2.503
2.498
HO
N
0.98
1.00
2.00
2.02
2.99
1.02
0.96
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)


HO
N
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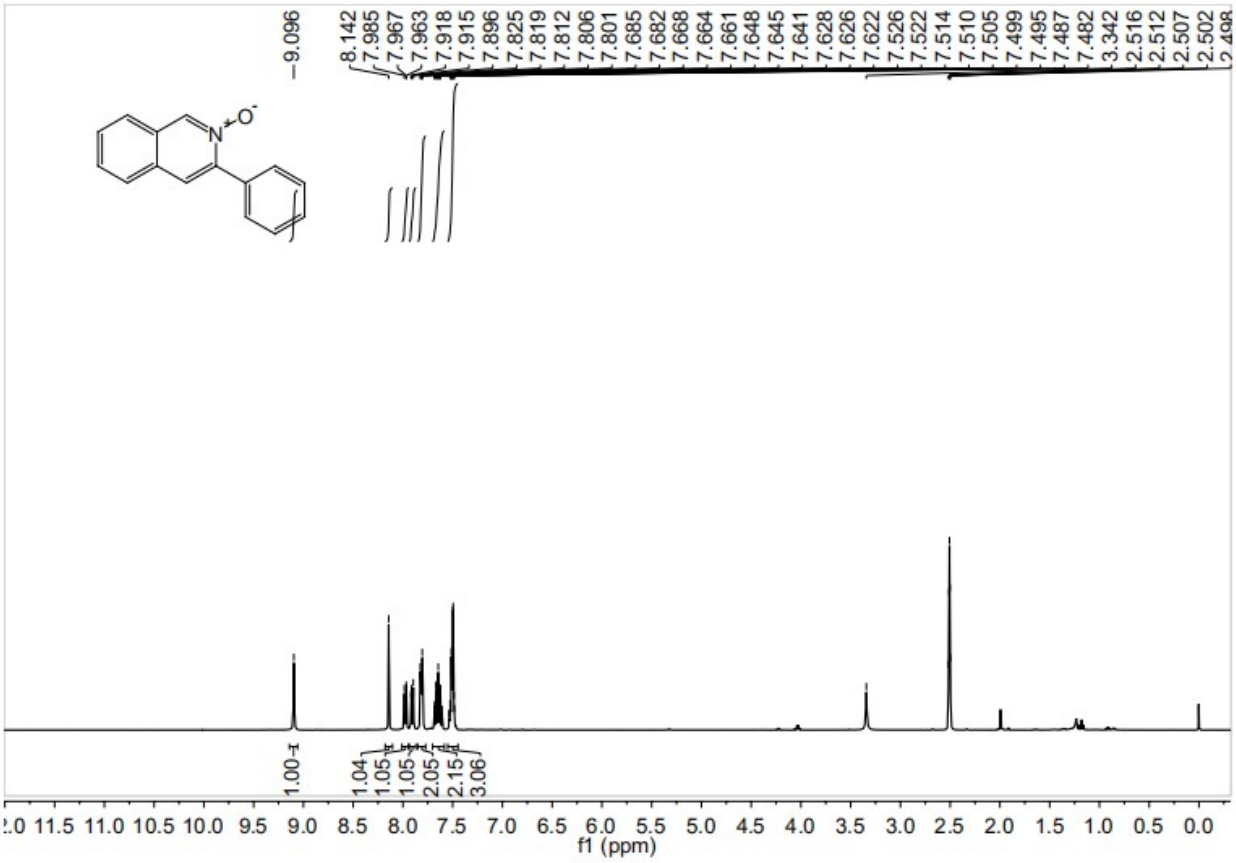
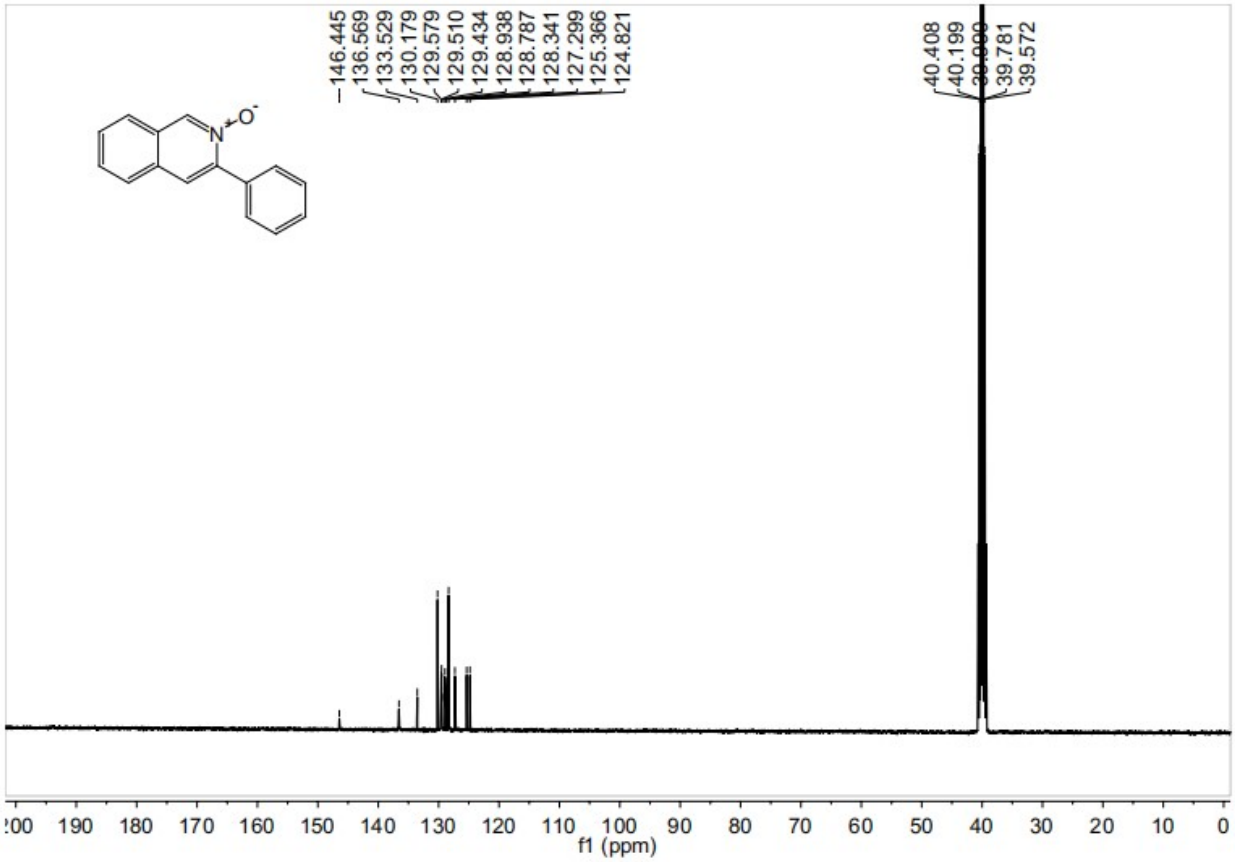
156.790
137.068
134.631
130.951
129.182
129.147
128.972
126.827
126.768
122.921
110.600
103.770
40.596
40.388
40.179
39.971
39.762
39.554
39.345
f1 (ppm)


N+
O-
9.096
8.142
7.985
7.967
7.963
7.918
7.915
7.896
7.825
7.819
7.812
7.806
7.801
7.685
7.682
7.668
7.664
7.661
7.648
7.645
7.641
7.628
7.626
7.622
7.526
7.522
7.514
7.510
7.505
7.499
7.495
7.487
7.482
3.342
2.516
2.512
2.507
2.502
1.00
1.04
1.05
1.05
2.05
2.15
3.06
f1 (ppm)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133.529
130.179
129.579
129.510
129.434
128.938
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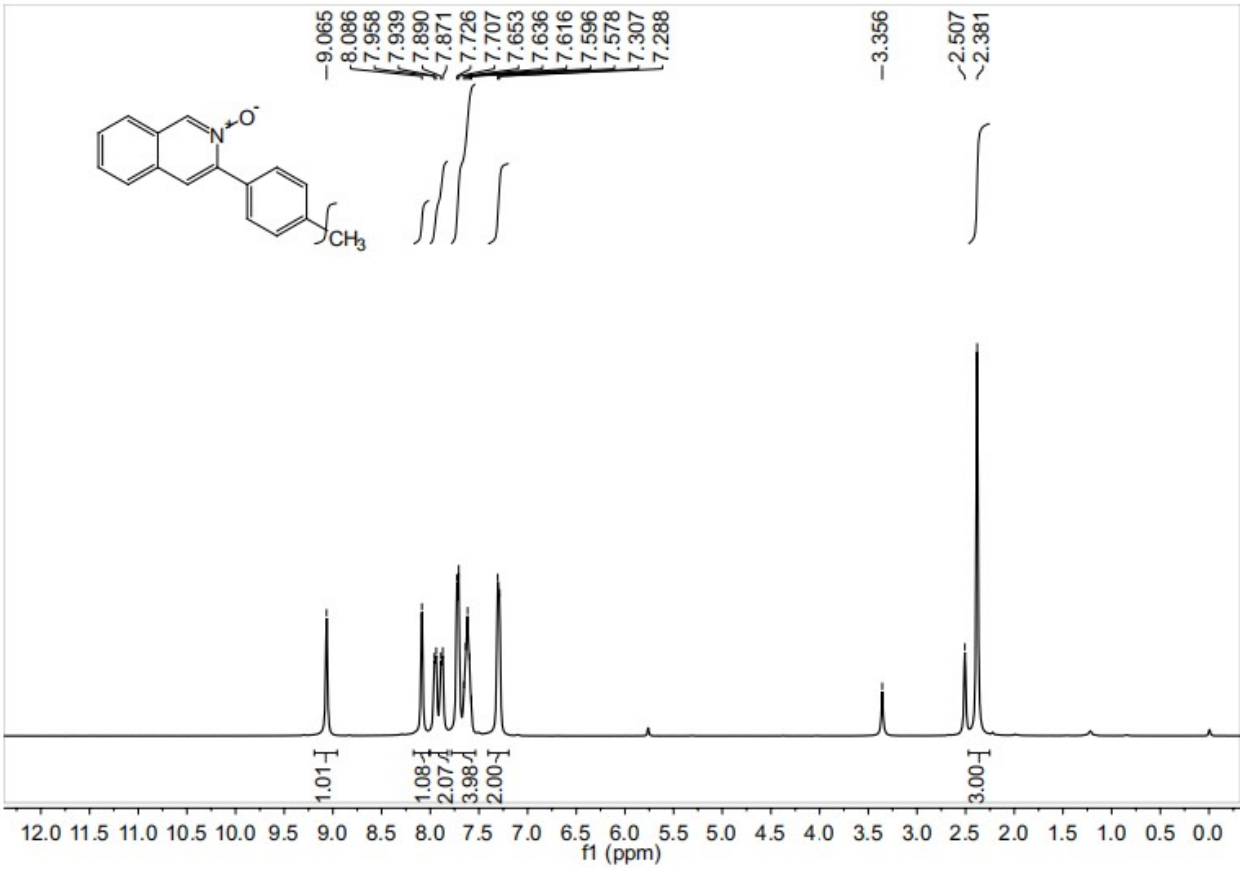
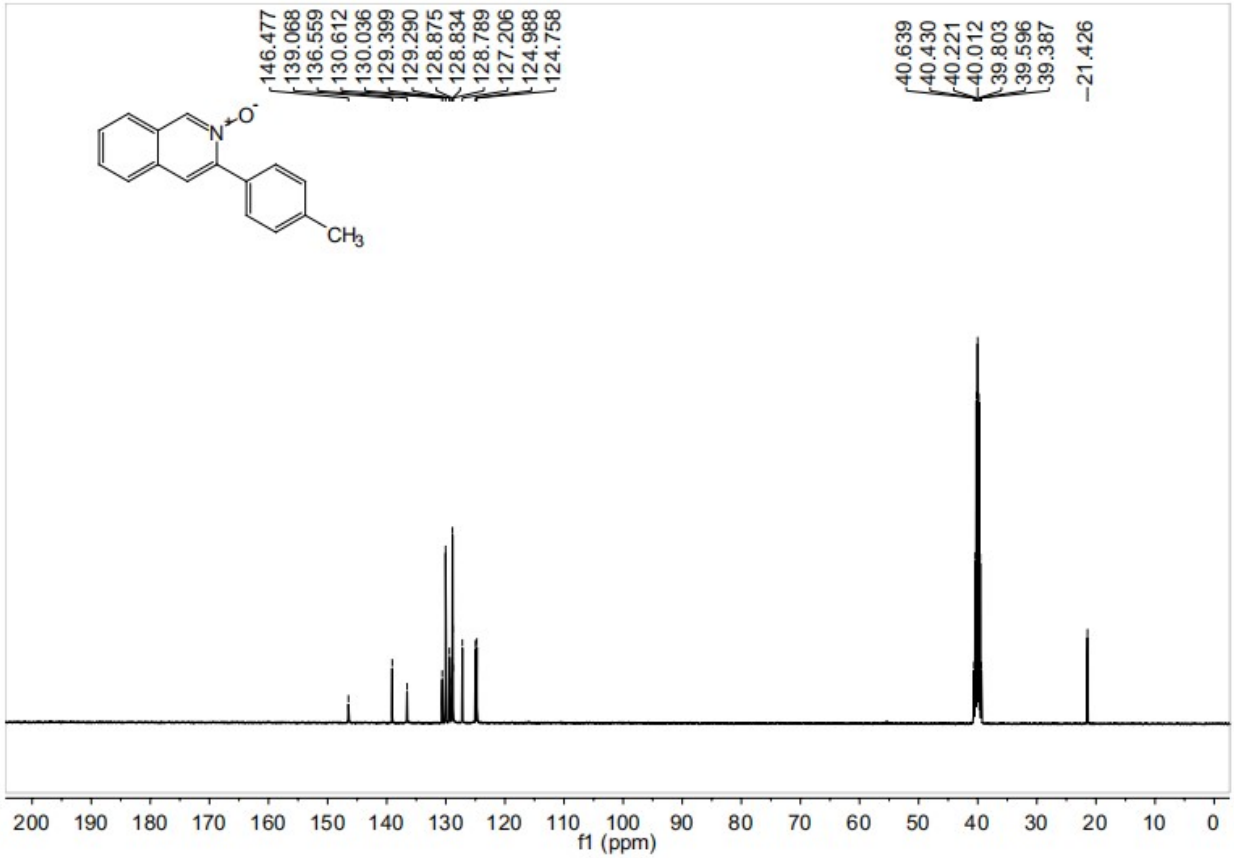
128.341
127.299
125.366
124.821
40.408
40.199
39.781
39.572
f1 (ppm)


9.065
8.086
7.958
7.939
7.890
7.871
7.726
7.707
7.653
7.636
7.616
7.596
7.578
7.307
7.288
3.356
2.507
2.381
CH3
1.01
1.08
2.07
3.98
2.00
3.00
f1 (ppm)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130.612
130.036
129.399
129.290
128.875
128.834
128.789
127.206
124.988
124.758
40.639
40.430
40.221
40.012
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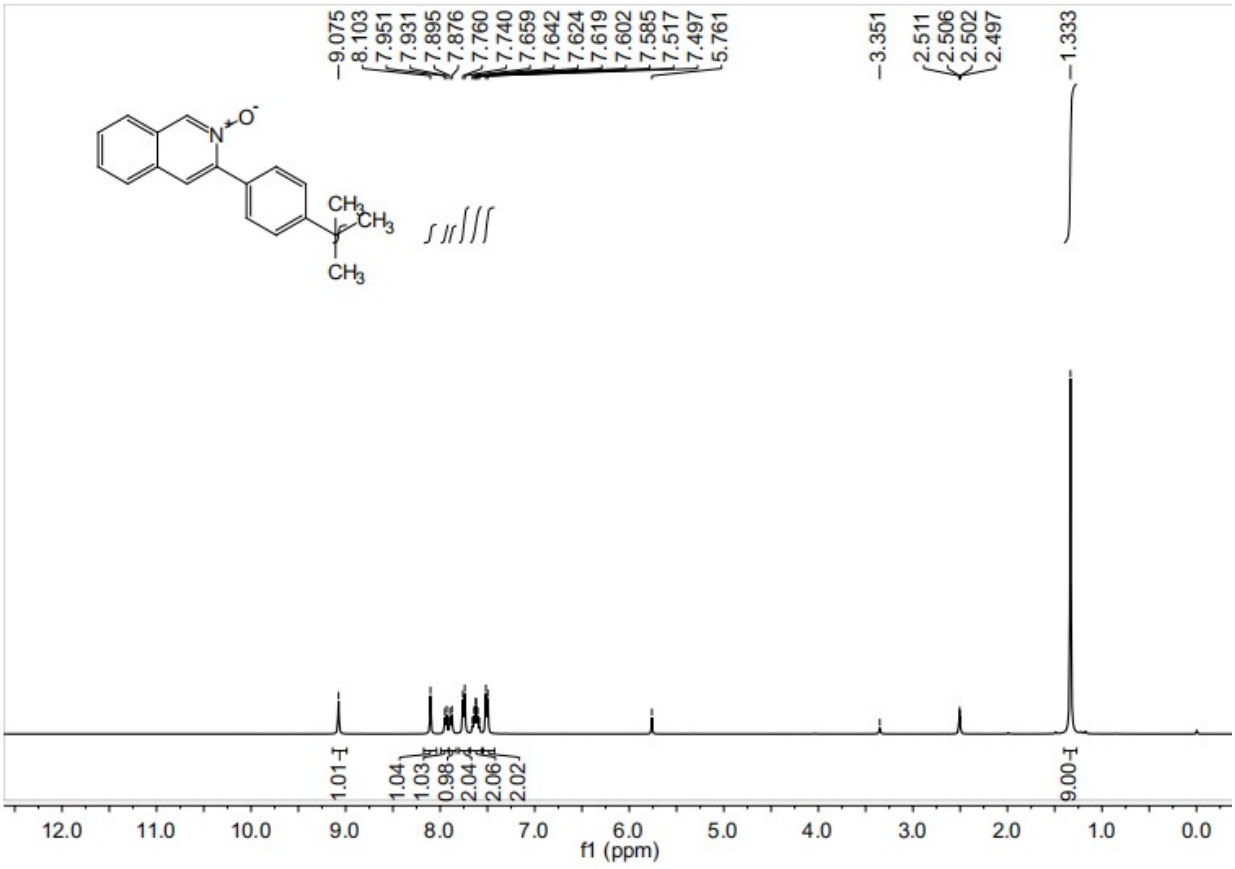
39.596
39.387
21.426
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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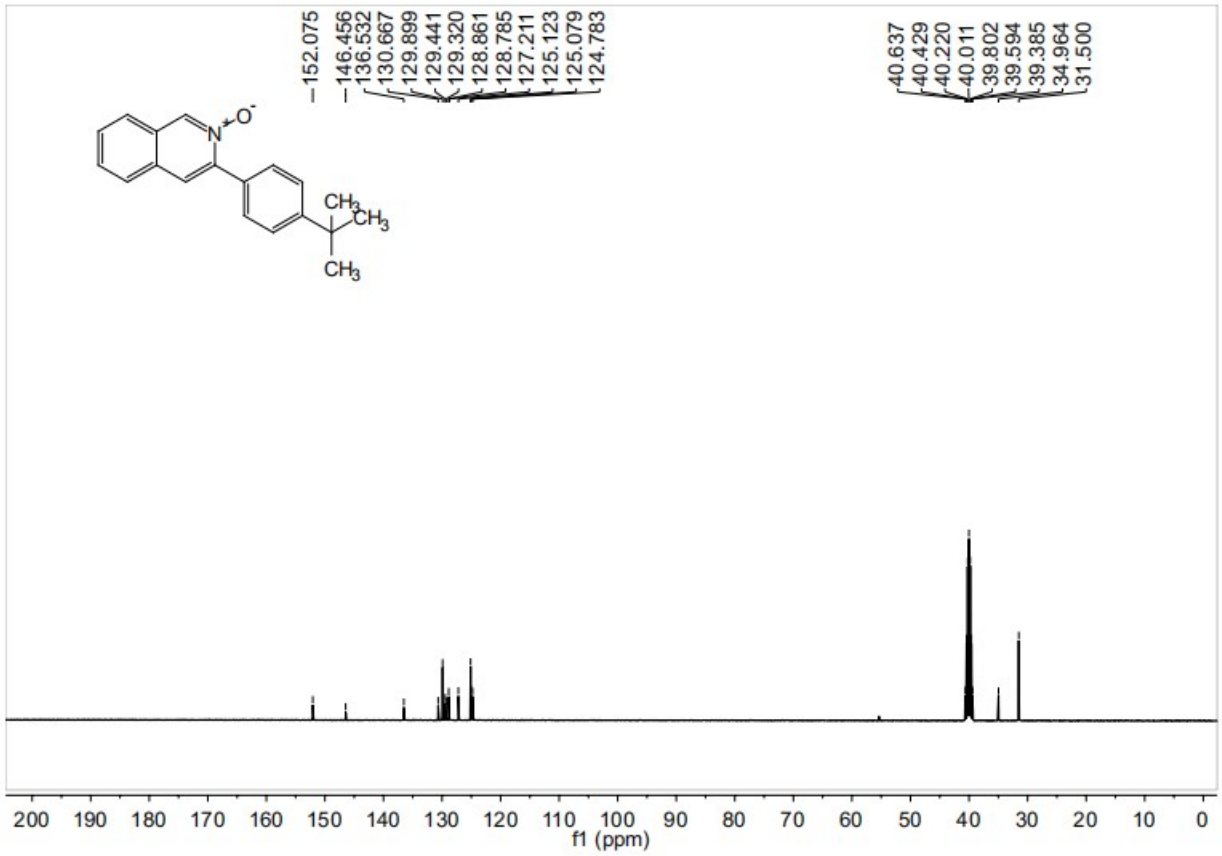
7.931
7.895
7.876
7.760
7.740
7.659
7.642
7.624
7.619
7.602
7.585
7.517
7.497
5.761
3.351
2.511
2.506
2.502
2.497
1.333
CH3
CH3
CH3
1.01
1.04
1.03
0.98
2.04
2.06
2.02
9.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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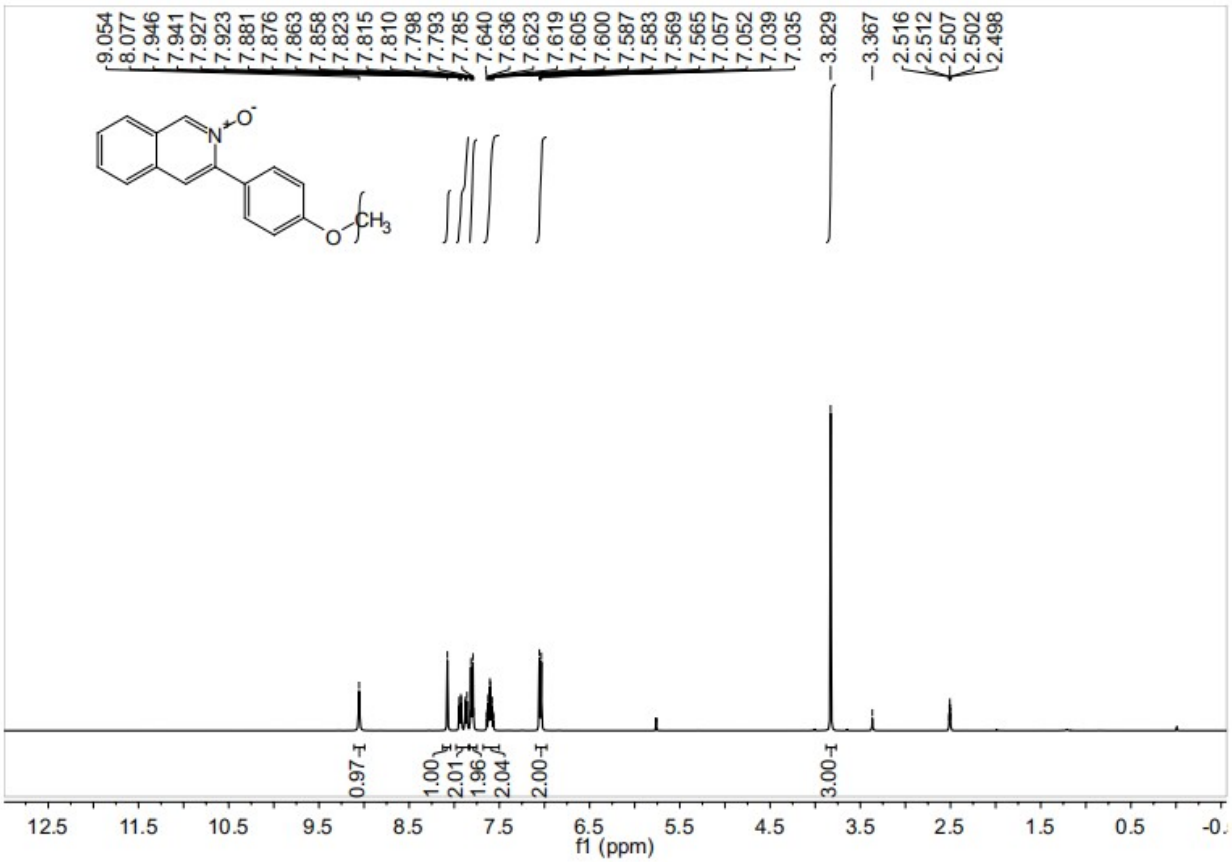
130.667
129.899
129.441
129.320
128.861
128.785
127.211
125.123
125.079
124.783
40.637
40.429
40.220
40.011
39.802
39.594
39.385
34.964
31.500
CH3
CH3
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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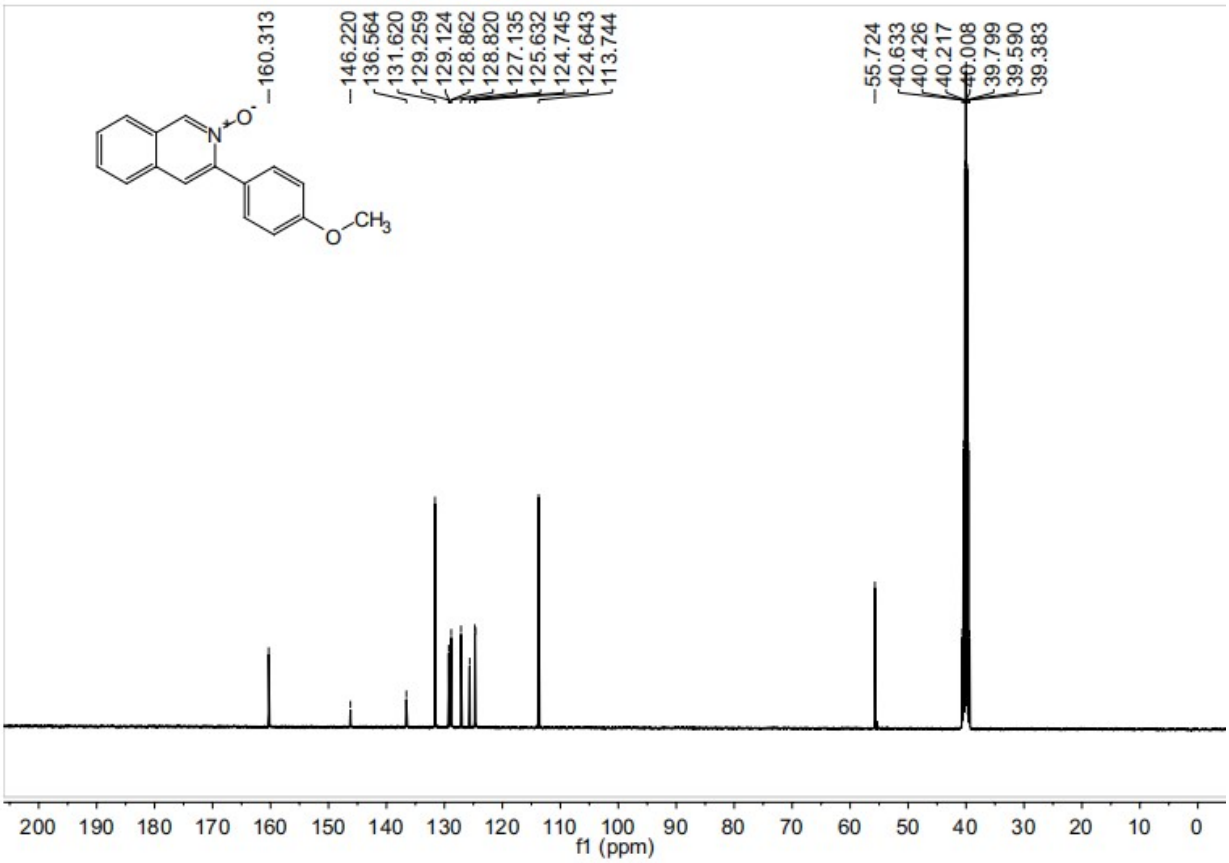
7.863
7.858
7.823
7.815
7.810
7.798
7.793
7.785
7.640
7.636
7.623
7.619
7.605
7.600
7.587
7.583
7.569
7.565
7.057
7.052
7.039
7.035
3.829
3.367
2.516
2.512
2.507
2.502
2.498
CH3
0.97
1.00
2.01
1.96
2.04
2.00
3.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5
f1 (ppm)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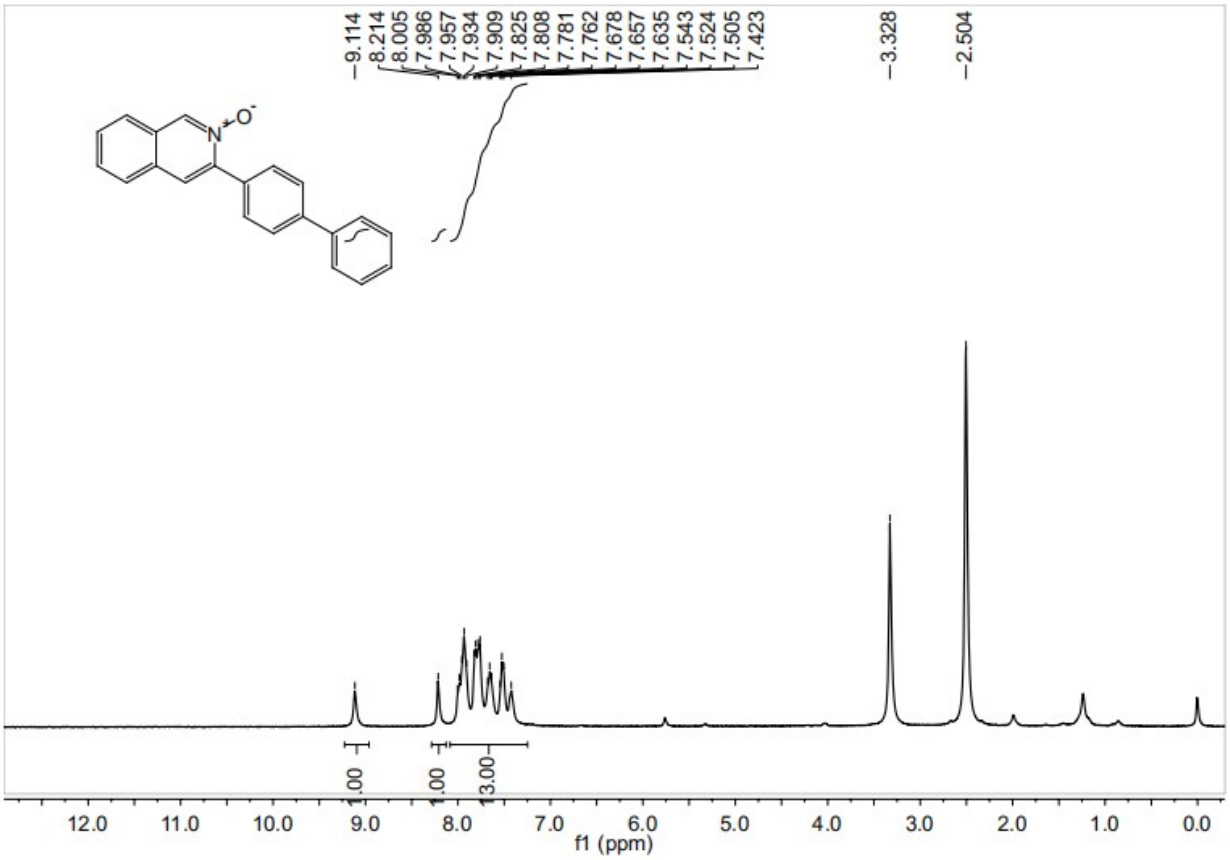
131.620
129.259
129.124
128.862
128.820
127.135
125.632
124.745
124.643
113.744
55.724
40.633
40.426
40.217
40.008
39.799
39.590
39.383
N+O-
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.214
8.005
7.986
7.957
7.934
7.909
7.825
7.808
7.781
7.762
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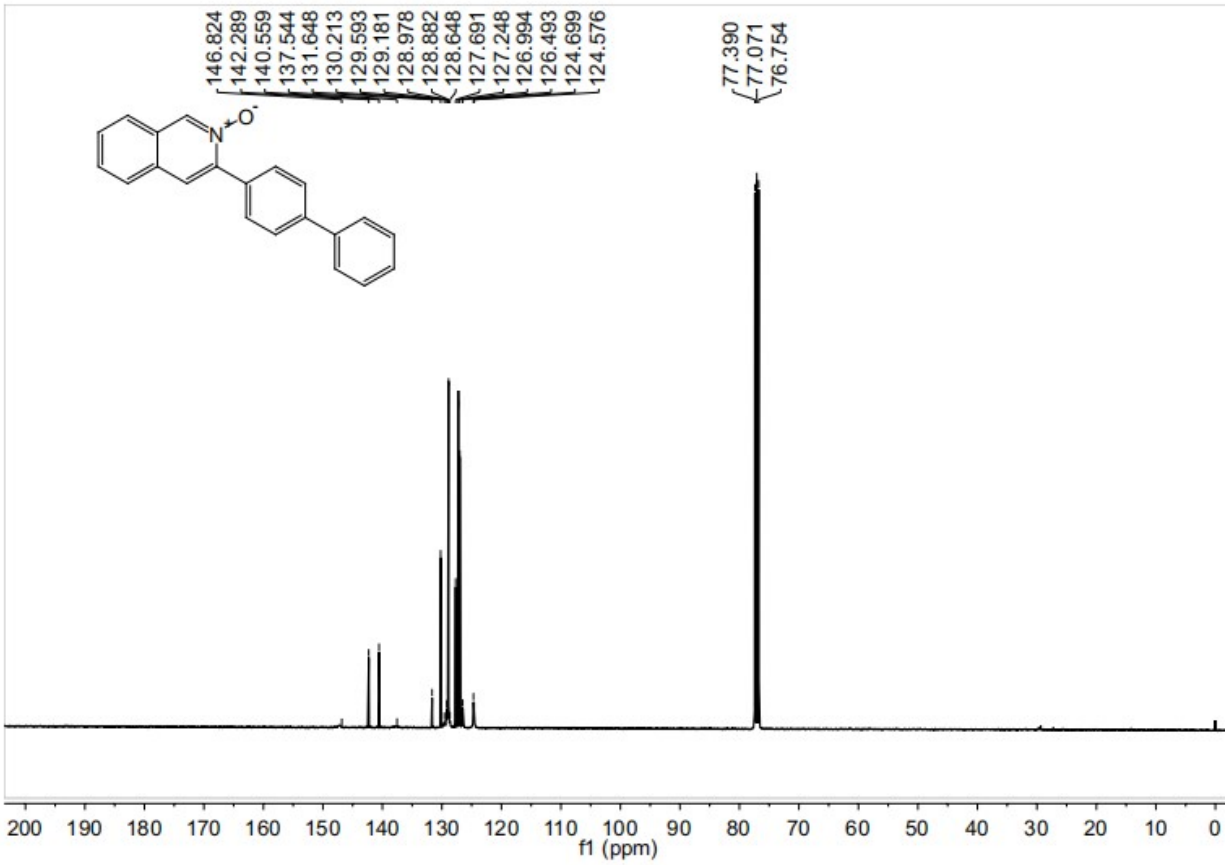
7.657
7.635
7.543
7.524
7.505
7.423
3.328
2.504
N+O-
1.00
1.00
3.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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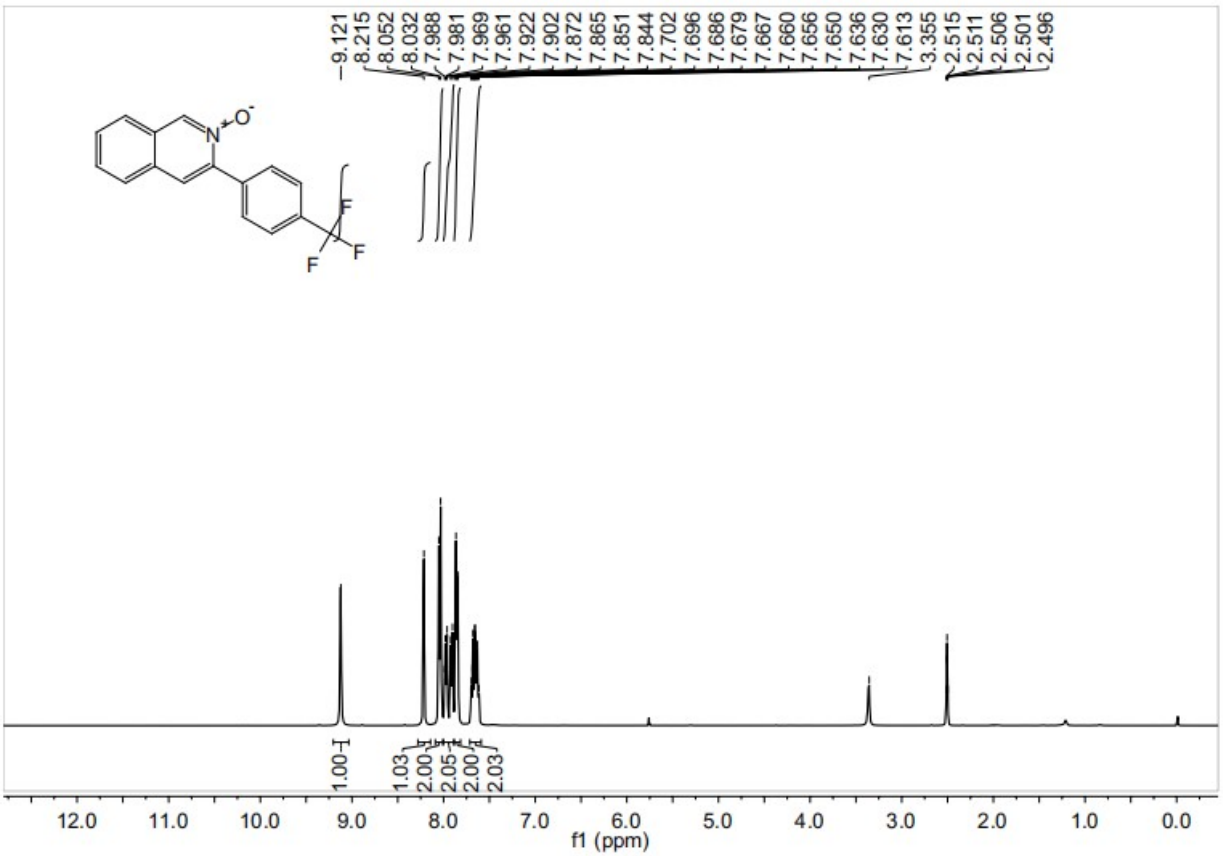
126.994
126.493
124.699
124.576
77.390
77.071
76.754
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.961
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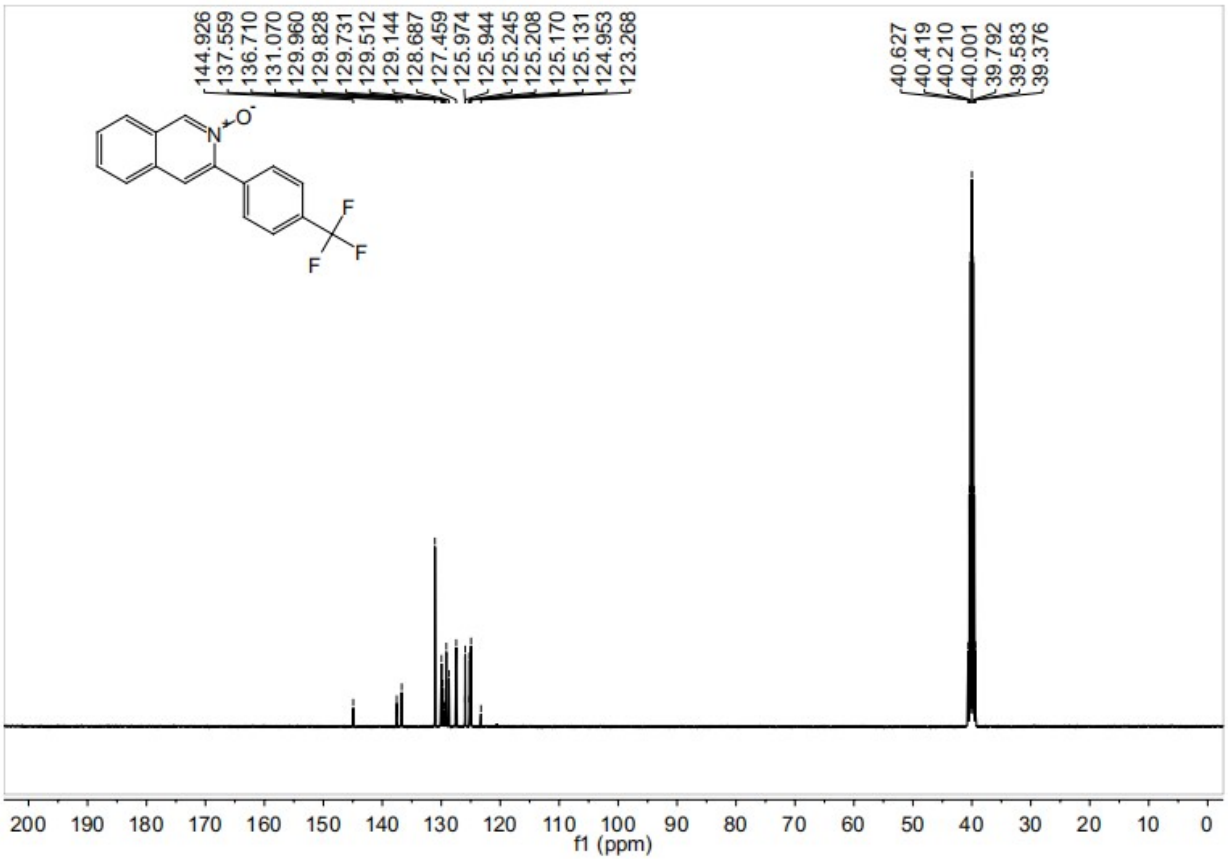
7.851
7.844
7.702
7.696
7.686
7.679
7.667
7.660
7.656
7.650
7.636
7.630
7.613
3.355
2.515
2.511
2.506
2.501
2.496
N
O
F
F
F
1.00
1.03
2.00
2.05
2.00
2.03
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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129.512
129.144
128.687
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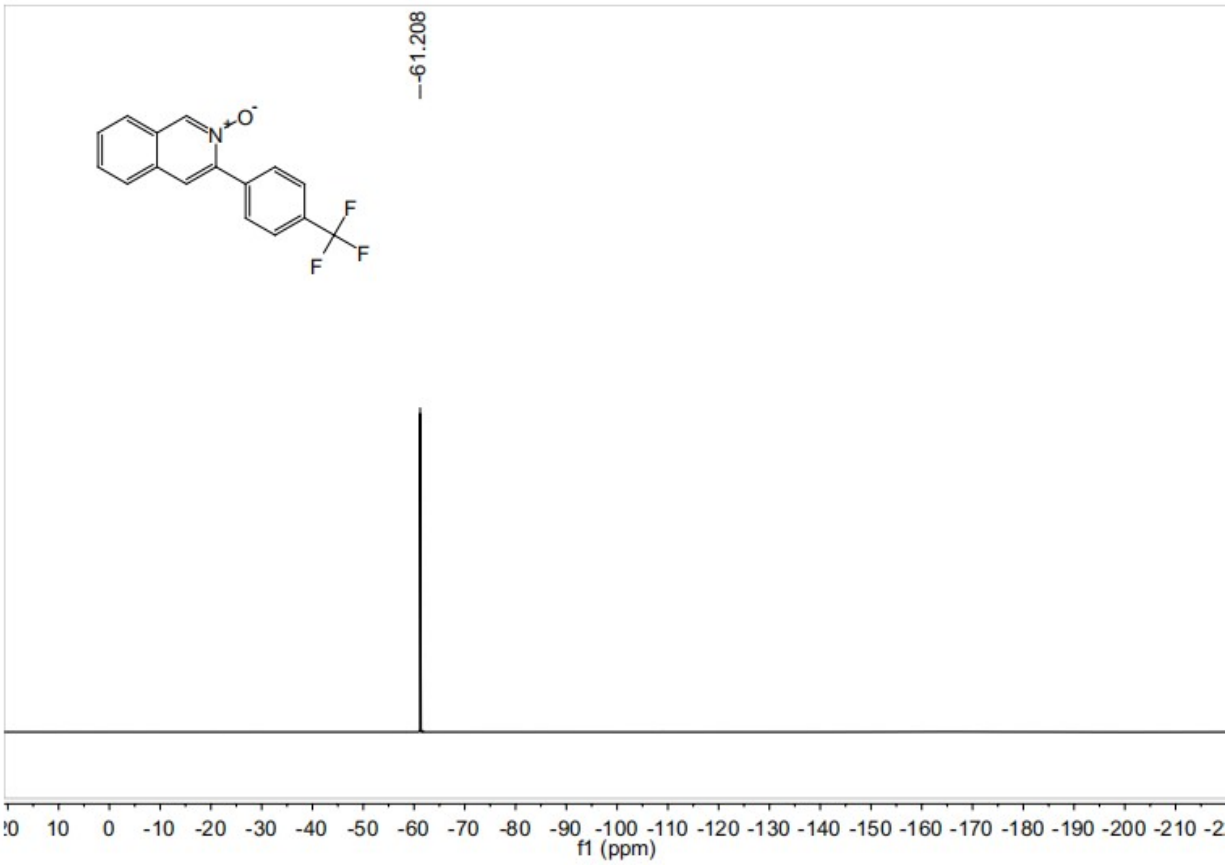
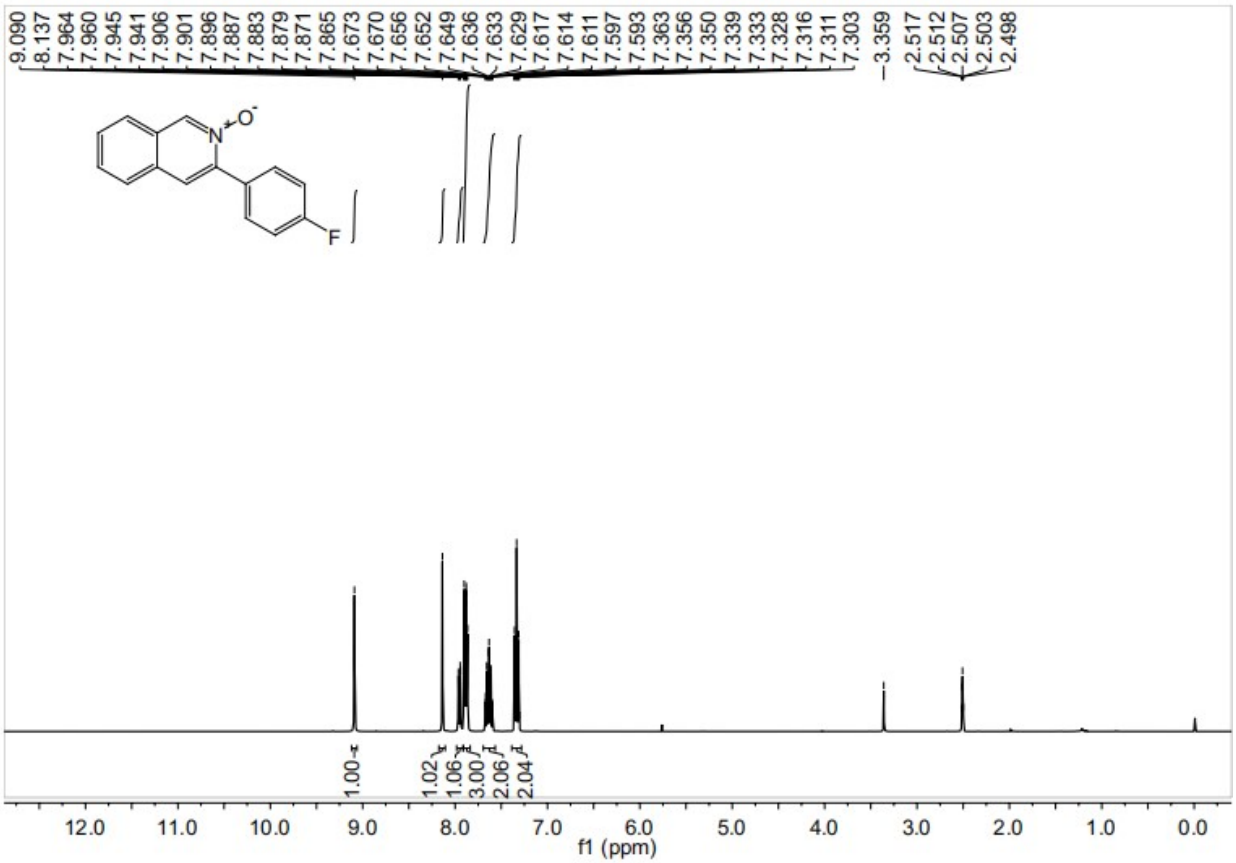
125.974
125.944
125.245
125.208
125.170
125.131
124.953
123.268
40.627
40.419
40.210
40.001
39.792
39.583
39.376
N+
O-
F
F
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-61.208
N+
O-
F
F
F
:0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -2
f1 (ppm)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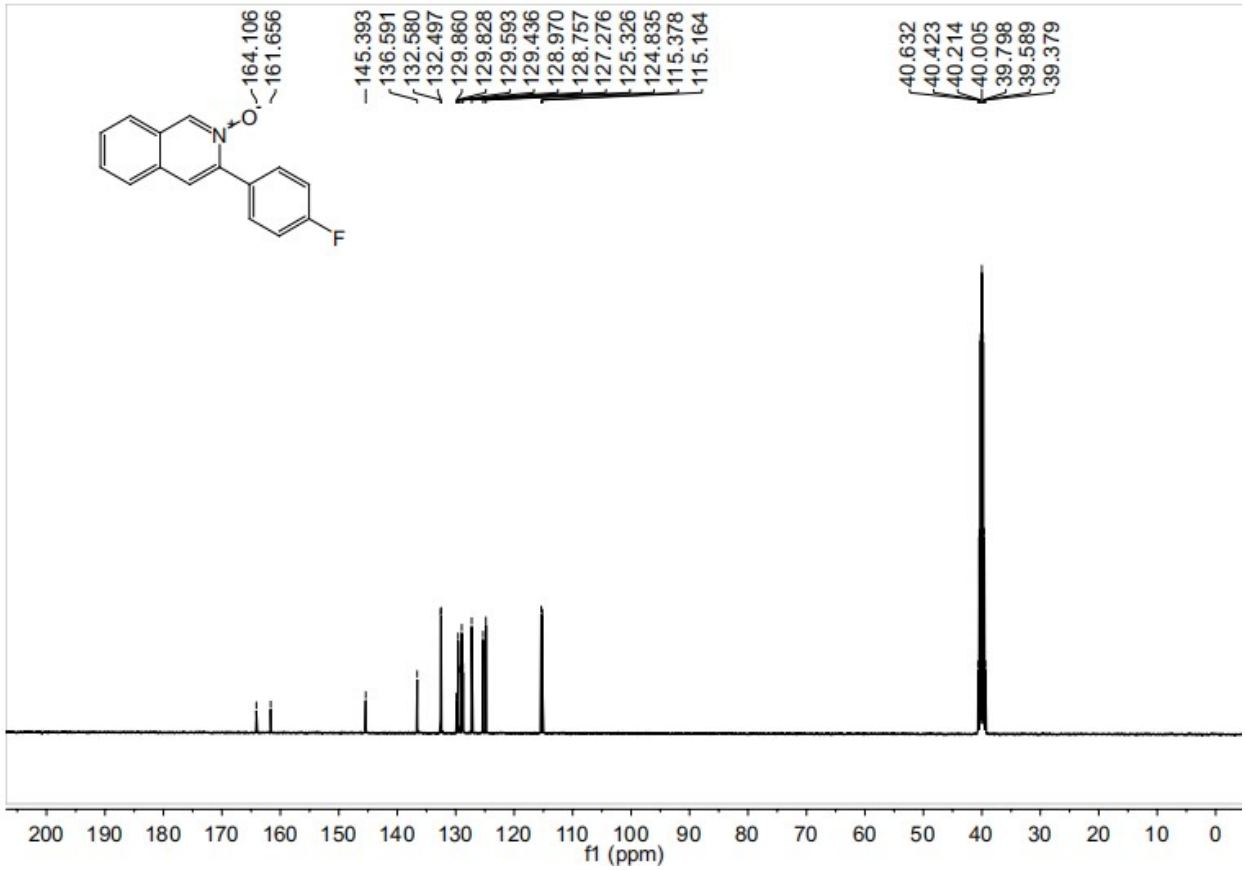
7.871
7.865
7.673
7.670
7.656
7.652
7.649
7.636
7.633
7.629
7.617
7.614
7.611
7.597
7.593
7.363
7.356
7.350
7.339
7.333
7.328
7.316
7.311
7.303
3.359
2.517
2.512
2.507
2.503
2.498
N+
O-
F
1.00
1.02
1.06
3.00
2.06
2.04
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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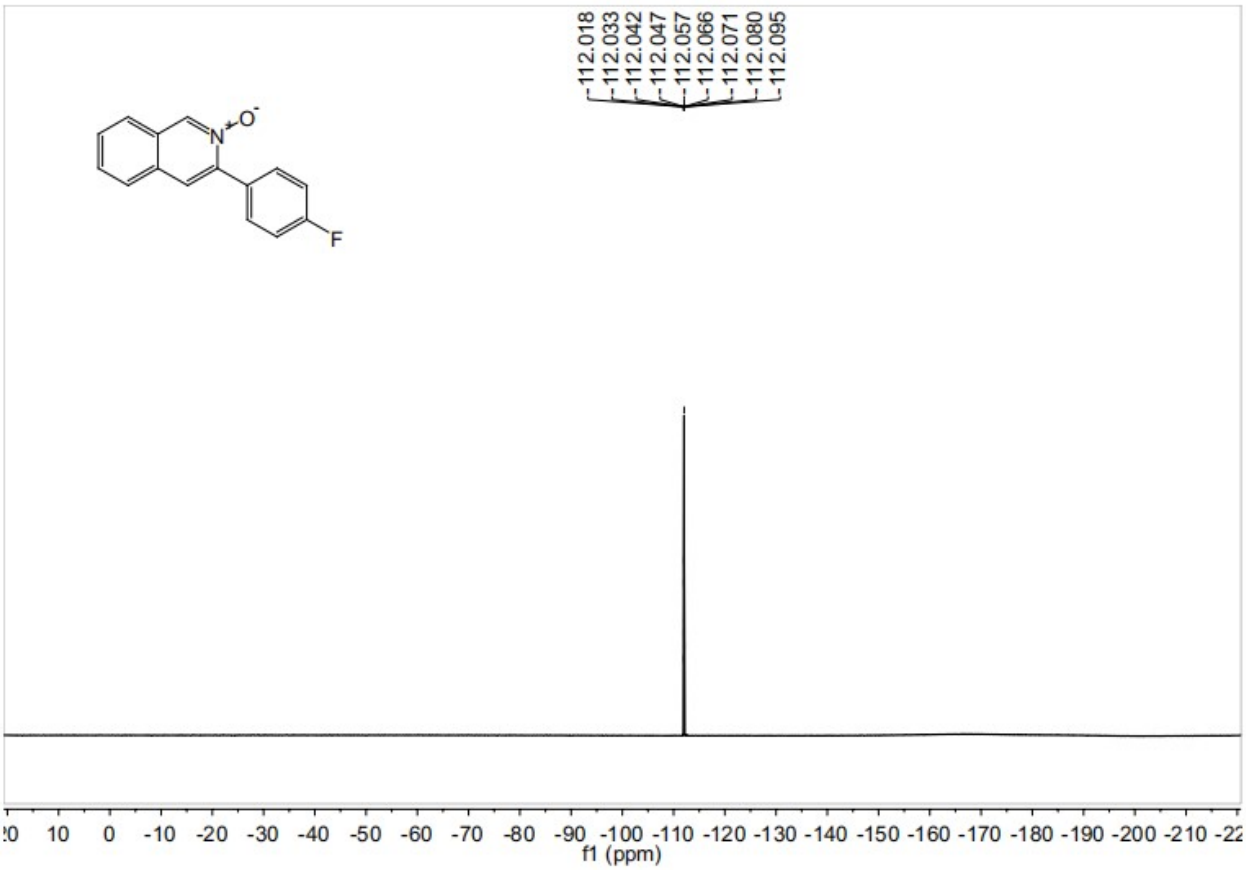
132.580
132.497
129.860
129.828
129.593
129.436
128.970
128.757
127.276
125.326
124.835
115.378
115.164
40.632
40.423
40.214
40.005
39.798
39.589
39.379
N+
O-
F
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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112.033
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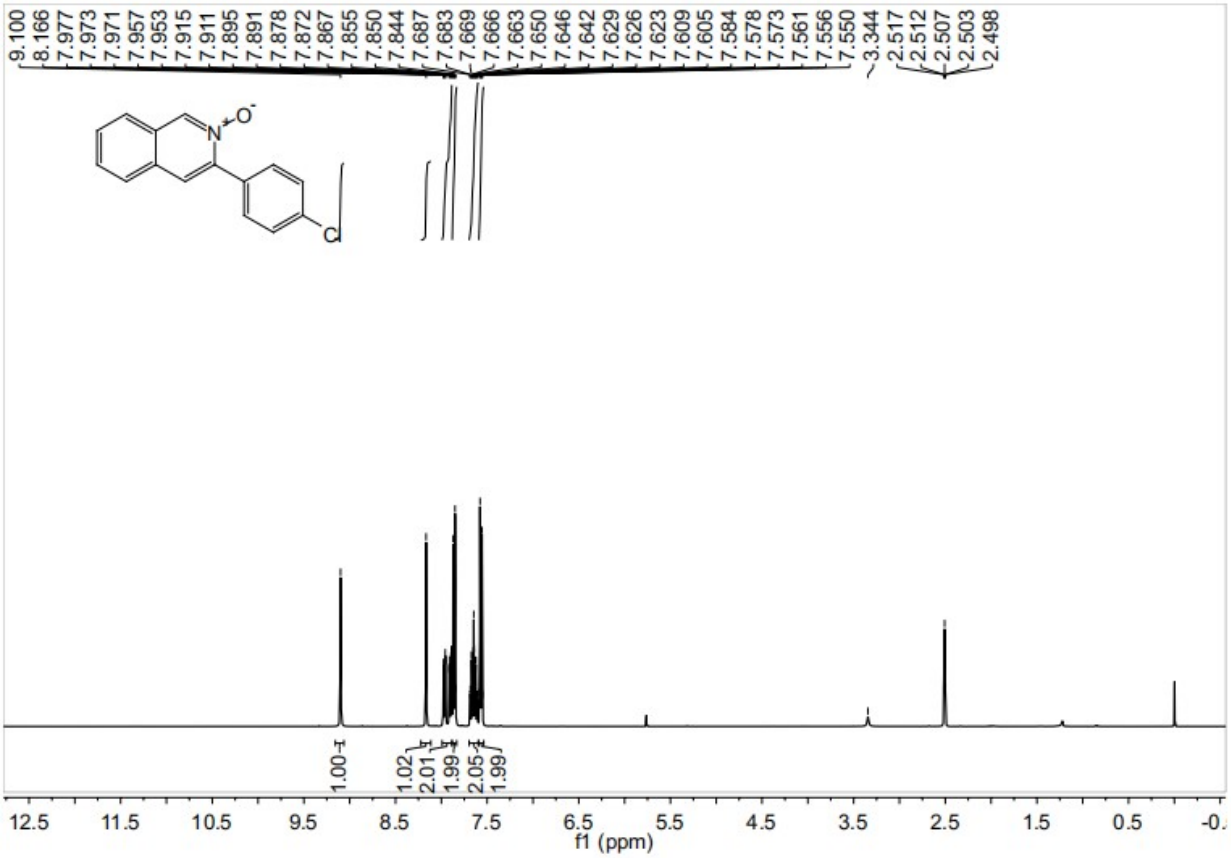
112.066
112.071
112.080
112.095
F
f1 (ppm)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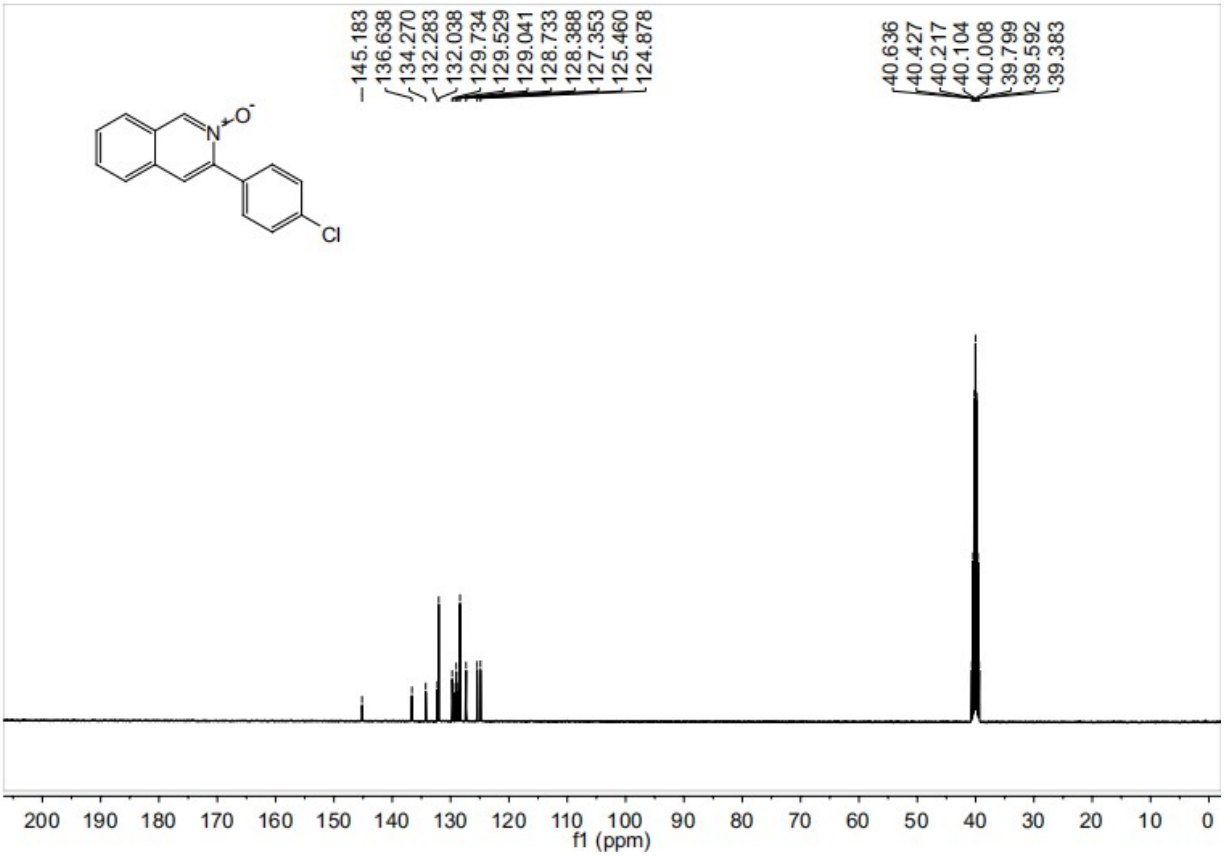
7.977
7.973
7.971
7.957
7.953
7.915
7.911
7.895
7.891
7.878
7.872
7.867
7.855
7.850
7.844
7.687
7.683
7.669
7.666
7.663
7.650
7.646
7.642
7.629
7.626
7.623
7.609
7.605
7.584
7.578
7.573
7.561
7.556
7.550
3.344
2.517
2.512
2.507
2.503
2.498
Cl
1.00
1.02
2.01
1.99
2.05
1.99
f1 (ppm)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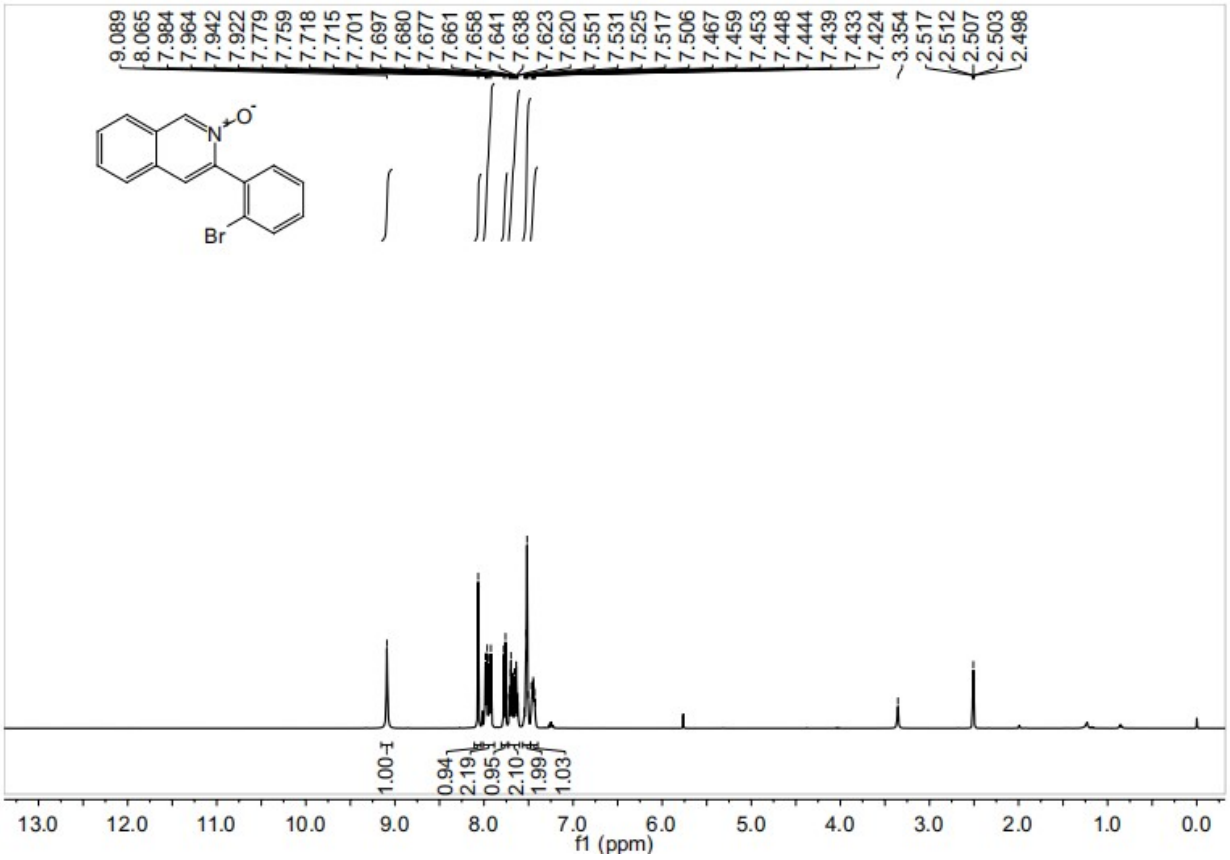
136.638
134.270
132.283
132.038
129.734
129.529
129.041
128.733
128.388
127.353
125.460
124.878
40.636
40.427
40.217
40.104
40.008
39.799
39.592
39.383
Cl
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.065
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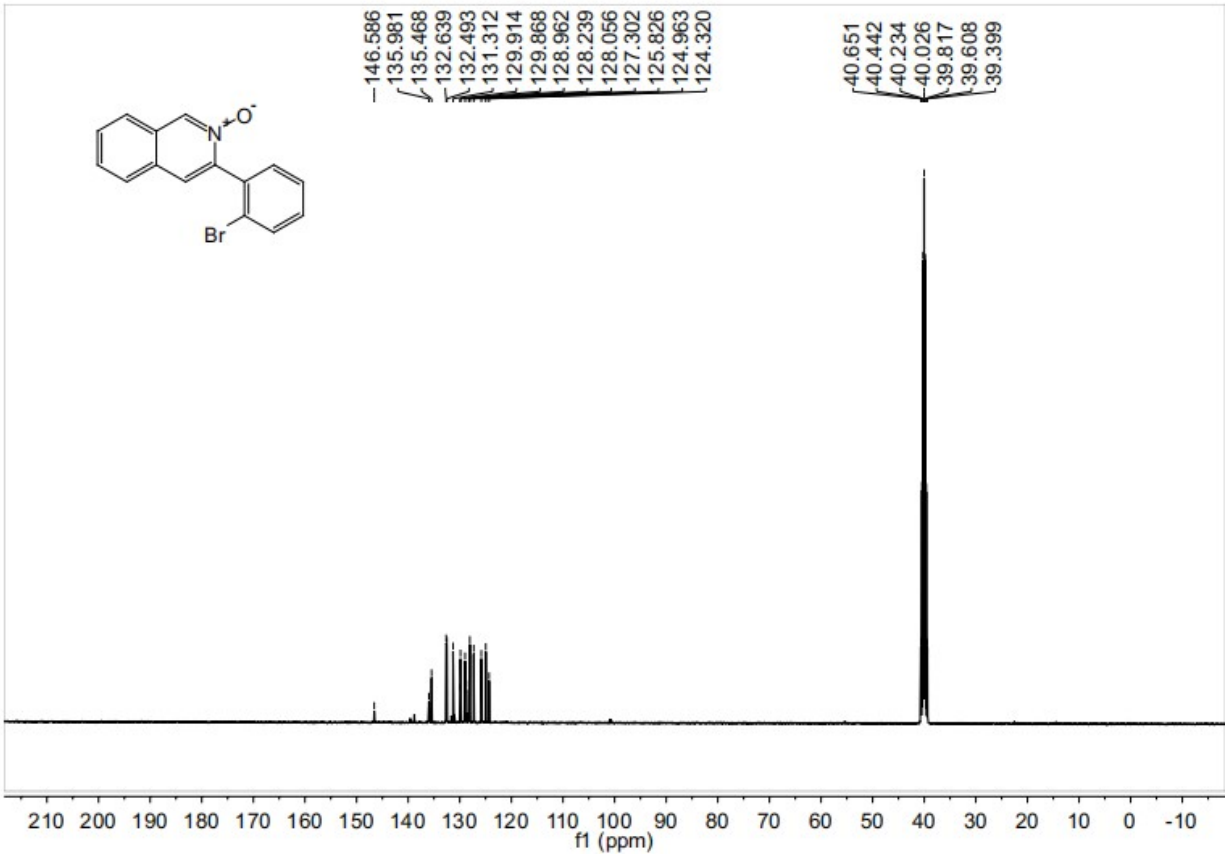
7.779
7.759
7.718
7.715
7.701
7.697
7.680
7.677
7.661
7.658
7.641
7.638
7.623
7.620
7.551
7.531
7.525
7.517
7.506
7.467
7.459
7.453
7.448
7.444
7.439
7.433
7.424
3.354
2.517
2.512
2.507
2.503
2.498
Br
1.00
0.94
2.19
0.95
2.10
1.99
1.03
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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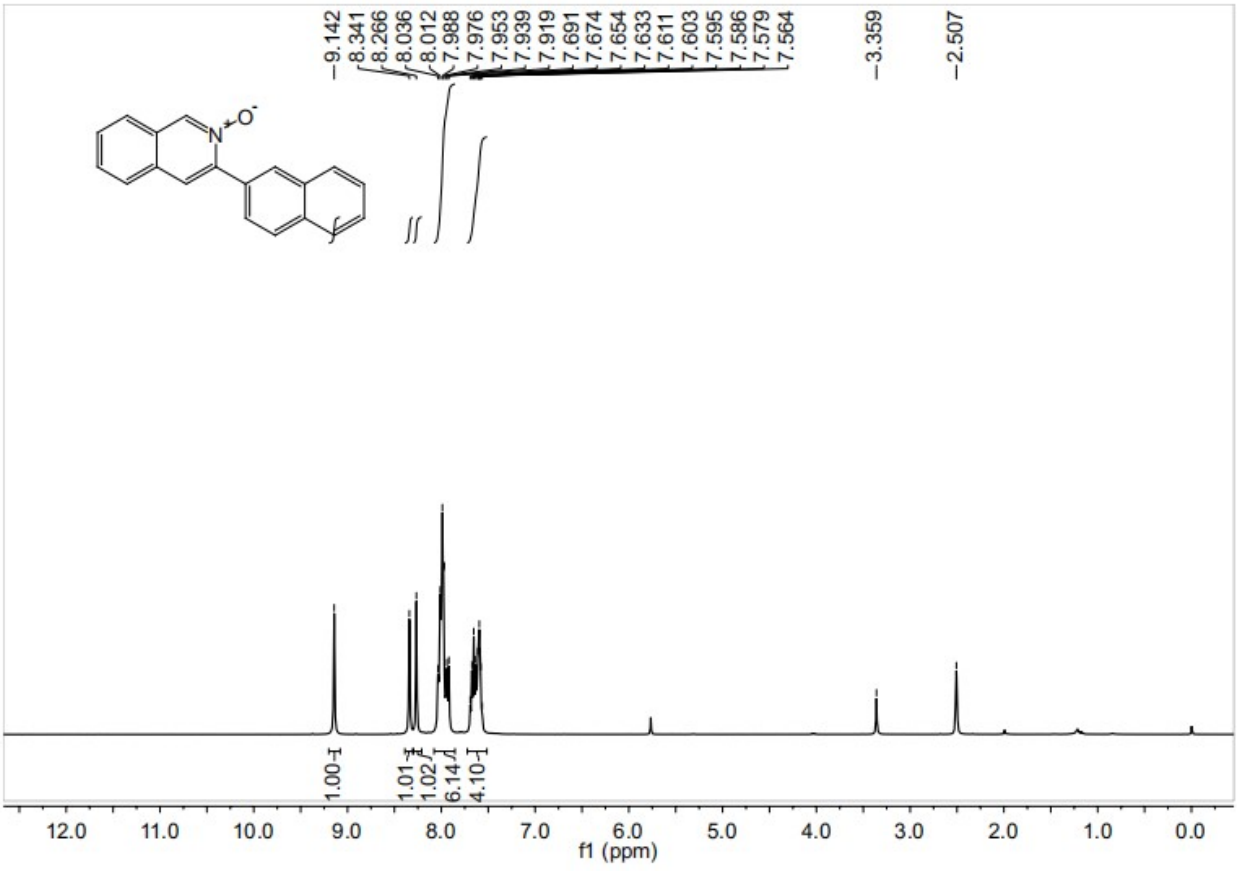
135.981
135.468
132.639
132.493
131.312
129.914
129.868
128.962
128.239
128.056
127.302
125.826
124.963
124.320
40.651
40.442
40.234
40.026
39.817
39.608
39.399
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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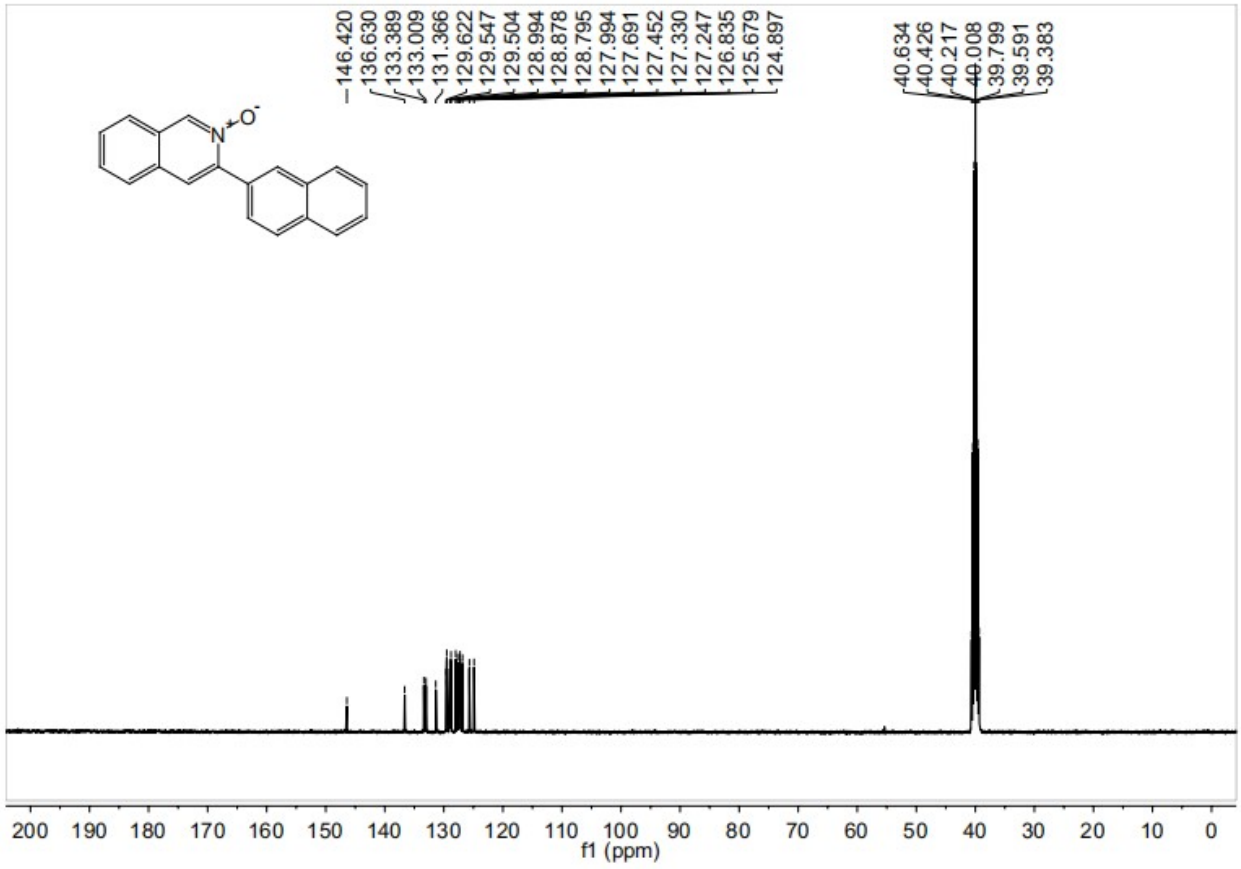
8.341
8.266
8.036
8.012
7.988
7.976
7.953
7.939
7.919
7.691
7.674
7.654
7.633
7.611
7.603
7.595
7.586
7.579
7.564
3.359
2.507
1.00
1.01
1.02
6.14
4.10
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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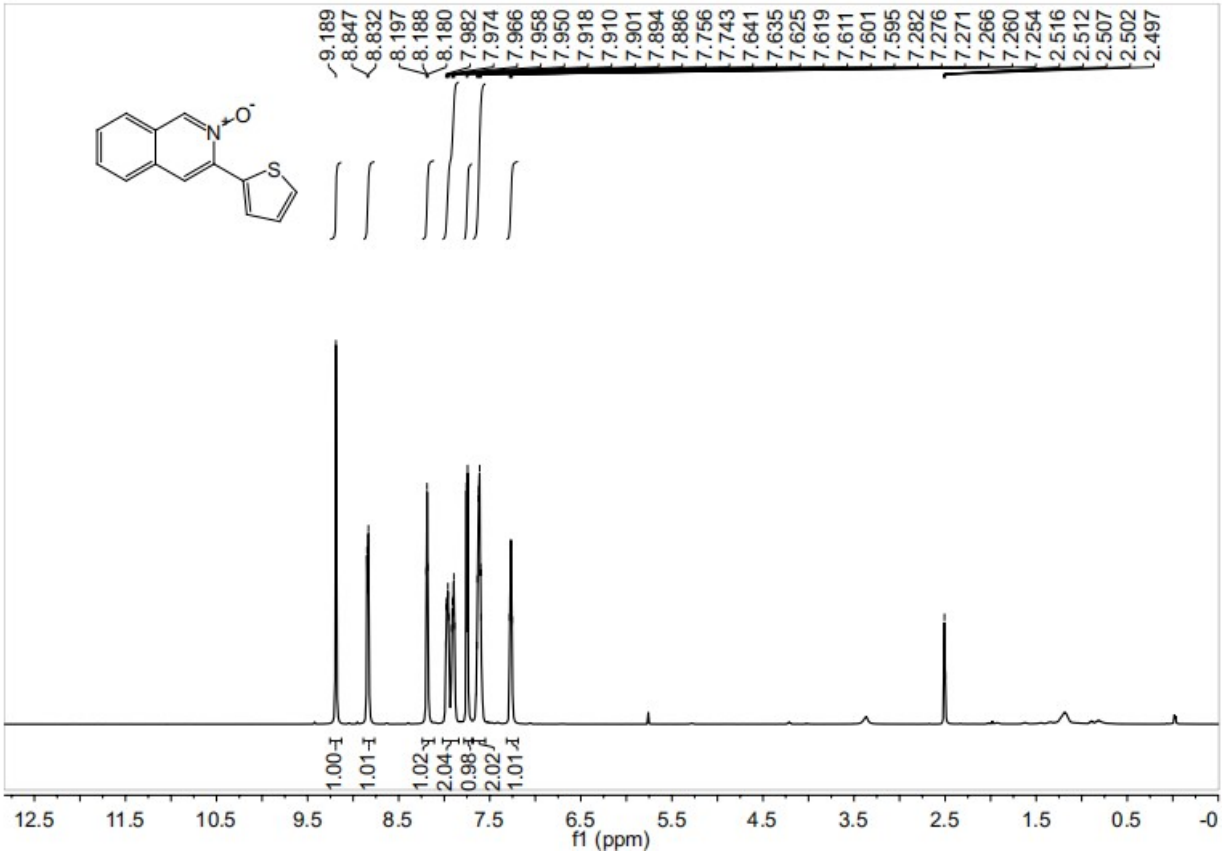
136.630
133.389
133.009
131.366
129.622
129.547
129.504
128.994
128.878
128.795
127.994
127.691
127.452
127.330
127.247
126.835
125.679
124.897
40.634
40.426
40.217
40.008
39.799
39.591
39.383
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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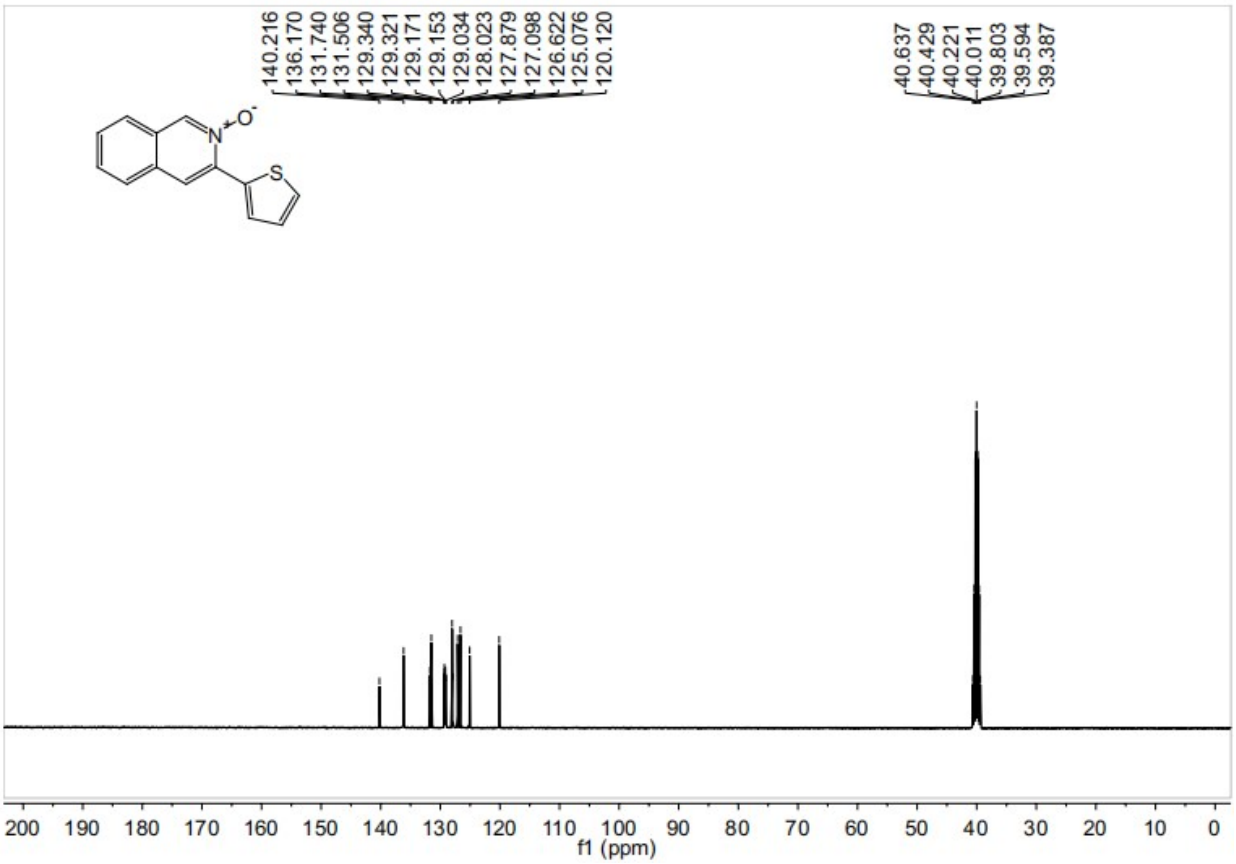
8.847
8.832
8.197
8.188
8.180
7.982
7.974
7.966
7.958
7.950
7.918
7.910
7.901
7.894
7.886
7.756
7.743
7.641
7.635
7.625
7.619
7.611
7.601
7.595
7.282
7.276
7.271
7.266
7.260
7.254
2.516
2.512
2.507
2.502
2.497
1.00
1.01
1.02
2.04
0.98
2.02
1.01
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0
f1 (ppm)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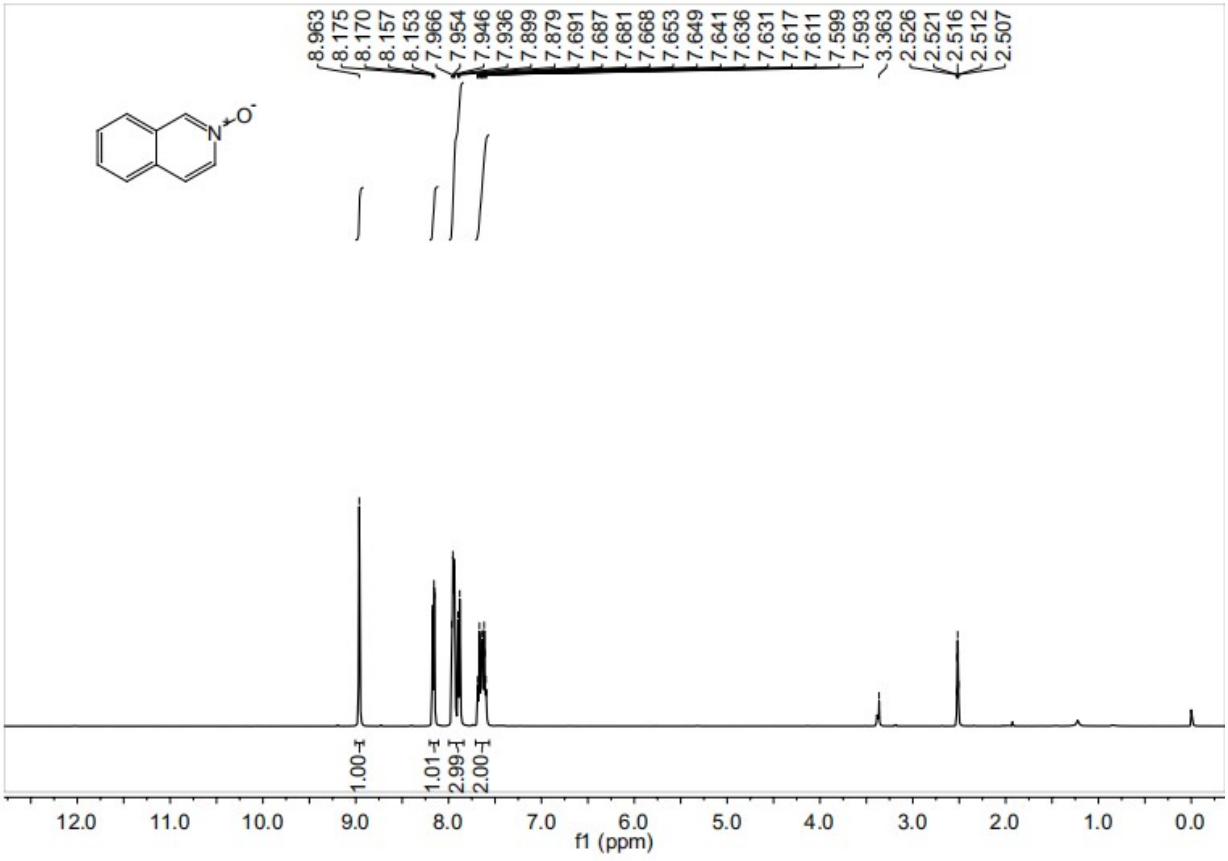
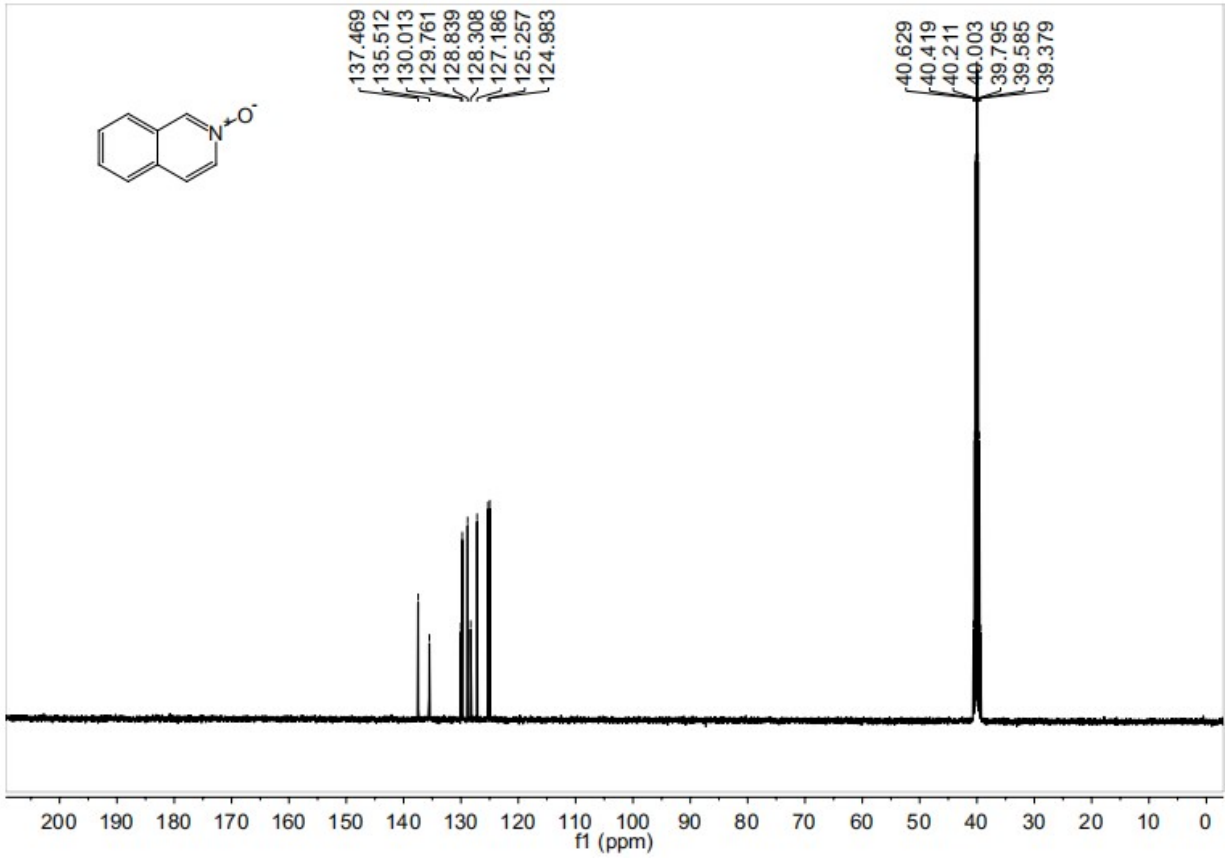
136.170
131.740
131.506
129.340
129.321
129.171
129.153
129.034
128.023
127.879
127.098
126.622
125.076
120.120
40.637
40.429
40.221
40.011
39.803
39.594
39.387
N+
O-
S
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.963
8.175
8.170
8.157
8.153
7.966
7.954
7.946
7.936
7.899
7.879
7.691
7.687
7.681
7.668
7.653
7.649
7.641
7.636
7.631
7.617
7.611
7.599
7.593
3.363
2.526
2.521
2.516
2.512
2.507
N+
O-
1.00
1.01
2.99
2.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)


137.469
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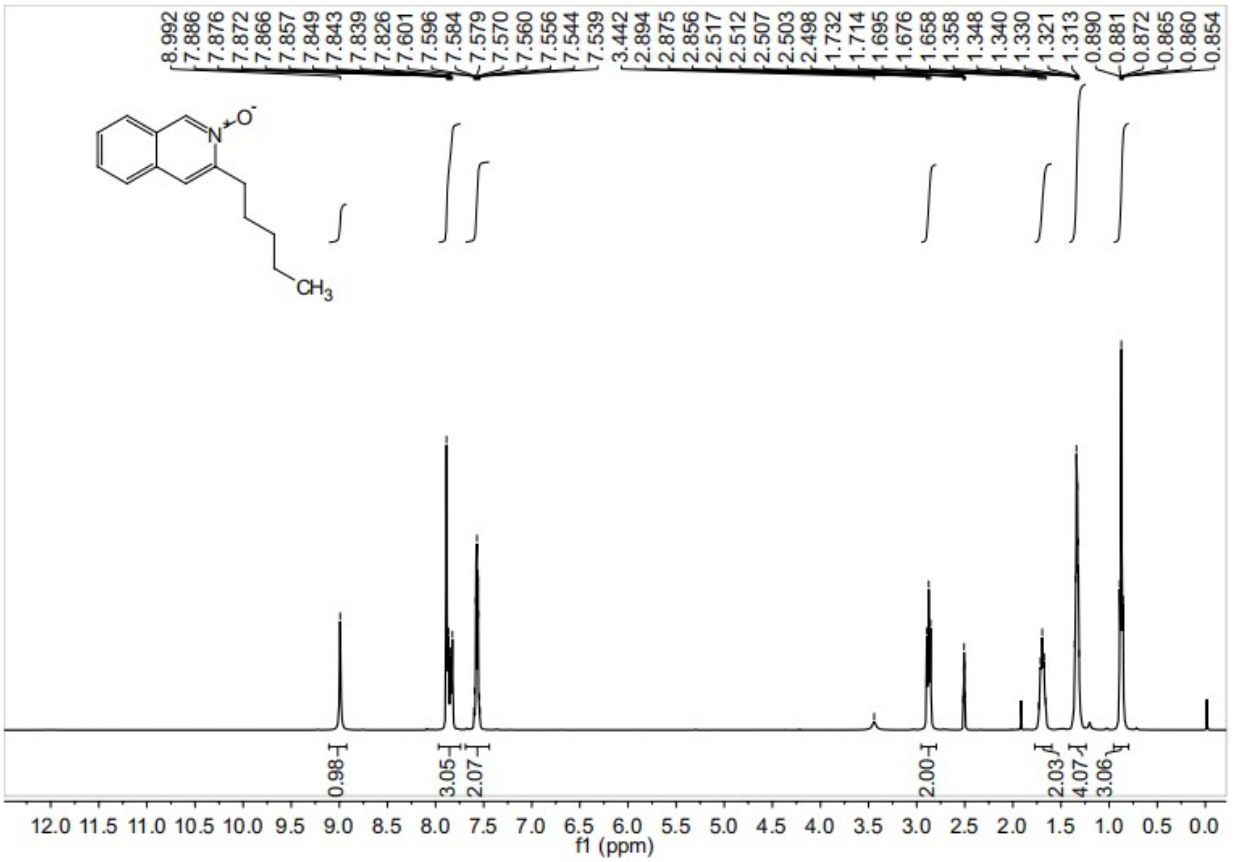
130.013
129.761
128.839
128.308
127.186
125.257
124.983
40.629
40.419
40.211
40.003
39.795
39.585
39.379
f1 (ppm)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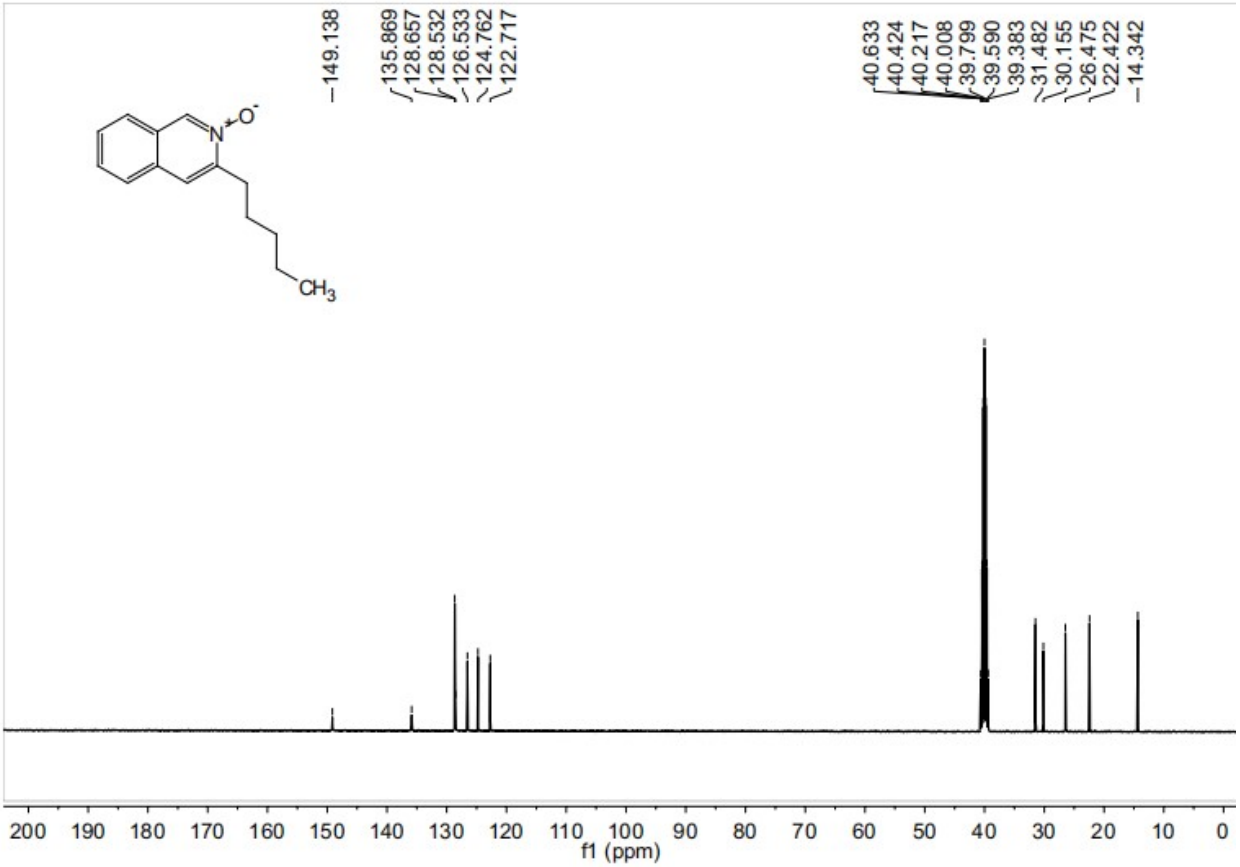
7.876
7.872
7.866
7.857
7.849
7.843
7.839
7.826
7.601
7.596
7.584
7.579
7.570
7.560
7.556
7.544
7.539
3.442
2.894
2.875
2.856
2.517
2.512
2.507
2.503
2.498
1.732
1.714
1.695
1.676
1.658
1.358
1.348
1.340
1.330
1.321
1.313
0.890
0.881
0.872
0.865
0.860
0.854
CH3
0.98
3.05
2.07
2.00
2.03
4.07
3.06
f1 (ppm)


149.138
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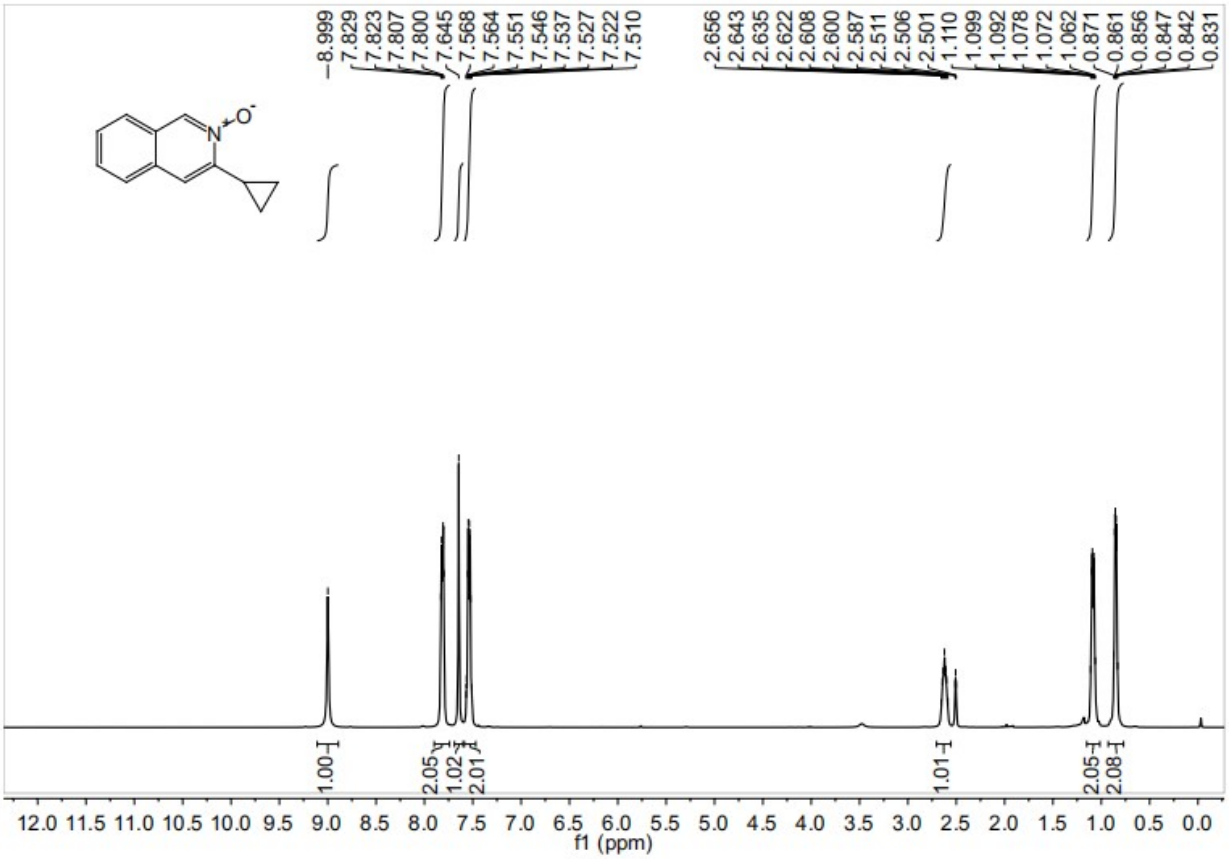
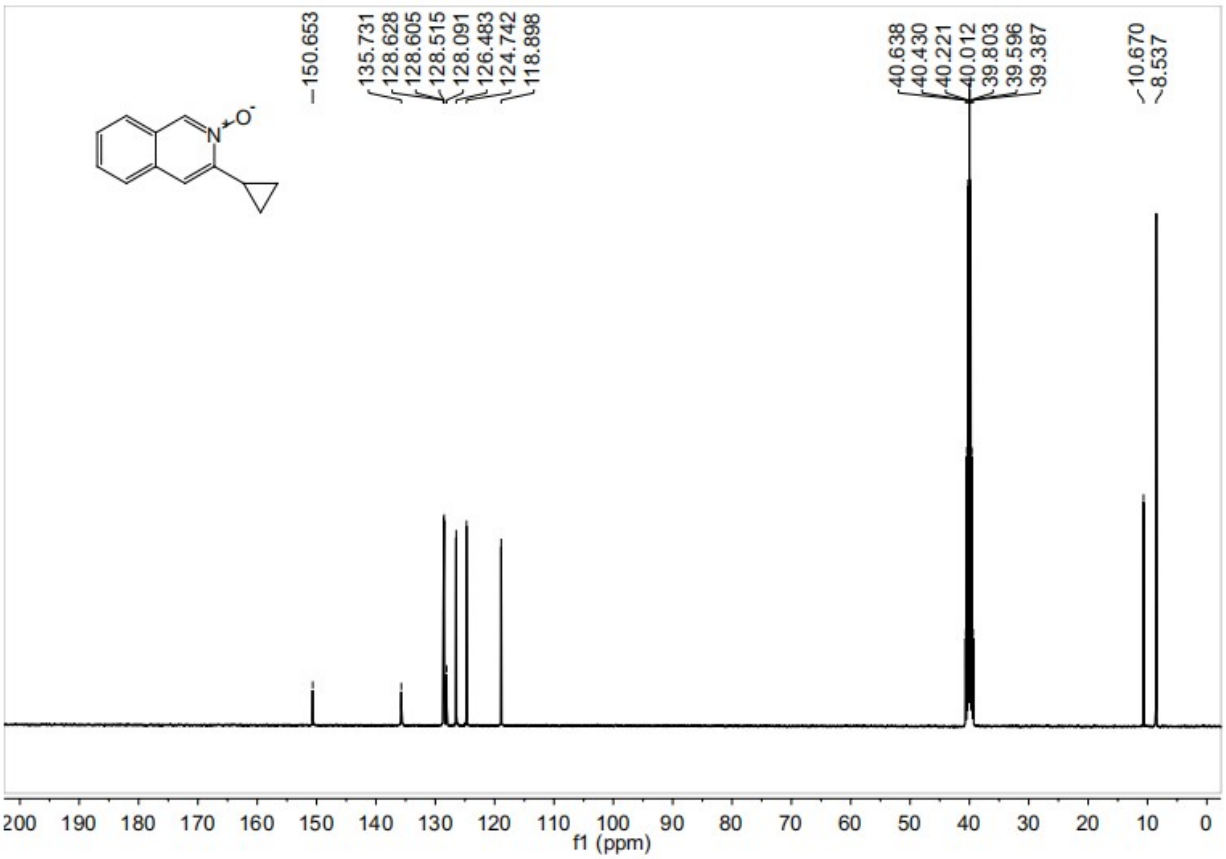
128.532
126.533
124.762
122.717
40.633
40.424
40.217
40.008
39.799
39.590
39.383
31.482
30.155
26.475
22.422
14.342
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.999
7.829
7.823
7.807
7.800
7.645
7.568
7.564
7.551
7.546
7.537
7.527
7.522
7.510
2.656
2.643
2.635
2.622
2.608
2.600
2.587
2.511
2.506
2.501
1.110
1.099
1.092
1.078
1.072
1.062
0.871
0.861
0.856
0.847
0.842
0.831
1.00
2.05
1.02
2.01
1.01
2.05
2.08
12.0 11.5 11.0 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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128.628
128.605
128.515
128.091
126.483
124.742
118.898
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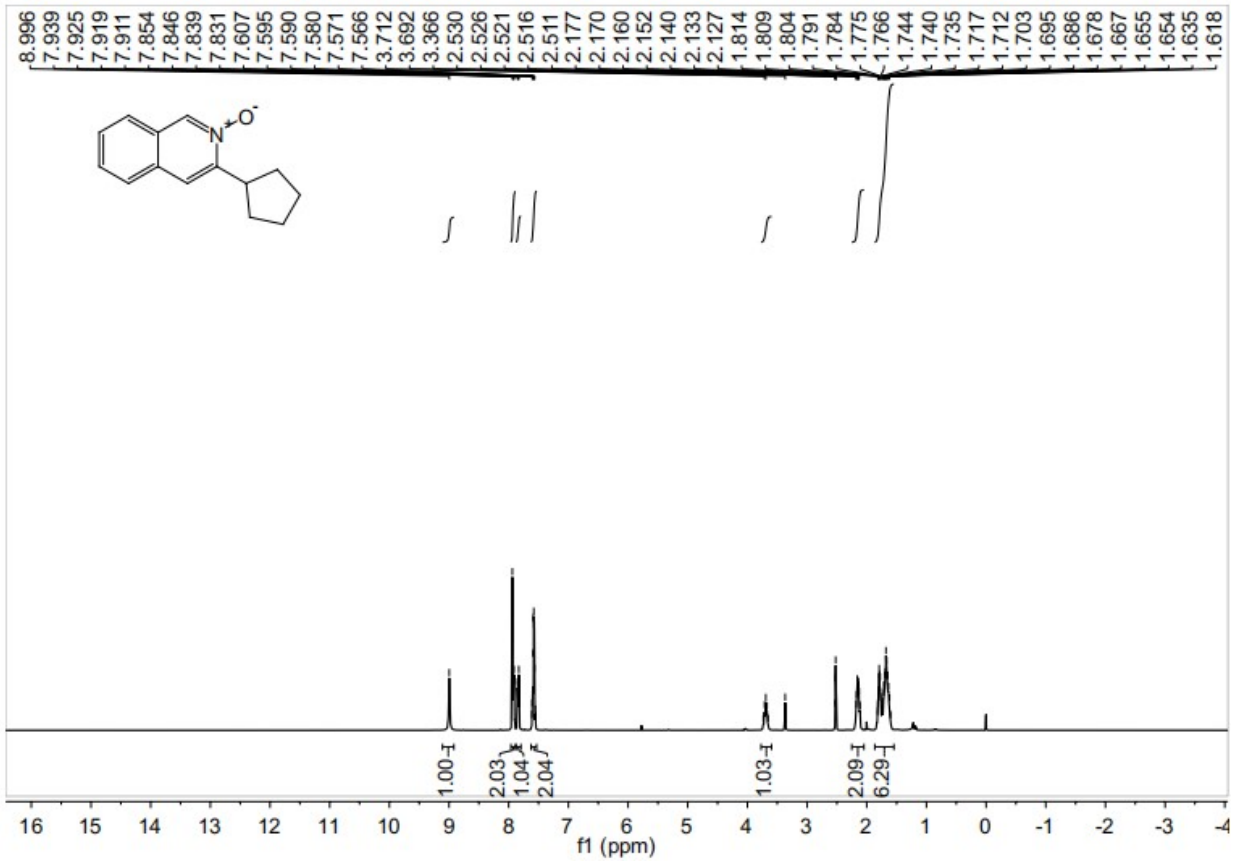
40.430
40.221
40.012
39.803
39.596
39.387
10.670
8.537
f1 (ppm)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7.919
7.911
7.854
7.846
7.839
7.831
7.607
7.595
7.590
7.580
7.571
7.566
3.712
3.692
3.366
2.530
2.526
2.521
2.516
2.511
2.177
2.170
2.160
2.152
2.140
2.133
2.127
1.814
1.809
1.804
1.791
1.784
1.775
1.766
1.744
1.740
1.735
1.717
1.712
1.703
1.695
1.686
1.678
1.667
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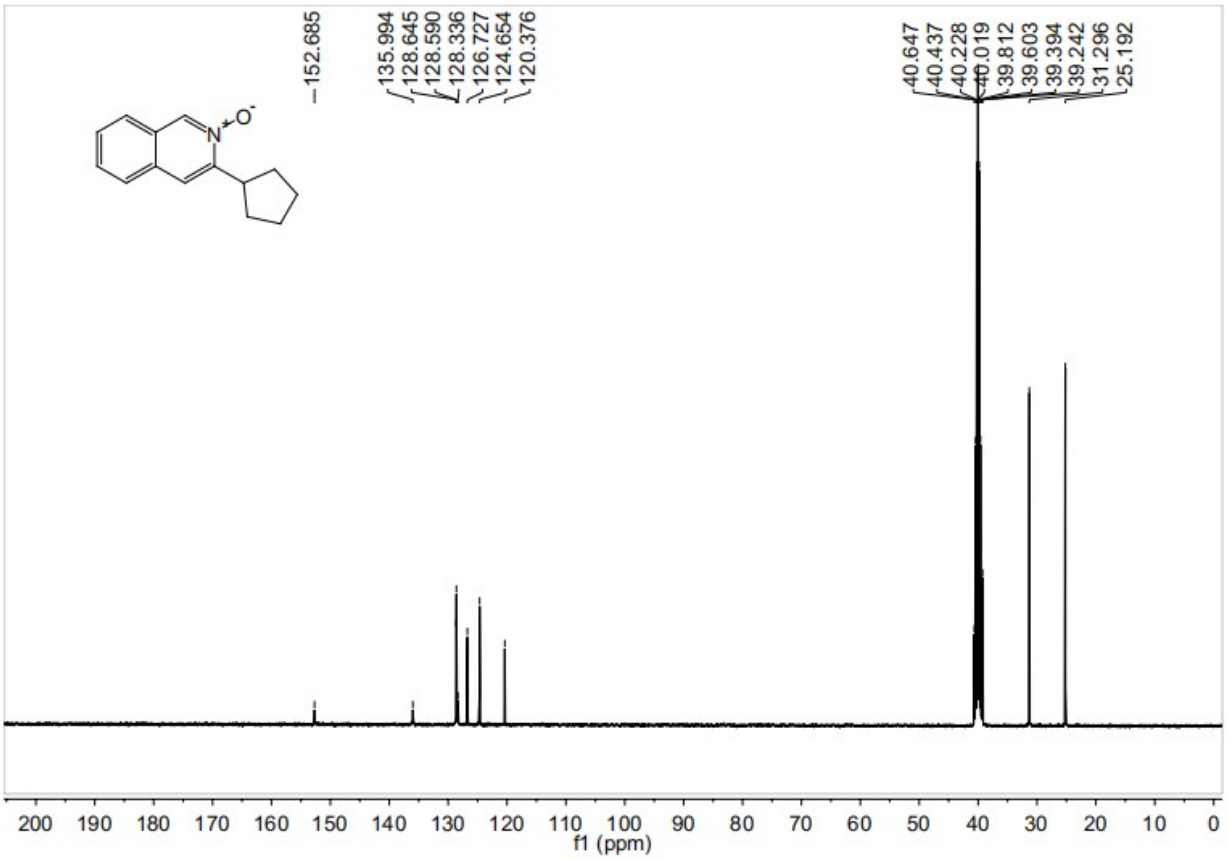
1.654
1.635
1.618
1.00
2.03
1.04
2.04
1.03
2.09
6.29
f1 (ppm)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126.727
124.654
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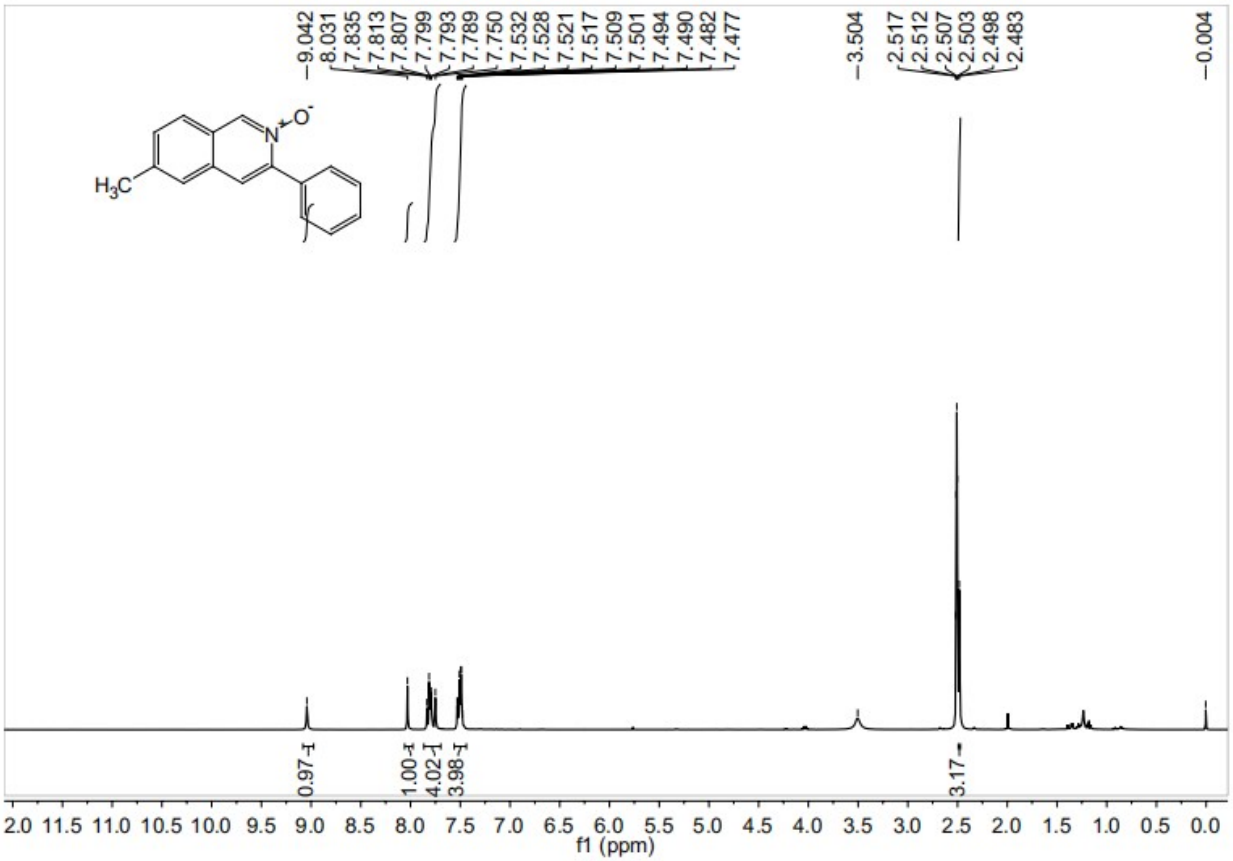
40.228
40.019
39.812
39.603
39.394
39.242
31.296
25.192
f1 (ppm)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7.789
7.750
7.532
7.528
7.521
7.517
7.509
7.501
7.494
7.490
7.482
7.477
3.504
2.517
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2.507
2.503
2.498
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0.004
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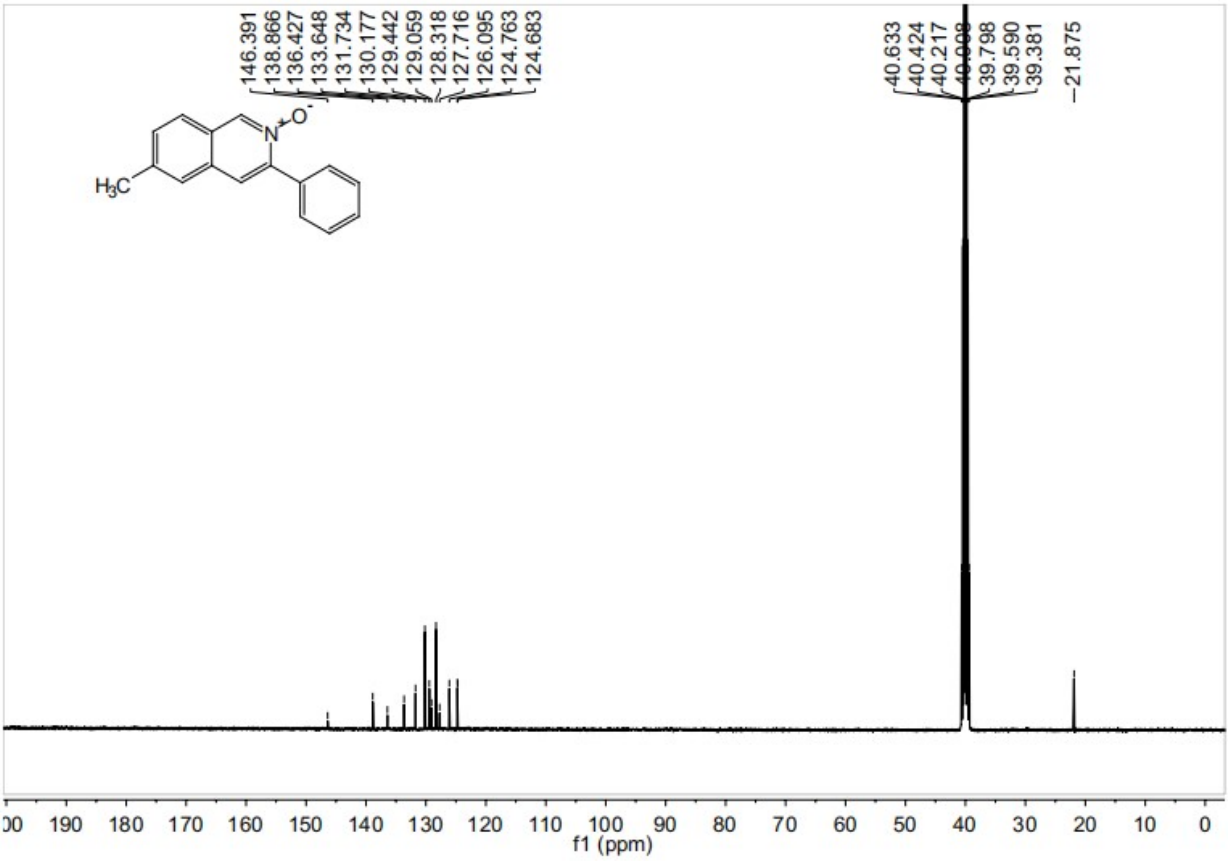
1.00
4.02
3.98
3.17
f1 (ppm)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136.427
133.648
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129.442
129.059
128.318
127.716
126.095
124.763
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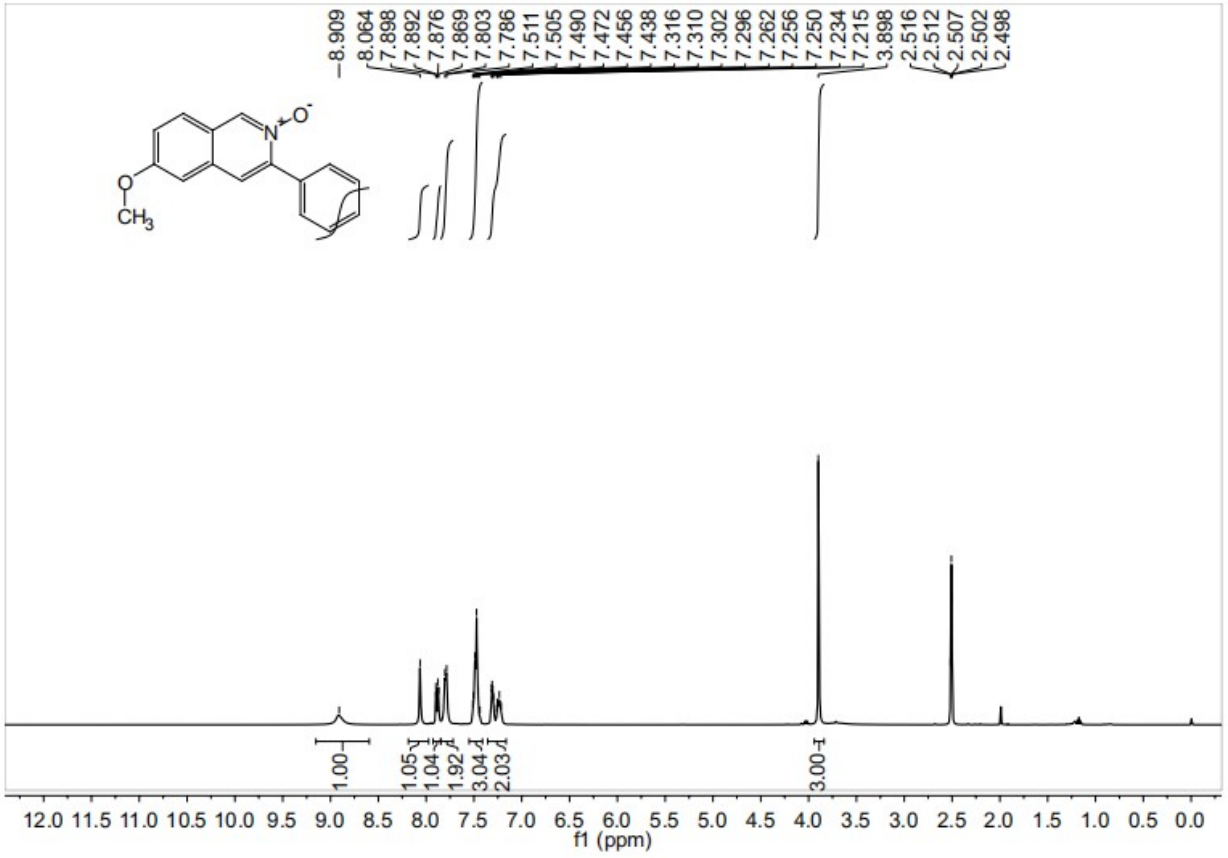
40.217
39.798
39.590
39.381
21.875
H3C
N+
O-
f1 (ppm)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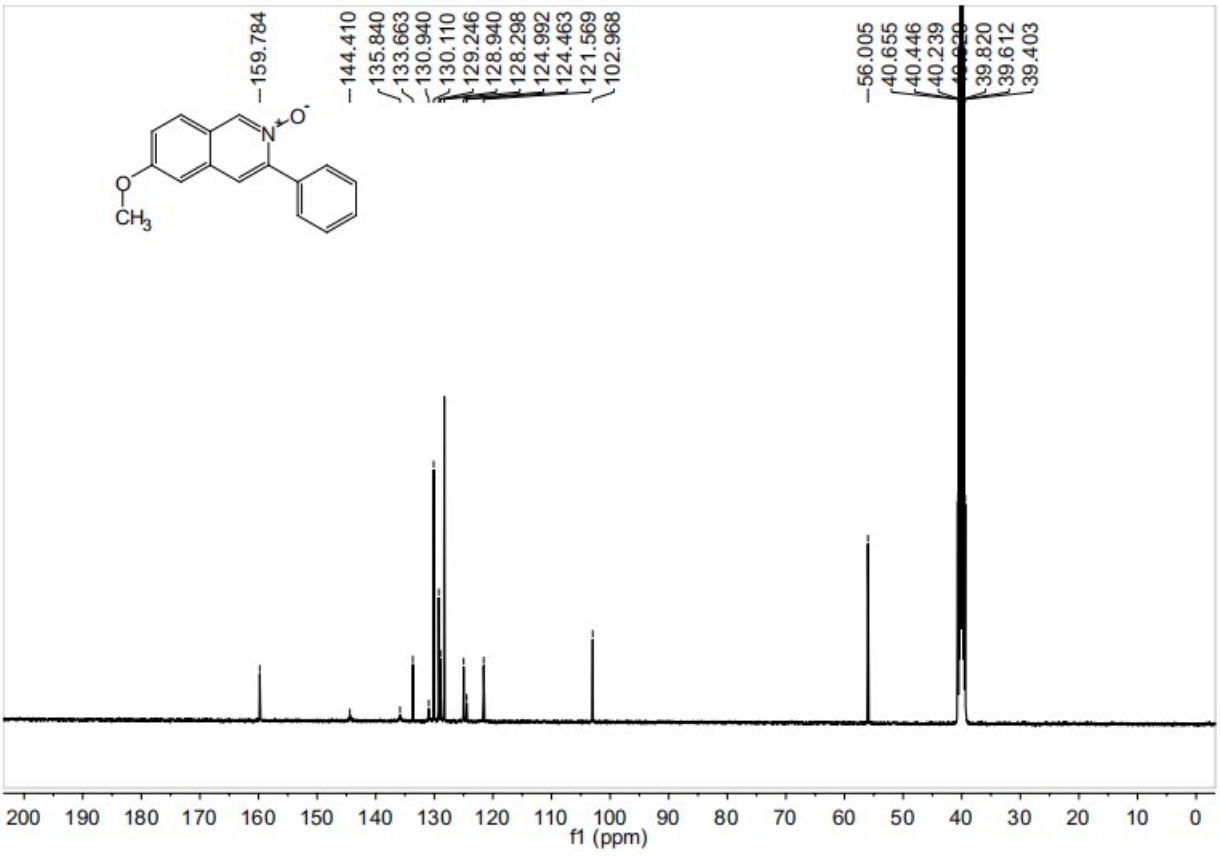
7.869
7.803
7.786
7.511
7.505
7.490
7.472
7.456
7.438
7.316
7.310
7.302
7.296
7.262
7.256
7.250
7.234
7.215
3.898
2.516
2.512
2.507
2.502
2.498
O
CH3
N+
O-
1.00
1.05
1.04
1.92
3.04
2.03
3.00
f1 (ppm)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128.940
128.298
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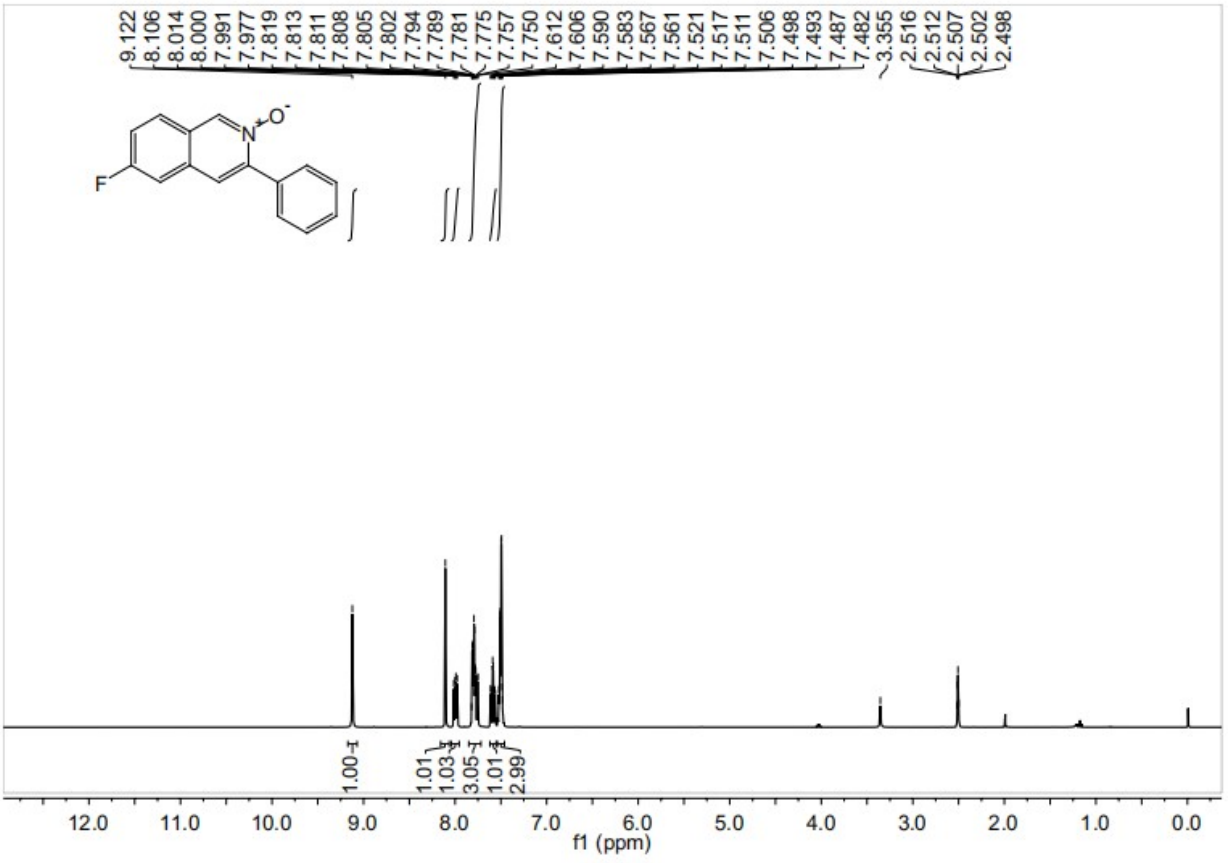
124.463
121.569
102.968
56.005
40.655
40.446
40.239
39.820
39.612
39.403
O
CH3
N+
O-
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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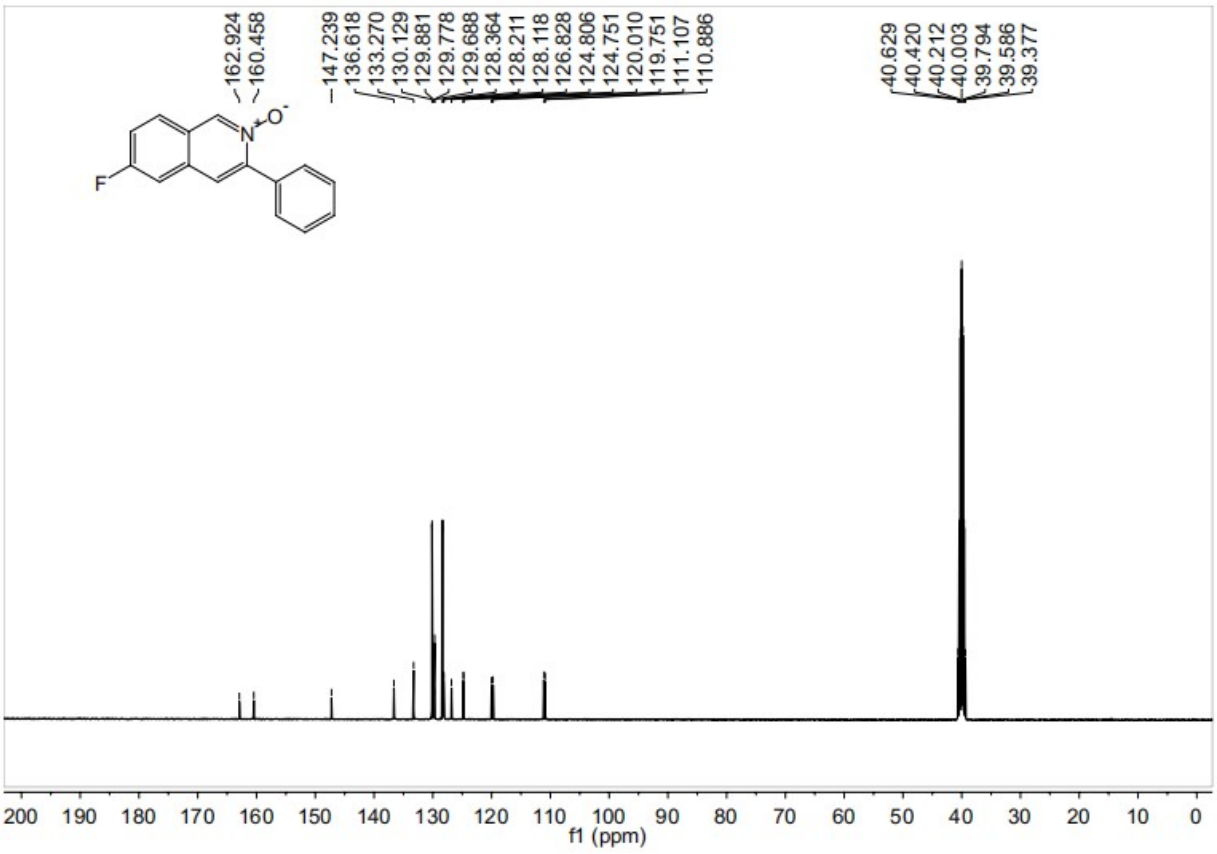
7.813
7.811
7.808
7.805
7.802
7.794
7.789
7.781
7.775
7.757
7.750
7.612
7.606
7.590
7.583
7.567
7.561
7.521
7.517
7.511
7.506
7.498
7.493
7.487
7.482
3.355
2.516
2.512
2.507
2.502
2.498
F
N+
O-
1.00
1.01
1.03
3.05
1.01
2.99
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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129.778
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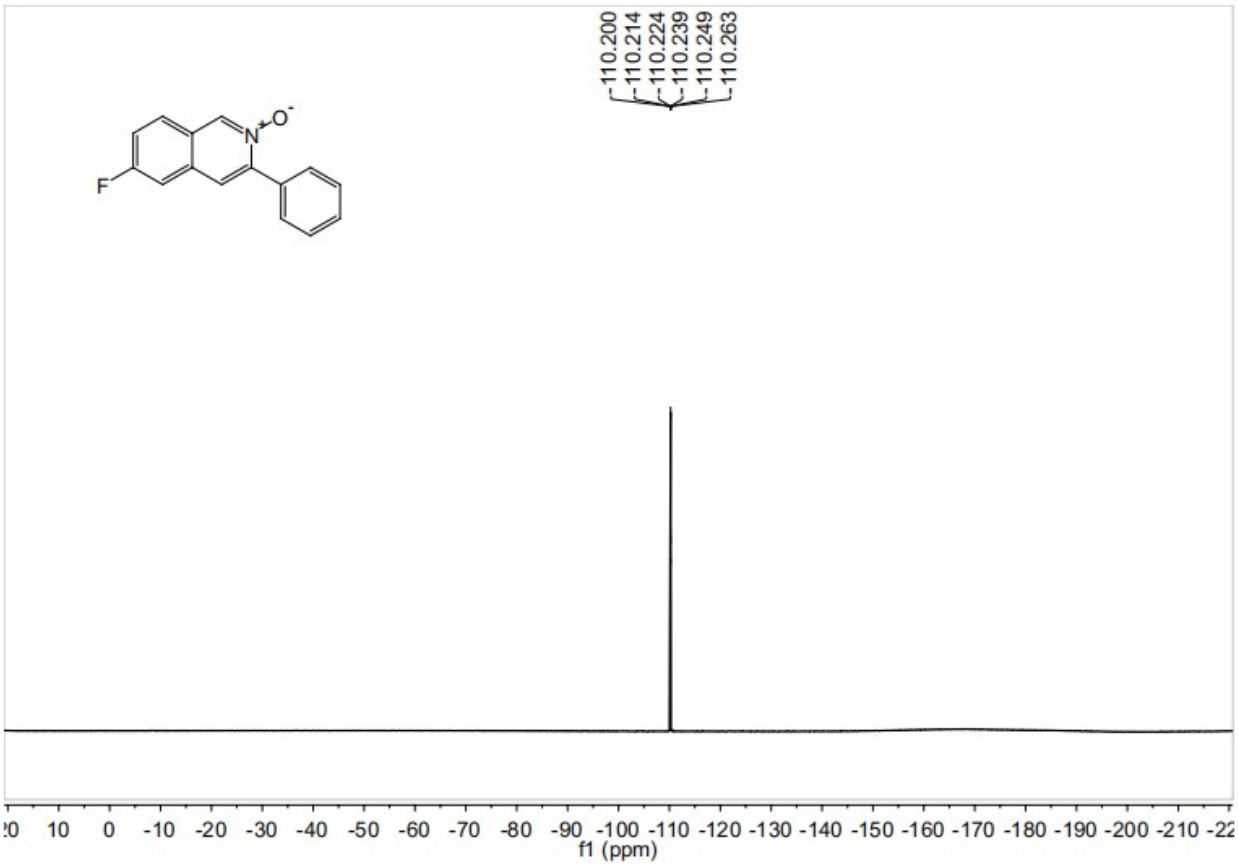
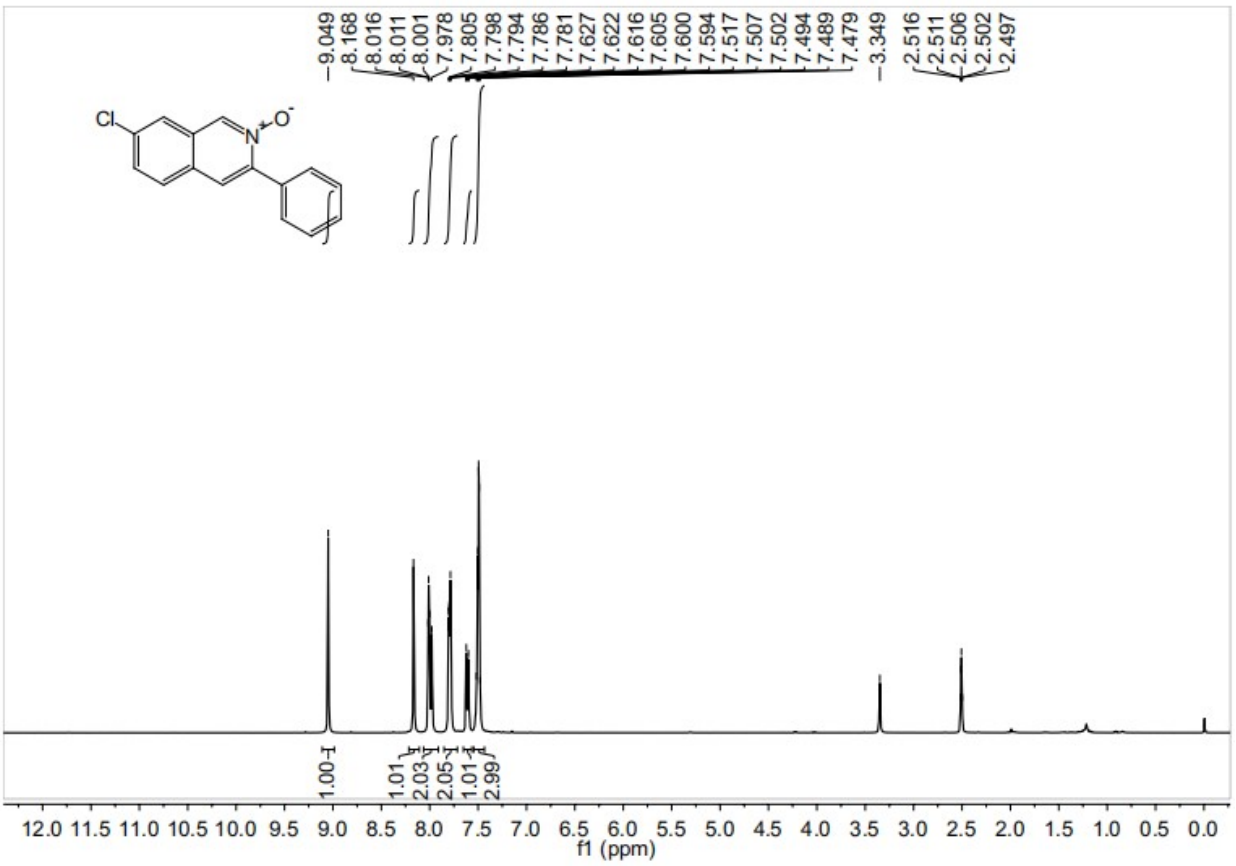
128.211
128.118
126.828
124.806
124.751
120.010
119.751
111.107
110.886
40.629
40.420
40.212
40.003
39.794
39.586
39.377
F
N+
O-
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


110.200
110.214
110.224
110.239
110.249
110.263
F
N+
O-
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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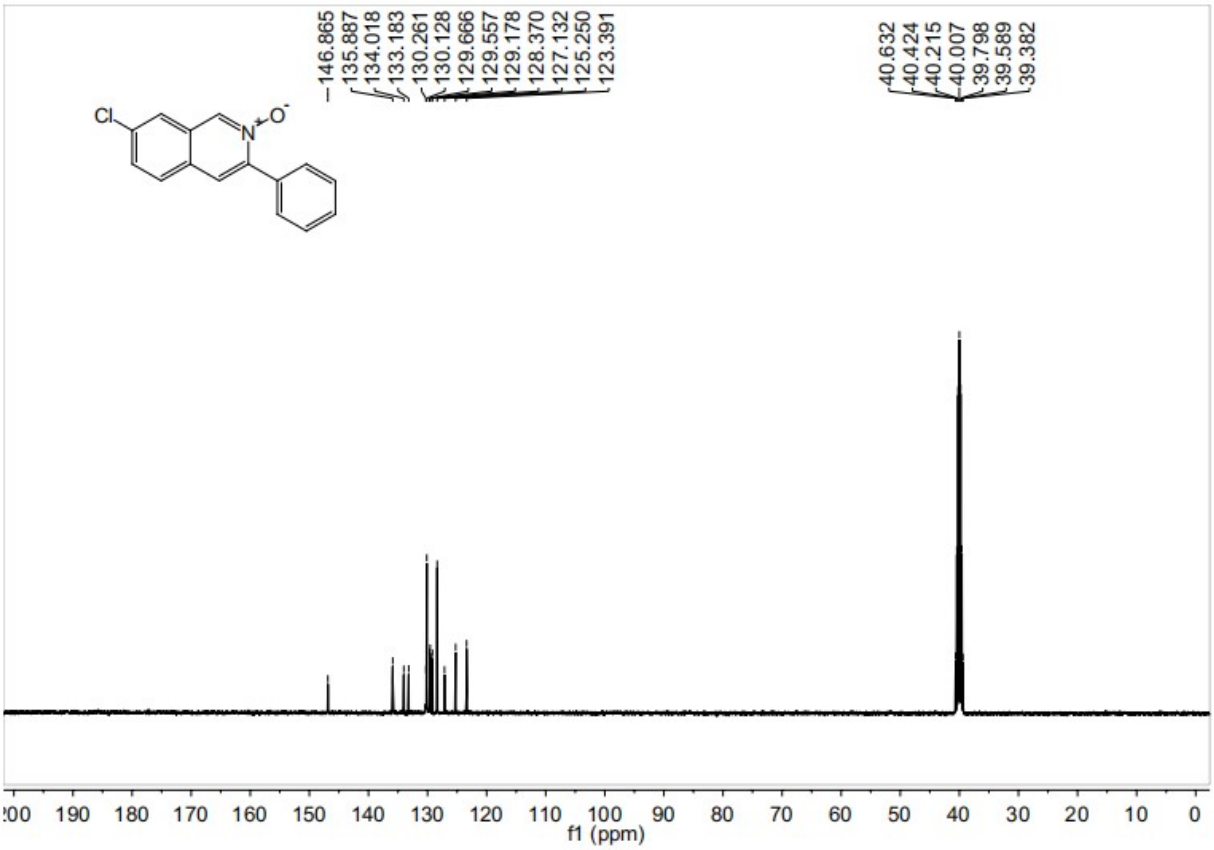
7.622
7.616
7.605
7.600
7.594
7.517
7.507
7.502
7.494
7.489
7.479
3.349
2.516
2.511
2.506
2.502
2.497
Cl
N
O
1.00
1.01
2.03
2.05
1.01
2.99
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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134.018
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130.128
129.666
129.557
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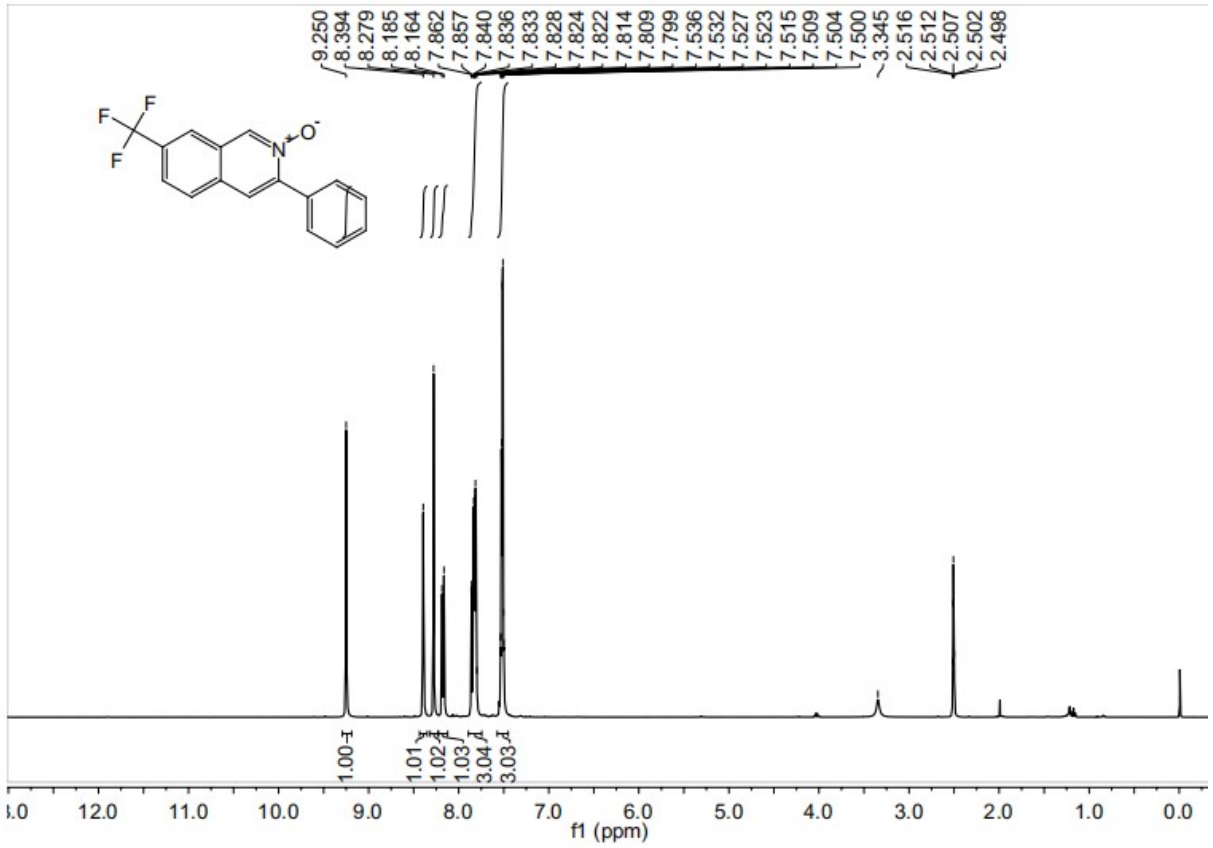
128.370
127.132
125.250
123.391
40.632
40.424
40.215
40.007
39.798
39.589
39.382
Cl
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.164
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7.857
7.840
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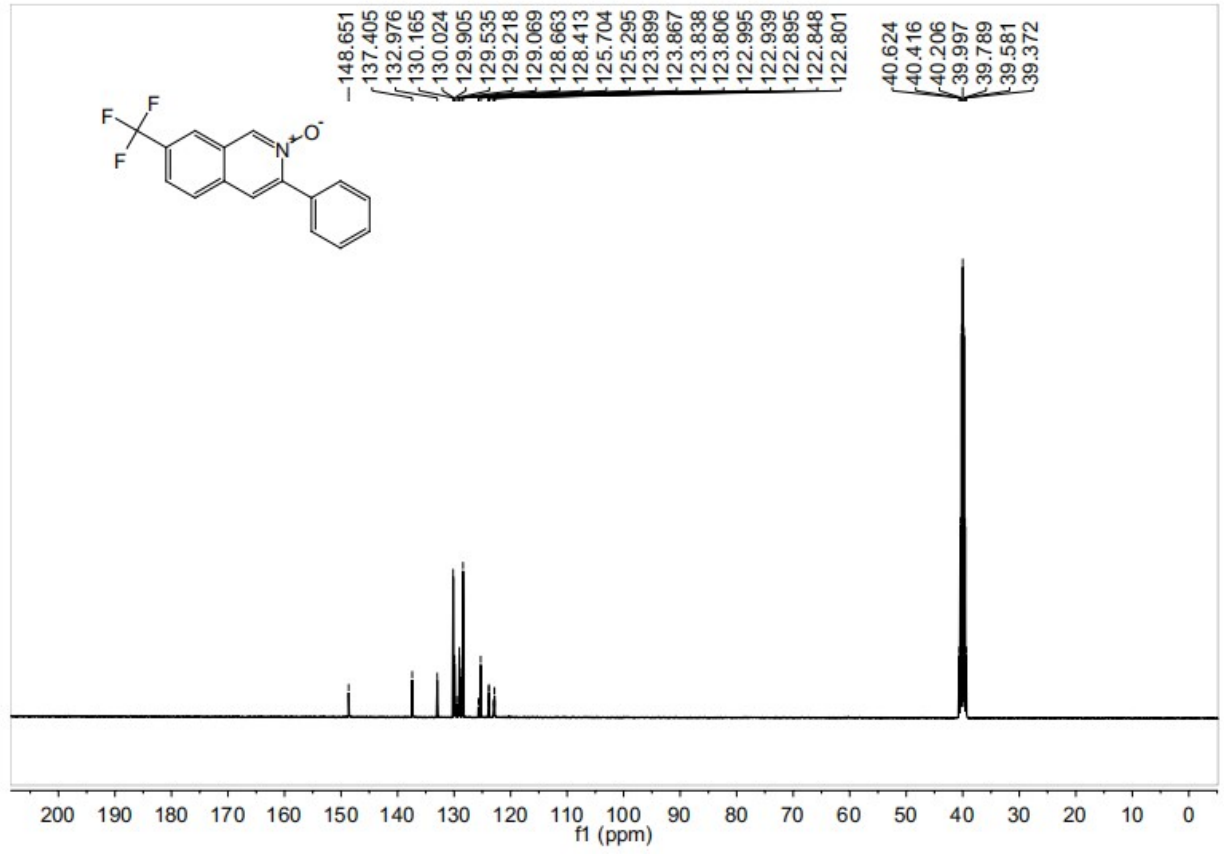
7.833
7.828
7.824
7.822
7.814
7.809
7.799
7.536
7.532
7.527
7.523
7.515
7.509
7.504
7.500
3.345
2.516
2.512
2.507
2.502
2.498
F
F
F
N
O
1.00
1.01
1.02
1.03
3.04
3.03
f1 (ppm)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128.413
125.704
125.295
123.899
123.867
123.838
123.806
122.995
122.939
122.895
122.848
122.801
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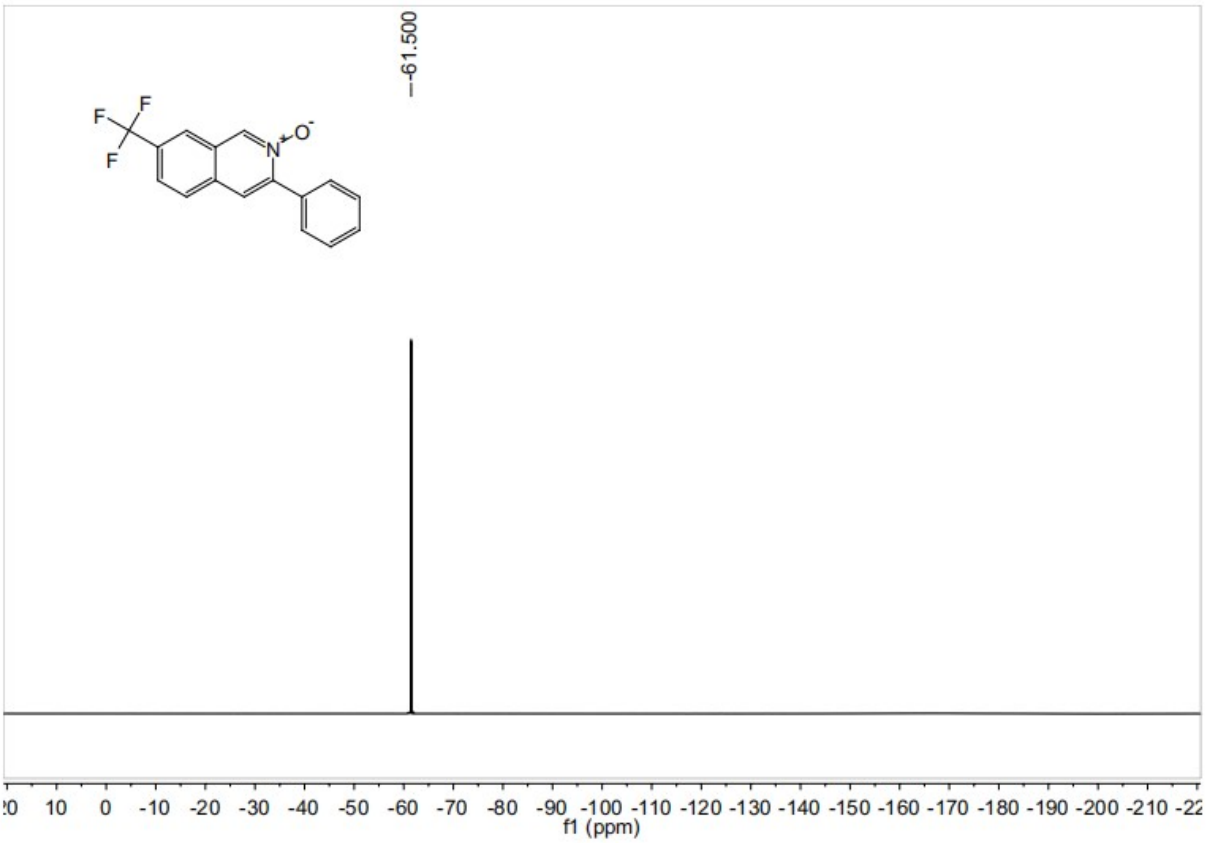
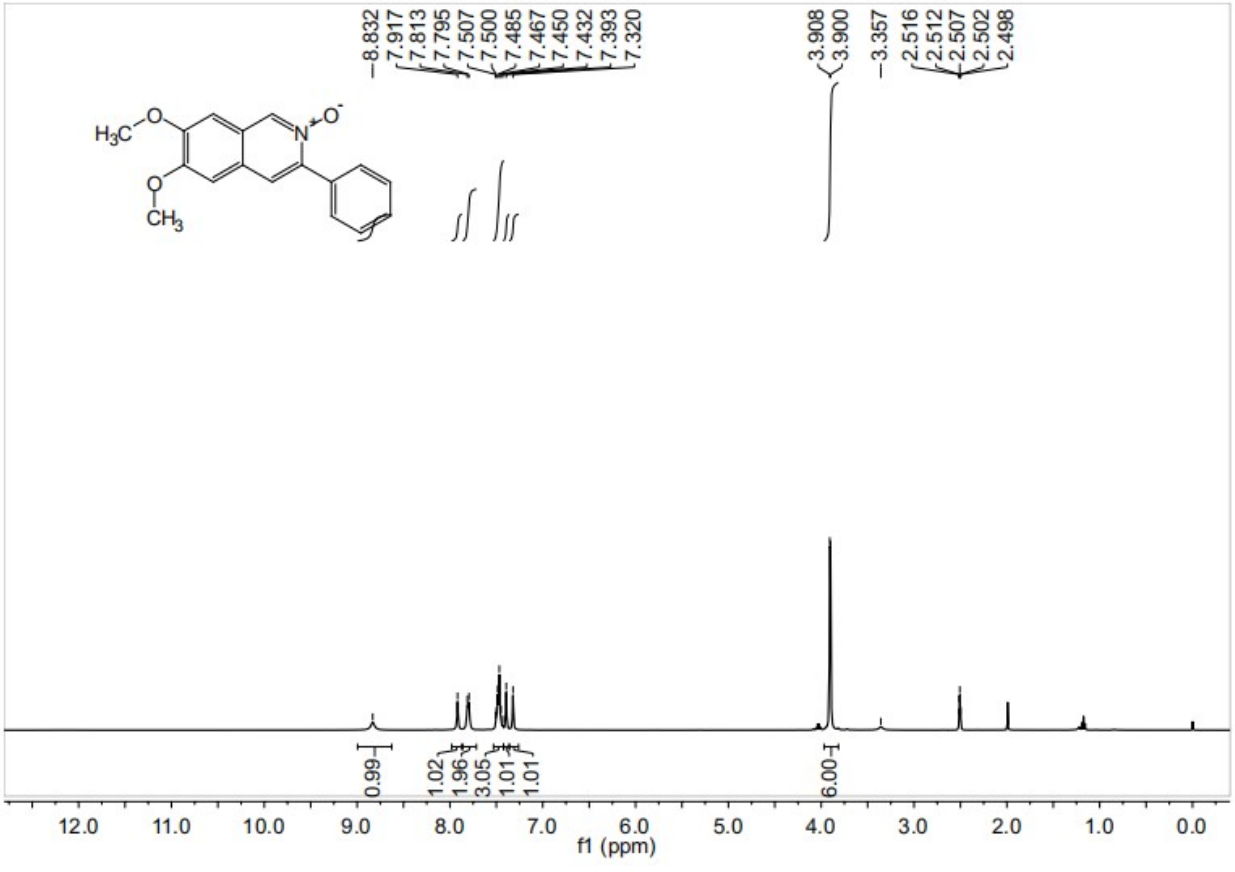
40.416
40.206
39.997
39.789
39.581
39.372
F
F
F
N
O
f1 (ppm)


-61.500
F
F
F
N+
O-
:0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22
f1 (ppm)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7.917
7.813
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7.507
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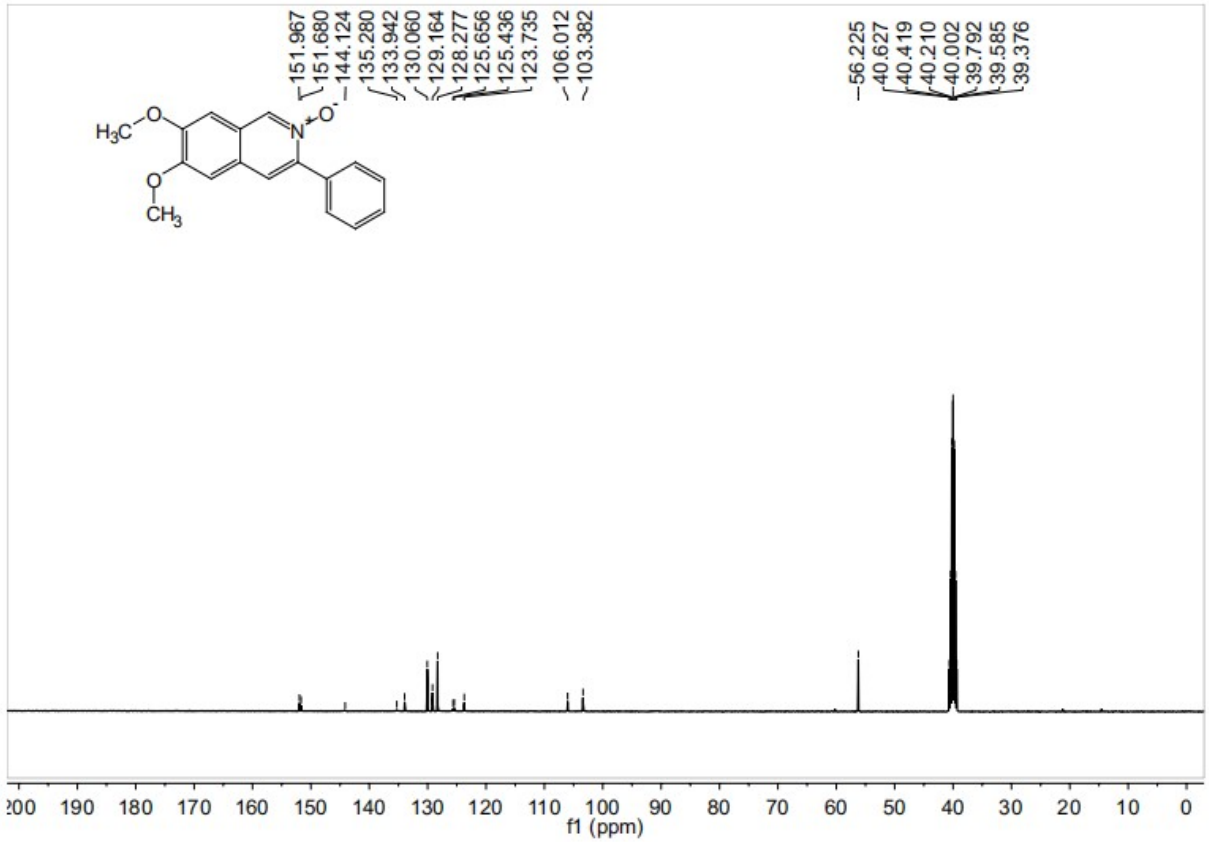
7.485
7.467
7.450
7.432
7.393
7.320
3.908
3.900
3.357
2.516
2.512
2.507
2.502
2.498
H3C
O
N+
O-
O
CH3
0.99
1.02
1.96
3.05
1.01
1.01
6.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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151.680
144.124
135.280
133.942
130.060
129.164
128.277
125.656
125.436
123.735
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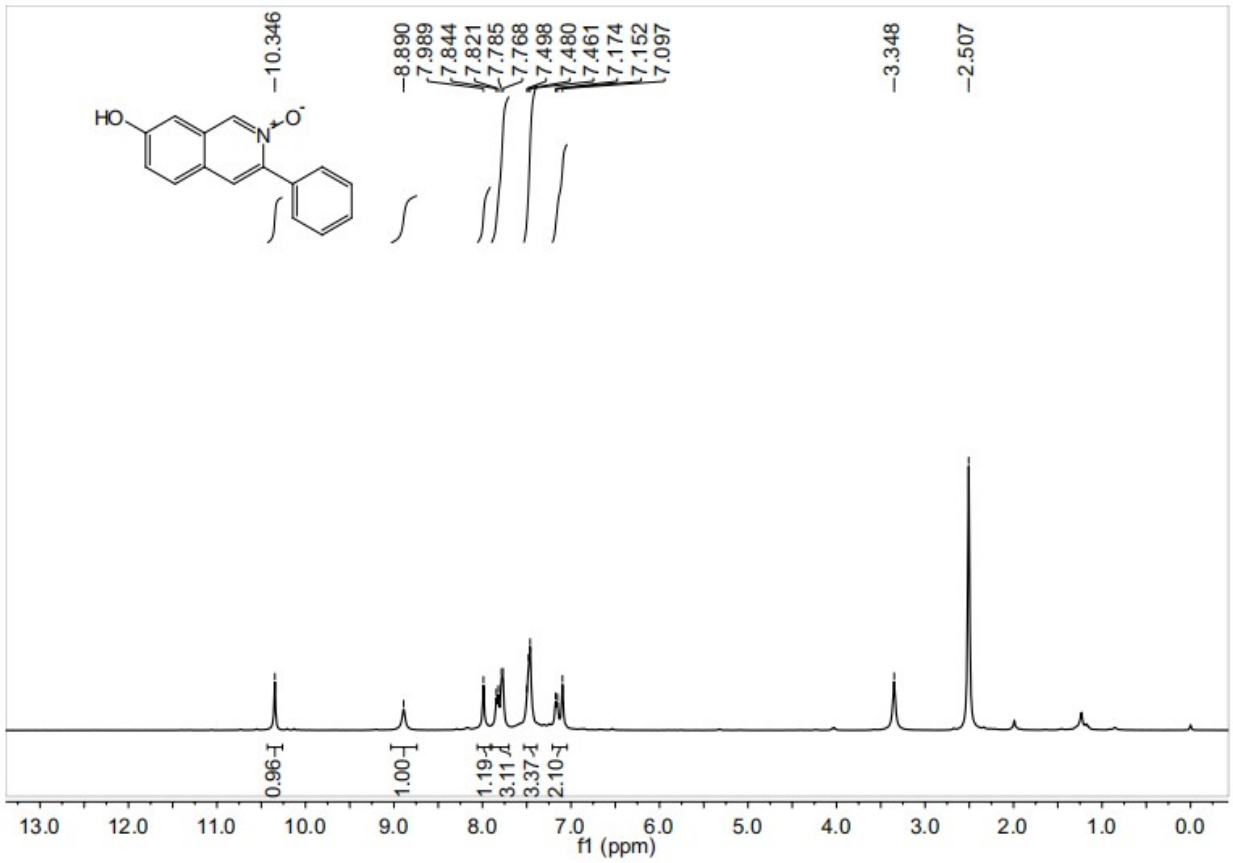
103.382
56.225
40.627
40.419
40.210
40.002
39.792
39.585
39.376
H3C
O
N+
O-
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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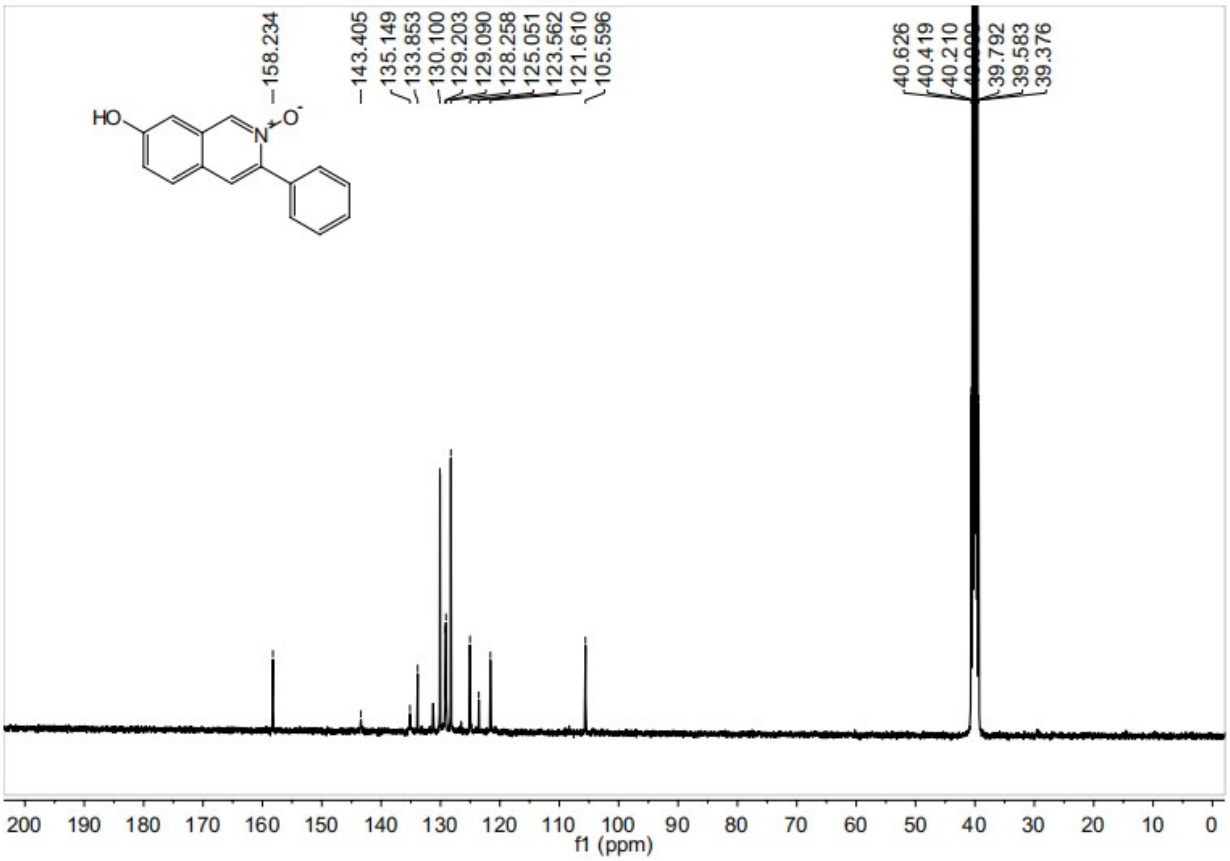
8.890
7.989
7.844
7.821
7.785
7.768
7.498
7.480
7.461
7.174
7.152
7.097
3.348
2.507
HO
N+
O-
0.96
1.00
1.19
3.11
3.37
2.10
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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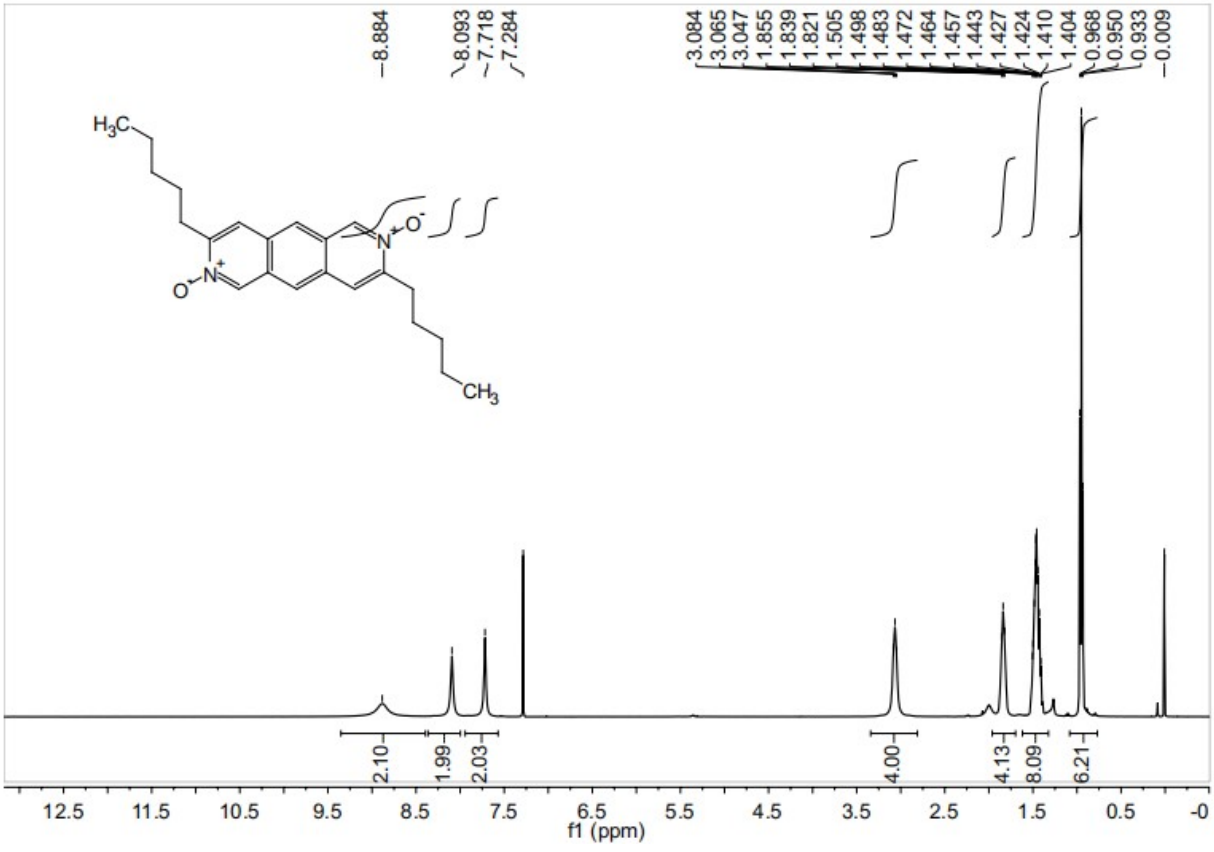
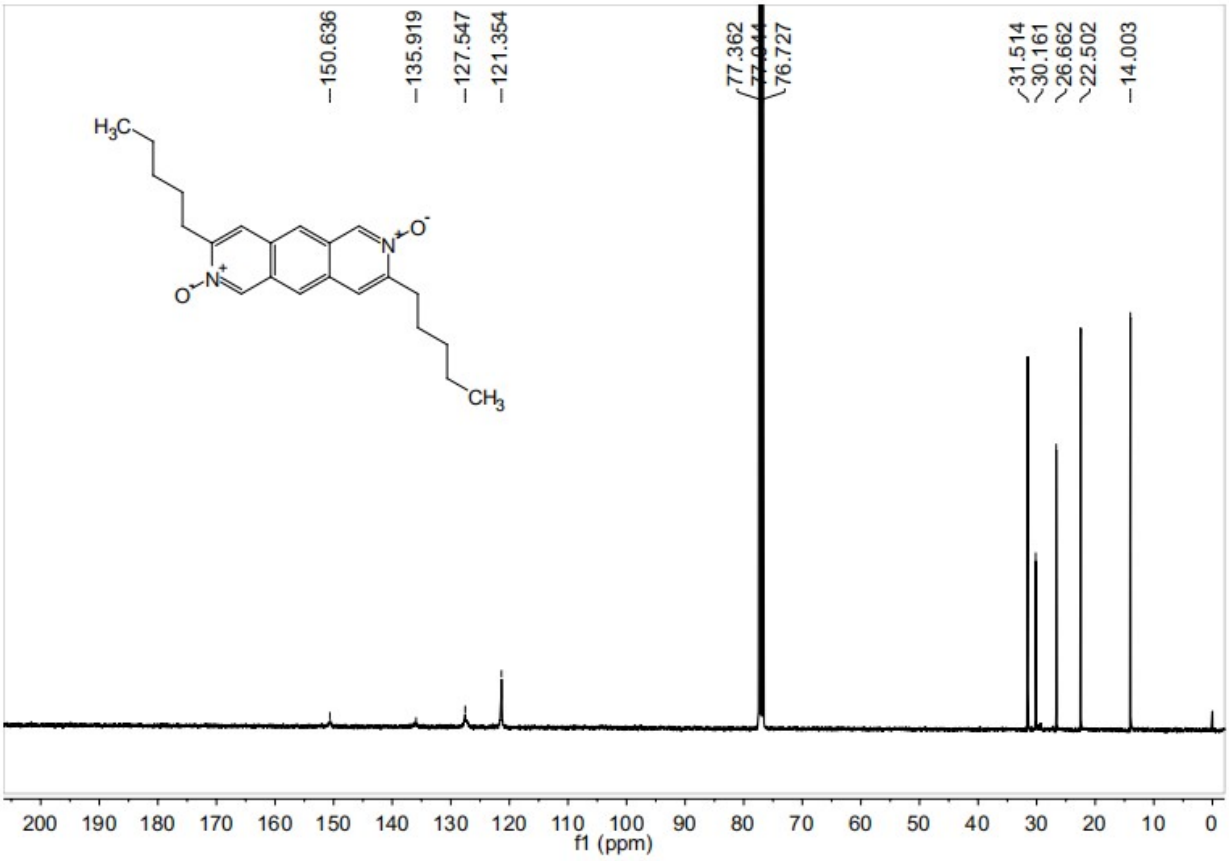
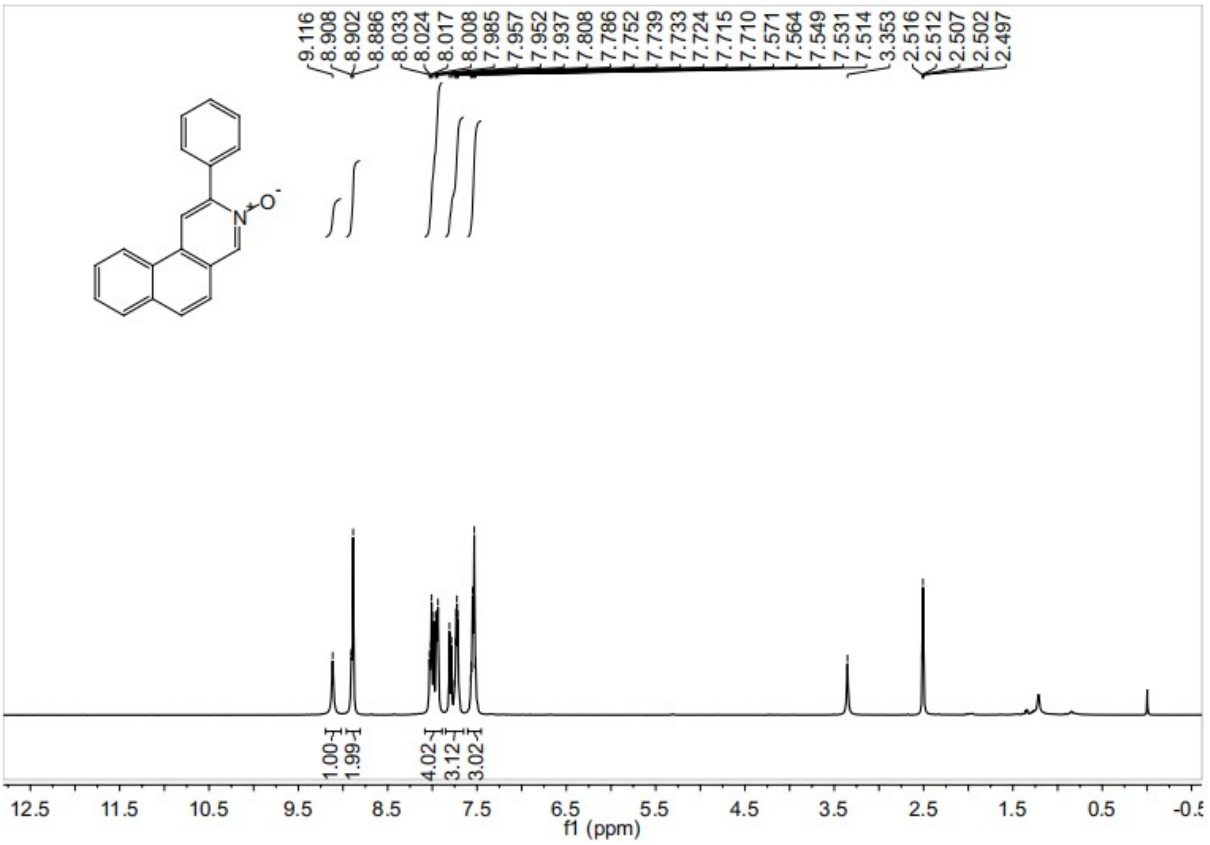
143.405
135.149
133.853
130.100
129.203
129.090
128.258
125.051
123.562
121.610
105.596
40.626
40.419
40.210
39.792
39.583
39.376
HO
N+
O-
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.884
8.093
7.718
7.284
3.084
3.065
3.047
1.855
1.839
1.821
1.505
1.498
1.483
1.472
1.464
1.457
1.443
1.427
1.424
1.410
1.404
0.968
0.950
0.933
-0.009
H3C
CH3
N+
O-
2.10
1.99
2.03
4.00
4.13
8.09
6.21
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0
f1 (ppm)


150.636
135.919
127.547
121.354
77.362
77.044
76.727
31.514
30.161
26.662
22.502
14.003
H3C
CH3
f1 (ppm)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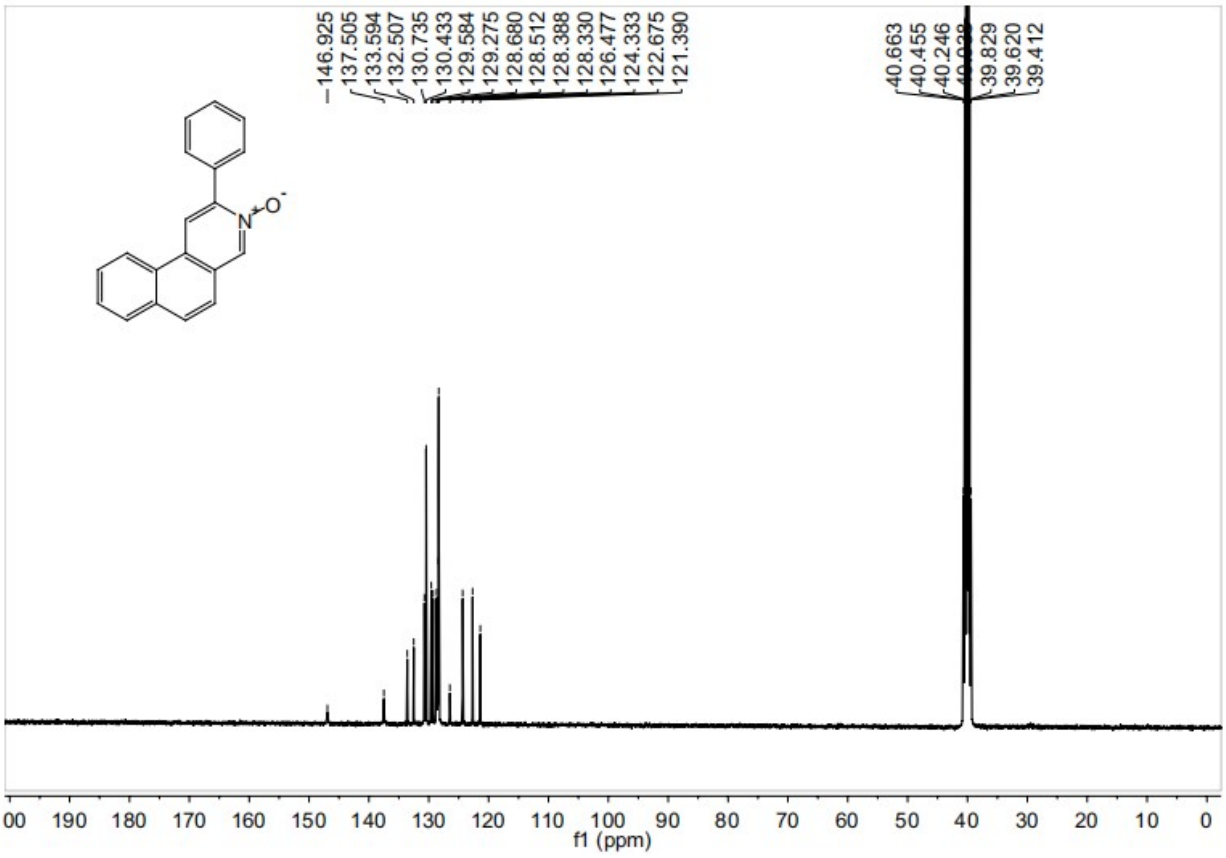
8.908
8.902
8.886
8.033
8.024
8.017
8.008
7.985
7.957
7.952
7.937
7.808
7.786
7.752
7.739
7.733
7.724
7.715
7.710
7.571
7.564
7.549
7.531
7.514
3.353
2.516
2.512
2.507
2.502
2.497
1.00
1.99
4.02
3.12
3.02
f1 (ppm)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130.735
130.433
129.584
129.275
128.680
128.512
128.388
128.330
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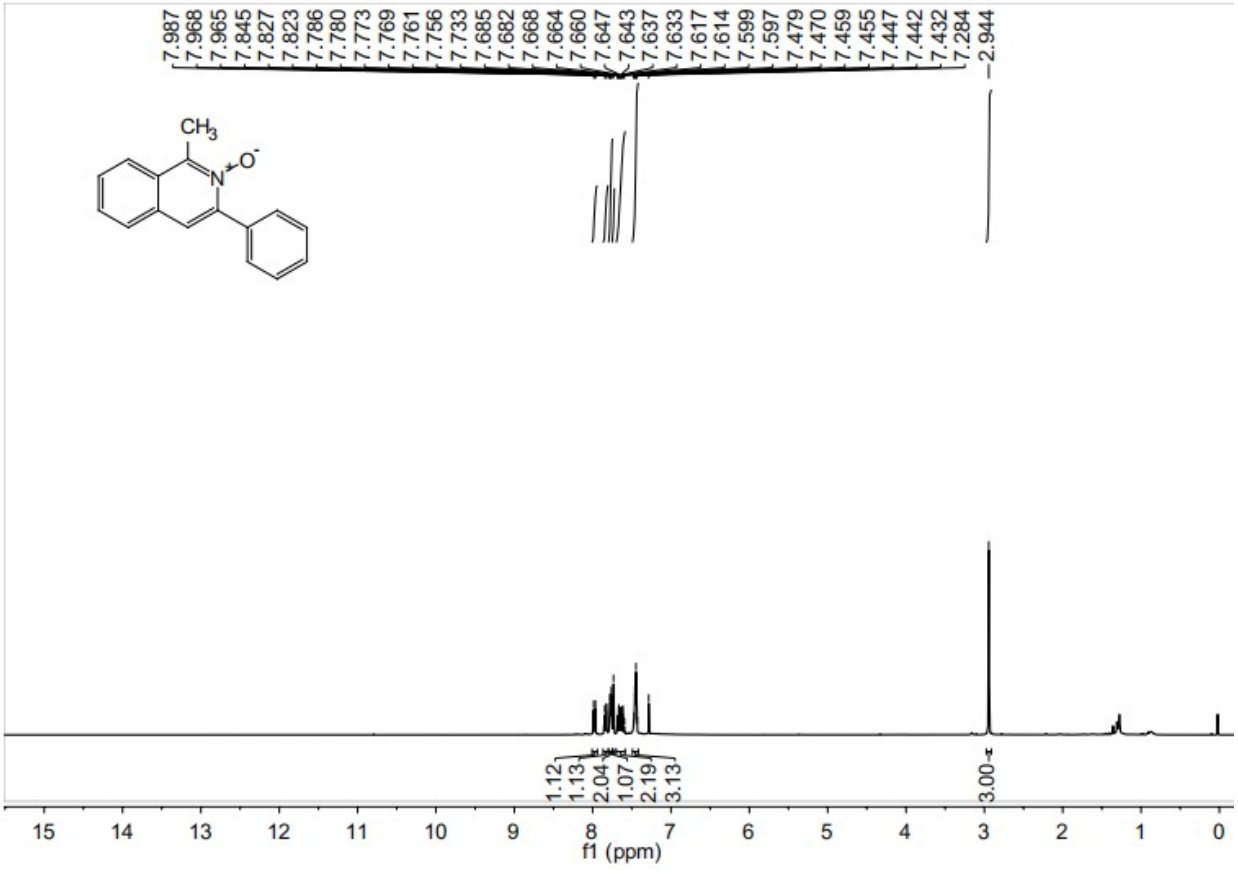
122.675
121.390
40.663
40.455
40.246
39.829
39.620
39.412
f1 (ppm)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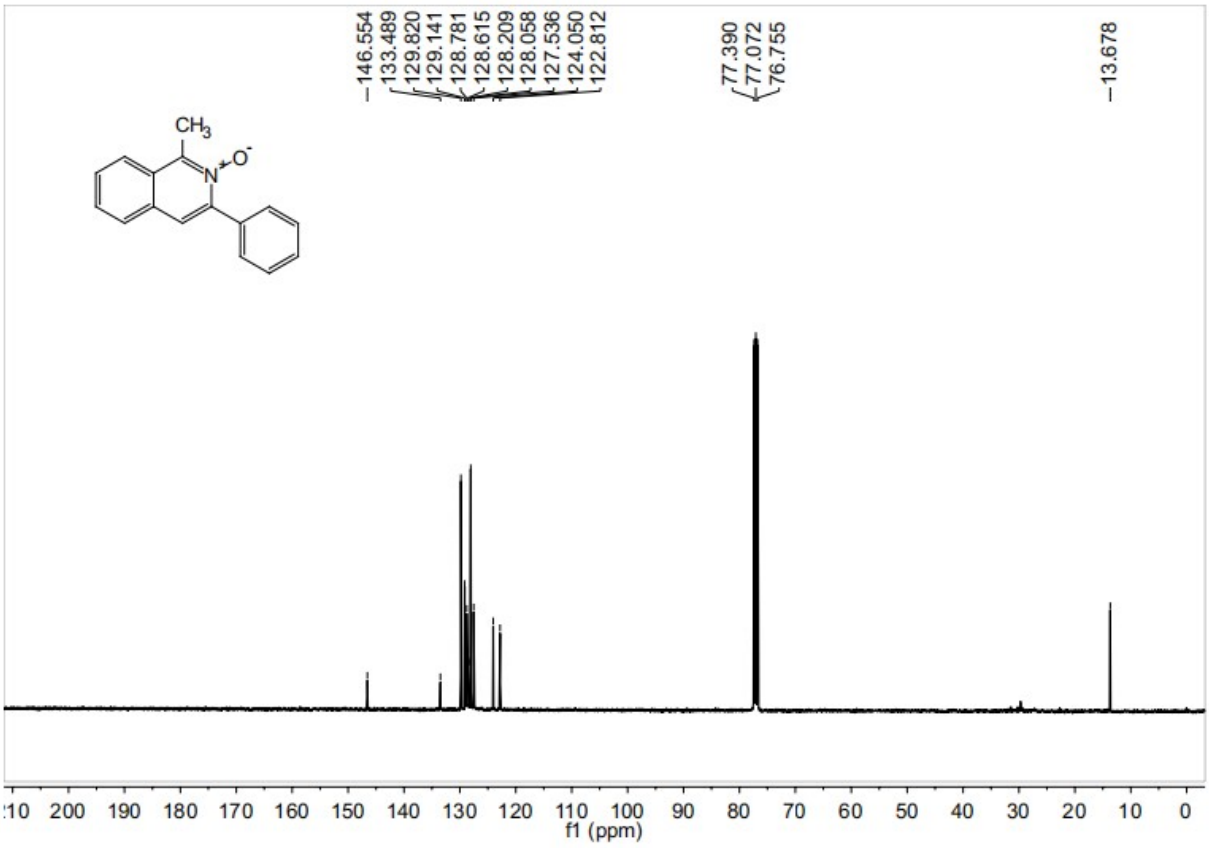
7.968
7.965
7.845
7.827
7.823
7.786
7.780
7.773
7.769
7.761
7.756
7.733
7.685
7.682
7.668
7.664
7.660
7.647
7.643
7.637
7.633
7.617
7.614
7.599
7.597
7.479
7.470
7.459
7.455
7.447
7.442
7.432
7.284
2.944
1.12
1.13
2.04
1.07
2.19
3.13
3.00
f1 (ppm)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128.615
128.209
128.058
127.536
124.050
122.812
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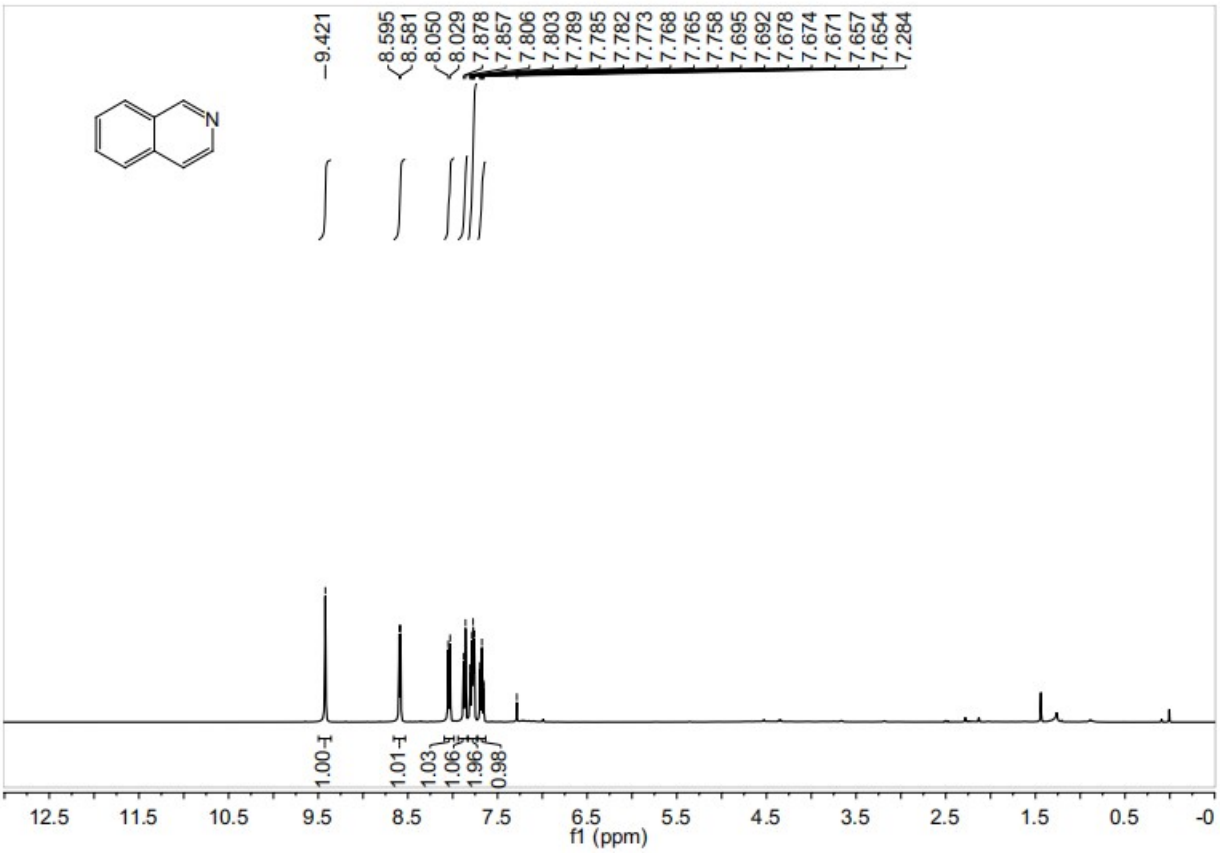
77.072
76.755
13.678
CH3
N+
O-
f1 (ppm)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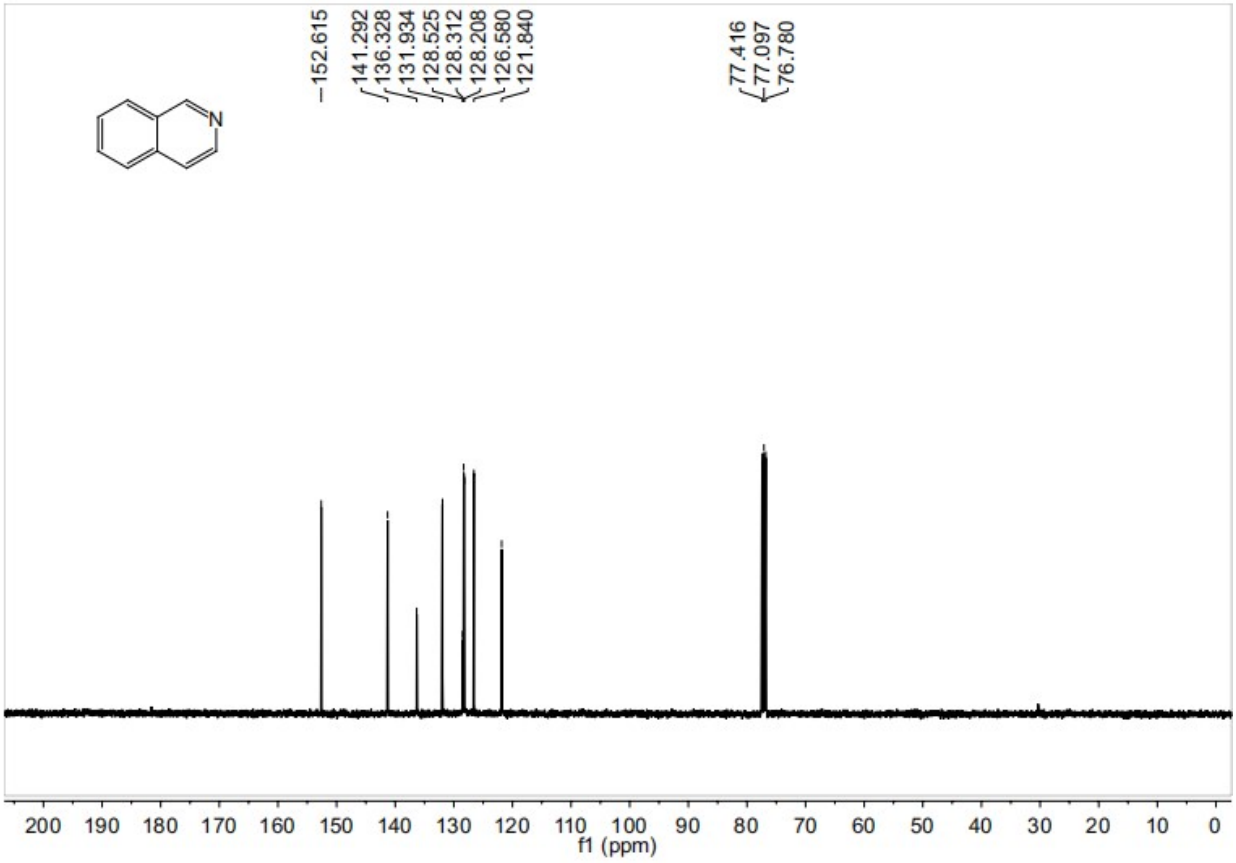
8.581
8.050
8.029
7.878
7.857
7.806
7.803
7.789
7.785
7.782
7.773
7.768
7.765
7.758
7.695
7.692
7.678
7.674
7.671
7.657
7.654
7.284
N
1.00
1.01
1.03
1.06
1.96
0.98
f1 (ppm)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128.525
128.312
128.208
126.580
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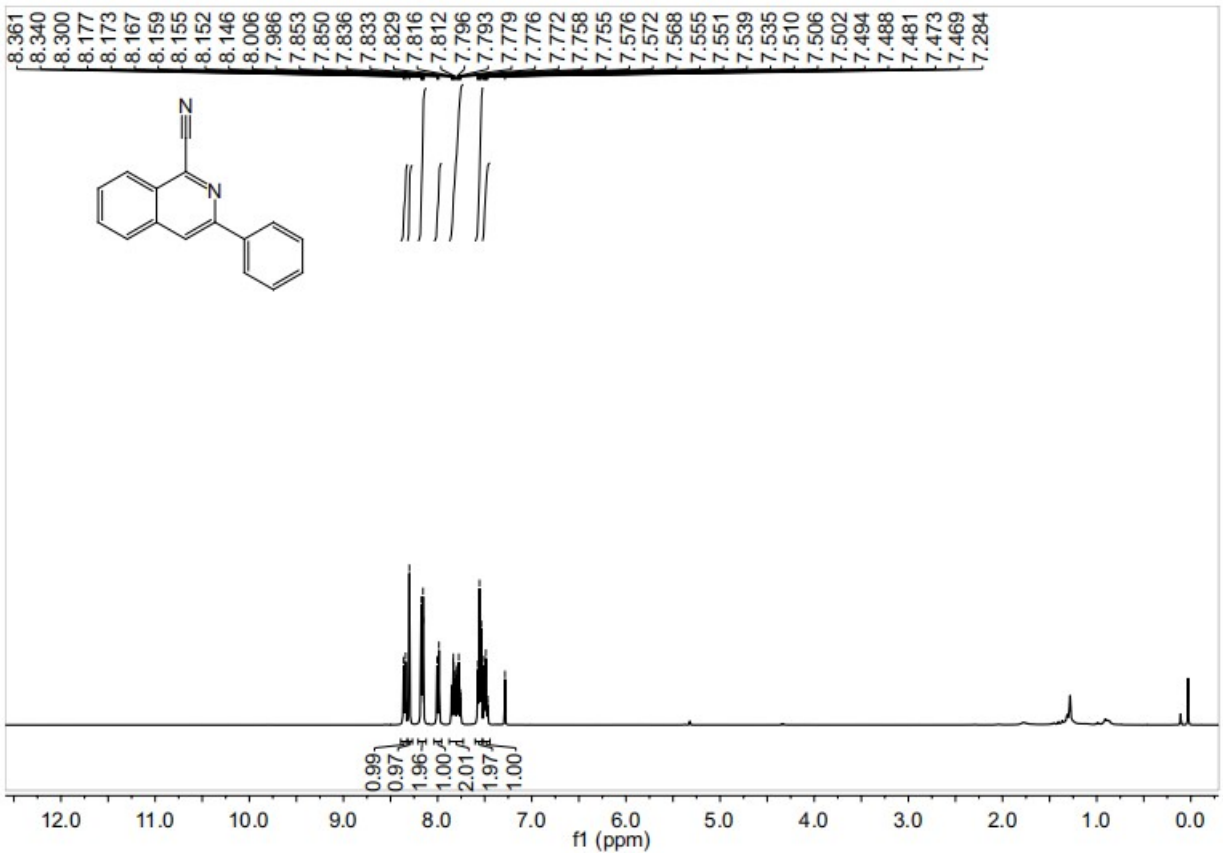
77.416
77.097
76.780
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.006
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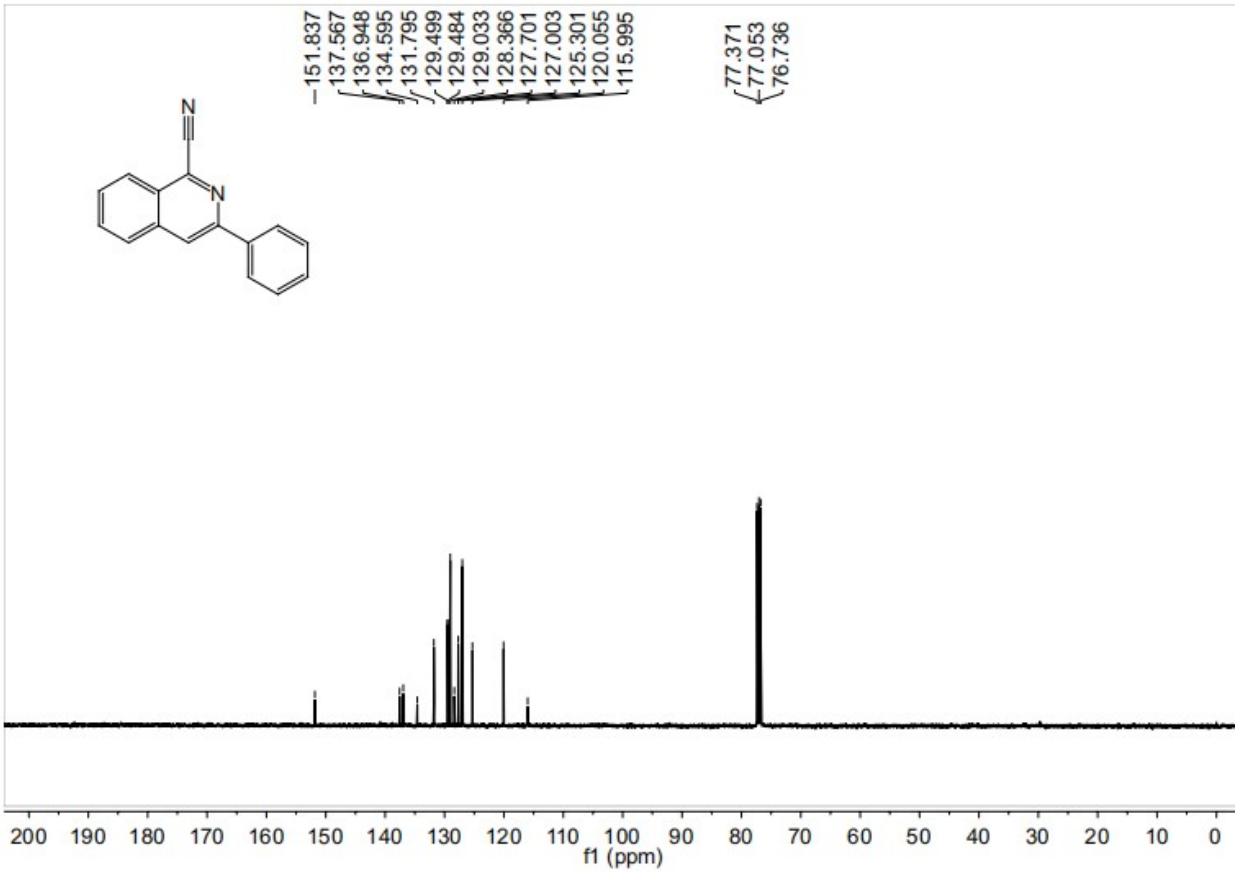
7.853
7.850
7.836
7.833
7.829
7.816
7.812
7.796
7.793
7.779
7.776
7.772
7.758
7.755
7.576
7.572
7.568
7.555
7.551
7.539
7.535
7.510
7.506
7.502
7.494
7.488
7.481
7.473
7.469
7.284
N
N
0.99
0.97
1.96
1.00
2.01
1.97
1.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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128.366
127.701
127.003
125.301
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115.995
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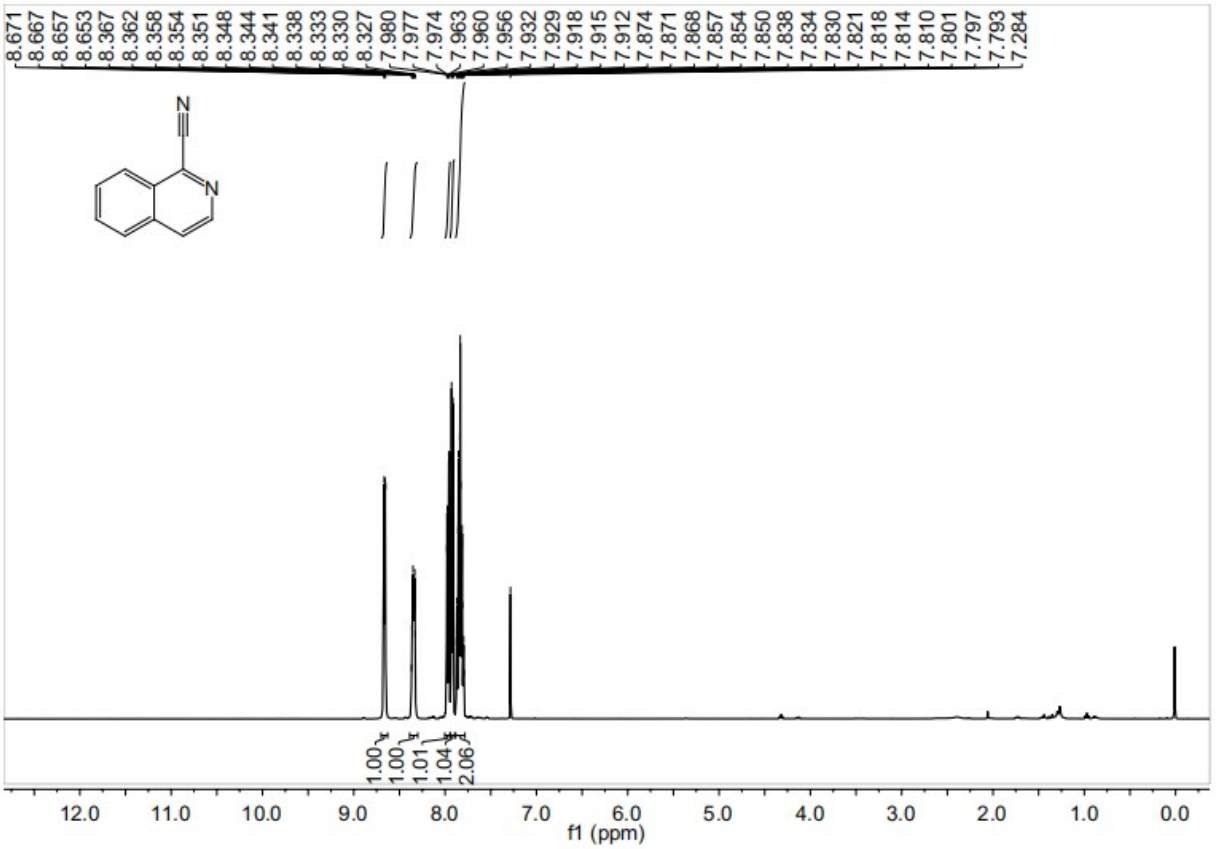
77.053
76.736
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.338
8.333
8.330
8.327
7.980
7.977
7.974
7.963
7.960
7.956
7.932
7.929
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7.915
7.912
7.874
7.871
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7.857
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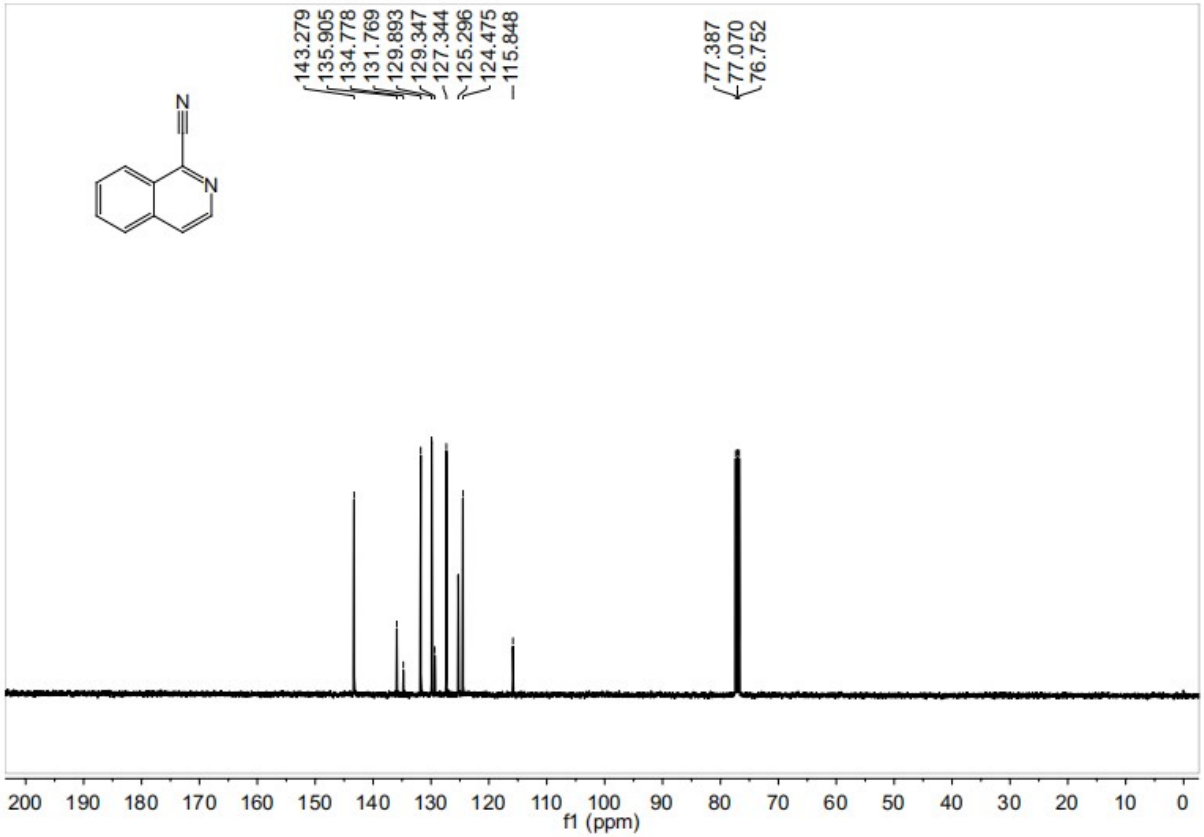
7.850
7.838
7.834
7.830
7.821
7.818
7.814
7.810
7.801
7.797
7.793
7.284
N
N
1.00
1.00
1.01
1.04
2.06
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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125.296
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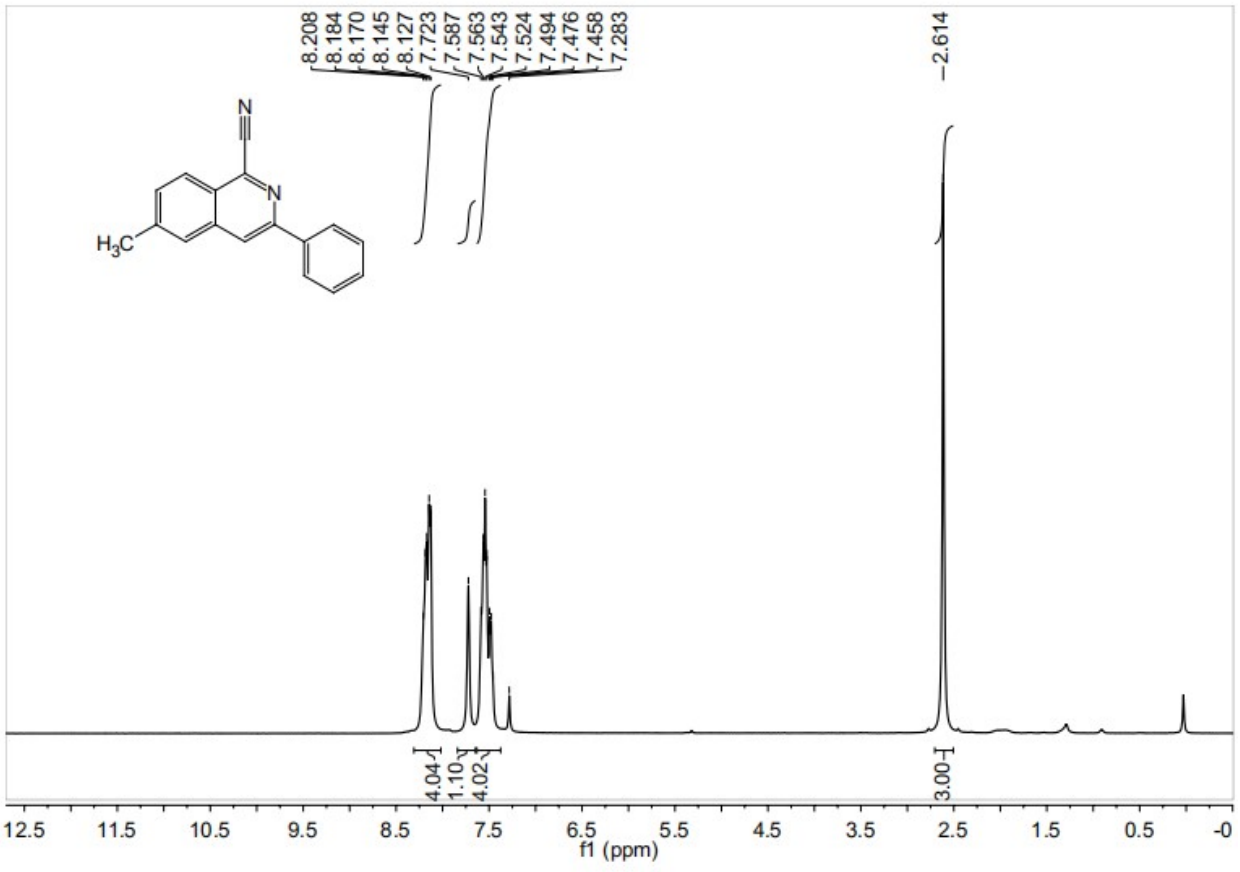
77.070
76.752
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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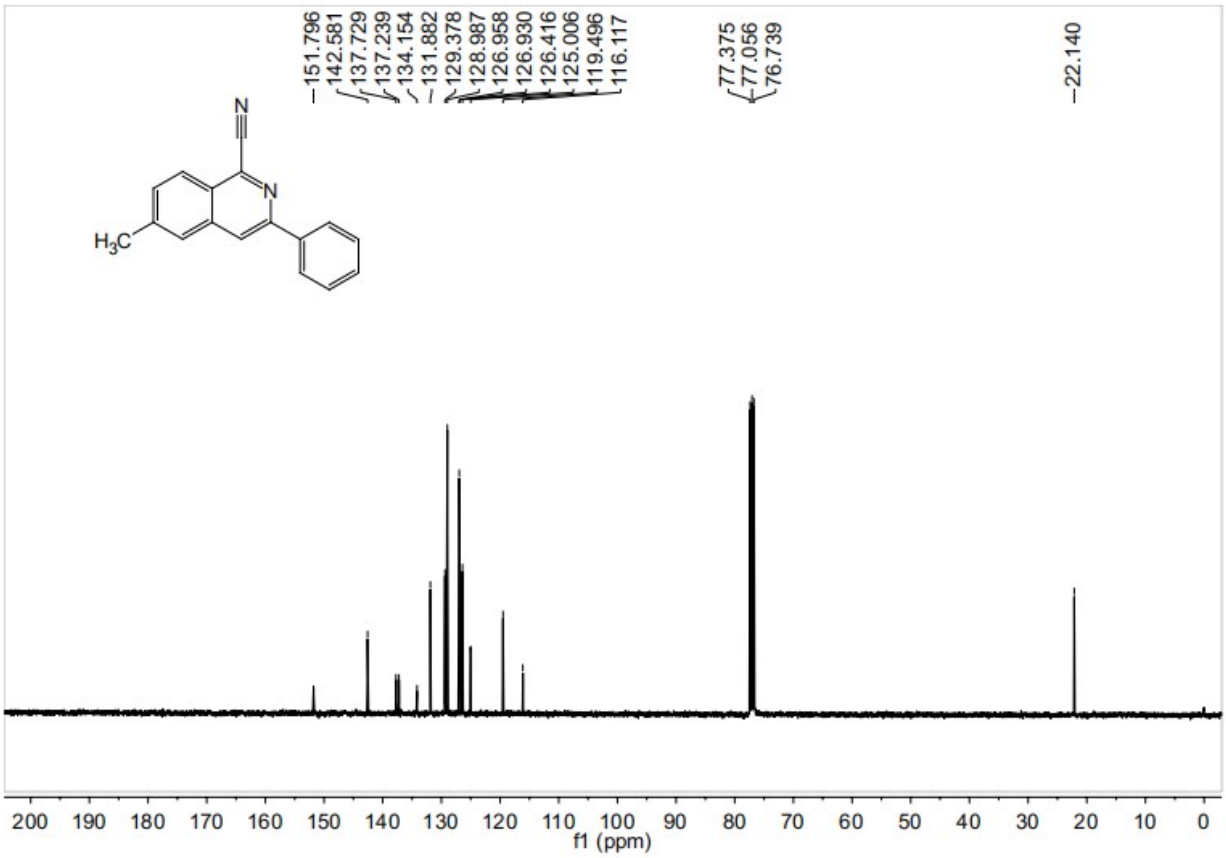
7.563
7.543
7.524
7.494
7.476
7.458
7.283
2.614
N
N
H3C
4.04
1.10
4.02
3.00
12.5 11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0
f1 (ppm)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119.496
116.117
77.375
77.056
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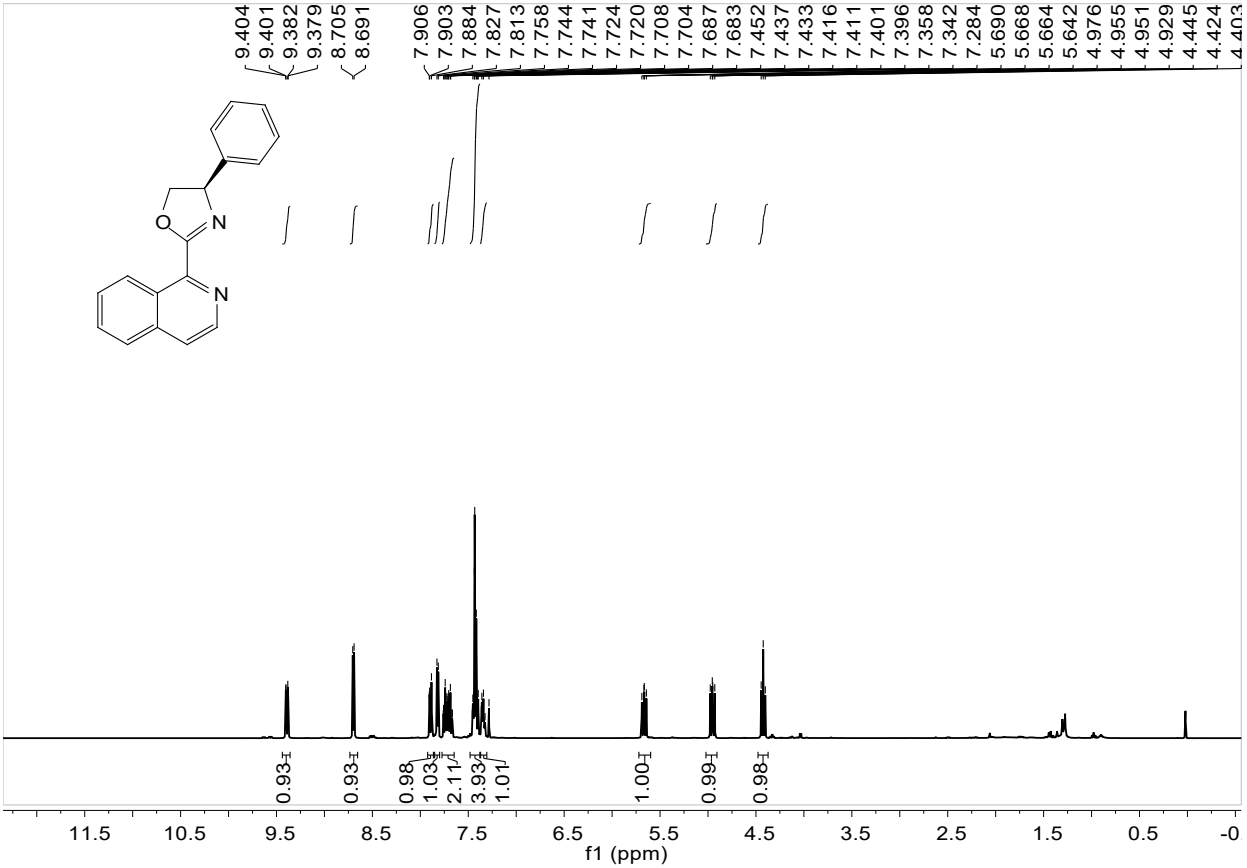
N
H3C
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.903
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7.744
7.741
7.724
7.720
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7.416
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7.401
7.396
7.358
7.342
7.284
5.690
5.668
5.664
5.642
4.976
4.955
4.951
4.929
4.445
4.424
O
N
N
0.93
0.93
0.98
1.03
2.11
3.93
1.01
1.00
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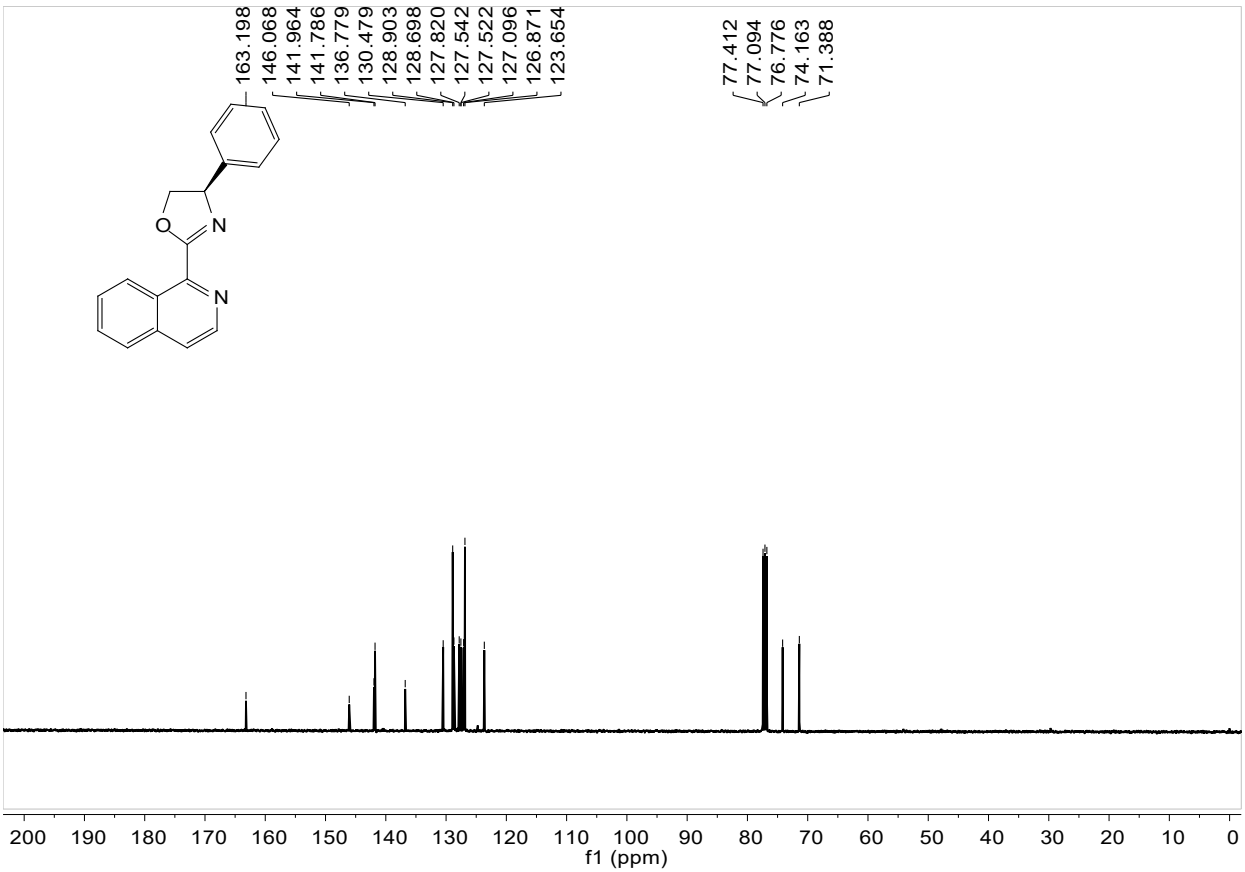
0.98
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0
f1 (ppm)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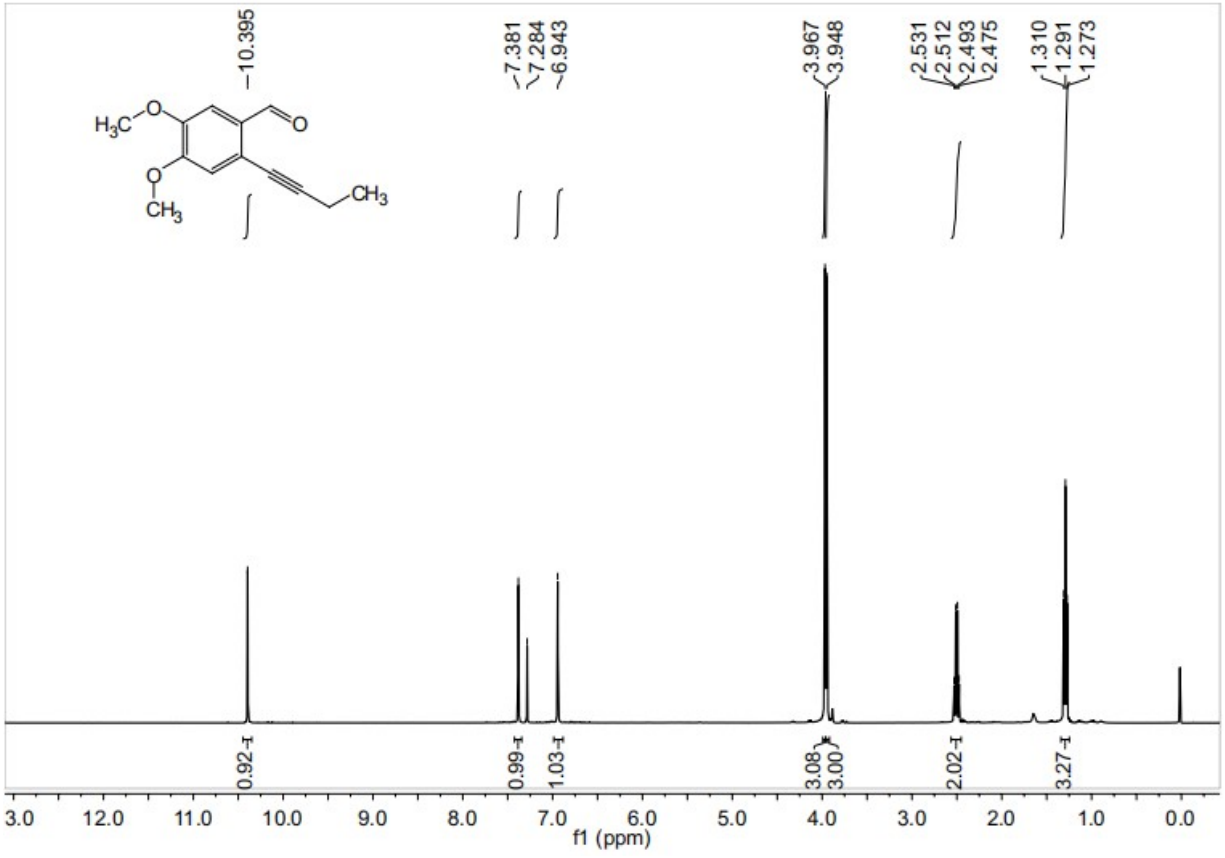
123.654
77.412
77.094
76.776
74.163
71.388
O
N
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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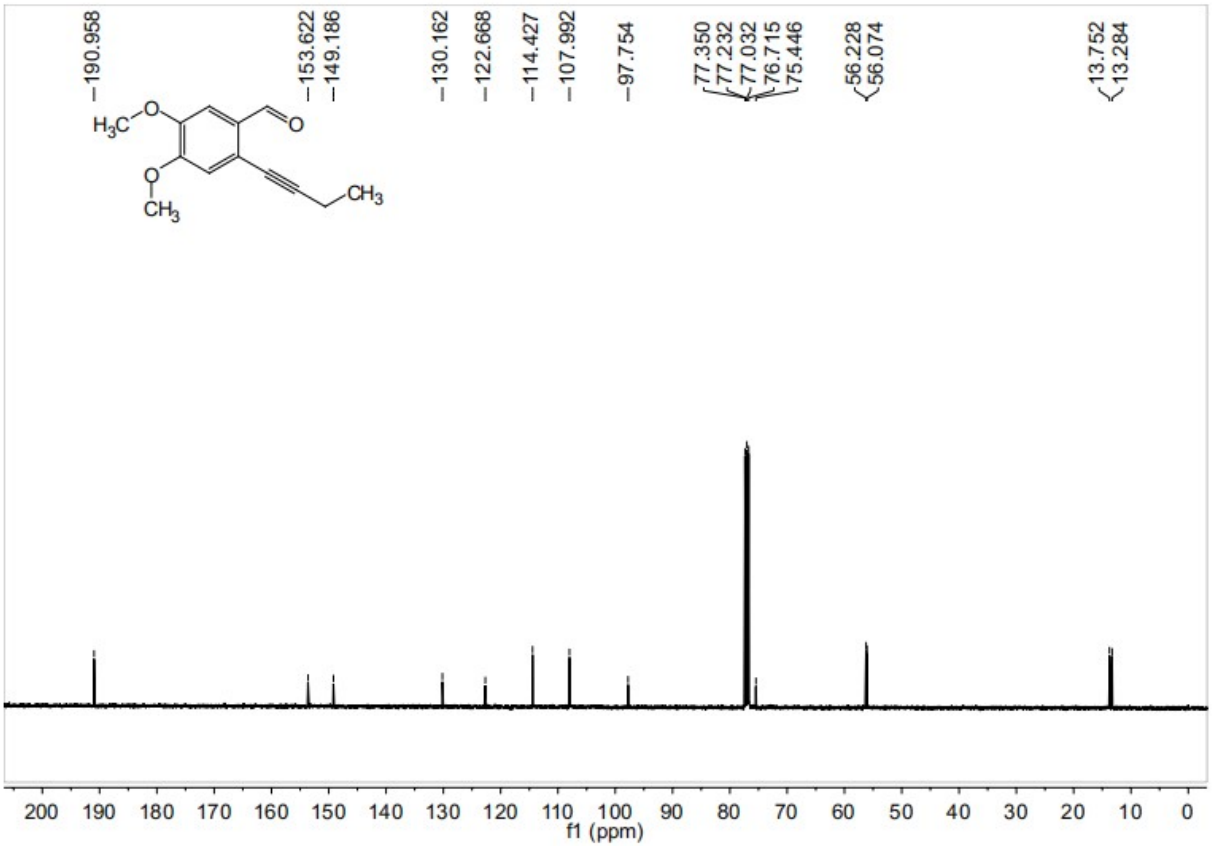
2.531
2.512
2.493
2.475
1.310
1.291
1.273
H3C
O
O
CH3
O
CH3
0.92
0.99
1.03
3.08
3.00
2.02
3.27
3.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)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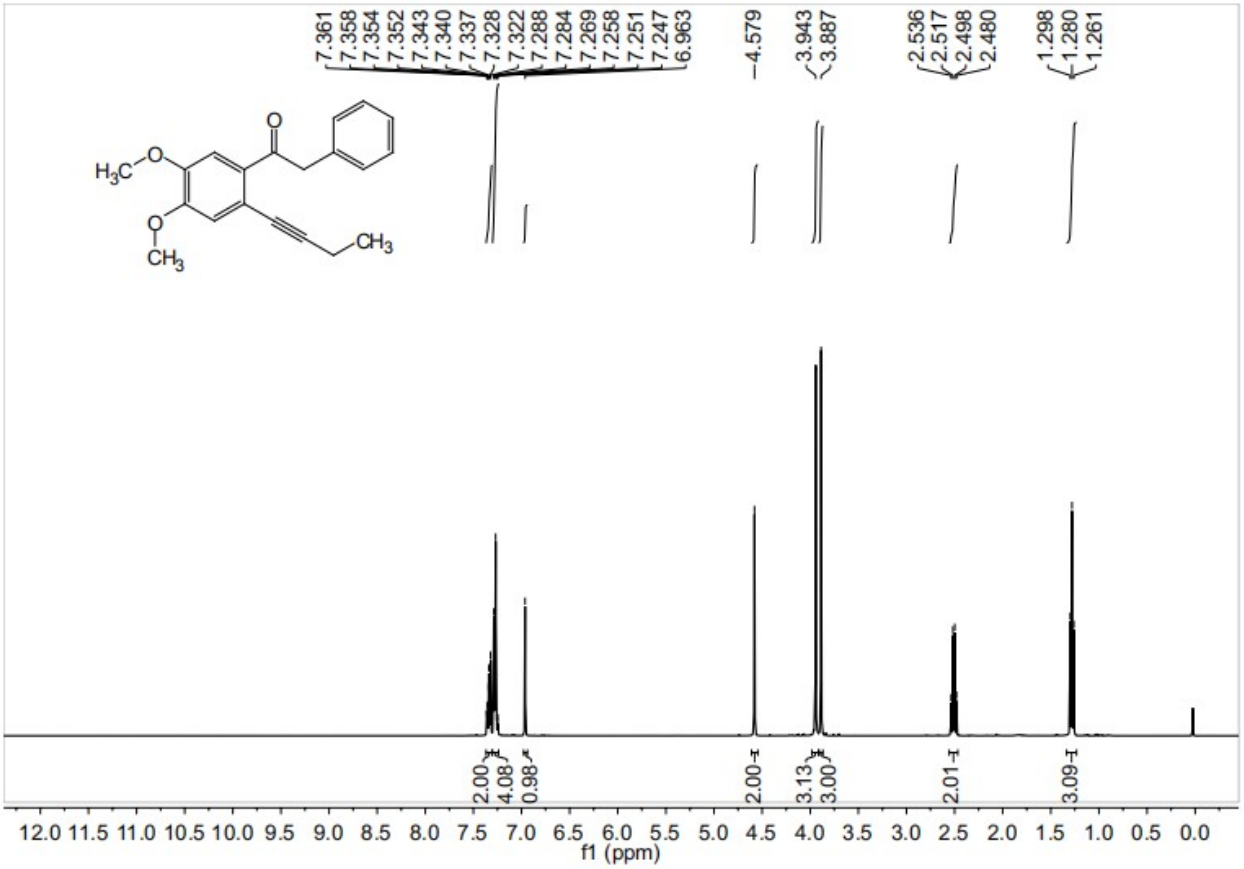
56.074
13.752
13.284
f1 (ppm)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7.284
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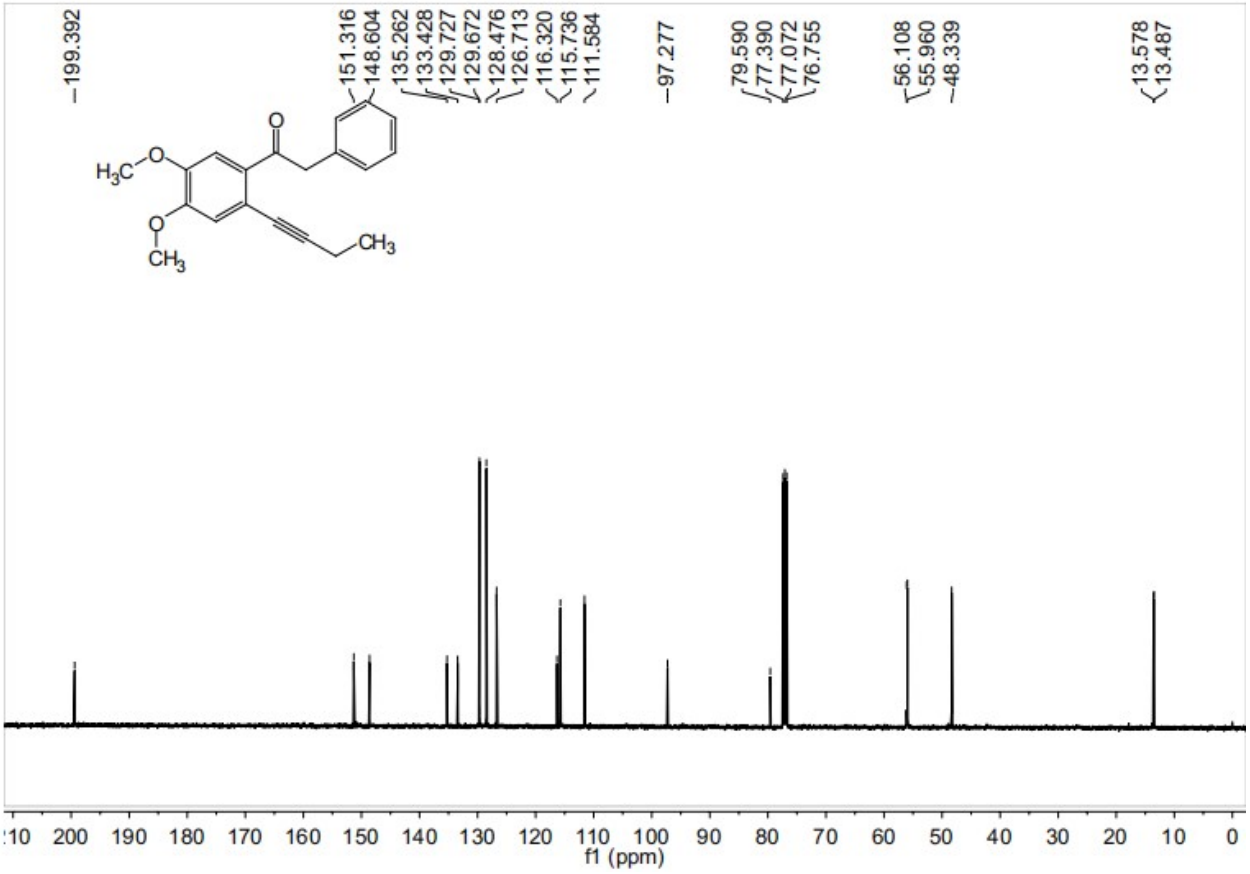
7.258
7.251
7.247
6.963
4.579
3.943
3.887
2.536
2.517
2.498
2.480
1.298
1.280
1.261
2.00
4.08
0.98
2.00
3.13
3.00
2.01
3.09
f1 (ppm)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148.604
135.262
133.428
129.727
129.672
128.476
126.713
116.320
115.736
111.584
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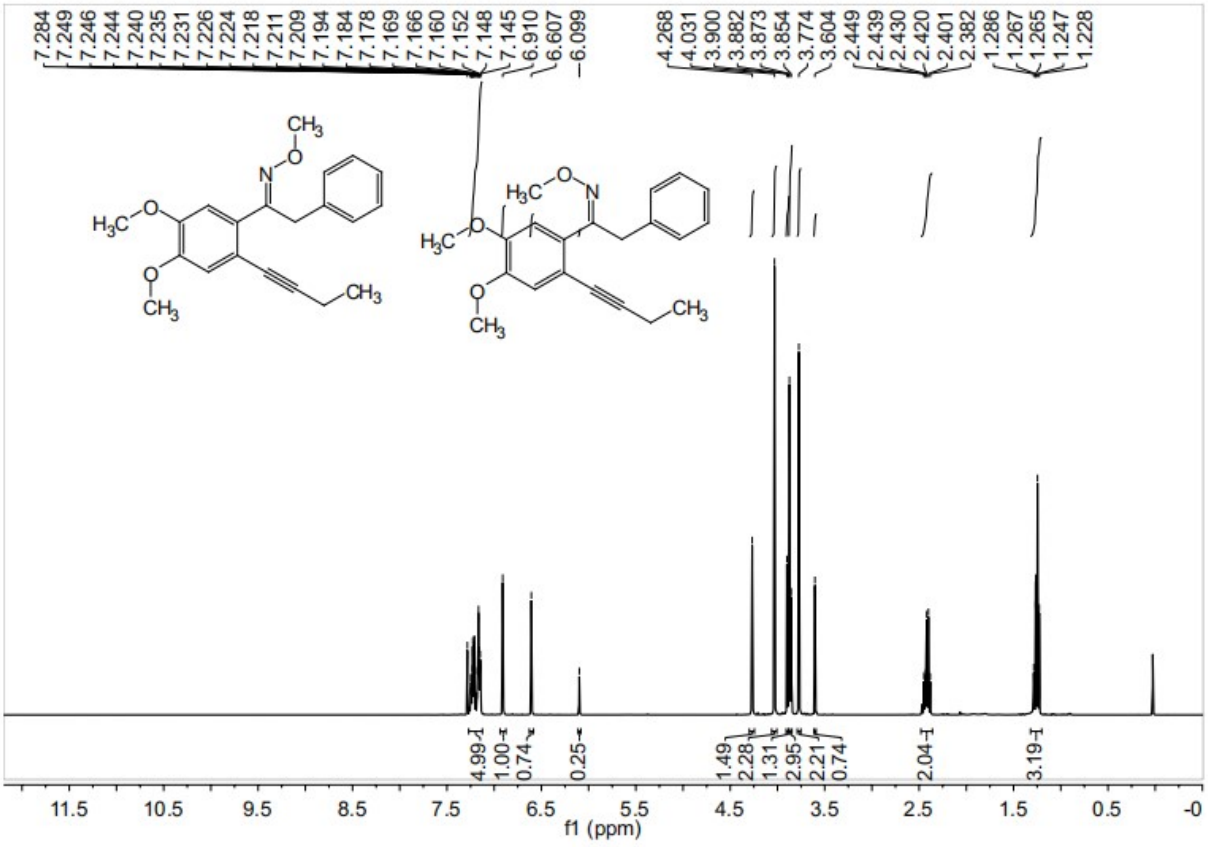
79.590
77.390
77.072
76.755
56.108
55.960
48.339
13.578
13.487
f1 (ppm)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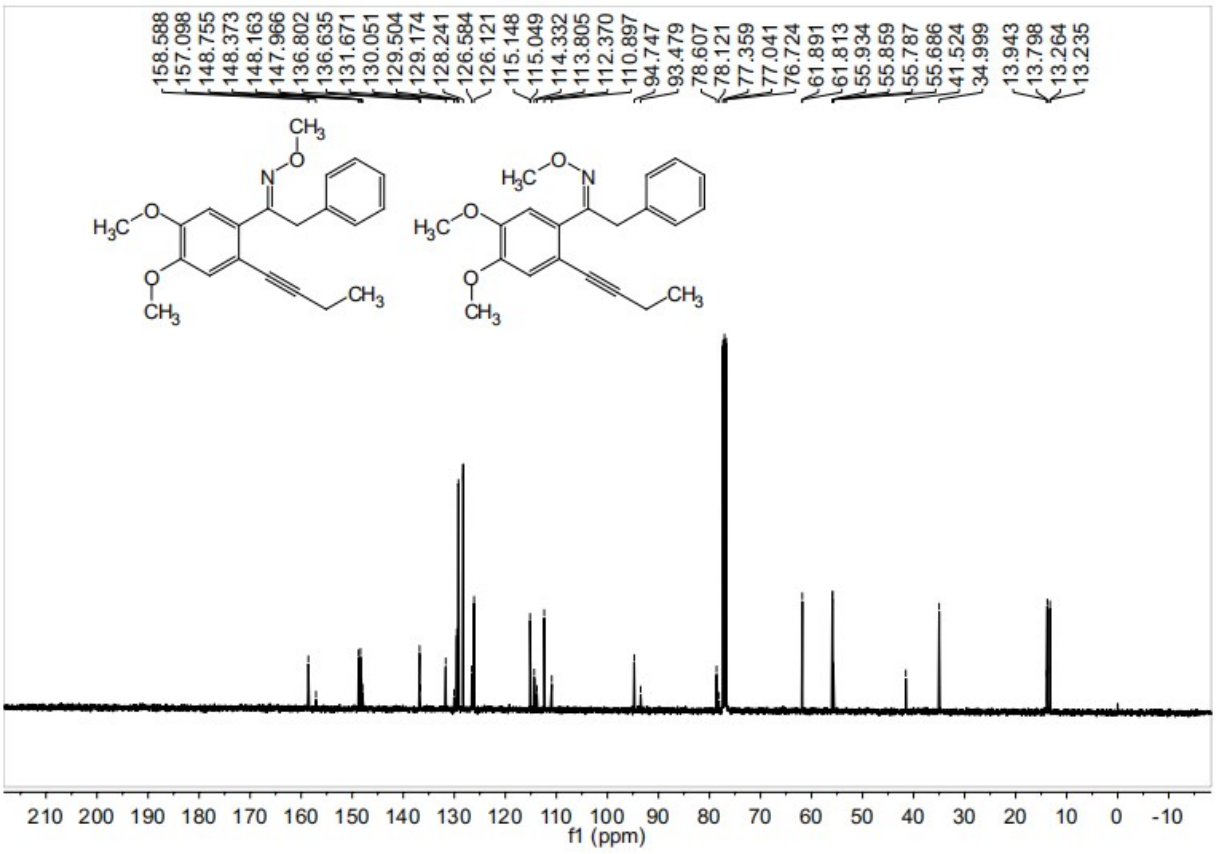
7.249
7.246
7.244
7.240
7.235
7.231
7.226
7.224
7.218
7.211
7.209
7.194
7.184
7.178
7.169
7.166
7.160
7.152
7.148
7.145
6.910
6.607
6.099
4.268
4.031
3.900
3.882
3.873
3.854
3.774
3.604
2.449
2.439
2.430
2.420
2.401
2.382
1.286
1.267
1.265
1.247
1.228
4.99
1.00
0.74
0.25
1.49
2.28
1.31
2.95
2.21
0.74
2.04
3.19
f1 (ppm)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148.755
148.373
148.163
147.966
136.802
136.635
131.671
130.051
129.504
129.174
128.241
126.584
126.121
115.148
115.049
114.332
113.805
112.370
110.897
94.747
93.479
78.607
78.121
77.359
77.041
76.724
61.891
61.813
55.934
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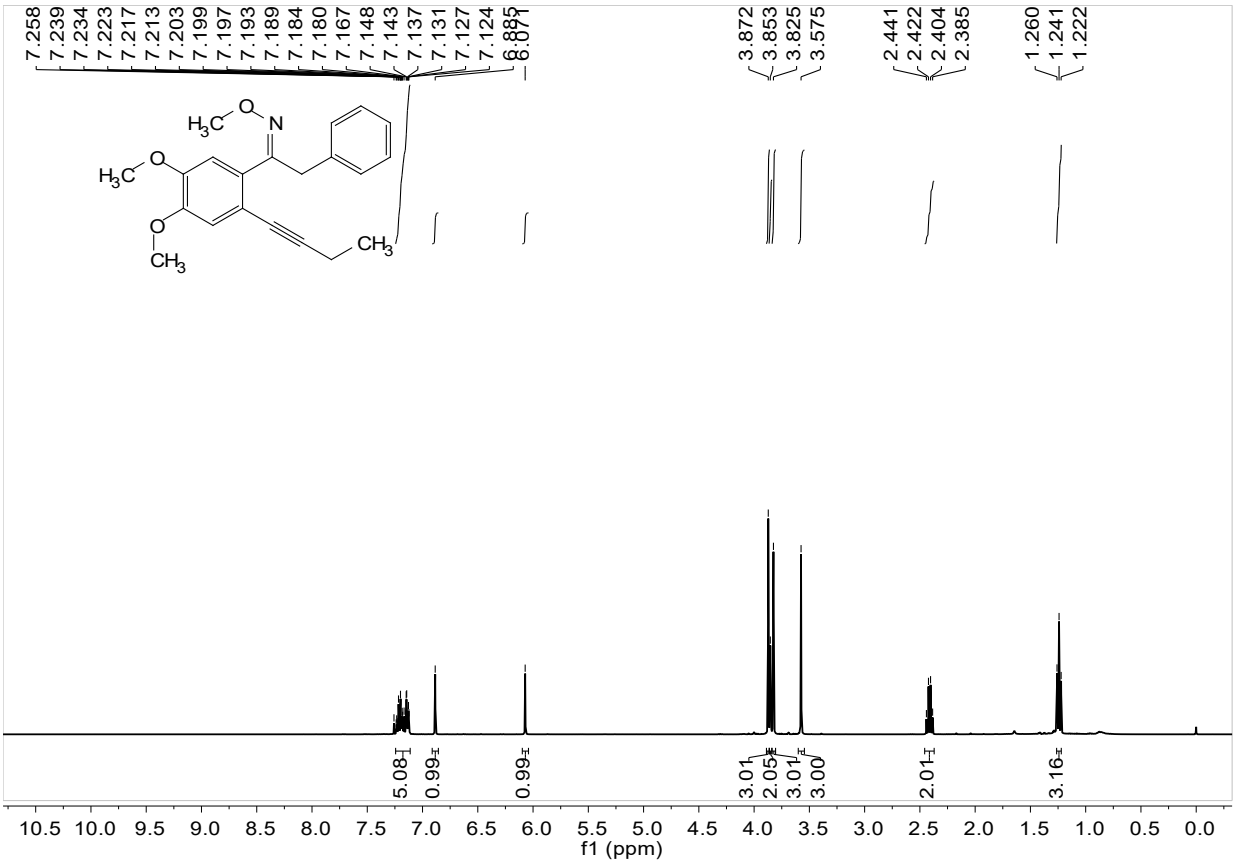
55.787
55.686
41.524
34.999
13.943
13.798
13.264
13.235
f1 (ppm)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7.239
7.234
7.223
7.217
7.213
7.203
7.199
7.197
7.193
7.189
7.184
7.180
7.167
7.148
7.143
7.137
7.131
7.127
7.124
6.885
6.871
3.872
3.853
3.825
3.575
2.441
2.422
2.404
2.385
1.260
1.241
1.222
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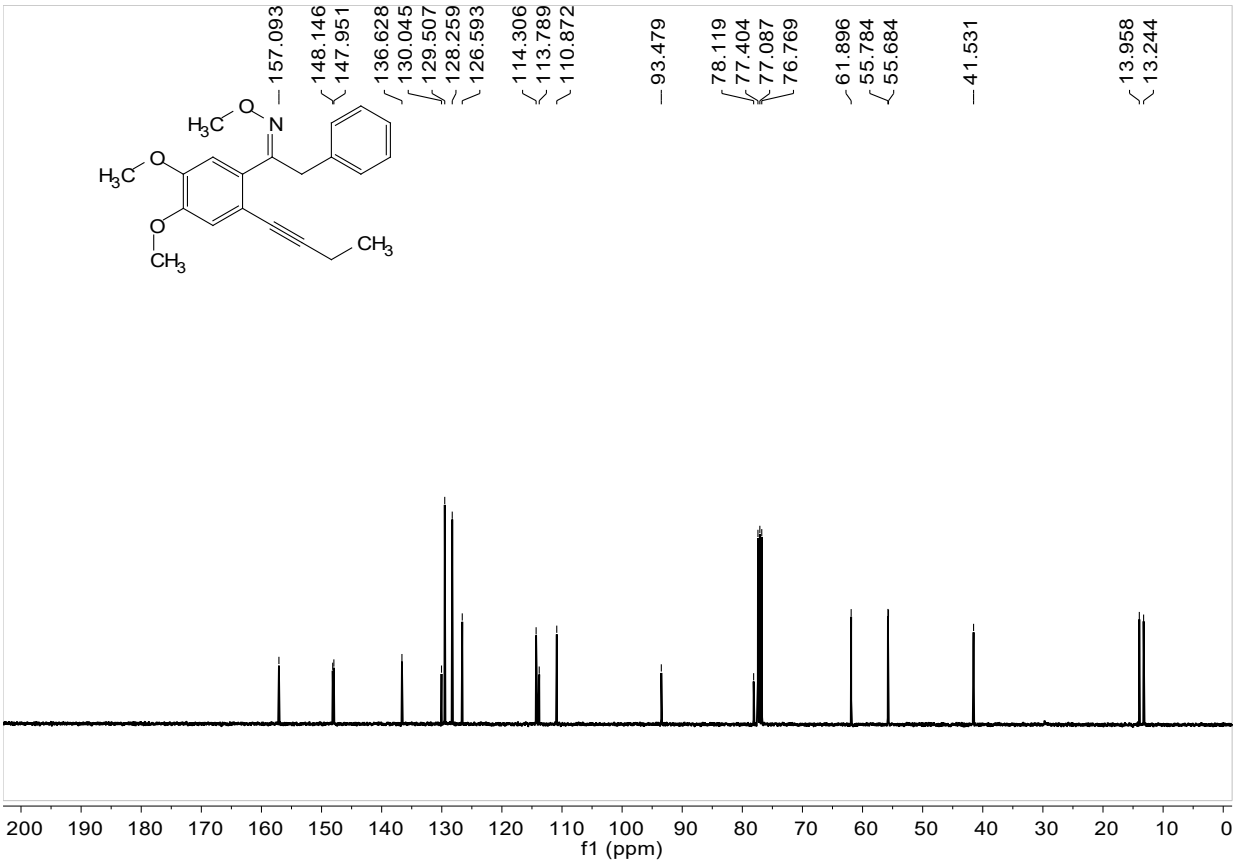
0.99
0.99
3.01
2.05
3.01
3.00
2.01
3.16
f1 (ppm)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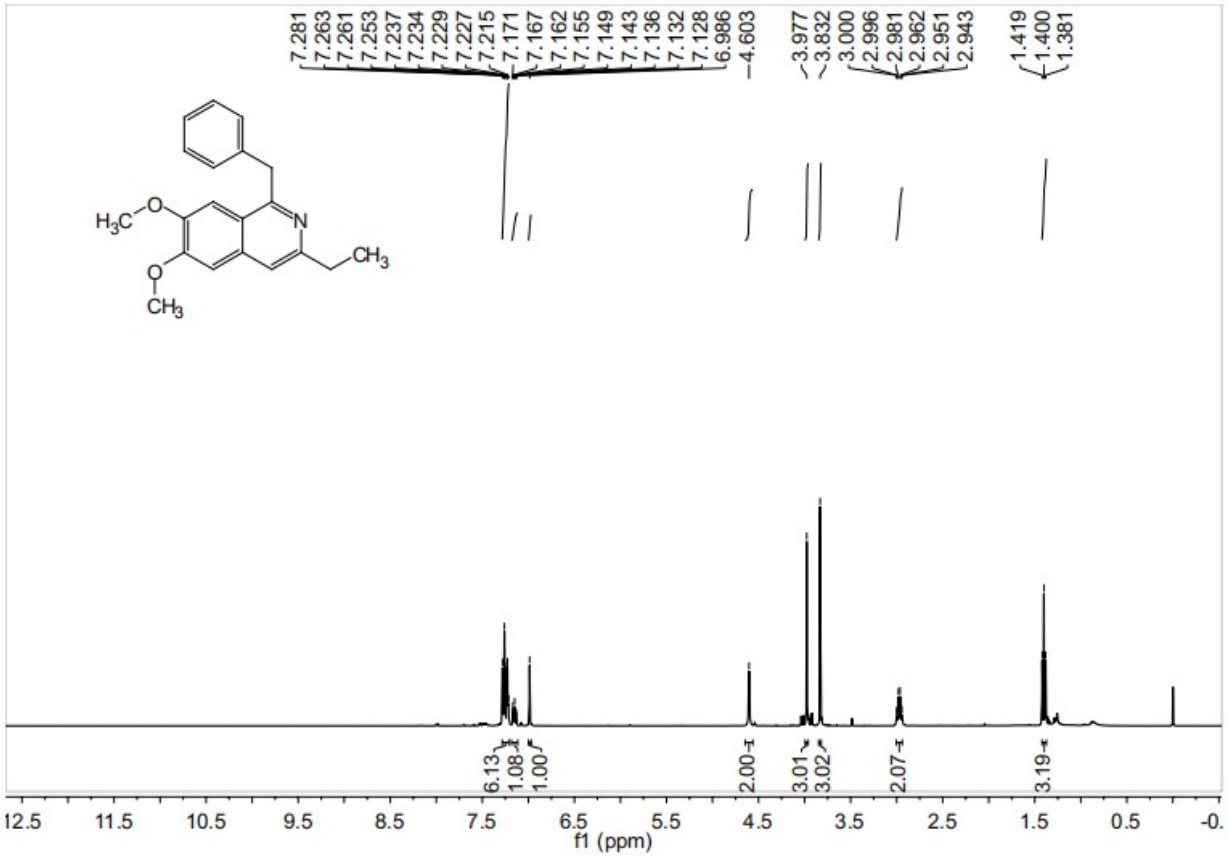
147.951
136.628
130.045
129.507
128.259
126.593
114.306
113.789
110.872
93.479
78.119
77.404
77.087
76.769
61.896
55.784
55.684
41.531
13.958
13.244
f1 (ppm)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7.263
7.261
7.253
7.237
7.234
7.229
7.227
7.215
7.171
7.167
7.162
7.155
7.149
7.143
7.136
7.132
7.128
6.986
4.603
3.977
3.832
3.000
2.996
2.981
2.962
2.951
2.943
1.419
1.400
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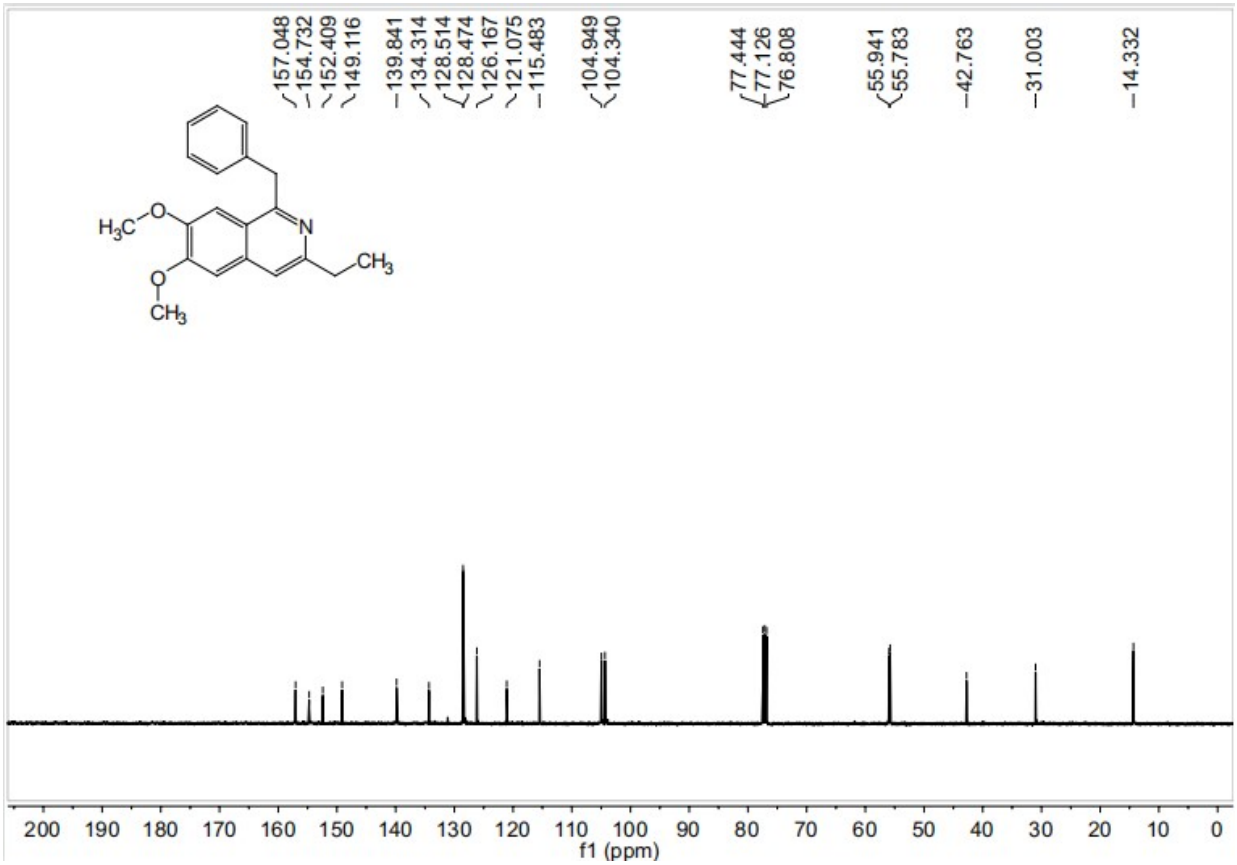
6.13
1.08
1.00
2.00
3.01
3.02
2.07
3.19
f1 (ppm)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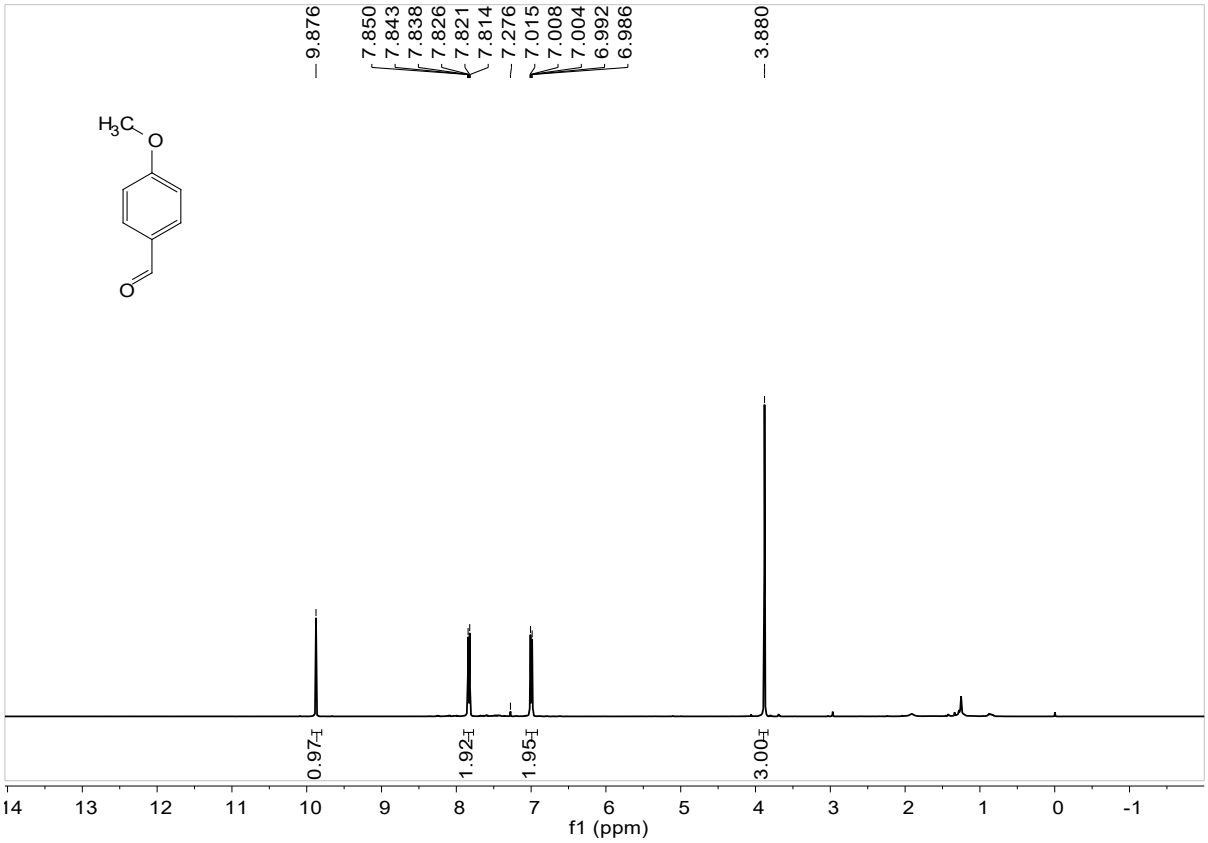
154.732
152.409
149.116
139.841
134.314
128.514
128.474
126.167
121.075
115.483
104.949
104.340
77.444
77.126
76.808
55.941
55.783
42.763
31.003
14.332
H3C
O
N
CH3
O
CH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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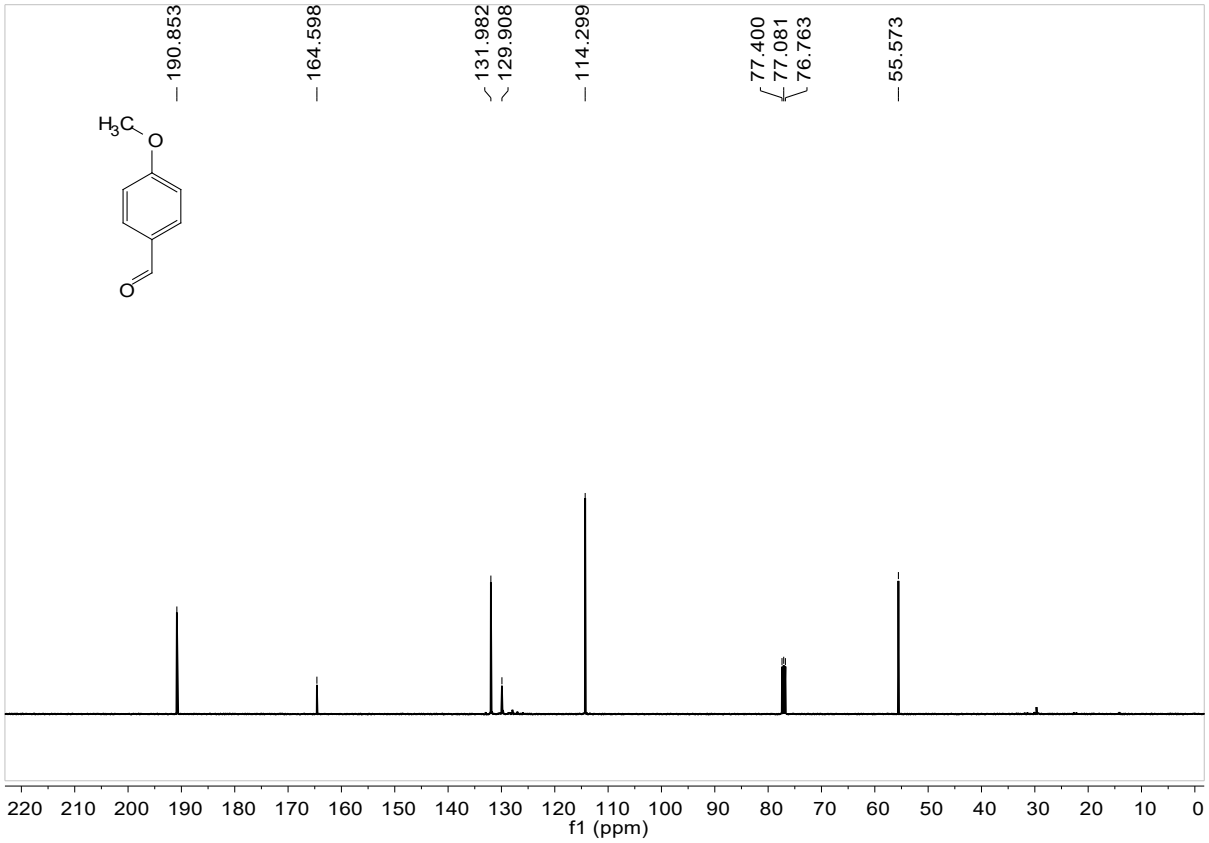
7.850
7.843
7.838
7.826
7.821
7.814
7.276
7.015
7.008
7.004
6.992
6.986
3.880
H3C
O
O
0.97
1.92
1.95
3.00
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)


190.853
164.598
131.982
129.908
114.299
77.400
77.081
76.763
55.573
H3C
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)