Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Copper-Catalyzed Tandem Aerobic Oxidative Cyclization for the Synthesis of the 4-Cyanoalkylpyrrolo[1,2-*a*]quinoxalines from 1-(2-Aminophenyl)pyrroles and Cyclobutanone Oxime Esters

Zhenyu An,[a] Yong Jiang,[b] Xin Guan,[a] Rulong Yan*[a]

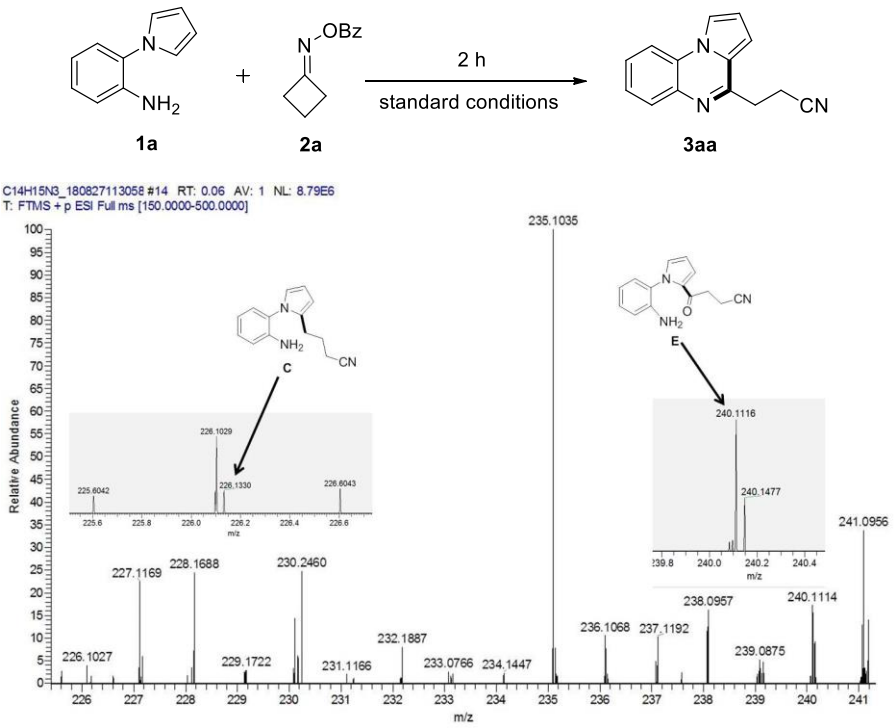
[a] State Key Laboratory of Applied Organic Chemistry, College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou, Gansu, China

[b] School of Chemistry and Chemical Engineering, Yangtze Normal University, Chongqing, China.

General remark

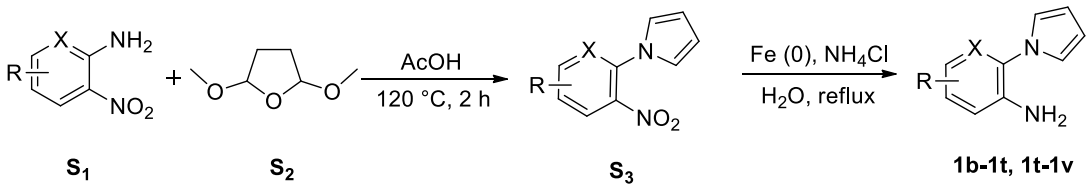
^{1}H NMR, and ^{13}C NMR spectra were recorded on Bruker 400M and Mercury 300M in $CDCl_3$ or DMSO. All ^{1}H NMR and ^{13}C NMR chemical shifts were given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. All compounds were further characterized by HRMS; copies of their ^{1}H NMR and ^{13}C NMR spectra were provided. Products were purified by flash chromatography on 200–300 mesh silica gels. All melting points were determined without correction. All reagents were purchased commercially and used as received, unless otherwise noted.

Figure S1. General procedure for trapping intermediates "C" and "E" by HRMS.



A mixture of 2-(1*H*-pyrrol-1-yl)aniline **1a** (1 equiv, 0.3 mmol), **2a** (1.2 equiv, 0.36 mmol), $Cu(OPiv)_2$ (10 mol %, 0.06 mmol), NMP (1-methyl-2-pyrrolidinone) (1 mL) were stirred at 80 ^{o}C under oxygen atmosphere for 2 h. The HRMS analysis indicates that intermediates **C** and **E** were captured in this reaction process. Unfortunately, the intermediate **D** can't be detected by HRMS analysis.

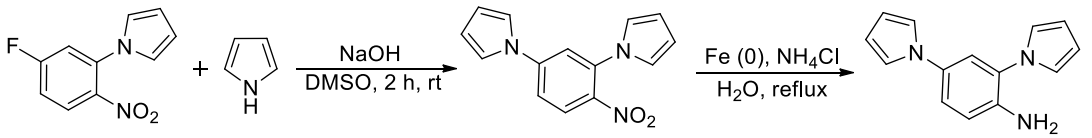
General procedure for the synthesis of 1b-1r and 1t-1v.[1]



S1 **S2** **S3** **1b-1t, 1t-1v**

Compound **1a** was purchased from commercial sources and used as received. Substituted 2-(1*H*-pyrrol-1-yl)anilines **1b-1r** and 2-(1*H*-pyrrol-1-yl)pyridin-3-amines **1t-1v** were prepared in the following method. A mixture of substituted **S1** (5 mmol) and **S2** (5 mmol) in acetic acid (25 mL) were refluxed for 2 h with vigorous stirring. After cooling, the reaction mixture was poured into water (100 mL) and extracted with ethyl acetate three times (3×20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and the solvent was removed in vacuo to afford **S3**. Then, the residue **S3** was added to iron powder (20 mmol) and NH_4Cl (2 mmol) in water (20 mL) and refluxed for 4 h. After cooling, the reaction mixture was poured into water (100 mL) and extracted with ethyl acetate three times (3×20 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and the solvent was removed in vacuo to afford a residue. The residue was purified by column chromatography on silica gel using petroleum ether/EtOAc as eluent to provide the desired product **1b-1r** and **1t-1v**.

General procedure for the synthesis of 1s.[2]



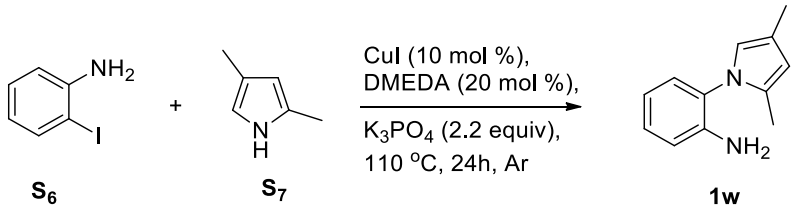
S4 **S5** **1s**

S4 was prepared from the method of synthesizing **S3**. Then, a mixture of **S4** (5 mmol), pyrrole (5 mmol) and NaOH (5 mmol) in DMSO (15 mL) was stirred vigorously for 2 h. Then, the reaction mixture was poured into water (60 mL) and extracted with ethyl acetate three times (3×30 mL). The combined organic layers were dried with Na_2SO_4 and the solvent was removed in vacuo to afford a residue **S5**.

The residue **S5** was added to iron powder (20 mmol) and NH_4Cl (2 mmol) in water

(60 mL) and refluxed for 4 h. After cooling, the reaction mixture was poured into water (100 mL) and extracted with ethyl acetate three times (3×60 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and the solvent was removed in vacuo to afford a residue. The residue was purified by column chromatography on silica gel to provide the desired product **1s** in 62% yield.

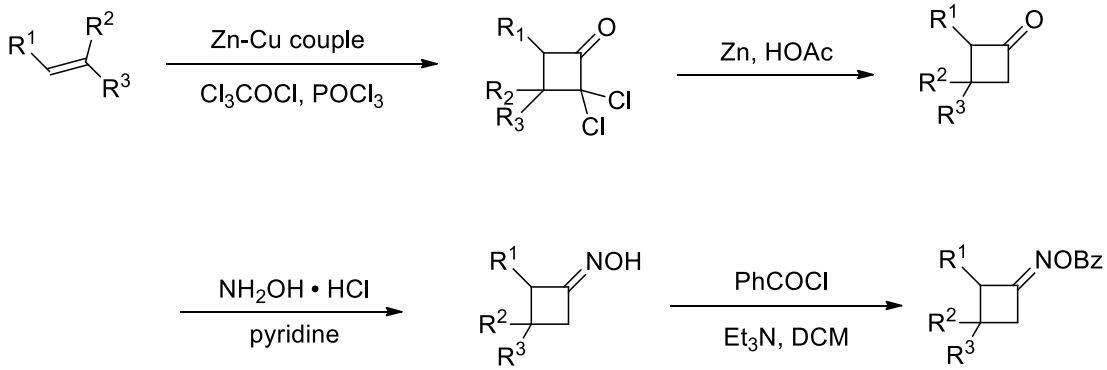
General procedure for the synthesis of 1w.[3]



S6 **S7** **1w**

Compounds **1w** were prepared in the following method. A screw-cap vial containing a stirring bar, was added 2-iodoanilines **S6** (5.0 mmol), CuI (10 mol %), DMEDA (*N*,*N*'-Dimethyl-1,2-ethanediamine, 20 mol %), K_3PO_4 (2.2 equiv), pyrrole **S7** (1.2 equiv), and toluene (2.0 mL). The mixture was stirred at 110 ^oC for 24 h under argon. The reaction mixture was diluted with ethyl acetate (50 mL) after cooling to room temperature. The mixture was filtered through a plug of silica gel and additional ethyl acetate was used to elute the silica gel. The filtrate was concentrated and the resulting residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate) to provide 2-(2,4-dimethyl-1*H*-pyrrol-1-yl)aniline **1w** in 79% yield.

General procedure for the synthesis of 2a-2e. [4]



Cyclobutanone *o*-benzoyl oximes were obtained from the corresponding cyclobutanones, which were commercial available or produced by the reduction of

α,*α*-dichlorocyclobutanones synthesized from the corresponding alkenes by the reported procedure[1]. The following experimental procedure is typical: to a 50 mL three-necked flask under argon were added alkene derivatives (5.0 mmol, 1.0 equiv), zinc-copper couple (960 mg, 15.0 mmol, 3.0 equiv), and anhydrous ether (10 mL). To this was added a solution of trichloroacetyl chloride (1.12 mL, 10.0 mmol, 2.0 equiv) and phosphorus oxychloride (0.51 mL, 5.5 mmol, 1.1 equiv) in ether (10 mL) over 1 h through an addition funnel. The suspension was stirred overnight at reflux. The resulting mixture was filtered through a pad of celite and washed with ether (20 mL). The organic solution was successively washed with water (30 mL), a saturated aqueous solution of $NaHCO_3$ (30 mL) and brine (30 mL), and dried over $MgSO_4$. Then the solution was filtered, concentrated and used in the next step without further purification.

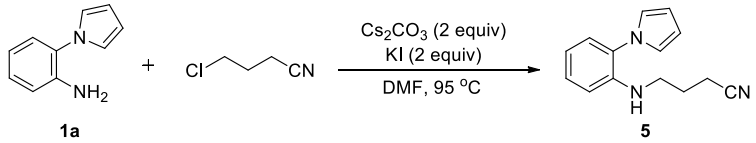
A mixture of 2,2-dichlorocyclobutanones (1.0 equiv) and zinc dust (4.0 equiv) in acetic acid (10 mL) was stirred at room temperature for 2 h and then heated at 80 ℃ for 5 h. The resulting mixture was allowed to cool to room temperature, and the solution was diluted with water (30 mL) and extracted with ether (3*20 mL). The organic phase was washed successively with a saturated solution of aqueous $NaHCO_3$ (3*30 mL), water (30 mL) and brine (30 mL), then dried over $MgSO_4$ and concentrated *in vacuum*. The crude material was purified by flash chromatography with a mixture of petroleum ether and ethyl acetate to afford various cyclobutanones.

A stirred solution of cyclobutanones (1.0 equiv) in pyridine (0.5 M) was added hydroxylamine hydrochloride (2.0 equiv) at rt. After stirring for 2 h, pyridine was removed under reduced pressure. The residue was diluted with water and extracted with EtOAc. The aqueous layer was extracted with EtOAc and the combined organic extracts were washed with brine, dried over $MgSO_4$, and evaporated under reduced pressure to give the crude material, which was used in the next step without further purification.

A mixture of cyclobutanone oxime (1.0 equiv), triethylamine (2.0 equiv) and DCM (0.5 M) in a 30 mL two-necked flask was added benzoyl chloride (1.5 equiv) at 0 ℃. After 6 h, water was added to the above solution, and the mixture was diluted with

diethyl ether. The organic layer was washed with water and dried over $MgSO_4$. The solvent was removed under vacuum and the residue was subjected to column chromatography on SiO_2 with EtOAc–hexane as an eluent to give cyclobutanone *O*-benzoyl oximes.

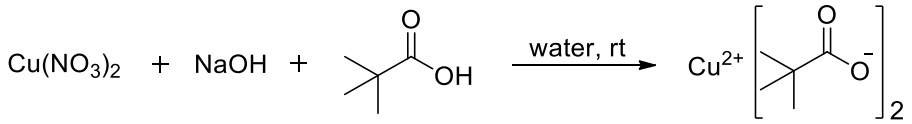
General procedure for the synthesis of 5. [5]



1a 5

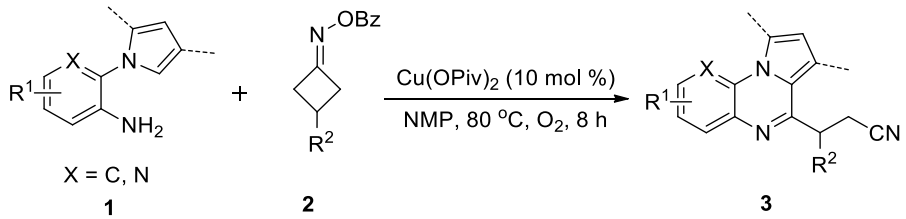
A mixture of 2-(1*H*-pyrrol-1-yl)aniline **1a** (1 equiv, 0.3 mmol), 4-chlorobutyronitrile (1.2 equiv, 0.36 mmol), Cs_2CO_3 (2 equiv, 0.6 mmol), KI (2 equiv, 0.6 mmol), DMF (N,N-Dimethylformamide) (1 mL) were stirred at 95 ^oC under air for 4 h (TLC monitored). Upon completion of the reaction, the reaction mixture was diluted with saturated brine (10 mL) and extracted with ethyl acetate (3 ×15 mL). The combined organic phase was dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum ether/ethyl acetate (10 : 1) to afford the desired product **5**.

General procedure for the synthesis of copper pivalate $Cu(OPiv)_2$. [6]



Pivalic acid (55 mmol, 5.61 g) and NaOH (50 mmol, 2 g) were dissolved in water (40 mL) with stirring for 1 h. The resulting mixture was filtered to remove unreacted pivalic acid, and the filtrate was added to an aqueous solution (40 mL) of $Cu(NO_3)_2 \cdot 3H_2O$ (25 mmol, 6.04 g). After stirring for 2 h, the dark green precipitate was formed, which was filtered, and washed with water (20 mL ×3), and dried in a vacuum oven at 100 ^oC for 12 h. Yield: 6.25 g, 94% (based on Cu).

General procedure for the synthesis of pyrrolo[1,2-*a*]quinoxaline derivatives.



A mixture of 2-(1*H*-pyrrol-1-yl)aniline **1a** (1 equiv, 0.3 mmol), **2a** (1.2 equiv, 0.36 mmol), $Cu(OPiv)_2$ (10 mol %, 0.06 mmol), NMP (1-methyl-2-pyrrolidinone) (1 mL) were stirred at 80 ^{o}C under oxygen atmosphere for 8 h (TLC monitored). Upon completion of the reaction, the reaction mixture was extracted with saturated brine (10 mL) and ethyl acetate (3×15 mL). The combined organic phase was dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum ether/ethyl acetate (10 : 1) to afford the desired product **3aa**.

The X-ray data of 3aa (CCDC 1842652)

An amount of 20 mg **3aa** were dissolved in tetrahydrofuran/petroleum ether (1:1) on the brown small reagent bottle (5 mL), which acted as good solvent, and a layer of ether was injected on the surface of tetrahydrofuran, and the cap is covered with a thin film, white crystals will be presented after seven days.

The data were collected at 296 K using a SuperNova (Dual) X-ray diffractometer equipped with a graphite monochromated Mo Kα radiation source (λ = 0.71073 Å) operation at 50 kV and 0.8 mA. Using Olex2[7], the structure was solved with the ShelXS[8] structure solution program using Direct Methods and refined with the ShelXL[9] refinement package using Least Squares minimisation. Nonhydrogen atoms were refined with anisotropic displacement parameters during the final cycles. All hydrogen atoms were placed by geometrical considerations and were added to the structure factor calculations.

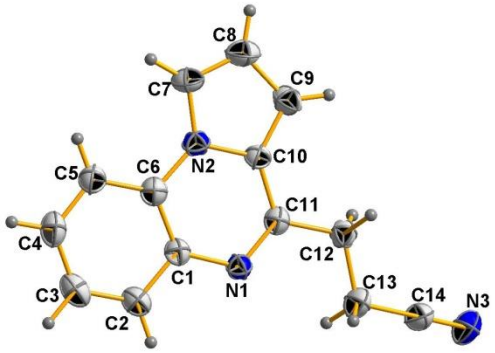
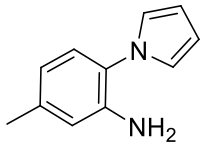


Figure S1. X-ray crystal structure of compound **3aa**, thermal ellipsoids are drawn at 30% probability level

Table S1. The crystal data and structure refinement for **3aa**

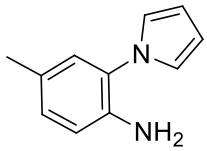
Identification code	3aa
Empirical formula	$C_{14}H_{11}N_3$
Formula weight	221.26
Temperature/K	295.9(3)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.5028(16)
b/Å	4.8074(7)
c/Å	23.494(6)
α/°	90.00
β/°	98.523(19)
γ/°	90.00
Volume/Å^3	1173.1(4)
Z	4
ρ_{calc}g/cm^3	1.253
μ/mm^{-1}	0.077
F(000)	464.0
Crystal size/mm^3	0.23 × 0.21 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	7.02 to 52.04
Index ranges	-12 ≤ h ≤ 6, -5 ≤ k ≤ 2, -28 ≤ l ≤
Reflections collected	3939
Independent reflections	2286 [R_{int} = 0.0448, R_{sigma} =
Data/restraints/parameters	2286/0/154
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0813, wR_2 = 0.1507
Final R indexes [all data]	R_1 = 0.1602, wR_2 = 0.1902
Largest diff. peak/hole / e Å^{-3}	0.17/-0.18

The data of products



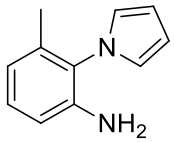
5-methyl-2-(1*H*-pyrrol-1-yl)aniline (1b)

Yellow solid (627.8 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.03-7.01 (d, *J* = 8.0 Hz, 1 H), 6.80-6.79 (m, 2 H), 6.60-6.56 (m, 2 H), 6.32-6.31 (m, 2 H), 3.62 (br s, 2 H), 2.30 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 141.9, 138.6, 127.0, 125.2, 121.9, 119.2, 116.6, 109.2, 21.2.



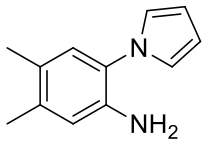
4-methyl-2-(1*H*-pyrrol-1-yl)aniline (1c)

Yellow solid (610.6 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.97-6.96 (m, 2 H), 6.83-6.82 (m, 2 H), 6.71-6.69 (d, *J* = 6.5 Hz, 1 H), 6.33-6.32 (m, 2 H), 3.57 (br s, 2 H), 2.26 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.3, 129.0, 127.9, 127.5, 127.4, 121.6, 116.2, 109.2, 20.2.



3-methyl-2-(1*H*-pyrrol-1-yl)aniline (1d)

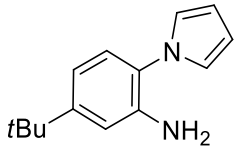
Yellow solid (626.9 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.09-7.05 (m, 2 H), 6.65-6.64 (m, 4 H), 6.36-6.35 (m, 2 H), 3.43 (br s, 2 H), 2.00 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.8, 136.9, 128.7, 126.7, 121.4, 119.6, 113.1, 109.3, 17.1.



4,5-dimethyl-2-(1*H*-pyrrol-1-yl)aniline (1e)

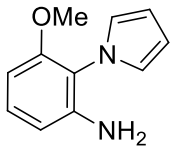
Yellow solid (610.6 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.91 (s, 1 H), 6.79-6.78 (m, 2 H), 6.58 (s, 1 H), 6.31-6.30 (m, 2 H), 3.49 (br s, 2 H), 2.20 (s, 3

H), 2.15 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.7, 137.1, 128.1, 126.7, 125.5, 122.0, 117.7, 109.3, 19.7, 18.8.



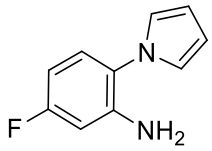
5-(*tert*-butyl)-2-(1*H*-pyrrol-1-yl)aniline (1f)

Yellow solid (727.6 mg, 68% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.07-7.04 (d, *J* = 8.8 Hz, 1 H), 6.82-6.78 (m, 4 H), 6.31-6.30 (m, 2 H), 3.62 (br s, 2 H), 1.31 (s, 9 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 151.8, 141.4, 126.6, 125.1, 121.7, 115.6, 113.2, 109.1, 34.5, 31.2.



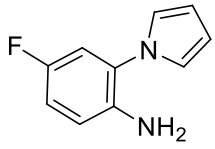
4-methoxy-2-(1*H*-pyrrol-1-yl)aniline (1g)

Yellow solid (694.6 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.11-7.07 (m, 1 H), 6.68-6.67 (m, 2 H), 6.39-6.33 (m, 4 H), 3.69 (s, 3 H), 3.56 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.2, 144.7, 129.0, 122.0, 116.1, 108.9, 108.2, 100.9, 55.7.



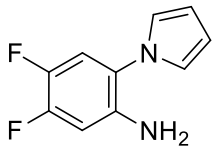
5-fluoro-2-(1*H*-pyrrol-1-yl)aniline (1h)

Yellow solid (589.4 mg, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.09-7.05 (m, 1 H), 6.77-6.76 (m, 2 H), 6.48-6.42 (m, 2 H), 6.33-6.32 (d, *J* = 2.4 Hz, 2 H), 3.77 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 164.0-161.5 (d, *J* = 243.1 Hz, 1 C), 144.0-143.9 (d, *J* = 11.7 Hz, 1 C), 128.6-128.5 (d, *J* = 10.7 Hz, 1 C), 123.6, 121.9, 109.6, 104.9-104.7 (d, *J* = 22.9 Hz, 1 C), 102.5-102.3 (d, *J* = 25.9 Hz, 1 C).



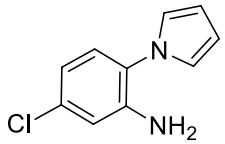
4-fluoro-2-(1*H*-pyrrol-1-yl)aniline (1i)

Yellow solid (589.6 mg, 67% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.91-6.87 (m, 2 H), 6.83-6.82 (d, *J* = 2.0 Hz, 2 H), 6.74-6.70 (m, 1 H), 6.35-6.34 (m, 2 H), 3.59 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.7-154.3 (d, *J* = 236.3 Hz, 1 C), 138.1-138.1(d, *J* = 2.4 Hz, 1 C), 127.7-127.6 (d, *J* = 9.5 Hz, 1 C), 121.5, 116.7-116.7 (d, *J* = 8.2 Hz, 1 C), 115.3-115.0 (d, *J* = 21.9 Hz, 1 C), 114.1-113.8 (d, *J* = 23.6 Hz, 1 C), 109.8.



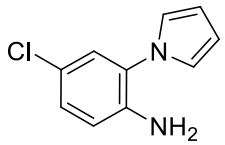
4,5-difluoro-2-(1*H*-pyrrol-1-yl)aniline (1j)

Yellow solid (611.1 mg, 63% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.03-6.99 (m, 1 H), 6.77 (s, 2 H), 6.61-6.55 (m, 1 H), 6.34 (s, 2 H), 3.64 (br s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 151.9-148.7 (d, *J* = 170.1 Hz, 1 C), 144.3-141.1 (d, *J* = 238.1 Hz, 1 C), 139.2-139.0 (d, *J* = 9.0 Hz, 1 C), 122.4-122.3 (d, *J* = 4.0 Hz, 1 C), 121.6, 116.0-115.8 (d, *J* = 18.9 Hz, 1 C), 109.8, 104.1-103.8 (d, *J* = 21.1 Hz, 1 C).



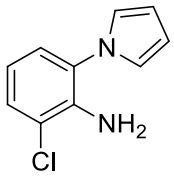
5-chloro-2-(1*H*-pyrrol-1-yl)aniline (1k)

Yellow solid (720.0 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.06-7.04 (d, *J* = 8.4 Hz, 1 H), 6.79-7.77 (m, 3 H), 6.75-6.72 (m, 1 H), 6.34-6.33 (m, 2 H), 3.77 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.2, 134.0, 128.2, 125.9, 121.6, 118.2, 115.6, 109.8.



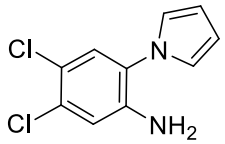
4-chloro-2-(1*H*-pyrrol-1-yl)aniline (1l)

Yellow solid (729.6 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.14-7.09 (m, 2 H), 6.81-6.80 (m, 2 H), 6.71-6.69 (d, *J* = 8.4 Hz, 1 H), 6.34-6.33 (m, 2 H), 3.72 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 140.7, 128.4, 128.0, 127.0, 122.6, 121.5, 116.9, 109.9.



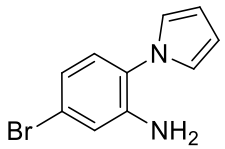
2-chloro-6-(1*H*-pyrrol-1-yl)aniline (1m)

Yellow solid (723.6 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.29-7.25 (m, 1 H), 7.08-7.06 (m, 1 H), 6.83-6.82 (m, 2 H), 6.73-6.69 (m, 1 H), 6.36-6.35 (m, 2 H), 4.12 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.4, 128.5, 127.9, 125.5, 121.5, 119.6, 117.5, 109.7,.



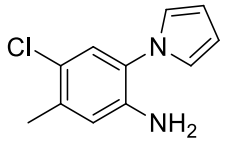
4,5-dichloro-2-(1*H*-pyrrol-1-yl)aniline (1n)

Yellow solid (757.1 mg, 67% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.22 (s, 1 H), 6.88 (s, 1 H), 6.79-6.77 (m, 2 H), 6.35-6.33 (m, 2 H), 3.79 (br s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 141.8, 132.2, 128.6, 126.9, 121.7, 120.8, 117.1, 110.4.



5-bromo-2-(1*H*-pyrrol-1-yl)aniline (1o)

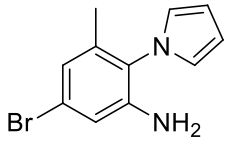
Yellow solid (810.8 mg, 69% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.00-6.97 (m, 1 H), 6.94-6.93 (m, 1 H), 6.90-6.86 (m, 1 H), 6.80-6.78 (m, 2 H), 6.34-6.33 (m, 2 H), 3.77 (br s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 143.6, 128.6, 126.6, 122.1, 121.8, 121.4, 118.7, 110.0.



4-chloro-5-methyl-2-(1*H*-pyrrol-1-yl)aniline (1p)

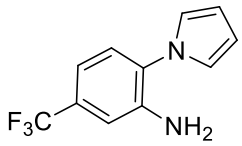
Yellow solid (729.6 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.10 (s, 1 H), 6.75-6.74 (m, 2 H), 6.57 (s, 1 H), 6.31-6.28 (m, 2 H), 3.55 (br s, 2 H), 2.28 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 140.3, 136.0, 128.4, 128.3, 127.0, 121.5,

117.8, 109.5, 19.7.



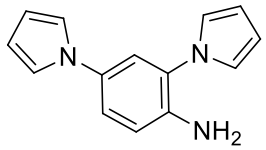
3-bromo-5-methyl-2-(1*H*-pyrrol-1-yl)aniline (1q)

Yellow solid (729.6 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.77 (s, 1 H), 6.75 (s, 1 H), 6.60-6.58 (m, 2 H), 6.35-6.33 (m, 2 H), 3.56 (br s, 2 H), 1.94 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 145.0, 138.7, 125.4, 122.1, 122.0, 121.2, 115.6, 109.6, 17.0.



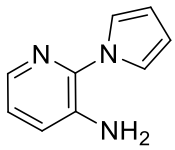
2-(1*H*-pyrrol-1-yl)-5-(trifluoromethyl)aniline (1r)

Yellow solid (723.2 mg, 64% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.25-7.21 (d, *J* = 10.2 Hz, 1 H), 7.03-7.01 (m, 2 H), 6.85-6.83 (m, 2 H), 6.38-6.36 (m, 2 H), 3.93 (br s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 142.4, 131.4-130.1 (q, *J* = 32.2 Hz, 1 C), 130.0, 127.6, 126.0-122.3 (d, *J* = 270.6 Hz, 1 C), 121.6, 115.2-115.1 (q, *J* = 3.7 Hz, 1 C), 113.0-112.9 (q, *J* = 3.7 Hz, 1 C), 110.3.



2,4-di(1*H*-pyrrol-1-yl)aniline (1s)

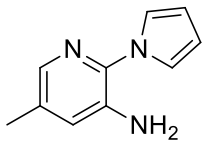
Yellow solid (691.3 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.22-7.19 (m, 2 H), 6.98-6.97 (m, 2 H), 6.87-6.86 (m, 2 H), 6.85-6.82 (d, *J* = 9.2 Hz, 1 H), 6.37-6.36 (m, 2 H), 6.31-6.30 (m, 2 H), 3.74 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 140.0, 132.7, 127.7, 121.6, 121.2, 120.0, 119.6, 116.7, 109.9, 109.8.



2-(1*H*-pyrrol-1-yl)pyridin-3-amine (1t)

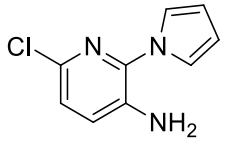
Yellow solid (667.8 mg, 81% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.92-7.90

(m, 1H), 7.15-7.14 (m, 2 H), 7.10-7.06 (m, 2 H), 6.36-6.35 (m, 2 H), 3.87 (br s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 139.8, 138.6, 136.1, 124.4, 123.1, 120.4, 110.2.



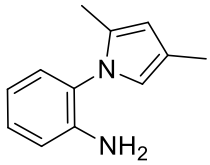
5-methyl-2-(1*H*-pyrrol-1-yl)pyridin-3-amine (1u)

Yellow solid (667.8 mg, 81% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.71 (s, 1H), 7.08-7.07 (m, 2 H), 6.87 (s, 1 H), 6.33-6.32 (m, 2 H), 3.81 (br s, 2 H), 2.25 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 138.7, 137.7, 135.8, 133.1, 124.9, 120.4, 109.8, 18.0.



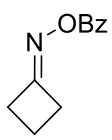
6-chloro-2-(1*H*-pyrrol-1-yl)pyridin-3-amine (1v)

Yellow solid (667.8 mg, 81% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.11-7.10 (m, 2H), 7.02-7.03 (m, 2 H), 6.33-6.32 (m, 2 H), 3.89 (br s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 138.4, 137.9, 134.9, 127.4, 123.1, 120.2, 110.5.



2-(2,4-dimethyl-1*H*-pyrrol-1-yl)aniline (1w)

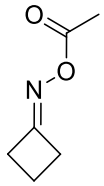
Yellow solid (734.7 mg, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.19-7.13 (m, 1H), 7.08-7.05 (m, 1 H), 6.77-6.72 (m, 2 H), 6.37 (s, 1 H), 5.88 (s, 1 H), 3.53 (br s, 2 H), 2.10 (d, *J* = 0.4 Hz, 3 H), 1.99 (d, *J* = 0.8 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.8, 129.8, 129.0, 128.7, 126.3, 119.0, 118.6, 118.1, 115.7, 108.9, 12.0, 11.9.



cyclobutanone *O*-benzoyl oxime (2a)

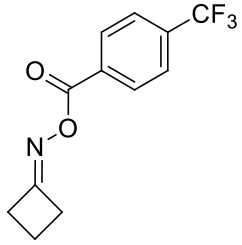
White solid (586 mg, 62% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.06-8.02

(m, 2 H), 7.60-7.54 (m, 1 H), 7.47-7.42 (m, 2 H), 3.15-3.08 (m, 4 H), 2.14-2.03 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ =169.0, 163.6, 132.8, 129.1, 128.5, 128.1, 31.4, 13.9.



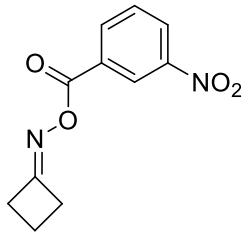
cyclobutanone *O*-acetyl oxime (2a-1)

White solid (464 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 3.08-3.00 (m, 4 H), 2.14 (s, 3 H), 2.11-2.03 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 168.4, 31.9, 31.7, 19.5, 14.3.



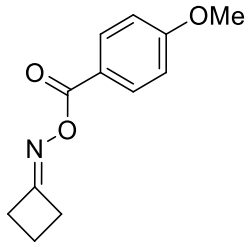
cyclobutanone *O*-(4-(trifluoromethyl)benzoyl) oxime (2a-2)

White solid (886 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.17-8.15 (d, *J* = 8.4 Hz, 2 H), 7.74-7.72 (d, *J* = 8.4 Hz, 2 H), 3.18-3.14 (m, 1 H), 2.19-2.11 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =170.0, 162.8, 135.0-134.1 (q, *J* = 32 Hz, 1 C), 132.2, 129.9, 125.5-12.4 (d, *J* = 4 Hz, 1 C), 124.8-122.0 (d, *J* = 271 Hz, 1 C), 31.8, 14.2.



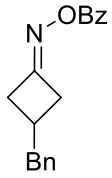
cyclobutanone *O*-(3-nitrobenzoyl) oxime (2a-3)

White solid (702 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.85-8.84 (m, 1 H), 8.47-8.44 (m, 1H), 8.40-8.38 (d, *J* = 8.0 Hz, 2 H), 7.73-7.69 (m, 1 H), 3.23-3.16 (m, 2 H), 2.21-2.13 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =170.4, 161.9, 148.1, 135.2, 130.7, 129.8, 127.6, 124.3, 31.8, 14.1.



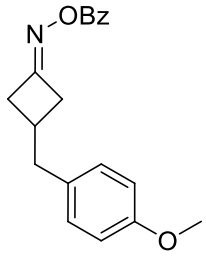
cyclobutanone *O*-(4-methoxybenzoyl) oxime (2a-4)

White solid (646 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.02-7.98 (m, 2 H), 6.95-6.91 (m, 2 H), 3.86 (s, 3 H), 3.15-3.10 (m, 4 H), 2.15-2.07 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =168.9, 163.9, 163.6, 131.7, 121.3, 113.8, 55.5, 31.9, 14.4.



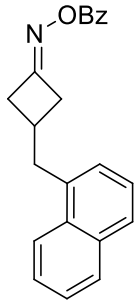
3-benzylcyclobutanone *O*-benzoyl oxime (2b)

White solid (804 mg, 58% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.05-8.02 (m, 2 H), 7.60-7.56 (m, 1 H), 7.47-7.42 (m, 2 H), 7.34-7.30 (m, 2 H), 7.26-7.17 (m, 3 H), 3.25-3.19 (m, 2 H), 2.92-2.74 (m, 5 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 166.8, 163.9, 139.2, 133.2, 129.5, 128.8, 128.5, 128.4, 128.3, 126.4, 41.6, 37.1, 29.3.



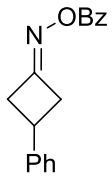
3-(4-methoxybenzyl)cyclobutanone *O*-benzoyl oxime (2c)

White solid (957 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.03-8.01 (m, 2 H), 7.57-7.53 (m, 1 H), 7.45-7.40 (m, 2 H), 7.09-7.07 (d, *J* = 8.6 Hz, 2 H), 6.85-6.83 (d, *J* = 8.6 Hz, 2 H), 3.77 (s, 3 H), 3.23-3.13 (m, 2 H), 2.84-2.67 (m, 5 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 167.0, 164.0, 158.2, 133.3, 131.3, 129.6, 129.5, 129.0, 128.5, 114.0, 55.3, 40.8, 37.1, 29.5.



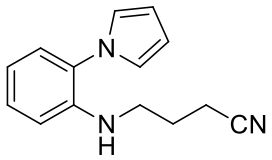
3-(naphthalen-2-ylmethyl)cyclobutanone *O*-benzoyl oxime (2d)

White solid (674 mg, 41% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.03-7.99 (m, 3 H), 7.87-7.85 (d, *J* = 7.8 Hz, 1 H), 7.76-7.74 (d, *J* = 8.2 Hz, 1 H), 7.57-7.49 (m, 3 H), 7.44-7.39 (m, 3 H), 7.28-7.23 (m, 1 H), 3.37-3.19 (m, 4 H), 2.99-2.83 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 166.9, 164.1, 135.2, 134.0, 133.3, 131.8, 129.7, 129.0, 128.9, 128.5, 127.4, 126.2, 125.8, 125.5, 123.4, 38.8, 37.6, 37.5, 28.5.



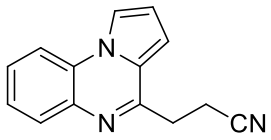
3-phenylcyclobutanone *O*-benzoyl oxime (2e)

White solid (779 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.08-8.05 (m, 2 H), 7.61-7.56 (m, 1 H), 7.48-7.43 (m, 2 H), 7.39-7.34 (m, 2 H), 7.30-7.26 (m, 3 H), 3.73-3.51 (m, 3 H), 3.29-3.18 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 165.9, 163.8, 142.8, 133.2, 129.5, 128.6, 128.4, 126.7, 126.2, 39.4, 39.3, 32.3.



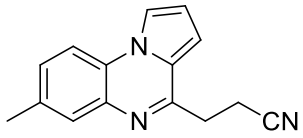
4-((2-(1*H*-pyrrol-1-yl)phenyl)amino)butanenitrile (5)

Yellow solid (734.7 mg, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.27-7.23 (m, 1H), 7.14-7.12 (m, 1 H), 6.77-6.72 (m, 4 H), 6.34-6.33 (m, 2 H), 3.76 (s, 1 H), 3.26-3.24 (m, 2 H), 2.38-2.34 (m, 2 H), 1.91-1.85 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.1, 129.0, 127.5, 127.2, 121.8, 119.0, 117.1, 111.0, 109.6, 41.9, 25.1, 14.6.



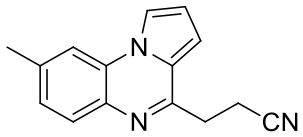
3-(pyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3aa)

Light yellow solid (53.0 mg, 80% yield), melting point: 118-120 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.93-7.90 (m, 2 H), 7.84-7.82 (m, 1 H), 7.53-7.48 (m, 1 H), 7.46-7.42 (m, 1 H), 6.89-6.86 (m, 2 H), 3.39-3.35 (m, 2 H), 3.08-3.04 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.7, 135.5, 129.8, 127.6, 127.3, 125.3, 125.2, 119.7, 114.7, 113.8, 113.7, 105.7, 29.9, 14.1; HRMS calcd for $C_{14}H_{12}N_3$ $[M+H]^+$ 222.1026; found: 222.1029.



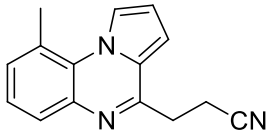
3-(7-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ba)

Light yellow solid (39.5 mg, 56% yield), melting point: 120-123 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.84 (s, 1 H), 7.69-7.66 (m, 2 H), 7.29-7.25 (m, 1 H), 6.81 (s, 2 H), 3.34-3.30 (m, 2 H), 3.04-3.00 (m, 2 H), 2.47 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.5, 135.3, 135.0, 129.4, 128.6, 125.1, 125.0, 119.8, 114.4, 113.4, 113.3, 105.3, 29.8, 21.0, 14.0; HRMS calcd for $C_{15}H_{14}N_3$ $[M+H]^+$ 236.1182; found: 236.1188.



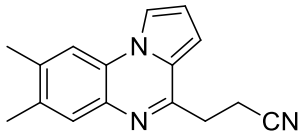
3-(8-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ca)

Light yellow solid (40.2 mg, 57% yield), melting point: 150-153 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.89-7.88 (m, 1 H), 7.79-7.77 (d, *J* = 8.4 Hz, 1 H), 7.62 (s, 1 H), 7.24-7.23 (d, *J* = 1.6 Hz, 1 H), 6.85-6.84 (d, *J* = 2.0 Hz, 2 H), 3.37-3.33 (m, 2 H), 3.06-3.03 (m, 2 H), 2.54 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.7, 138.1, 133.4, 129.3, 127.0, 126.5, 125.3, 119.8, 114.3, 113.7, 113.6, 105.3, 29.9, 21.8, 14.1; HRMS calcd for $C_{15}H_{14}N_3$ $[M+H]^+$ 236.1182; found: 236.1176.



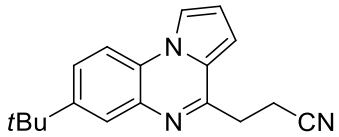
3-(9-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3da)

Light yellow solid (52.2 mg, 74% yield), melting point: 116-118 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.27-8.26 (m, 1 H), 7.78-7.75 (m, 1 H), 7.29-7.25 (m, 2 H), 6.87-6.85 (m, 1 H), 6.83-6.81 (m, 1 H), 3.33-3.30 (m, 2 H), 3.04-3.01 (m, 2 H), 2.89 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.2, 137.0, 131.0, 128.1, 127.5, 126.4, 125.3, 124.6, 120.2, 119.8, 112.9, 104.9, 29.6, 23.8, 13.9; HRMS calcd for $C_{15}H_{14}N_3$ $[M+H]^+$ 236.1182; found: 236.1188.



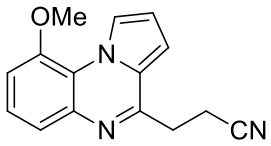
3-(7,8-dimethylpyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ea)

Light yellow solid (33.6 mg, 45% yield), melting point: 159-160 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.85-7.84 (m, 1 H), 7.66 (s, 1 H), 7.57 (s, 1 H), 6.83-6.82 (d, *J* = 2.0 Hz, 2 H), 3.36-3.32 (m, 2 H), 3.05-3.01 (m, 2 H), 2.42 (s, 3 H), 2.37 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 150.7, 137.1, 134.2, 133.6, 129.7, 125.3, 125.2, 119.9, 114.2, 114.1, 113.4, 105.2, 29.9, 20.3, 19.6, 14.3; HRMS calcd for $C_{16}H_{16}N_3$ $[M+H]^+$ 250.1339; found: 250.1334.



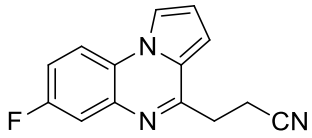
3-(7-(*tert*-butyl)pyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3fa)

Light yellow solid (39.8 mg, 48% yield), melting point: 134-137 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.92-7.88 (m, 2 H), 7.77-7.74 (d, *J* = 8.8 Hz, 1 H), 7.57-7.54 (m, 1 H), 6.86-6.83 (m, 2 H), 3.38-3.34 (m, 2 H), 3.07-3.03 (m, 2 H), 1.41 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.6, 148.5, 135.1, 125.9, 125.3, 125.2, 125.0, 119.7, 114.4, 113.5, 113.2, 105.4, 34.6, 31.4, 30.0, 14.3; HRMS calcd for $C_{18}H_{20}N_3$ $[M^+H]^+$ 278.1652; found: 278.1659.



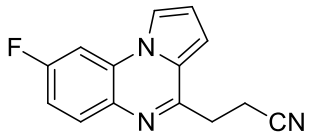
3-(9-methoxypyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ga)

Light yellow solid (52.0 mg, 69% yield), melting point: 121-124 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.70-8.69 (m, 1 H), 7.51-7.49 (d, *J* = 8.0 Hz, 1 H), 7.33-7.29 (m, 1 H), 7.00-6.98 (d, *J* = 8.0 Hz, 1 H), 6.86-6.85 (m, 1 H), 6.79-6.77 (m, 1 H), 4.03 (s, 3 H), 3.33-3.30 (m, 2 H), 3.03-3.00 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.8, 149.6, 137.5, 125.6, 124.3, 122.3, 121.5, 119.8, 118.5, 112.5, 108.9, 104.8, 56.1, 29.7, 14.0; HRMS calcd for $C_{15}H_{14}N_3O$ $[M^+H]^+$ 252.1132; found: 252.1138.



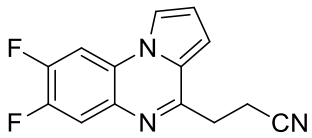
3-(7-fluoropyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ha)

Yellow solid (52.3 mg, 73% yield), melting point: 126-128 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.87 (s, 1 H), 7.86-7.74 (m, 1 H), 7.58-7.55 (m, 1 H), 7.24-7.19 (m, 1 H), 6.89-6.85 (m, 2 H), 3.37-3.33 (m, 2 H), 3.06-3.03 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 161.0-158.6 (d, *J* = 243 Hz, 1 C), 153.0, 136.6-136.5 (d, *J* = 11 Hz, 1 C), 125.1-119.8 (d, *J* = 528 Hz, 1 C), 123.9, 115.4, 115.2, 115.0, 114.9, 114.8, 113.9, 106.1, 29.9, 14.0; HRMS calcd for $C_{14}H_{11}FN_3$ $[M+H]^+$ 240.0932; found: 240.0937.



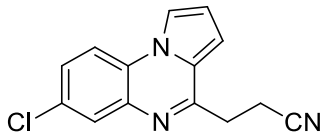
3-(8-fluoropyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ia)

Light yellow solid (47.5 mg, 71% yield), melting point: 120-123 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.88-7.87 (m, 1 H), 7.78-7.75 (m, 1 H), 7.59-7.56 (m, 1 H), 7.24-7.19 (m, 1 H), 6.89-6.85 (m, 2 H), 3.37-3.34 (m, 2 H), 3.06-3.03 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.9, 158.5, 152.9, 136.6-136.5 (d, *J* = 11 Hz, 1 C), 125.0-119.7 (d, *J* = 534 Hz, 1 C), 123.9, 115.3, 115.1, 114.9, 114.8-114.7 (d, *J* = 10 Hz, 1 C), 113.9, 106.0, 29.8, 13.9; HRMS calcd for $C_{14}H_{11}FN_3$ $[M+H]^+$ 240.0932; found: 240.0938.



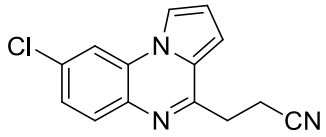
3-(7,8-difluoropyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ja)

Light yellow solid (60.9 mg, 79% yield), melting point: 145-146 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6, ppm): δ = 8.42-8.37 (m, 1 H), 8.35-8.34 (d, *J* = 1.6 Hz, 1 H), 7.79-7.74 (m, 1 H), 7.10-7.09 (m, 1 H), 6.91-6.90 (m, 1 H), 3.32-3.29 (m, 2 H), 3.03-3.00 (m, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6, ppm): δ = 153.5, 149.8-148.2 (dd, *J* = 154 Hz, 15 Hz, 1 C), 147.4-145.7 (dd, *J* = 150 Hz, 14 Hz, 1 C), 131.7-123.7 (dd, *J* = 801 Hz, 10 Hz, 1 C), 124.3, 120.6, 117.1, 116.4-116.2 (d, *J* = 18 Hz, 1 C), 114.3, 107.3, 104.0, 103.7, 29.2, 13.5; HRMS calcd for $C_{14}H_{10}F_2N_3$ $[M+H]^+$ 258.0838; found: 258.0830.



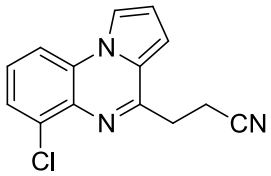
3-(7-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ka)

Light yellow solid (48.2 mg, 63% yield), melting point: 147-150 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.91-7.90 (d, *J* = 2.4 Hz, 1 H), 7.90-7.89 (m, 1 H), 7.77-7.74 (d, *J* = 8.8 Hz, 1 H), 7.47-7.44 (m, 1 H), 6.91-6.87 (m, 2 H), 3.39-3.35 (m, 2 H), 3.07-3.03 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.9, 136.3, 130.4, 129.2, 127.6, 125.9, 125.2, 119.7, 115.0, 114.8, 114.2, 106.3, 29.8, 13.9; HRMS calcd for $C_{14}H_{11}ClN_3$ $[M+H]^+$ 256.0636; found: 256.0630.



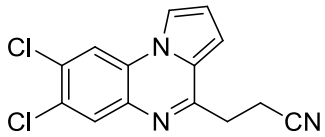
3-(8-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3la)

Light yellow solid (53.6 mg, 70% yield), melting point: 200-203 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.78 (m, 3 H), 7.37-7.34 (m, 1 H), 6.88 (s, 2 H), 3.37-3.33 (m, 2 H), 3.06-3.02 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.8, 133.9, 132.9, 130.8, 127.8, 125.6, 125.1, 119.7, 114.9, 114.3, 113.8, 106.1, 29.8, 13.9; HRMS calcd for $C_{14}H_{11}ClN_3$ $[M+H]^+$ 256.0636; found: 256.0643.



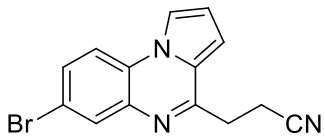
3-(6-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ma)

Light yellow solid (36.0 mg, 47% yield), melting point: 138-140 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.89-7.88 (m, 1 H), 7.71-7.69 (m, 1 H), 7.50-7.48 (m, 1 H), 7.38-7.34 (m, 1 H), 6.90-6.87 (m, 2 H), 3.40-3.36 (m, 2 H), 3.13-3.10 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.1, 134.2, 132.3, 128.3, 127.2, 125.9, 125.2, 119.8, 115.3, 114.4, 112.4, 106.2, 29.9, 13.8; HRMS calcd for $C_{14}H_{11}ClN_3$ $[M+H]^+$ 256.0636; found: 256.0642.



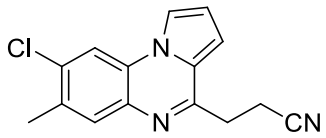
3-(7,8-dichloropyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3na)

Light yellow solid (58.9 mg, 68% yield), melting point: 141-143 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d_6, ppm): δ = 8.60 (s, 1 H), 8.48-8.47 (d, *J* = 2.0 Hz, 1 H), 7.94 (s, 1 H), 7.15-7.14 (d, *J* = 3.6 Hz, 1 H), 6.94-6.92 (m, 1 H), 3.35-3.31 (m, 2 H), 3.05-3.01 (m, 2 H); ^{13}C NMR (100 MHz, DMSO-d_6, ppm): δ = 154.7, 134.6, 129.7, 129.6, 127.3, 126.6, 124.6, 120.6, 117.6, 116.8, 114.6, 108.0, 29.2, 13.5; HRMS calcd for $C_{14}H_{10}Cl_2N_3$ $[M+H]^+$ 290.0247; found: 290.0240.



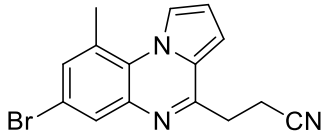
3-(7-bromopyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3oa)

Light yellow solid (48.4 mg, 54% yield), melting point: 156-158 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.04-8.03 (d, *J* = 1.6 Hz, 1 H), 7.86 (s, 1 H), 7.66-7.64 (d, *J* = 8.8 Hz, 1 H), 7.56-7.53 (m, 1 H), 6.89-6.86 (m, 2 H), 3.37-3.33 (m, 2 H), 3.05-3.02 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.8, 136.5, 132.1, 130.2, 126.2, 125.1, 119.7, 117.7, 114.9, 114.2, 106.3, 29.7, 13.8; HRMS calcd for $C_{14}H_{11}BrN_3$ $[M+H]^+$ 300.0131; found: 300.0138.



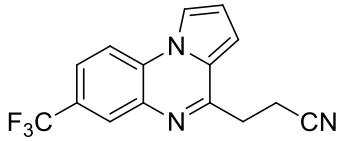
3-(8-chloro-7-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3pa)

Light yellow solid (46.0 mg, 57% yield), melting point: 176-178 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.80-7.79 (m, 1 H), 7.80 (s, 1 H), 7.74 (s, 1 H), 6.86-6.83 (m, 2 H), 3.36-3.32 (m, 2 H), 3.05-3.01 (m, 2 H), 2.47 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.8, 134.0, 133.3, 133.2, 131.1, 125.9, 125.0, 119.7, 114.7, 114.0, 113.9, 105.9, 29.8, 19.8, 13.9; HRMS calcd for $C_{15}H_{13}ClN_3$ $[M+H]^+$ 270.0793; found: 270.0798.



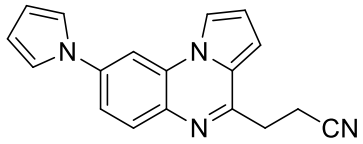
3-(9-bromo-7-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3qa)

Light yellow solid (59.2 mg, 63% yield), melting point: 141-144 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.26-8.25 (m, 1 H), 7.95-7.94 (d, *J* = 2.4 Hz, 1 H), 7.41-7.40 (d, *J* = 2.0 Hz, 1 H), 6.93-6.92 (m, 1 H), 6.88-6.86 (m, 1 H), 3.37-3.34 (m, 2 H), 3.06-3.02 (m, 2 H), 2.88 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.3, 138.2, 133.3, 130.5, 127.3, 126.7, 126.5, 120.5, 119.8, 117.1, 113.6, 105.7, 29.6, 23.7, 13.9; HRMS calcd for $C_{15}H_{13}BrN_3$ $[M+H]^+$ 314.0288; found: 314.0284.



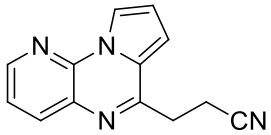
3-(7-(trifluoromethyl)pyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3ra)

Light yellow solid (64.2 mg, 74% yield), melting point: 162-165 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.21-8.20 (d, *J* = 1.2 Hz, 1 H), 7.97-7.96 (m, 1 H), 7.92-7.90 (d, *J* = 8.4 Hz, 1 H), 7.73-7.71 (m, 1 H), 7.00-6.92 (m, 2 H), 3.41-3.37 (m, 2 H), 3.10-3.06 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 153.2, 135.1, 129.4, 127.5-127.2 (q, *J* = 18 Hz, 1 C), 125.4, 125.2-122.5 (d, *J* = 270 Hz, 1 H), 124.0-123.9 (d, *J* = 3.0 Hz, 1 H), 119.6, 115.4, 114.7, 114.4, 106.8, 29.8, 13.8; HRMS calcd for $C_{15}H_{11}F_3N_3$ $[M+H]^+$ 290.0900; found: 290.0908.



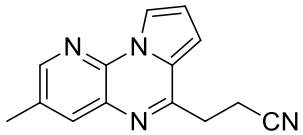
3-(8-(1*H*-pyrrol-1-yl)pyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3sa)

Light yellow solid (68.6 mg, 80% yield), melting point: 170-173 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.97-7.95 (d, *J* = 8.7 Hz, 1 H), 7.93-7.92 (m, 1 H), 7.79-7.78 (d, *J* = 8.7 Hz, 1 H), 7.50-7.47 (m, 1 H), 7.22-7.21 (m, 2 H), 6.92-6.91 (d, *J* = 1.8 Hz, 2 H), 6.44-6.43 (m, 2 H), 3.41-3.37 (m, 2 H), 3.10-3.06 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.2, 139.7, 133.2, 131.1, 128.0, 125.4, 119.8, 119.6, 117.8, 114.8, 114.3, 111.3, 106.1, 105.1, 29.9, 14.1; HRMS calcd for $C_{18}H_{15}N_4$ $[M+H]^+$ 287.1291; found: 287.1298.



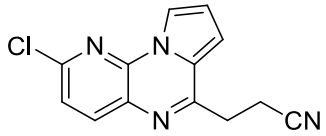
3-(pyrido[3,2-*e*]pyrrolo[1,2-*a*]pyrazin-6-yl)propanenitrile (3ta)

Light yellow solid (36.0 mg, 54% yield), melting point: 143-145 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.52-8.50 (m, 1 H), 8.37-8.36 (m, 1 H), 8.19-8.17 (m, 1 H), 7.43-7.40 (m, 1 H), 6.94-6.93 (m, 1 H), 6.89-6.88 (m, 1 H), 3.39-3.35 (m, 2 H), 3.07-3.03 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.7, 146.7, 139.3, 137.0, 130.2, 126.6, 121.5, 119.6, 115.9, 114.2, 107.2, 29.7, 14.0; HRMS calcd for $C_{13}H_{11}N_4$ $[M+H]^+$ 223.0978; found: 223.0982.



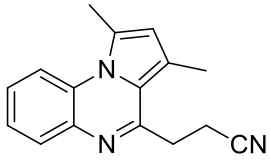
3-(3-methylpyrido[3,2-*e*]pyrrolo[1,2-*a*]pyrazin-6-yl)propanenitrile (3ua)

Light yellow solid (30.4 mg, 43% yield), melting point: 158-160 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.34-8.33 (m, 2 H), 8.00-7.99 (d, *J* = 1.2 Hz, 1 H), 6.92-6.91 (m, 1 H), 6.87-6.86 (m, 1 H), 3.38-3.35 (m, 2 H), 3.06-3.02 (m, 2 H), 2.49 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.6, 147.3, 137.4, 137.0, 131.3, 129.9, 126.6, 119.6, 115.7, 113.9, 106.9, 29.7, 18.1, 14.0; HRMS calcd for $C_{14}H_{13}N_4$ $[M+H]^+$ 237.1135; found: 237.1140.



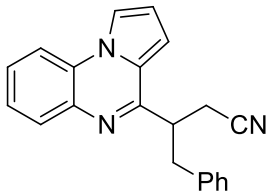
3-(2-chloropyrido[3,2-*e*]pyrrolo[1,2-*a*]pyrazin-6-yl)propanenitrile (3va)

Light yellow solid (35.3 mg, 46% yield), melting point: 184-186 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.36-8.35 (d, *J* = 1.2 Hz, 1 H), 8.16-8.14 (d, *J* = 8.4 Hz, 1 H), 7.43-7.41 (d, *J* = 8.4 Hz, 1 H), 6.98-6.92 (m, 2 H), 3.42-3.38 (m, 2 H), 3.09-3.05 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.9, 147.7, 139.6, 138.7, 129.1, 126.7, 122.0, 119.6, 116.4, 114.8, 107.6, 29.8, 13.9; HRMS calcd for $C_{13}H_{10}ClN_4$ $[M+H]^+$ 257.0589; found: 257.0594.



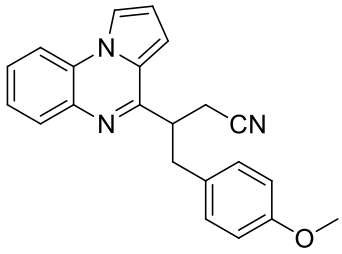
3-(1,3-dimethylpyrrolo[1,2-*a*]quinoxalin-4-yl)propanenitrile (3wa)

Light yellow solid (52.3 mg, 70% yield), melting point: 162-165 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.18-8.15, (m, 1 H), 7.84-7.82 (m, 1 H), 7.40-7.34 (m, 2 H), 6.38 (s, 1 H), 3.47-3.43 (m, 2 H), 3.06-3.02 (m, 2 H), 2.88 (s, 3 H), 2.57 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.0, 136.4, 129.9, 129.3, 127.8, 126.2, 124.4, 123.2, 120.2, 118.4, 116.3, 115.0, 31.1, 17.7, 14.7, 14.0; HRMS calcd for $C_{16}H_{16}N_3$ $[M+H]^+$ 250.1339; found: 250.1331.



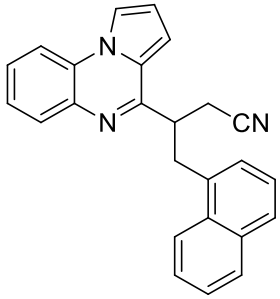
4-phenyl-3-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butanenitrile (3ab)

Colorless oil (60.6 mg, 65% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.96-7.92, (m, 2 H), 7.84-7.82 (m, 1 H), 7.53-7.48 (m, 1 H), 7.46-7.42 (m, 1 H), 7.28-7.22 (m, 2 H), 7.21-7.18 (m, 3 H), 6.85-6.82 (m, 2 H), 3.86-3.79 (m, 1 H), 3.40-3.35 (m, 1 H), 3.11-3.02 (m, 2 H), 2.78-2.72 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.0, 138.2, 135.6, 130.0, 129.1, 128.7, 127.7, 127.3, 126.9, 125.4, 125.3, 119.2, 114.8, 113.8, 113.7, 105.7, 42.4, 40.2, 20.0; HRMS calcd for $C_{21}H_{18}N_3$ $[M+H]^+$ 312.1495; found: 312.1490.



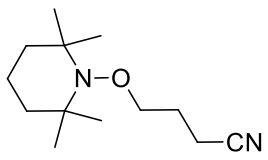
4-(4-methoxyphenyl)-3-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butanenitrile (3ac)

Colorless oil (53.2 mg, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.95-7.91, (m, 2 H), 7.84-7.82 (m, 1 H), 7.52-7.41 (m, 2 H), 7.10-7.08 (d, *J* = 8.6 Hz, 2 H), 6.85-6.82 (m, 2 H), 6.80-6.78 (d, *J* = 8.6 Hz, 2 H), 3.82-3.76 (m, 4 H), 3.34-3.29 (m, 1 H), 3.08-2.97 (m, 2 H), 2.77-2.72 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 158.5, 155.2, 135.6, 130.2, 130.0, 127.6, 127.3, 125.4, 125.2, 119.2, 114.8, 114.7, 114.1, 113.8, 113.7, 105.7, 55.3, 42.6, 39.2, 19.9; HRMS calcd for $C_{22}H_{20}N_3O$ $[M+H]^+$ 342.1601; found: 342.1606.



4-(naphthalen-2-yl)-3-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butanenitrile (3ad)

Colorless oil (45.5 mg, 42% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.13-8.11, (d, *J* = 8.4 Hz, 1 H), 7.99-7.97 (m, 1 H), 7.85-7.84 (m, 2 H), 7.80-7.77 (m, 1 H), 7.71-7.69 (m, 1 H), 7.56-7.52 (m, 1 H), 7.51-7.43 (m, 3 H), 7.30-7.25 (m, 2 H), 6.71-6.70 (m, 1 H), 6.59-6.58 (m, 1 H), 4.05-3.98 (m, 1 H), 3.78-3.72 (m, 1 H), 3.60-3.55 (m, 1 H), 3.16-3.09 (m, 1 H), 2.83-2.77 (m, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.5, 135.7, 134.3, 134.0, 131.9, 129.9, 129.1, 127.7, 127.6, 127.2, 126.3, 125.8, 125.7, 125.4, 125.3, 125.2, 123.3, 119.1, 114.9, 114.8, 113.7, 105.7, 41.3, 37.5, 20.9; HRMS calcd for $C_{25}H_{20}N_3$ $[M+H]^+$ 362.1652; found: 362.1656.



4-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)butanenitrile (4)

Colorless oil (42.3 mg, 63% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 3.86-3.83, (m, 2 H), 2.51-2.47 (m, 2 H), 1.92-1.86 (m, 2 H), 1.55-1.43 (m, 6 H), 1.15 (s, 6 H), 1.09 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 119.7, 73.6, 59.8, 39.6, 33.1, 25.1, 20.1, 17.1, 14.5; HRMS calcd for $C_{13}H_{25}N_2O$ $[M+H]^+$ 225.1962; found: 225.1967.

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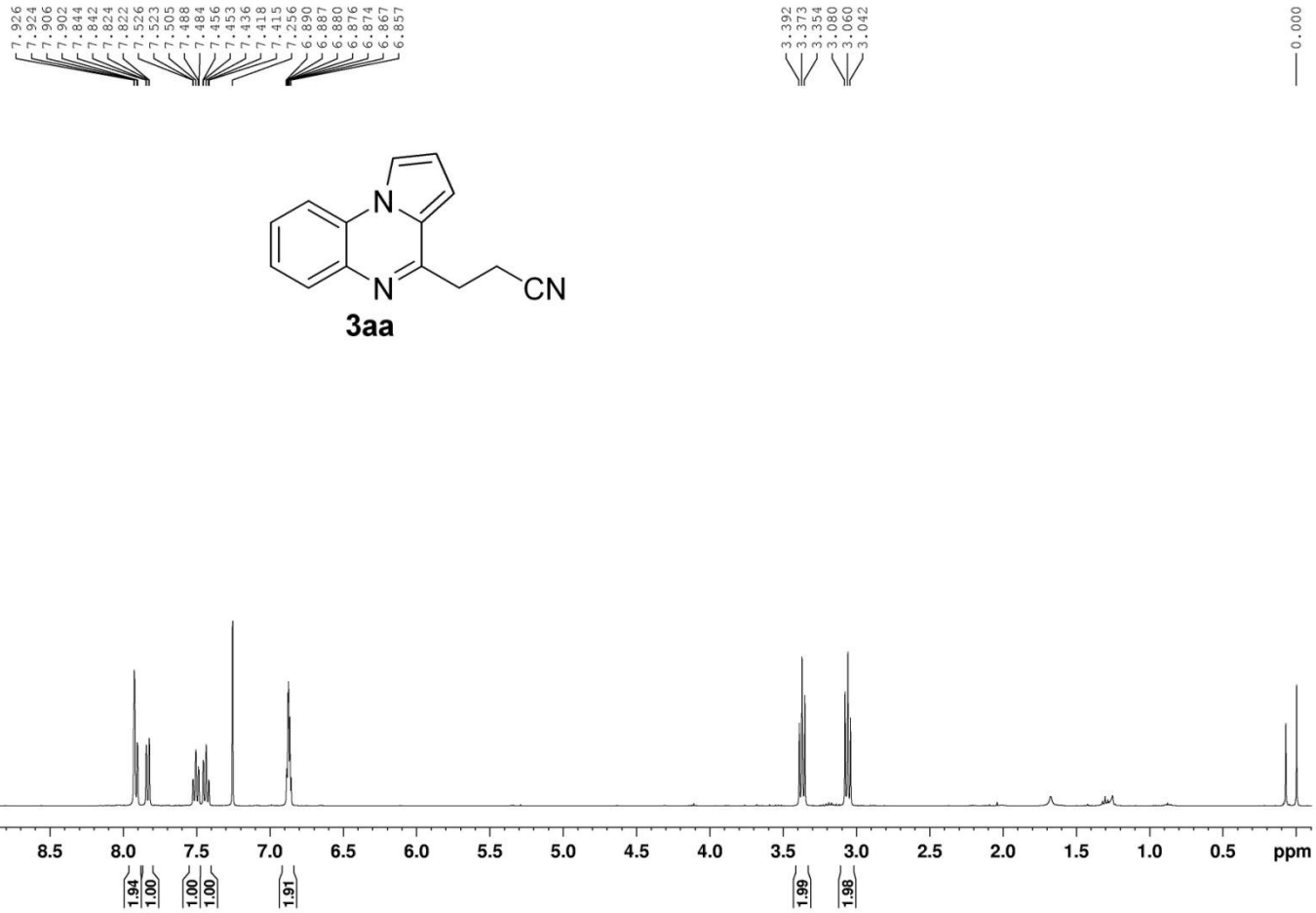
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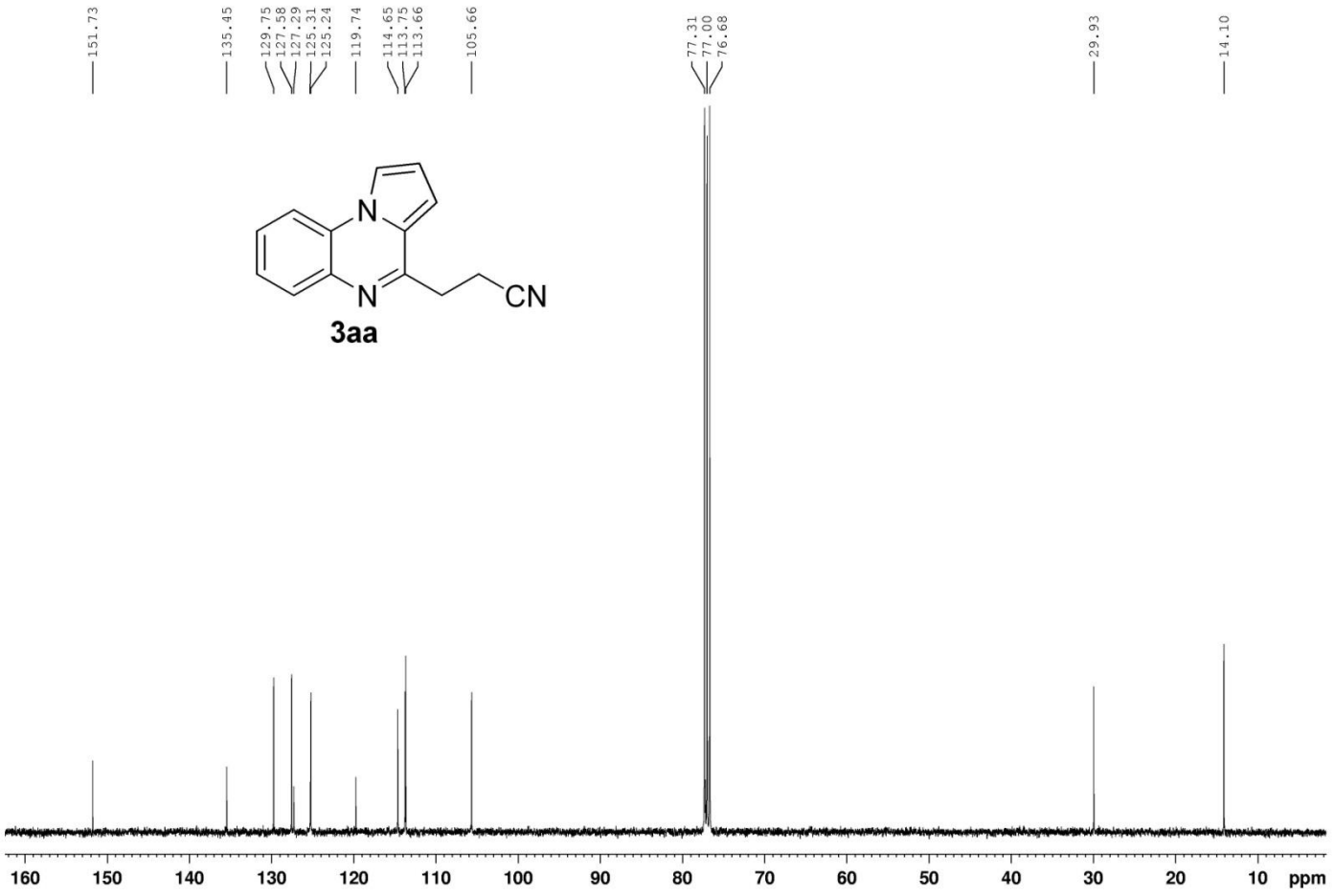
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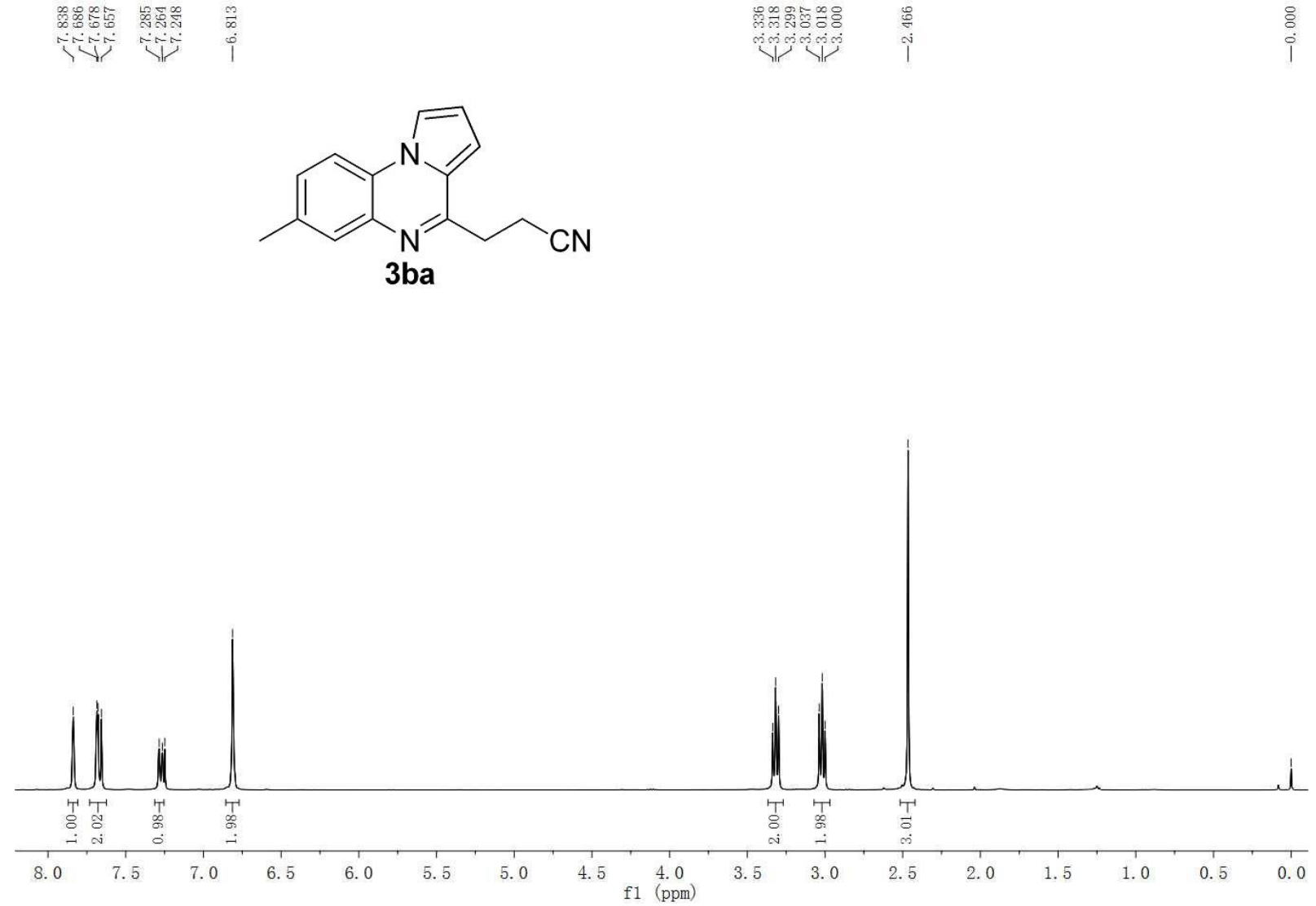
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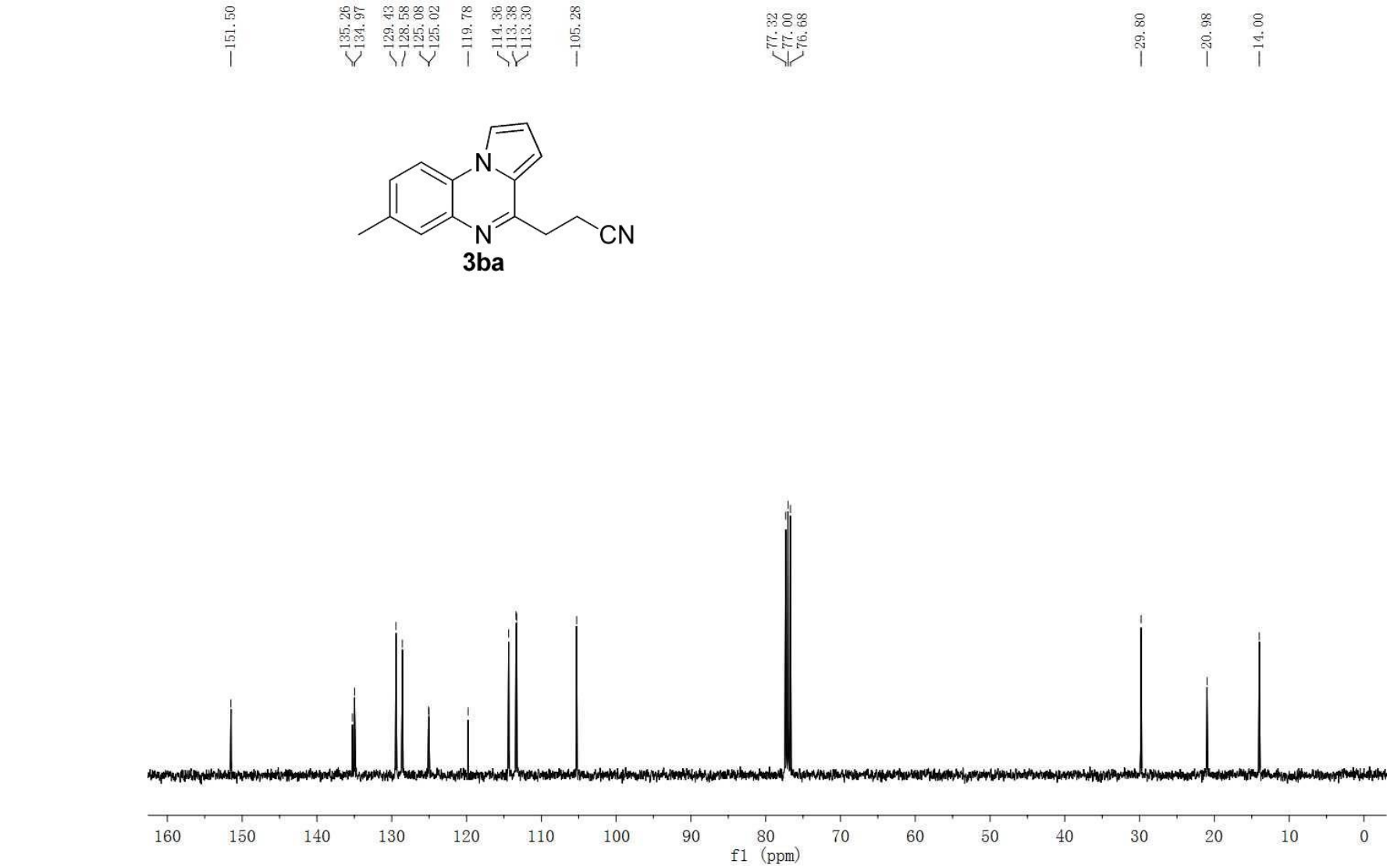
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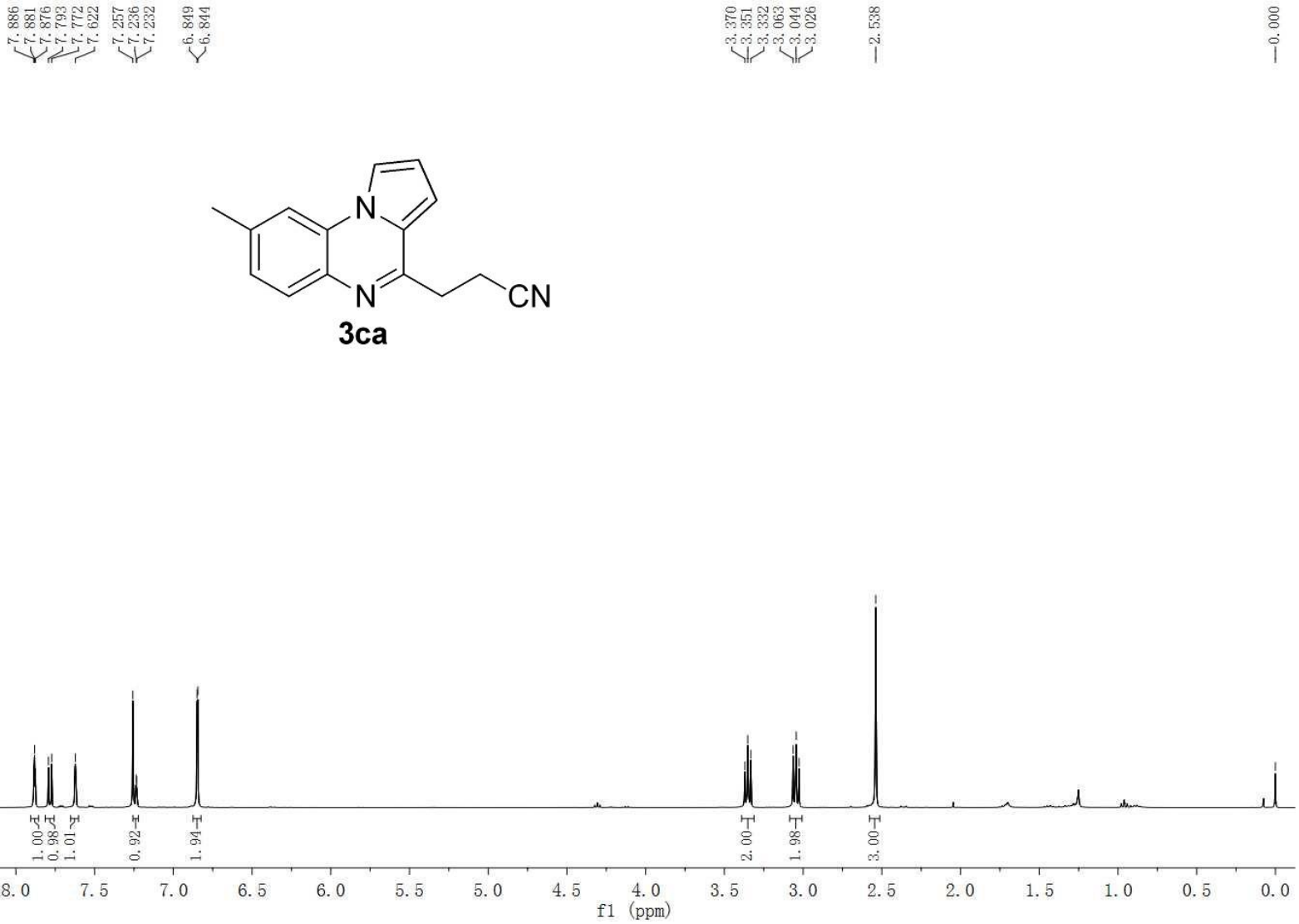
f1 (ppm)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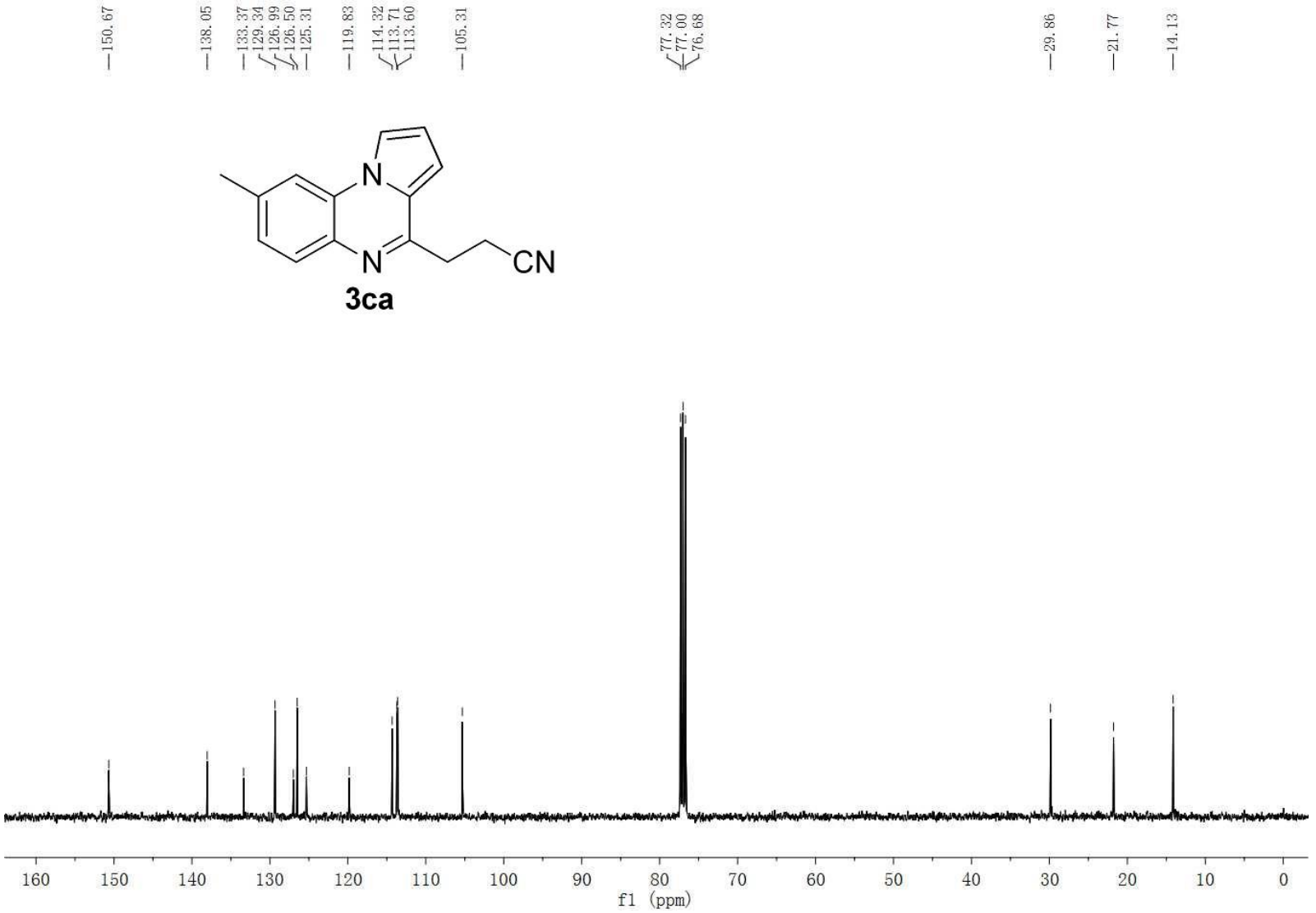
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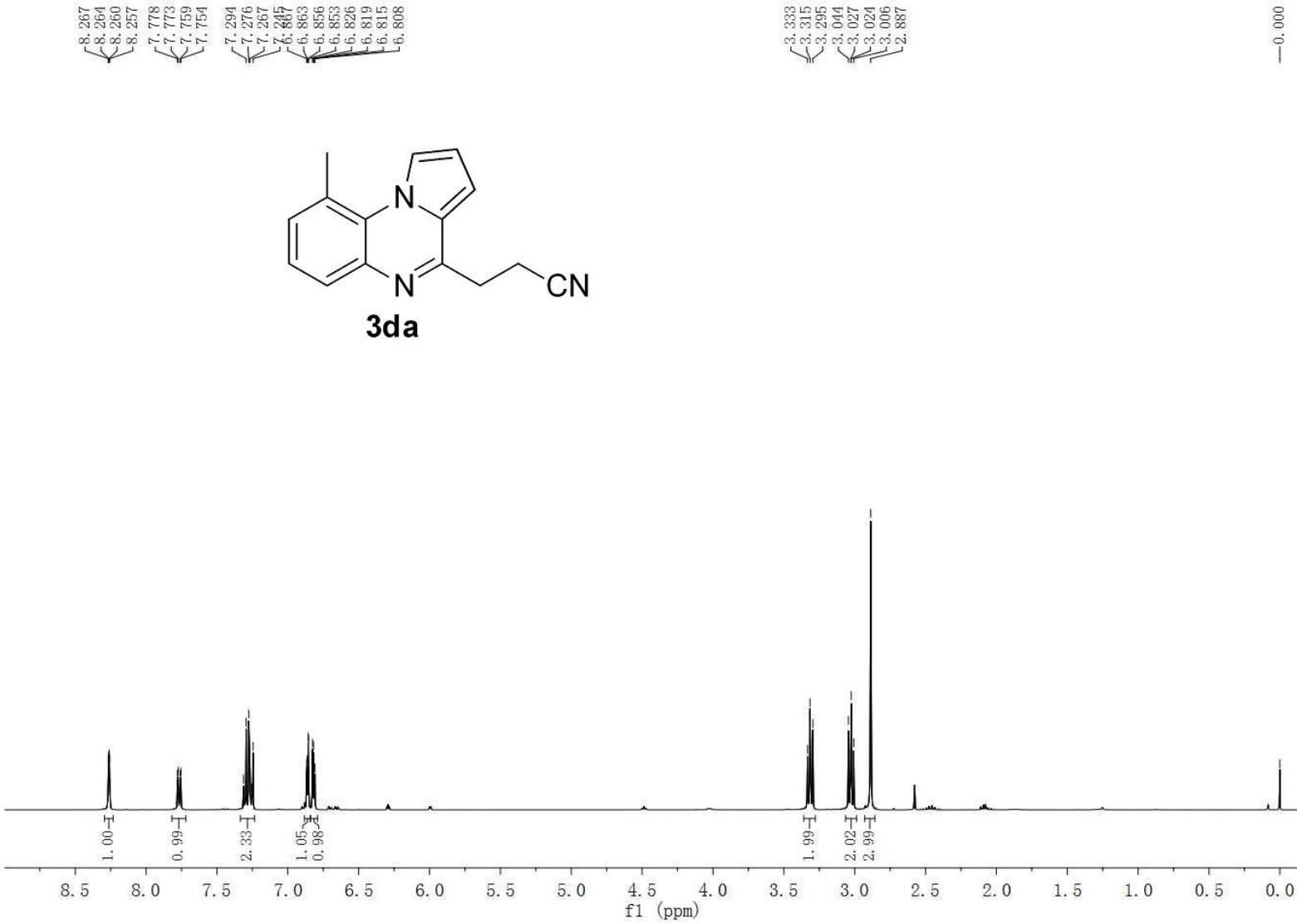
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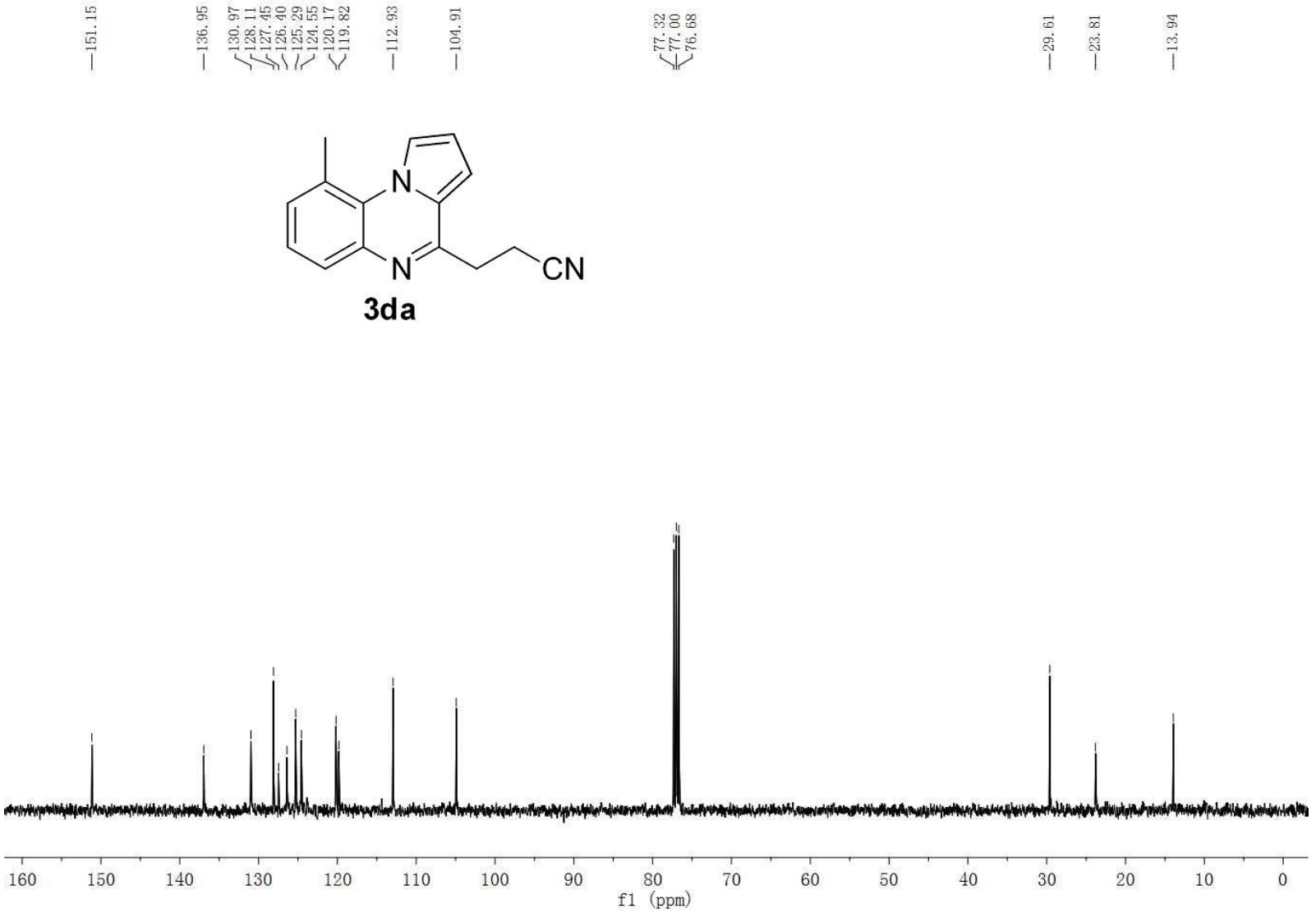
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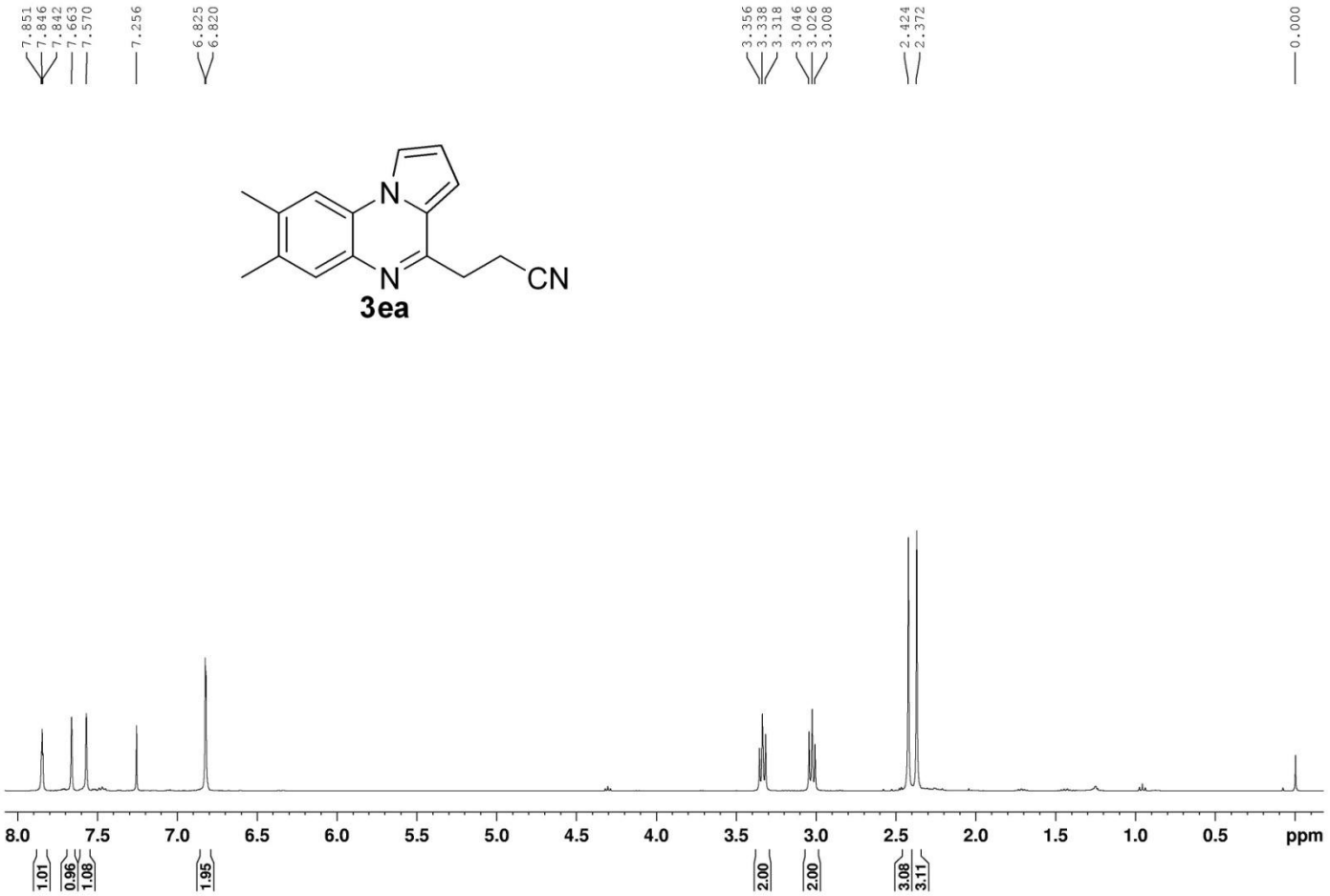
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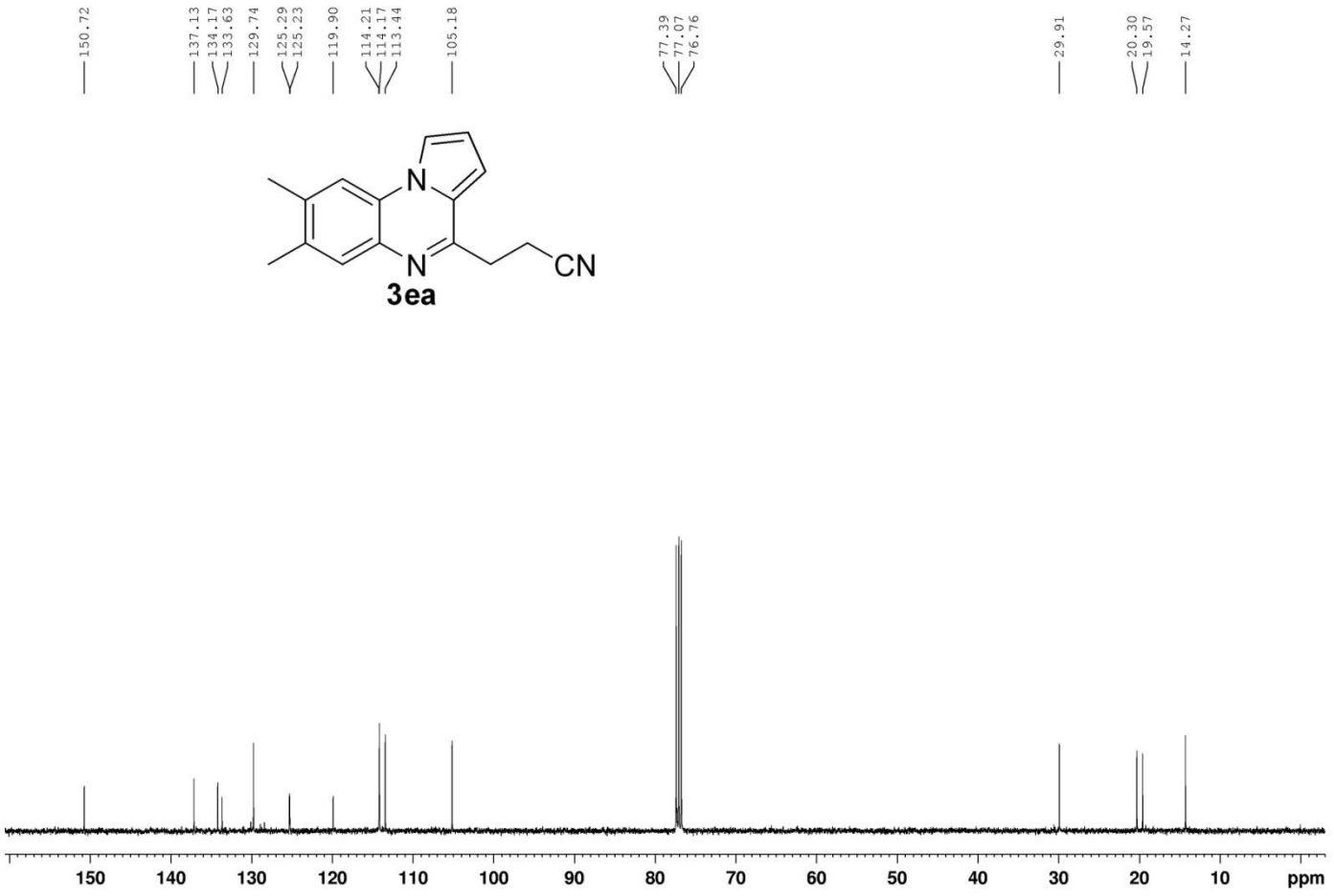
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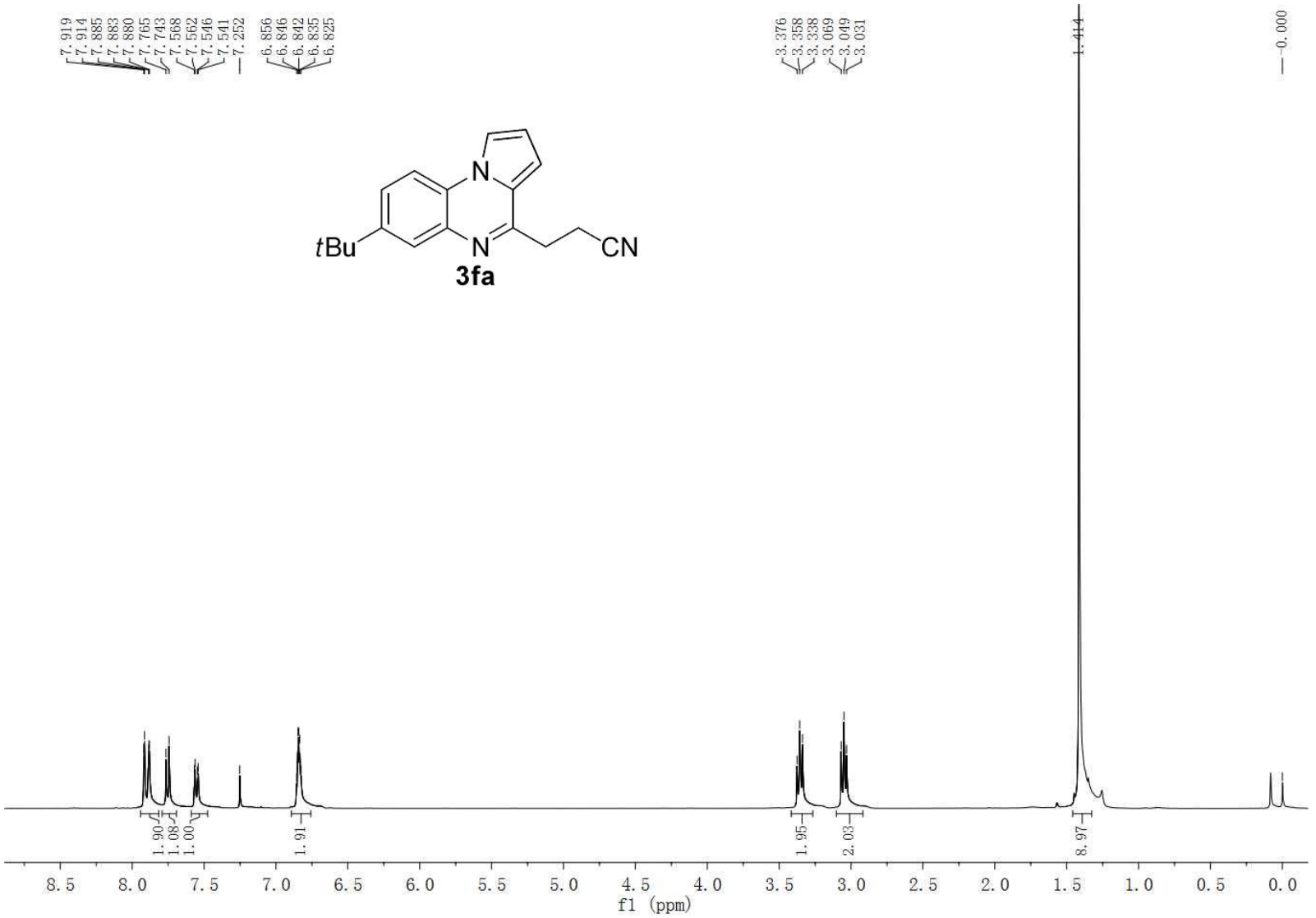
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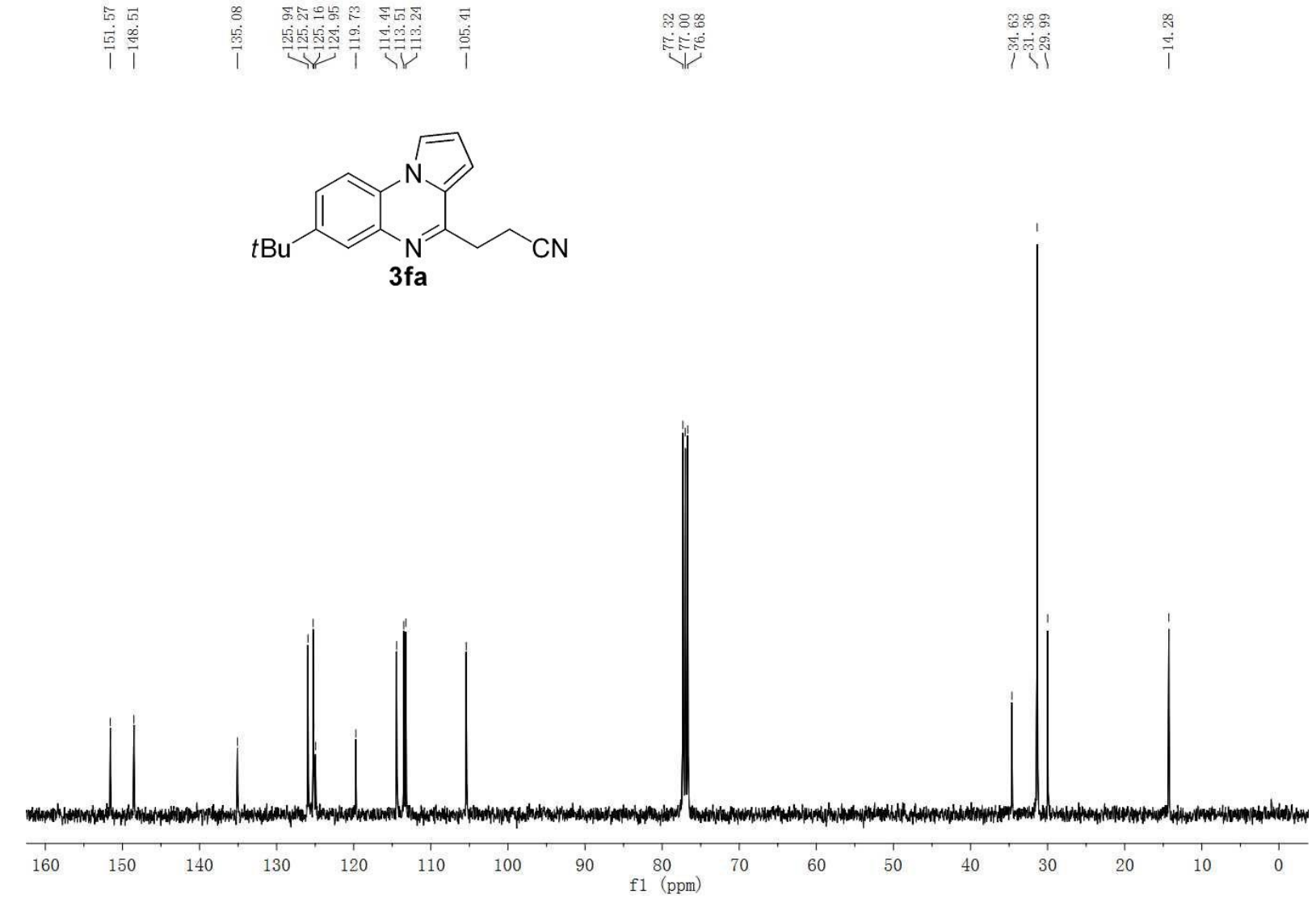
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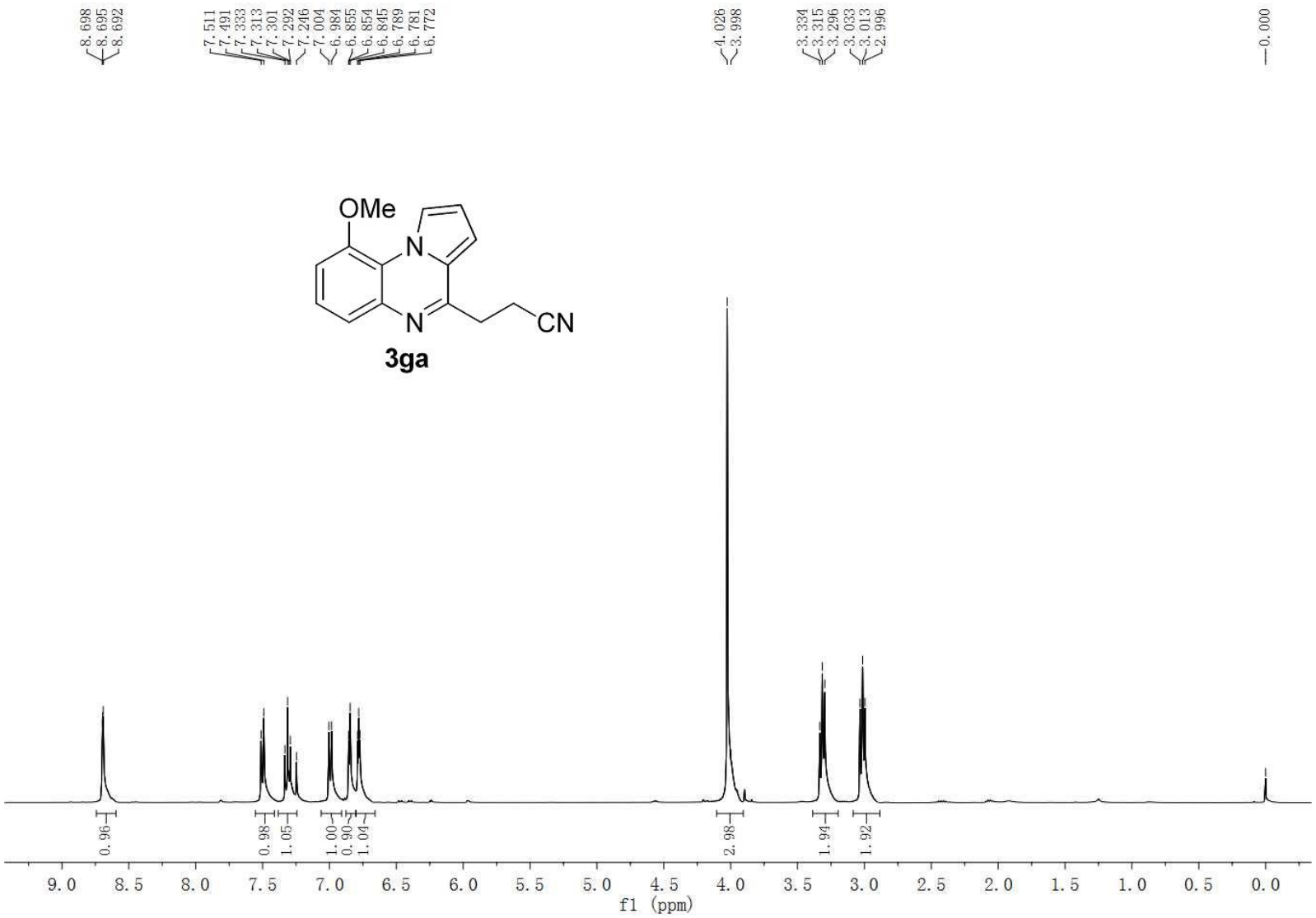
f1 (ppm)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7.301
7.292
7.246
7.004
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6.855
6.854
6.845
6.789
6.781
6.772
4.026
3.998
3.334
3.315
3.296
3.033
3.013
2.996
0.000
OMe
N
N
CN
3ga
0.96
0.98
1.05
1.00
0.90
1.04
2.98
1.94
1.92
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
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1.5
1.0
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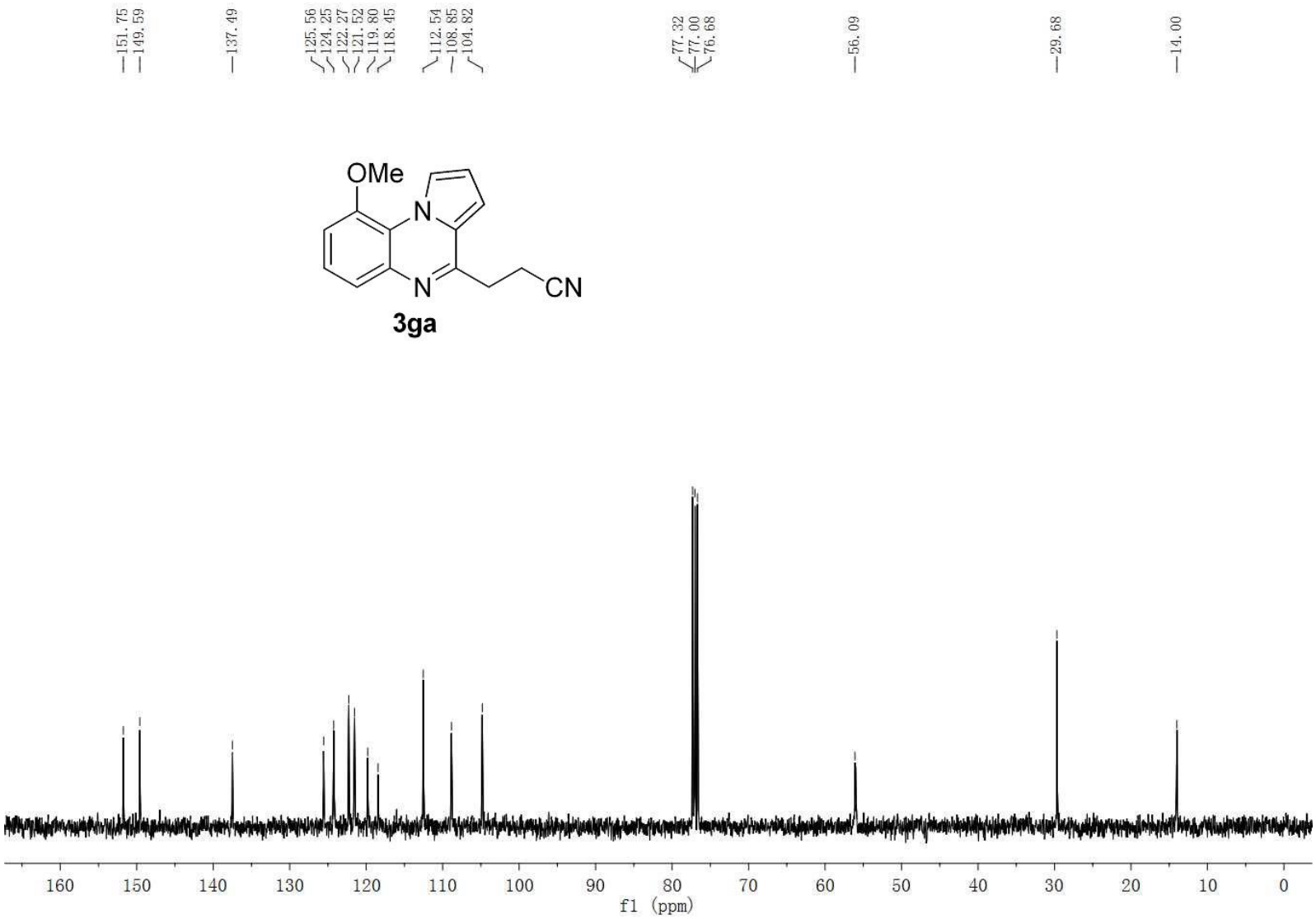
f1 (ppm)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119.80
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112.54
108.85
104.82
77.32
77.00
76.68
56.09
29.68
14.00
OMe
N
N
CN
3ga
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140
130
120
110
100
90
80
70
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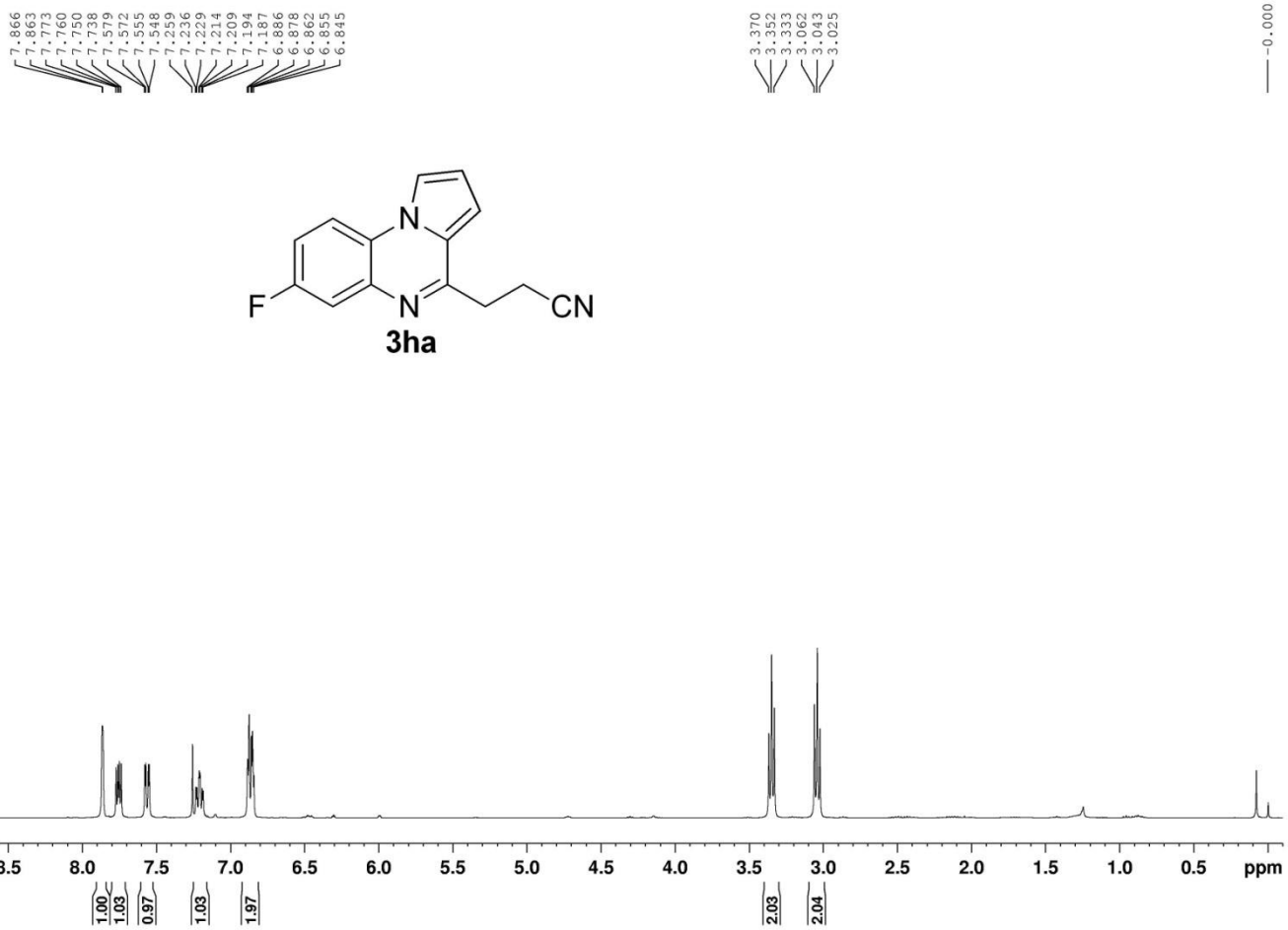
50
40
30
20
10
0
f1 (ppm)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7.229
7.214
7.209
7.194
7.187
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6.878
6.862
6.855
6.845
3.370
3.352
3.333
3.062
3.043
3.025
-0.000
N
F
N
CN
3ha
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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0.5
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1.03
1.97
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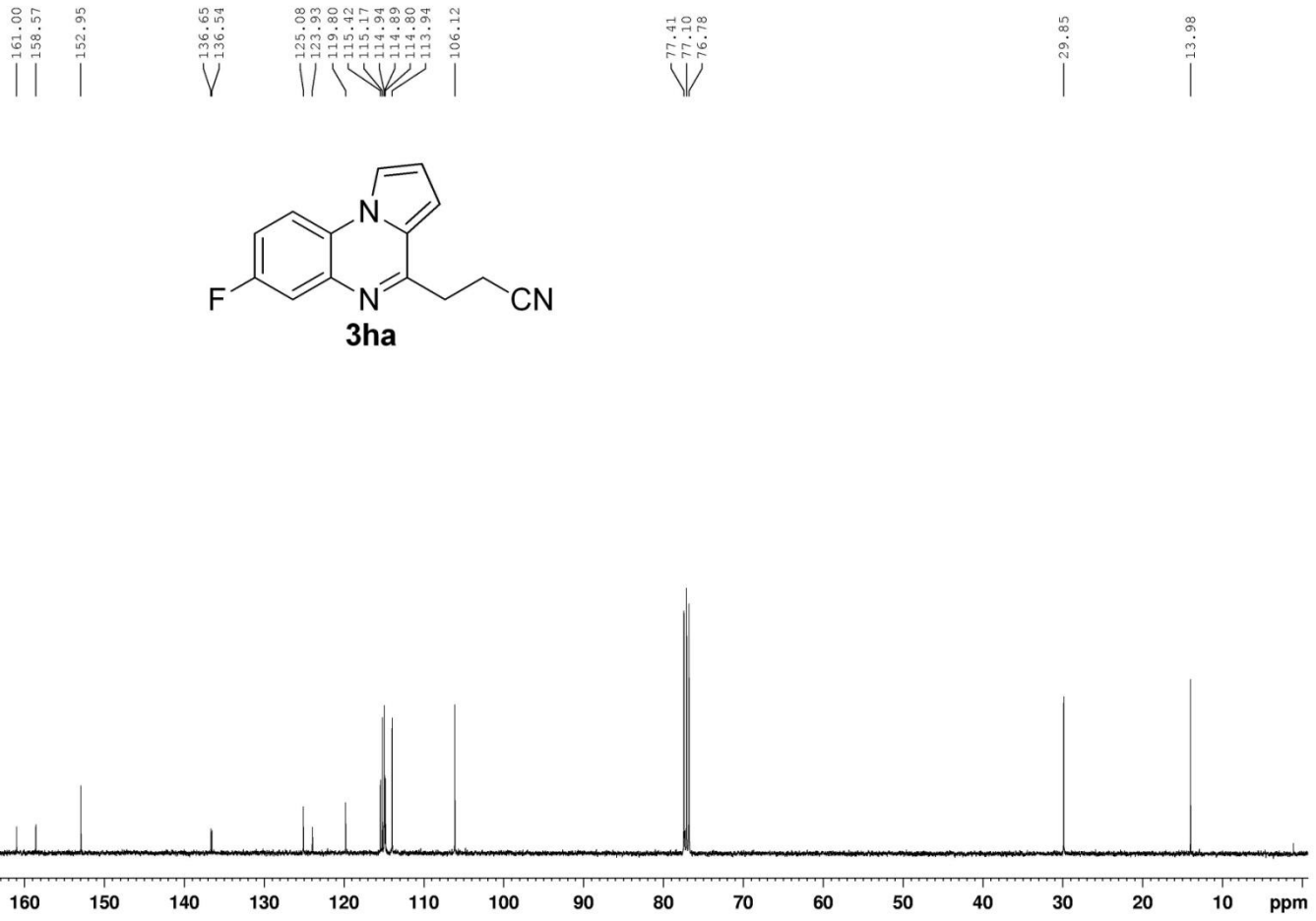
2.04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115.17
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114.89
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113.94
106.12
77.41
77.10
76.78
29.85
13.98
N
F
N
CN
3ha
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.875
7.872
7.868
7.865
7.781
7.769
7.759
7.746
7.587
7.579
7.563
7.556
7.258
7.222
6.890
6.883
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6.857
6.848
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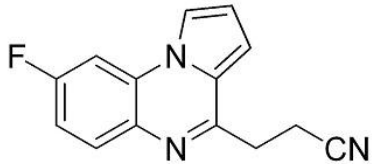
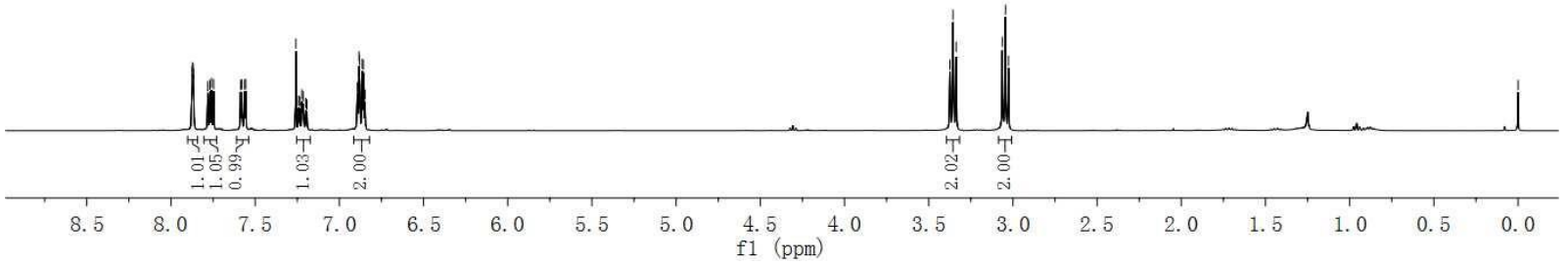
3.356
3.337
3.063
3.044
3.026
0.000


F
N
N
CN

3ia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2.02
2.00
8.5
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7.5
7.0
6.5
6.0
5.5
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4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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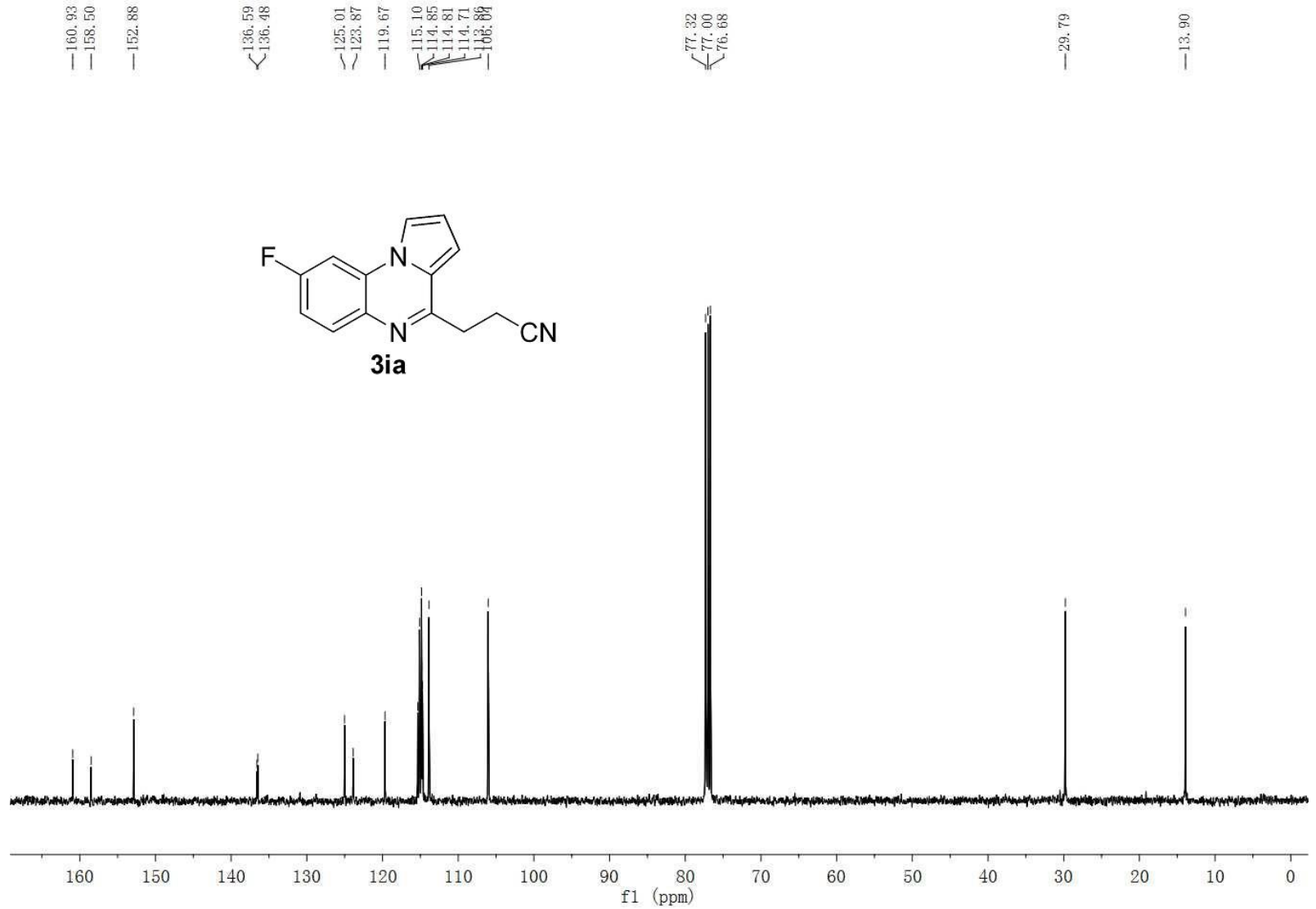
0.0
f1 (ppm)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136.48
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115.10
114.85
114.81
114.71
106.04
77.32
77.00
76.68
29.79
13.90
F
N
N
CN
3ia
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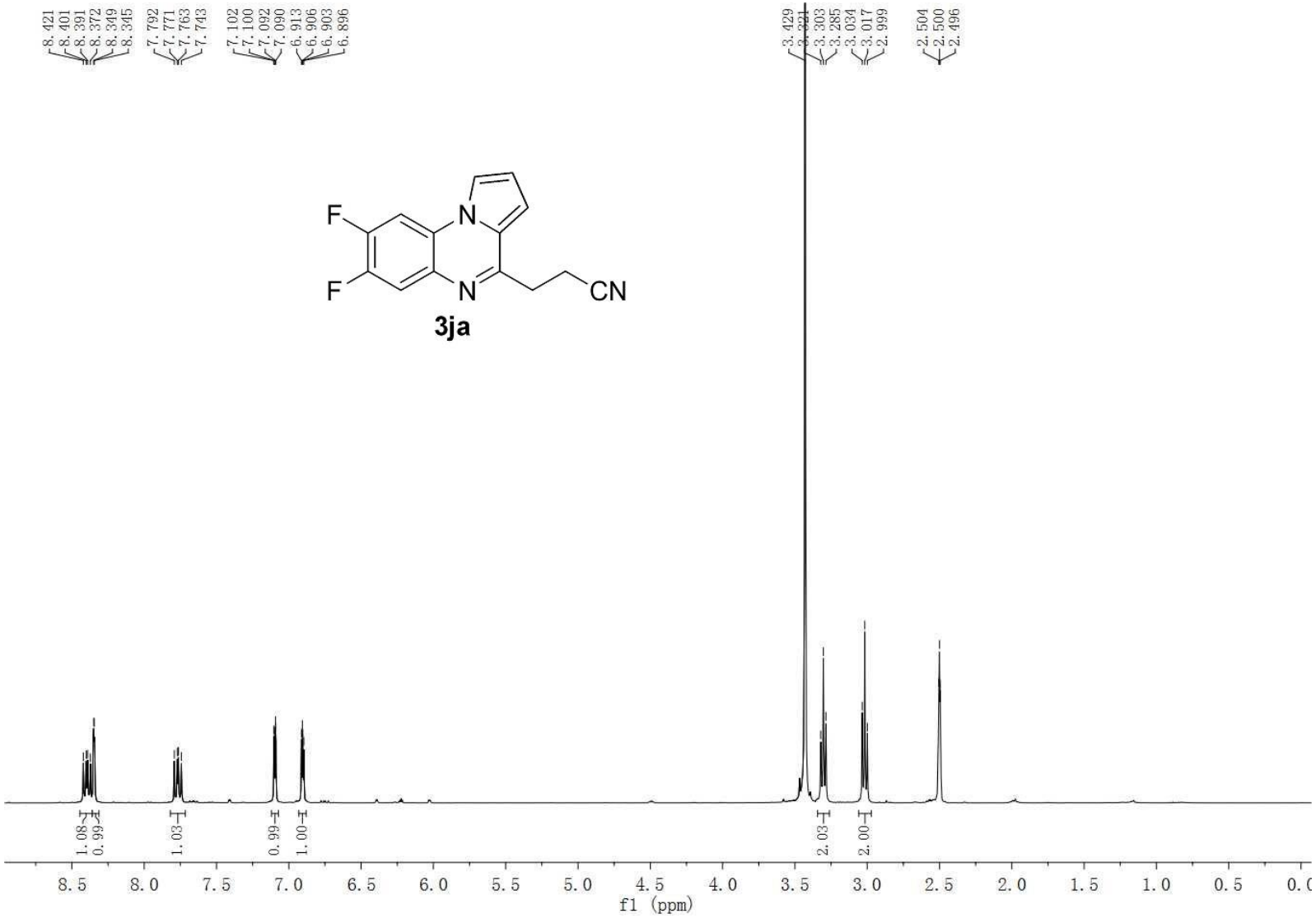
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.345
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7.771
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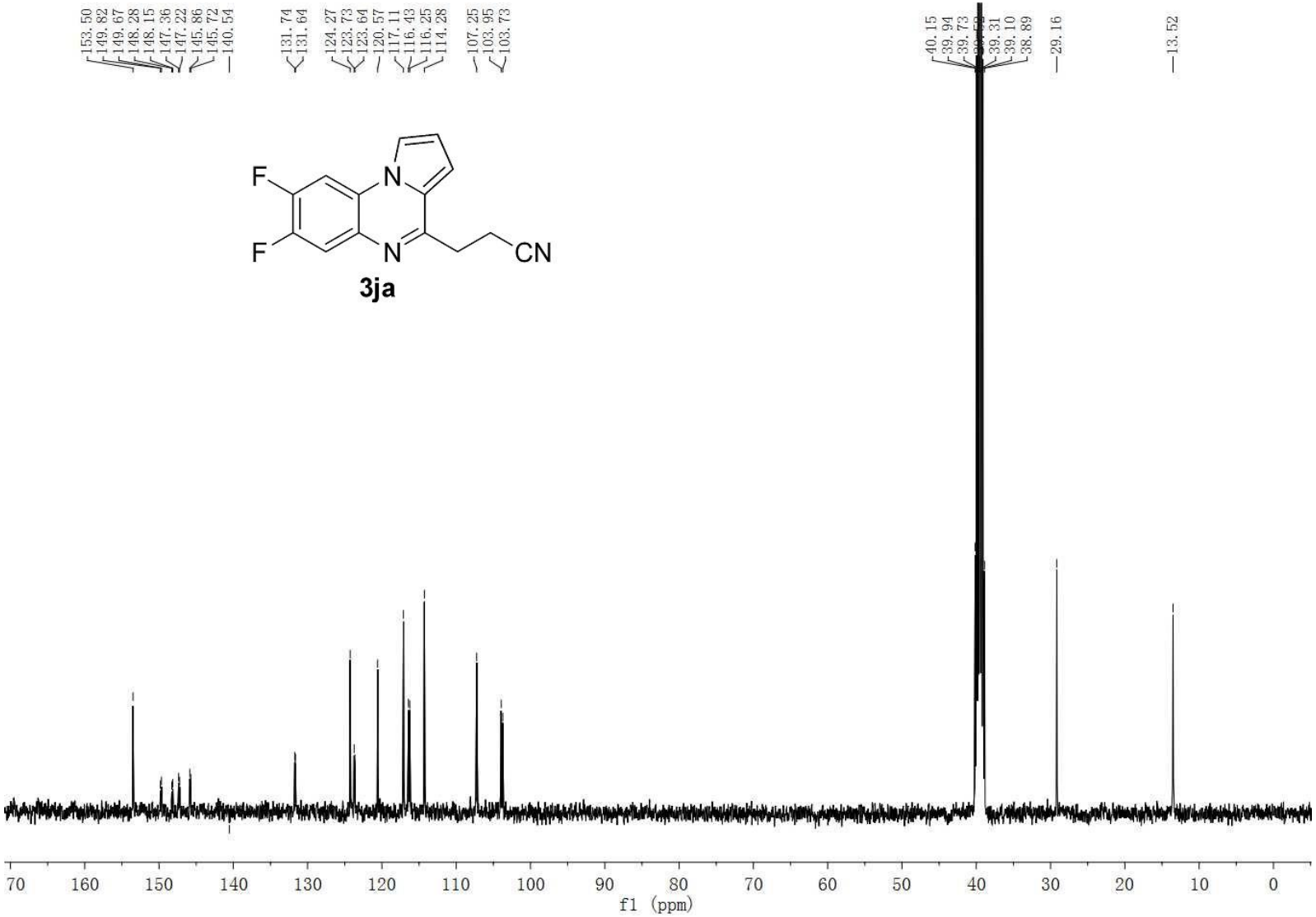
7.743
7.102
7.100
7.092
7.090
6.913
6.906
6.903
6.896
3.429
3.303
3.285
3.034
3.017
2.999
2.504
2.500
2.496
F
F
N
N
CN
3ja
1.08
0.99
1.03
0.99
1.00
2.03
2.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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149.82
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148.15
147.36
147.22
145.86
145.72
140.54
131.74
131.64
124.27
123.73
123.64
120.57
117.11
116.43
116.25
114.28
107.25
103.95
103.73
40.15
39.94
39.73
39.31
39.10
38.89
29.16
13.52
F
F
N
N
CN
3ja
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150
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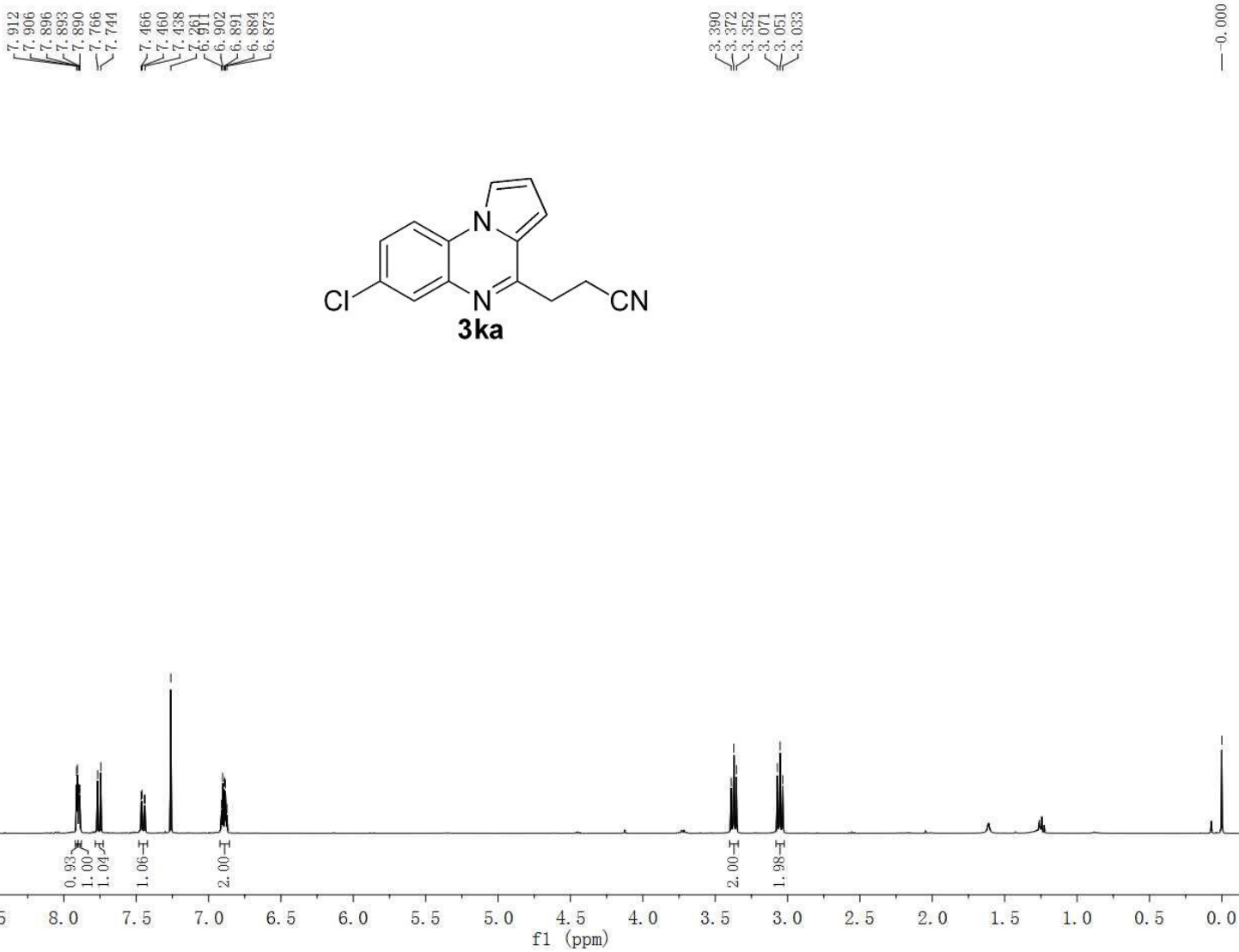
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.466
7.460
7.438
7.261
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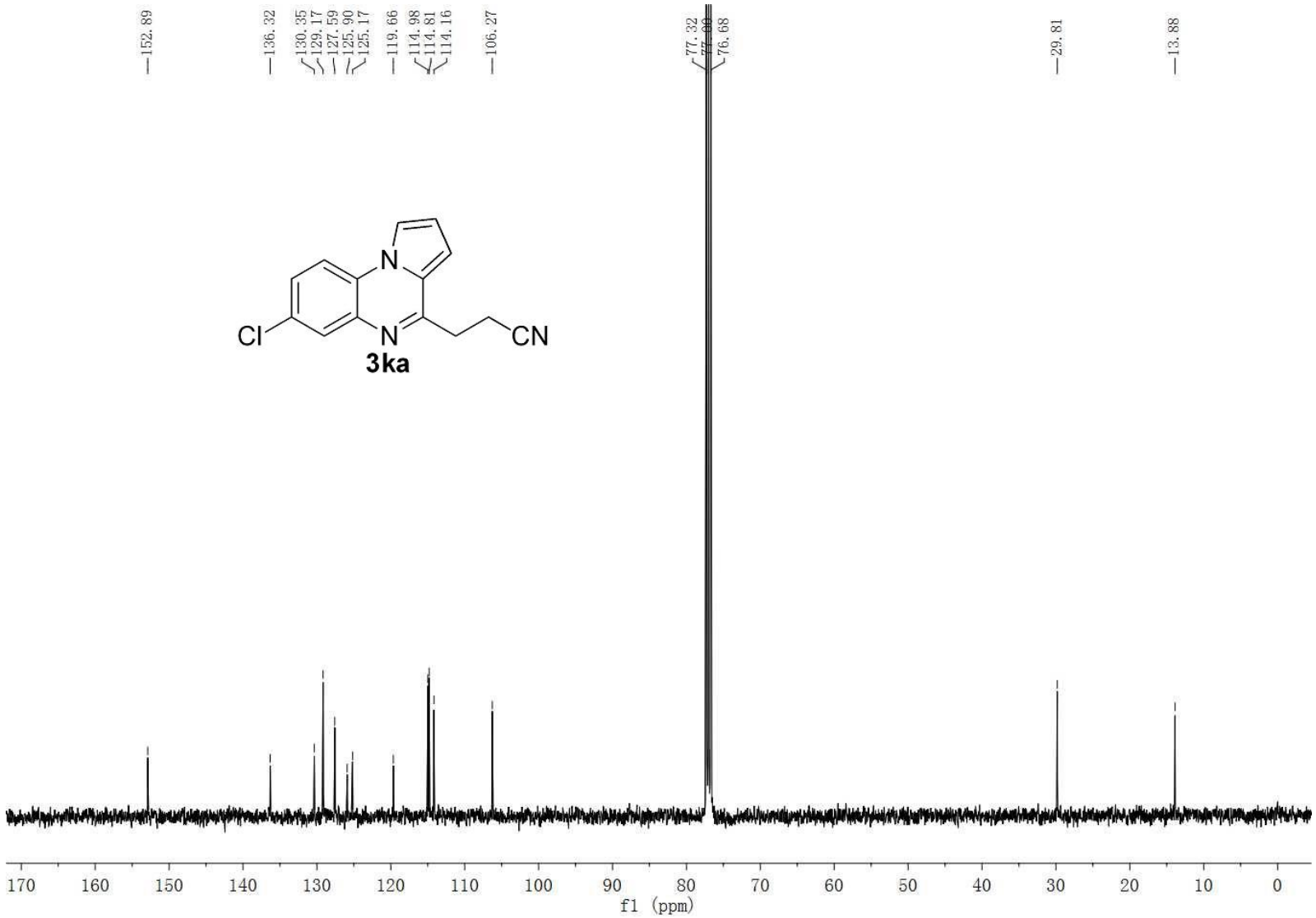
6.902
6.891
6.884
6.873
3.390
3.372
3.352
3.071
3.051
3.033
0.000
Cl
N
N
CN
3ka
0.93
1.00
1.04
1.06
2.00
2.00
1.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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127.59
125.90
125.17
119.66
114.98
114.81
114.16
106.27
77.32
77.00
76.68
29.81
13.88
N
N
Cl
CN
3ka
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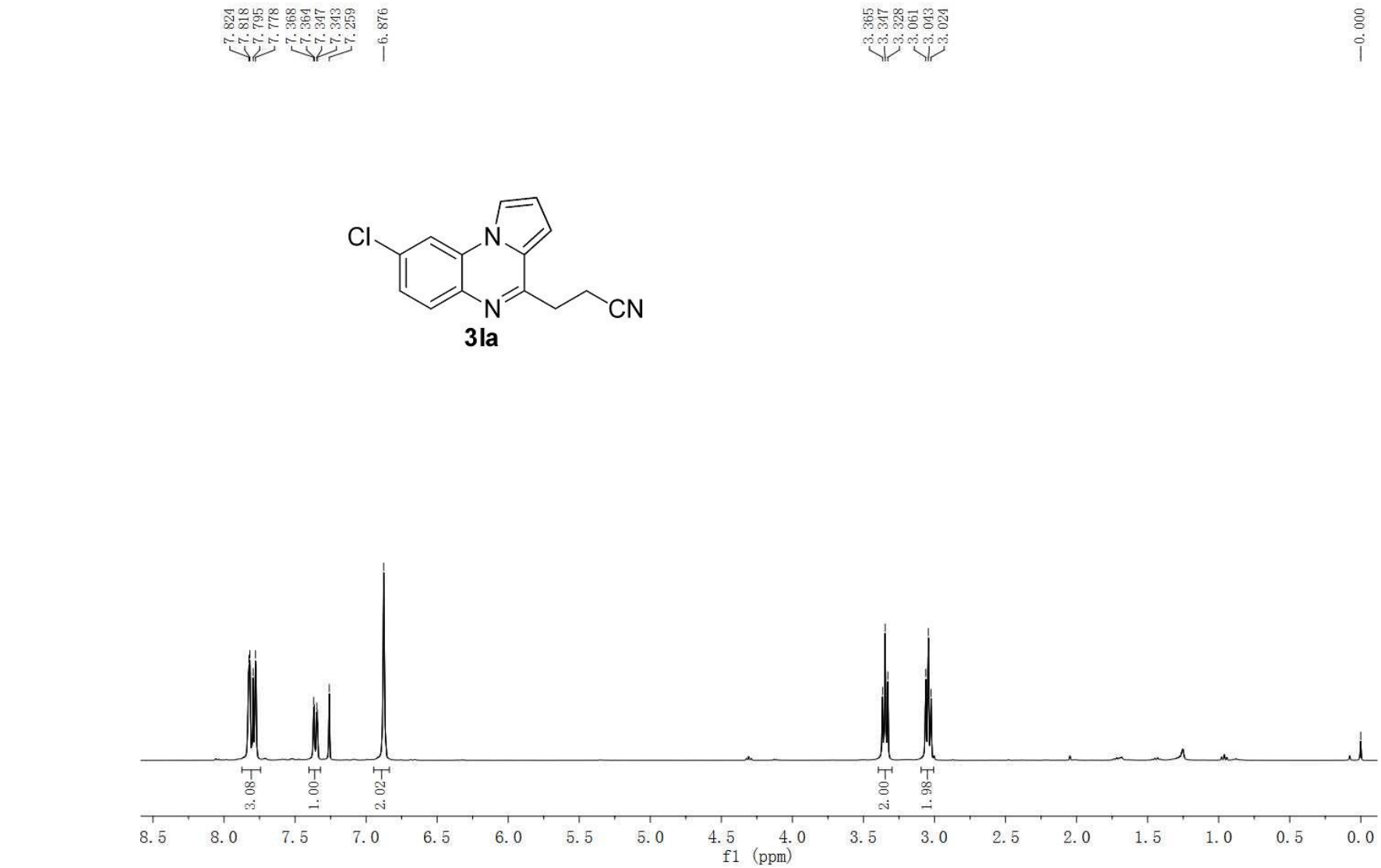
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.343
7.259
6.876
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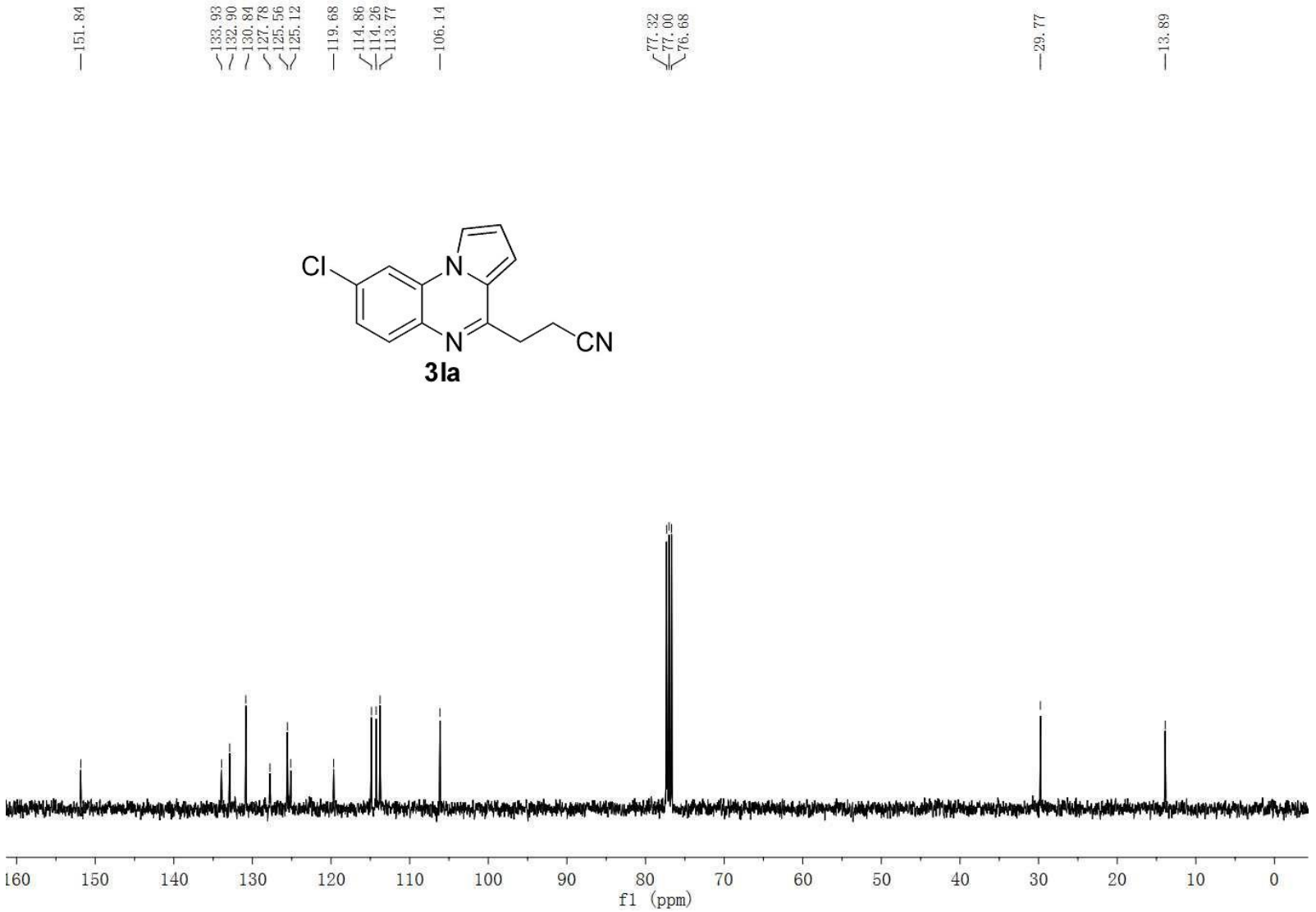
3.347
3.328
3.061
3.043
3.024
0.000
Cl
N
N
CN
3.08
1.00
2.02
2.00
1.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3la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119.68
114.86
114.26
113.77
106.14
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77.00
76.68
29.77
13.89
Cl
N
N
CN
3la
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130
120
110
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90
80
70
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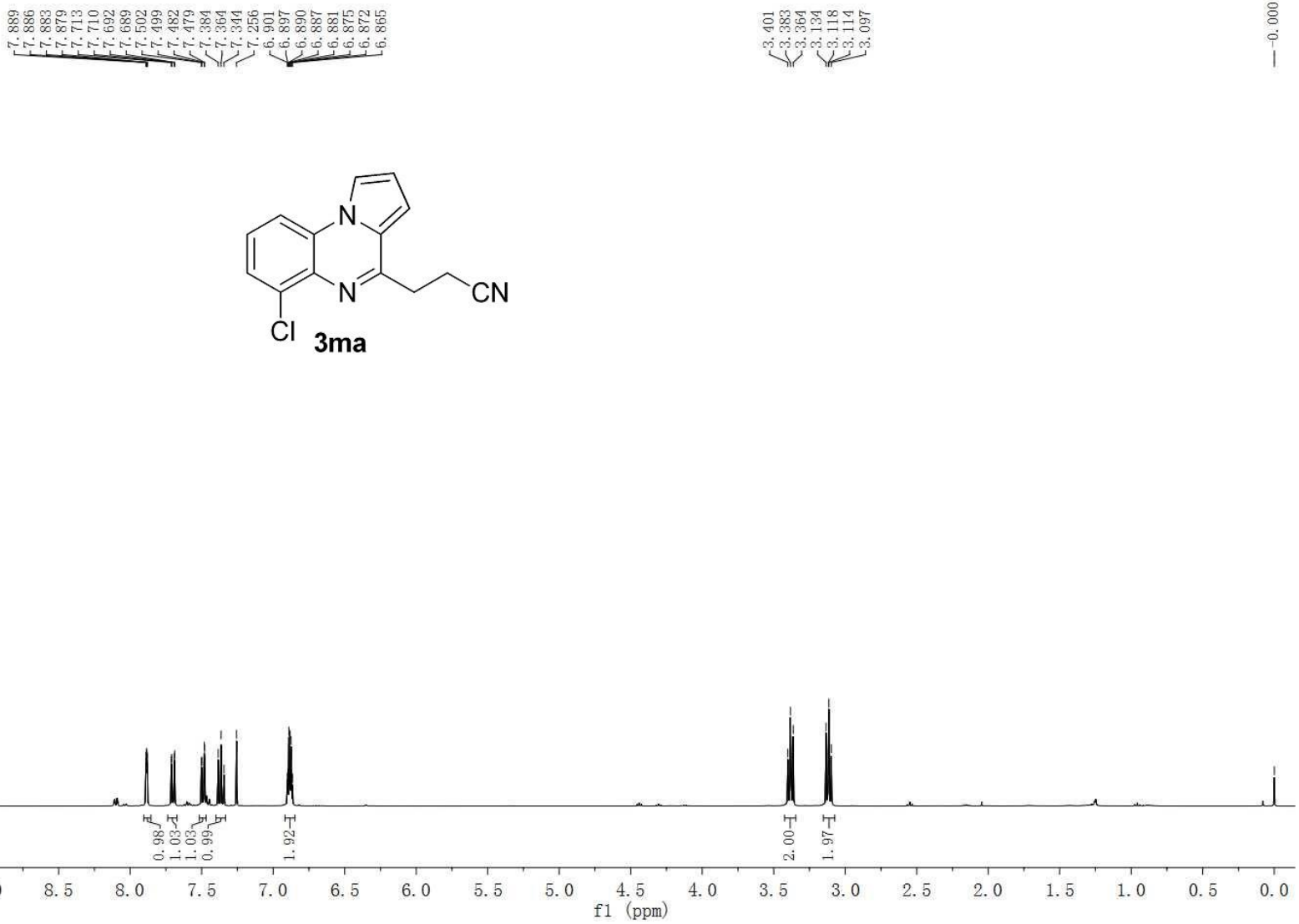
50
40
30
20
10
0
f1 (ppm)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7.384
7.364
7.344
7.256
6.901
6.897
6.890
6.887
6.881
6.875
6.872
6.865
3.401
3.383
3.364
3.134
3.118
3.114
3.097
0.000
N
N
CN
Cl
3ma
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1.03
0.99
1.92
2.00
1.97
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8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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2.0
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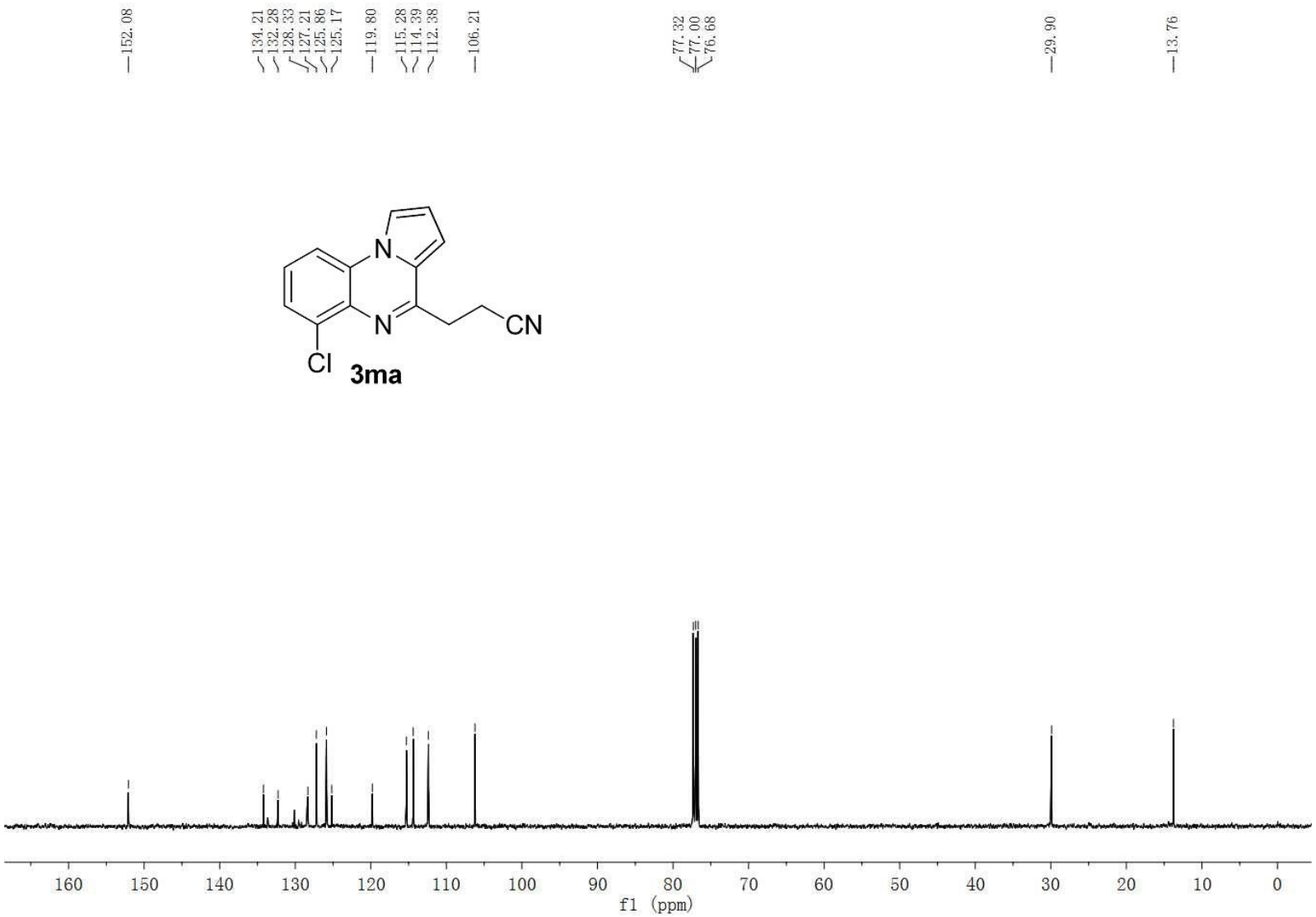
0.0
f1 (ppm)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115.28
114.39
112.38
106.21
77.32
77.00
76.68
29.90
13.76
N
N
CN
Cl
3ma
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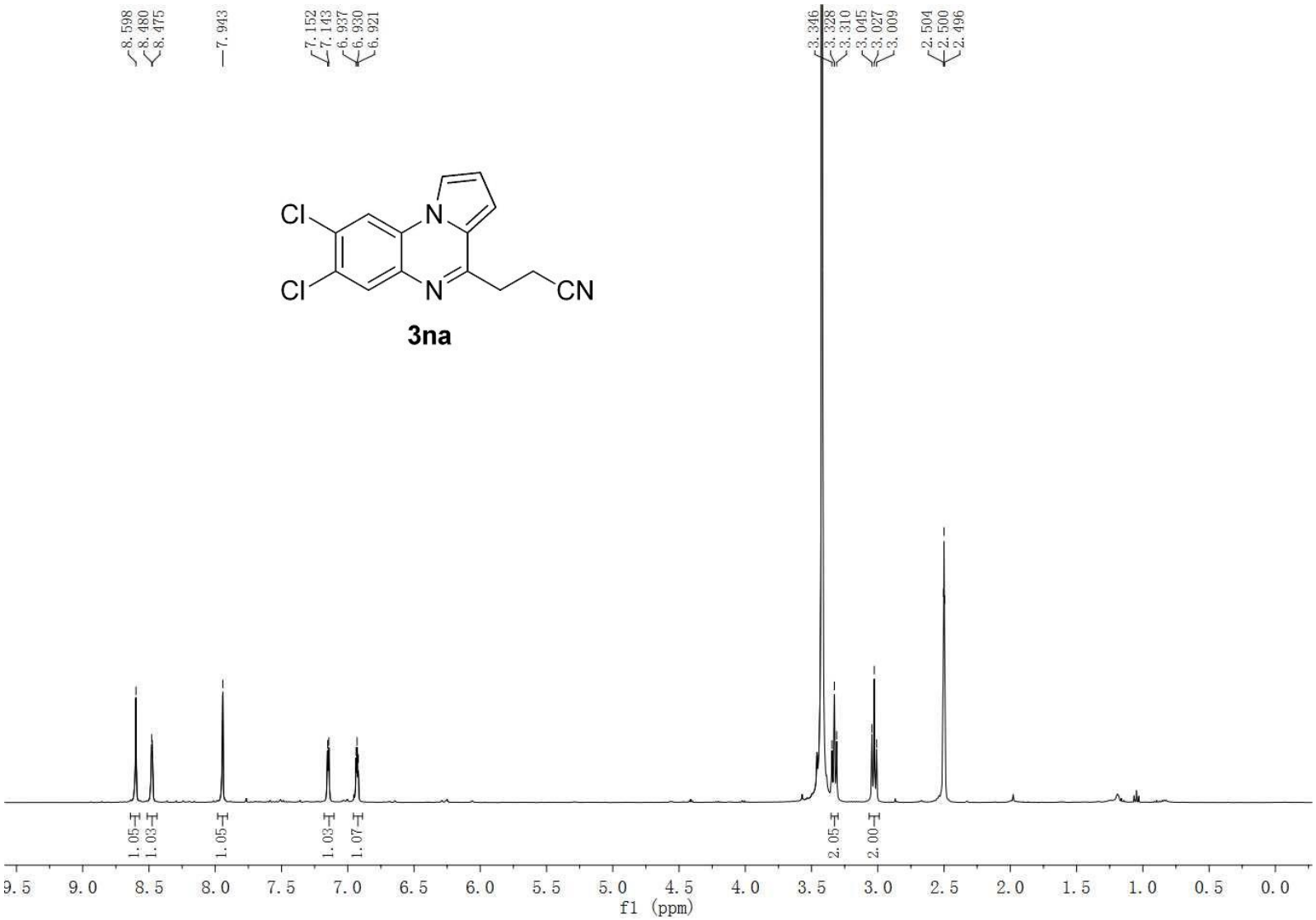
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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3.328
3.310
3.045
3.027
3.009
2.504
2.500
2.496
Cl
Cl
N
N
CN
3na
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1.03
1.05
1.03
1.07
2.05
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
3.0
2.5
2.0
1.5
1.0
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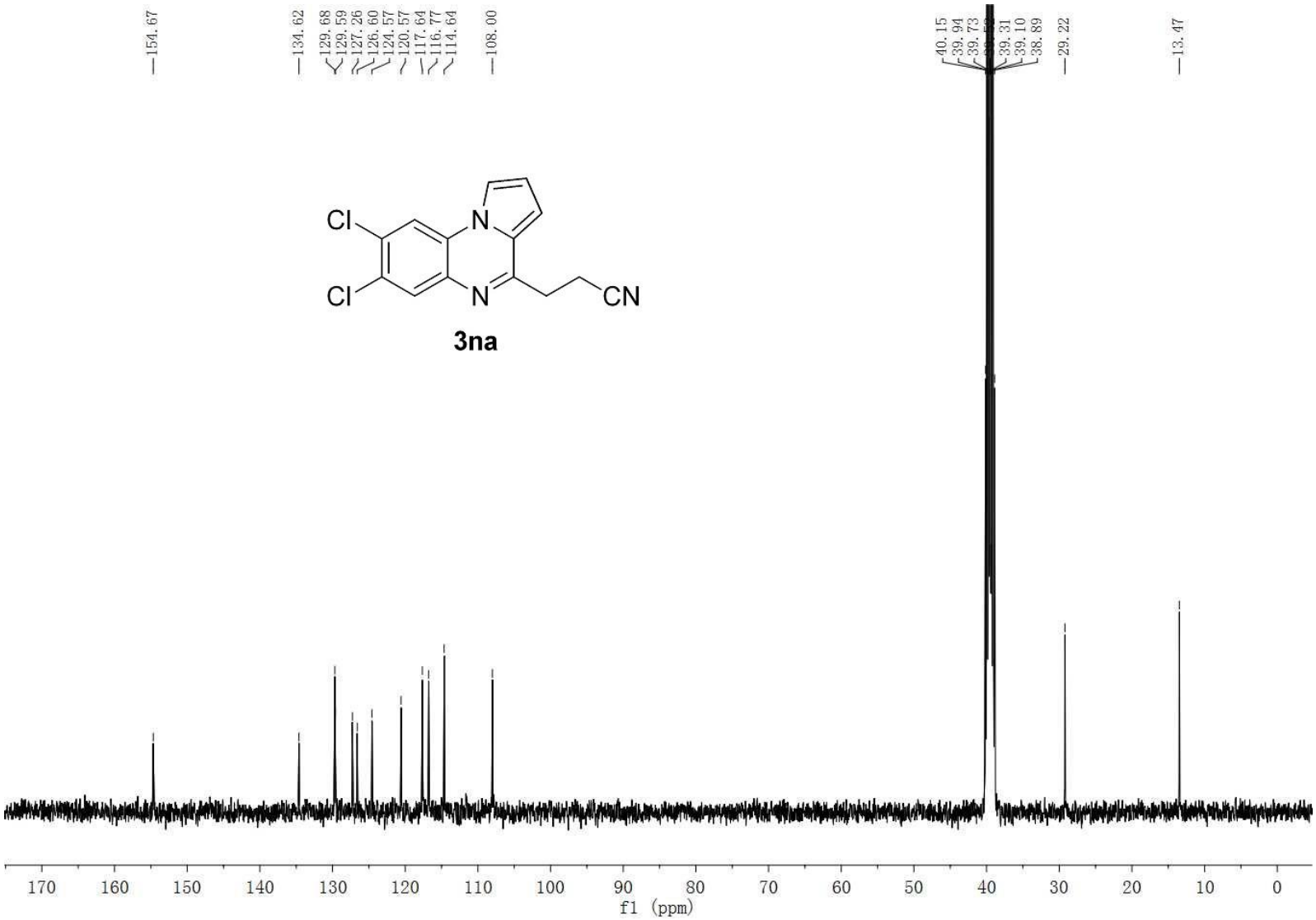
f1 (ppm)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120.57
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116.77
114.64
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40.15
39.94
39.73
39.31
39.10
38.89
29.22
13.47
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Cl
N
N
CN
3na
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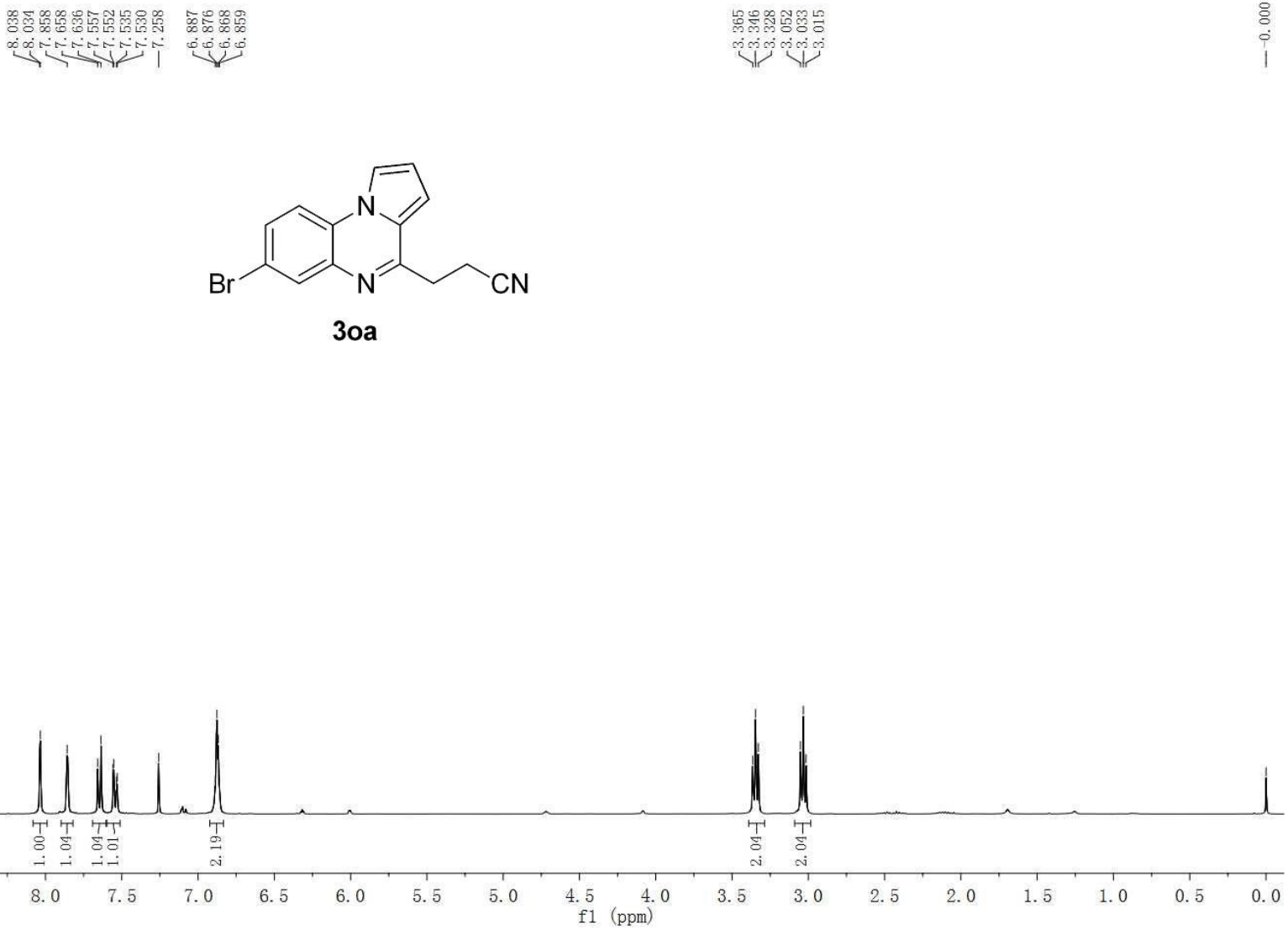
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.535
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6.887
6.876
6.868
6.859
3.365
3.346
3.328
3.052
3.033
3.015
0.000
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Br
N
CN
3oa
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1.04
1.04
1.01
2.19
2.04
2.04
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7.0
6.5
6.0
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2.0
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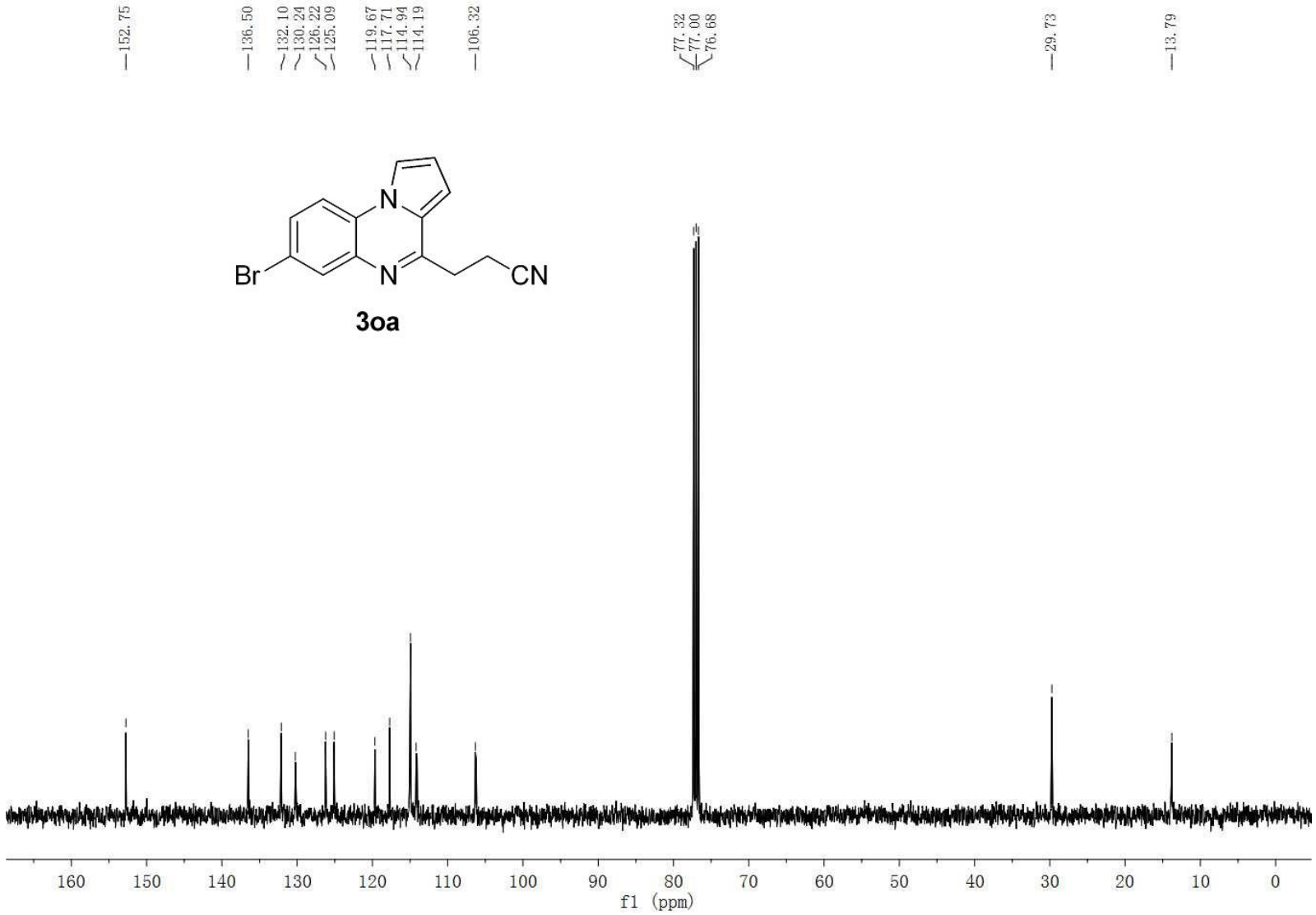
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117.71
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114.19
106.32
77.32
77.00
76.68
29.73
13.79
Br
N
N
CN
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130
120
110
100
90
80
70
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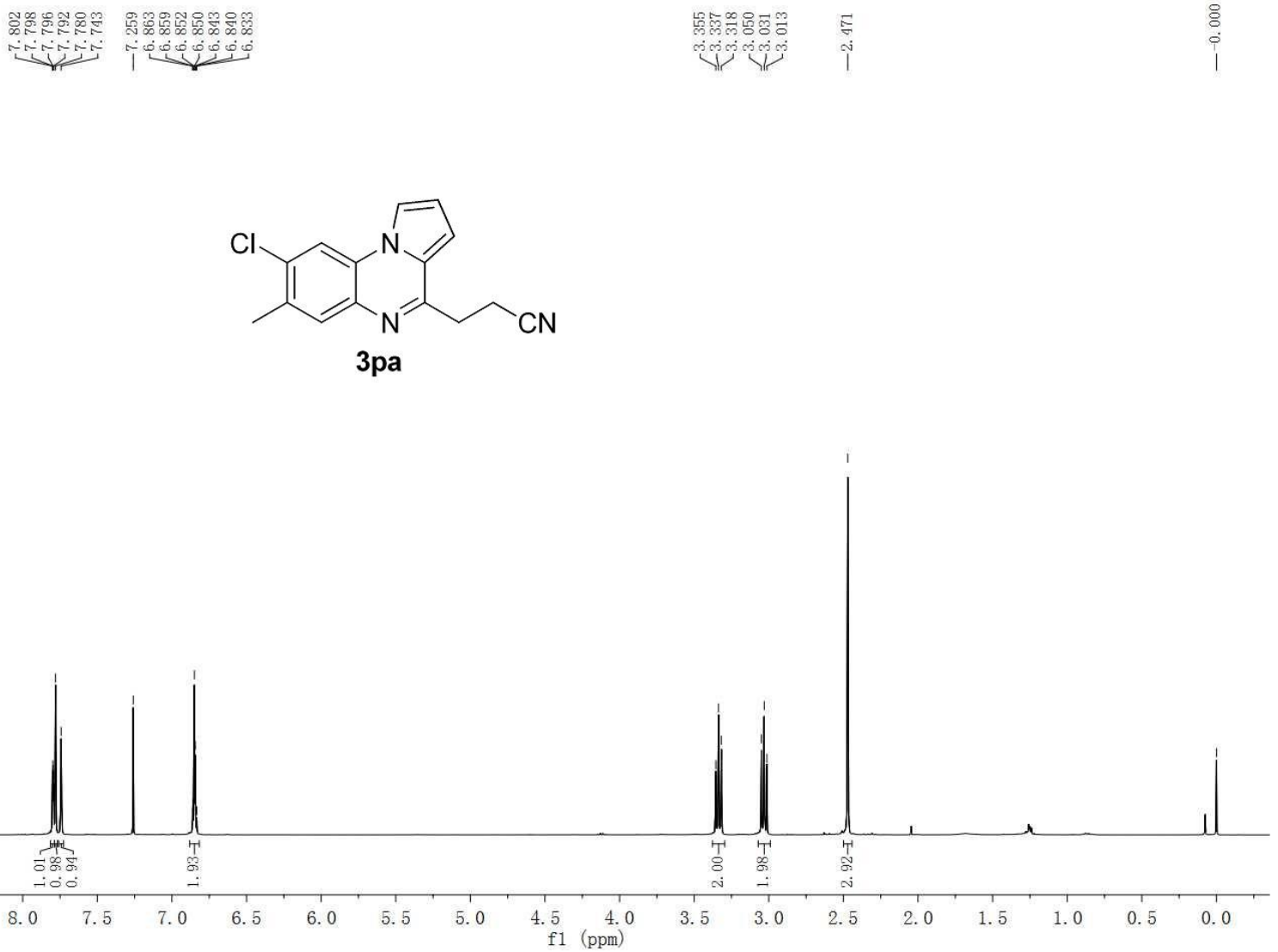
50
40
30
20
10
0
f1 (ppm)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6.840
6.833
3.355
3.337
3.318
3.050
3.031
3.013
2.471
0.000
Cl
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N
CN
3pa
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0.98
0.94
1.93
2.00
1.98
2.92
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
1.5
1.0
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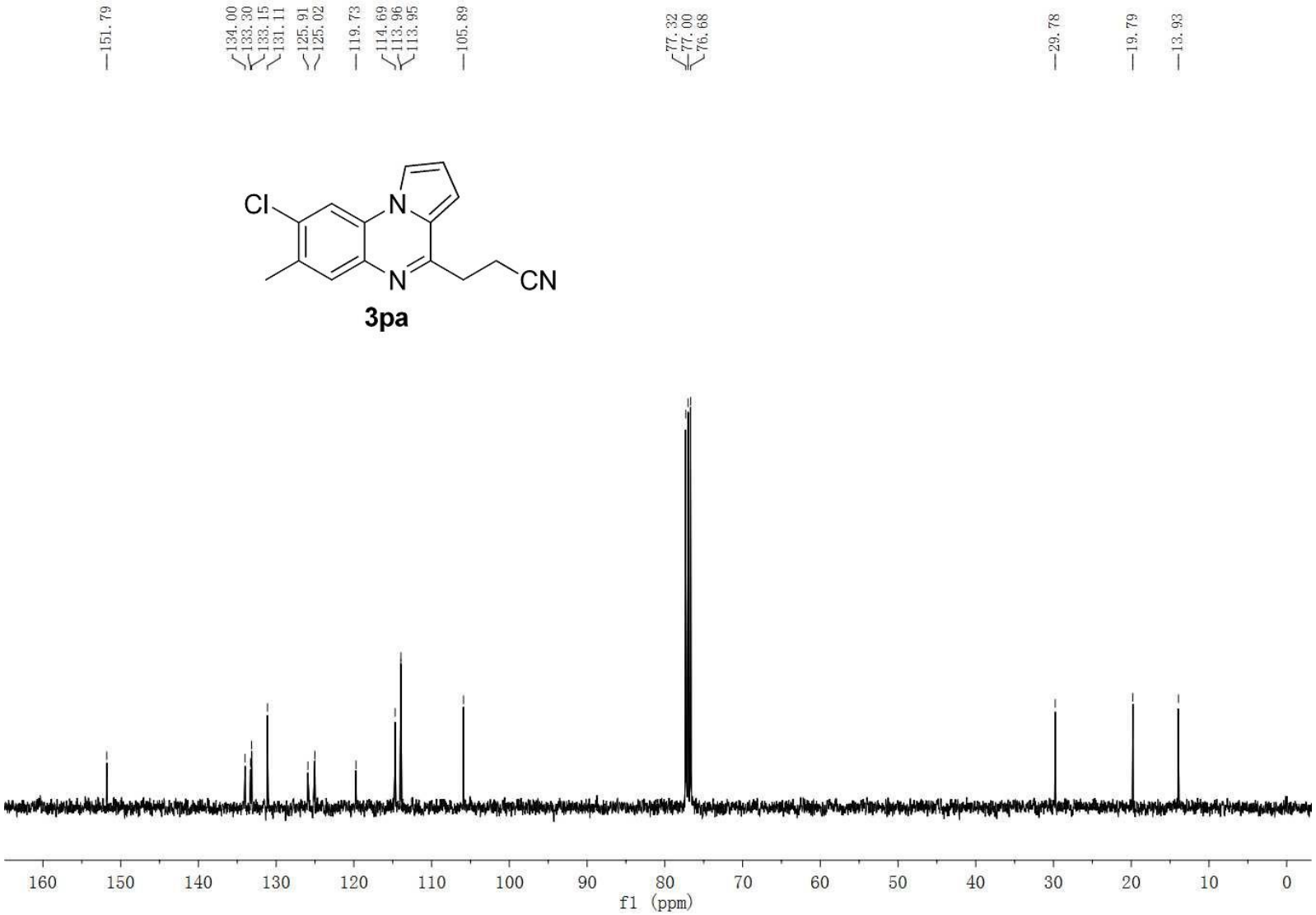
0.0
f1 (ppm)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113.96
113.95
105.89
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77.00
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29.78
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N
N
CN
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90
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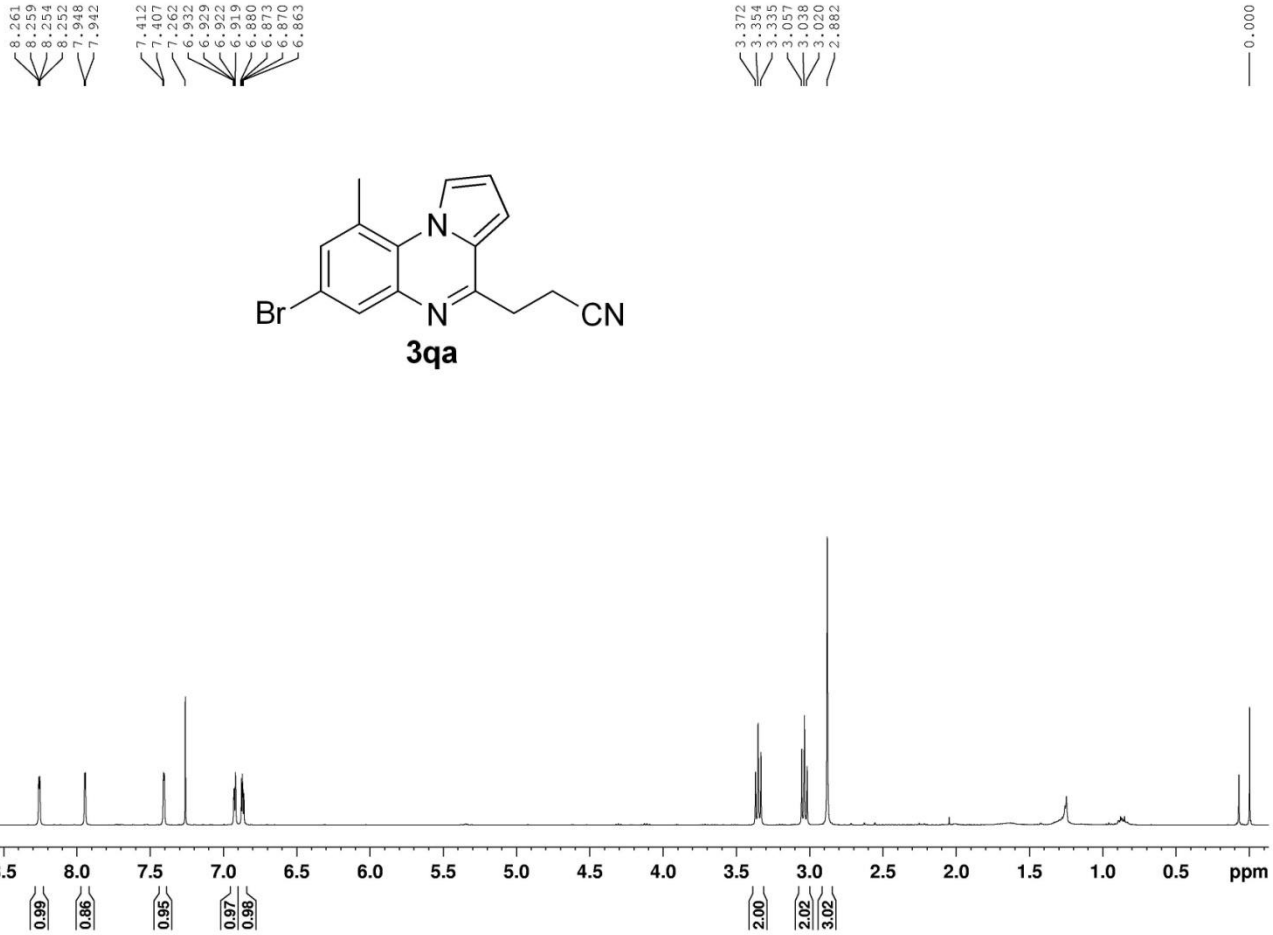
50
40
30
20
10
0
f1 (ppm)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7.407
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6.929
6.922
6.919
6.880
6.873
6.870
6.863
3.372
3.354
3.335
3.057
3.038
3.020
2.882
0.000
N
N
Br
CN
3qa
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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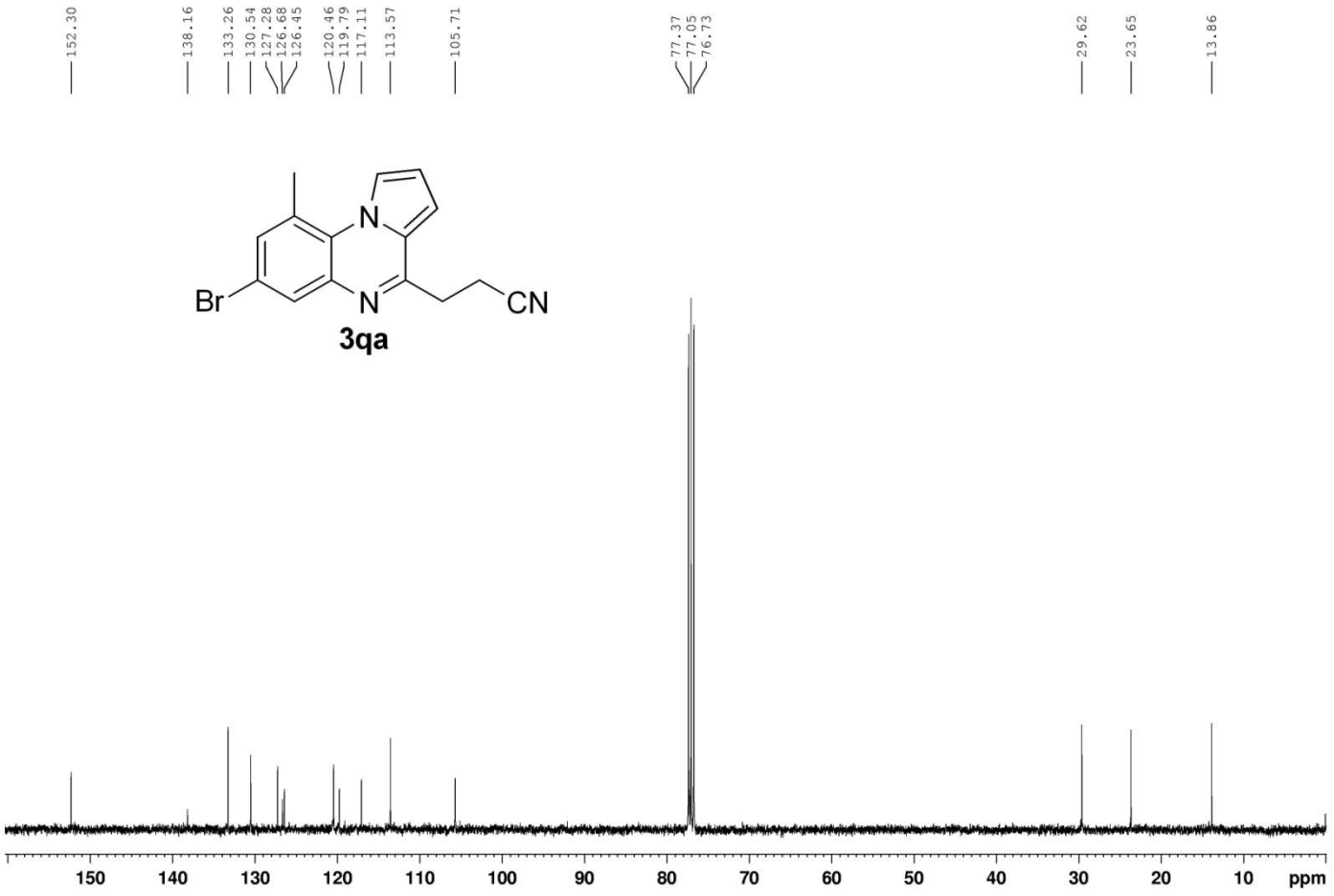
0.95
0.97
0.98
2.00
2.02
3.02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120.46
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117.11
113.57
105.71
77.37
77.05
76.73
29.62
23.65
13.86
N
Br
N
CN
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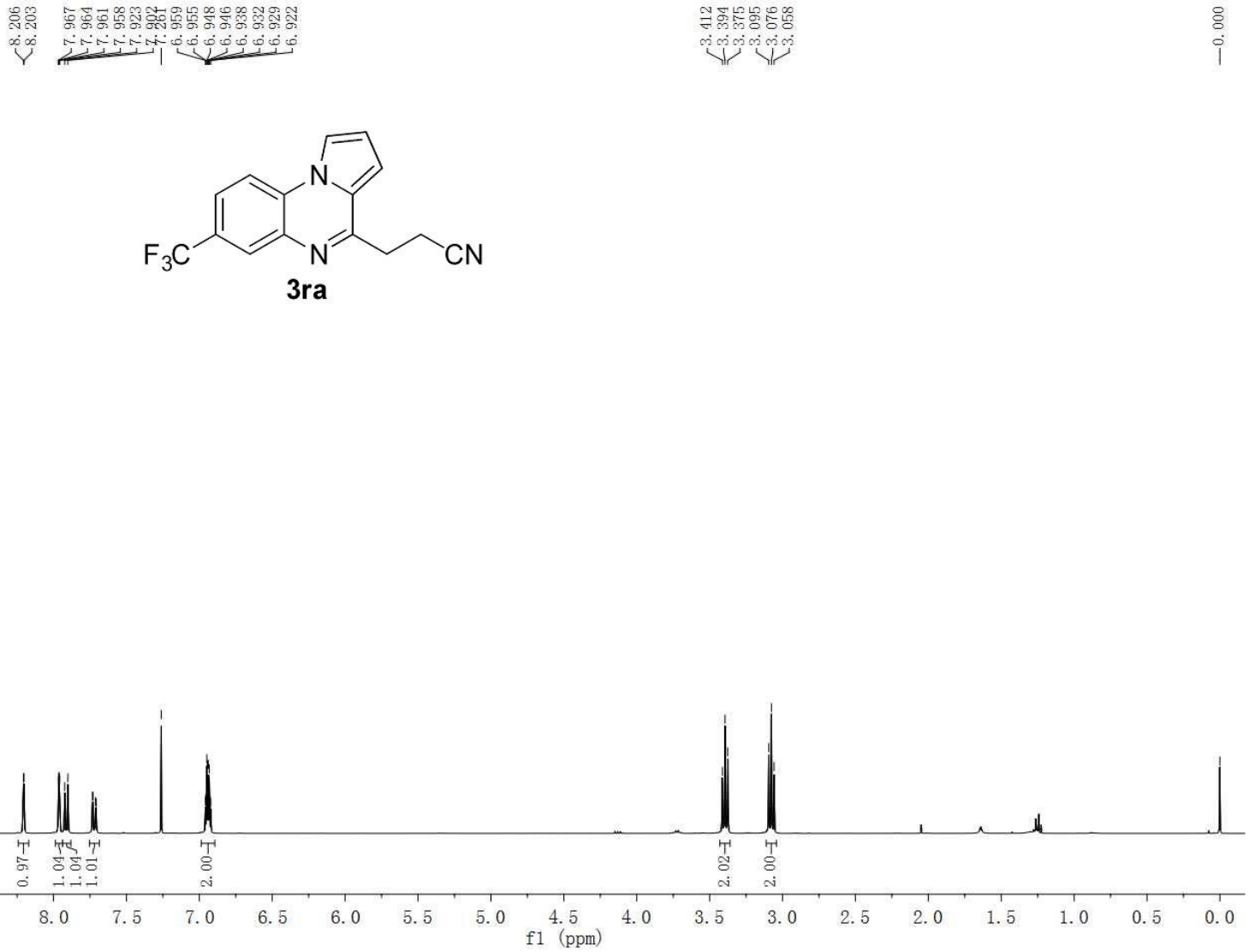
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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6.946
6.938
6.932
6.929
6.922
3.412
3.394
3.375
3.095
3.076
3.058
0.000
F3C
N
N
CN
3ra
0.97
1.04
1.04
1.01
2.00
2.02
2.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.5
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2.5
2.0
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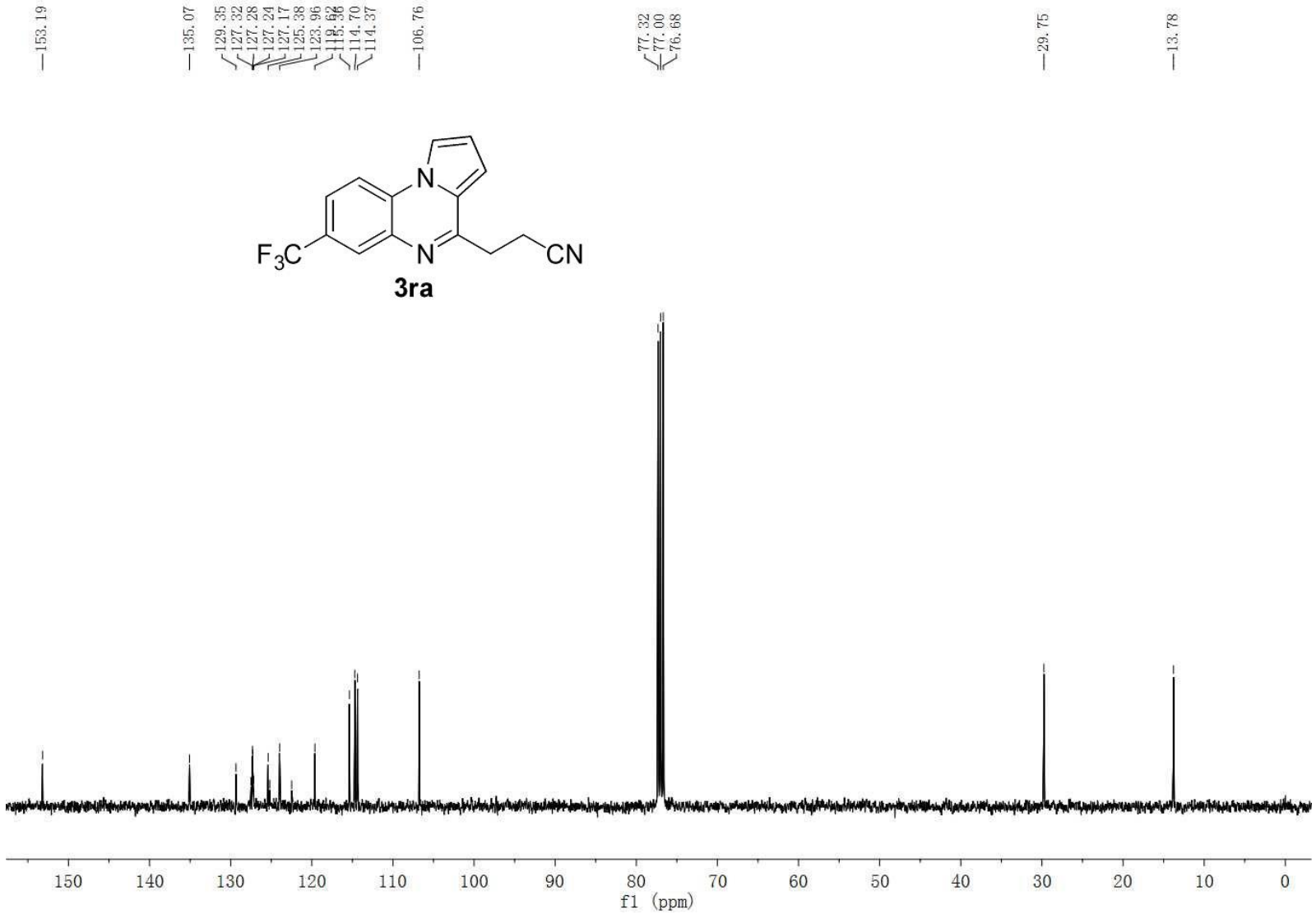
f1 (ppm)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135.07
129.35
127.32
127.28
127.24
127.17
125.38
123.96
114.70
114.37
106.76
77.32
77.00
76.68
29.75
13.78
N
N
F3C
CN
3ra
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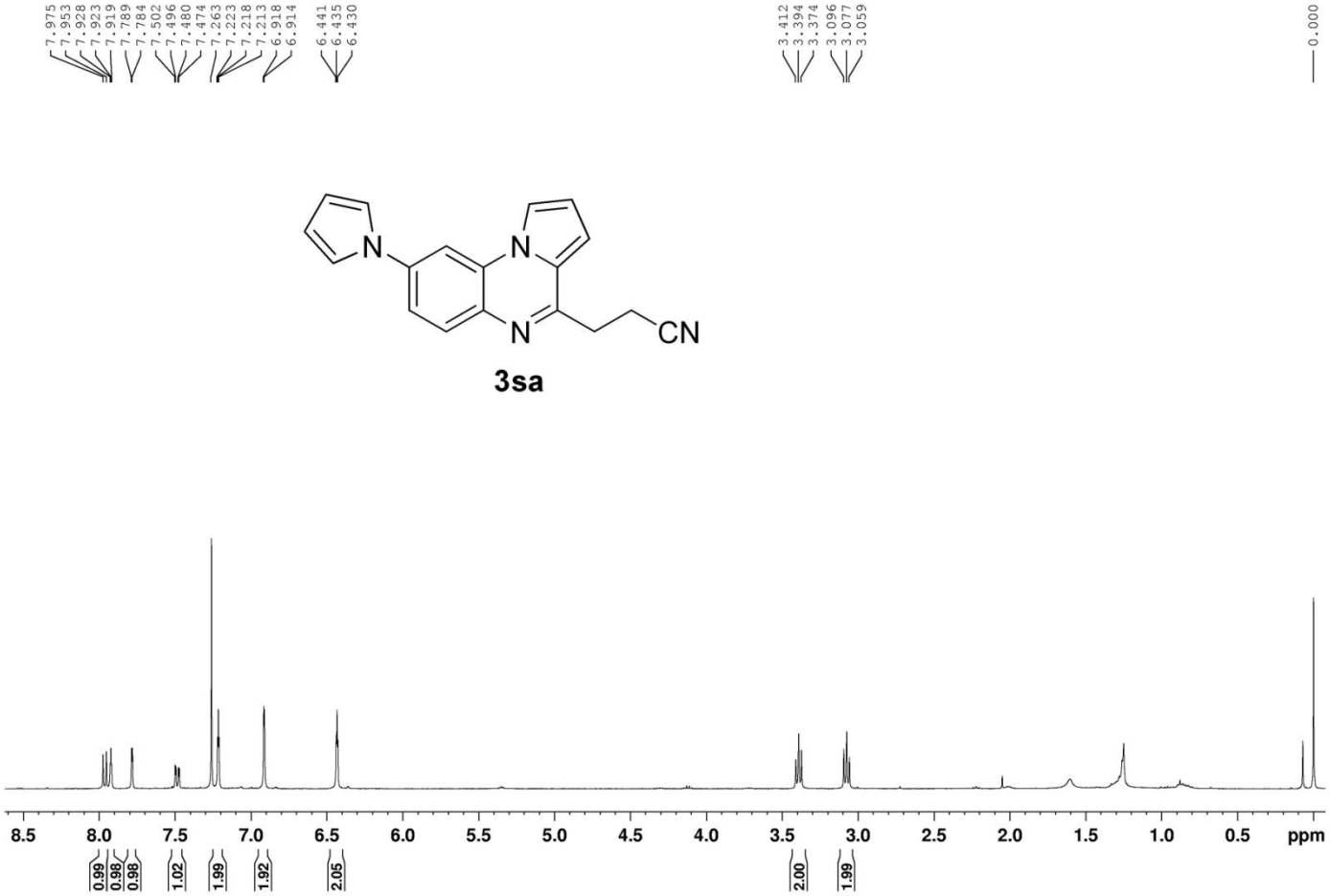
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.928
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7.784
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7.496
7.480
7.474
7.263
7.223
7.218
7.213
6.918
6.914
6.441
6.435
6.430
3.412
3.394
3.374
3.096
3.077
3.059
0.000
N
N
N
CN
3sa
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
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0.5
ppm
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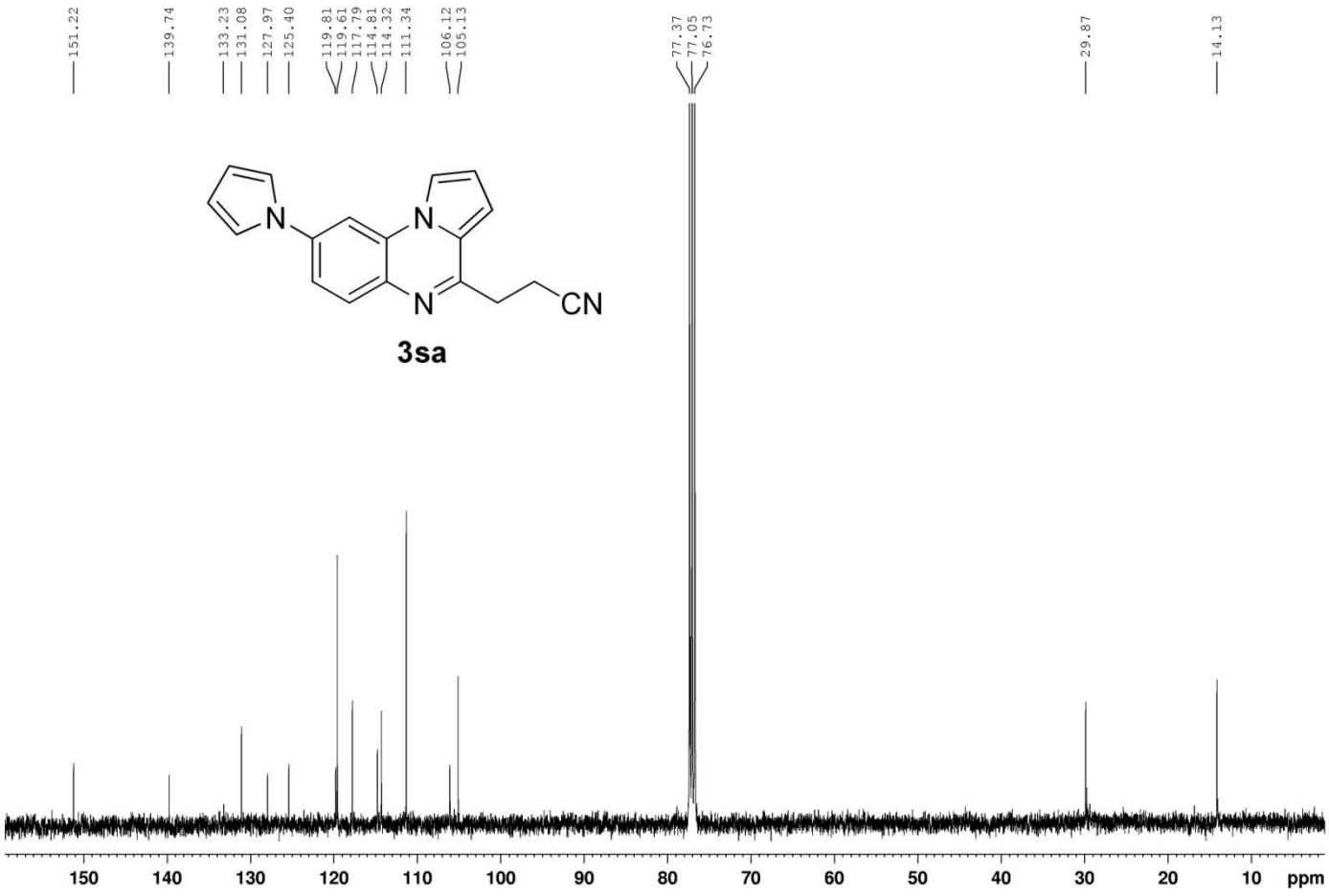
0.98
0.98
1.02
1.99
1.92
2.05
2.00
1.99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133.23
131.08
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119.61
117.79
114.81
114.32
111.34
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105.13
77.37
77.05
76.73
29.87
14.13
N
N
N
CN
3sa
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.520
8.516
8.508
8.504
8.372
8.369
8.366
8.363
8.191
8.187
8.171
8.167
7.432
7.421
7.412
7.401
7.265
6.941
6.938
6.931
6.928
6.893
6.886
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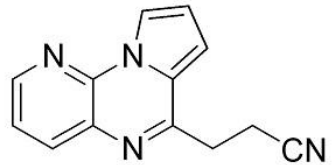
3.351
3.068
3.049
3.031
0.000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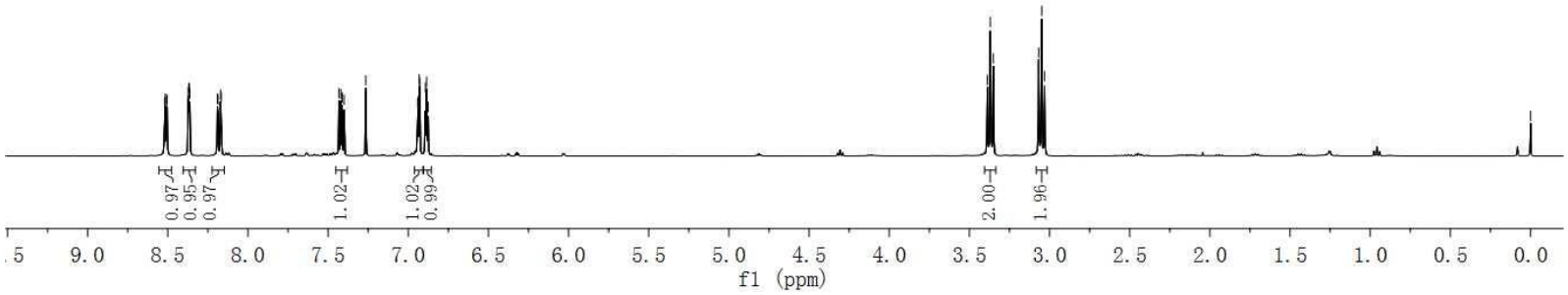
N
N
CN

3ta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0.95
0.97
1.02
1.02
0.99
2.00
1.96
9.0
8.5
8.0
7.5
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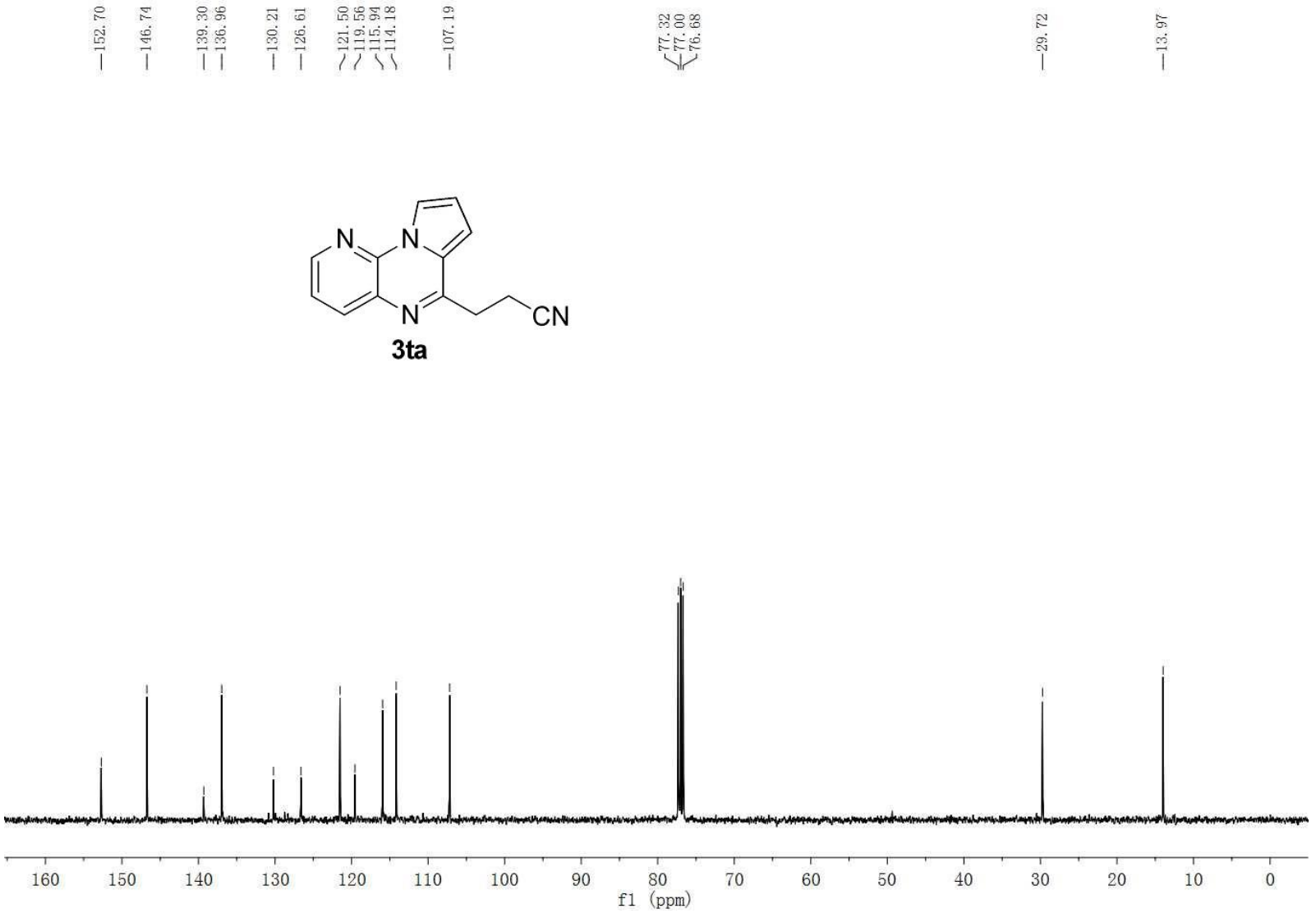
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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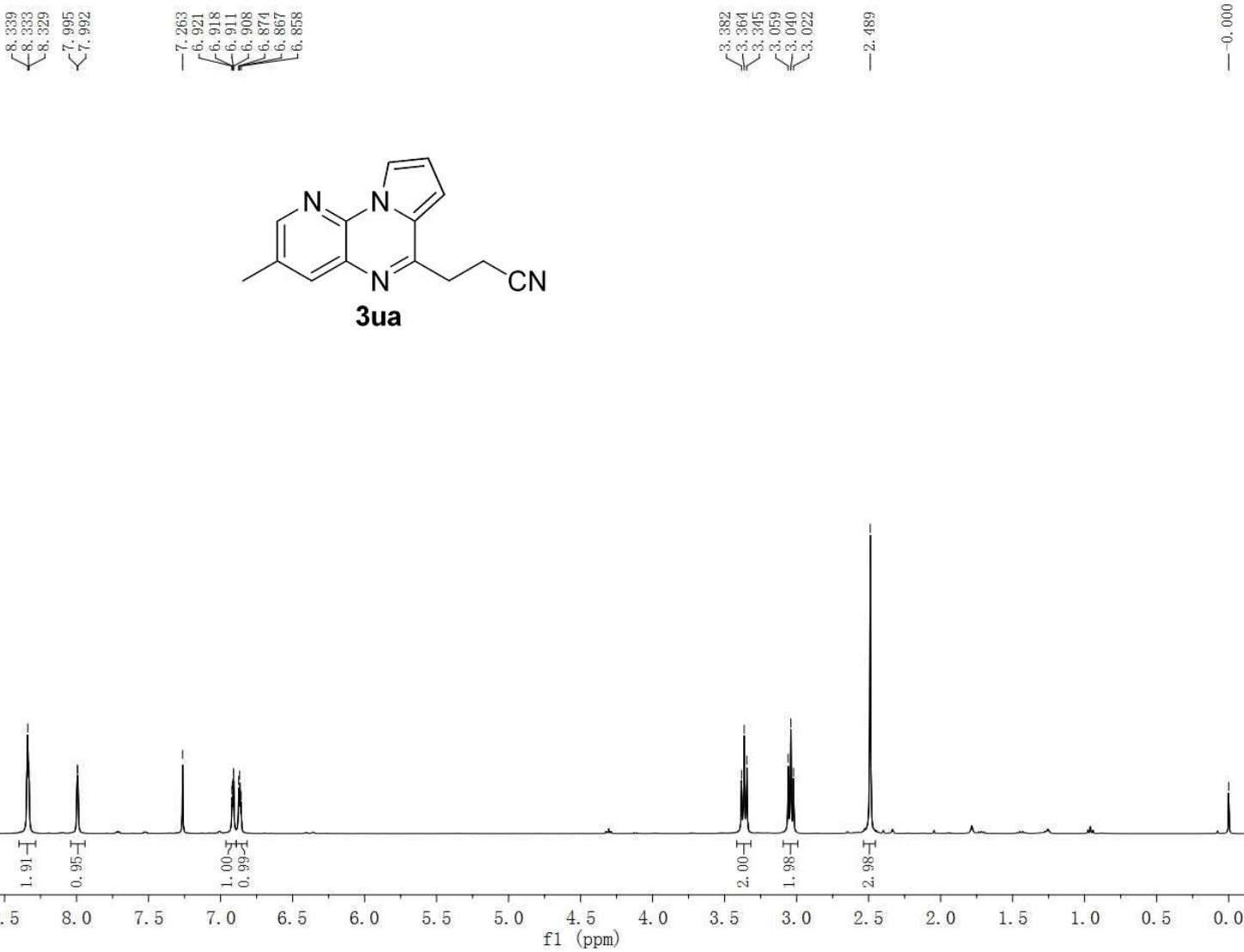
146.74
139.30
136.96
130.21
126.61
121.50
119.56
115.94
114.18
107.19
77.32
77.00
76.68
29.72
13.97
N
N
N
CN
3ta
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.263
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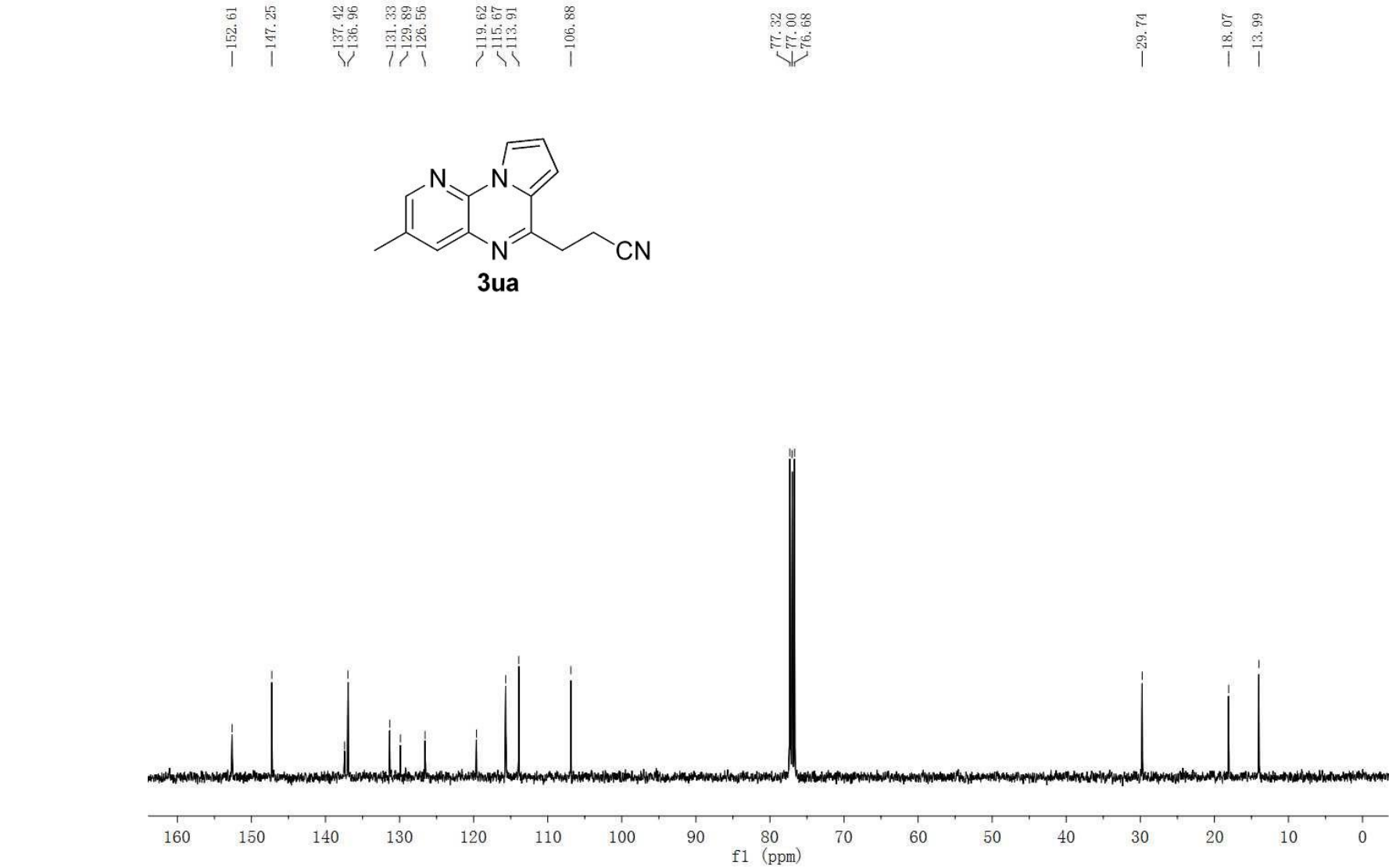
6.918
6.911
6.908
6.874
6.867
6.858
3.382
3.364
3.345
3.059
3.040
3.022
2.489
0.000
N
N
N
CN
3ua
1.91
0.95
1.00
0.99
2.00
1.98
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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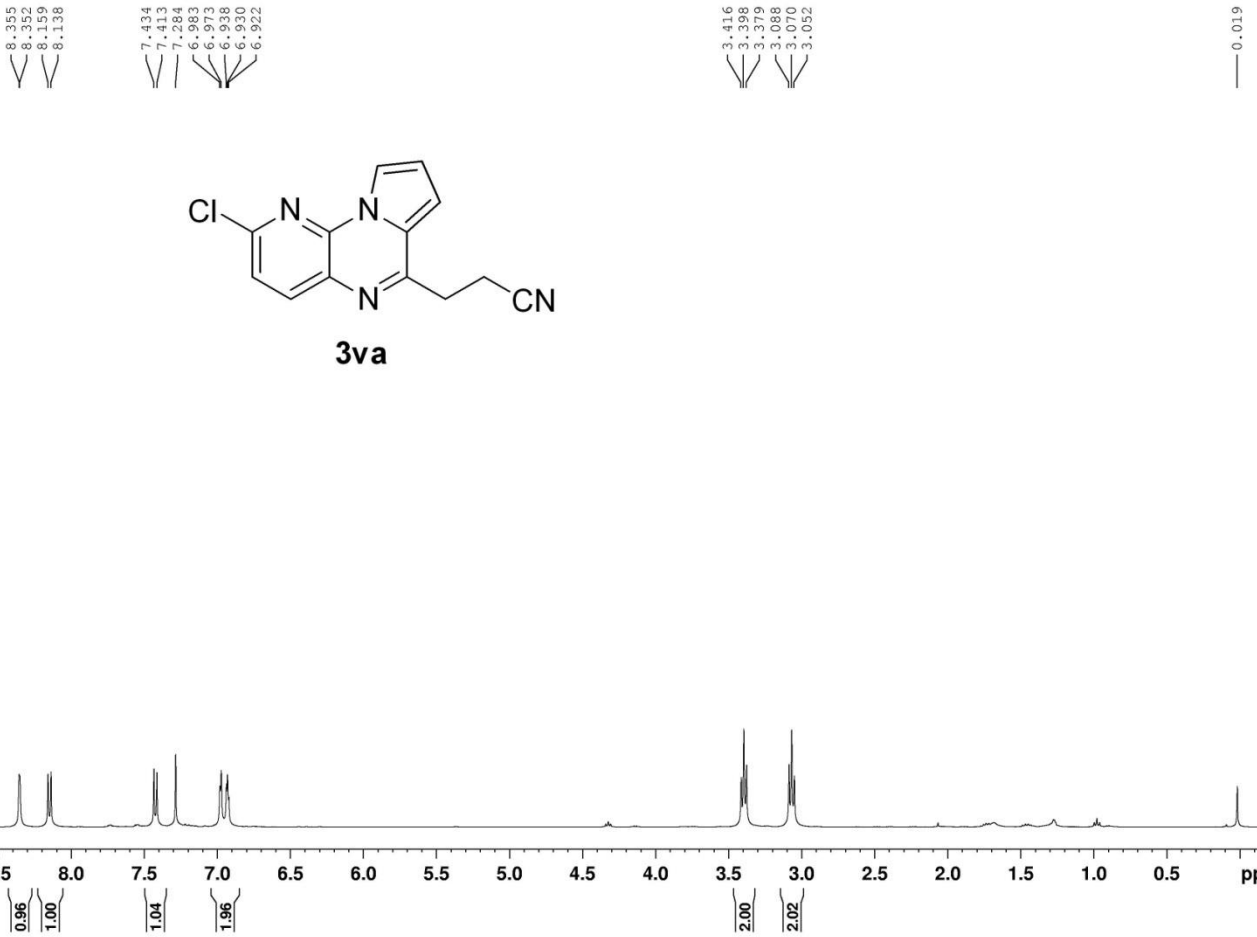
137.42
136.96
131.33
129.89
126.56
119.62
115.67
113.91
106.88
77.32
77.00
76.68
29.74
18.07
13.99
N
N
N
CN
3ua
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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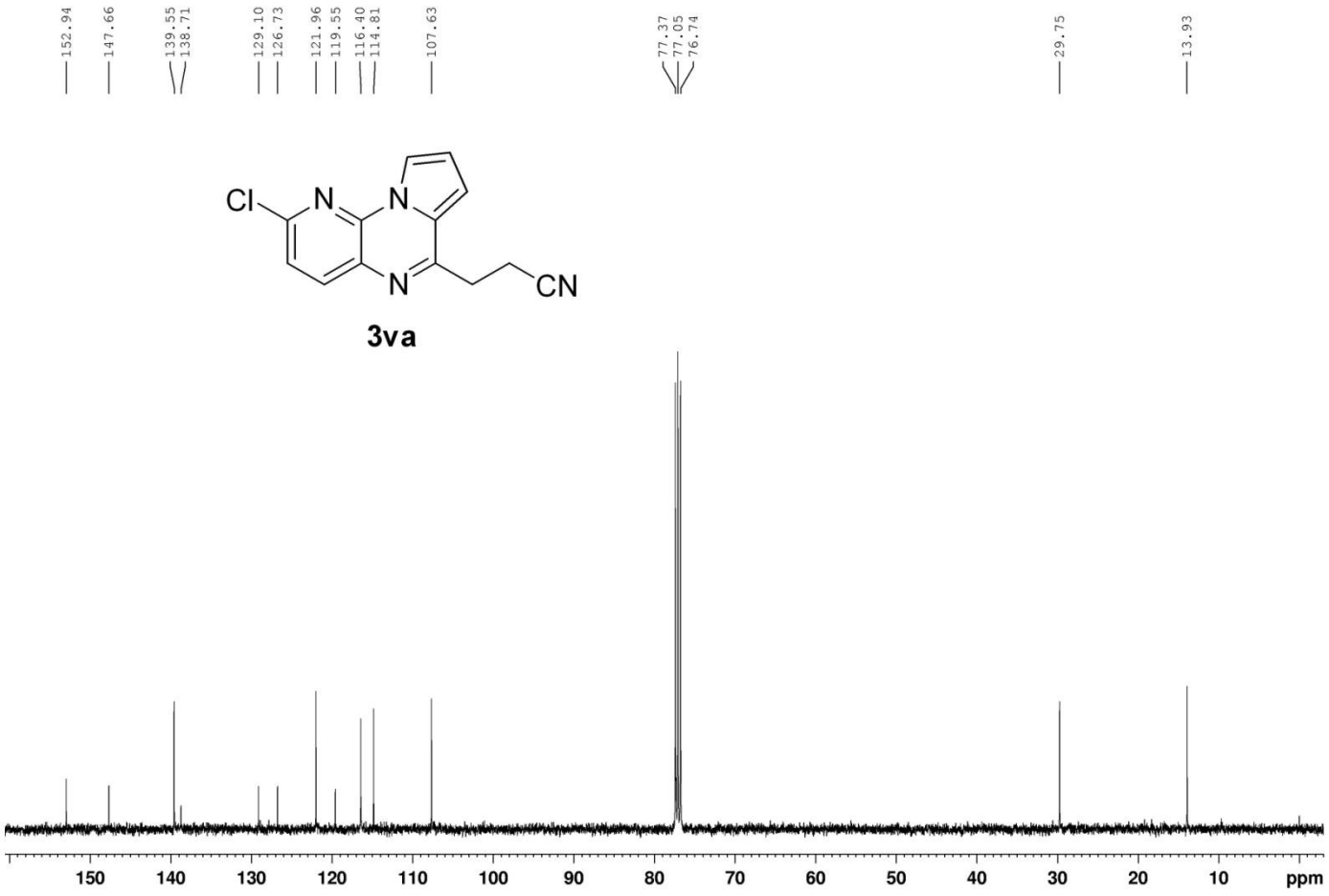
8.352
8.159
8.138
7.434
7.413
7.284
6.983
6.973
6.938
6.930
6.922
3.416
3.398
3.379
3.088
3.070
3.052
0.019
Cl
N
N
N
CN
3va
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.96
1.00
1.04
1.96
2.00
2.02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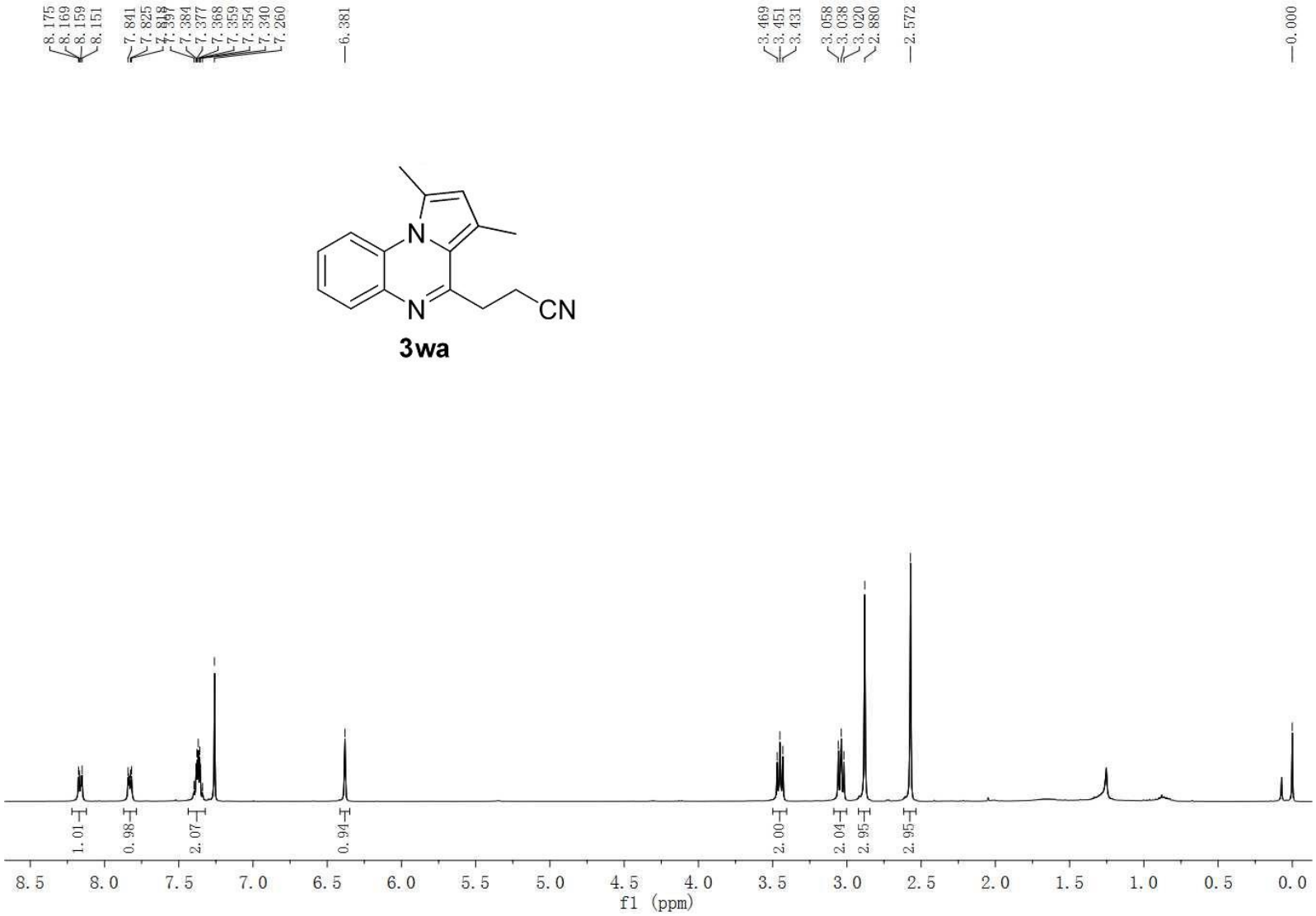
129.10
126.73
121.96
119.55
116.40
114.81
107.63
77.37
77.05
76.74
29.75
13.93
Cl
N
N
N
CN
3va
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.169
8.159
8.151
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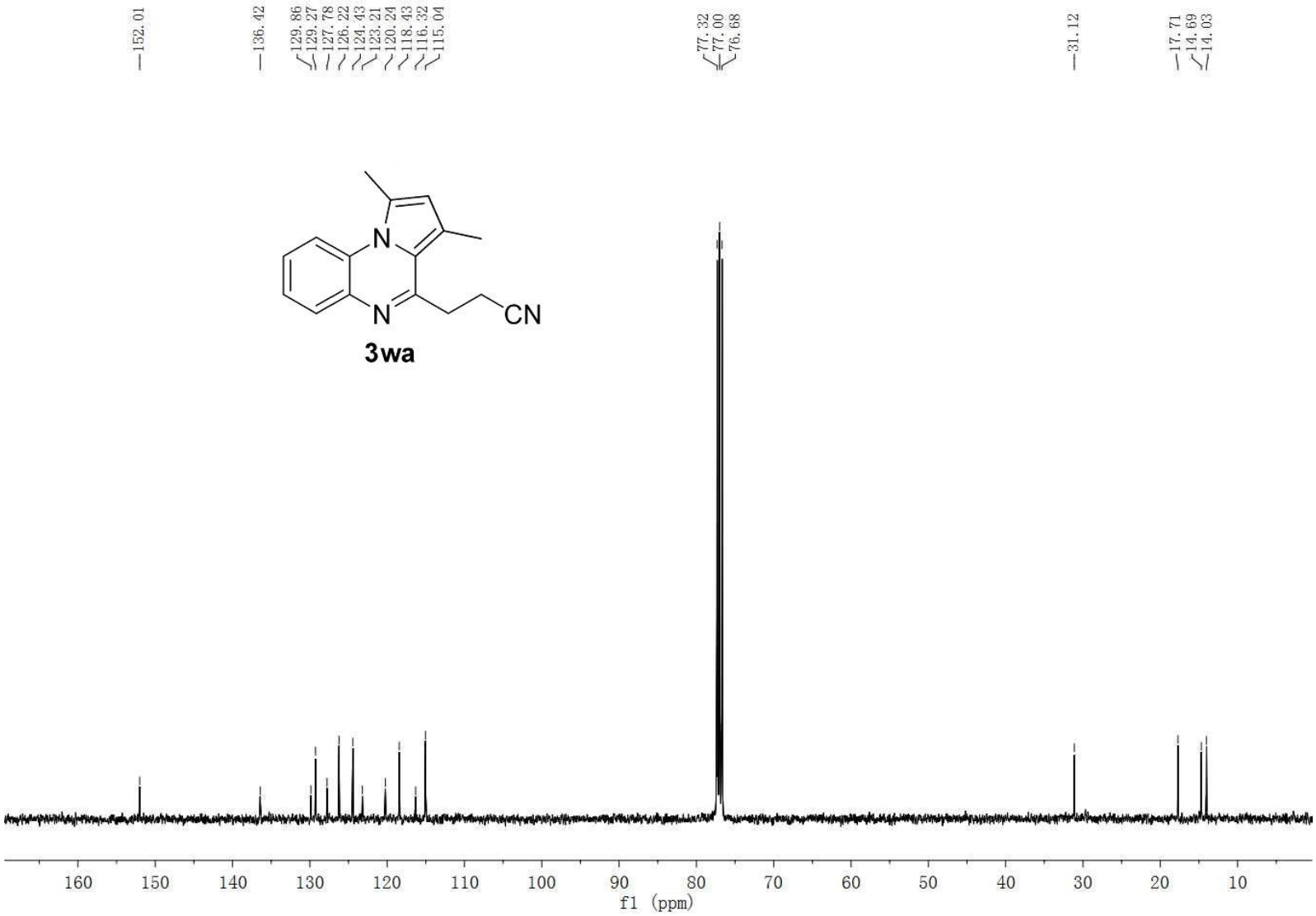
7.825
7.397
7.384
7.377
7.368
7.359
7.354
7.340
7.260
6.381
3.469
3.451
3.431
3.058
3.038
3.020
2.880
2.572
0.000
N
N
CN
3wa
1.01
0.98
2.07
0.94
2.00
2.04
2.95
2.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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136.42
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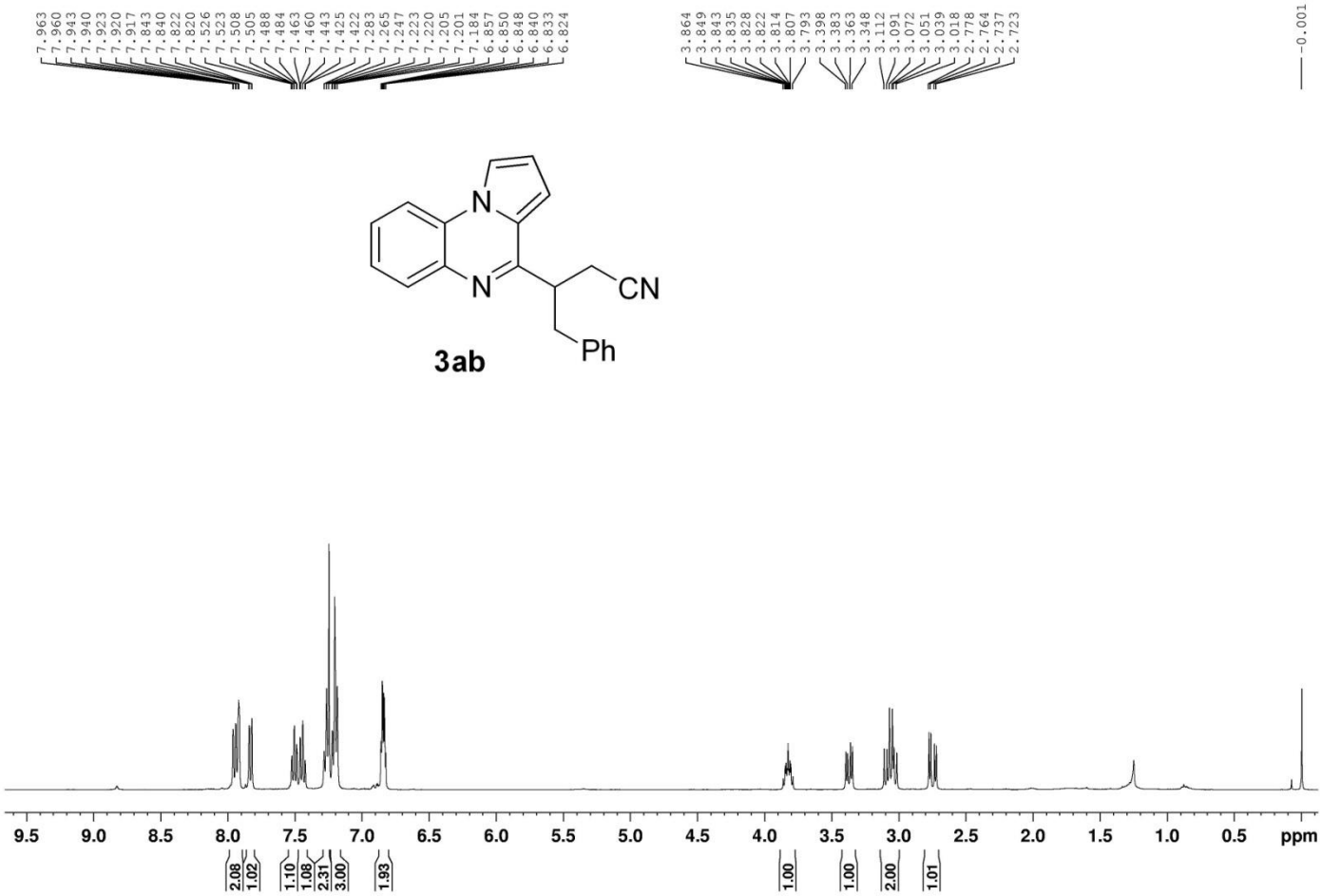
126.22
124.43
123.21
120.24
118.43
116.32
115.04
77.32
77.00
76.68
31.12
17.71
14.69
14.03
N
N
CN
3wa
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.920
7.917
7.843
7.840
7.822
7.820
7.526
7.523
7.508
7.505
7.488
7.484
7.463
7.460
7.443
7.425
7.422
7.283
7.265
7.247
7.223
7.220
7.205
7.201
7.184
6.857
6.850
6.848
6.840
6.833
6.824
3.864
3.849
3.843
3.835
3.828
3.822
3.814
3.807
3.793
3.398
3.383
3.363
3.348
3.112
3.091
3.072
3.051
3.039
3.018
2.778
2.764
2.737
2.723
-0.001
N
N
CN
Ph
3ab
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
ppm
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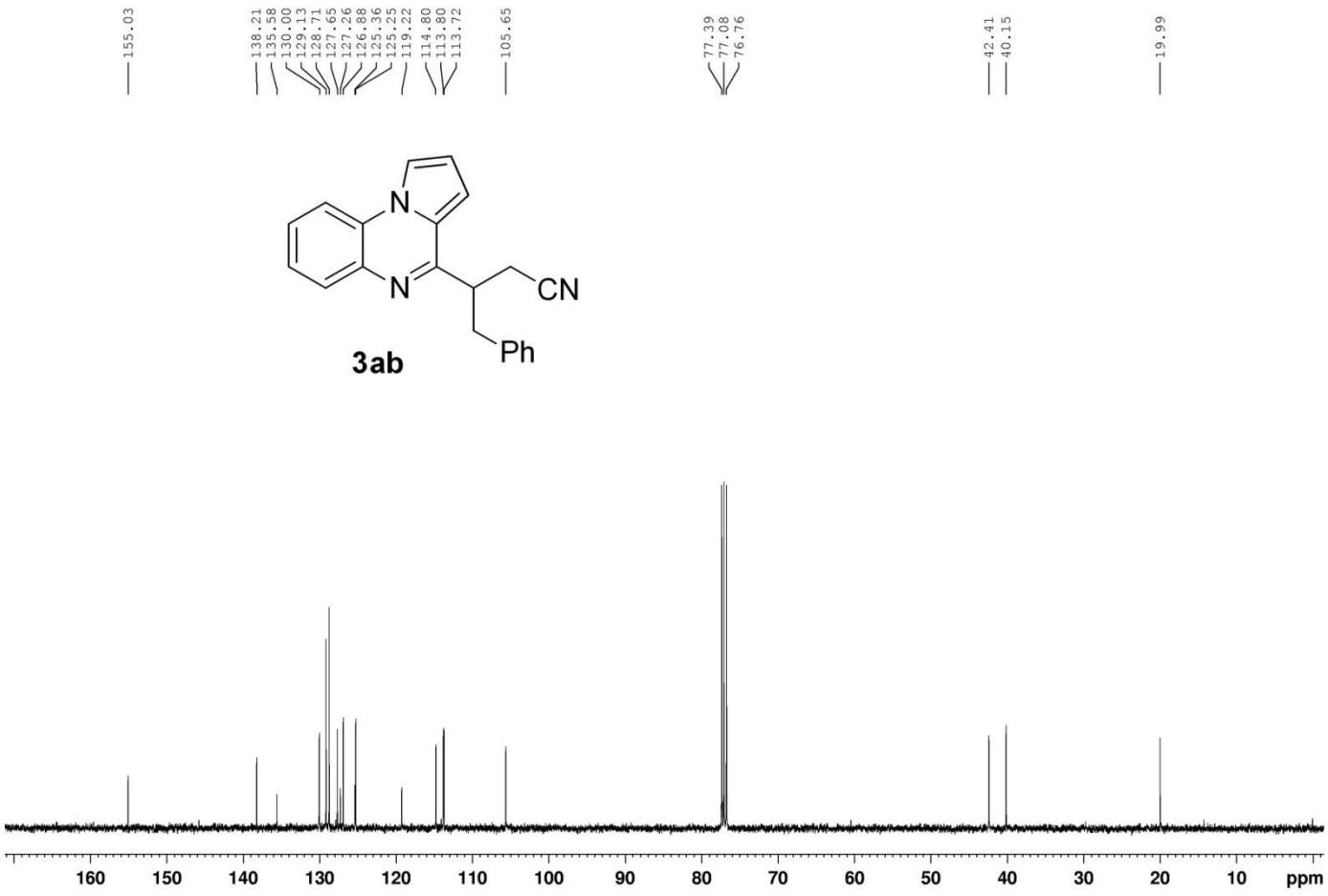
1.02
1.10
1.08
2.31
3.00
1.93
1.00
1.00
2.00
1.01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127.26
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125.36
125.25
119.22
114.80
113.80
113.72
105.65
77.39
77.08
76.76
42.41
40.15
19.99
N
N
CN
Ph
3ab
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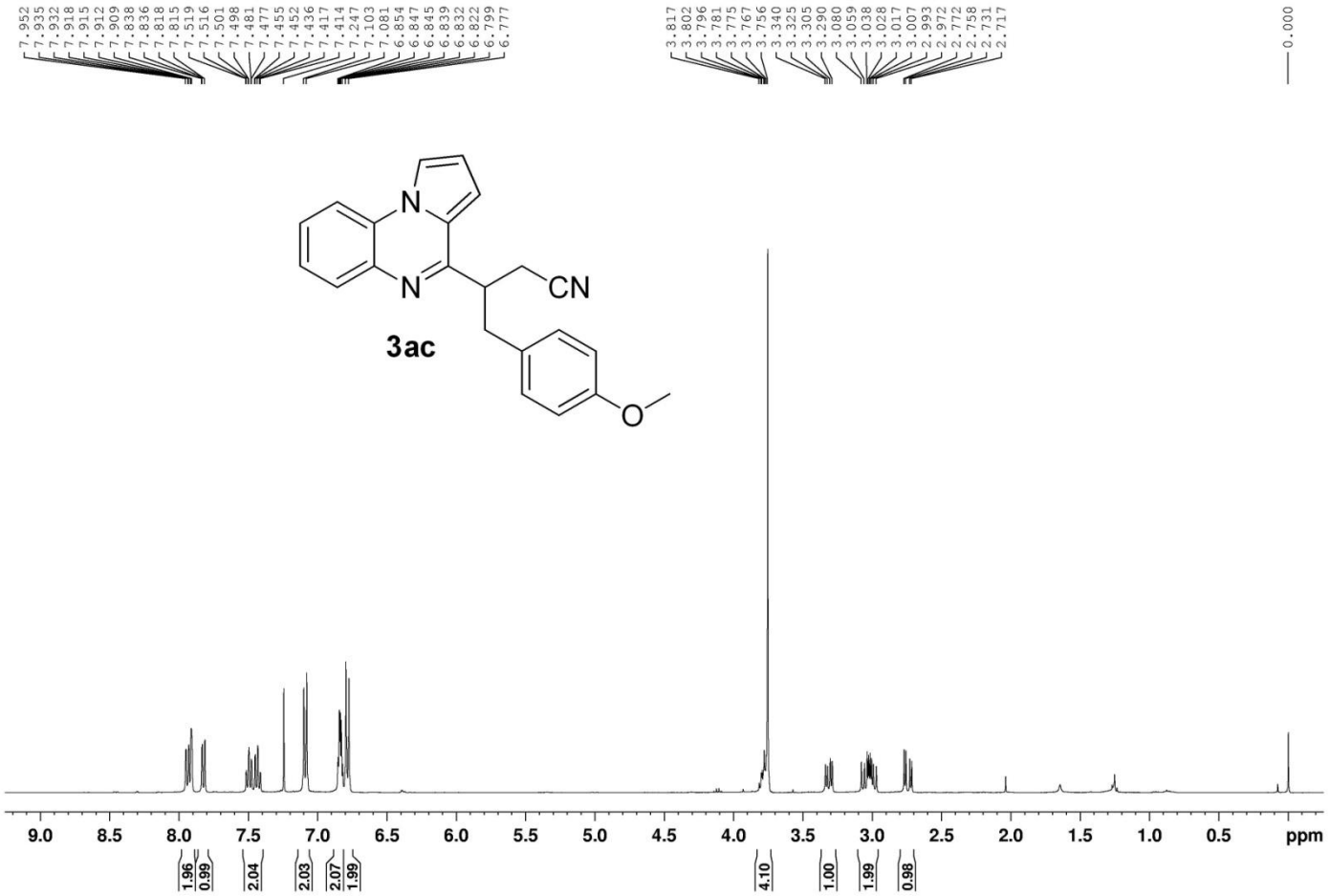
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.815
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7.516
7.501
7.498
7.481
7.477
7.455
7.452
7.436
7.417
7.414
7.247
7.103
7.081
6.854
6.847
6.845
6.839
6.832
6.822
6.799
6.777
3.817
3.802
3.796
3.781
3.775
3.767
3.756
3.340
3.325
3.305
3.290
3.080
3.059
3.038
3.028
3.017
3.007
2.993
2.972
2.772
2.758
2.731
2.717
0.000
N
N
CN
3ac
O
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
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ppm
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0.99
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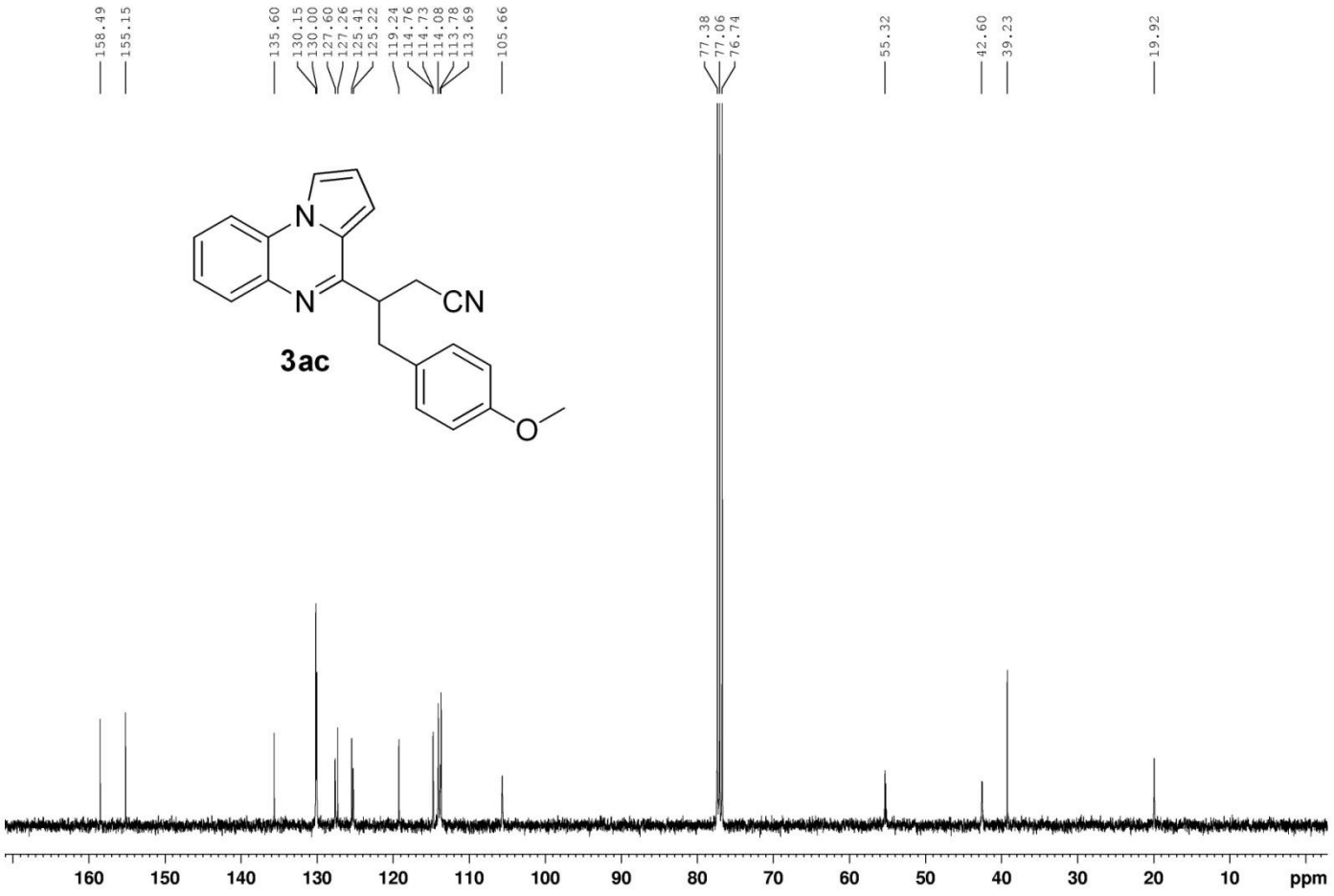
2.03
2.07
1.99
4.10
1.00
1.99
0.98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125.41
125.22
119.24
114.76
114.73
114.08
113.78
113.69
105.66
77.38
77.06
76.74
55.32
42.60
39.23
19.92
N
N
CN
O
3ac
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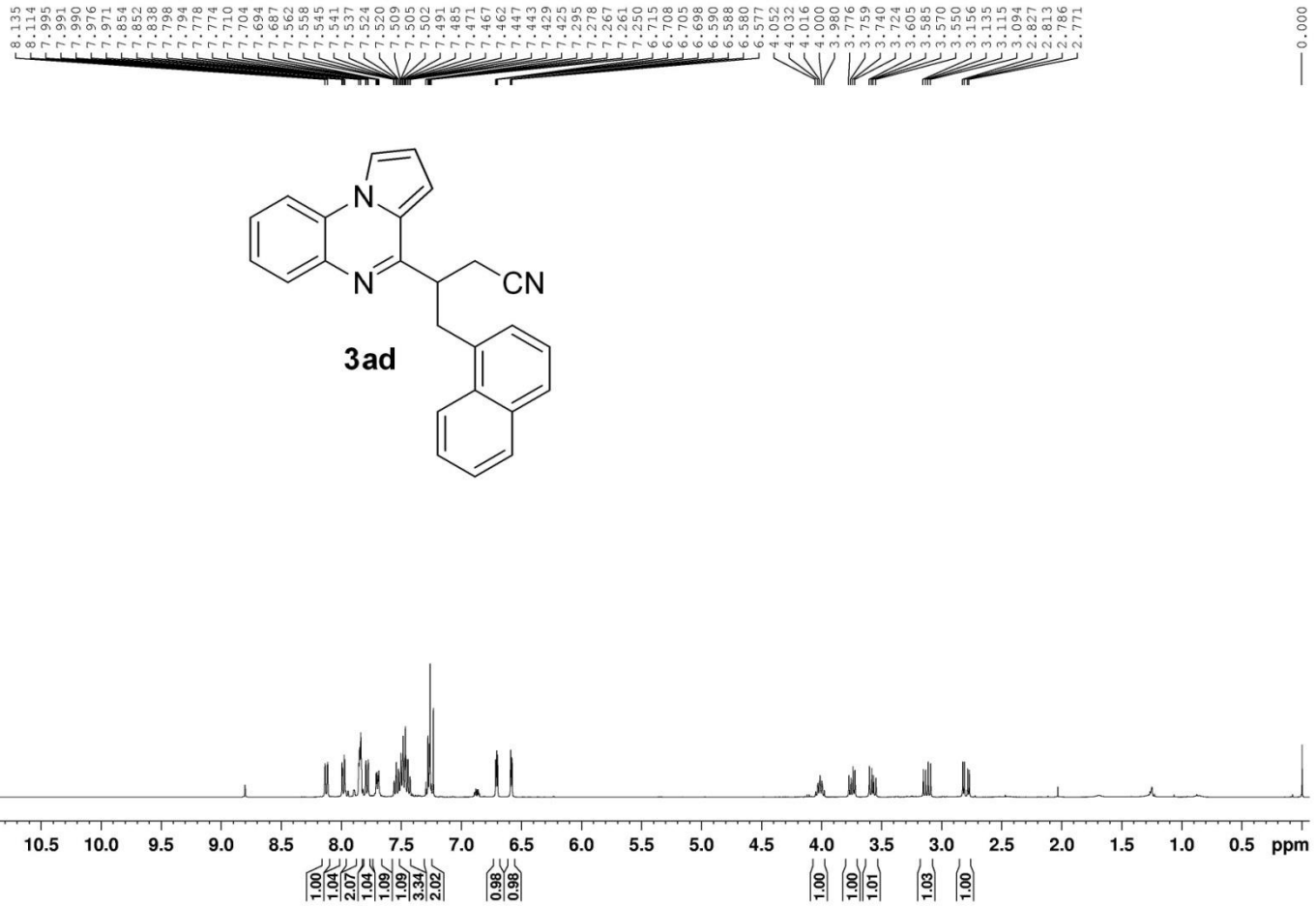
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.794
7.778
7.774
7.710
7.704
7.694
7.687
7.562
7.558
7.545
7.541
7.537
7.524
7.520
7.509
7.505
7.502
7.491
7.485
7.471
7.467
7.462
7.447
7.443
7.429
7.425
7.295
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7.267
7.261
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6.708
6.705
6.698
6.590
6.588
6.580
6.577
4.052
4.032
4.016
4.000
3.980
3.776
3.759
3.740
3.724
3.605
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3.570
3.550
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3.135
3.115
3.094
2.827
2.813
2.786
2.771
0.000
N
N
CN
3ad
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
ppm
1.00
1.04
2.07
1.04
1.09
1.09
3.34
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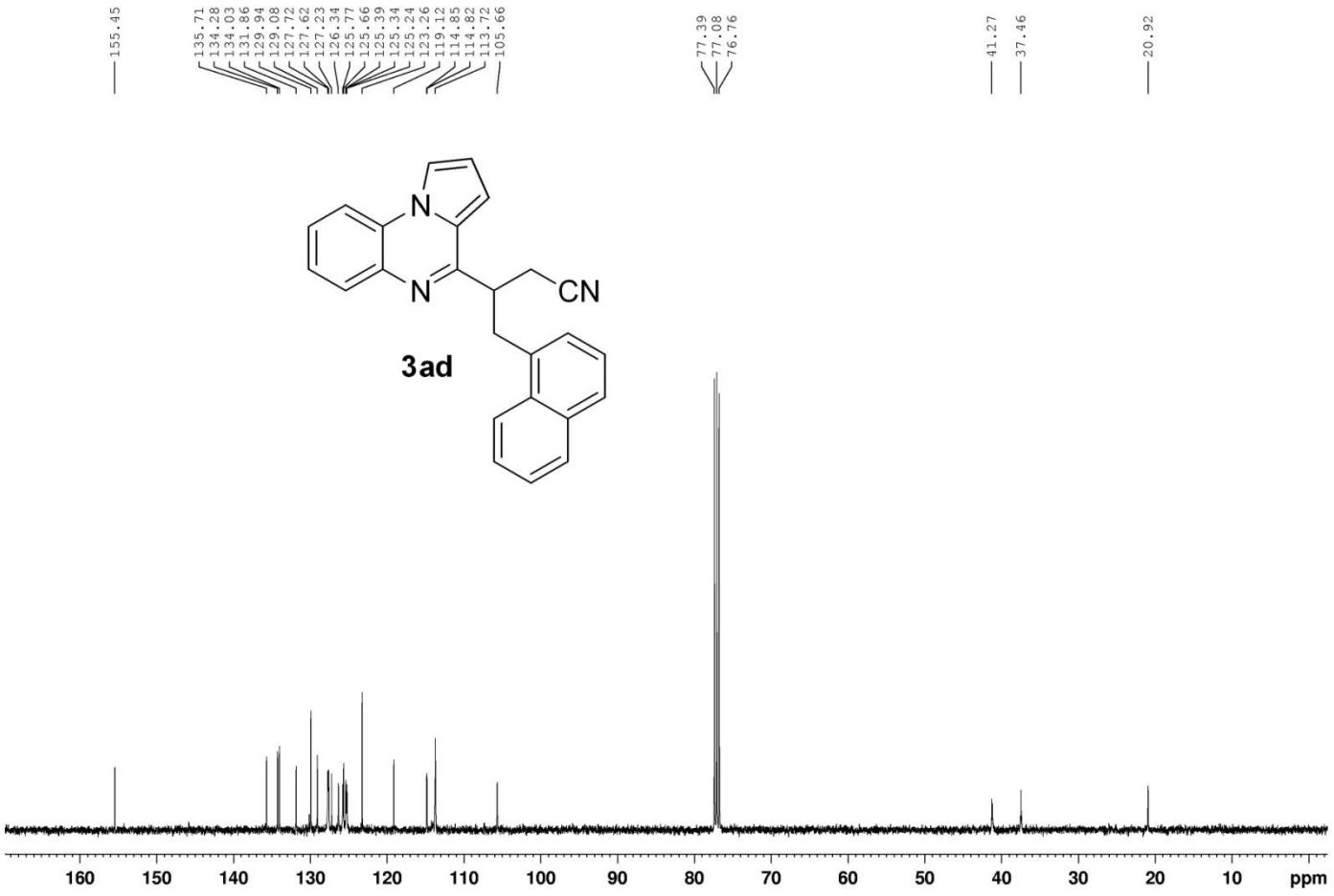
0.98
1.00
1.00
1.01
1.03
1.00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126.34
125.77
125.66
125.39
125.34
125.24
123.26
119.12
114.85
114.82
113.72
105.66
77.39
77.08
76.76
41.27
37.46
20.92
N
N
CN
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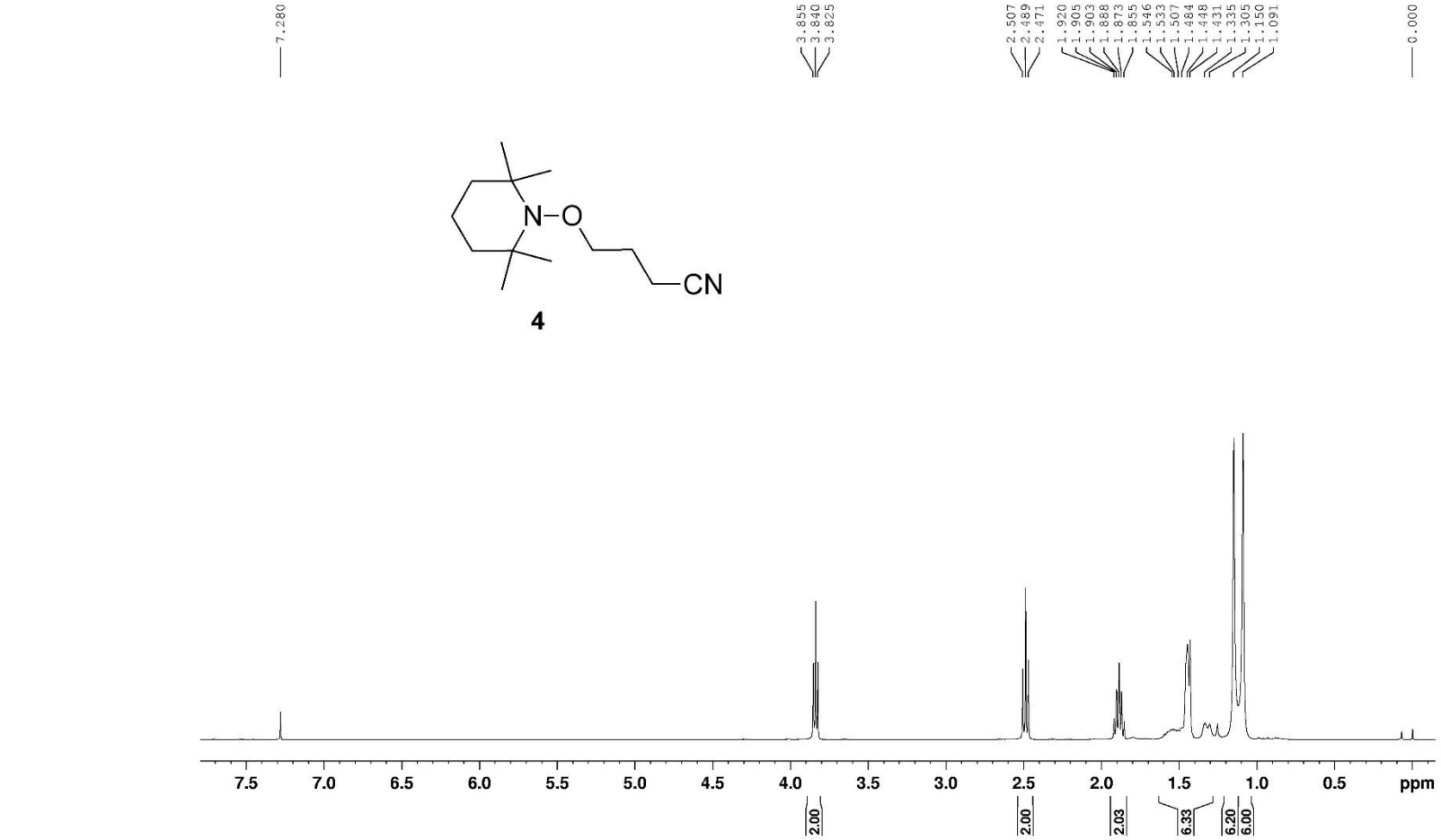
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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3.825
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2.489
2.471
1.920
1.905
1.903
1.888
1.873
1.855
1.546
1.533
1.507
1.484
1.448
1.431
1.335
1.305
1.150
1.091
0.000
N–O
CN
4
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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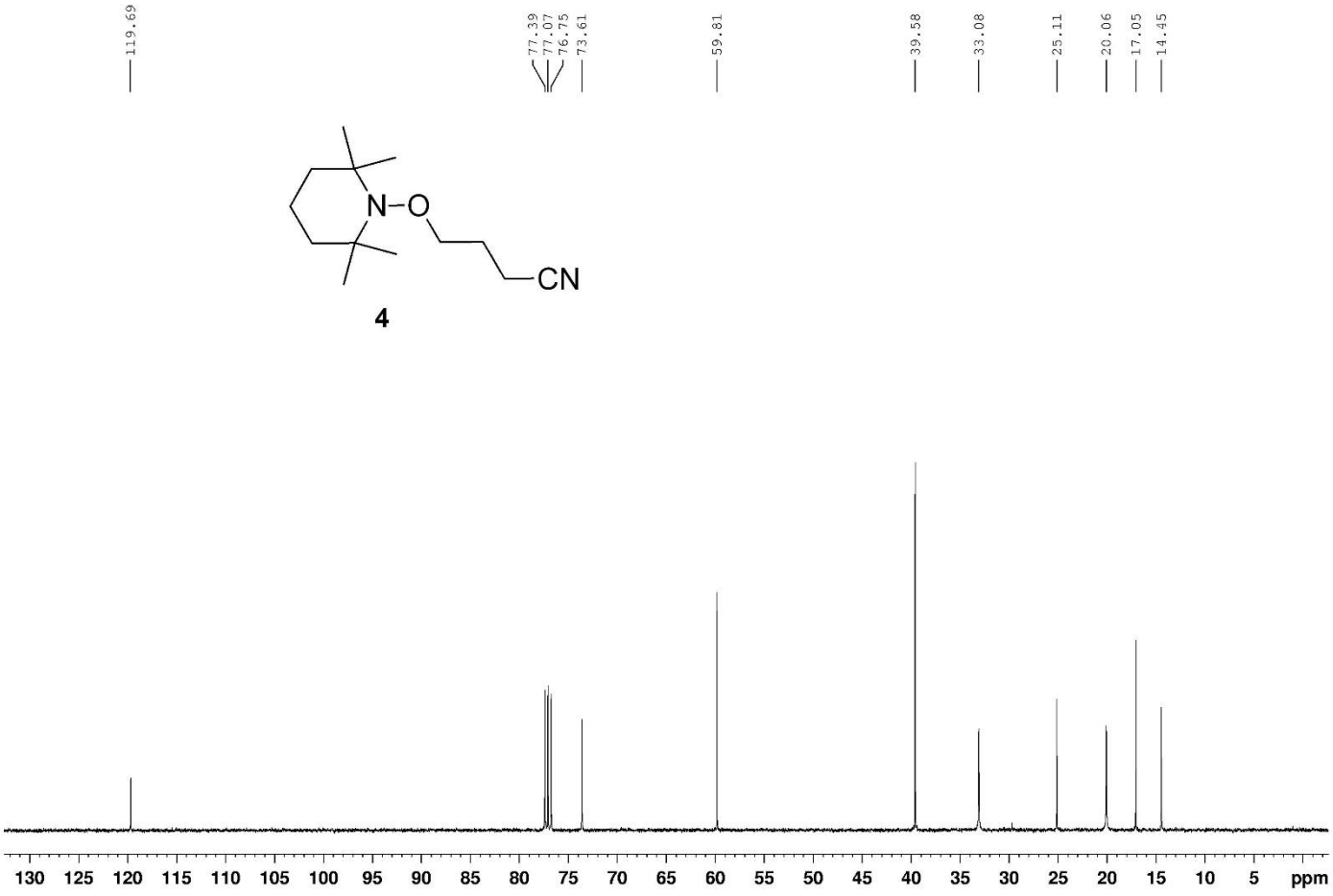
2.00
2.03
6.33
6.20
6.00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76.75
73.61
59.81
39.58
33.08
25.11
20.06
17.05
14.45
N–O
CN
4
130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 ppm