Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

$FeCl_3$-Catalyzed Synthesis of Pyrrolo[1,2-*a*]quinoxaline Derivatives from 1-(2-Aminophenyl)pyrroles through Annulation and Cleavage of Cyclic Ethers

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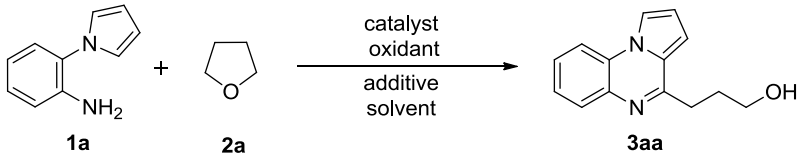
General remark

^{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 reactions were carried out under argon atmosphere in oven-dried glassware, unless otherwise noted. Tetrahydrofuran (THF) was distilled prior to use and stored over activated molecular sieves. All reagents were purchased commercially and used as received, unless otherwise noted.

Table S1. Optimization of Reaction Conditions [a]



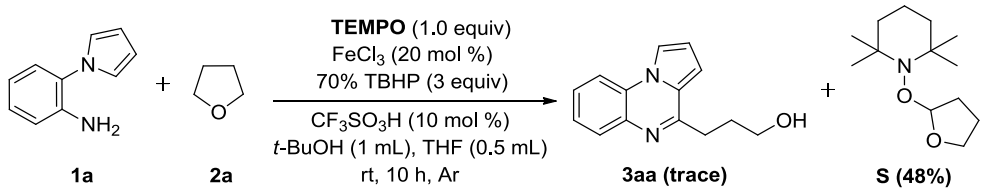
1a 2a 3aa

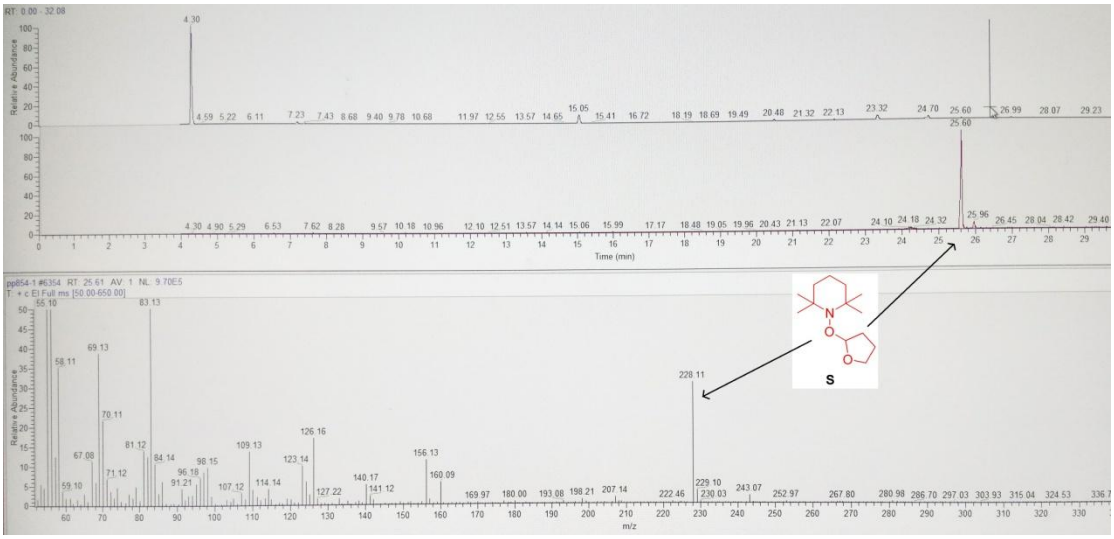
entry	catalyst (mol %)	oxidant (equiv)	additive (mol %)	solvent	T/℃	yield (%) [b]
1	$FeCl_3$ (10)	TBHP (2) [c]	-	THF	60	46
2	$Cu(OAc)_2$ (10)	TBHP (2) [c]	-	THF	60	0
3	$Pd(OAc)_2$ (10)	TBHP (2) [c]	-	THF	60	0
4	$FeCl_2$ (10)	TBHP (2) [c]	-	THF	60	38
5	$FeBr_3$ (10)	TBHP (2) [c]	-	THF	60	34
6	$Fe(OTf)_3$ (10)	TBHP (2) [c]	-	THF	60	30
7	$FeCl_3$ (20)	TBHP (2) [c]	-	THF	60	50
8	$FeCl_3$ (20)	TBHP (2) [c]	-	THF	100	32
9	$FeCl_3$ (20)	TBHP (2) [c]	-	THF	25	58
10	$FeCl_3$ (20)	DTBP (2) [d]	-	THF	25	38
11	$FeCl_3$ (20)	$K_2S_2O_8$ (2)	-	THF	25	trace
12	$FeCl_3$ (20)	DDQ (2) [d]	-	THF	25	0
13	$FeCl_3$ (20)	TBHP (2) [e]	-	THF	25	72
14	$FeCl_3$ (20)	TBHP (3) [e]	-	THF	25	80

15	$FeCl_3$ (20)	TBHP (3) [e]	-	MeCN/THF (1:1)	25	35
16	$FeCl_3$ (20)	TBHP (3) [e]	-	CH_3NO_2/THF(1:1)	25	50
17	$FeCl_3$ (20)	TBHP (3) [e]	-	*t*BuOH/THF (1:1)	25	84
18	$FeCl_3$ (20)	TBHP (3) [e]	-	*i*PrOH/THF (1:1)	25	70
19	$FeCl_3$ (20)	TBHP (3) [e]	-	*t*BuOH [f]	25	31
20	$FeCl_3$ (20)	TBHP (3) [e]	-	*t*BuOH/THF (2:1)	25	89
21	$FeCl_3$ (20)	TBHP (3) [e]	CF_3COOH (10)	*t*BuOH/THF (2:1)	25	84
22	**$FeCl_3$** (20)	**TBHP (3)** [e]	**CF_3SO_3H (10)**	***t*BuOH/THF (2:1)**	**25**	**94**
	$FeCl_3$ (20)	TBHP (3) [e]	CF_3SO_3H (10)	*t*BuOH/THF (2:1)	25	78 [g]
23	$FeCl_3$ (20)	TBHP (3) [e]	CF_3SO_3H (20)	*t*BuOH/THF (2:1)	25	80
24	-	TBHP (3) [e]	CF_3SO_3H (10)	*t*BuOH/THF (2:1)	25	0
25	$FeCl_3$ (20)	-	CF_3SO_3H (10)	*t*BuOH/THF (2:1)	25	0

[a] Reaction conditions: **1a** (0.3 mmol), catalyst (20 mol %), oxidant (3 equiv), additive (10 mol %), solvent (1.5 mL), rt, 10 h, Ar. [b]Yields of isolated products. [c] 5.5 M TBHP in decane. [d] DTBP = di-*tert*-butyl peroxide, DDQ = dichloro-5,6-dicyano-1,4-benzoquinone. [e] 70% TBHP in water. [f] THF (5 equiv). [g] Under O_2. Entry in bold highlights optimized reaction conditions, and the reaction time was monitored by TLC.

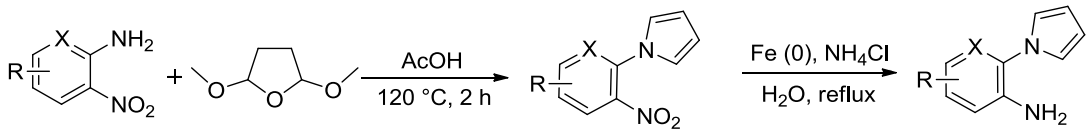
General procedure radical trapping experiment.





A mixture of 1-(2-aminophenyl)pyrrole **1a** (1 equiv, 0.3 mmol), 2,2,6,6-tetramethyl-1-piperidinyloxy TEMPO (1.0 equiv, 0.3 mmol), $FeCl_3$ (20 mol %, 0.06 mmol), TBHP (3.0 equiv, 0.9 mmol, 70% in water), CF_3SO_3H (10 mol %, 0.03mmol), tetrahydrofuran **2a** (0.5 mL), *tert*-butyl alcohol (1 mL) were stirred at ambient temperature under argon atmosphere for 10 h (TLC monitored). Upon completion of the reaction, the reaction mixture was extracted with ethyl acetate and saturated brine. All organic phase obtained were dried over anhydrous Na_2SO_4 and filtered. The resulting was analyzed by GC-MS. Then the intermediate **S** was isolated in 48% (based on TEMPO) by column chromatography on silica gel using petroleum ether/EtOAc as eluent (100:1), which was identified by ^1H NMR, ^{13}C NMR.

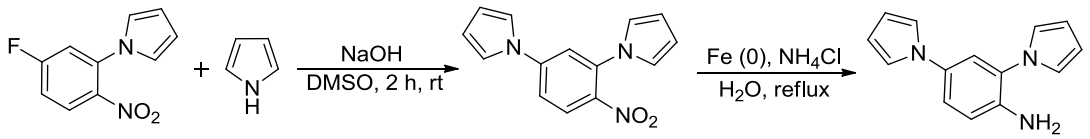
General procedure for the synthesis of 1b-1r and 1t.[1]



S_1 **S_2** **S_3** **1b-1o, 1t**

Compound **1a** was purchased from commercial sources and used as received. Substituted 2-(1*H*-pyrrol-1-yl)anilines **1b-1r** and **1t** were prepared in the following method. A mixture of substituted **S_1** (5 mmol) and **S_2** (5 mmol) in acetic acid (25 mL) was 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 **S_3**. Then, the residue **S_3** 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**.

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

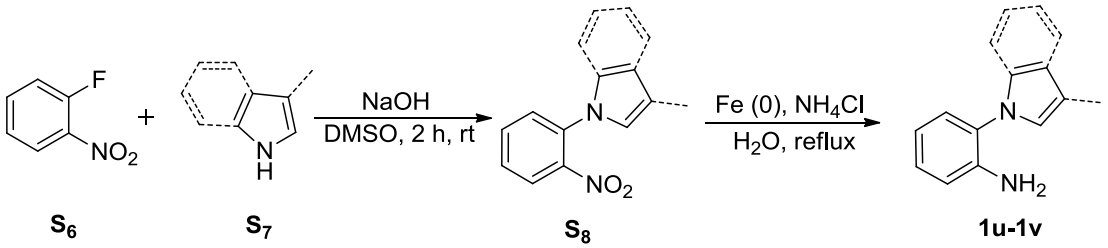


S_4 **S_5** **1s**

S_4 was prepared from the method of synthesizing **S_3**. Then, a mixture of **S_4** (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 **S_5**.

The residue **S_5** 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**.

General procedure for the synthesis of 1u-1v.[2]

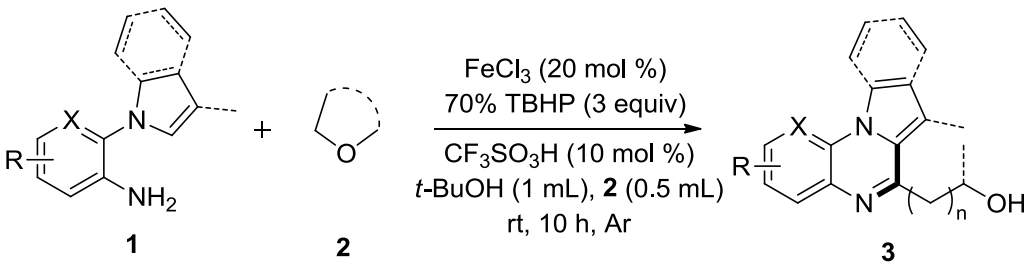


S_6 **S_7** **S_8** **1u-1v**

To a well-stirred solution of *N*-heterocycle **S_7** (5.0 mmol) in DMSO (5.0 mL), NaOH (5.0 mmol) and 1-fluoro-2-nitrobenzene **S_6** (5.0 mmol) were added slowly. The reaction mixture was stirred vigorously for 2 h at room temperature until no more starting material was detected by TLC analysis. The reaction mixture was extracted with ethyl acetate and saturated brine. Then the organic phase was combined and dried with anhydrous Na_2SO_4. The solvent was evaporated to obtain desired products **S_8** which were directly used for next step without further purification.

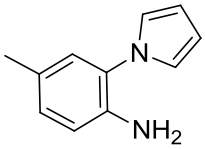
The residue **S_8** was added to iron powder (20 mmol) and NH_4Cl (2 mmol) in water (60 mL) and refluxed for 4 h. After cooling, the reaction mixture was poured into water (100 mL) and extracted with ethyl acetate three times (3×60 mL). The combined organic layers were dried with anhydrous Na_2SO_4 and the solvent was removed in vacuo to afford the residue. The residue was purified by column chromatography on silica gel to provide the desired products **1u** and **1v**.

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



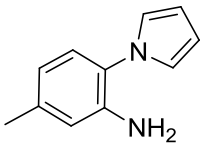
A mixture of 2-(1*H*-pyrrol-1-yl)aniline **1a** (1 equiv, 0.3 mmol), $FeCl_3$ (20 mol %, 0.06 mmol), 70% TBHP (3.0 equiv, 0.9 mmol), CF_3SO_3H (10 mol %, 0.03mmol), cyclic ethers **2a** (0.5 mL), *tert*-butyl alcohol (1 mL) were stirred at ambient temperature under argon atmosphere for 10 h (TLC monitored). Upon completion of the reaction, the reaction mixture was then extracted with ethyl acetate and saturated brine. 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 (1:1) to afford the desired **3aa**.

The data of products



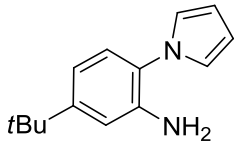
4-methyl-2-(1*H*-pyrrol-1-yl)aniline (1b)

White 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.



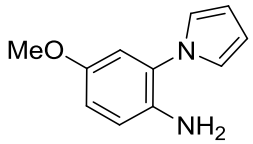
5-methyl-2-(1*H*-pyrrol-1-yl)aniline (1c)

White 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.



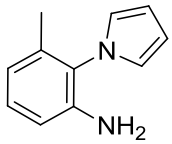
5-(*tert*-butyl)-2-(1*H*-pyrrol-1-yl)aniline (1d)

White 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.



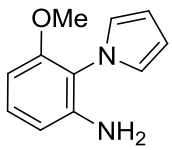
4-methoxy-2-(1*H*-pyrrol-1-yl)aniline (1e)

White solid (695.6 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.85-6.84 (m, 2 H), 6.79-6.73 (m, 3 H), 6.34-6.33 (m, 2 H), 3.74 (s, 3 H), 3.44 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.5, 135.5, 128.1, 121.7, 117.3, 114.8, 112.5, 109.5, 55.9.



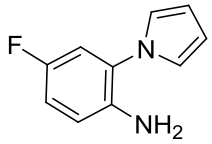
3-methyl-2-(1*H*-pyrrol-1-yl)aniline (1f)

White 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.



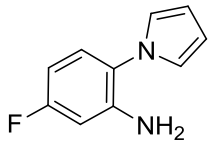
3-methoxy-2-(1*H*-pyrrol-1-yl)aniline (1g)

White 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.



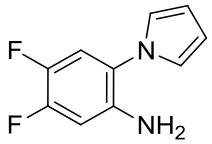
4-fluoro-2-(1*H*-pyrrol-1-yl)aniline (1h)

White 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.



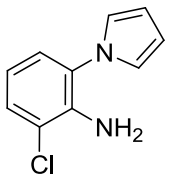
5-fluoro-2-(1*H*-pyrrol-1-yl)aniline (1i)

White 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).



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

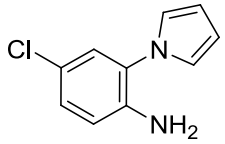
White solid (611.1 mg, 63% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.03-6.99 (m, 1 H), 6.77 (s, 2 H), 6.61-6.55 (m, 1 H), 6.34 (s, 2 H), 3.64 (br s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 151.9-148.7 (d, *J* = 170.1 Hz, 1 C), 144.3-141.1 (d, *J* = 238.1 Hz, 1 C), 139.2-139.0 (d, *J* = 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).



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

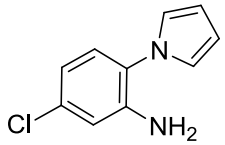
White solid (723.6 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.29-7.25

(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,.



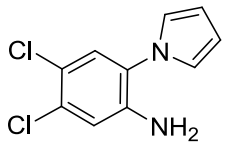
4-chloro-2-(1*H*-pyrrol-1-yl)aniline (1l)

White 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.



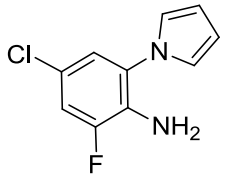
5-chloro-2-(1*H*-pyrrol-1-yl)aniline (1m)

White 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.



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

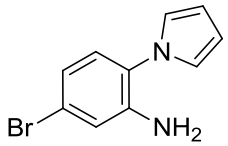
White solid (757.1 mg, 67% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.22 (s, 1 H), 6.88 (s, 1 H), 6.79-6.77 (m, 2 H), 6.35-6.33 (m, 2 H), 3.79 (br s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 141.8, 132.2, 128.6, 126.9, 121.7, 120.8, 117.1, 110.4.



4-chloro-2-fluoro-6-(1*H*-pyrrol-1-yl)aniline (1o)

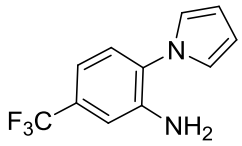
White solid (630.0 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.05-7.02 (m, 1 H), 6.99-6.98 (m, 1 H), 6.83-6.82 (m, 2 H), 6.36-6.35 (m, 2 H), 3.80 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.5-150.1 (d, *J* = 241.2 Hz, 1 C),

130.0-129.8 (d, *J* = 13.9 Hz, 1 C), 129.0-128.9 (d, *J* = 6.2 Hz, 1 C), 124.5, 122.4-122.4 (d, *J* = 3.3 Hz, 1 C), 121.3, 115.0-114.8 (d, *J* = 22.2 Hz, 1 C), 110.2.



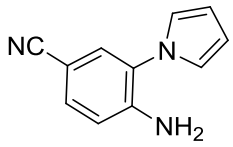
5-bromo-2-(1*H*-pyrrol-1-yl)aniline (1p)

White 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.



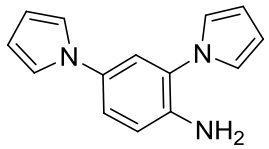
2-(1*H*-pyrrol-1-yl)-5-(trifluoromethyl)aniline (1q)

White 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.



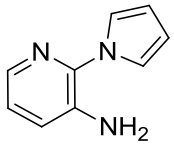
4-amino-3-(1*H*-pyrrol-1-yl)benzonitrile (1r)

White solid (539.8 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.43-7.41 (m, 2 H), 6.81-6.78 (m, 3 H), 6.38-6.36 (m, 2 H), 4.31 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.5, 132.7, 131.2, 126.8, 121.4, 119.2, 115.7, 110.4, 100.2.



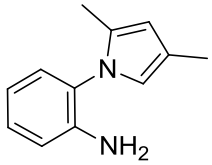
2,4-di(1*H*-pyrrol-1-yl)aniline (1s)

White 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.



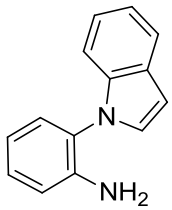
2-(1*H*-pyrrol-1-yl)pyridin-3-amine (1t)

White 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.



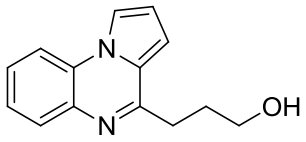
2-(2,4-dimethyl-1*H*-pyrrol-1-yl)aniline (1u)

White 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.



2-(1*H*-indol-1-yl)aniline (1v)

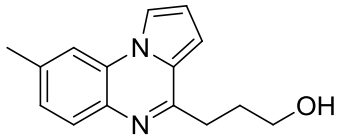
White solid (884.0 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.70-7.68 (m, 1 H), 7.26-7.13 (m, 6 H), 6.87-6.82 (m, 2 H), 6.69-6.68 (d, *J* = 3.0 Hz, 1 H), 3.56 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.2, 136.4, 129.2, 128.7, 128.6, 128.6, 124.9, 122.2, 121.0, 120.2, 118.6, 116.3, 110.8, 103.2.



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

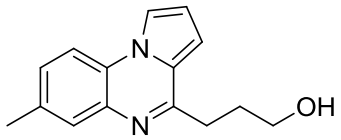
Yellow oil (61.0 mg, 90% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.92-7.87 (m, 2 H), 7.83-7.81 (m, 1 H), 7.48-7.46 (m, 1 H), 7.43-7.41 (m, 1 H), 6.96-6.94 (m, 1 H), 6.86-6.85 (m, 1 H), 4.75 (br s, 1 H), 3.83-3.80 (m, 2 H), 3.26-3.23 (m, 2 H), 2.21-2.14 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.7, 135.1, 129.0, 127.2, 127.1,

125.8, 125.2, 114.7, 113.7, 113.6, 106.8, 62.7, 32.8, 29.6; HRMS calcd for $C_{14}H_{15}N_2O$ $[M+H]^+$ 227.1179; found: 227.1182.



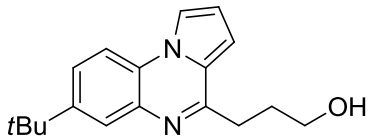
3-(8-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ba).

Yellow oil (51.1 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.89-7.88 (m, 1 H), 7.78-7.76 (d, *J* = 8.4 Hz, 1 H), 7.62 (s, 1 H), 7.26-7.22 (m, 1 H), 6.93-6.92 (m, 1 H), 6.85-6.84 (m, 1 H), 3.82-3.80 (m, 2 H), 3.25-3.22 (m, 2 H), 2.53 (s, 3 H), 2.20-2.14 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.6, 137.7, 133.0, 128.7, 126.9, 126.5, 125.9, 114.4, 113.7, 133.6, 106.5, 62.7, 32.8, 29.5, 21.8; HRMS calcd for $C_{15}H_{17}N_2O$ $[M+H]^+$ 241.1336; found: 241.1330.



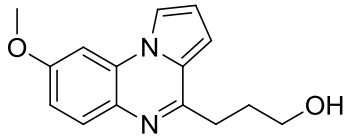
3-(7-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ca)

Light yellow solid (47.5 mg, 66% yield), melting point: 108-110 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.87-7.86 (m, 1 H), 7.70-7.68 (m, 2 H), 7.29-7.26 (m, 1 H), 6.93-6.92 (m, 1 H), 6.83-6.82 (m, 1 H), 3.83-3.80 (m, 2 H), 3.25-3.22 (m, 2 H), 2.46 (s, 3 H), 2.20-2.13 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.5, 135.1, 134.8, 128.7, 128.4, 125.7, 125.0, 114.6, 113.5, 113.4, 106.7, 62.7, 32.8, 29.6, 21.0; HRMS calcd for $C_{15}H_{17}N_2O$ $[M+H]^+$ 241.1336; found: 241.1141.



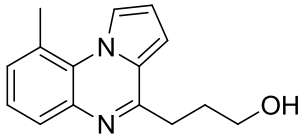
3-(7-(*tert*-butyl)pyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3da)

Yellow oil (46.5 mg, 55% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.91-7.89 (m, 2 H), 7.78-7.76 (d, *J* = 8.8 Hz, 1 H), 7.56-7.53 (m, 1 H), 6.94-6.93 (m, 1 H), 6.85-6.83 (m, 1 H), 4.59 (br s, 1 H), 3.84-3.81 (m, 2 H), 3.26-3.23 (m, 2 H), 2.21-2.15 (m, 2 H), 1.40 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.5, 148.6, 134.9, 125.8, 125.4, 124.9, 114.4, 113.5, 113.3, 106.5, 62.7, 34.7, 32.8, 31.4, 29.8; HRMS calcd for $C_{18}H_{23}N_2O$ $[M+H]^+$ 283.1805; found: 283.1811.



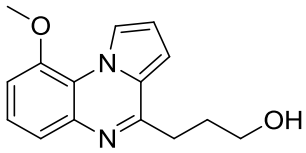
3-(8-methoxypyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ea)

Light yellow solid (50.7 mg, 66% yield), melting point: 105-108 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.80 (m, 2 H), 7.26-7.23 (m, 1 H), 7.02-7.00 (m, 1 H), 6.92-6.90 (m, 1 H), 6.86-6.85 (m, 1 H), 3.94 (s, 3 H), 3.82-3.79 (m, 2 H), 3.24-3.20 (m, 2 H), 2.19-2.13 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 158.9, 153.9, 130.1, 129.4, 127.9, 125.8, 114.3, 113.8, 112.7, 106.4, 97.7, 62.7, 55.8, 32.7, 29.6; HRMS calcd for $C_{15}H_{17}N_2O_2$ $[M+H]^+$ 257.1285; found: 257.1280.



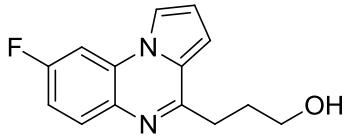
3-(9-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3fa).

Yellow oil (36.2 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.30-8.29 (d, *J* = 1.6 Hz, 1 H), 7.77-7.75 (m, 1 H), 7.31-7.26 (m, 2 H), 6.97-6.96 (m, 1 H), 6.84-6.82 (m, 1 H), 4.93 (br s, 1 H), 3.83-3.80 (m, 2 H), 3.24-3.21 (m, 2 H), 2.91 (s, 3 H), 2.20-2.14 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 155.8, 136.3, 130.1, 126.9, 126.8, 126.5, 124.9, 124.1, 119.8, 112.6, 105.9, 61.8, 32.0, 29.9, 23.4; HRMS calcd for $C_{15}H_{17}N_2O$ $[M+H]^+$ 241.1336; found: 241.1330.



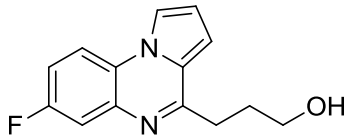
3-(9-methoxypyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ga)

Light yellow solid (48.6 mg, 63% yield), melting point: 101-103 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.68-8.67 (d, *J* = 5.6 Hz, 1 H), 7.49-7.46 (m, 1 H), 7.30-7.24 (m, 1 H), 6.97-6.92 (m, 2 H), 6.76-6.75 (m, 1 H), 5.19 (br s, 1 H), 3.99 (s, 3 H), 3.82-3.79 (m, 2 H), 3.22-3.18 (m, 2 H), 2.18-2.12 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.7, 149.6, 137.1, 126.1, 124.2, 122.3, 120.8, 118.3, 112.5, 108.5, 106.0, 62.4, 56.0, 32.5, 29.7; HRMS calcd for $C_{15}H_{17}N_2O_2$ $[M+H]^+$ 257.1285; found: 257.1279.



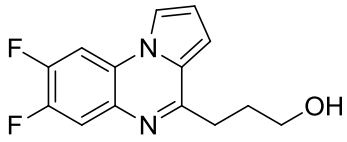
3-(8-fluoropyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ha)

Light yellow solid (60.0 mg, 82% yield), melting point: 108-111 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.86-7.83 (m, 1 H), 7.79-7.78 (m, 1 H), 7.48-7.45 (m, 1 H), 7.14-7.09 (m, 1 H), 6.95-6.93 (m, 1 H), 6.88-6.86 (m, 1 H), 4.47 (br s, 1 H), 3.82-3.80 (m, 2 H), 3.23-3.19 (m, 2 H), 2.20-2.13 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 162.4-159.9 (d, *J* = 246 Hz, 1 C), 155.9-155.8 (d, *J* = 3 Hz, 1 C), 131.7-131.7 (d, *J* = 2 Hz, 1 C), 130.8-130.7 (d, *J* = 9 Hz, 1 C), 127.9-127.7 (d, *J* = 11 Hz, 1 C), 125.5, 114.8, 114.2, 113.2-112.9 (d, *J* = 23 Hz, 1 C), 107.0, 100.6-100.4 (d, *J* = 26 Hz, 1 C), 62.6, 32.6, 29.6; HRMS calcd for $C_{14}H_{14}FN_2O$ $[M+H]^+$ 245.1085; found: 245.1081.



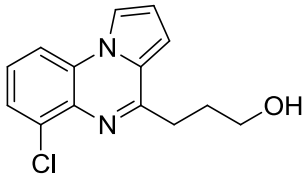
3-(7-fluoropyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ia)

Yellow oil (62.2 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.87-7.86 (m, 1 H), 7.78-7.75 (m, 1 H), 7.57-7.54 (m, 1 H), 7.23-7.18 (m, 1 H), 6.97-6.95 (m, 1 H), 6.86-6.84 (m, 1 H), 4.25 (br s, 1 H), 3.82-3.79 (m, 2 H), 3.23-3.20 (m, 2 H), 2.20-2.13 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 161.0-158.6 (d, *J* = 269 Hz, 1 C), 158.0, 136.5-136.4 (d, *J* = 12 Hz, 1 C), 125.6, 123.9, 115.0, 114.9, 114.7, 114.5-114.3 (d, *J* = 22 Hz, 1 C), 113.9, 107.2, 62.5, 32.6, 29.7; HRMS calcd for $C_{14}H_{14}FN_2O$ $[M+H]^+$ 245.1085; found: 245.1079.



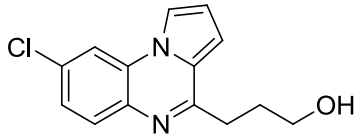
3-(7,8-difluoropyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ja)

Light yellow solid (70.7 mg, 90% yield), melting point: 134-136 ^{o}C. ^{1}H NMR (400 MHz, DMSO, ppm): δ = 8.46-8.41 (m, 1 H), 8.36-8.35 (m, 1 H), 7.83-7.78 (m, 1 H), 7.05-7.04 (m, 1 H), 6.91-6.90 (m, 1 H), 4.57-4.54 (m, 1 H), 3.55-3.51 (m, 2 H), 3.01-2.97 (m, 2 H), 1.98-1.91 (m, 2 H); ^{13}C NMR (100 MHz, DMSO, ppm): δ = 158.3, 150.4-149.0 (dd, *J* = 127 Hz, *J* = 14 Hz, 1 C), 147.9-146.6 (dd, *J* = 124 Hz, *J* = 14 Hz, 1 C), 133.2-133.1 (d, *J* = 7 Hz, 1 C), 125.6, 124.5-124.4 (d, *J* = 10 Hz, 1 C), 117.6, 117.1-117.0 (d, *J* = 17 Hz, 1 C), 114.9, 107.9, 104.7-104.5 (d, *J* = 23 Hz, 1 C), 61.3, 32.1, 31.6; HRMS calcd for $C_{14}H_{13}F_2N_2O$ $[M+H]^+$ 263.0991; found: 263.0981.



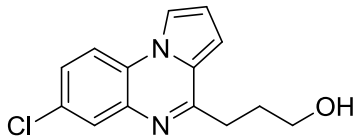
3-(6-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ka)

Yellow solid (46.8 mg, 60% yield), melting point: 94-96 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.81-7.80 (m, 1 H), 7.62-7.59 (m, 1 H), 7.41-7.38 (m, 1 H), 7.28-7.24 (m, 1 H), 6.91-6.90 (m, 1 H), 6.81-6.80 (m, 1 H), 5.03 (br s, 1 H), 3.84-3.81 (m, 2 H), 3.24-3.21 (m, 2 H), 2.20-2.14 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 157.3, 133.2, 132.0, 128.0, 126.6, 125.6, 125.5, 115.2, 114.2, 112.2, 107.3, 62.6, 32.6, 29.0; HRMS calcd for $C_{14}H_{14}ClN_2O$ $[M+H]^+$ 261.0789; found: 261.0794.



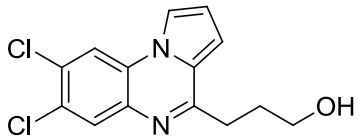
3-(8-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3la)

Light yellow solid (51.7 mg, 66% yield), melting point: 88-90 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.84-7.83 (m, 1 H), 7.79-7.77 (m, 2 H), 7.36-7.33 (m, 1 H), 6.96-6.95 (m, 1 H), 6.87-6.86 (m, 1 H), 4.37 (br s, 1 H), 3.82-3.79 (m, 2 H), 3.23-3.19 (m, 2 H), 2.19-2.13 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.9, 133.7, 132.6, 130.2, 127.7, 125.7, 125.6, 114.9, 114.3, 113.8, 107.3, 62.6, 32.6, 29.6; HRMS calcd for $C_{14}H_{14}ClN_2O$ $[M+H]^+$ 261.0789; found: 261.0781.



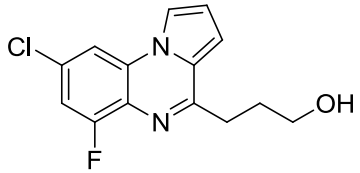
3-(7-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ma)

Light yellow solid (71.0 mg, 91% yield), melting point: 115-118 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.87-7.86 (d, *J* = 2.0 Hz, 2 H), 7.75-7.72 (d, *J* = 8.8 Hz, 1 H), 7.43-7.40 (m, 1 H), 6.97-6.96 (m, 1 H), 6.88-6.86 (m, 1 H), 4.21 (br s, 1 H), 3.82-3.79 (m, 2 H), 3.24-3.20 (m, 2 H), 2.19-2.13 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 158.0, 136.1, 130.4, 128.5, 127.2, 125.8, 125.7, 115.0, 114.8, 114.1, 107.4, 62.6, 32.6, 29.6; HRMS calcd for $C_{14}H_{14}ClN_2O$ $[M+H]^+$ 261.0789; found: 261.0784.



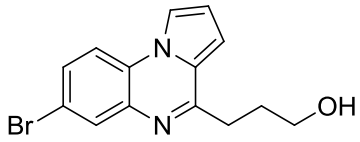
3-(7,8-dichloropyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3na)

Light yellow solid (66.2 mg, 75% yield), melting point: 130-133 ^{o}C. ^{1}H NMR (300 MHz, DMSO-d_6, ppm): δ = 8.58 (s, 1 H), 8.46-8.45 (d, *J* = 1.5 Hz, 1 H), 7.94 (s, 1 H), 7.08-7.06 (m, 1 H), 6.91-6.89 (m, 1 H), 4.57-4.54 (m, 1 H), 3.56-3.50 (m, 2 H), 3.01-2.96 (m, 2 H), 1.99-1.90 (m, 2 H); ^{13}C NMR (75 MHz, DMSO, ppm): δ = 158.5, 135.1, 129.4, 128.9, 126.9, 126.4, 124.9, 117.1, 116.5, 114.3, 107.6, 60.4, 31.2, 30.6; HRMS calcd for $C_{14}H_{13}Cl_2N_2O$ $[M+H]^+$ 295.0400; found: 295.0392.



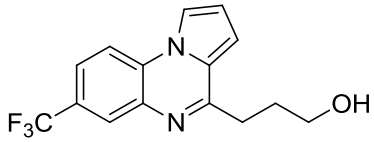
3-(8-chloro-6-fluoropyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3oa)

Yellow oil (61.7 mg, 74% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.77-7.75 (m, 1 H), 7.52-7.51 (m, 1 H), 7.10-7.06 (m, 1 H), 6.98-6.97 (m, 1 H), 6.87-6.85 (m, 1 H), 4.57 (s, 1 H), 3.83-3.80 (m, 2 H), 3.23-3.18 (m, 2 H), 2.20-2.12 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 159.6-156.2 (d, *J* = 256 Hz, 1 C), 157.1, 132.1-131.9 (d, *J* = 11.3 Hz, 1 C), 128.6-128.5 (d, *J* = 5.3 Hz, 1 C), 125.7, 123.9-123.7 (d, *J* = 13.5 Hz, 1 C), 115.2, 114.6, 112.3-112.0 (d, *J* = 22.5 Hz, 1 C), 109.6-109.5 (d, *J* = 4.5 Hz, 1 C), 108.1, 62.4, 32.7, 29.7; HRMS calcd for $C_{14}H_{13}ClFN_2O$ $[M+H]^+$ 279.0695; found: 279.0688.



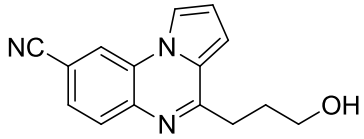
3-(7-bromopyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3pa)

Light yellow solid (61.1 mg, 67% yield), melting point: 130-133 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.06-8.05 (d, *J* = 1.8 Hz, 1 H), 7.90-7.89 (m, 1 H), 7.71-7.68 (d, *J* = 8.7 Hz, 1 H), 7.59-7.55 (m, 1 H), 6.99-6.97 (m, 1 H), 6.89-6.87 (m, 1 H), 4.08 (br s, 1 H), 3.83-3.79 (m, 2 H), 3.25-3.21 (m, 2 H), 2.21-2.13 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 158.2, 134.6, 130.7, 130.0, 128.8, 126.3, 125.6, 115.3, 115.2, 114.5, 107.9, 62.5, 32.5, 29.5; HRMS calcd for $C_{14}H_{14}BrN_2O$ $[M+H]^+$ 305.0284; found: 305.0278.



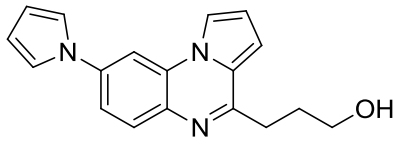
3-(7-(trifluoromethyl)pyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3qa)

Light yellow solid (85.6 mg, 97% yield), melting point: 110-113 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.18 (s, 1 H), 7.96-7.89 (m, 2 H), 7.72-7.69 (d, *J* = 8.7 Hz, 1 H), 7.02-7.01 (d, *J* = 3.9 Hz, 1 H), 6.93-6.91 (m, 1 H), 3.89 (br s, 1 H), 3.84-3.80 (m, 2 H), 3.26-3.22 (m, 2 H), 2.23-2.15 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 158.4, 135.0, 129.3, 127.6-126.3 (q, *J* = 32.3 Hz, 1 C), 126.7-126.6 (d, *J* = 4.5 Hz, 1 C),126.0, 125.7-122.1 (d, *J* = 269.3 Hz, 1 C), 123.6-123.5 (d, *J* = 3.0 Hz, 1 C), 115.3, 114.7, 114.4, 107.9, 62.5, 32.5, 29.6; HRMS calcd for $C_{15}H_{14}F_3N_2O$ $[M+H]^+$ 295.1053; found: 295.1043.



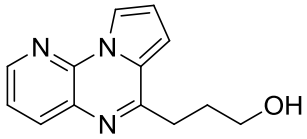
4-(3-hydroxypropyl)pyrrolo[1,2-*a*]quinoxaline-8-carbonitrile (3ra)

Light yellow solid (62.7 mg, 83% yield), melting point: 147-149 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.13-8.12 (d, *J* = 1.8 Hz, 1 H), 7.96-7.93 (m, 2 H), 7.68-7.67 (m, 1 H), 7.07-7.06 (m, 1 H), 6.96-6.93 (m, 1 H), 3.84-3.80 (m, 2 H), 3.65 (br s, 1 H), 3.27-3.23 (m, 2 H), 2.23-2.14 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 160.0, 138.1, 129.9, 128.0, 127.3, 125.8, 118.4, 118.1, 115.7, 114.9, 109.7, 108.6, 62.3, 32.5, 29.6; HRMS calcd for $C_{15}H_{14}N_3O$ $[M+H]^+$ 252.1132; found: 252.1139.



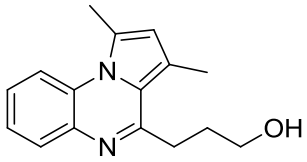
3-(8-(1H-pyrrol-1-yl)pyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3sa)

Yellow oil (82.9 mg, 95% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.94-7.89 (m, 2 H), 7.77-7.76 (d, *J* = 2.4 Hz, 1 H), 7.47-7.44 (m, 1 H), 7.21-7.19 (m, 1 H), 6.97-6.96 (m, 1 H), 6.90-6.89 (m, 1 H), 6.43-6.41 (m, 1 H), 4.39 (br s, 1 H), 3.84-3.80 (m, 2 H), 3.27-3.22 (m, 2 H), 2.22-2.14 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 156.1, 139.2, 132.8, 130.1, 127.6, 125.7, 119.5, 117.5, 114.6, 114.1, 111.2, 107.1, 104.9, 62.5, 32.5, 29.7; HRMS calcd for $C_{18}H_{18}N_3O$ $[M+H]^+$ 292.1445; found: 292.1439.



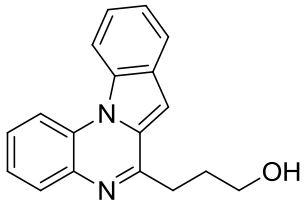
3-(pyrido[3,2-*e*]pyrrolo[1,2-*a*]pyrazin-6-yl)propan-1-ol (3ta)

Yellow oil (35.4 mg, 52% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.50-8.48 (m, 1 H), 8.38-8.37 (m, 1 H), 8.17-8.14 (m, 1 H), 7.42-7.38 (m, 1 H), 7.02-7.00 (m, 1 H), 6.89-6.87 (m, 1 H), 4.17 (br s, 1 H), 3.83-3.80 (m, 2 H), 3.25-3.21 (m, 2 H), 2.22-2.14 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 157.9, 146.3, 139.3, 136.3, 130.1, 127.2, 121.5, 115.9, 114.2, 108.3, 62.4, 32.4, 29.8; HRMS calcd for $C_{13}H_{14}N_3O$ $[M+H]^+$ 228.1132; found: 228.1127.



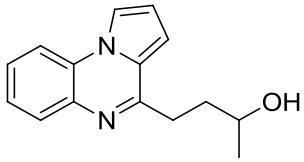
3-(1,3-dimethylpyrrolo[1,2-*a*]quinoxalin-4-yl)propan-1-ol (3ua)

Light yellow solid (34.3 mg, 45% yield), melting point: 109-113 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.19-8.15 (m, 1 H), 7.82-7.79 (m, 1 H), 7.37-7.34 (m, 2 H), 6.40 (s, 1 H), 3.81-3.77 (m, 2 H), 3.35-3.31 (m, 2 H), 2.89 (s, 3 H), 2.59 (s, 3 H), 2.19-2.13 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 157.0, 135.9, 129.7, 128.3, 127.9, 125.9, 124.4, 123.5, 118.7, 117.5, 115.0, 62.5, 33.9, 29.6, 17.7, 14.9; HRMS calcd for $C_{16}H_{19}N_2O$ $[M+H]^+$ 255.1492; found: 255.1486.



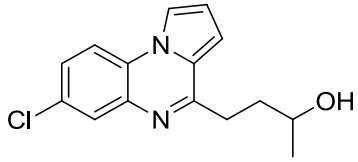
3-(indolo[1,2-*a*]quinoxalin-6-yl)propan-1-ol (3va)

Light yellow solid (39.7 mg, 48% yield), melting point: 84-86 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.41-8.36 (m, 2 H), 7.92-7.90 (d, *J* = 7.8 Hz, 2 H), 7.56-7.49 (m, 2 H), 7.44-7.35 (m, 2 H), 7.17 (s, 1 H), 3.86-3.82 (m, 2 H), 3.30-3.25 (m, 2 H), 2.26-2.18 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 158.2, 134.9, 132.9, 130.1, 129.3, 129.2, 128.9, 128.0, 124.4, 124.0, 122.7, 122.6, 114.6, 114.5, 100.2, 62.5, 32.7, 29.5; HRMS calcd for $C_{18}H_{17}N_2O$ $[M+H]^+$ 277.1336; found: 277.1330.



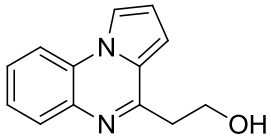
4-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butan-2-ol (3ab)

Yellow oil (56.2 mg, 78% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.91-7.87 (m, 2 H), 7.82-7.79 (m, 1 H), 7.43-7.39 (m, 2 H), 6.95-6.93 (m, 1 H), 6.86-6.83 (m, 1 H), 4.92 (br s, 1 H), 4.00-3.94 (m, 1 H), 3.28-3.17 (m, 2 H), 2.08-2.02 (m, 2 H), 1.29-1.26 (d, *J* = 6.3 Hz, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 156.9, 135.0, 128.9, 127.1, 125.7, 125.1, 114.6, 113.6, 113.5, 106.7, 67.5, 35.9, 31.8, 23.6; HRMS calcd for $C_{15}H_{17}N_2O$ $[M+H]^+$ 241.1336; found: 241.1329.



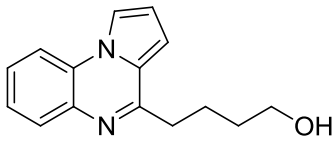
4-(7-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)butan-2-ol (3jb)

Yellow oil (60.0 mg, 73% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.89-7.88 (d, *J* = 1.5 Hz, 2 H), 7.76-7.73 (d, *J* = 8.7 Hz, 1 H), 7.44-7.41 (m, 1 H), 7.00-6.97 (d, *J* = 3.9 Hz, 1 H), 6.88-6.86 (m, 1 H), 4.37 (br s, 1 H), 3.95 (m, 1 H), 3.32-3.13 (m, 2 H), 2.09-1.99 (m, 2 H), 1.28-1.27 (d, *J* = 6.0 Hz, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 158.1, 136.0, 130.2, 128.4, 127.1, 125.7, 125.6, 114.9, 114.7, 114.0, 107.3, 67.4, 35.9, 31.7, 23.6; HRMS calcd for $C_{15}H_{16}ClN_2O$ $[M+H]^+$ 275.0946; found: 275.0938.



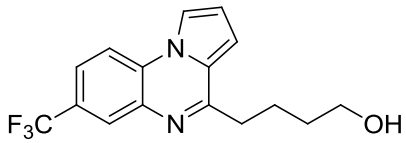
2-(pyrrolo[1,2-*a*]quinoxalin-4-yl)ethanol (3ac)

Light yellow solid (54.1 mg, 85% yield), melting point: 121-123 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.93-7.83 (m, 3 H), 7.50-7.43 (m, 2 H), 6.91-6.85 (m, 2 H), 4.67 (br s, 1 H), 4.21 (m, 2 H), 3.26-3.22 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 156.1, 135.0, 129.3, 129.1, 127.2, 125.7, 125.1, 114.6, 113.7, 113.6, 106.4, 60.3, 35.3; HRMS calcd for $C_{13}H_{13}N_2O$ $[M+H]^+$ 213.1023; found: 213.1016.



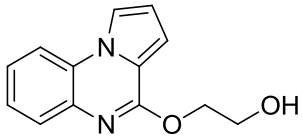
4-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butan-1-ol (3ad)

Yellow oil (51.8 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.91-7.89 (m, 2 H), 7.83-7.81 (m, 1 H), 7.49-7.39 (m, 2 H), 6.93-6.91 (m, 1 H), 6.86-6.84 (m, 1 H), 3.72-3.69 (m, 2 H), 3.11-3.07 (m, 2 H), 2.09-2.01 (m, 2 H), 1.79-1.72 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 157.0, 135.6, 129.2, 127.3, 127.1, 125.9, 125.2, 114.3, 113.7, 113.6, 106.4, 62.0, 34.5, 32.4, 23.4; HRMS calcd for $C_{15}H_{17}N_2O$ $[M+H]^+$ 241.1336; found: 241.1329.



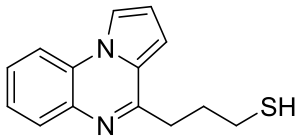
4-(7-(trifluoromethyl)pyrrolo[1,2-a]quinoxalin-4-yl)butan-1-ol (3nd)

Light yellow solid (61.0 mg, 66% yield), melting point: 114-116 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.17 (s, 1 H), 7.92-7.86 (m, 2 H), 7.69-7.65 (m, 1 H), 6.98-6.96 (m, 1 H), 6.90-6.88 (m, 1 H), 3.74-3.70 (m, 2 H), 3.10-3.05 (m, 2 H), 2.78 (br s, 1 H), 2.08-1.98 (m, 2 H), 1.80-1.71 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 158.6, 135.3, 129.3, 127.0-126.7 (q, *J* = 33.0 Hz, 1 C), 126.7-126.6 (d, *J* = 3.8 Hz, 1 C), 125.9, 125.7-122.1 (d, *J* = 270.8 Hz, 1 C), 123.4-123.3 (d, *J* = 3.8 Hz, 1 C), 115.0, 114.5, 114.2, 107.5, 62.0, 34.5, 32.3, 23.6; HRMS calcd for $C_{16}H_{16}F_3N_2O$ $[M+H]^+$ 309.1209; found: 309.1199.



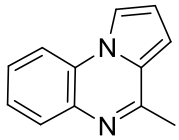
2-(pyrrolo[1,2-*a*]quinoxalin-4-yloxy)ethanol (3ae)

Colorless oil (30.9 mg, 45% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 8.04-8.02 (m, 1 H), 7.97-7.96 (m, 1 H), 7.87-7.85 (m, 1 H), 7.56-7.52 (m, 1 H), 7.46-7.26 (m, 1 H), 7.12-7.11 (m, 1 H), 6.91-6.89 (m, 1 H), 6.11 (s, 1 H), 4.35-4.27 (m, 2H), 4.22-4.14 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 151.5, 135.2, 130.6, 128.2, 127.8, 125.2, 123.7, 114.4, 114.0, 113.6, 107.4, 103.4, 65.6; HRMS calcd for $C_{16}H_{14}BN_2$ $[M+H]^+$ 229.0972; found: 229.0980.



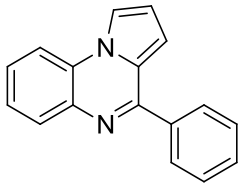
3-(pyrrolo[1,2-*a*]quinoxalin-4-yl)propane-1-thiol (3ag)

Colorless oil (32.1 mg, 44% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.88 (s, 2 H), 7.82-7.79 (d, *J* = 7.5 Hz, 1 H), 7.46-7.40 (m, 2 H), 6.92-6.82 (m, 2 H), 3.14-3.10 (m, 2H), 2.89-2.84 (m, 2 H), 2.37-2.30 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 156.1, 135.8, 129.4, 127.2, 126.9, 125.9, 125.0, 114.2, 113.6, 113.5, 106.2, 38.5, 33.9, 27.4; HRMS calcd for $C_{16}H_{14}BN_2$ $[M+H]^+$ 243.0951; found: 243.0945.



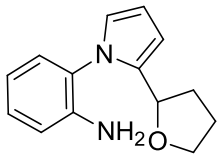
4-methylpyrrolo[1,2-*a*]quinoxaline (4)

Light yellow solid (36.0 mg, 66% yield), melting point: 132-133 °C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.91-7.88 (m, 2 H), 7.82-7.78 (m, 1 H), 7.46-7.41 (m, 2 H), 6.88-6.82 (m, 2 H), 2.72 (s, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 153.6, 135.9, 129.2, 127.3, 126.8, 126.2, 125.1, 114.2, 113.6, 113.4, 106.4, 22.0; HRMS calcd for $C_{12}H_{11}N_2$ $[M+H]^+$ 183.0917; found: 183.0910.



4-phenylpyrrolo[1,2-*a*]quinoxaline (5)

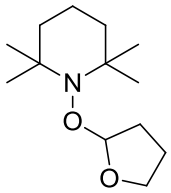
Light yellow solid (42.4 mg, 58% yield), melting point: 99-100 °C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 8.05-7.97 (m, 4 H), 7.96-7.84 (m, 1 H), 7.55-7.42 (m, 5 H), 6.99-6.97 (m, 1 H), 6.89-6.86 (m, 1 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 154.4, 138.5, 136.2, 130.2, 129.7, 128.6, 127.4, 127.1, 125.4, 125.2, 114.5, 113.9, 113.6, 108.6; HRMS calcd for $C_{17}H_{13}N_2$ $[M+H]^+$ 245.1073; found: 245.1080.



2-(2-(tetrahydrofuran-2-yl)-1*H*-pyrrol-1-yl)aniline (6)

White solid (20.5 mg, 30% yield), melting point: 88-90 °C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.28-7.25 (m, 1 H), 7.14-7.13 (m, 1 H), 6.96-6.91 (m, 1 H), 6.82-6.76 (m, 1 H), 6.73-6.70 (m, 1 H), 6.30-6.29 (m, 1 H), 5.98-5.97(m, 1 H), 4.51-4.47 (m, 1 H), 3.68-3.64 (m, 2 H), 1.95-1.84 (m, 2 H), 1.82-1.69 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 135.7, 129.3, 125.4, 124.6, 119.0, 115.4, 114.6,

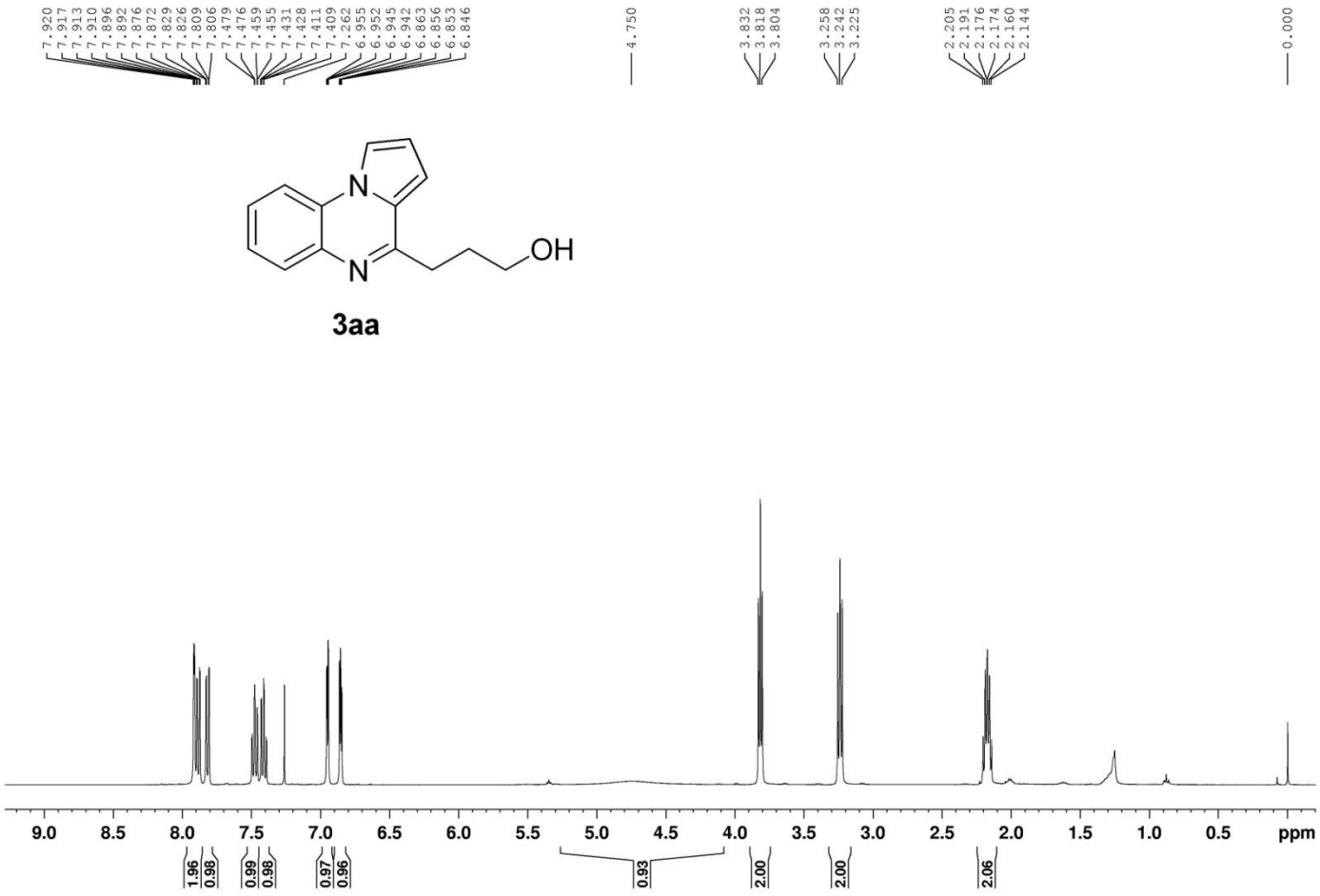
114.1, 109.9, 104.0, 62.7, 50.8, 31.9, 28.5; HRMS calcd for $C_{14}H_{17}N_2O$ $[M+H]^+$ 229.1336; found: 229.1333.



2,2,6,6-tetramethyl-1-((tetrahydrofuran-2-yl)oxy)piperidine (S) [3]

Colorless oil (32.7 mg, 48% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 5.37-5.34 (m, 1 H), 3.91-3.78 (m, 2 H), 2.04-1.88 (m, 3 H), 1.83-1.74 (m, 1 H), 1.60-1.42 (m, 5 H), 1.33-1.31 (m, 1 H), 1.22 (s, 3 H), 1.11 (s, 3 H), 1.07 (s, 3 H), 1.04 (s, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 109.5, 66.6, 60.1, 58.5, 40.0, 39.6, 33.8, 33.3, 31.2, 23.9, 20.4, 20.0, 17.2.

[1] C.-X. Xie, L. Feng, W.-L. Li, X.-J. Ma, X.-K. Ma, Y.-H. Liu, and C. Ma. *Org. Biomol. Chem*., 2016, **14**, 8529.
[2] Z.-Y. Zhang, C.-X. Xie, X.-C. Tan, G.-L. Song, L.-L. Wen, H. G, and C. Ma, *Org. Chem. Front.*, 2015, **2**, 942.
[3] (a) D. Liu, C. Liu, H. Li, and A. Lei, *Chem. Commun.*, 2014, **50**, 3623; (b) S. Pan, J. Liu, H. Li, Z. Wang, X. Guo and Z. Li, *Org. Lett.*, 2010, **12**, 1932.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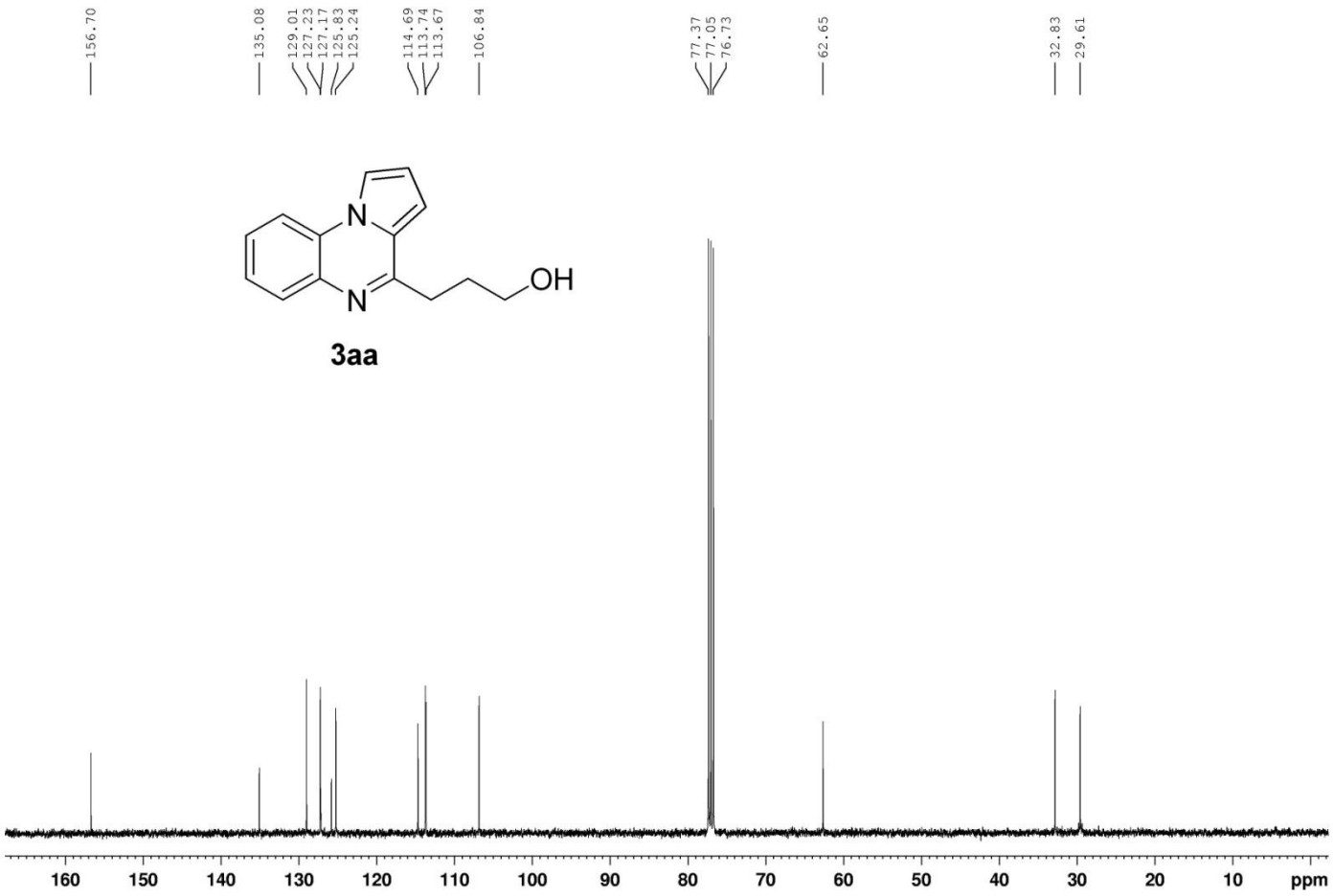
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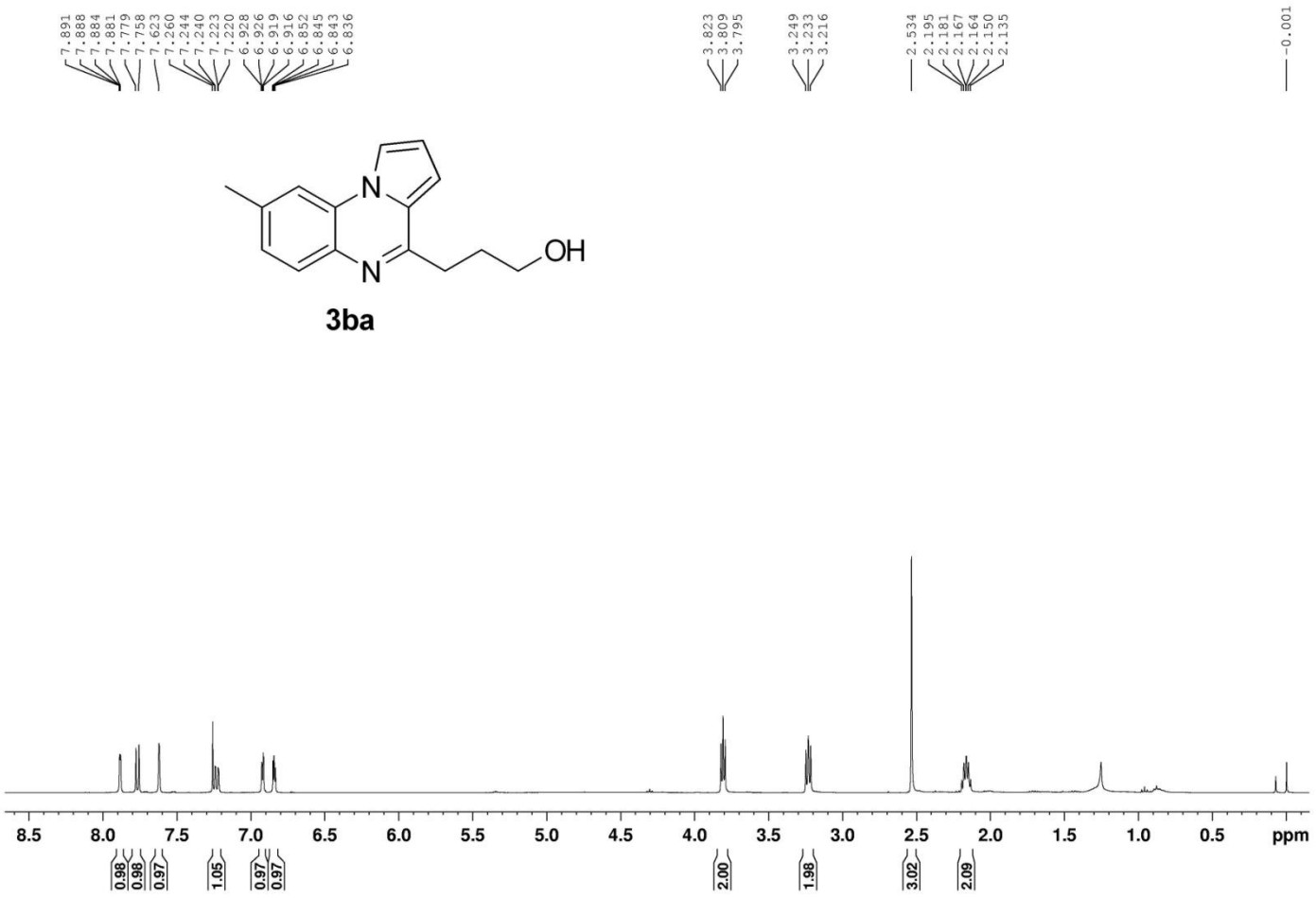
ppm

3aa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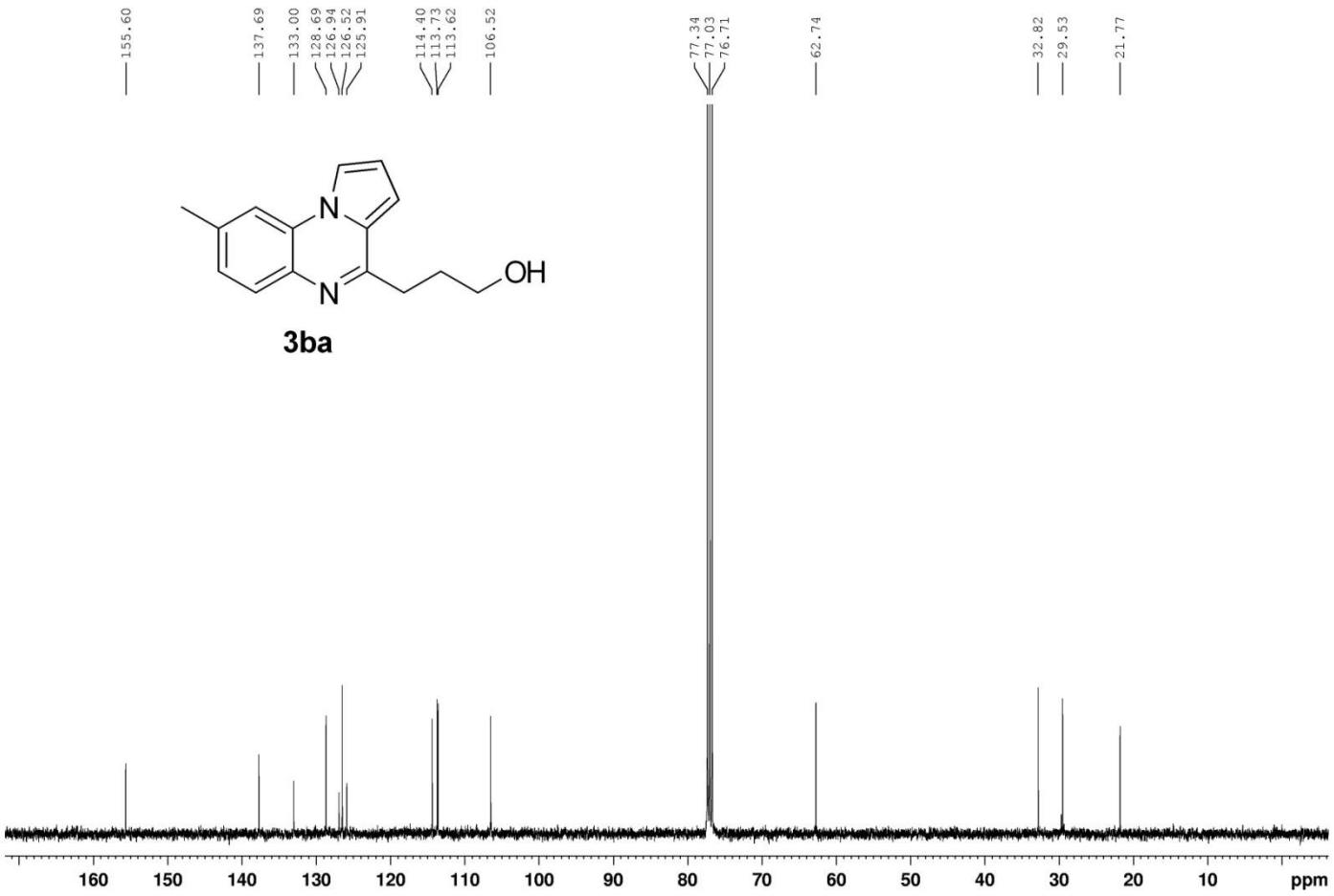
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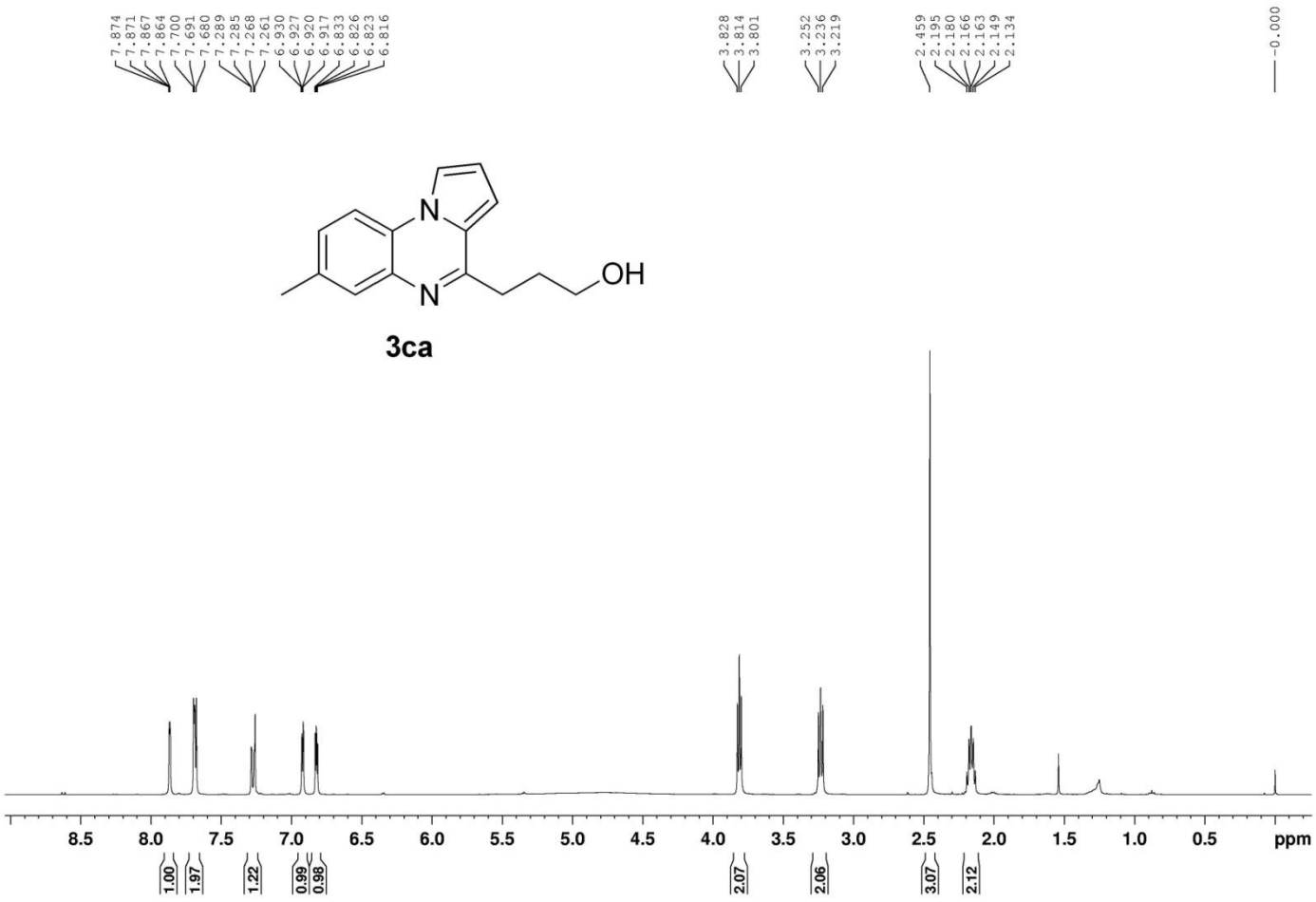
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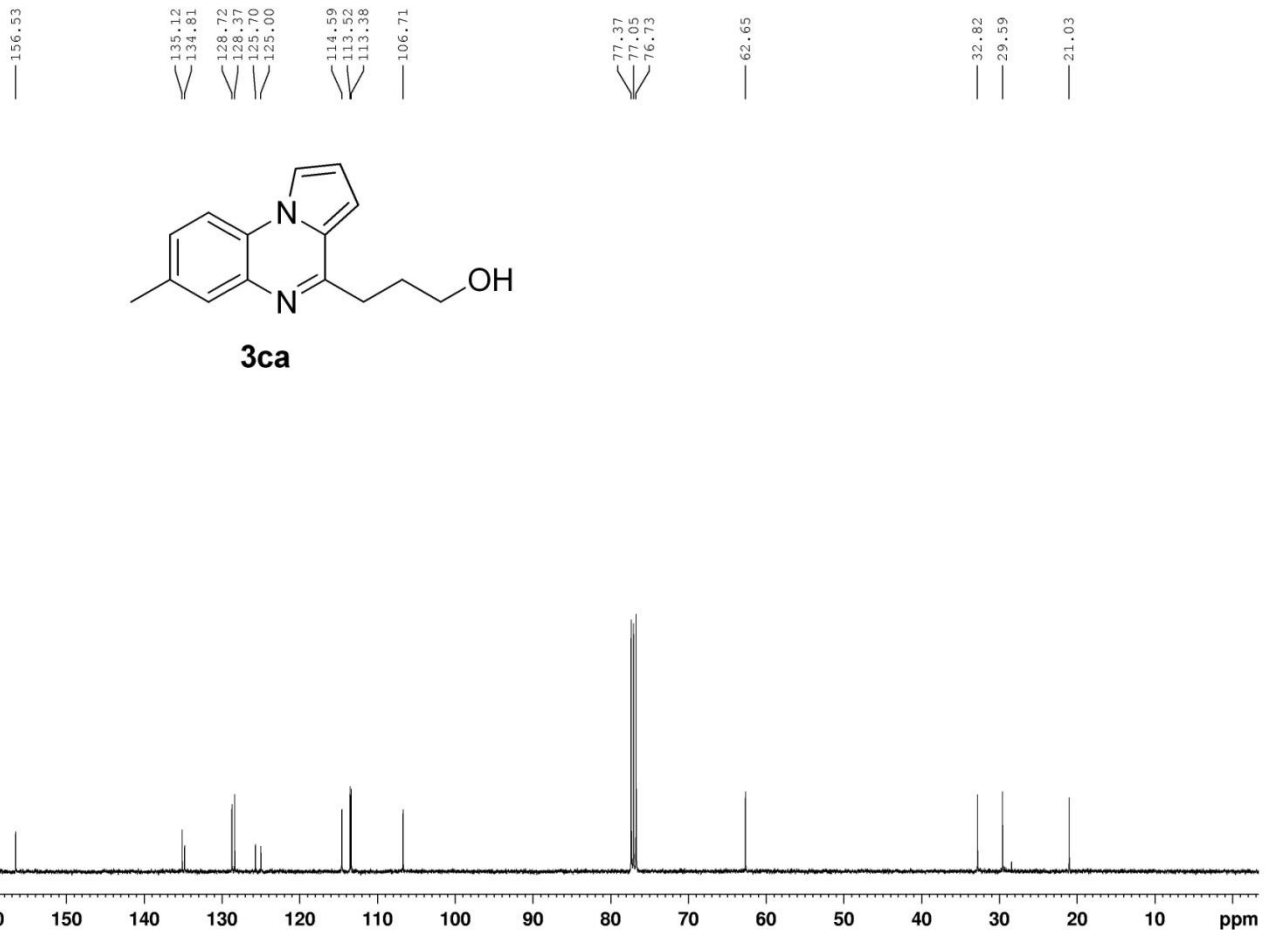
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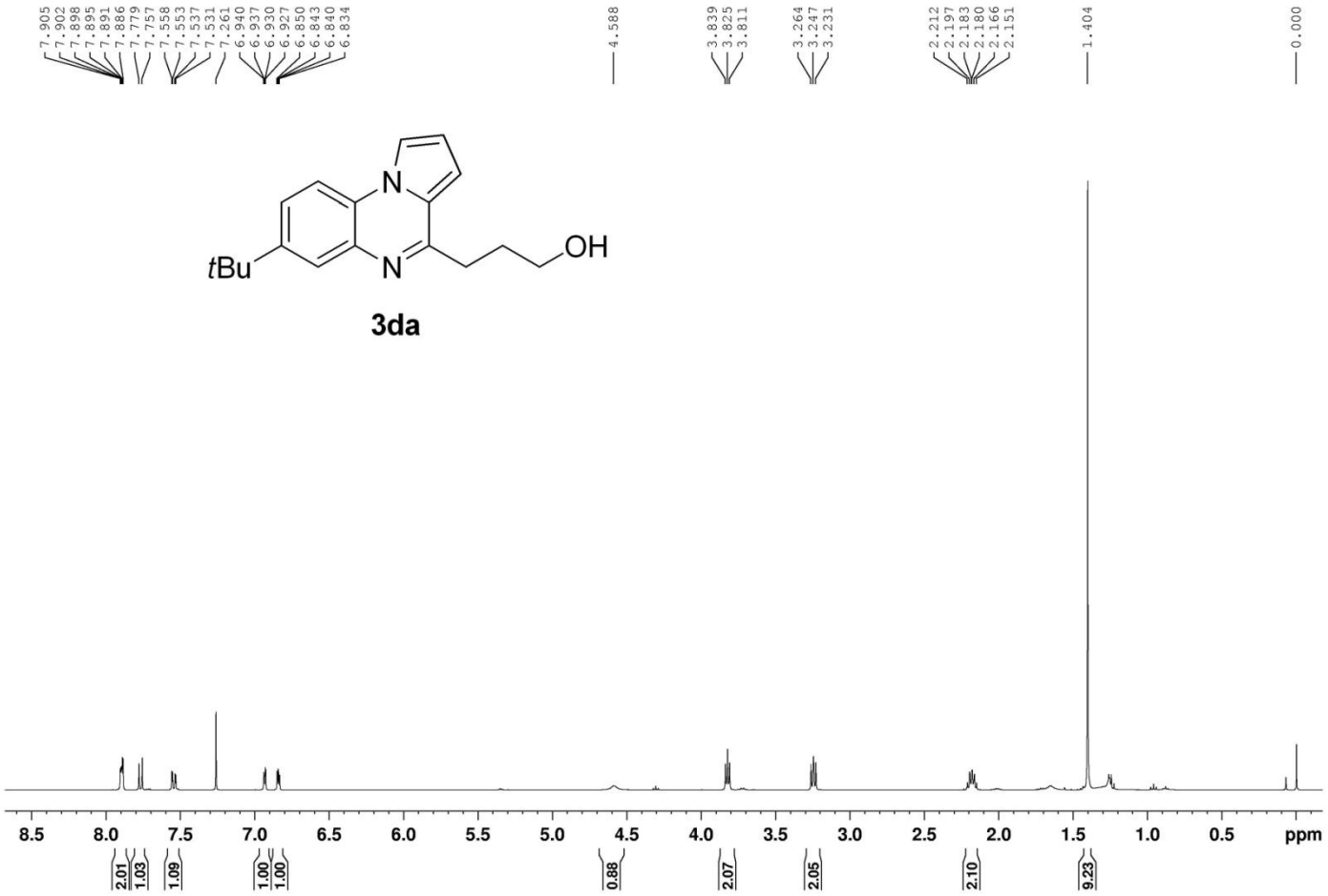
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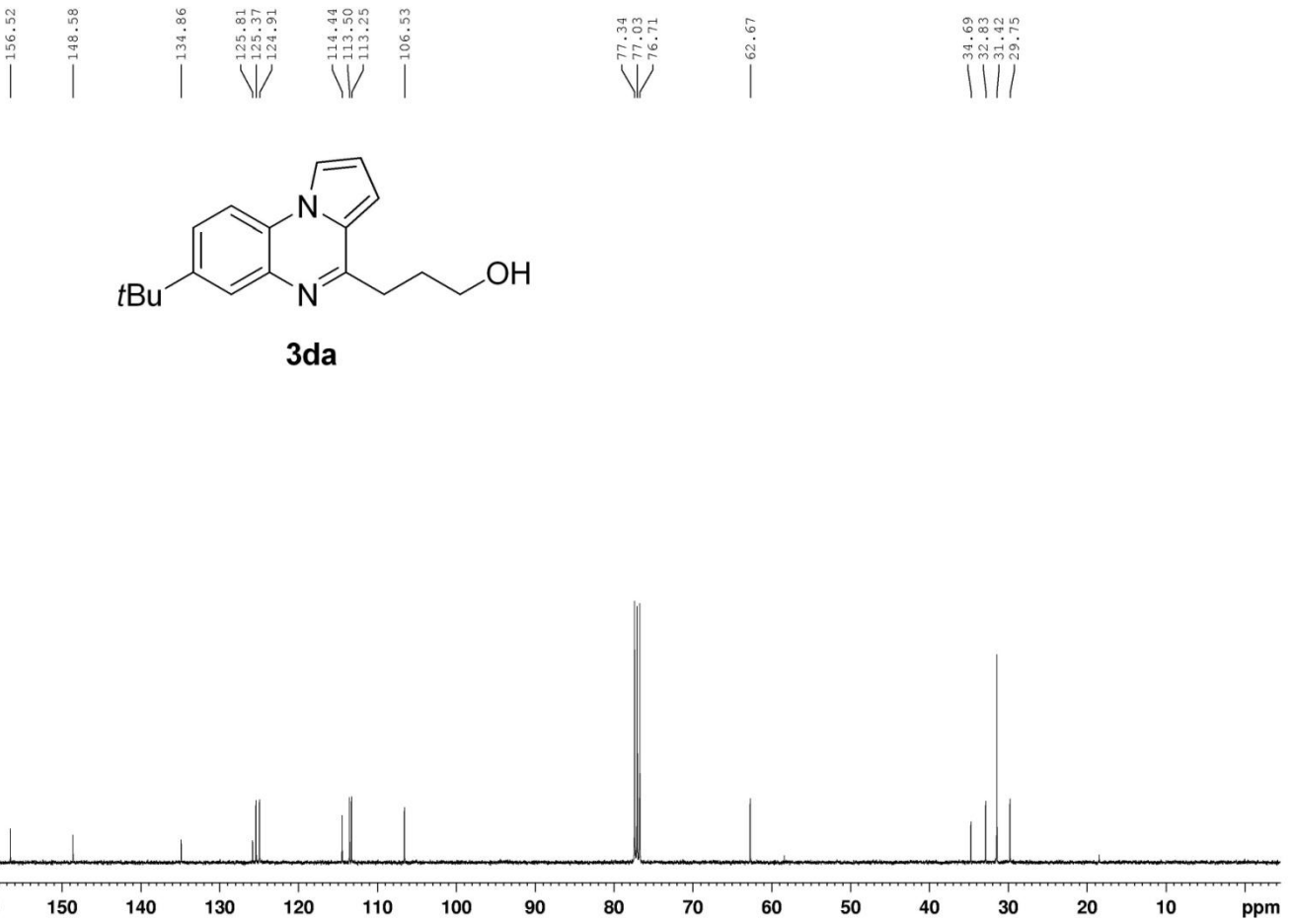
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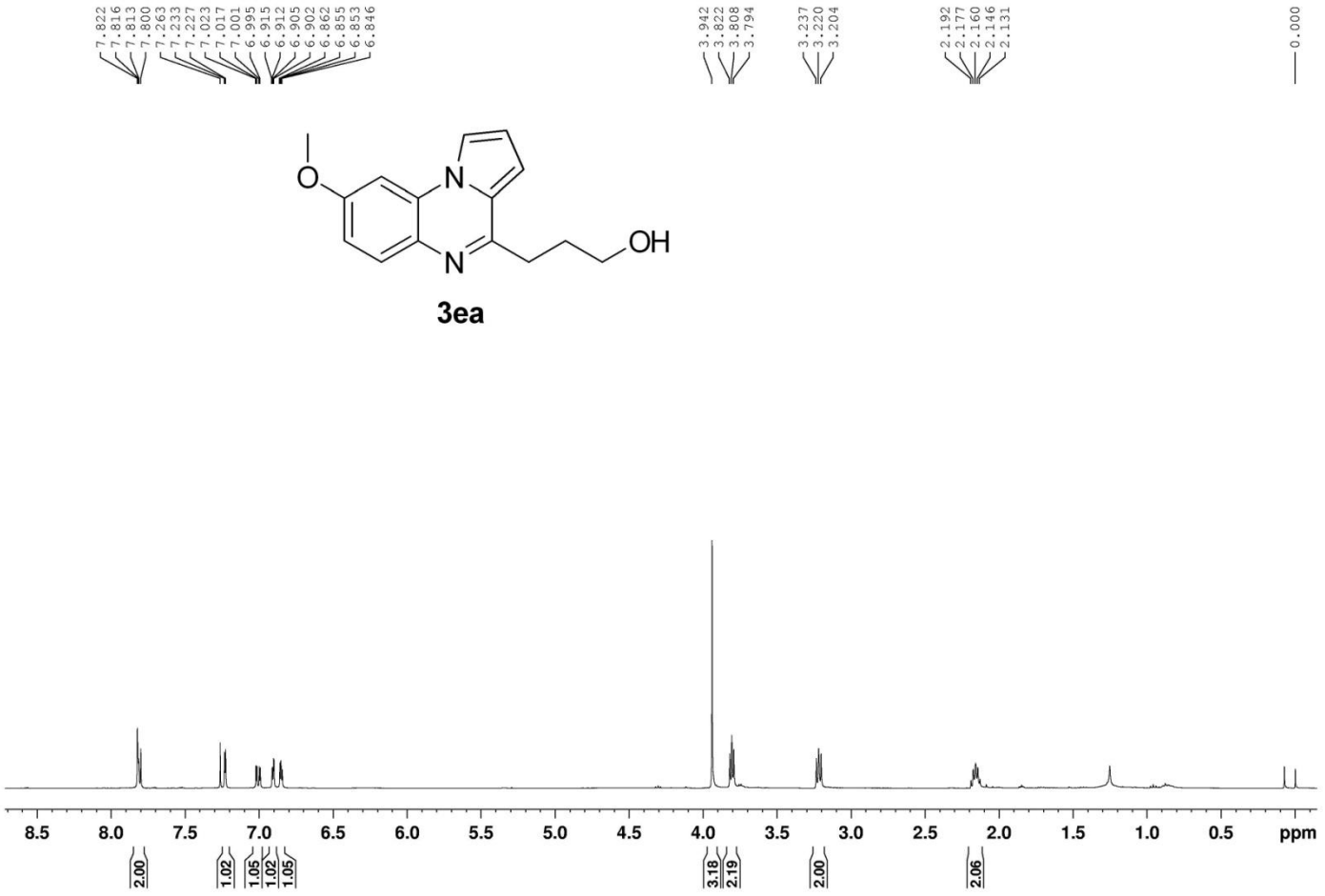
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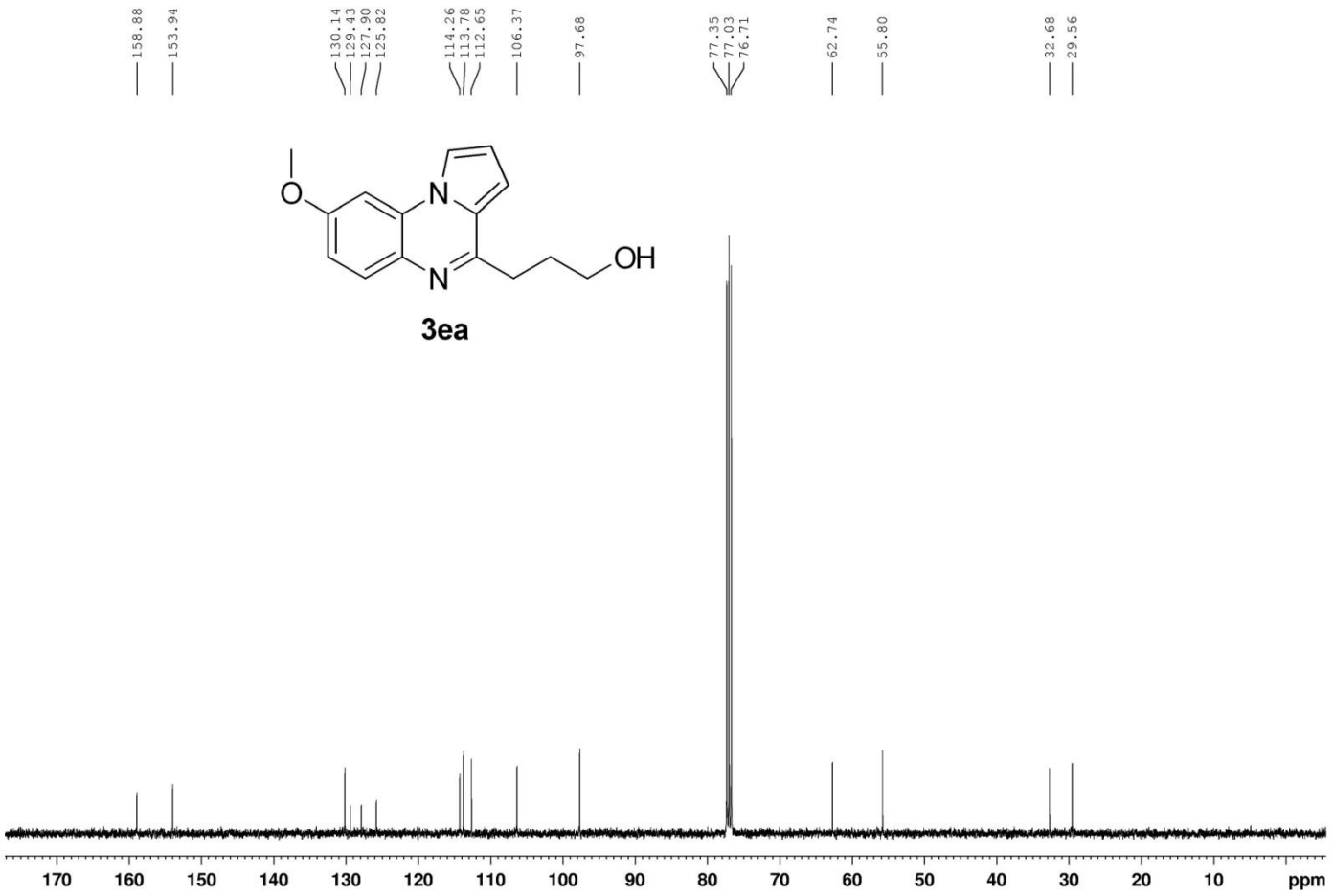
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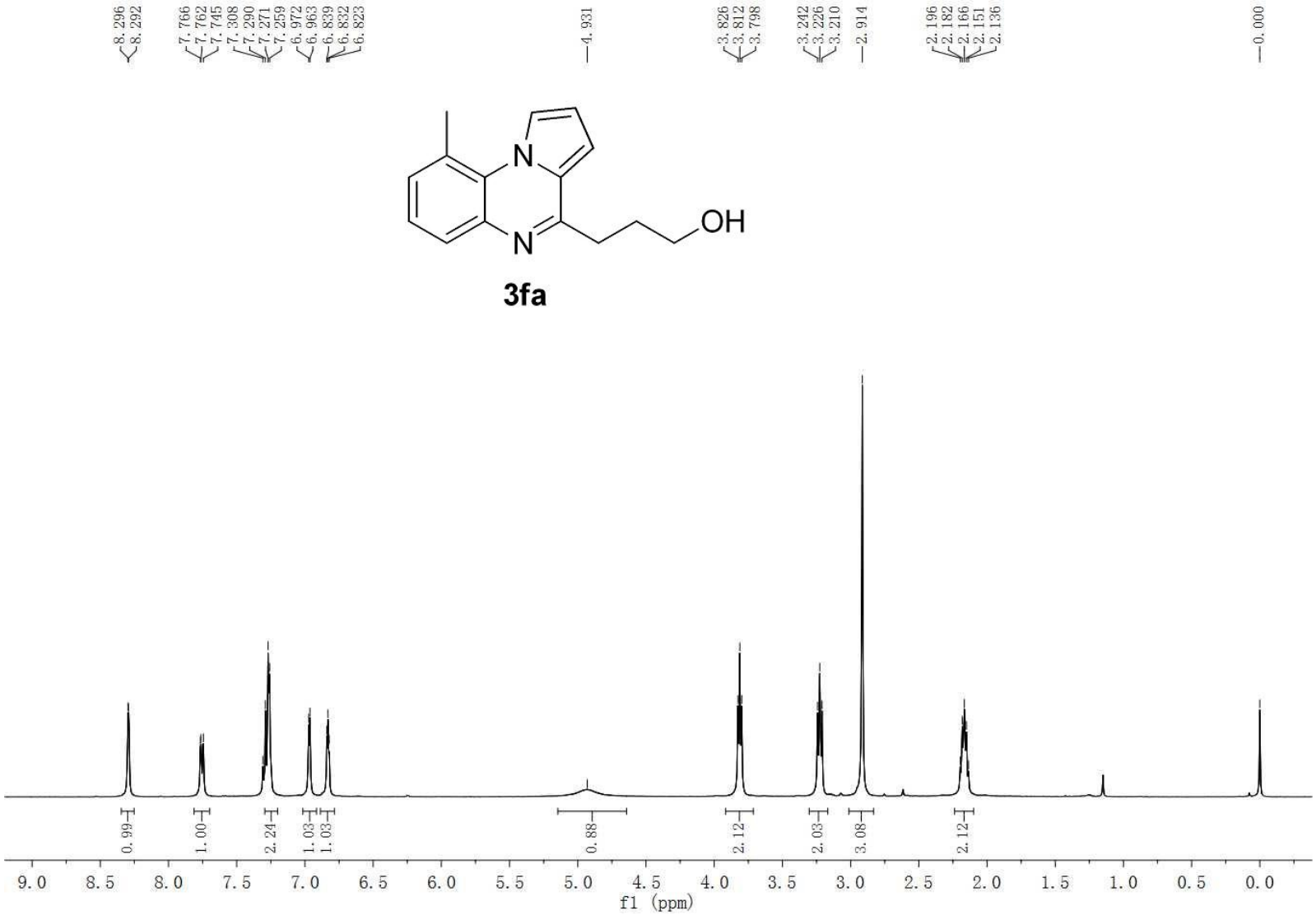
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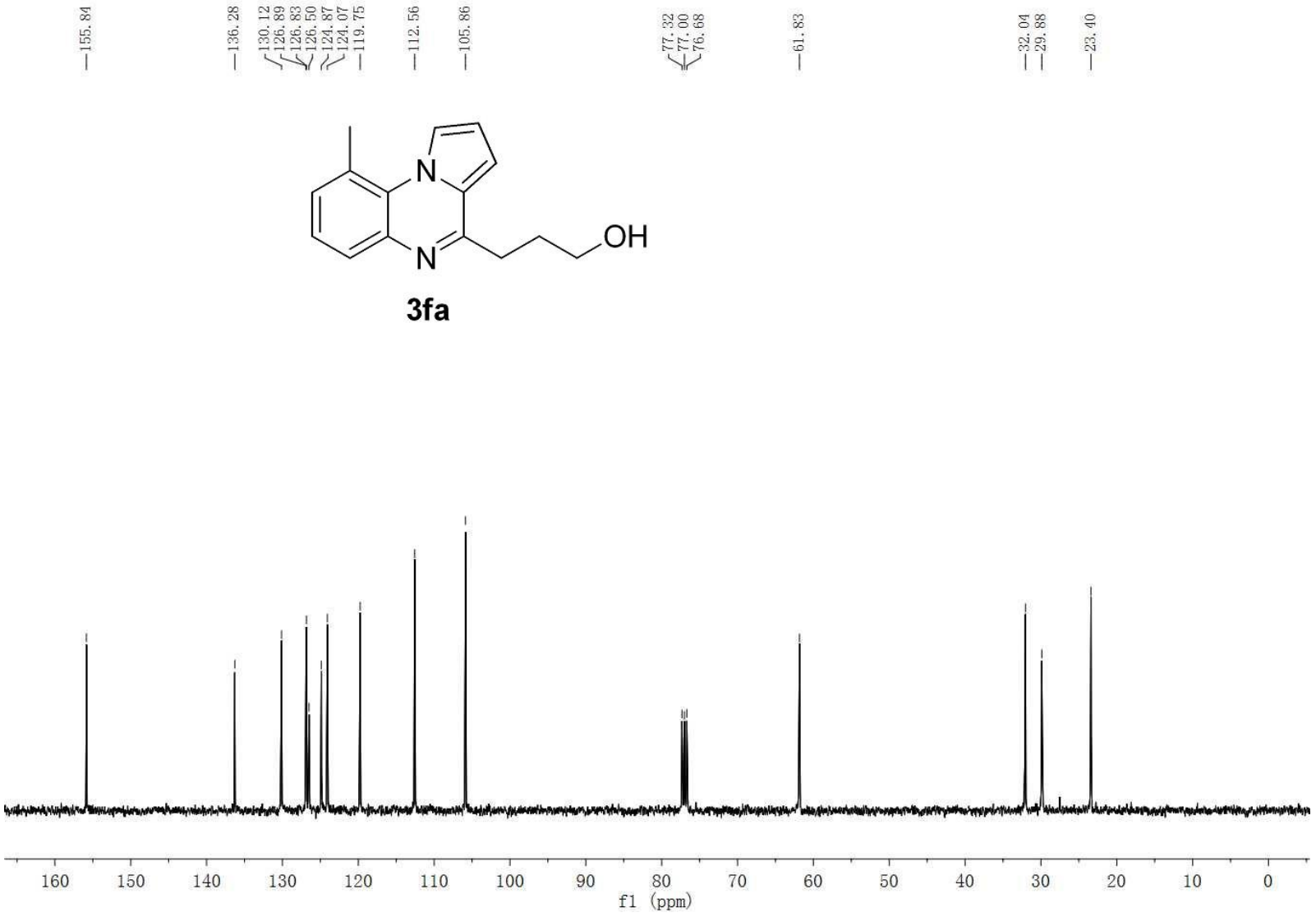
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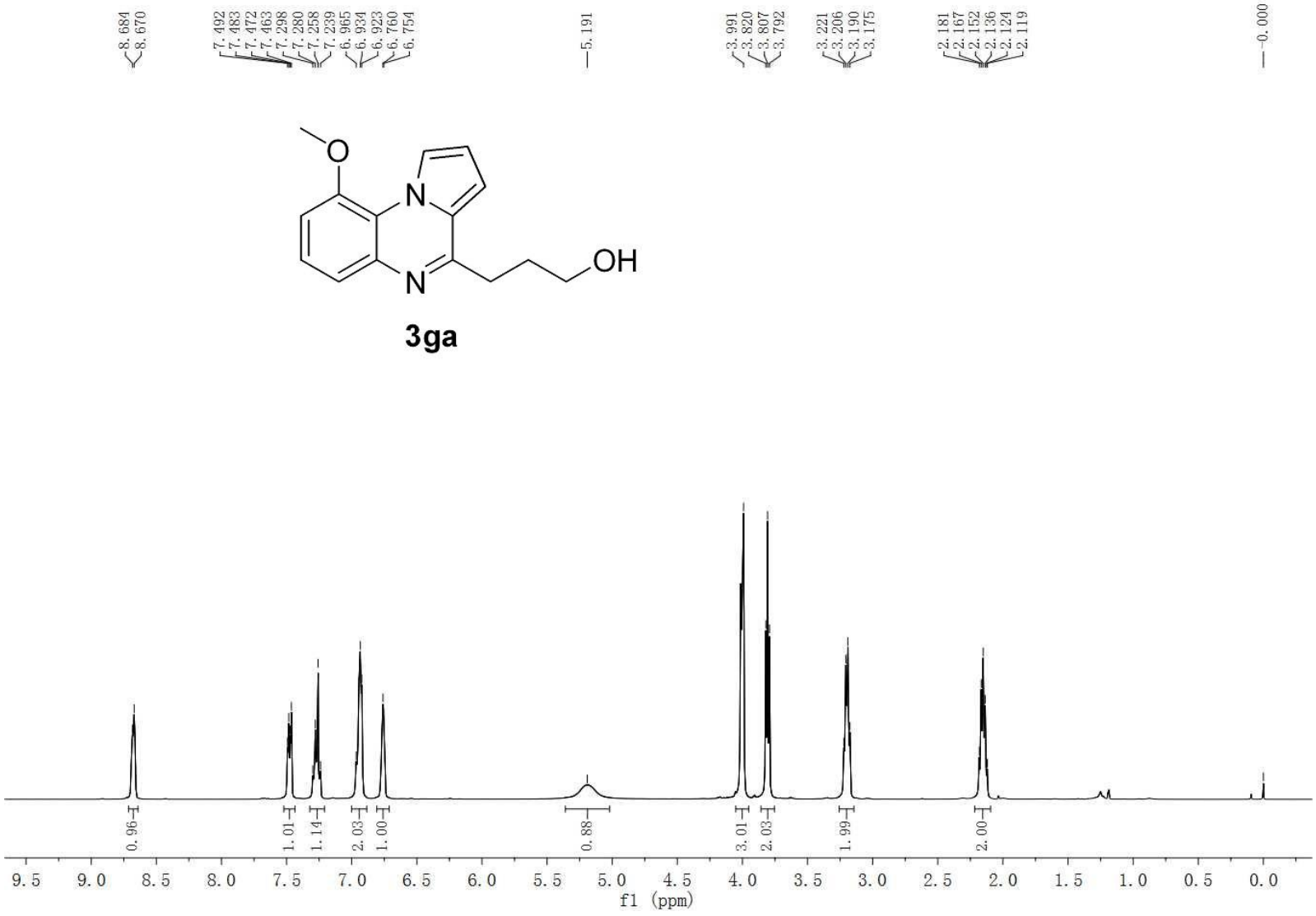
3fa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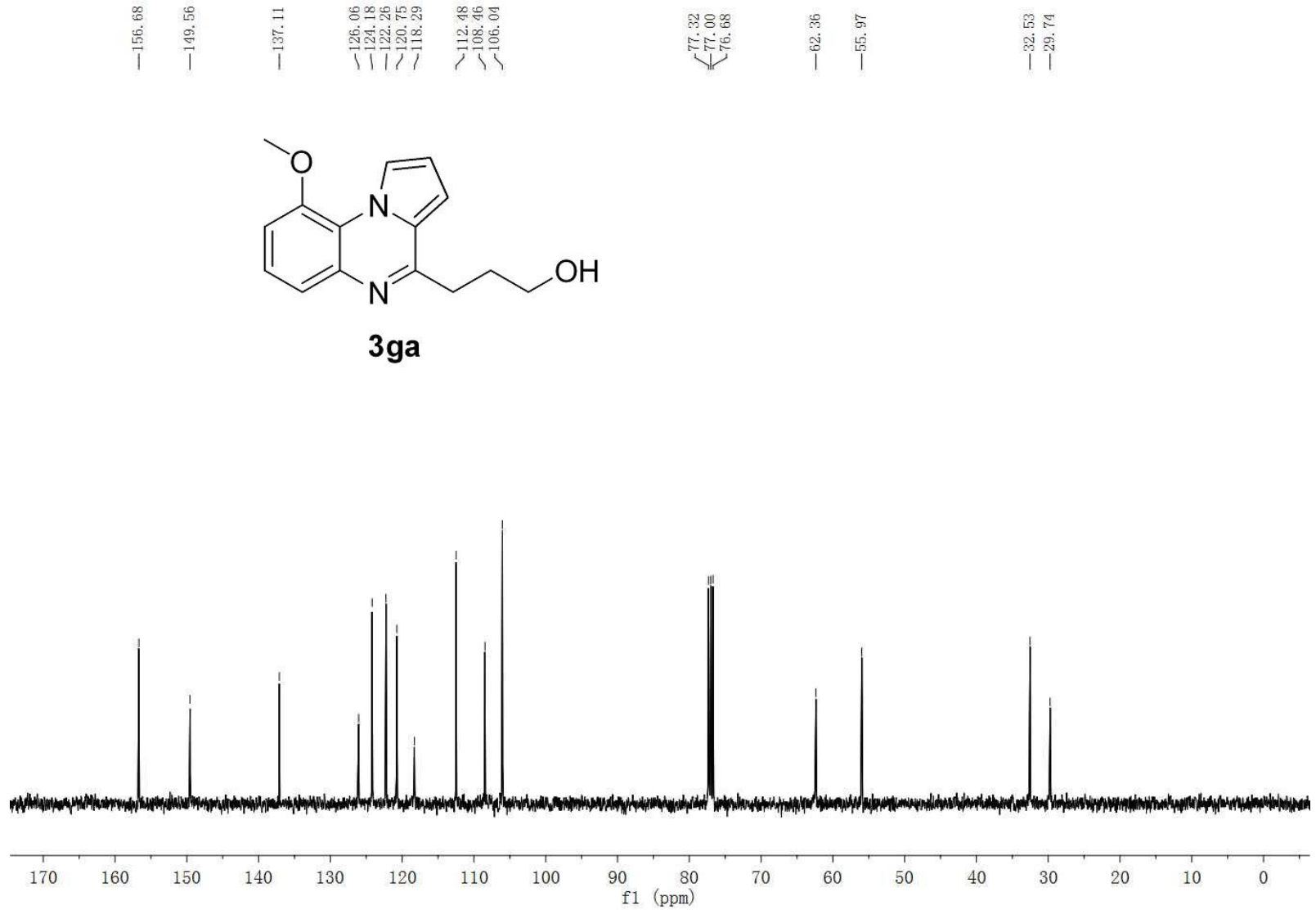
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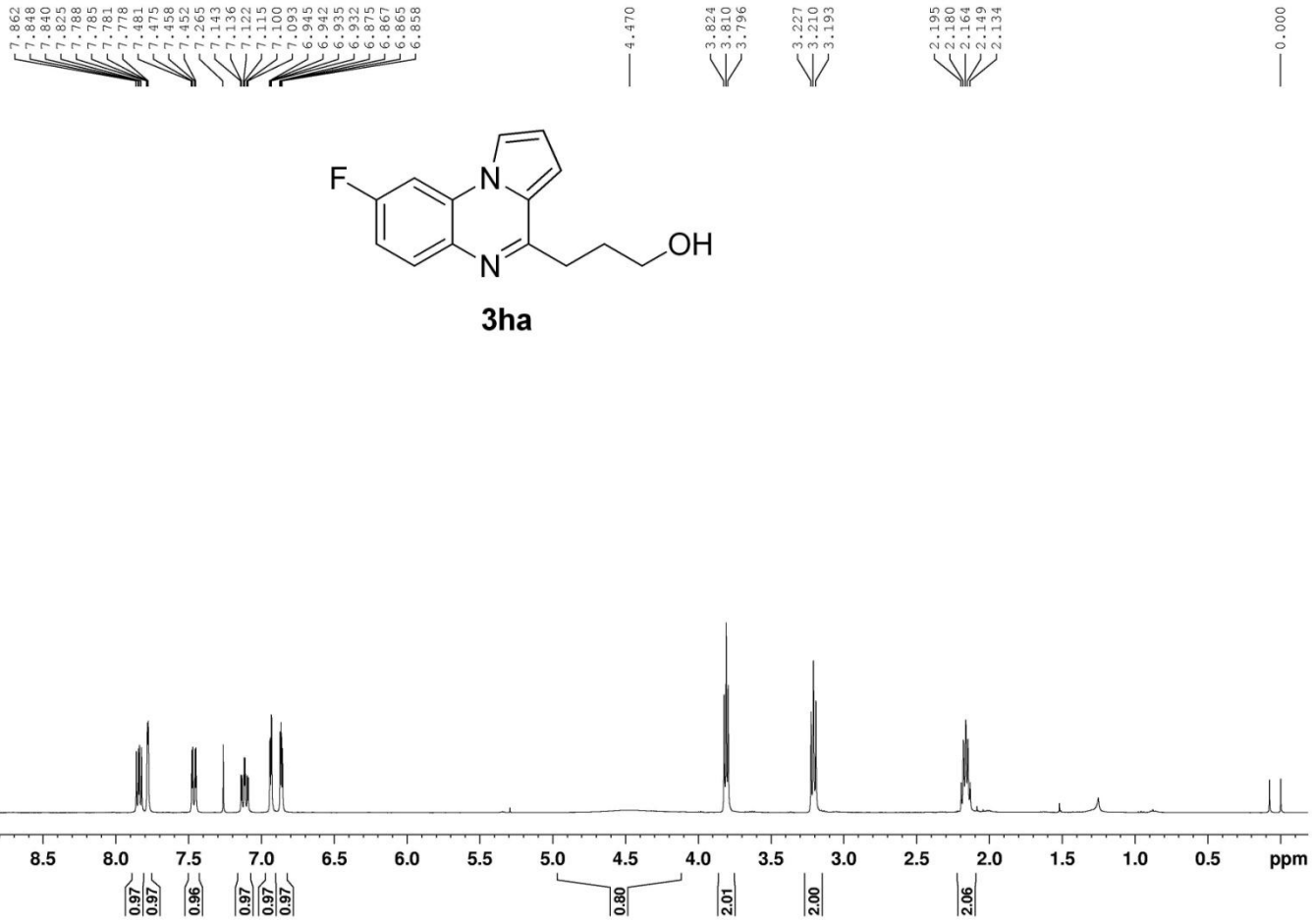
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2.164
2.149
2.134
0.000
F
N
N
OH
3ha
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
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0.97
0.96
0.97
0.97
0.97
0.80
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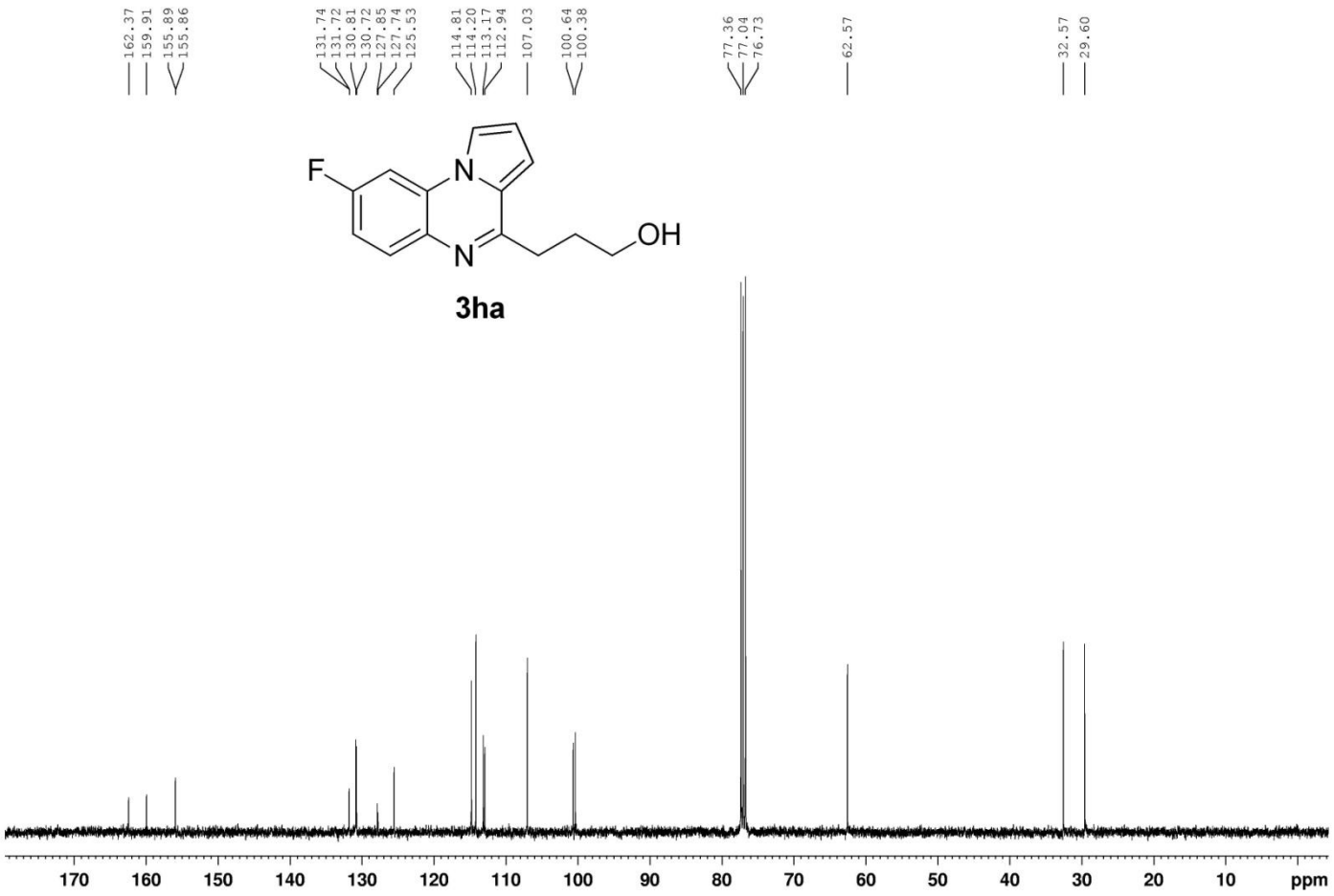
2.00
2.06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159.91
155.89
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131.74
131.72
130.81
130.72
127.85
127.74
125.53
114.81
114.20
113.17
112.94
107.03
100.64
100.38
77.36
77.04
76.73
62.57
32.57
29.60
F
N
N
OH
3ha
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.873
7.870
7.867
7.864
7.782
7.769
7.759
7.747
7.570
7.563
7.546
7.539
7.263
7.225
7.218
7.205
7.203
7.198
7.183
7.176
6.965
6.963
6.955
6.953
6.857
6.850
6.847
6.840
4.245
3.822
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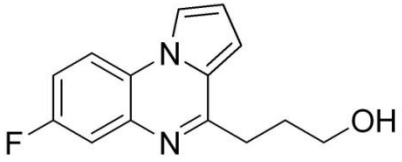
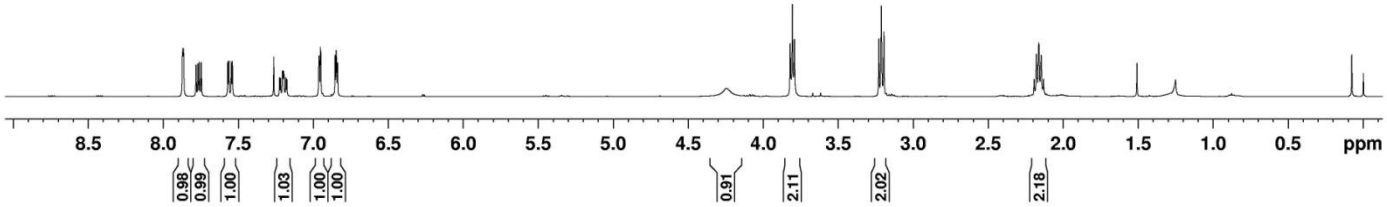
3.794
3.231
3.215
3.198
2.196
2.181
2.164
2.149
2.133
0.000


N
F
N
OH

3ia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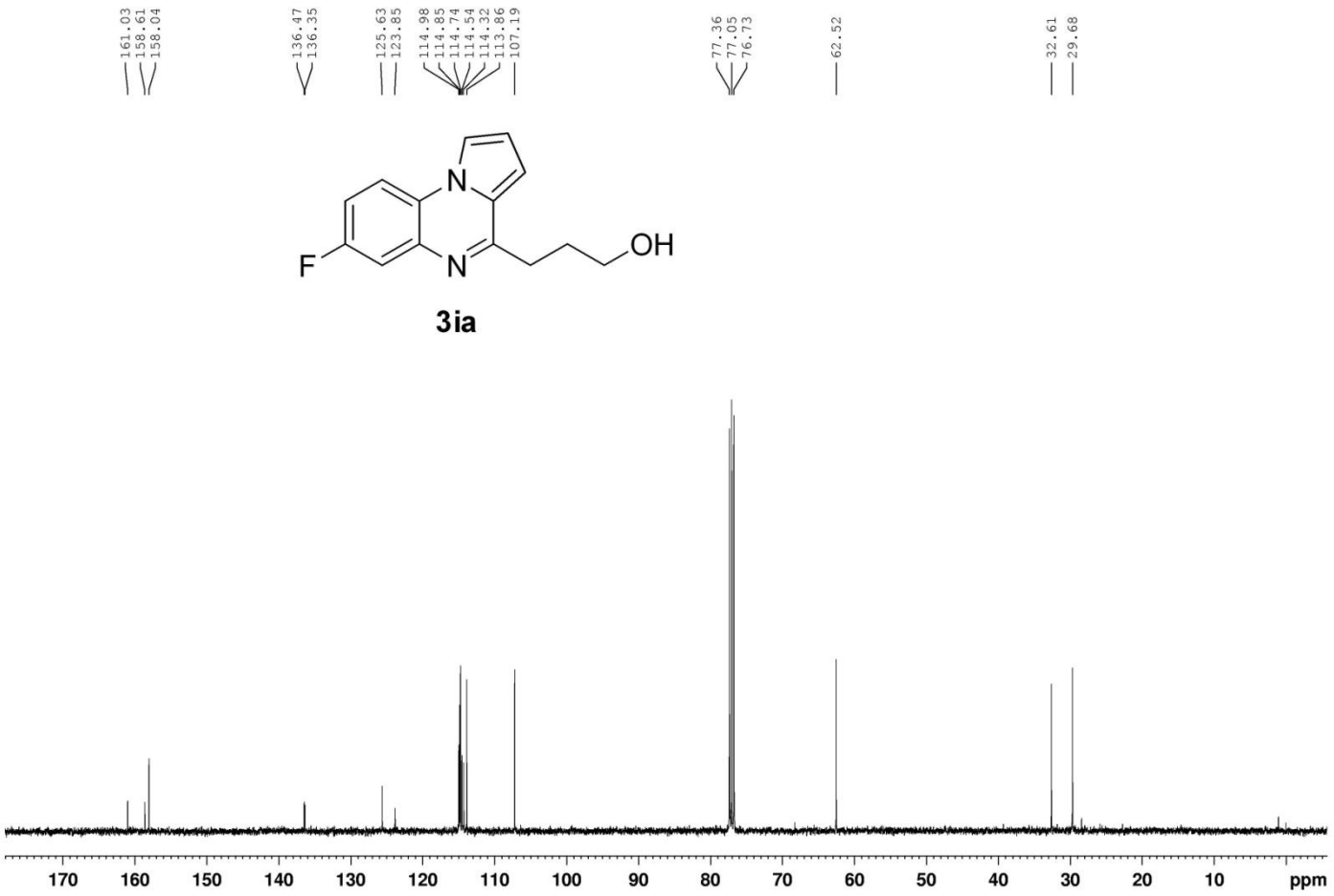
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
0.98
0.99
1.00
1.03
1.00
1.00
0.91
2.11
2.02
2.18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158.61
158.04
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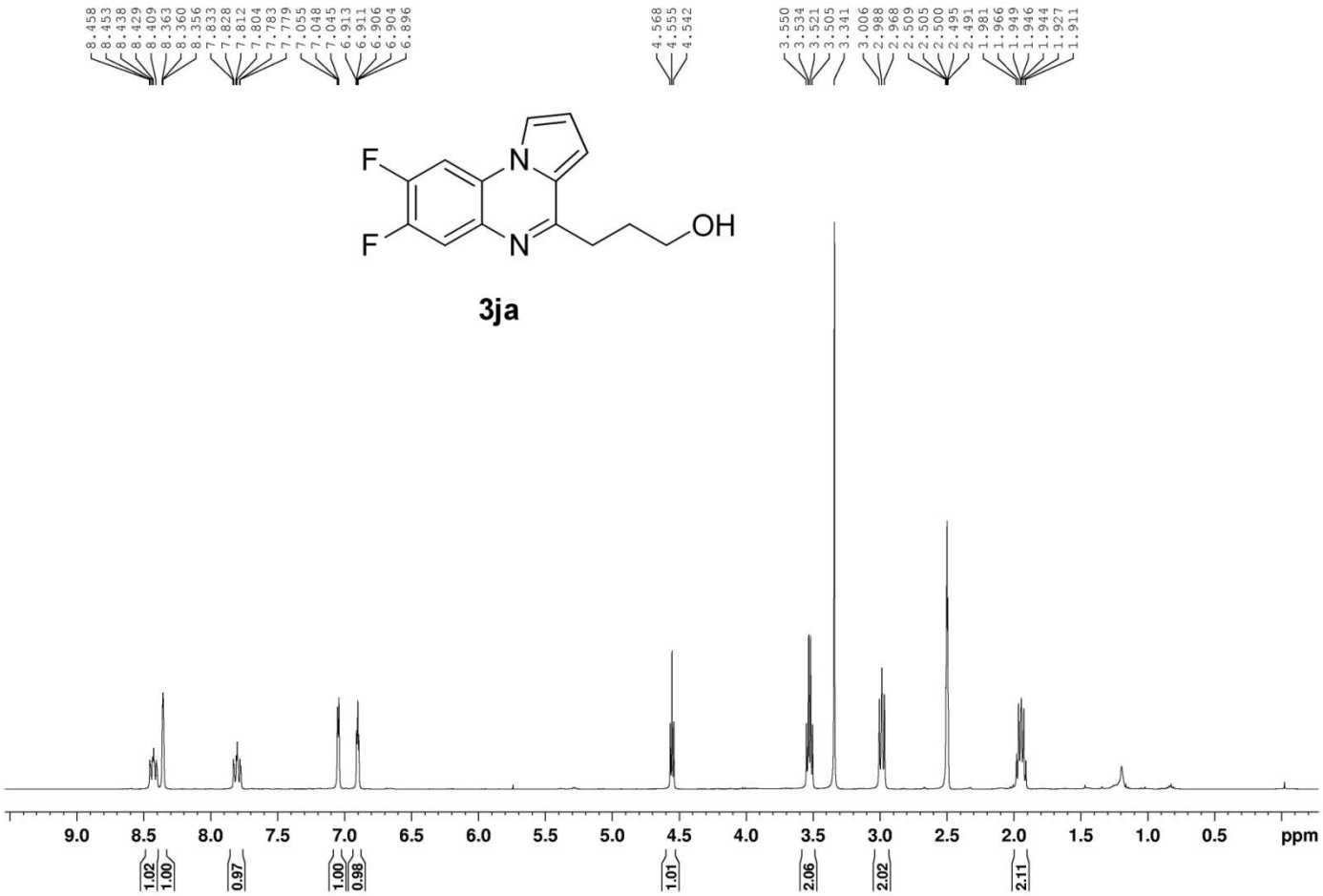
136.35
125.63
123.85
114.98
114.85
114.74
114.54
114.32
113.86
107.19
77.36
77.05
76.73
62.52
32.61
29.68
N
N
F
OH
3ia
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.453
8.438
8.429
8.409
8.363
8.360
8.356
7.833
7.828
7.812
7.804
7.783
7.779
7.055
7.048
7.045
6.913
6.911
6.906
6.904
6.896
4.568
4.555
4.542
3.550
3.534
3.521
3.505
3.341
3.006
2.988
2.968
2.509
2.505
2.500
2.495
2.491
1.981
1.966
1.949
1.946
1.944
1.927
1.911
F
F
N
N
OH
3ja
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
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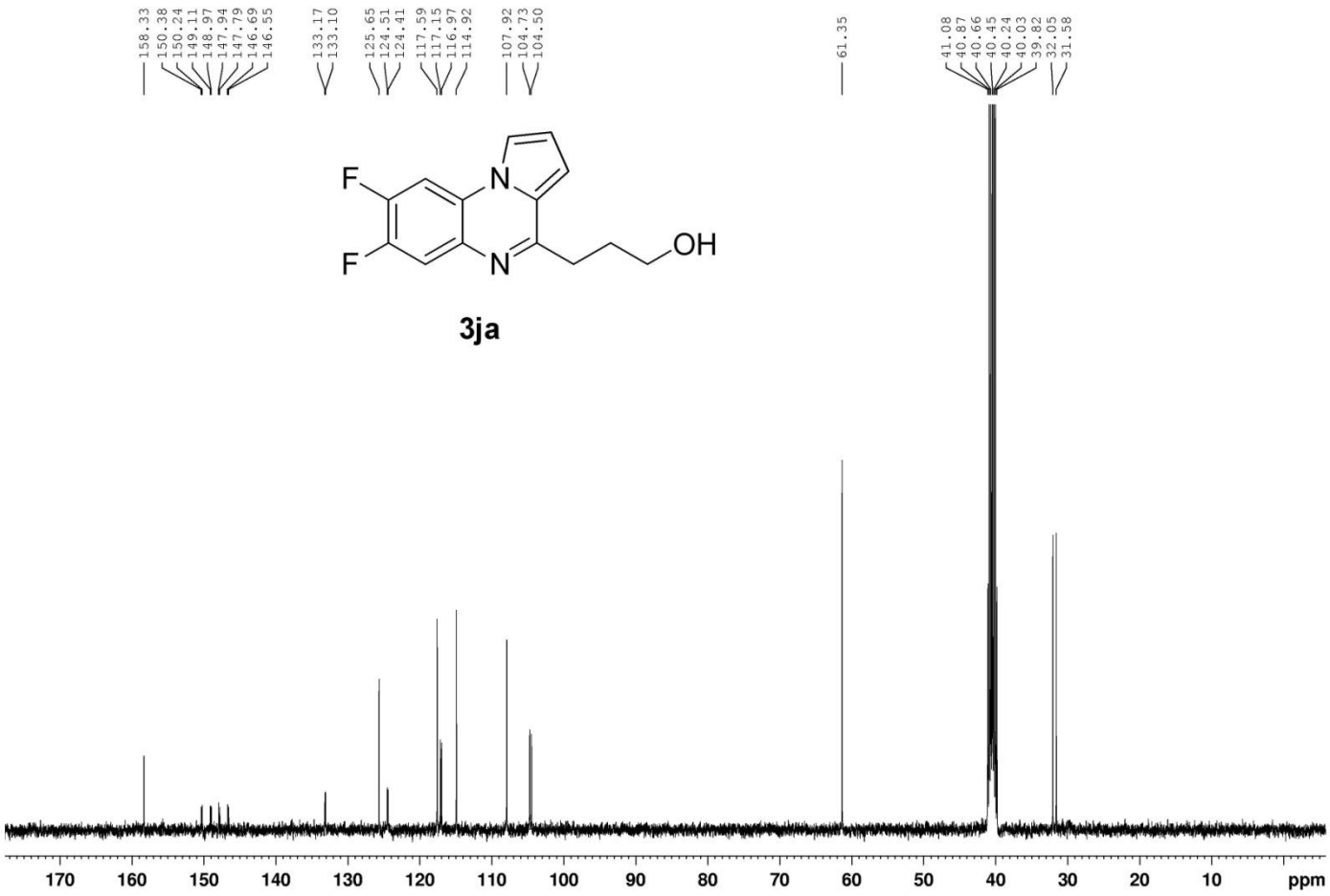
ppm
1.02
1.00
0.97
1.00
0.98
1.01
2.06
2.02
2.11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148.97
147.94
147.79
146.69
146.55
133.17
133.10
125.65
124.51
124.41
117.59
117.15
116.97
114.92
107.92
104.73
104.50
61.35
41.08
40.87
40.66
40.45
40.24
40.03
39.82
32.05
31.58
F
F
N
N
OH
3ja
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.811
7.808
7.804
7.801
7.616
7.613
7.595
7.592
7.407
7.403
7.387
7.384
7.281
7.274
7.261
7.241
6.913
6.910
6.903
6.899
6.814
6.807
6.804
6.797
5.032
3.838
3.825
3.812
3.240
3.224
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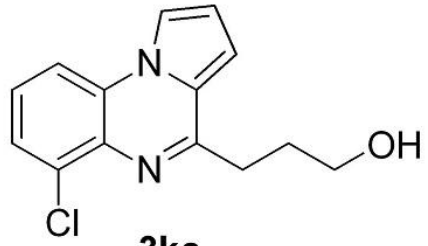
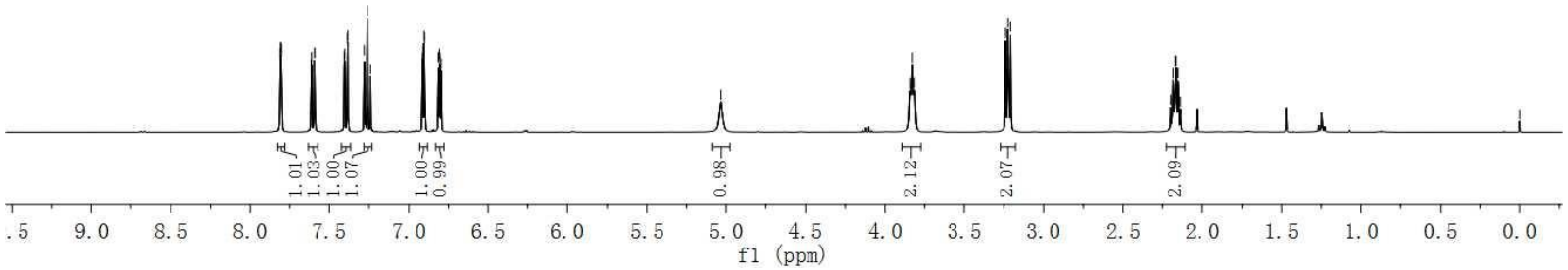
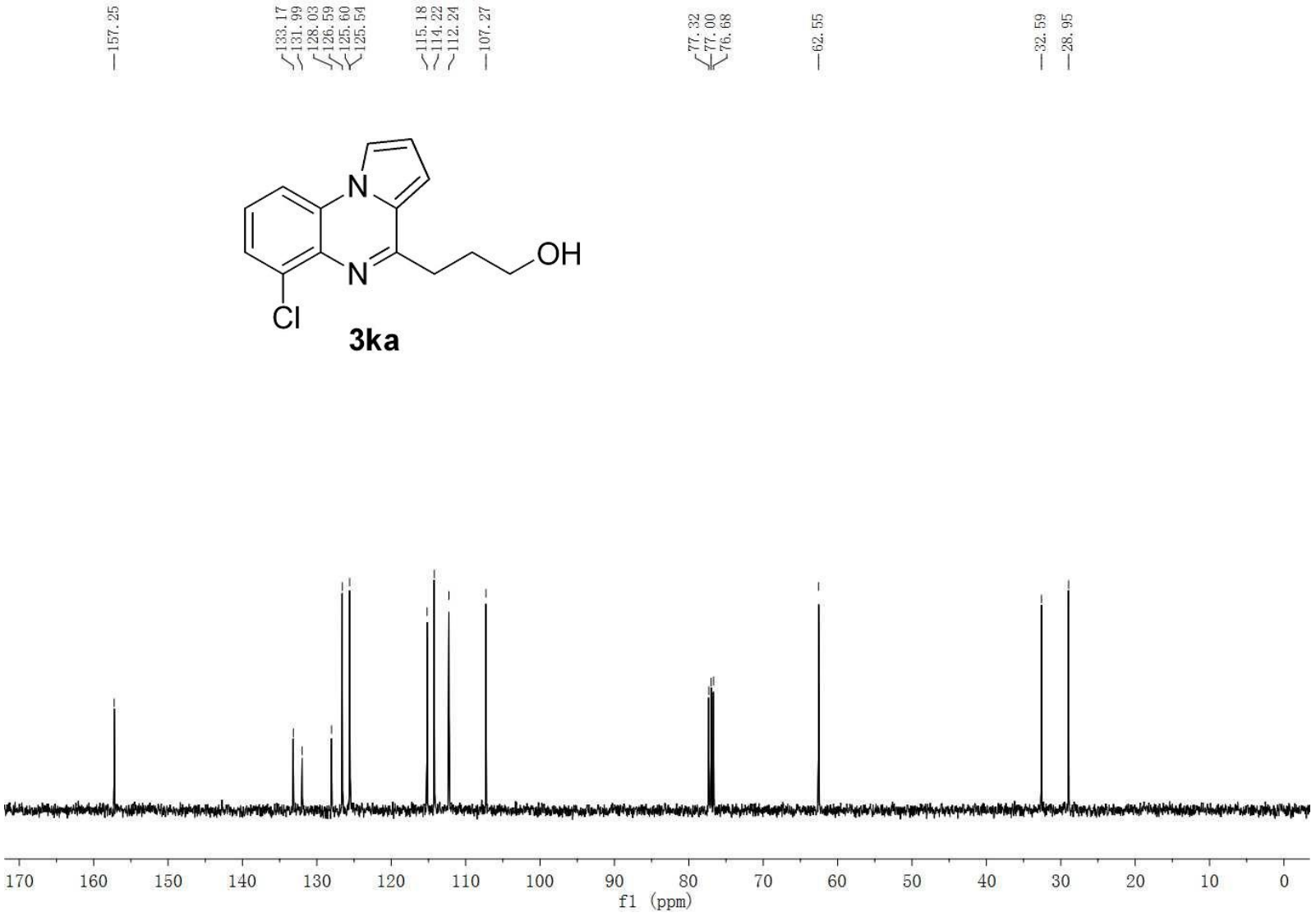
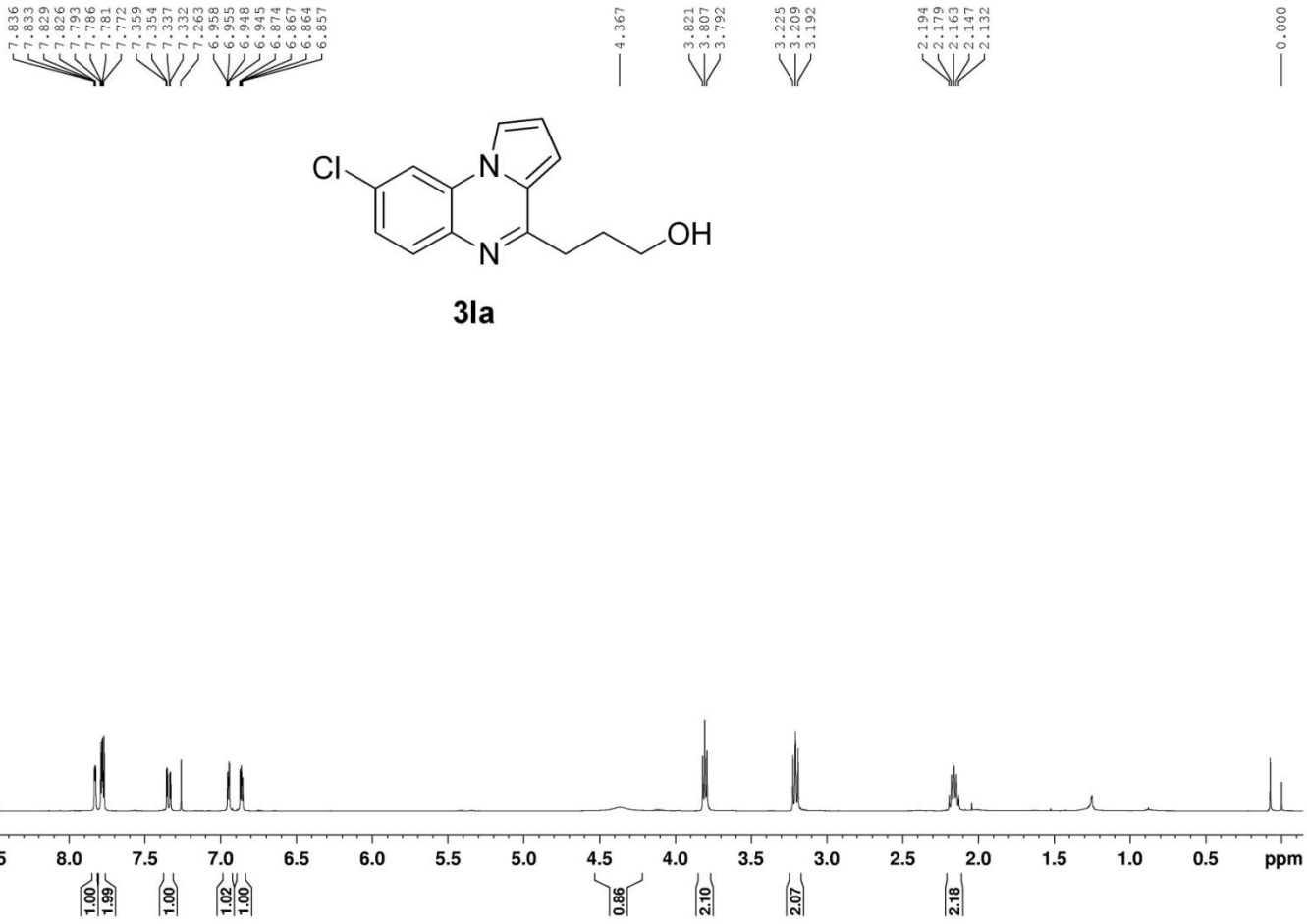
2.183
2.170
2.167
2.153
2.138
0.000

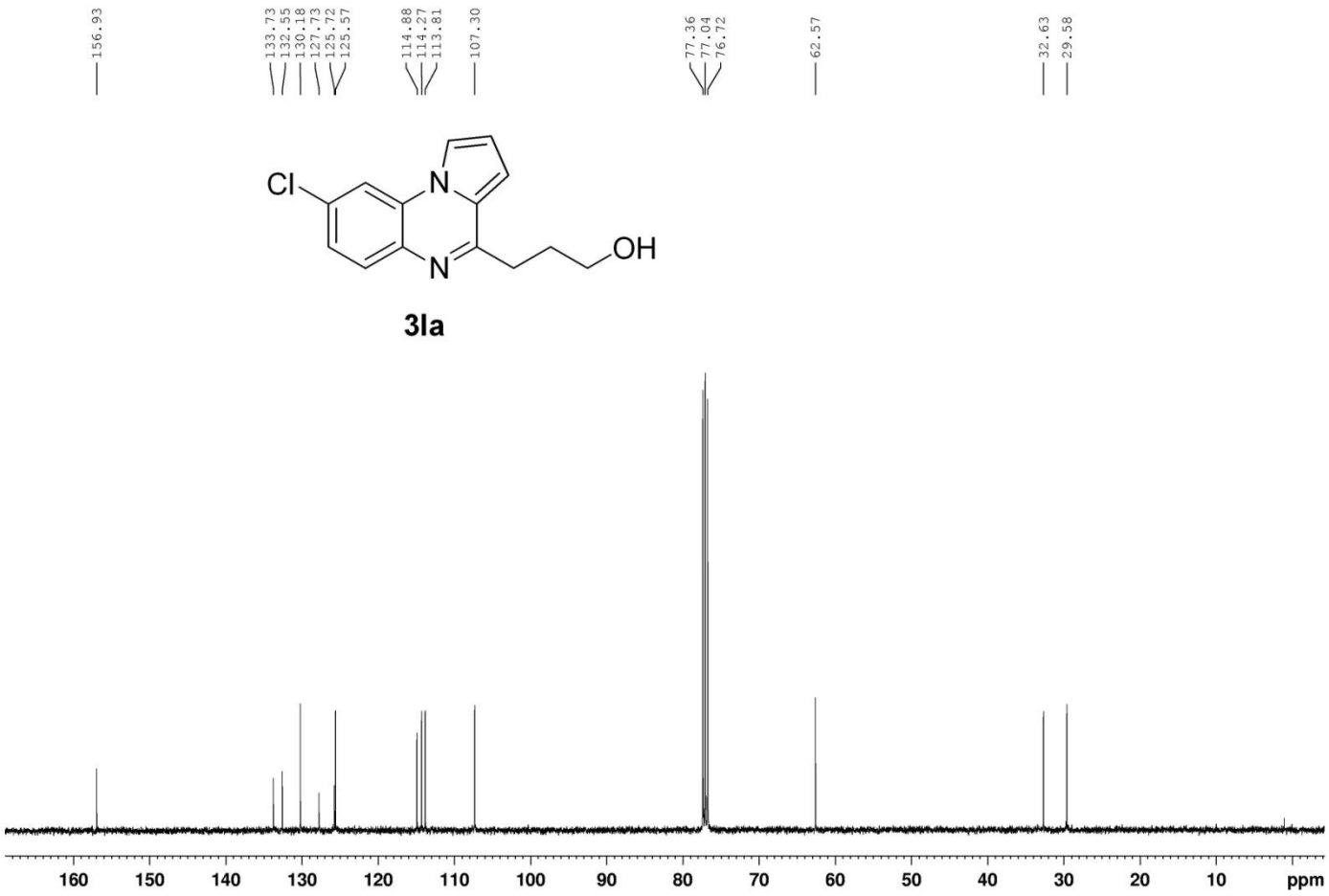

N
N
OH
Cl

3ka

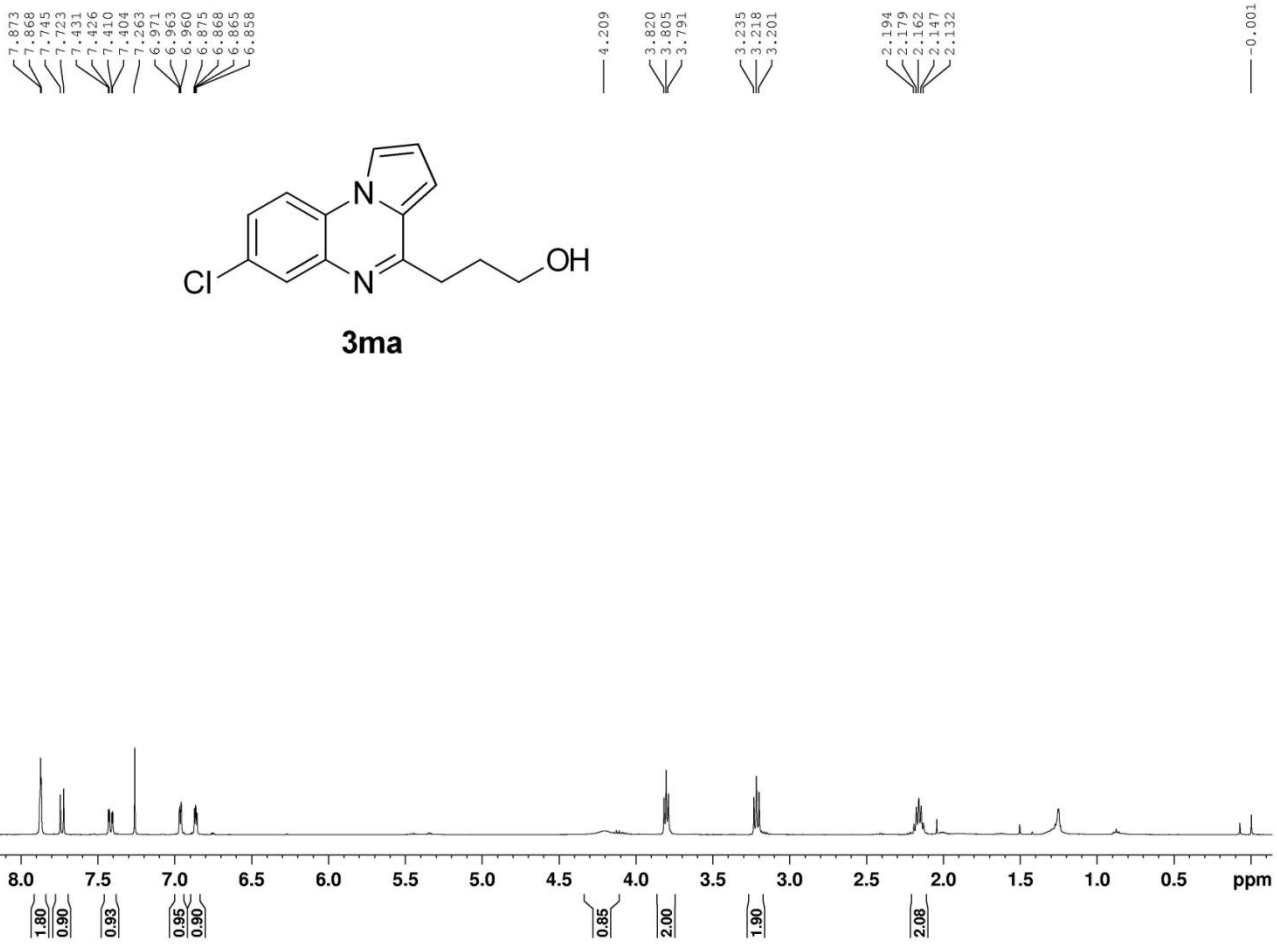

1.01
1.03
1.00
1.07
1.00
0.99
0.98
2.12
2.07
2.09
.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


157.25
133.17
131.99
128.03
126.59
125.60
125.54
115.18
114.22
112.24
107.27
77.32
77.00
76.68
62.55
32.59
28.95
N
N
OH
Cl
3ka
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.836
7.833
7.829
7.826
7.793
7.786
7.781
7.772
7.359
7.354
7.337
7.332
7.263
6.958
6.955
6.948
6.945
6.874
6.867
6.864
6.857
4.367
3.821
3.807
3.792
3.225
3.209
3.192
2.194
2.179
2.163
2.147
2.132
0.000
Cl
N
N
OH
3Ia
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
1.99
1.00
1.02
1.00
0.86
2.10
2.07
2.18


156.93
133.73
132.55
130.18
127.73
125.72
125.57
114.88
114.27
113.81
107.30
77.36
77.04
76.72
62.57
32.63
29.58
Cl
N
N
OH
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3Ia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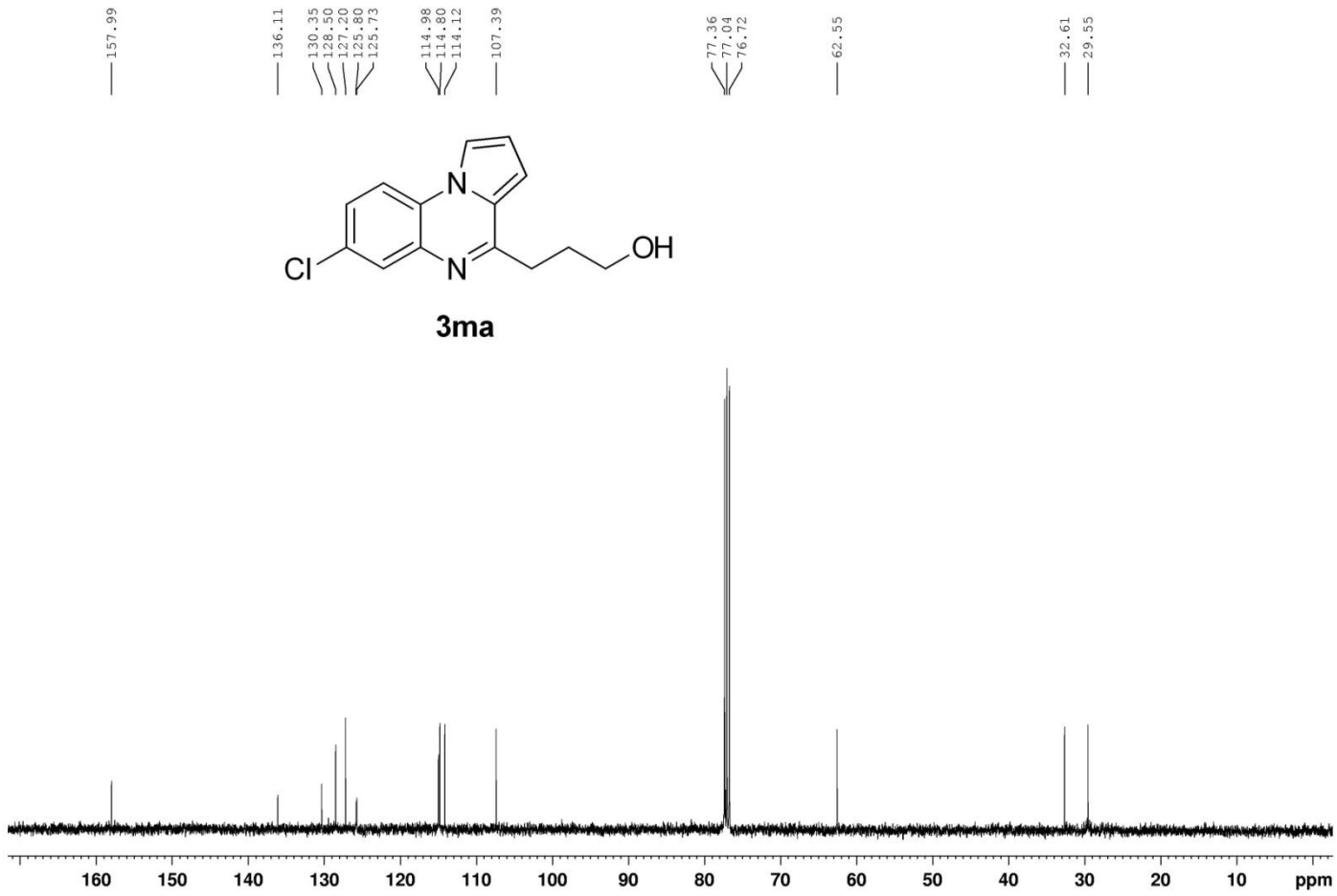
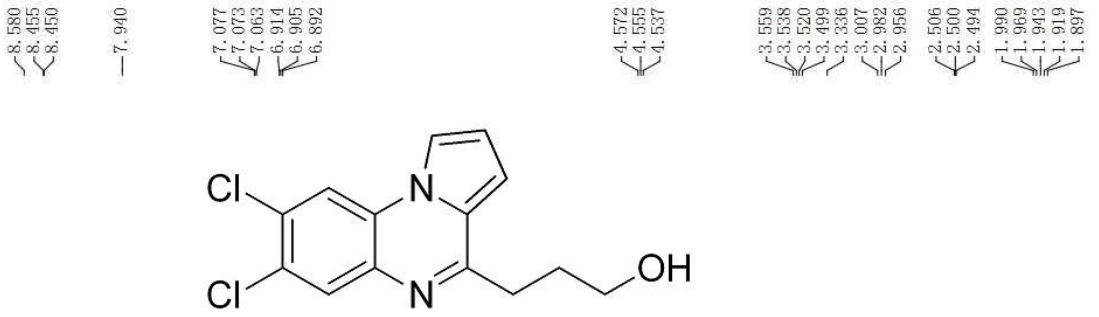
7.745
7.723
7.431
7.426
7.410
7.404
7.263
6.971
6.963
6.960
6.875
6.868
6.865
6.858
4.209
3.820
3.805
3.791
3.235
3.218
3.201
2.194
2.179
2.162
2.147
2.132
-0.001
N
N
Cl
OH
3ma
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.80
0.90
0.93
0.95
0.90
0.85
2.00
1.90
2.08


157.99
136.11
130.35
128.50
127.20
125.80
125.73
114.98
114.80
114.12
107.39
77.36
77.04
76.72
62.55
32.61
29.55
N
N
Cl
OH
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3ma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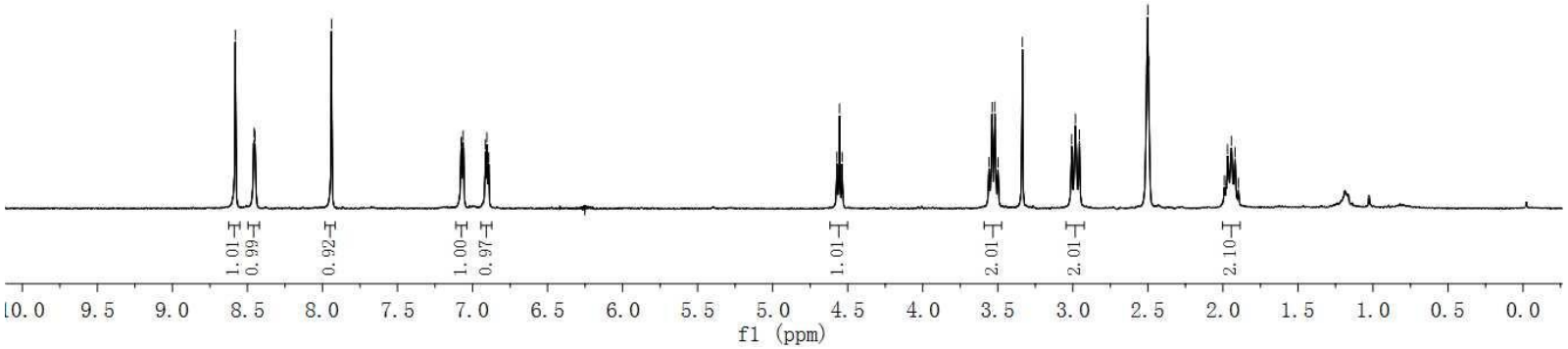
8.455
8.450
7.940
7.077
7.073
7.063
6.914
6.905
6.892
4.572
4.555
4.537
3.559
3.538
3.520
3.499
3.336
3.007
2.982
2.956
2.506
2.500
2.494
1.990
1.969
1.943
1.919
1.897
Cl
Cl
N
N
OH

3na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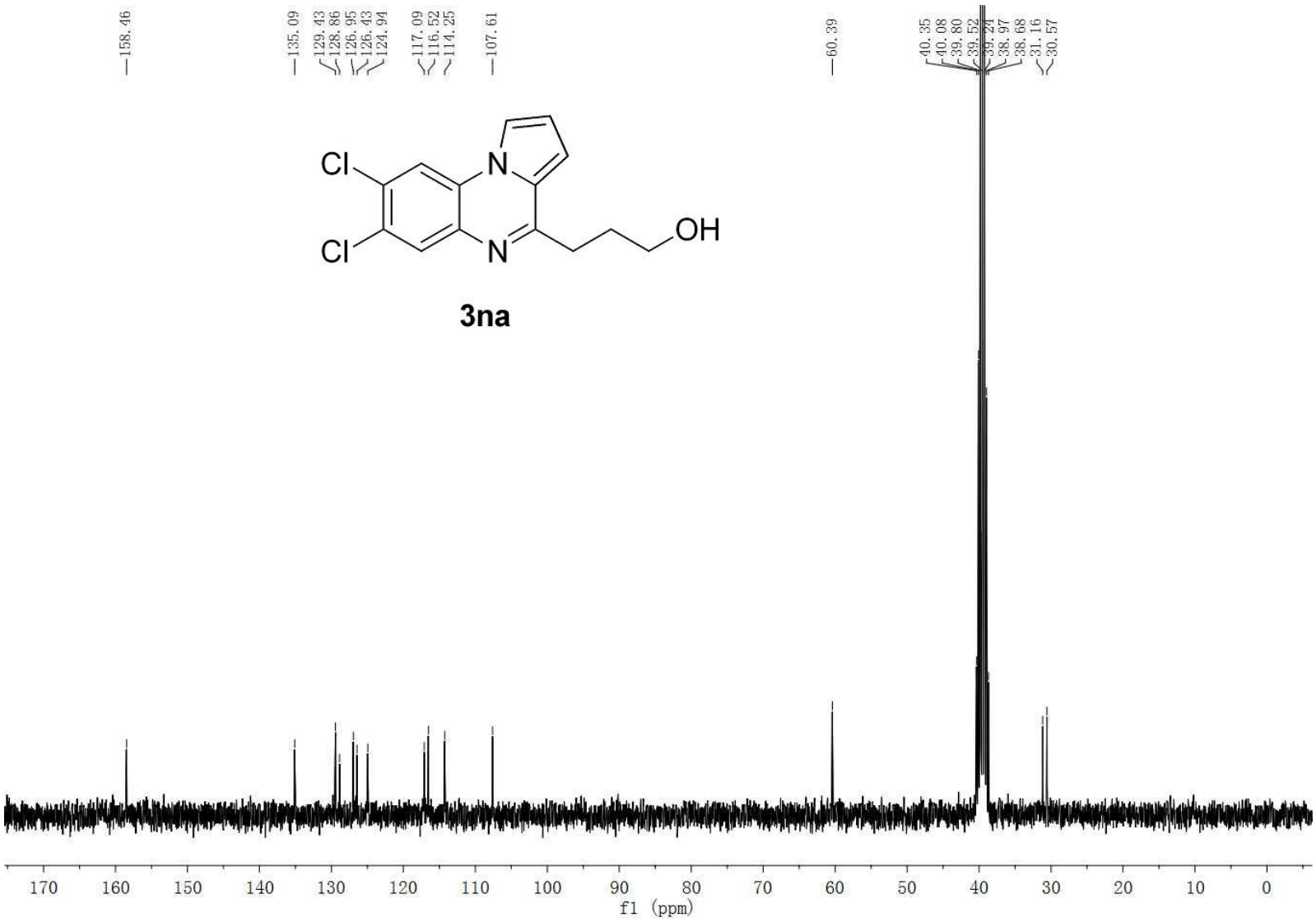
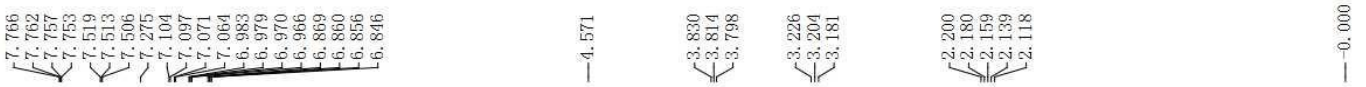
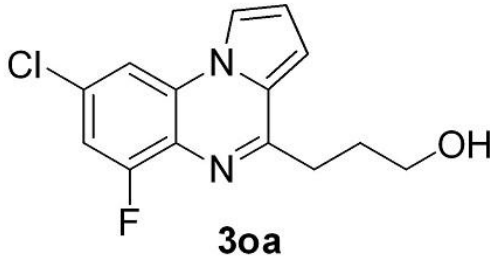
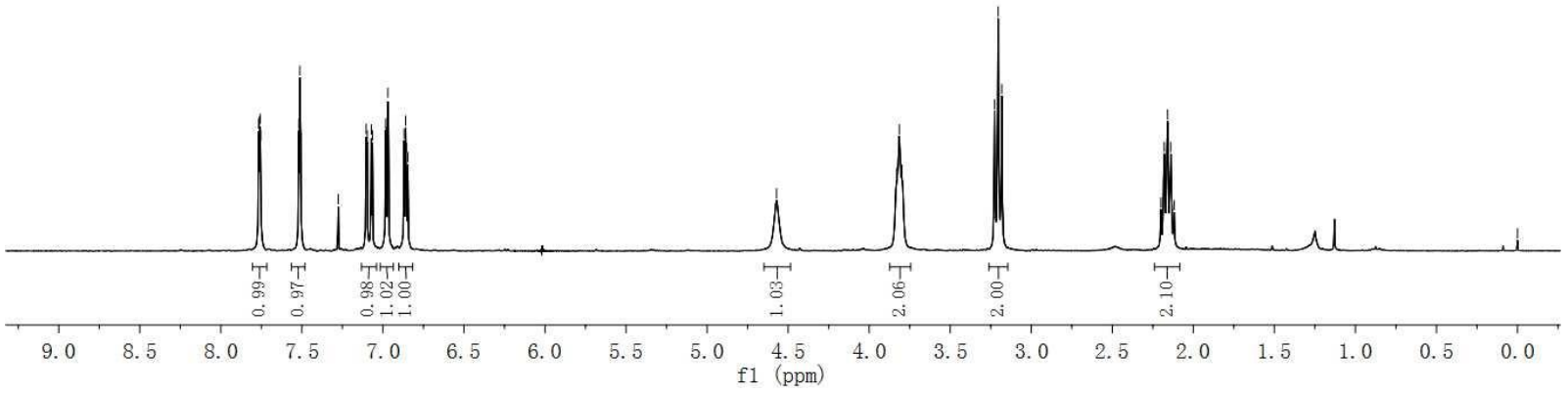
0.99
2.26
2.00
0.97
4.10
2.01
2.01
2.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

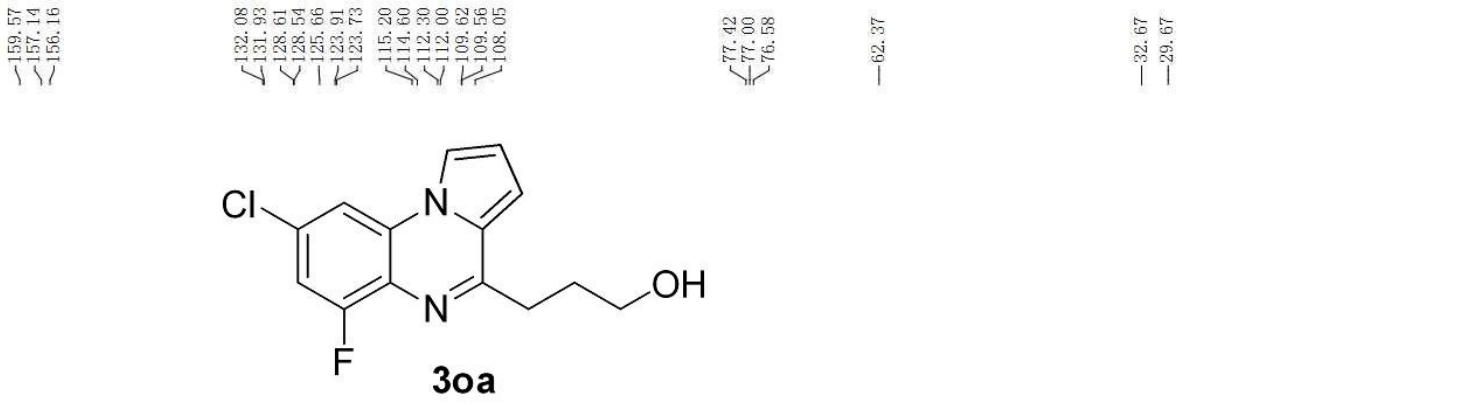

158.46
135.09
129.43
128.86
126.95
126.43
124.94
117.09
116.52
114.25
107.61
60.39
40.35
40.08
39.80
39.52
39.24
38.97
38.68
31.16
30.57
Cl
Cl
N
N
OH
3na
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.766
7.762
7.757
7.753
7.519
7.513
7.506
7.275
7.104
7.097
7.071
7.064
6.983
6.979
6.970
6.966
6.869
6.860
6.856
6.846
4.571
3.830
3.814
3.798
3.226
3.204
3.181
2.200
2.180
2.159
2.139
2.118
0.000


Cl
N
N
OH
F

3oa


0.99
0.97
0.98
1.02
1.00
1.03
2.06
2.00
2.10
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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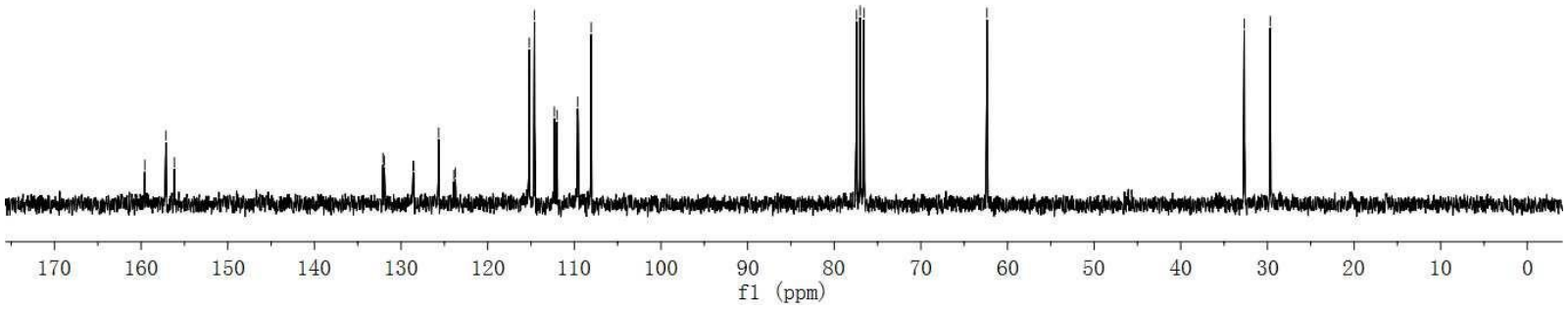
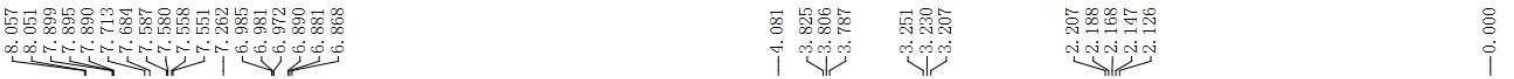
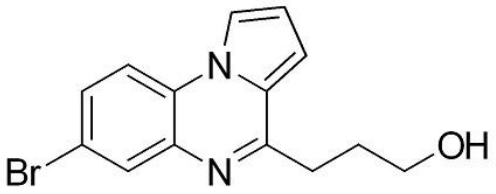
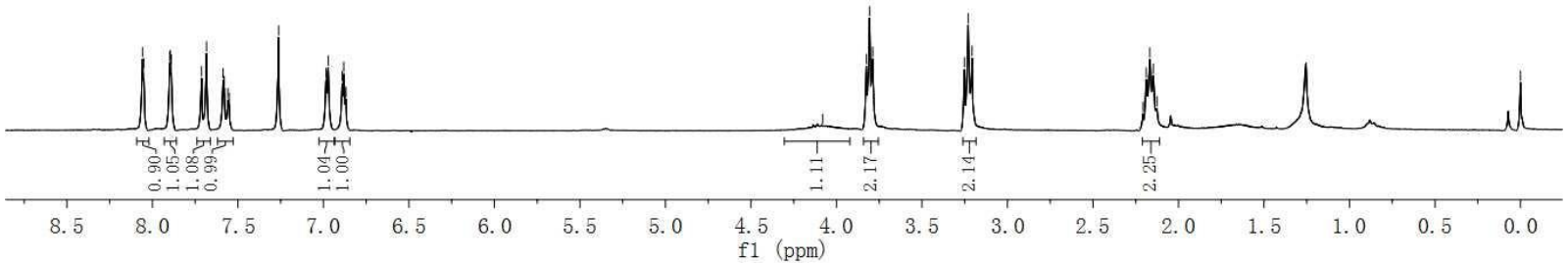
157.14
156.16
132.08
131.93
128.61
128.54
125.66
123.91
123.73
115.20
114.60
112.30
112.00
109.62
109.56
108.05
77.42
77.00
76.58
62.37
32.67
29.67
Cl
N
N
OH
F
3oa


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

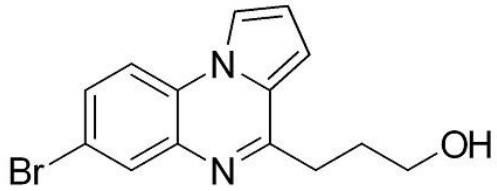

8.057
8.051
7.899
7.895
7.890
7.713
7.684
7.587
7.580
7.558
7.551
7.262
6.985
6.981
6.972
6.890
6.881
6.868
4.081
3.825
3.806
3.787
3.251
3.230
3.207
2.207
2.188
2.168
2.147
2.126
0.000


N
N
Br
OH

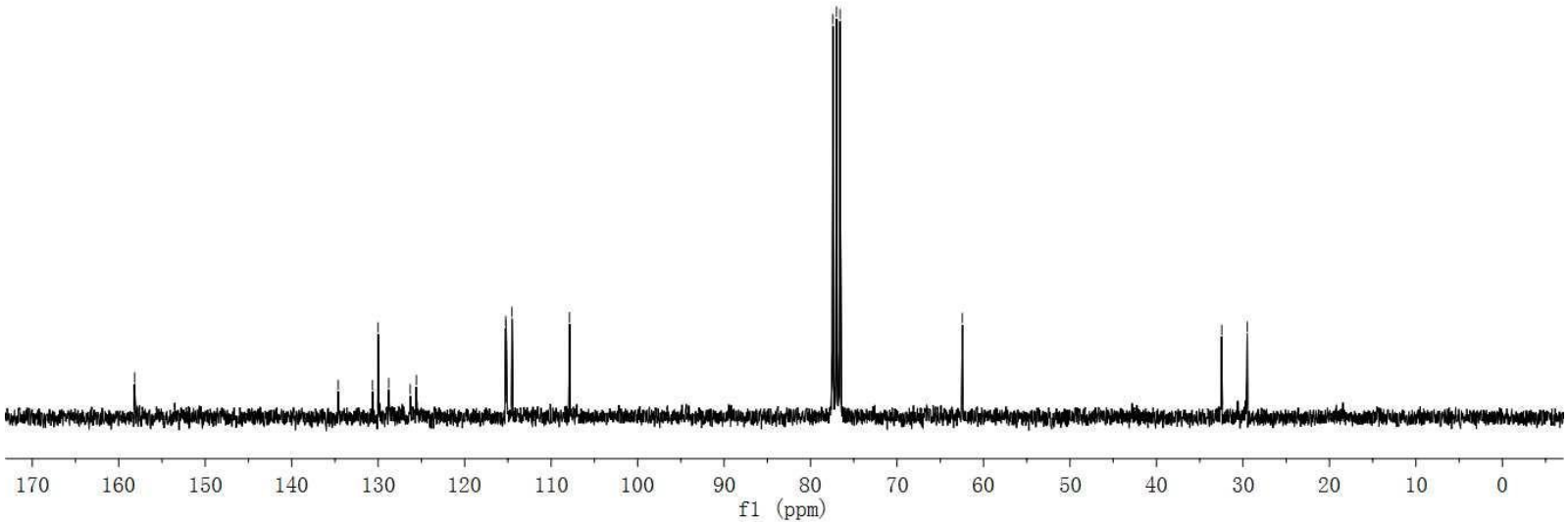
3pa

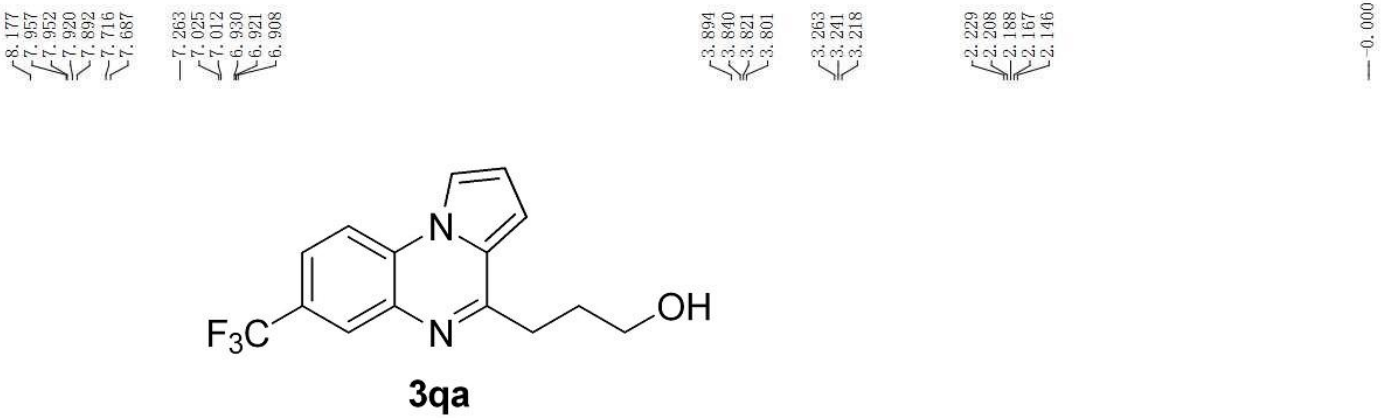

0.90
1.05
1.08
0.99
1.04
1.00
1.11
2.17
2.14
2.25
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

158.17
134.62
130.66
130.01
128.78
126.29
125.58
115.25
115.20
114.53
107.88
77.42
77.00
76.58
62.46
32.45
29.50



3pa

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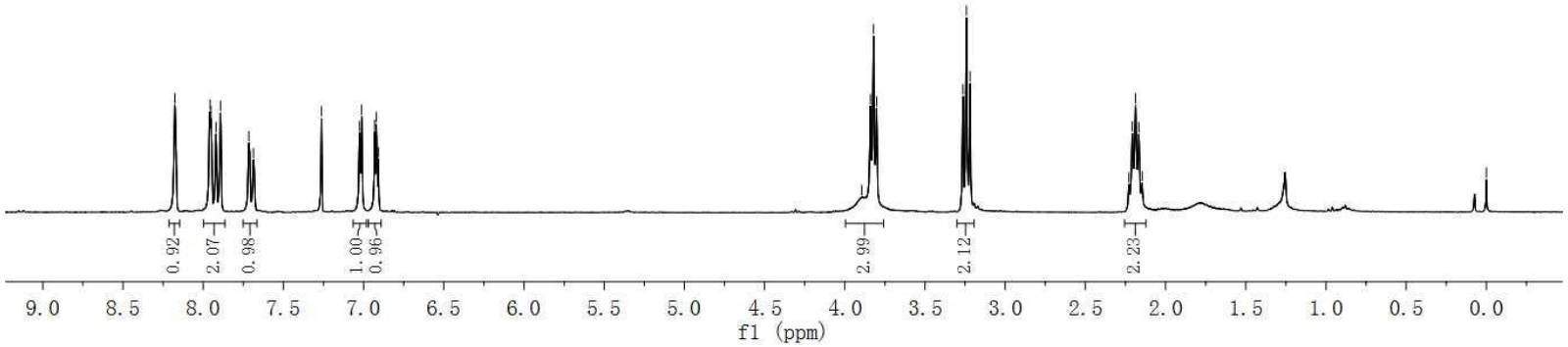
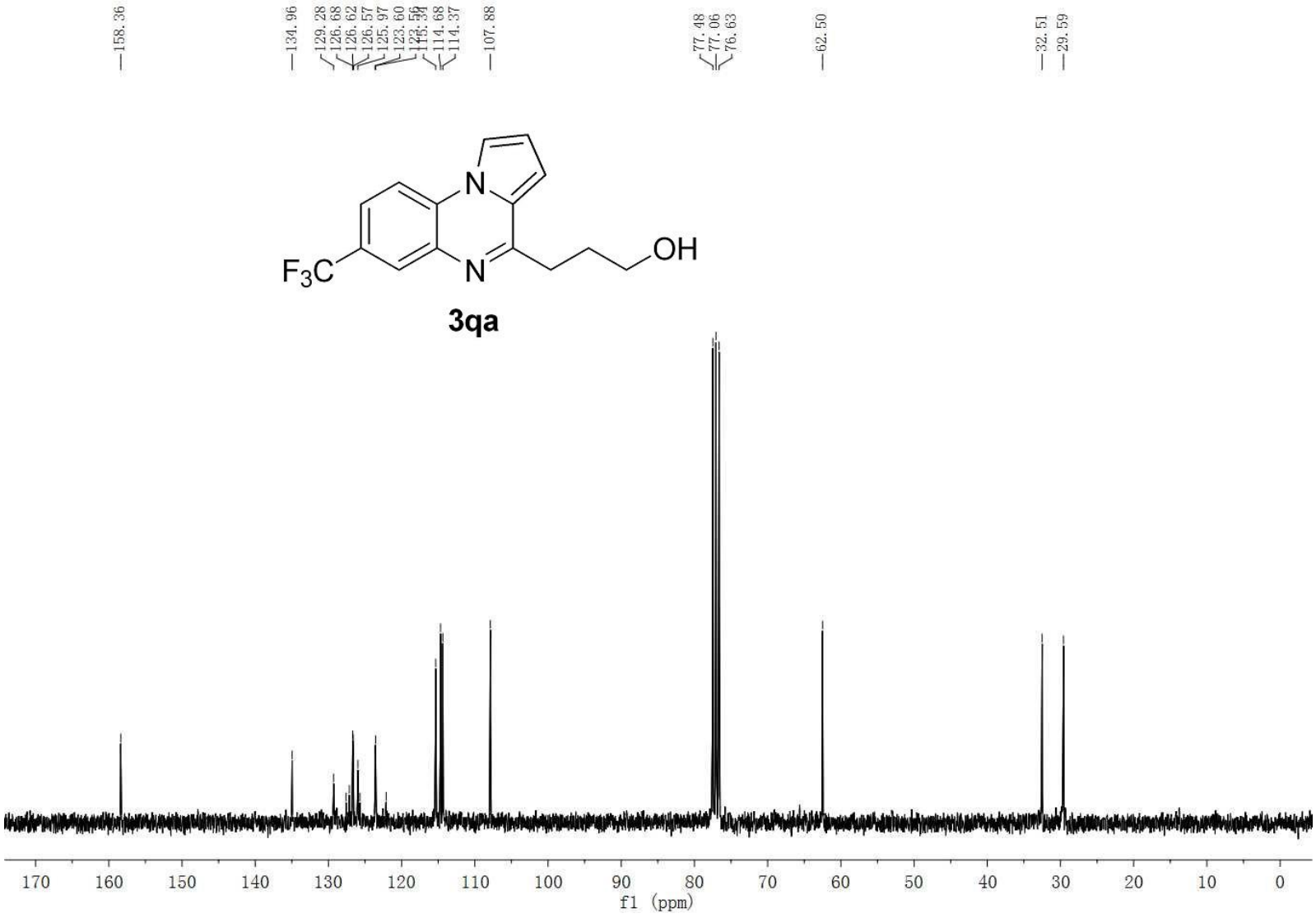
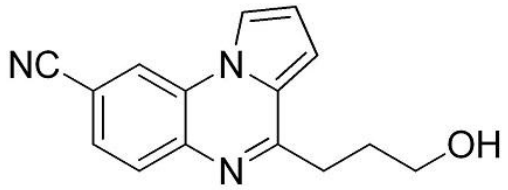
7.952
7.920
7.892
7.716
7.687
7.263
7.025
7.012
6.930
6.921
6.908
3.894
3.840
3.821
3.801
3.263
3.241
3.218
2.229
2.208
2.188
2.167
2.146
0.000
N
N
F3C
OH
3qa

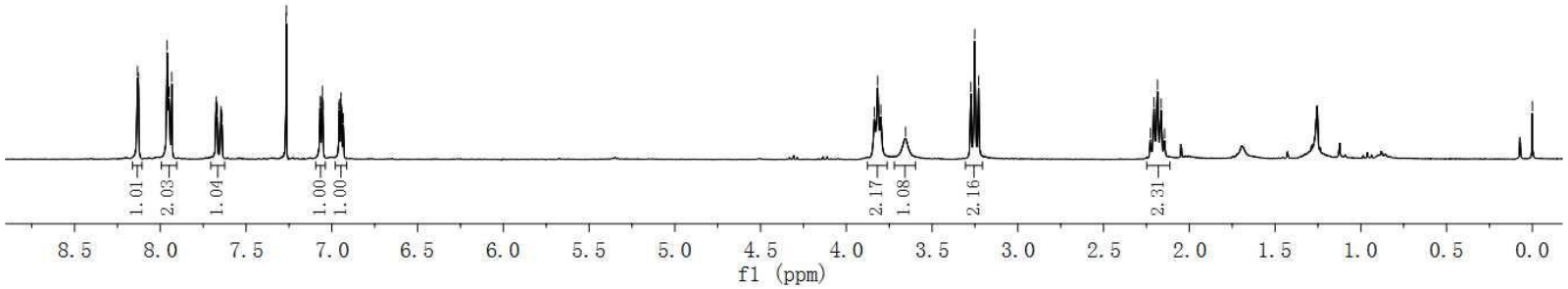

0.92
2.07
0.98
1.00
0.96
2.99
2.12
2.23
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

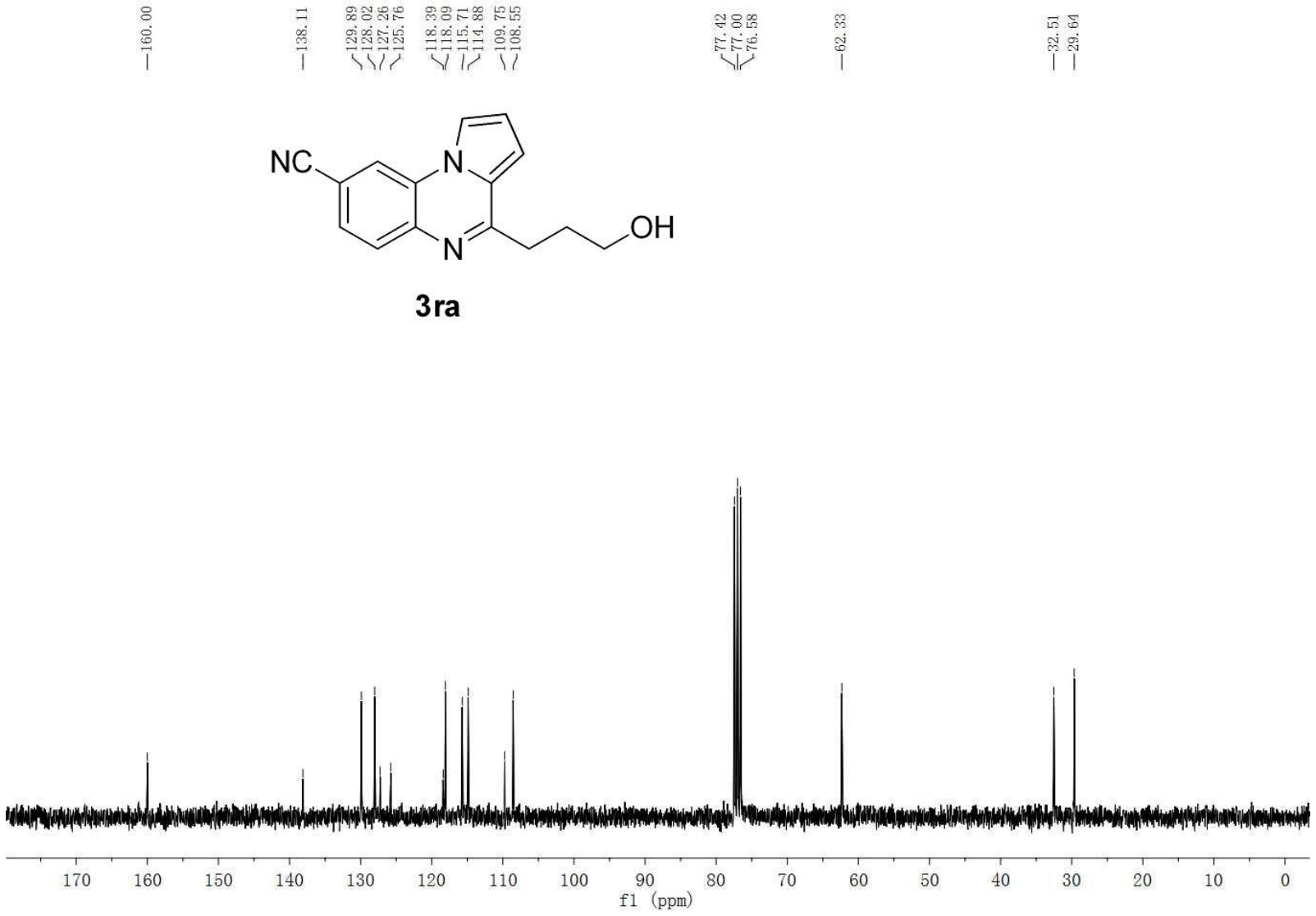

158.36
134.96
129.28
126.68
126.62
126.57
125.97
123.60
114.68
114.37
107.88
77.48
77.06
76.63
62.50
32.51
29.59
N
N
F3C
OH
3qa
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.133
8.127
7.960
7.954
7.948
7.933
7.676
7.674
7.670
7.267
7.265
7.068
7.064
7.057
7.055
7.051
6.958
6.956
6.948
6.946
6.942
6.935
6.933
3.836
3.818
3.799
3.654
3.273
3.251
3.228
2.227
2.206
2.185
2.165
2.144
0.000

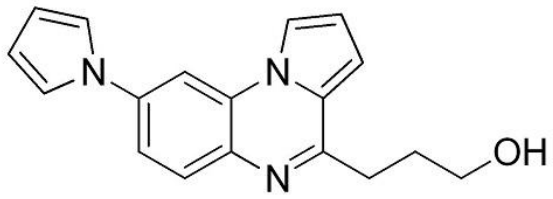

NC
N
N
OH

3ra

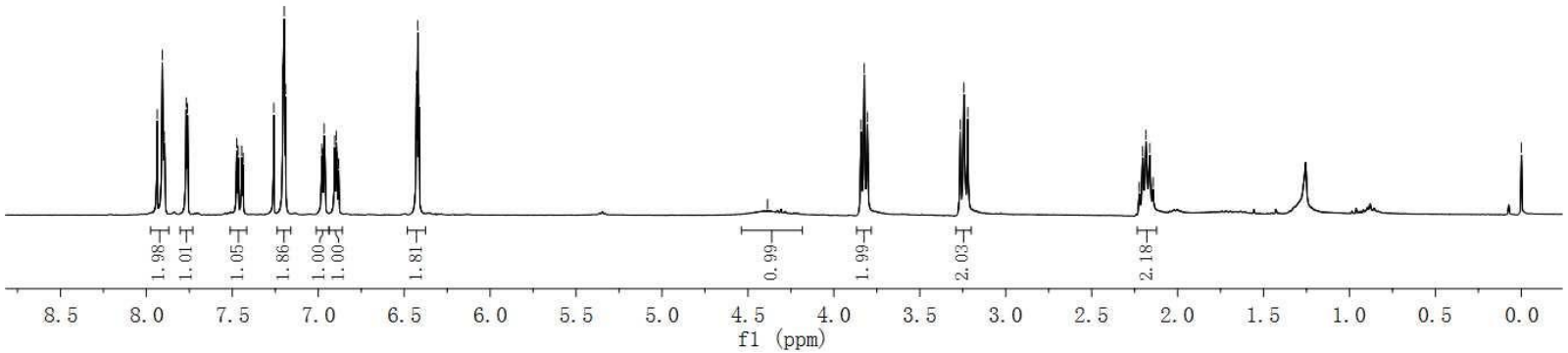

1.01
2.03
1.04
1.00
1.00
2.17
1.08
2.16
2.31
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

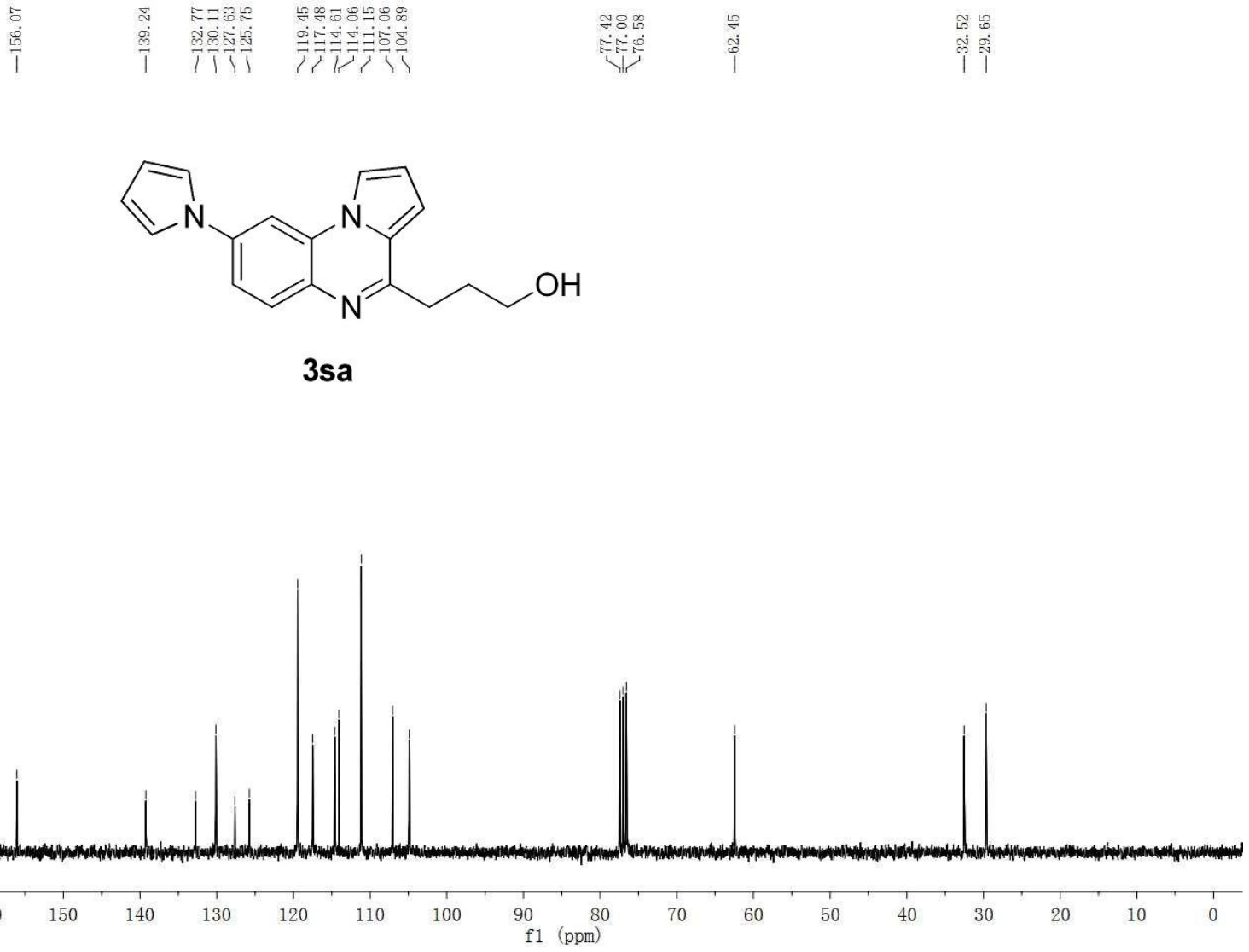

160.00
138.11
129.89
128.02
127.26
125.76
118.39
118.09
115.71
114.88
109.75
108.55
77.42
77.00
76.58
62.33
32.51
29.64
NC
N
N
OH
3ra
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.937
7.907
7.902
7.897
7.893
7.768
7.760
7.474
7.258
7.205
7.198
7.190
6.966
6.962
6.904
6.885
6.428
6.421
6.414
4.386
3.842
3.823
3.804
3.265
3.243
3.220
2.223
2.204
2.184
2.162
2.142
0.000

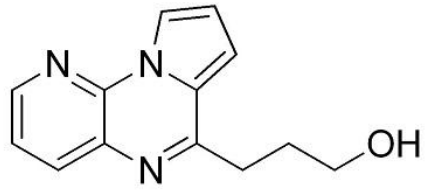

N
N
N
OH

3sa

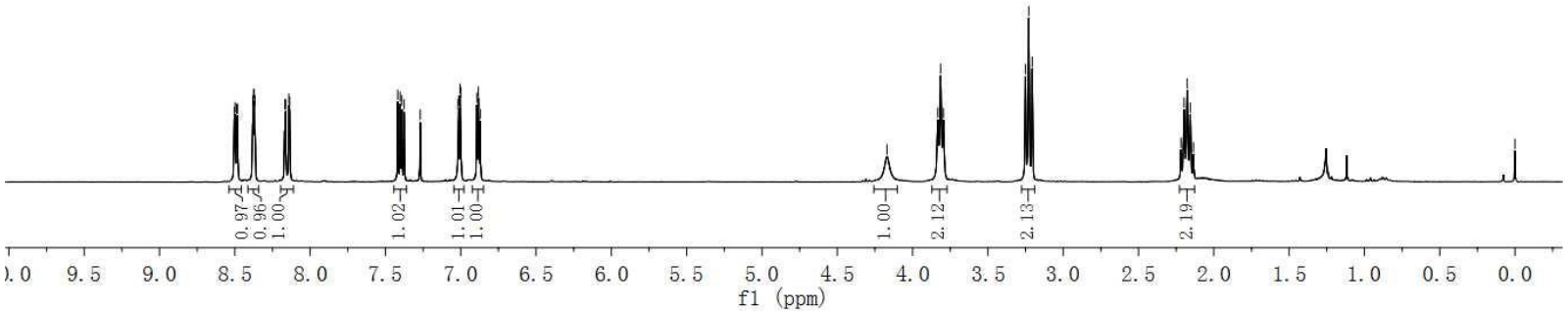

1.98
1.01
1.05
1.86
1.00
1.00
1.81
0.99
1.99
2.03
2.18
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

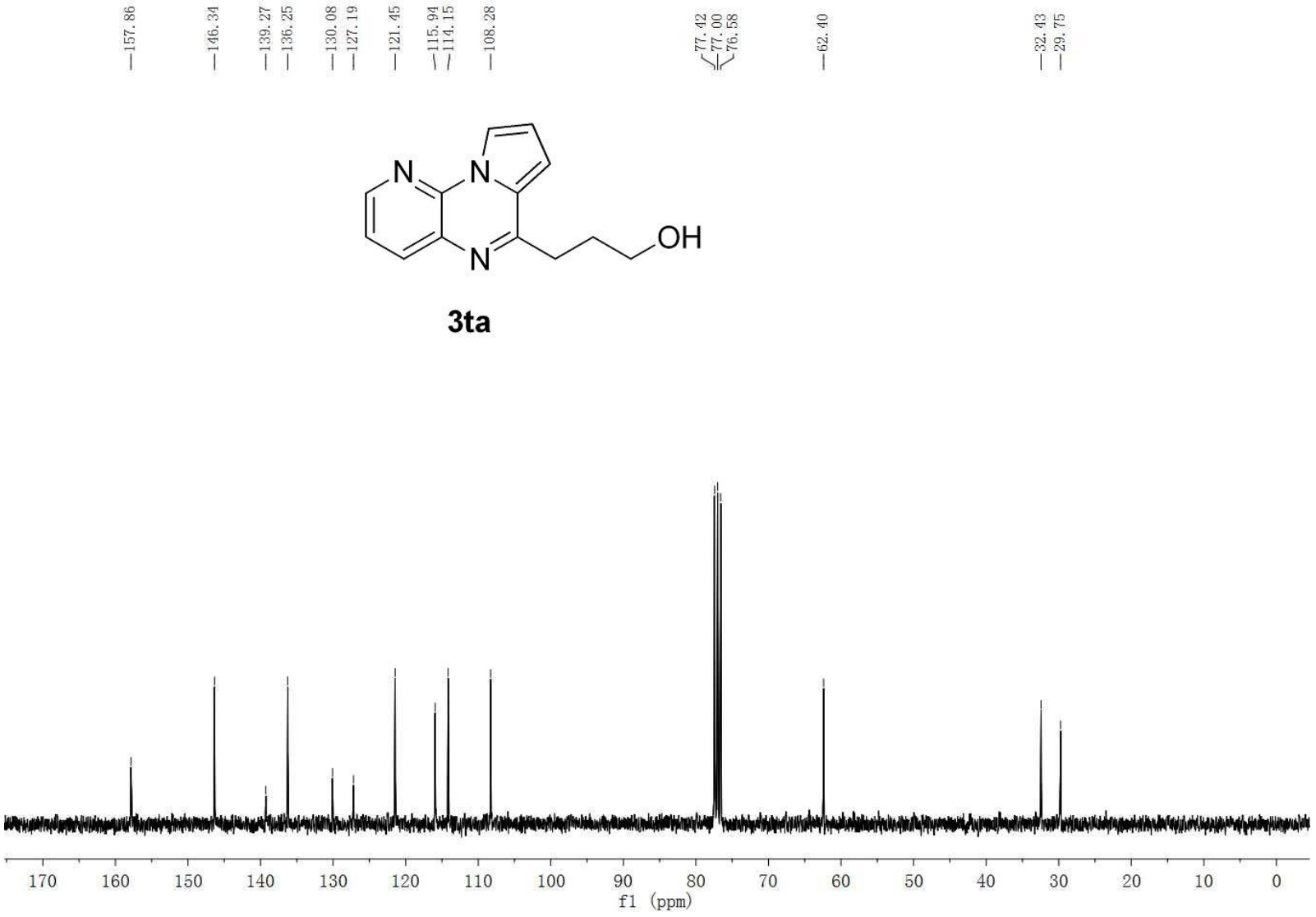

156.07
139.24
132.77
130.11
127.63
125.75
119.45
117.48
114.61
114.06
111.15
107.06
104.89
77.42
77.00
76.58
62.45
32.52
29.65
N
N
N
OH
3sa
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.503
8.498
8.488
8.482
8.380
8.376
8.371
8.367
8.168
8.162
8.141
8.136
7.418
7.403
7.392
7.376
7.269
7.018
7.013
7.004
7.000
6.893
6.883
6.880
6.870
4.170
3.833
3.814
3.795
3.251
3.229
3.206
2.218
2.198
2.177
2.156
2.135
0.000

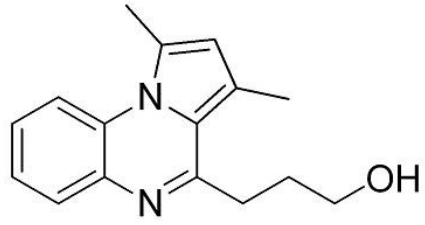

N
N
N
OH

3ta

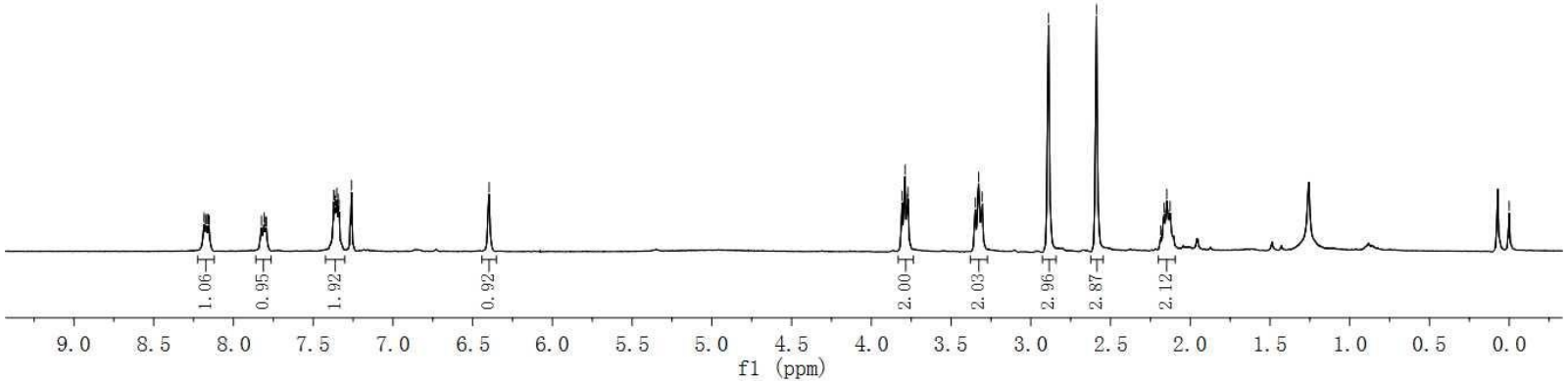

0.97
0.96
1.00
1.02
1.01
1.00
1.00
2.12
2.13
2.19
f1 (ppm)

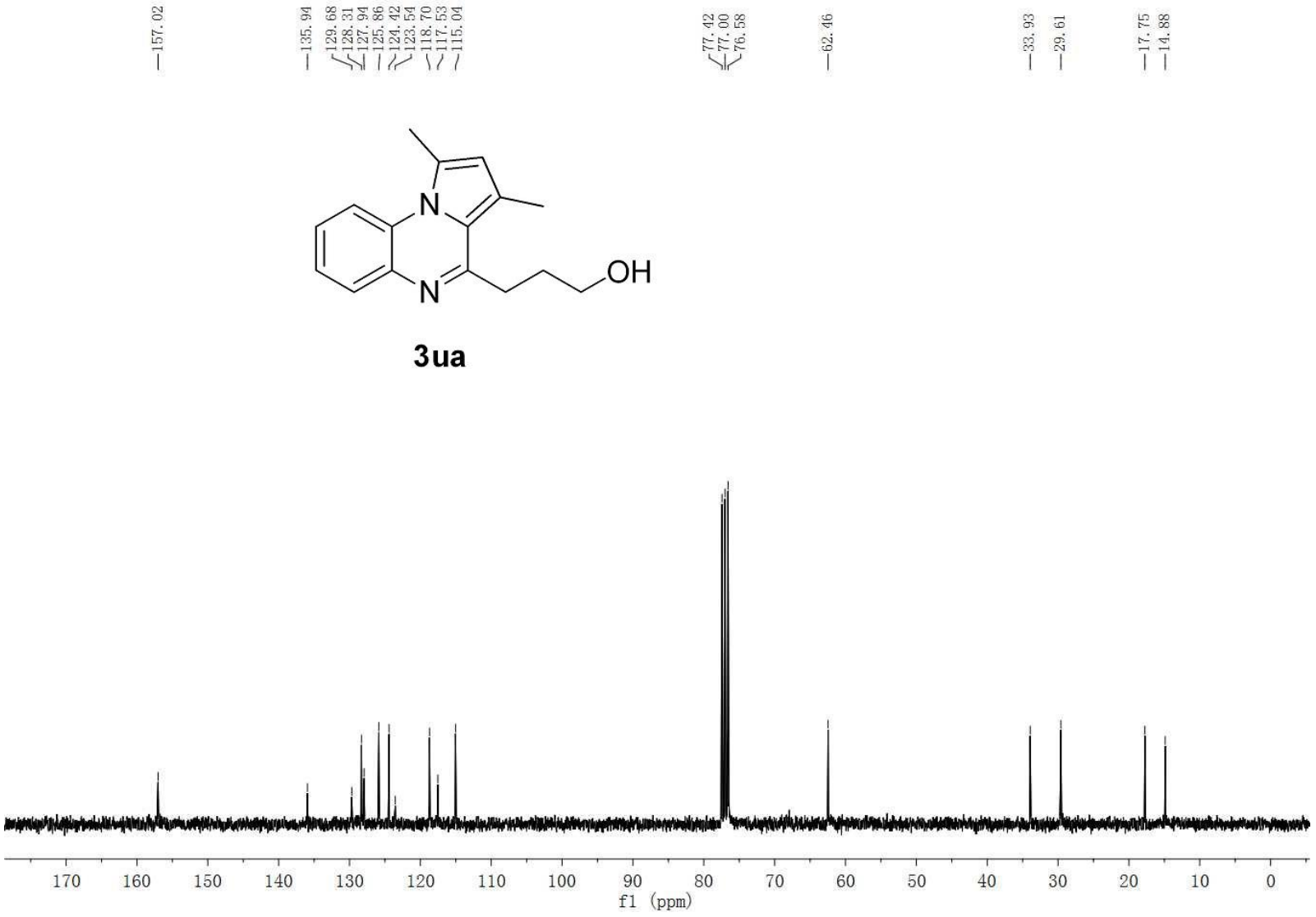

157.86
146.34
139.27
136.25
130.08
127.19
121.45
115.94
114.15
108.28
77.42
77.00
76.58
62.40
32.43
29.75
N
N
N
OH
3ta
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.185
8.176
8.169
8.159
8.152
7.824
7.808
7.793
7.371
7.367
7.362
7.352
7.343
7.338
7.259
6.397
3.807
3.788
3.774
3.770
3.348
3.327
3.305
2.889
2.588
2.185
2.164
2.147
2.126
0.000

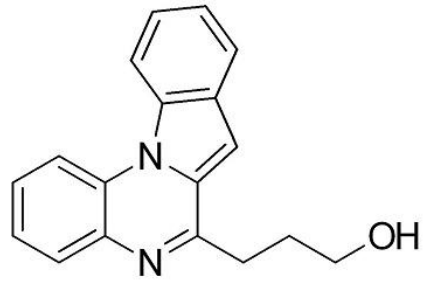

N
N
OH

3ua

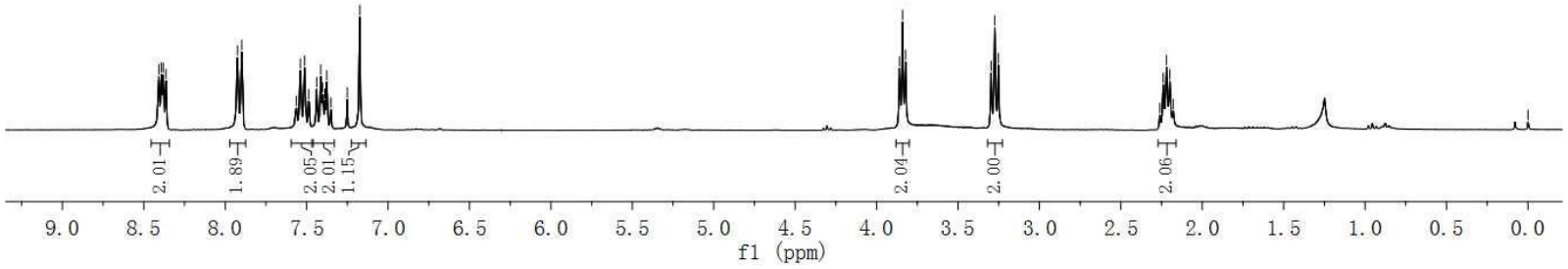

1.06
0.95
1.92
0.92
2.00
2.03
2.96
2.87
2.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

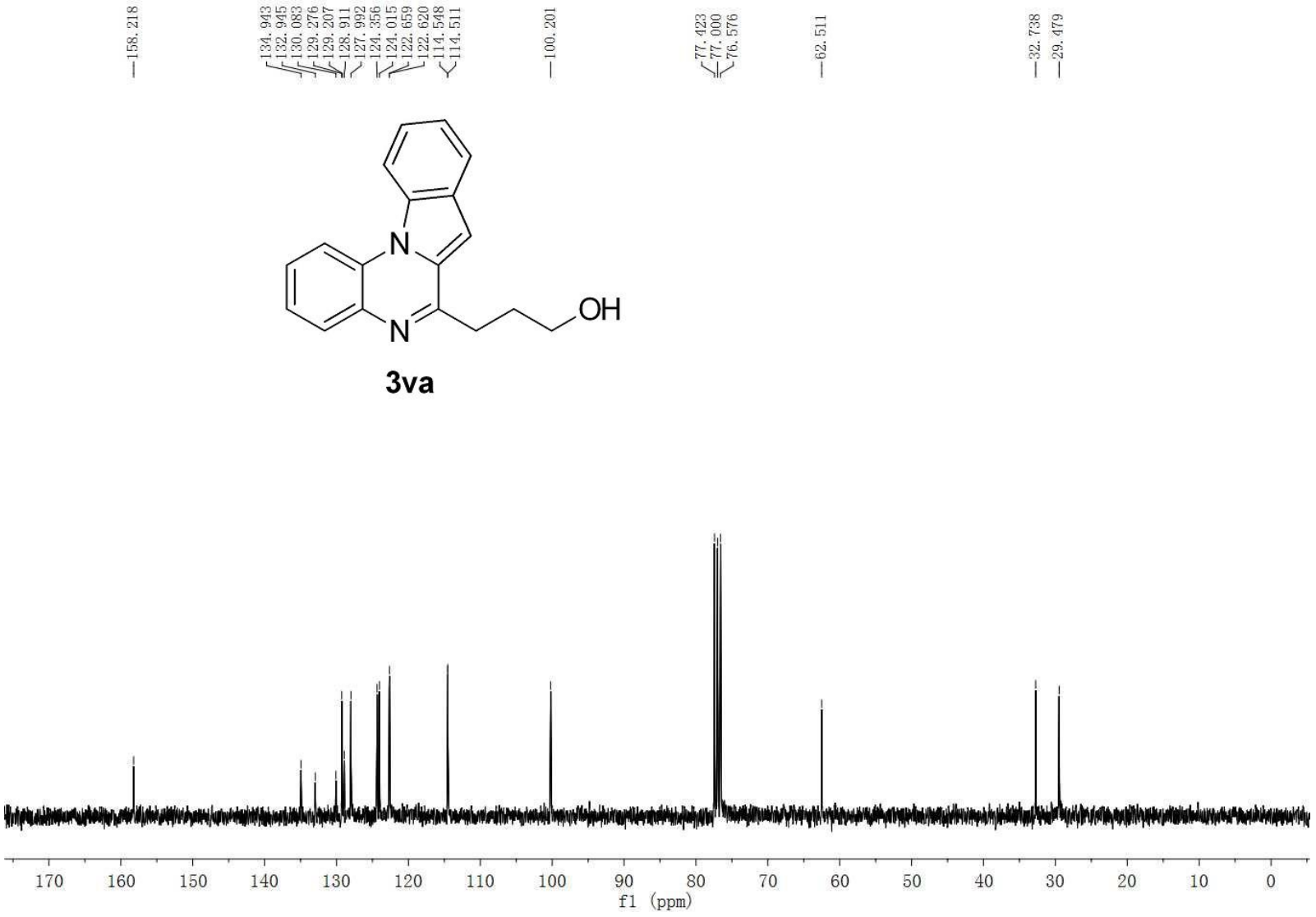

157.02
135.94
129.68
128.31
127.94
125.86
124.42
123.54
118.70
117.53
115.04
77.42
77.00
76.58
62.46
33.93
29.61
17.75
14.88
N
N
OH
3ua
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

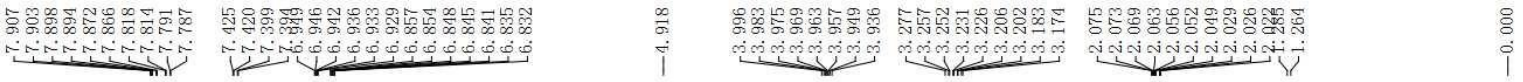

8.408
8.392
8.381
8.363
7.924
7.898
7.563
7.538
7.512
7.488
7.438
7.413
7.401
7.388
7.377
7.350
7.250
7.173
3.859
3.840
3.822
3.297
3.275
3.252
2.261
2.240
2.220
2.199
2.178
0.000

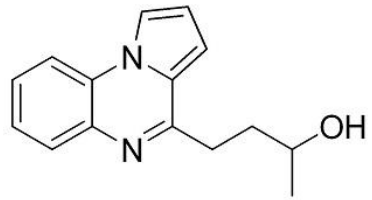

N
N
OH

3va

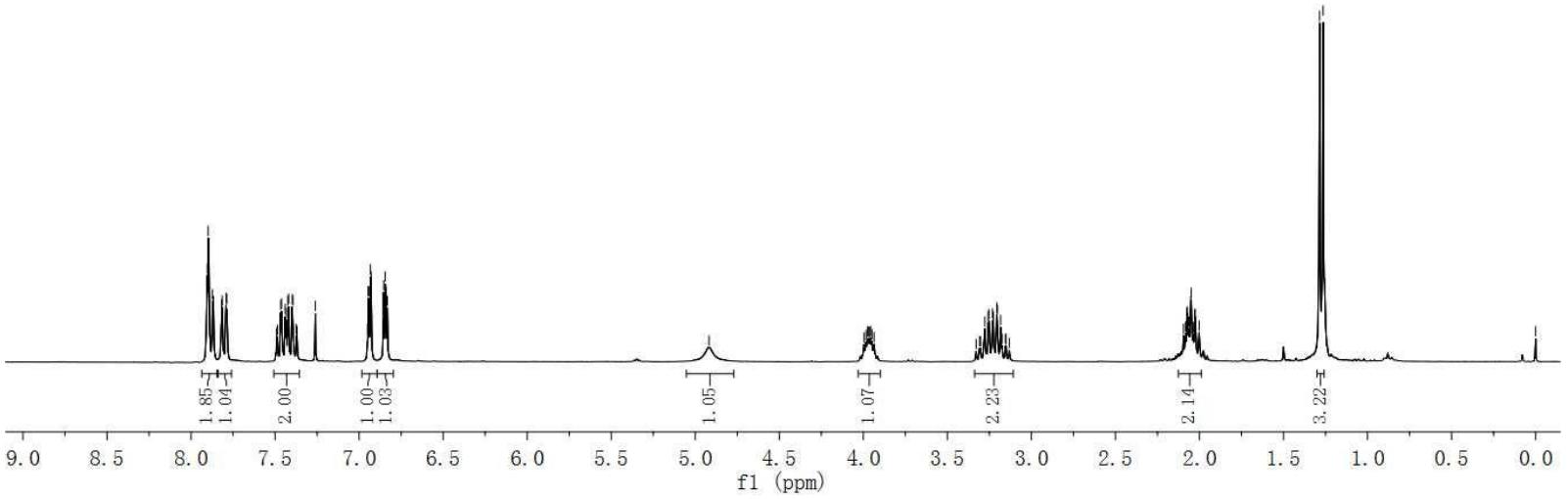

2.01
1.89
2.05
2.01
1.15
2.04
2.00
2.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

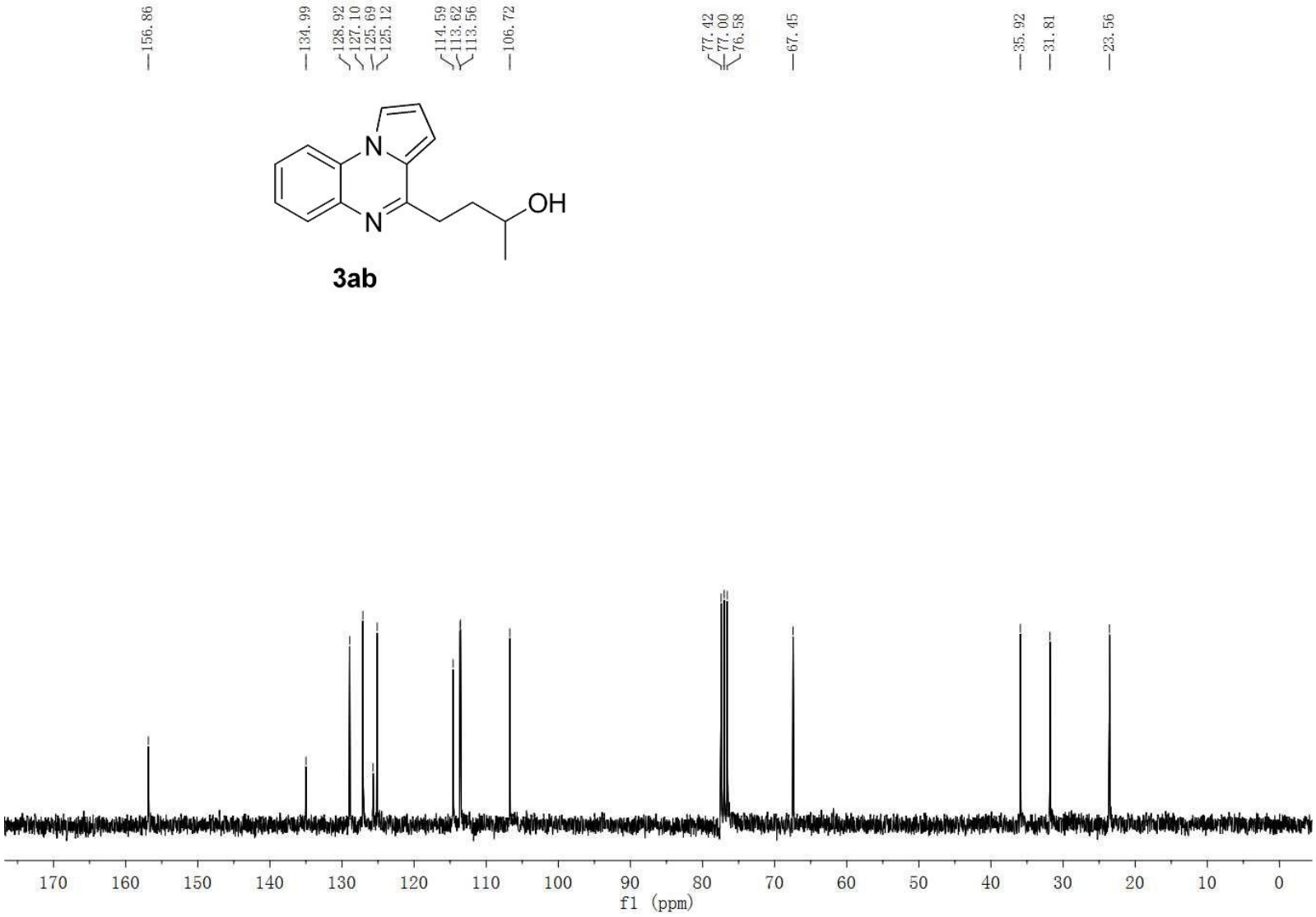

158.218
134.943
132.945
130.083
129.276
129.207
128.911
127.992
124.356
124.015
122.659
122.620
114.548
114.511
100.201
77.423
77.000
76.576
62.511
32.738
29.479
N
N
OH
3va
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

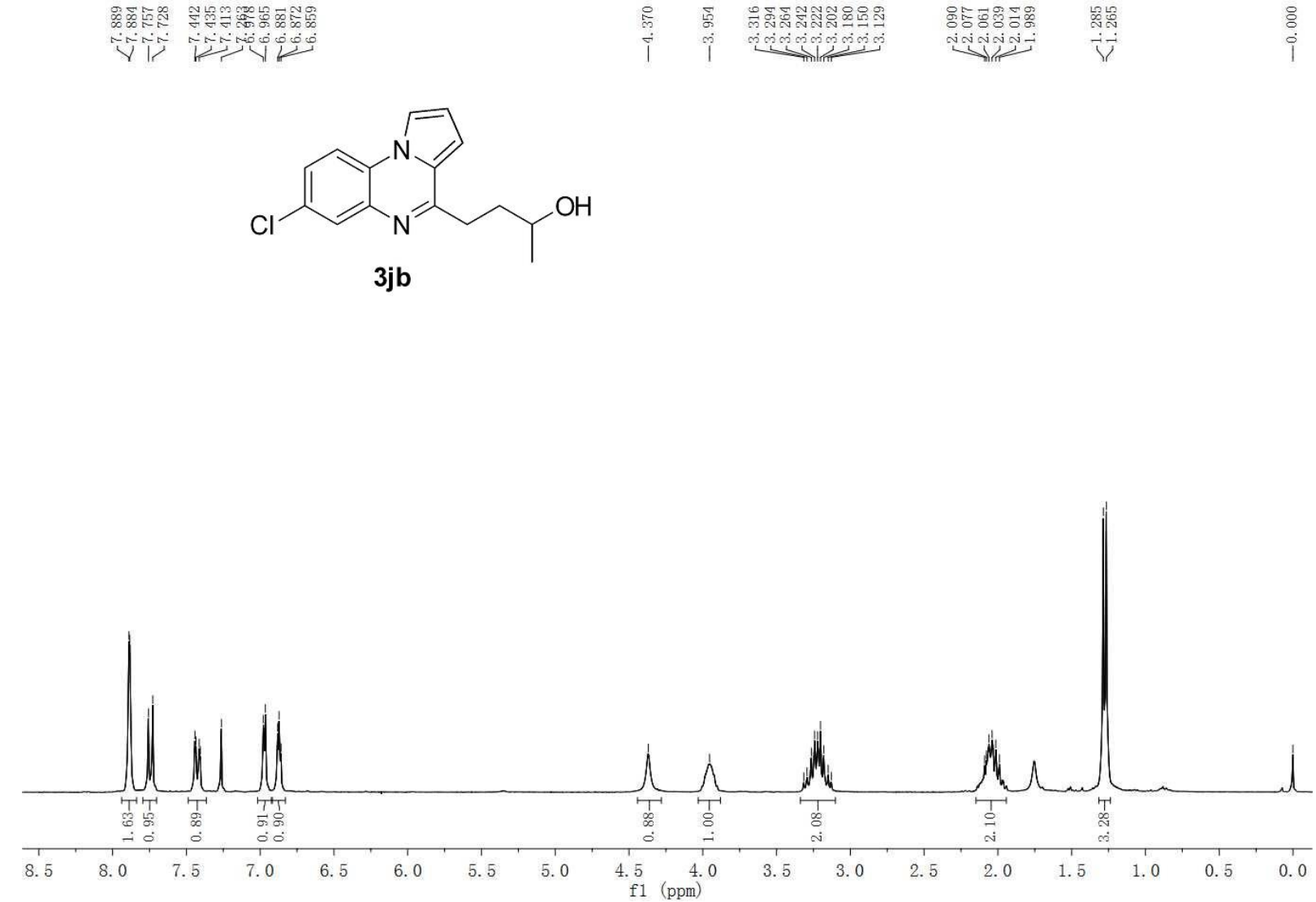

7.907
7.903
7.898
7.894
7.872
7.866
7.818
7.814
7.791
7.787
7.425
7.420
7.399
6.946
6.942
6.936
6.933
6.929
6.857
6.854
6.848
6.845
6.841
6.835
6.832
4.918
3.996
3.983
3.975
3.969
3.963
3.957
3.949
3.936
3.277
3.257
3.252
3.231
3.226
3.206
3.202
3.183
3.174
2.075
2.073
2.069
2.063
2.056
2.052
2.049
2.029
2.026
1.264
0.000


N
N
OH

3ab

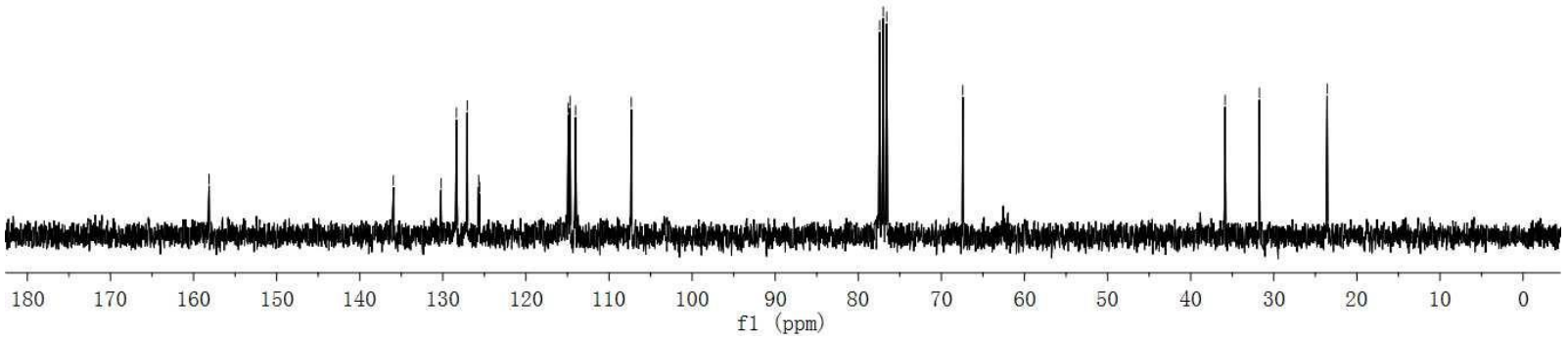

1.85
1.04
2.00
1.00
1.03
1.05
1.07
2.23
2.14
3.22
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


156.86
134.99
128.92
127.10
125.69
125.12
114.59
113.62
113.56
106.72
77.42
77.00
76.58
67.45
35.92
31.81
23.56
N
N
OH
3ab
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

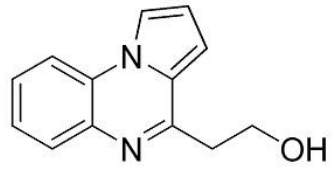

7.889
7.884
7.757
7.728
7.442
7.435
7.413
7.263
6.965
6.881
6.872
6.859
4.370
3.954
3.316
3.294
3.264
3.242
3.222
3.202
3.180
3.150
3.129
2.090
2.077
2.061
2.039
2.014
1.989
1.285
1.265
0.000
Cl
N
N
OH
3jb
1.63
0.95
0.89
0.91
0.90
0.88
1.00
2.08
2.10
3.28
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


158.13
135.95
130.22
128.36
127.06
125.68
125.57
114.90
114.69
114.03
107.32
77.42
77.00
76.58
67.42
35.86
31.73
23.57
N
N
Cl
OH

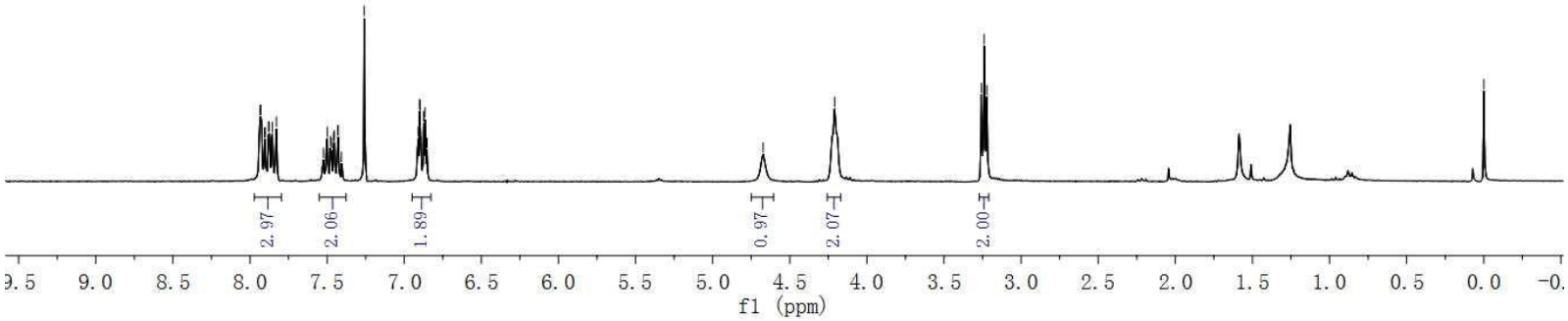
3jb


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

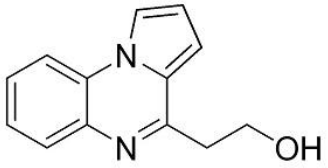

7.934
7.930
7.906
7.902
7.880
7.875
7.855
7.829
7.499
7.431
7.429
7.259
6.909
6.900
6.898
6.874
6.865
6.852
4.673
4.209
3.257
3.239
3.222
0.000


N
N
OH

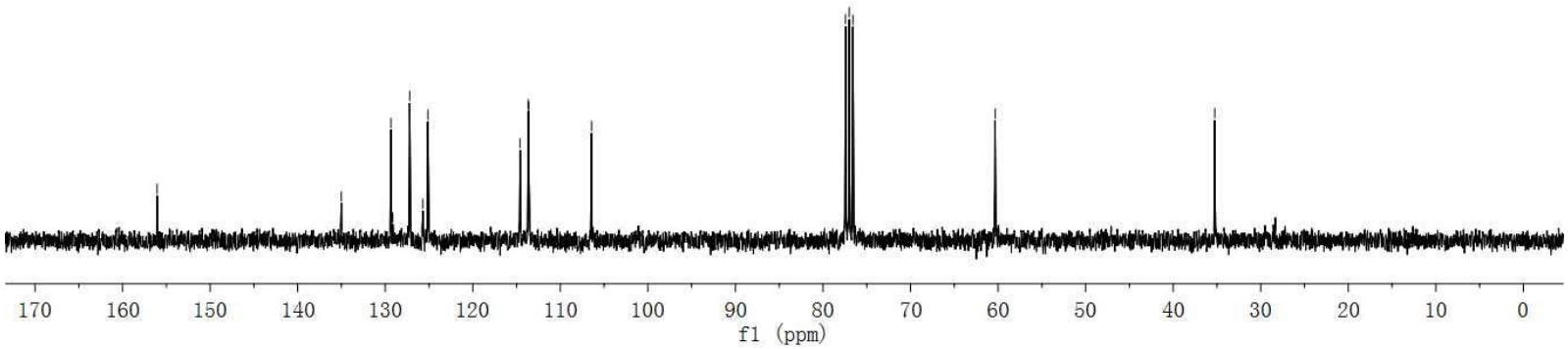
3ac


2.97
2.06
1.89
0.97
2.07
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

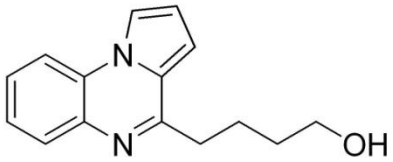
156.06
135.01
129.34
129.13
127.21
125.71
125.13
114.60
113.66
113.62
106.43
77.42
77.00
76.58
60.33
35.25



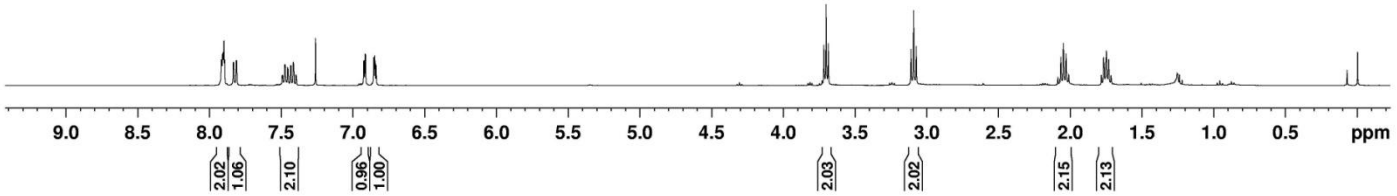
3ac




7.917
7.914
7.909
7.906
7.902
7.899
7.894
7.833
7.830
7.813
7.810
7.493
7.489
7.475
7.471
7.455
7.451
7.435
7.431
7.415
7.412
7.397
7.394
7.260
6.925
6.922
6.915
6.912
6.855
6.848
6.845
6.838
3.717
3.702
3.686
3.110
3.092
3.074
2.086
2.069
2.051
2.032
2.014
1.786
1.770
1.754
1.751
1.735
1.718
0.000


N
N
OH

3ad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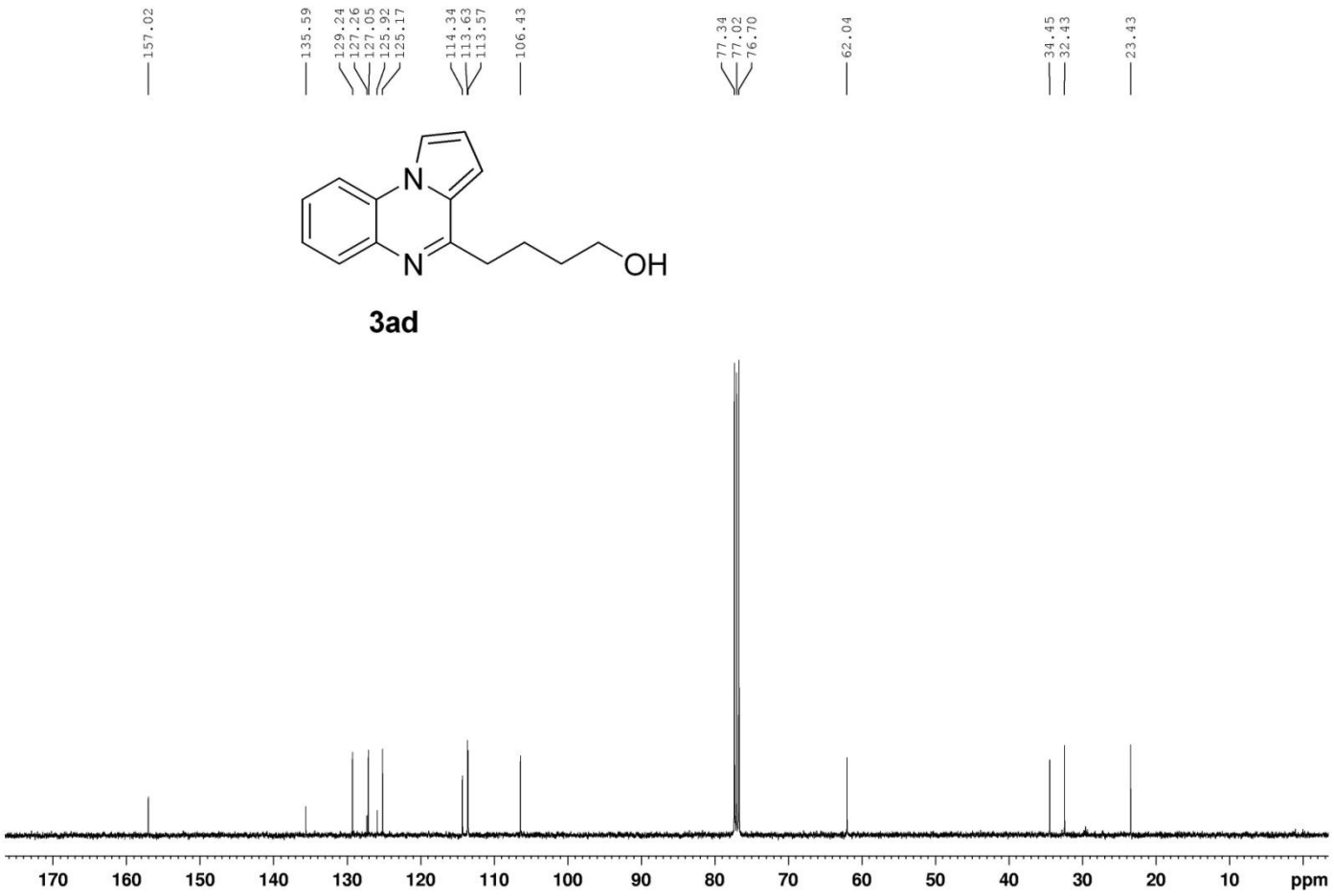
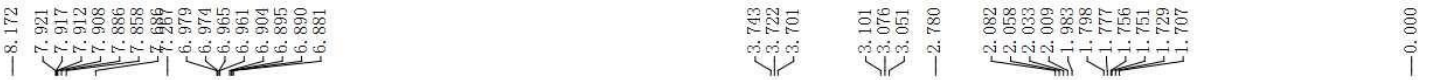
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.02
1.06
2.10
0.96
1.00
2.03
2.02
2.15
2.13


157.02
135.59
129.24
127.26
127.05
125.92
125.17
114.34
113.63
113.57
106.43
77.34
77.02
76.70
62.04
34.45
32.43
23.43
N
N
OH
3ad
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.172
7.921
7.917
7.912
7.908
7.886
7.858
6.979
6.974
6.965
6.961
6.904
6.895
6.890
6.881
3.743
3.722
3.701
3.101
3.076
3.051
2.780
2.082
2.058
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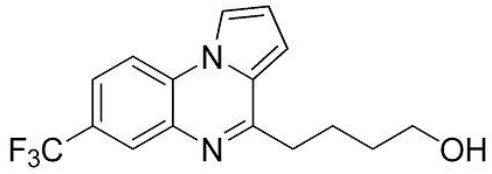
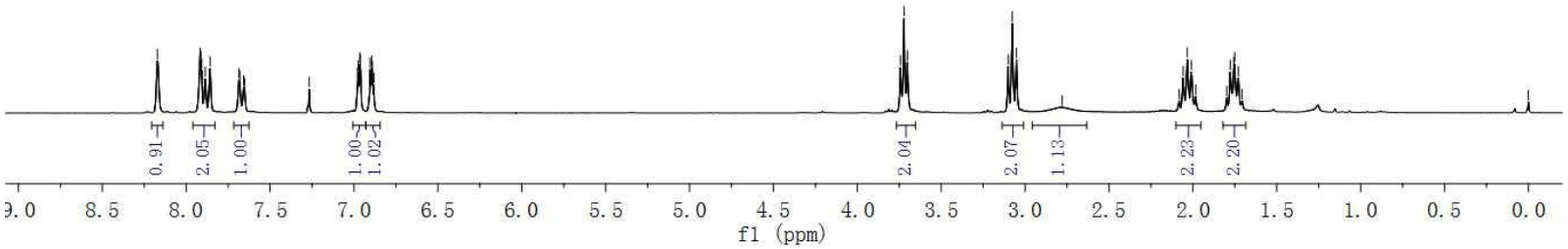
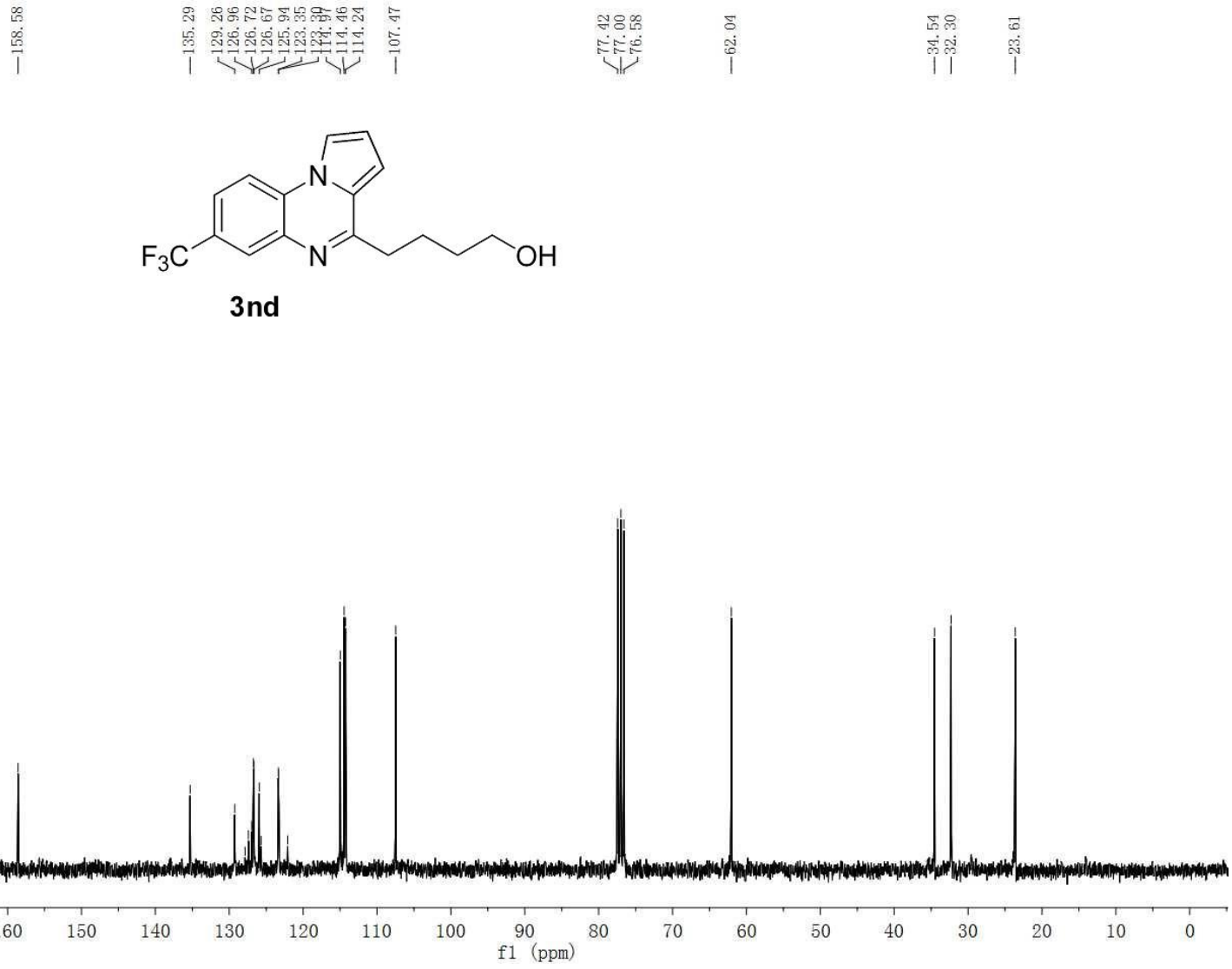
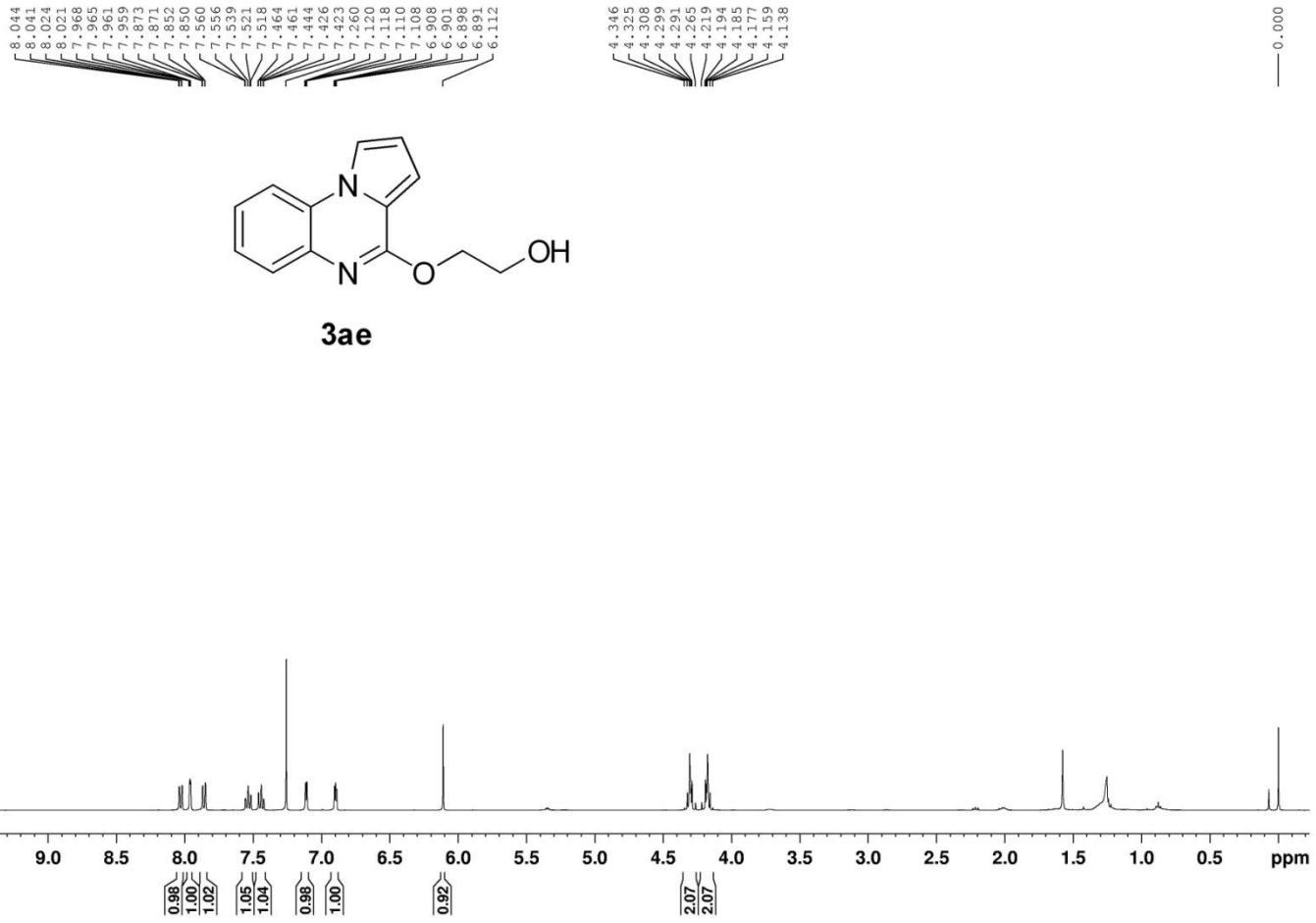
2.009
1.983
1.798
1.777
1.756
1.751
1.729
1.707
0.000

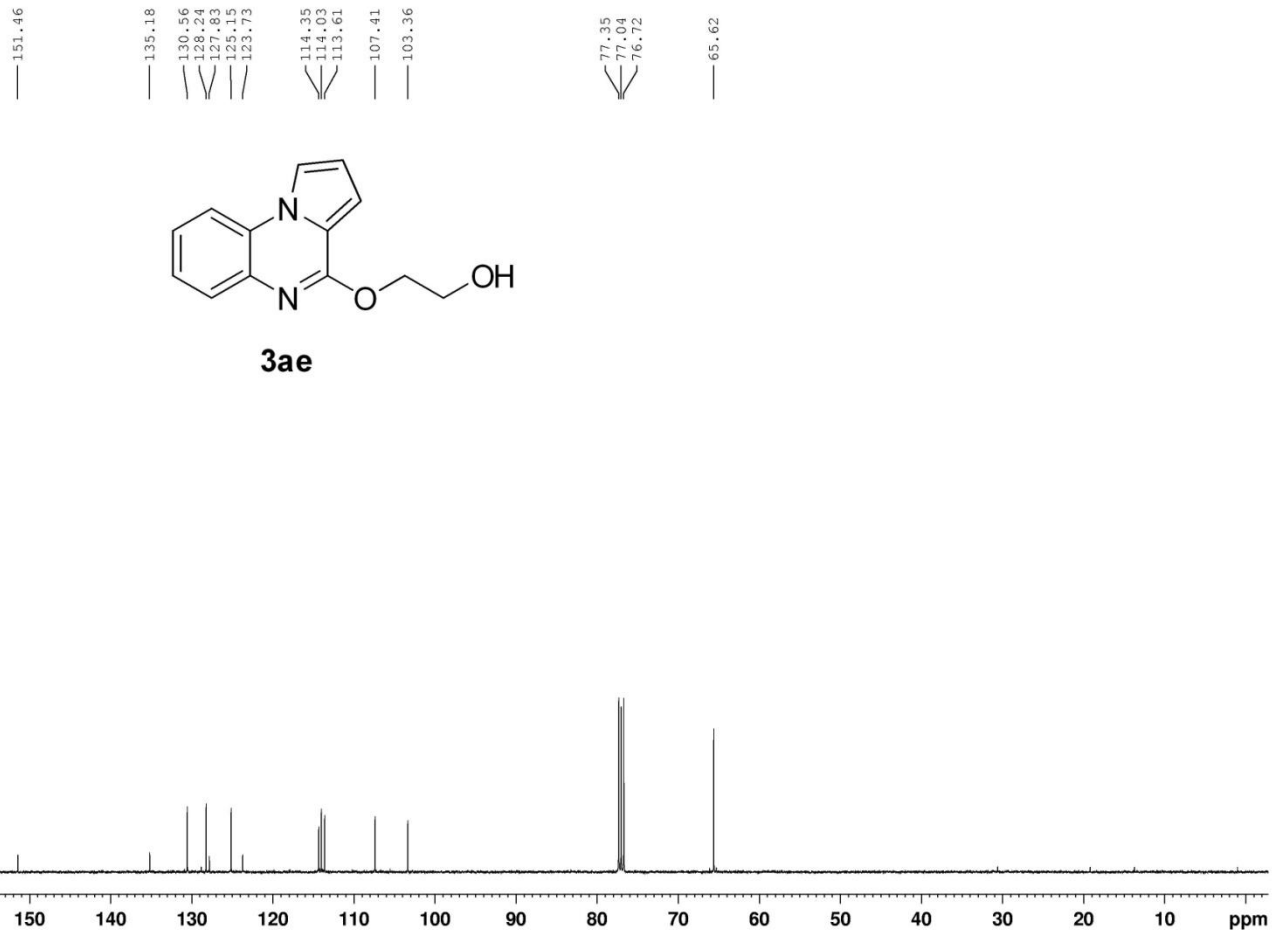

N
N
F3C
OH

3nd


0.91
2.05
1.00
1.00
1.02
2.04
2.07
1.13
2.23
2.20
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

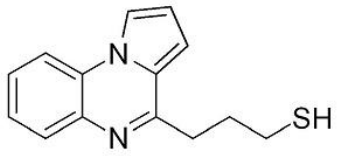

158.58
135.29
129.26
126.96
126.72
126.67
125.94
123.35
114.46
114.24
107.47
77.42
77.00
76.58
62.04
34.54
32.30
23.61
N
N
F3C
OH
3nd
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.044
8.041
8.024
8.021
7.968
7.965
7.961
7.959
7.873
7.871
7.852
7.850
7.560
7.556
7.539
7.521
7.518
7.464
7.461
7.444
7.426
7.423
7.260
7.120
7.118
7.110
7.108
6.908
6.901
6.898
6.891
6.112
4.346
4.325
4.308
4.299
4.291
4.265
4.219
4.194
4.185
4.177
4.159
4.138
0.000
N
N
O
OH
3ae
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
0.98
1.00
1.02
1.05
1.04
0.98
1.00
0.92
2.07
2.07

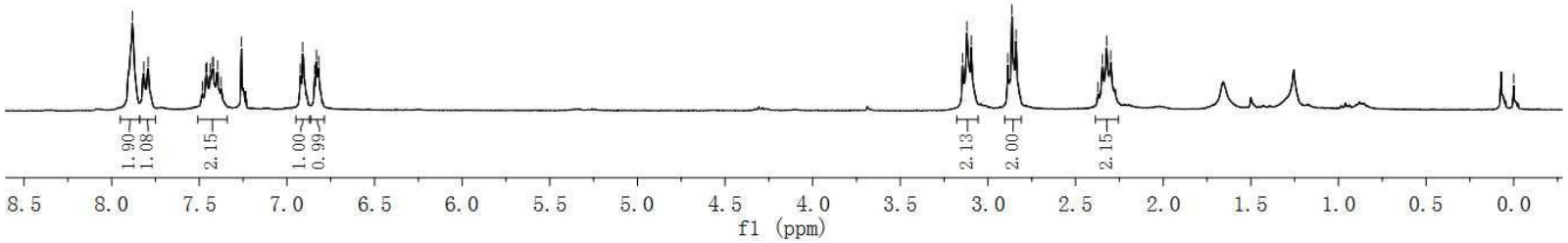

151.46
135.18
130.56
128.24
127.83
125.15
123.73
114.35
114.03
113.61
107.41
103.36
77.35
77.04
76.72
65.62
N
N
O
OH
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

3ae

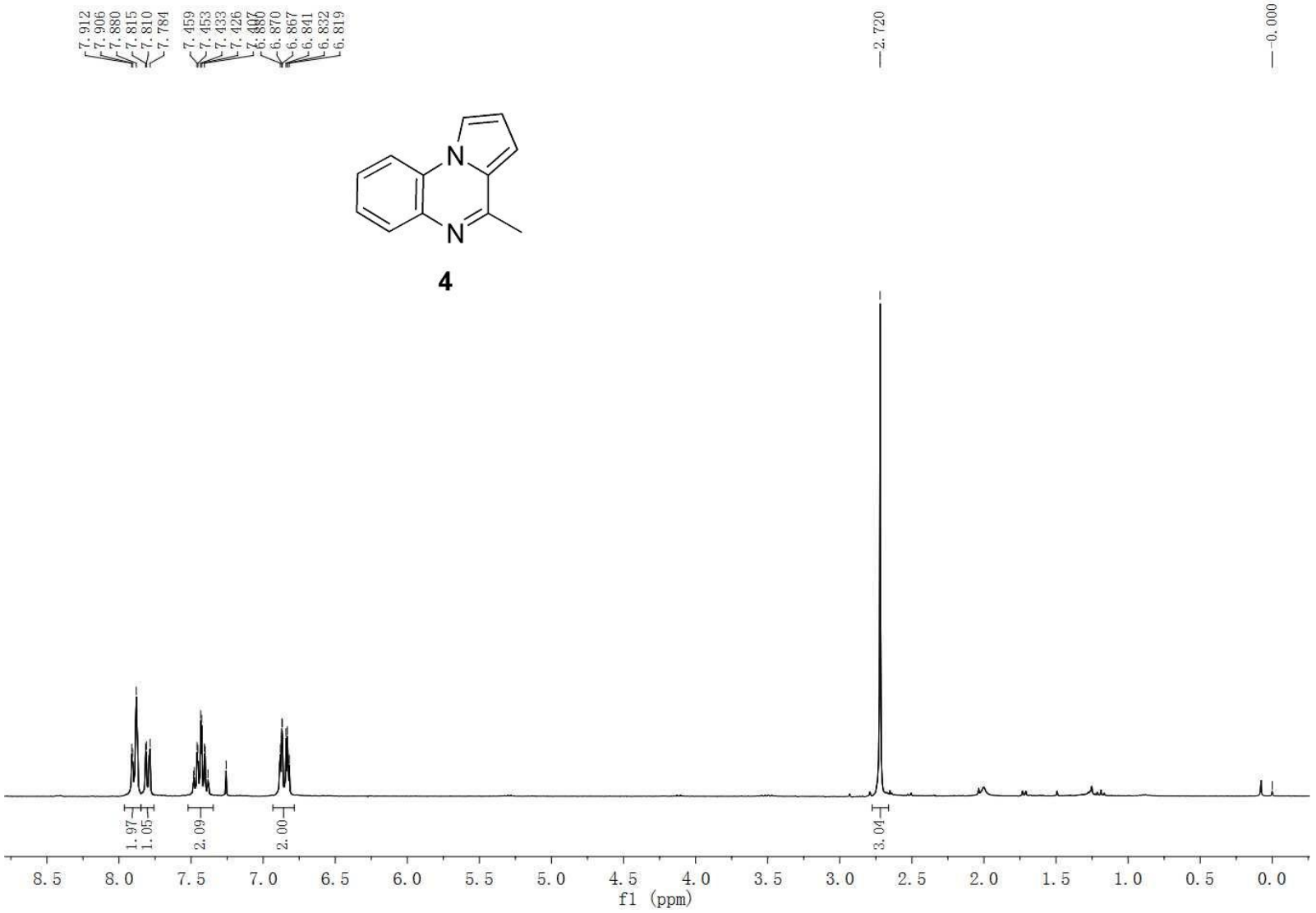

7.881
7.817
7.792
7.457
7.425
7.420
7.395
7.259
6.910
6.841
6.831
6.818
3.144
3.120
3.095
2.886
2.863
2.839
2.372
2.347
2.323
2.299
0.000

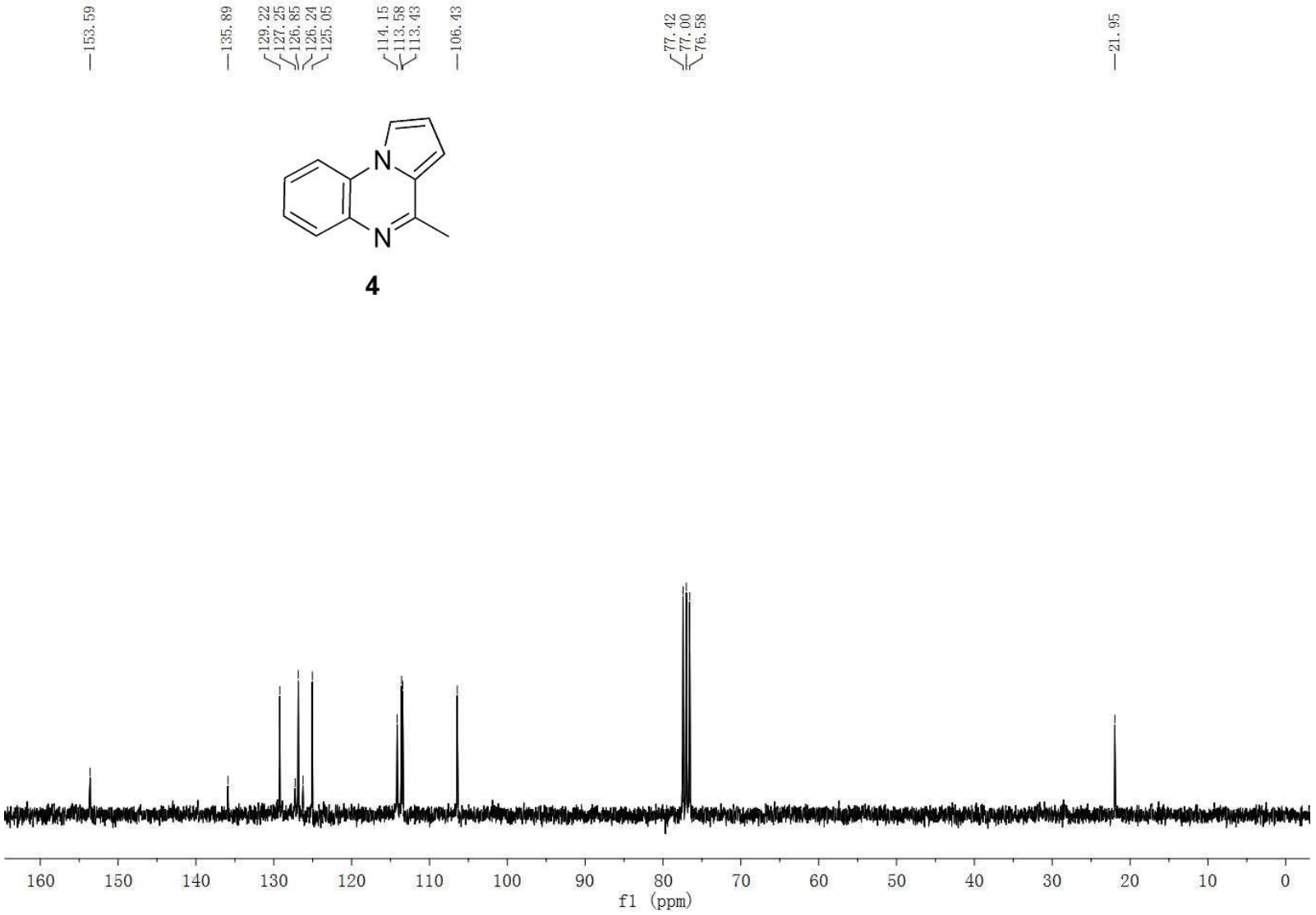

N
N
SH

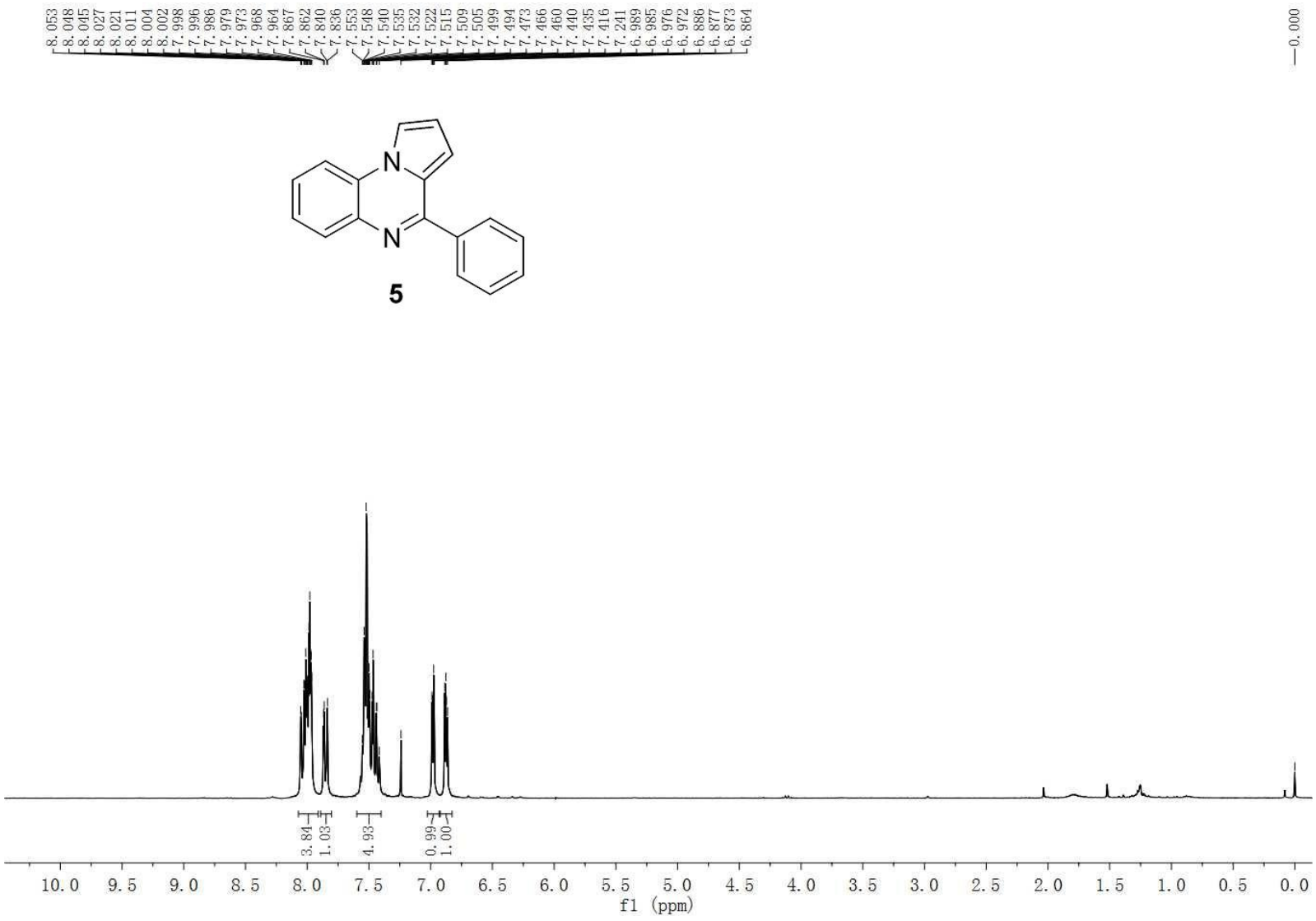
3ag

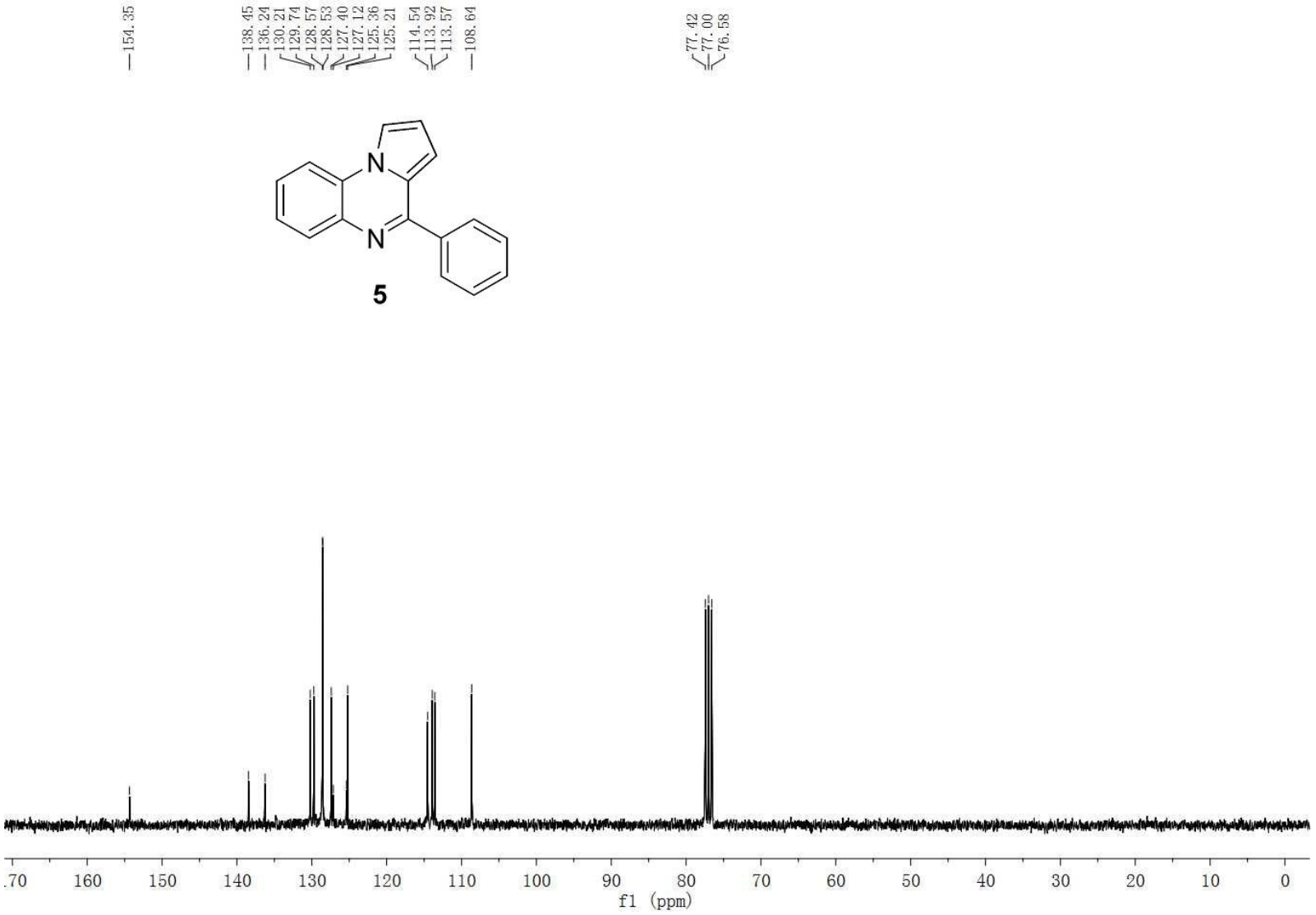

1.90
1.08
2.15
1.00
0.99
2.13
2.00
2.15
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

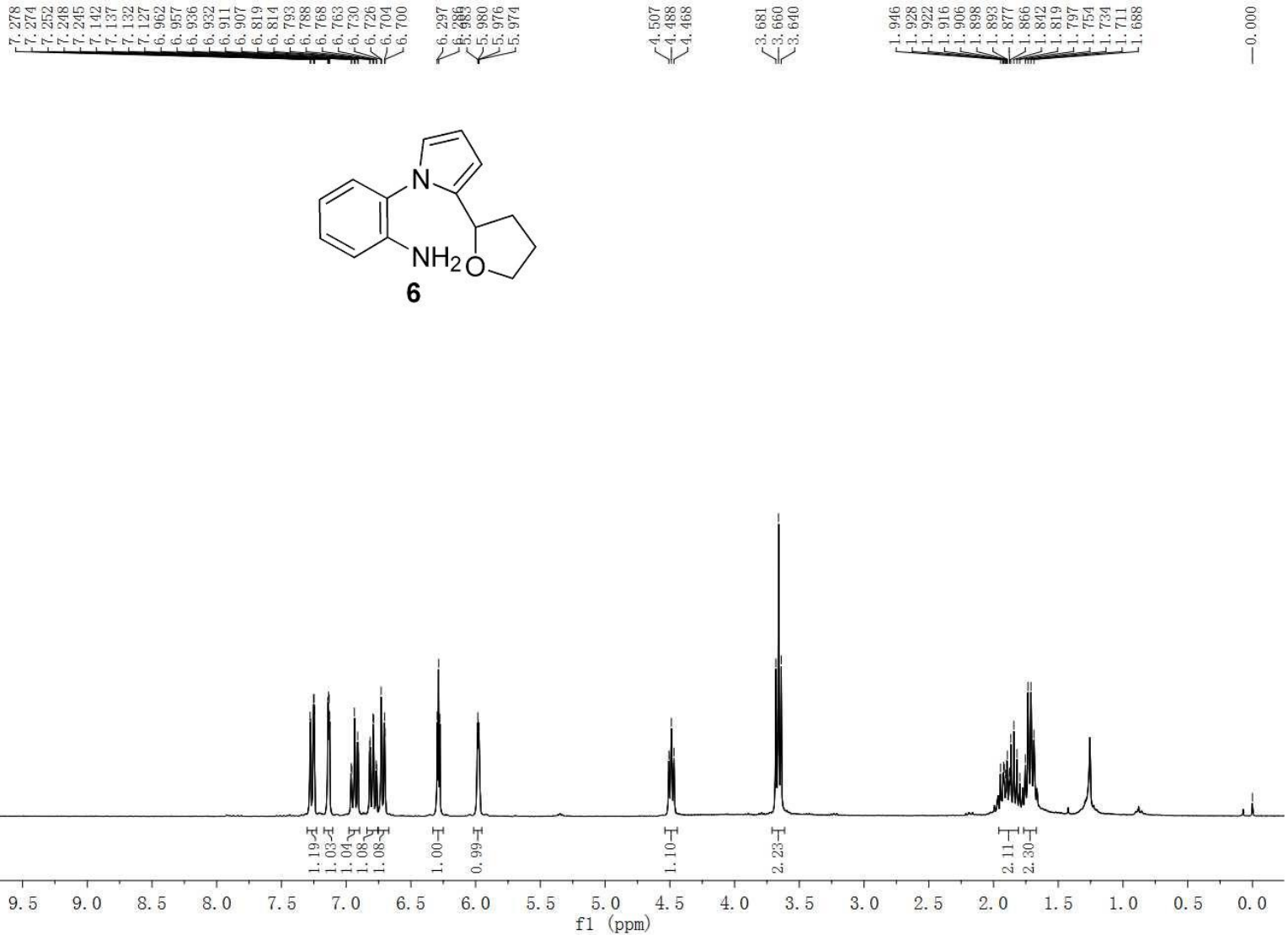

156.10
135.84
129.42
127.18
126.93
125.87
125.02
114.18
113.55
113.50
106.24
77.42
77.00
76.58
38.46
33.94
27.37
N
N
SH
3ag
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

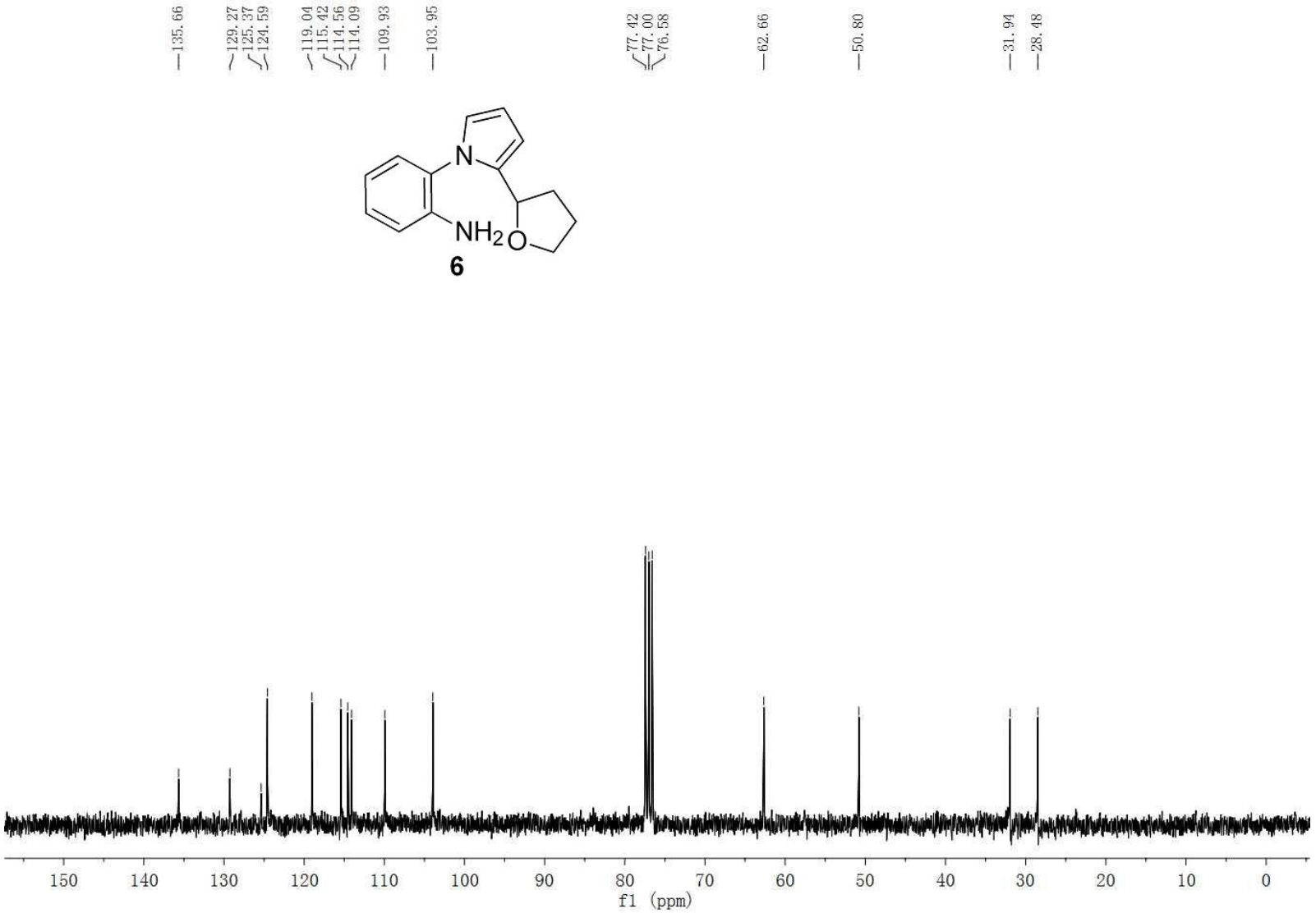

7.912
7.906
7.880
7.815
7.810
7.784
7.459
7.453
7.433
7.426
6.870
6.867
6.841
6.832
6.819
2.720
0.000
N
N
4
1.97
1.05
2.09
2.00
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

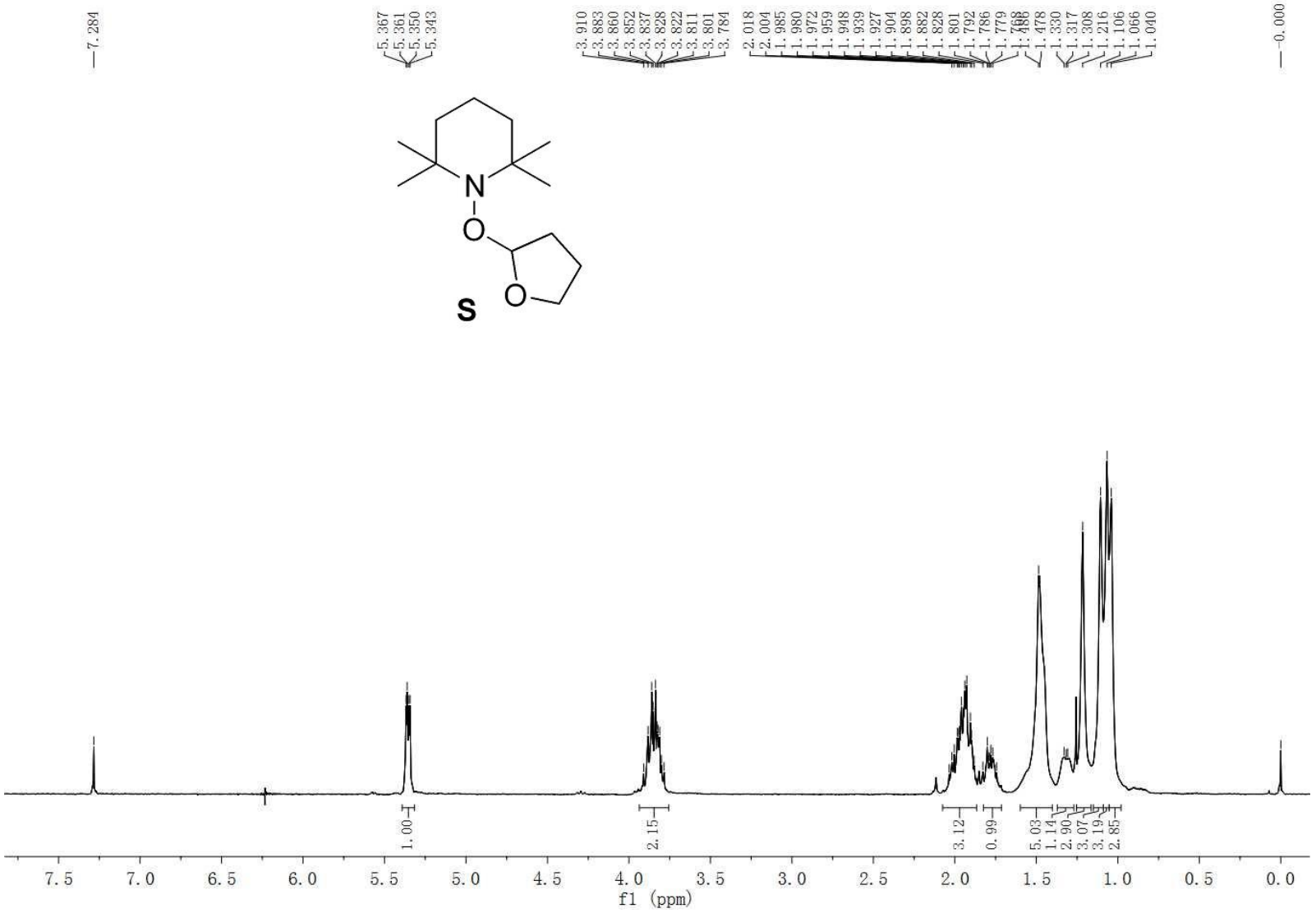

153.59
135.89
129.22
127.25
126.85
126.24
125.05
114.15
113.58
113.43
106.43
77.42
77.00
76.58
21.95
N
N
4
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

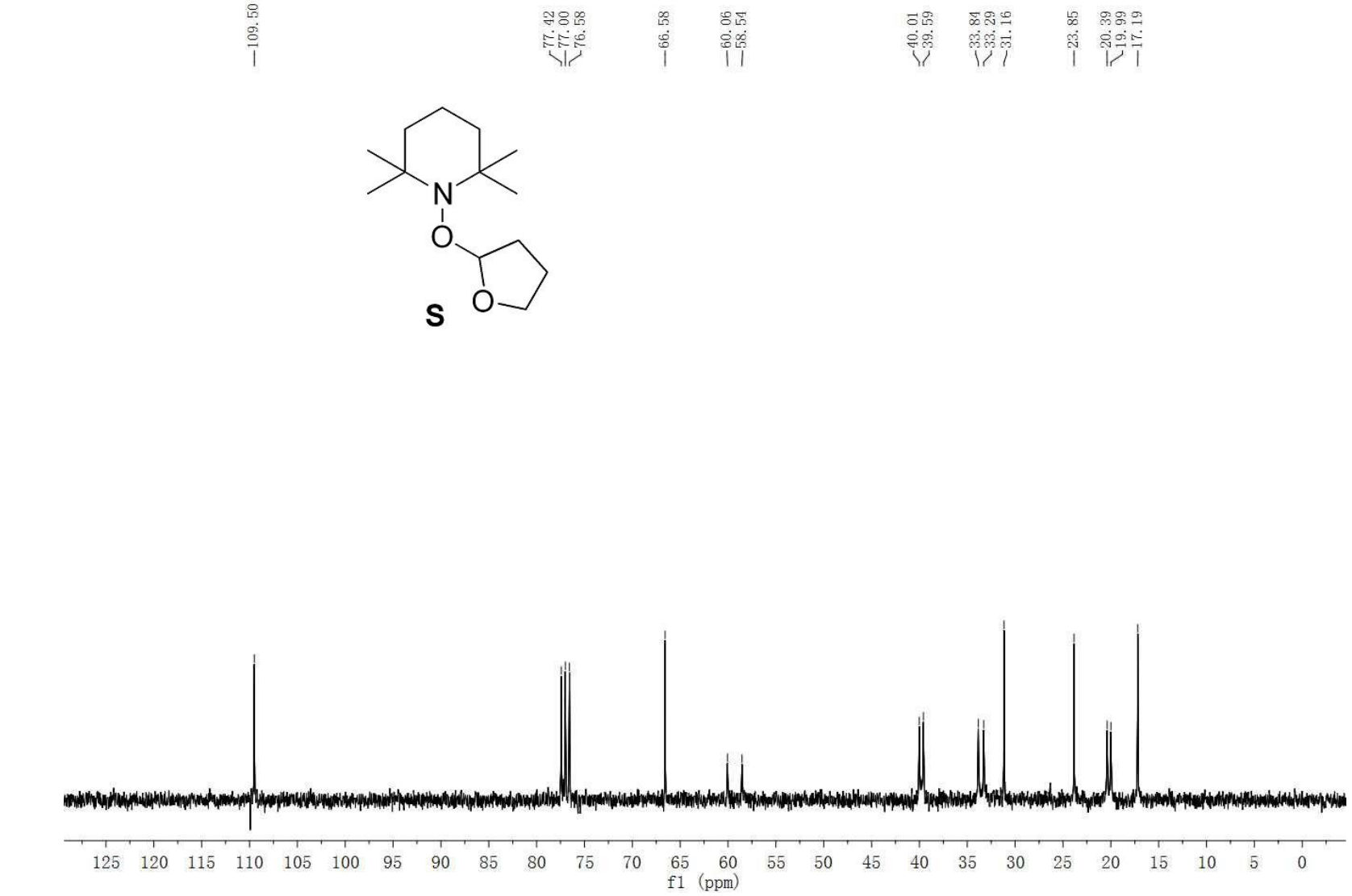

8.053
8.048
8.045
8.027
8.021
8.011
8.004
8.002
7.998
7.996
7.986
7.979
7.973
7.968
7.964
7.867
7.862
7.840
7.836
7.553
7.548
7.540
7.535
7.532
7.522
7.515
7.509
7.505
7.499
7.494
7.473
7.466
7.460
7.440
7.435
7.416
7.241
6.989
6.985
6.976
6.972
6.886
6.877
6.873
6.864
0.000
N
N
5
3.84
1.03
4.93
0.99
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


154.35
138.45
136.24
130.21
129.74
128.57
128.53
127.40
127.12
125.36
125.21
114.54
113.92
113.57
108.64
77.42
77.00
76.58
N
N
5
f1 (ppm)


7.278
7.274
7.252
7.248
7.245
7.142
7.137
7.132
7.127
6.962
6.957
6.936
6.932
6.911
6.907
6.819
6.814
6.793
6.788
6.768
6.763
6.730
6.726
6.704
6.700
6.297
5.980
5.976
5.974
4.507
4.488
4.468
3.681
3.660
3.640
1.946
1.928
1.922
1.916
1.906
1.898
1.893
1.877
1.866
1.842
1.819
1.797
1.754
1.734
1.711
1.688
0.000
N
NH2
O
6
1.19
1.03
1.04
1.08
1.08
1.00
0.99
1.10
2.23
2.11
2.30
f1 (ppm)


135.66
129.27
125.37
124.59
119.04
115.42
114.56
114.09
109.93
103.95
77.42
77.00
76.58
62.66
50.80
31.94
28.48
N
NH2
O
6
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.284
5.367
5.361
5.350
5.343
3.910
3.883
3.860
3.852
3.837
3.828
3.822
3.811
3.801
3.784
2.018
2.004
1.985
1.980
1.972
1.959
1.948
1.939
1.927
1.904
1.898
1.882
1.828
1.801
1.792
1.786
1.779
1.478
1.330
1.317
1.308
1.216
1.106
1.066
1.040
0.000
N
O
O
S
1.00
2.15
3.12
0.99
5.03
1.14
2.90
3.07
3.19
2.85
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)


109.50
77.42
77.00
76.58
66.58
60.06
58.54
40.01
39.59
33.84
33.29
31.16
23.85
20.39
19.99
17.19
N
O
O
S
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 0
f1 (ppm)