Supporting Information

Copper-catalyzed oxidative cyclization of 2-(1*H*-pyrrol-1-yl)aniline and alkylsilyl peroxides: a route to pyrrolo[1,2-*a*]quinoxalines

Zhenyu An,[‡,a] Man Miao,[‡,a] Fengkai Sun,[a] Xiao-Bing Lan,[a] Jian-Qiang Yu,[a] Xiaoli Guo,*[,a] and Jian Zhang*[,a,b]

[a] College of Pharmacy, Ningxia Characteristic Traditional Chinese Medicine Modern Engineering Research Center, Ningxia Medical University, Yinchuan, Ningxia Hui Autonomous Region, China.

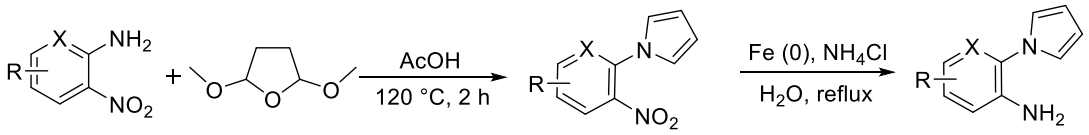
[b] State Key Laboratory of Oncogenes and Related Genes, Key Laboratory of Cell Differentiation and Apoptosis of Chinese Ministry of Education, Shanghai Jiao Tong University School of Medicine, Shanghai, China.

1. General Information

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker 400M and Mercury 600M in $CDCl_3$. 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.

2. Experimental Section

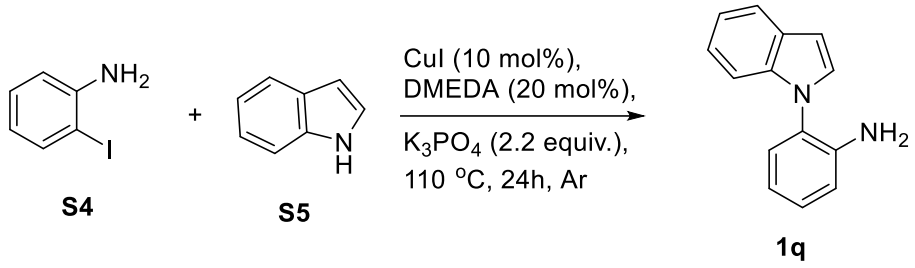
General procedure for the synthesis of 1b-1p.[1]



S1 **S2** **S3** **1a-1p**

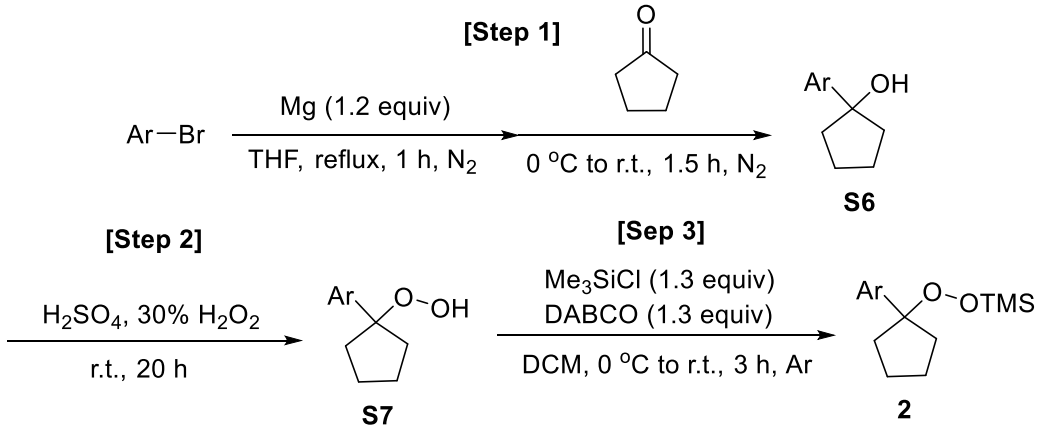
Compound **1a** was purchased from commercial sources and used as received. Substituted 2-(1*H*-pyrrol-1-yl)anilines **1b-1p** were prepared in the following method. A mixture of substituted **S1** (5 mmol) and **S2** (5 mmol) in acetic acid (25 mL) were refluxed for 2 h with vigorous stirring. After 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/ethyl acetate as eluent to provide the desired product **1b-1p**.

General procedure for the synthesis of 2-(1*H*-indol-1-yl)aniline 1q[2]:



A screw-cap vial containing a stirring bar, was added 2-iodoanilines **S1** (2.0 mmol), CuI (10 mol%), DMEDA (*N*,*N*′-Dimethyl-1,2-ethanediamine, 20 mol%), K_3PO_4 (2.2 equiv), pyrrole **S2** (1.2 equiv), and toluene (2.0 mL). The mixture was stirred at 110 °C 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-(1*H*-pyrrol-1-yl)aniline.

General procedure for the synthesis of 2a-2j. [3]



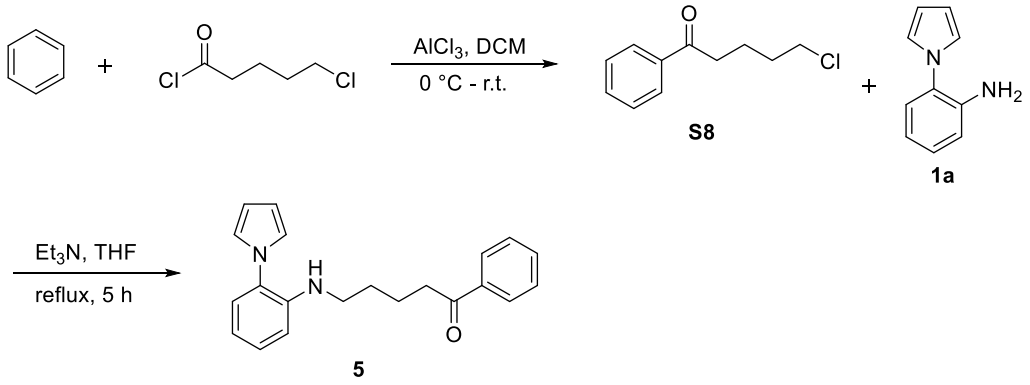
[Step 1] To flame-dried Mg turnings (1.44 g, 60 mmol, 1.2 equiv) in anhydrous THF (100 mL) was added ArBr (60 mmol, 1.2 equiv) carefully under N_2 atmosphere. After being refluxed for 1 h, the obtained ArMgBr/THF solution was cooled down to 0 °C and then cyclopentanone (4.4 mL, 50 mmol, 1.0 equiv) was added dropwisely. After being stirred at r.t. for 1.5 h, the reaction mixture was quenched with sat. NH_4Cl aq. at 0 °C and extracted with a solution of hexane/ethyl acetate (4/1) three times. The combined organic layer was dried over Na_2SO_4 and concentrated. The crude product **S6** was used for the next step without further purification.

[Step 2] To **S6** in a flask was added a solution of H_2SO_4/30% H_2O_2 aq. (1.5 mL/50

mL) slowly. After being stirred vigorously at room temperature for 20 h, the reaction mixture was diluted with H_2O (100 mL) and then extracted with CH_2Cl_2 three times. The combined organic layer was dried over Na_2SO_4 and concentrated. The residue was purified by flash column chromatography on silica gel (hexane/CH_2Cl_2 = 1/1) to afford hydroperoxide **S7** as a pale-yellow oil.

[Step 3] To a solution of **S7** (33 mmol, 1.0 equiv) and 1,4-diazabicyclo[2.2.2]octane (DABCO, 4.8 g, 43 mmol, 1.3 equiv) in anhydrous CH_2Cl_2 (100 mL) was added Me_3SiCl (5.4 mL, 43 mmol, 1.3 equiv) at 0 °C under argon atmosphere. After being stirred at r.t. for 3 h, the reaction mixture was diluted with hexane (80 mL) and passed through a celite pad to remove white precipitates, eluting with hexane. The obtained filtrate was concentrated and purified by flash column chromatography on silica gel (hexane/ethyl acetate = 20/1) to afford trimethyl((1-phenylcyclopentyl)peroxy)silanes **2** as a colorless oil.

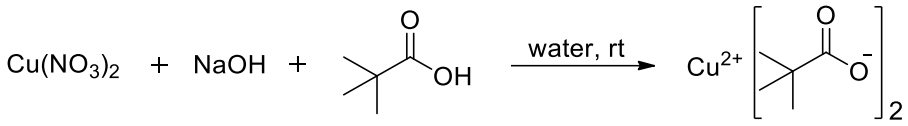
General procedure for the synthesis of 5. [4]



A flame-dry round-bottom flask equipped with a magnetic stirbar was charged with 50 mL of CH_2Cl_2 and cooled via an ice bath. $AlCl_3$ (24 mmol, 1.2 equiv) was added, followed by addition of the benzene (20 mmol, 1 equiv) dropwise. The stirred suspension becomes a clear, slightly brown solution over the course of 30 min. 5-Chloropentanoyl chloride (24 mmol, 1.2 equiv) was then added dropwise to the solution. The reaction was warmed to room temperature, stirred overnight and quenched by adding ice pieces at 0 ºC. Upon completion of reaction, the aqueous phase was separated and extracted with CH_2Cl_2. The combined organic phase was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to afford crude product **S8**. The crude material was used in the next step without further purification.

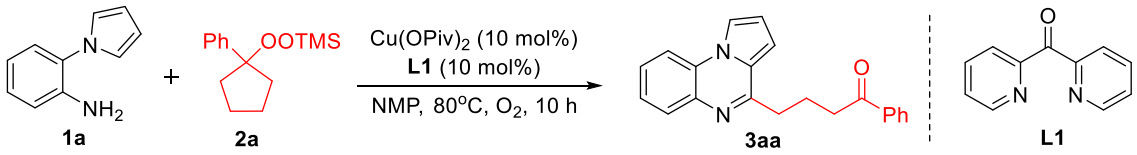
Triethyl amine (12 mmol, 1.2 equiv) was then added to a solution of 2-(1*H*-pyrrol-1-yl)aniline **1a** (11 mmol, 1.1 equiv) and **S8** (10 mmol) in THF (20 mL) and the mixture was warmed to reflux for 5 h. The mixture was cooled to ambient temperature and water was added. Then, the mixture was extracted twice with ethyl acetate and the organic layers were combined, washed with brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. Purification by flash column chromatography on silica gel (petroleum ether/ethyl acetate) gave the desired **5**.

General procedure for the synthesis of copper pivalate $Cu(OPiv)_2$.[5]



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 °C 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, 0.2 mmol), **2a** (2.0 equiv, 0.4 mmol), $Cu(OPiv)_2$ (10 mol%, 0.02 mmol), ligand **L1** (10 mol%, 0.02 mmol), NMP (3 mL) were stirred at 80 °C under oxygen atmosphere for 10 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 3na (CCDC 2287787)

An amount of 20 mg **3na** were dissolved in acetonitrile/petroleum ether (8:1) 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 crystal was kept at 149.98(10) K during data collection. Using Olex2, the structure was solved with the ShelXS structure solution program using Intrinsic Phasing and refined with the ShelXL 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.

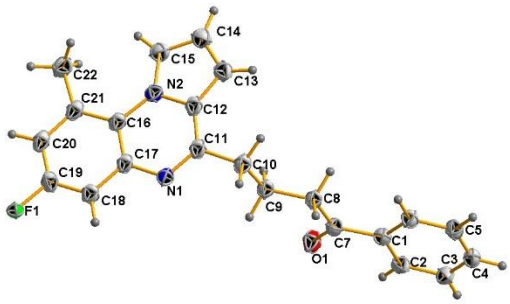


Figure S1. X-ray crystal structure of compound **3na**, thermal ellipsoids are drawn at 30% probability level

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

Identification code	**3na**
Empirical formula	$C_{22}H_{19}FN_2O$
Formula weight	346.39
Temperature/K	149.98(10)
Crystal system	monoclinic
Space group	P21/c
a/Å	7.38752(8)
b/Å	13.87031(12)
c/Å	16.86229(17)
α/°	90
β/°	102.3714(10)
γ/°	90

Volume/Å3	1687.71(3)
Z	4
ρcalcg/cm3	1.363
μ/mm-1	0.744
F(000)	728.0
Crystal size/mm3	0.18 × 0.15 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.334 to 154.956
Index ranges	-9 ≤ h ≤ 9, -17 ≤ k ≤ 14, -21 ≤ l ≤
Reflections collected	18850
Independent reflections	3410 [Rint = 0.0398, Rsigma =
Data/restraints/parameters	3410/0/236
Goodness-of-fit on F2	1.053
Final R indexes [I>=2σ (I)]	R1 = 0.0383, wR2 = 0.0989
Final R indexes [all data]	R1 = 0.0398, wR2 = 0.1000
Largest diff. peak/hole / e Å-3	0.18/-0.27

References

[1] (a) 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; (b) O. G. Kulinkovich *Chem. Rev.*, 2003, **103**, 2597.

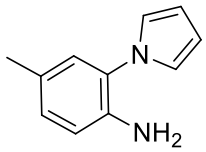
[2] Y. Wang, and Q. Zhu, *Adv. Synth. Catal.*, 2012, **354**, 1902.

[3] (a) R. Sakamoto, S. Sakurai, and K. Maruoka, *Chem. Eur. J.*, 2017, **23**, 9030; (b) R. Sakamoto, T. Kato, S. Sakurai, and K. Maruoka, *Org. Lett.*, 2018, **20**, 1400; (c) T. Seihara, S. Sakurai, T. Kato, R. Sakamoto, and K. Maruoka, *Org. Lett.*, 2019, *21*, 2477; (d) S. Sakurai, S. Tsuzuki, R. Sakamoto, and K. Maruoka, *J. Org. Chem.* 2020, **85**, 3973.

[4] (a) J. Wang, Y. Wang, D. Liu, and W. Zhang, *Adv. Synth. Catal.*, 2015, **357**, 3262; (b) B. Yang, K. Chansaenpak, H. Wu, L. Zhu, M. Wang, Z. Li, and H. Lu, *Chem. Commun.*, 2017, **53**, 3497.

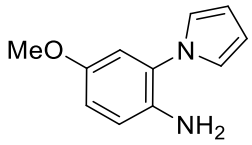
[5] L.-H. Xie and S. M. Paik, *Chem. Eur. J.*, 2011, **17**, 13653.

Characterization data of products



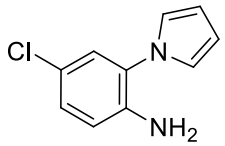
4-methyl-2-(1*H*-pyrrol-1-yl)aniline (1b)

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.



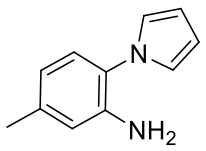
4-methoxy-2-(1*H*-pyrrol-1-yl)aniline (1c)

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.



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

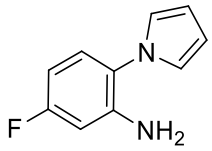
Yellow solid (729.6 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.14-7.09 (m, 2 H), 6.81-6.80 (m, 2 H), 6.71-6.69 (d, J = 8.4 Hz, 1 H), 6.34-6.33 (m, 2 H), 3.72 (br s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 140.7, 128.4, 128.0, 127.0, 122.6, 121.5, 116.9, 109.9.



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

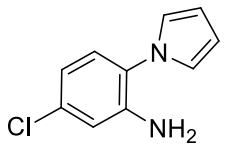
Yellow solid (627.8 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.03-7.01 (d, J = 8.0 Hz, 1 H), 6.80-6.79 (m, 2 H), 6.60-6.56 (m, 2 H), 6.32-6.31 (m, 2 H), 3.62

(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.



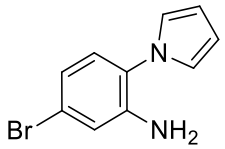
5-fluoro-2-(1*H*-pyrrol-1-yl)aniline (1f)

Yellow solid (589.4 mg, 67% 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), 144.5 (d, *J* = 11.7 Hz, 1 C), 128.6 (d, *J* = 10.7 Hz, 1 C), 123.6, 121.9, 109.6, 104.8 (d, *J* = 22.9 Hz, 1 C), 102.4 (d, *J* = 25.9 Hz, 1 C).



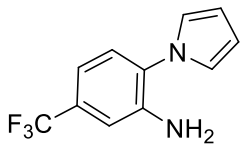
5-chloro-2-(1*H*-pyrrol-1-yl)aniline (1g)

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.



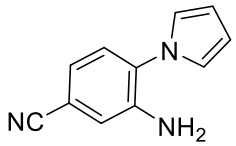
5-bromo-2-(1*H*-pyrrol-1-yl)aniline (1h)

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.



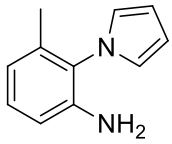
2-(1*H*-pyrrol-1-yl)-5-(trifluoromethyl)aniline (1i)

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, 131.3 (q, J = 32.2 Hz, 1 C), 130.0, 127.6, 124.2, 121.6, 115.2 (q, J = 3.7 Hz, 1 C), 113.0 (q, J = 3.7 Hz, 1 C), 110.3.



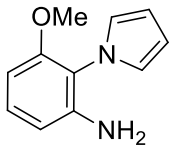
4-amino-3-(1*H*-pyrrol-1-yl)benzonitrile (1j)

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.



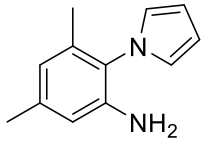
3-methyl-2-(1*H*-pyrrol-1-yl)aniline (1k)

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, 3 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.



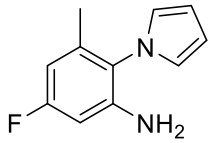
4-methoxy-2-(1*H*-pyrrol-1-yl)aniline (1l)

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.



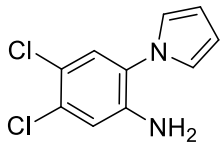
4,5-dimethyl-2-(1*H*-pyrrol-1-yl)aniline (1m)

Yellow solid (610.6 mg, 66% 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.



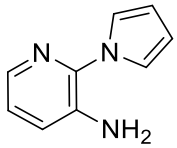
5-fluoro-3-methyl-2-(1*H*-pyrrol-1-yl)aniline (1n)

Yellow solid (589 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.65-6.64 (m, 2 H), 6.40-6.34 (m, 4 H), 3.64 (br s, 2 H), 2.00 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 163.8, 161.3, 145.3 (d, J = 12.3 Hz, 1 C), 139.0 (d, J = 10.5 Hz, 1 C), 121.7, 109.6, 106.1 (d, J = 22.5 Hz, 1 C), 99.6 (d, J = 25.7 Hz, 1 C), 17.4.



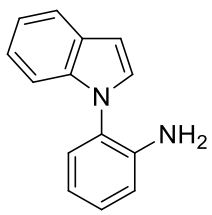
4,5-dichloro-2-(1*H*-pyrrol-1-yl)aniline (1o)

Yellow solid (760.5 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.



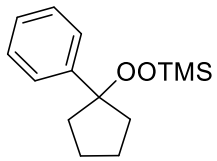
2-(1*H*-pyrrol-1-yl)pyridin-3-amine (1p)

Yellow solid (636 mg, 80% 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.



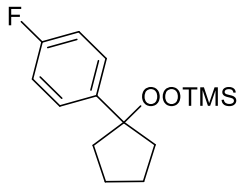
2-(1*H*-indol-1-yl)aniline (1q)

White solid (269.1 mg, 58% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.69-7.67 (m, 1 H), 7.22-7.11 (m, 6 H), 6.82-6.78 (m, 2 H), 6.67-6.66 (d, J = 23.1 Hz, 1 H), 3.48 (br, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.2, 136.5, 129.3, 128.7, 128.6, 124.9, 122.3, 121.1, 120.3, 118.6, 116.3, 110.9, 103.3, 102.6.



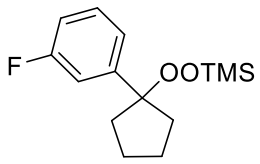
trimethyl((1-phenylcyclopentyl)peroxy)silane (2a)

Colorless oil (3.63 g, 29% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.47-7.46 (m, 2 H), 7.34-7.32 (m, 2 H), 7.26-7.24 (m, 1 H), 2.38-2.35 (m, 2 H), 1.94-1.88 (m, 4 H), 1.79-1.75 (m, 2 H), 0.10 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 144.5, 128.0, 127.2, 127.0, 95.4, 36.9, 24.6, -0.9.



((1-(4-fluorophenyl)cyclopentyl)peroxy)trimethylsilane (2b)

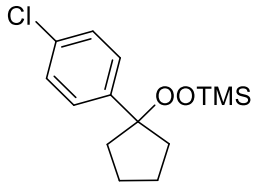
Colorless oil (3.48 g, 26% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.42-7.39 (m, 2 H), 7.02-6.97 (m, 2 H), 2.36-2.30 (m, 2 H), 1.90-1.84 (m, 4 H), 1.76-1.74 (m, 2 H), 0.08 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 161.7 (d, J = 243.2 Hz, 1 C), 140.0, 128.6 (d, J = 7.9 Hz, 1 C), 114.6 (d, J = 21.1 Hz, 1 C), 94.7, 36.7, 24.3, -1.2.



((1-(3-fluorophenyl)cyclopentyl)peroxy)trimethylsilane (2c)

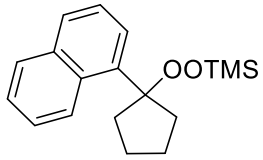
Colorless oil (3.22 g, 24% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.25-7.21 (m, 1 H), 7.18-7.12 (m, 2 H), 6.92-6.87 (m, 1 H), 2.30-2.24 (m, 2 H), 1.89-1.78 (m, 4 H), 1.80-1.71 (m, 2 H), 0.08 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 162.8 (d, J = 242.5 Hz, 1 C), 147.3 (d, J = 6.7 Hz, 1 C), 129.3 (d, J = 8.0 Hz, 1 C), 122.2 (d, J = 2.7 Hz, 1 C), 114.0 (d, J = 22.0 Hz, 1 C), 113.7 (d, J = 21.1 Hz, 1 C), 94.8, 36.9, 24.5,

-1.1.



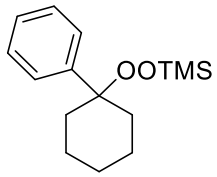
((1-(4-chlorophenyl)cyclopentyl)peroxy)trimethylsilane (2d)

Colorless oil (3.98 g, 28% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.37-7.34 (m, 2 H), 7.28-7.24 (m, 2 H), 2.31-2.26 (m, 2 H), 1.87-1.80 (m, 4 H), 1.76-1.72 (m, 2 H), 0.08 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.9, 132.7, 128.3, 128.0, 94.7, 36.7, 24.4, -1.1.



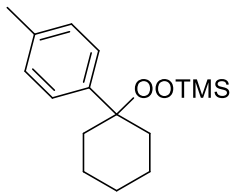
trimethyl((1-(naphthalen-1-yl)cyclopentyl)peroxy)silane (2e)

Colorless oil (3.02 g, 20% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 8.59-8.56 (m, 1 H), 7.88-7.85 (m, 1 H), 7.80-7.77 (m, 1 H), 7.64-7.61 (m, 1 H), 7.51-7.47 (m, 2 H), 7.44-7.40 (m, 1 H), 2.66-2.61 (m, 2 H), 2.29-2.21 (m, 2 H), 1.96-1.92 (m, 2 H), 1.79-1.74 (m, 2 H), 0.02 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 139.7, 134.7, 132.2, 128.8, 128.6, 127.3, 125.2, 125.2, 125.0, 124.7, 96.0, 36.8, 24.5, -1.1.



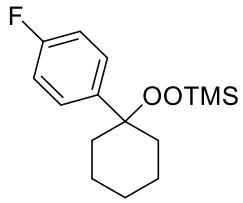
trimethyl((1-phenylcyclohexyl)peroxy)silane (2f)

Colorless oil (3.56 g, 27% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.46-7.43 (m, 2 H), 7.33-7.28 (m, 2 H), 7.24-7.21 (m, 1 H), 2.03-1.96 (m, 2 H), 1.80-1.71 (m, 4 H), 1.69-1.62 (m, 2 H), 1.58-1.52 (m, 2 H), 0.03 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 148.9, 128.0, 126.9, 125.9, 75.7, 39.3, 26.0, 22.7, -1.0.



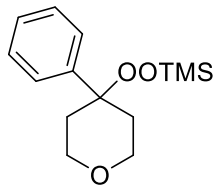
trimethyl((1-(*p*-tolyl)cyclohexyl)peroxy)silane (2g)

Colorless oil (3.48 g, 25% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.37 (d, J = 8.4 Hz, 2 H), 7.17 (d, J = 8.4 Hz, 2 H), 2.36 (s, 3 H), 2.16-2.12 (m, 2 H), 1.88-1.81 (m, 2 H), 1.77-1.66 (m, 3 H), 1.56-1.51 (m, 2 H), 1.36-1.29 (m, 1 H), 0.18 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 142.6, 136.4, 128.7, 126.2, 84.1, 34.6, 25.8, 22.4, 21.2, -0.9.



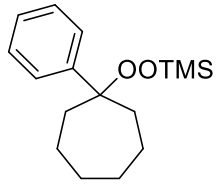
((1-(4-fluorophenyl)cyclohexyl)peroxy)trimethylsilane (2h)

Colorless oil (3.10 g, 22% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.45-7.40 (m, 2 H), 7.03-6.98 (m, 2 H), 2.14-2.10 (m, 1 H), 2.00-1.95 (m, 1 H), 1.83-1.65 (m, 5 H), 1.57-1.51 (m, 2 H), 1.33-1.23 (m, 1 H), 0.16 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 161.9 (d, J = 243.2 Hz, 1 C), 141.5, 127.9 (d, J = 7.8 Hz, 1 C), 114.7 (d, J = 20.9 Hz, 1 C), 83.8, 34.7, 25.7, 22.3, -1.0.



trimethyl((4-phenyltetrahydro-2*H*-pyran-4-yl)peroxy)silane (2i)

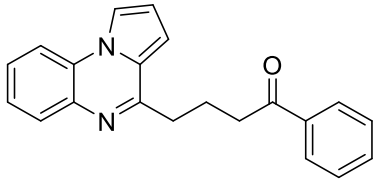
Colorless oil (2.66 g, 20% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 7.45-7.43 (m, 2 H), 7.37-7.33 (m, 2 H), 7.28-7.26 (m, 1 H), 3.86-3.77 (m, 4 H), 2.16-2.05 (m, 4 H), 0.13 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 144.0, 128.0, 127.1, 125.7, 81.3, 63.6, 34.2, -1.1.



trimethyl((1-phenylcycloheptyl)peroxy)silane (2j)

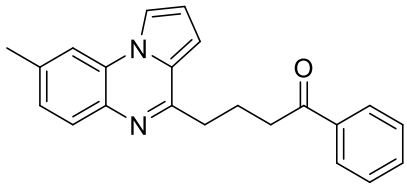
Colorless oil (2.36 g, 17% yield). H NMR (400 MHz, $CDCl_3$, ppm): δ 7.48-7.45 (m, 2 H), 7.36-7.30 (m, 2 H), 7.26-7.22 (m, 1 H), 2.13-2.02 (m, 4 H), 1.83-1.77 (m, 2 H),

1.70-1.65 (m, 2 H), 1.61-1.49 (m, 4 H), -0.04 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 146.7, 127.8, 126.4, 126.1, 88.6, 38.1, 30.2, 23.1, -1.0.



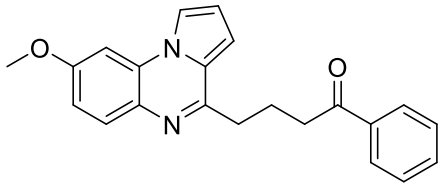
1-phenyl-4-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butan-1-one (3aa)

Colorless oil (43.3 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.96-7.95 (m, 2 H), 7.92-7.86 (m, 2 H), 7.83-7.80 (m, 1 H), 7.56-7.51 (m, 1 H), 7.49-7.39 (m, 4 H), 7.01-6.99 (m, 1 H),6.85-6.83 (m, 1 H), 3.18-3.11 (m, 4 H), 2.43-2.33 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 200.1, 156.7, 137.2, 136.1, 133.1, 129.6, 128.7, 128.2, 127.5, 127.1, 126.1, 125.2, 114.3, 113.8, 113.7, 106.6, 38.2, 35.0, 22.8; HRMS calcd for $C_{21}H_{19}N_2O$ $[M+H]^+$ 315.1492; found: 315.1494.



4-(8-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3ba)

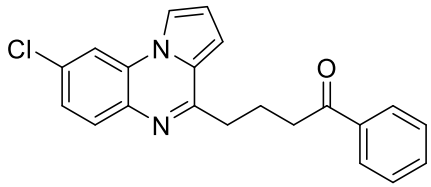
White solid (38.1 mg, 58% yield), melting point: 100-103 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.98-7.96 (m, 2 H), 7.87-7.86 (m, 1 H), 7.79 (d, *J* = 8.4 Hz, 1 H), 7.63 (s, 1 H), 7.56-7.52 (m, 1 H), 7.46-7.42 (m, 2 H), 7.25-7.22 (m, 1 H), 6.98-6.96 (m, 1 H), 6.84-6.82 (m, 1 H), 3.17-3.10 (m, 4 H), 2.54 (s, 3 H), 2.41-2.34 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 200.2, 155.6, 137.5, 137.2, 134.0, 133.1, 129.3, 128.7, 128.2, 127.2, 126.5, 126.2, 114.0, 113.9, 113.6, 106.3, 38.2, 34.9, 22.8, 21.9; HRMS calcd for $C_{22}H_{21}N_2O$ $[M+H]^+$ 329.1649; found: 329.1650.



4-(8-methoxypyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3ca)

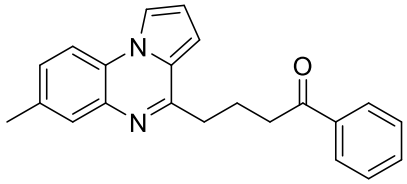
Colorless oil (31.0 mg, 45% yield). ^{1}H NMR (600 MHz, $CDCl_3$, ppm): 7.98-7.96 (m, 2 H), 7.83 (d, *J* = 9.0 Hz, 1 H), 7.80-7.79 (m, 1 H), 7.55-7.53 (m, 1 H), 7.45-7.43 (m,

2 H), 7.24 (d, *J* = 2.4 Hz, 1 H), 7.03-7.01 (m, 1 H),6.96-6.95 (m, 1 H), 6.85-6.84 (m, 1 H), 3.94 (s, 3 H), 3.16-3.14 (m, 2 H), 3.12-3.10 (m, 2 H), 2.39-2.34 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ = 200.2, 158.9, 154.0, 137.2, 133.0, 130.8, 130.5, 128.7, 128.3, 128.2, 126.1, 113.9, 113.8, 112.7, 106.1, 97.8, 55.9, 38.2, 34.8, 22.8; HRMS calcd for $C_{22}H_{21}N_2O_2$ $[M+H]^+$ 345.1598; found: 345.1599.



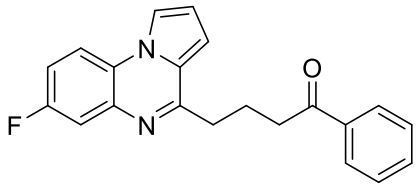
4-(8-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3da)

White solid (44.5 mg, 64% yield), melting point: 103-104ºC. ^{1}H NMR (600 MHz, $CDCl_3$, ppm): 7.96 (d, *J* = 8.4 Hz, 2 H), 7.81-7.79 (m, 3 H), 7.55-7.52 (m, 1 H), 7.45-7.42 (m, 2 H), 7.36-7.34 (m, 1 H), 7.00 (d, *J* = 4.2 Hz, 1 H),6.85-6.84 (m, 1 H), 3.16-3.14 (m, 2 H), 3.12-3.10 (m, 2 H), 2.40-2.34 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ = 200.0, 156.9, 137.2, 134.7, 133.1, 132.4, 130.8, 128.7, 128.2, 128.0, 126.0, 125.5, 114.6, 114.3, 113.9, 107.1, 38.1, 34.8, 22.5; HRMS calcd for $C_{21}H_{18}ClN_2O$ $[M+H]^+$ 349.1102; found: 349.1105.



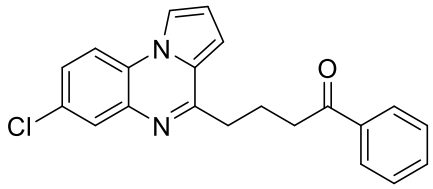
4-(7-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3ea)

Colorless oil (40.7 mg, 62% yield). ^{1}H NMR (600 MHz, $CDCl_3$, ppm): 7.98-7.96 (m, 2 H), 7.86-7.85 (m, 1 H), 7.72-7.70 (m, 2 H), 7.56-7.53 (m, 1 H), 7.45-7.43 (m, 2 H), 7.29-7.27 (m, 1 H), 6.98-6.97 (m, 1 H),6.82-6.81 (m, 1 H), 3.17-3.14 (m, 2 H), 3.14-3.11 (m, 2 H), 2.48 (s, 3 H), 2.40-2.35 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ = 200.2, 156.6, 137.2, 136.0, 135.0, 133.0, 129.5, 128.7, 128.2, 128.2, 126.0, 125.3, 114.1, 113.5, 113.4, 106.3, 38.2, 34.9, 22.7, 21.2; HRMS calcd for $C_{22}H_{21}N_2O$ $[M+H]^+$ 329.1649; found: 329.1651.



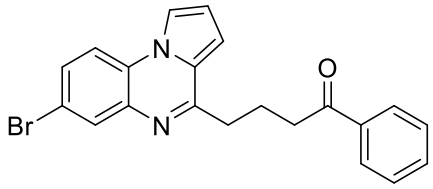
4-(7-fluoropyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3fa)

Colorless oil (41.8 mg, 63% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.98-7.95 (m, 2 H), 7.84-7.83 (m, 1 H), 7.77-7.73 (m, 1 H), 7.57-7.52 (m, 2 H), 7.46-7.42 (m, 2 H), 7.21-7.16 (m, 1 H), 7.01-7.00 (m, 1 H), 6.84-6.82 (m, 1 H), 3.17-3.10 (m, 4 H), 2.41-2.33 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 200.0, 159.9 (d, J = 241.9 Hz, 1 C), 157.9, 137.2 (d, J = 11.4 Hz, 1 C), 137.1, 133.1, 128.7, 128.2, 125.8, 124.1, 114.9 (d, J = 11.5 Hz, 1 C), 114.7 (d, J = 24.7 Hz, 1 C), 114.8, 114.5, 113.8, 107.0, 38.0, 34.9, 22.6; HRMS calcd for $C_{21}H_{18}FN_2O$ $[M+H]^+$ 333.1398; found: 333.1397.



4-(7-chloropyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3ga)

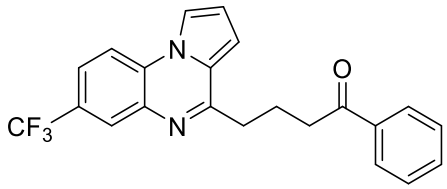
White solid (41.8 mg, 60% yield), melting point: 98-100^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$, ppm): 7.98-7.95 (m, 2 H), 7.87-7.86 (m, 1 H), 7.75-7.73 (d, J = 9.0 Hz, 1 H), 7.57-7.54 (m, 2 H), 7.46-7.44 (m, 2 H), 7.42-7.41 (m, 1 H), 7.21-7.16 (m, 1 H), 7.02-7.01 (m, 1 H), 6.86-6.85 (m, 1 H), 3.17-3.15 (m, 2 H), 3.13-3.11 (m, 2 H), 2.39-2.35 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): 200.0, 157.9, 137.2, 137.0, 133.1, 130.3, 129.1, 128.7, 128.2, 127.1, 126.1, 126.0, 114.9, 114.7, 114.1, 107.2, 38.1, 34.8, 22.5; HRMS calcd for $C_{21}H_{18}ClN_2O$ $[M+H]^+$ 349.1102; found: 349.1106.



4-(7-bromopyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3ha)

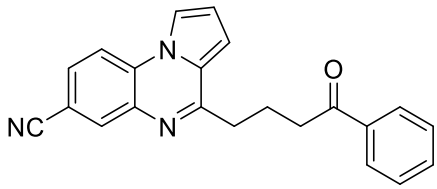
Colorless oil (43.1 mg, 55% yield). ^{1}H NMR (600 MHz, $CDCl_3$, ppm): 7.97-7.96 (m, 3 H), 7.84-7.83 (m, 1 H), 7.74 (d, J = 8.4 Hz, 1 H), 7.56-7.53 (m, 1 H), 7.51-7.49 (m, 1 H), 7.46-7.43 (m, 2 H), 7.02-7.01 (m, 1 H),6.87-6.86 (m, 1 H), 3.17-3.14 (m, 2 H),

3.12-3.10 (m, 2 H), 2.40-2.35 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ = 200.0, 157.1, 137.2, 135.1, 133.1, 131.0, 128.7, 128.4, 128.4, 128.2, 126.1, 120.2, 116.9, 114.6, 114.3, 107.2, 38.1, 34.9, 22.5; HRMS calcd for $C_{22}H_{18}BrN_2O$ $[M+H]^+$ 393.0597; found: 393.0592.



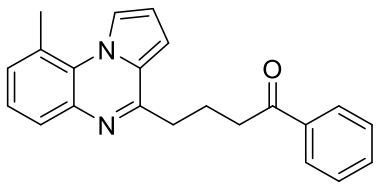
1-phenyl-4-(7-(trifluoromethyl)pyrrolo[1,2-*a*]quinoxalin-4-yl)butan-1-one (3ia)

Colorless oil (53.5 mg, 70% yield). ^{1}H NMR (600 MHz, $CDCl_3$, ppm): 8.16 (s, 1 H), 7.98-7.96 (m, 2 H), 7.92-7.91 (m, 1 H), 7.88 (d, *J* = 8.4 Hz, 1 H), 7.68-7.66 (m, 1 H), 7.56-7.53 (m, 1 H), 7.45-7.43 (m, 2 H), 7.06-7.05 (m, 1 H), 6.90-6.89 (m, 1 H), 3.18-3.16 (m, 2 H), 3.15-3.13 (m, 2 H), 2.41-2.37 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ = 200.0, 158.2, 137.2, 135.8, 133.1, 129.6, 128.7, 128.2, 127.2, 126.2, 124.2 (q, *J* = 270.3 Hz, 1 C), 123.5, 123.4, 115.0, 114.7, 114.4, 107.6, 38.0, 34.8, 22.4; HRMS calcd for $C_{22}H_{18}F_3N_2O$ $[M+H]^+$ 383.1366; found: 383.1362.



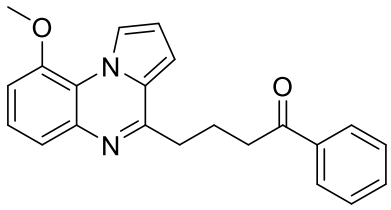
4-(4-oxo-4-phenylbutyl)pyrrolo[1,2-*a*]quinoxaline-7-carbonitrile (3ja)

White solid (52.9 mg, 78% yield), melting point: 137-139^{o}C. ^{1}H NMR (600 MHz, $CDCl_3$, ppm): 8.13 (d, *J* = 1.8 Hz, 1 H), 7.97-7.96 (m, 2 H), 7.91-7.90 (m, 1 H), 7.85 (d, *J* = 8.4 Hz, 1 H), 7.67-7.65 (m, 1 H), 7.57-7.55 (m, 1 H), 7.47-7.44 (m, 2 H),7.08-7.07 (m, 1 H), 6.93-6.91 (m, 1 H), 3.18-3.16 (m, 2 H), 3.14-3.11 (m, 2 H), 2.40-2.35 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ = 199.8, 158.7, 137.0, 135.9, 134.1, 133.2, 130.3, 129.7, 128.7, 128.1, 126.1, 118.6, 115.3, 115.2, 114.9, 108.4, 108.2, 37.9, 34.7, 22.2; HRMS calcd for $C_{22}H_{18}N_3O$ $[M+H]^+$ 340.1444; found: 340.1444.



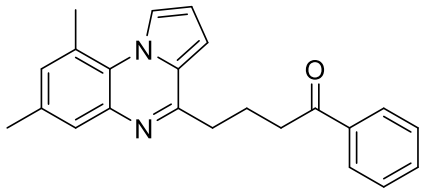
4-(9-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3ka)

White solid (35.4 mg, 54% yield), melting point: 84-85°C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 8.25-8.24 (m, 1 H), 7.97-7.95 (m, 2 H), 7.79-7.77 (m, 1 H), 7.54-7.49 (m, 1 H), 7.44-7.40 (m, 2 H), 7.30-7.22 (m, 2 H), 7.02-7.01 (m, 1 H), 6.82-6.80 (m, 1 H), 3.16-3.09 (m, 4 H), 2.89 (s, 3 H), 2.41-2.33 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 200.1, 156.1, 137.6, 137.1, 133.0, 130.6, 128.6, 128.2, 128.0, 127.7, 127.3, 125.4, 124.5, 120.0, 112.9, 105.9, 38.1, 34.7, 24.0, 22.6; HRMS calcd for $C_{22}H_{21}N_2O$ $[M+H]^+$ 329.1648; found: 329.1649.



4-(9-methoxypyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3la)

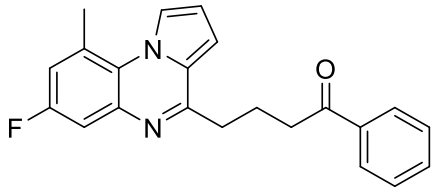
White solid (20.6 mg, 30% yield), melting point: 102-103°C. ^{1}H NMR (600 MHz, 3$CDCl_3$, ppm): 8.71-8.70 (m, 1 H), 7.97-7.96 (m, 2 H), 7.54-7.51 (m, 2 H), 7.44-7.41 (m, 2 H), 7.33-7.31 (m, 1 H), 7.02-7.01 (m, 1 H), 7.01-6.99 (m, 1 H),6.80-6.79 (m, 1 H), 4.04 (s, 3 H), 3.16-3.13 (m, 2 H), 3.13-3.11 (m, 2 H), 2.40-2.35 (m, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ = 200.2, 156.8, 149.9, 138.3, 137.1, 133.0, 128.6, 128.2, 126.5, 124.3, 122.1, 121.6, 118.8, 112.6, 108.7, 105.9, 56.3, 38.2, 34.8, 22.8; HRMS calcd for $C_{22}H_{21}N_2O_2$ $[M+H]^+$ 345.1598; found: 345.1598.



4-(7,9-dimethylpyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3ma)

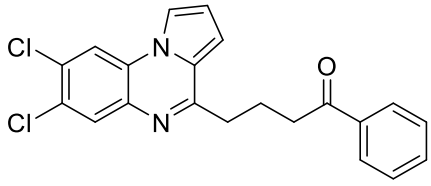
White solid (45.8 mg, 67% yield), melting point: 106-108°C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 8.23-8.22 (m, 1 H), 7.98-7.95 (m, 2 H), 7.58 (s, 1 H), 7.55-7.51 (m, 1 H), 7.45-7.41 (m, 2 H), 7.07 (s, 1 H),7.00-6.98 (m, 1 H), 6.80-6.78 (m, 1 H), 3.16-3.13 (m, 2 H), 3.12-3.08 (m, 2 H), 2.87 (s, 3 H), 2.42 (s, 3 H), 2.40-2.33 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 200.2, 156.0, 137.7, 137.2, 134.1, 133.0, 131.8,

128.6, 128.2, 128.0, 127.3, 125.6, 125.1, 119.7, 112.7, 105.7, 38.2, 34.7, 23.8, 22.7, 20.8; HRMS calcd for $C_{23}H_{23}N_2O$ $[M+H]^+$ 343.1805; found: 343.1807.



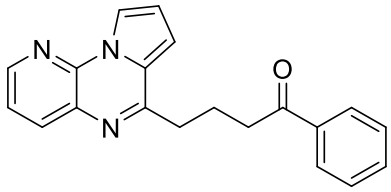
4-(7-fluoro-9-methylpyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3na)

White solid (47.1 mg, 68% yield), melting point: 103-105°C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 8.24-8.23 (m, 1 H), 7.98-7.96 (m, 2 H), 7.57-7.53 (m, 1 H), 7.47-7.43 (m, 3 H), 7.06-7.04 (m, 1 H), 7.03-7.00 (m, 1 H),6.84-6.82 (m, 1 H), 3.18-3.14 (m, 2 H), 3.13-3.09 (m, 2 H), 2.91 (s, 3 H), 2.40-2.33 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 200.1, 158.7 (d, J = 241.4 Hz, 1 C), 157.3, 139.0 (d, J = 11.8 Hz, 1 C), 137.1, 133.1, 128.7, 128.2, 127.4 (d, J = 8.7 Hz, 1 C), 127.2, 124.4, 120.0, 117.7 (d, J = 23.4 Hz, 1 C), 113.1 (d, J = 21.5 Hz, 1 C), 113.1, 106.4, 38.1, 34.7, 24.1, 22.6; HRMS calcd for $C_{22}H_{20}FN_2O$ $[M+H]^+$ 347.1554; found: 347.1552.



4-(7,8-dichloropyrrolo[1,2-*a*]quinoxalin-4-yl)-1-phenylbutan-1-one (3oa)

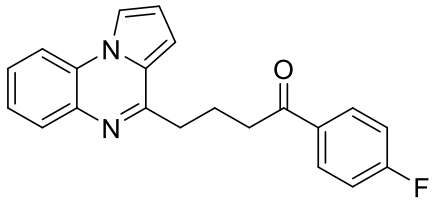
Colorless oil (46.6 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.98-7.96 (m, 3 H), 7.91 (s, 1 H), 7.83-7.81 (m, 1 H), 7.58-7.54 (m, 1 H), 7.48-7.44 (m, 2 H), 7.04-7.03 (m, 1 H), 6.89-6.87 (m, 1 H), 3.18-3.14 (m, 2 H), 3.13-3.10 (m, 2 H), 2.40-2.35 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 200.0, 158.1, 137.1, 135.5, 133.2, 130.6, 130.5, 128.7, 128.7, 128.2, 126.6, 125.9, 115.4, 114.9, 114.6, 107.7, 37.97, 34.8, 22.3; HRMS calcd for $C_{21}H_{17}Cl_2N_2O$ $[M+H]^+$ 383.0712; found: 383.0715.



1-phenyl-4-(pyrido[3,2-*e*]pyrrolo[1,2-*a*]pyrazin-6-yl)butan-1-one (3pa)

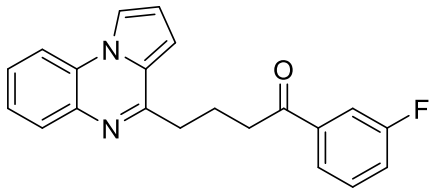
Colorless oil (25.8 mg, 41% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 8.49-8.48 (m,

1 H), 8.36-8.35 (m, 1 H), 8.17-8.14 (m, 1 H), 7.97-7.95 (m, 2 H), 7.56-7.52 (m, 1 H), 7.46-7.38 (m, 3 H), 7.06-7.05 (m, 1 H), 6.88-6.86 (m, 1 H), 3.18-3.12 (m, 4 H), 2.42-2.35 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 199.9, 157.8, 146.3, 139.6, 137.1, 136.8, 133.1, 130.9, 128.7, 128.2, 127.5, 121.5, 115.7, 114.2, 108.1, 38.0, 34.8, 22.6; HRMS calcd for $C_{20}H_{18}N_3O$ $[M+H]^+$ 316.1444; found: 316.1447.



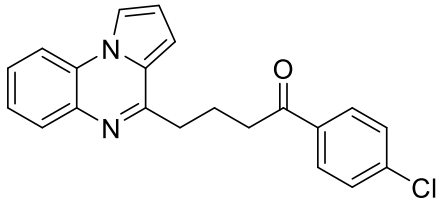
1-(4-fluorophenyl)-4-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butan-1-one (3ab)

White solid (45.2 mg, 68% yield), melting point: 107-109^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 8.02-7.98 (m, 2 H), 7.92-7.89 (m, 2 H), 7.85-7.82 (m, 1 H), 7.51-7.40 (m, 2 H), 7.13-7.08 (m, 2 H), 7.00-6.99 (m, 1 H), 6.86-6.85 (m, 1 H), 3.16-3.11 (m, 4 H), 2.42-2.34 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 198.5, 165.8 (d, J = 252.8 Hz, 1 C), 156.5, 136.0, 133.6, 130.9 (d, J = 9.1 Hz, 1 C), 129.6, 127.5, 127.2, 126.1, 125.2, 115.7 (d, J = 21.6 Hz, 1 C), 114.4, 113.8, 113.8, 106.6, 38.0, 34.8, 22.7; HRMS calcd for $C_{21}H_{18}FN_2O$ $[M+H]^+$ 333.1398; found: 333.1398.



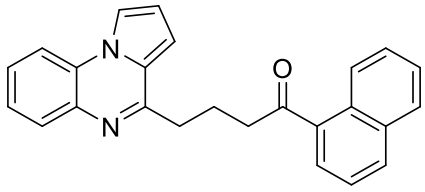
1-(3-fluorophenyl)-4-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butan-1-one (3ac)

Colorless oil (41.8 mg, 63% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.91-7.87 (m, 2 H), 7.80-7.78 (m, 1 H), 7.74-7.71 (m, 1 H), 7.67-7.63 (m, 1 H), 7.47-7.36 (m, 3 H), 7.24-7.19 (m, 1 H), 6.98-6.96 (m, 1 H), 6.84-6.82 (m, 1 H), 3.14-3.10 (m, 4 H), 2.41-2.34 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 198.8, 162.9 (d, J = 246.2 Hz, 1 C), 156.4, 139.1 (d, J = 5.0 Hz, 1 C), 135.9, 130.3 (d, J = 7.6 Hz, 1 C), 129.5, 127.4, 127.1, 126.0, 125.2, 123.9, 120.0 (d, J =21.3 Hz, 1 C), 114.9 (d, J = 22.2 Hz, 1 C), 114.4, 113.7, 113.7, 106.5, 38.2, 34.7, 22.5; HRMS calcd for $C_{21}H_{18}FN_2O$ $[M+H]^+$ 333.1398; found: 333.1399.



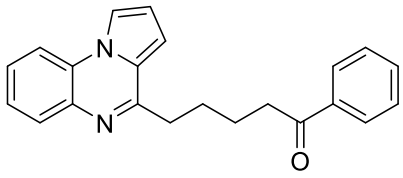
1-(4-chlorophenyl)-4-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butan-1-one (3ad)

White solid (45.2 mg, 65% yield), melting point: 104-106°C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.92-7.88 (m, 4 H), 7.85-7.82 (m, 1 H), 7.51-7.40 (m, 4 H), 6.99-6.98 (m, 1 H), 6.86-6.85 (m, 1 H), 3.15-3.10 (m, 4 H), 2.41-2.34 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 198.9, 156.5, 139.5, 136.0, 135.4, 129.7, 129.6, 129.0, 127.5, 127.2, 126.1, 125.3, 114.4, 113.8, 113.8, 106.6, 38.1, 34.8, 22.6; HRMS calcd for $C_{21}H_{18}ClN_2O$ $[M+H]^+$ 349.1102; found: 349.1106.



1-(naphthalen-1-yl)-4-(pyrrolo[1,2-*a*]quinoxalin-4-yl)butan-1-one (3ae)

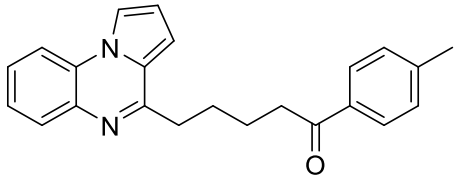
White solid (48.0 mg, 66% yield), melting point: 128-130°C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 8.61-8.58 (m, 1 H), 7.92-7.87 (m, 2 H), 7.85-7.80 (m, 3 H), 7.76-7.73 (m, 1 H), 7.56-7.52 (m, 1 H), 7.50-7.46 (m, 1 H), 7.44-7.35 (m, 3 H), 6.96-6.95 (m, 1 H), 6.80-6.79 (m, 1 H), 3.23-3.19 (m, 2 H), 3.16-3.12 (m, 2 H), 2.46-2.39 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 204.3, 156.5, 136.1, 135.9, 134.0, 132.5, 130.2, 129.5, 128.4, 127.9, 127.6, 127.3, 127.0, 126.4, 126.0, 125.8, 125.1, 124.4, 114.3, 113.7, 113.6, 106.5, 41.6, 34.9, 23.1; HRMS calcd for $C_{25}H_{21}N_2O$ $[M+H]^+$ 365.1648; found: 365.1644.



1-phenyl-5-(pyrrolo[1,2-*a*]quinoxalin-4-yl)pentan-1-one (3af)

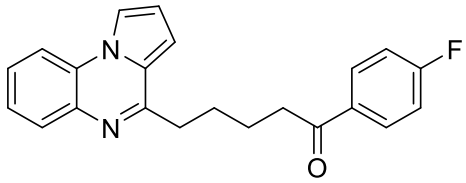
Colorless oil (40.7 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.96-7.89 (m, 4 H), 7.83-7.80 (m, 1 H), 7.55-7.51 (m, 1 H), 7.46-7.39 (m, 4 H), 6.92-6.91 (m, 1 H), 6.85-6.84 (m, 1 H), 3.10-3.04 (m, 4 H), 2.05-1.99 (m, 2 H), 1.97-1.91 (m, 2 H); ^{13}C

NMR (100 MHz, $CDCl_3$, ppm): δ = 200.3, 157.1, 137.1, 136.1, 133.0, 129.5, 128.7, 128.2, 127.4, 127.1, 126.1, 125.2, 114.3, 113.8, 113.6, 106.4, 38.5, 35.6, 28.1, 24.5; HRMS calcd for $C_{22}H_{21}N_2O$ $[M+H]^+$ 329.1648; found: 329.1652.



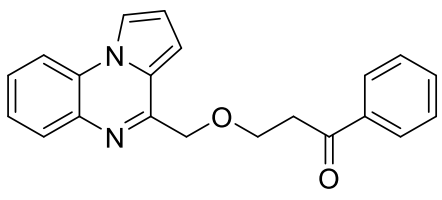
5-(pyrrolo[1,2-*a*]quinoxalin-4-yl)-1-(*p*-tolyl)pentan-1-one (3ag)

Colorless oil (36.3 mg, 53% yield). ^1H NMR (400 MHz, $CDCl_3$, ppm): 7.91-7.78 (m, 5 H), 7.46-7.38 (m, 2 H), 7.22-7.20 (m, 2 H), 6.91-6.89 (m, 1 H), 6.83-6.82 (m, 1 H), 3.09-3.00 (m, 4 H), 2.38 (s, 3 H), 2.05-1.89 (m, 4 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 200.0, 157.0, 143.7, 136.0, 134.6, 129.5, 129.3, 128.3, 127.3, 127.0, 126.0, 125.1, 114.3, 113.7, 113.6, 106.4, 38.4, 35.6, 28.1, 24.6, 21.7; HRMS calcd for $C_{23}H_{23}N_2O$ $[M+H]^+$ 343.1805; found: 343.1810.



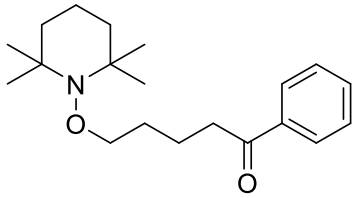
1-(4-fluorophenyl)-5-(pyrrolo[1,2-*a*]quinoxalin-4-yl)pentan-1-one (3ah)

White solid (44.3 mg, 64% yield), melting point: 113-115ºC. ^1H NMR (400 MHz, $CDCl_3$, ppm): 7.95-7.89 (m, 3 H), 7.87-7.86 (m, 1 H), 7.79-7.76 (m, 1 H), 7.46-7.37 (m, 2 H), 7.09-7.04 (m, 2 H), 6.90-6.89 (m, 1 H), 6.83-6.81 (m, 1 H), 3.08-3.05 (m, 2 H), 3.02-2.98 (m, 2 H), 2.05-1.97 (m, 2 H), 1.94-1.87 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 198.6, 165.7 (d, J = 252.8 Hz, 1 C), 156.9, 135.9, 133.4, 130.7 (d, J = 9.2 Hz, 1 C), 129.4, 127.3, 127.0, 125.9, 125.1, 115.5 (d, J = 21.6 Hz, 1 C), 114.3, 113.7, 113.6, 106.3, 38.3, 35.5, 27.9, 24.4; HRMS calcd for $C_{22}H_{20}FN_2O$ $[M+H]^+$ 347.1554; found: 347.1559.



1-phenyl-3-(pyrrolo[1,2-*a*]quinoxalin-4-ylmethoxy)propan-1-one (3ai)

Colorless oil (28.5 mg, 45% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): 7.99-7.97 (m, 2 H), 7.93-7.90 (m, 2 H), 7.85-7.83 (m, 1 H), 7.57-7.53 (m, 1 H), 7.50-7.40 (m, 4 H), 7.02-7.01 (m, 1 H), 6.87-6.85 (m, 1 H), 3.19-3.13 (m, 4 H), 2.42-2.35 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ 200.4, 156.9, 137.3, 136.2, 133.3, 129.8, 128.9, 128.4, 127.6, 127.4, 126.3, 125.4, 114.6, 114.0, 113.9, 106.9, 38.3, 35.2, 23.0; HRMS calcd for $C_{22}H_{21}N_2O$ $[M+H]^+$ 331.1441; found: 331.1445.

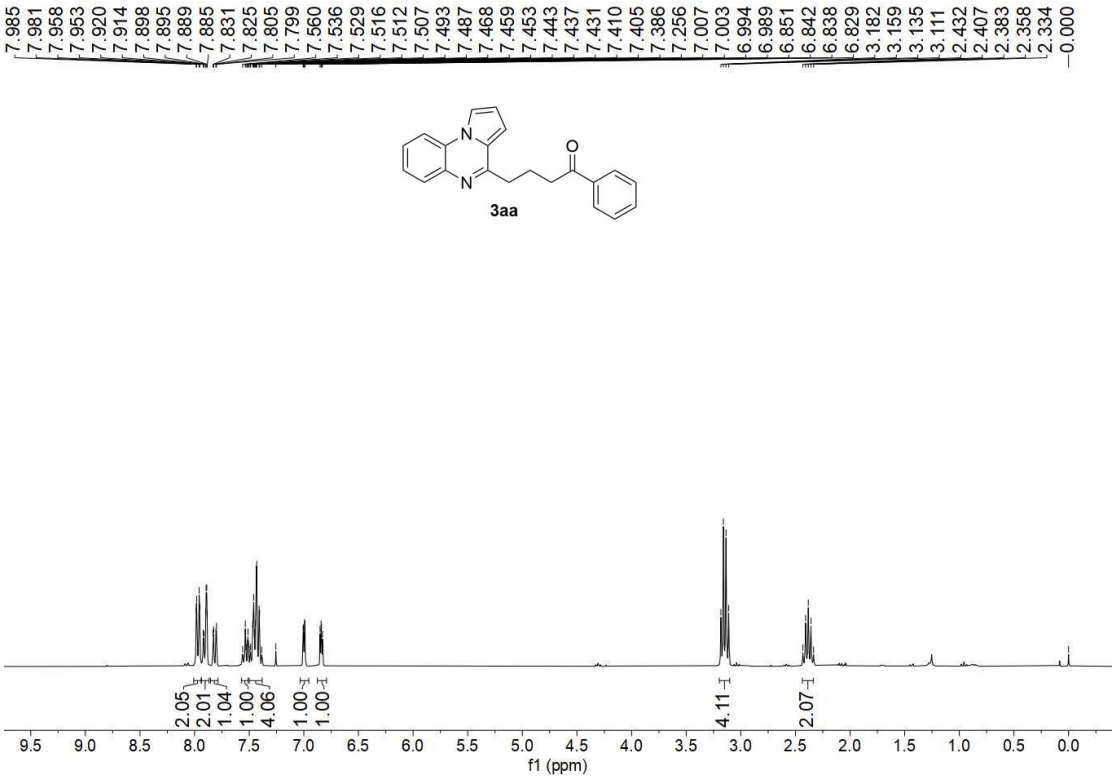


1-phenyl-5-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)pentan-1-one (4)

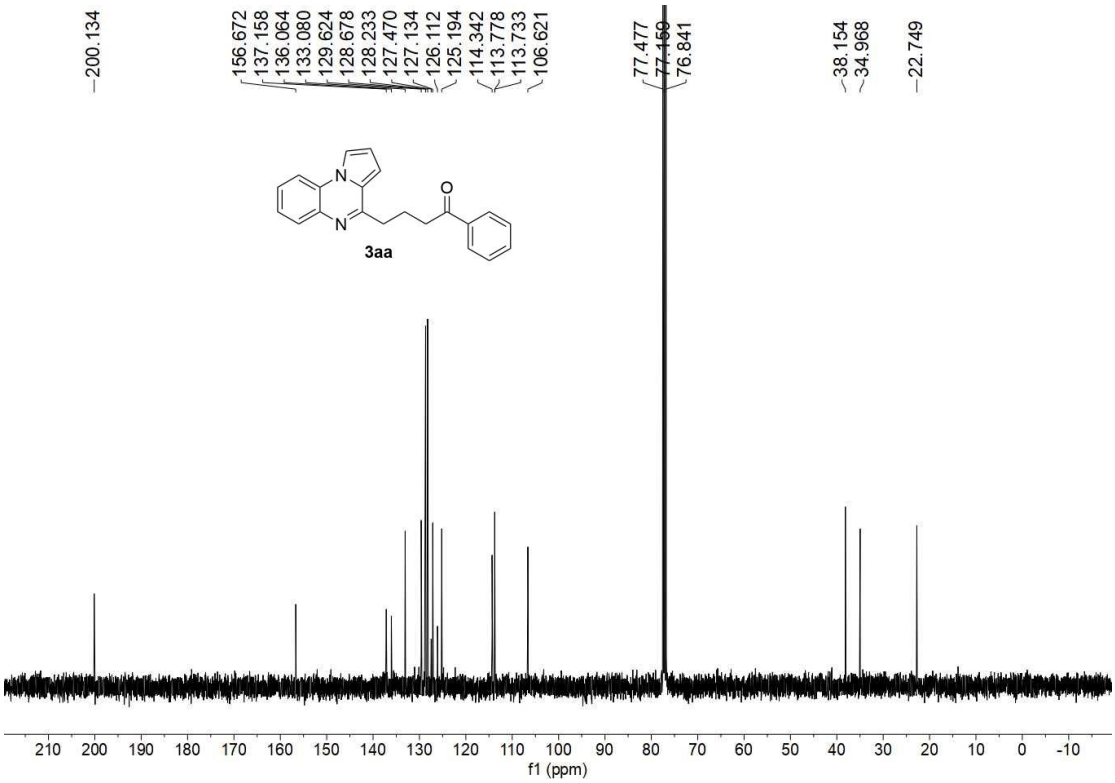
Colorless oil (29.8 mg, 47% yield). ^{1}H NMR (600 MHz, $CDCl_3$, ppm): 7.97-7.96 (m, 2 H), 7.56-7.54 (m, 1 H), 7.47-7.44 (m, 2 H), 3.80-3.78 (m, 2 H), 3.03-3.00 (m, 2 H), 1.87-1.81 (m, 2 H), 1.65-1.60 (m, 2 H), 1.56-1.51 (m, 1 H), 1.47-1.43 (m, 4 H), 1.32-1.26 (m, 1 H), 1.15 (s, 6 H), 1.09 (s, 6 H); ^{13}C NMR (150 MHz, $CDCl_3$, ppm): δ = 200.4, 137.2, 133.0, 128.7, 128.2, 76.6, 59.8, 39.7, 38.7, 33.2, 28.6, 21.6, 20.3, 17.3; HRMS calcd for $C_{20}H_{32}NO_2$ $[M+H]^+$ 318.2428; found: 318.2430.

Copies of NMR spectra

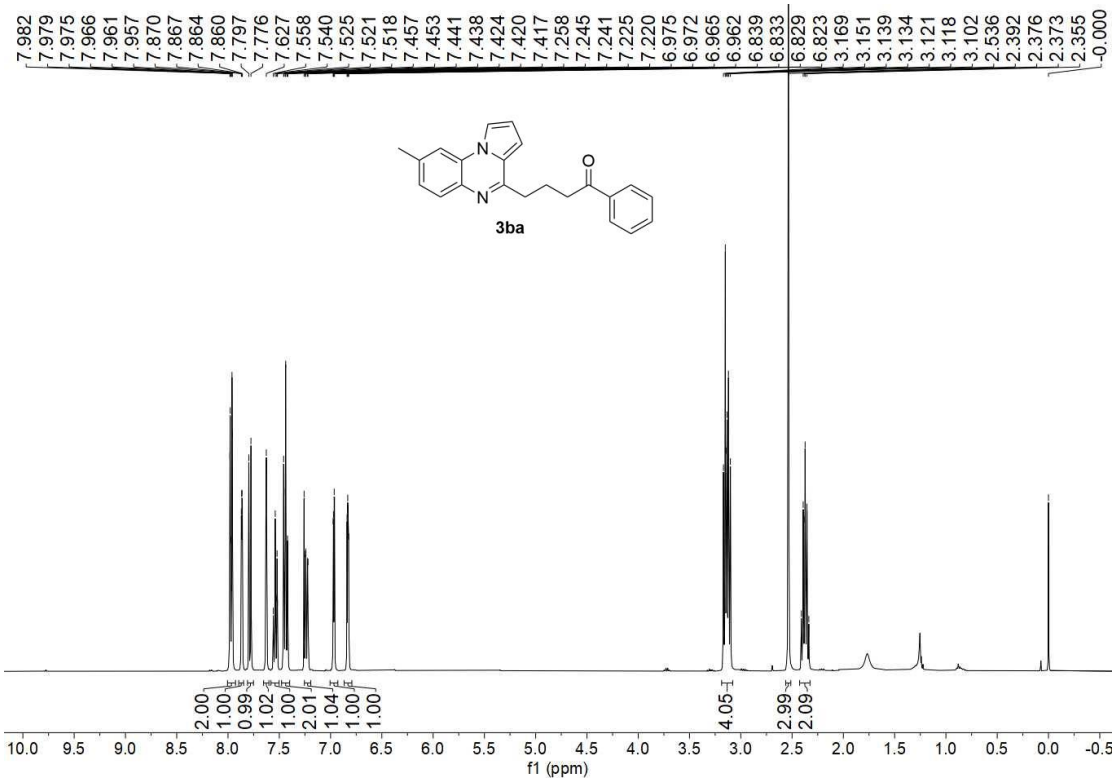
^{1}H NMR (400MHz, $CDCl_3$) of compound **3aa**



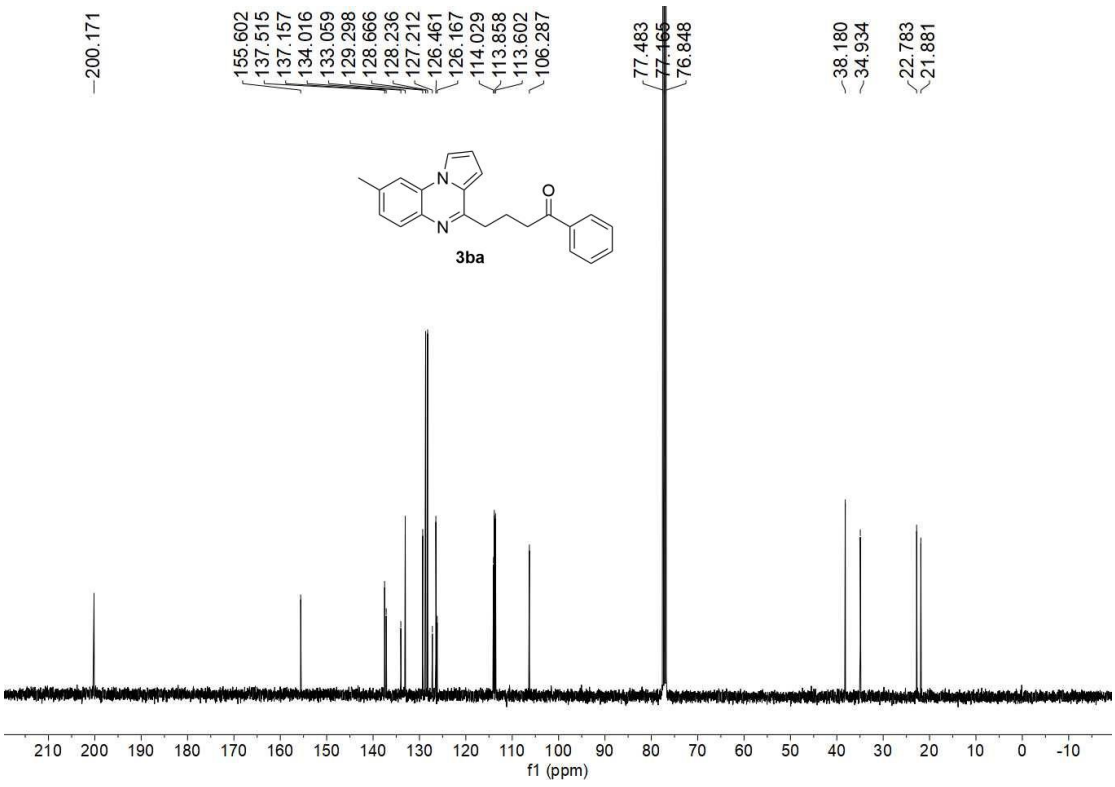
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3aa**



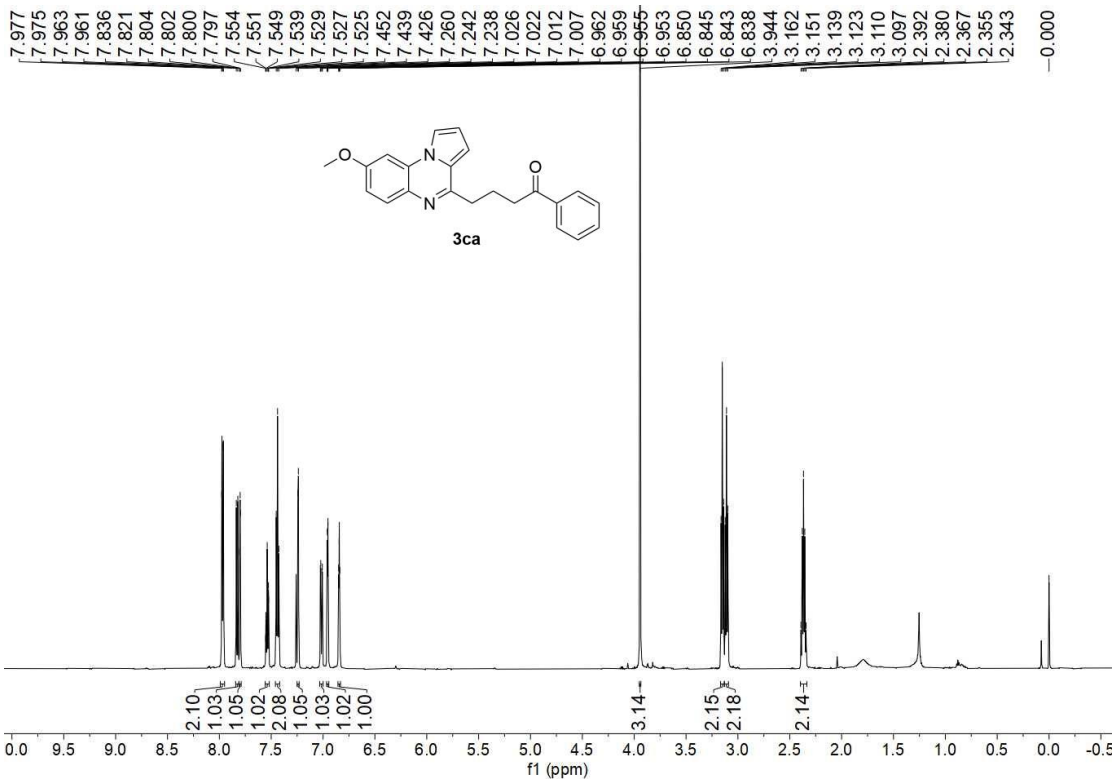
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ba**



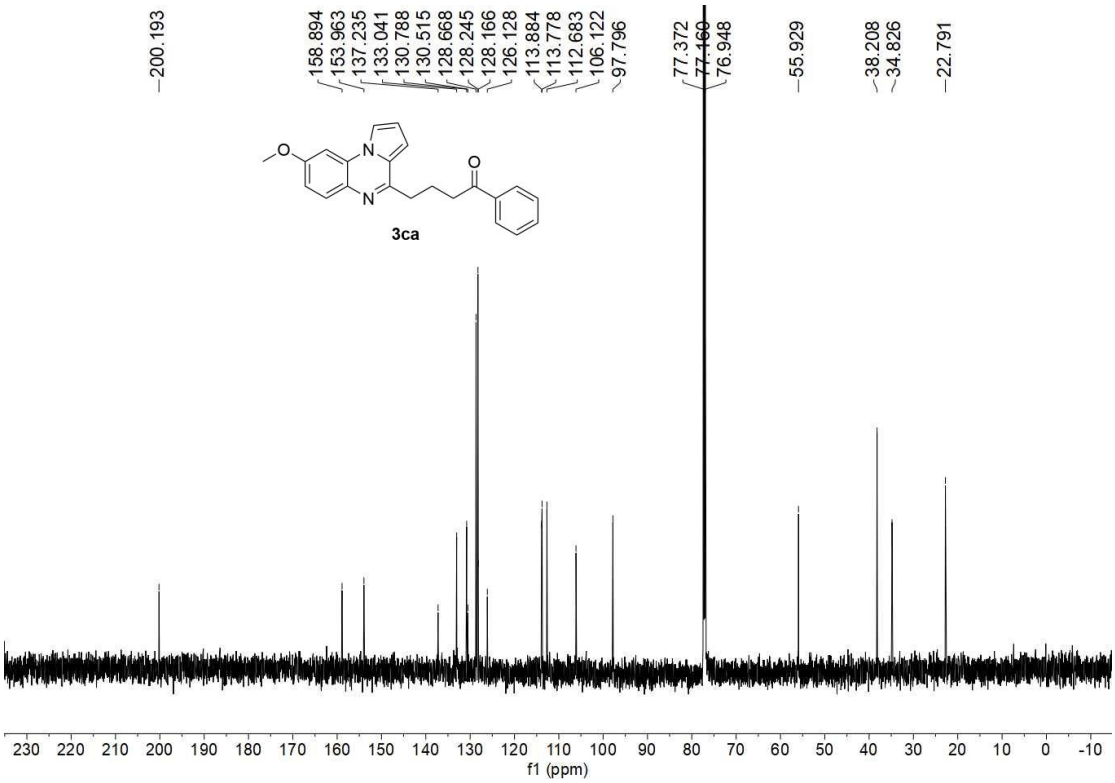
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ba**



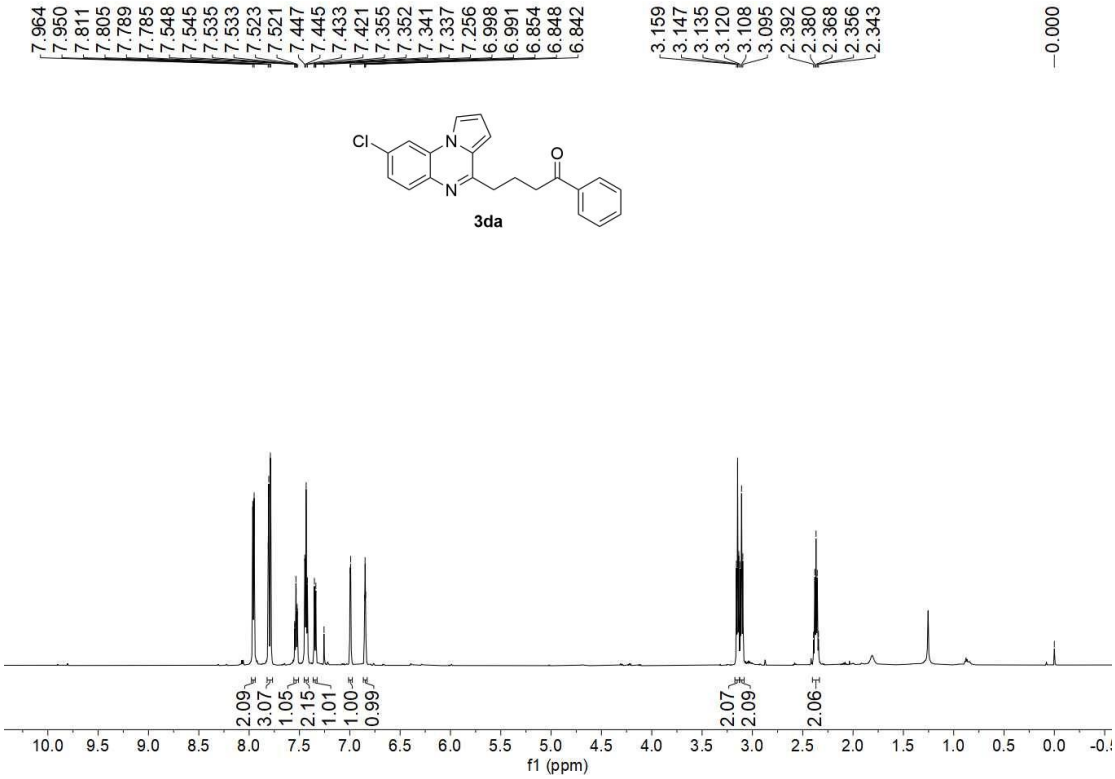
^{1}H NMR (600MHz, $CDCl_3$) of compound **3ca**



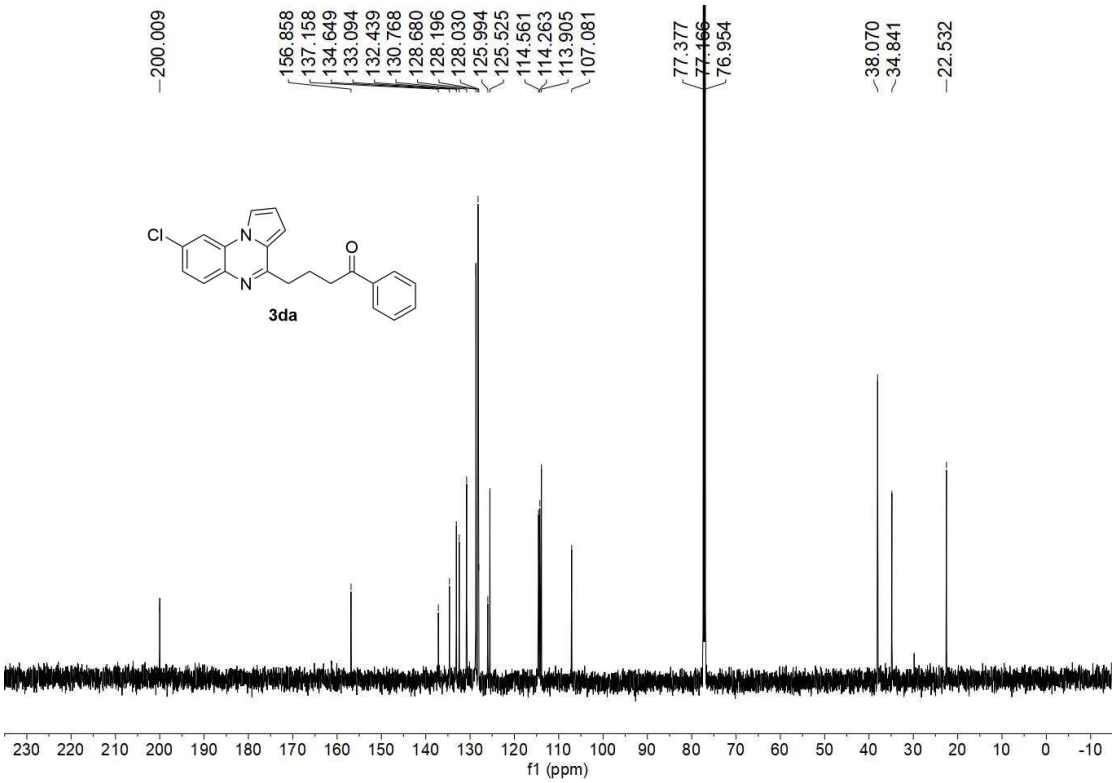
^{13}C NMR (150 MHz, $CDCl_3$) of compound **3ca**



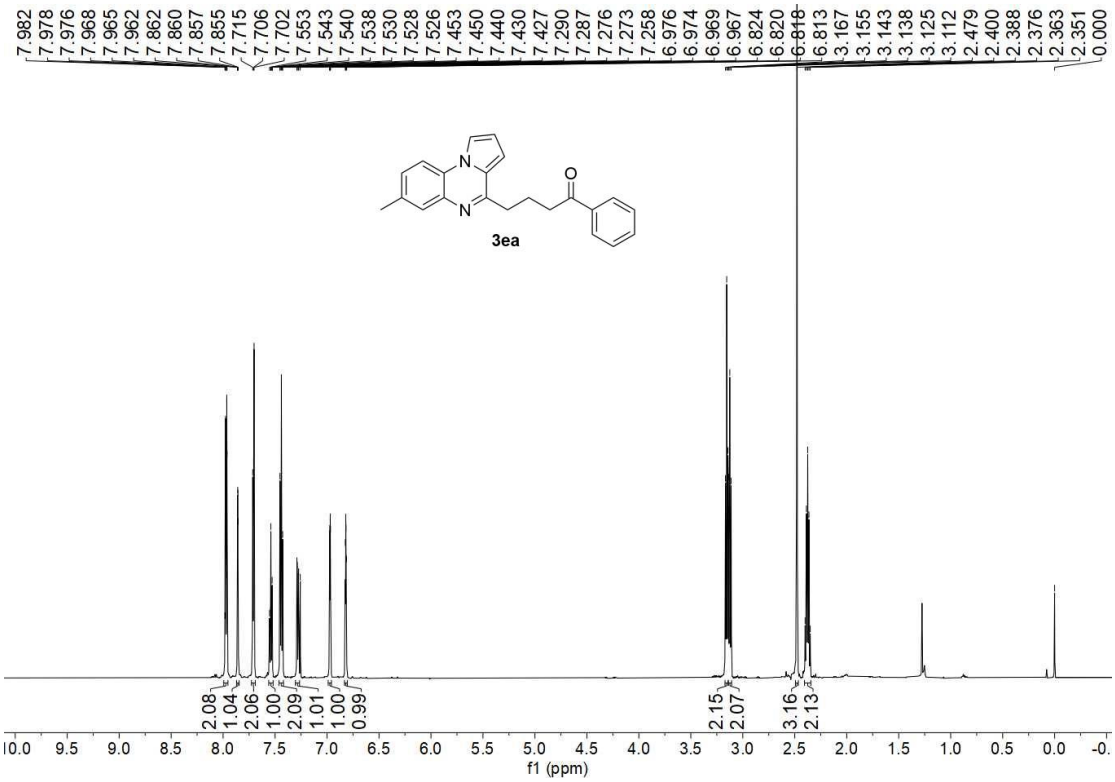
^{1}H NMR (600MHz, $CDCl_3$) of compound **3da**



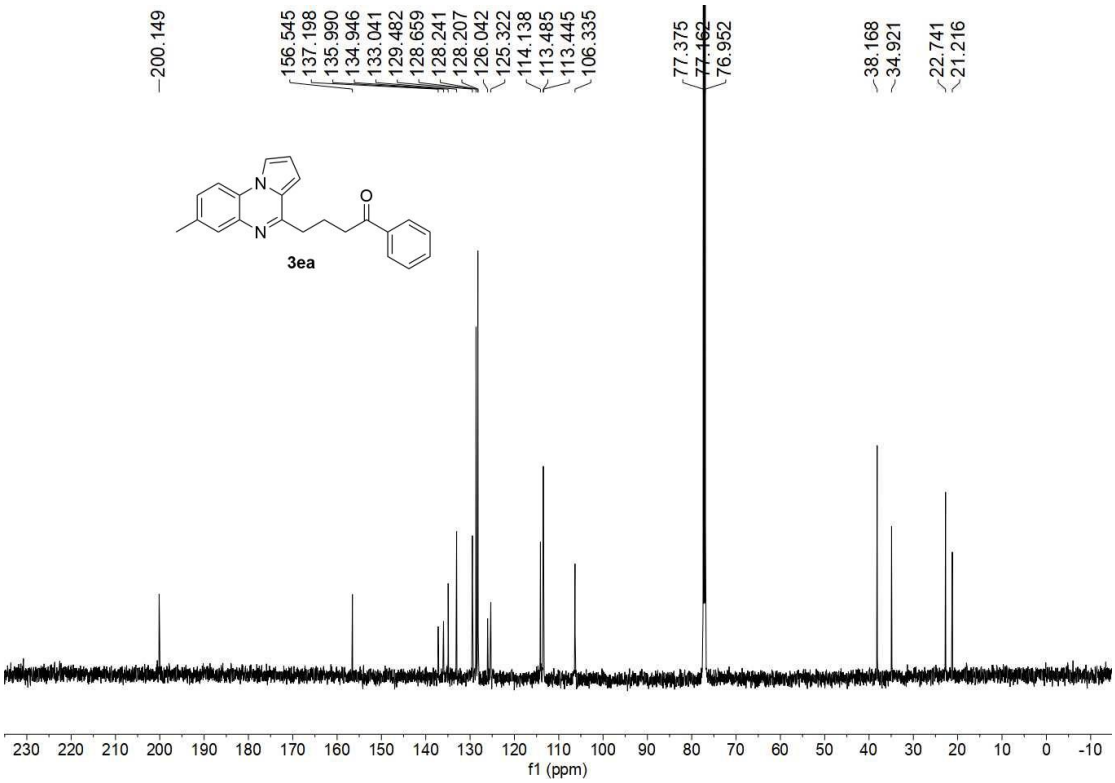
^{13}C NMR (150 MHz, $CDCl_3$) of compound **3da**



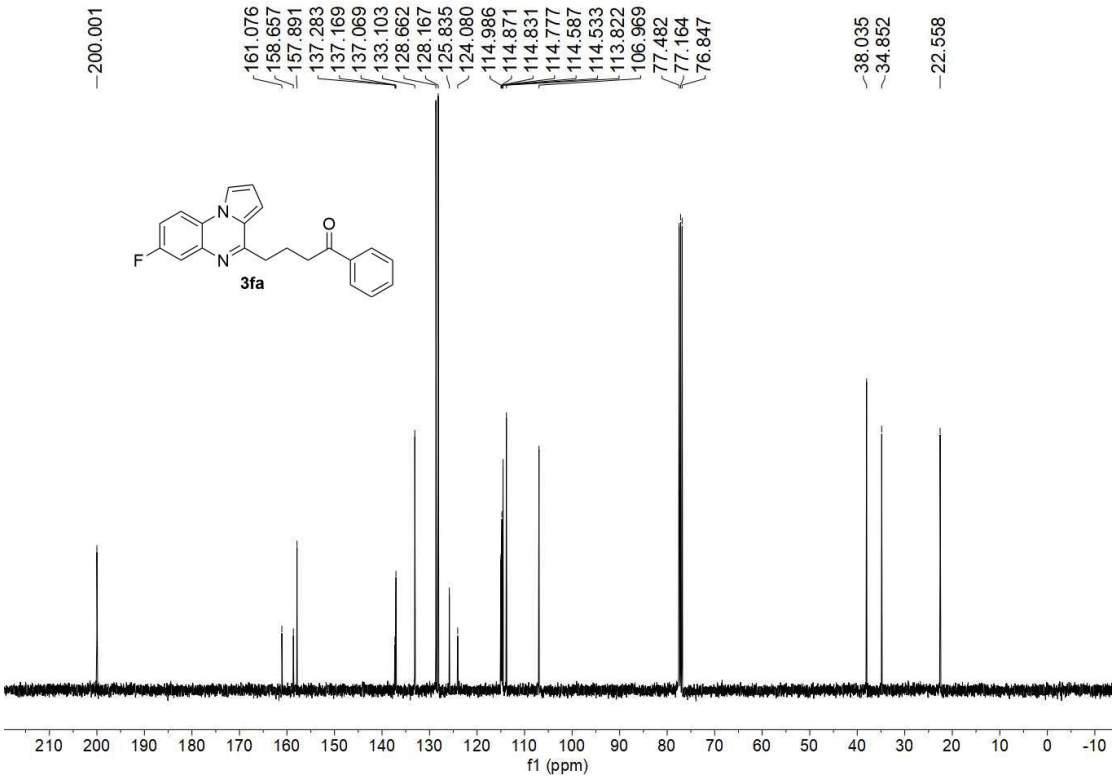
^{1}H NMR (600MHz, $CDCl_3$) of compound **3ea**



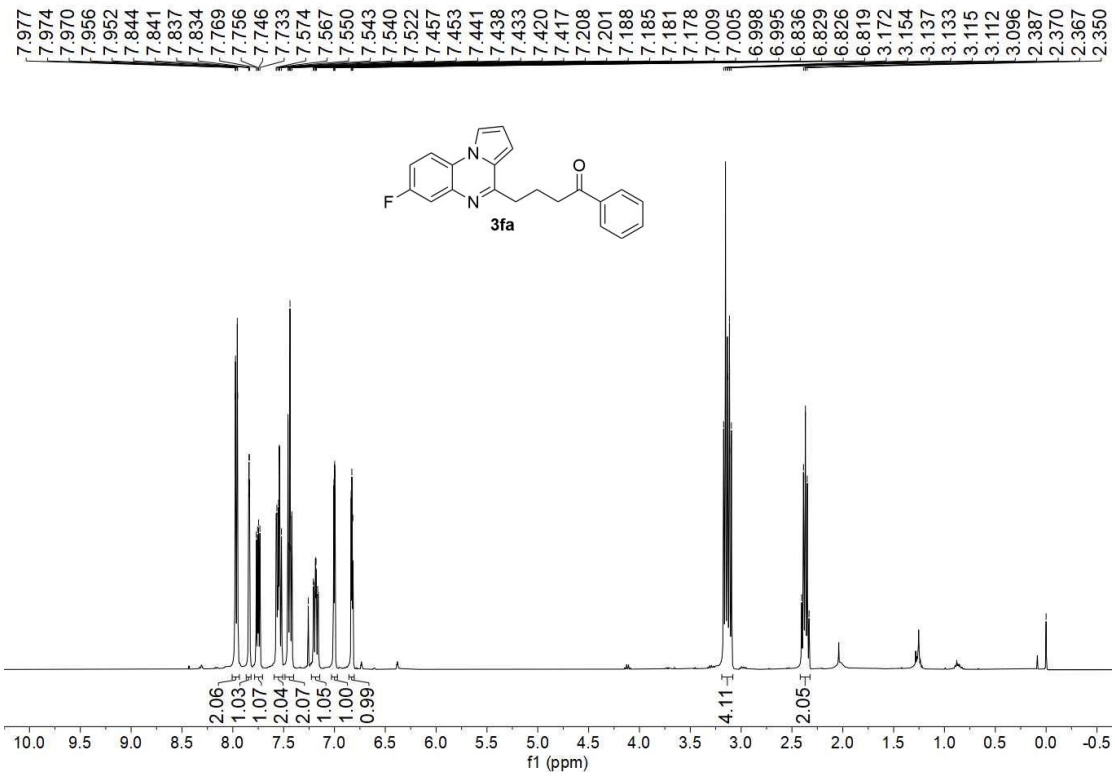
^{13}C NMR (150 MHz, $CDCl_3$) of compound **3ea**



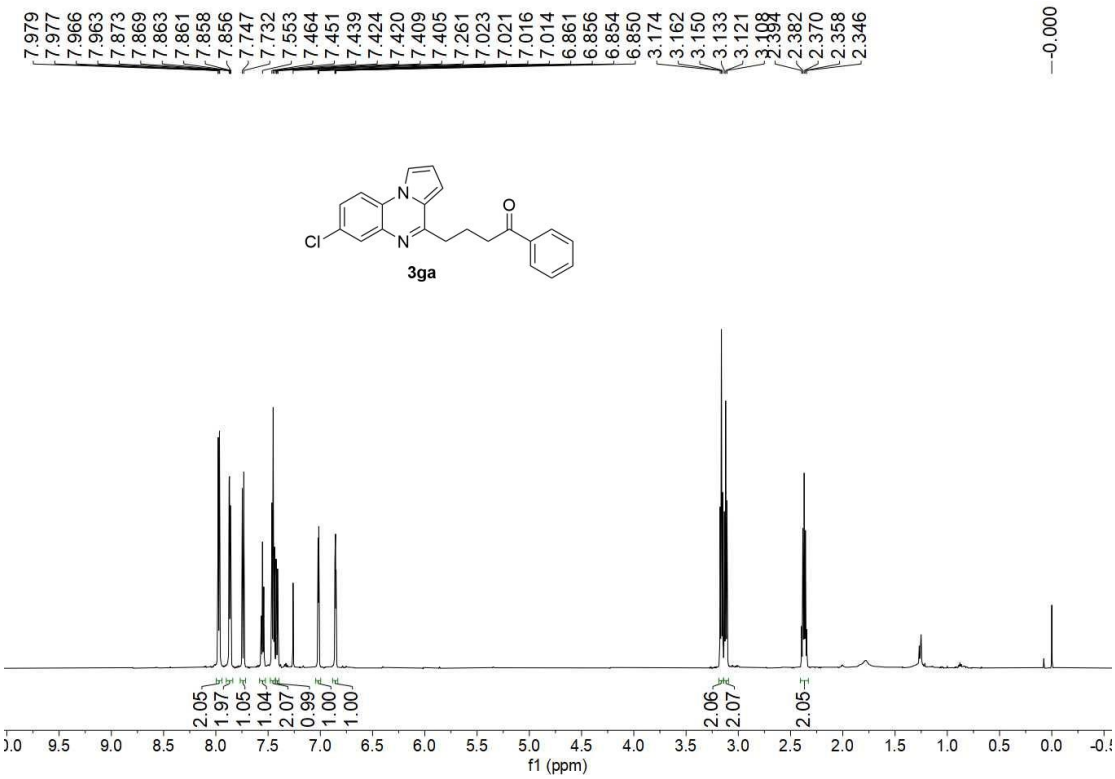
^{1}H NMR (400MHz, $CDCl_3$) of compound **3fa**



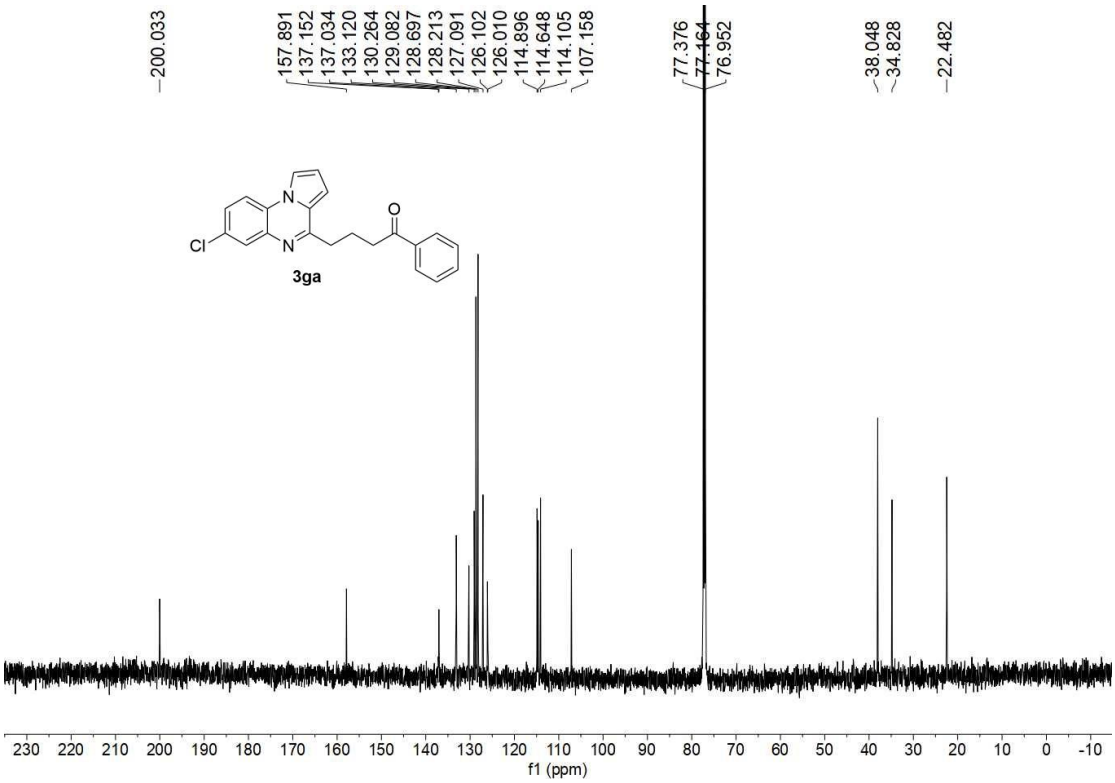
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3fa**



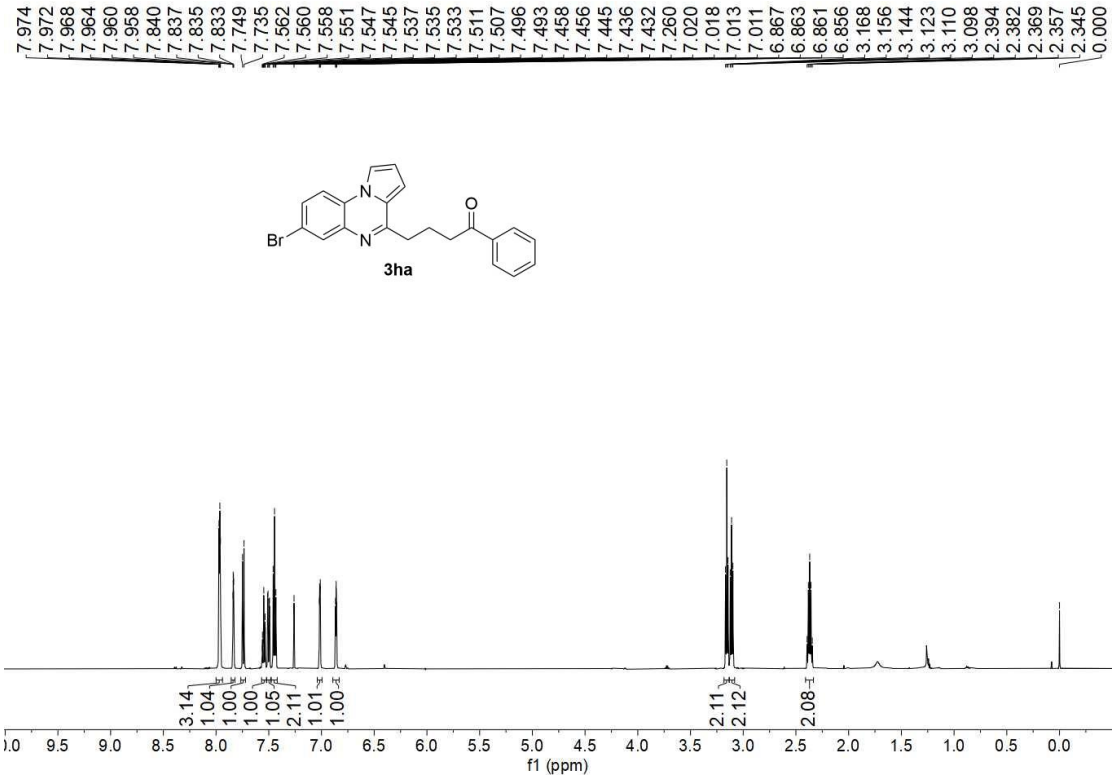
^{1}H NMR (600MHz, $CDCl_3$) of compound **3ga**



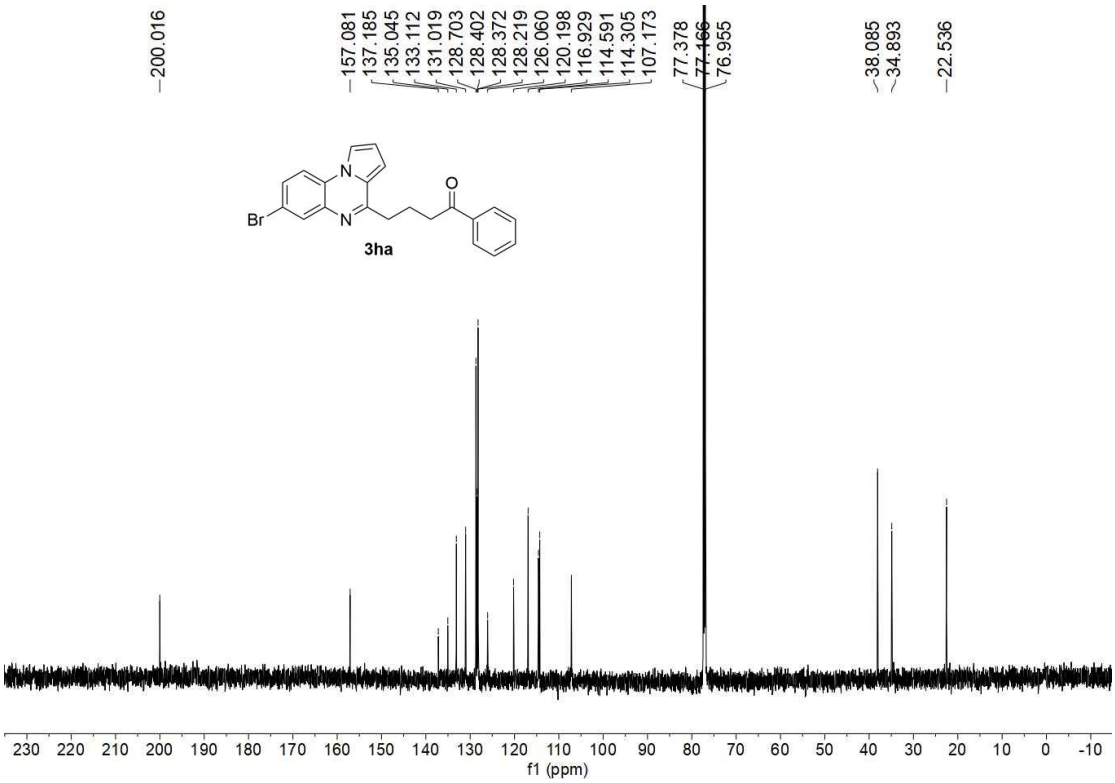
^{13}C NMR (150 MHz, $CDCl_3$) of compound **3ga**



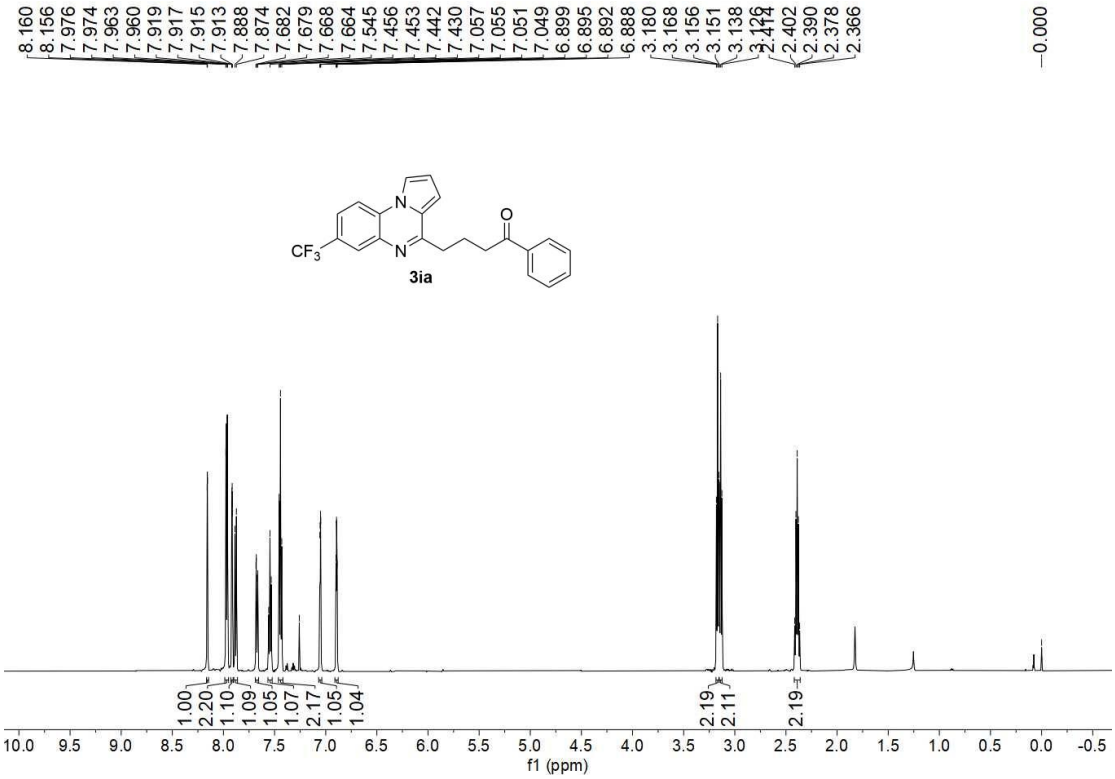
^{1}H NMR (600MHz, $CDCl_3$) of compound **3ha**



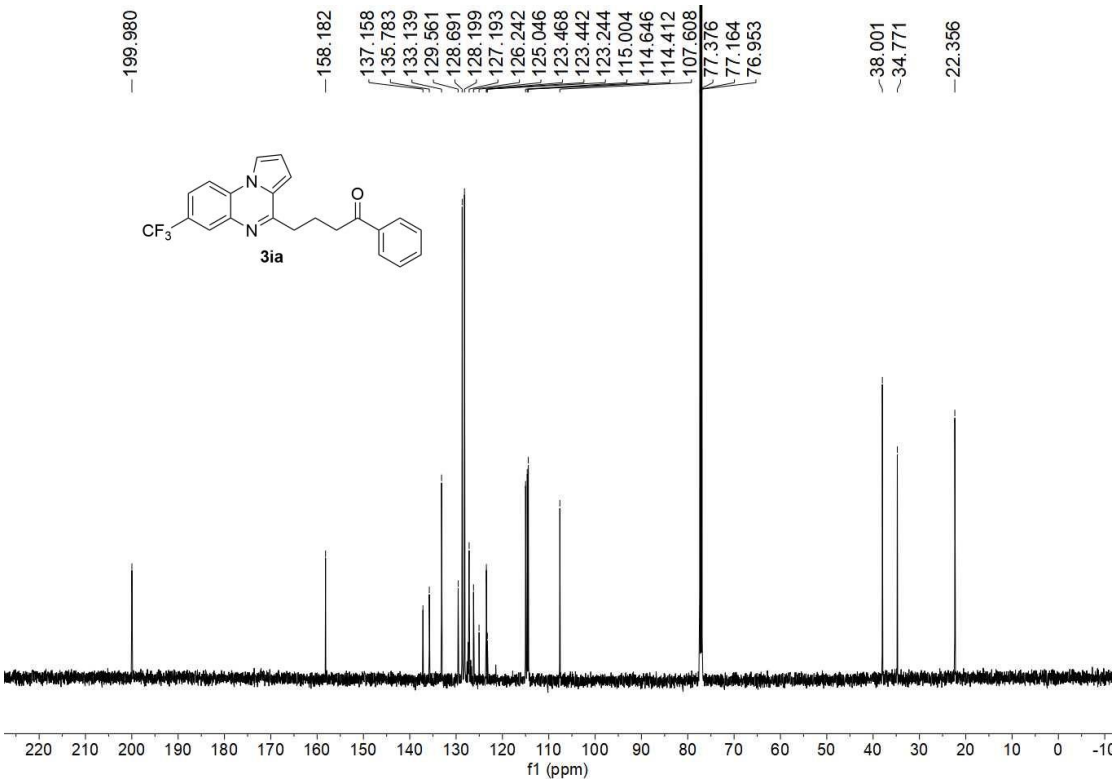
^{13}C NMR (150 MHz, $CDCl_3$) of compound **3ha**



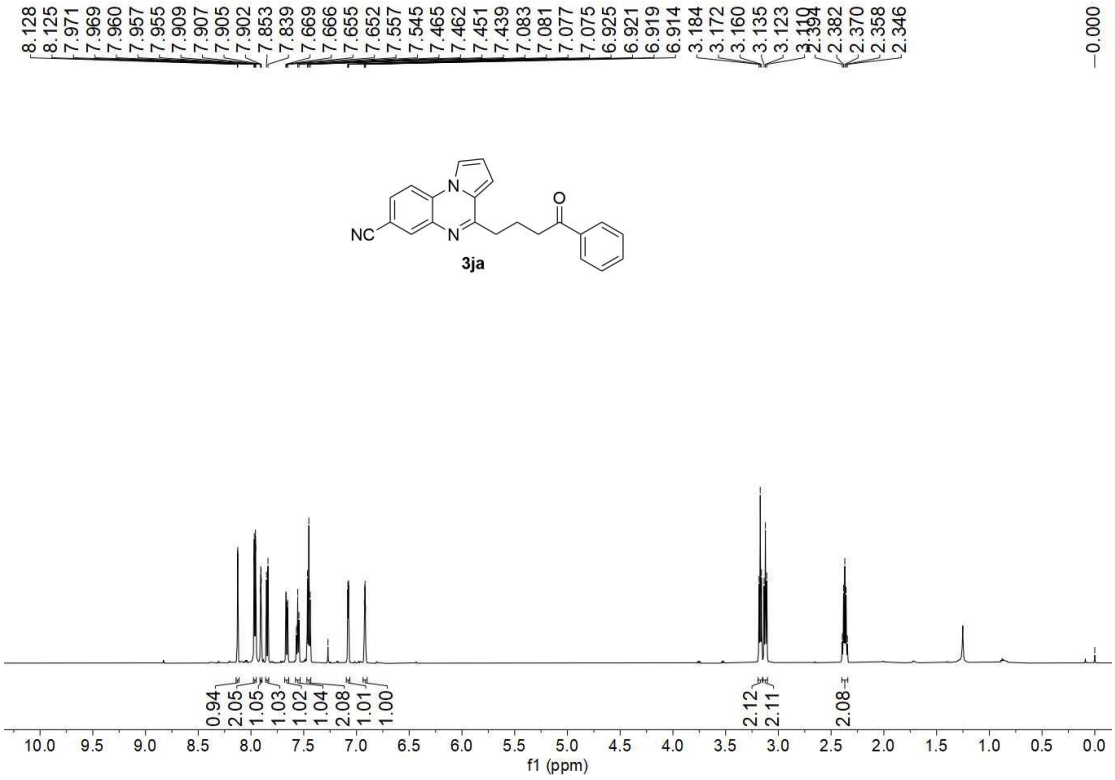
^{1}H NMR (600MHz, $CDCl_3$) of compound **3ia**



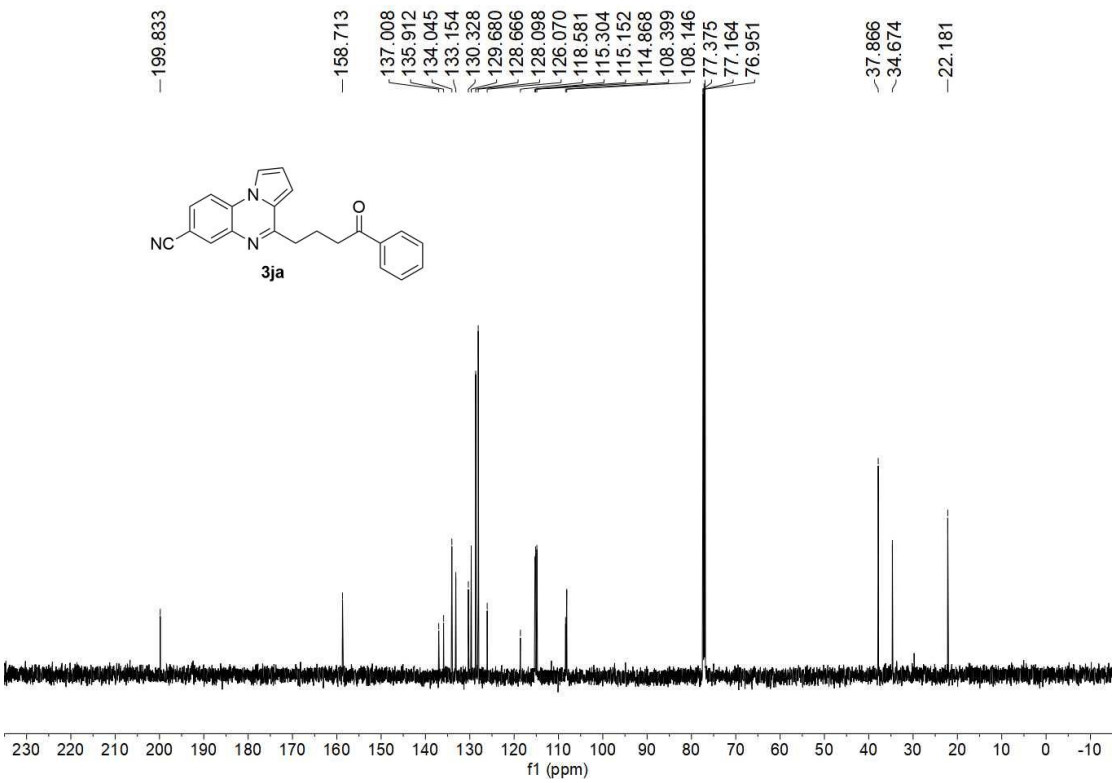
^{13}C NMR (150 MHz, $CDCl_3$) of compound **3ia**



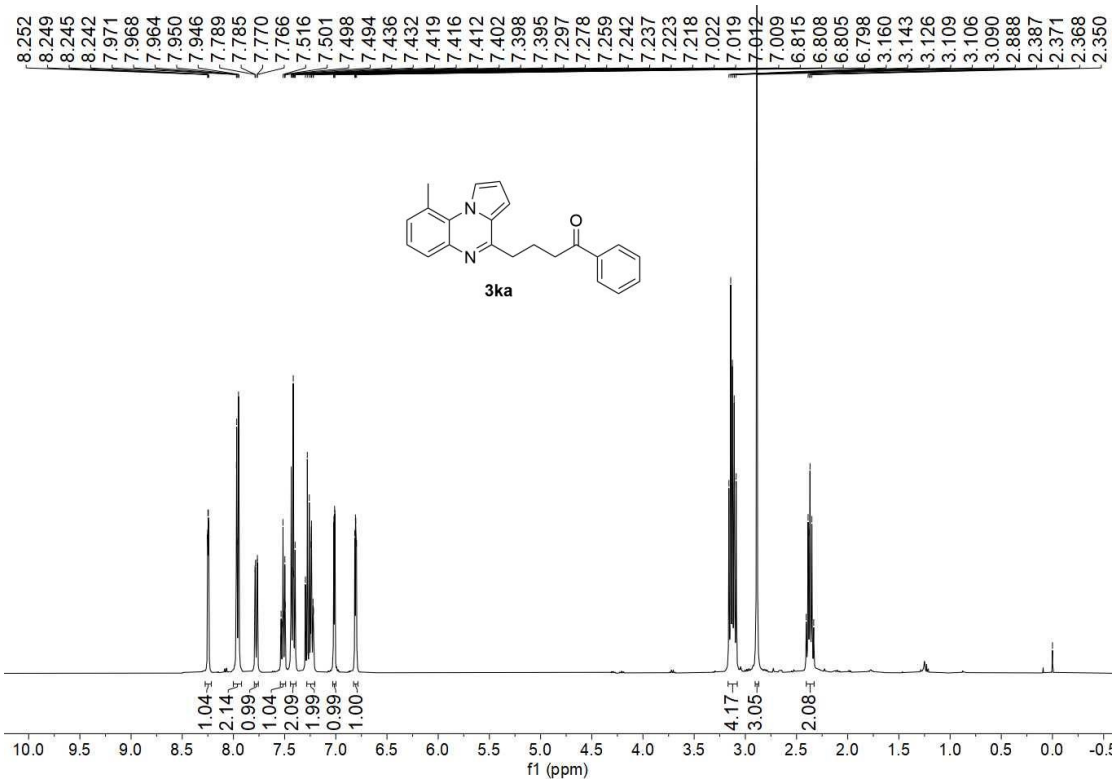
^{1}H NMR (600MHz, $CDCl_3$) of compound **3ja**



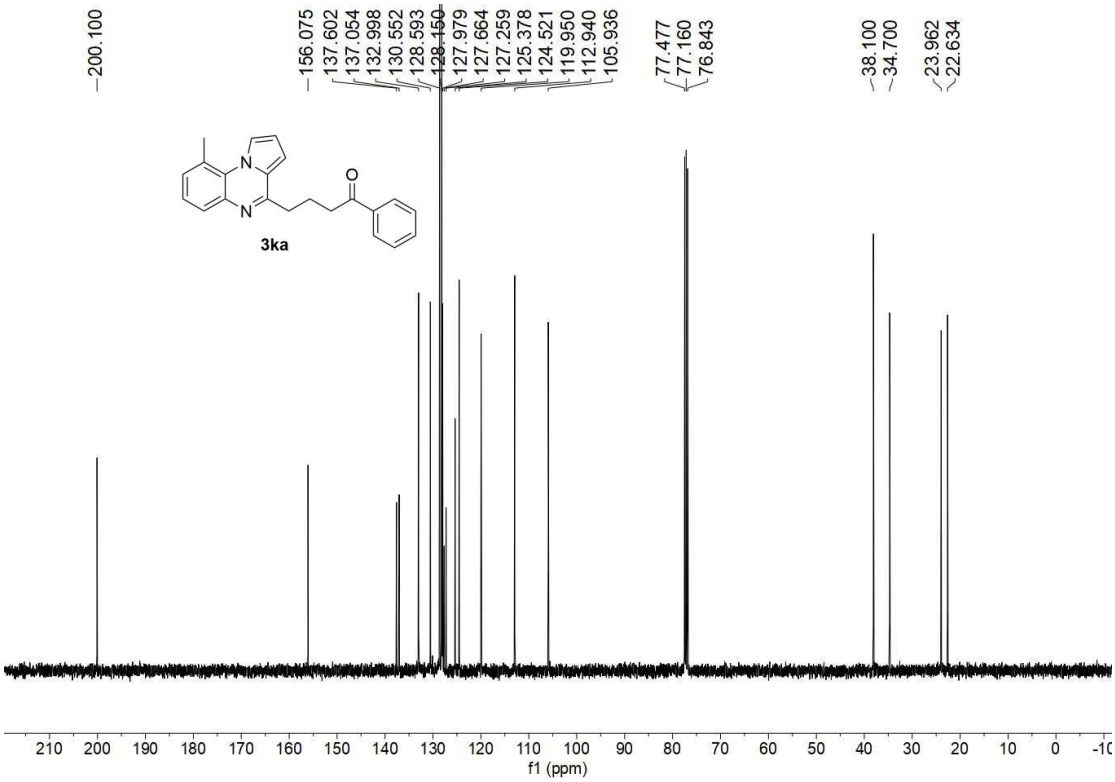
^{13}C NMR (150 MHz, $CDCl_3$) of compound **3ja**



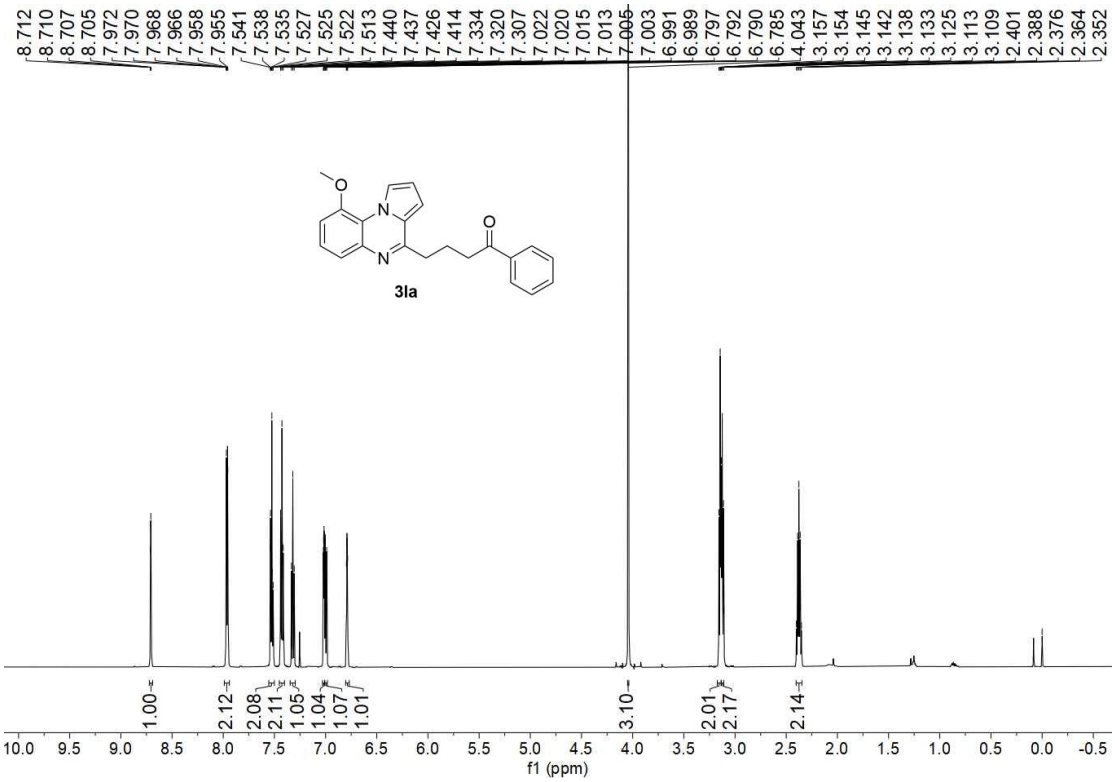
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ka**



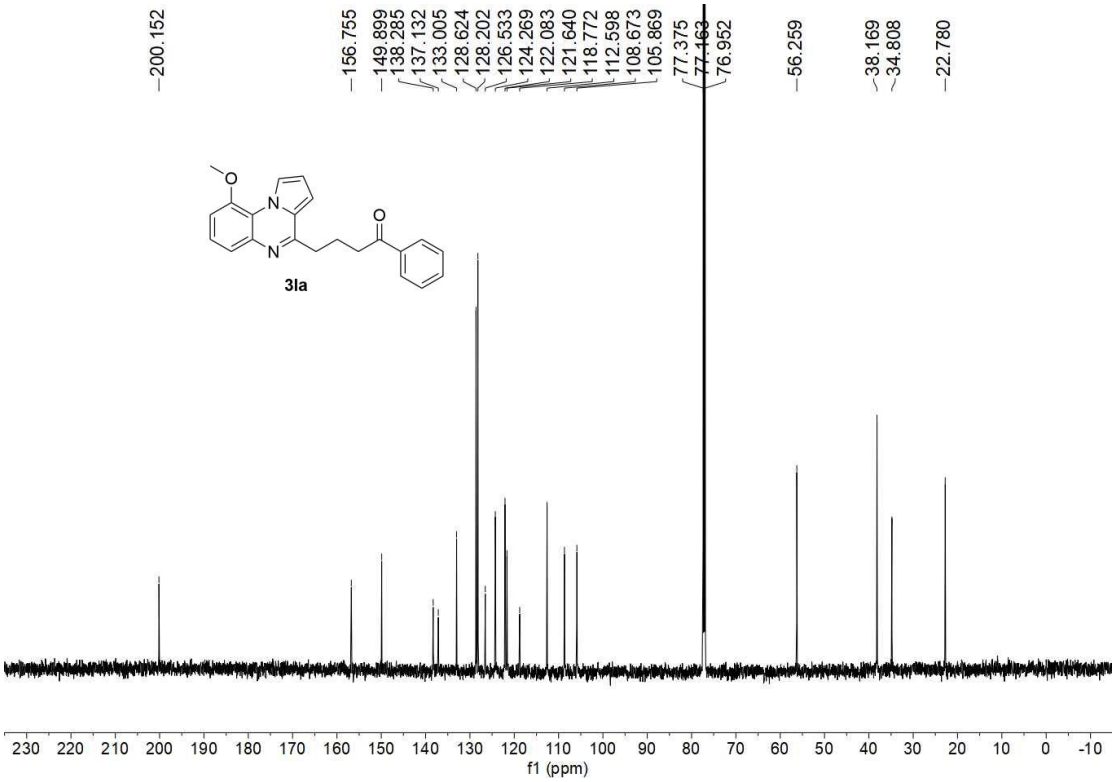
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ka**



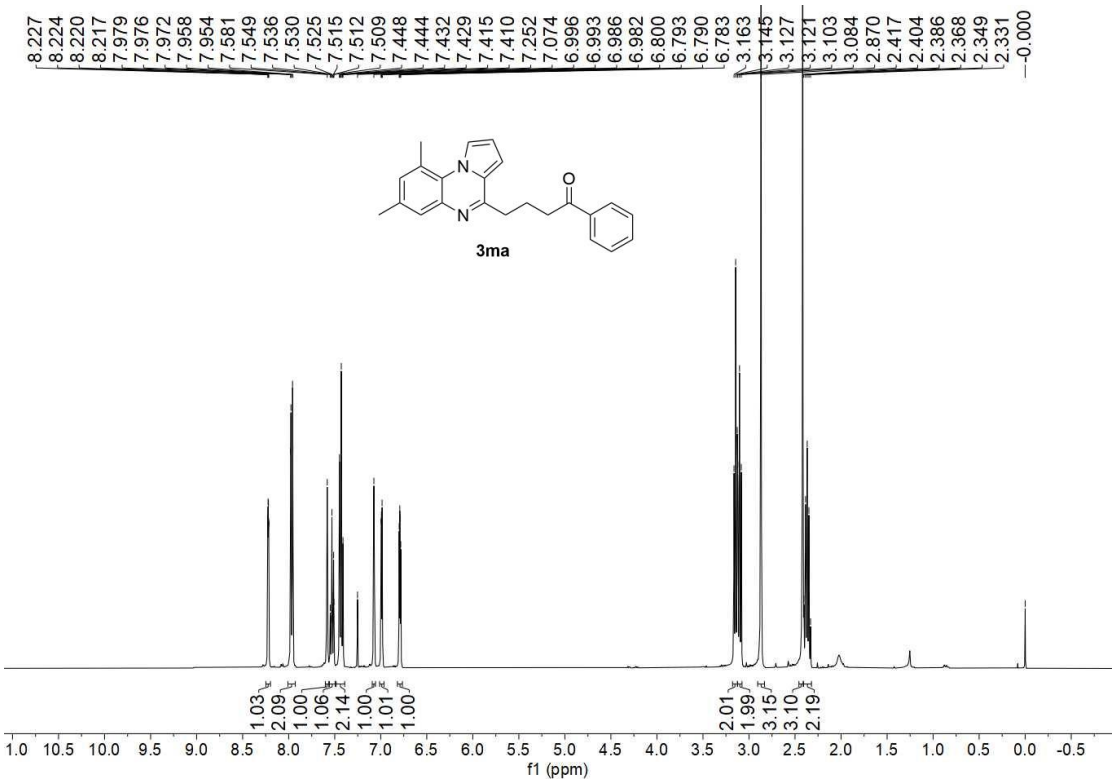
^{1}H NMR (600MHz, $CDCl_3$) of compound **3la**



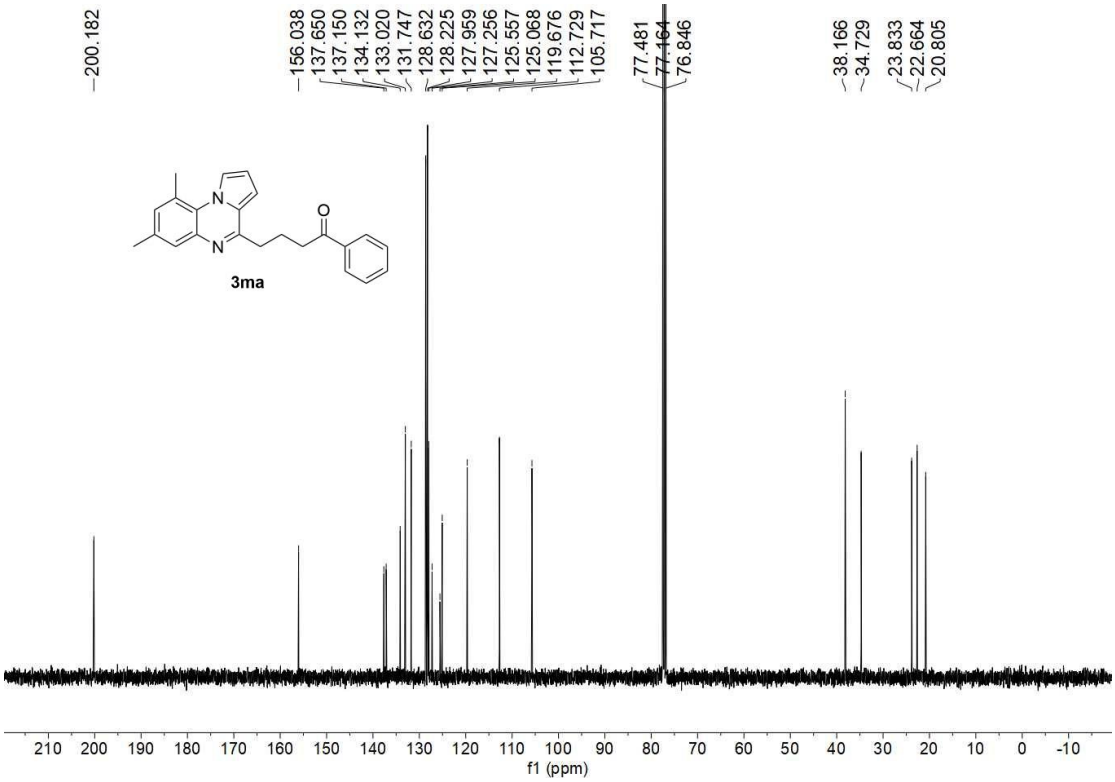
^{13}C NMR (150 MHz, $CDCl_3$) of compound **3la**



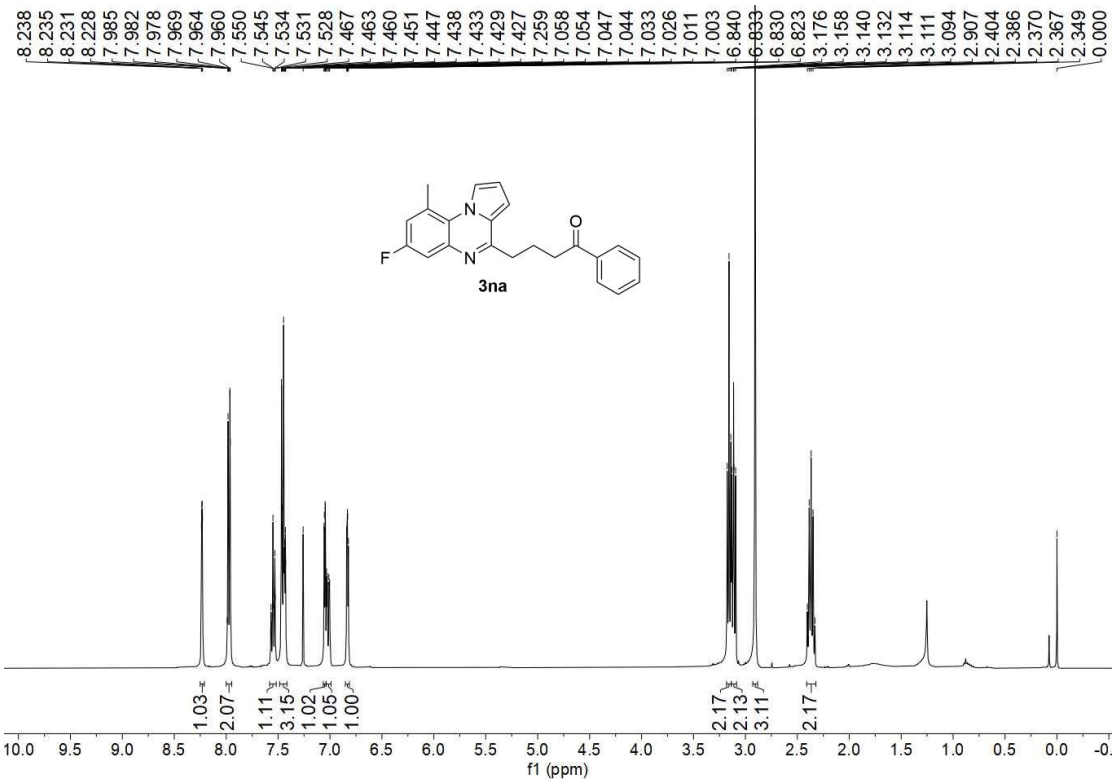
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ma**



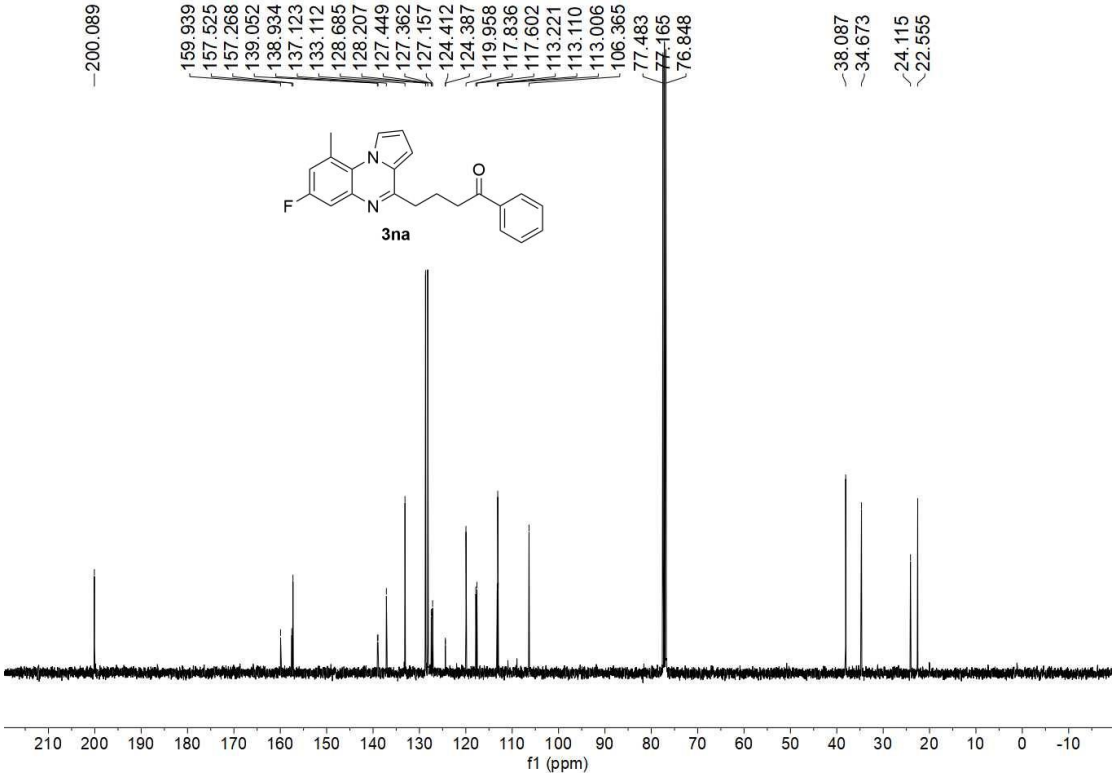
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ma**



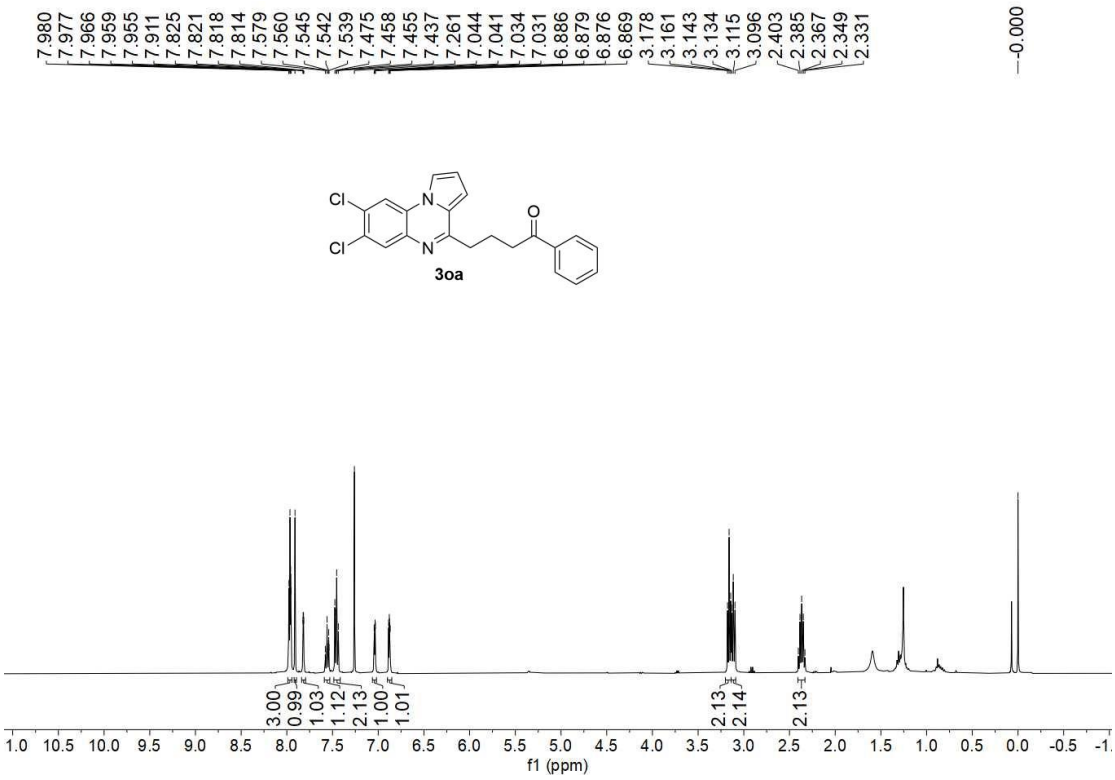
^{1}H NMR (400MHz, $CDCl_3$) of compound **3na**



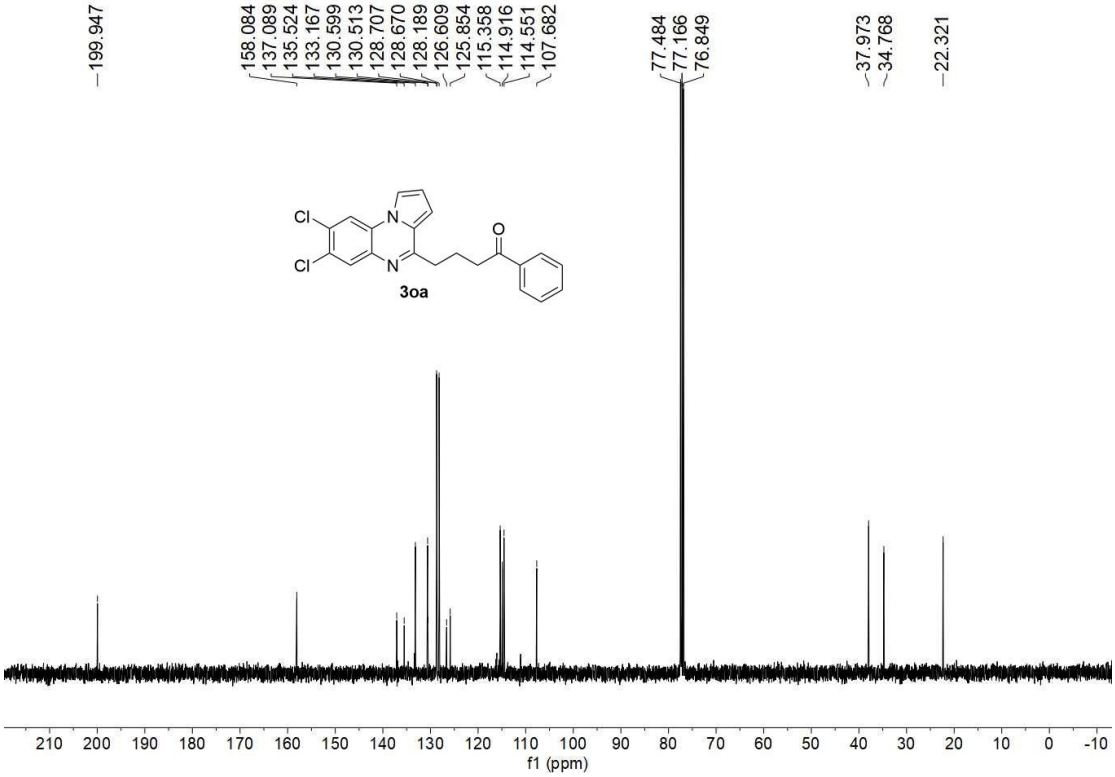
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3na**



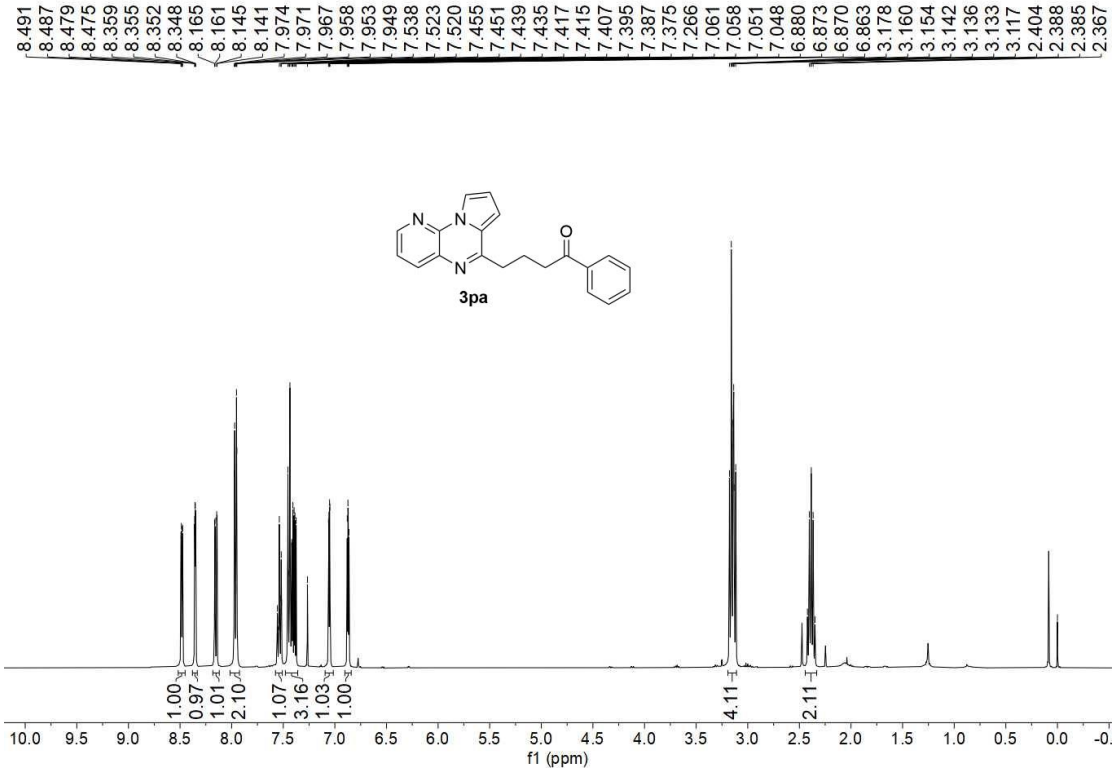
^{1}H NMR (400MHz, $CDCl_3$) of compound **3oa**



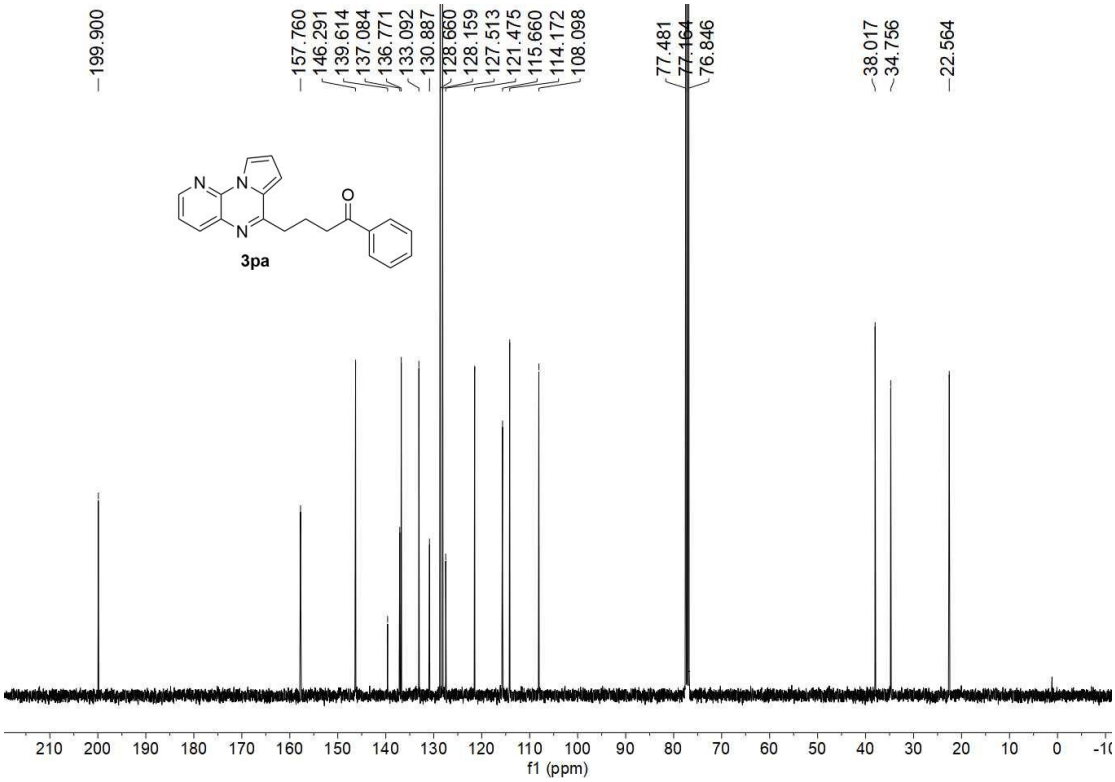
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3oa**



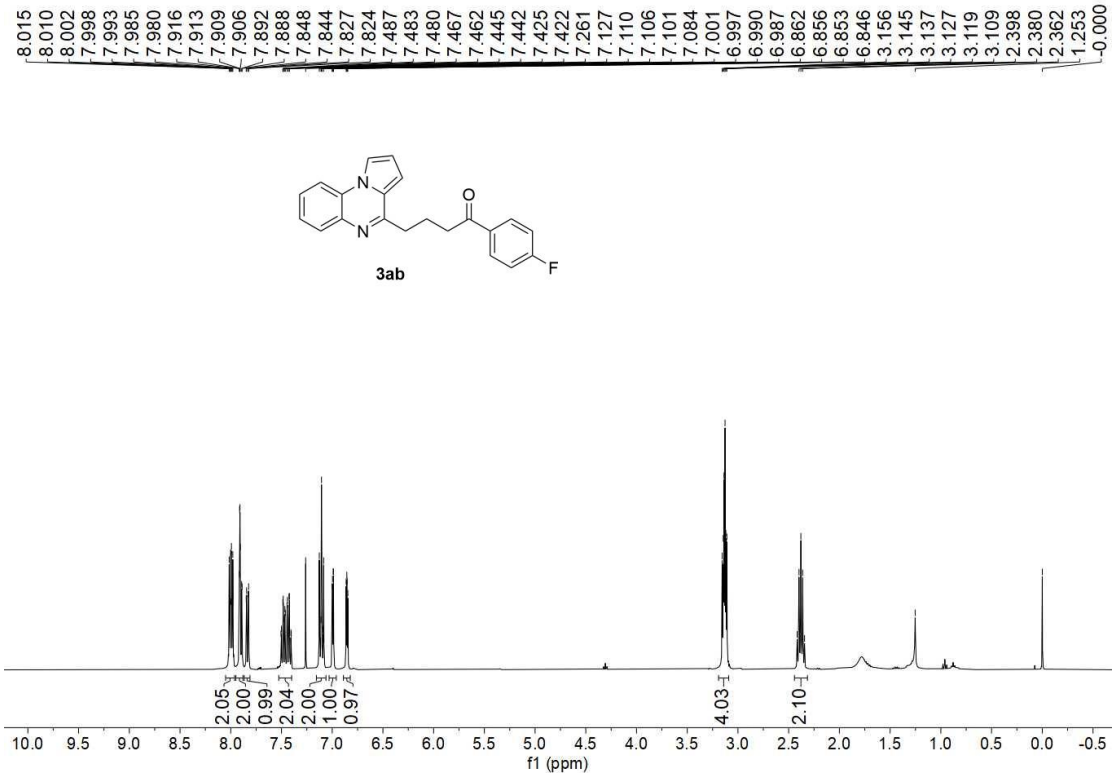
^{1}H NMR (400MHz, $CDCl_3$) of compound **3pa**



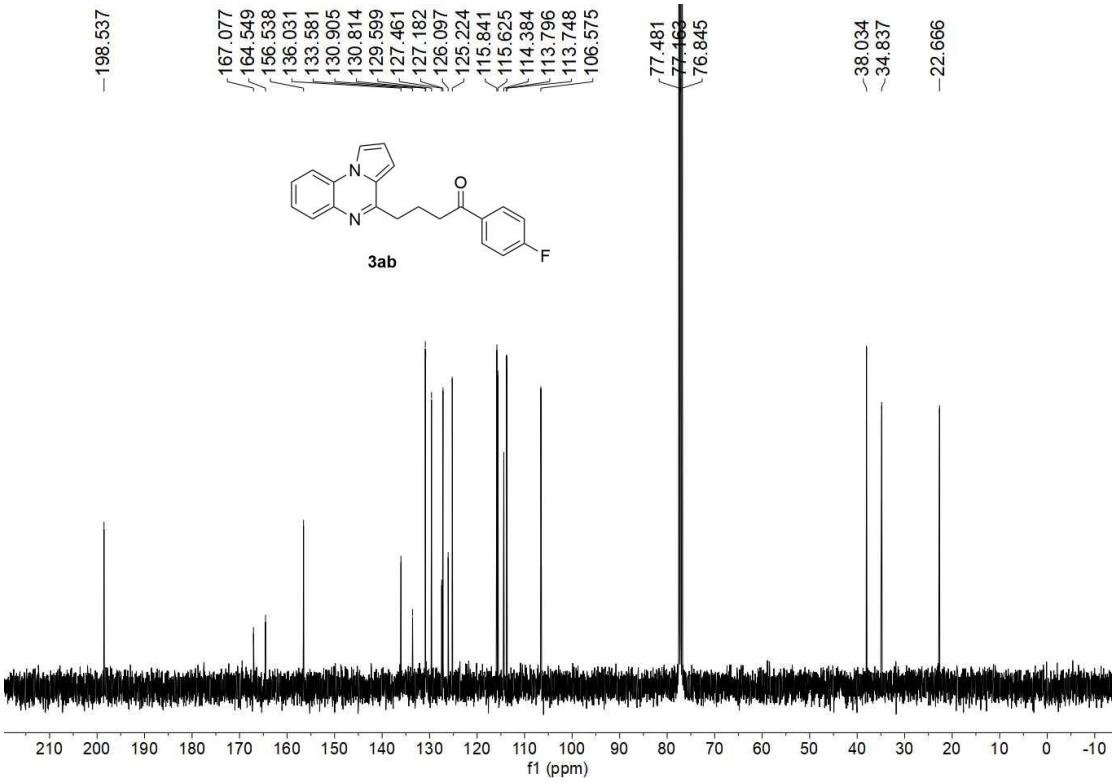
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3pa**



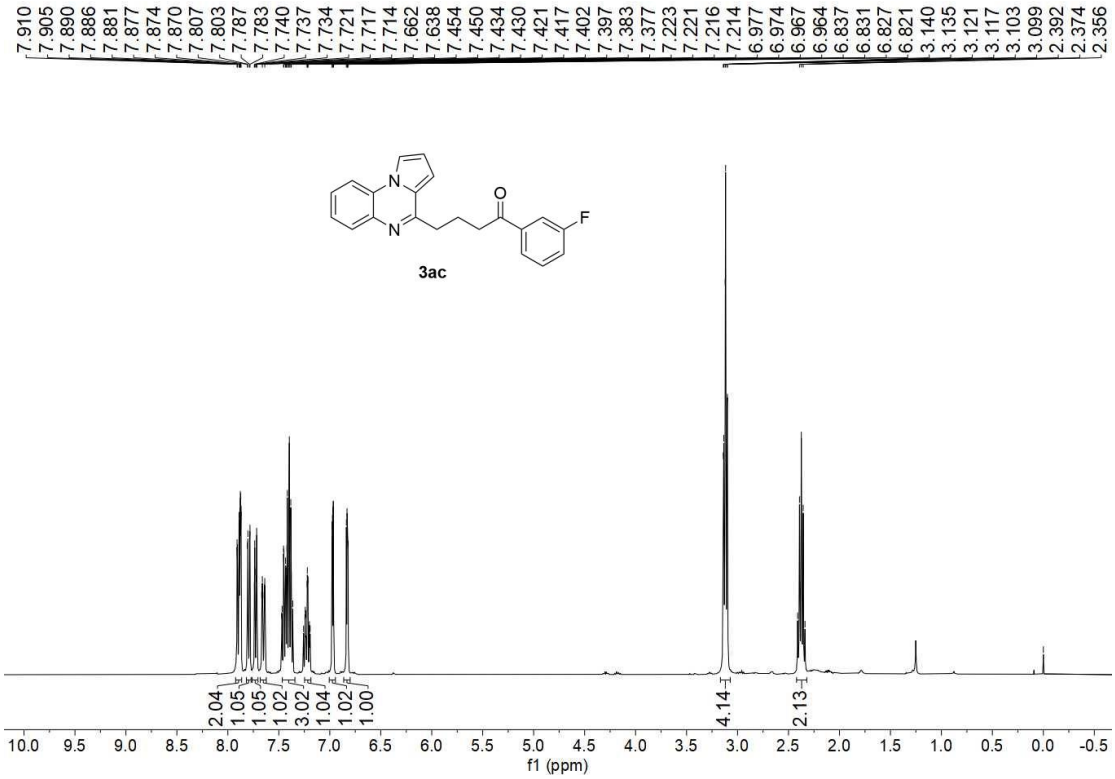
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ab**



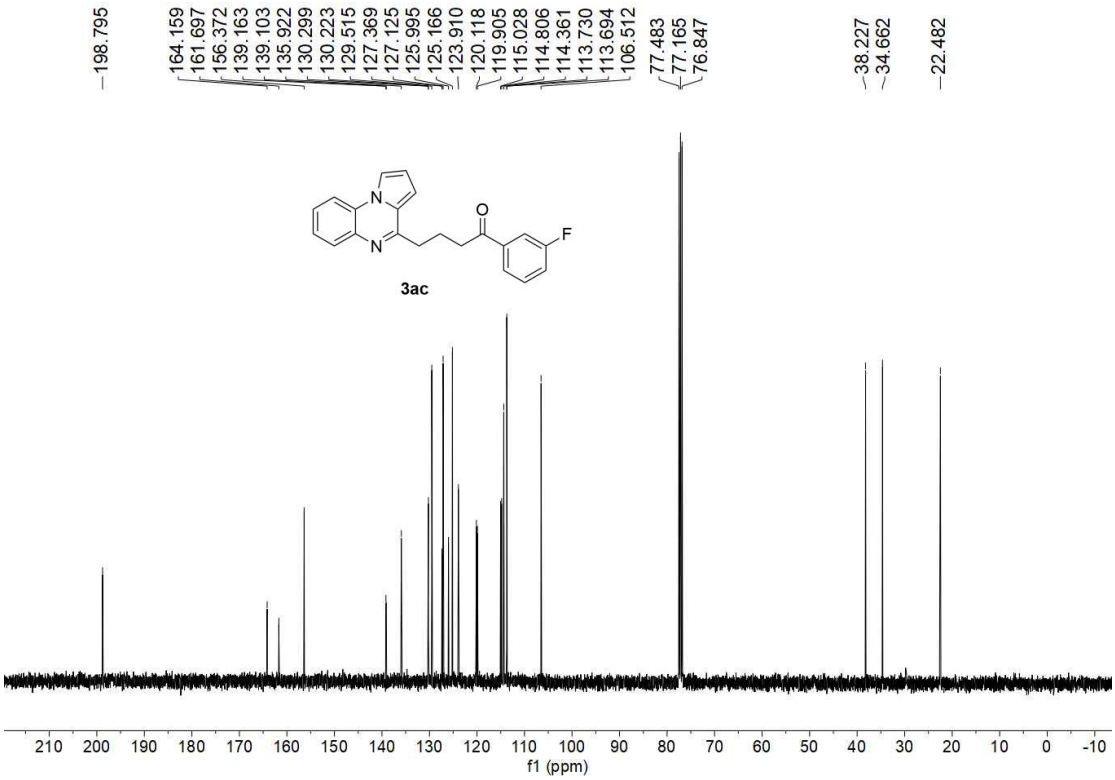
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ab**



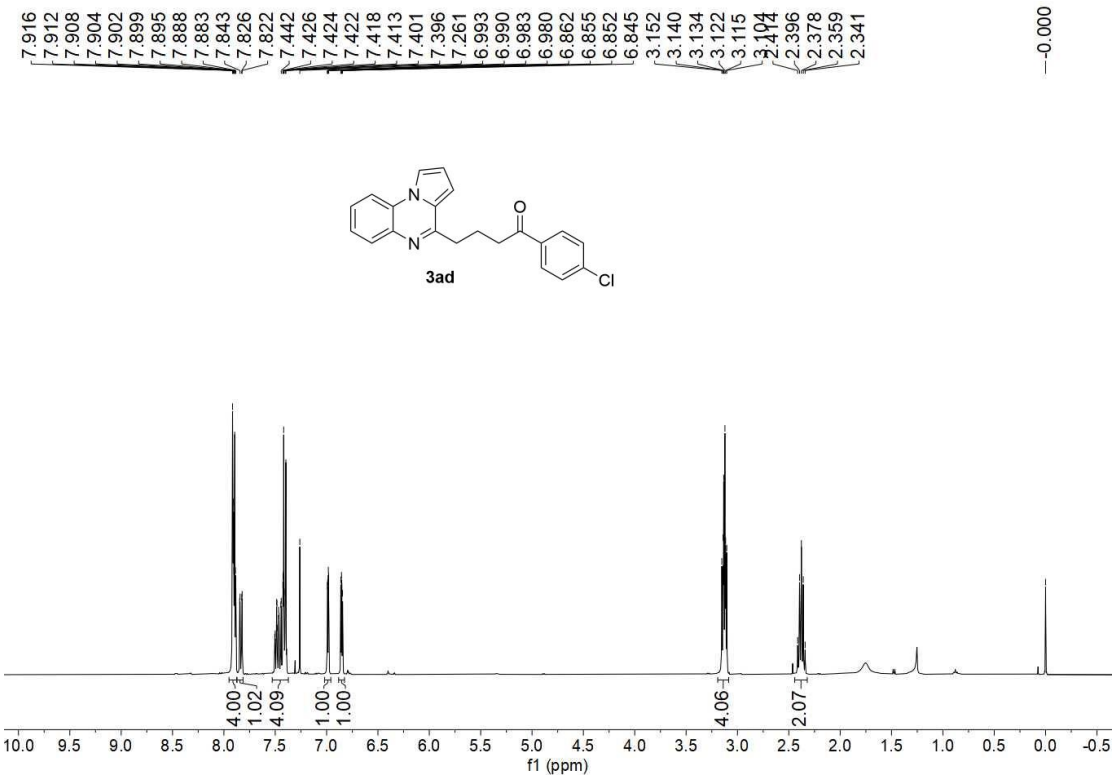
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ac**



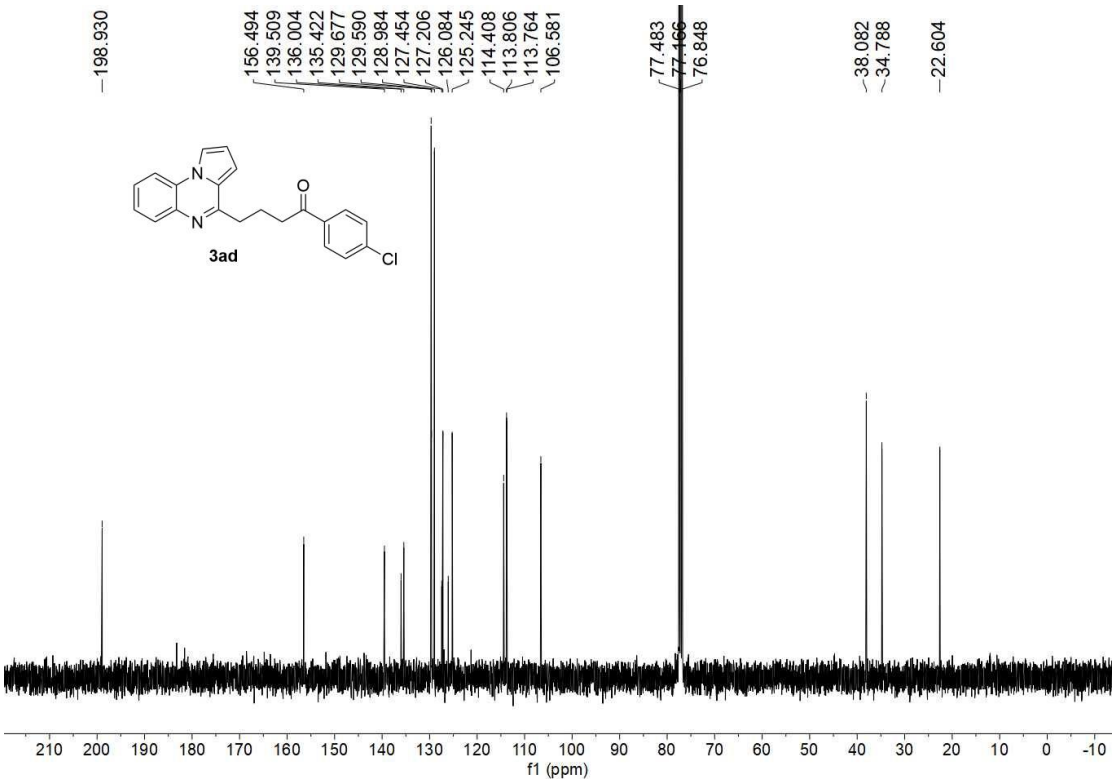
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ac**



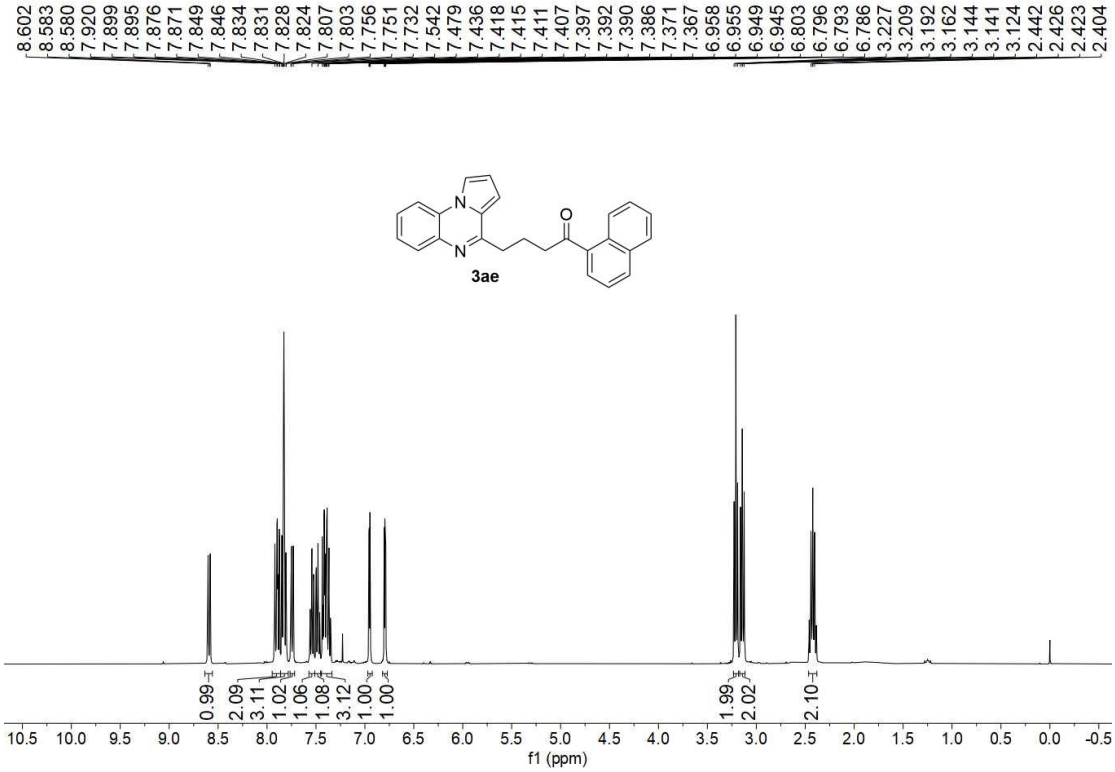
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ad**



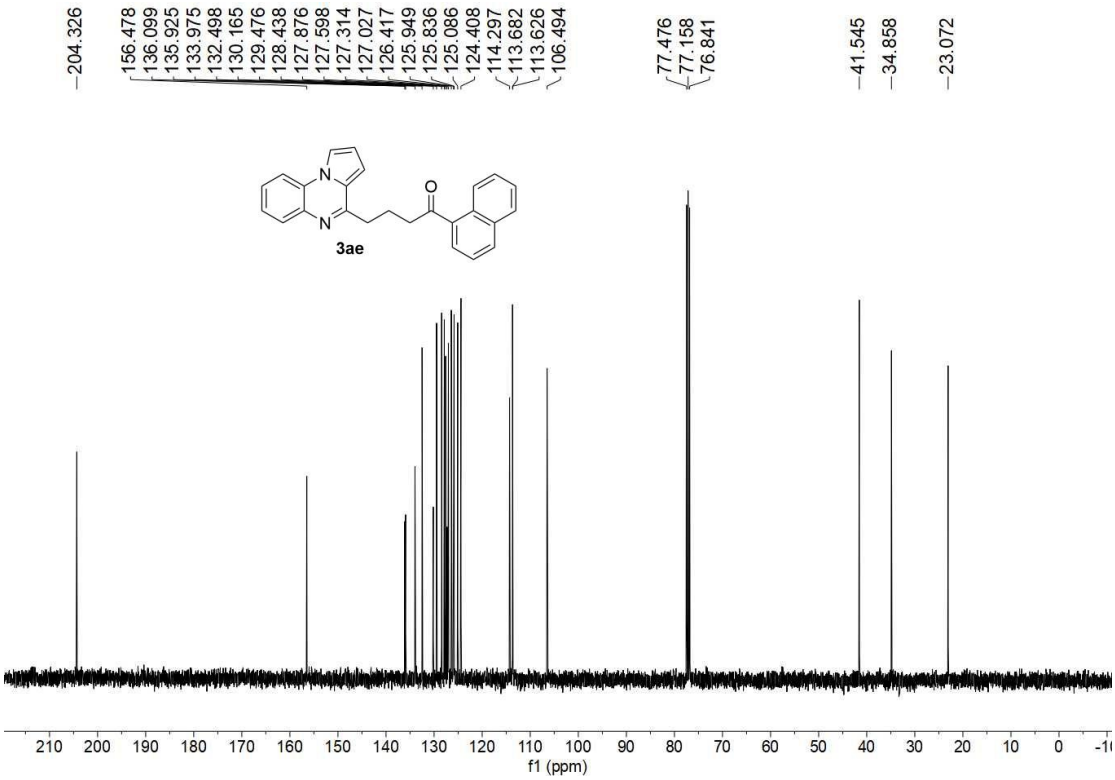
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ad**



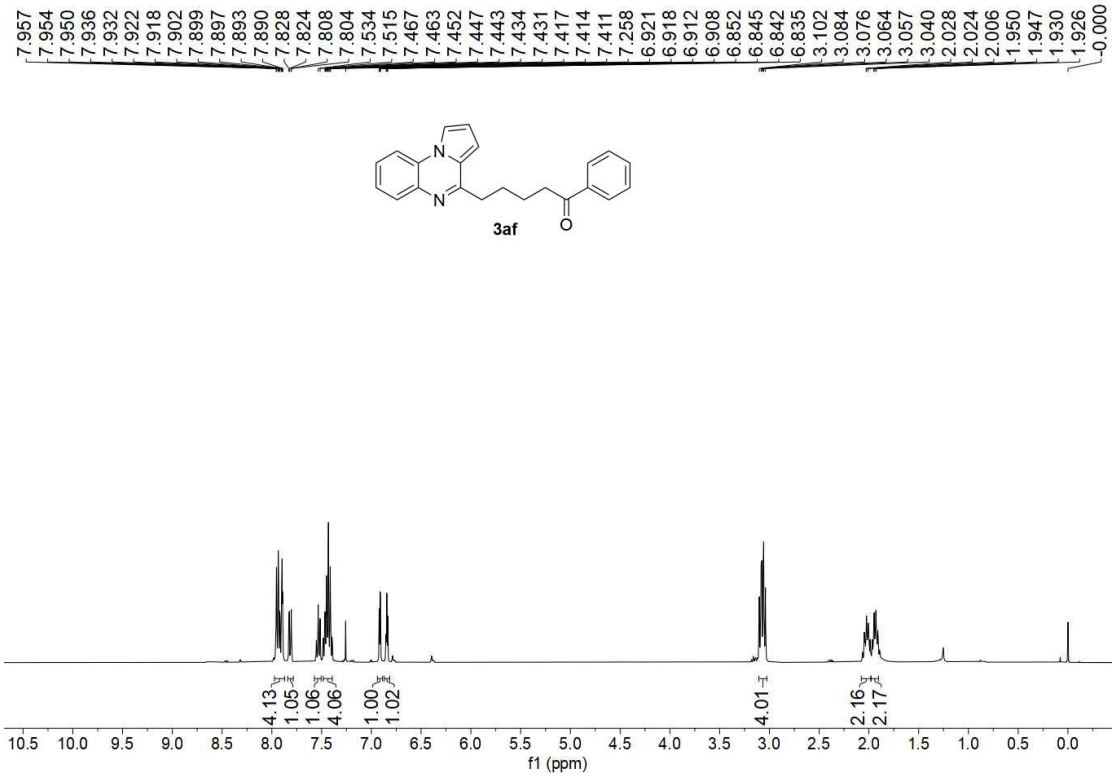
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ae**



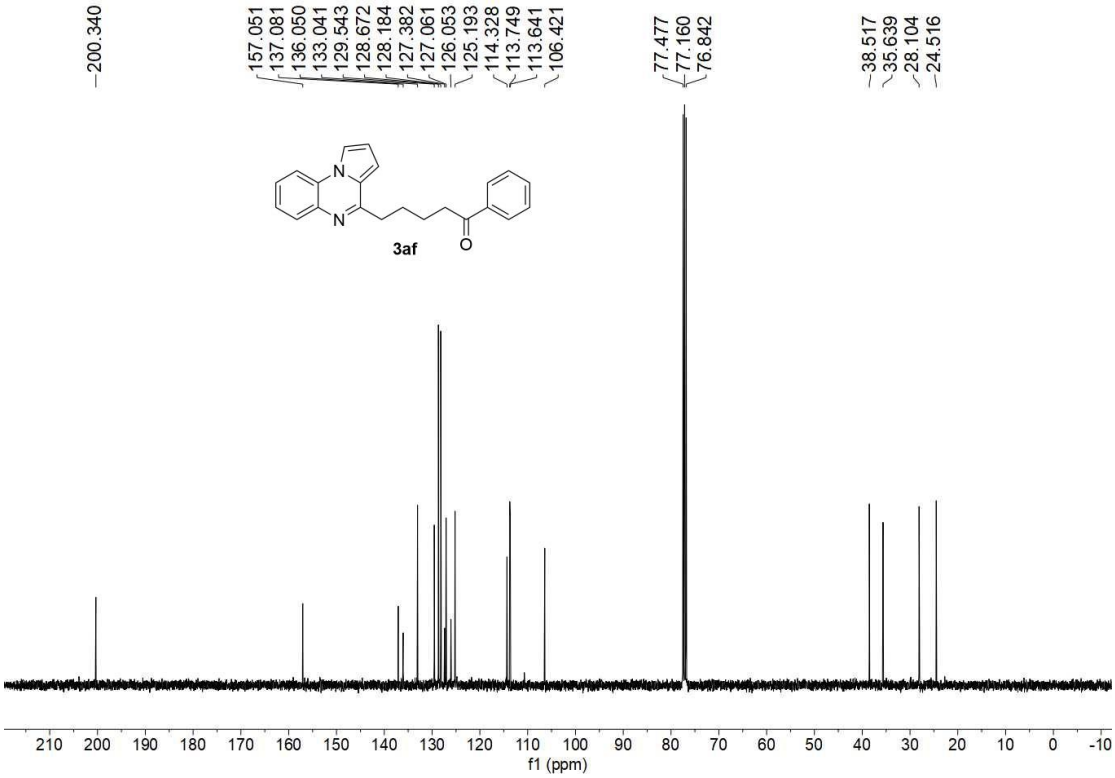
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ae**



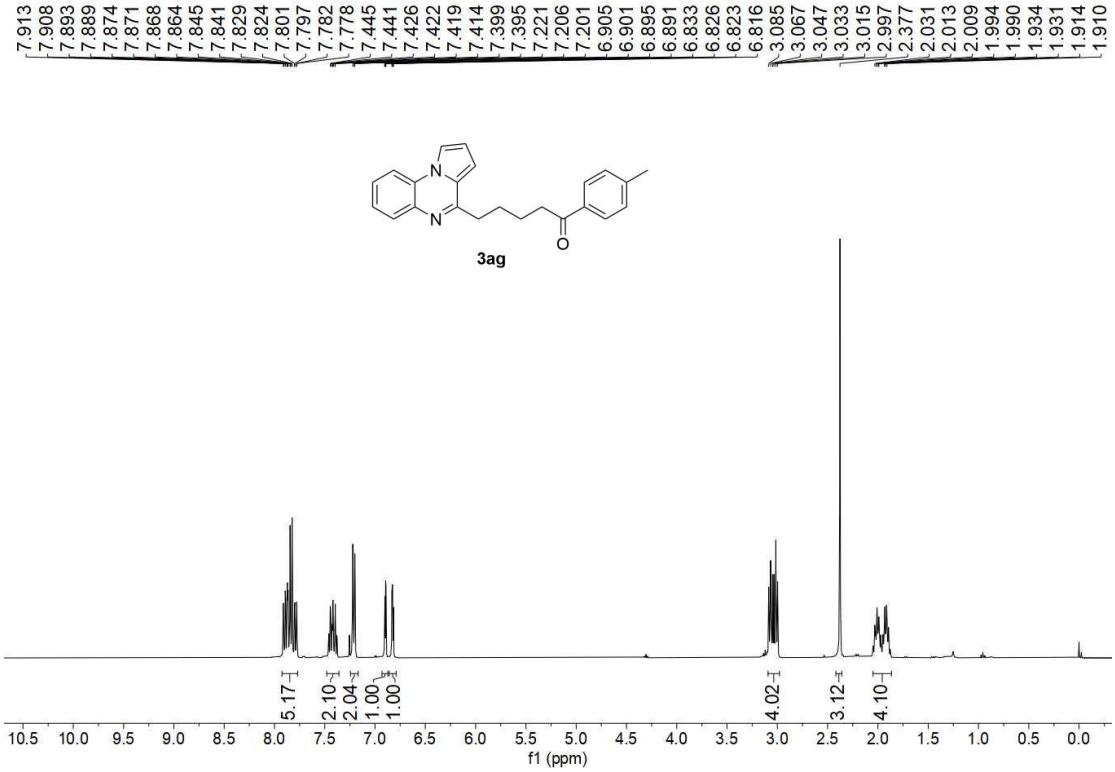
^{1}H NMR (400MHz, $CDCl_3$) of compound **3af**



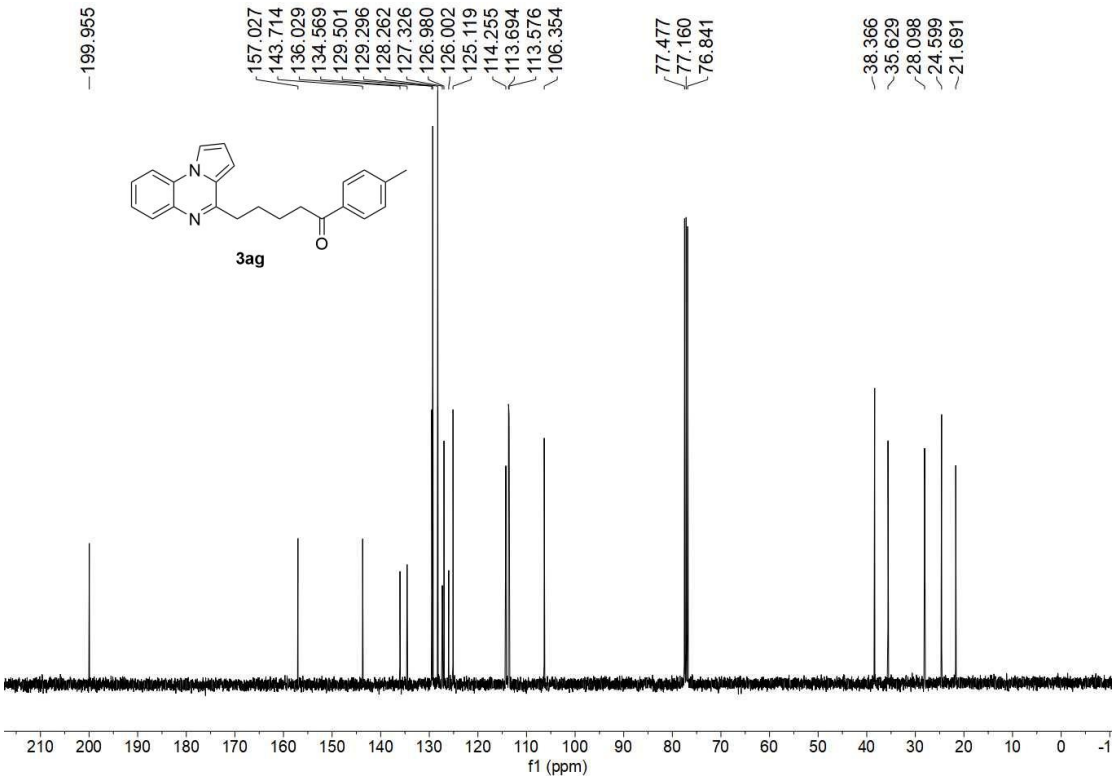
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3af**



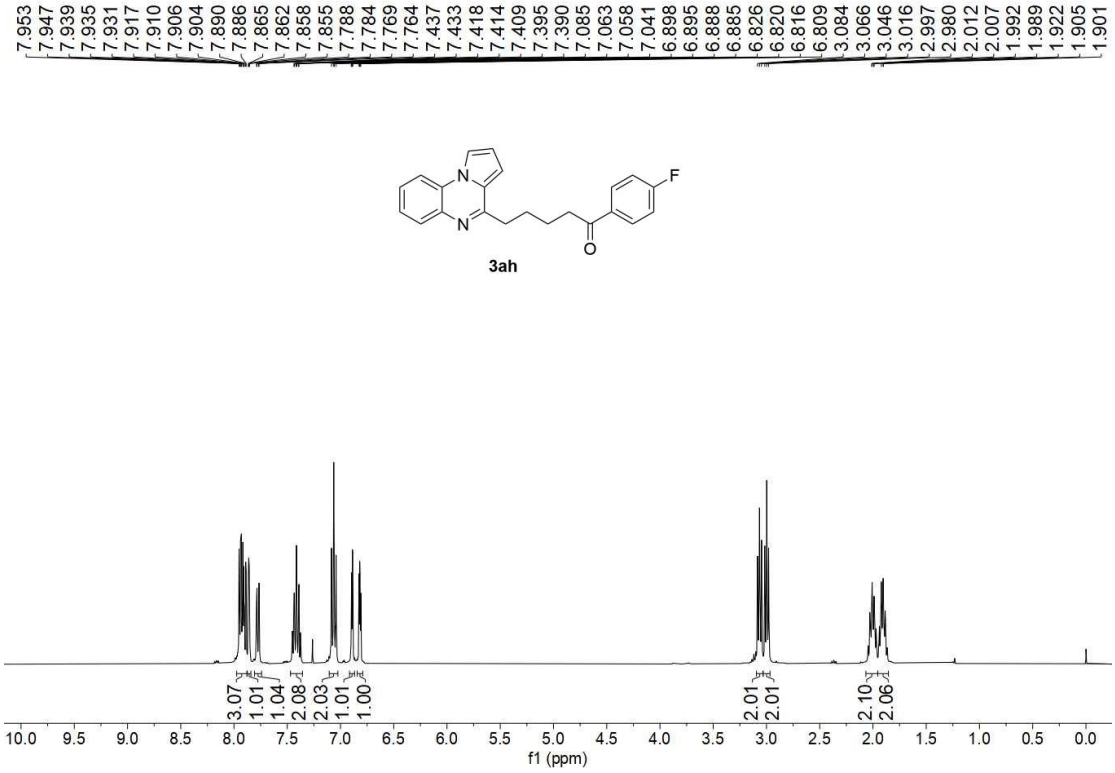
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ag**



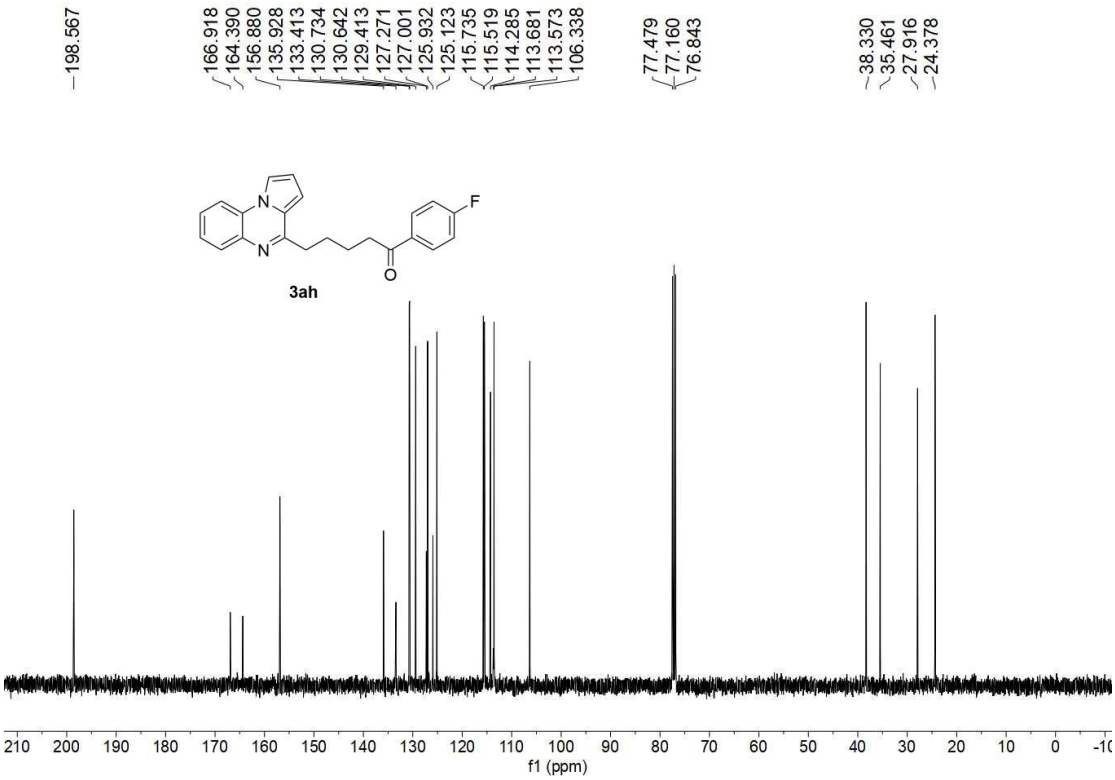
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ag**



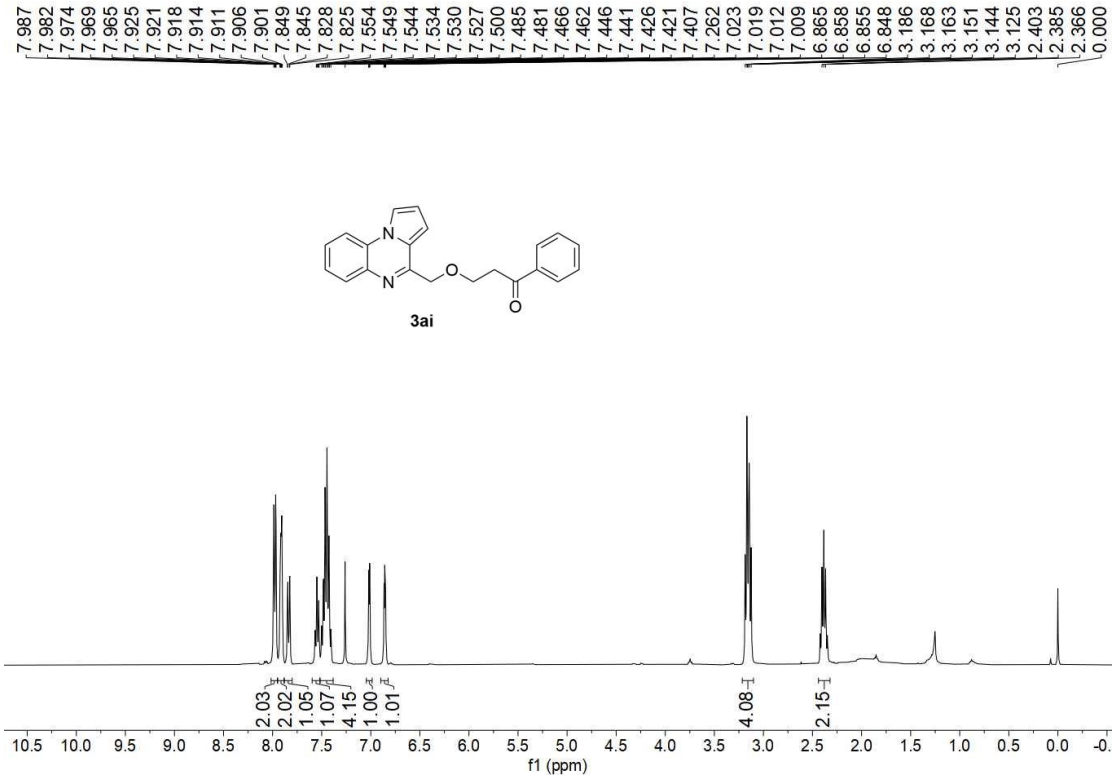
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ah**



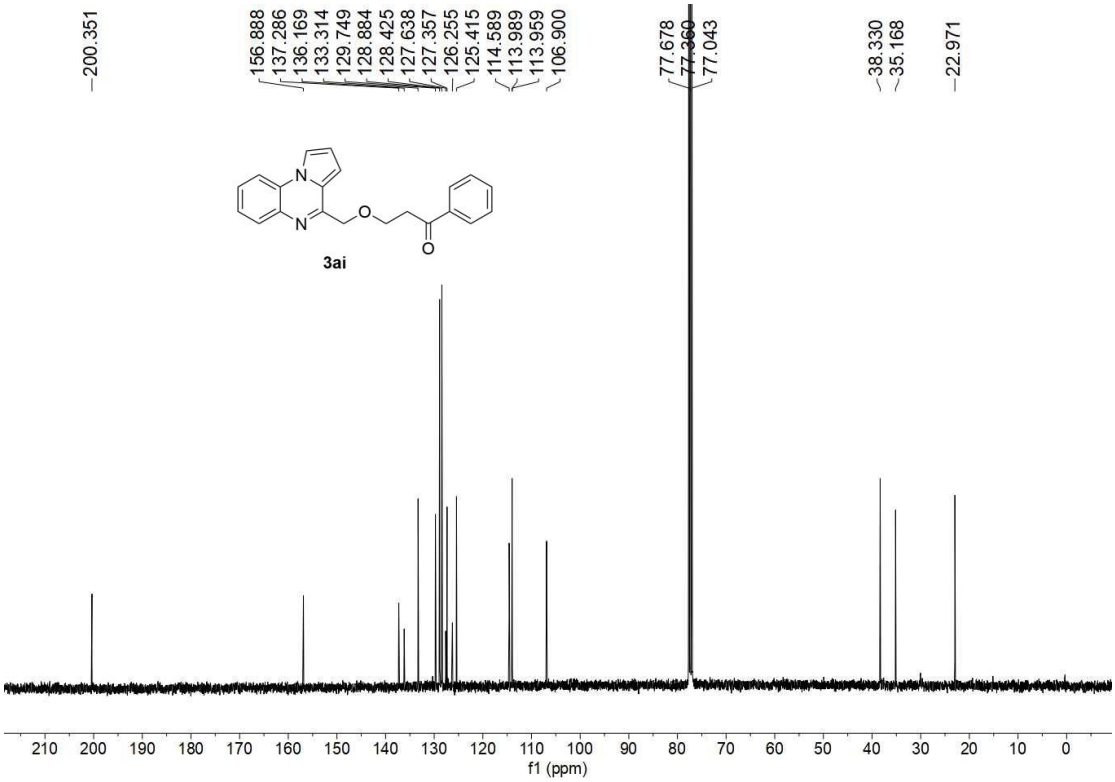
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ah**



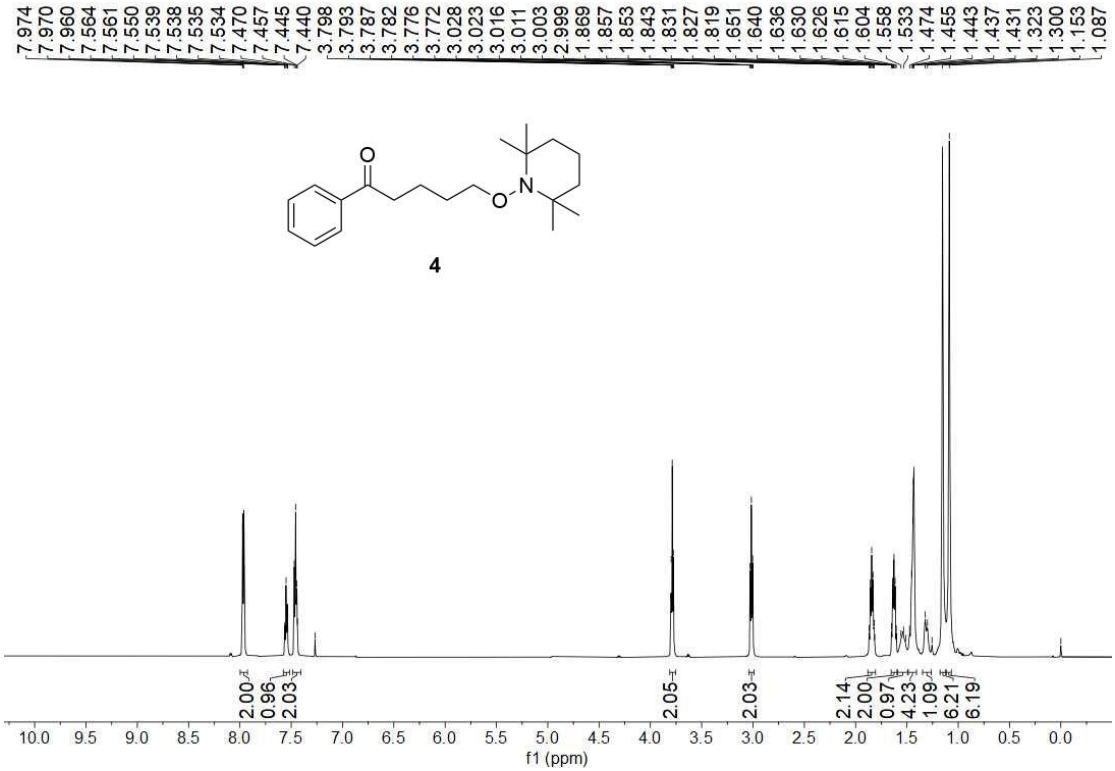
^{1}H NMR (400MHz, $CDCl_3$) of compound **3ai**



^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ai**



^{1}H NMR (600MHz, $CDCl_3$) of compound **4**



^{13}C NMR (150 MHz, $CDCl_3$) of compound **4**