Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Regioselective remote C5 cyanoalkoxylation and cyanoalkylation of 8-aminoquinolines with azobisisobutyronitrile

*Chunxia Wen,[a] Ronglin Zhong,[b] Zengxin Qin,[a] Mengfei Zhao[a] and Jizhen Li *[a]*

[a]Department of Organic Chemistry, College of Chemistry, Jilin University, 2519 Jiefang Road, Changchun, 130023, China

[b]Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, College of Chemistry, Jilin University, Changchun, 130023, China.

Corresponding author E-mail: ljz@jlu.edu.cn

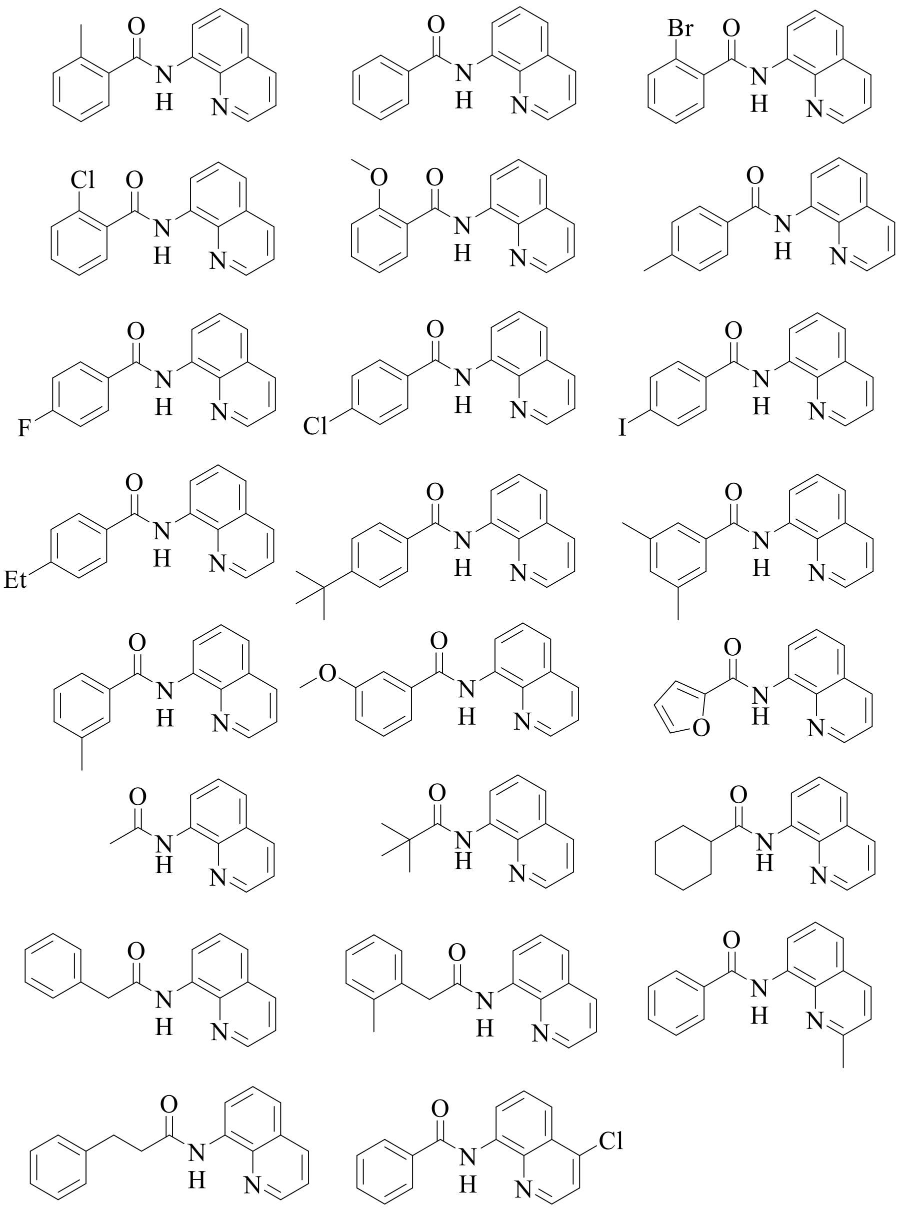
Contents

1. General information

All reagents, starting materials, and solvents were purchased from commercial sources and used without treatment, unless otherwise indicated. All the solvents were dried and newly distilled. NMR spectra were obtained on a Bruker AMX 400 system using chloroform-d as deuterated solvents. The ^{1}H-NMR spectra were recorded at 400 MHz in $CDCl_3$, and the ^{13}C-NMR spectra were recorded at 100 MHz in $CDCl_3$. All shifts were given in ppm. All coupling constants (*J* values) were reported in Hertz (Hz). Single crystal X-ray diffraction data were collected using a Bruker-AXS SMART APEX2 CCD diffractometer (Mo Kα, λ = 0.71073 Å). High-Resolution Liquid Chromatography-Mass Spectrometry was recorded on the Bruker MicrOTOF QII. Column chromatography was performed on silica gel 100-200 mesh or 200-300 mesh. Ethyl acetate and petroleum ether were used for column chromatography.

2. Preparation of starting materials[1]

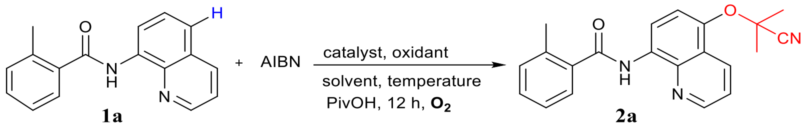
Preparation of starting materials: 8-aminoquinoline (0.72 g, 5.0 mmol) was dissolved in 10 mL of dichloromethane and cooled to 0 °C using an ice bath. NEt_3 (0.55 g, 5.5 mmol) was added to the 8-aminoquinoline solution followed by the corresponding acid chloride (5.5 mmol) dropwise. The mixture was stirred for 10 h at room temperature. Then, the mixture was washed with sat. $NaHCO_3$ (50 mL), and was extracted with dichloromethane for three times (3 x 40 mL). The organic layer was dried over Na_2SO_4. After filtration and evaporation, the amides were purified by column chromatography through silica gel.



3. Experimental section

3.1 Optimization of reaction conditions

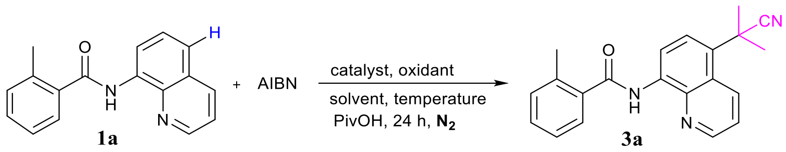
Table S1 Optimization for C5-selective cyanoalkoxylation reaction[a]



Entry	Catalyst	Oxidant	Temp (°C)	Solvent	Yield[b] (%)
1[c, d]	$Cu(OAc)_2$	$PhI(OAc)_2$	90	CH_3CN	25
2[c, d]	$Cu(OAc)_2$	TBHP	90	CH_3CN	30
3[c, d]	$Cu(OAc)_2$	$K_2S_2O_8$	90	CH_3CN	40
4[d]	$Cu(OAc)_2$	$K_2S_2O_8$	90	CH_3CN	50
5	$Cu(OAc)_2$	$K_2S_2O_8$	90	CH_3CN	60
6	$Cu(OAc)_2$	/	90	CH_3CN	trace
7	$Cu(NO_3)_2\cdot 3H_2O$	$K_2S_2O_8$	90	CH_3CN	trace
8	$NiSO_4$	$K_2S_2O_8$	90	CH_3CN	15
9	[Ru]	$K_2S_2O_8$	90	CH_3CN	n.r
10	$Cu(OAc)_2$	$K_2S_2O_8$	80	CH_3CN	66
11	$Cu(OAc)_2$	$K_2S_2O_8$	75	CH_3CN	68
12	**$Cu(OAc)_2$**	**$K_2S_2O_8$**	**70**	**CH_3CN**	**70**
13	$Cu(OAc)_2$	$K_2S_2O_8$	60	CH_3CN	64
14	$Cu(OAc)_2$	$K_2S_2O_8$	100	CH_3CN	45
15	$Cu(OAc)_2$	$K_2S_2O_8$	70	1,4-dioxane	n.r
16	$Cu(OAc)_2$	$K_2S_2O_8$	70	DCE	10
17	$Cu(OAc)_2$	$K_2S_2O_8$	70	DCM	15
18	$Cu(OAc)_2$	$K_2S_2O_8$	70	CH_3OH	20
19	$Cu(OAc)_2$	$K_2S_2O_8$	70	Toluene	n.r
20	$Cu(OAc)_2$	$K_2S_2O_8$	70	DMF	10
21[e]	$Cu(OAc)_2$	$K_2S_2O_8$	70	CH_3CN	n.r
22	$Cu(OAc)_2$	$PhI(OAc)_2$	90	CH_3CN	20

[a] Reaction conditions: **1a** (0.2 mmol), AIBN (4.0 equiv), catalyst (0.1 equiv), oxidant (1.0 equiv), PivOH (0.2 equiv), solvent (2.0 mL), under O_2 for 12 h. [b] Isolated yield. [c] Under air. [d] Oxidant (2.0 equiv). [e] Under N_2. [Ru]= [Ru (p-cymene) $Cl_2]_2$. n.r. = no reaction.

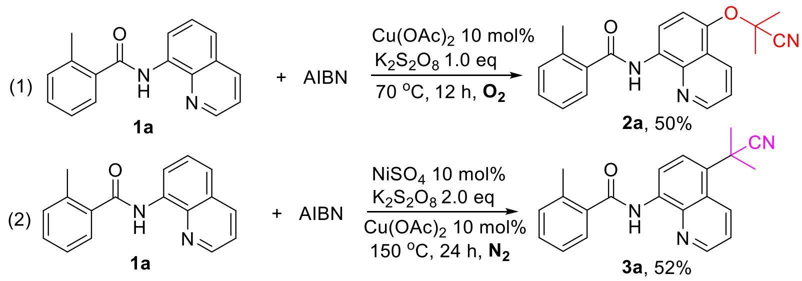
Table S2 Optimization for C5-selective cyanoalkylation reaction[a]



Entry	Catalyst	Oxidant	Solvent	Temp (°C)	Yield[b] (%)
1	$NiSO_4$	$PhI(OAc)_2$	CH_3CN	90	n.r
2	$NiSO_4$	$K_2S_2O_8$	CH_3CN	90	24
3	$NiSO_4$	Ag_2CO_3	CH_3CN	90	n.r
4	$NiSO_4$	$(NH_4)_2S_2O_8$	CH_3CN	90	n.r
5	$NiSO_4$	$K_2S_2O_8$	1,4-dioxane	90	trace
6	$NiSO_4$	$K_2S_2O_8$	THF	90	28
7	$NiSO_4$	$K_2S_2O_8$	DMSO	90	20
8	$NiSO_4$	$K_2S_2O_8$	CH_3CN/H_2O(1/1)	90	n.r
9	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(15/1)	90	27
10	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(10/1)	90	30
11	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(5/1)	90	32
12	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	90	35
13	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(1/1)	90	30
14	$NiCl_2$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	90	20
15	$Ni(OTf)_2$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	90	22
16	$Ni(dppf)_2Cl_2$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	90	20
17[c]	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	90	22
18[d]	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	90	45
19[d]	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	120	50
20[d]	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	140	60
21[d]	**$NiSO_4$**	**$K_2S_2O_8$**	**CH_3CN/DMSO(3/1)**	**150**	**67**
22[d]	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	160	57
23[e]	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	150	50
24	$NiSO_4$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	150	42
25	$Cu(OAc)_2$	$K_2S_2O_8$	CH_3CN/DMSO(3/1)	150	trace

[a] Reaction conditions: 1a (0.2 mmol), AIBN (4.0 equiv), catalyst (10 mol%), PivOH (2.0 equiv), oxidant (2.0 equiv), solvent (2.0 mL), under N_2 for 24 h. [b] Isolated yield. [c] Added 10 mol% $Cu(OTf)_2$. [d] Added 10 mol% $Cu(OAc)_2$. [e] Added 10 mol% $Fe(acac)_3$. n.r. = no reaction.

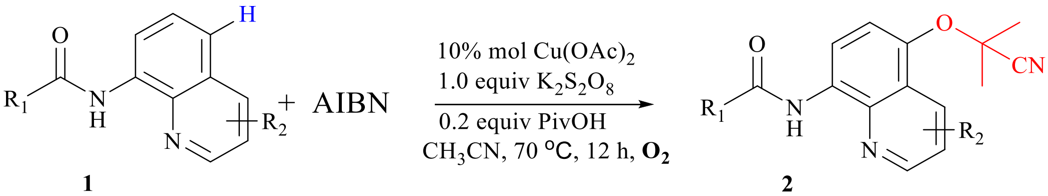
3.2 Control conditions (without PivOH)



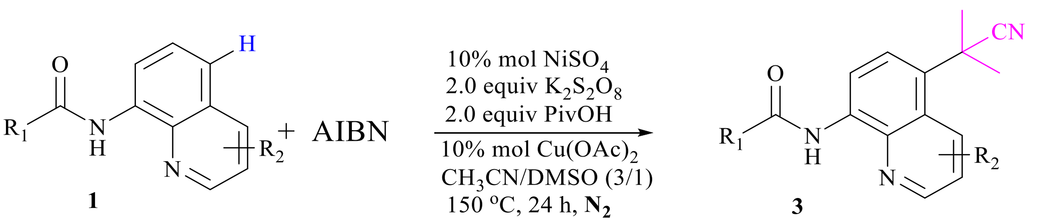
Scheme S1 Control conditions without PivOH

According to previous literatures, the C5 position activation of quinoline usually required weak acidity, which could promote the addition of free radicals. [2] We carried out control experiments without PivOH, and the results showed corresponding yields decreased, which indicated that pivalic acid was favorable to the reaction.

3.3 General procedures for C5-selective cyanoalkoxylation and cyanoalkylation of N-(8-quinolinyl) amides

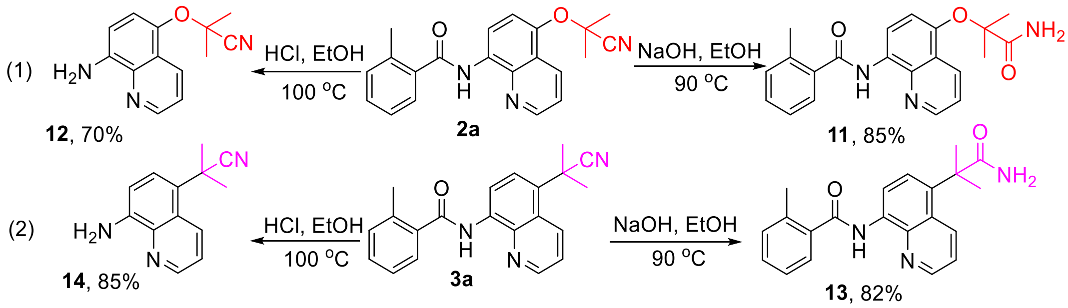


N-(8-quinolinyl) amide **1** (0.2 mmol, 1.0 equiv), AIBN (0.8 mmol, 4.0 equiv), $Cu(OAc)_2$ (0.02 mmol, 0.1 equiv), PivOH (0.04 mmol, 0.2 equiv) were mixed in CH_3CN (2.0 mL) and stirred in a dried Schlenk tube under oxygen atmosphere at 70 °C for 12 h. After completion of the reaction (TLC monitored), it was cooled to room temperature and transferred to a round bottom flask after dilution with CH_2Cl_2 dried over anhydrous Na_2SO_4. The solvent was concentrated under reduced pressure and further purified by flash chromatography (SiO_2, petroleum ether/ethyl acetate gradient), yielding the target product **2**.



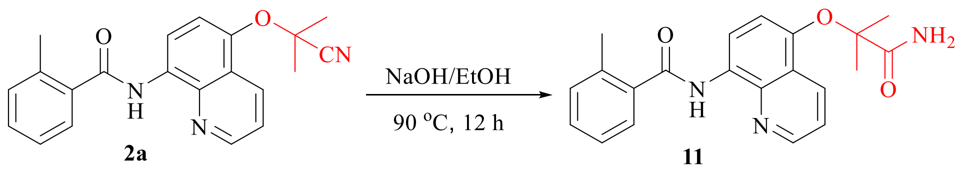
N-(8-quinolinyl) amide **1** (0.2 mmol, 1.0 equiv), AIBN (0.8 mmol, 4.0 equiv), $NiSO_4$ (0.02 mmol, 0.1 equiv), PivOH (0. 4 mmol, 2.0 equiv), $Cu(OAc)_2$ (0.02 mmol, 0.1 equiv) were mixed in CH_3CN/DMSO (1.5 mL/0.5 mL) and stirred in a dried Schlenk tube under nitrogen atmosphere at 150 °C for 24 h. After completion of the reaction (TLC monitored), the organic layer was washed with H_2O, and was extracted with dichloromethane. Then, the organic layer was dried over anhydrous Na_2SO_4, and resulting organic solution was concentrated under reduced pressure and further purified by flash chromatography (SiO_2, petroleum ether/ethyl acetate gradient), yielding the target product **3**.

3.4 Synthetic transformations of 2a and 3a

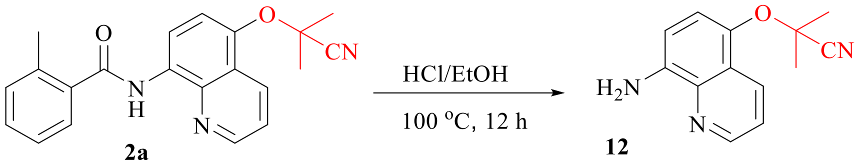


Scheme S2 Functional groups transformation.

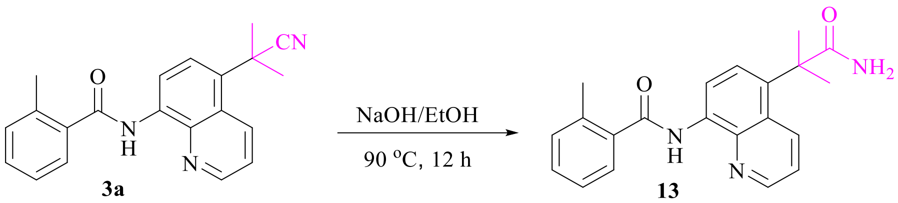
To demonstrate the potential application, the transformations of the products were also investigated (Scheme S2). Upon treatment of **2a** and **3a** with NaOH in EtOH at 90 °C for 12 h, the corresponding amide derivatives **11** and **13** were obtained in 85% yield and 82% yield, respectively. In addition, the 8-aminoquinoline directing group of **2a** and **3a** could be easily removed by simple acid hydrolysis, giving the corresponding product **12** in 70% yield and **14** in 85% yield, respectively.



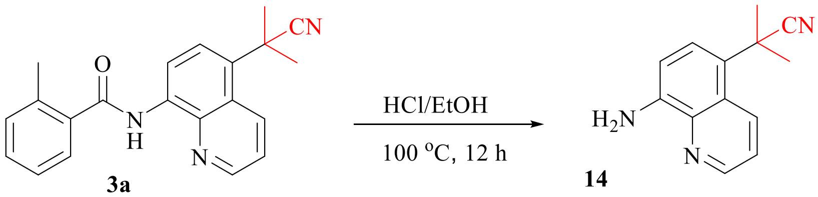
To a solution of **2a** (0.2 mmol, 1.0 equiv) in 2.0 mL of EtOH, NaOH (0.8 mmol, 4.0 equiv) was added. The mixture was stirred at 90 °C for 12 h. Upon completion of room temperature and evaporation of the solvent under reduced pressure, the residue was purified by column chromatography (petroleum ether/EtOAc=2:1) to afford pure **11** as a white solid in 85% yield.



To a solution of **2a** (0.2 mmol, 1.0 equiv) in 4.0 mL of EtOH, concentrated HCl (2.0 mL) was added. The mixture was stirred at 100 °C for 12 h. Upon completion of room temperature and evaporation of the solvent under reduced pressure, the residue was purified by column chromatography (petroleum ether/EtOAc=5:1) to afford pure **12** as a pale yellow solid in 70% yield.



To a solution of **3a** (0.2 mmol, 1.0 equiv) in 2.0 mL of EtOH, NaOH (0.8 mmol, 4.0 equiv) was added. The mixture was stirred at 90 °C for 12 h. Upon completion of room temperature and evaporation of the solvent under reduced pressure, the residue was purified by column chromatography (petroleum ether/EtOAc=2:1) to afford pure **13** as a white solid in 82% yield.



To a solution of **3a** (0.2 mmol, 1.0 equiv) in 4.0 mL of EtOH, concentrated HCl (2.0 mL) was added. The mixture was stirred at 100 °C for 12 h. Upon completion of room temperature and evaporation of the solvent under reduced pressure, the residue was purified by column chromatography (petroleum ether/EtOAc=5:1) to afford pure **14** as a pale yellow solid in 85% yield.

4. The single crystal X-ray diffraction studies of N-(5-((2-cyanopropan-2-yl)oxy)quinolin-8-yl)-2-methylbenzamide 2a

Single-crystal X-ray structure of **2a**

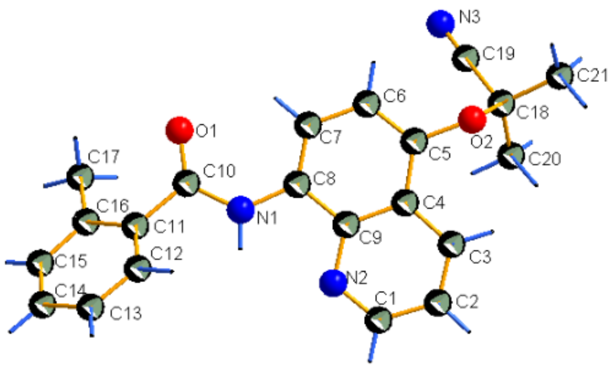


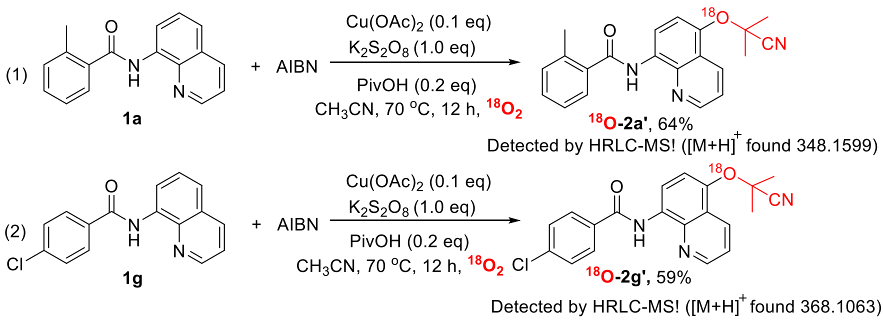
Table S3. Crystal data and structure refinement for **2a**.

Identification code	**2a**	
Empirical formula	$C_{21}H_{19}N_3O_2$	
Formula weight	345.39	
Temperature	150 (2) K	
Crystal system	Orthorhombic	
Space group	Pna21	
Unit cell dimensions	a = 12.4892 (11) A	alpha = 90 deg.
	b = 7.3635 (6) A	beta = 90 deg.
	c = 18.9497 (17) A	gamma = 90 deg.
Volume	1742.7 (3) A^3	
Z, Calculated density	4, 1.316 Mg/m^3	
Absorption coefficient	0.087 mm^-1	
F (000)	728.0	

Crystal size	0.220 x 0.200 x 0.180 mm
Theta range for data collection	3.262 to 52.75 deg.
Limiting indices	-15<=h<=15, -9<=k<=4, -23<=l<=21
Reflections collected	9497
Independent reflections	3459 [Rint = 0.0519, Rsigma = 0.0425]
Data / restraints / parameters	3459 / 1 / 239
Goodness-of-fit on F^2	1.049
Final R indices [I>2 sigma (I)]	R1 = 0.0403, wR2 = 0.0896
R indices (all data)	R1 = 0.0526, wR2 = 0.0957
Largest diff. peak and hole	0.19 and -0.17 e.A^-3
Flack parameter	-0.5(7)

5. Mechanism investigation

5.1 Isotopic labeling experiments



N-(8-quinolinyl) amide **1** (0.2 mmol, 1.0 equiv), AIBN (0.8 mmol, 4.0 equiv), $Cu(OAc)_2$ (0.02 mmol, 0.1 equiv), PivOH (0.04 mmol, 0.2 equiv) were mixed in CH_3CN (2.0 mL) and stirred in a dried Schlenk tube under $^{18}O_2$ atmosphere at 70 °C for 12 h. After completion of the reaction (TLC monitored), it was cooled to room temperature and transferred to a round bottom flask after dilution with CH_2Cl_2. The solvent was concentrated under reduced pressure and further purified by flash chromatography (SiO_2, petroleum ether/ethyl acetate gradient), providing the product ^{18}O-**2a**' and ^{18}O-**2g**' (isolated yields 64% and 59%). The product ^{18}O-**2a**' (peak 3.7 min) was analyzed by HRMS. HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O^{18}O$: 348.1592, found: 348.1599. The product ^{18}O-**2g**' (peak 4.05 min) was analyzed by HRMS. HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}ClN_3O^{18}O$: 368.1046, found: 368.1063.

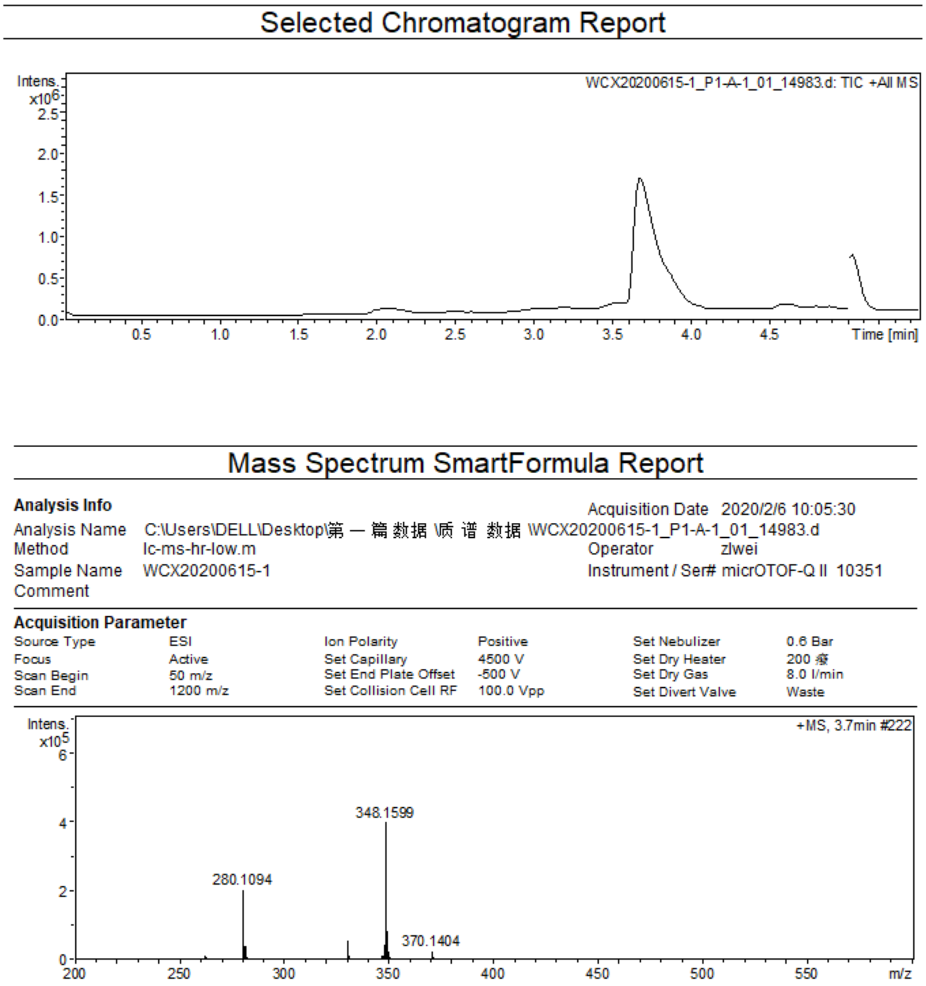


Figure S1 LC-MS analysis of the ^{18}O-labled product **2a'.**

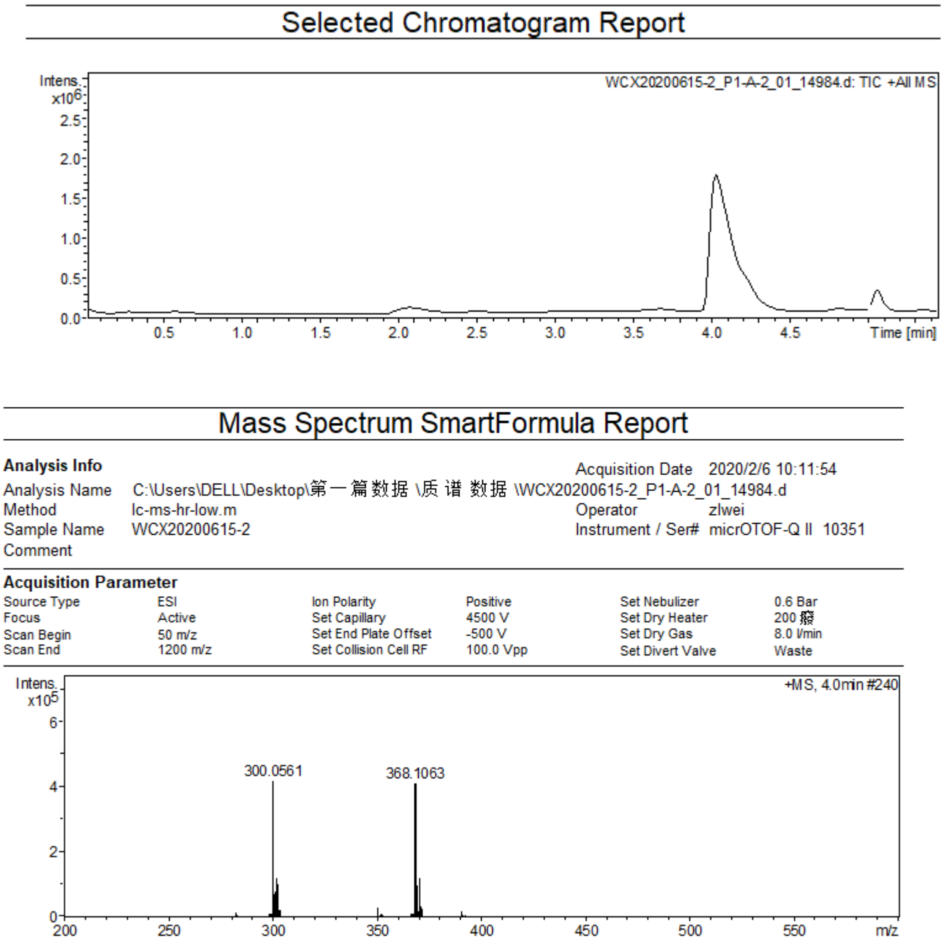


Figure S2 LC-MS analysis of the ^{18}O-labled product **2g’**.

5.2 Unreacted substrates.

Several quinoline analogues were undertaken under the standard conditions (Figure S3). Quinoline analogues without an amido bond (**4**, **5**) were ineffective. However, substrates N-methyl-N-(8-quinolinyl) benzamide (**6**), the naphthylamide derivatives (**7**) and (**8**) were inactive in the reaction. These results indicated 8-aminoquinoline amide skeleton and free NH were necessary for cyanoalkoxylation and cyanoalkylation reactions.

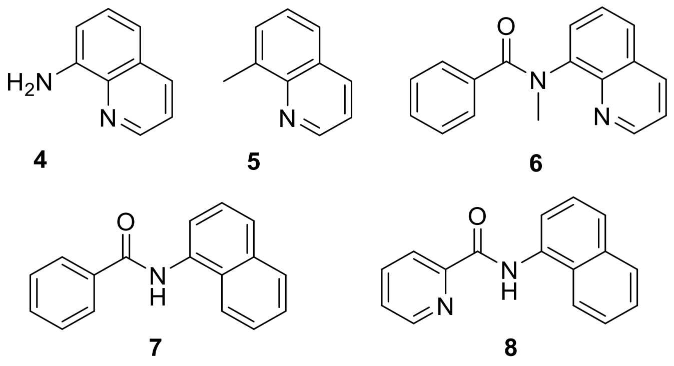
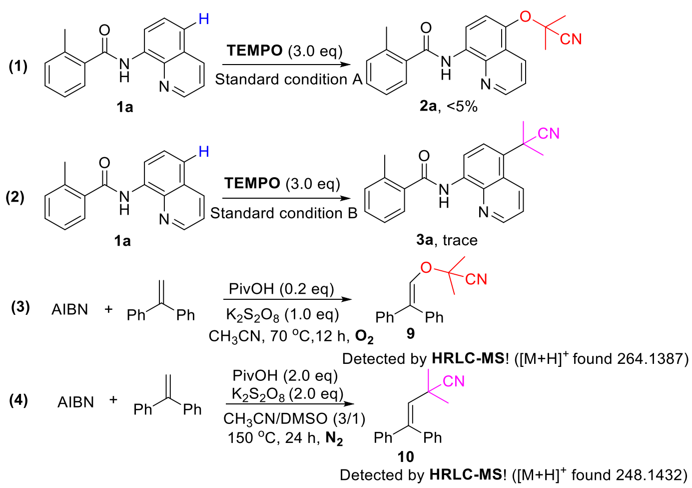


Figure S3 Unreacted substrates.

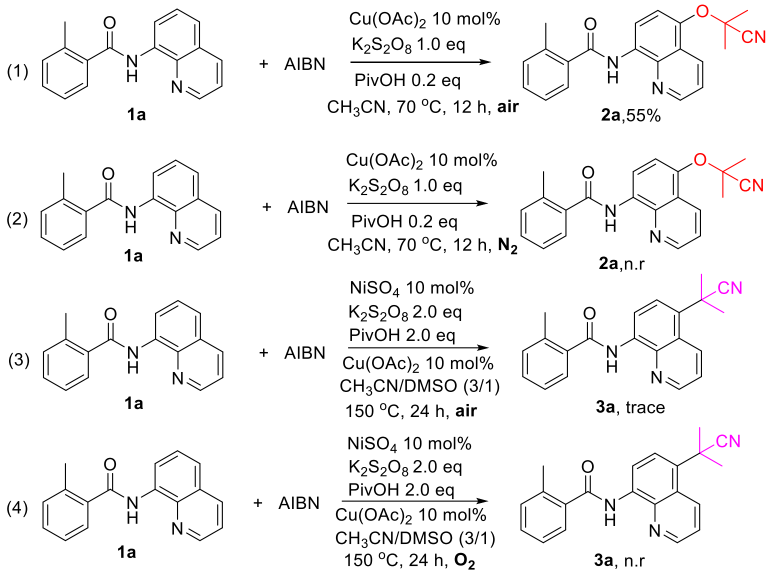
To gain insight into the reaction mechanisms, some control experiments were carried out (Scheme S3). Only a trace of the desired products **2a** and **3a** was obtained in the presence of radical scavenger TEMPO (3.0 equiv.), which implied the involvement of free radical in the reaction pathway (eq 1 and eq 2). Furthermore, we tried to capture cyanopropyloxyl radical and cyanopropyl radical by using 3.0 equiv. 1, 1-diphenylethylene, and radical coupling products **9** and **10** were detected *via* LC-MS (eq 3 and eq 4).



Scheme S3 Investigation of the radical pathway.

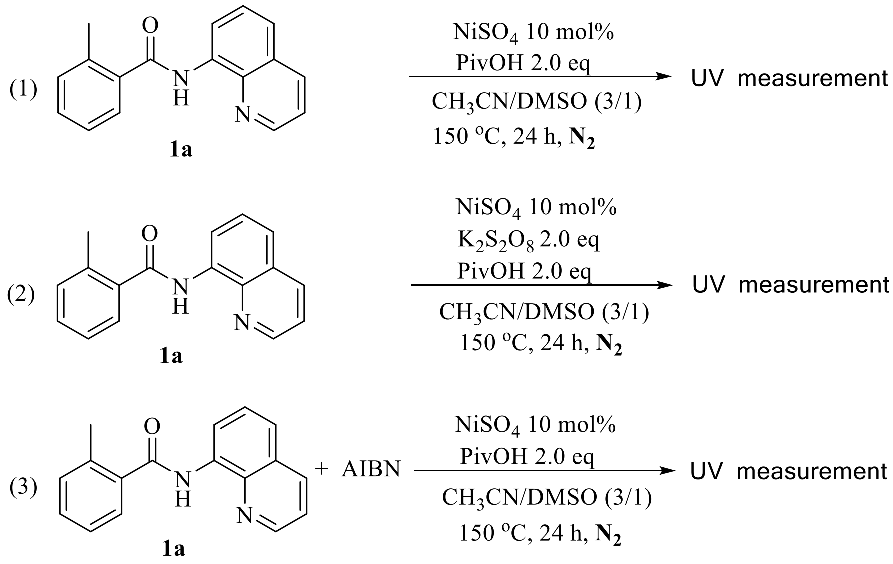
5.3 Radical control experiments.

We performed control experiments through changing the gas composition under standard conditions (Scheme S4). For the cyanoalkoxylation reaction, the yield of product **2a** decreased under air (eq 1), and cyanoalkoxylation did not occur under nitrogen atmosphere (eq 2). For the cyanoalkylation reaction, only trace of product **3a** was obtained under air (eq 3), product **3a** was completely undetectable under oxygen atmosphere (eq 4). The results showed that gas composition was an important factor for the formation of different radicals.



Scheme S4 Radical control experiments.

5.4 Study of Ni valence number change by UV.



Scheme S5 Mechanism research.

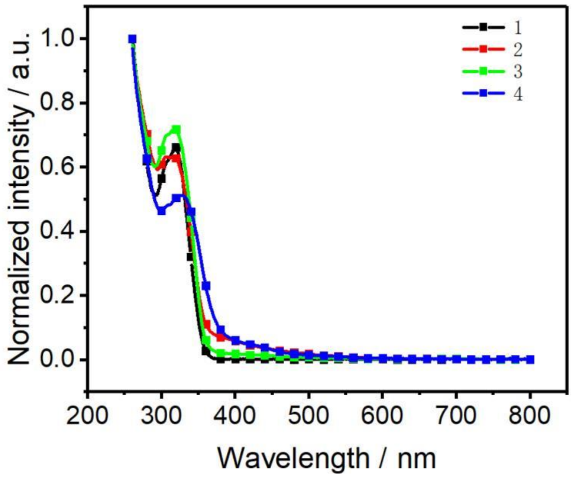
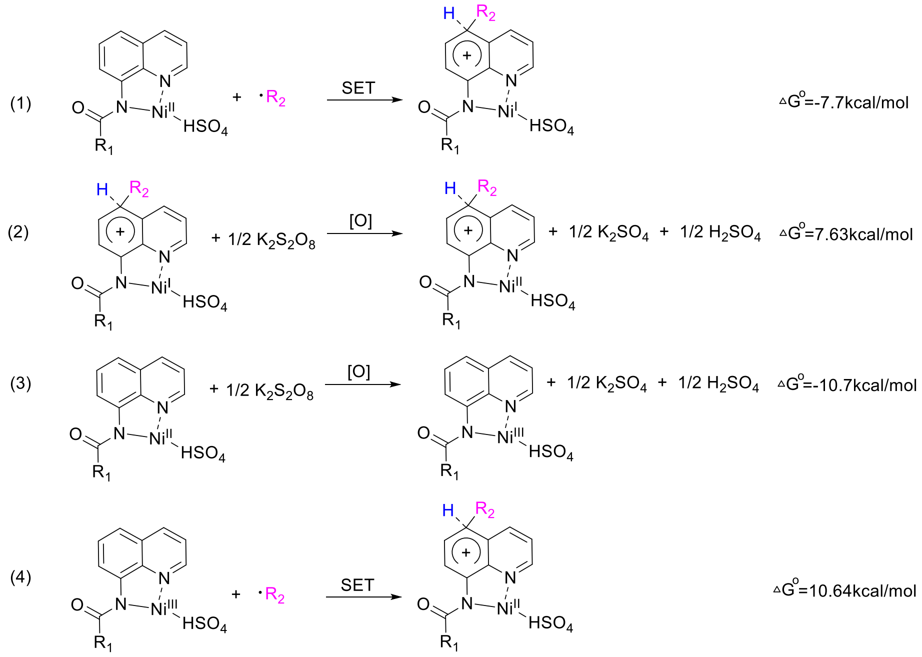


Figure S4 UV absorption of three reaction solutions.

After the above reactions were completed (Scheme S5), we tested the UV absorption wavelength of the above three reaction solutions after filtration. First, we tested the UV absorption wavelength of substrate **1a** dissolved in CH_3CN/DMSO (3/1) solvent, and the measured spectrum was **black** as shown in **line 1** for a reference; the spectrum of the first reaction solution was **red** as shown in **line 2**; the spectrum of the second reaction solution was **green** as shown in **line 3**; the third reaction solution was plotted in **blue** as shown in **line 4** (Figure S4). According to the changes of the maximum absorption wavelength of the three reaction solutions, only **the third reaction was red shifted** (about at 330 nm，**line 4**), while the second reaction did not change. Therefore, we suspected that the reaction mechanism might be that the SET process firstly took place, and divalent nickel converted into monovalent nickel preferentially.

5.5 Computational details for cyanoalkylation reaction.

All geometry optimizations were performed by the B3PW91-D3 functional[3, 4] in gas phase, where the D3 denotes the third-generation dispersion correction by Grimme and co-workers.[5] The Stuttgart-Dresden-Bonn basis sets[6] were employed for valence electrons of Ni and Cu with effective core potentials representing their core electrons and 6-311+G(d) basis sets were used for other atoms. Solvation effect (acetonitrile) was evaluated with polarizable continuum model (PCM).[7] In this work, thermal correction and entropy contribution to the Gibbs energy were evaluated at 298.15 K and 1 atm. All these calculations were carried out with Gaussian 09 program.[8]



Scheme S6 The Gibbs energy of reaction for the SET and oxidation process of Ni^{II} complex.

There are two plausible pathways for conversion of Ni^{II} complex. In the first pathway, the Ni^{II} complex firstly converts to a Ni^{I} complex through a SET process (eq 1), and then the reductive Ni^{I} is oxidized by the $K_2S_2O_8$ (eq 2). In the second pathway, the Ni^{II} complex is firstly oxidized by the $K_2S_2O_8$ (eq 3) to a Ni^{III} complex, and then a SET process occurs (eq 4). As shown in Scheme S6, the Gibbs energy of reaction (ΔG°) of eq (1) is -7.7 kcal/mol suggesting that this SET process is exoergonic and will occur easily. However, ΔG° of eq 4 is 10.6 kcal/mol, suggesting this SET process is endoergonic and such SET process is difficult to occur. These results indicate that the SET process would occur prior to the oxidation process, which is consistent with the experimental results as shown in Figure S4 about the study of Ni valence state change.

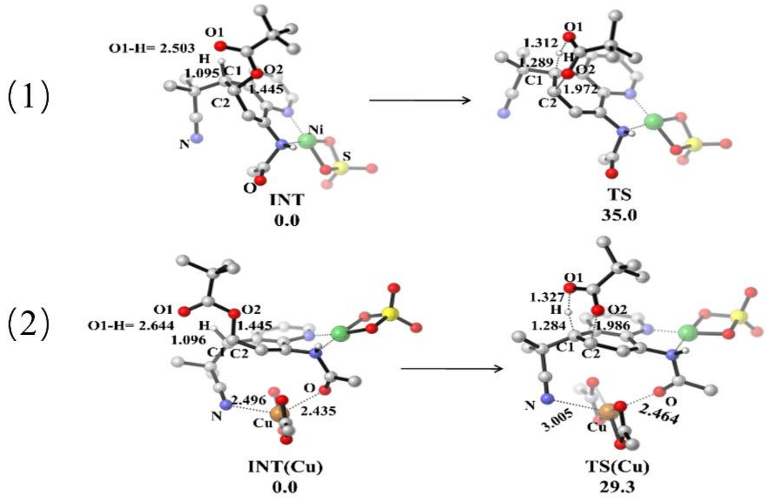
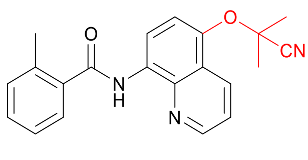


Figure S5 The geometry and energy change in the elementary step of proton transfer in the absence(1)/presence(2) of $Cu(OAc)_2$.

It is interesting that yield of the reaction increased with cooperation of the $Cu(OAc)_2$. To understand the effect of $Cu(OAc)_2$, we calculated the Gibbs energy of activation ($\Delta G^{o‡}$) in the absence/presence of $Cu(OAc)_2$ as shown in Figure S5. Results showed that the $\Delta G^{o‡}$ decreases 4.7 kcal/mol in the presence of $Cu(OAc)_2$, which was consistent with the experimental results that yield of the reaction increased in the presence of the $Cu(OAc)_2$. As shown in the structure of **TS(Cu)**, the Cu−N distance was 3.005 Å and Cu−O distance was 2.464 Å, respectively. It indicateed that the coordination between cyano and carbonyl groups and Cu^{II} stabilized the TS(Cu) more than INT(Cu), which decreased the $\Delta G^{o‡}$.[9]

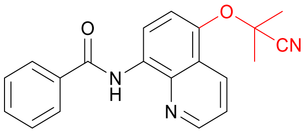
6. Characterization data of products

2a:



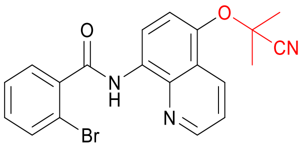
White solid, isolated yield: 70%; ^{1}H NMR (400 Hz, $CDCl_3$) δ: 10.07 (s, 1H), 8.91 (d, J = 8.6 Hz, 1H), 8.80 (dd, J = 4.2, 1.7 Hz, 1H), 8.47 (dd, J = 8.5, 1.7 Hz, 1H), 7.67 (d, J = 7.4 Hz, 1H), 7.55 (d, J = 8.6 Hz, 1H), 7.49 (dd, J = 8.5, 4.2 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.33 (t, J = 7.3 Hz, 2H), 2.60 (s, 3H), 1.85 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.07 (s), 148.79 (s), 144.72 (s), 139.21 (s), 136.69 (s), 136.57 (s), 131.56 (s), 131.38 (s), 131.31 (s), 130.34 (s), 127.25 (s), 126.02 (s), 123.40 (s), 121.52 (s), 120.68 (s), 116.22 (s), 116.02 (s), 72.74 (s), 27.54 (s), 20.20 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_2$: 346.1550, found: 346.1548.

2b:



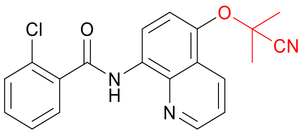
White solid, isolated yield: 54%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.59 (s, 1H), 8.90 (d, J = 8.6 Hz, 1H), 8.87 (d, J = 4.1 Hz, 1H), 8.47 (dd, J = 8.4, 1.3 Hz, 1H), 8.06 (d, J = 6.5 Hz, 2H), 7.58 – 7.49 (m, 5H), 1.83 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.37 (s), 148.83 (s), 144.68 (s), 139.35 (s), 131.86 (s), 131.36 (s), 130.51 (s), 129.70 (s), 128.82 (s), 127.26 (s), 123.58 (s), 123.40 (s), 121.56 (s), 116.19 (s), 116.06 (s), 72.69 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{17}N_3O_2$: 332.1394, found: 332.1391.

2c:



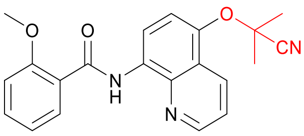
White solid, isolated yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.17 (s, 1H), 8.92 (d, J = 8.5 Hz, 1H), 8.81 (d, J = 3.9 Hz, 1H), 8.47 (d, J = 8.4 Hz, 1H), 7.70 (t, J = 8.3 Hz, 2H), 7.56 (d, J = 8.5 Hz, 1H), 7.50 (dd, J = 8.4, 4.1 Hz, 1H), 7.45 (t, J = 7.5 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 1.85 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.76 (s), 148.90 (s), 145.02 (s), 139.21 (s), 138.23 (s), 133.69 (s), 131.54 (s), 131.31 (s), 131.07 (s), 129.61 (s), 127.68 (s), 123.35 (s), 121.59 (s), 120.65 (s), 119.69 (s), 116.41 (s), 115.99 (s), 72.69 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}BrN_3O_2$: 410.0499, 412.0478, found: 410.0492, 412.0477.

2d:



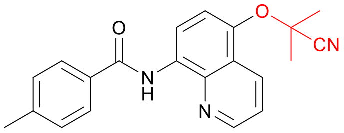
White solid, isolated yield: 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.37 (s, 1H), 8.93 (d, J = 8.6 Hz, 1H), 8.82 (d, J = 3.7 Hz, 1H), 8.48 (d, J = 8.4 Hz, 1H), 7.82 (dd, J = 7.2, 1.8 Hz, 1H), 7.56 (d, J = 8.6 Hz, 1H), 7.53 – 7.47 (m, 2H), 7.47 – 7.40 (m, 2H), 1.85 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.73 (s), 148.92 (s), 145.00 (s), 139.26 (s), 135.72 (s), 131.56 (s), 131.28 (s), 131.19 (s), 131.15 (s), 130.53 (s), 130.14 (s), 127.19 (s), 123.34 (s), 121.58 (s), 120.66 (s), 116.45 (s), 116.00 (s), 72.69 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}ClN_3O_2$: 366.1004, found: 366.1002.

2e:



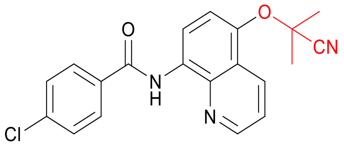
White solid, isolated yield: 73%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 12.23 (s, 1H), 8.99 (d, J = 8.6 Hz, 1H), 8.87 (d, J = 2.8 Hz, 1H), 8.43 (d, J = 8.4 Hz, 1H), 8.34 (d, J = 7.7 Hz, 1H), 7.55 – 7.44 (m, 3H), 7.12 (t, J = 7.5 Hz, 1H), 7.05 (d, J = 8.2 Hz, 1H), 4.16 (s, 3H), 1.82 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.47 (s), 157.71 (s), 148.79 (s), 144.46 (s), 139.75 (s), 133.18 (s), 132.55 (s), 132.28 (s), 131.09 (s), 123.41 (s), 122.18 (s), 121.35 (s), 121.28 (s), 120.83 (s), 116.65 (s), 116.33 (s), 111.61 (s), 72.67 (s), 56.11 (s), 27.50 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_3$: 362.1499, found: 362.1494.

2f:



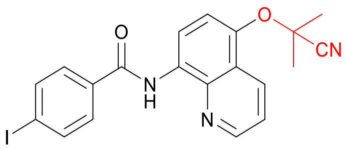
White solid, isolated yield: 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.56 (s, 1H), 8.89 (d, *J* = 8.6 Hz, 1H), 8.87 (dd, *J* = 4.6, 2.1 Hz, 1H), 8.46 (d, *J* = 8.5 Hz, 1H), 7.97 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 1H), 7.51 (dd, *J* = 8.5, 4.3 Hz, 1H), 7.34 (d, *J* = 7.9 Hz, 2H), 2.45 (s, 3H), 1.83 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.36, 148.78, 144.56, 142.37, 139.34, 132.25, 131.50, 131.33, 129.48, 127.27, 123.40, 121.52, 120.72, 116.24, 115.95, 72.70, 27.52, 21.55. HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_2$: 346.1550, found: 346.1549.

2g:



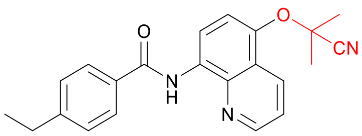
White solid, isolated yield: 65%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.55 (s, 1H), 8.86 (dd, *J* = 5.0, 3.4 Hz, 2H), 8.47 (dd, *J* = 8.5, 1.5 Hz, 1H), 8.00 (d, *J* = 8.5 Hz, 2H), 7.55 – 7.49 (m, 4H), 1.84 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.22 (s), 148.89 (s), 144.86 (s), 139.29 (s), 138.14 (s), 133.43 (s), 131.41 (s), 131.05 (s), 129.08 (s), 128.69 (s), 123.35 (s), 121.62 (s), 120.65 (s), 116.15 (s), 115.99 (s), 72.66 (s), 27.52 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}ClN_3O_2$: 366.1004, found: 366.1001.

2h:



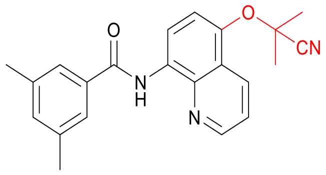
White solid, isolated yield: 70% ; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.57 (s, 1H), 8.95 – 8.82 (m, 2H), 8.49 (d, *J* = 8.3 Hz, 1H), 7.91 (d, *J* = 8.3 Hz, 2H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.53 (dd, *J* = 12.4, 6.4 Hz, 2H), 1.85 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.49 (s), 148.91 (s), 144.87 (s), 139.25 (s), 138.03 (s), 134.46 (s), 131.42 (s), 130.99 (s), 128.82 (s), 123.34 (s), 121.65 (s), 120.65 (s), 119.11 (s), 116.13 (s), 115.95 (s), 72.67 (s), 27.50 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}IN_3O_2$: 458.0360, found: 458.0359.

2i:



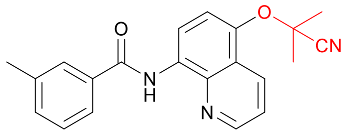
White solid, isolated yield: 69%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.57 (s, 1H), 8.90 (d, *J* = 8.6 Hz, 1H), 8.86 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.46 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.99 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 1H), 7.50 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.37 (d, *J* = 8.1 Hz, 2H), 2.75 (q, *J* = 7.6 Hz, 2H), 1.83 (s, 6H), 1.29 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.37 (s), 148.77 (s), 148.58 (s), 144.54 (s), 139.34 (s), 132.51 (s), 131.54 (s), 131.32 (s), 128.30 (s), 127.37 (s), 123.40 (s), 121.52 (s), 120.73 (s), 116.26 (s), 115.93 (s), 72.70 (s), 28.87 (s), 27.52 (s), 15.34 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{21}N_3O_2$: 360.1707, found: 360.1702.

2j:



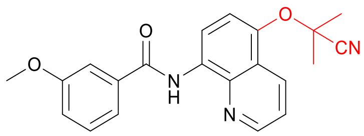
White solid, isolated yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.51 (s, 1H), 8.89 (d, *J* = 8.7 Hz, 2H), 8.47 (d, *J* = 8.4 Hz, 1H), 7.64 (s, 2H), 7.56 – 7.48 (m, 2H), 7.20 (s, 1H), 2.43 (s, 6H), 1.83 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.78 (s), 148.83 (s), 144.57 (s), 139.33 (s), 138.48 (s), 135.09 (s), 133.51 (s), 131.48 (s), 131.34 (s), 124.98 (s), 123.38 (s), 121.53 (s), 119.10 (s), 116.19 (s), 116.03 (s), 72.69 (s), 27.50 (s), 21.37 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{21}N_3O_2$: 360.1707, found: 360.1705.

2k:



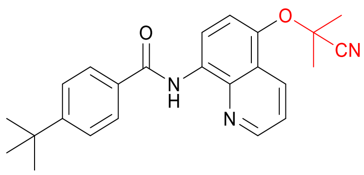
White solid, isolated yield: 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.56 (s, 1H), 8.91 (d, *J* = 8.7 Hz, 1H), 8.88 (d, *J* = 3.9 Hz, 1H), 8.48 (d, *J* = 8.4 Hz, 1H), 7.88 (s, 1H), 7.85 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 1H), 7.52 (dd, *J* = 8.5, 4.3 Hz, 1H), 7.46 – 7.37 (m, 2H), 2.48 (s, 3H), 1.84 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.60 (s), 148.81 (s), 144.62 (s), 139.36 (s), 138.71 (s), 135.09 (s), 132.62 (s), 131.47 (s), 131.34 (s), 128.66 (s), 128.05 (s), 124.18 (s), 123.39 (s), 121.53 (s), 120.72 (s), 116.23 (s), 116.05 (s), 72.69 (s), 27.54 (s), 21.50 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_2$: 346.1550, found: 346.1548.

2l:



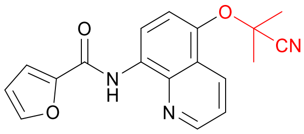
White solid, isolated yield: 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.58 (s, 1H), 8.89 (d, *J* = 8.6 Hz, 1H), 8.87 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.47 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.62 (dd, *J* = 4.0, 2.0 Hz, 2H), 7.55 (d, *J* = 8.6 Hz, 1H), 7.51 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.45 (t, *J* = 8.1 Hz, 1H), 7.12 (dd, *J* = 7.8, 2.1 Hz, 1H), 3.91 (s, 3H), 1.84 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.20 (s), 160.02 (s), 148.85 (s), 144.70 (s), 139.35 (s), 136.58 (s), 131.36 (s), 131.33 (s), 129.80 (s), 123.39 (s), 121.56 (s), 120.70 (s), 119.04 (s), 118.05 (s), 116.16 (s), 116.05 (s), 112.65 (s), 72.68 (s), 55.53 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_3$: 362.1499, found: 362.1495.

2m:



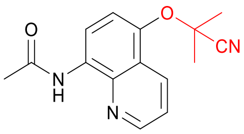
White solid, isolated yield: 58%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.58 (s, 1H), 8.90 (d, *J* = 8.6 Hz, 1H), 8.86 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.47 (dd, *J* = 8.5, 1.6 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.8 Hz, 3H), 7.51 (dd, *J* = 8.5, 4.2 Hz, 1H), 1.84 (s, 6H), 1.38 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.39 (s), 155.40 (s), 148.77 (s), 144.54 (s), 139.35 (s), 132.26 (s), 131.55 (s), 131.33 (s), 127.12 (s), 125.77 (s), 123.42 (s), 121.52 (s), 120.72 (s), 116.32 (s), 115.95 (s), 72.71 (s), 35.03 (s), 31.20 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{24}H_{25}N_3O_2$: 388.2020, found: 388.2020.

2n:



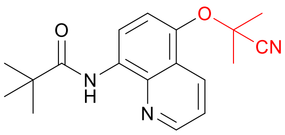
White solid, isolated yield: 50%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.64 (s, 1H), 8.91 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.84 (d, *J* = 8.6 Hz, 1H), 8.47 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.63 (s, 1H), 7.55 – 7.50 (m, 2H), 7.30 (d, *J* = 3.4 Hz, 1H), 6.59 (dd, *J* = 3.5, 1.7 Hz, 1H), 1.84 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 156.29 (s), 148.94 (s), 148.28 (s), 144.78 (s), 144.52 (s), 139.25 (s), 131.28 (s), 130.94 (s), 123.37 (s), 121.56 (s), 120.69 (s), 116.19 (s), 116.02 (s), 115.15 (s), 112.47 (s), 72.64 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{18}H_{16}N_3O_3$: 322.1186, found: 322.1181.

2o:



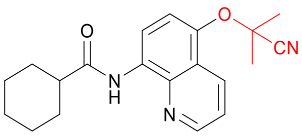
White solid, isolated yield: 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.67 (s, 1H), 8.85 (d, *J* = 1.6 Hz, 1H), 8.75 (d, *J* = 8.5 Hz, 1H), 8.48 (d, *J* = 8.4 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 2.37 (s, 3H), 1.85 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.70 (s), 148.67 (s), 144.46 (s), 138.79 (s), 131.29 (s), 131.25 (s), 123.26 (s), 121.48 (s), 120.70 (s), 116.04 (s), 115.90 (s), 72.65 (s), 27.47 (s), 25.04 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{15}H_{15}N_3O_2$: 270.1237, found: 270.1235.

2p:



White solid, isolated yield: 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.15 (s, 1H), 8.84 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.76 (d, *J* = 8.6 Hz, 1H), 8.44 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.49 (dd, *J* = 8.5, 4.3 Hz, 2H), 1.81 (s, 6H), 1.43 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 177.09 (s), 148.77 (s), 144.31 (s), 139.28 (s), 131.52 (s), 131.23 (s), 123.34 (s), 121.45 (s), 120.74 (s), 116.26 (s), 115.58 (s), 72.72 (s), 40.26 (s), 27.72 (s), 27.44 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{18}H_{21}N_3O_2$: 312.1707, found: 312.1707.

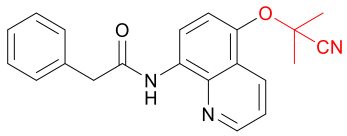
2q:



White solid, isolated yield: 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.78 (s, 1H), 8.86 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.79 (d, *J* = 8.6 Hz, 1H), 8.47 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.51 (dd, *J* = 8.5, 4.1 Hz, 2H), 2.54 – 2.44

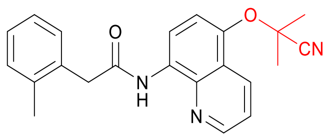
(m, 1H), 2.10 (d, J = 13.2 Hz, 2H), 1.93 – 1.87 (m, 2H), 1.84 (s, 6H), 1.72 – 1.60 (m, 3H), 1.44 – 1.32 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 174.75 (s), 148.62 (s), 144.27 (s), 139.05 (s), 131.51 (s), 131.29 (s), 123.35 (s), 121.40 (s), 120.71 (s), 116.39 (s), 115.88 (s), 72.71 (s), 46.86 (s), 29.77 (s), 27.51 (s), 25.77 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{23}N_3O_2$: 338.1863, found: 338.1858.

2r:



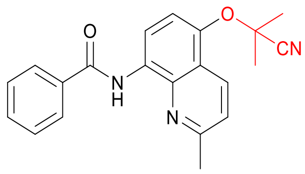
White solid, isolated yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.78 (s, 1H), 8.78 – 8.67 (m, 2H), 8.39 (dd, J = 8.4, 1.2 Hz, 1H), 7.47 – 7.38 (m, 6H), 7.35 – 7.31 (m, 1H), 3.88 (s, 2H), 1.79 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.47 (s), 148.73 (s), 144.61 (s), 139.01 (s), 134.62 (s), 131.18 (s), 131.13 (s), 129.53 (s), 129.00 (s), 127.38 (s), 123.23 (s), 121.43 (s), 120.68 (s), 116.02 (s), 115.85 (s), 72.68 (s), 45.27 (s), 27.46 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_2$: 346.1550, found: 346.1549.

2s:



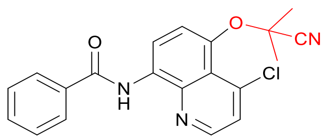
White solid, isolated yield: 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.72 (s, 1H), 8.71 (d, J = 8.6 Hz, 1H), 8.65 (d, J = 3.0 Hz, 1H), 8.39 (d, J = 8.4 Hz, 1H), 7.49 – 7.34 (m, 4H), 7.28 (d, J = 5.8 Hz, 2H), 3.90 (s, 2H), 2.40 (s, 3H), 1.80 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.38 (s), 148.73 (s), 144.58 (s), 139.05 (s), 137.26 (s), 133.09 (s), 131.11 (s), 130.80 (s), 130.60 (s), 127.83 (s), 126.65 (s), 123.21 (s), 121.38 (s), 120.67 (s), 116.09 (s), 115.81 (s), 72.68 (s), 43.18 (s), 27.48 (s), 19.72 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{21}N_3O_2$: 360.1707, found: 360.1704.

2t:



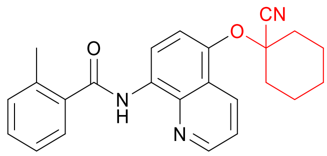
White solid, isolated yield: 58%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.66 (s, 1H), 8.86 (d, J = 8.6 Hz, 1H), 8.34 (d, J = 8.6 Hz, 1H), 8.07 (dd, J = 7.7, 1.4 Hz, 2H), 7.60 – 7.54 (m, 3H), 7.47 (d, J = 8.6 Hz, 1H), 7.37 (d, J = 8.6 Hz, 1H), 2.78 (s, 3H), 1.83 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.24 (s), 157.90 (s), 144.78 (s), 138.85 (s), 135.28 (s), 131.76 (s), 131.46 (s), 130.85 (s), 128.82 (s), 127.23 (s), 122.33 (s), 121.53 (s), 117.41 (s), 116.04 (s), 115.53 (s), 72.69 (s), 27.56 (s), 25.38 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_2$: 346.1550, found: 346.1548.

2u:



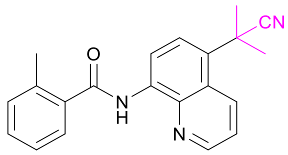
White solid, isolated yield: 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.68 (s, 1H), 8.97 (d, J = 8.7 Hz, 1H), 8.67 (d, J = 4.7 Hz, 1H), 8.06 (d, J = 6.7 Hz, 2H), 7.71 (d, J = 8.7 Hz, 1H), 7.60 – 7.52 (m, 4H), 1.83 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.37 (s), 148.83 (s), 144.68 (s), 139.35 (s), 131.86 (s), 131.36 (s), 130.51 (s), 129.70 (s), 128.82 (s), 127.26 (s), 123.58 (s), 123.40 (s), 121.56 (s), 116.19 (s), 116.06 (s), 72.69 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}ClN_3O_2$: 366.1004, found: 366.1003.

2v:



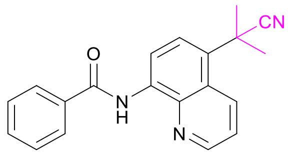
White solid, isolated yield: 30%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.05 (s, 1H), 8.89 (d, *J* = 8.7 Hz, 1H), 8.80 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.52 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.67 (d, *J* = 7.4 Hz, 1H), 7.55 (d, *J* = 8.6 Hz, 1H), 7.49 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.41 (t, *J* = 6.8 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 2H), 2.60 (s, 3H), 2.41 – 2.30 (m, 2H), 2.00 (t, *J* = 10.2 Hz, 2H), 1.90 – 1.82 (m, 2H), 1.72 – 1.64 (m, 3H), 1.47 – 1.33 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.05 (s), 148.74 (s), 144.40 (s), 139.30 (s), 136.68 (s), 136.61 (s), 131.37 (s), 131.34 (s), 131.24 (s), 130.32 (s), 127.26 (s), 126.01 (s), 123.27 (s), 121.43 (s), 119.90 (s), 116.01 (s), 115.79 (s), 37.98 (s), 35.98 (s), 24.53 (s), 22.45 (s), 20.21 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{24}H_{24}N_3O_2$: 386.1863, found: 386.1859.

3a:



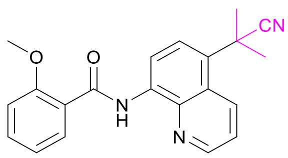
White solid, isolated yield: 67%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.34 (s, 1H), 8.94 (dd, *J* = 8.8, 1.4 Hz, 1H), 8.89 (d, *J* = 8.3 Hz, 1H), 8.84 (dd, *J* = 4.1, 1.4 Hz, 1H), 7.68 (d, *J* = 7.7 Hz, 1H), 7.62 – 7.56 (m, 2H), 7.42 (t, *J* = 6.9 Hz, 1H), 7.34 (t, *J* = 7.7 Hz, 2H), 2.60 (s, 3H), 1.96 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.29 (s), 147.89 (s), 139.43 (s), 136.76 (s), 136.40 (s), 135.42 (s), 134.83 (s), 133.19 (s), 131.45 (s), 130.49 (s), 129.84 (s), 127.29 (s), 126.07 (s), 125.32 (s), 124.15 (s), 121.56 (s), 115.33 (s), 33.93 (s), 28.91 (s), 20.24 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O$: 330.1601, found: 330.1593.

3b:



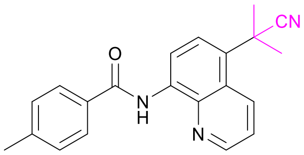
White solid, isolated yield: 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.90 (s, 1H), 8.98 (d, *J* = 8.8 Hz, 1H), 8.94 – 8.91 (m, 2H), 8.11 (d, *J* = 6.7 Hz, 2H), 7.67 – 7.56 (m, 5H), 1.98 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.55 (s), 147.93 (s), 139.58 (s), 135.26 (s), 134.91 (s), 133.24 (s), 132.03 (s), 129.74 (s), 128.86 (s), 127.33 (s), 125.33 (s), 124.84 (s), 124.22 (s), 121.59 (s), 115.38 (s), 33.93 (s), 28.90 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{17}N_3O$: 316.1444, found: 316.1445.

3c:



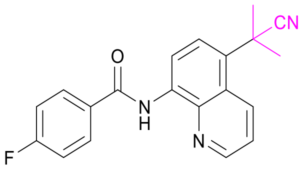
White solid, isolated yield: 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 12.45 (s, 1H), 8.99 (d, *J* = 8.3 Hz, 1H), 8.96 – 8.91 (m, 2H), 8.34 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.62 – 7.58 (m, 1H), 7.57 – 7.50 (m, 2H), 7.15 (t, *J* = 7.2 Hz, 1H), 7.09 (d, *J* = 8.3 Hz, 1H), 4.21 (s, 3H), 1.96 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.78 (s), 157.78 (s), 147.82 (s), 140.07 (s), 136.47 (s), 133.33 (s), 133.02 (s), 132.39 (s), 129.34 (s), 125.38 (s), 124.95 (s), 124.37 (s), 122.18 (s), 121.35 (s), 121.31 (s), 116.12 (s), 111.64 (s), 56.16 (s), 33.88 (s), 28.92 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_2$: 346.1550, found: 346.1550.

3d:



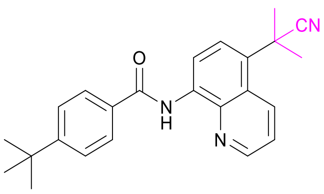
White solid, isolated yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.85 (s, 1H), 8.95 (dd, *J* = 8.8, 1.3 Hz, 1H), 8.92 (dd, *J* = 4.1, 1.3 Hz, 1H), 8.89 (d, *J* = 8.3 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 2H), 7.63 (dd, *J* = 8.7, 4.2 Hz, 1H), 7.57 (d, *J* = 8.3 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.47 (s, 3H), 1.97 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.53 (s), 147.88 (s), 142.57 (s), 139.58 (s), 135.37 (s), 133.21 (s), 132.10 (s), 129.52 (s), 127.34 (s), 125.31 (s), 124.86 (s), 124.23 (s), 121.55 (s), 115.28 (s), 33.91 (s), 28.90 (s), 21.59 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O$: 330.1601, found: 330.1593.

3e:



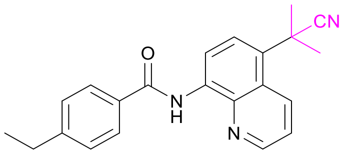
White solid, isolated yield: 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.83 (s, 1H), 8.95 (dd, *J* = 8.8, 1.4 Hz, 1H), 8.91 (dd, *J* = 4.2, 1.4 Hz, 1H), 8.86 (d, *J* = 8.3 Hz, 1H), 8.12 – 8.07 (m, 2H), 7.63 (dd, *J* = 8.8, 4.2 Hz, 1H), 7.57 (d, *J* = 8.3 Hz, 1H), 7.22 (d, *J* = 8.6 Hz, 2H), 1.96 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 166.33 (s), 164.37 (s), 163.81 (s), 147.95 (s), 139.50 (s), 135.09 (s), 133.28 (s), 131.07 (d, *J* = 3.1 Hz), 129.86 (s), 129.71 (d, *J* = 9.0 Hz), 125.31 (s), 124.81 (s), 124.19 (s), 121.63 (s), 116.03 (s), 115.81 (s), 115.35 (s), 33.93 (s), 28.88 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}FN_3O$: 334.1350, found: 334.1349.

3f:



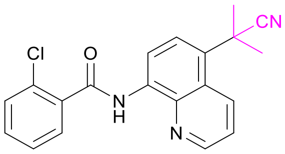
White solid, isolated yield: 72%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.86 (s, 1H), 8.95 (dd, *J* = 8.7, 1.4 Hz, 1H), 8.90 (dd, *J* = 8.3, 4.8 Hz, 2H), 8.03 (d, *J* = 8.5 Hz, 2H), 7.62 (dd, *J* = 8.7, 4.2 Hz, 1H), 7.60 – 7.56 (m, 3H), 1.96 (s, 6H), 1.38 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.54 (s), 155.59 (s), 147.86 (s), 139.59 (s), 135.40 (s), 133.21 (s), 132.10 (s), 129.55 (s), 127.19 (s), 125.81 (s), 125.32 (s), 124.85 (s), 124.23 (s), 121.54 (s), 115.28 (s), 35.06 (s), 33.92 (s), 31.20 (s), 28.90 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{24}H_{25}N_3O$: 372.2070, found: 372.2066.

3g:



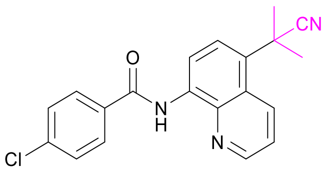
White solid, isolated yield: 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.86 (s, 1H), 8.95 (dd, *J* = 8.8, 1.3 Hz, 1H), 8.92 (dd, *J* = 4.2, 1.3 Hz, 1H), 8.89 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 2H), 7.63 (dd, *J* = 8.8, 4.2 Hz, 1H), 7.57 (d, *J* = 8.3 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 2H), 2.76 (q, *J* = 7.6 Hz, 2H), 1.96 (s, 6H), 1.30 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.58 (s), 148.79 (s), 147.88 (s), 139.59 (s), 135.38 (s), 133.21 (s), 132.34 (s), 129.55 (s), 128.35 (s), 127.45 (s), 125.32 (s), 124.86 (s), 124.24 (s), 121.55 (s), 115.29 (s), 33.92 (s), 28.90 (s), 15.36 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{21}N_3O$: 344.1757, found: 344.1749.

3h:



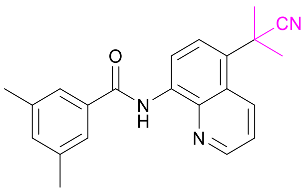
White solid, isolated yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.64 (s, 1H), 9.14 – 8.73 (m, 3H), 7.82 (d, *J* = 6.0 Hz, 1H), 7.74 – 7.30 (m, 5H), 7.57 – 7.39 (m, 3H), 1.97 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.99 (s), 148.01 (s), 139.45 (s), 135.60 (s), 135.12 (s), 133.16 (s), 131.69 (s), 131.19 (s), 130.58 (s), 130.24 (s), 130.14 (s), 127.21 (s), 125.31 (s), 124.78 (s), 124.13 (s), 121.61 (s), 115.74 (s), 33.95 (s), 28.90 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}ClN_3O$: 350.1055, found: 350.1050.

3i:



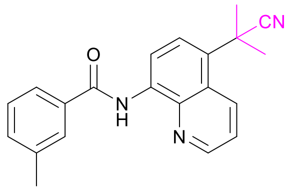
White solid, isolated yield: 64%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.85 (s, 1H), 8.96 (dd, *J* = 8.8, 1.3 Hz, 1H), 8.92 (d, *J* = 4.1 Hz, 1H), 8.87 (d, *J* = 8.3 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 2H), 7.64 (dd, *J* = 8.7, 4.2 Hz, 1H), 7.58 (d, *J* = 8.3 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 1.97 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.43 (s), 147.98 (s), 139.51 (s), 138.34 (s), 135.00 (s), 133.31 (s), 133.27 (s), 130.01 (s), 129.13 (s), 128.75 (s), 125.33 (s), 124.78 (s), 124.19 (s), 121.66 (s), 115.46 (s), 33.95 (s), 28.89 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}ClN_3O$: 350.1055, found: 350.1049.

3j:



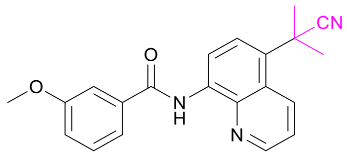
White solid, isolated yield: 58%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.79 (s, 1H), 8.99 – 8.92 (m, 2H), 8.89 (d, *J* = 8.3 Hz, 1H), 7.67 (s, 2H), 7.63 (dd, *J* = 8.7, 4.2 Hz, 1H), 7.57 (d, *J* = 8.3 Hz, 1H), 7.23 (s, 1H), 2.45 (s, 6H), 1.96 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 166.04 (s), 147.92 (s), 139.63 (s), 138.56 (s), 135.42 (s), 134.99 (s), 133.68 (s), 133.22 (s), 129.60 (s), 125.34 (s), 125.07 (s), 124.87 (s), 124.25 (s), 121.55 (s), 115.41 (s), 33.93 (s), 28.91 (s), 21.39 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{21}N_3O$: 344.1757, found: 344.1749.

3k:



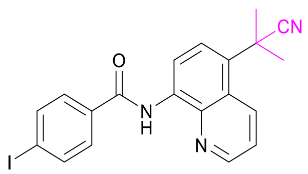
White solid, isolated yield: 61%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.87 (s, 1H), 8.98 (dd, J = 8.8, 1.4 Hz, 1H), 8.95 (dd, J = 4.2, 1.4 Hz, 1H), 8.92 (d, J = 8.3 Hz, 1H), 7.94 – 7.87 (m, 2H), 7.65 (dd, J = 8.7, 4.2 Hz, 1H), 7.60 (d, J = 8.3 Hz, 1H), 7.50 – 7.41 (m, 2H), 2.52 (s, 3H), 1.99 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.79 (s), 147.92 (s), 139.60 (s), 138.75 (s), 135.33 (s), 134.92 (s), 133.22 (s), 132.79 (s), 129.66 (s), 128.71 (s), 128.09 (s), 125.32 (s), 124.85 (s), 124.25 (s), 124.23 (s), 121.57 (s), 115.38 (s), 33.93 (s), 28.90 (s), 21.52 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O$: 330.1601, found: 330.1602.

3l:



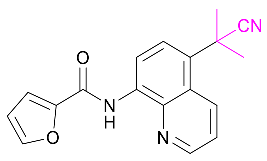
White solid, isolated yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.87 (s, 1H), 8.95 (dd, J = 8.8, 1.3 Hz, 1H), 8.92 (dd, J = 4.1, 1.3 Hz, 1H), 8.89 (d, J = 8.3 Hz, 1H), 7.66 – 7.61 (m, 3H), 7.58 (d, J = 8.3 Hz, 1H), 7.47 (t, J = 8.1 Hz, 1H), 7.14 (dd, J = 9.1, 1.9 Hz, 1H), 3.92 (s, 3H), 1.97 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.40 (s), 160.03 (s), 147.94 (s), 139.56 (s), 136.39 (s), 135.23 (s), 133.24 (s), 129.85 (s), 129.79 (s), 125.32 (s), 124.82 (s), 124.21 (s), 121.60 (s), 119.10 (s), 118.17 (s), 115.40 (s), 112.72 (s), 55.54 (s), 33.94 (s), 28.90 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O_2$: 346.1550, found: 346.1541.

3m:



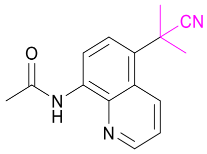
White solid, isolated yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.86 (s, 1H), 8.99 (dd, J = 8.8, 1.4 Hz, 1H), 8.92 (dd, J = 4.2, 1.4 Hz, 1H), 8.85 (d, J = 8.3 Hz, 1H), 7.91 (d, J = 8.5 Hz, 2H), 7.81 (d, J = 8.5 Hz, 2H), 7.65 (dd, J = 8.8, 4.2 Hz, 1H), 7.59 (d, J = 8.3 Hz, 1H), 1.96 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 164.81 (s), 147.89 (s), 139.29 (s), 138.08 (s), 134.81 (s), 134.27 (s), 133.63 (s), 130.18 (s), 128.91 (s), 125.39 (s), 124.75 (s), 124.29 (s), 121.68 (s), 115.96 (s), 99.22 (s), 33.96 (s), 28.88 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{16}IN_3O$: 442.0411, found: 442.0407.

3n:



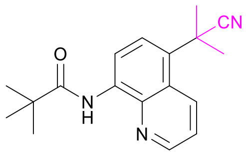
White solid, isolated yield: 45% ;^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.90 (s, 1H), 8.96 (s, 1H), 8.94 (dd, J = 5.4, 1.4 Hz, 1H), 8.83 (d, J = 8.3 Hz, 1H), 7.67 – 7.60 (m, 2H), 7.56 (d, J = 8.4 Hz, 1H), 7.31 (d, J = 3.5 Hz, 1H), 6.60 (dd, J = 3.5, 1.7 Hz, 1H), 1.96 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 156.48 (s), 148.19 (s), 148.04 (s), 144.68 (s), 139.45 (s), 133.16 (s), 129.86 (s), 124.15 (s), 121.61 (s), 121.09 (s), 120.24 (s), 115.48 (s), 115.40 (s), 112.54 (s), 33.93 (s), 28.89 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{18}H_{16}N_3O_2$: 306.1237, found: 306.1234.

3o:



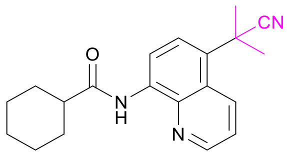
White solid, isolated yield: 64%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.91 (s, 1H), 8.91 (dd, J = 8.8, 1.3 Hz, 1H), 8.85 (dd, J = 4.1, 1.3 Hz, 1H), 8.71 (d, J = 8.3 Hz, 1H), 7.59 (dd, J = 8.8, 4.2 Hz, 1H), 7.50 (d, J = 8.3 Hz, 1H), 2.36 (s, 3H), 1.93 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.92 (s), 147.73 (s), 139.04 (s), 135.17 (s), 133.16 (s), 129.48 (s), 125.21 (s), 124.83 (s), 124.14 (s), 121.49 (s), 115.20 (s), 33.86 (s), 28.86 (s), 25.19 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{15}H_{15}N_3O$: 254.1288, found: 254.1283.

3p:



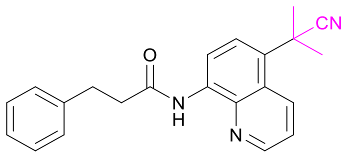
White solid, isolated yield: 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.39 (s, 1H), 8.91 (dd, J = 8.7, 1.1 Hz, 1H), 8.88 (dd, J = 4.1, 1.2 Hz, 1H), 8.74 (d, J = 8.3 Hz, 1H), 7.59 (dd, J = 8.7, 4.2 Hz, 1H), 7.51 (d, J = 8.3 Hz, 1H), 1.93 (s, 6H), 1.43 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 177.41 (s), 147.83 (s), 139.60 (s), 135.38 (s), 133.13 (s), 129.26 (s), 125.23 (s), 124.85 (s), 124.16 (s), 121.41 (s), 115.01 (s), 40.39 (s), 33.86 (s), 28.88 (s), 27.70 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{18}H_{21}N_3O$: 296.1757, found: 296.1750.

3q:



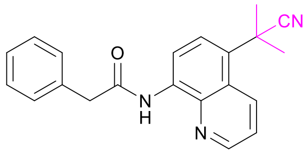
White solid, isolated yield: 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.99 (s, 1H), 8.89 (d, J = 8.9 Hz, 1H), 8.85 (d, J = 4.2 Hz, 1H), 8.71 (d, J = 8.3 Hz, 1H), 7.57 (dd, J = 8.7, 4.2 Hz, 1H), 7.48 (d, J = 8.3 Hz, 1H), 2.51 – 2.41 (m, 1H), 2.05 (dd, J = 13.2, 2.1 Hz, 2H), 1.90 (s, 6H), 1.89 – 1.83 (m, 2H), 1.66 – 1.55 (m, 3H), 1.40 – 1.27 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 175.11 (s), 147.60 (s), 139.13 (s), 135.16 (s), 133.53 (s), 129.40 (s), 125.30 (s), 124.81 (s), 124.30 (s), 121.43 (s), 115.65 (s), 46.84 (s), 33.87 (s), 29.72 (s), 28.88 (s), 25.77 (s), 25.73 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{23}N_3O$: 322.1915, found: 322.1914.

3r:



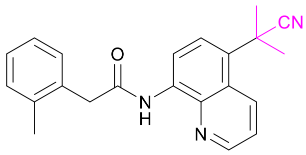
White solid, isolated yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.91 (s, 1H), 8.91 (dd, J = 8.8, 1.4 Hz, 1H), 8.82 (dd, J = 4.1, 1.4 Hz, 1H), 8.74 (d, J = 8.3 Hz, 1H), 7.58 (dd, J = 8.8, 4.1 Hz, 1H), 7.51 (d, J = 8.3 Hz, 1H), 7.30 (d, J = 4.4 Hz, 4H), 7.21 (dd, J = 8.8, 4.5 Hz, 1H), 3.15 (t, 2H), 2.90 (t, 2H), 1.94 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 170.94 (s), 147.71 (s), 140.64 (s), 139.09 (s), 135.07 (s), 133.14 (s), 129.50 (s), 128.59 (s), 128.39 (s), 126.30 (s), 125.21 (s), 124.83 (s), 124.15 (s), 121.48 (s), 115.29 (s), 39.74 (s), 33.87 (s), 31.42 (s), 28.87 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{21}N_3O$: 344.1757, found: 344.1753.

3s:



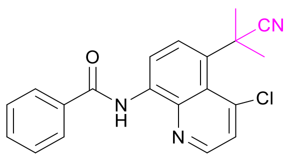
White solid, isolated yield: 56%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.03 (s, 1H), 8.88 (dd, J = 8.8, 1.4 Hz, 1H), 8.74 (dd, J = 4.1, 1.3 Hz, 1H), 8.71 (d, J = 8.3 Hz, 1H), 7.54 (dd, J = 8.8, 4.2 Hz, 1H), 7.48 (d, J = 8.3 Hz, 1H), 7.45 – 7.39 (m, 4H), 7.36 – 7.31 (m, 1H), 3.90 (s, 2H), 1.91 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.69 (s), 147.75 (s), 139.23 (s), 135.03 (s), 134.50 (s), 133.07 (s), 129.67 (s), 129.54 (s), 129.01 (s), 127.41 (s), 125.16 (s), 124.78 (s), 124.05 (s), 121.41 (s), 115.16 (s), 45.37 (s), 33.86 (s), 28.85 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}N_3O$: 330.1601, found: 330.1601.

3t:



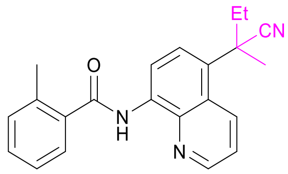
White solid, isolated yield: 59% ; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 9.97 (s, 1H), 8.86 (dd, J = 8.8, 1.4 Hz, 1H), 8.70 (d, J = 8.3 Hz, 1H), 8.67 (dd, J = 4.2, 1.4 Hz, 1H), 7.52 (dd, J = 8.8, 4.2 Hz, 1H), 7.48 (d, J = 8.3 Hz, 1H), 7.36 (dd, J = 7.2, 3.3 Hz, 1H), 7.28 (t, J = 4.5 Hz, 3H), 3.90 (s, 2H), 2.39 (s, 3H), 1.91 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 169.60 (s), 147.74 (s), 139.20 (s), 137.23 (s), 134.96 (s), 133.09 (s), 133.03 (s), 130.81 (s), 130.60 (s), 129.67 (s), 127.86 (s), 126.65 (s), 125.15 (s), 124.78 (s), 124.07 (s), 121.39 (s), 115.19 (s), 43.28 (s), 33.86 (s), 28.84 (s), 19.71 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{21}N_3O$: 344.1757, found: 344.1754.

3u:



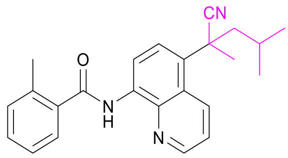
White solid, isolated yield: 40%;^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.94 (s, 1H), 8.92 (d, J = 8.5 Hz, 1H), 8.70 (d, J = 4.6 Hz, 1H), 8.06 (d, J = 6.8 Hz, 2H), 7.80 (d, J = 8.6 Hz, 1H), 7.70 (d, J = 4.6 Hz, 1H), 7.61 – 7.54 (m, 3H), 2.05 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 165.61 (s), 146.75 (s), 141.76 (s), 140.94 (s), 135.68 (s), 134.78 (s), 132.16 (s), 130.00 (s), 128.90 (s), 127.85 (s), 127.32 (s), 125.79 (s), 125.66 (s), 125.56 (s), 115.91 (s), 35.91 (s), 32.00 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{20}H_{17}ClN_3O$: 350.1055, found: 350.1055.

3v:



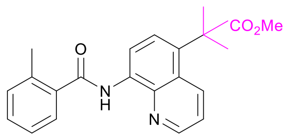
White solid, isolated yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.35 (s, 1H), 8.96 – 8.87 (m, 2H), 8.83 (dd, J = 4.1, 1.4 Hz, 1H), 7.68 (d, J = 7.7 Hz, 1H), 7.62 – 7.54 (m, 2H), 7.42 (t, J = 7.5 Hz, 1H), 7.33 (t, J = 7.6 Hz, 2H), 2.60 (s, 3H), 2.38 (dd, J = 14.1, 7.3 Hz, 1H), 2.10 (dd, J = 14.1, 7.3 Hz, 1H), 1.94 (s, 3H), 1.10 (t, J = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 168.31 (s), 147.85 (s), 139.45 (s), 136.76 (s), 136.40 (s), 135.29 (s), 133.11 (s), 131.45 (s), 130.49 (s), 128.91 (s), 127.29 (s), 126.07 (s), 125.41 (s), 125.22 (s), 124.10 (s), 121.45 (s), 115.32 (s), 39.54 (s), 33.74 (s), 25.74 (s), 20.25 (s), 9.52 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{22}N_3O$: 344.1757, found: 344.1755.

3w:



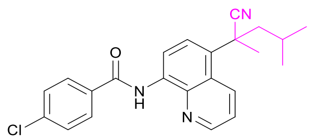
White solid, isolated yield: 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.35 (s, 1H), 8.93 – 8.85 (m, 2H), 8.82 (dd, J = 4.1, 1.3 Hz, 1H), 7.67 (t, J = 7.9 Hz, 2H), 7.57 (dd, J = 8.8, 4.1 Hz, 1H), 7.45 – 7.38 (m, 1H), 7.33 (t, J = 7.6 Hz, 2H), 2.60 (s, 3H), 2.27 (dd, J = 14.2, 5.7 Hz, 1H), 2.02 (s, 3H), 1.95 (dd, J = 14.2, 6.0 Hz, 1H), 1.90 – 1.82 (m, 1H), 1.04 (d, J = 6.6 Hz, 3H), 0.85 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.25 (s), 147.82 (s), 139.42 (s), 136.77 (s), 136.41 (s), 135.30 (s), 133.16 (s), 131.45 (s), 130.49 (s), 129.47 (s), 127.28 (s), 126.07 (s), 125.42 (s), 125.36 (s), 124.56 (s), 121.40 (s), 115.35 (s), 49.31 (s), 39.04 (s), 26.84 (s), 25.76 (s), 24.05 (s), 23.95 (s), 20.26 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{24}H_{25}N_3O$: 372.2070, found: 372.2077.

3x:



White solid, isolated yield: 57%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 8.89 (d, J = 8.2 Hz, 1H), 8.75 (dd, J = 4.1, 1.4 Hz, 1H), 8.21 (dd, J = 8.7, 1.4 Hz, 1H), 7.64 (dd, J = 15.5, 7.9 Hz, 2H), 7.45 – 7.38 (m, 2H), 7.32 (t, J = 7.4 Hz, 2H), 3.58 (s, 3H), 2.59 (s, 3H), 1.75 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.99 (s), 168.16 (s), 147.40 (s), 139.34 (s), 136.69 (s), 136.65 (s), 134.96 (s), 134.14 (s), 132.74 (s), 131.36 (s), 130.31 (s), 127.25 (s), 126.11 (s), 126.01 (s), 124.00 (s), 121.29 (s), 115.78 (s), 52.49 (s), 45.84 (s), 27.54 (s), 20.20 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{22}N_2O_3$: 363.1703, found: 363.1726.

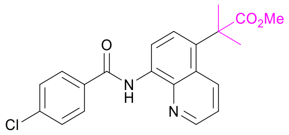
3y:



White solid, isolated yield: 48%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.85 (s, 1H), 8.90 (dd, J = 5.0, 3.7 Hz, 2H), 8.86 (d, J = 8.3 Hz, 1H), 8.02 (d, J = 8.5 Hz, 2H), 7.66 (d, J = 8.3 Hz, 1H), 7.62 (dd, J = 8.5, 4.5

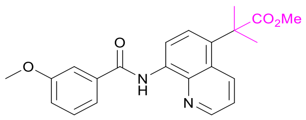
Hz, 1H), 7.53 (d, J = 8.5 Hz, 2H), 2.27 (dd, J = 14.2, 5.7 Hz, 1H), 2.02 (s, 3H), 1.94 (dd, J = 14.2, 5.9 Hz, 1H), 1.89 – 1.82 (m, 1H), 1.03 (d, J = 6.6 Hz, 3H), 0.83 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.41 (s), 147.89 (s), 139.50 (s), 138.31 (s), 134.89 (s), 133.31 (s), 129.67 (s), 129.12 (s), 128.75 (s), 125.42 (s), 125.38 (s), 124.51 (s), 121.48 (s), 115.51 (s), 49.32 (s), 39.01 (s), 26.76 (s), 25.74 (s), 23.98 (d, J = 9.8 Hz). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{23}H_{22}ClN_3O$: 392.1524, found: 392.1533.

3z:



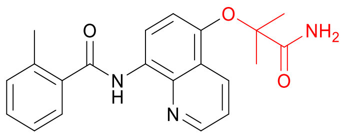
White solid, isolated yield: 50%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.80 (s, 1H), 8.87 – 8.82 (m, 2H), 8.24 (dd, J = 8.7, 1.4 Hz, 1H), 8.02 (d, J = 8.6 Hz, 2H), 7.63 (d, J = 8.2 Hz, 1H), 7.52 (d, J = 8.5 Hz, 2H), 7.47 (dd, J = 8.7, 4.2 Hz, 1H), 3.58 (s, 3H), 1.75 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.91 (s), 164.31 (s), 147.42 (s), 139.39 (s), 138.12 (s), 135.15 (s), 133.69 (s), 133.53 (s), 132.96 (s), 129.06 (s), 128.73 (s), 126.16 (s), 124.07 (s), 121.36 (s), 116.04 (s), 52.49 (s), 45.87 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{19}ClN_2O_3$: 383.1157, found: 383.1171.

3aa:



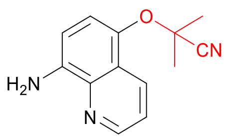
White solid, isolated yield: 54%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.81 (s, 1H), 8.86 (dd, J = 19.0, 6.1 Hz, 2H), 8.23 (d, J = 8.7 Hz, 1H), 7.66 – 7.61 (m, 3H), 7.49 – 7.43 (m, 2H), 7.13 (d, J = 8.2 Hz, 1H), 3.92 (s, 3H), 3.58 (s, 3H), 1.76 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 178.99 (s), 165.25 (s), 160.01 (s), 147.44 (s), 139.52 (s), 136.68 (s), 134.90 (s), 133.96 (s), 132.79 (s), 129.78 (s), 126.13 (s), 124.05 (s), 121.31 (s), 119.08 (s), 118.02 (s), 115.83 (s), 112.68 (s), 55.52 (s), 52.48 (s), 45.86 (s), 27.53 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{22}H_{22}N_2O_4$: 379.1652, found: 379.1674.

11:



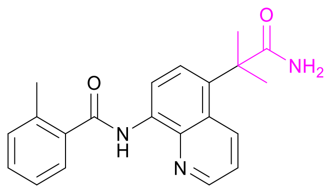
White solid, isolated yield: 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.03 (s, 1H), 8.84 (d, J = 8.6 Hz, 1H), 8.80 (dd, J = 4.1, 1.4 Hz, 1H), 8.53 (dd, J = 8.5, 1.4 Hz, 1H), 7.66 (d, J = 7.3 Hz, 1H), 7.49 (dd, J = 8.5, 4.2 Hz, 1H), 7.40 (t, J = 7.3 Hz, 1H), 7.32 (t, J = 7.2 Hz, 2H), 7.10 (d, J = 8.5 Hz, 1H), 6.70 (s, 1H), 5.56 (s, 1H), 2.60 (s, 3H), 1.64 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 177.24 (s), 168.05 (s), 148.70 (s), 144.85 (s), 139.30 (s), 136.63 (s), 136.58 (s), 131.50 (s), 131.37 (s), 130.44 (s), 130.33 (s), 127.24 (s), 126.02 (s), 123.40 (s), 121.37 (s), 116.03 (s), 115.29 (s), 82.54 (s), 25.03 (s), 20.21 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{21}N_3O_3$: 364.1656, found: 364.1654.

12:



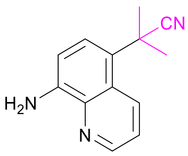
Pale yellow solid, isolated yield: 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.79 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.34 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.43 – 7.38 (m, 2H), 6.87 (d, *J* = 8.3 Hz, 1H), 1.76 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.58 (s), 145.52 (s), 139.28 (s), 136.57 (s), 130.20 (s), 127.24 (s), 125.97 (s), 122.84 (s), 121.14 (s), 113.11 (s), 73.33 (s), 25.70 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{13}H_{14}N_3O$: 228.1131, found: 228.1128.

13:



White solid, isolated yield: 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.28 (s, 1H), 8.87 (d, *J* = 8.2 Hz, 1H), 8.76 (d, *J* = 2.9 Hz, 1H), 8.39 (d, *J* = 8.6 Hz, 1H), 7.70 – 7.62 (m, 2H), 7.45 (dd, *J* = 8.7, 4.1 Hz, 1H), 7.40 (t, *J* = 7.1 Hz, 1H), 7.31 (t, *J* = 7.5 Hz, 2H), 5.17 (d, *J* = 21.6 Hz, 2H), 2.58 (s, 3H), 1.73 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 180.48 (s), 168.27 (s), 147.85 (s), 139.50 (s), 136.70 (s), 136.46 (s), 134.81 (s), 134.70 (s), 134.04 (s), 131.43 (s), 130.45 (s), 127.27 (s), 126.24 (s), 126.06 (s), 124.70 (s), 121.51 (s), 115.56 (s), 46.45 (s), 27.88 (s), 20.24 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{21}H_{22}N_3O_2$: 348.1707, found: 348.1705.

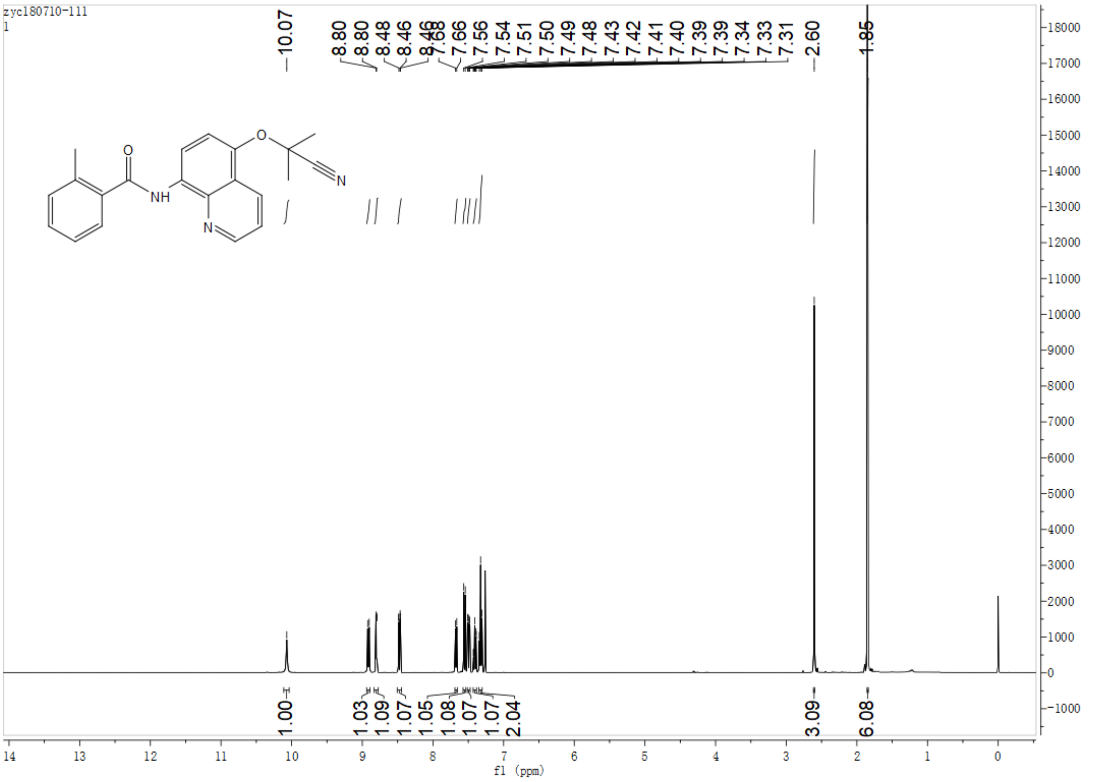
14:

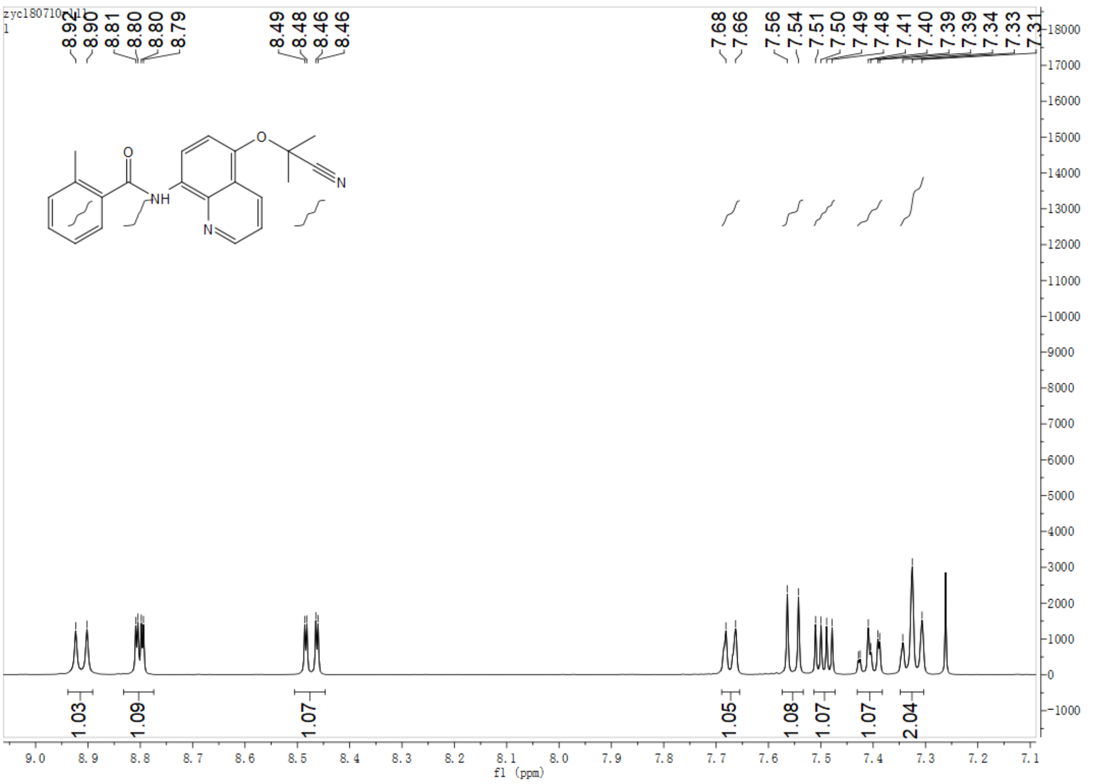


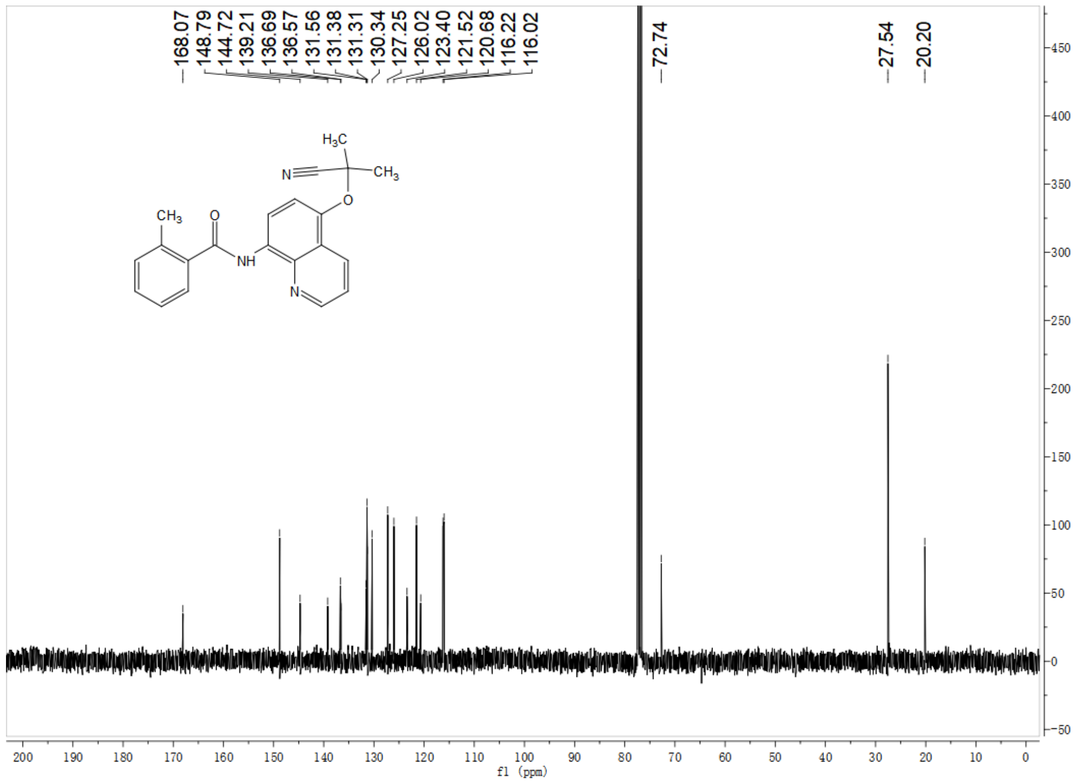
Pale yellow solid, isolated yield: 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.80 (dd, *J* = 10.2, 1.8 Hz, 2H), 7.51 (dd, *J* = 8.7, 4.2 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 6.85 (d, *J* = 8.1 Hz, 1H), 5.20 (s, 2H), 1.90 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ: 146.98 (s), 144.62 (s), 139.17 (s), 132.70 (s), 125.99 (s), 125.29 (s), 124.21 (s), 123.53 (s), 121.23 (s), 108.18 (s), 33.63 (s), 28.92 (s). HRMS (ESI): m/z: calcd for $[M+H]^+$ $C_{13}H_{14}N_3$: 212.1182, found: 212.1180.

7. ^{1}H and ^{13}C NMR spectra

2a:

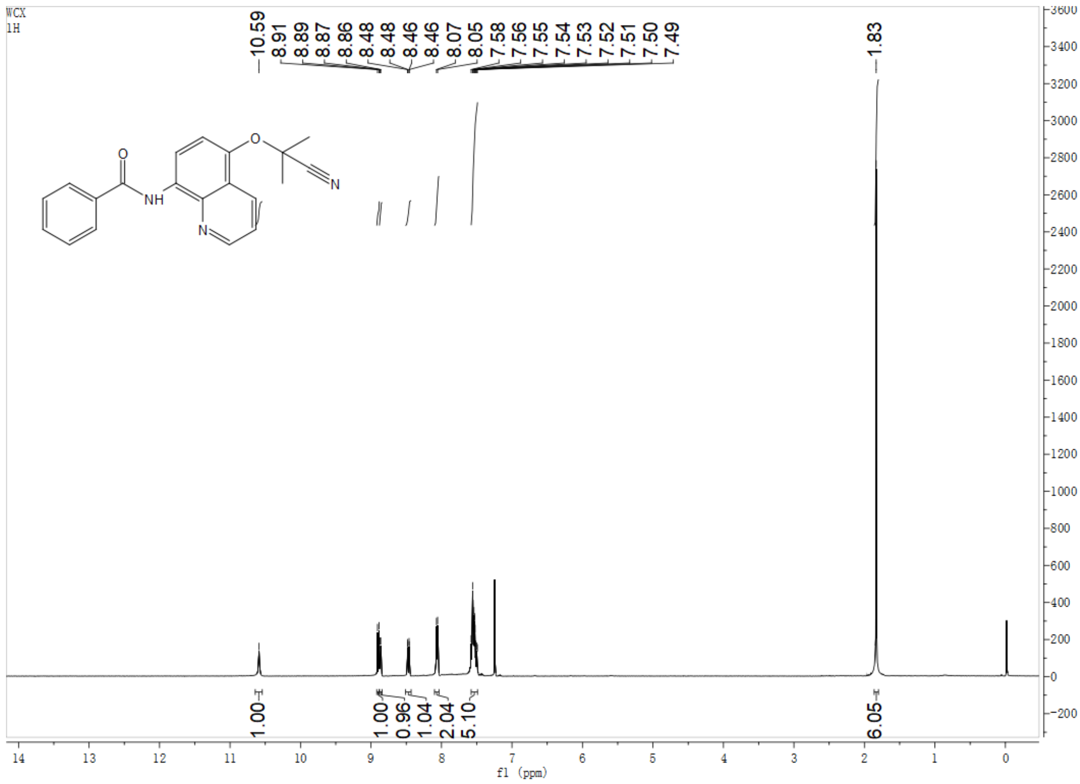




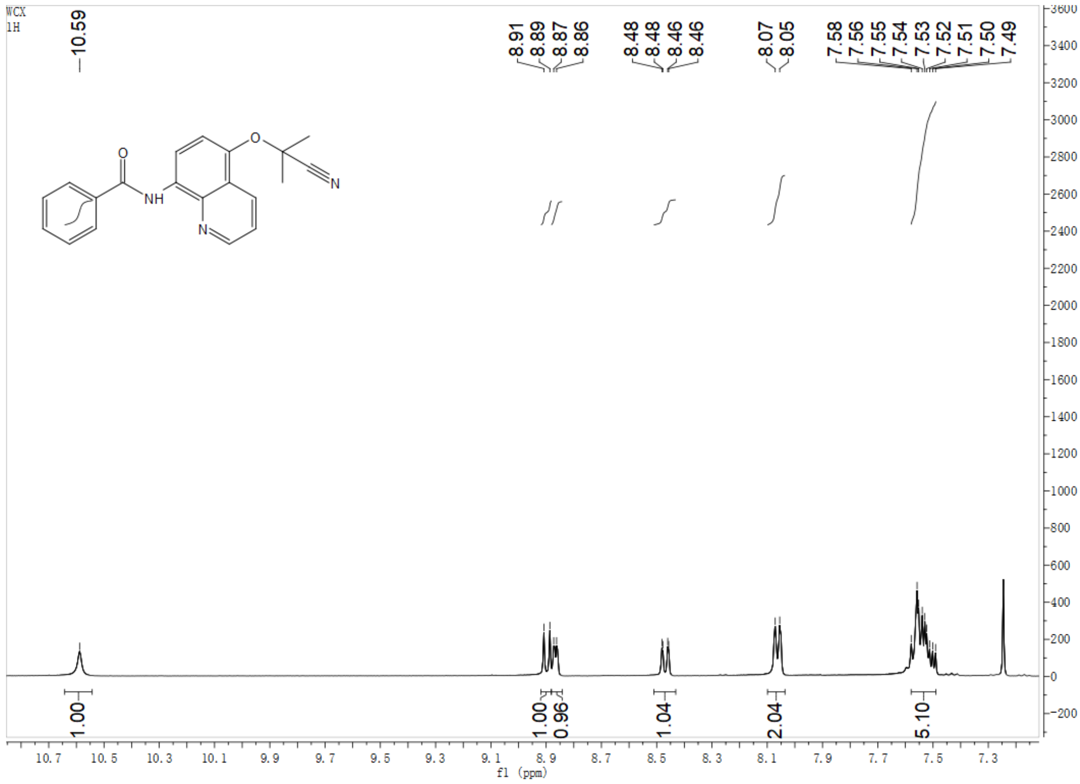


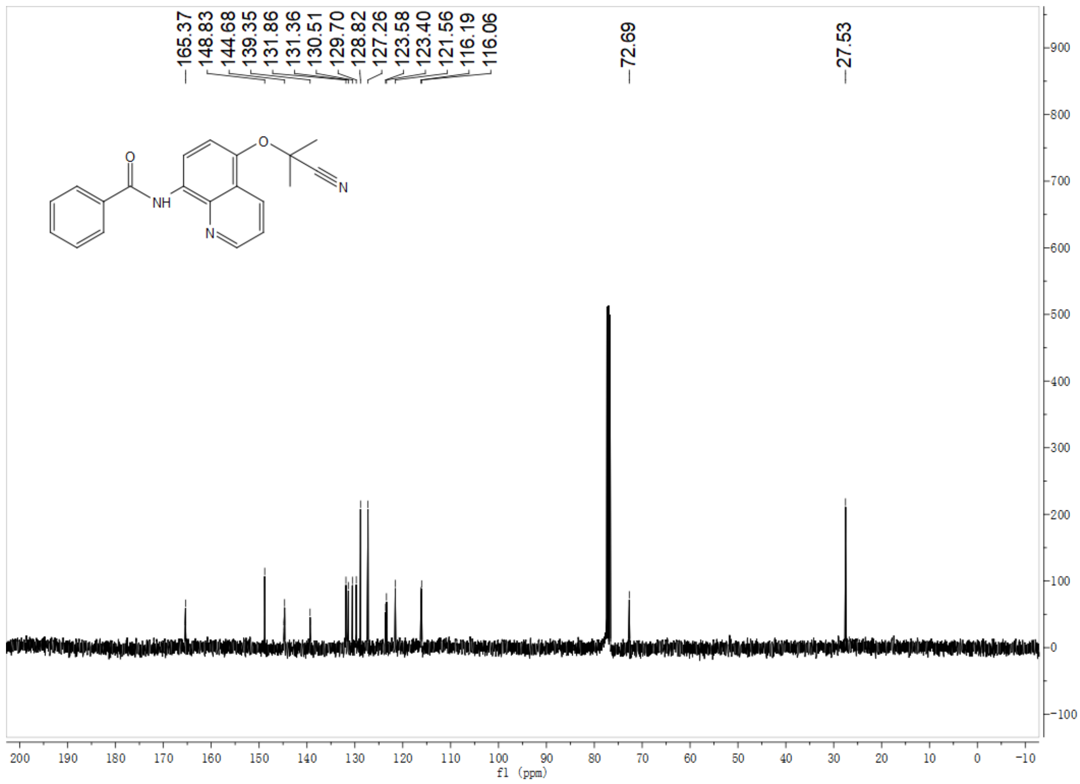
168.07
148.79
144.72
139.21
136.69
136.57
131.56
131.38
131.31
130.34
127.25
126.02
123.40
121.52
120.68
116.22
116.02
72.74
27.54
20.20
f1 (ppm)

2b:

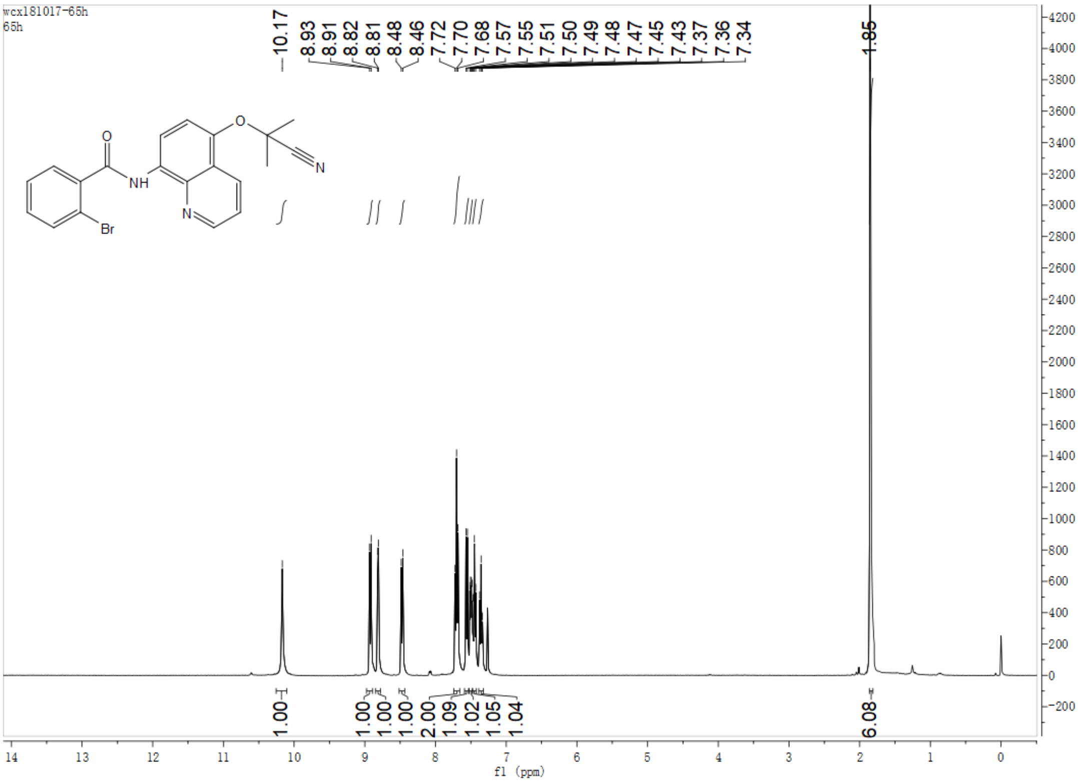


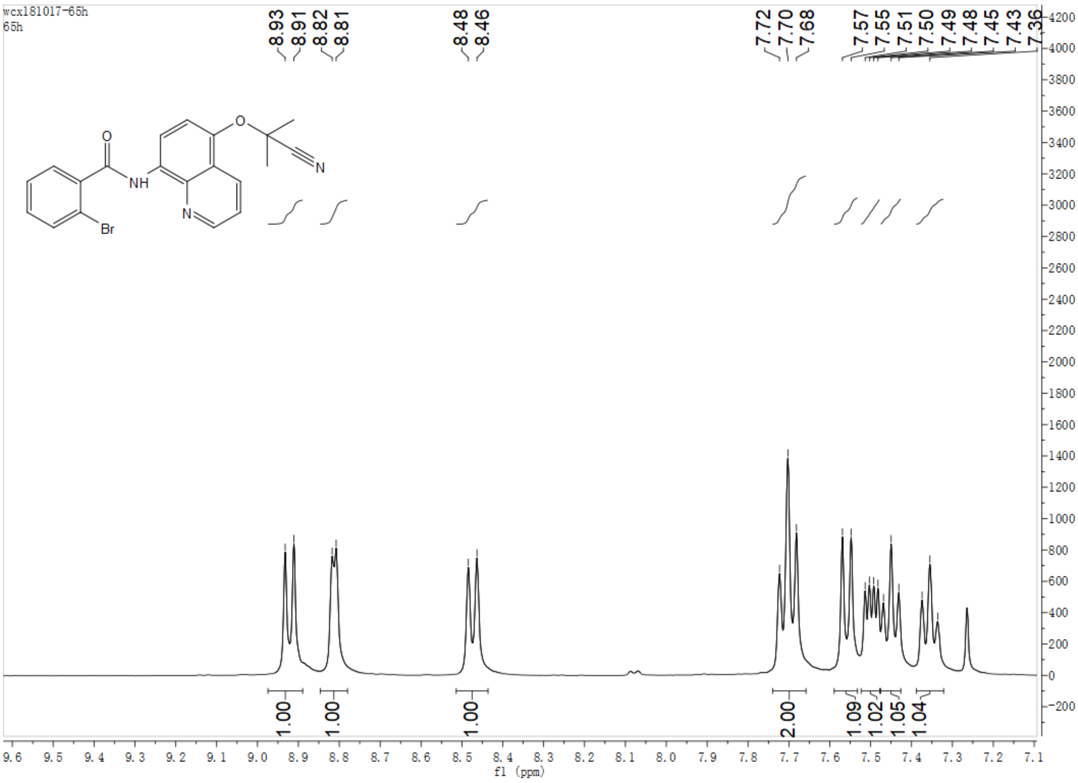
WCX
1H
10.59
8.91
8.89
8.87
8.86
8.48
8.48
8.46
8.46
8.07
8.05
7.58
7.56
7.55
7.54
7.53
7.52
7.51
7.50
7.49
1.83
1.00
1.00
0.96
1.04
2.04
5.10
6.05
f1 (ppm)

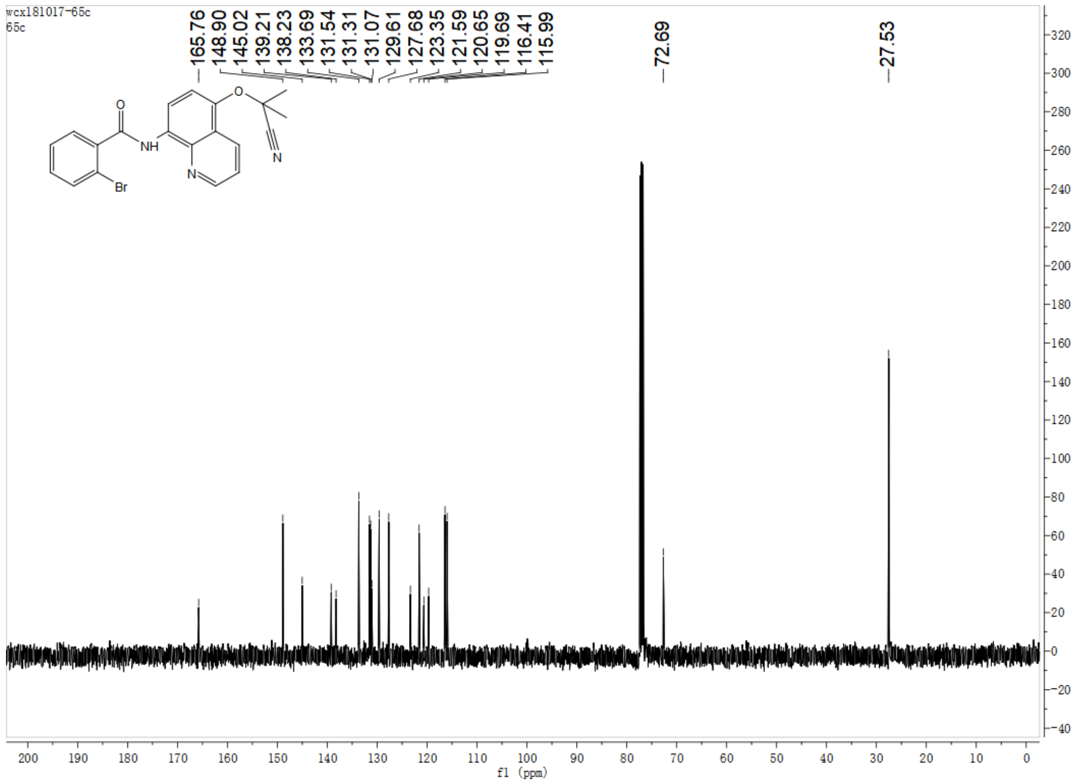

WCX
1H
10.59
8.91
8.89
8.87
8.86
8.48
8.48
8.46
8.46
8.07
8.05
7.58
7.56
7.55
7.54
7.53
7.52
7.51
7.50
7.49
1.00
1.00
0.96
1.04
2.04
5.10
f1 (ppm)


165.37
148.83
144.68
139.35
131.86
131.36
130.51
129.70
128.82
127.26
123.58
123.40
121.56
116.19
116.06
72.69
27.53
f1 (ppm)

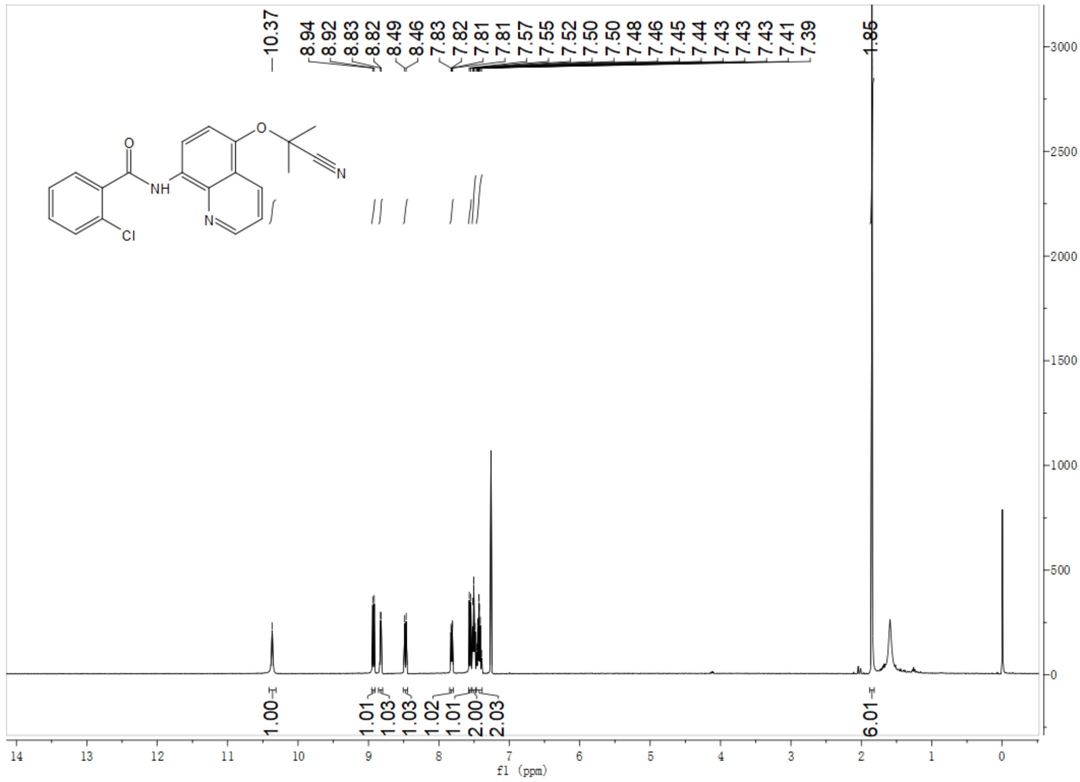
2c:

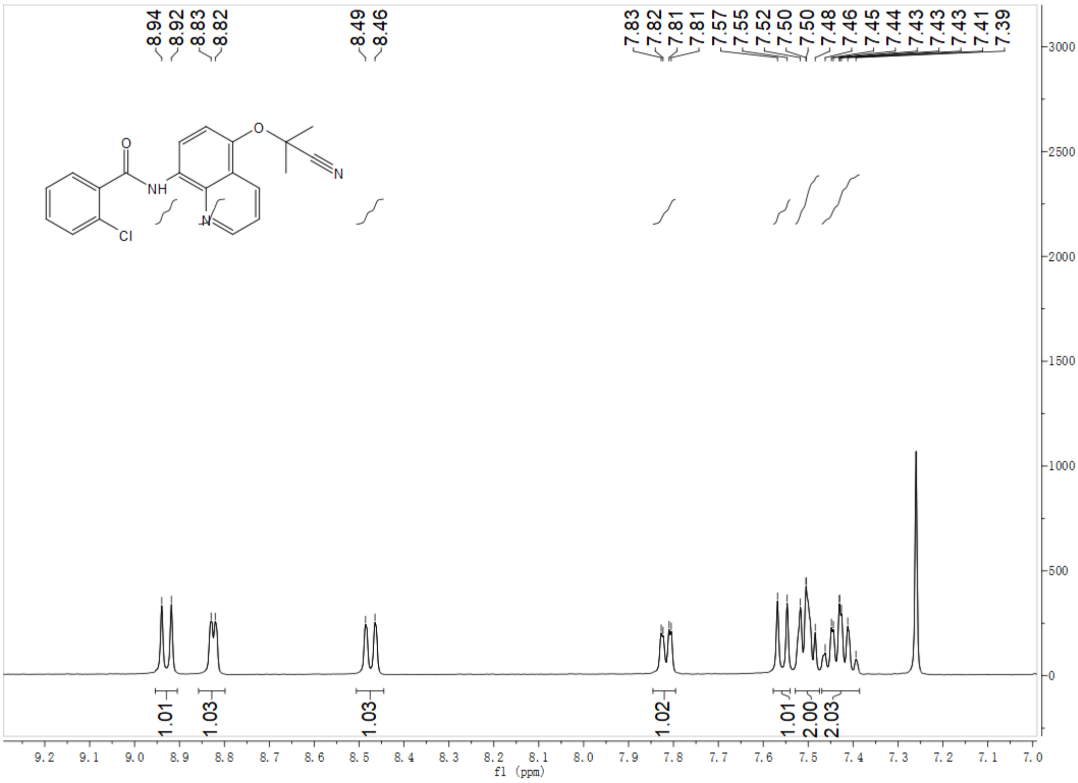


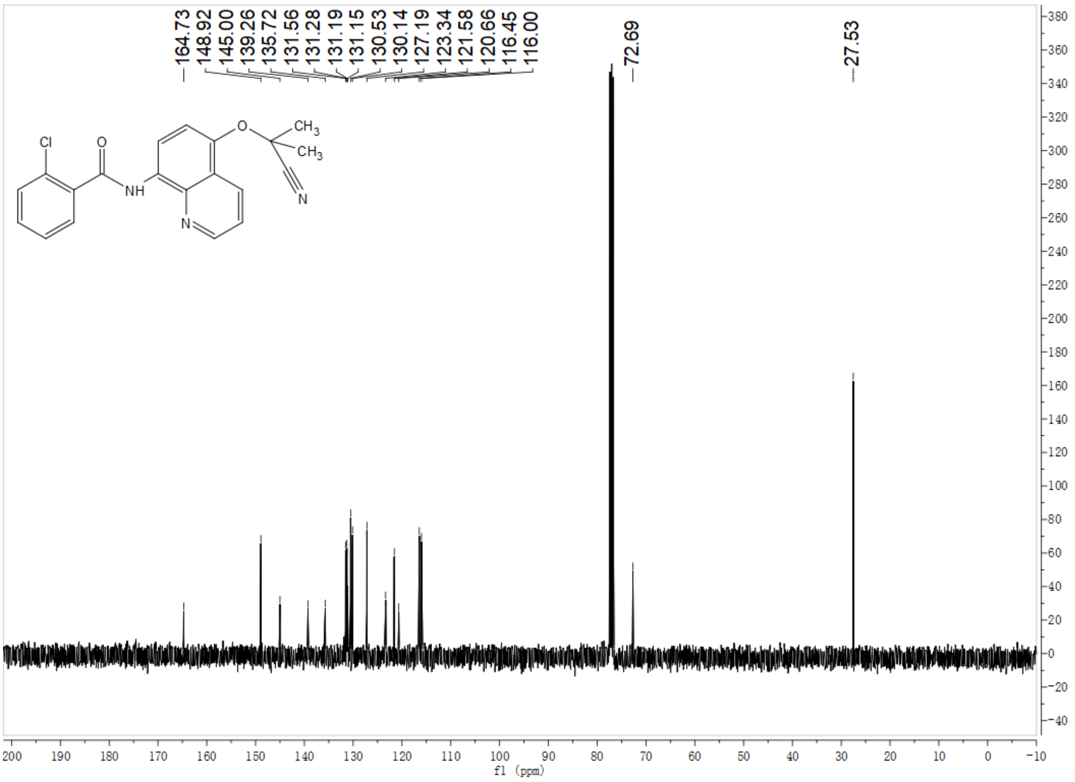



wcx181017-65c
65c
165.76
148.90
145.02
139.21
138.23
133.69
131.54
131.31
131.07
129.61
127.68
123.35
121.59
120.65
119.69
116.41
115.99
72.69
27.53
O
NH
N
Br
O
N
f1 (ppm)

2d:


10.37
8.94
8.92
8.83
8.82
8.49
8.46
7.83
7.82
7.81
7.81
7.57
7.55
7.52
7.50
7.50
7.48
7.46
7.45
7.44
7.43
7.43
7.43
7.41
7.39
1.85
O
NH
N
Cl
O
N
1.00
1.01
1.03
1.03
1.02
1.01
2.00
2.03
6.01
f1 (ppm)


8.94
8.92
8.83
8.82
8.49
8.46
7.83
7.82
7.81
7.81
7.57
7.55
7.52
7.50
7.50
7.48
7.46
7.45
7.44
7.43
7.43
7.43
7.41
7.39
1.01
1.03
1.03
1.02
1.01
2.00
2.03
O
NH
N
Cl
f1 (ppm)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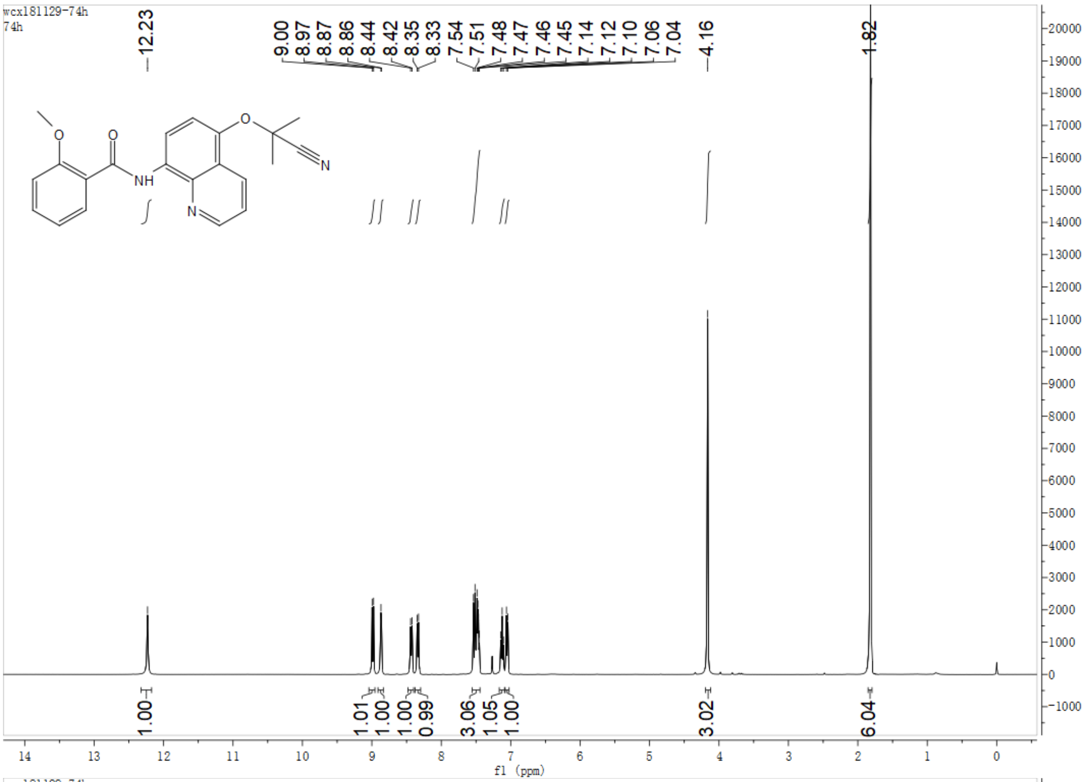
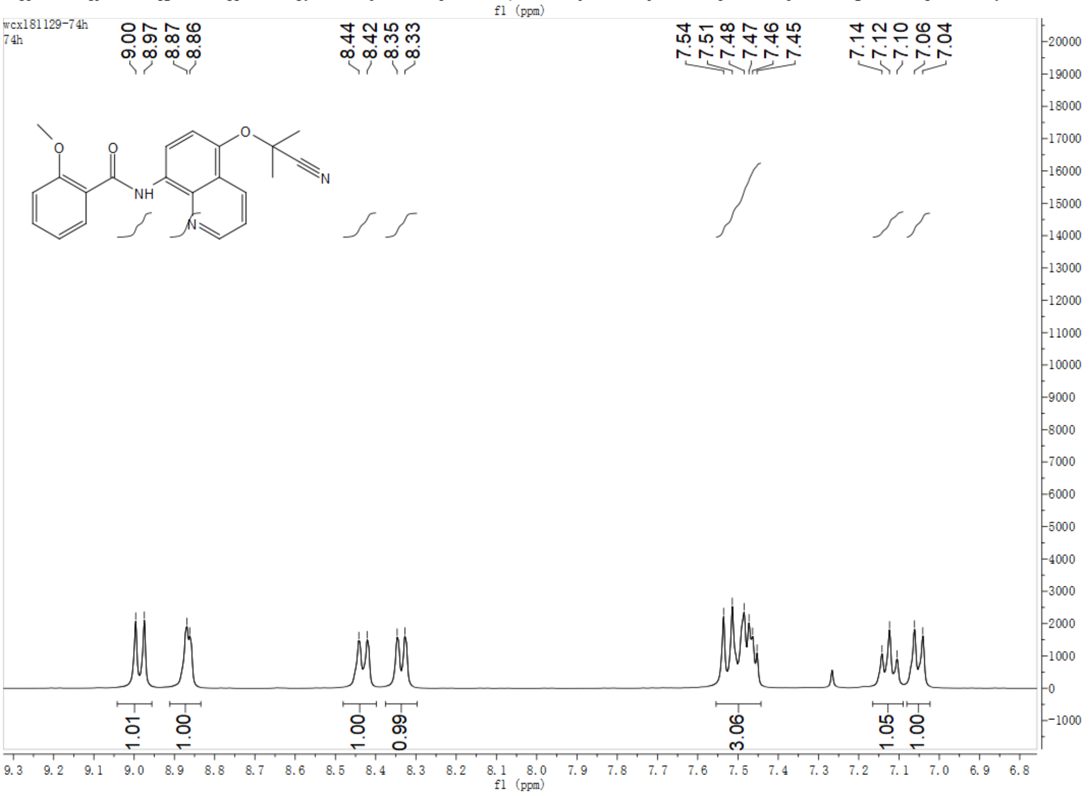
148.92
145.00
139.26
135.72
131.56
131.28
131.19
131.15
130.53
130.14
127.19
123.34
121.58
120.66
116.45
116.00
72.69
27.53
Cl
O
NH
N
O
CH3
CH3
N
f1 (ppm)

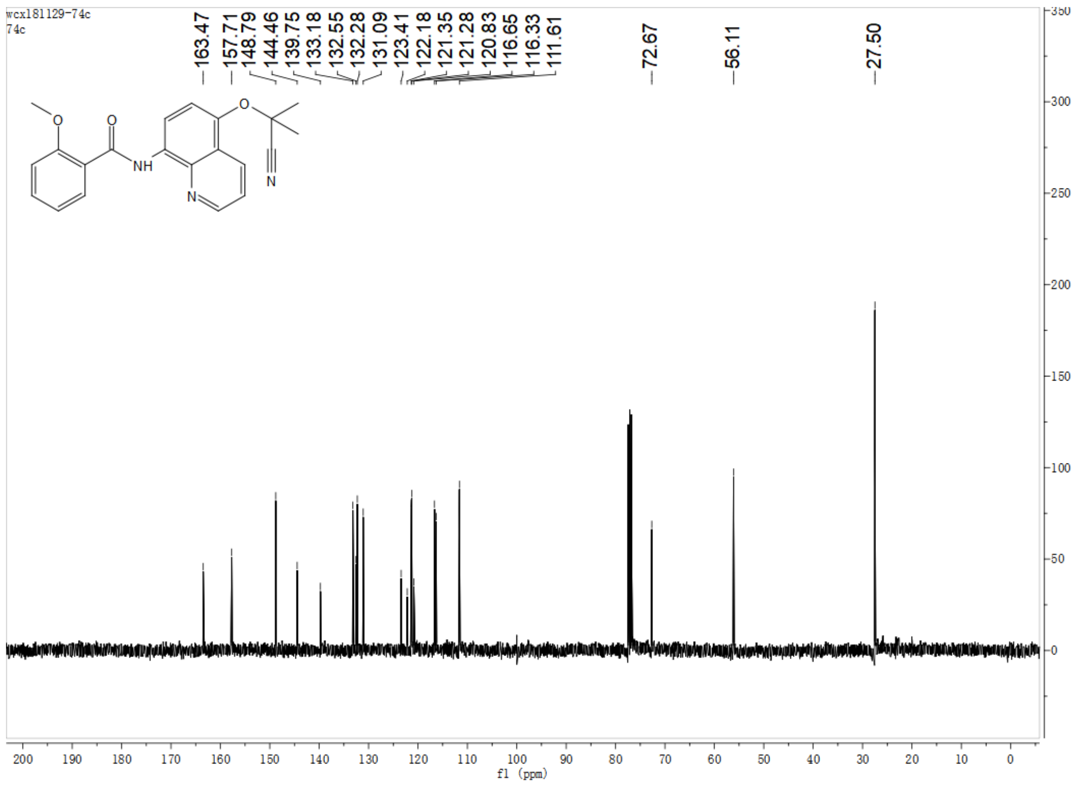
2e:



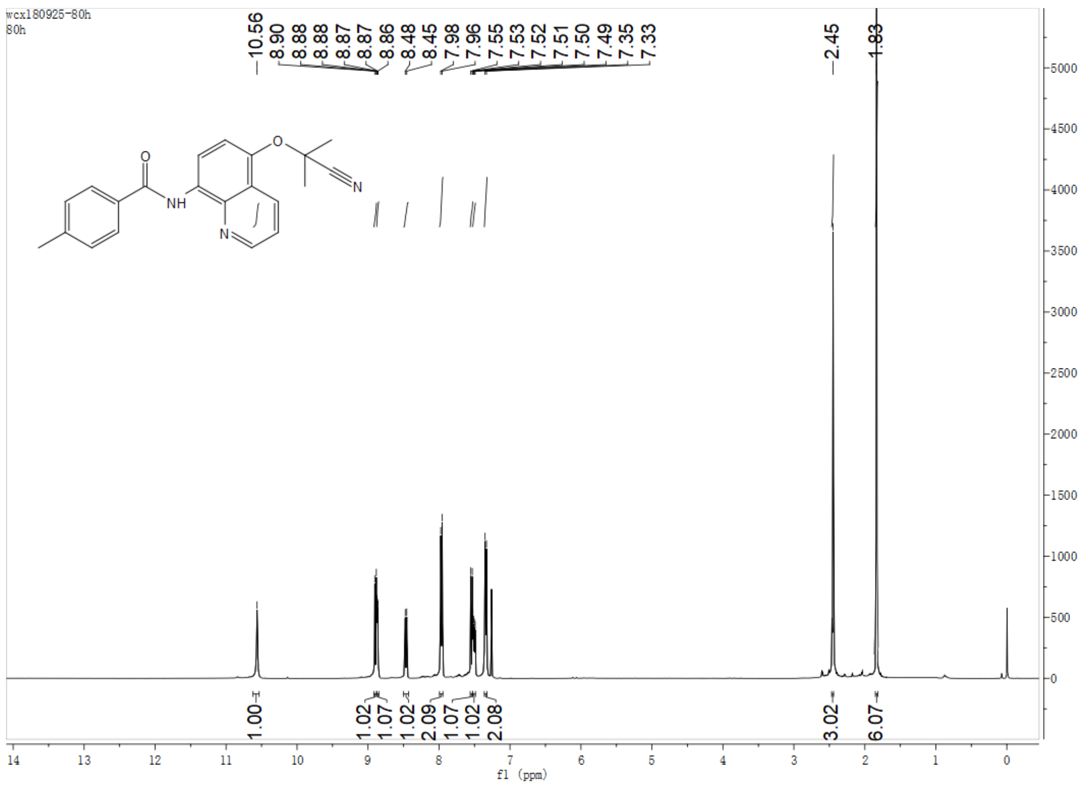
wcx181129-74h
74h
12.23
9.00
8.97
8.87
8.86
8.44
8.42
8.35
8.33
7.54
7.51
7.48
7.47
7.46
7.45
7.14
7.12
7.10
7.06
7.04
4.16
1.82
1.00
1.01
1.00
1.00
0.99
3.06
1.05
1.00
3.02
6.04
f1 (ppm)

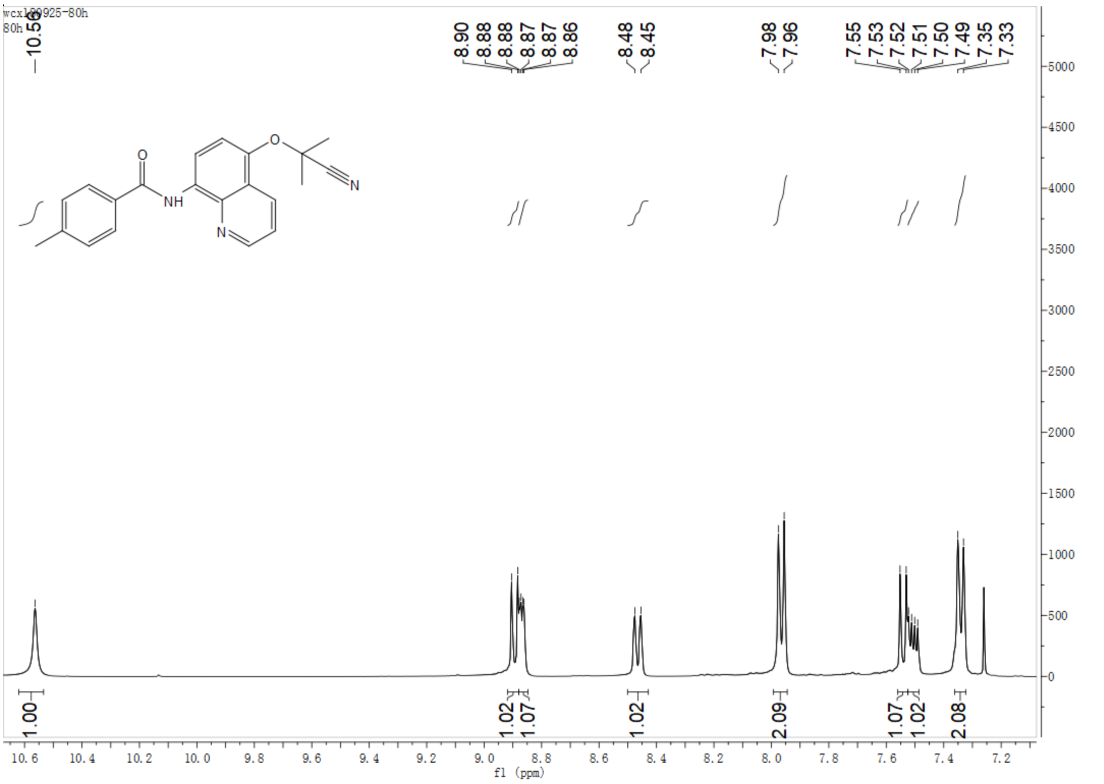


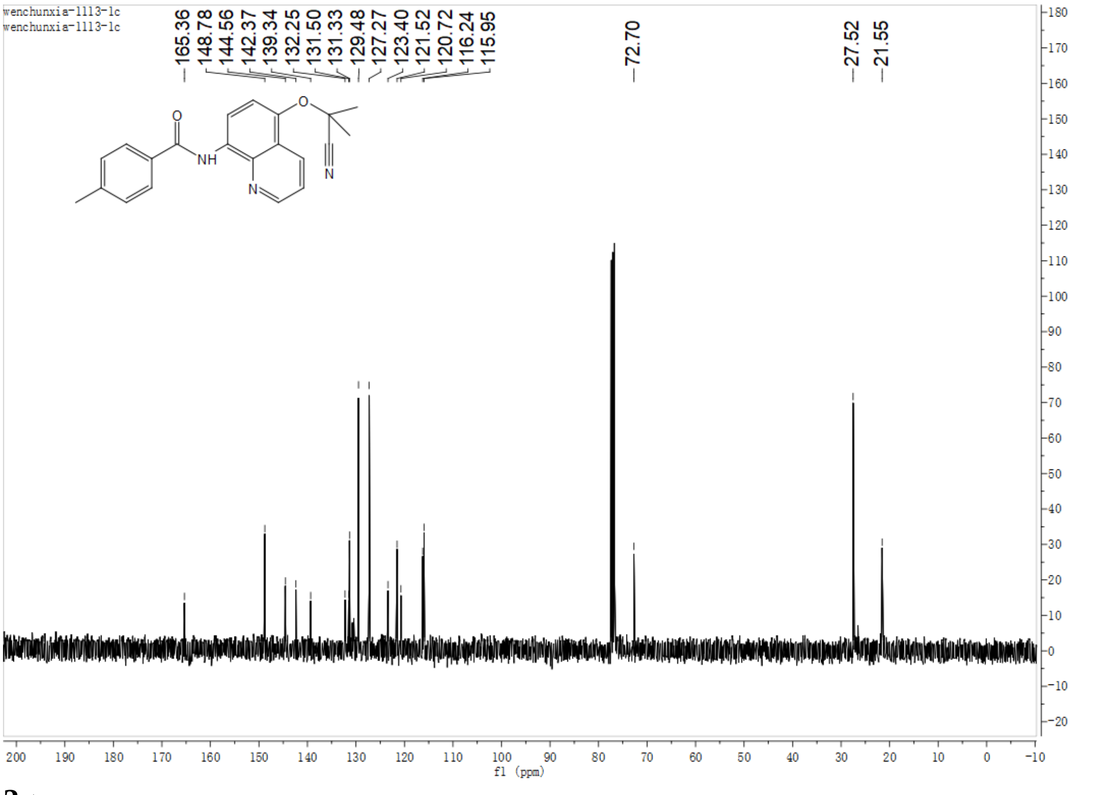
wcx181129-74h
74h
9.00
8.97
8.87
8.86
8.44
8.42
8.35
8.33
7.54
7.51
7.48
7.47
7.46
7.45
7.14
7.12
7.10
7.06
7.04
1.01
1.00
1.00
0.99
3.06
1.05
1.00
f1 (ppm)



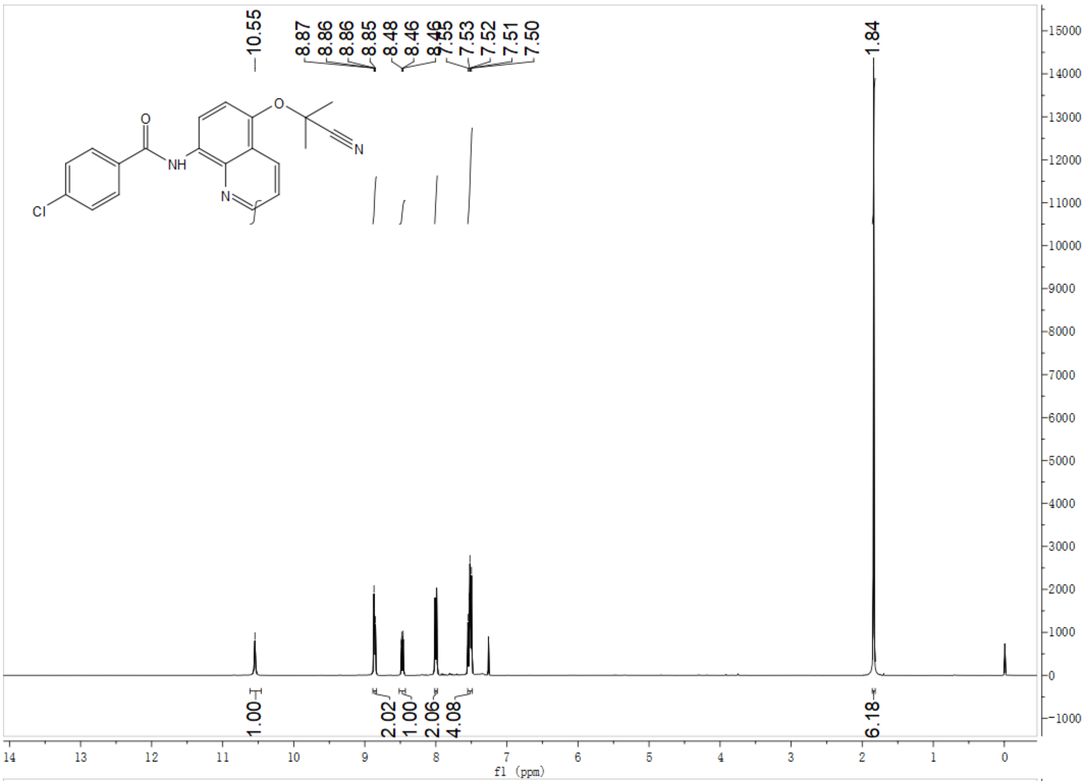
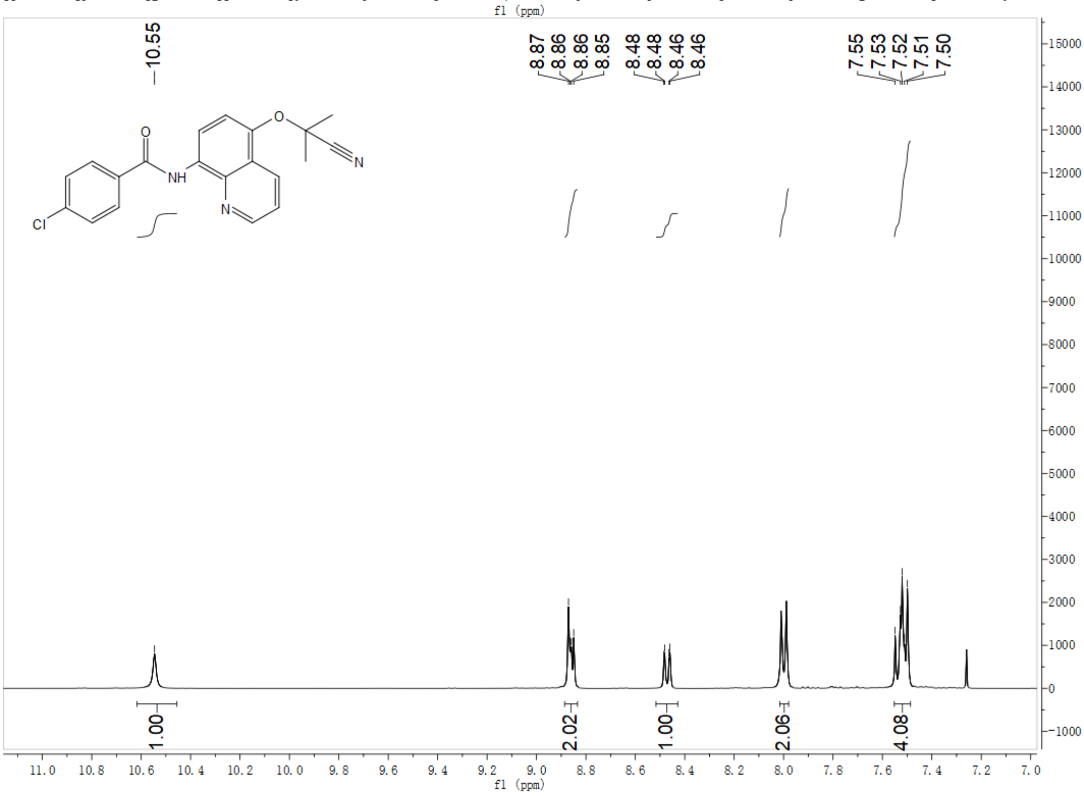
2f:

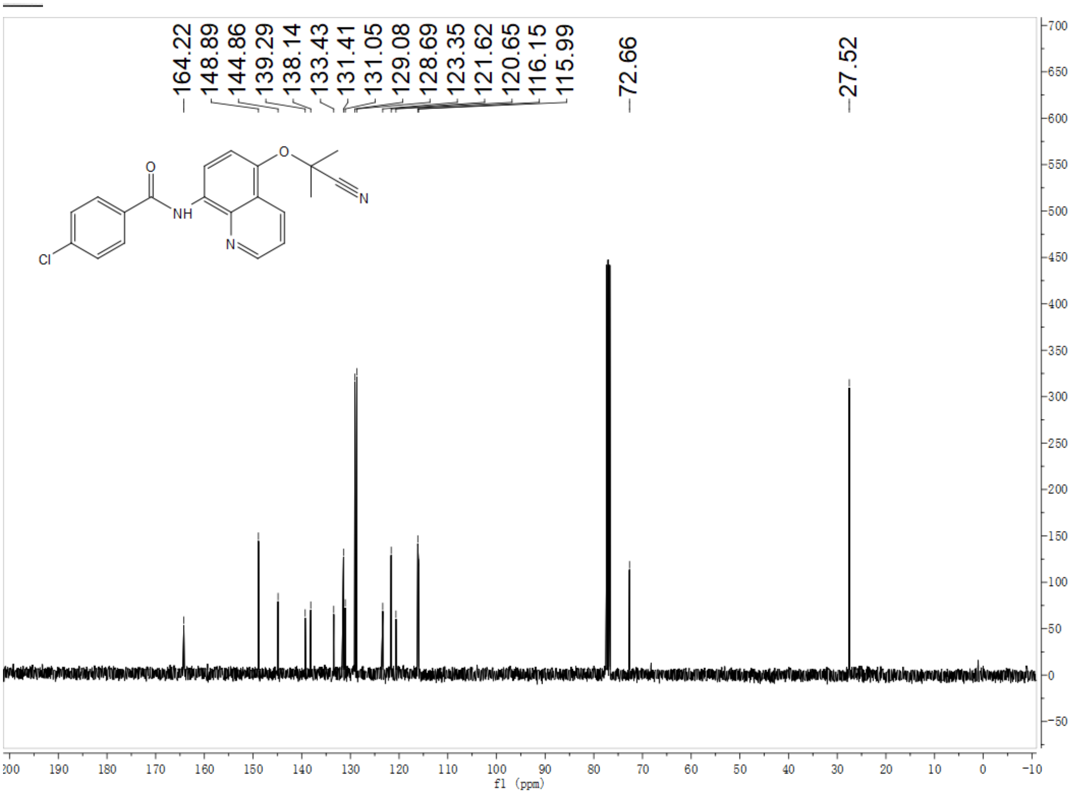



wcxl90925-80h
80h
10.56
8.90
8.88
8.88
8.87
8.87
8.86
8.48
8.45
7.98
7.96
7.55
7.53
7.52
7.51
7.50
7.49
7.35
7.33
O
NH
N
O
N
1.00
1.02
1.07
1.02
2.09
1.07
1.02
2.08
f1 (ppm)

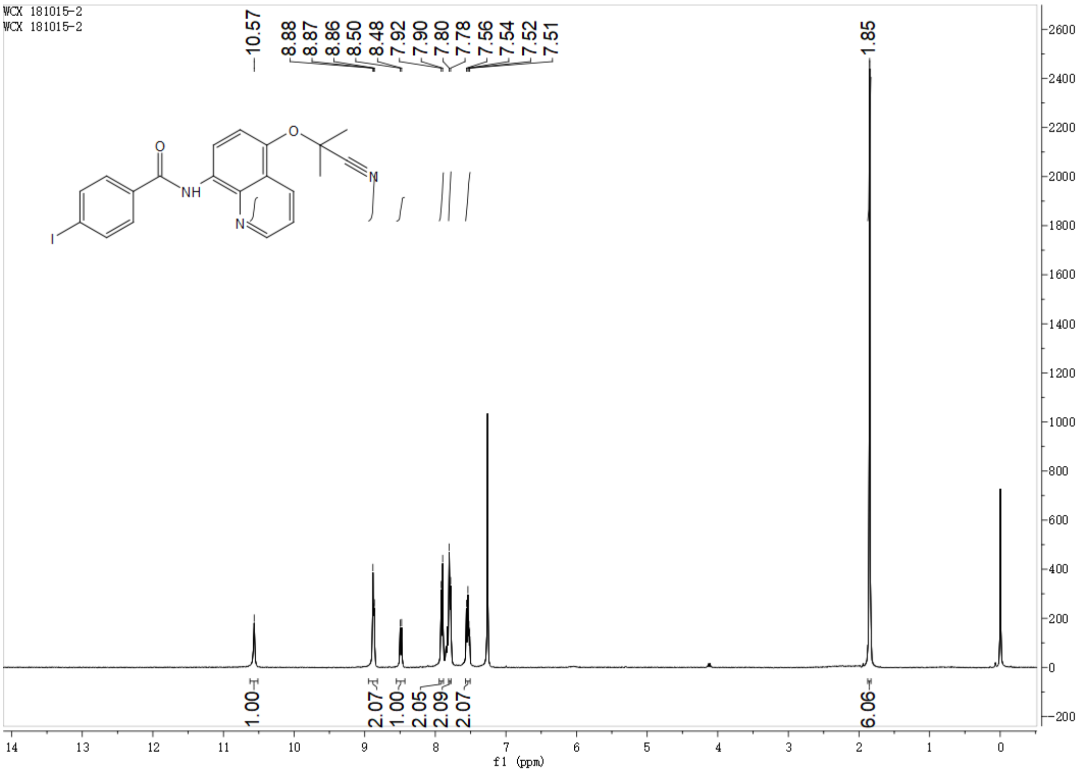

wenchunxia-1113-1c
wenchunxia-1113-1c
165.36
148.78
144.56
142.37
139.34
132.25
131.50
131.33
129.48
127.27
123.40
121.52
120.72
116.24
115.95
72.70
27.52
21.55
O
NH
N
O
N
f1 (ppm)

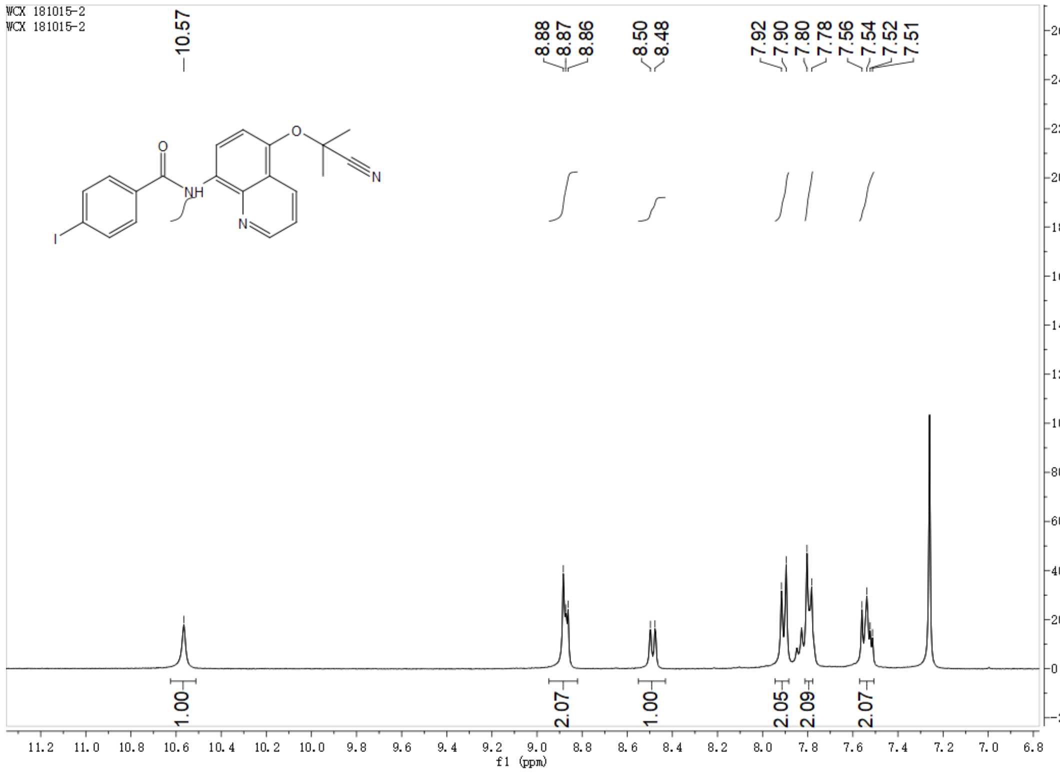
2g:

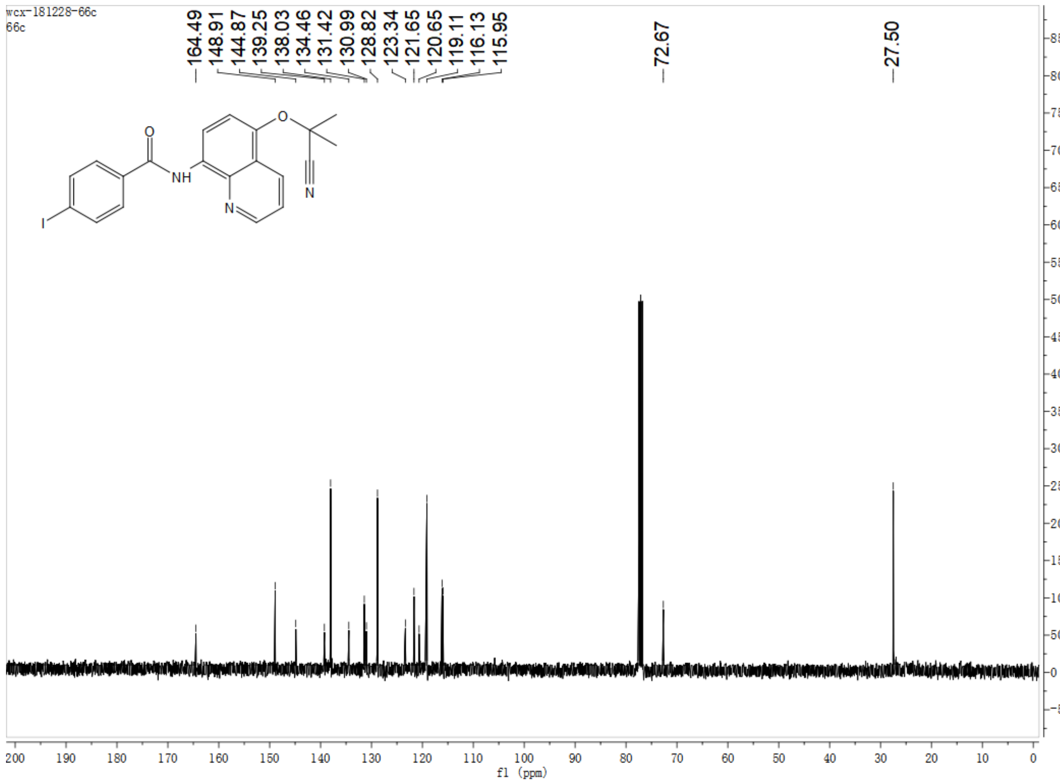

10.55
8.87
8.86
8.86
8.85
8.48
8.46
8.46
7.55
7.53
7.52
7.51
7.50
1.84
1.00
2.02
1.00
2.06
4.08
6.18
f1 (ppm)
O
NH
Cl
N
O
N

10.55
8.87
8.86
8.86
8.85
8.48
8.48
8.46
8.46
7.55
7.53
7.52
7.51
7.50
1.00
2.02
1.00
2.06
4.08
f1 (ppm)
O
NH
Cl
N
O
N


164.22
148.89
144.86
139.29
138.14
133.43
131.41
131.05
129.08
128.69
123.35
121.62
120.65
116.15
115.99
72.66
27.52
O
NH
N
O
N
Cl
f1 (ppm)

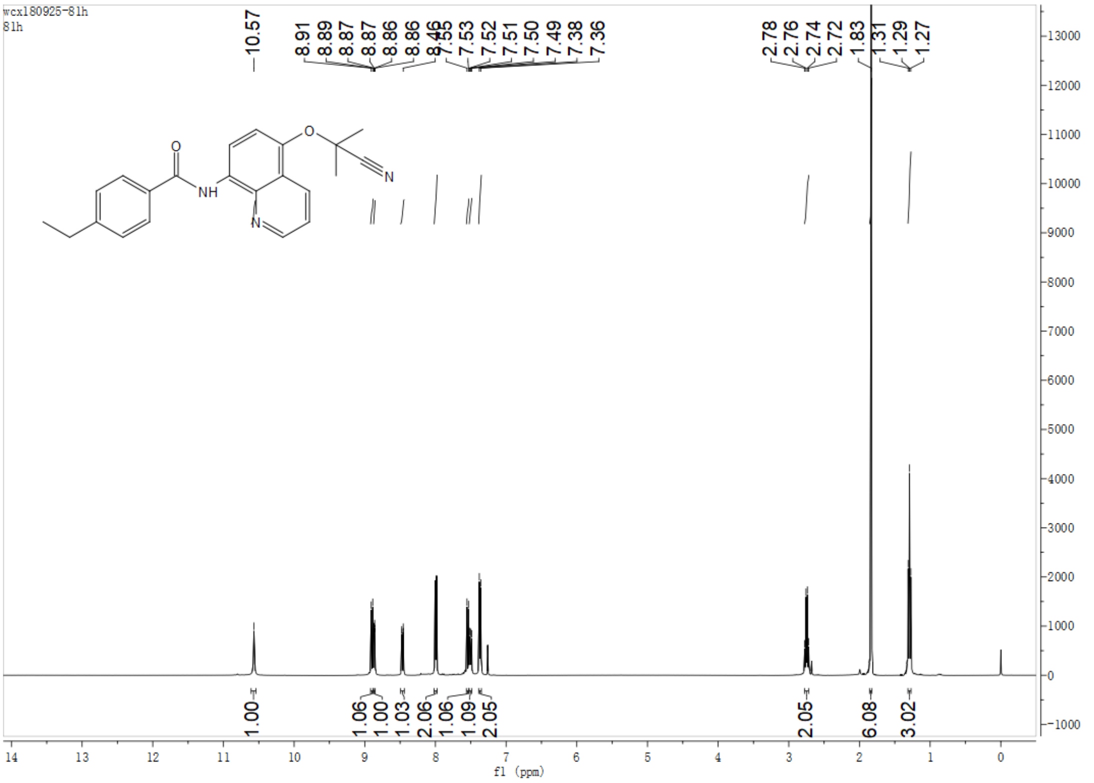
2h:

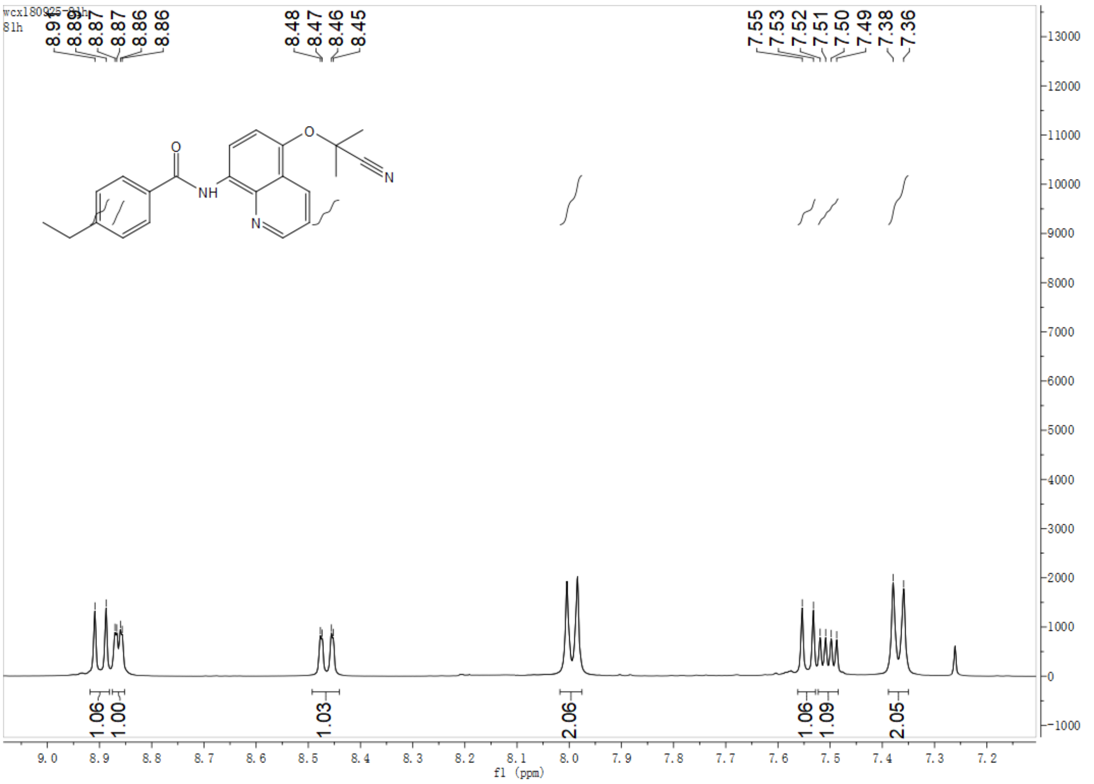

WCX 181015-2
WCX 181015-2
10.57
8.88
8.87
8.86
8.50
8.48
7.92
7.90
7.80
7.78
7.56
7.54
7.52
7.51
1.85
O
NH
N
O
N
I
1.00
2.07
1.00
2.05
2.09
2.07
6.06
f1 (ppm)

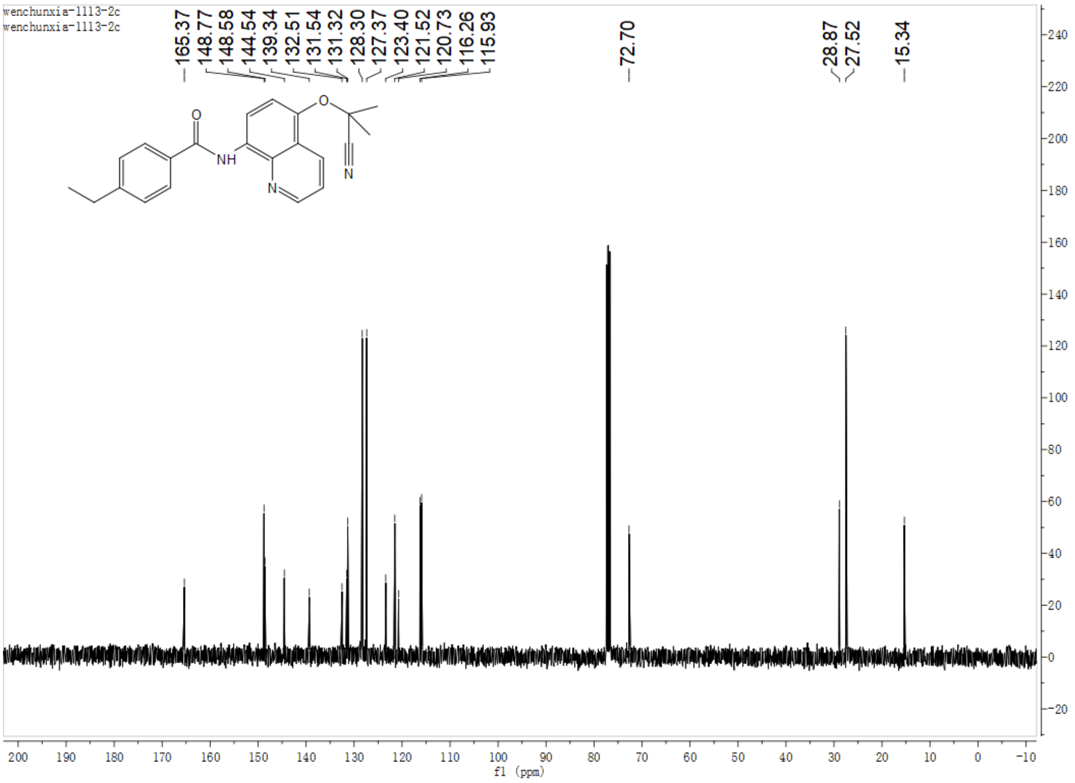

WCX 181015-2
WCX 181015-2
10.57
8.88
8.87
8.86
8.50
8.48
7.92
7.90
7.80
7.78
7.56
7.54
7.52
7.51
1.00
2.07
1.00
2.05
2.09
2.07
f1 (ppm)


wcx-181228-66c
66c
164.49
148.91
144.87
139.25
138.03
134.46
131.42
130.99
128.82
123.34
121.65
120.65
119.11
116.13
115.95
72.67
27.50
f1 (ppm)

2i:






wenchunxia-1113-2c
wenchunxia-1113-2c
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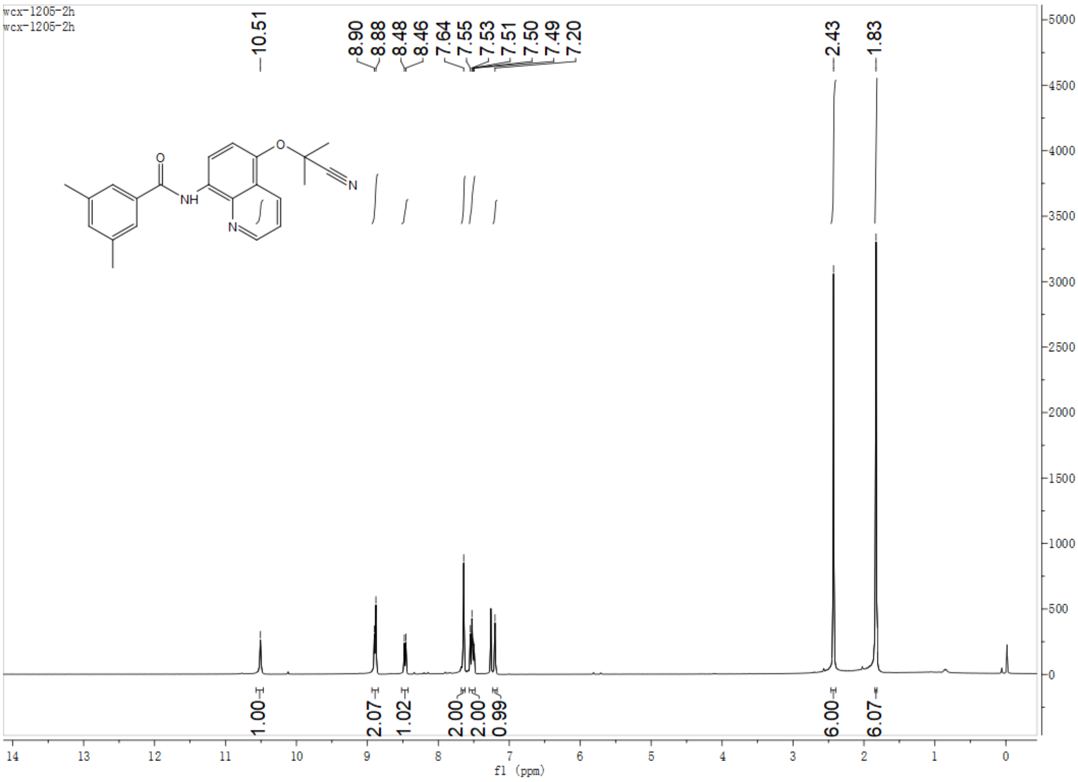
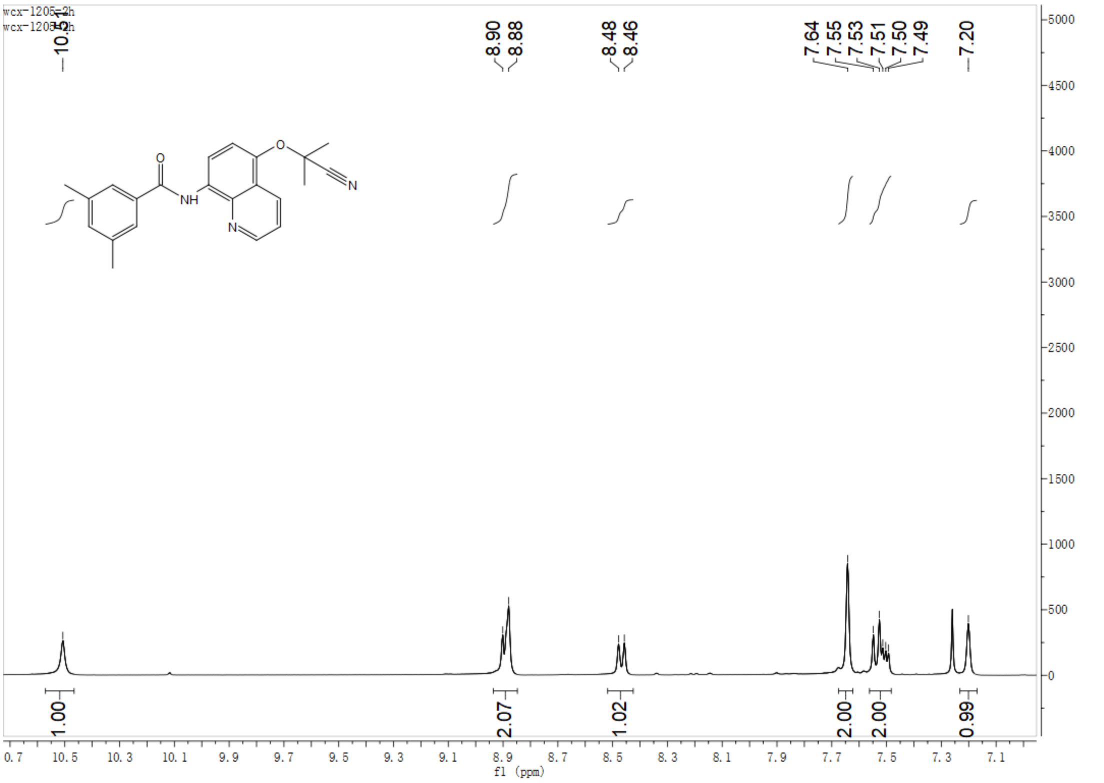
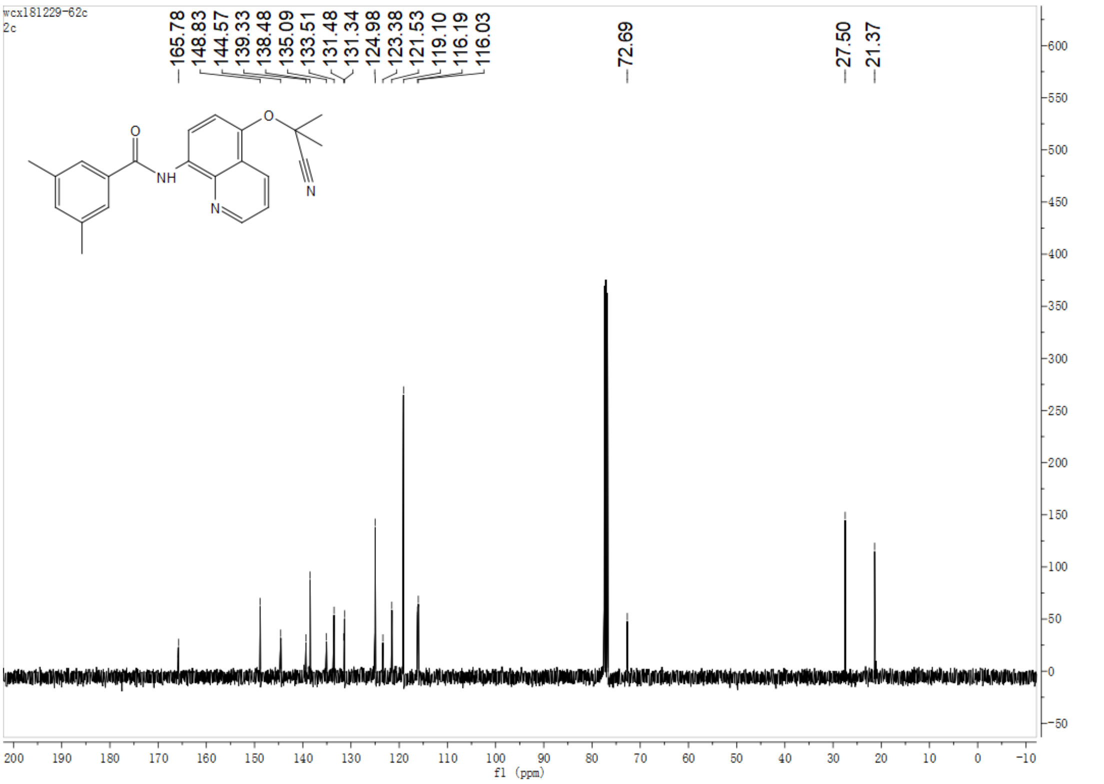
148.77
148.58
144.54
139.34
132.51
131.54
131.32
128.30
127.37
123.40
121.52
120.73
116.26
115.93
72.70
28.87
27.52
15.34
f1 (ppm)

2j:


wcx-1205-2h
wcx-1205-2h
10.51
8.90
8.88
8.48
8.46
7.64
7.55
7.53
7.51
7.50
7.49
7.20
2.43
1.83
1.00
2.07
1.02
2.00
2.00
0.99
6.00
6.07
f1 (ppm)


wcx-1205-2h
10.51
8.90
8.88
8.48
8.46
7.64
7.55
7.53
7.51
7.50
7.49
7.20
1.00
2.07
1.02
2.00
2.00
0.99
f1 (ppm)


wcx181229-62c
2c
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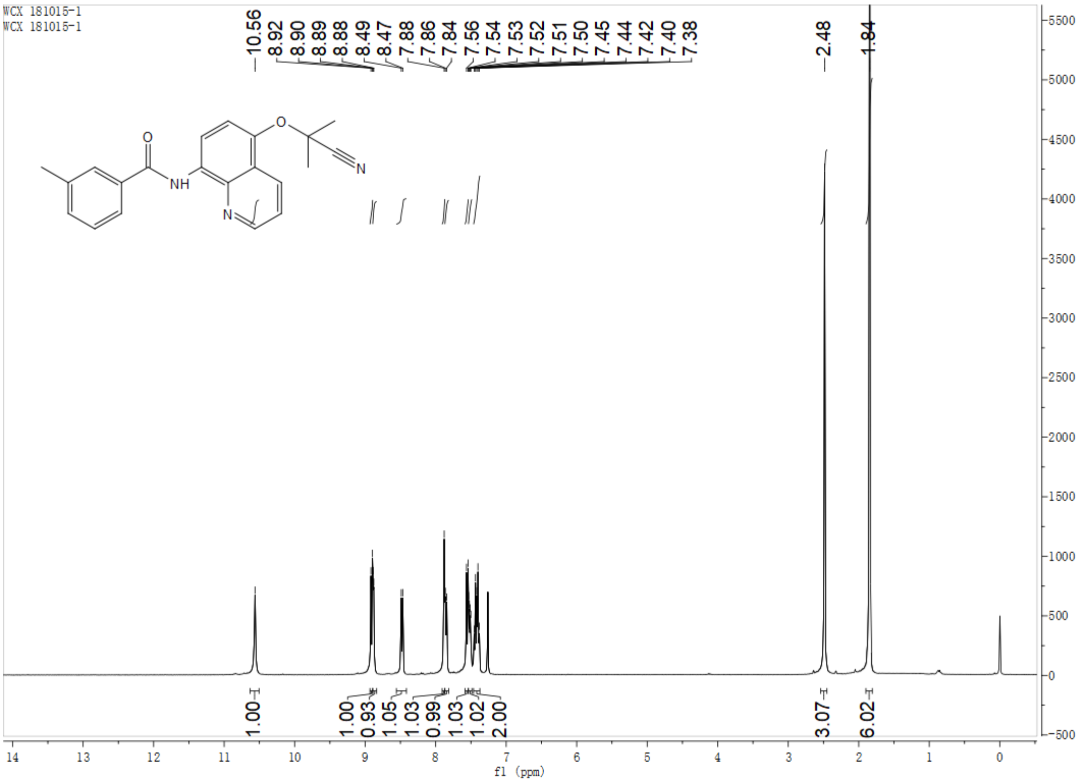
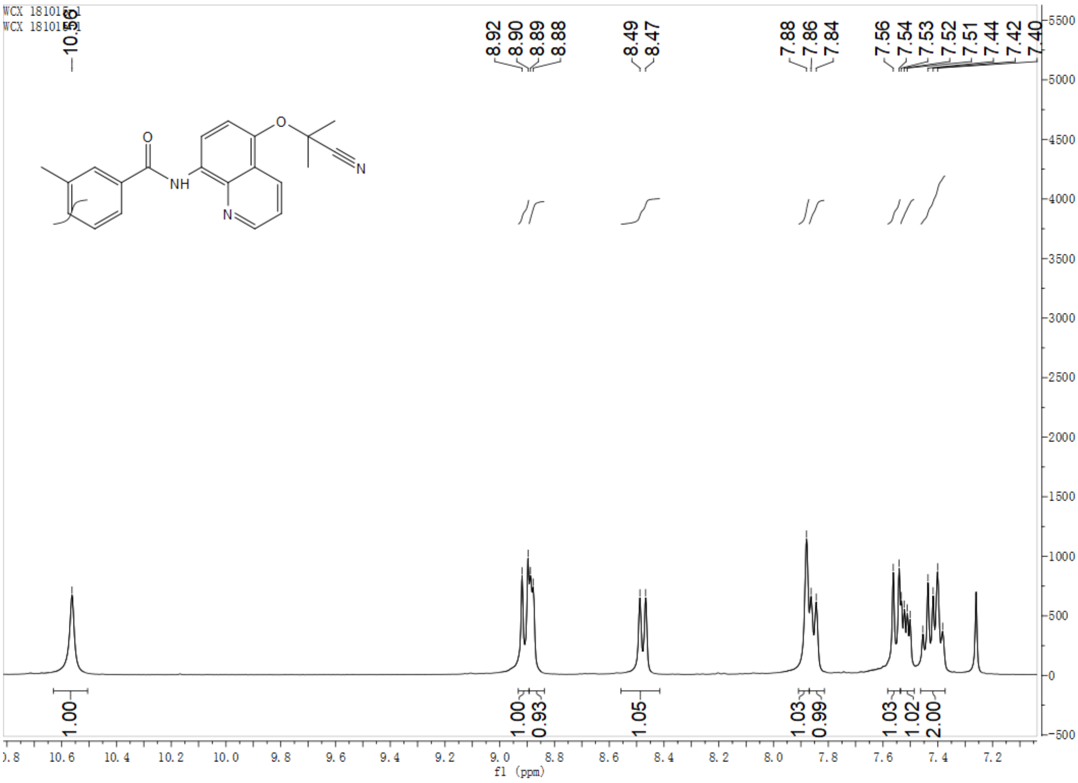
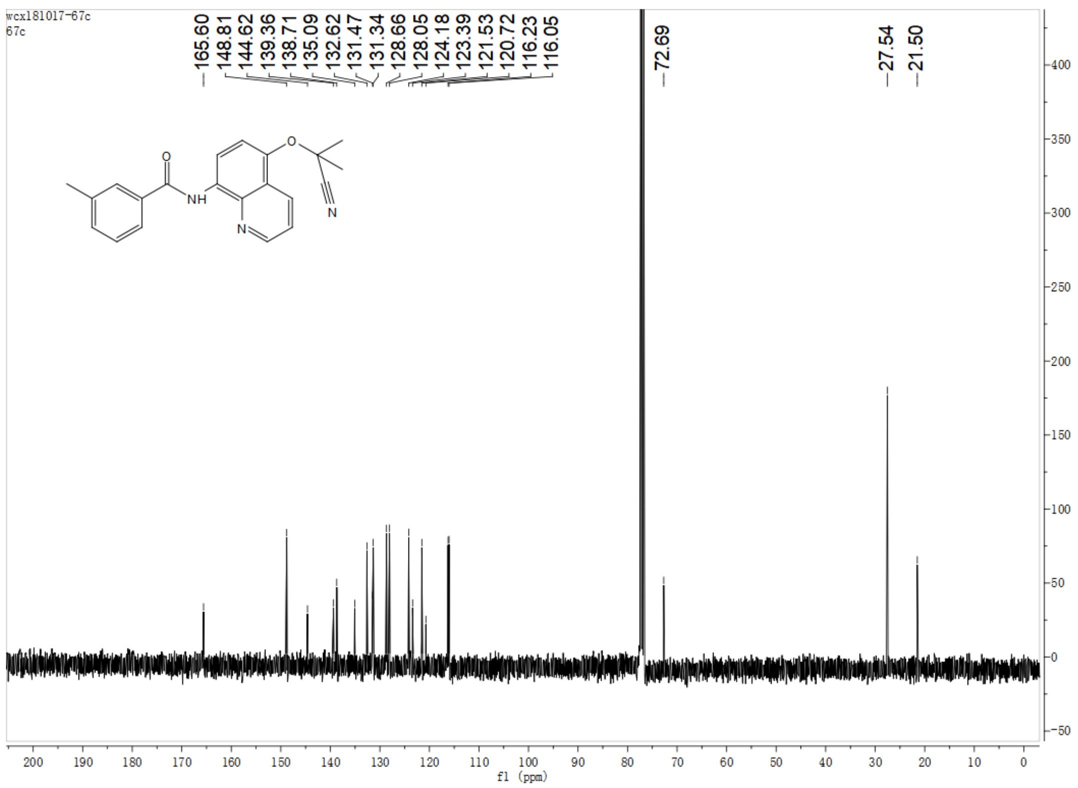
148.83
144.57
139.33
138.48
135.09
133.51
131.48
131.34
124.98
123.38
121.53
119.10
116.19
116.03
72.69
27.50
21.37
f1 (ppm)

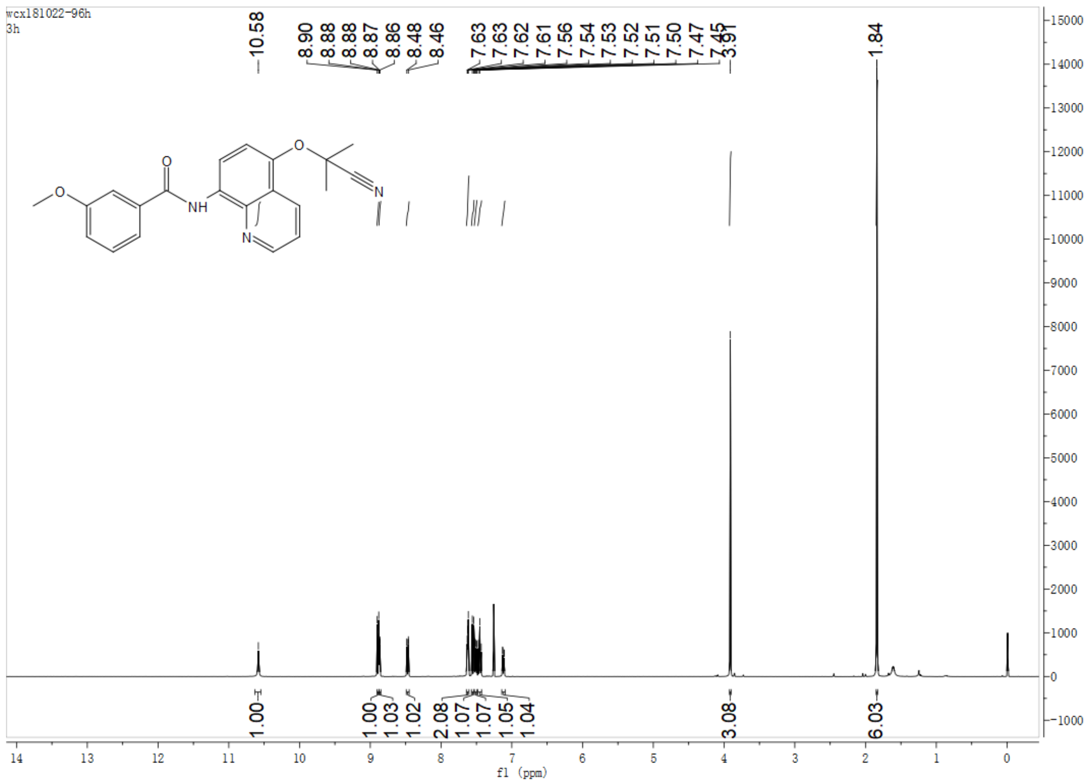
2k:

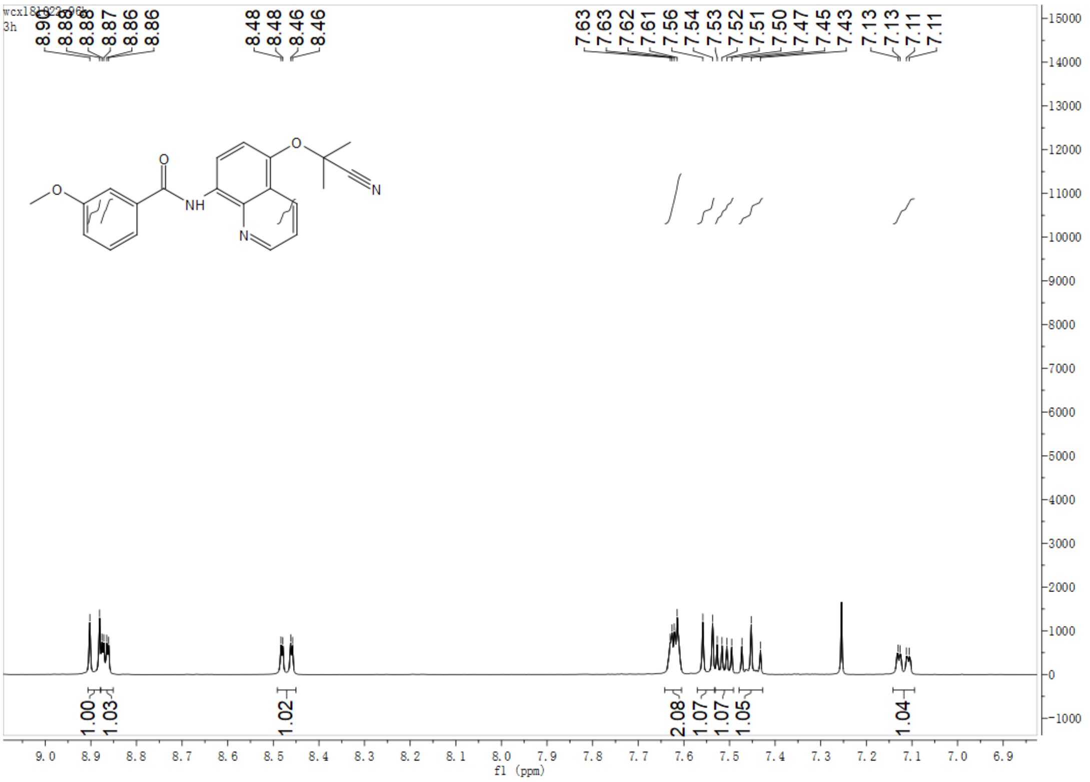

WCX 181015-1
WCX 181015-1
10.56
8.92
8.90
8.89
8.88
8.49
8.47
7.88
7.86
7.84
7.56
7.54
7.53
7.52
7.51
7.50
7.45
7.44
7.42
7.40
7.38
2.48
1.84
O
NH
N
O
N
1.00
1.00
0.93
1.05
1.03
0.99
1.03
1.02
2.00
3.07
6.02
f1 (ppm)

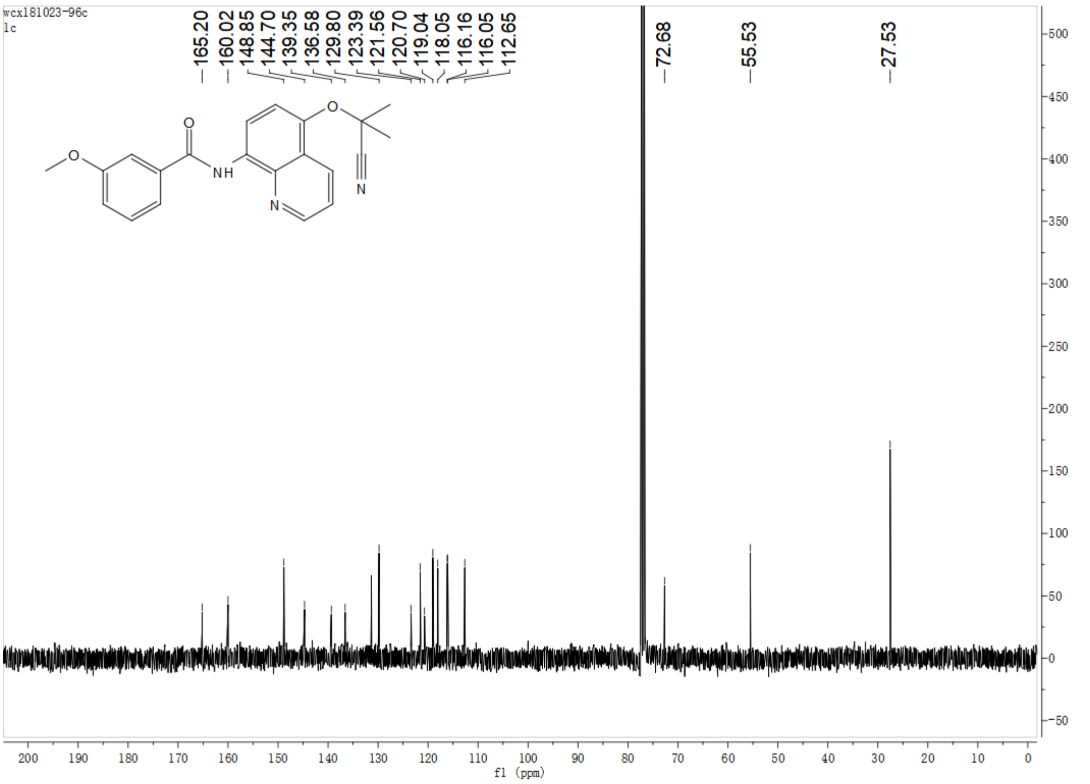

10.56
8.92
8.90
8.89
8.88
8.49
8.47
7.88
7.86
7.84
7.56
7.54
7.53
7.52
7.51
7.44
7.42
7.40
O
NH
N
O
N
1.00
1.00
0.93
1.05
1.03
0.99
1.03
1.02
2.00
f1 (ppm)



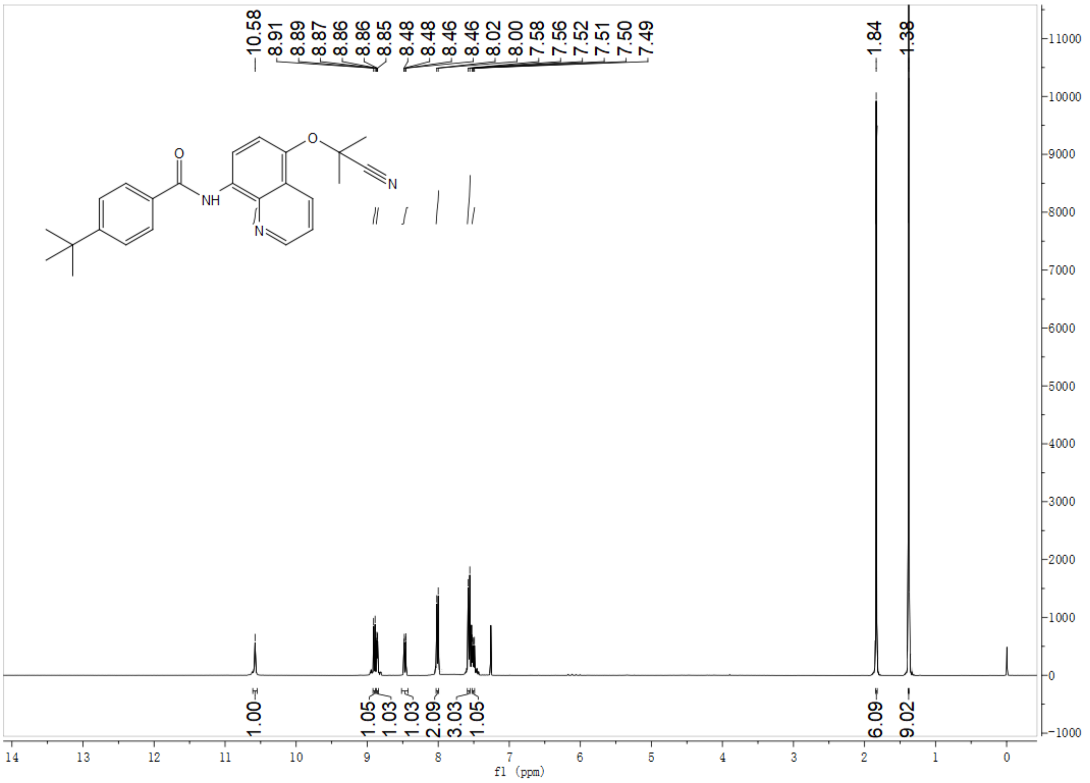
2l:



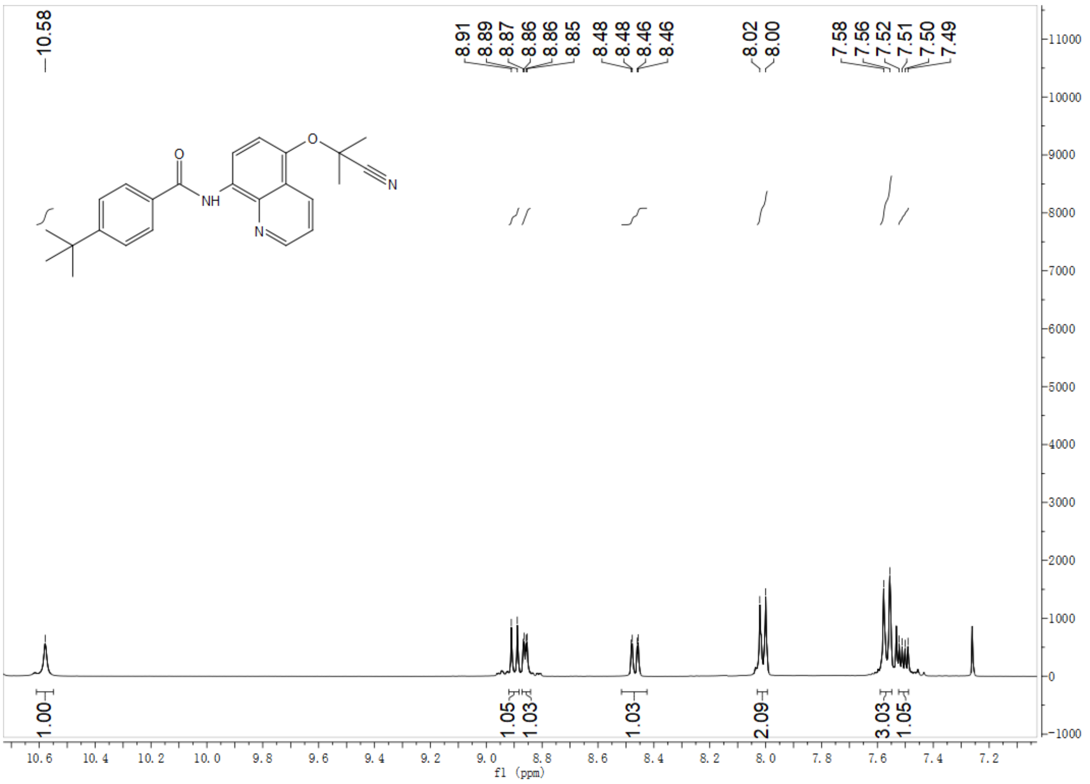

wcx181023-96h
3h
8.90
8.88
8.88
8.87
8.86
8.86
8.48
8.48
8.46
8.46
7.63
7.63
7.62
7.61
7.56
7.54
7.53
7.52
7.51
7.50
7.47
7.45
7.43
7.13
7.13
7.11
7.11
O
NH
N
O
N
1.00
1.03
1.02
2.08
1.07
1.07
1.05
1.04
f1 (ppm)


wcx181023-96c
1c
165.20
160.02
148.85
144.70
139.35
136.58
129.80
123.39
121.56
120.70
119.04
118.05
116.16
116.05
112.65
72.68
55.53
27.53
O
NH
N
O
N
f1 (ppm)

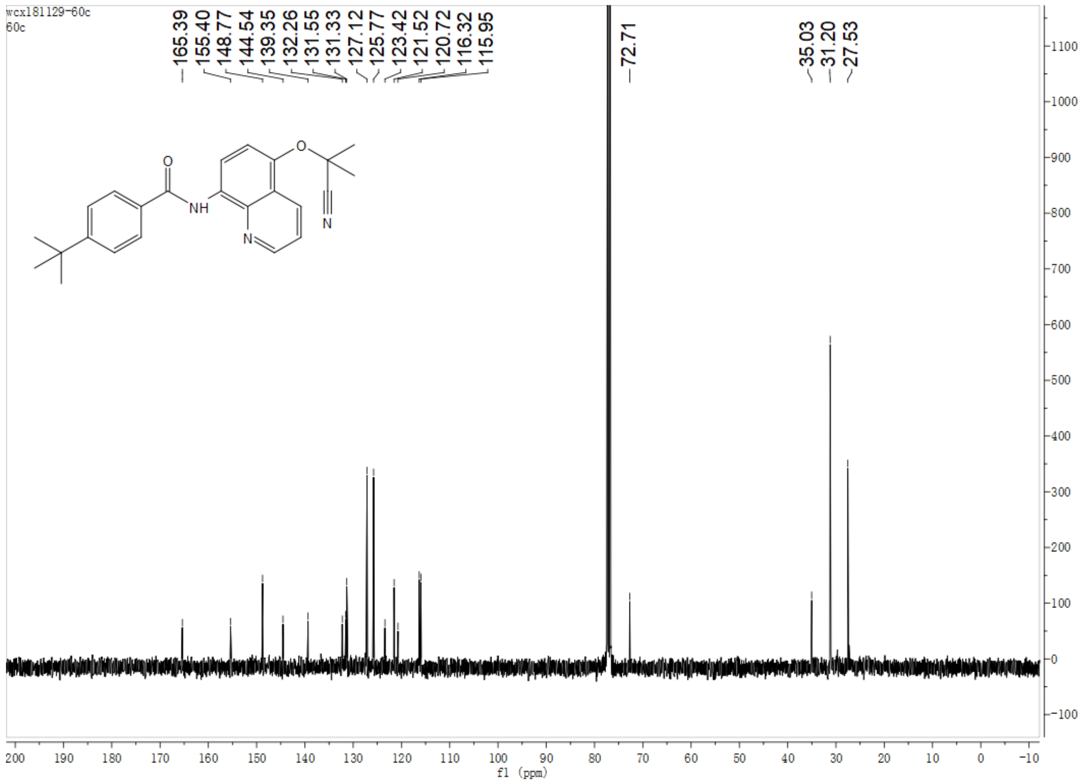
2m:



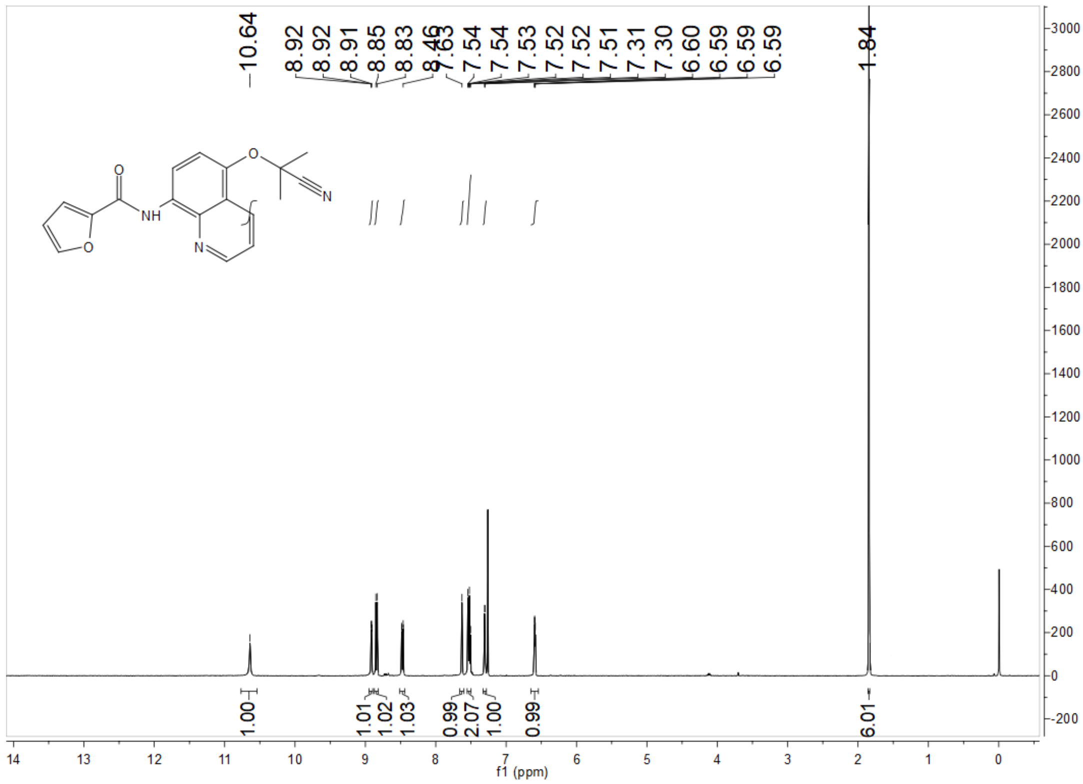
10.58
8.91
8.89
8.87
8.86
8.86
8.85
8.48
8.48
8.46
8.46
8.02
8.00
7.58
7.56
7.52
7.51
7.50
7.49
1.84
1.38
1.00
1.05
1.03
1.03
2.09
3.03
1.05
6.09
9.02
f1 (ppm)

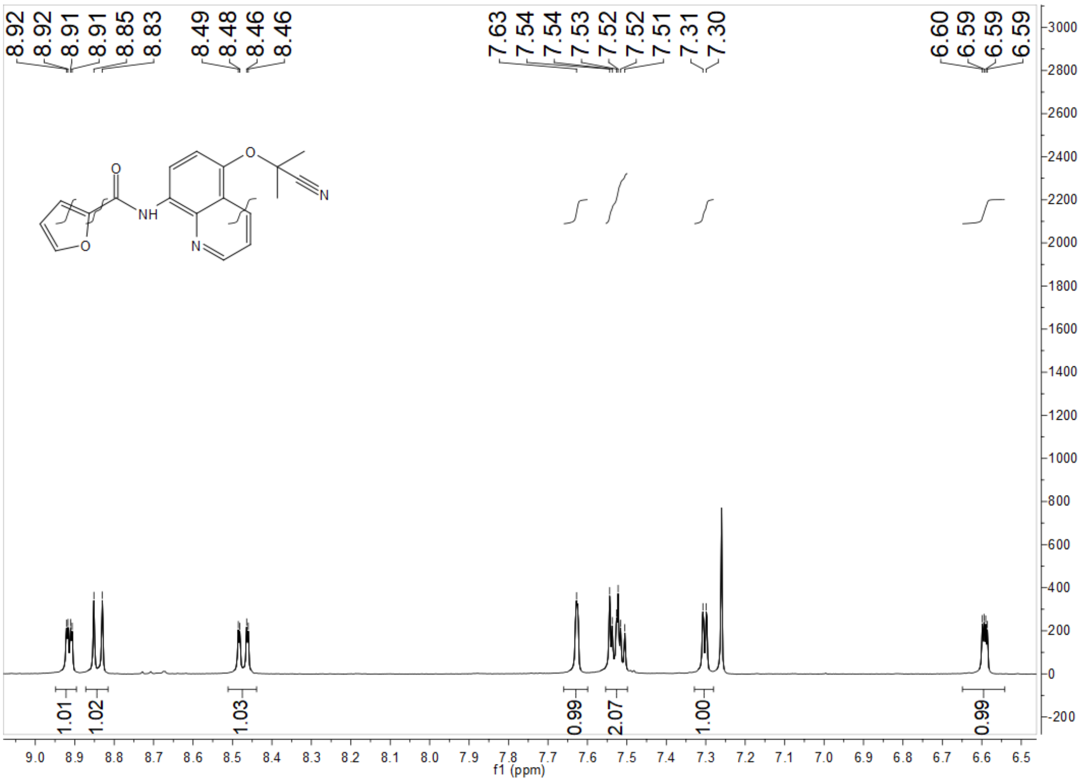


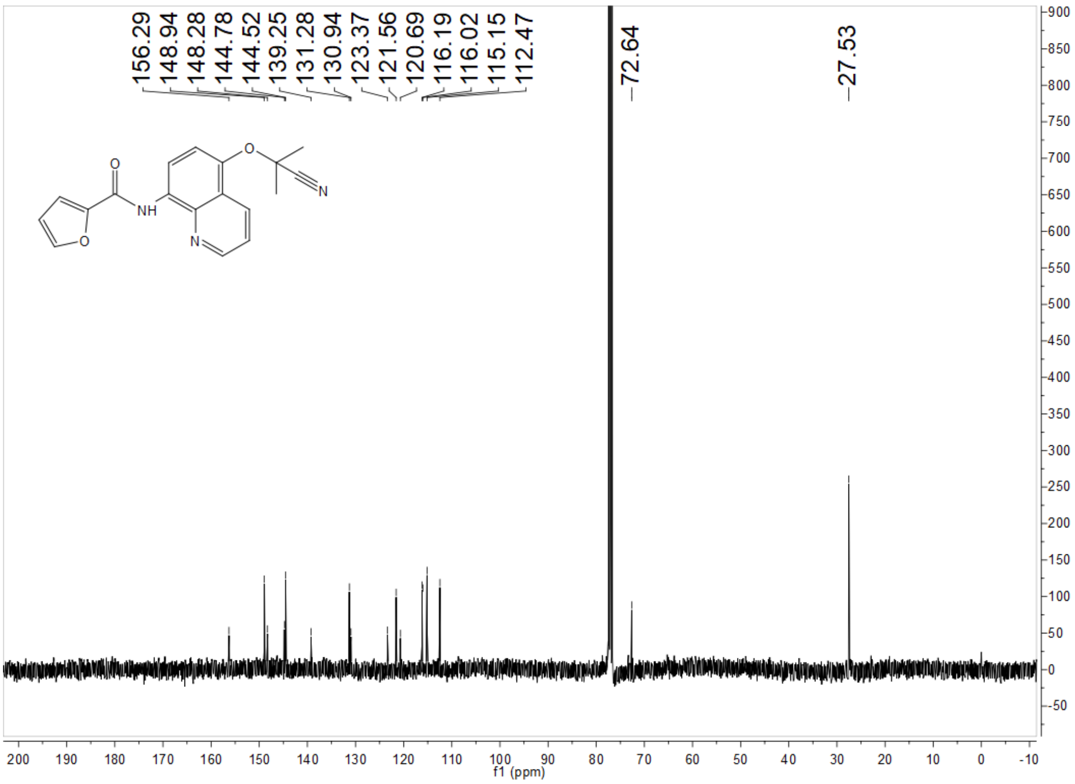
10.58
8.91
8.89
8.87
8.86
8.86
8.85
8.48
8.48
8.46
8.46
8.02
8.00
7.58
7.56
7.52
7.51
7.50
7.49
1.00
1.05
1.03
1.03
2.09
3.03
1.05
f1 (ppm)



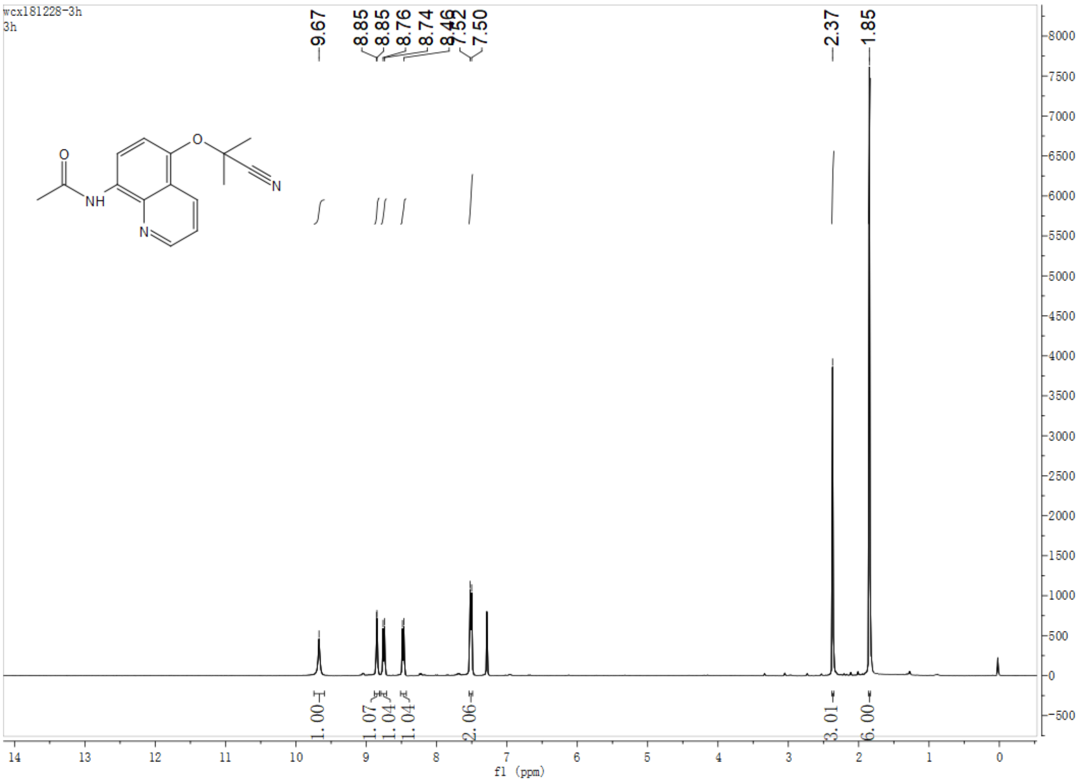
2n:

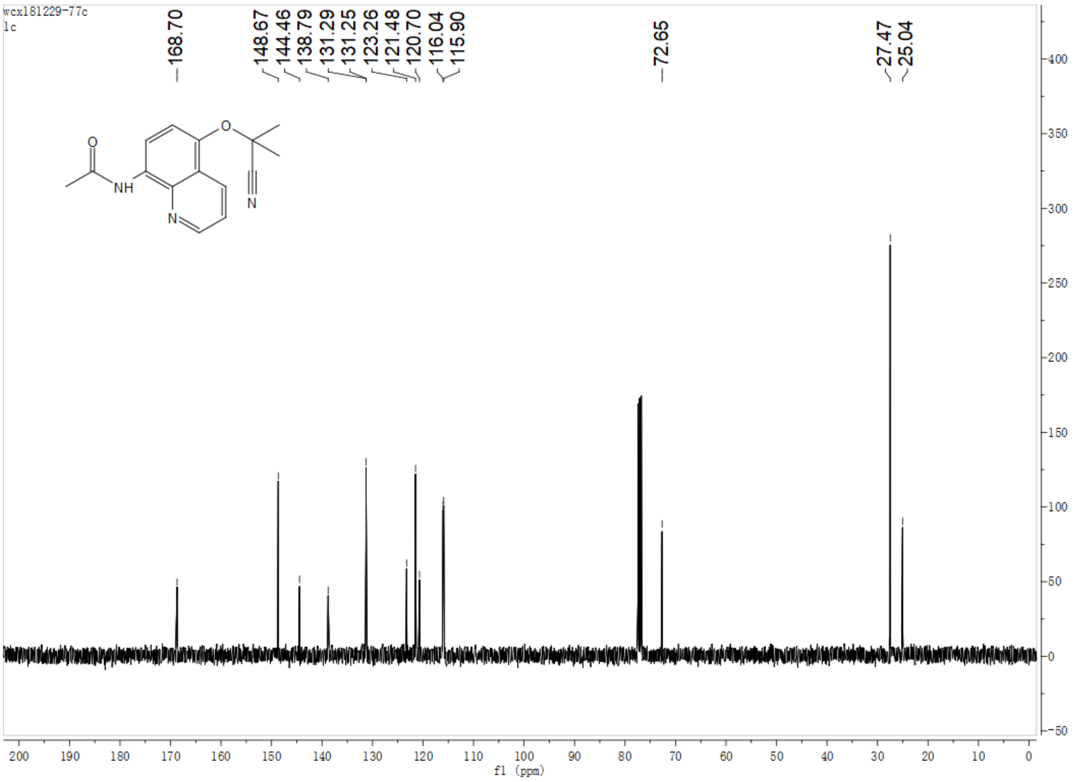



8.92
8.92
8.91
8.91
8.85
8.83
8.49
8.48
8.46
8.46
7.63
7.54
7.54
7.53
7.52
7.52
7.51
7.31
7.30
6.60
6.59
6.59
6.59
1.01
1.02
1.03
0.99
2.07
1.00
0.99
f1 (ppm)

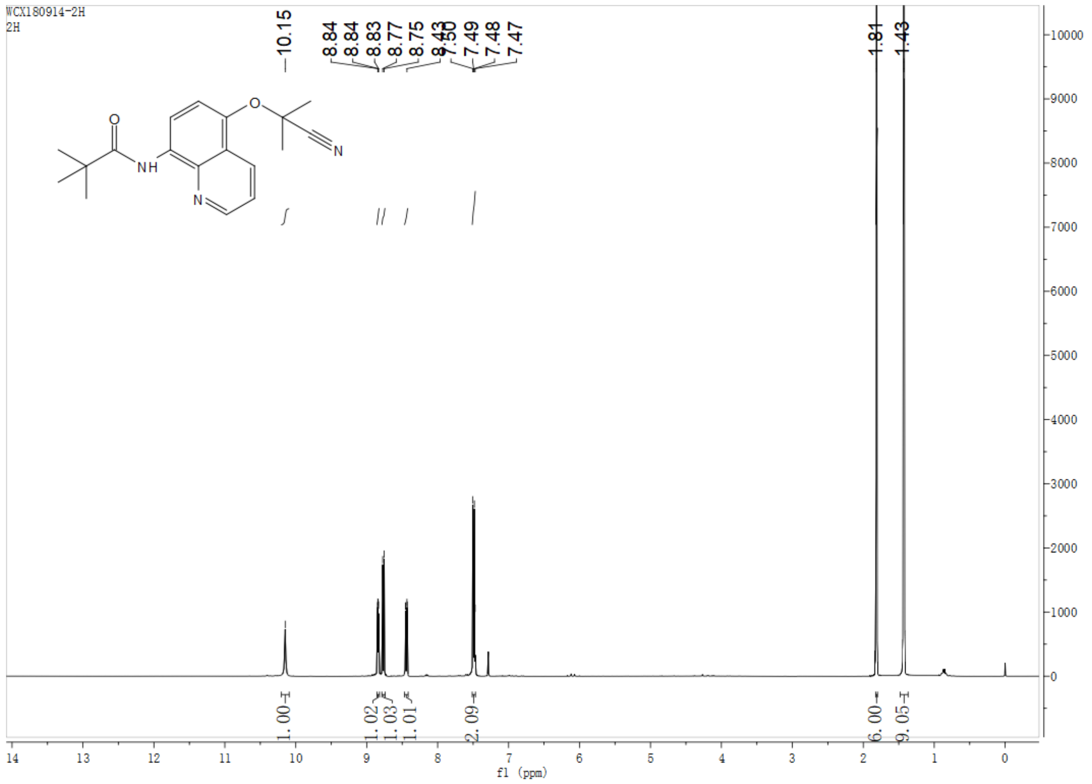

156.29
148.94
148.28
144.78
144.52
139.25
131.28
130.94
123.37
121.56
120.69
116.19
116.02
115.15
112.47
72.64
27.53
f1 (ppm)

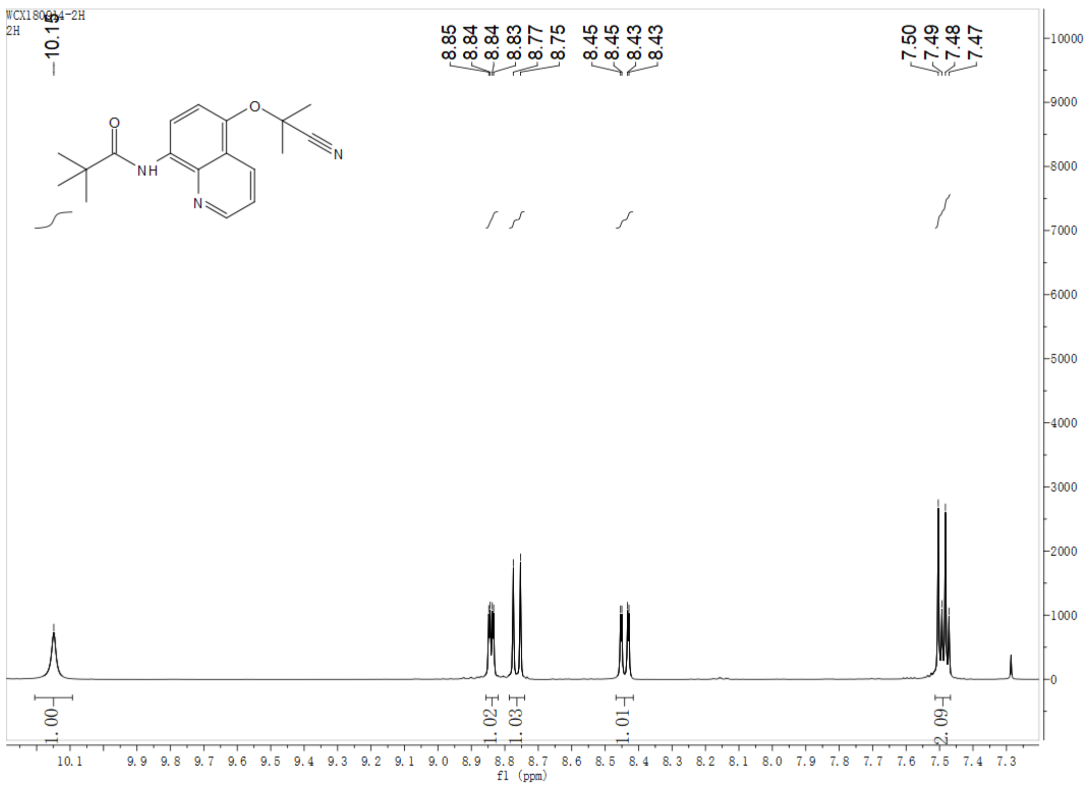
2o:

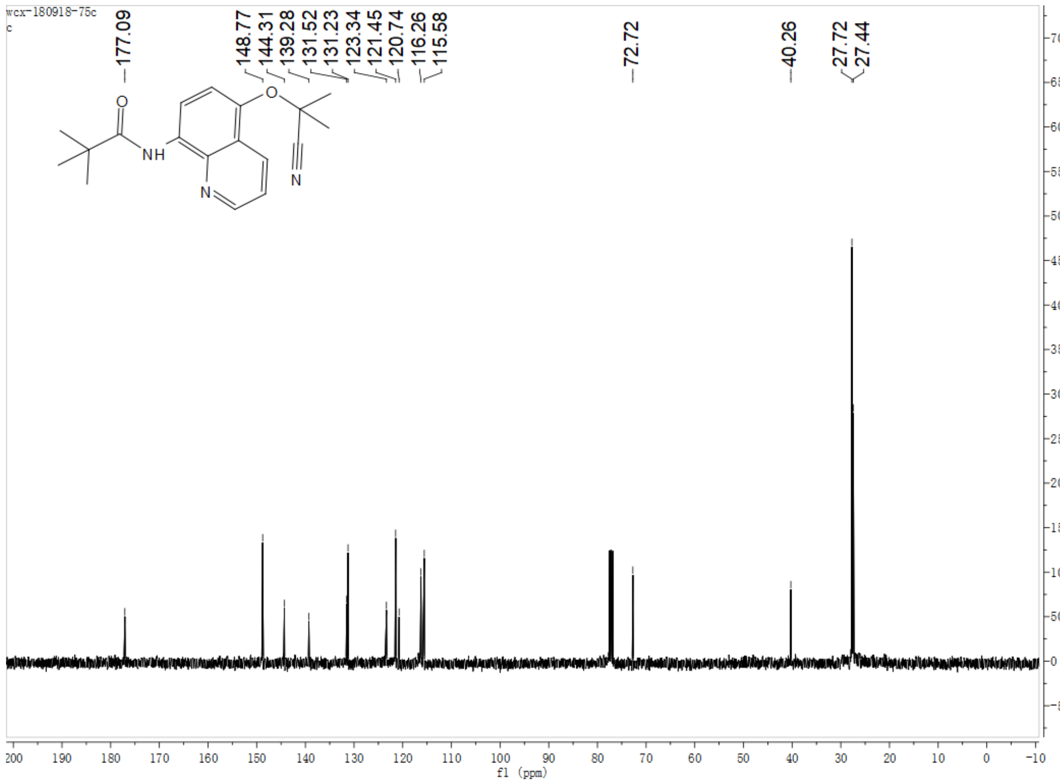

wcx181228-3h
3h
9.67
8.85
8.85
8.76
8.74
8.46
7.52
7.50
2.37
1.85
1.00
1.07
1.04
1.04
2.06
3.01
6.00
f1 (ppm)


wcx181229-77c
1c
168.70
148.67
144.46
138.79
131.29
131.25
123.26
121.48
120.70
116.04
115.90
72.65
27.47
25.04
f1 (ppm)

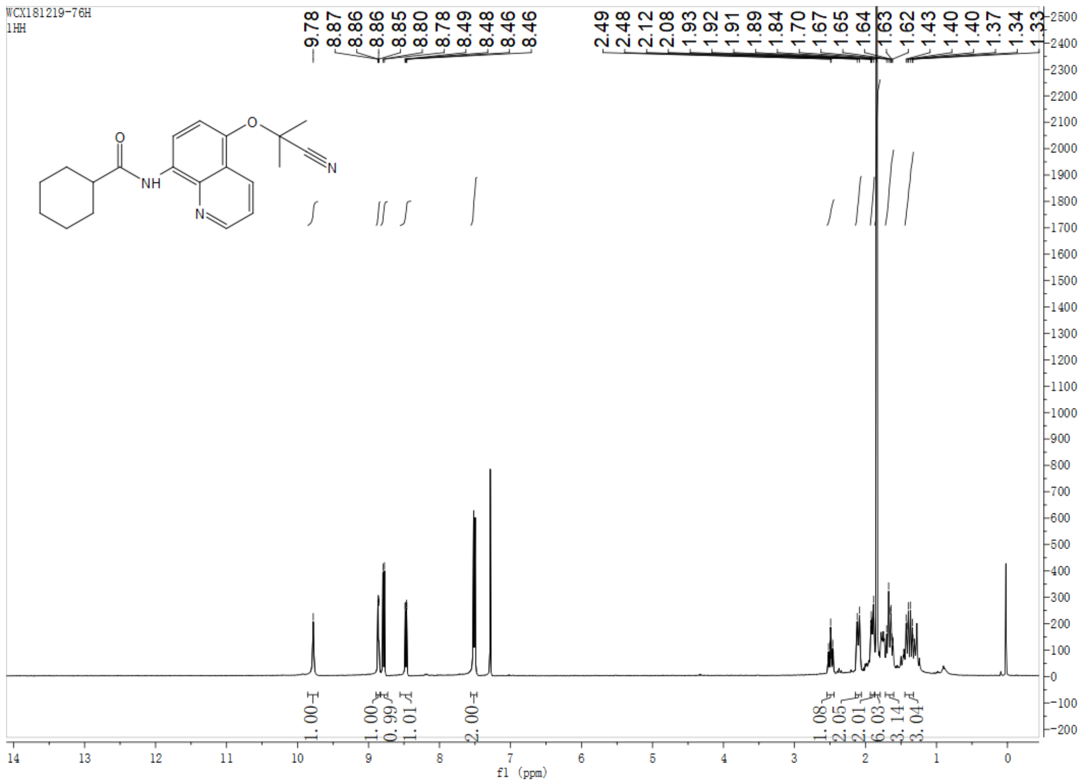
2p:


WCX180914-2H
2H
10.15
8.84
8.84
8.83
8.77
8.75
8.43
7.50
7.49
7.48
7.47
1.81
1.43
1.00
1.02
1.03
1.01
2.09
6.00
9.05
f1 (ppm)


WCX180914-2H
2H
10.15
8.85
8.84
8.84
8.83
8.77
8.75
8.45
8.45
8.43
8.43
7.50
7.49
7.48
7.47
1.00
1.02
1.03
1.01
2.09
f1 (ppm)


wcx-180918-75c
c
177.09
148.77
144.31
139.28
131.52
131.23
123.34
121.45
120.74
116.26
115.58
72.72
40.26
27.72
27.44
O
NH
N
O
N
f1 (ppm)

2q:


WCX181219-76H
1HH
9.78
8.87
8.86
8.86
8.85
8.80
8.78
8.49
8.48
8.46
8.46
2.49
2.48
2.12
2.08
1.93
1.92
1.91
1.89
1.84
1.70
1.67
1.65
1.64
1.63
1.62
1.43
1.40
1.40
1.37
1.34
1.33
O
NH
N
O
N
1.00
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1.01
2.00
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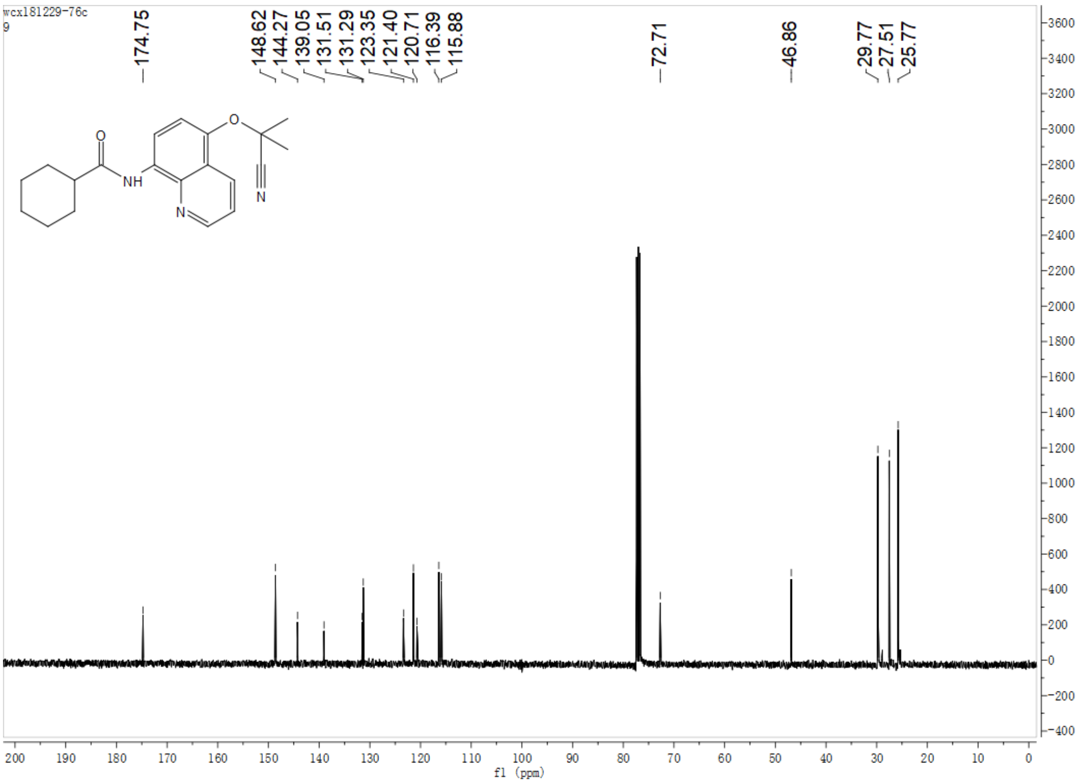
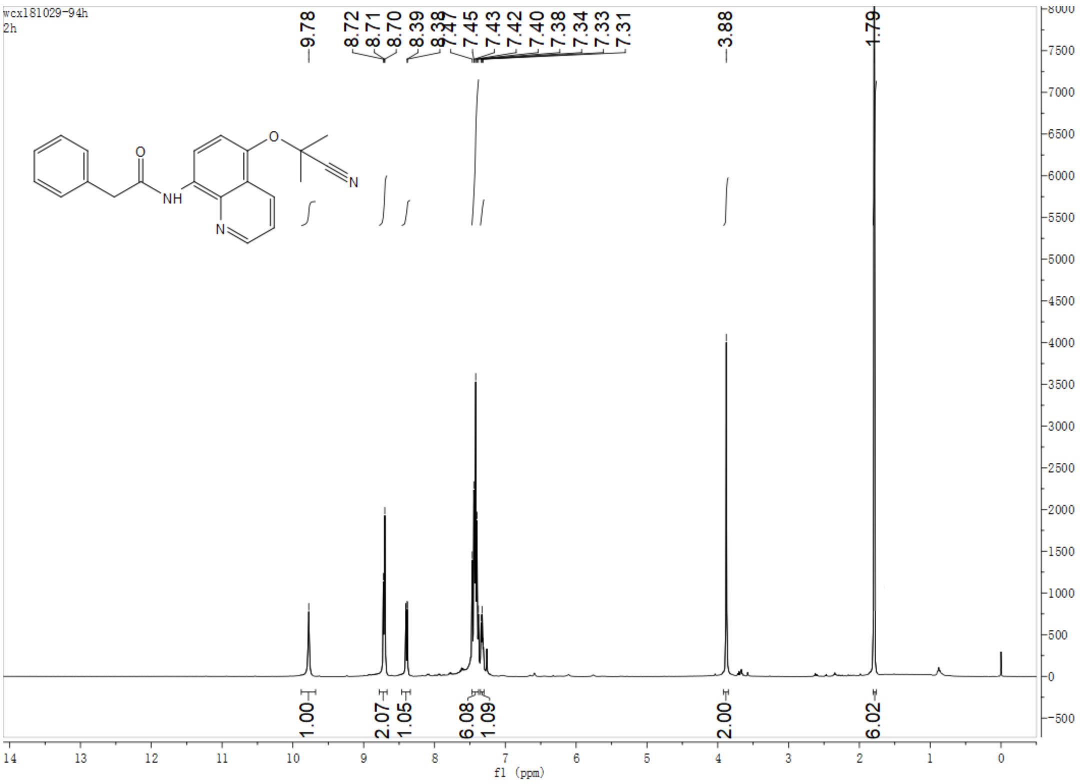
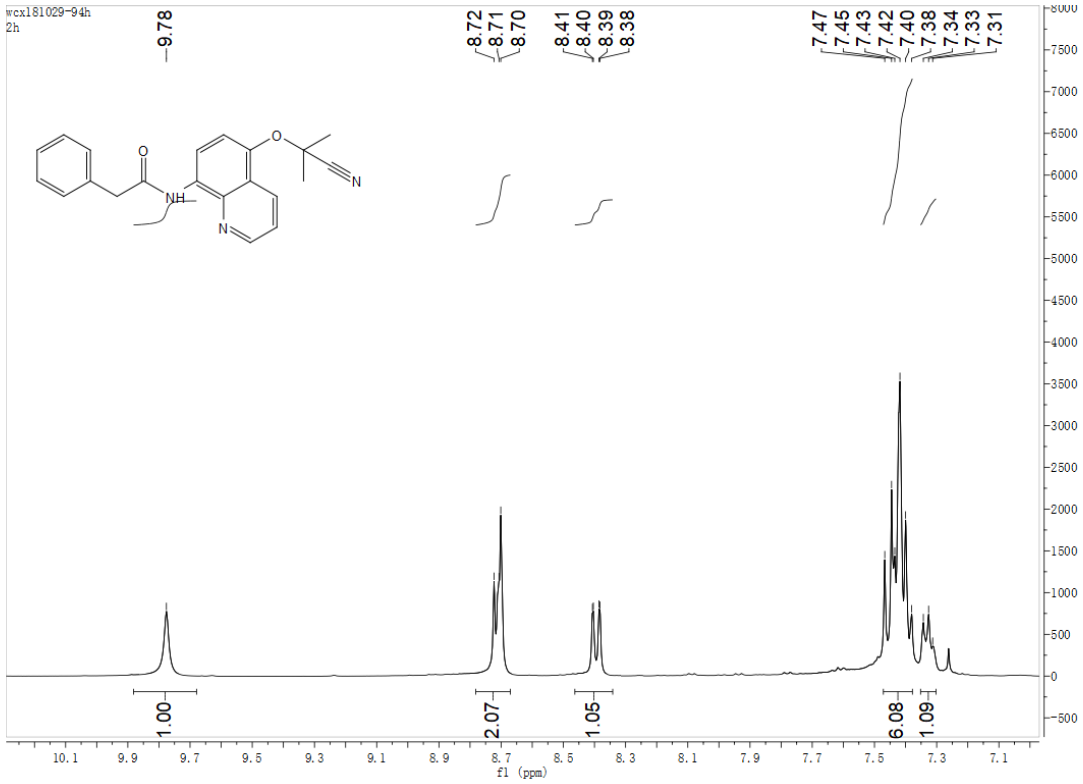
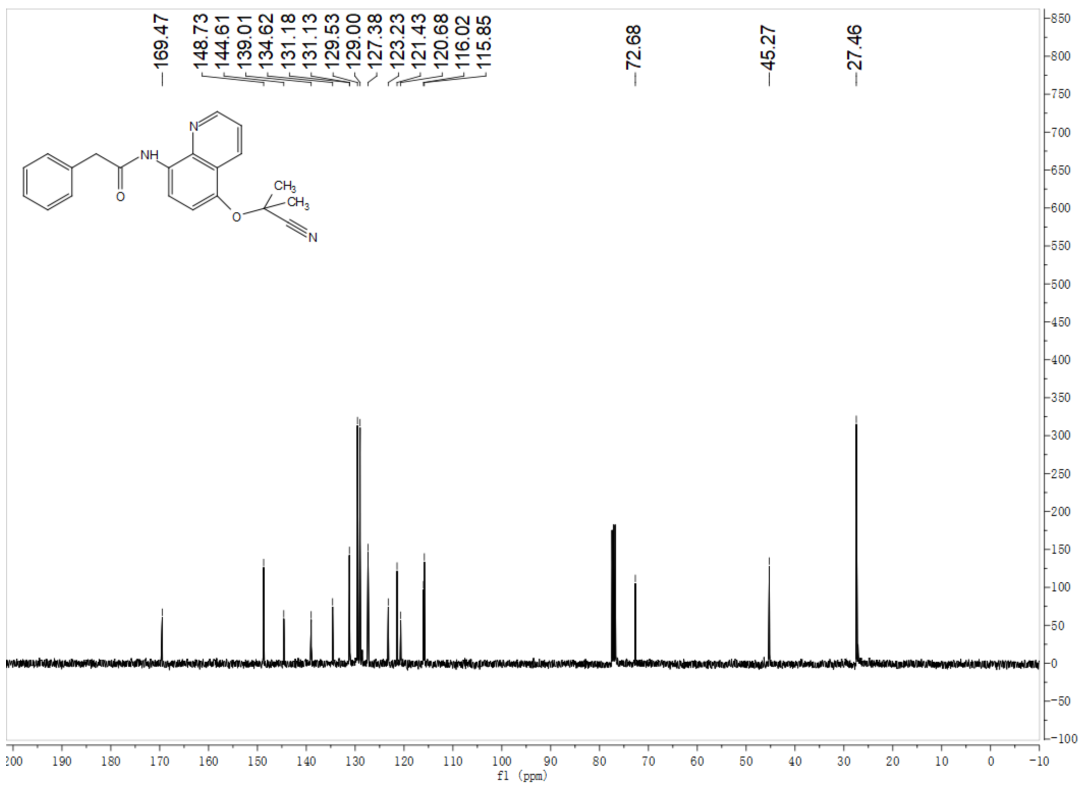
3.14
3.04
f1 (ppm)



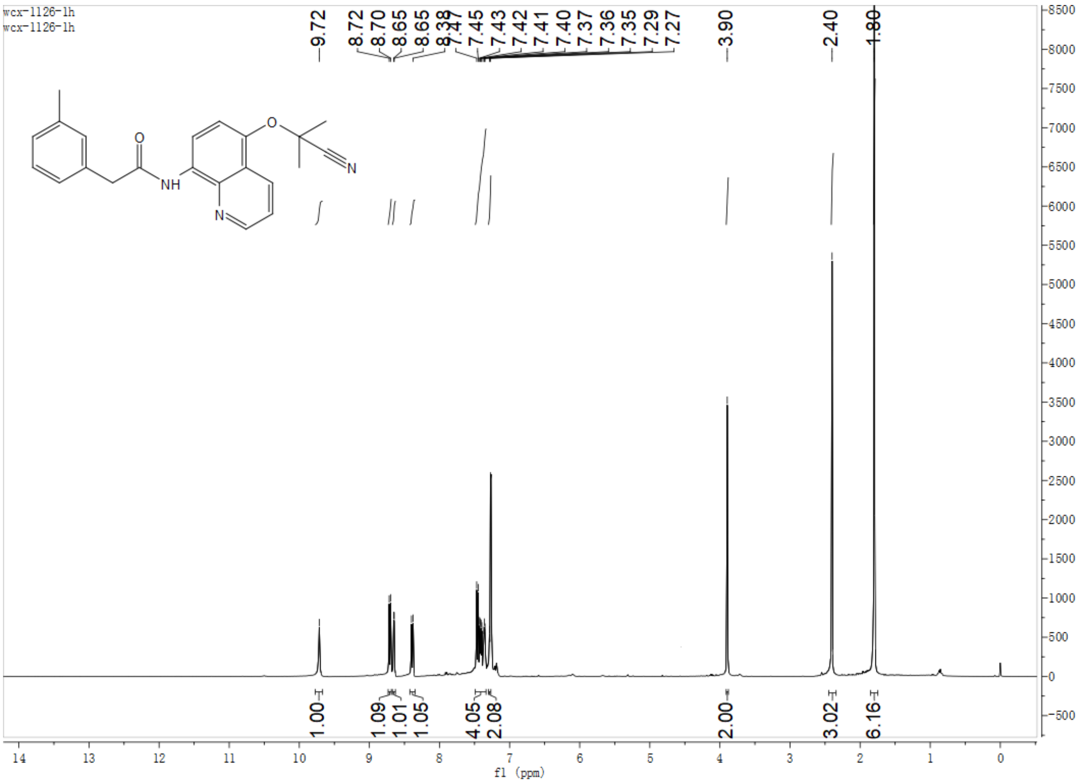
2r:

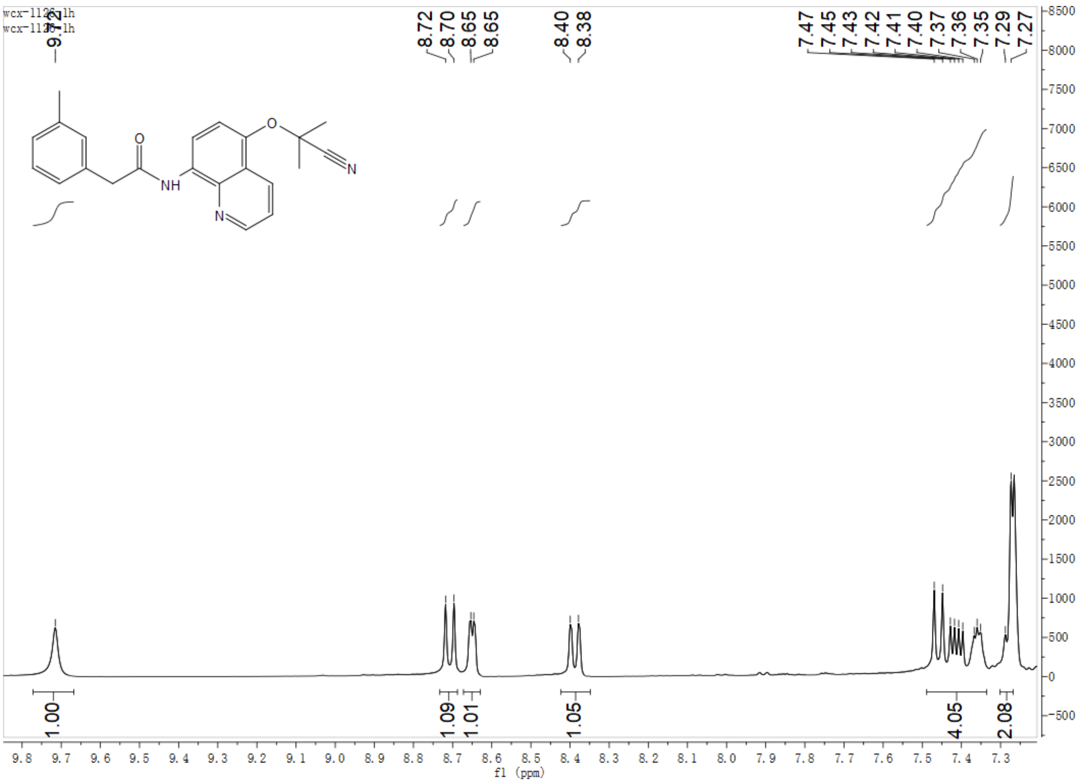


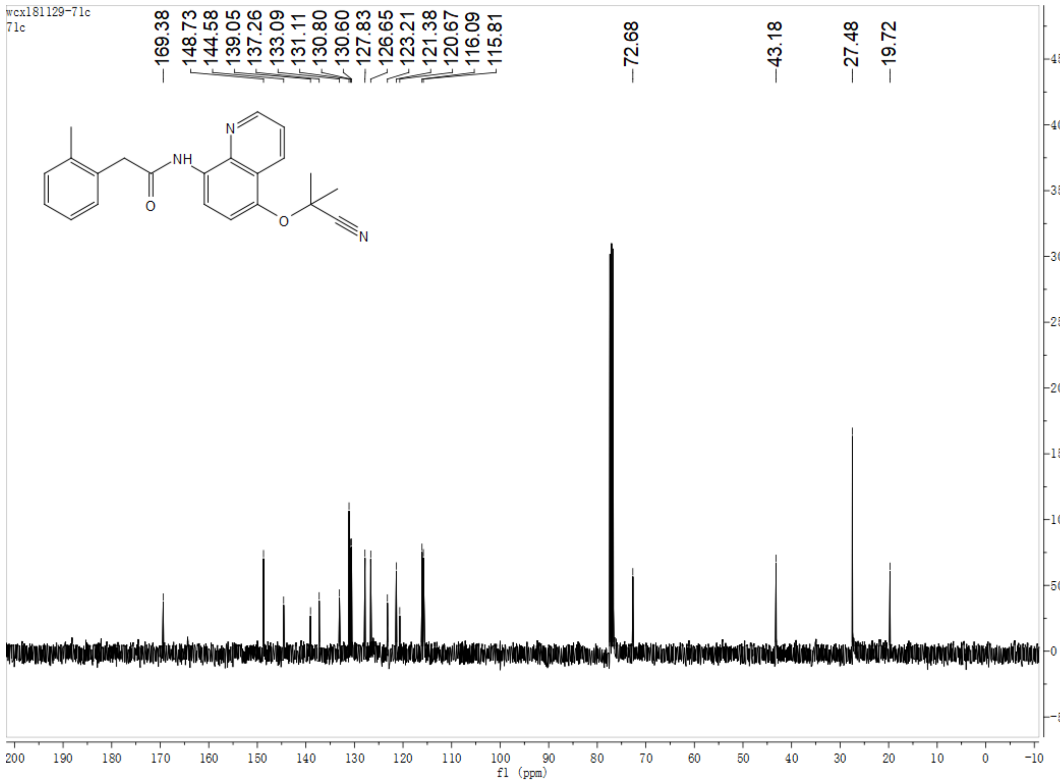

wcx181029-94h
2h
9.78
8.72
8.71
8.70
8.41
8.40
8.39
8.38
7.47
7.45
7.43
7.42
7.40
7.38
7.34
7.33
7.31
O
NH
N
N
1.00
2.07
1.05
6.08
1.09
f1 (ppm)


169.47
148.73
144.61
139.01
134.62
131.18
131.13
129.53
129.00
127.38
123.23
121.43
120.68
116.02
115.85
72.68
45.27
27.46
N
NH
O
CH_3
CH_3
O
N
f1 (ppm)

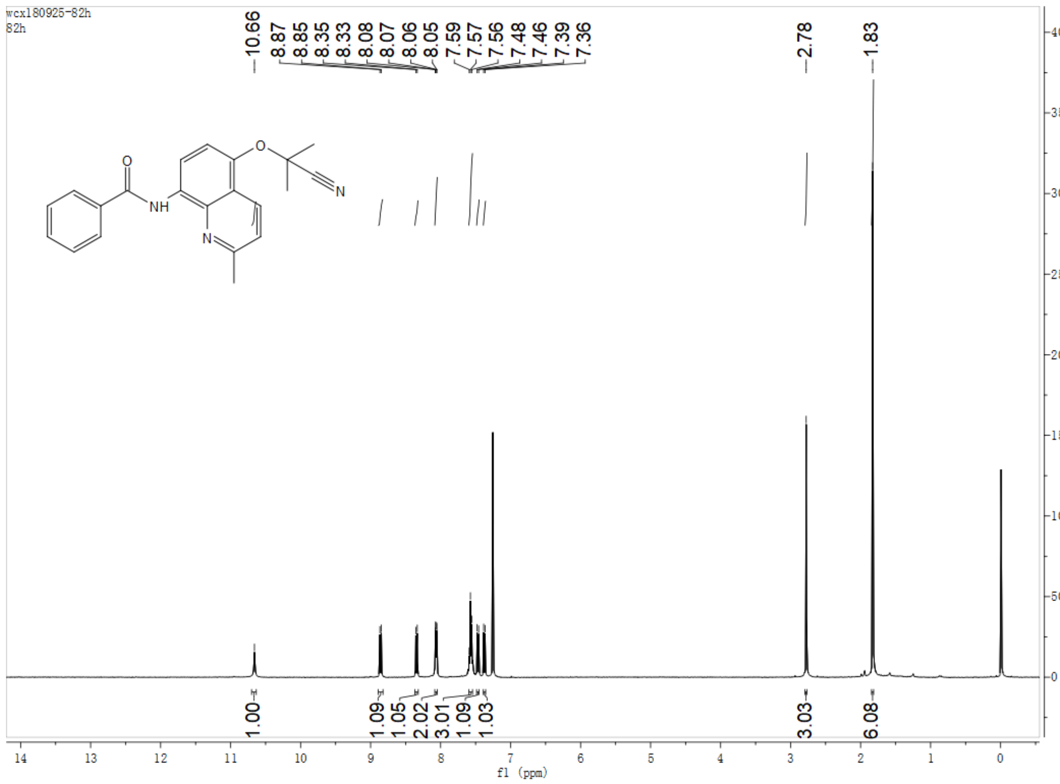
2s:

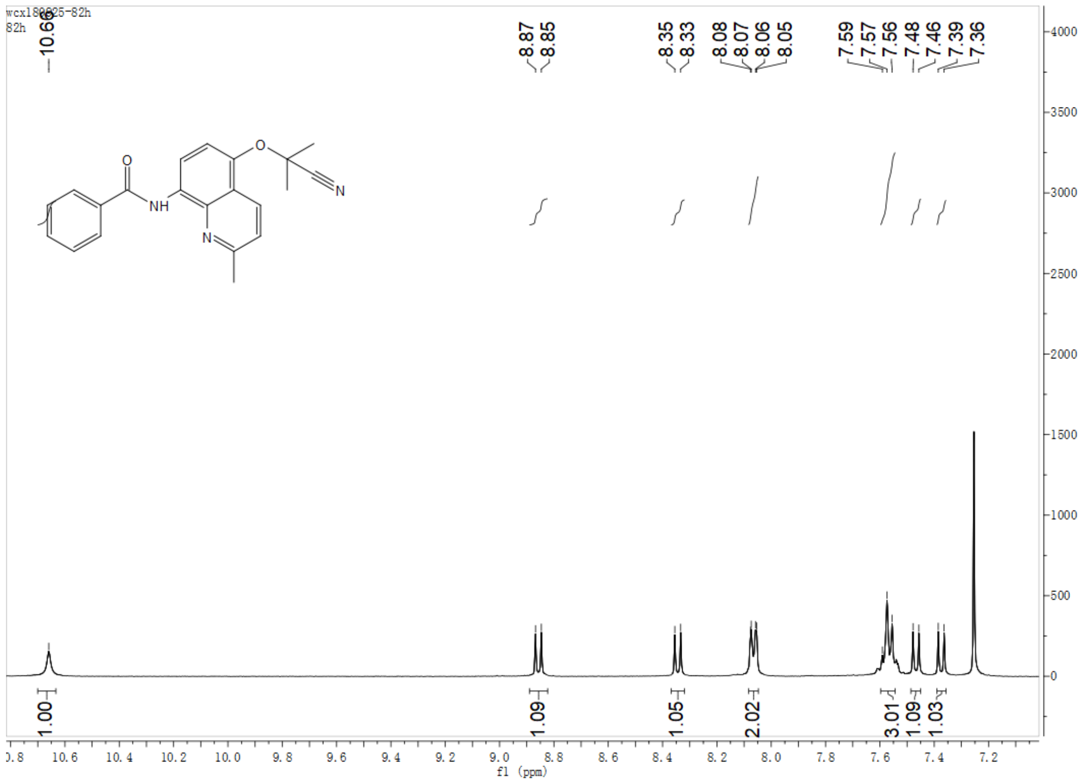


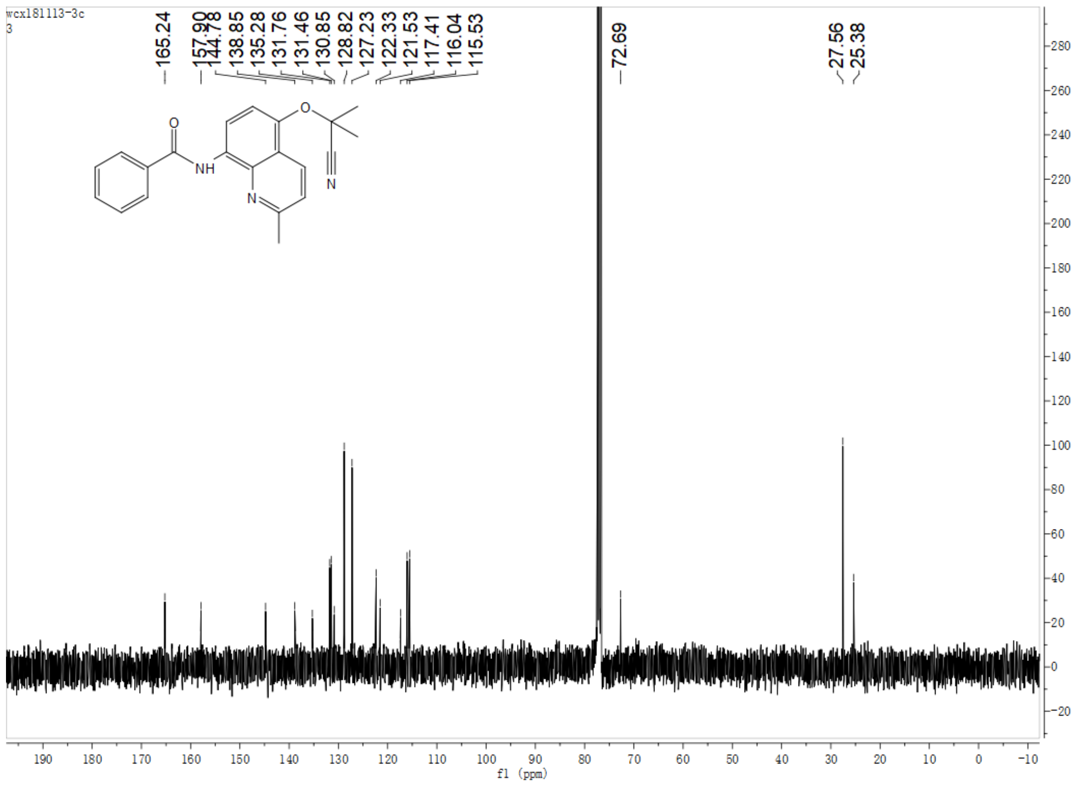




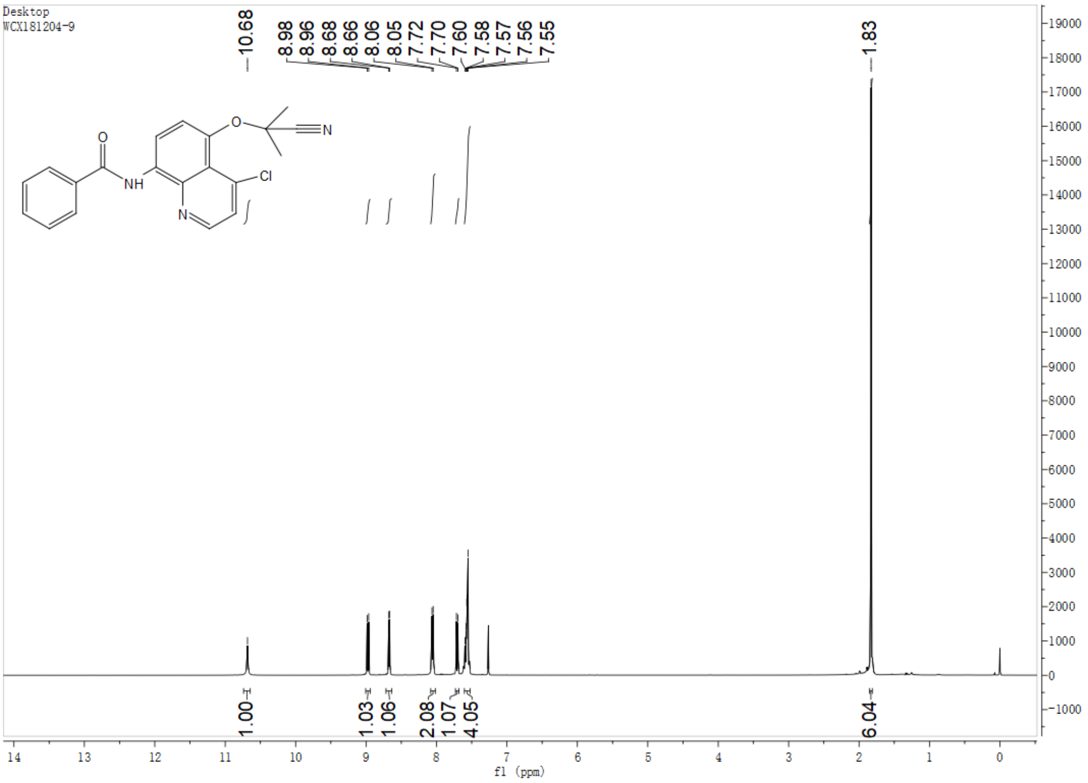
2t:

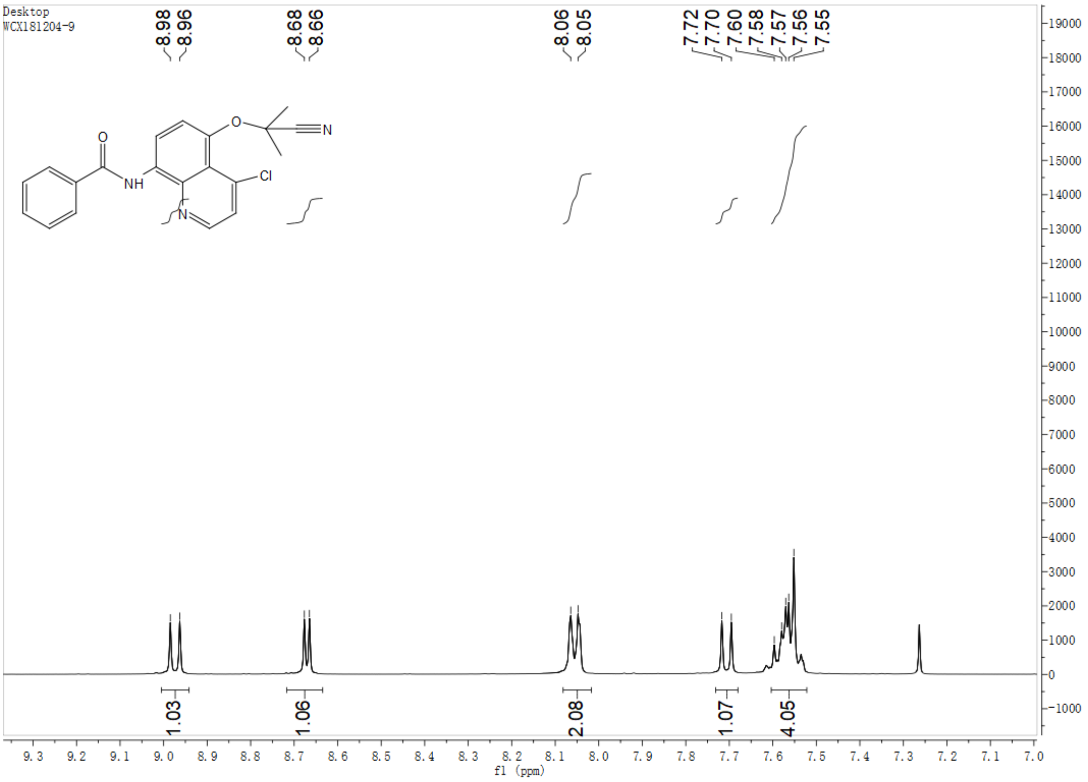


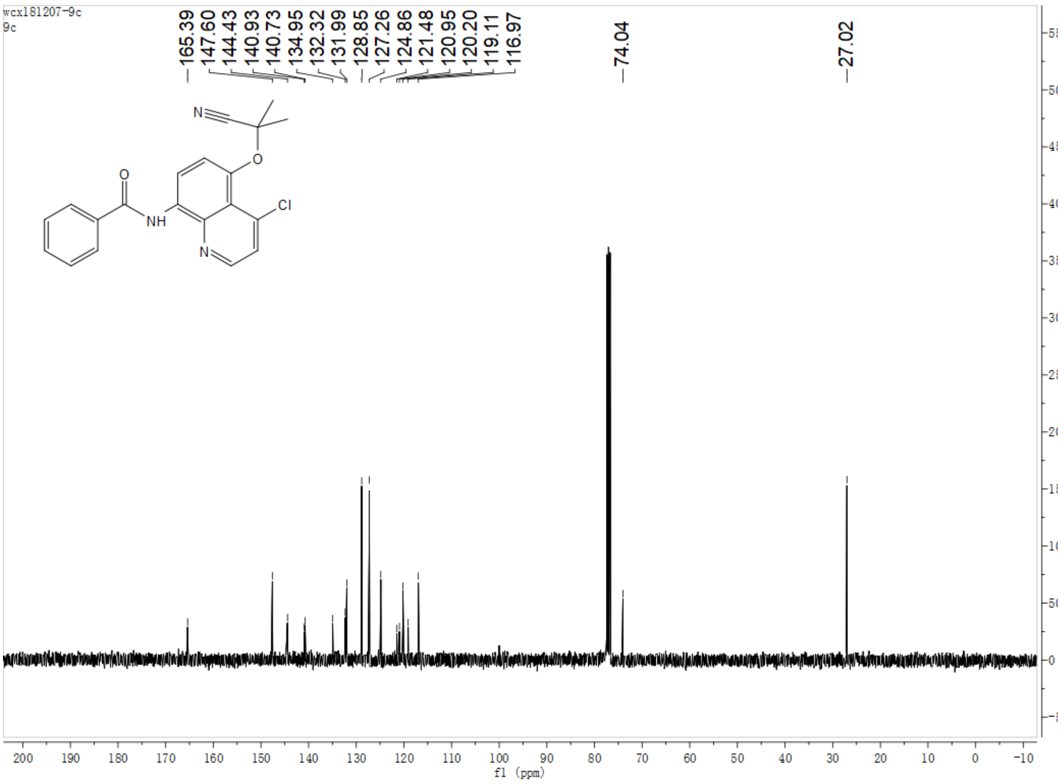




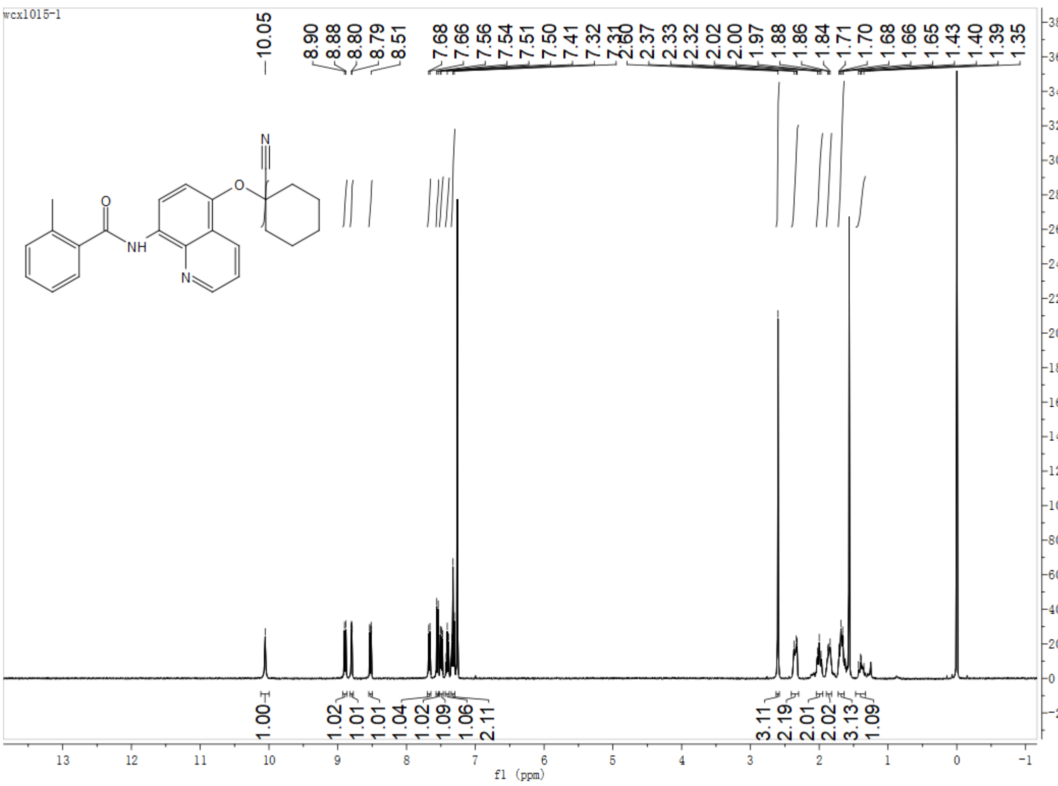
2u:

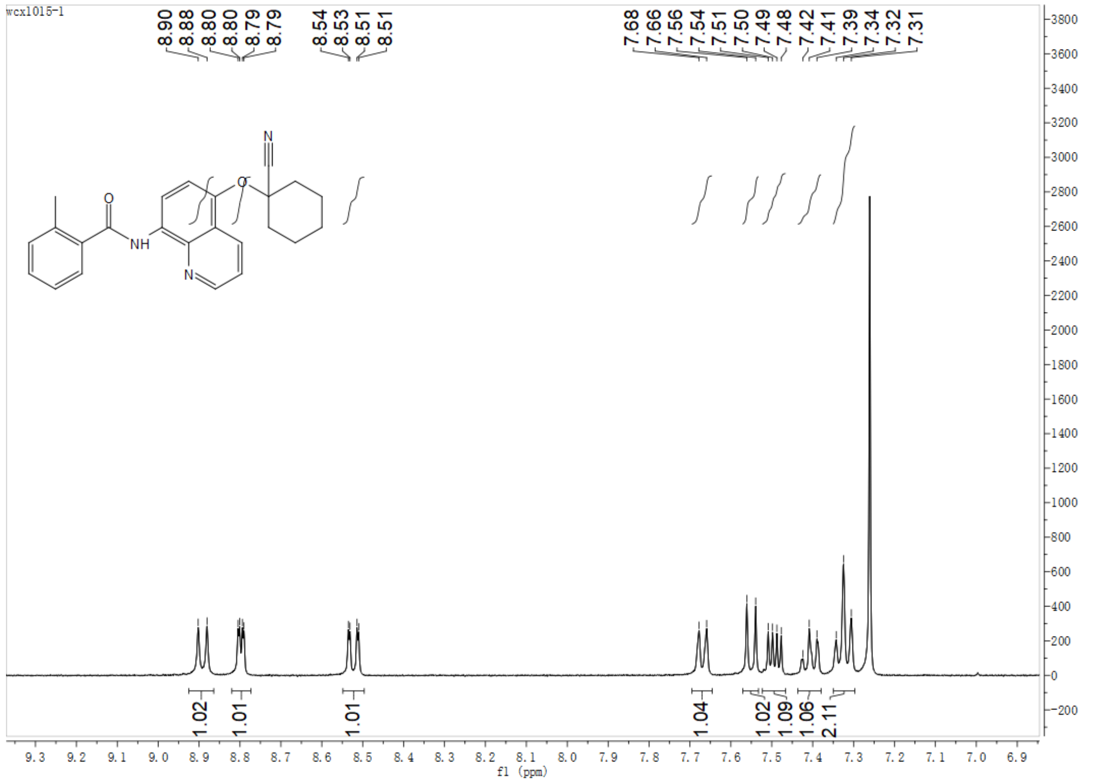

Desktop
WCX181204-9
10.68
8.98 8.96 8.68 8.66 8.06 8.05 7.72 7.70 7.60 7.58 7.57 7.56 7.55
1.83
O
NH
N
O
N
Cl
1.00
1.03
1.06
2.08
1.07
4.05
6.04
f1 (ppm)

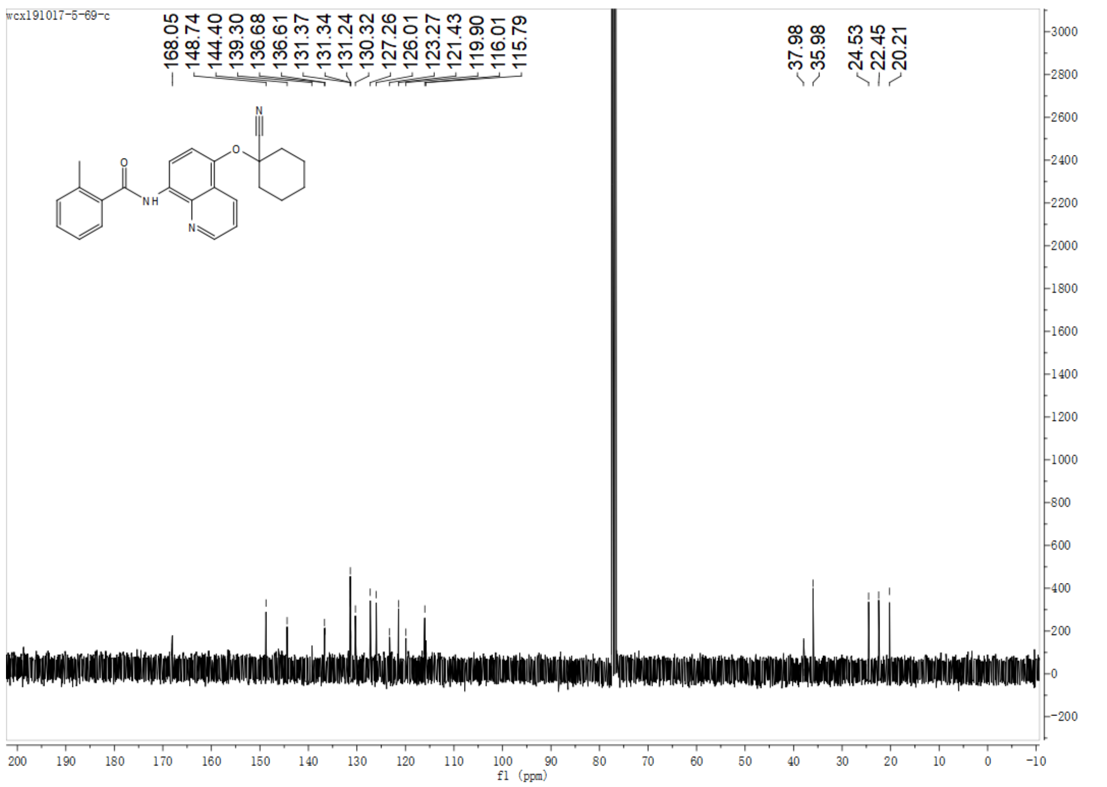

Desktop
WCX181204-9
8.98 8.96
8.68 8.66
8.06 8.05
7.72 7.70 7.60 7.58 7.57 7.56 7.55
O
NH
N
O
N
Cl
1.03
1.06
2.08
1.07
4.05
f1 (ppm)



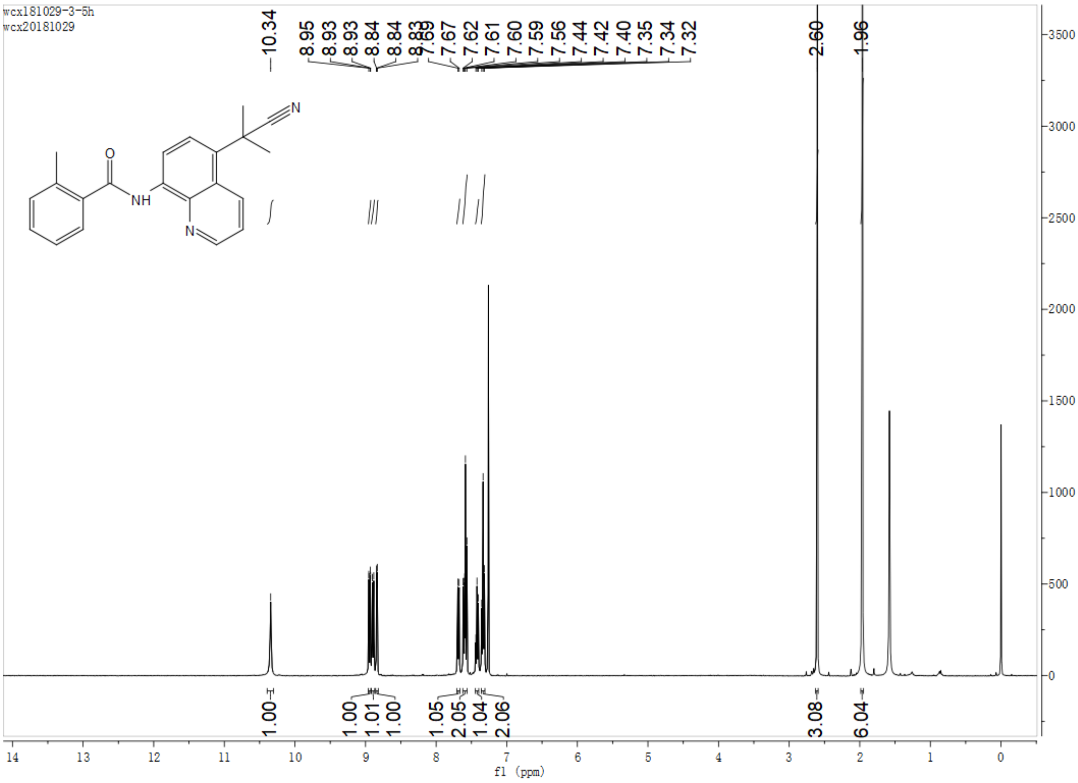
2v:

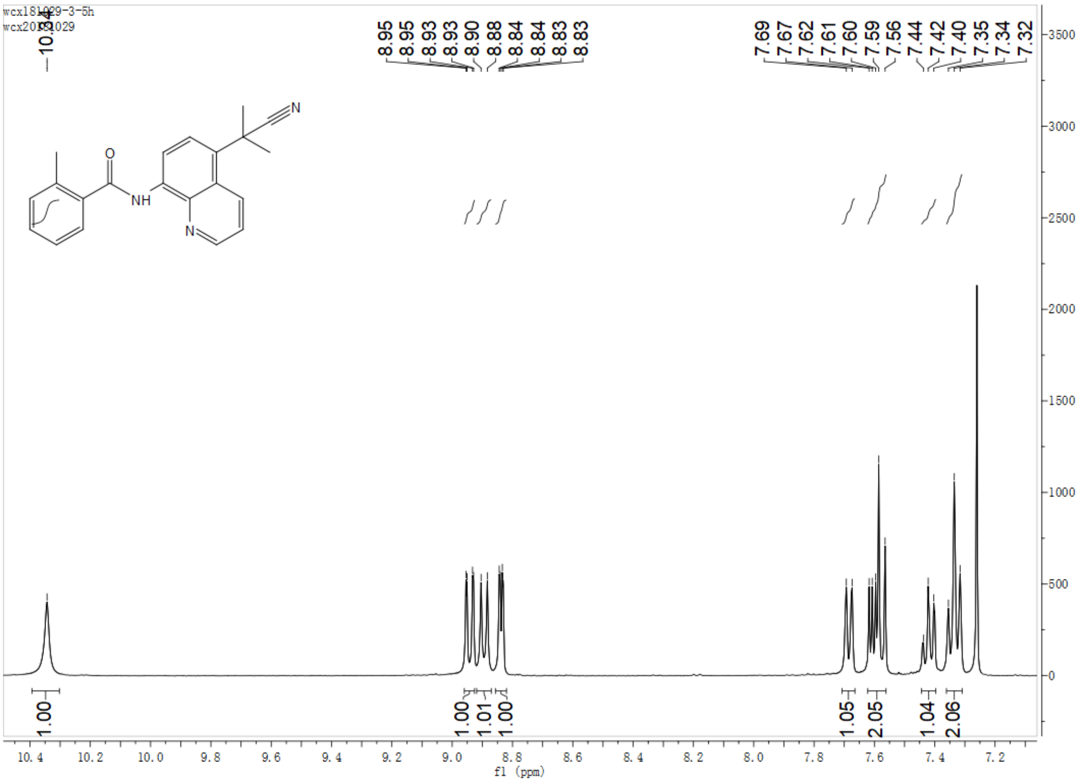


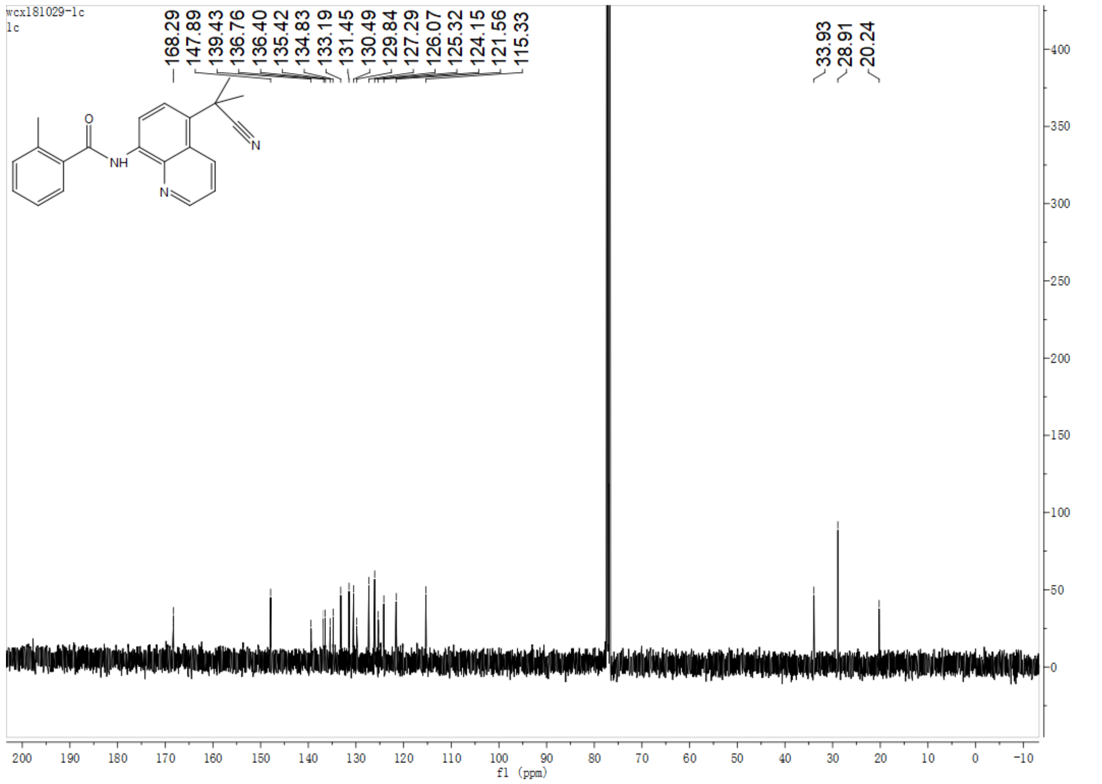

wcx1015-1
8.90 8.88 8.80 8.80 8.79 8.79
8.54 8.53 8.51 8.51
7.68 7.66 7.56 7.54 7.51 7.50 7.49 7.48 7.42 7.41 7.39 7.34 7.32 7.31
1.02 1.01 1.01 1.04 1.02 1.09 1.06 2.11
fl (ppm)


wcx191017-5-69-c
168.05 148.74 144.40 139.30 136.68 136.61 131.37 131.34 131.24 130.32 127.26 126.01 123.27 121.43 119.90 116.01 115.79
37.98 35.98 24.53 22.45 20.21
fl (ppm)

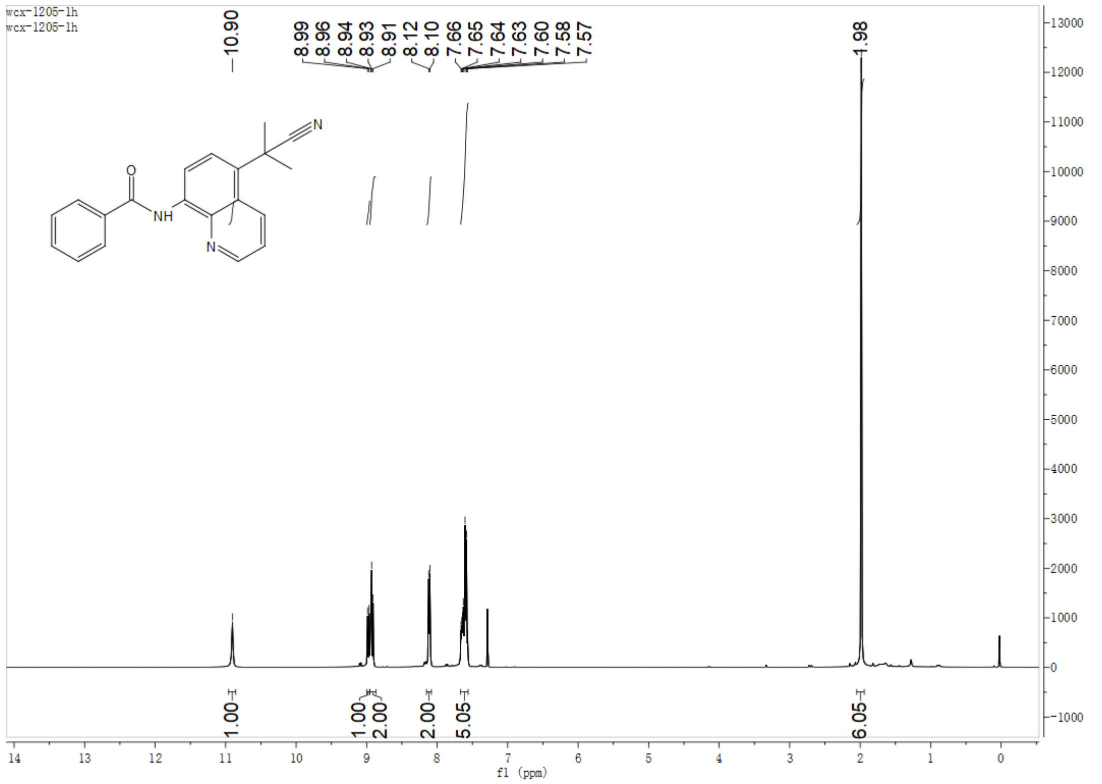
3a:

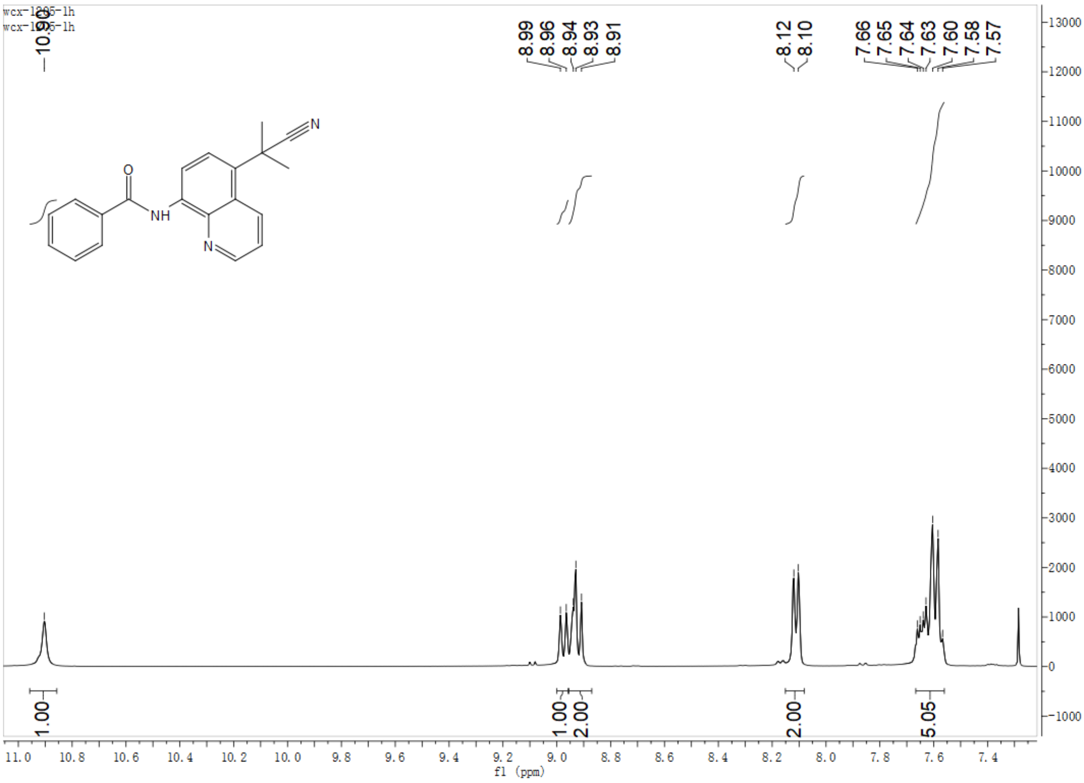


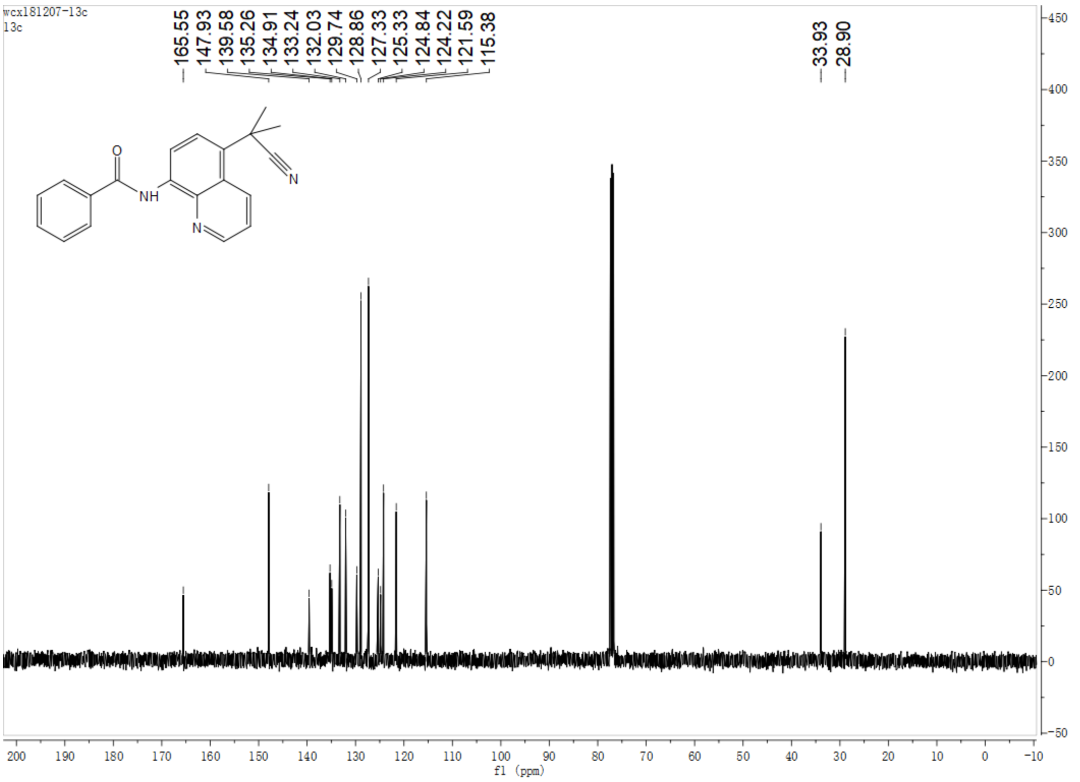



wcx181029-1c
1c
168.29
147.89
139.43
136.76
136.40
135.42
134.83
133.19
131.45
130.49
129.84
127.29
126.07
125.32
124.15
121.56
115.33
33.93
28.91
20.24
f1 (ppm)

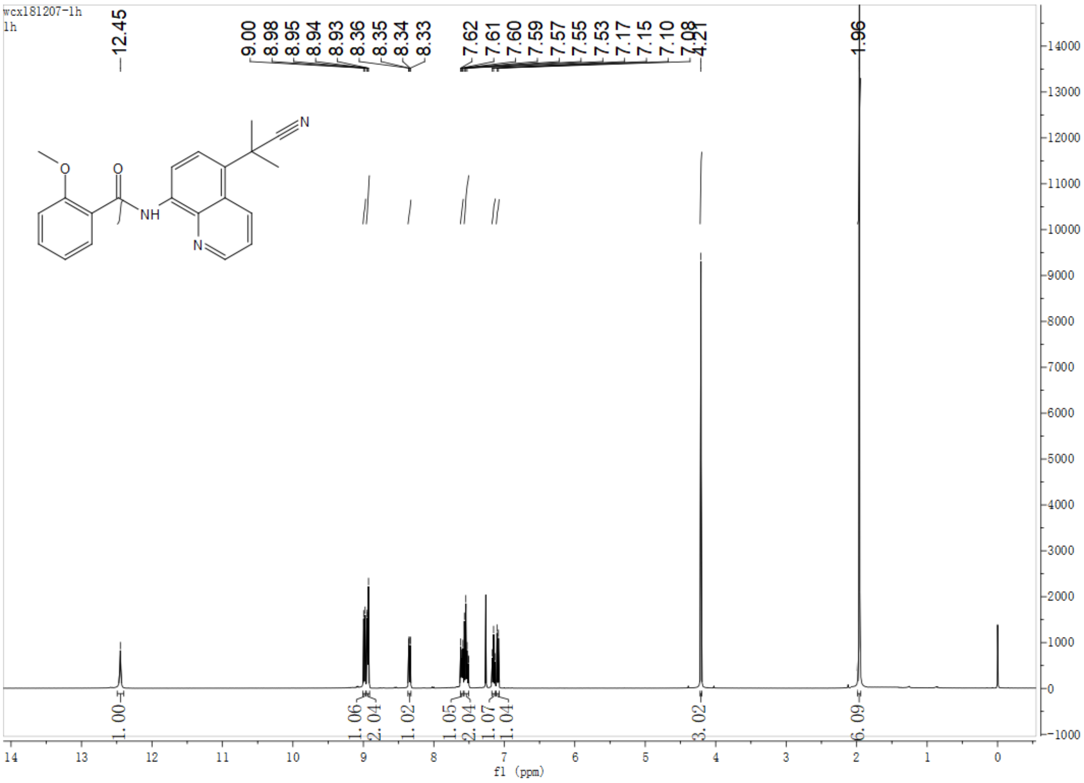
3b:

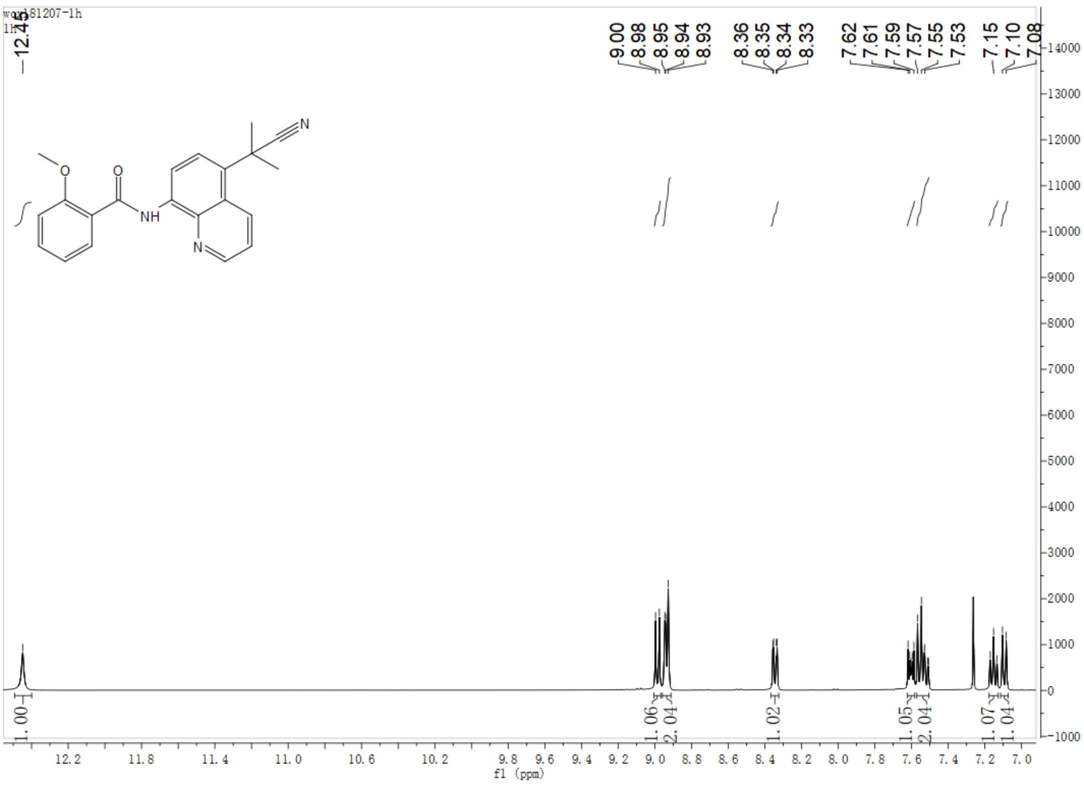

wcx-1205-1h
wcx-1205-1h
10.90
8.99
8.96
8.94
8.93
8.91
8.12
8.10
7.66
7.65
7.64
7.63
7.60
7.58
7.57
1.98
1.00
1.00
2.00
2.00
5.05
6.05
f1 (ppm)

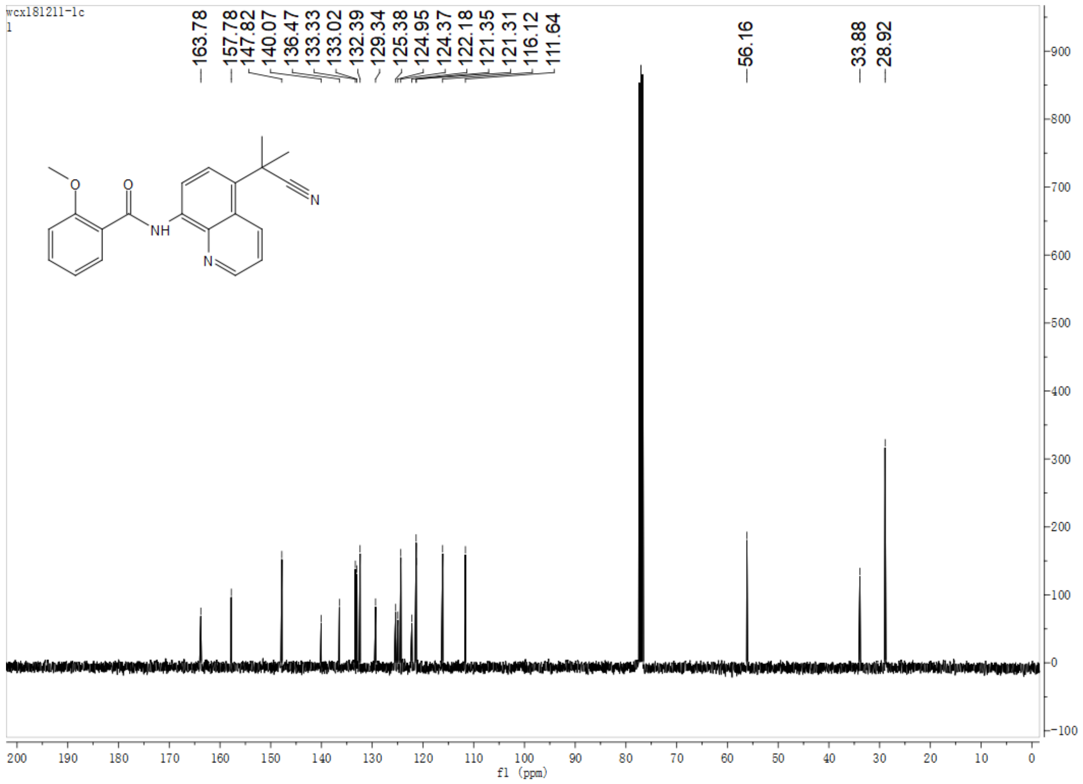




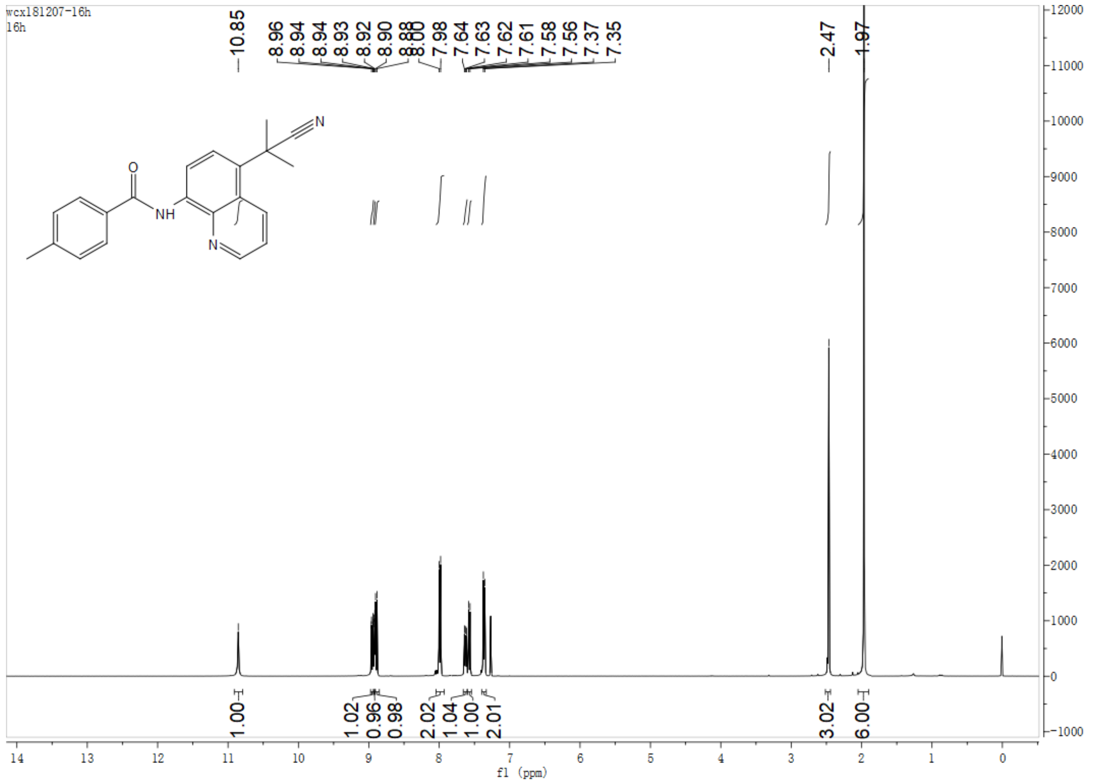
3c:

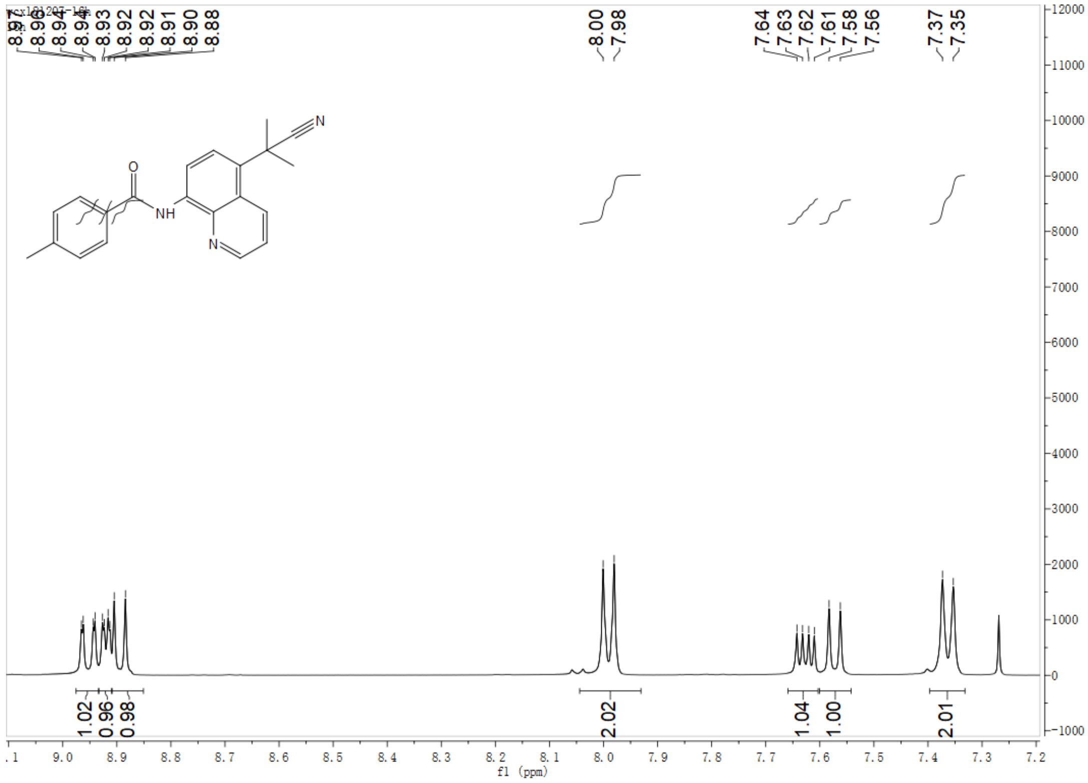

wcx181207-1h
1h
12.45
9.00
8.98
8.95
8.94
8.93
8.36
8.35
8.34
8.33
7.62
7.61
7.60
7.59
7.57
7.55
7.53
7.17
7.15
7.10
7.08
4.21
1.96
N
O
O
NH
N
1.00
1.06
2.04
1.02
1.05
2.04
1.07
1.04
3.02
6.09
fl (ppm)

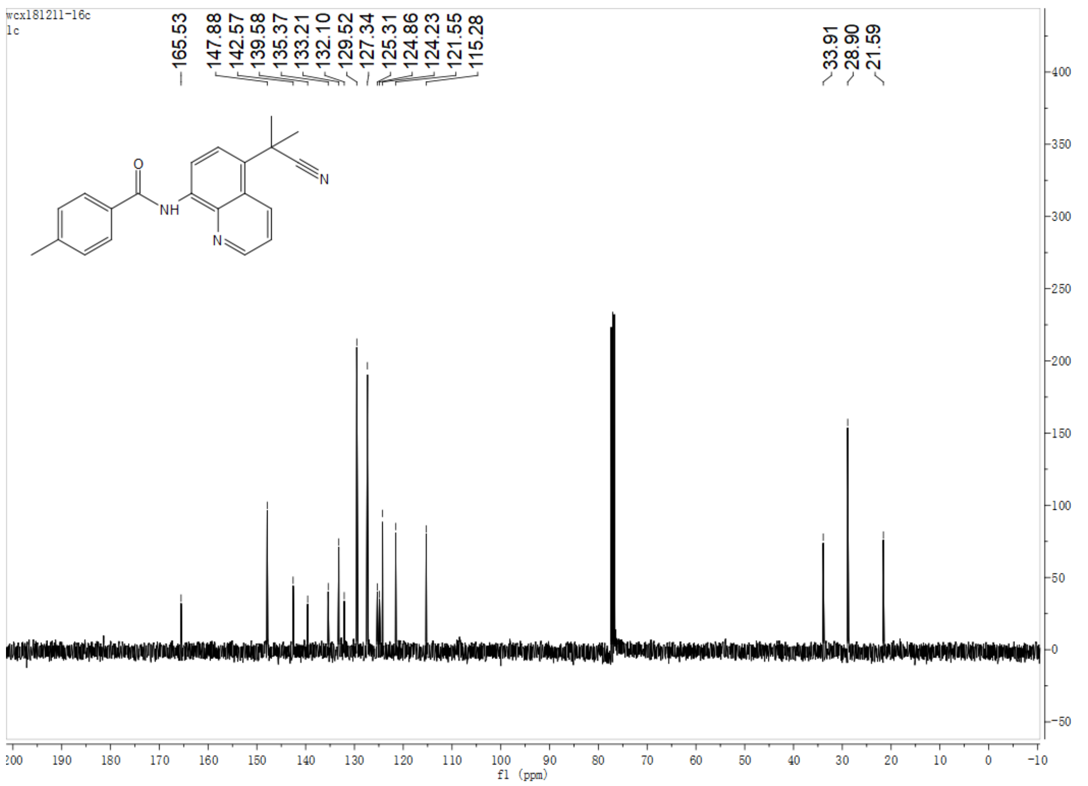

wcx181207-1h
1h
12.45
9.00
8.98
8.95
8.94
8.93
8.36
8.35
8.34
8.33
7.62
7.61
7.59
7.57
7.55
7.53
7.15
7.10
7.08
N
O
O
NH
N
1.00
1.06
2.04
1.02
1.05
2.04
1.07
1.04
fl (ppm)


wcx181211-1c
1
163.78
157.78
147.82
140.07
136.47
133.33
133.02
132.39
129.34
125.38
124.95
124.37
122.18
121.35
121.31
116.12
111.64
56.16
33.88
28.92
O
NH
N
f1 (ppm)

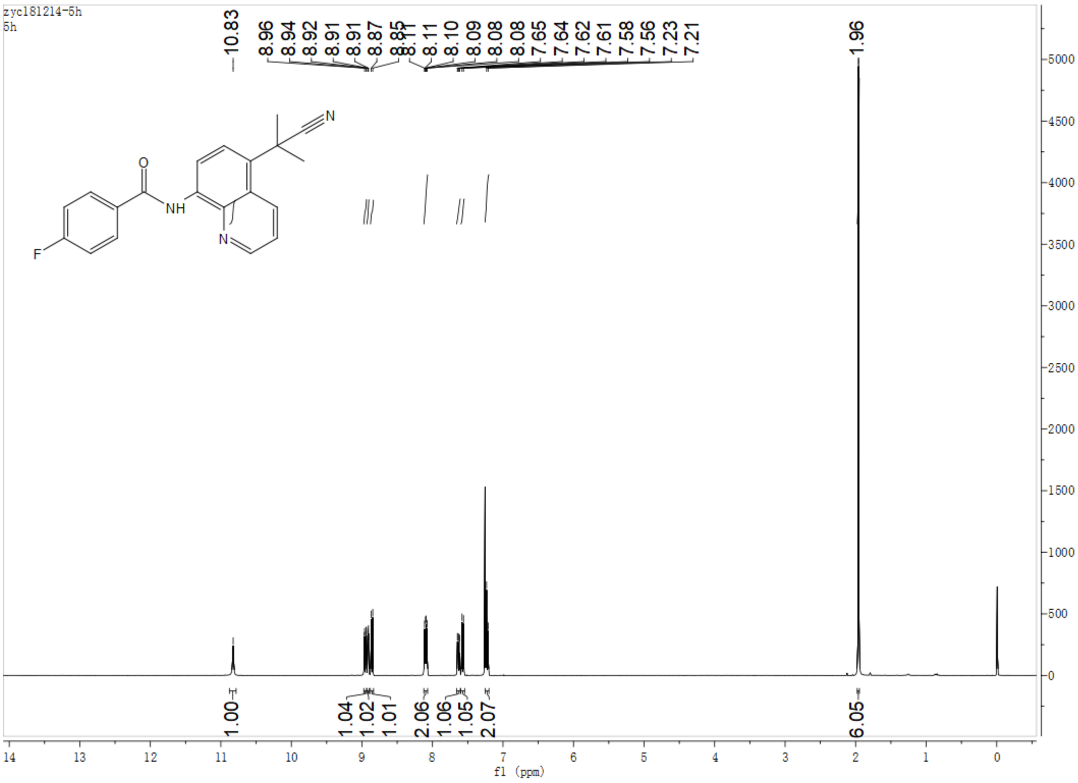
3d:

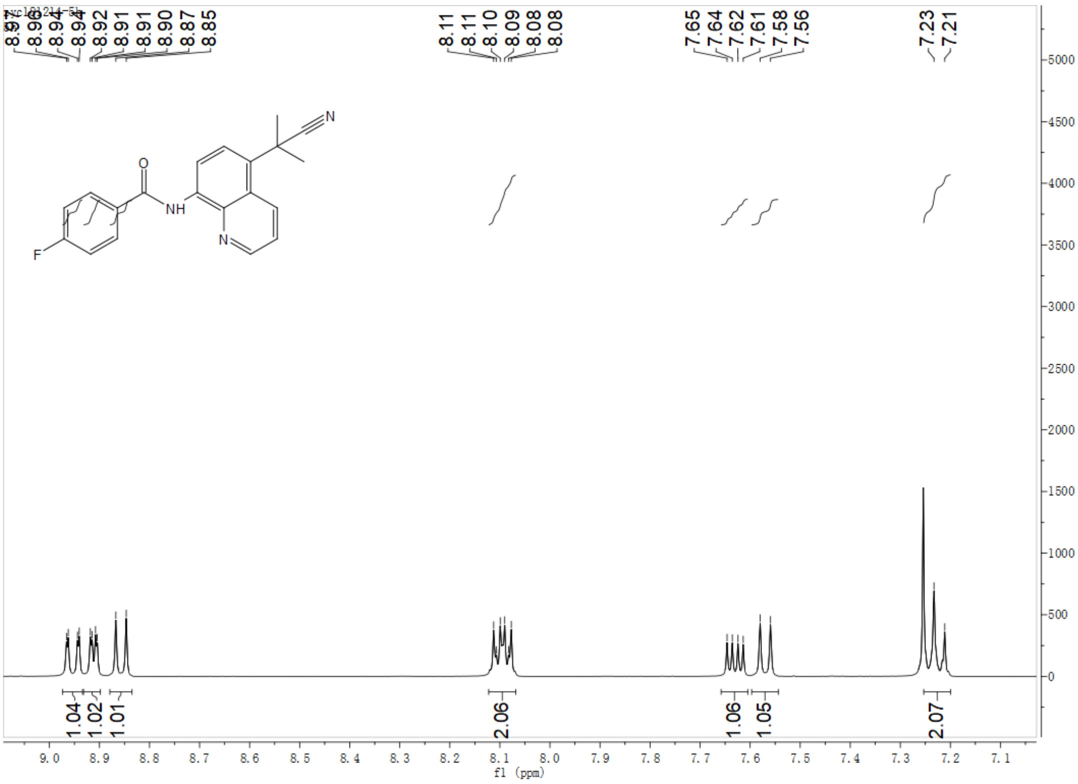

wcx181207-16h
16h
10.85
8.96
8.94
8.94
8.93
8.92
8.90
8.88
8.00
7.98
7.64
7.63
7.62
7.61
7.58
7.56
7.37
7.35
2.47
1.97
O
NH
N
1.00
1.02
0.96
0.98
2.02
1.04
1.00
2.01
3.02
6.00
f1 (ppm)

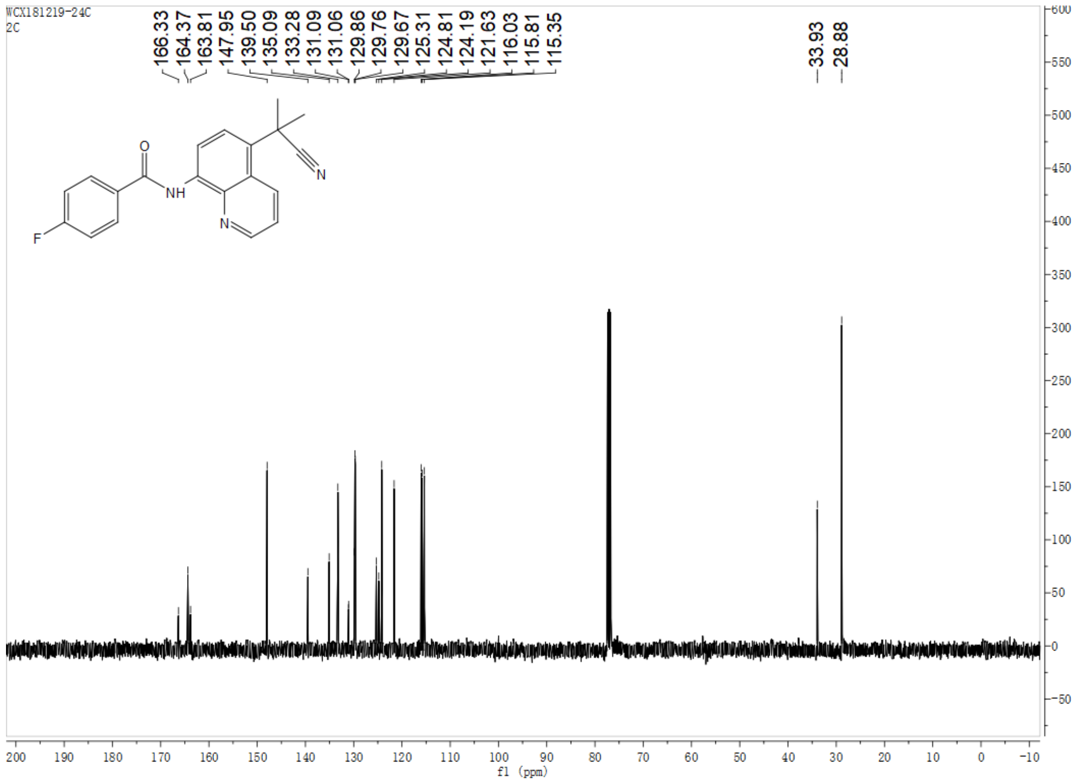




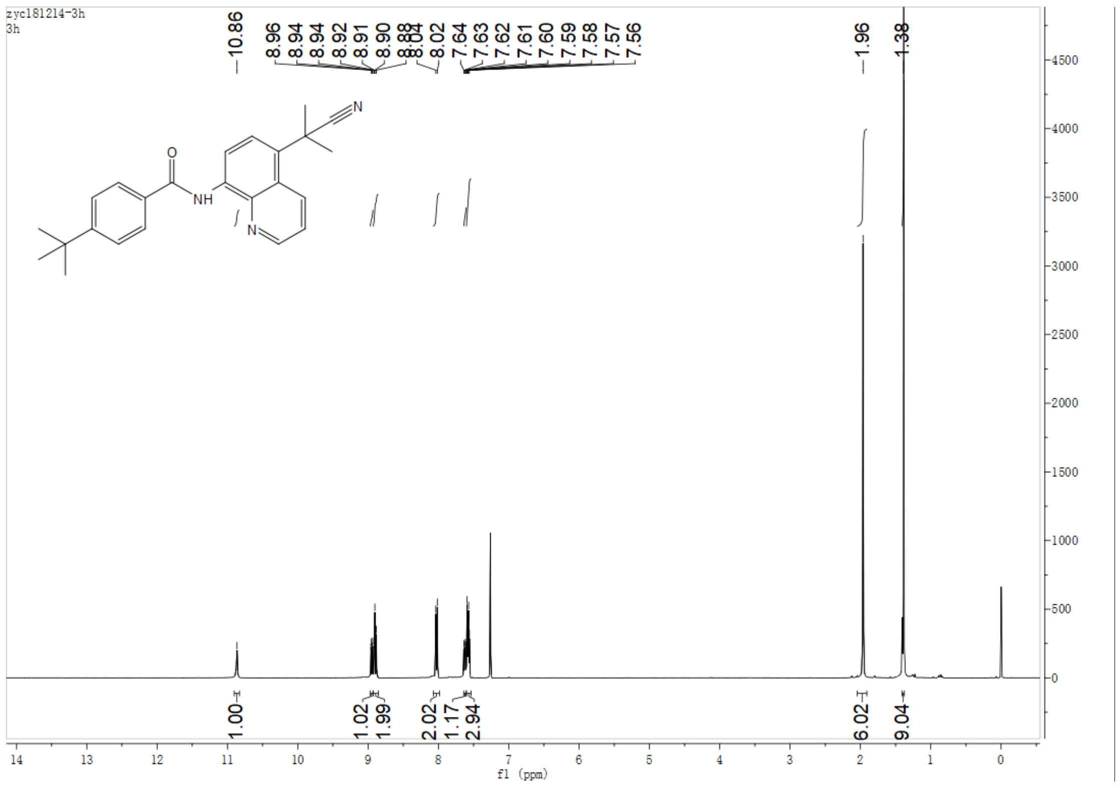
3e:

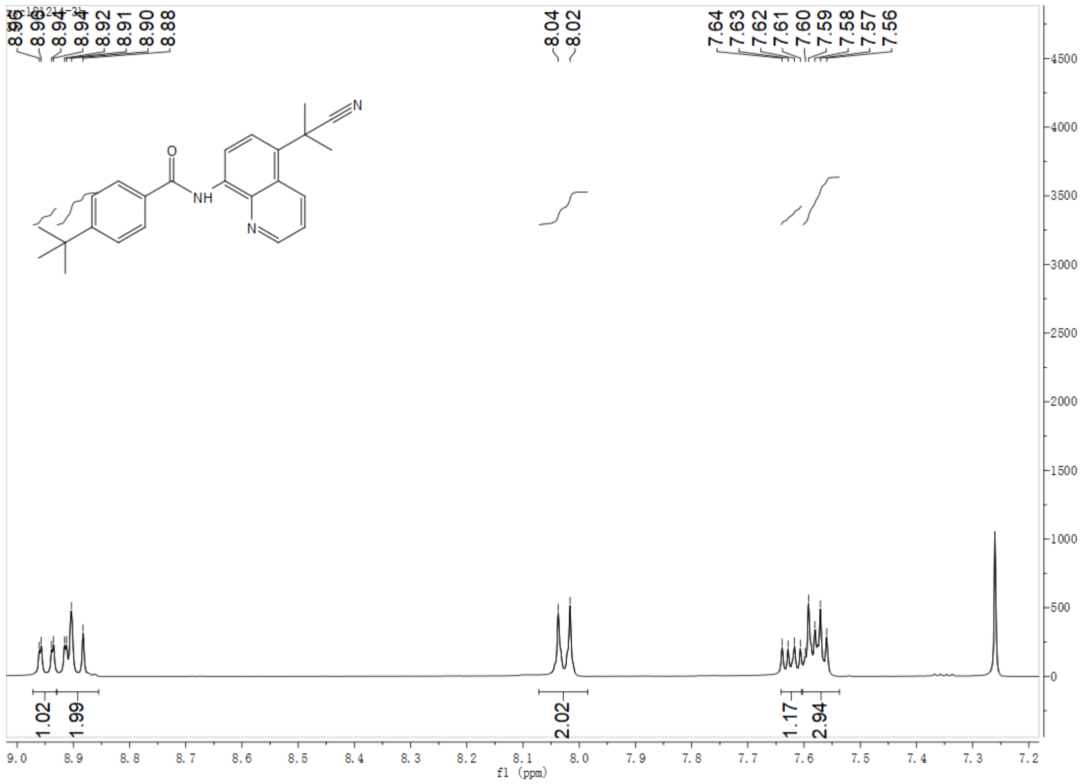


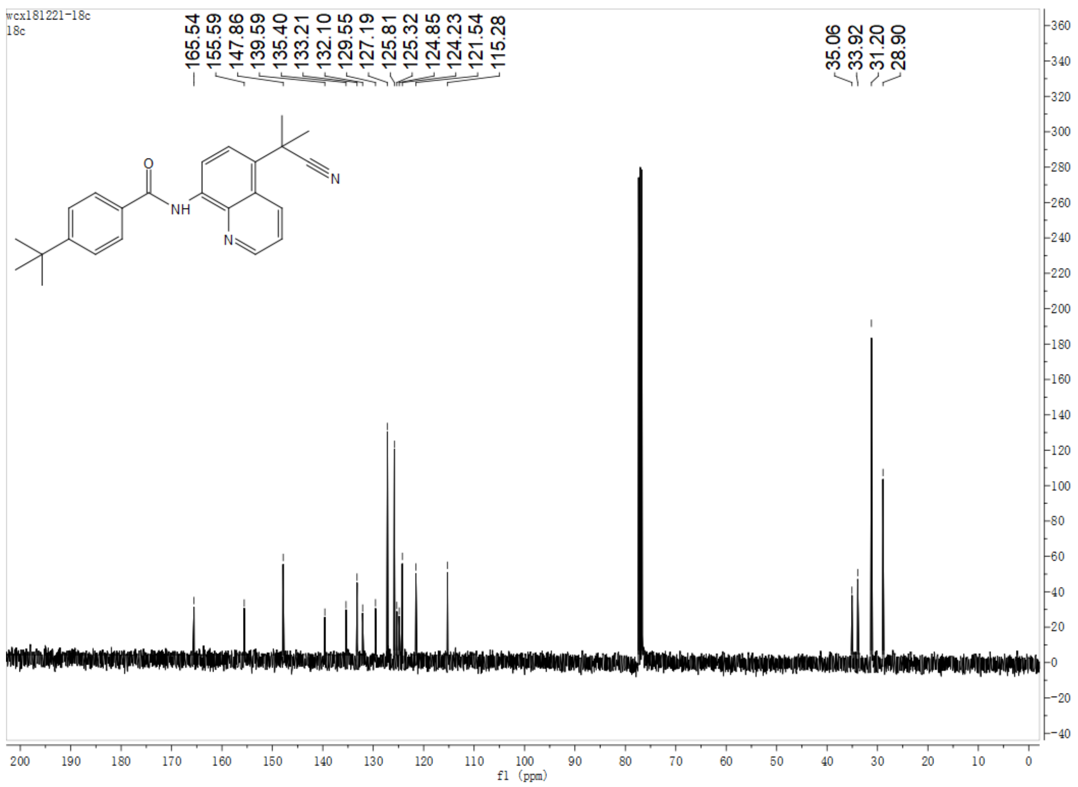



WCX181219-24C
2C
166.33
164.37
163.81
147.95
139.50
135.09
133.28
131.09
131.06
129.86
129.76
129.67
125.31
124.81
124.19
121.63
116.03
115.81
115.35
33.93
28.88
O
NH
N
F
N
f1 (ppm)

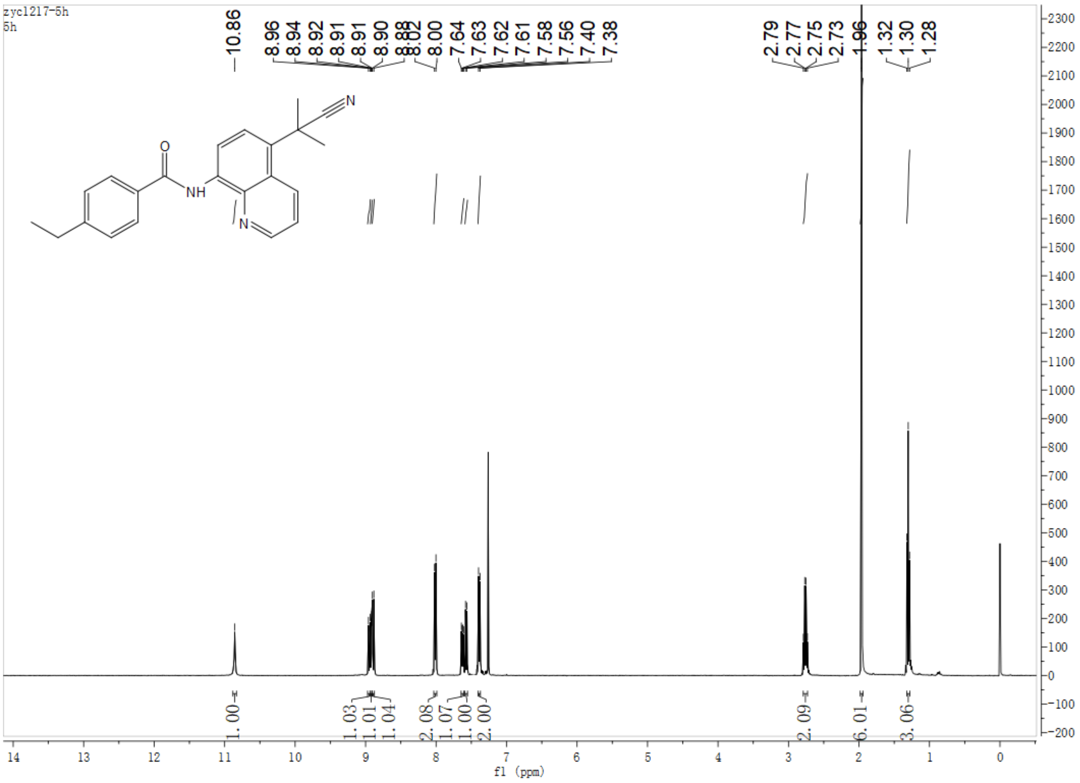
3f:

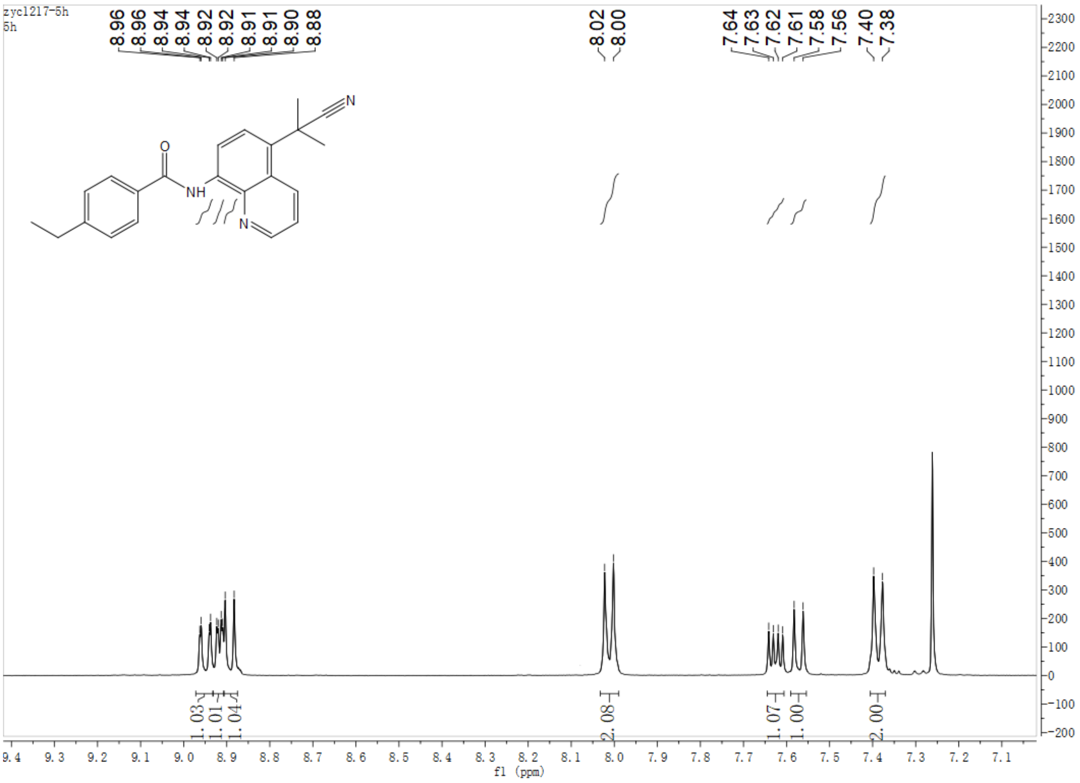

zyc181214-3h
3h
10.86
8.96
8.94
8.94
8.92
8.91
8.90
8.88
8.04
8.02
7.64
7.63
7.62
7.61
7.60
7.59
7.58
7.57
7.56
1.96
1.38
N
O
NH
N
1.00
1.02
1.99
2.02
1.17
2.94
6.02
9.04
f1 (ppm)

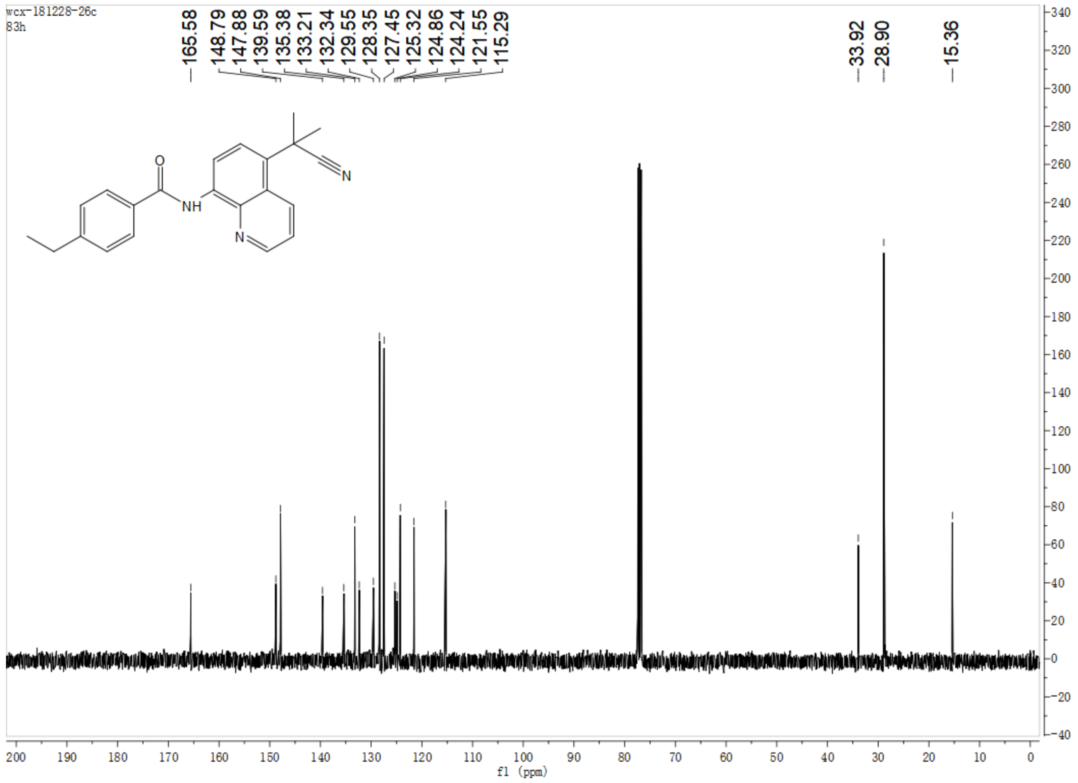




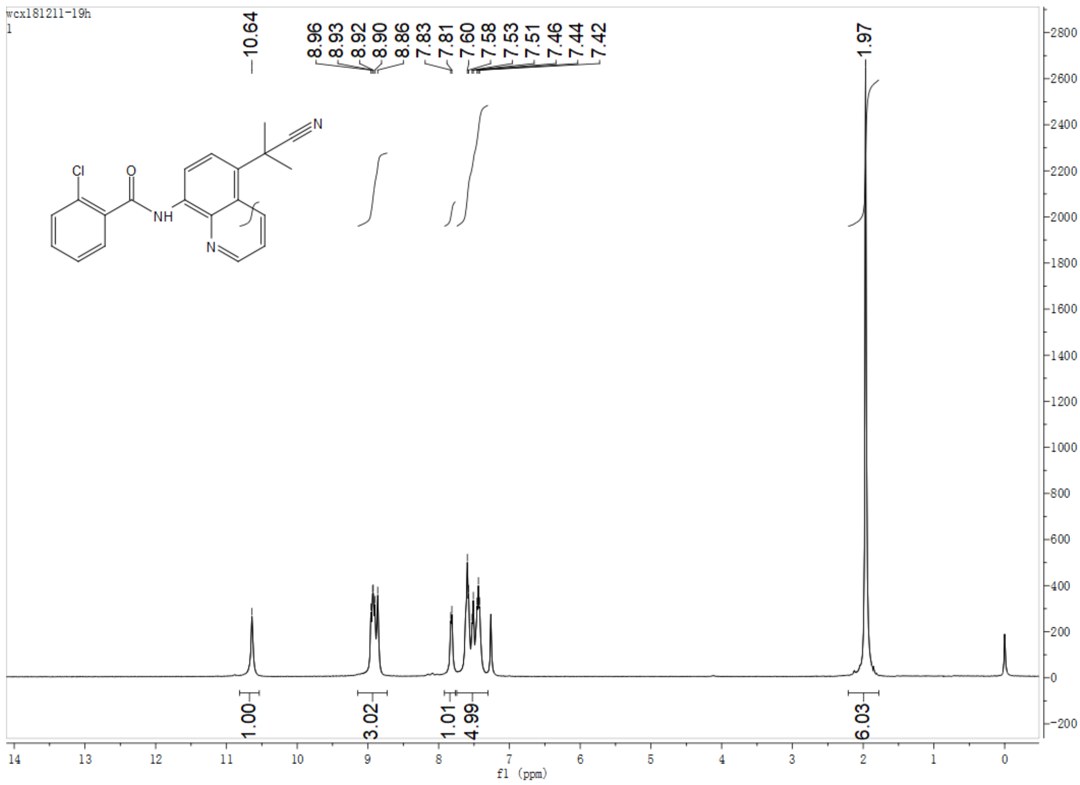
3g:

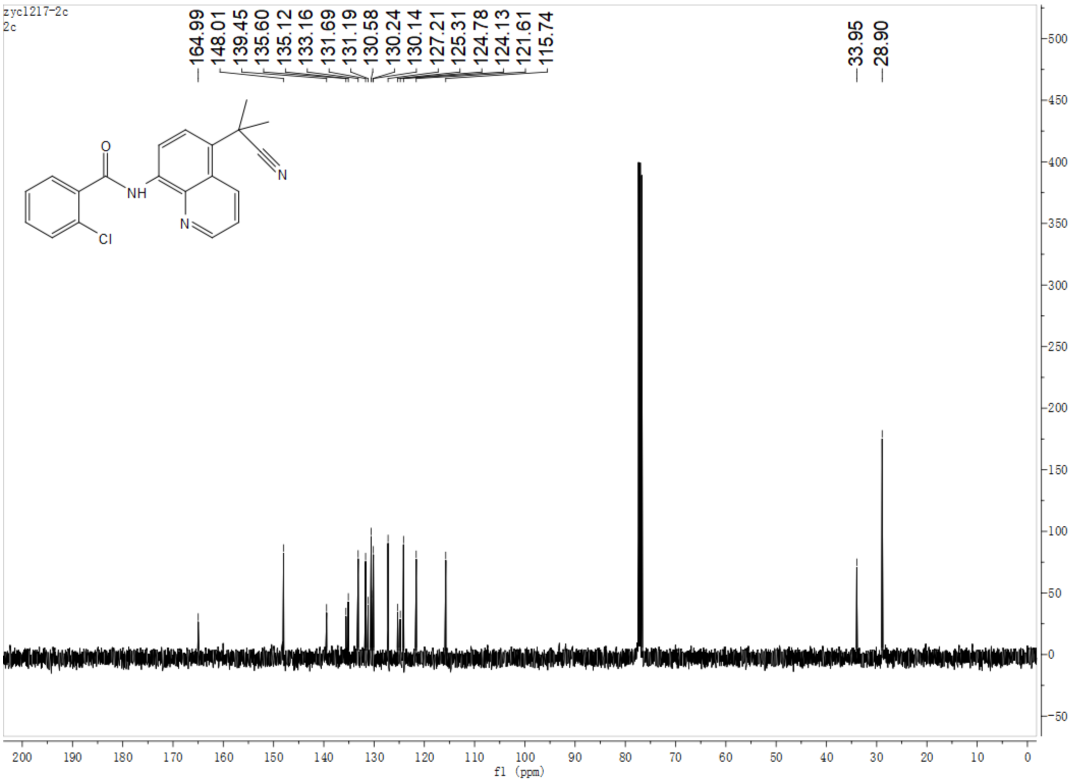




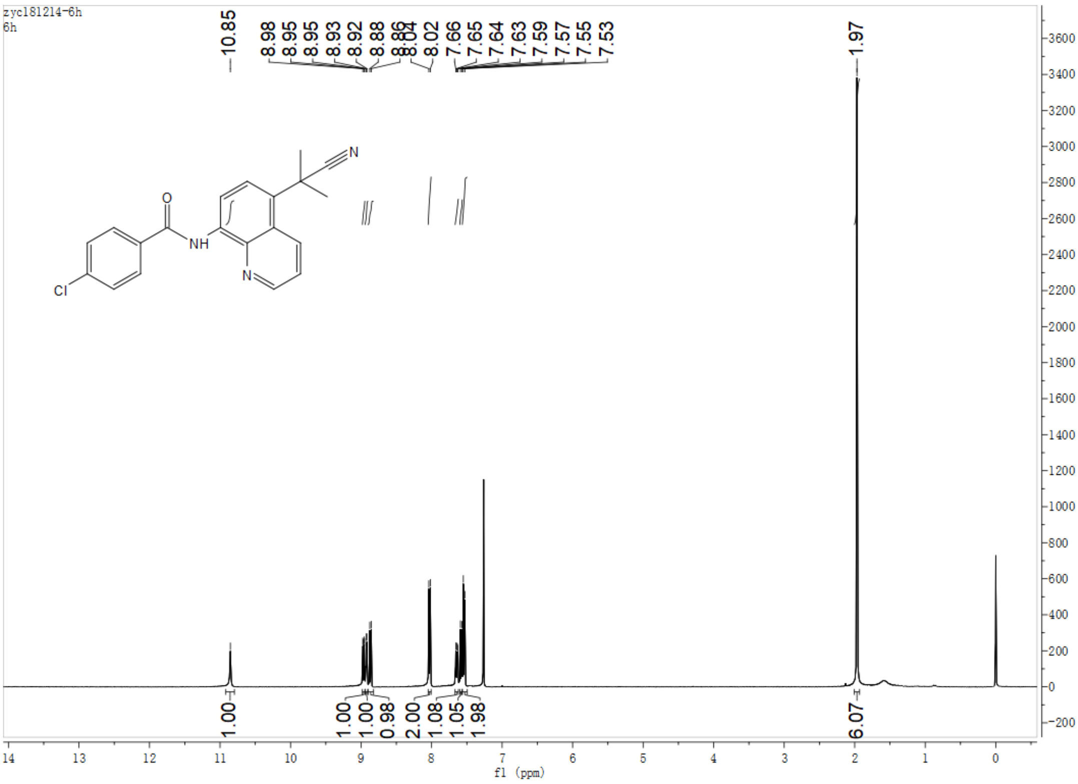

wcx-181228-26c
83h
165.58
148.79
147.88
139.59
135.38
133.21
132.34
129.55
128.35
127.45
125.32
124.86
124.24
121.55
115.29
33.92
28.90
15.36
O
NH
N
N
f1 (ppm)

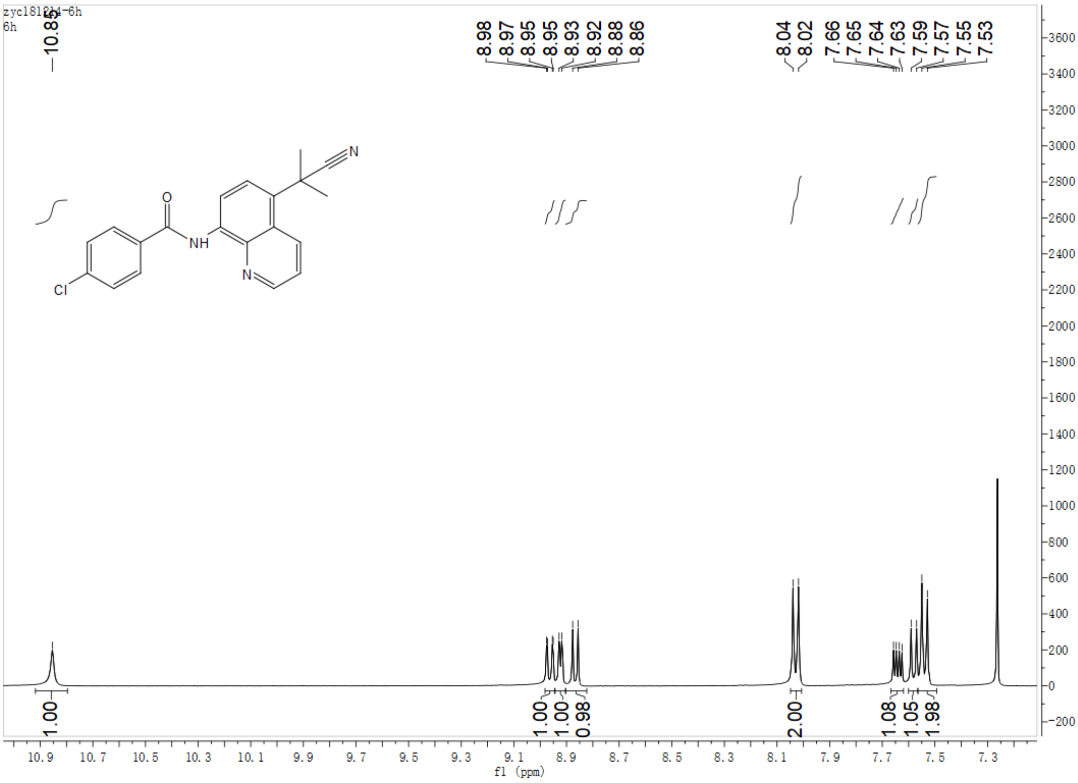
3h:

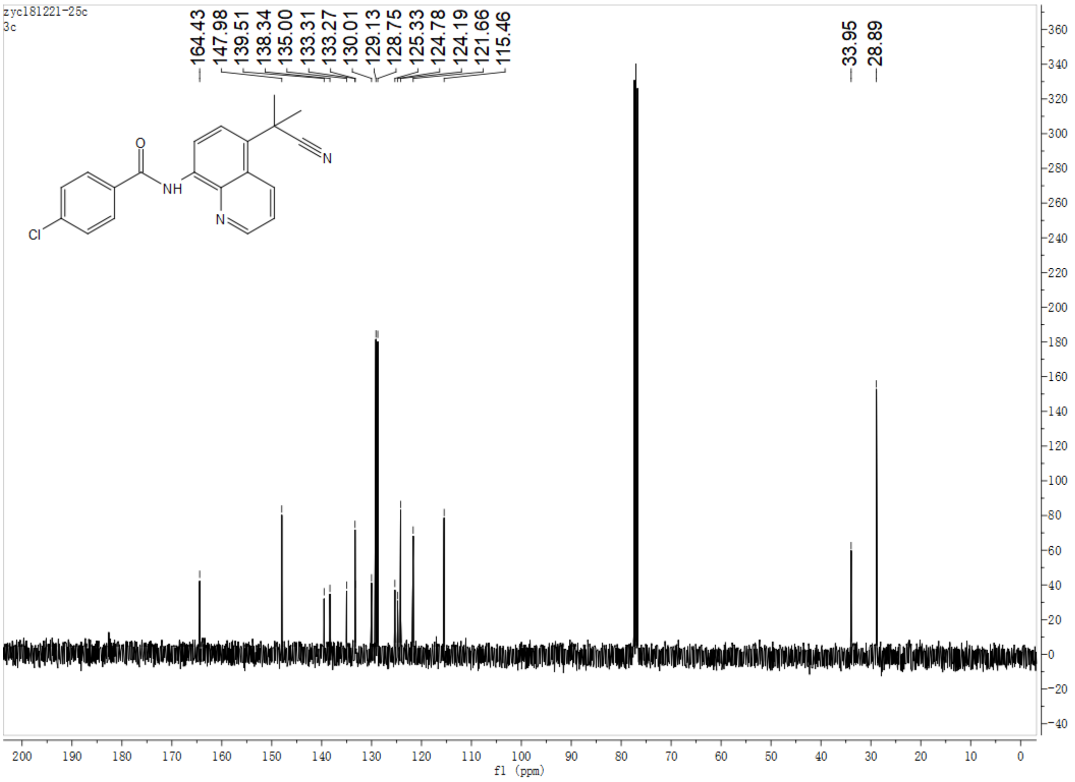

wcx181211-19h
1
10.64
8.96
8.93
8.92
8.90
8.86
7.83
7.81
7.60
7.58
7.53
7.51
7.46
7.44
7.42
1.97
Cl
O
NH
N
N
1.00
3.02
1.01
4.99
6.03
f1 (ppm)


zyc1217-2c
2c
164.99
148.01
139.45
135.60
135.12
133.16
131.69
131.19
130.58
130.24
130.14
127.21
125.31
124.78
124.13
121.61
115.74
33.95
28.90
f1 (ppm)

3i:


zyc181214-6h
6h
10.85
8.98
8.95
8.95
8.93
8.92
8.88
8.86
8.04
8.02
7.66
7.65
7.64
7.63
7.59
7.57
7.55
7.53
1.97
1.00
1.00
1.00
0.98
2.00
1.08
1.05
1.98
6.07
f1 (ppm)


zyc181214-6h
6h
10.85
8.98
8.97
8.95
8.93
8.92
8.88
8.86
8.04
8.02
7.66
7.65
7.64
7.63
7.59
7.57
7.55
7.53
1.00
1.00
1.00
0.98
2.00
1.08
1.05
1.98
O
NH
N
N
Cl
f1 (ppm)


zyc181221-25c
3c
164.43
147.98
139.51
138.34
135.00
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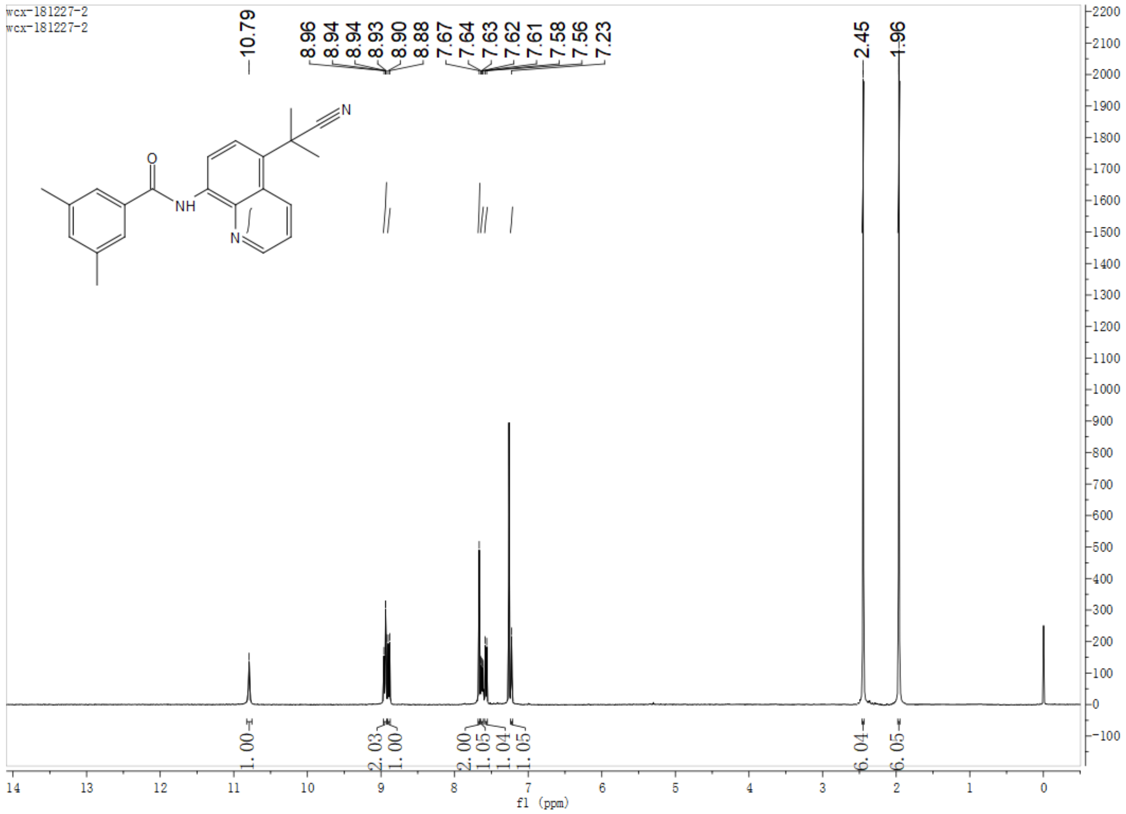
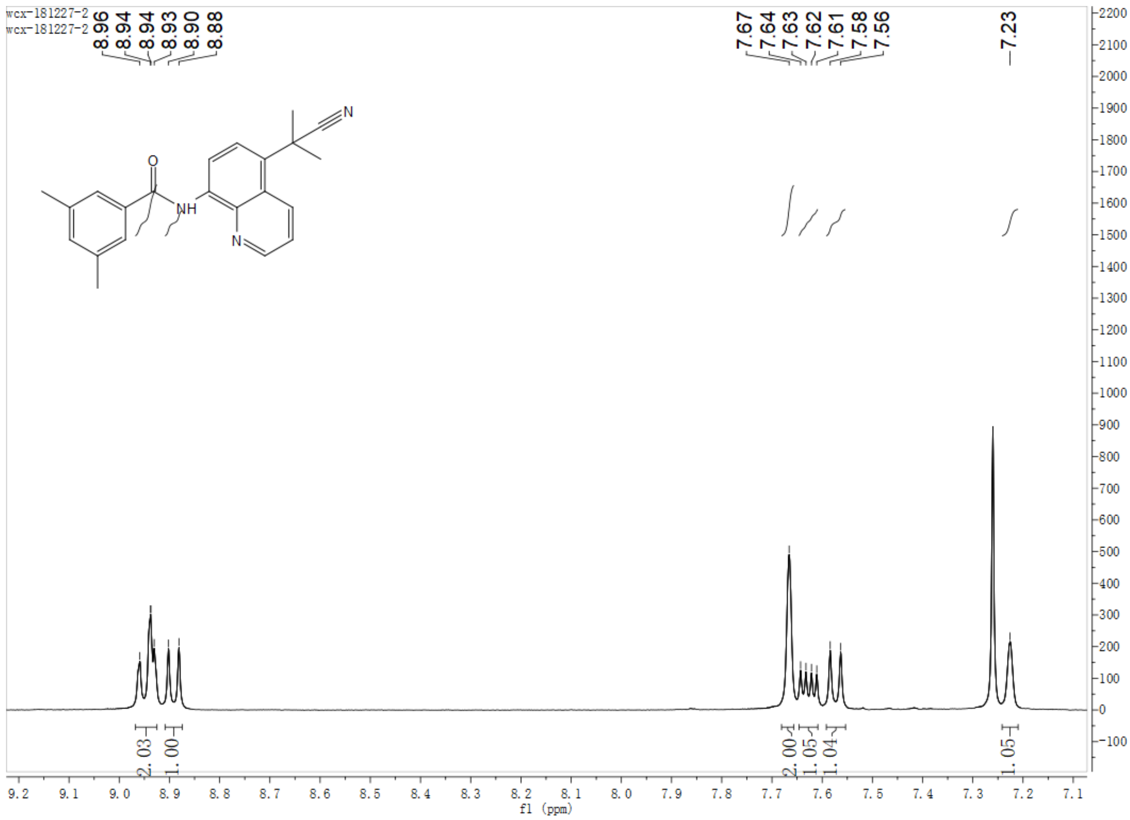
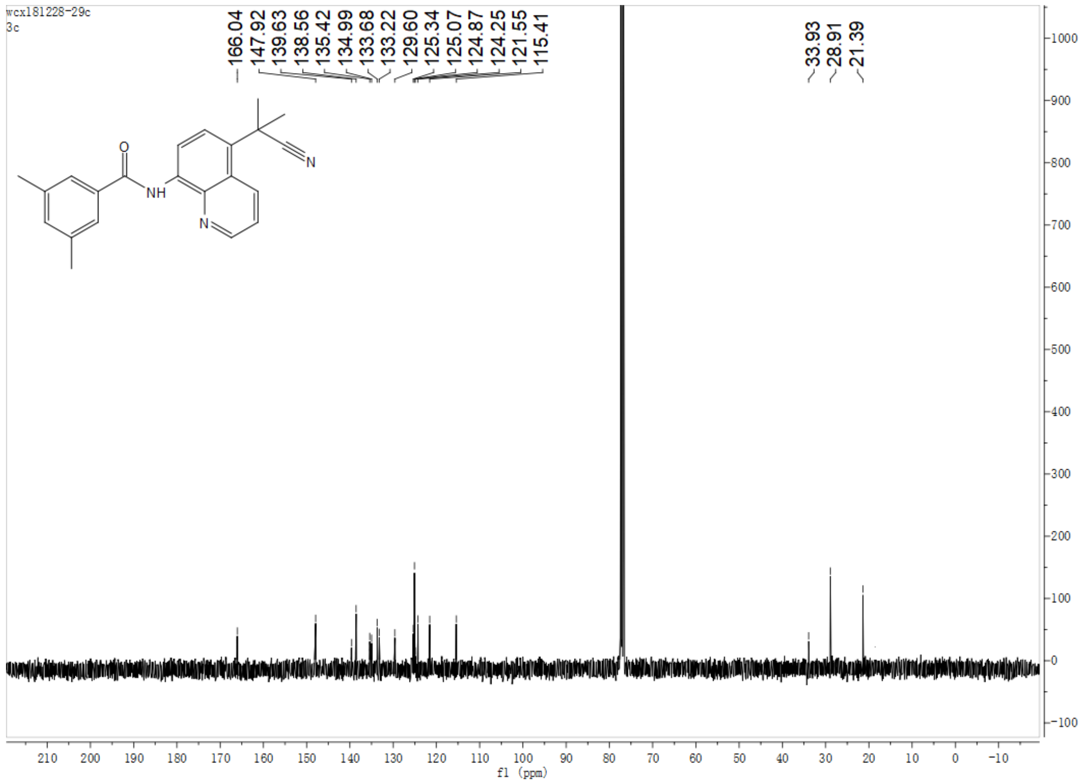
133.27
130.01
129.13
128.75
125.33
124.78
124.19
121.66
115.46
33.95
28.89
O
NH
N
N
Cl
f1 (ppm)

3j:


wcx-181227-2
wcx-181227-2
10.79
8.96
8.94
8.94
8.93
8.90
8.88
7.67
7.64
7.63
7.62
7.61
7.58
7.56
7.23
2.45
1.96
1.00
2.03
1.00
2.00
1.05
1.04
1.05
6.04
6.05
f1 (ppm)


wcx-181227-2
wcx-181227-2
8.96
8.94
8.94
8.93
8.90
8.88
7.67
7.64
7.63
7.62
7.61
7.58
7.56
7.23
2.03
1.00
2.00
1.05
1.04
1.05
f1 (ppm)


wcx181228-29c
3c
166.04
147.92
139.63
138.56
135.42
134.99
133.68
133.22
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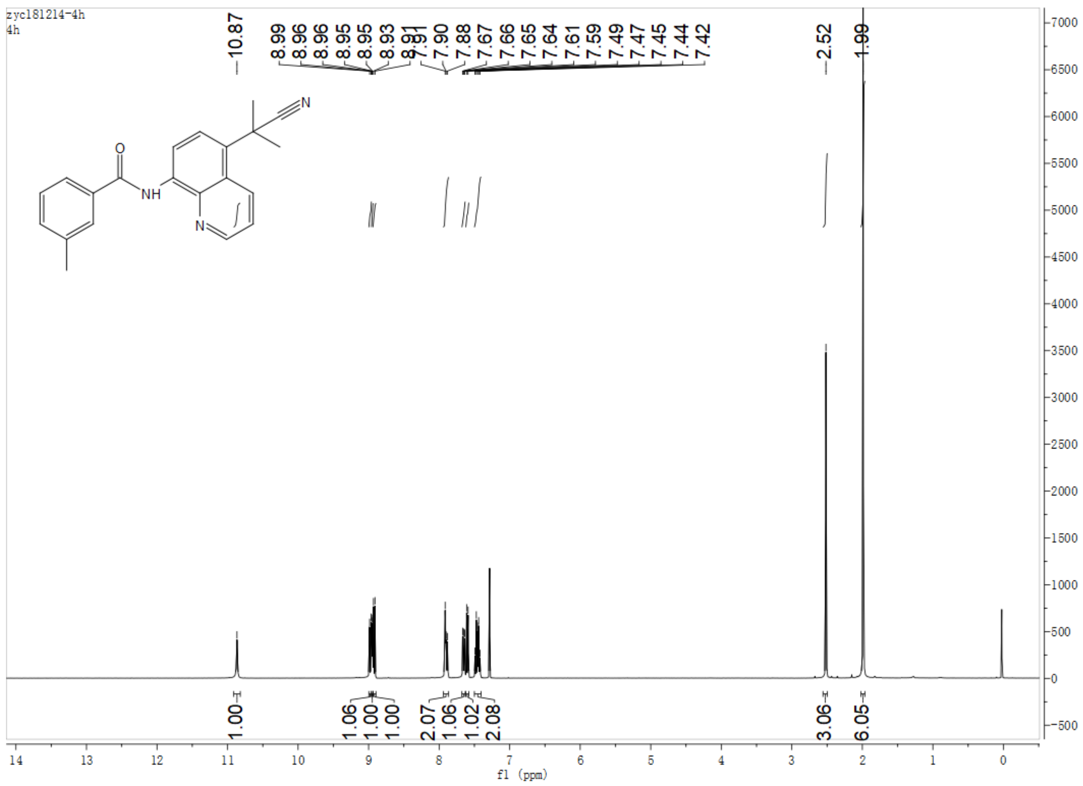
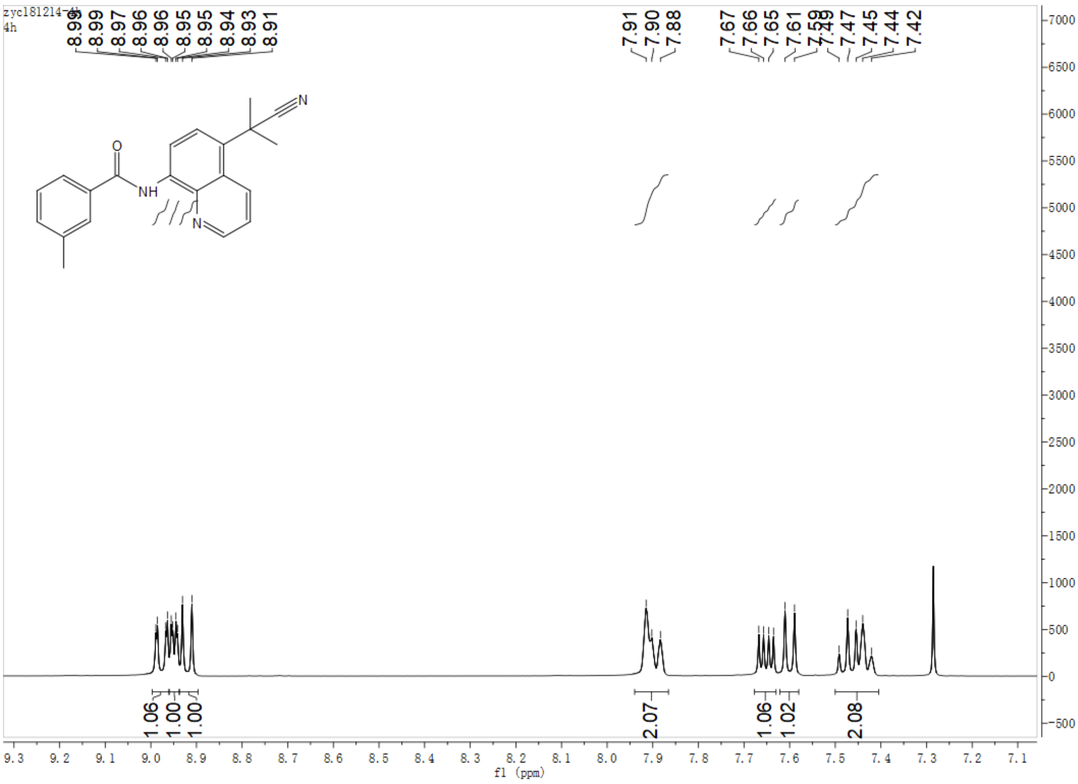
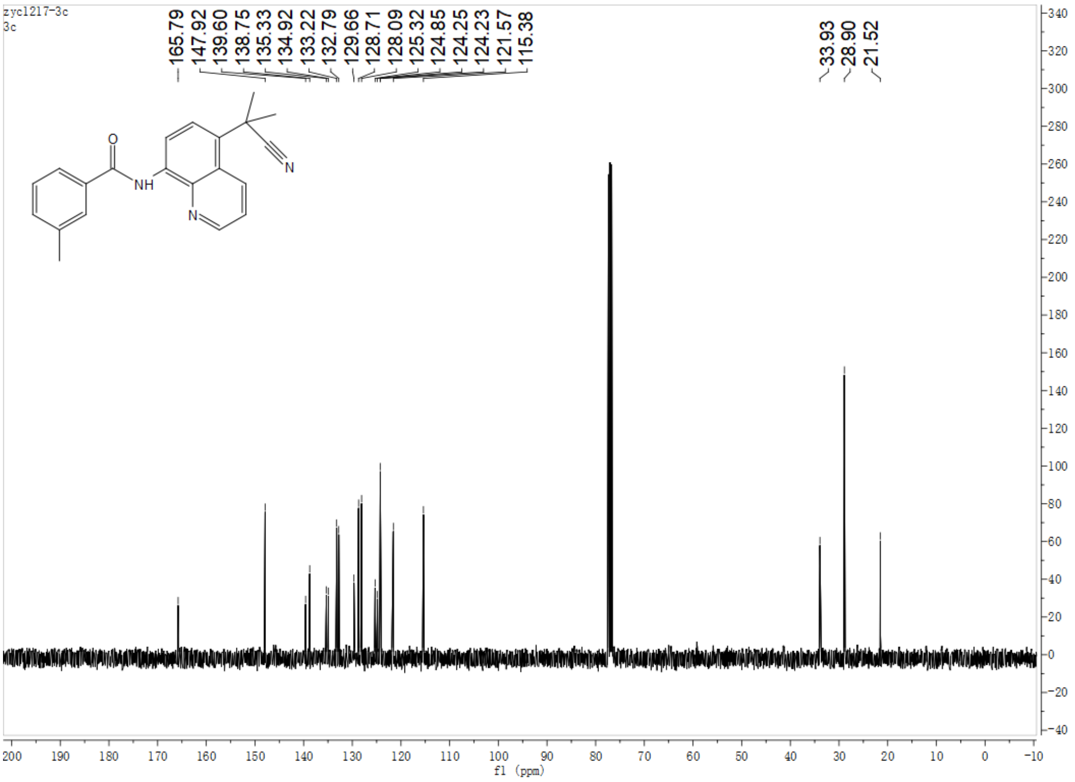
125.34
125.07
124.87
124.25
121.55
115.41
33.93
28.91
21.39
f1 (ppm)

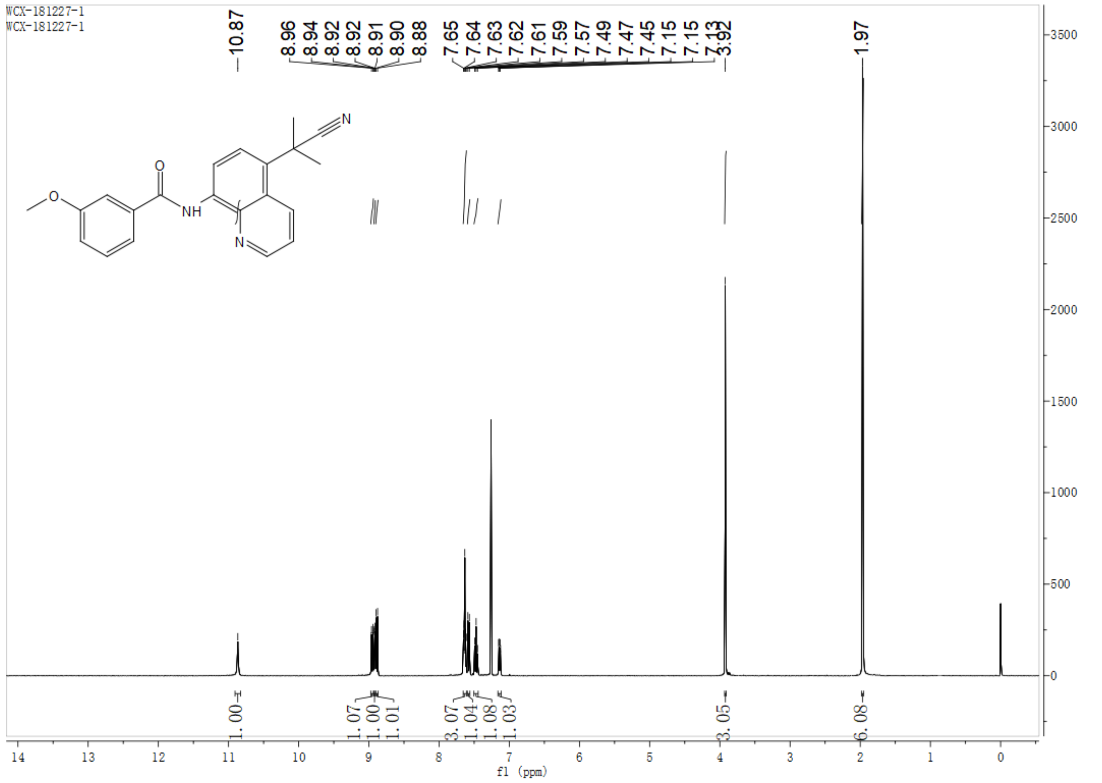
3k:

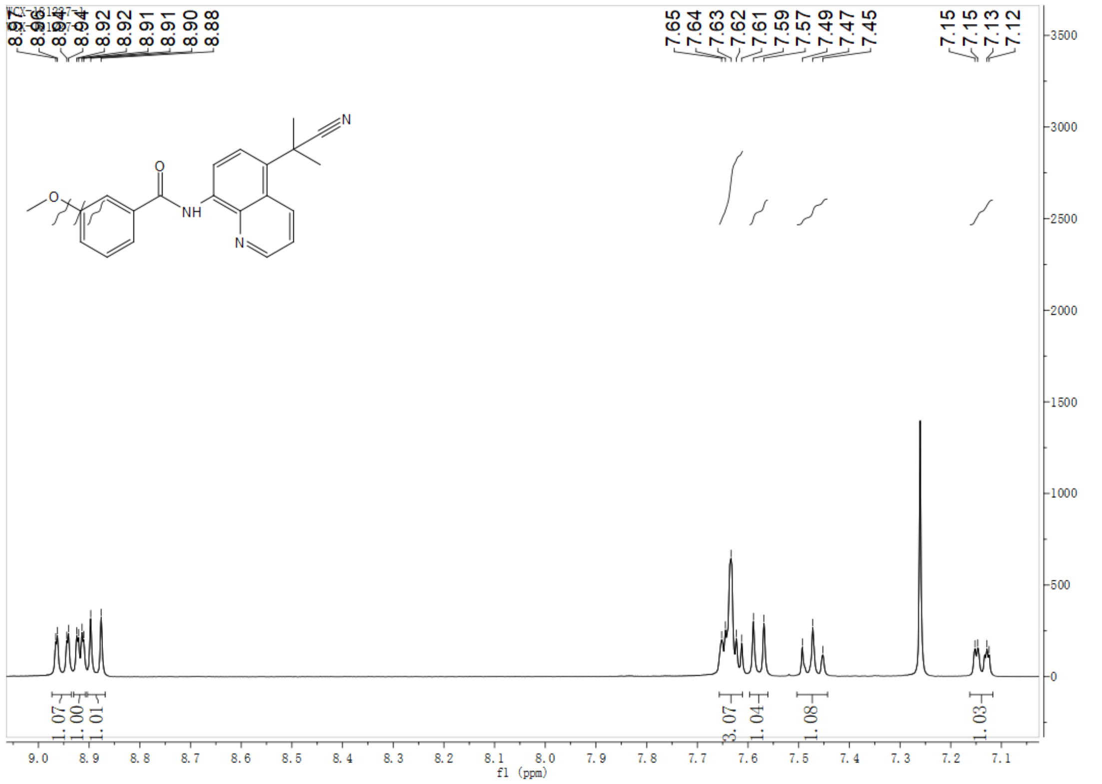

zyc181214-4h
4h
10.87
8.99
8.96
8.96
8.95
8.95
8.93
8.91
7.91
7.90
7.88
7.67
7.66
7.65
7.64
7.61
7.59
7.49
7.47
7.45
7.44
7.42
2.52
1.99
1.00
1.06
1.00
1.00
2.07
1.06
1.02
2.08
3.06
6.05
f1 (ppm)

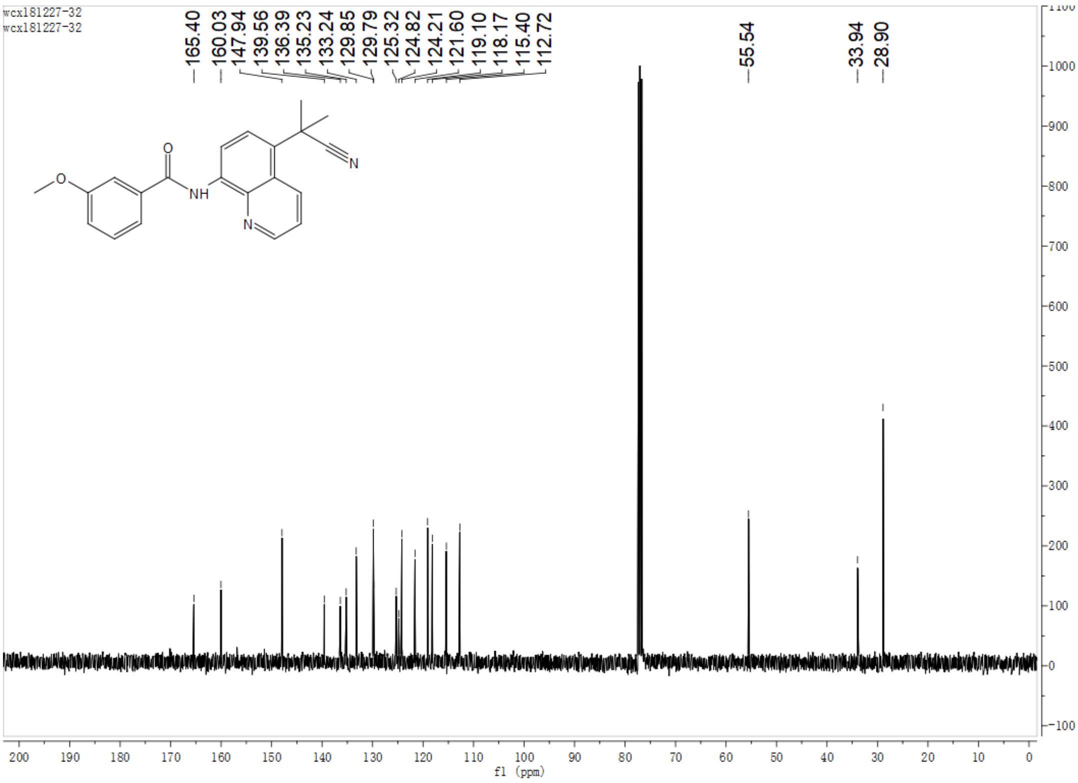

zyc181214-4h
4h
8.99
8.99
8.97
8.96
8.96
8.95
8.95
8.94
8.93
8.91
7.91
7.90
7.88
7.67
7.66
7.65
7.61
7.59
7.49
7.47
7.45
7.44
7.42
O
NH
N
N
1.06
1.00
1.00
2.07
1.06
1.02
2.08
f1 (ppm)


zyc1217-3c
3c
165.79
147.92
139.60
138.75
135.33
134.92
133.22
132.79
129.66
128.71
128.09
125.32
124.85
124.25
124.23
121.57
115.38
33.93
28.90
21.52
O
NH
N
N
f1 (ppm)

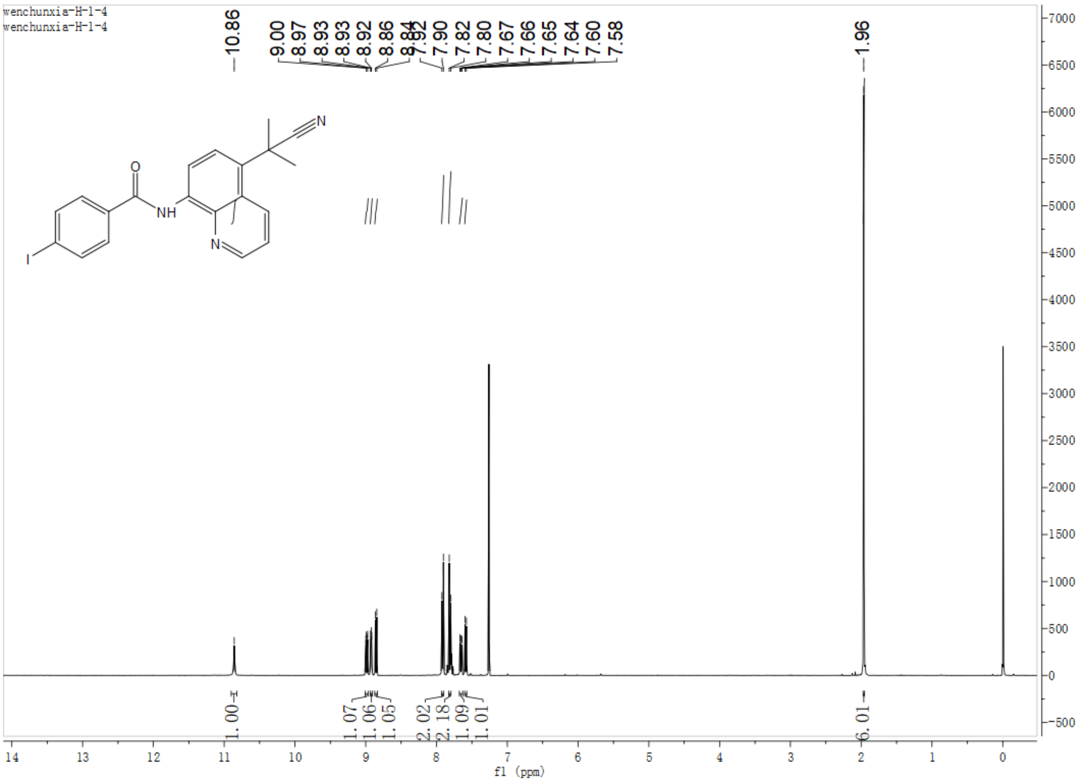
3l:

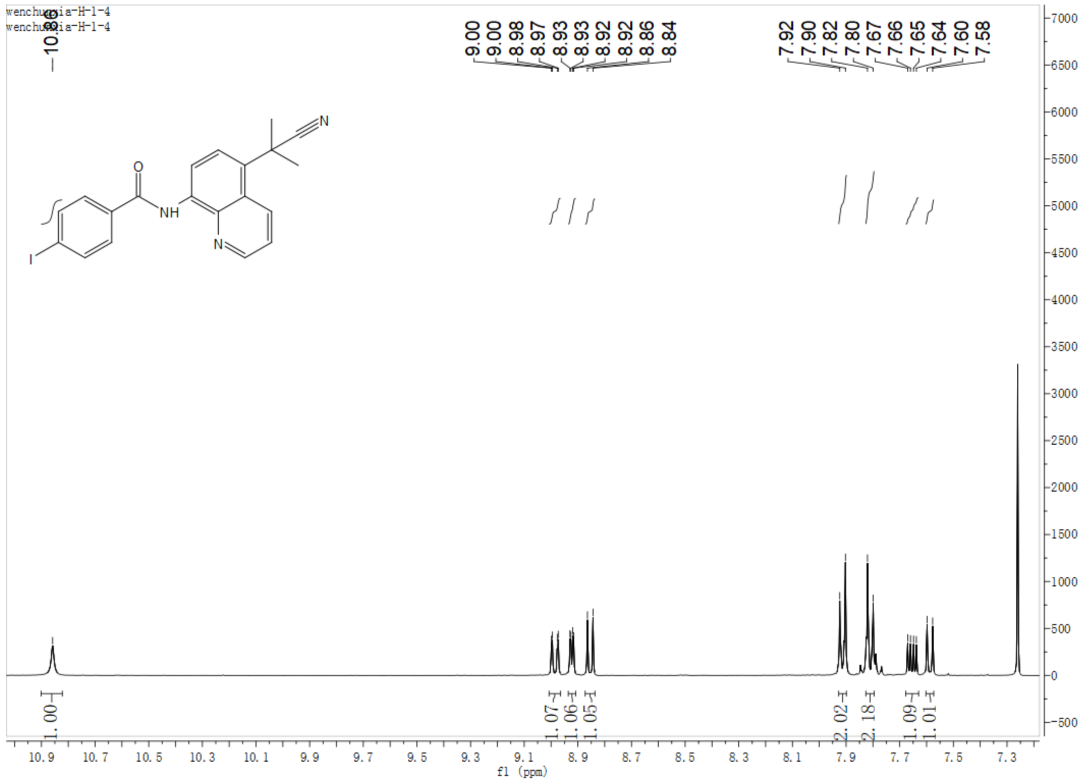


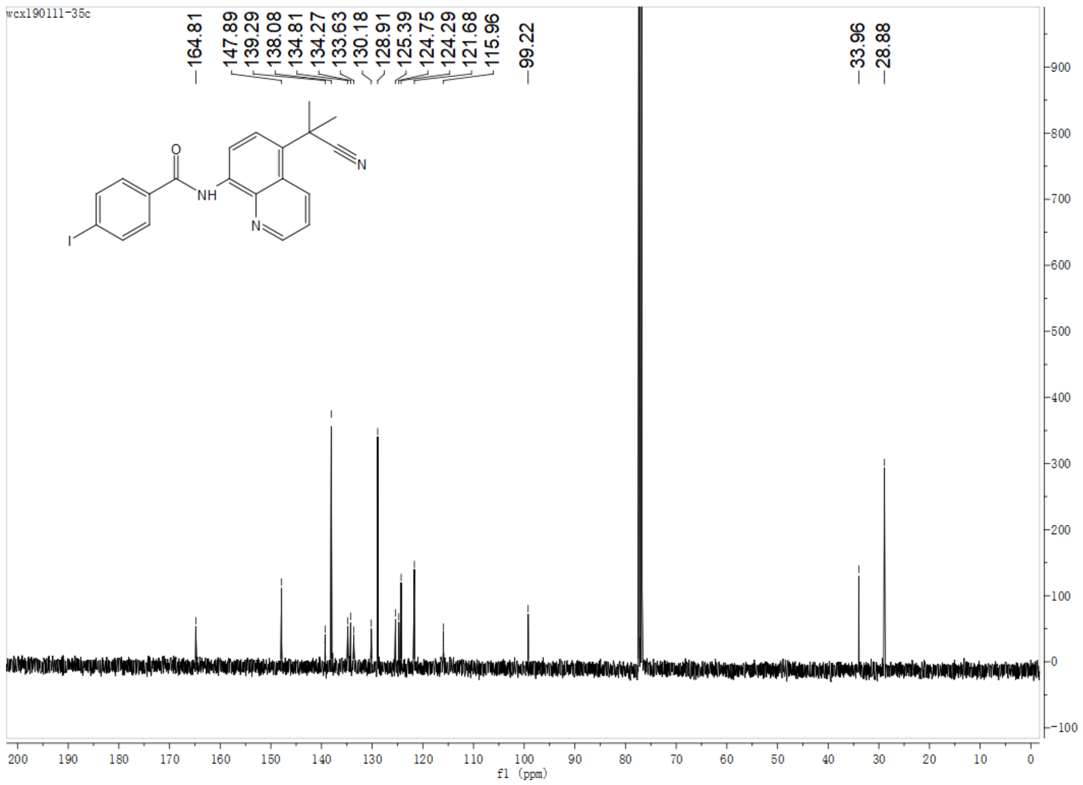



wcx181227-32
wcx181227-32
165.40
160.03
147.94
139.56
136.39
135.23
133.24
129.85
129.79
125.32
124.82
124.21
121.60
119.10
118.17
115.40
112.72
55.54
33.94
28.90
O
NH
N
N
f1 (ppm)

3m:


wenchunxia-H-1-4
wenchunxia-H-1-4
10.86
9.00
8.97
8.93
8.93
8.92
8.86
8.84
7.92
7.90
7.82
7.80
7.67
7.66
7.65
7.64
7.60
7.58
1.96
O
NH
N
N
I
1.00
1.07
1.06
1.05
2.02
2.18
1.09
1.01
6.01
f1 (ppm)


wenchuxia-H-1-4
wenchuxia-H-1-4
10.86
9.00
9.00
8.98
8.97
8.93
8.93
8.92
8.92
8.86
8.84
7.92
7.90
7.82
7.80
7.67
7.66
7.65
7.64
7.60
7.58
O
NH
N
N
I
1.00
1.07
1.06
1.05
2.02
2.18
1.09
1.01
f1 (ppm)


wcx190111-35c
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139.29
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134.27
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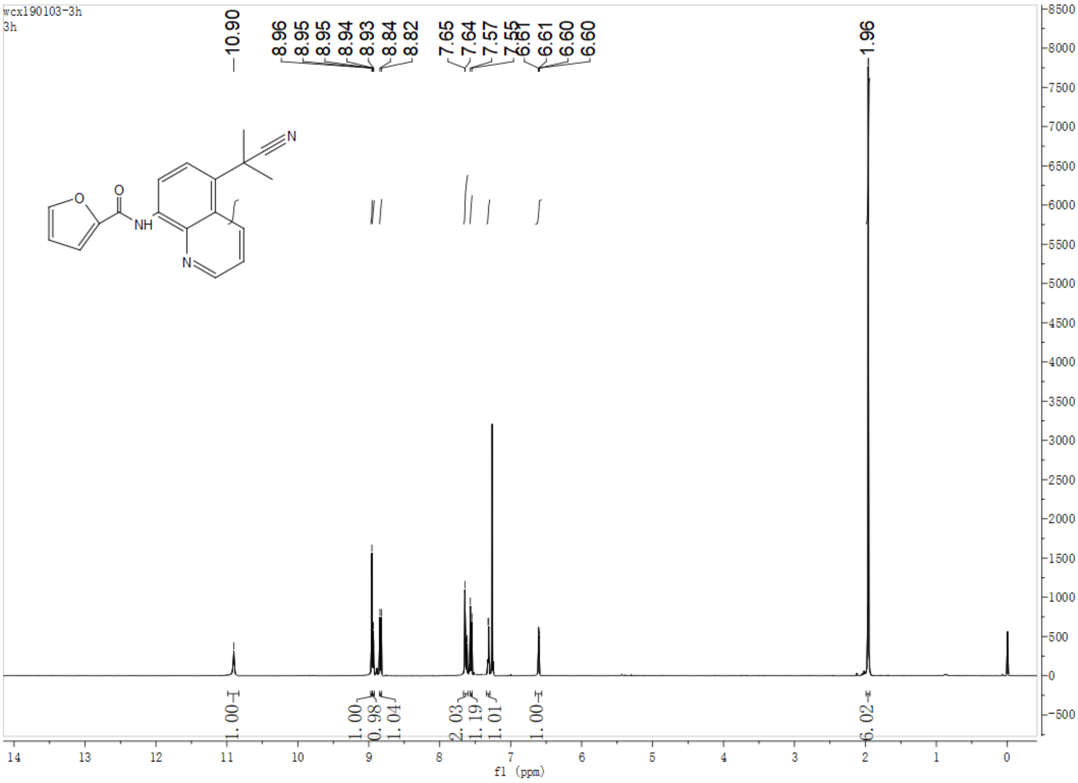
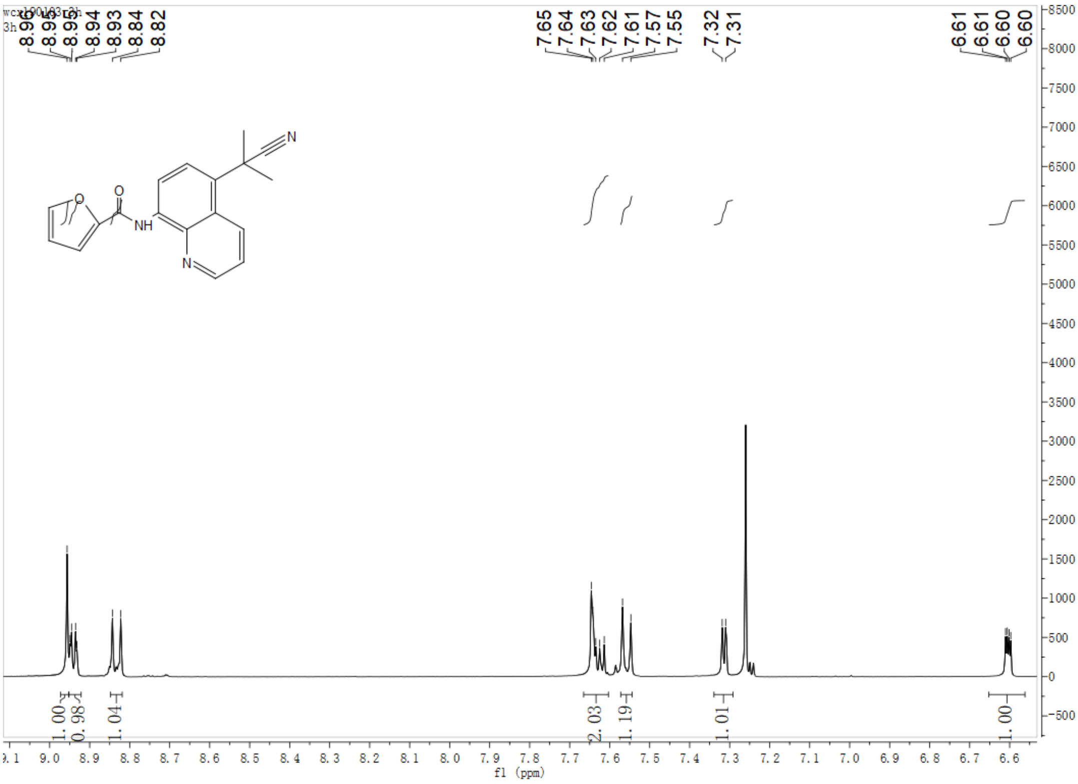
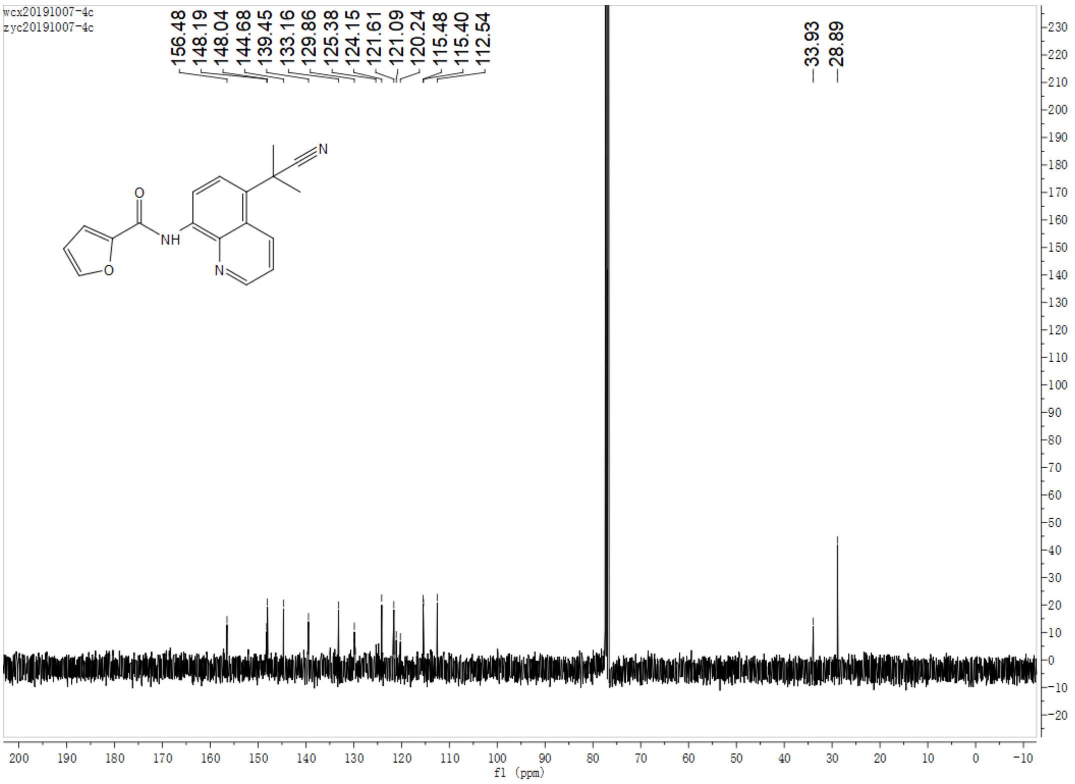
130.18
128.91
125.39
124.75
124.29
121.68
115.96
99.22
33.96
28.88
O
NH
N
N
I
f1 (ppm)

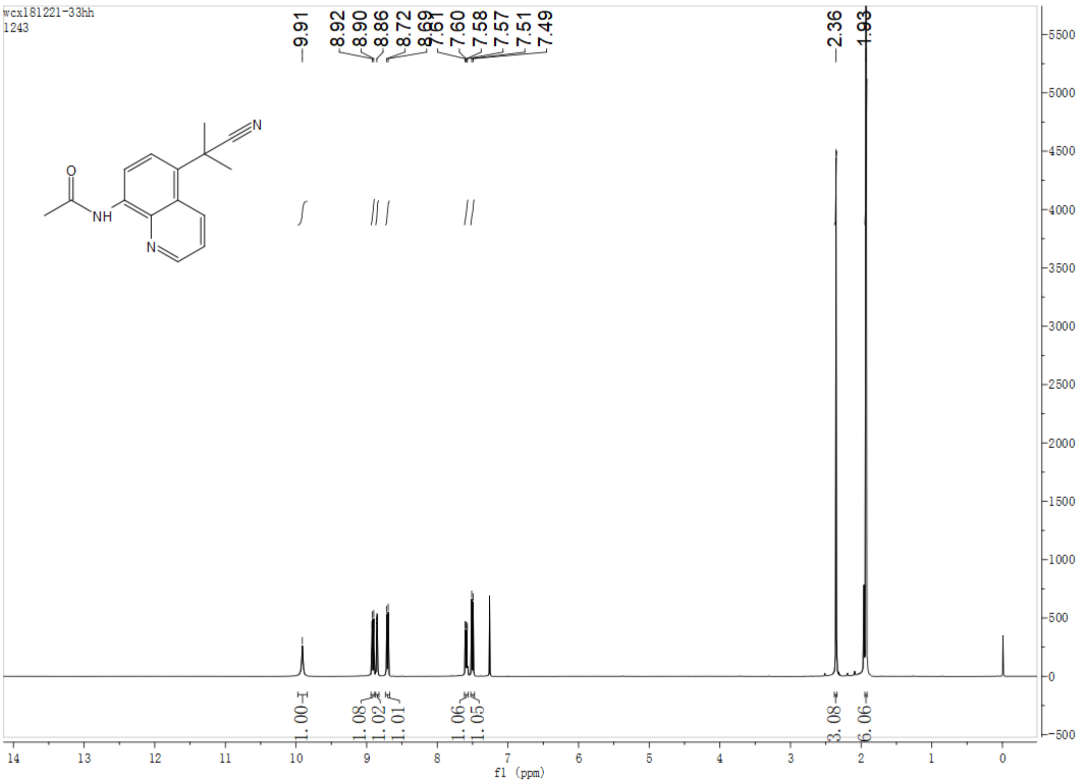
3n:

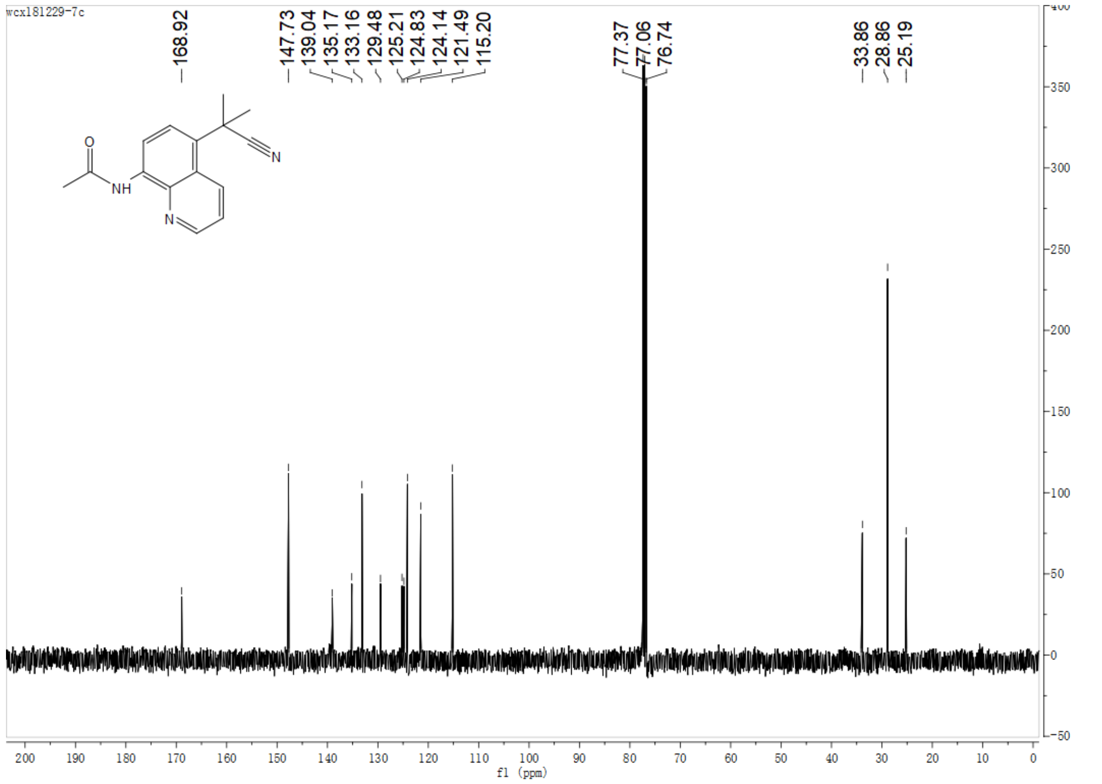




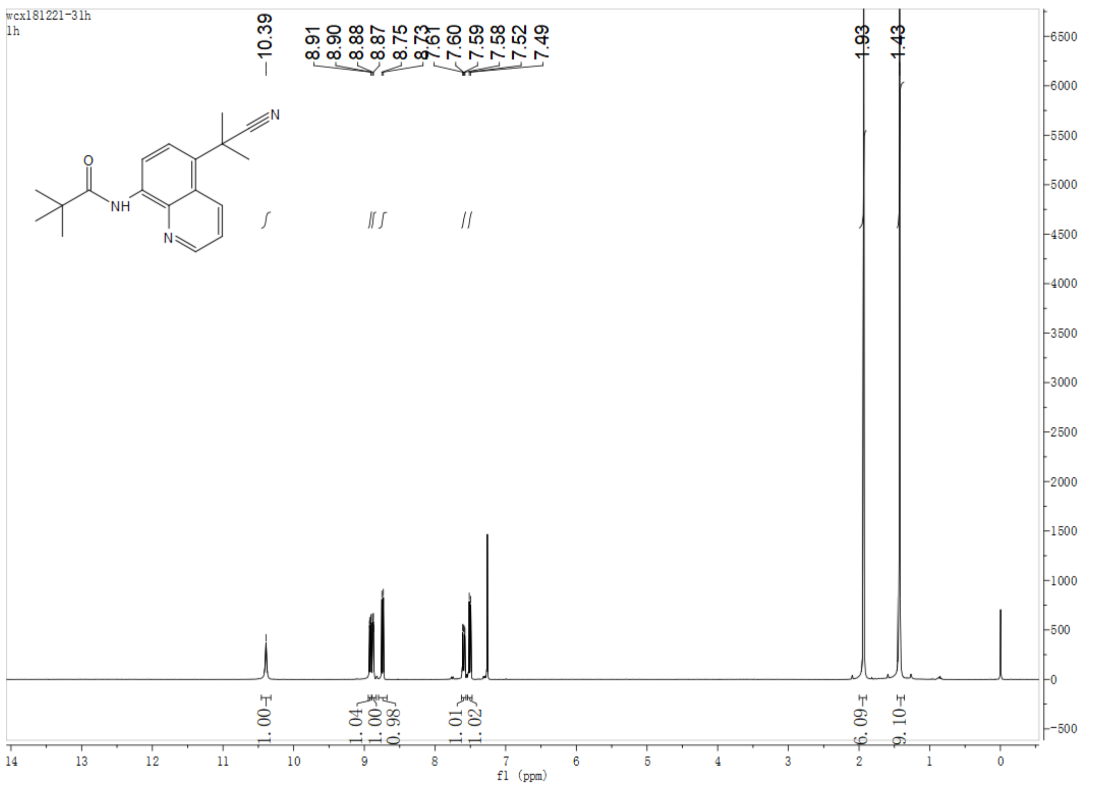

wcx20191007-4c
zyc20191007-4c
156.48
148.19
148.04
144.68
139.45
133.16
129.86
125.38
124.15
121.61
121.09
120.24
115.48
115.40
112.54
33.93
28.89
NH
O
N
f1 (ppm)

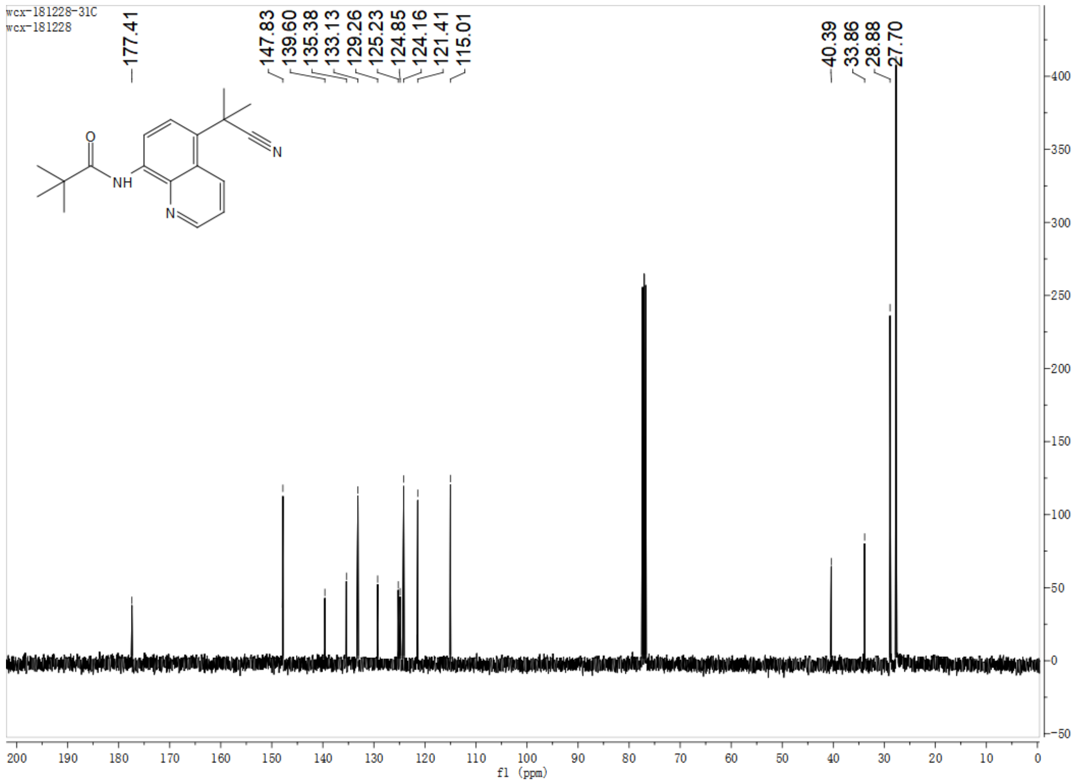
3o:


wcx181221-33hh
1243
9.91
8.92
8.90
8.86
8.72
8.69
7.61
7.60
7.58
7.57
7.51
7.49
2.36
1.93
NH
N
1.00
1.08
1.02
1.01
1.06
1.05
3.08
6.06
f1 (ppm)

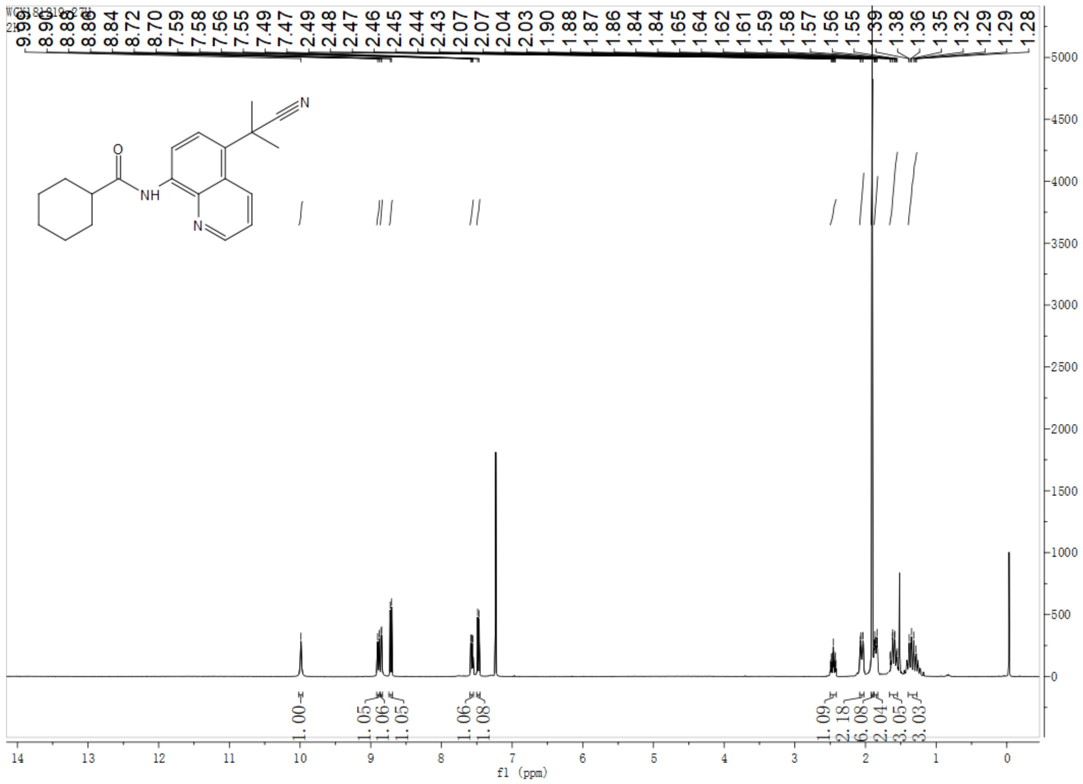


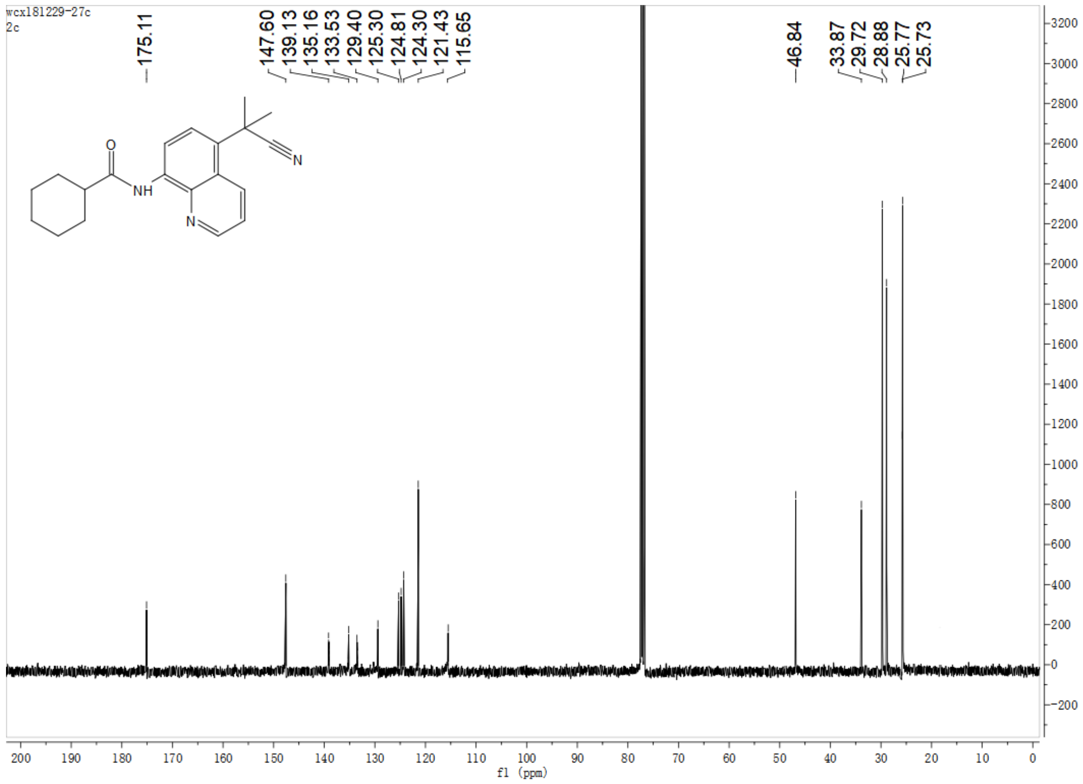
3p:



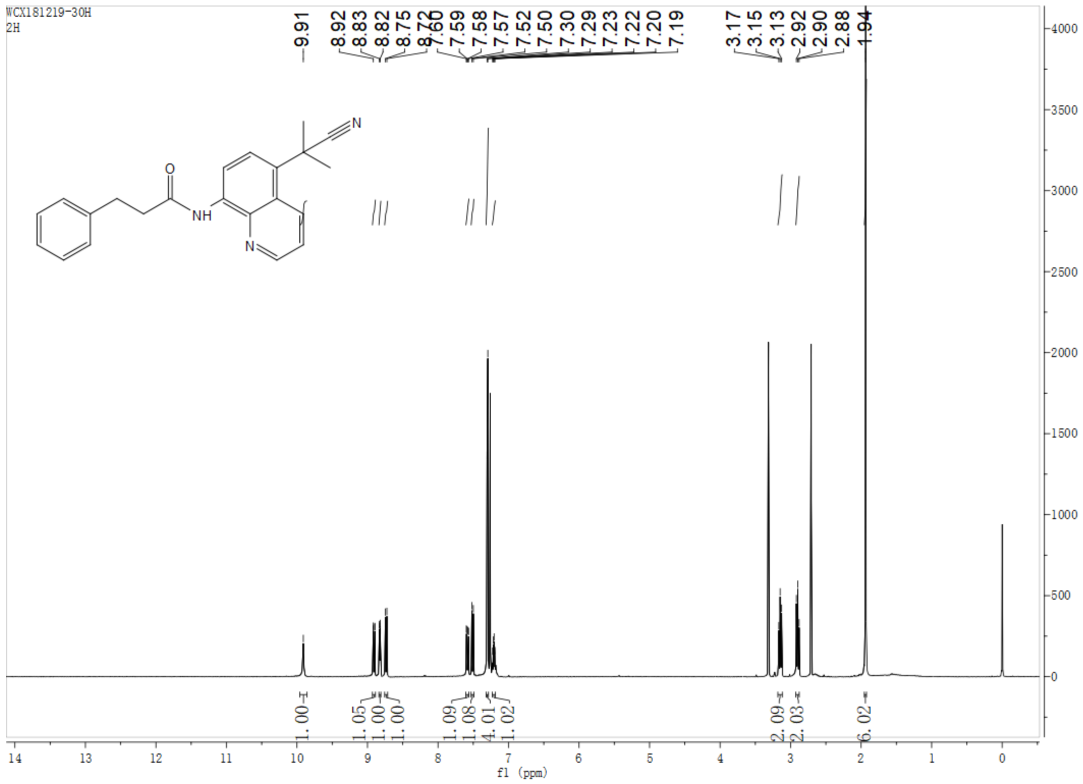


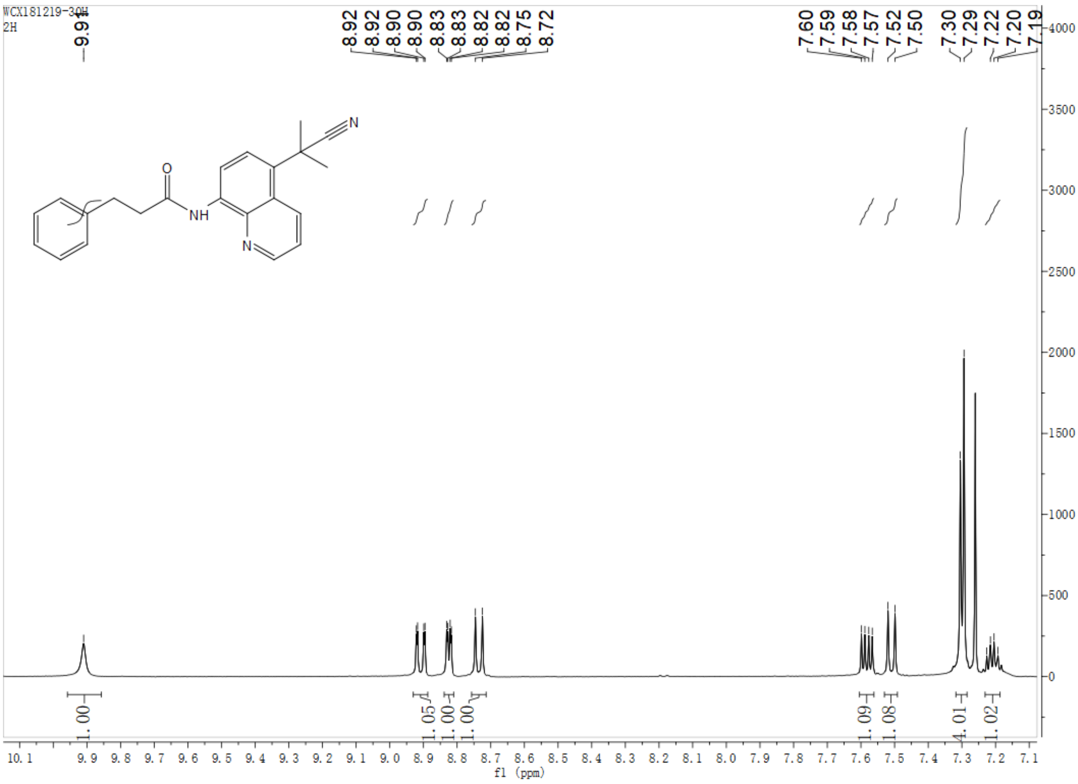
3q:

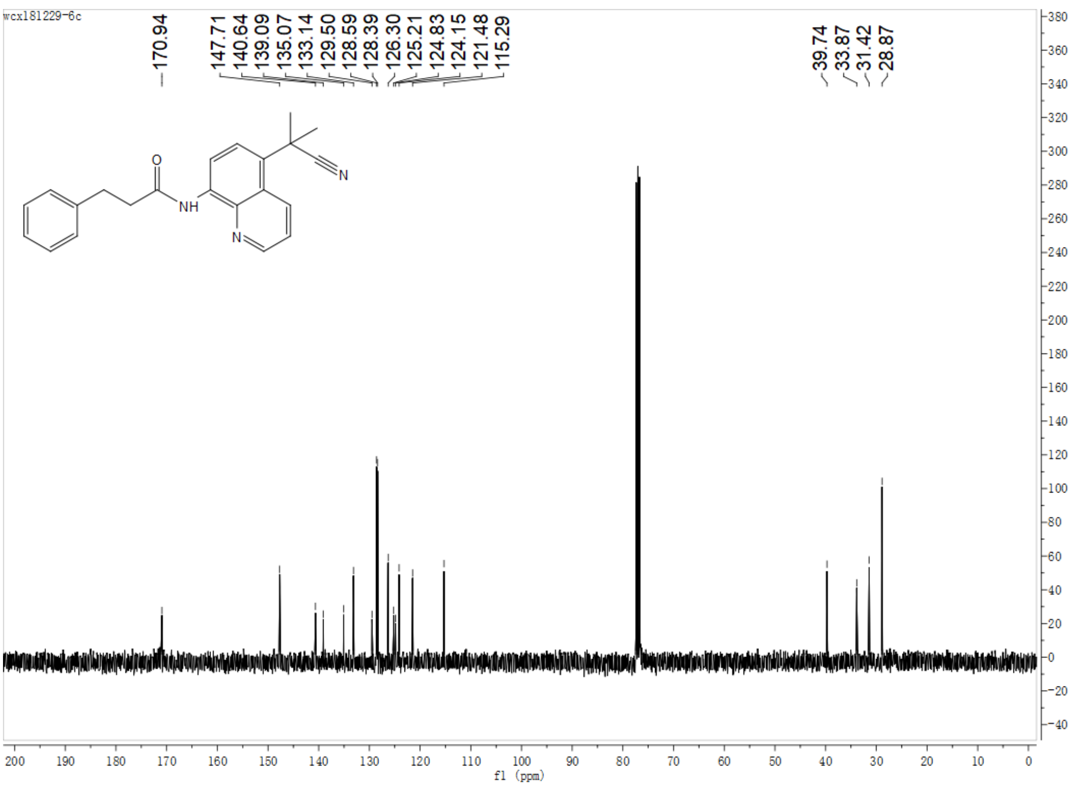




3r:




WCX181219-30H
2H
9.91
8.92
8.92
8.90
8.90
8.83
8.83
8.82
8.82
8.75
8.72
7.60
7.59
7.58
7.57
7.52
7.50
7.30
7.29
7.22
7.20
7.19
O
NH
N
N
1.00
1.05
1.00
1.00
1.09
1.08
4.01
1.02
f1 (ppm)


wcx181229-6c
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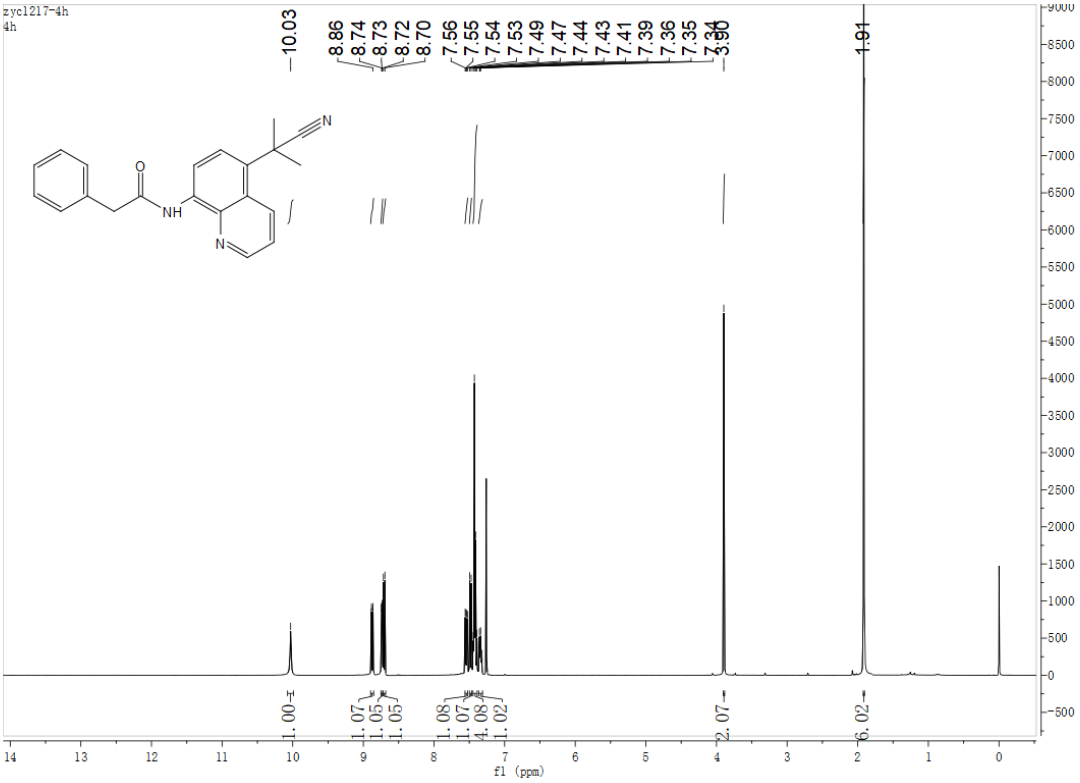
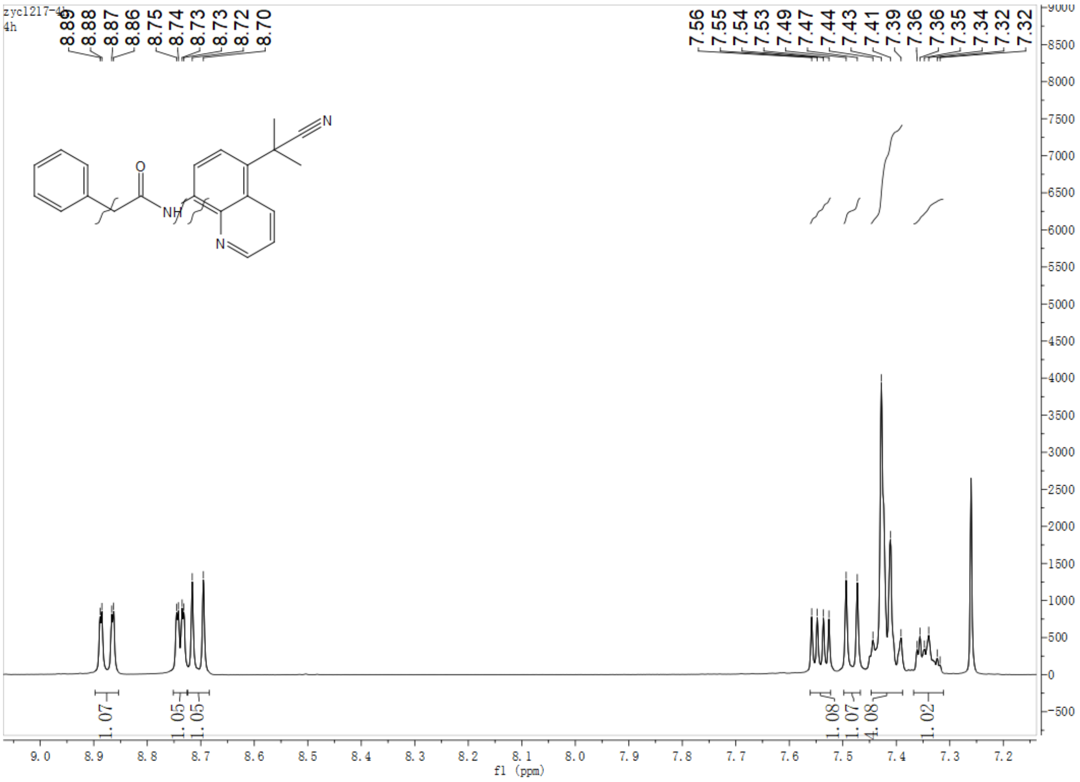
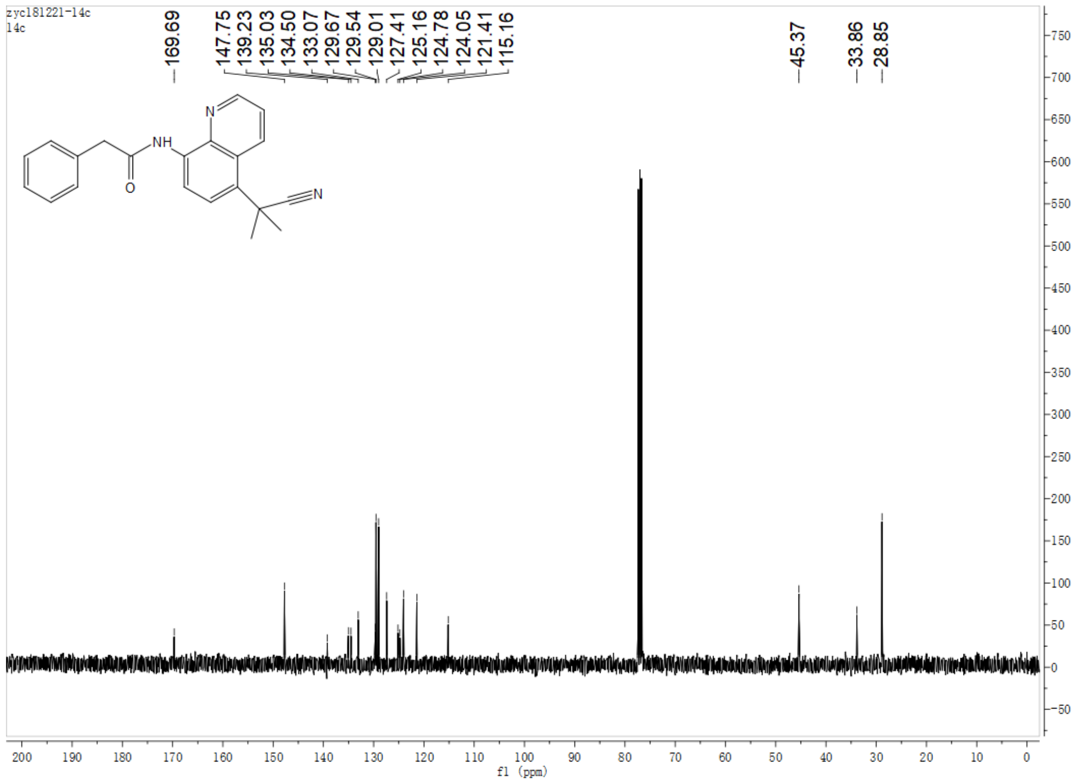
147.71
140.64
139.09
135.07
133.14
129.50
128.59
128.39
126.30
125.21
124.83
124.15
121.48
115.29
39.74
33.87
31.42
28.87
O
NH
N
N
f1 (ppm)

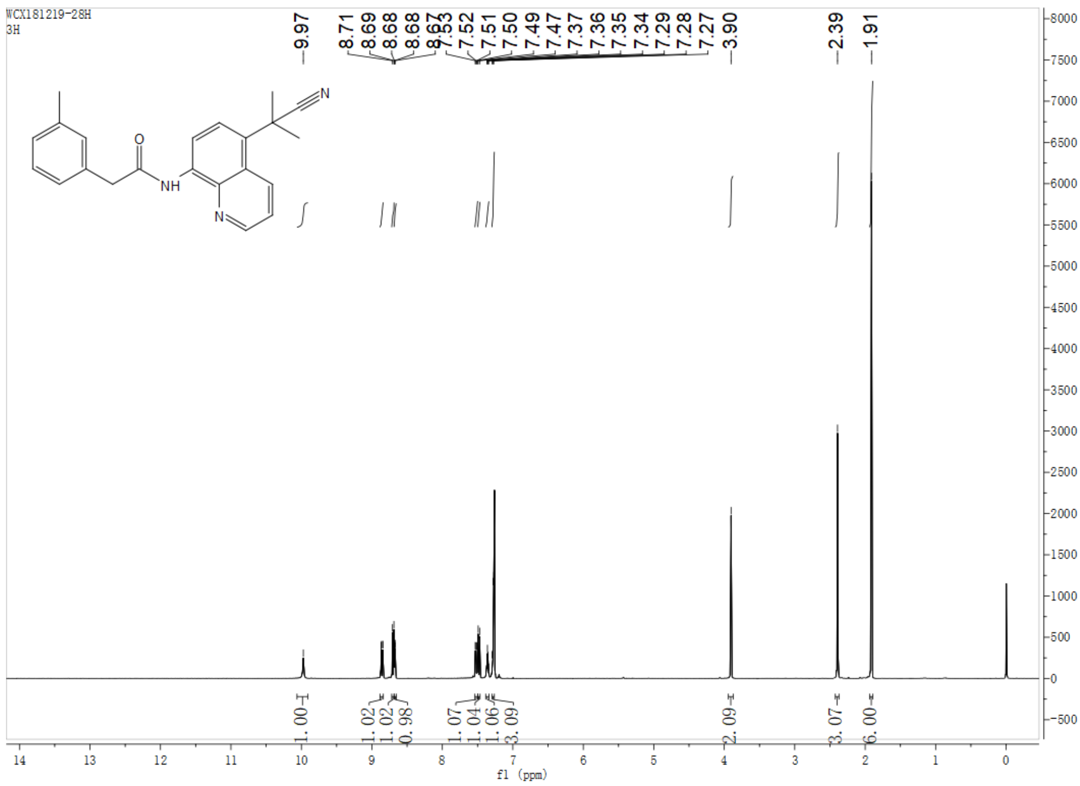
3s:

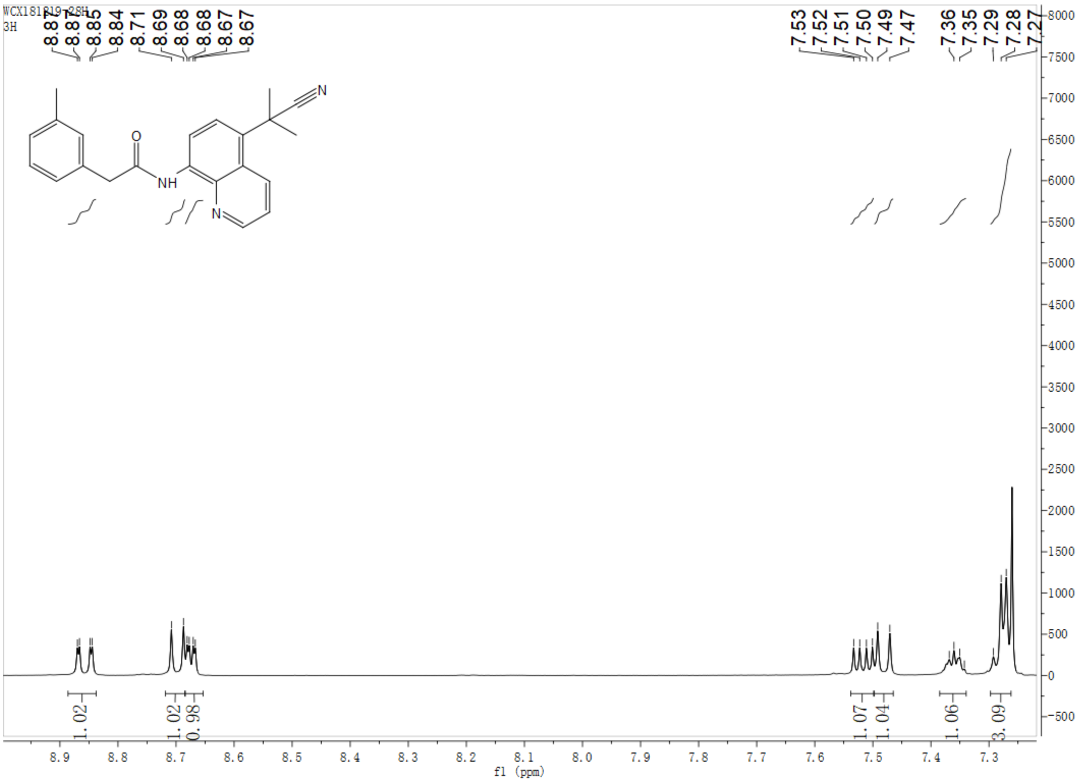


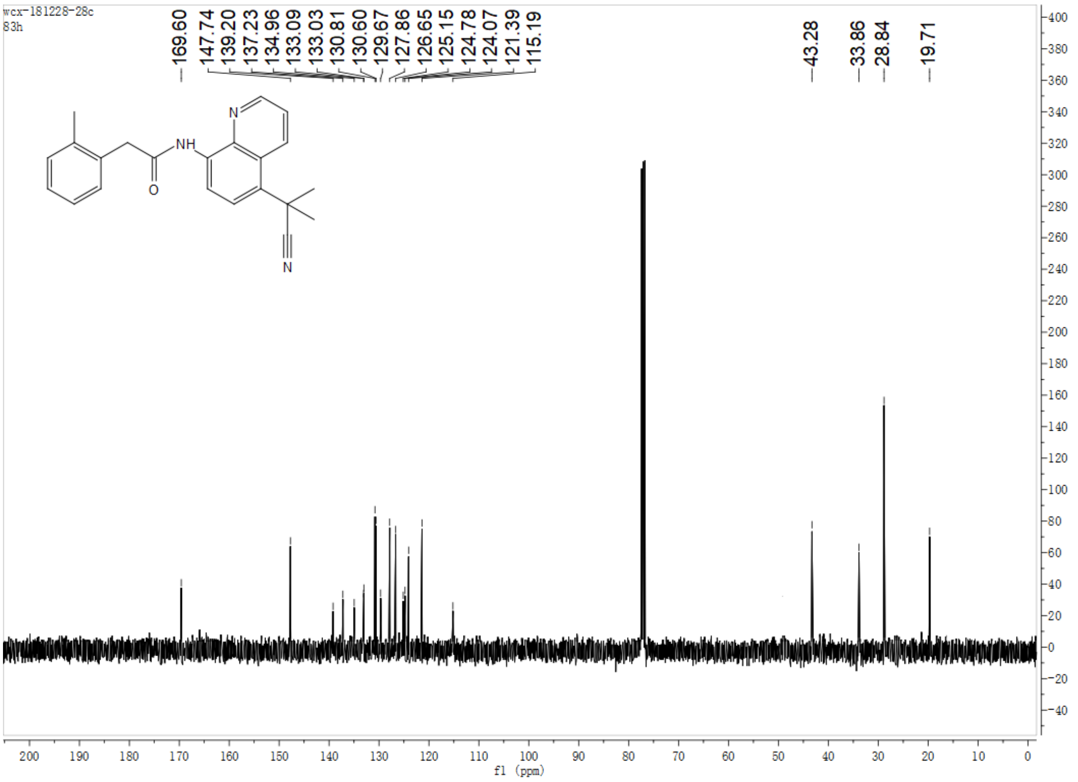




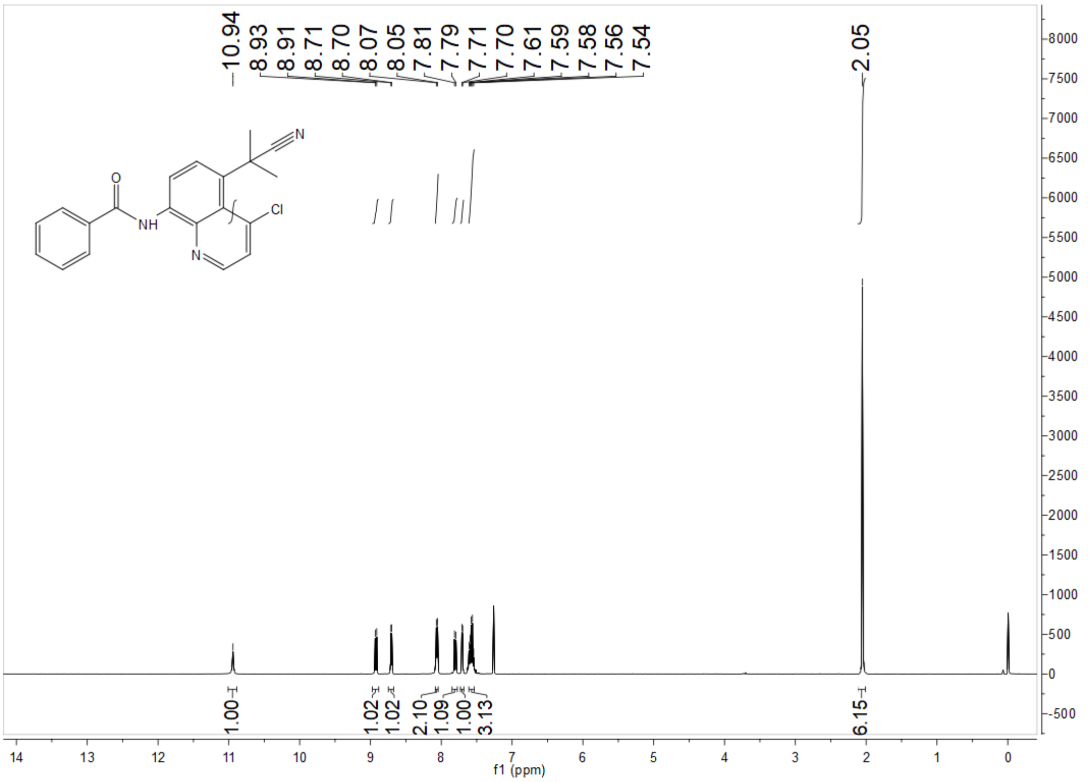
3t:



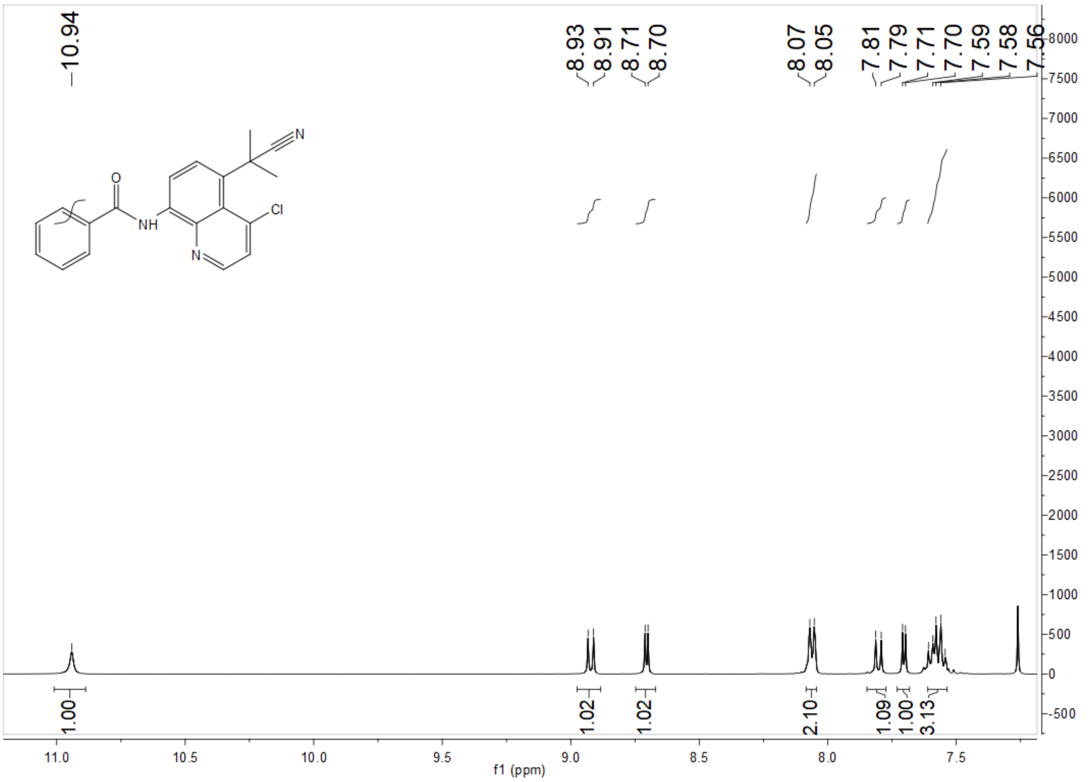




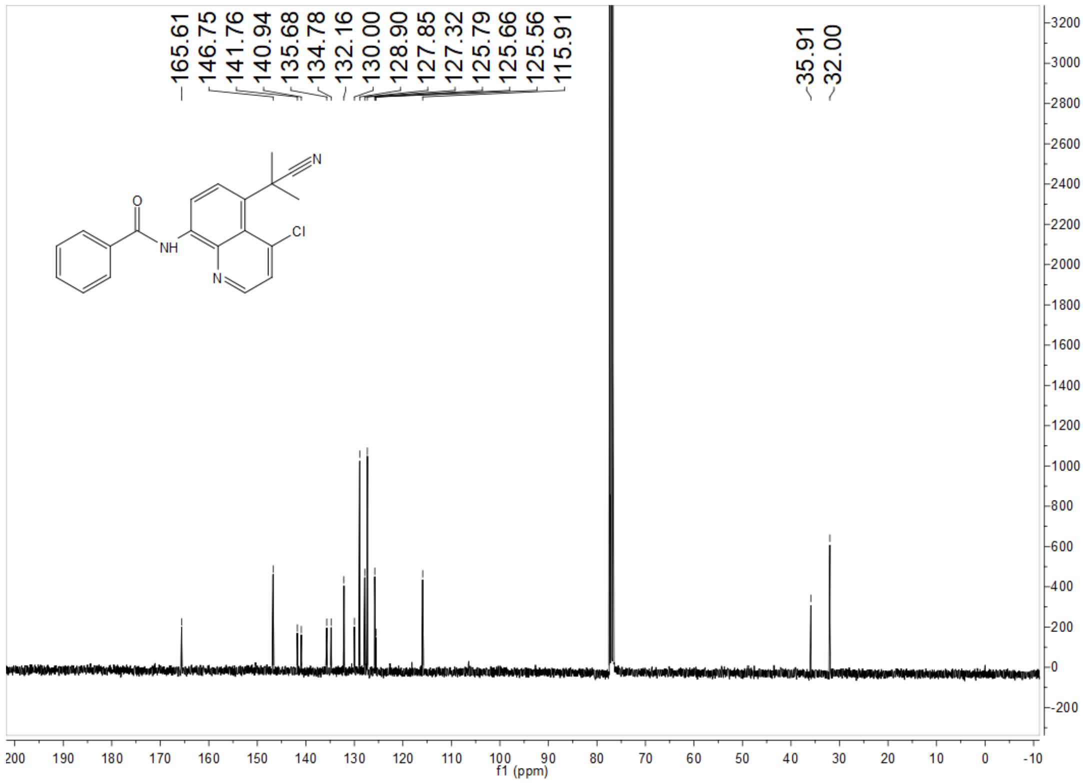
3u:



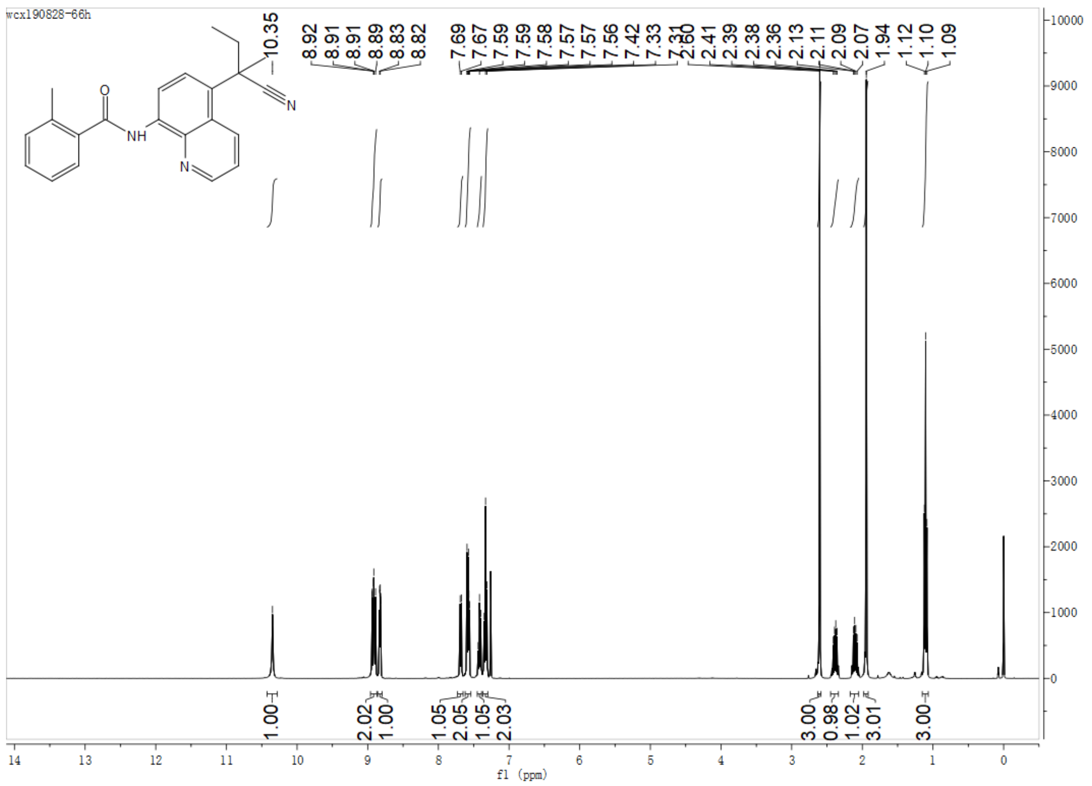
10.94
8.93
8.91
8.71
8.70
8.07
8.05
7.81
7.79
7.71
7.70
7.61
7.59
7.58
7.56
7.54
2.05
O
NH
N
N
Cl
1.00
1.02
1.02
2.10
1.09
1.00
3.13
6.15
f1 (ppm)

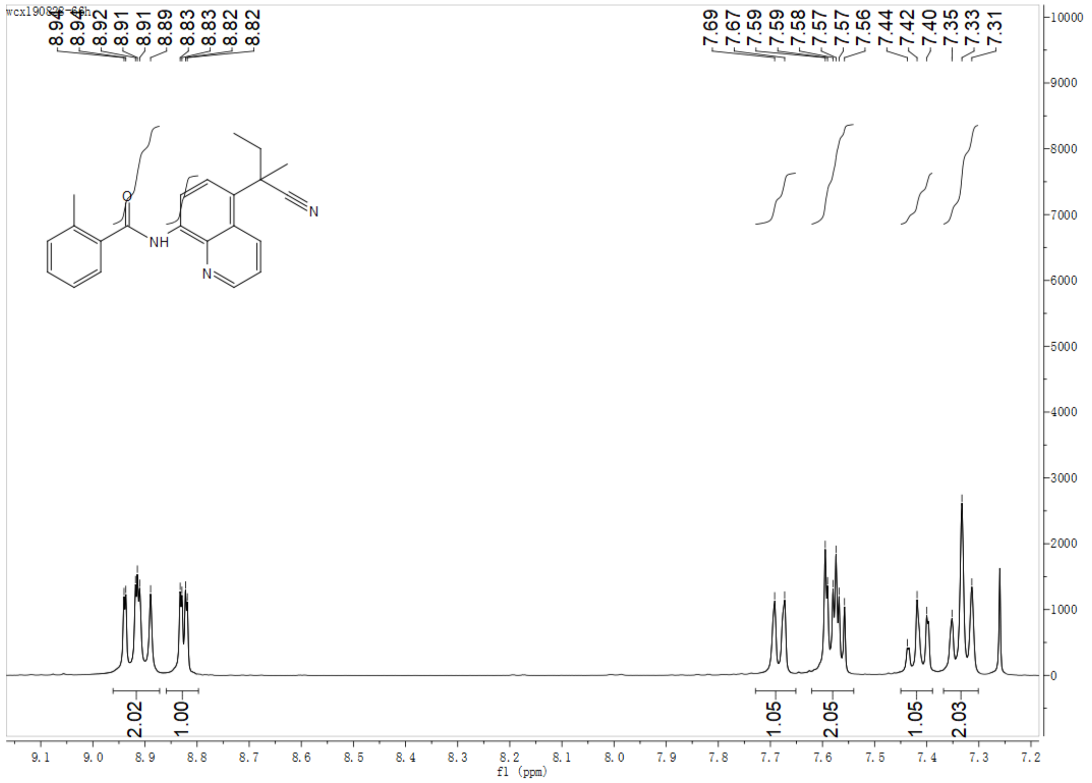


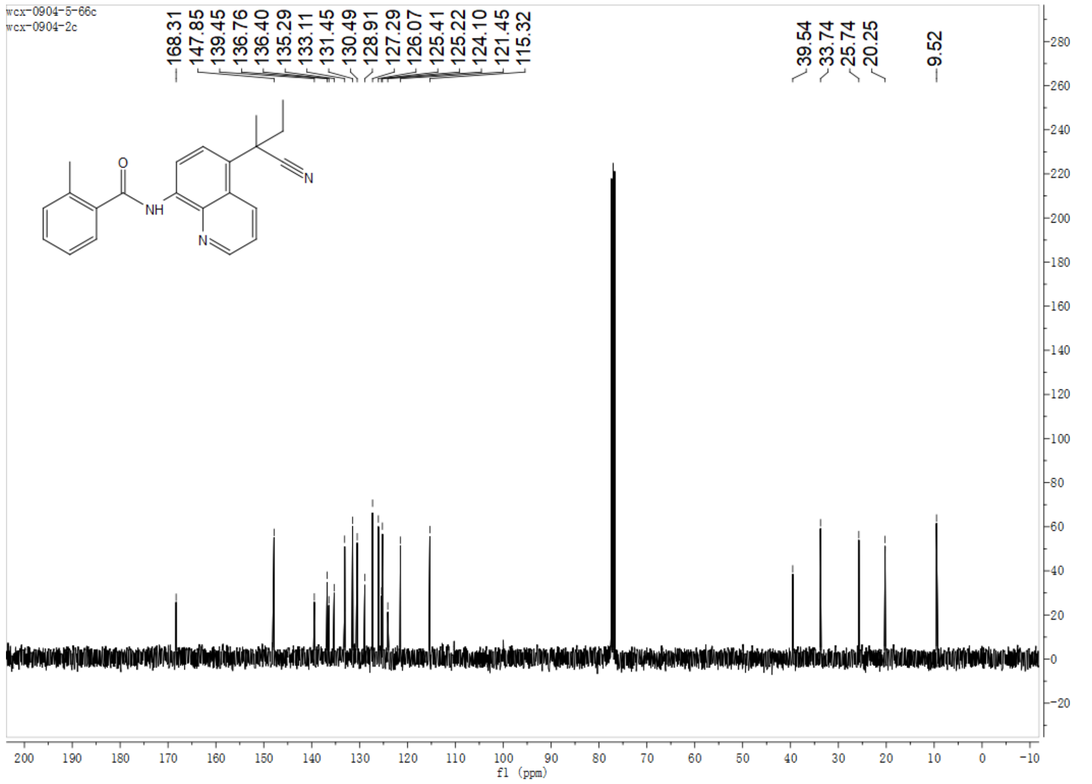
10.94
8.93
8.91
8.71
8.70
8.07
8.05
7.81
7.79
7.71
7.70
7.59
7.58
7.56
O
NH
N
N
Cl
1.00
1.02
1.02
2.10
1.09
1.00
3.13
f1 (ppm)



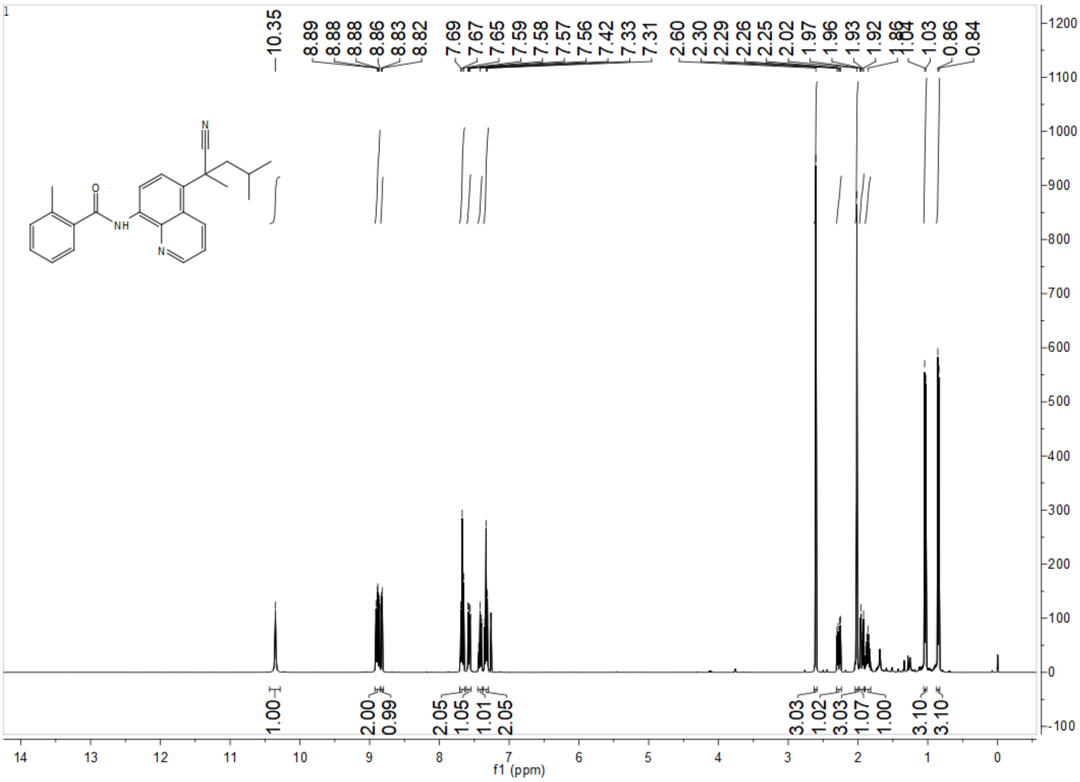
3v:

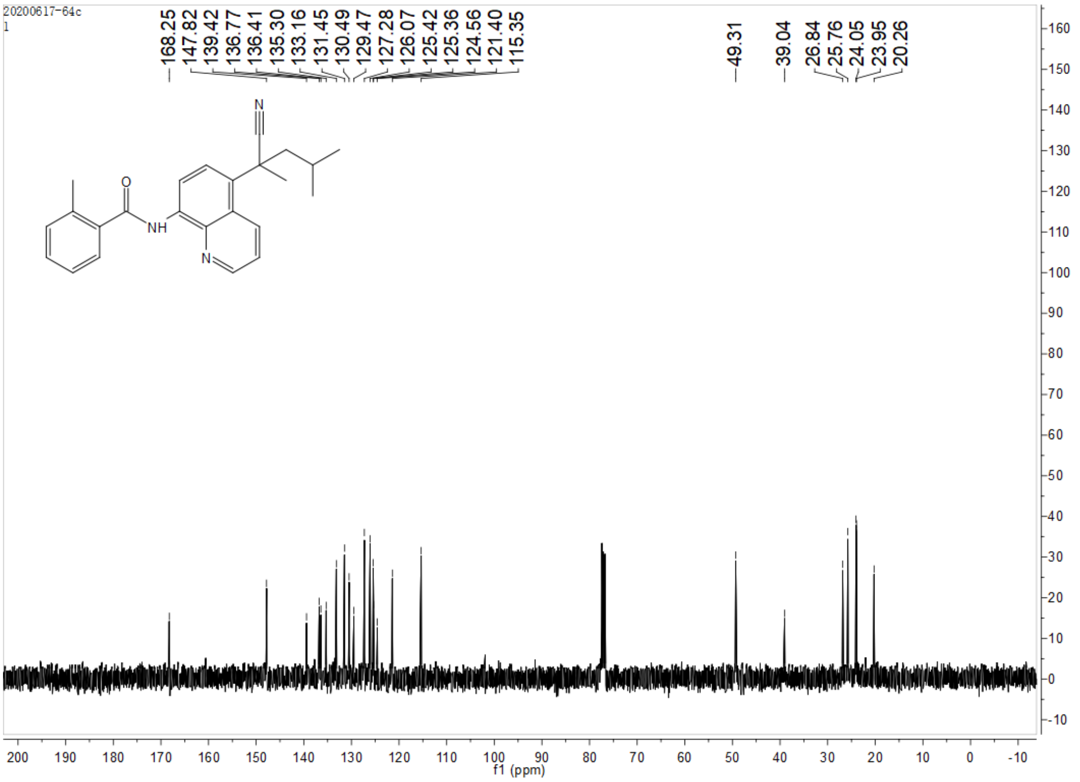




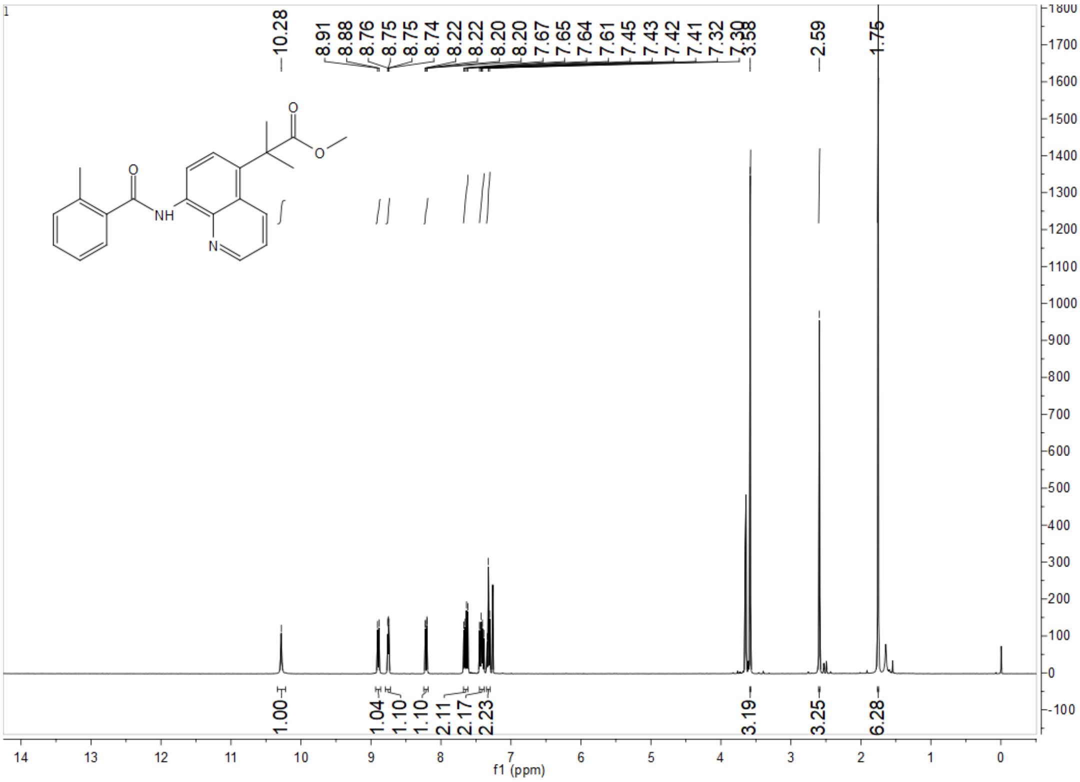


3w:

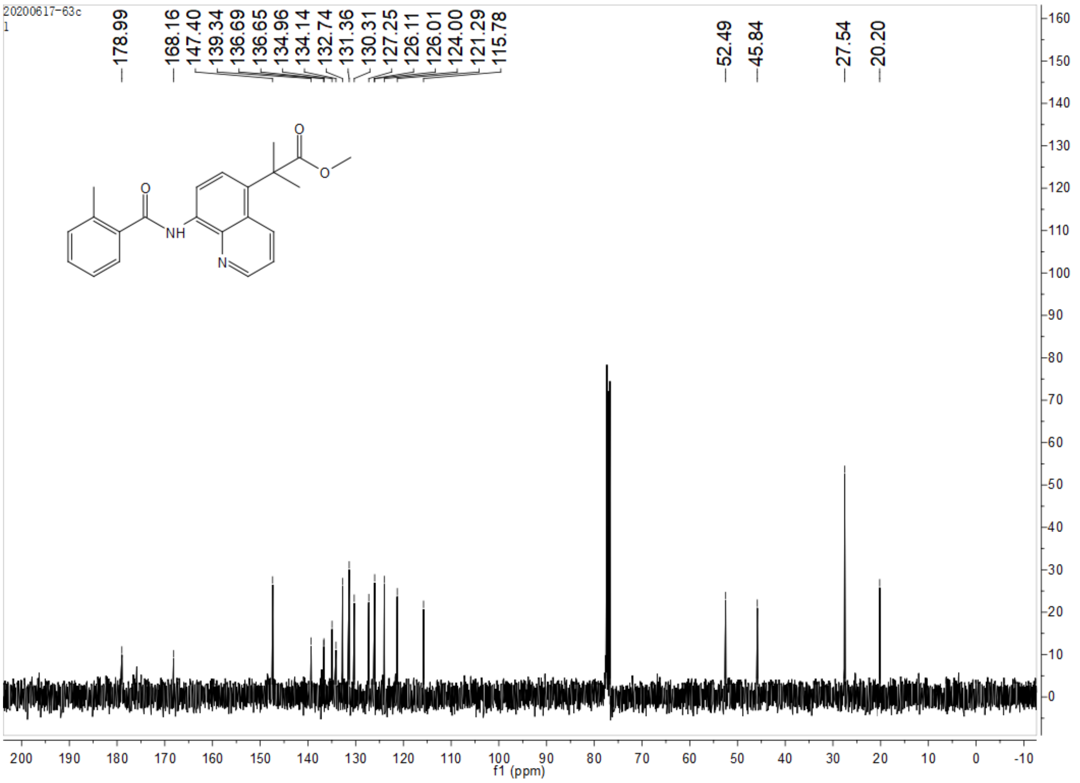




3x:

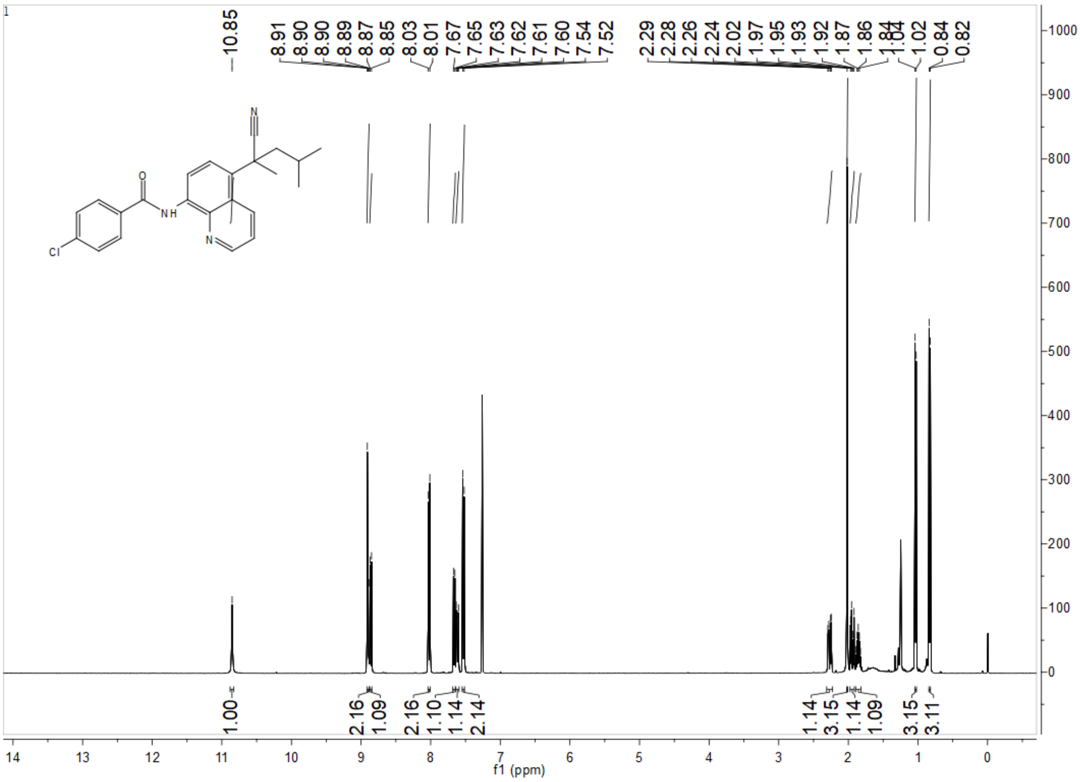


10.28
8.91
8.88
8.76
8.75
8.75
8.74
8.22
8.22
8.20
8.20
7.67
7.65
7.64
7.61
7.45
7.43
7.42
7.41
7.32
7.30
3.58
2.59
1.75
NH
N
O
1.00
1.04
1.10
1.10
2.11
2.17
2.23
3.19
3.25
6.28
f1 (ppm)

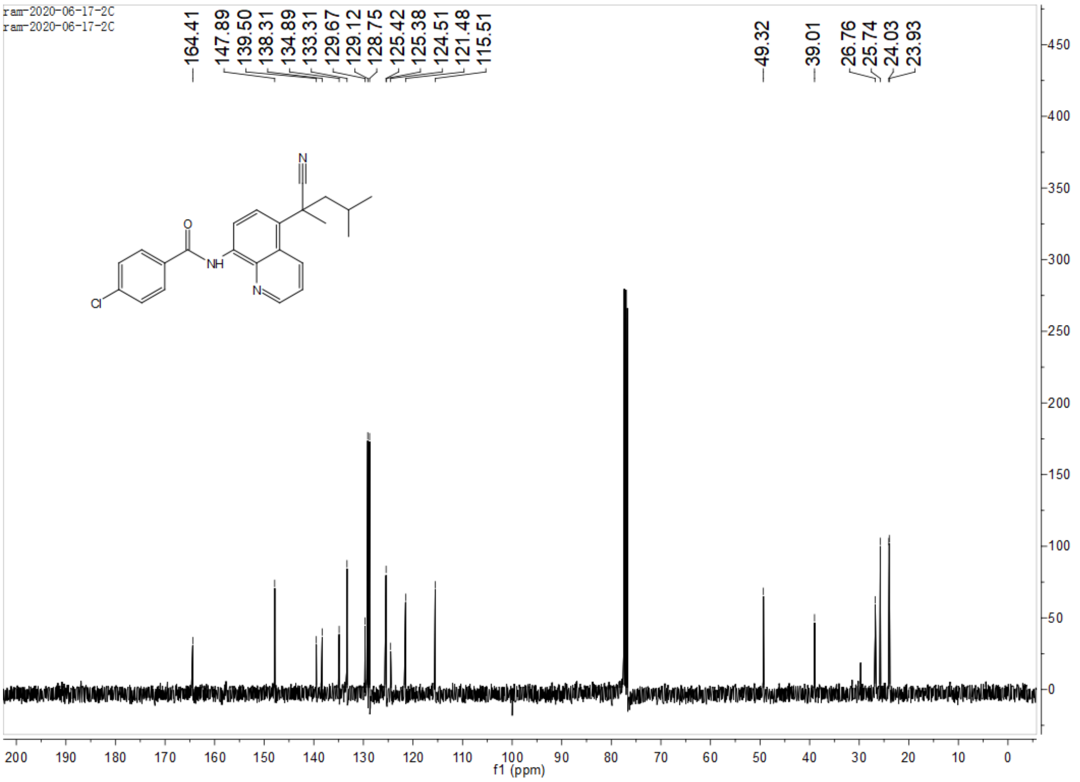


20200617-63c
178.99
168.16
147.40
139.34
136.69
136.65
134.96
134.14
132.74
131.36
130.31
127.25
126.11
126.01
124.00
121.29
115.78
52.49
45.84
27.54
20.20
NH
N
O
f1 (ppm)

3y:

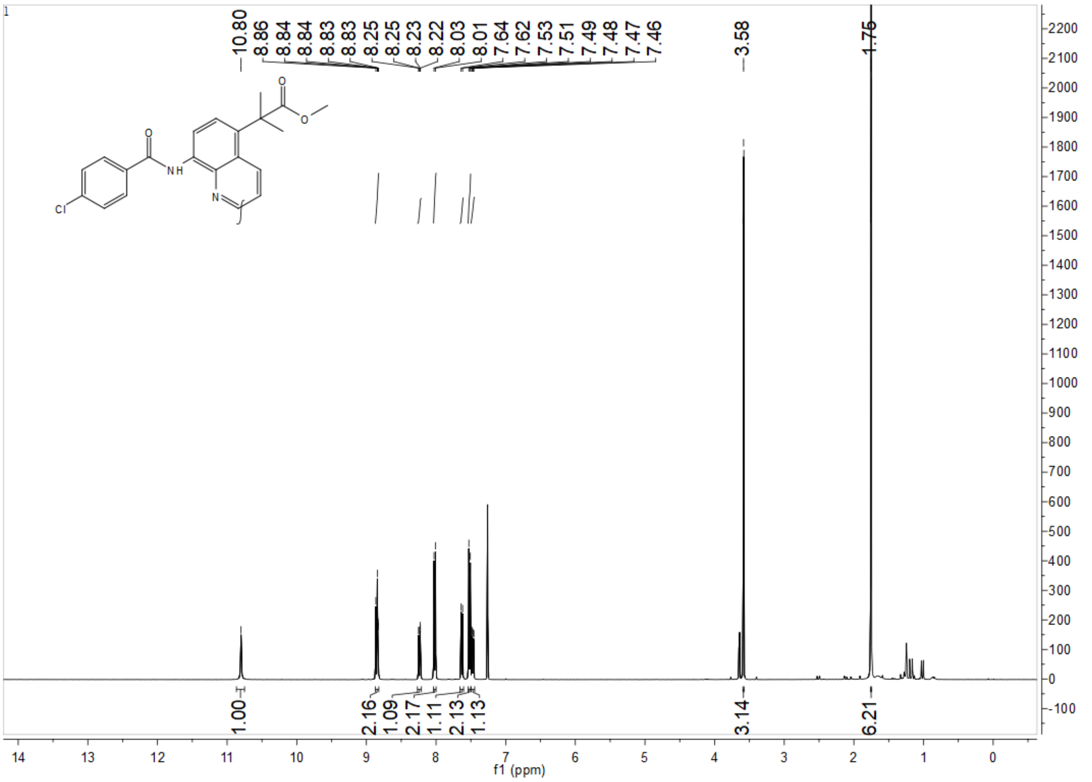


10.85
8.91
8.90
8.90
8.89
8.87
8.85
8.03
8.01
7.67
7.65
7.63
7.62
7.61
7.60
7.54
7.52
2.29
2.28
2.26
2.24
2.02
1.97
1.95
1.93
1.92
1.87
1.86
1.84
1.04
1.02
0.84
0.82
1.00
2.16
1.09
2.16
1.10
1.14
2.14
1.14
3.15
1.14
1.09
3.15
3.11
f1 (ppm)

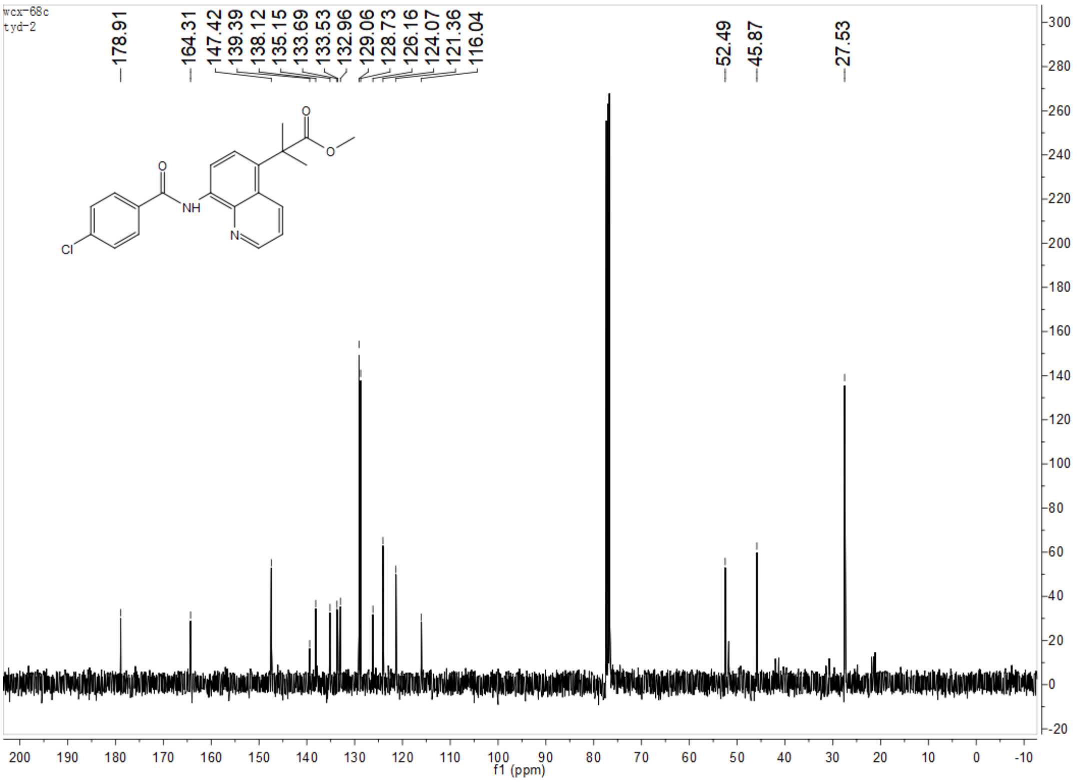


164.41
147.89
139.50
138.31
134.89
133.31
129.67
129.12
128.75
125.42
125.38
124.51
121.48
115.51
49.32
39.01
26.76
25.74
24.03
23.93
f1 (ppm)

3z:

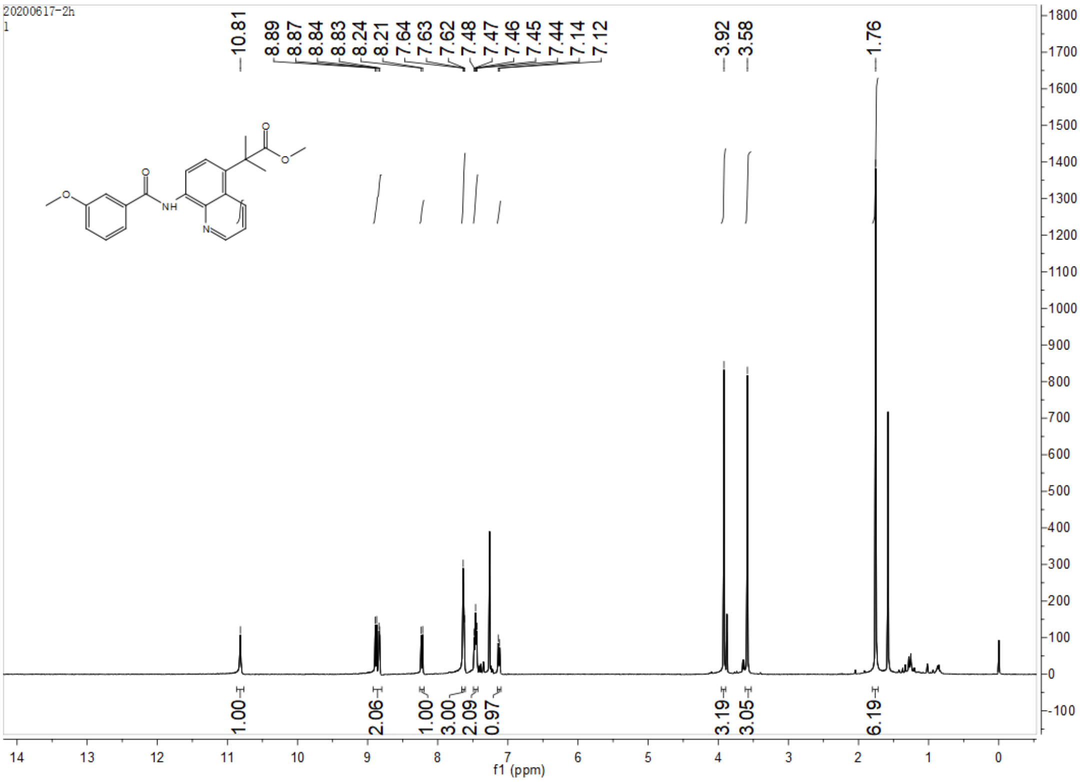


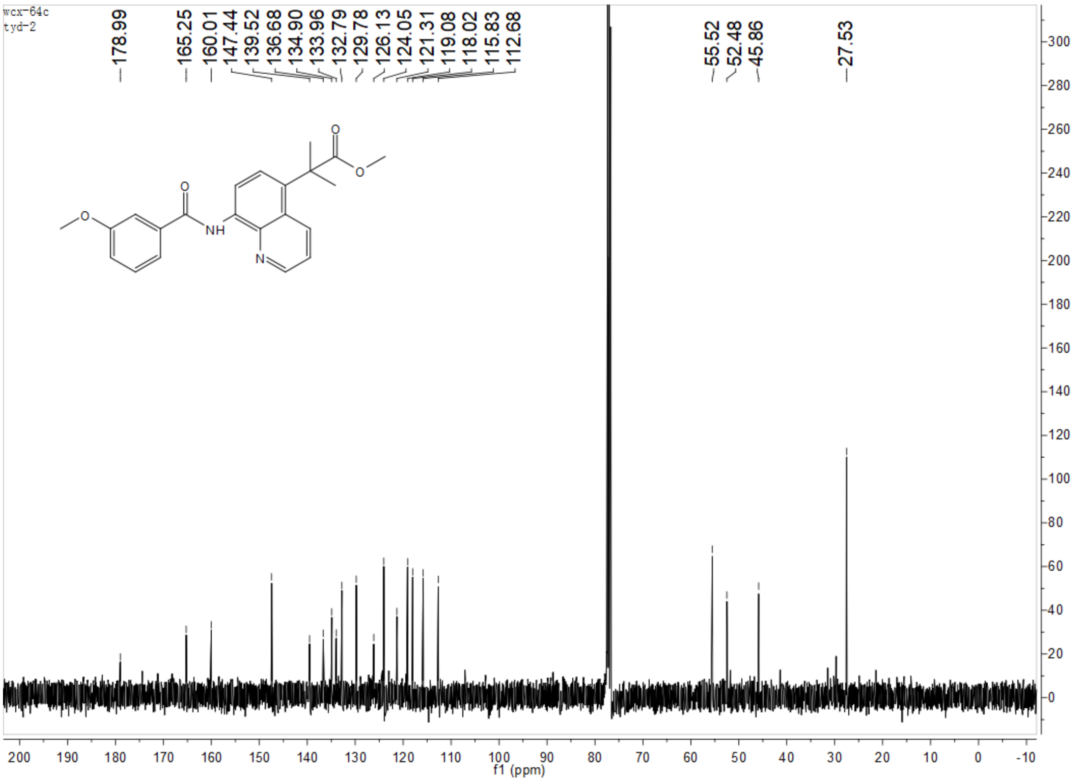
10.80
8.86
8.84
8.84
8.83
8.83
8.25
8.25
8.23
8.22
8.03
8.01
7.64
7.62
7.53
7.51
7.49
7.48
7.47
7.46
3.58
1.75
1.00
2.16
1.09
2.17
1.11
2.13
1.13
3.14
6.21
f1 (ppm)



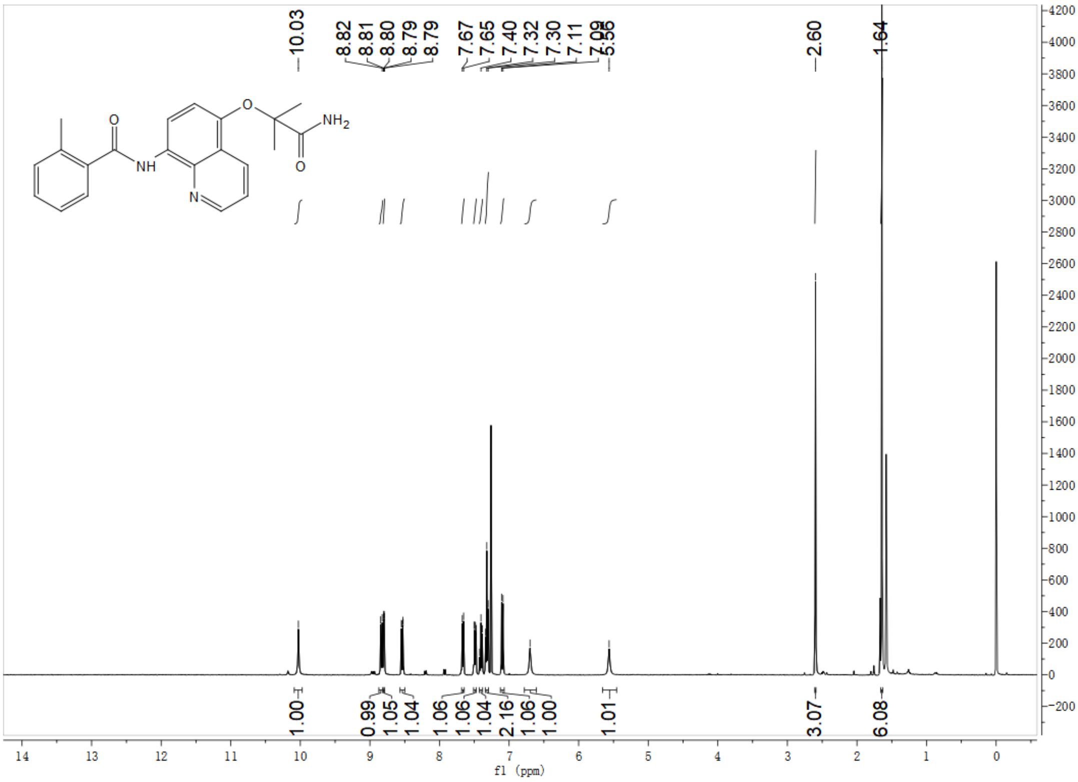
wcx-68c
tyd-2
178.91
164.31
147.42
139.39
138.12
135.15
133.69
133.53
132.96
129.06
128.73
126.16
124.07
121.36
116.04
52.49
45.87
27.53
f1 (ppm)

3aa:

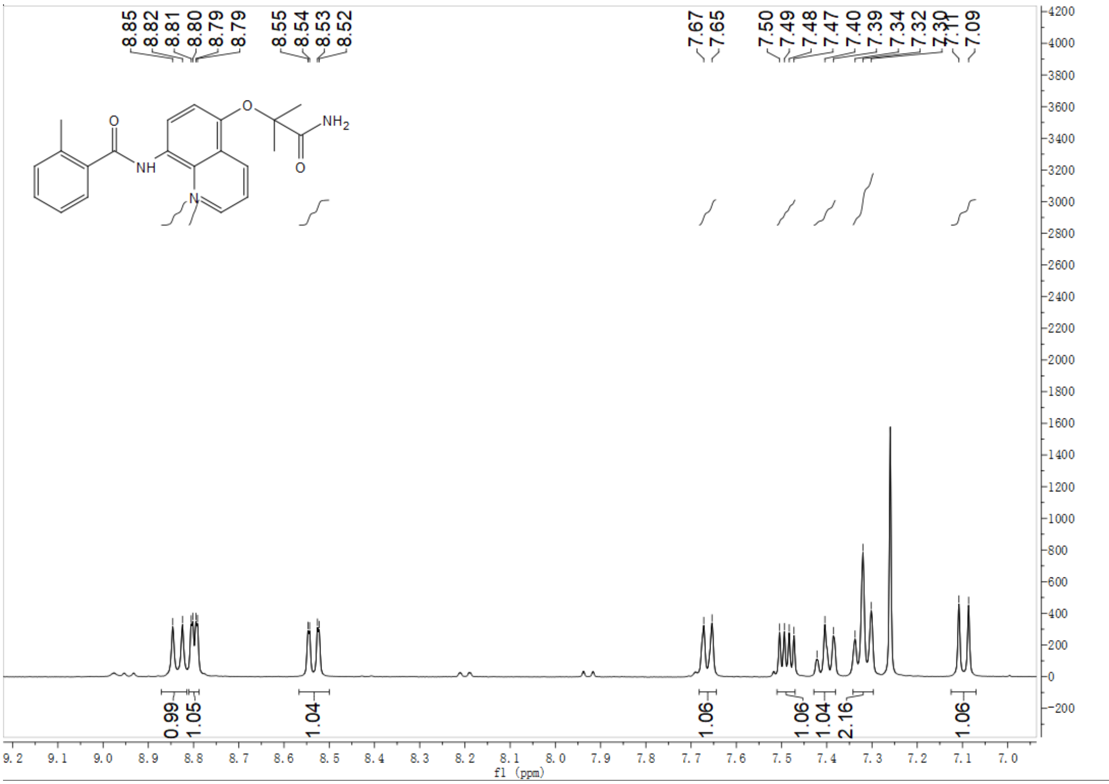

20200617-2h
1
10.81
8.89
8.87
8.84
8.83
8.24
8.21
7.64
7.63
7.62
7.48
7.47
7.46
7.45
7.44
7.14
7.12
3.92
3.58
1.76
1.00
2.06
1.00
3.00
2.09
0.97
3.19
3.05
6.19
f1 (ppm)


wcx-64c
tyd-2
178.99
165.25
160.01
147.44
139.52
136.68
134.90
133.96
132.79
129.78
126.13
124.05
121.31
119.08
118.02
115.83
112.68
55.52
52.48
45.86
27.53
f1 (ppm)

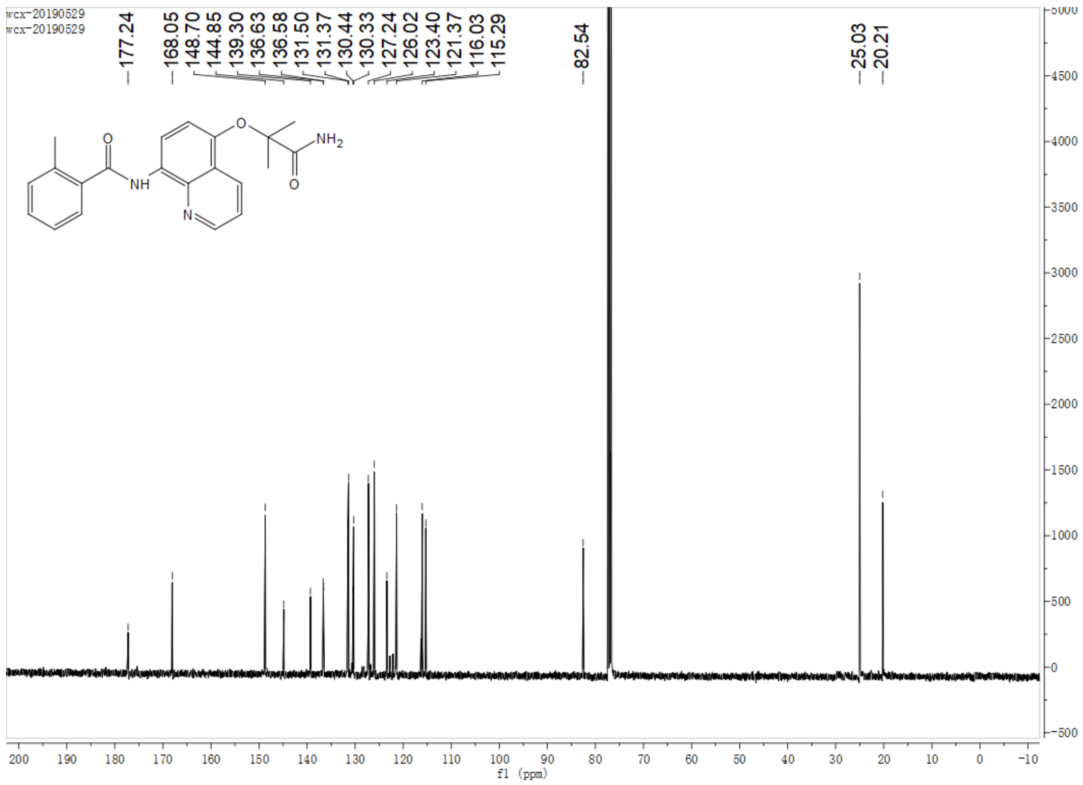
11:



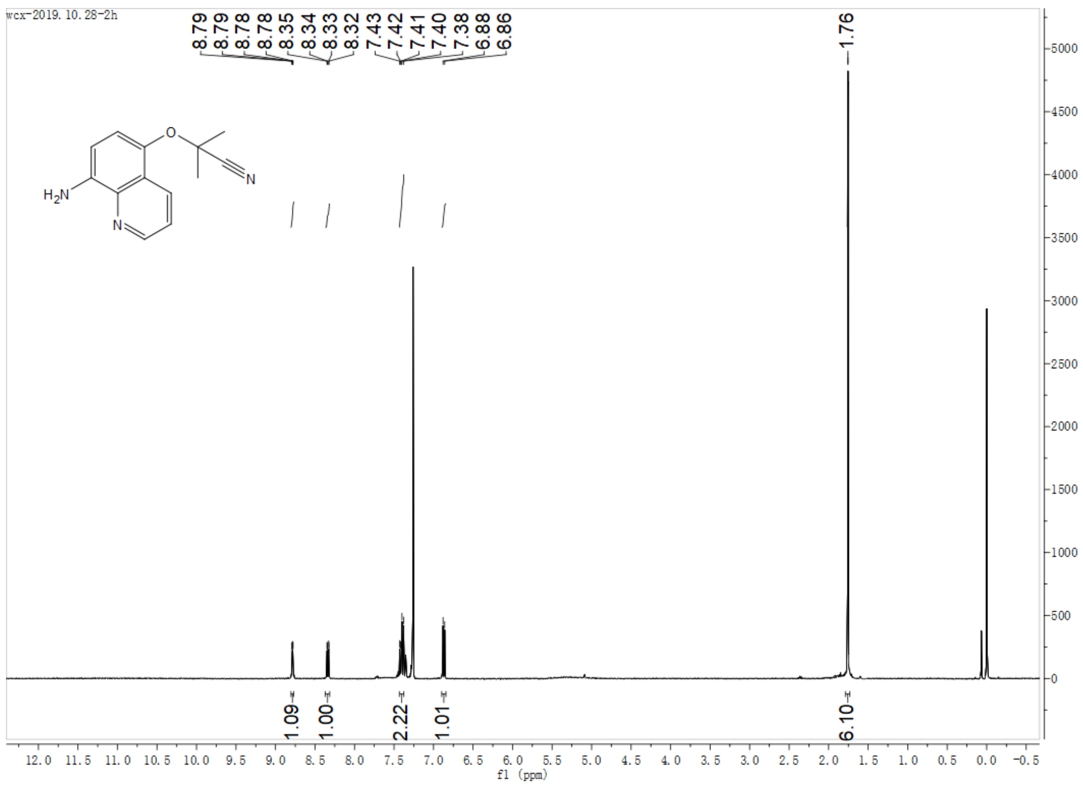
10.03
8.82
8.81
8.80
8.79
8.79
7.67
7.65
7.40
7.32
7.30
7.11
7.09
5.56
2.60
1.64
NH$_2$
O
NH
N
1.00
0.99
1.05
1.04
1.06
1.06
1.04
2.16
1.06
1.00
1.01
3.07
6.08
f1 (ppm)

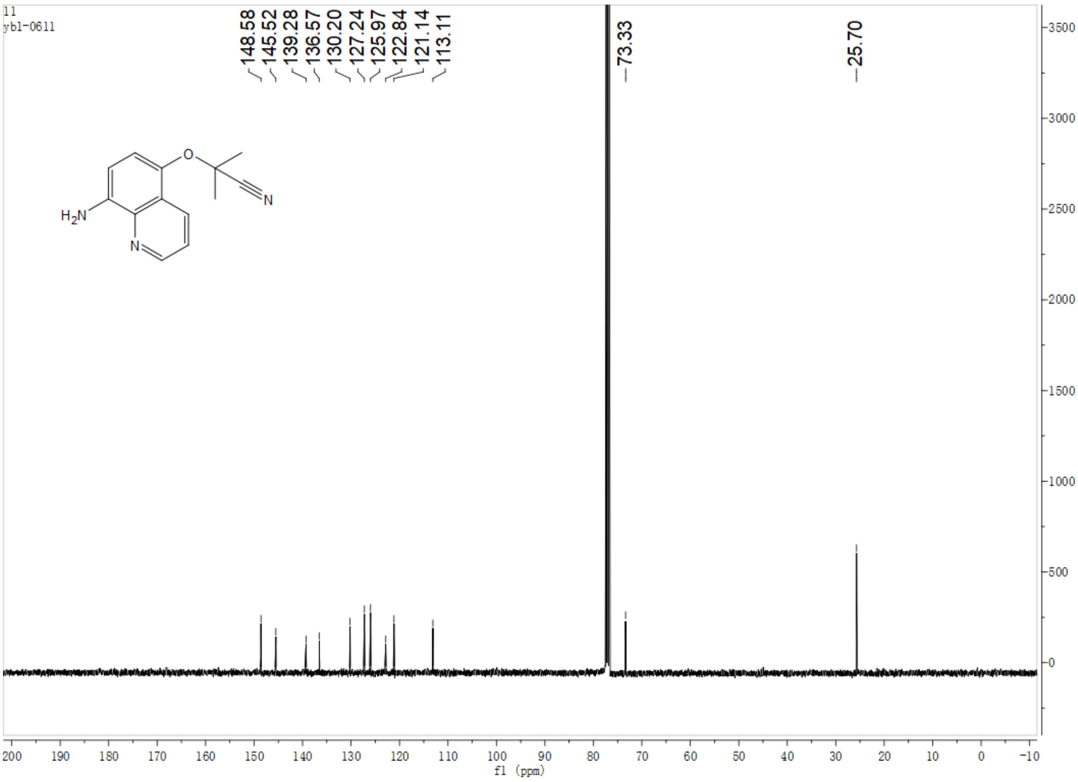


8.85
8.82
8.81
8.80
8.79
8.79
8.55
8.54
8.53
8.52
7.67
7.65
7.50
7.49
7.48
7.47
7.40
7.39
7.34
7.32
7.30
7.11
7.09
NH$_2$
O
NH
N
0.99
1.05
1.04
1.06
1.06
1.04
2.16
1.06
f1 (ppm)

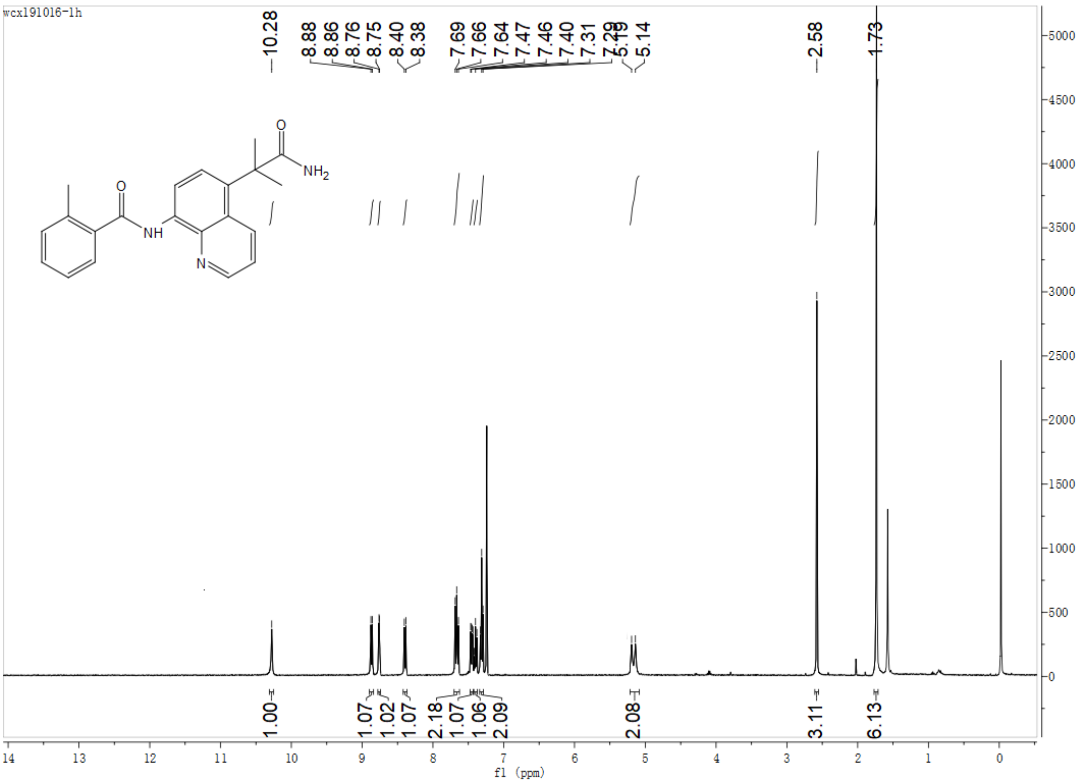

wcx-20190529
wcx-20190529
177.24
168.05
148.70
144.85
139.30
136.63
136.58
131.50
131.37
130.44
130.33
127.24
126.02
123.40
121.37
116.03
115.29
82.54
25.03
20.21
O
NH
N
O
NH2
O
f1 (ppm)

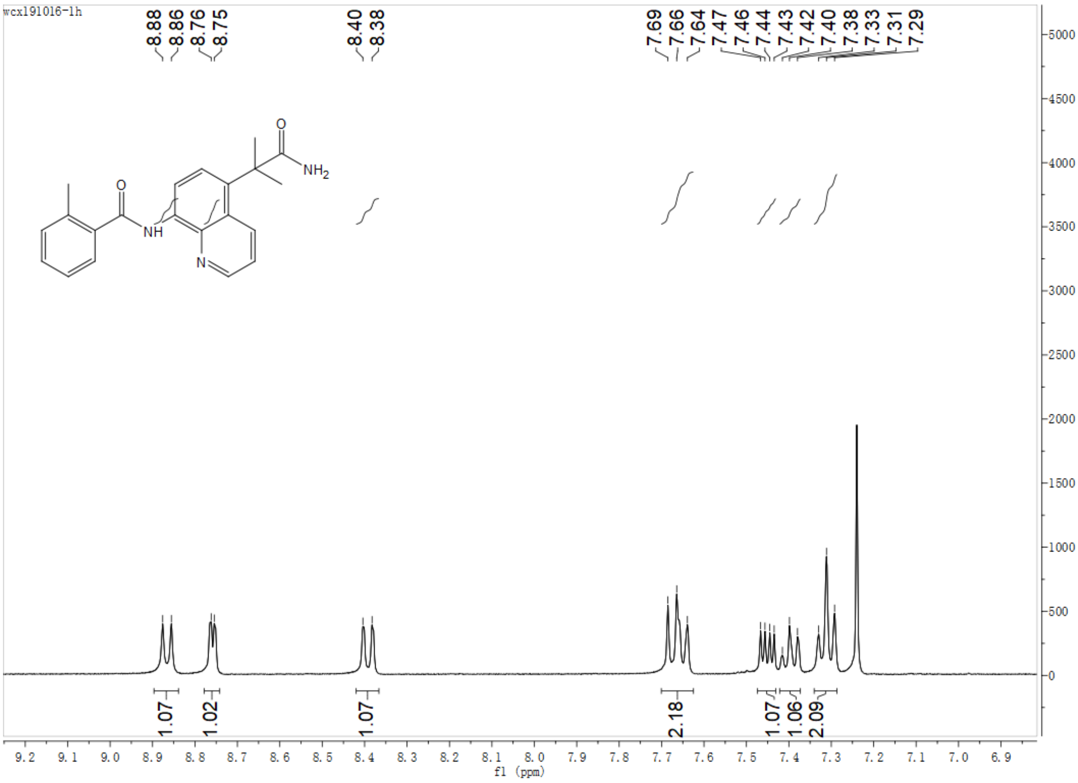
12:

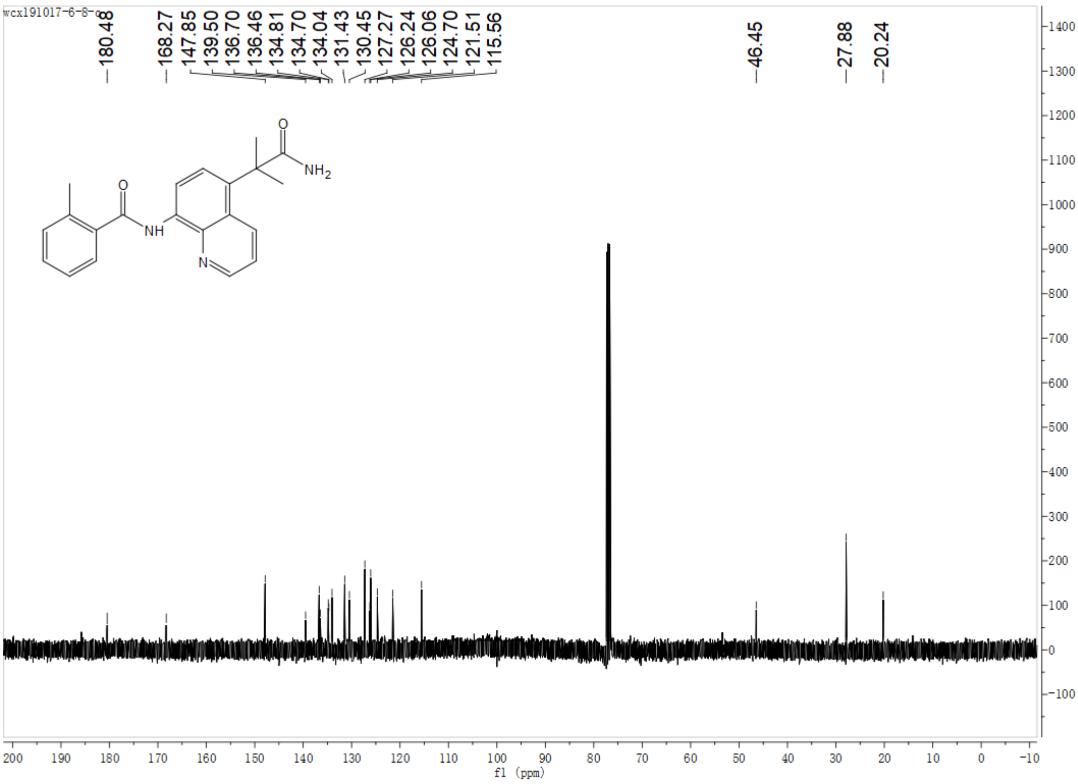

wcx-2019.10.28-2h
8.79
8.79
8.78
8.78
8.35
8.34
8.33
8.32
7.43
7.42
7.41
7.40
7.38
6.88
6.86
1.76
O
N
H2N
N
1.09
1.00
2.22
1.01
6.10
f1 (ppm)


11
ybl-0611
148.58
145.52
139.28
136.57
130.20
127.24
125.97
122.84
121.14
113.11
73.33
25.70
H2N
N
O
N
f1 (ppm)

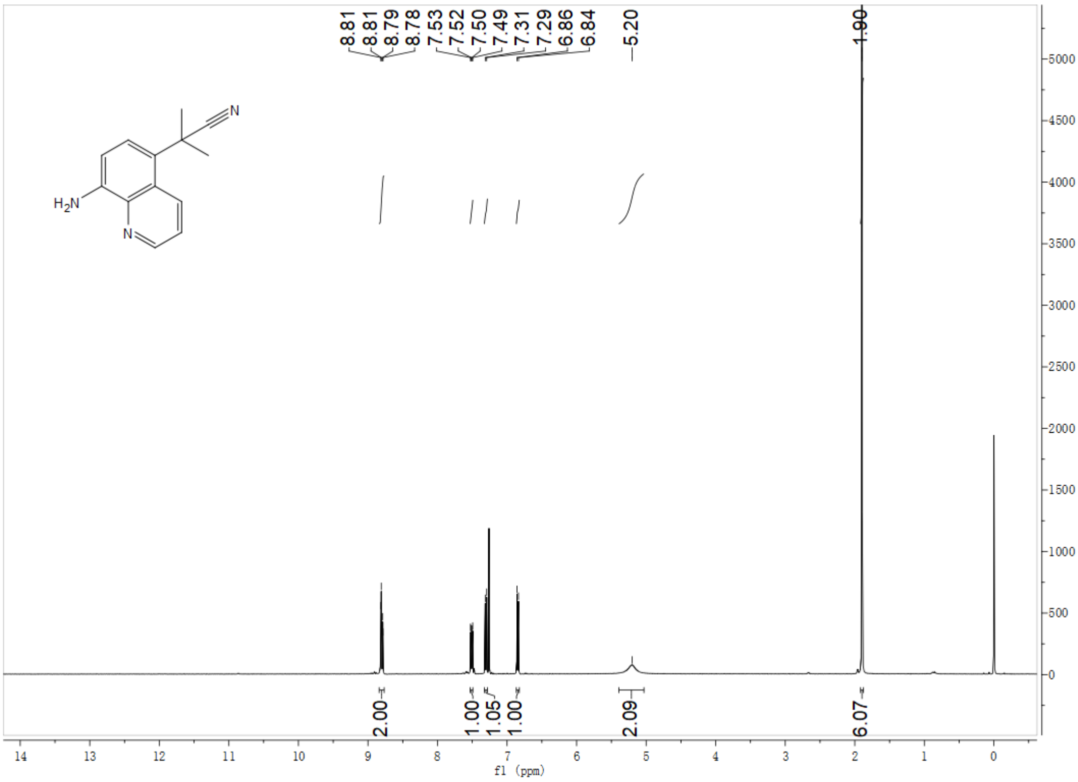
13:

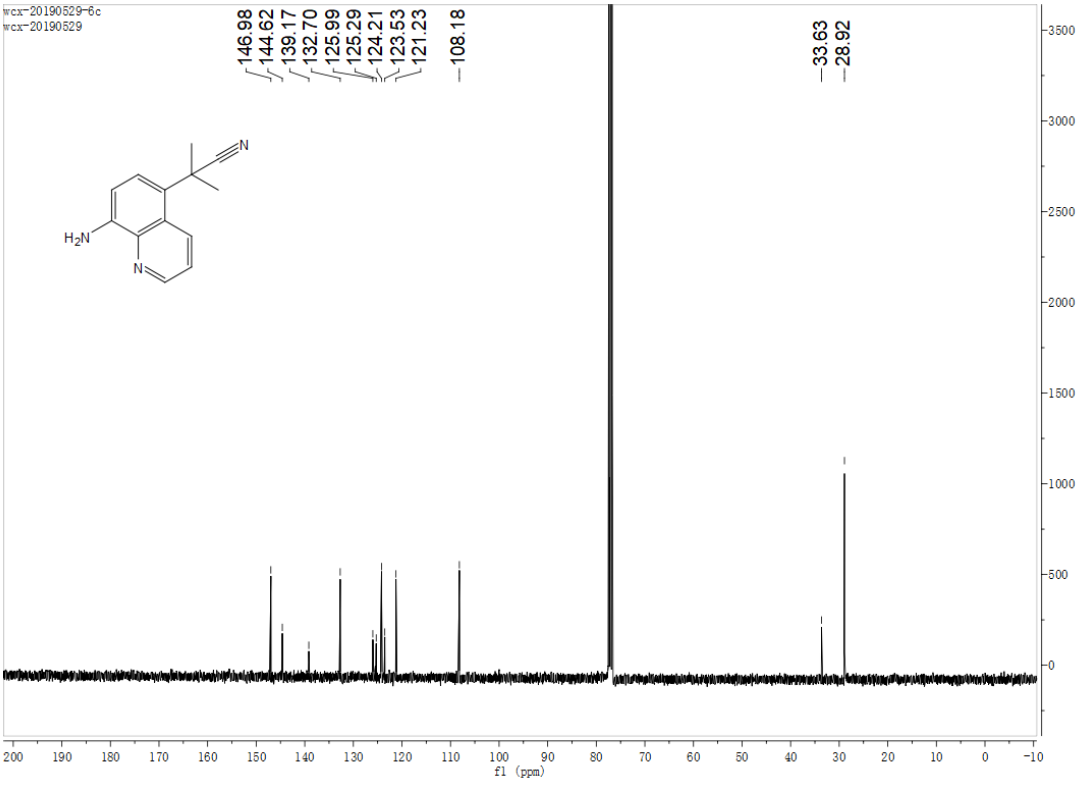

wcx191016-1h
10.28
8.88
8.86
8.76
8.75
8.40
8.38
7.69
7.66
7.64
7.47
7.46
7.40
7.31
7.29
5.19
5.14
2.58
1.73
O
NH2
O
NH
N
1.00
1.07
1.02
1.07
2.18
1.07
1.06
2.09
2.08
3.11
6.13
f1 (ppm)


wcx191016-1h
8.88
8.86
8.76
8.75
8.40
8.38
7.69
7.66
7.64
7.47
7.46
7.44
7.43
7.42
7.40
7.38
7.33
7.31
7.29
O
NH2
O
NH
N
1.07
1.02
1.07
2.18
1.07
1.06
2.09
f1 (ppm)


wcx191017-6-8-c
180.48
168.27
147.85
139.50
136.70
136.46
134.81
134.70
134.04
131.43
130.45
127.27
126.24
126.06
124.70
121.51
115.56
46.45
27.88
20.24
O
NH2
O
NH
N
f1 (ppm)

14:


8.81
8.81
8.79
8.78
7.53
7.52
7.50
7.49
7.31
7.29
6.86
6.84
5.20
1.90
H2N
N
N
2.00
1.00
1.05
1.00
2.09
6.07
f1 (ppm)


wcx-20190529-6c
wcx-20190529
146.98
144.62
139.17
132.70
125.99
125.29
124.21
123.53
121.23
108.18
33.63
28.92
H2N
N
N
f1 (ppm)

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