Heterogeneous Single-Site copper in Hierarchical MOF Microspheres Enables Sustainable Urea-Functionalization of Quinoline N-Oxides

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1. General information

1.1 Materials

Unless otherwise specified, all reagents and solvents were obtained from commercial suppliers and used without further purification. All reagents were weighed and handled in air at room temperature.

1.2 Characterizations

X-ray diffraction (XRD) patterns were collected with an X-ray powder diffractometer (D/Max 2400, Japan). N_2 adsorption-desorption isotherms were recorded using an automated gas sorption analyzer (BET, Autosorb-iQ-C, USA). The morphology characterizations were carried out with scanning electron microscopy (SEM, Nova. Nano SEM 450, USA), high-resolution transmission electron microscopy (HRTEM, Jem-2100F), and high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM, FEI Themis Z). X-ray photoelectron spectroscopy (XPS) measurement was performed with a non-monochromatic Al Kα X-ray source and a hemispherical energy analyzer (Escalab 250Xi, Thermo Fisher). X-ray absorption fine structure (XAFS) measurement was measured at Beijing Synchrotron Radiation Facility, China. The copper and aluminium contents in the sample were determined by inductively coupled plasma mass spectrometry (ICP-MS, NexION 300D) after microwave digestion. Elemental analysis for C, H, N, and O was performed on an Elementar Vario EL analyzer. C, H, and N contents were measured using the CHNS operation mode, and O content was measured using the separate O mode. Mass spectra were performed on a spectrometer operating on ESI-TOF.

NMR Experimental Details: ^{1}H NMR spectra were recorded at 400 MHz and ^{13}C NMR spectra were recorded at 100 MHz by using a Bruker Avance 400 spectrometer. Chemical shifts were calibrated using residual undeuterated solvent as an internal reference (^{1}H NMR: $CDCl_3$ 7.26 ppm, ^{13}C NMR: $CDCl_3$ 77.0 ppm, ^{1}H NMR: DMSO 2.50 ppm, ^{13}C NMR: 40.0 ppm). The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Chromatographic purifications were carried out on a Biotage Isolera Four instrument. Sample Preparation: all compounds were prepared for NMR analysis by dissolving approximately 5-15mg of sample in 0.6 mL of deuterated dimethyl sulfoxide (DMSO-d_6). The residual solvent signals were used as an internal reference. Measurement Parameters: all NMR spectra were acquired on a Bruker Avance 400 spectrometer equipped with a 5 mm PABBO BB-1H/D probe. ^{1}H NMR spectra: operating frequency 400.13 MHz, measurement temperature 293.3 K, using the zg30 pulse

program. The specific parameters were as follows: spectral width (SW) 20.03 ppm, acquisition time (AQ) 4.09 s, relaxation delay (D1) 1.0 s, number of scans (NS) 16, and 90° pulse width (P1) 17.8 μs. ^{13}C NMR spectra: Operating frequency 100.62 MHz, measurement temperature 294.1 K, using the zgpg30 pulse program. The specific parameters were as follows: spectral width (SW) 238.90 ppm, acquisition time (AQ) 1.36 s, relaxation delay (D1) 2.0 s, number of scans (NS) 500-1000，and 90° pulse width (P1) 76.3 μs, with composite pulse ^{1}H decoupling (Waltz16) applied during acquisition. Data Processing and Integration: the acquired free induction decays (FIDs) were processed using MestReNova software. Exponential line broadening (LB = 0.3 Hz for ^{1}H NMR; LB = 1.0 Hz for ^{13}C NMR) was applied, followed by zero-filling to 65536 points, and subsequent Fourier transformation. Manual phase and baseline corrections were applied to all spectra. For ^{1}H NMR spectra, peak integration was performed manually on the phase- and baseline-corrected spectra.

2. Preparation and characterization of MOF-based catalyst

2.1 Syntheses of MOF catalysts

The MOF-253 was synthesized and purified according to a traditional solvothermal method reported in the literature[1]. $AlCl_3 \cdot 6H_2O$ (151 mg, 0.625 mmol) and 2,2′-bipyridine-5,5′-dicarboxylic acid (306 mg, 1.25 mmol) were dissolved in 10 mL DMF, sealed in a Teflon-lined autoclave, and hydrothermally treated at 120°C for 24 h. The product was centrifuged, washed with DMF and methanol (3-day soaking), then vacuum-dried at 80°C for 12 h.

The MOF-253-Cu was prepared by simple impregnation method. Typically, a mixture of 100 mg MOF-253 and $Cu(BF_4)_2$ (molar ratio 1:0.4) was dispersed in 3 mL acetonitrile and stirred at room temperature for 12 h. The blue product was centrifuged, washed (MeCN/EtOH), and dried under vacuum at 80°C for 12 h.

MOF-253-M (M = $Zn(BF_4)_2$, $Co(BF_4)_2$, $Cu(NO_3)_2$, $Cu(SO_4)_2$) were prepared analogously to MOF-253-Cu with the corresponding metal salts instead of $Cu(BF_4)_2$.

2.2 MOF Catalysts characterization data

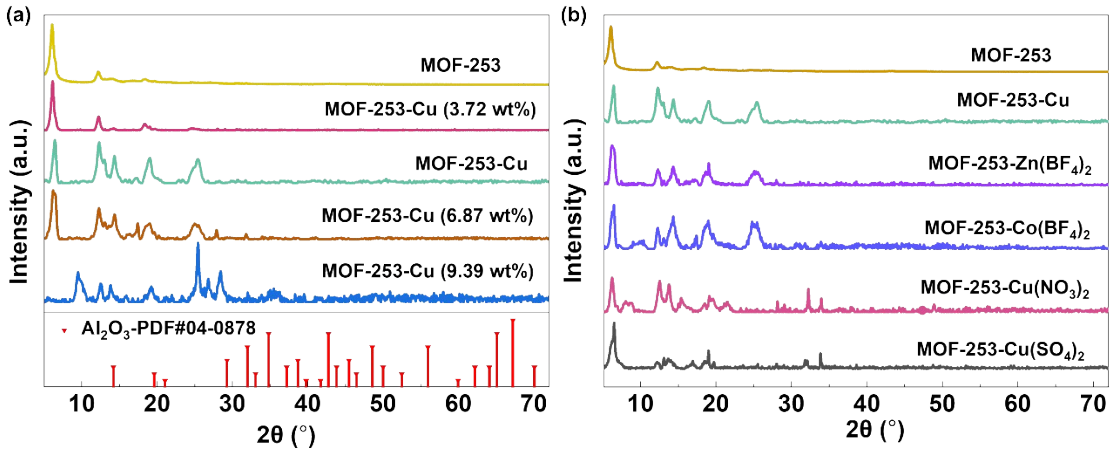


Figure S1. XRD patterns of MOF-253 and its metalated derivatives.

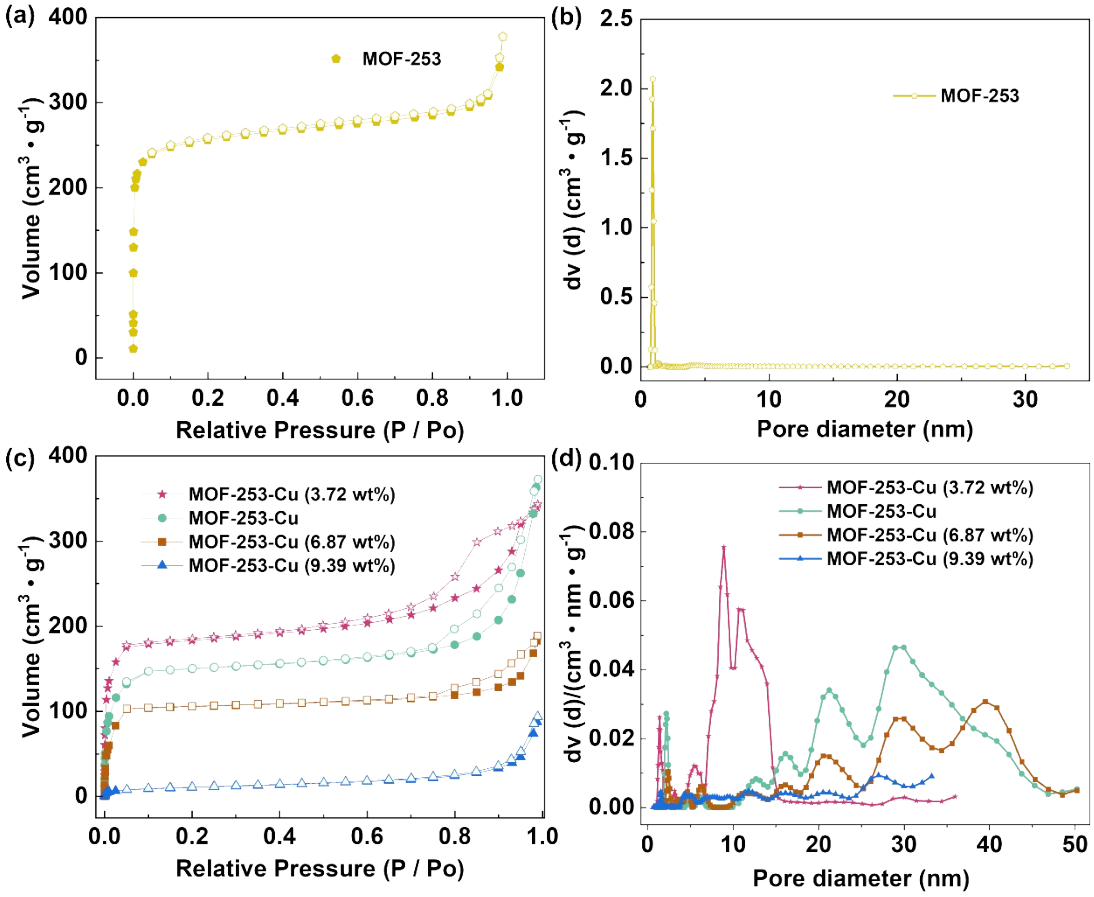


Figure S2. N_2 adsorption–desorption isotherms and corresponding pore size distribution profiles of various samples.

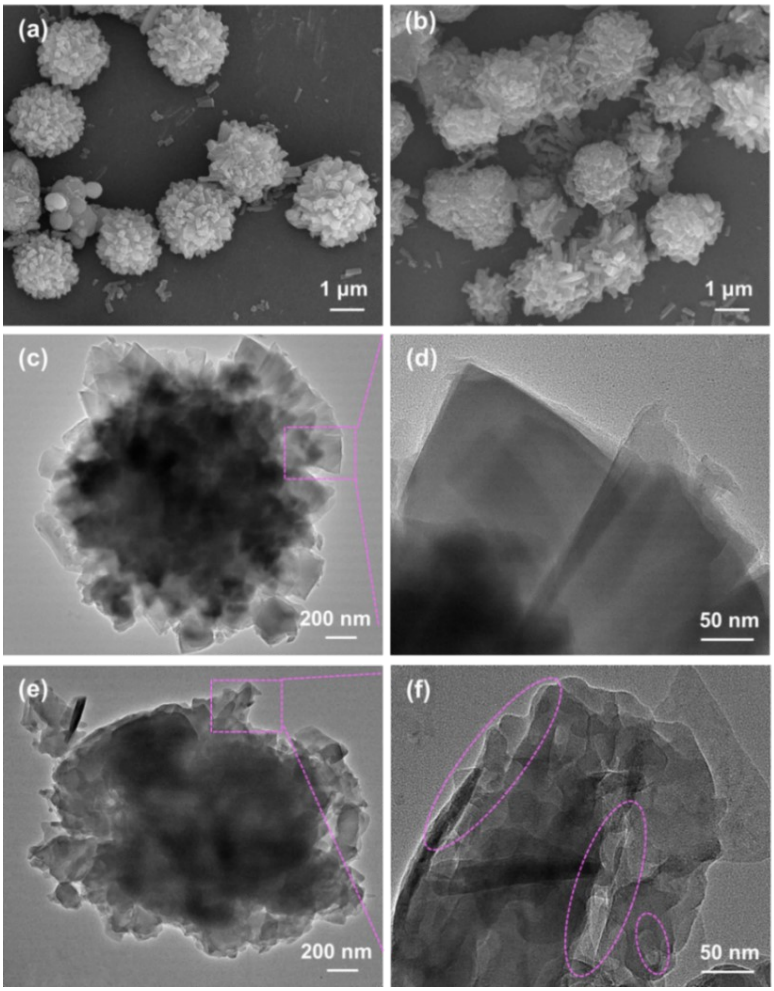


Figure S3. SEM images of (a) pristine MOF-253 and (b) MOF-253-Cu. TEM images of (c, d) pristine MOF-253 and (e, f) MOF-253-Cu.

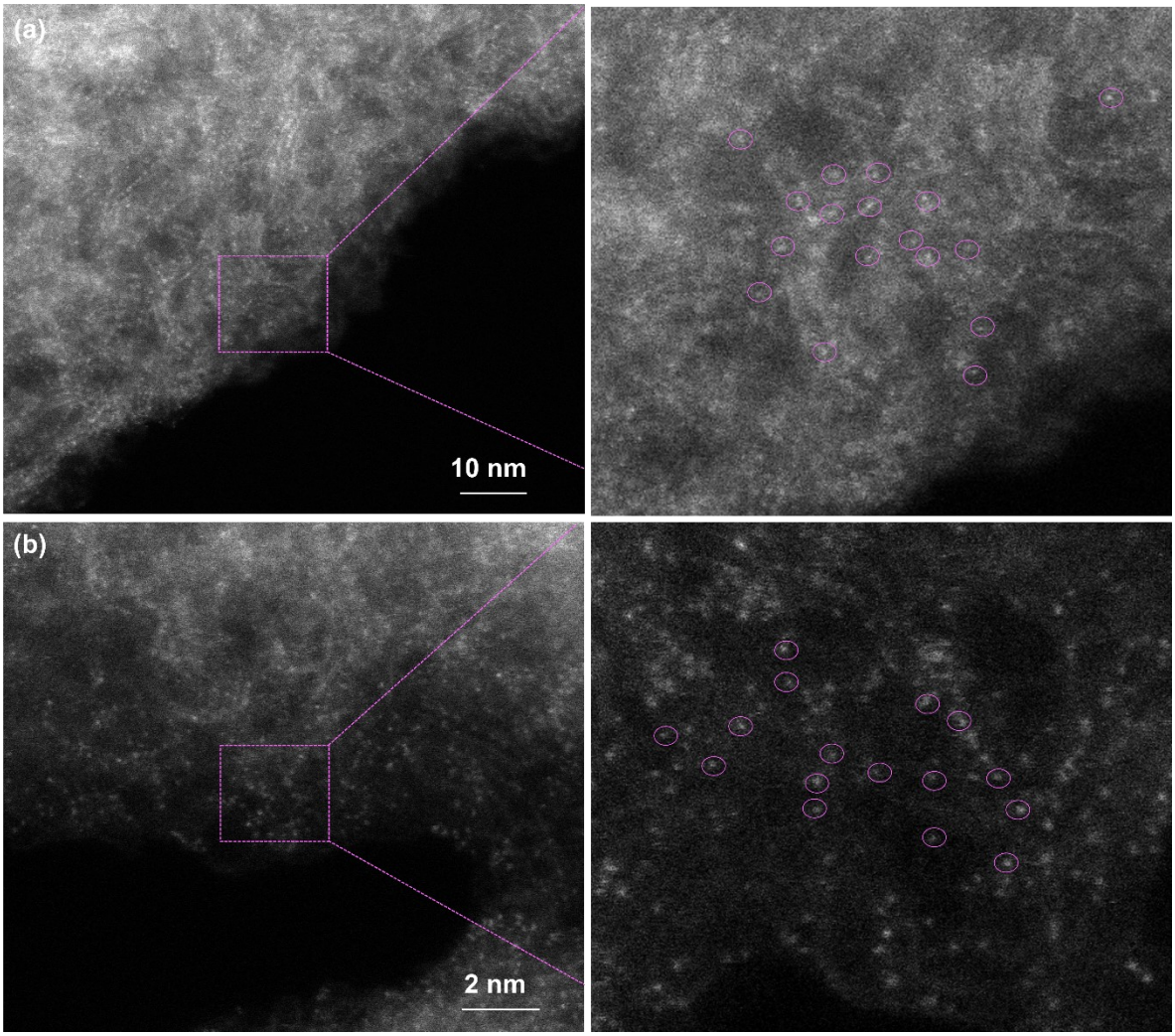


Figure S4. HAADF-STEM images of MOF-253-Cu.

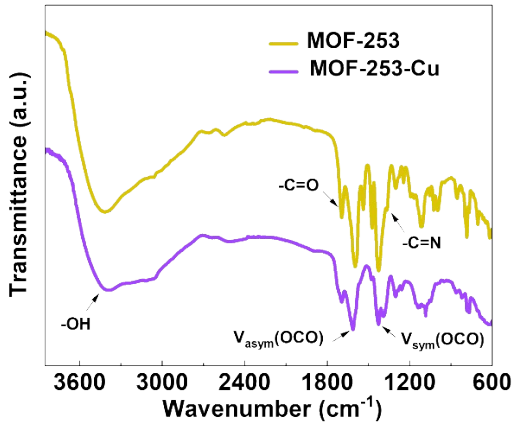


Figure S5. Infrared spectroscopy of pristine MOF-253 and MOF-253-Cu.

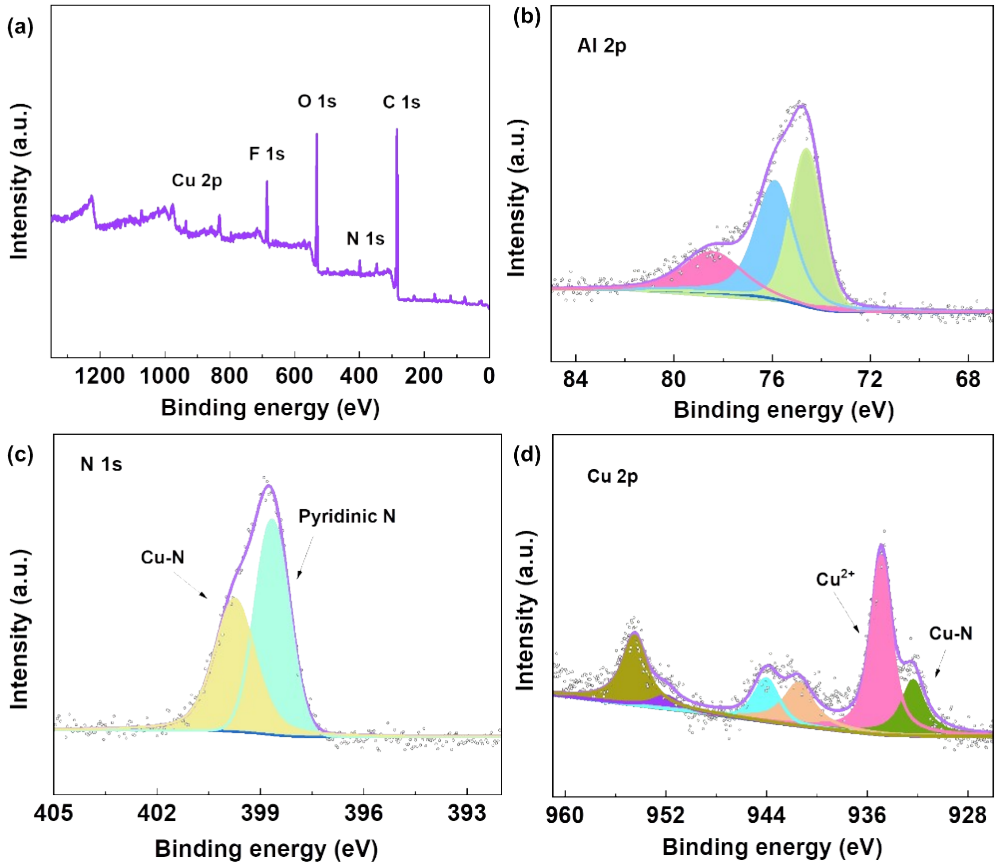


Figure S6. XPS spectra of the MOF-253-Cu. (a) full survey spectrum, (b) Al 2p, (c) N 1s, and (d) Cu 2p.

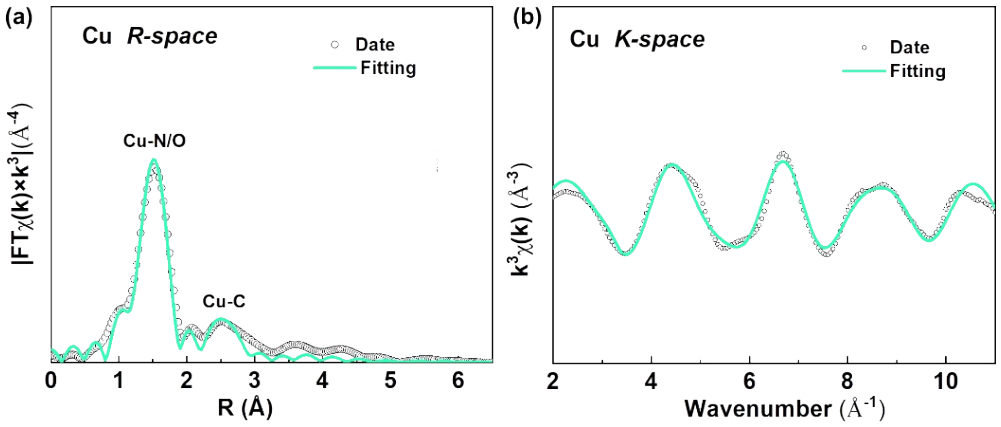


Figure S7. (a) EXAFS fitting curve of MOF-253-Cu in R-space and K-space.

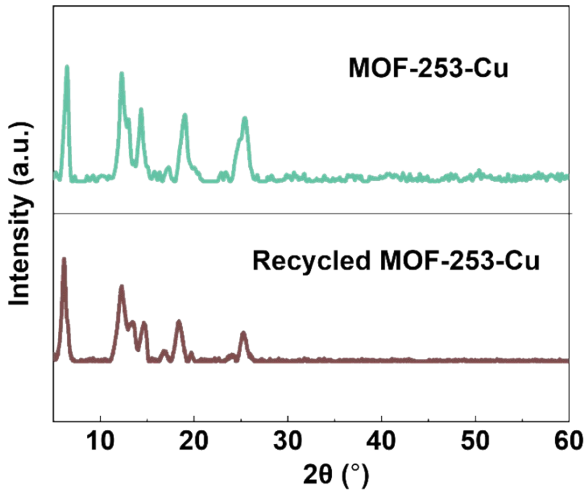


Figure S8. Comparison of XRD patterns for MOF-253-Cu before and after 8 catalytic cycles

Table S1. Elemental analysis of MOF-253 and MOF-253-Cu[a]

Name	Al	Cu	C	H	N	O	C/Al	C/N
MOF-253	9.21	/	50.63	2.35	9.98	26.69	5.497	5.073
MOF-253-Cu	7.49	5.43	37.81	1.78	7.32	21.25	5.048	5.165

[a]After microwave digestion, Cu and Al contents were determined by ICP-MS. Elemental analysis for C, H, N, and O was performed, with C/H/N measured in CHNS mode and O measured separately in O mode.

Table S2. Surface area and copper loading content of various samples.

Materials	Cu (wt%)	Surface area (m^2/g)
MOF-253	/	1001
MOF-253-Cu (3.72 wt%)	3.72	392
MOF-253-Cu	5.43	327
MOF-253-Cu (6.87 wt%)	6.87	226
MOF-253-Cu (9.39 wt%)	9.39	89

Table S3. EXAFS fitting parameters at the Cu K–edge for various samples

Sample	Shell	*CN*[a]	*R*(Å)[b]	σ^2(Å^2)[c]	ΔE_0(eV)[d]	*R* factor
Cu foil	Cu-Cu	12*	2.54±0.01	0.0086	4.0	0.0025
Cu_2O	Cu-O	2*	1.85±0.01	0.0025	6.9	0.0140
	Cu-Cu	12*	3.04±0.01	0.0199	8.7	
CuO	Cu-O	4*	1.95±0.01	0.0046	-1.1	0.0195
	Cu-Cu	10*	2.90±0.01	0.0224	-7.8	
	Cu-Cu	2*	3.56±0.01	0.0057	10.9	
CuPc	Cu-N	4*	1.94±0.01	0.0023	4.9	0.0099
	Cu-N/O	**4.0±0.3**	**1.94±0.01**	**0.0036**	**7.7**	
MOF-253-Cu	**Cu-C**	**3.5±1.4**	**2.84±0.01**	**0.0050**	**1.6**	**0.0159**
	Cu-C	**10.6±4.3**	**3.18±0.01**	**0.0011**	**9.5**	

[a]*CN*, coordination number; [b]*R*, distance between absorber and backscatter atoms; [c]σ^2, Debye-Waller factor to account for both thermal and structural disorders; [d]ΔE_0, inner potential correction; *R* factor indicates the goodness of the fit. S_0^2 was fixed to 0.835, according to the experimental EXAFS fit of Cu foil by fixing CN as the known crystallographic value. Fitting range: $2.0 \le k$ (/Å) ≤ 12.0 and $1 \le R$ (Å) ≤ 3.0 (Cu foil); $2.0 \le k$ (/Å) ≤ 12.0 and $1.0 \le R$ (Å) ≤ 3.0 (Cu_2O); $2.0 \le k$ (/Å) ≤ 12.0 and $1.0 \le R$ (Å) ≤ 3.6 (CuO); $2.0 \le k$ (/Å) ≤ 12.0 and $1.0 \le R$ (Å) ≤ 2.0 (CuPc); $2.0 \le k$ (/Å) ≤ 10.0 and $1.0 \le R$ (Å) ≤ 2.9 (MOF-253-Cu). A reasonable range of EXAFS fitting parameters: $0.600 < S_0^2 < 1.000$; $CN > 0$; $\sigma^2 > 0$ Å^2; $|\Delta E_0| < 15$ eV; *R* factor < 0.02.

3. MOF-253-Cu-Catalyzed Synthesis of Quinoline-Urea Derivatives

3.1 Synthesis of Quinoline N-oxides

The quinolone compound (3.0 mmol) was dissolved in 20 mL of CH_2Cl_2 in a 100 mL round-bottom flask. Subsequently, m-chloroperbenzoic acid (4.5 mmol) was added dropwise to the flask at 0 °C, and the mixed solution was reacted at 30 °C for 6 hrs. After the reaction was complete, saturated Na_2SO_3 solution was used to wash the reaction solution. The solution was separated via extraction, and the organic phase was further concentrated under vacuum. The crude product was purified by silica gel column chromatography to obtain the pyridine/quinoline N-oxide.

3.2 General procedure for the synthesis of quinoline-urea derivatives 3

Quinoline-*N*-oxides **1** (0.3 mmol), carbodiimide **2** (0.36 mmol), MOF-253-Cu (6 mg), and dimethyl sulfoxide (DMSO, 2.5 mL) were added to a 15 mL glass tube at room temperature. The mixture was then stirred at 40 °C for 15 hours. After completion of the reaction, the solvent DMSO was removed under reduced pressure with a recovery rate of 95%, and the crude product was purified by silica gel column chromatography to afford the desired product **3**.

3.3 Large-scale synthesis of 3a, 3c and 3l

Quinoline-N-oxide **1a** (10.0 mmol), N, N'-dicyclohexylcarbodiimide **2a** (12.0 mmol), MOF-253-Cu catalyst (200.0 mg), and DMSO (80.0 mL) were charged into a 150 mL glass reactor under ambient conditions. The reaction mixture was maintained under continuous agitation at 40°C for 15 h. Upon completion, the system was cooled to ambient temperature and subjected to HPLC analysis, affording the target urea derivative **3a** in 89% yield.

4-methylquinoline 1-oxide (**1c**, 10.0 mmol) underwent ureidation under identical reaction conditions to deliver 1,3-dicyclohexyl-1-(4-methylquinolin-2-yl) urea **3c** in 85% yield. Parallel treatment of 4-chloroquinoline 1-oxide (**1l**, 10.0 mmol) via the same ureidation protocol offered 1-(4-chloroquinolin-2-yl)-1,3-dicyclohexylurea **3l** with 82% yield.

3.4 Calculating of green chemistry metrics

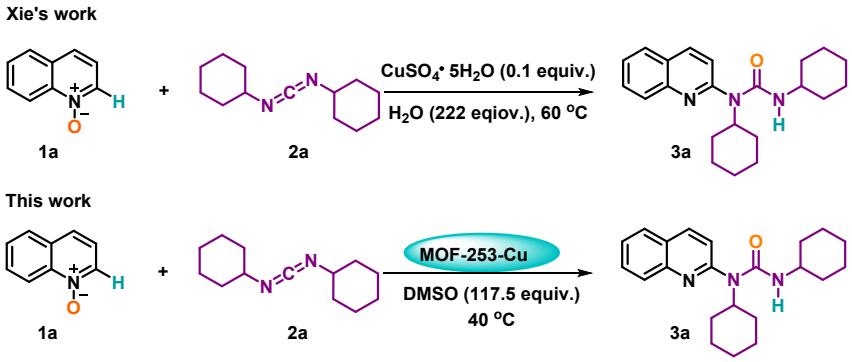


Table S4. Comparison of reaction conditions

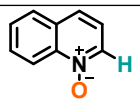
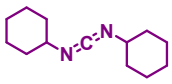
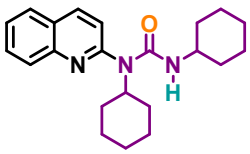
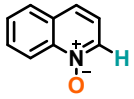
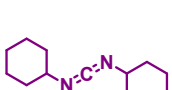
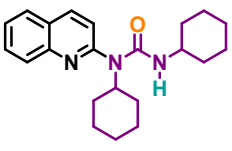
method	Substrate	Catalyst	solvent	product
Xie's work	 **M = 145.2** 145.2 X 1 = 145.2  **M = 206.2** 206.2 X 1 = 206.2	$CuSO_4 \cdot 5H_2O$ **M = 249.61** 246.91X0.1=24.69	H_2O (M = 18) 18 X222.2=3999.6	 **M = 351.4** 351.4 X 0.92 = 323.3
This work	 **M = 145.2** 145.2 X 1 = 145.2  **M = 206.2** 206.2 X 1 = 206.2	MOF-253-Cu (6 mg) **Filtration and Recovery**	DMSO (M = 78) 78X117.5=9165	 **M = 351.4** 351.4 X 0.95 = 333.8

Table S5. Calculation of green chemistry metrics

$$AE = \frac{\text{MW of product}}{\text{MW of stoichiometric reactants}} \times 100\%$$

$$= \frac{351.4}{145.2 + 206.2} \times 100\% = \mathbf{100\%}$$ Xie's work

$$= \frac{351.4}{145.2 + 206.2} \times 100\% = \mathbf{100\%}$$ this work

$$RME = \frac{\text{Mass of product}}{\text{Total mass of inputs}} \times 100\%$$

$$= \frac{0.3 \times 351.4 \times 0.92/1000}{(0.3 \times 145.2 + 0.36 \times 206.2 + 0.03 \times 249.61)/1000 + (6.2 \times 1 + 15 \times 0.9)*0.05 + 2} \times 100\%$$

$$= \mathbf{3.11\%}$$ Xie's work

$$= \frac{0.3 \times 351.4 \times 0.95/1000}{(0.3 \times 145.2 + 0.36 \times 206.2)/1000 + 2.5 \times 1.1 \times 0.05} \times 100\%$$ this work

$$= \mathbf{39.2\%}$$

$$\text{E-factor} = \frac{\text{Total Mass of Inputs - Mass of Product}}{\text{Mass of Product}} \times 100\%$$

$$= \frac{10366 - 323.3}{323.3} = \mathbf{31}$$ Xie's work

$$= \frac{850.9 - 333.8}{333.8} = \mathbf{1.55}$$ this work

4. Mechanism Research

4.1 Reaction quinoline under standard conditions

Quinoline **4a** (0.3 mmol), *N, N'*-dicyclohexylcarbodiimide (DCC, 0.36 mmol), MOF-253-Cu (6 mg), and DMSO (2.5 mL) were added to a 15 mL glass tube at room temperature. The mixture was then stirred at 40 ℃ for 15 hours. After completion, the mixture was cooled to room temperature and analyzed by HPLC. No target product **3a** was detected.

4.2 Radical trapped experiment

Quinoline-*N*-oxide **1a** (0.3 mmol), *N,N'*-dicyclohexylcarbodiimide (DCC, 0.36 mmol), MOF-253-Cu (6 mg), 2,2,6,6-tetramethyl-1-piperidyloxy (TEMPO, 0.6 mmol), and DMSO (2.5 mL) were added to a 15 mL glass tube at room temperature. The mixture was then stirred at 40 ℃ for 15 hours. After completion, the mixture was cooled to room temperature and analyzed by HPLC. The product **3a** was obtained in 85% yield.

Following the identical protocol but substituting TEMPO with butylated hydroxytoluene (BHT, 0.6 mmol) while maintaining all other parameters constant, the analogous transformation proceeded to provide **3a** in 81% yield (as determined by HPLC).

4.3 KSCN poisoning experiment

Quinoline-*N*-oxide **1a** (0.3 mmol), *N,N′*-dicyclohexylcarbodiimide (DCC, 0.36 mmol), MOF-253-Cu (6 mg), KSCN (0.36 mmol, 1.2 equiv.), and DMSO (2.5 mL) were added to a 15 mL glass tube at room temperature. The mixture was then stirred at 40 ℃ for 15 hours. After completion, the mixture was cooled to room temperature and analyzed by TLC.

4.4 KIE Experiment

Quinoline-*N*-oxide **1a** and 2-d_1-quinoline *N*-oxide **1a-d$_1$** (1:1) (totally 0.3 mmol, deuteration ratio has been calculated), *N,N′*-dicyclohexylcarbodiimide (DCC, 0.36 mmol), MOF-253-Cu (6 mg), and DMSO (2.5 mL) were added to a 15 mL glass tube at room temperature. The mixture was stirred at 40 ℃ for 3 hours. After cooling to room temperature, residual starting material (mixture of 2-d_1-quinoline-*N*-oxide and quinolone-*N*-oxide) was recovered by column chromatography on silica gel (200-300 mesh), which was characterized by ^{1}H NMR spectroscopy. The average k_H / k_D = 1.10 was calculated based on the isolated yields. Representative ^{1}H NMR spectra copy was shown below:

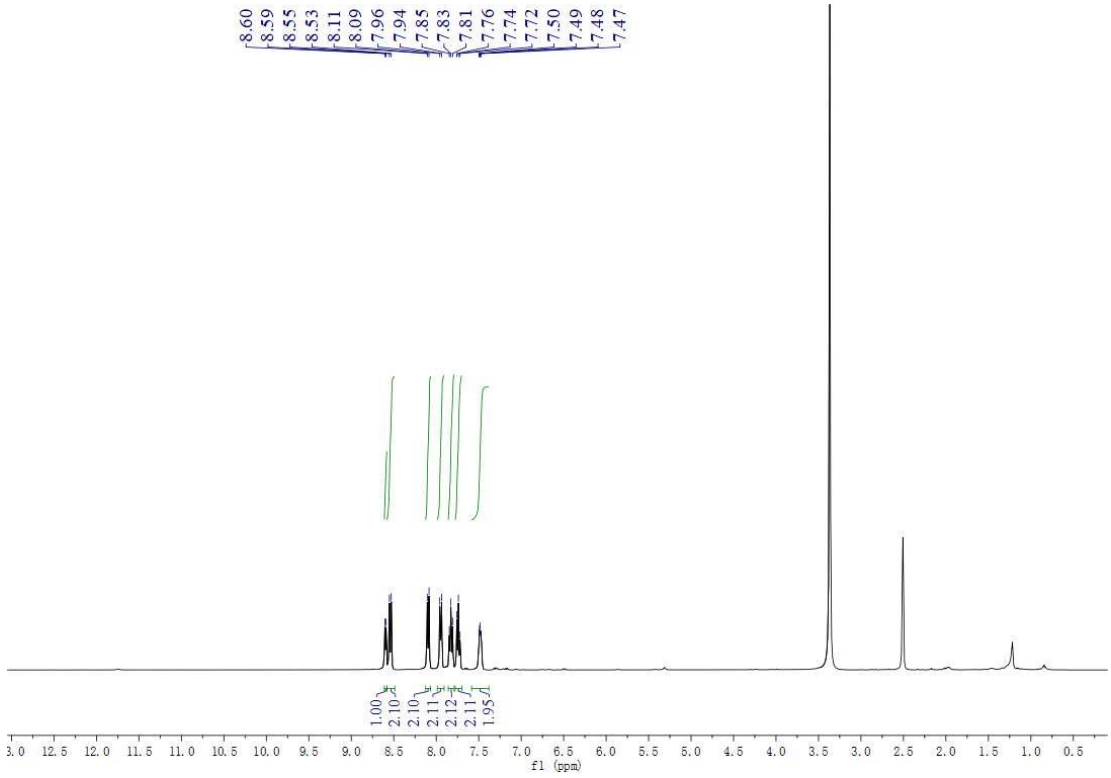


Figure S9. Local ^{1}H NMR ($CDCl_3$, 400 MHz) image for the reaction of **1a**, **1a-d$_1$** and DCC

4.5 Role of $^{18}O_2$

Quinoline-*N*-oxide **1a** (0.3 mmol), *N,N'*-dicyclohexylcarbodiimide (DCC, 0.36 mmol), MOF-253-Cu (6 mg), and DMSO (2.5 mL) were added to a 15 mL glass tube with an ^{18}O balloon at room temperature. The mixture was then stirred at 40 ℃ for 15 hours. After completion, the mixture was cooled to room temperature and analyzed by HPLC-MS. No target **^{18}O-3a** was detected.

5. Computational Details

5.1 Computational details and figures

Geometry optimizations were performed using Gaussian 16, Revision C.01[2], with the unrestricted B3LYP functional[3, 4] and the 6-31G(d) basis set[5] for lighter atoms, while the LANL2DZ basis set was employed for Cu[6-8]. Dispersion corrections were included using Grimme's D3 model[9] with Becke-Johnson damping factors[10]. Harmonic vibrational frequency calculations were conducted at the same level of theory to confirm the nature of stationary points as either minima or transition states and to provide thermodynamic corrections. Subsequent single-point calculations were performed on above optimized geometries at M06 functional[11] using the 6-311+G(d, p) basis set[12, 13], incorporating solvent effects via the SMD model[14] in dimethyl sulfoxide. The solvation enthalpies were obtained by combining the solvent-corrected energies from these calculations with enthalpic corrections derived from the frequency calculations.

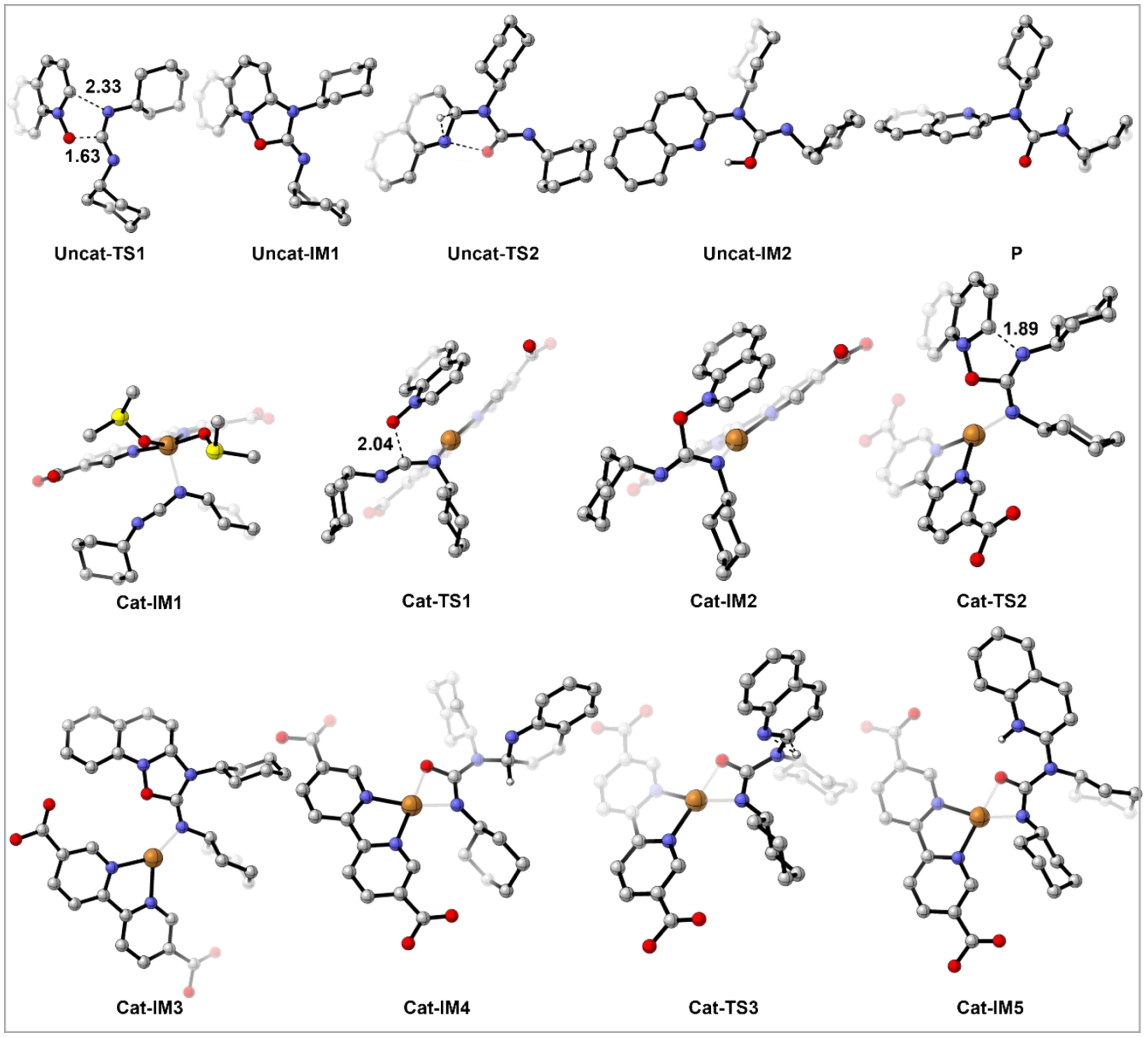


Figure S10. Optimized structures and selected geometric parameters for the uncatalyzed and catalyzed reactions between quinoline N-oxide and DCC.

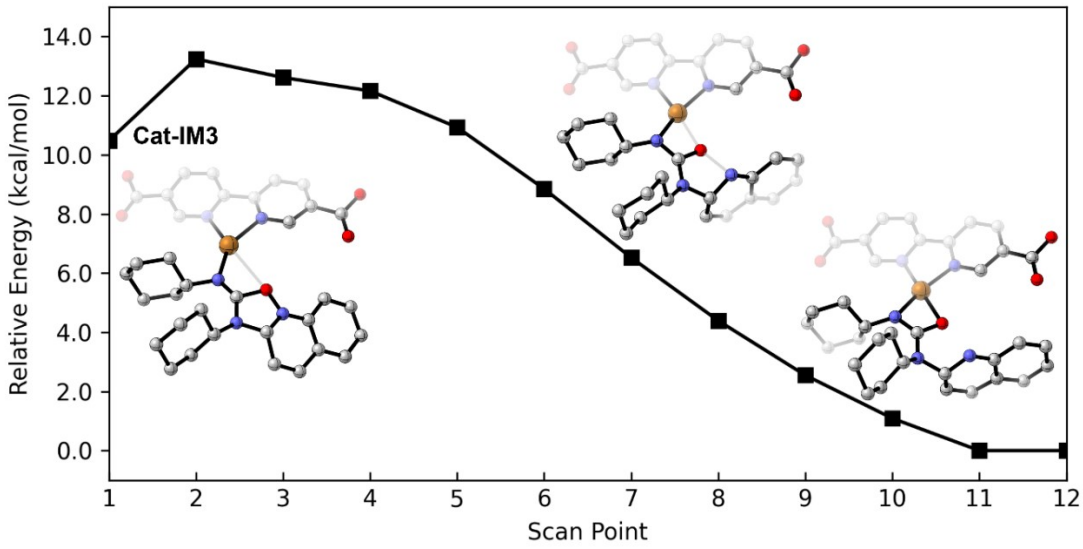


Figure S11. Computed linear scan of the N–O bond fragmentation pathway from intermediate Cat-IM3.

5.2 Coordinates and energies

Cartesian coordinates (Å) of geometries optimized at B3LYP-D3(BJ)/6-31G(d) (H, C, N, O, etc.) and LANL2DZ (Cu). Single-point energies E_{sol} (Hartree) were computed at M06/6-311+G(d,p) (H, C, N, O, etc.) and LANL2DZ (Cu) using the SMD solvation model for dimethyl sulfoxide. Gibbs free energies G_{sol} (Hartree) were computed by E_{sol} with the corrections from the frequency calculations.

Quinoline
$\boldsymbol{E}_{sol}$ = -476.8822
$\boldsymbol{G}_{sol}$ = -476.7740

O	1.570207	-2.114709	-0.000384
N	1.307332	-0.866403	0.000138
C	2.294504	0.059090	0.000160
C	2.023935	1.433196	0.000177
C	0.729101	1.899684	0.000008
C	-0.331320	0.958682	-0.000172
C	-0.032679	-0.431654	0.000095
H	0.508884	2.961568	-0.000405
H	2.867236	2.115190	-0.000089
H	3.288754	-0.365354	0.000777
C	-1.050113	-1.402639	-0.000036
C	-2.367924	-0.997461	0.000066
C	-2.694469	0.378750	-0.000020
C	-1.700969	1.332380	-0.000314
H	-0.753144	-2.443267	0.000407
H	-3.160582	-1.738712	0.000754
H	-3.736560	0.683015	0.000914
H	-1.947964	2.389875	-0.000034

DCC
$\boldsymbol{E}_{sol}$ = -617.8375
$\boldsymbol{G}_{sol}$ = -617.5407

N	-0.581114	-0.820564	-0.476650
C	0.445328	-1.027294	0.164200
N	1.496105	-1.360583	0.694736
C	2.588484	-0.496710	1.159682
C	3.871306	-0.861389	0.391609
C	3.817747	-0.388941	-1.065781
H	4.025105	-1.943580	0.446526
H	4.718265	-0.383804	0.901934
C	3.561817	1.122086	-1.147422
H	3.015150	-0.925206	-1.587457
H	4.752842	-0.646945	-1.575442
C	2.273287	1.507659	-0.408135
H	3.507268	1.444463	-2.193433
H	4.411760	1.655362	-0.697645
C	2.290269	1.008563	1.045083
H	1.410876	1.085985	-0.936804
H	2.138291	2.595450	-0.416884
H	1.338742	1.231948	1.542779
H	3.070405	1.544332	1.602003
H	2.737619	-0.749436	2.216346
C	-1.890584	-0.506527	0.104629
C	-2.984556	-1.196797	-0.717125
C	-4.383492	-0.831433	-0.204831
H	-2.828440	-2.280525	-0.693238
H	-2.872531	-0.882747	-1.762886
C	-4.592158	0.688680	-0.184418
H	-4.513632	-1.226800	0.812434
H	-5.146031	-1.314809	-0.825690
C	-3.496354	1.384799	0.633797
H	-5.581352	0.932912	0.219364
H	-4.568838	1.069450	-1.214846
C	-2.097814	1.015390	0.122426
H	-3.588184	1.085705	1.687344
H	-3.628252	2.472344	0.606277
H	-1.958810	1.390179	-0.899755
H	-1.320667	1.480941	0.739782
H	-1.944210	-0.875722	1.140388

Catalyst
$\boldsymbol{E}_{sol}$ = -2175.6790
$\boldsymbol{G}_{sol}$ = -2175.3823

C	-2.759954	-3.391009	-0.149195
C	3.088745	-3.247736	0.189698
C	-3.337990	-2.124384	-0.256370
C	-1.369961	-3.499004	-0.063483
C	1.705486	-3.422504	0.111009
C	3.613219	-1.954855	0.177432
C	-2.499047	-1.012792	-0.291090
C	-0.590641	-2.342314	-0.075745
C	0.881233	-2.303090	0.022512
C	2.732080	-0.875667	0.088836
N	1.412586	-1.051603	0.015124
N	-1.175610	-1.121735	-0.187830
H	-3.386133	-4.276109	-0.128177
H	3.752394	-4.102410	0.257682
C	-4.808196	-1.846017	-0.297981
H	-0.908216	-4.474948	0.020373
H	1.284691	-4.420349	0.116035
C	5.074545	-1.631650	0.248999
H	-2.900800	-0.017009	-0.408880
H	3.098972	0.143111	0.077025
Cu	0.069366	0.454433	-0.105691
O	-1.426553	1.716083	-0.244644
S	-1.918509	2.742593	0.847049
O	1.507576	1.754823	-0.075353

S	1.393386	3.301778	-0.352881
O	5.489151	-0.493772	0.221300
O	5.825657	-2.733183	0.342784
H	6.761663	-2.468552	0.384871
O	-5.253081	-0.717915	-0.234434
O	-5.531701	-2.961995	-0.395324
H	-6.476290	-2.725382	-0.408414
C	-2.814214	3.958738	-0.148158
H	-3.533894	3.437098	-0.782215
H	-3.313877	4.656544	0.528353
H	-2.077223	4.487833	-0.753204
C	-3.314182	1.926895	1.671726
H	-2.906842	1.111653	2.272445
H	-4.028326	1.546885	0.936627
H	-3.785019	2.660168	2.332051
C	2.111176	3.506330	-2.001620
H	3.080355	3.004453	-2.035994
H	2.214578	4.575604	-2.203935
H	1.418145	3.060487	-2.717124
C	2.726711	3.975383	0.667238
H	2.441134	3.831657	1.710284
H	2.821248	5.042130	0.449063
H	3.652526	3.441732	0.442950

DMSO

E_{sol} = -553.1352

G_{sol} = -553.0839

O	-0.000608	1.505864	0.388053
S	-0.000071	0.243111	-0.440744
C	-1.357450	-0.821882	0.180525
H	-1.264725	-0.928899	1.264261
H	-1.322149	-1.796011	-0.314455
H	-2.294677	-0.316664	-0.059226
C	1.358072	-0.820885	0.180534
H	2.295125	-0.315484	-0.059431
H	1.323024	-1.795102	-0.314332
H	1.265672	-0.927931	1.264304

Uncat-TS1

E_{sol} = -1094.6894

G_{sol} = -1094.2592

O	-0.418970	-1.215859	1.288350
N	-1.684224	-0.757180	1.194864
C	-1.906123	0.425488	1.793641
C	-3.124950	1.103612	1.562969
C	-4.009281	0.613640	0.640688
C	-3.719829	-0.586529	-0.072588
C	-2.499228	-1.261326	0.197665
H	-4.943535	1.129269	0.440624
H	-3.317786	2.018789	2.108787
H	-1.234043	0.676124	2.597456
C	-2.137134	-2.422085	-0.505436
C	-2.995213	-2.909994	-1.473342
C	-4.219732	-2.267181	-1.751493
C	-4.574674	-1.125785	-1.061007
H	-1.194991	-2.900974	-0.275142
H	-2.720573	-3.802622	-2.026170
H	-4.879676	-2.670751	-2.512154
H	-5.511196	-0.618225	-1.271833
N	-0.099283	0.981790	0.430597
C	0.585523	-0.087624	0.672358
N	1.785201	-0.487609	0.565532
C	2.252500	-1.794190	1.001995
C	2.142164	-2.819822	-0.147256
C	3.044508	-2.448879	-1.330447
H	1.097105	-2.884668	-0.470152
H	2.424716	-3.810218	0.237439
C	4.505695	-2.293606	-0.885728
H	2.692840	-1.500866	-1.753396
H	2.963460	-3.206136	-2.119920
C	4.631383	-1.281818	0.261851
H	5.130565	-1.988347	-1.733892
H	4.886701	-3.270016	-0.551238
C	3.723643	-1.661668	1.438095
H	4.335559	-0.289202	-0.095807
H	5.673692	-1.211238	0.595688
H	3.794353	-0.911711	2.233553
H	4.050299	-2.620890	1.863577
H	1.668506	-2.166585	1.854239
C	0.639176	2.206975	0.181307
C	-0.255648	3.416358	0.478988
C	0.450899	4.741596	0.168045
H	-0.572519	3.385176	1.529303
H	-1.166244	3.323819	-0.128843
C	0.956968	4.780149	-1.280569
H	1.305173	4.863096	0.848819
H	-0.223019	5.585118	0.360750
C	1.857149	3.574721	-1.582519
H	1.492267	5.718038	-1.471419
H	0.094935	4.764736	-1.962566
C	1.141826	2.253683	-1.273700
H	2.768598	3.644300	-0.972345
H	2.182111	3.593462	-2.629682
H	0.274286	2.132023	-1.936333
H	1.803626	1.398803	-1.440638
H	1.526934	2.253276	0.836434

Uncat-IM1

E_{sol} = -1094.7271

G_{sol} = -1094.2920

O	0.368199	-1.407802	-1.027299
N	1.612417	-0.740582	-1.329123
C	1.226365	0.671020	-1.304468
C	2.414689	1.577740	-1.156785
C	3.544840	1.133973	-0.592723
C	3.657643	-0.235324	-0.107716
C	2.625332	-1.146445	-0.416361
H	4.400985	1.792209	-0.471308
H	2.310882	2.595715	-1.514163
C	2.667700	-2.451310	0.072118

C	3.740045	-2.855411	0.868553
C	4.780154	-1.973120	1.166059
C	4.733549	-0.670788	0.673752
H	1.863503	-3.134542	-0.169947
H	3.761967	-3.870792	1.252302
H	5.616406	-2.296207	1.777247
H	5.528157	0.032901	0.906781
N	0.261573	0.678174	-0.184427
C	-0.376857	-0.546858	-0.217484
N	-1.462415	-0.855973	0.351080
C	-1.965297	-2.228191	0.261805
C	-2.910436	-2.474808	1.448886
C	-4.166702	-1.598645	1.362192
H	-2.372644	-2.281878	2.383543
H	-3.197503	-3.535149	1.451395
C	-4.903836	-1.808705	0.032095
H	-3.863777	-0.548571	1.446067
H	-4.833529	-1.811465	2.206110
C	-3.970931	-1.570532	-1.163709
H	-5.776824	-1.147715	-0.028243
H	-5.287132	-2.838699	-0.010913
C	-2.715825	-2.447106	-1.068624
H	-3.667420	-0.516608	-1.180600
H	-4.497090	-1.767912	-2.105195
H	-2.036308	-2.249949	-1.904408
H	-3.003133	-3.505713	-1.131702
H	-1.133777	-2.946047	0.311469
C	-0.502202	1.853427	0.237210
C	-1.153090	2.594440	-0.941434
C	-2.009894	3.764853	-0.439775
H	-1.760058	1.891311	-1.523129
H	-0.373100	2.983052	-1.611747
C	-1.191436	4.718325	0.441223
H	-2.850738	3.365673	0.143464
H	-2.445060	4.304100	-1.288671
C	-0.532399	3.969136	1.607540
H	-1.828086	5.526637	0.818451
H	-0.410386	5.192610	-0.169923
C	0.330661	2.802819	1.106943
H	-1.314985	3.578600	2.272605
H	0.075240	4.655058	2.208335
H	1.173163	3.196995	0.526520
H	0.760143	2.240179	1.941946
H	-1.305447	1.438001	0.854864
H	0.707510	0.878355	-2.251258

Uncat-TS2

$\boldsymbol{E}_{\mathbf{sol}}$ = -1094.6848

$\boldsymbol{G}_{\mathbf{sol}}$ = -1094.2582

O	-0.335114	-1.428084	-0.891963
N	-1.876028	-0.537157	0.704230
C	-1.303499	0.677006	0.263587
C	-2.117320	1.666565	-0.454446
C	-3.418195	1.401366	-0.714665
C	-4.012041	0.151546	-0.313770
C	-3.204161	-0.775716	0.403092
H	-4.026776	2.113880	-1.264272
H	-1.644337	2.581446	-0.783397
C	-3.744976	-2.003553	0.827843
C	-5.062489	-2.314402	0.534554
C	-5.865326	-1.401548	-0.171922
C	-5.347693	-0.182234	-0.588014
H	-3.095239	-2.687394	1.361965
H	-5.478492	-3.264945	0.851948
H	-6.897198	-1.653157	-0.395279
H	-5.968121	0.521395	-1.135367
N	0.053551	0.598288	0.179688
C	0.554617	-0.684836	-0.414623
N	1.852887	-0.749462	-0.383148
C	2.432413	-1.923107	-1.029481
C	3.922134	-1.654637	-1.295478
C	4.712615	-1.516240	0.011988
H	4.021243	-0.744198	-1.898137
H	4.333299	-2.483953	-1.888142
C	4.540043	-2.755921	0.901124
H	4.340855	-0.634725	0.547566
H	5.775077	-1.343603	-0.200583
C	3.055891	-3.043346	1.170375
H	5.082585	-2.626079	1.846080
H	4.989594	-3.625724	0.399251
C	2.269705	-3.176932	-0.139656
H	2.629181	-2.218282	1.753335
H	2.947426	-3.953569	1.773368
H	1.204192	-3.334148	0.051710
H	2.633302	-4.051423	-0.698411
H	1.924718	-2.122624	-1.984161
C	0.956232	1.752284	0.271317
C	0.514672	2.757966	1.341305
C	1.562557	3.870150	1.491339
H	0.368272	2.235772	2.294354
H	-0.448354	3.215061	1.075288
C	1.846783	4.558562	0.149166
H	2.493143	3.432344	1.876050
H	1.227292	4.601669	2.235286
C	2.273883	3.541472	-0.917462
H	2.617524	5.327308	0.275754
H	0.938482	5.078047	-0.189196
C	1.227870	2.431431	-1.081693
H	3.229617	3.087472	-0.623224
H	2.446863	4.041627	-1.876924
H	0.304729	2.861317	-1.493225
H	1.575297	1.666720	-1.781360
H	1.901233	1.302687	0.586901
H	-1.719660	0.664819	1.446252

Uncat-IM2

$\boldsymbol{E}_{\mathbf{sol}}$ = -1094.8204

$\boldsymbol{G}_{\mathbf{sol}}$ = -1094.3860

O	-0.02584	-2.06720	0.58362
N	2.12325	-0.81064	0.36903

C	1.42557	0.27435	0.03612
C	2.07907	1.39354	-0.57895
C	3.42813	1.34720	-0.79481
C	4.18669	0.20287	-0.43215
C	3.46515	-0.88294	0.14251
H	3.92907	2.18692	-1.26900
H	1.51095	2.25064	-0.89980
C	4.16458	-2.06130	0.49943
C	5.52576	-2.14640	0.29471
C	6.24362	-1.06838	-0.27307
C	5.58217	0.08717	-0.63111
H	3.60493	-2.88119	0.93732
H	6.05514	-3.05258	0.57305
H	7.31439	-1.15551	-0.42645
H	6.12072	0.92190	-1.07156
N	0.06015	0.28008	0.28608
C	-0.70301	-0.92434	0.47002
N	-1.97374	-0.83464	0.49890
C	-2.74880	-2.05592	0.69676
C	-4.11791	-1.66982	1.28120
C	-4.94732	-0.84600	0.28773
H	-3.96794	-1.10993	2.21121
H	-4.65996	-2.58958	1.54049
C	-5.12141	-1.58960	-1.04388
H	-4.42994	0.10346	0.10539
H	-5.92537	-0.60353	0.72044
C	-3.76360	-1.98628	-1.64046
H	-5.68479	-0.97256	-1.75448
H	-5.71892	-2.49752	-0.87526
C	-2.93564	-2.80353	-0.64068
H	-3.20719	-1.07868	-1.90464
H	-3.90525	-2.55564	-2.56697
H	-1.95274	-3.05052	-1.05429
H	-3.44603	-3.75481	-0.43547
H	-2.23226	-2.72933	1.39475
C	-0.74250	1.52910	0.30480
C	-1.15894	2.01891	-1.09012
C	-2.15534	3.17910	-0.95674
H	-1.61291	1.17932	-1.62514
H	-0.29660	2.34986	-1.68093
C	-1.59088	4.30386	-0.07823
H	-3.08293	2.80068	-0.50624
H	-2.42135	3.56218	-1.94822
C	-1.18963	3.78024	1.30798
H	-2.32368	5.11264	0.02104
H	-0.70842	4.73908	-0.56927
C	-0.17004	2.63481	1.20293
H	-2.08674	3.41898	1.82849
H	-0.77581	4.59027	1.91887
H	0.77303	3.03927	0.82336
H	0.04325	2.21581	2.19252
H	-1.66812	1.19974	0.77771
H	0.96020	-1.84524	0.61221

P

E_{sol} = -1094.8419

G_{sol} = -1094.4082

O	0.64190	-2.12298	0.81626
N	-2.11064	-0.27470	-0.73975
C	-1.32350	-0.37762	0.30604
C	-1.77396	-0.79085	1.59266
C	-3.09989	-1.08878	1.76256
C	-3.99195	-0.97513	0.66404
C	-3.43863	-0.55243	-0.58373
H	-3.48021	-1.40597	2.72978
H	-1.06121	-0.87369	2.40266
C	-4.29317	-0.42398	-1.70751
C	-5.63772	-0.70252	-1.59610
C	-6.18601	-1.11970	-0.35940
C	-5.37854	-1.25335	0.74889
H	-3.84898	-0.10464	-2.64429
H	-6.28588	-0.60339	-2.46164
H	-7.24777	-1.33506	-0.28843
H	-5.79258	-1.57412	1.70111
N	0.04737	-0.01508	0.12934
C	0.98236	-0.98412	0.50066
N	2.30164	-0.59507	0.50509
C	3.35536	-1.60253	0.64371
C	3.53829	-2.42643	-0.64519
C	4.10515	-1.57634	-1.78886
H	2.57651	-2.87054	-0.91612
H	4.22692	-3.25454	-0.42992
C	5.42461	-0.90421	-1.38290
H	3.37278	-0.80513	-2.06579
H	4.25052	-2.19392	-2.68191
C	5.25837	-0.07025	-0.10447
H	5.80486	-0.27767	-2.19796
H	6.18141	-1.68084	-1.20407
C	4.66712	-0.90937	1.04015
H	4.60957	0.79306	-0.31679
H	6.21996	0.35387	0.20572
H	4.50347	-0.29233	1.93067
H	5.38937	-1.68761	1.31565
H	3.02926	-2.26980	1.44458
C	0.41857	1.40133	-0.07688
C	0.70310	2.10468	1.26367
C	1.20462	3.53805	1.04871
H	1.42925	1.52282	1.83955
H	-0.23060	2.11569	1.84166
C	0.22701	4.34990	0.19018
H	2.18286	3.50405	0.54721
H	1.36939	4.02770	2.01502
C	-0.07503	3.63017	-1.13058
H	0.62835	5.35144	-0.00217
H	-0.71075	4.48706	0.74599
C	-0.60042	2.20672	-0.89358
H	0.84038	3.58644	-1.73786
H	-0.80790	4.19719	-1.71502
H	-1.54942	2.25959	-0.34941
H	-0.81175	1.69417	-1.83377

H	1.33670	1.40318	-0.68114
H	2.55735	0.27115	0.06157

Cat-IM1

E_{sol} = -2793.5432

G_{sol} = -2792.9219

H	3.661383	2.986816	-0.372465
H	3.018743	3.758038	-1.869280
C	3.075992	3.814261	-0.780092
H	3.514302	4.762523	-0.458530
O	0.726618	2.538022	-0.901614
S	1.395995	3.713911	-0.103641
H	0.841313	5.202694	-1.912162
C	0.692615	5.217621	-0.830269
H	1.187092	6.083354	-0.382716
H	-0.368551	5.231610	-0.576617
C	2.634158	-0.267361	3.310100
C	-3.178403	-0.876883	3.442523
C	3.104346	0.317643	2.132749
C	1.258423	-0.412405	3.492802
C	-1.793929	-0.745251	3.558672
C	-3.822173	-0.332972	2.330113
C	2.173554	0.729640	1.181162
C	0.382231	0.045713	2.507328
C	-1.088891	-0.076535	2.558188
C	-3.057388	0.354219	1.384649
N	-1.736619	0.472795	1.501062
N	0.861882	0.621466	1.376521
H	3.332266	-0.601879	4.069162
H	-3.750314	-1.406011	4.196267
C	4.540815	0.580126	1.824464
H	0.879763	-0.869575	4.398384
H	-1.278917	-1.179283	4.406663
C	-5.286493	-0.466527	2.055149
H	2.498359	1.144059	0.238242
H	-3.518380	0.805056	0.514200
Cu	-0.509717	1.209725	0.016112
O	-2.061438	1.827089	-1.011046
S	-1.963997	1.859970	-2.580047
O	-5.790636	-0.097980	1.016350
O	-5.939986	-1.042469	3.071081
H	-6.881552	-1.107057	2.832945
O	4.892577	1.250751	0.872420
O	5.365841	0.013953	2.706842
H	6.281836	0.237397	2.464387
C	-2.283126	3.594044	-2.993174
H	-2.413731	3.677208	-4.074930
H	-3.173619	3.934457	-2.460992
H	-1.404855	4.158658	-2.682600
C	-3.547928	1.145693	-3.095588
H	-3.520116	0.081844	-2.860687
H	-3.654188	1.282682	-4.174448
H	-4.356995	1.639104	-2.553239
N	-0.305853	-0.700322	-1.136912
C	0.852849	-1.157669	-1.231018
N	2.004098	-1.498472	-1.148622
C	3.106009	-1.728124	-2.104373
C	4.416677	-1.254606	-1.463501
C	4.800250	-2.108120	-0.248363
H	4.344243	-0.196381	-1.192511
H	5.197622	-1.331058	-2.229024
C	4.868485	-3.598549	-0.608310
H	4.052818	-1.965374	0.544055
H	5.760036	-1.765414	0.151931
C	3.551363	-4.081328	-1.231127
H	5.106978	-4.192708	0.279566
H	5.687503	-3.759012	-1.321462
C	3.161367	-3.227133	-2.443718
H	2.751598	-4.032416	-0.480702
H	3.634099	-5.129294	-1.534638
H	2.199489	-3.545720	-2.860253
H	3.907376	-3.346394	-3.238564
H	2.897412	-1.147915	-3.010175
C	-1.507274	-1.569528	-1.238110
C	-1.536202	-2.651979	-0.153987
C	-2.836129	-3.464066	-0.246254
H	-1.433051	-2.193406	0.834724
H	-0.670621	-3.313616	-0.291553
C	-3.010382	-4.078471	-1.641340
H	-3.687544	-2.803000	-0.028678
H	-2.841218	-4.244801	0.520702
C	-2.939758	-3.006969	-2.737629
H	-3.961139	-4.616293	-1.701734
H	-2.219031	-4.820345	-1.810078
C	-1.646843	-2.184564	-2.635009
H	-3.807328	-2.337403	-2.642424
H	-3.009535	-3.464607	-3.728888
H	-0.779392	-2.832362	-2.820210
H	-1.614614	-1.395584	-3.395797
H	-2.353354	-0.895431	-1.066946

Cat-TS1

E_{sol} = -2164.0998

G_{sol} = -2163.4960

O	0.87235	-2.12744	-1.83851
N	-0.37073	-2.48697	-1.62477
C	-0.64175	-3.69142	-1.09803
C	-1.95999	-4.09990	-0.85856
H	-2.12612	-5.08533	-0.43977
C	-3.01197	-3.26103	-1.16557
H	-4.03943	-3.56014	-0.98685
C	-2.74489	-1.98559	-1.72220
C	-3.76906	-1.06856	-2.07901
H	-4.80072	-1.36723	-1.92741
C	-3.45376	0.16829	-2.59929
H	-4.24453	0.85443	-2.88325
C	-2.10355	0.54554	-2.78447
C	-1.07360	-0.31773	-2.45930
H	-0.03680	-0.07485	-2.65046
H	-1.87174	1.51422	-3.21486

H	0.22925	-4.30267	-0.90276
C	-1.39188	-1.58632	-1.92787
C	0.07477	4.66146	0.21441
C	-5.00657	1.86217	0.88037
C	1.17699	3.81758	0.06442
C	-1.18793	4.10647	0.43040
C	-3.84821	2.63471	0.77099
C	-4.89658	0.47221	0.88718
C	0.97776	2.43913	0.16053
C	-1.32212	2.71954	0.49864
C	-2.60813	2.00460	0.67798
C	-3.62218	-0.09337	0.82863
N	-2.51788	0.64707	0.72677
N	-0.23204	1.92102	0.37338
H	0.20338	5.73643	0.15578
H	-5.98196	2.33201	0.94174
C	2.57223	4.28868	-0.20877
H	-2.04864	4.75444	0.53928
H	-3.92330	3.71455	0.74861
C	-6.05559	-0.47248	0.86939
H	1.81667	1.75859	0.05561
H	-3.50998	-1.16998	0.85382
Cu	-0.67856	-0.04355	0.50449
O	-5.92483	-1.64666	0.58726
O	-7.20842	0.13135	1.16236
H	-7.92667	-0.52519	1.12166
O	3.49174	3.52283	-0.40224
O	2.65761	5.62215	-0.21643
H	3.58008	5.87397	-0.39967
N	0.85104	-1.13184	0.61803
C	1.72580	-1.02336	-0.34745
N	2.73948	-0.57365	-0.80587
C	3.58345	-0.71459	-1.99453
C	4.40410	0.56969	-2.17489
C	5.41726	0.76367	-1.04060
H	3.73563	1.43377	-2.24718
H	4.92424	0.48300	-3.13570
C	6.32626	-0.46194	-0.88075
H	4.87540	0.95126	-0.10437
H	6.00970	1.66231	-1.23421
C	5.50898	-1.74432	-0.67119
H	7.01621	-0.31519	-0.04407
H	6.94583	-0.57429	-1.78001
C	4.48907	-1.94862	-1.79725
H	4.98566	-1.69017	0.29405
H	6.16789	-2.61647	-0.61780
H	3.86443	-2.83199	-1.62963
H	5.01045	-2.09975	-2.74979
H	2.90625	-0.88192	-2.83820
C	1.39575	-1.50091	1.96634
C	2.31614	-0.40589	2.52594
C	2.85838	-0.81514	3.90416
H	1.76341	0.53956	2.59135
H	3.15139	-0.24924	1.83365
C	3.57566	-2.16893	3.84070
H	2.02849	-0.87143	4.62076
H	3.53454	-0.03581	4.26845
C	2.65404	-3.25548	3.27474
H	3.92575	-2.45534	4.83646
H	4.46802	-2.07980	3.20683
C	2.10620	-2.86451	1.89446
H	1.81654	-3.42579	3.96362
H	3.18585	-4.20807	3.18830
H	2.93334	-2.79297	1.17700
H	1.40723	-3.61940	1.51918
H	0.51542	-1.60202	2.60984

Cat-IM2

$\boldsymbol{E}_{\mathbf{sol}}$ = -2164.1064

$\boldsymbol{G}_{\mathbf{sol}}$ = -2163.5009

O	0.86104	-1.81559	-1.67919
N	-0.41159	-2.31074	-1.49649
C	-0.56265	-3.53074	-0.97443
C	-1.84426	-4.04261	-0.76176
C	-2.94590	-3.28171	-1.11206
C	-2.77634	-2.00475	-1.69636
C	-1.45475	-1.49585	-1.88395
H	-3.95165	-3.65006	-0.93632
H	-1.94655	-5.03038	-0.32940
H	0.35003	-4.06160	-0.73430
C	-1.22746	-0.22116	-2.43890
C	-2.32276	0.53848	-2.80335
C	-3.64267	0.06062	-2.62634
C	-3.86822	-1.18473	-2.08318
H	-0.21594	0.12558	-2.60103
H	-2.16440	1.51503	-3.24868
H	-4.47927	0.67905	-2.93250
H	-4.87341	-1.56099	-1.93101
C	-0.04603	4.75711	0.13304
C	-4.96967	1.72775	0.86849
C	1.09204	3.97030	-0.05128
C	-1.27016	4.13563	0.38462
C	-3.84775	2.54658	0.73470
C	-4.79381	0.34512	0.93301
C	0.96239	2.58303	0.04410
C	-1.32789	2.74267	0.45232
C	-2.57693	1.97108	0.67537
C	-3.49228	-0.15670	0.91898
N	-2.42069	0.62587	0.79086
N	-0.20862	1.99428	0.29132
H	0.02613	5.83744	0.07836
H	-5.96640	2.15378	0.89984
C	2.45551	4.51377	-0.34602
H	-2.15755	4.73876	0.53044
H	-3.97365	3.61923	0.65961
C	-5.90439	-0.65288	0.92375
H	1.83298	1.94862	-0.08281
H	-3.32766	-1.22332	1.00332
Cu	-0.53002	-0.01330	0.56944
O	-5.72195	-1.82010	0.63286

O	-7.08407	-0.11066	1.22878
H	-7.76764	-0.80341	1.19351
O	3.41721	3.79977	-0.52924
O	2.46536	5.85128	-0.38129
H	3.37288	6.14736	-0.57193
N	0.87365	-1.27249	0.63516
C	1.62634	-1.56458	-0.44916
N	2.88796	-1.57509	-0.54635
C	3.63128	-1.73449	-1.78727
C	3.74605	-0.34095	-2.46580
C	4.58320	0.64024	-1.63739
H	2.74074	0.05294	-2.66162
H	4.21815	-0.50555	-3.44115
C	5.96904	0.05824	-1.32725
H	4.06522	0.87067	-0.69741
H	4.67531	1.58827	-2.17600
C	5.86496	-1.30985	-0.64020
H	6.53650	0.75431	-0.70186
H	6.53048	-0.04859	-2.26483
C	5.02520	-2.29395	-1.46429
H	5.40923	-1.19014	0.35120
H	6.86180	-1.73025	-0.47619
H	4.92305	-3.25253	-0.94466
H	5.52257	-2.50191	-2.41917
H	3.08897	-2.40554	-2.46627
C	1.50740	-1.36853	1.97531
C	2.50613	-0.22002	2.24368
C	3.03606	-0.31064	3.68099
H	2.00549	0.74237	2.08151
H	3.32769	-0.29529	1.52733
C	3.66310	-1.68151	3.96232
H	2.21433	-0.13087	4.38739
H	3.76731	0.48791	3.84213
C	2.66764	-2.81329	3.68039
H	4.00546	-1.73180	5.00001
H	4.55135	-1.81183	3.33015
C	2.14197	-2.74698	2.23960
H	1.82575	-2.74783	4.38258
H	3.13602	-3.78836	3.84613
H	2.96673	-2.90264	1.53923
H	1.39443	-3.53044	2.06485
H	0.67405	-1.25105	2.67851

Cat-TS2

E_{sol} = -2164.0863

G_{sol} = -2163.4787

O	0.650863	-0.402476	-1.504397
N	1.464766	-1.380088	-2.102306
C	2.702269	-0.798840	-2.334698
C	3.812258	-1.697919	-2.550586
C	3.707667	-2.993105	-2.159001
C	2.500146	-3.497666	-1.560025
C	1.366866	-2.653200	-1.501588
H	4.540350	-3.676027	-2.298302
H	4.709754	-1.305130	-3.009879
H	2.653029	0.110687	-2.924376
C	0.165729	-3.096408	-0.943823
C	0.099660	-4.375888	-0.399571
C	1.215354	-5.226956	-0.441264
C	2.395296	-4.797578	-1.029767
H	-0.705181	-2.454003	-0.968930
H	-0.824086	-4.723539	0.052423
H	1.147206	-6.225834	-0.025402
H	3.256635	-5.455954	-1.082267
C	-4.710540	3.131239	-1.035931
C	-5.152669	-2.419489	0.703687
C	-3.400934	3.608737	-1.102472
C	-4.937946	1.818944	-0.617794
C	-5.162953	-1.090501	0.281082
C	-3.934657	-3.021822	1.023444
C	-2.360594	2.747759	-0.749677
C	-3.852168	1.012989	-0.276109
C	-3.960861	-0.389726	0.187061
C	-2.771358	-2.257867	0.932625
N	-2.783741	-0.985532	0.522413
N	-2.586063	1.495595	-0.351791
H	-5.538108	3.778166	-1.304301
H	-6.074506	-2.985597	0.775726
C	-3.022869	4.996072	-1.521797
H	-5.951136	1.442153	-0.556755
H	-6.100659	-0.617250	0.019155
C	-3.785853	-4.454868	1.427323
H	-1.334153	3.092899	-0.794057
H	-1.815134	-2.696166	1.194231
Cu	-1.187553	0.169174	0.267126
O	-2.703971	-4.996576	1.523613
O	-4.964695	-5.040492	1.647531
H	-4.810764	-5.969553	1.895166
O	-1.873219	5.377136	-1.540132
O	-4.091382	5.726532	-1.856978
H	-3.789394	6.614510	-2.117925
N	0.586100	0.789412	0.407448
C	1.421857	0.257029	-0.492041
N	2.684514	0.118874	-0.682579
C	3.856591	0.511903	0.095523
C	4.914479	1.164363	-0.808802
C	6.129962	1.582311	0.031155
H	4.479307	2.027096	-1.325595
H	5.231051	0.448294	-1.575203
C	6.708655	0.393930	0.809498
H	5.828938	2.371330	0.733586
H	6.888027	2.021828	-0.623636
C	5.640359	-0.272379	1.685991
H	7.549207	0.723304	1.426978
H	7.110149	-0.343364	0.101560
C	4.419419	-0.699421	0.858644
H	5.319585	0.428892	2.468479
H	6.052182	-1.145469	2.201075
H	3.636067	-1.119679	1.499843
H	4.702449	-1.476005	0.140726

H	3.549197	1.261054	0.825173
C	0.876558	1.965441	1.256528
C	1.577564	3.115817	0.518101
C	1.755585	4.320126	1.454949
H	0.987888	3.397510	-0.362570
H	2.557678	2.802231	0.148495
C	2.486933	3.922126	2.742529
H	0.769909	4.733171	1.706943
H	2.296990	5.110681	0.927355
C	1.740490	2.802489	3.478104
H	2.595847	4.791957	3.396586
H	3.504784	3.586990	2.497972
C	1.551817	1.565559	2.587326
H	0.757181	3.171236	3.798510
H	2.275386	2.510119	4.386851
H	2.520648	1.094043	2.401367
H	0.928875	0.814422	3.084888
H	-0.118639	2.334948	1.538343

Cat-IM3

$\boldsymbol{E}_{sol}$ = -2164.0878

$\boldsymbol{G}_{sol}$ = -2163.4803

H	4.14859	1.06453	-1.26023
H	5.21163	2.44010	0.74809
C	3.78036	1.04331	-0.21384
C	4.92052	1.39780	0.69395
C	5.62141	0.42243	1.30154
N	3.28818	-0.29106	0.05958
H	6.49427	0.66712	1.89808
C	5.23930	-0.97151	1.20618
C	3.97066	-1.31639	0.60762
C	5.99758	-2.00678	1.75344
C	3.49016	-2.64570	0.59911
H	6.94793	-1.77402	2.22206
H	2.55254	-2.89968	0.12822
C	5.53925	-3.32362	1.71128
C	4.28641	-3.63536	1.13286
H	6.14890	-4.11731	2.12944
H	3.94766	-4.66329	1.07822
O	1.94013	-0.35082	-0.20076
C	-5.82608	-1.44815	0.25927
C	-1.54679	-5.23196	-0.69190
C	-5.41040	-0.14266	0.51952
C	-4.86408	-2.40880	-0.04613
C	-2.63058	-4.39028	-0.46122
C	-0.27651	-4.67020	-0.84291
C	-4.04526	0.14466	0.45256
C	-3.51592	-2.04363	-0.08580
C	-2.42786	-3.00842	-0.38343
C	-0.16039	-3.28078	-0.78996
N	-1.19551	-2.47298	-0.55766
N	-3.12162	-0.76985	0.15416
H	-6.87869	-1.70429	0.29326
H	-1.67803	-6.30693	-0.73847
C	-6.33556	0.98066	0.85708
H	-5.17262	-3.42380	-0.26104
H	-3.61582	-4.81498	-0.31974
C	0.96851	-5.47044	-1.00524
H	-3.70847	1.15424	0.64895
H	0.79941	-2.80789	-0.95345
Cu	-1.04491	-0.44878	-0.18455
O	2.08431	-4.99544	-0.88447
O	0.72134	-6.75452	-1.27609
H	1.56971	-7.22333	-1.36082
O	-5.95389	2.11505	1.05424
O	-7.61391	0.58429	0.91159
H	-8.16136	1.35796	1.13216
N	0.19570	1.10231	-0.12987
C	1.46510	0.99597	-0.16645
N	2.55090	1.82979	-0.12446
C	2.70542	3.24302	-0.61956
C	2.46806	4.29242	0.47426
C	2.79188	5.69392	-0.06867
H	3.09088	4.05353	1.34332
H	1.43201	4.27127	0.82316
C	2.02252	5.98540	-1.36324
H	3.87022	5.76988	-0.26254
H	2.56130	6.43910	0.69785
C	2.32680	4.93354	-2.43737
H	2.27743	6.98224	-1.73392
H	0.94358	5.99604	-1.15489
C	1.98538	3.51641	-1.94615
H	3.39062	4.98140	-2.70448
H	1.76632	5.13913	-3.35379
H	2.28715	2.76591	-2.68655
H	0.90366	3.43309	-1.83161
H	3.77551	3.29833	-0.85363
C	-0.49735	2.39821	0.06531
C	-1.09537	2.45296	1.47685
C	-1.82987	3.78569	1.69267
H	-0.29736	2.32438	2.21692
H	-1.78433	1.60892	1.61013
C	-2.88835	4.04300	0.61169
H	-1.09419	4.60167	1.68335
H	-2.28581	3.79319	2.68710
C	-2.29046	3.94054	-0.79793
H	-3.32855	5.03434	0.75538
H	-3.71603	3.33157	0.72000
C	-1.56169	2.60607	-1.01612
H	-1.57856	4.76306	-0.95400
H	-3.06976	4.05963	-1.55642
H	-2.27620	1.77361	-0.98103
H	-1.09778	2.57091	-2.00811
H	0.21842	3.21100	-0.01336

Cat-IM4

$\boldsymbol{E}_{sol}$ = -2164.1161

$\boldsymbol{G}_{sol}$ = -2163.5104

H	-2.55497	-1.61705	-0.01624
H	-3.73939	-1.23201	2.24139

C	-3.15247	-0.70102	0.18416
C	-4.12162	-1.12926	1.23120
C	-5.40402	-1.43983	0.91272
N	-3.66020	-0.43692	-1.13905
H	-6.10511	-1.78688	1.66519
C	-5.85035	-1.27068	-0.43190
C	-4.89522	-0.74540	-1.42494
C	-7.15479	-1.54975	-0.84636
C	-5.33884	-0.52260	-2.78816
H	-7.87643	-1.93677	-0.13461
H	-4.60830	-0.13269	-3.48823
C	-7.52920	-1.32395	-2.16746
C	-6.62554	-0.80771	-3.14274
H	-8.54930	-1.54477	-2.46855
H	-6.97215	-0.65048	-4.15795
O	-0.22420	1.29810	0.04390
C	5.54995	-2.14420	-0.84256
C	4.71383	3.63441	-0.53168
C	4.37841	-2.89038	-0.70473
C	5.47889	-0.75233	-0.77995
C	5.04756	2.28155	-0.61504
C	3.38180	4.00107	-0.33101
C	3.17714	-2.20980	-0.50813
C	4.24428	-0.13762	-0.57096
C	4.03998	1.32620	-0.49457
C	2.42192	2.99287	-0.21880
N	2.75262	1.70358	-0.29843
N	3.11485	-0.88055	-0.43072
H	6.49910	-2.64477	-0.99677
H	5.47738	4.39864	-0.62121
C	4.31384	-4.38398	-0.73397
H	6.37868	-0.16050	-0.89143
H	6.07800	1.98796	-0.77119
C	2.90779	5.41619	-0.22331
H	2.25368	-2.76363	-0.40812
H	1.37572	3.23128	-0.06270
Cu	1.43919	0.21171	-0.08776
O	1.74646	5.70674	-0.04005
O	3.91290	6.29290	-0.35219
H	3.54487	7.19016	-0.27240
O	3.28369	-4.99852	-0.55430
O	5.50922	-4.93575	-0.97185
H	5.40507	-5.90342	-0.97289
N	-0.17671	-0.88013	0.30816
C	-0.90192	0.22987	0.32695
N	-2.24353	0.33322	0.62665
C	-2.87481	1.66546	0.89043
C	-2.94263	2.58125	-0.33831
C	-3.69034	3.87872	0.00468
H	-3.43461	2.05658	-1.16570
H	-1.92389	2.80879	-0.66283
C	-3.04481	4.58795	1.20270
H	-4.73888	3.64821	0.24072
H	-3.70455	4.53493	-0.87089
C	-2.97510	3.66082	2.42177
H	-3.60752	5.49349	1.45026
H	-2.03114	4.91052	0.93032
C	-2.22689	2.35821	2.09511
H	-3.99320	3.42252	2.75868
H	-2.47980	4.16091	3.25972
H	-2.23288	1.67879	2.95491
H	-1.18301	2.58424	1.85974
H	-3.90484	1.41115	1.17921
C	-0.44331	-2.09267	1.08685
C	0.65587	-2.30313	2.14330
C	0.44687	-3.60207	2.93290
H	0.67680	-1.43407	2.81106
H	1.62918	-2.33981	1.64080
C	0.33108	-4.81106	1.99617
H	-0.46759	-3.51742	3.53567
H	1.27105	-3.73682	3.64015
C	-0.80102	-4.60982	0.98120
H	0.15841	-5.72249	2.57635
H	1.27655	-4.95397	1.45624
C	-0.59463	-3.32091	0.17606
H	-1.76206	-4.55895	1.51287
H	-0.86522	-5.46331	0.29963
H	0.30547	-3.41486	-0.44330
H	-1.41872	-3.16828	-0.53663
H	-1.37673	-1.95549	1.65367

Cat-TS3

E_{sol} = -2164.1022

G_{sol} = -2163.4994

H	-3.543876	-0.677893	-0.305779
H	-5.118834	1.132876	1.161320
C	-3.404737	0.520297	-0.089682
C	-4.782832	0.947649	0.151078
C	-5.631648	1.067860	-0.909637
N	-2.971962	0.224265	-1.396328
H	-6.655768	1.389310	-0.745609
C	-5.198954	0.788352	-2.238390
C	-3.850661	0.310950	-2.419261
C	-6.031450	0.915224	-3.363359
C	-3.390755	-0.049934	-3.713867
H	-7.048773	1.271397	-3.238841
H	-2.376210	-0.417544	-3.816715
C	-5.549229	0.584296	-4.619458
C	-4.229076	0.101600	-4.795478
H	-6.194410	0.689886	-5.485445
H	-3.884112	-0.153228	-5.791578
O	-0.309845	1.566380	0.233394
C	5.183368	-2.343786	-0.709979
C	4.756410	3.481255	-0.610703
C	3.968355	-3.003054	-0.518477
C	5.204787	-0.948976	-0.710904
C	4.988157	2.105746	-0.660247
C	3.459319	3.950687	-0.398119
C	2.817927	-2.236427	-0.334277
C	4.016827	-0.244109	-0.519072

C	3.916215	1.231087	-0.495891
C	2.428524	3.020830	-0.242015
N	2.662383	1.707978	-0.292224
N	2.841458	-0.902925	-0.333105
H	6.094597	-2.912898	-0.855002
H	5.572207	4.184371	-0.734044
C	3.805261	-4.490084	-0.492878
H	6.140194	-0.424130	-0.858353
H	5.991430	1.732562	-0.822900
C	3.096181	5.401186	-0.322669
H	1.865111	-2.724950	-0.184153
H	1.406478	3.341586	-0.072831
Cu	1.253904	0.322491	-0.048206
O	1.963129	5.783369	-0.135555
O	4.164885	6.192833	-0.485109
H	3.869632	7.118198	-0.424732
O	2.732206	-5.027933	-0.322285
O	4.967204	-5.125969	-0.677679
H	4.801281	-6.084673	-0.649162
N	-0.461372	-0.620820	0.360002
C	-1.049930	0.535437	0.460637
N	-2.406154	0.753462	0.842093
C	-2.728504	1.036814	2.273273
C	-1.507289	1.578134	3.027167
C	-1.894535	1.919252	4.474581
H	-1.107864	2.454086	2.510810
H	-0.720357	0.811964	3.035209
C	-2.498883	0.713032	5.202600
H	-2.616583	2.746081	4.468476
H	-1.009920	2.285298	5.004074
C	-3.694926	0.143286	4.430633
H	-2.804137	0.996800	6.213906
H	-1.734091	-0.067671	5.312812
C	-3.305668	-0.197852	2.984913
H	-4.511542	0.877668	4.423336
H	-4.085184	-0.751766	4.923966
H	-4.170666	-0.595373	2.439885
H	-2.543306	-0.985939	2.986514
H	-3.478389	1.836500	2.261695
C	-1.068586	-1.932092	0.559955
C	-0.407103	-2.663067	1.737043
C	-1.000511	-4.064859	1.928443
H	-0.514001	-2.059581	2.645628
H	0.670286	-2.743118	1.545947
C	-0.919929	-4.886379	0.635306
H	-2.050129	-3.973000	2.240224
H	-0.478721	-4.574992	2.743610
C	-1.611795	-4.157588	-0.524008
H	-1.376014	-5.869345	0.786062
H	0.132481	-5.062364	0.378049
C	-1.019883	-2.757552	-0.734262
H	-2.686389	-4.068576	-0.309866
H	-1.526244	-4.735234	-1.449456
H	0.022998	-2.848792	-1.061885
H	-1.545162	-2.213742	-1.527041
H	-2.126995	-1.782456	0.826680

Cat-IM5

E_{sol} = -2164.2163

G_{sol} = -2163.6051

H	-2.620184	-0.440652	-0.117010
H	-3.862286	3.483066	0.496001
C	-3.063404	1.500636	0.151792
C	-4.069775	2.423808	0.528572
C	-5.284170	1.959717	0.976073
N	-3.344560	0.187177	0.243613
H	-6.046733	2.672000	1.276487
C	-5.566578	0.572608	1.072701
C	-4.544791	-0.334014	0.685228
C	-6.803626	0.050211	1.519691
C	-4.749120	-1.722644	0.720770
H	-7.587831	0.736651	1.821688
H	-3.973313	-2.411186	0.397803
C	-7.001047	-1.314126	1.561197
C	-5.974313	-2.196155	1.155901
H	-7.949116	-1.716355	1.900186
H	-6.148532	-3.266462	1.182252
O	-0.987559	-0.224663	-0.774823
C	5.442276	-2.239563	0.033176
C	0.583990	-5.467047	-0.492187
C	5.195983	-0.868328	0.100768
C	4.366922	-3.114491	-0.133415
C	1.817244	-4.819710	-0.390994
C	-0.584250	-4.705783	-0.582500
C	3.878926	-0.421278	-0.011518
C	3.074629	-2.601526	-0.225679
C	1.856138	-3.425366	-0.382256
C	-0.468872	-3.317019	-0.601155
N	0.711813	-2.708592	-0.500998
N	2.853364	-1.259544	-0.164750
H	6.456256	-2.615144	0.111898
H	0.527333	-6.549807	-0.488123
C	6.249222	0.177073	0.301824
H	4.542627	-4.181592	-0.189156
H	2.726391	-5.401613	-0.305203
C	-1.968434	-5.270846	-0.622733
H	3.665001	0.638101	0.030996
H	-1.345368	-2.689757	-0.698858
Cu	0.909988	-0.733475	-0.349614
O	-2.961350	-4.576021	-0.537822
O	-1.967067	-6.599634	-0.747722
H	-2.888049	-6.914504	-0.761574
O	5.983726	1.354609	0.410387
O	7.476453	-0.350295	0.348461
H	8.117696	0.369757	0.483350
N	0.482873	1.182505	0.032015
C	-0.750677	0.989283	-0.333250
N	-1.813416	1.915679	-0.280943
C	-1.756781	3.192546	-1.110536
C	-0.910080	2.994078	-2.373108

C	-1.027399	4.235171	-3.274841
H	-1.247118	2.098248	-2.906468
H	0.138461	2.838159	-2.100977
C	-0.662802	5.521132	-2.522371
H	-2.055787	4.310157	-3.651098
H	-0.384823	4.103724	-4.150406
C	-1.505083	5.680121	-1.250662
H	-0.798920	6.387741	-3.175726
H	0.401524	5.498228	-2.251420
C	-1.357775	4.451444	-0.337093
H	-2.561055	5.812298	-1.521818
H	-1.209704	6.577861	-0.700087
H	-1.963699	4.560730	0.568781
H	-0.316812	4.381427	-0.015011
H	-2.789908	3.317444	-1.448522
C	1.033036	2.245506	0.878653
C	2.086927	3.074512	0.132178
C	2.730260	4.120671	1.052152
H	1.635849	3.553812	-0.741755
H	2.864572	2.405880	-0.256791
C	3.326541	3.468924	2.305133
H	1.972260	4.858746	1.348684
H	3.498249	4.667839	0.497781
C	2.261138	2.667447	3.062890
H	3.756761	4.233131	2.959077
H	4.151024	2.806128	2.009605
C	1.607326	1.613460	2.158701
H	1.487584	3.350325	3.438024
H	2.693412	2.176251	3.940126
H	2.356214	0.860730	1.879981
H	0.806999	1.083726	2.689002
H	0.207758	2.900432	1.178065

6. Characterization data of various products

1,3-dicyclohexyl-1-(quinolin-2-yl)urea **(3a)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.20 (d, *J* = 8.8 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.67 (t, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 8.8 Hz, 1H), 4.35 – 4.28 (m, 1H), 3.55- 3.53 (m, 1H), 1.80 – 1.55 (m, 12H), 1.28 – 1.06 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.7, 154.9, 146.8, 137.9, 130.1, 128.0, 127.8, 125.5, 125.3, 118.9, 56.4, 49.5, 33.8, 32.9, 31.5, 26.4, 25.8, 25.7, 25.1, 24.9.

1,3-dicyclohexyl-1-(3-methylquinolin-2-yl)urea **(3b)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.17 (s, 1H), 7.90 (t, *J* = 8.8 Hz, 2H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 5.67 (d, J = 7.6 Hz, 1H), 4.17 (t, J = 7.6 Hz, 1H), 3.49 – 3.44 (m, 1H), 2.30 (s, 3H), 1.76 – 1.50 (m, 10H), 1.28 – 0.83 (m, 10H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.3, 153.9, 146.1, 138.3, 131.6, 129.1, 129.0, 128.0, 127.4, 126.9, 56.5, 49.6, 33.4, 31.9, 26.1, 25.8, 25.7, 18.2.

1,3-dicyclohexyl-1-(4-methylquinolin-2-yl)urea **(3c)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.98 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.67 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.07 (s, 1H), 4.30 – 4.23 (m, 1H), 3.55 – 3.50 (m, 1H), 2.61 (s, 3H), 1.77 – 1.50 (m, 12H), 1.30 – 1.02 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.7, 154.7, 146.7, 145.9, 129.9, 128.4, 125.7, 125.3, 124.4, 119.3, 56.5, 49.4, 32.9, 31.5, 26.4, 25.8, 25.7, 25.1, 18.8.

1,3-dicyclohexyl-1-(5-methylquinolin-2-yl)urea **(3d)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.31 (d, *J* = 9.2 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 8.8 Hz, 2H), 7.23 (d, *J* = 8.8 Hz, 1H), 4.33 – 4.26 (m, 1H), 3.54 – 3.52 (m, 1H), 2.61 (s, 3H), 1.76 – 1.51 (m, 12H), 1.25 – 1.05 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.7, 154.6, 147.1, 134.9, 134.6, 129.8, 126.3, 126.0, 124.7, 118.8, 56.4, 49.5, 32.9, 31.5, 26.4, 25.8, 25.7, 25.1, 18.7.

1,3-dicyclohexyl-1-(7-methylquinolin-2-yl)urea **(3e)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.14 (d, *J* = 8.8 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.59 (s, 1H), 7.29 (t, *J* = 6.8 Hz, 2H), 7.12 (d, *J* = 8.8 Hz, 1H), 4.30 – 4.27 (m, 1H), 3.53 – 3.49 (m, 1H), 2.48 (s, 3H), 1.76 – 1.54 (m, 12H), 1.25 – 1.02 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.7, 154.9, 147.0, 139.9, 137.6, 127.7, 127.4, 127.0, 123.5, 118.1, 56.4, 49.5, 32.9, 26.4, 25.8, 25.7, 25.2, 21.8.

1,3-dicyclohexyl-1-(8-methylquinolin-2-yl)urea **(3f)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.16 (d, *J* = 6.8 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 4.2 Hz, 1H), 7.41 (d, *J* = 6.0 Hz, 1H), 7.35 (t, *J* = 6.4 Hz, 1H), 7.21 (d, J = 6.4 Hz, 1H), 4.32 – 4.27 (m, 1H), 3.52 (s, 1H), 2.63 (s, 3H), 1.87 – 1.53 (m, 12H), 1.29 – 1.07 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.9, 154.0, 145.5, 138.1, 135.1, 126.0, 125.3, 125.1, 118.8, 56.8, 49.7, 33.2, 31.5, 26.5, 25.9, 25.8, 25.4, 18.2.

1,3-dicyclohexyl-1-(5-methoxyquinolin-2-yl)urea **(3g)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.34 (d, *J* = 8.4 Hz, 1H), 7.58 (t, *J* = 8.0 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 8.8 Hz, 1H), 7.14 (d, *J* = 9.2 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 1H), 4.31 – 4.27 (m, 1H), 3.96 (s, 3H), 3.53 - 3.51 (m, 1H), 1.79 – 1.51 (m, 12H), 1.25 – 1.00 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.7, 155.3, 155.2, 147.8, 132.1, 130.4, 120.1, 117.5, 116.9, 104.2, 56.3, 49.5, 32.8, 31.4, 26.4, 25.8, 25.7, 25.1; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{23}H_{32}N_3O_2$: 382.2489; found: 382.2481.

1,3-dicyclohexyl-1-(6-methoxyquinolin-2-yl)urea **(3h)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*)

δ 8.16 (d, *J* = 8.8 Hz, 1H), 7.76 (d, *J* = 9.2 Hz, 1H), 7.35 (d, *J* = 6.0 Hz, 2H), 7.20 (d, *J* = 8.8 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 4.21 (t, J = 10.2 Hz, 1H), 3.87 (s, 3H), 3.49 (d, J = 7.6 Hz, 1H), 1.74 – 1.49 (m, 12H), 1.22 – 0.96 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 157.3, 155.9, 152.7, 142.6, 137.1, 129.4, 127.1, 122.2, 121.1, 106.4, 56.5, 56.0, 49.4, 33.1, 31.8, 26.4, 25.8, 25.2.

1,3-dicyclohexyl-1-(8-methoxyquinolin-2-yl)urea **(3i)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.05 (d, *J* = 7.2 Hz, 1H), 8.22 (d, *J* = 8.8 Hz, 1H), 7.43 – 7.36 (m, 2H), 7.32 (d, *J* = 9.2 Hz, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 4.13 (t, J = 12.0 Hz, 1H), 3.95 (s, 3H), 3.56 (t, J = 3.2 Hz, 1H), 2.12 – 2.02 (m, 2H), 1.83 – 1.55 (m, 10H), 1.30 – 1.11 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.5, 154.3, 154.0, 138.4, 137.2, 126.0, 125.7, 117.7, 109.6, 58.1, 56.2, 49.2, 33.2, 31.2, 26.6, 25.9, 25.7, 24.9.

1,3-dicyclohexyl-1-(6-fluoroquinolin-2-yl)urea **(3j)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.19 (d, *J* = 9.2 Hz, 1H), 7.85 (dd, *J* = 8.8 Hz, 1H), 7.70 (d, J = 9.2 Hz, 1H), 7.57 (t, *J* = 8.8 Hz, 1H), 7.23 (d, *J* = 8.8 Hz, 1H), 7.17 (d, *J* = 7.6 Hz, 1H), 4.29 (s, 1H), 3.50 (s, 1H), 1.75 – 1.51 (m, 12H), 1.26 – 1.01 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 158.1, 155.8, 154.5, 144.0, 137.4, 130.5, 130.5, 126.1, 120.4, 119.8, 119.5, 111.5, 111.3, 56.5, 49.7, 32.9, 31.6, 26.4, 25.8, 25.8, 25.3; ^{19}F NMR (376 MHz, DMSO-*d6*) δ -116.3.

1,3-dicyclohexyl-1-(8-fluoroquinolin-2-yl)urea **(3k)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.22 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H), 7.48 (t, *J* = 8.8 Hz, 1H), 7.40 (dd, *J* = 7.6, 4.8 Hz, 1H), 7.24 (d, *J* = 9.2 Hz, 1H), 4.36 – 4.30 (m, 1H), 3.54 - 3.52 (m, 1H), 1.89 – 1.52 (m, 12H), 1.28 – 1.05 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 157.9, 155.6, 155.1, 137.8, 136.5, 136.4, 126.9, 124.7, 124.6, 123.9, 118.9, 114.5, 114.4, 56.5, 49.7, 32.9, 31.3, 26.4, 25.8, 25.8, 25.2; ^{19}F NMR (376 MHz, DMSO-*d6*) δ -127.9; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{22}H_{29}FN_3O$: 370.2289; found: 370.2286.

1-(4-chloroquinolin-2-yl)-1,3-dicyclohexylurea **(3l)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.05 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 8.4 Hz, 1H), 7.76 (t, J = 6.4 Hz, 1H), 7.57 (t, *J* = 6.4 Hz, 1H), 7.38 (d, *J* = 6.4 Hz, 1H), 7.31 (d, J = 3.2 Hz, 1H), 4.37 (s, 1H), 3.54 (d, J = 4.0 Hz, 1H), 1.75 – 1.53 (m, 12H), 1.28 – 1.07 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.5, 154.6, 147.6, 141.6, 131.4, 128.5, 126.3, 123.9, 123.0, 118.3, 56.0, 49.8, 32.8, 31.3, 26.3, 25.8, 25.7, 25.2.

1-(6-chloroquinolin-2-yl)-1,3-dicyclohexylurea **(3m)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.14 (d, *J* = 8.8 Hz, 1H), 7.97 (d, *J* = 1.2 Hz, 1H), 7.76 (d, J = 8.8 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.19 (d, J = 8.8 Hz, 1H), 4.36 – 4.35 (m, 1H), 3.53 – 3.51 (m, 1H), 1.78 – 1.52 (m, 12H), 1.25 – 1.05 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.6, 155.3, 145.5, 137.0, 130.4, 129.7, 128.9, 126.7, 125.9, 119.1, 56.0, 49.7, 32.8, 31.3, 26.3, 25.8, 25.7, 25.2.

1-(7-chloroquinolin-2-yl)-1,3-dicyclohexylurea **(3n)[15]**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.17 (d, *J* = 8.8 Hz, 1H), 7.87 (d, *J* = 8.8 Hz, 1H), 7.76 (s, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.43 (d, *J* = 8.8 Hz, 1H), 7.13 (d, *J* = 9.2 Hz, 1H), 4.39 – 4.37 (m, 1H), 3.54 - 3.52 (m, 1H), 1.83 – 1.54 (m, 12H), 1.30 – 1.09 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.8, 155.5, 147.6, 137.6, 134.5, 129.9, 126.2, 125.0, 123.6, 117.8, 55.8, 49.8, 32.7, 31.2, 26.3, 25.8, 25.7, 25.2.

1-(8-chloroquinolin-2-yl)-1,3-dicyclohexylurea **(3o)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.23 (d, *J* = 8.8 Hz, 1H), 8.18 (d, *J* = 7.6 Hz, 1H), 7.83 (d, J = 7.6 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 9.2 Hz, 1H), 4.33 (t, J = 12.0 Hz, 1H), 3.55 - 3.51 (m, 1H), 2.07 – 1.99 (m, 3H), 1.86 – 1.55 (m, 9H), 1.31 – 1.06 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*)

δ 155.5, 142.5, 138.4, 130.6, 130.0, 127.4, 126.2, 125.0, 118.2, 57.2, 49.8, 33.1, 31.0, 26.6, 25.9, 25.8, 25.2; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{22}H_{29}ClN_3O$: 386.1994; found: 386.1997.

1-(5-bromoquinolin-2-yl)-1,3-dicyclohexylurea **(3p)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.26 (d, *J* = 8.8 Hz, 1H), 7.77 – 7.71 (m, 2H), 7.61 - 7.53 (m, 2H), 7.26 (d, *J* = 9.2 Hz, 1H), 4.42 – 4.38 (m, 1H), 3.55 - 3.53 (m, 1H), 1.83 – 1.59 (m, 12H), 1.29 – 1.08 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.7, 155.5, 148.0, 136.3, 130.8, 128.3, 123.9, 121.3, 119.1, 55.9, 49.8, 32.7, 31.2, 26.4, 25.8, 25.7, 25.2.

1-(6-bromoquinolin-2-yl)-1,3-dicyclohexylurea **(3q)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.13 (d, *J* = 9.2 Hz, 1H), 7.75 (d, J = 8.8 Hz, 1H), 7.68 (d, J = 9.2 Hz, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.18 (d, *J* = 8.8 Hz, 1H), 4.36 – 4.35 (m, 1H), 3.54 – 3.52 (m, 1H), 1.78 – 1.53 (m, 12H), 1.25 – 1.03 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.6, 155.3, 145.7, 136.9, 132.9, 129.9, 129.8, 126.5, 118.9, 117.1, 56.0, 49.7, 33.8, 31.3, 26.3, 25.8, 25.7, 25.2, 24.9.

1,3-dicyclohexyl-1-(4-nitroquinolin-2-yl)urea **(3r)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.10 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.83 (t, J = 8.0 Hz, 1H), 7.76 (s, 1H), 7.66 – 7.61 (m, 2H), 4.45 (s, 1H), 3.55 (s, 1H), 1.85 – 1.61 (m, 12H), 1.26 – 1.08 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.2, 154.4, 153.4, 148.6, 131.7, 128.3, 127.2, 122.7, 115.5, 112.7, 100.0, 56.1, 49.9, 32.7, 31.1, 26.3, 25.7, 25.2; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{22}H_{29}N_4O_3$: 397.2234; found: 397.2238.

ethyl 2-(1,3-dicyclohexylureido)quinoline-6-carboxylate **(3s)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.48 (s, 3H), 8.27 (d, *J* = 9.2 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.12 (d, *J* = 9.2 Hz, 1H), 4.47 (t, J = 10.2 Hz, 1H), 4.36 (dd, J = 14.4, 7.2 Hz, 2H), 3.55 (t, J = 4.0 Hz, 1H), 1.85 – 1.57 (m, 12H), 1.36 (t, J = 7.2 Hz, 3H), 1.27 – 1.08 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 166.1, 156.5, 155.2, 149.6, 138.7, 130.6, 129.3, 127.5, 125.0, 123.7, 116.7, 61.2, 55.4, 49.9, 32.6, 31.0, 26.3, 25.8, 25.7, 25.1, 14.7; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{25}H_{34}N_3O_3$: 424.2595; found: 424.2591.

1,3-dicyclohexyl-1-(4,7-dichloroquinolin-2-yl)urea **(3t)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.03 (d, J = 8.8 Hz, 1H), 7.83 (s, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.25 (s, 1H), 4.40 (s, 1H), 3.56 – 3.54 (m, 1H), 1.83 – 1.55 (m, 12H), 1.25 – 1.07 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.5, 155.0, 148.3, 141.5, 136.0, 126.7, 126.0, 121.2, 116.9, 55.7, 49.9, 32.7, 31.0, 26.2, 25.7, 25.1; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{22}H_{28}Cl_2N_3O$: 420.1604; found: 420.1605.

1-(4-chloro-6-fluoroquinolin-2-yl)-1,3-dicyclohexylurea **(3u)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.93 – 7.91 (m, 1H), 7.78 – 7.68 (m, 2H), 7.42 – 7.24 (m, 2H), 4.34 (s, 1H), 3.54 (s, 1H), 1.76 – 1.57 (m, 12H), 1.27 – 1.07 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 158.7, 155.4, 154.2, 144.7, 140.9, 131.4, 131.3, 123.9, 121.1, 120.8, 119.5, 108.0, 107.8, 56.1, 49.8, 32.8, 31.3, 26.3, 25.7, 25.2; ^{19}F NMR (376 MHz, DMSO-*d6*) δ -114.1; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{22}H_{28}ClFN_3O$: 404.1899; found: 404.1894.

1-(benzo[*h*]quinolin-2-yl)-1,3-dicyclohexylurea **(3v)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.99 (d, *J* = 8.0 Hz, 1H), 8.28 (d, *J* = 8.8 Hz, 1H), 8.02 (d, J = 7.2 Hz, 1H), 7.84 (dd, *J* = 12.8, 8.8 Hz, 2H), 7.76 – 7.70 (m, 2H), 7.32 (d, J = 8.4 Hz, 1H), 7.06 (d, J = 7.6 Hz, 1H), 4.34 – 4.39 (m, 1H), 3.56 - 3.54 (m, 1H), 1.83 – 1.75 (m, 8H), 1.67 – 1.52 (m, 4H), 1.22 – 1.02 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 155.9, 154.2, 144.6, 138.1, 134.0, 130.8, 128.5, 128.5, 127.3, 126.0, 125.8, 124.1, 123.0, 119.5, 56.4, 49.7, 33.0, 31.7, 26.5, 26.0,

25.8, 25.3.

1,3-dicyclohexyl-1-(isoquinolin-1-yl)urea **(3w)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.41 (d, J = 5.6 Hz, 1H), 7.98 (d, *J* = 8.8 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 5.6 Hz, 1H), 7.74 (t, J = 7.6 Hz, 1H), 7.63 (t, J = 7.6 Hz, 1H), 5.37 (d, J = 7.6 Hz, 1H), 4.28 (s, 1H), 3.44 – 3.42 (m, 1H), 1.76 – 1.47 (m, 12H), 1.27 – 0.85 (m, 8H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 156.0, 153.3, 141.9, 138.1, 130.8, 128.1, 127.8, 127.4, 125.8, 121.1, 56.5, 49.5, 33.2, 32.0, 26.0, 25.7, 25.5; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{22}H_{30}N_3O$: 352.2383; found: 352.2385.

1,3-diisopropyl-1-(quinolin-2-yl)urea **(3x)**[15]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.21 (d, *J* = 9.2 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 1H), 7.26 (d, *J* = 7.6 Hz, 1H), 7.20 (d, *J* = 8.8 Hz, 1H), 4.69 – 4.62 (m, 1H), 1.25 (d, *J* = 6.8 Hz, 6H), 1.05 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 156.7, 155.2, 147.2, 138.7, 130.9, 128.6, 128.4, 126.4, 126.2, 119.9, 49.1, 43.1, 23.5, 22.1.

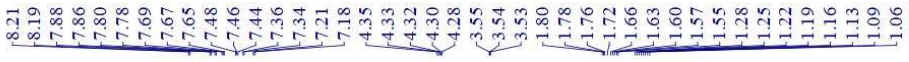
3-(*tert*-butyl)-1-ethyl-1-(quinolin-2-yl)urea **(3y)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 10.77 (s, 1H), 8.33 (d, *J* = 9.2 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 5.6 Hz, 2H), 7.46 (t, *J* = 8.4 Hz, 2H), 4.03 (q, *J* = 6.8 Hz, 2H), 1.41 (s, 9H), 1.18 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 154.7, 154.4, 145.0, 139.3, 130.9, 128.0, 126.4, 125.2, 124.0, 113.8, 50.6, 29.3, 14.4; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{16}H_{22}N_3O$: 272.1757; found: 272.1760.

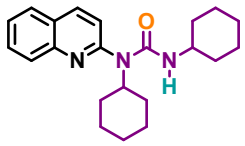
N-(*p*-tolyl)quinolin-2-amine **(3z)**[16]: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.31 (s, 1H), 8.02 (d, J = 8.8 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.65 (d, J = 8.8 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.26 (t, *J* = 7.2 Hz, 1H), 7.13 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.8 Hz, 1H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 154.8, 147.5, 139.4, 137.2, 130.3, 129.9, 129.5, 128.0, 126.7, 123.9, 123.0, 119.0, 114.6, 21.0.

heptan-2-yl 2-((5-chloro-2-(1,3-dicyclohexylureido)quinolin-8-yl)oxy)acetate **(3aa)**: ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.38 (d, *J* = 7.6 Hz, 1H), 8.32 (d, *J* = 9.2 Hz, 1H), 7.44 – 7.39 (m, 2H), 7.11 (d, *J* = 8.4 Hz, 1H), 5.00 (s, 2H), 4.92 – 4.86 (m, 1H), 4.25 (t, *J* = 11.6 Hz, 1H), 3.54 – 3.53 (m, 1H), 2.05 – 1.99 (m, 2H), 1.85 – 1.76 (m, 7H), 1.66 – 1.42 (m, 7H), 1.43 – 1.13 (m, 15H), 0.78 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-*d6*) δ 168.6, 155.2, 154.6, 151.8, 138.6, 134.4, 124.5, 123.0, 122.4, 118.4, 112.5, 71.9, 66.6, 57.5, 55.4, 49.6, 35.6, 33.8, 33.0, 32.9, 31.5, 31.0, 26.5, 25.8, 25.7, 25.2, 24.8, 22.4, 20.1, 14.2; HRMS (ESI): m/z $[M+H]^+$ calcd for $C_{31}H_{45}ClN_3O_4$: 558.3093; found: 558.3091.

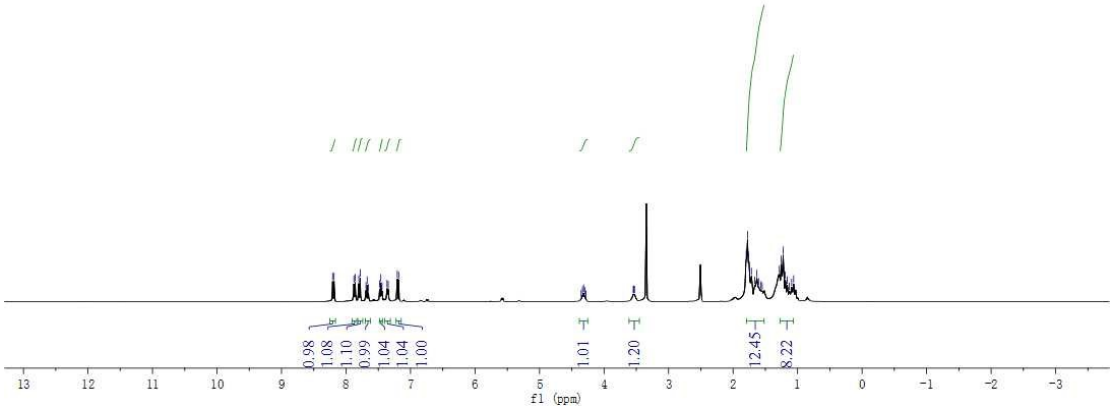
7. [1]H and [13]C NMR spectra

[1]H NMR of **3a**

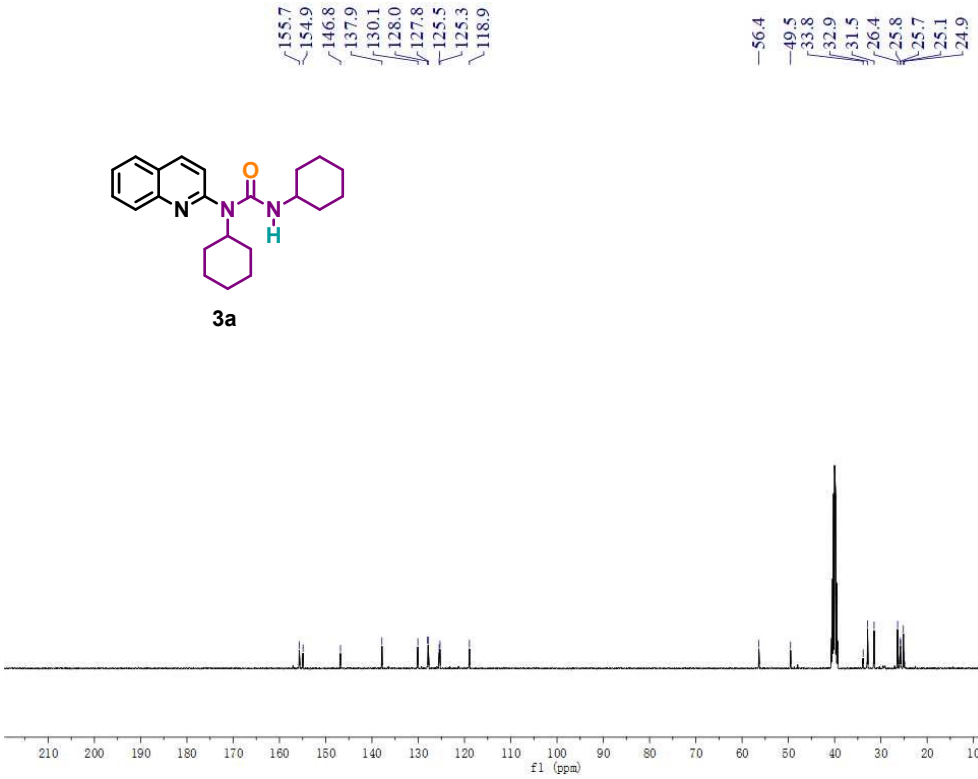




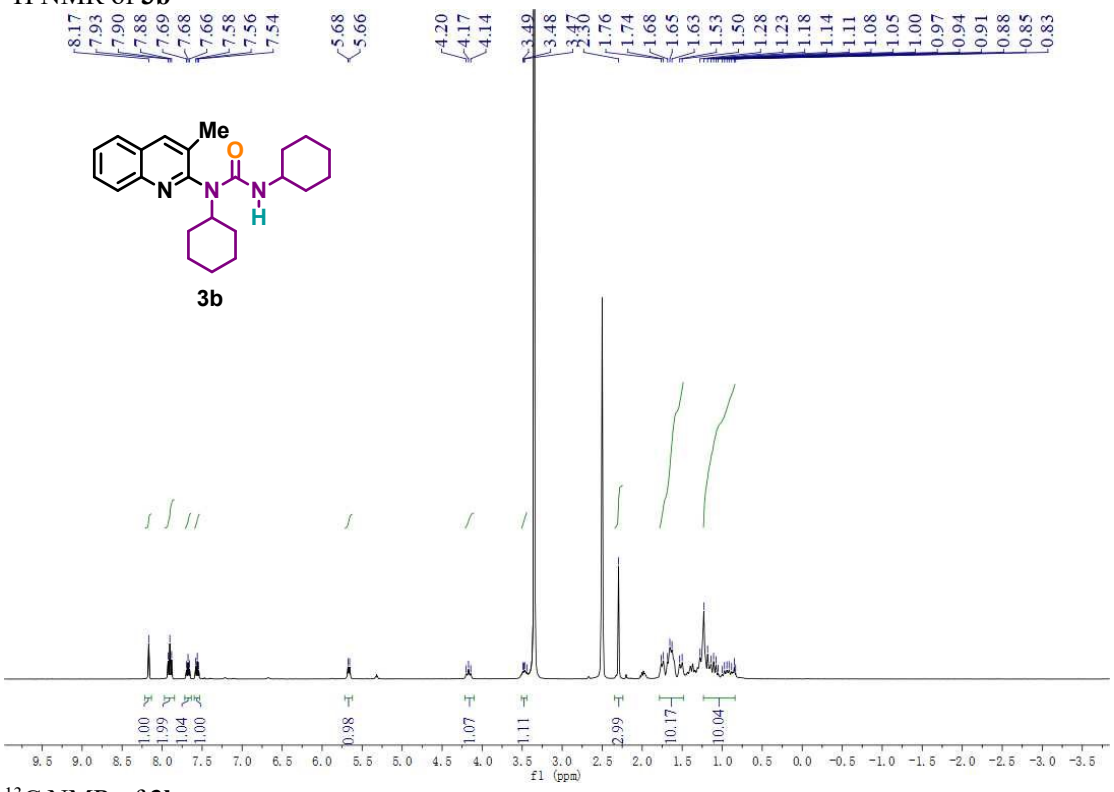
3a



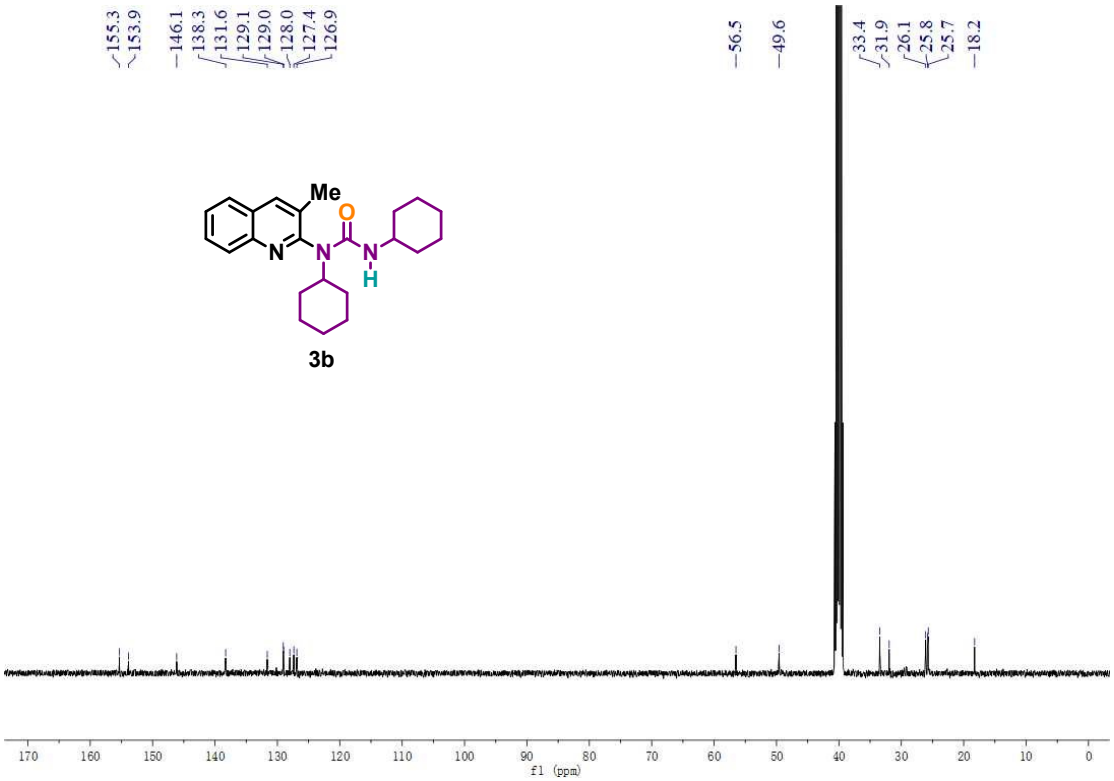
[13]C NMR of **3a**



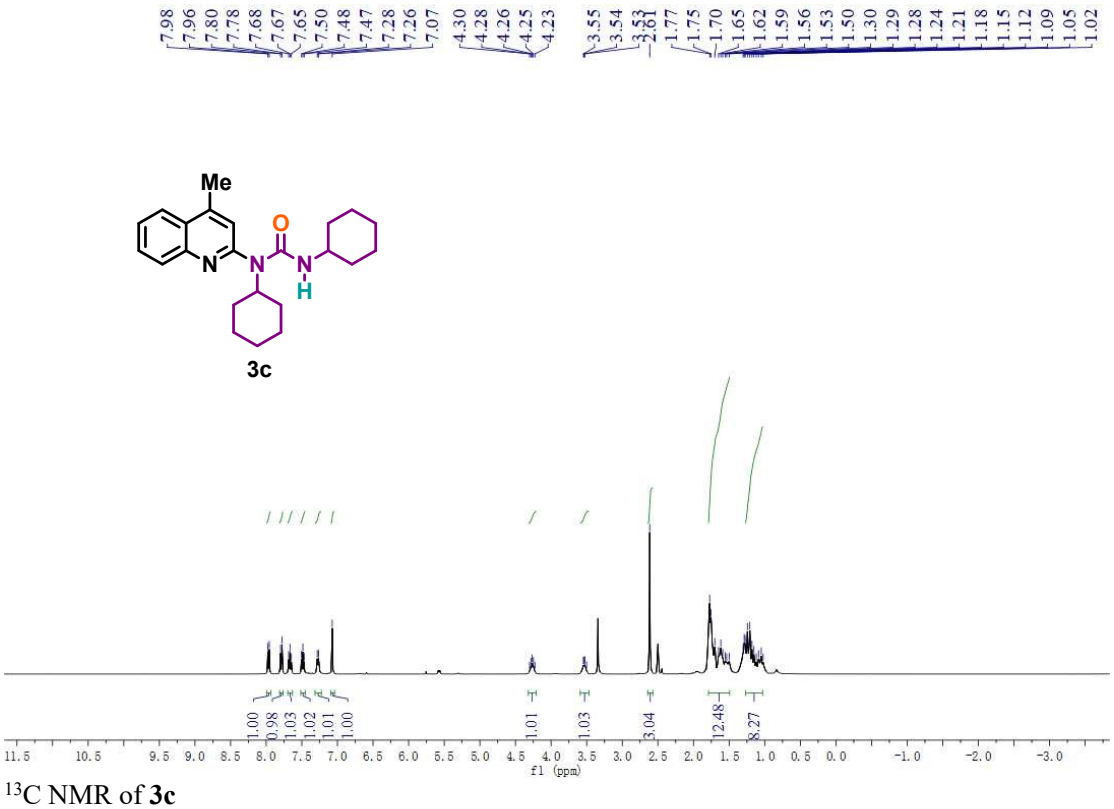
^{1}H NMR of **3b**



^{13}C NMR of **3b**

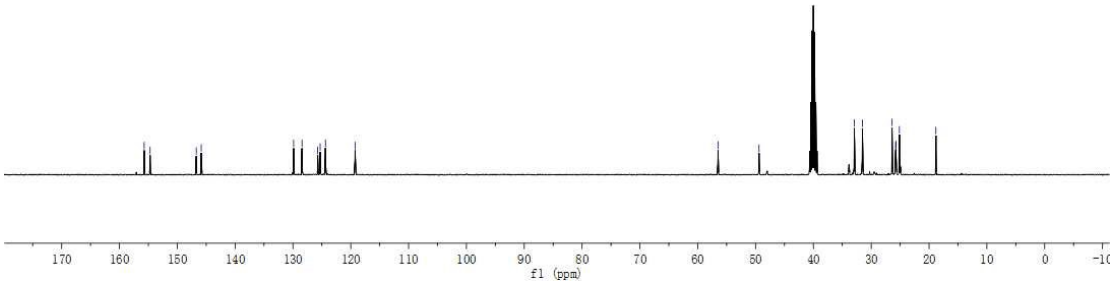


^{1}H NMR of **3c**

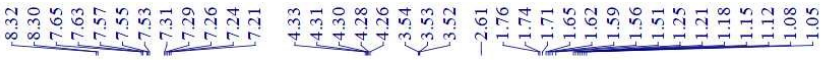


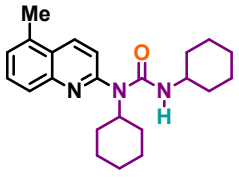
^{13}C NMR of **3c**

3c

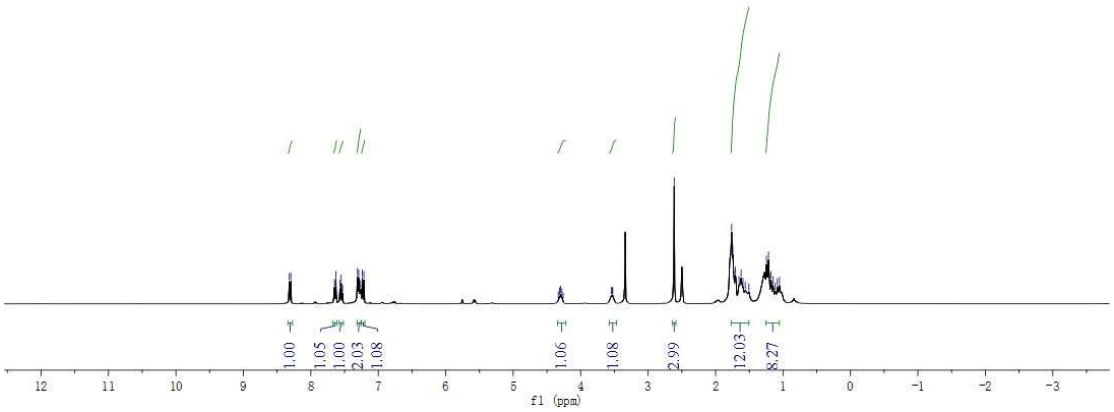


^{1}H NMR of **3d**

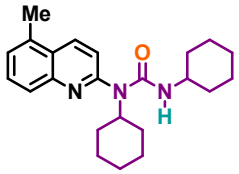




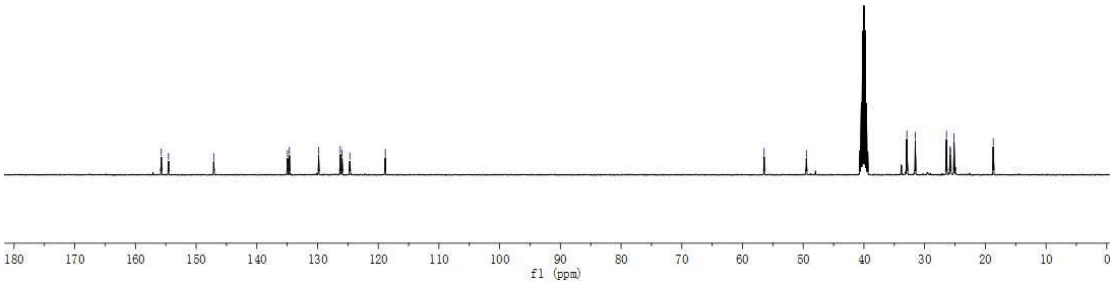
3d



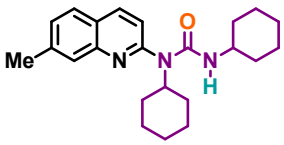
^{13}C NMR of **3d**



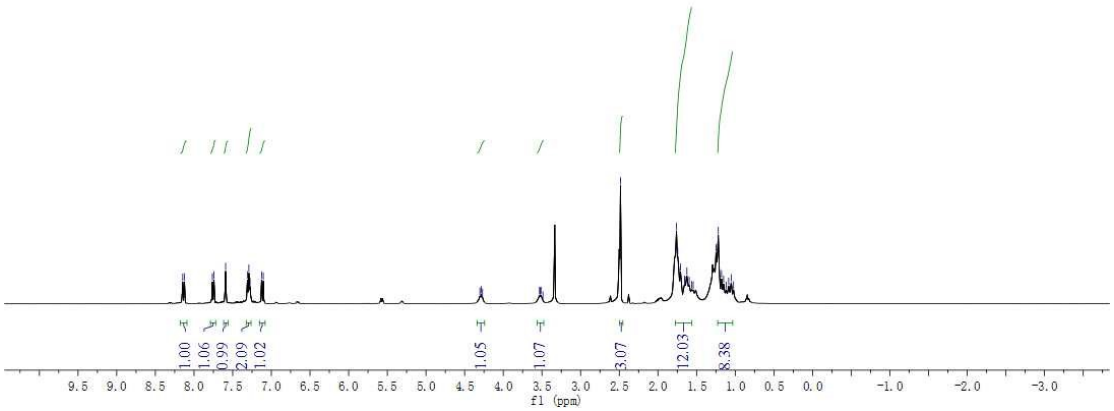
3d



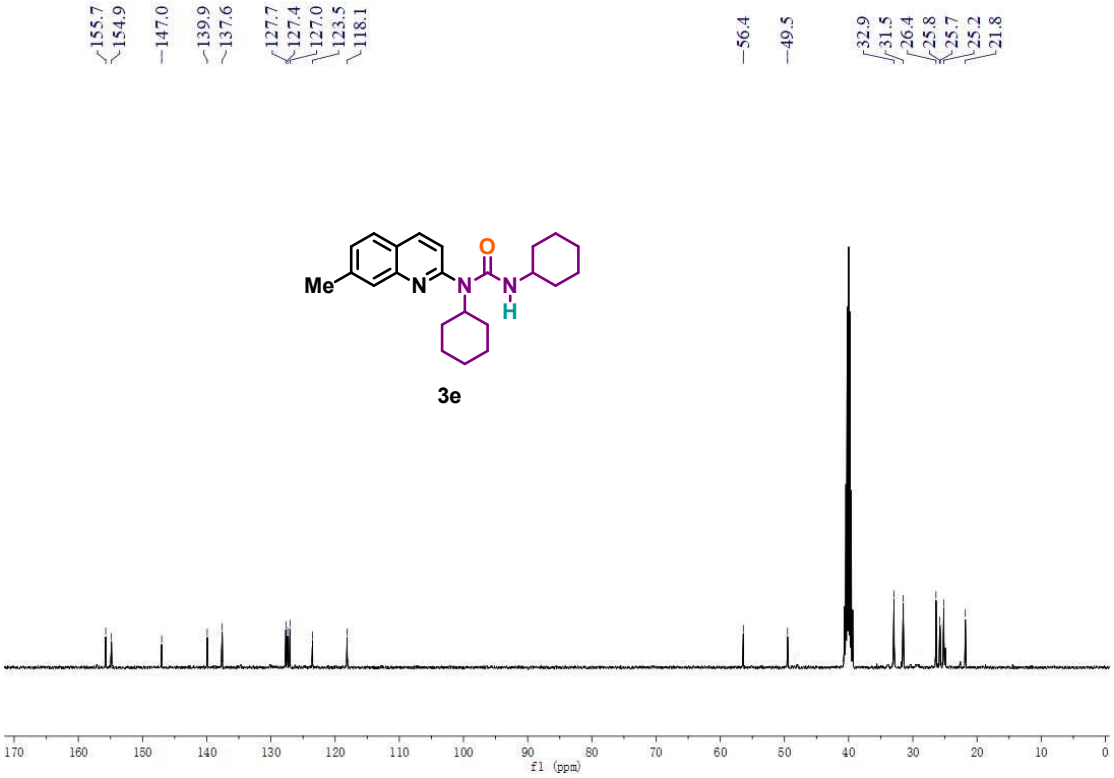
^{1}H NMR of **3e**



3e



^{13}C NMR of **3e**



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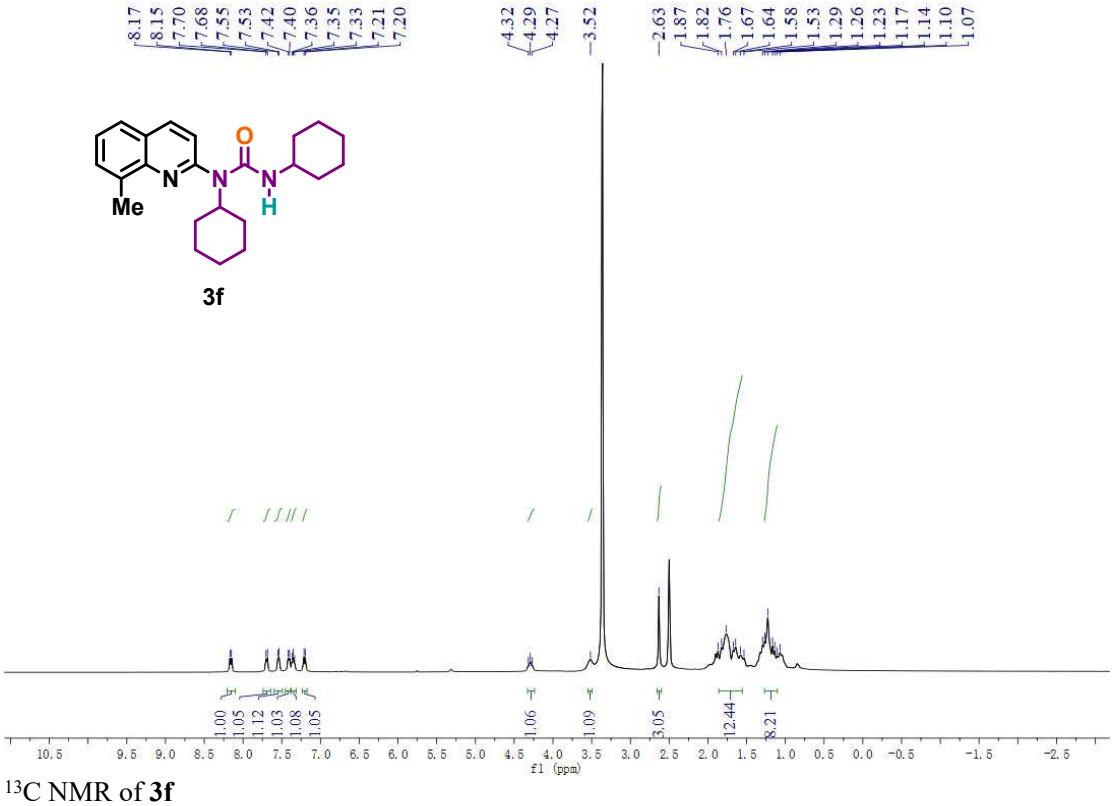

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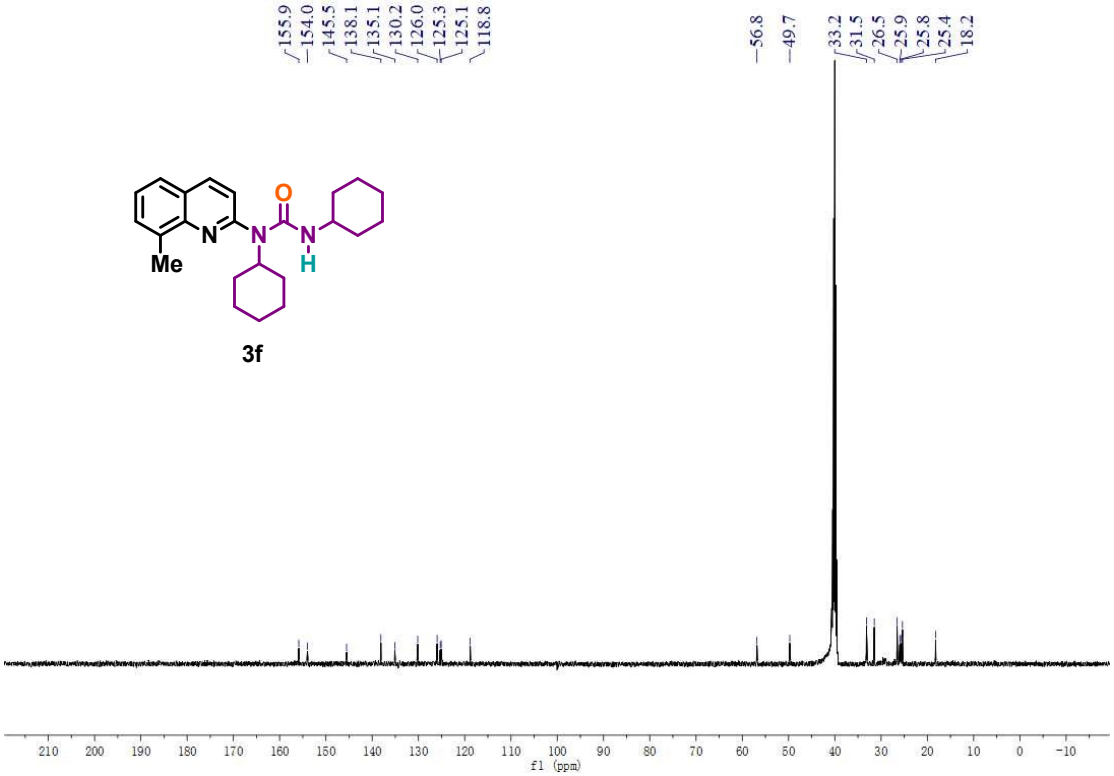

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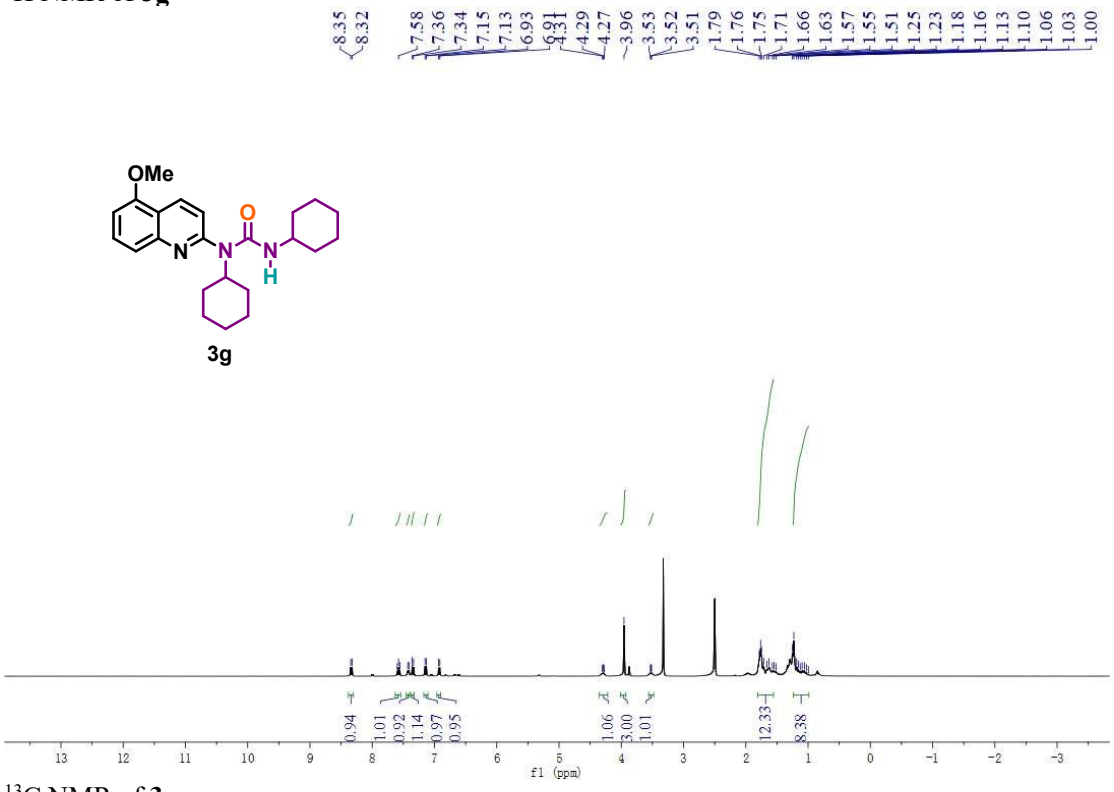

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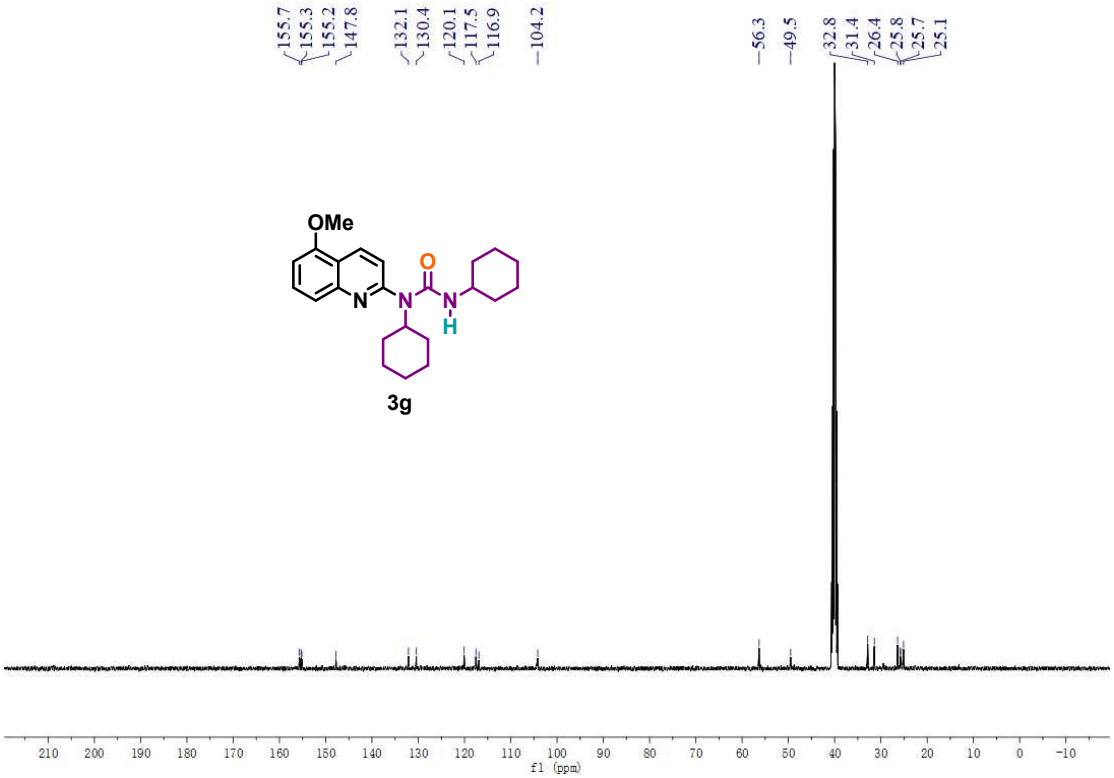

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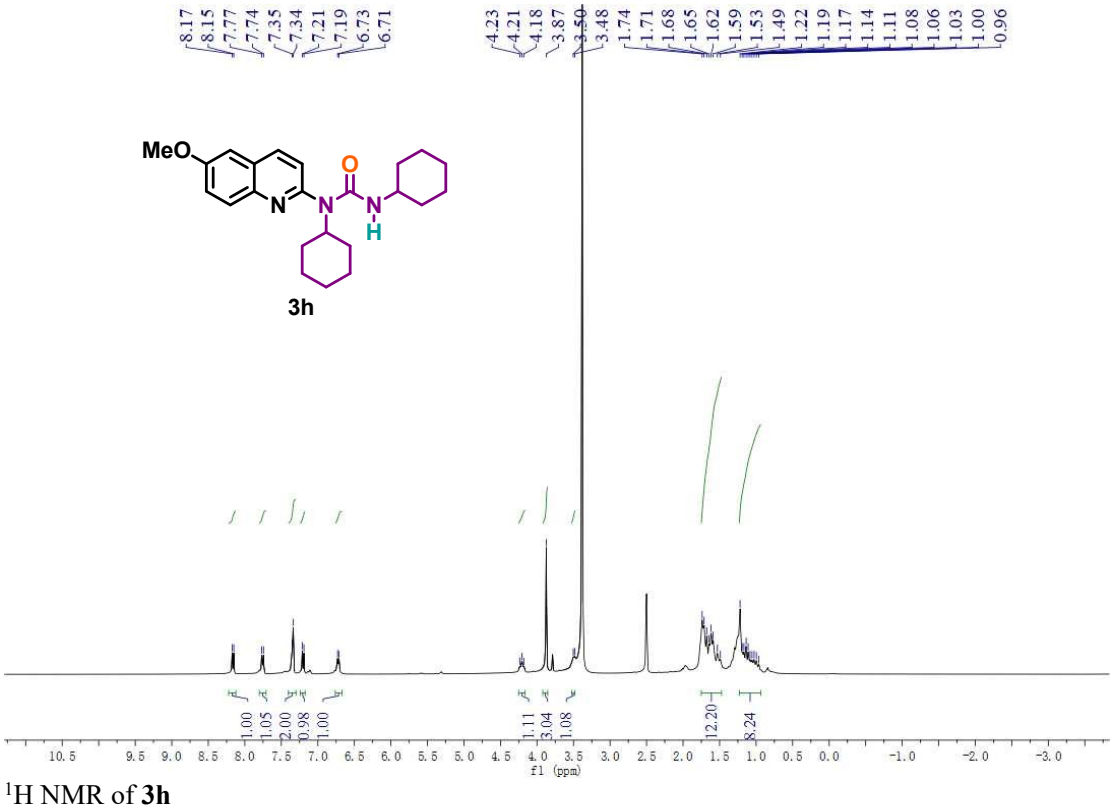
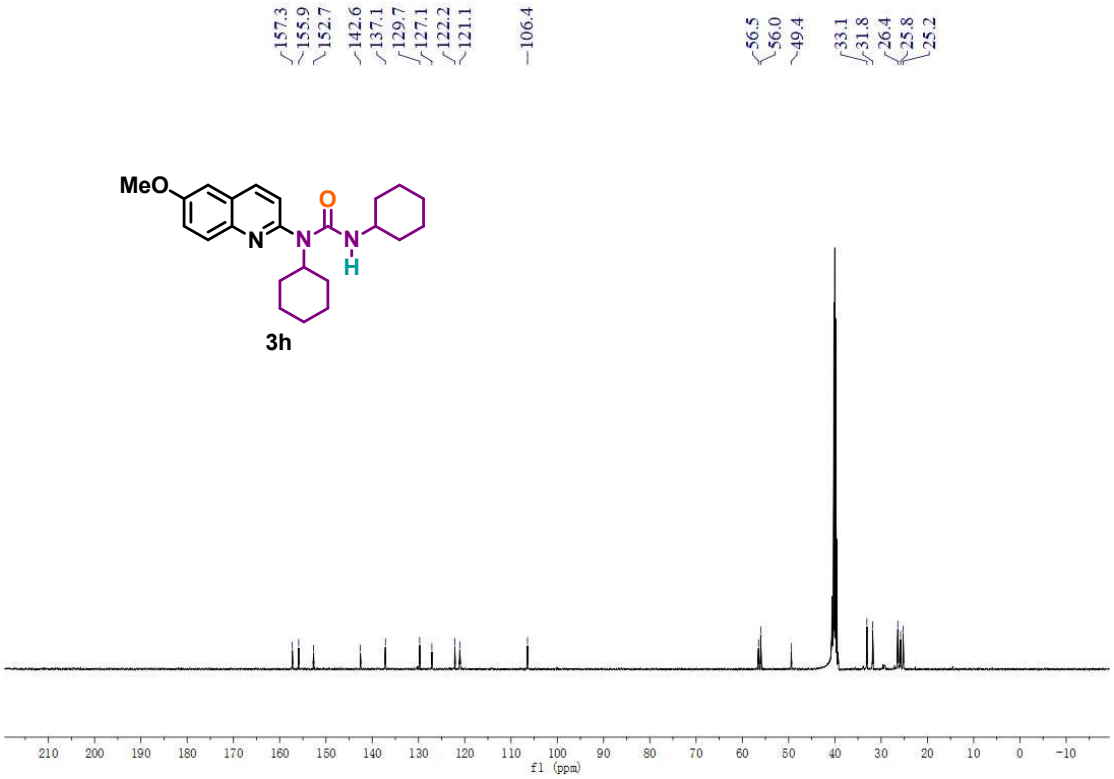


^{1}H NMR of **3h**



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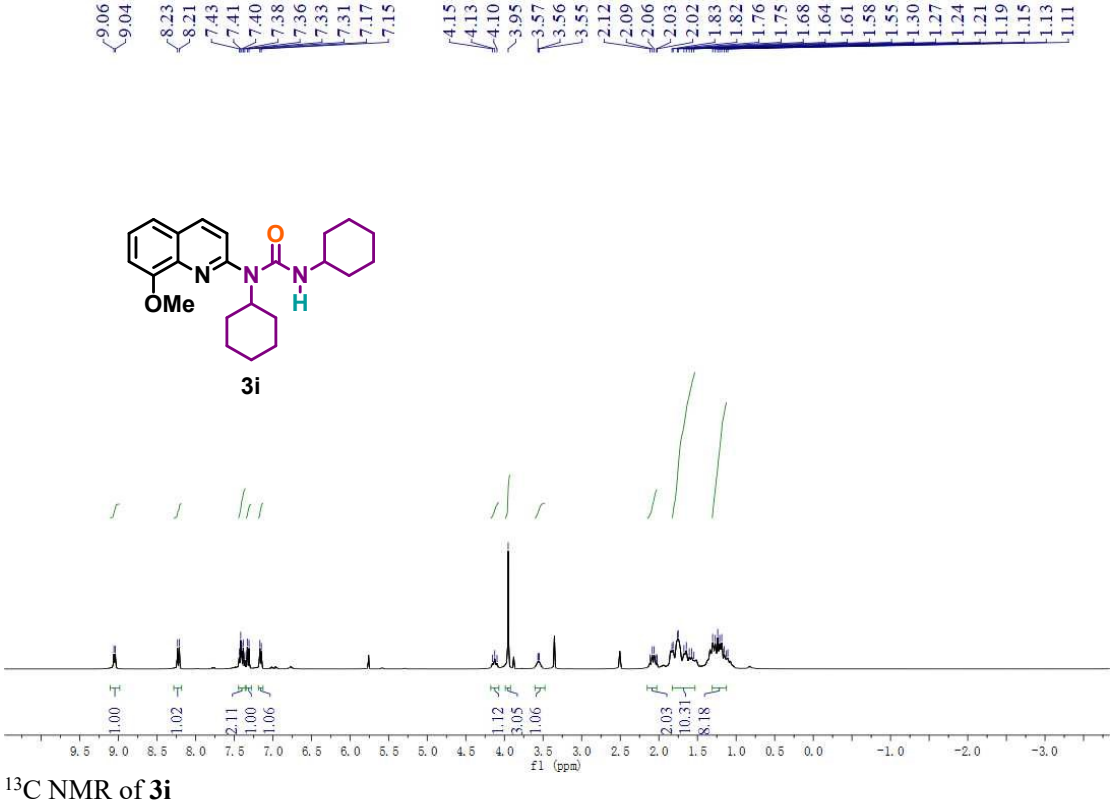

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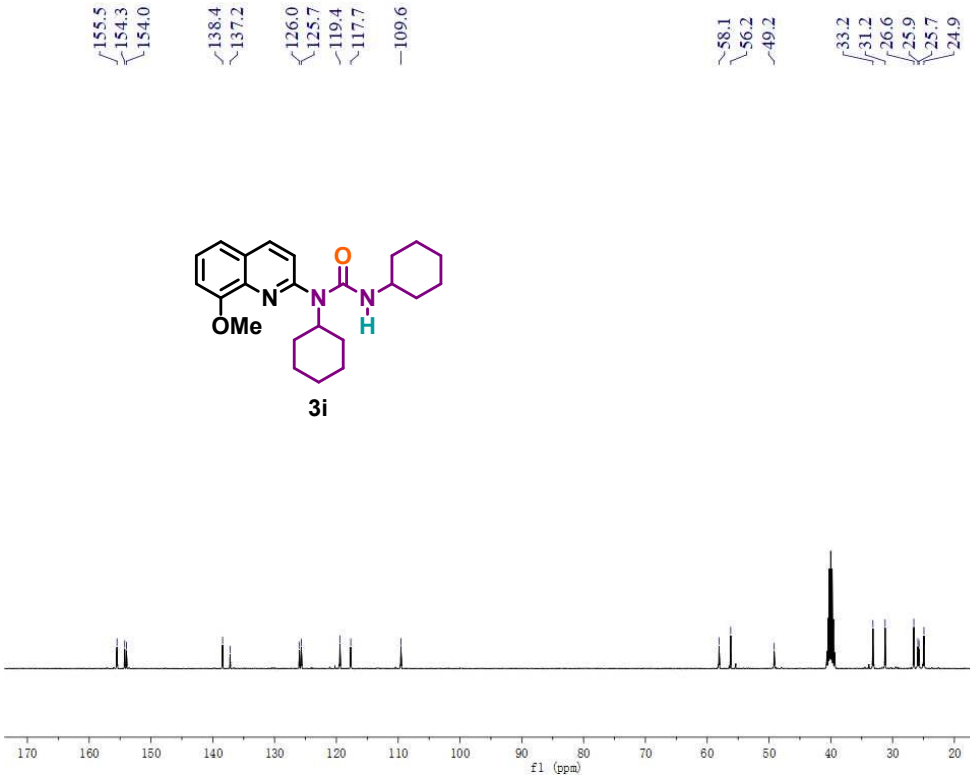

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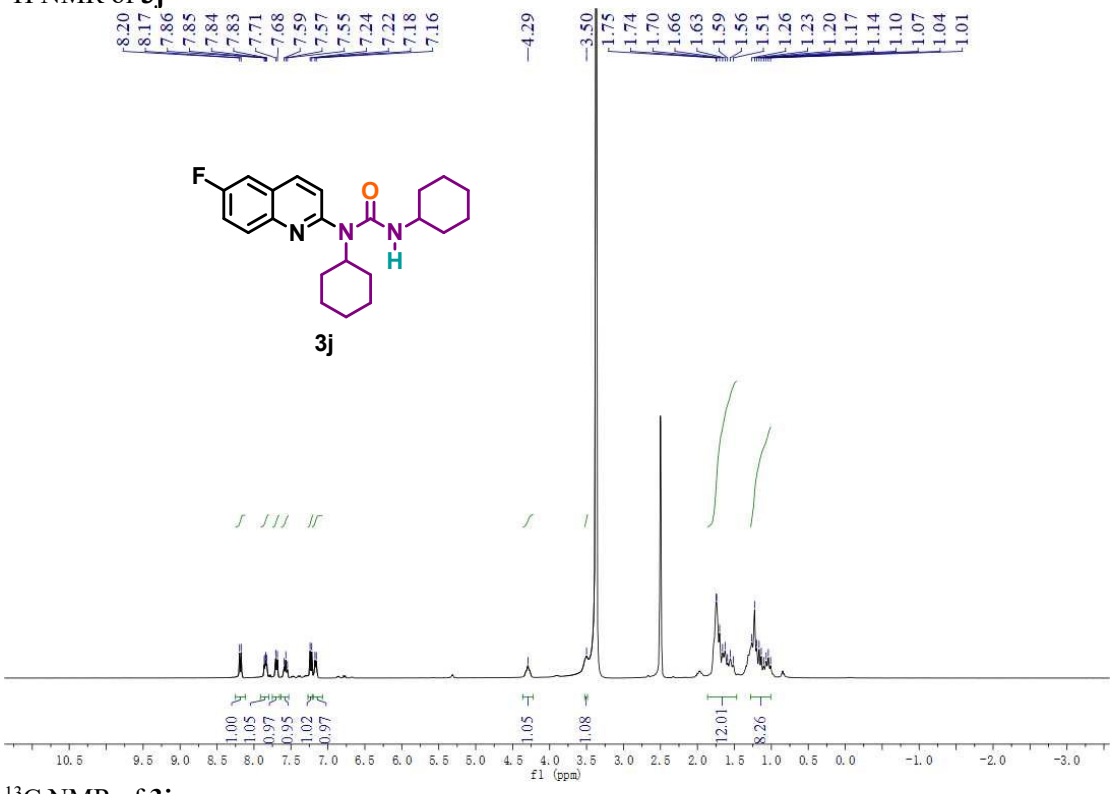

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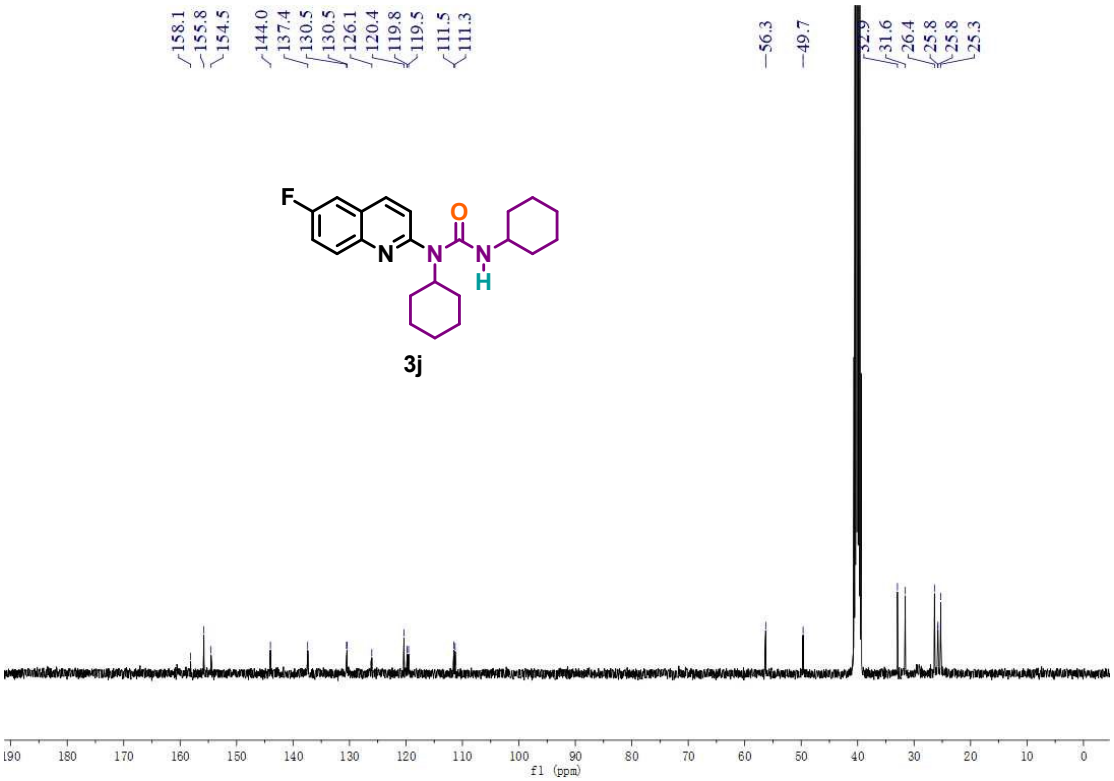

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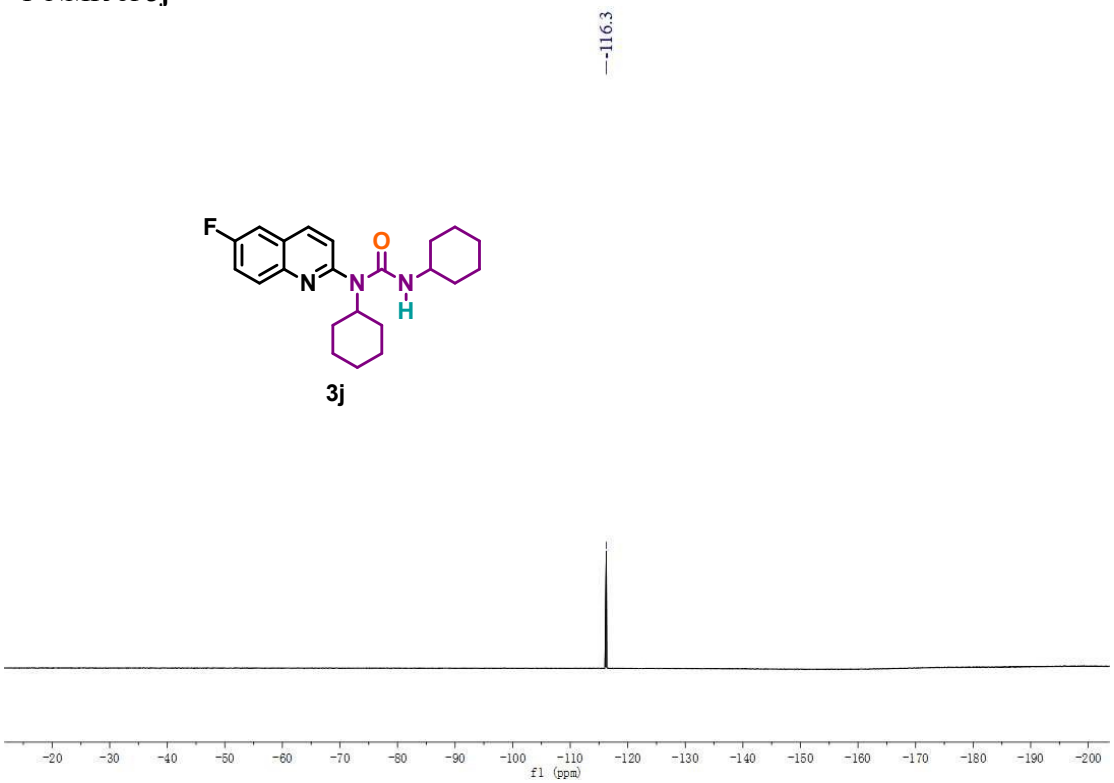

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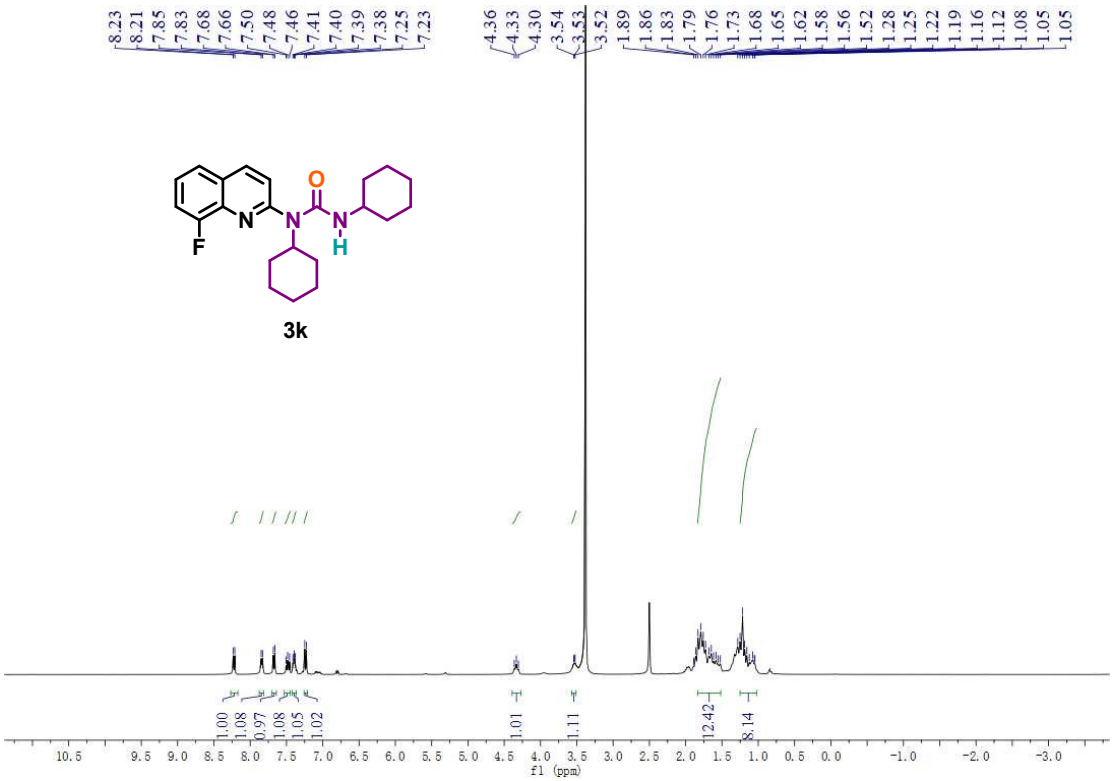

3k

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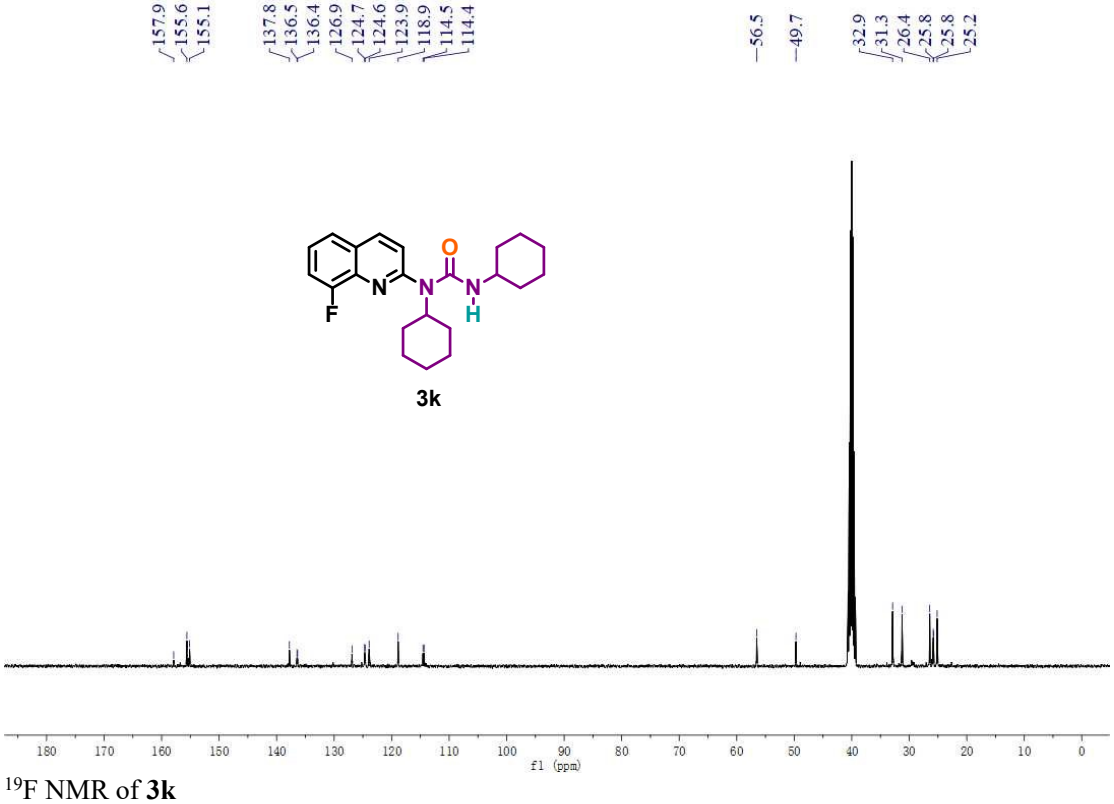

3k

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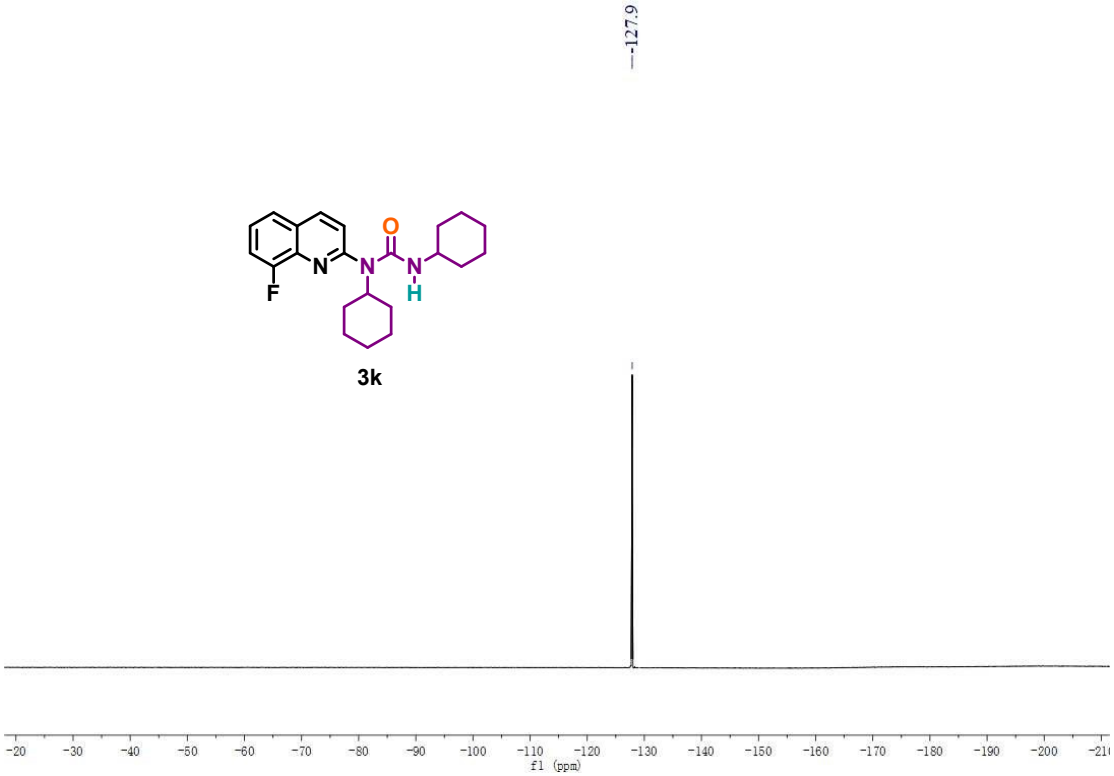
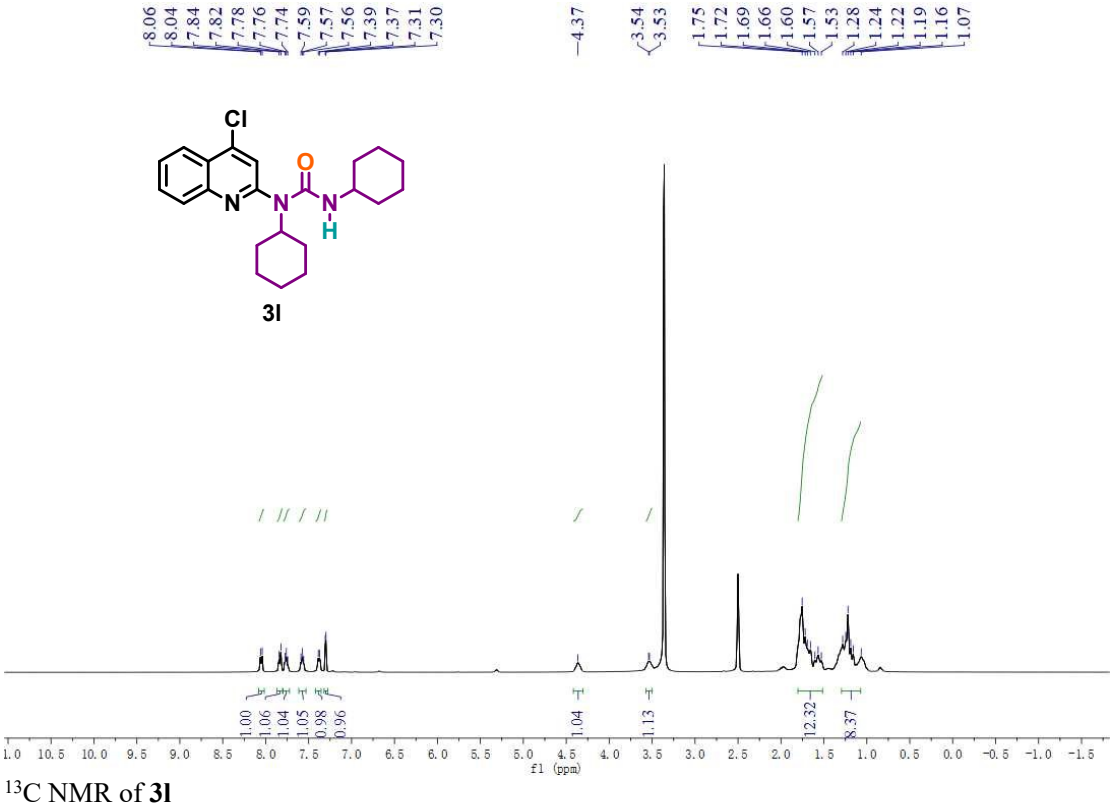


^{1}H NMR of **3l**



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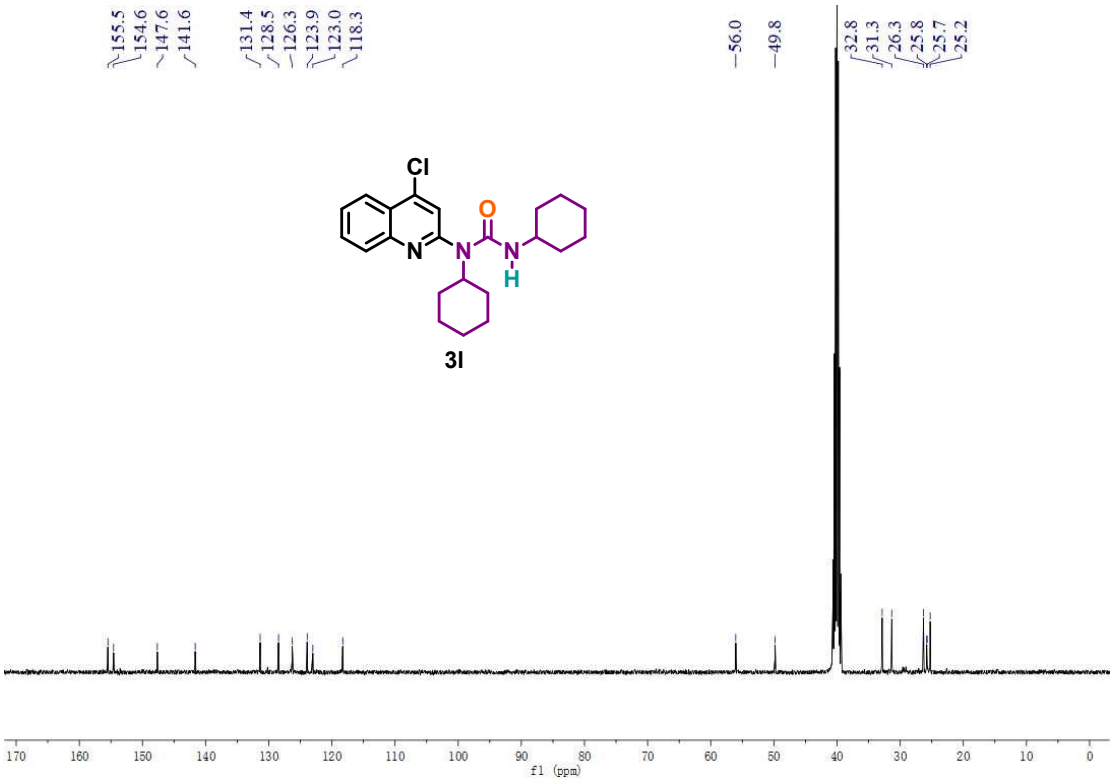

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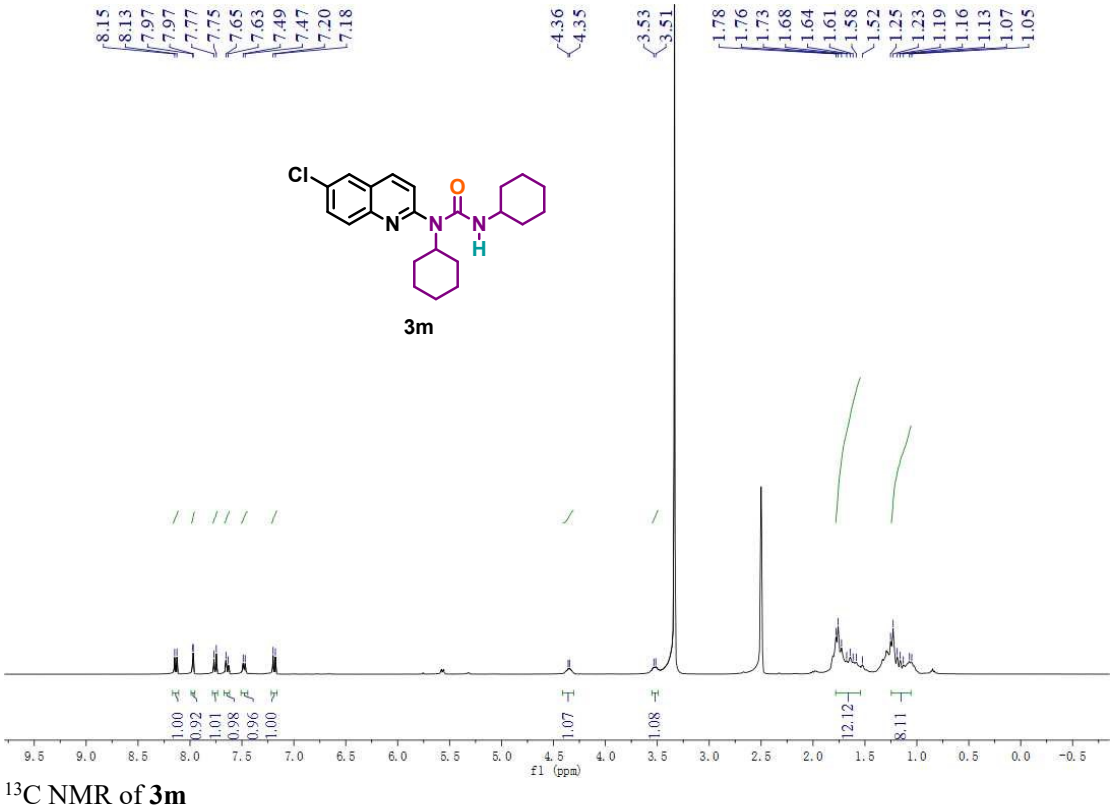

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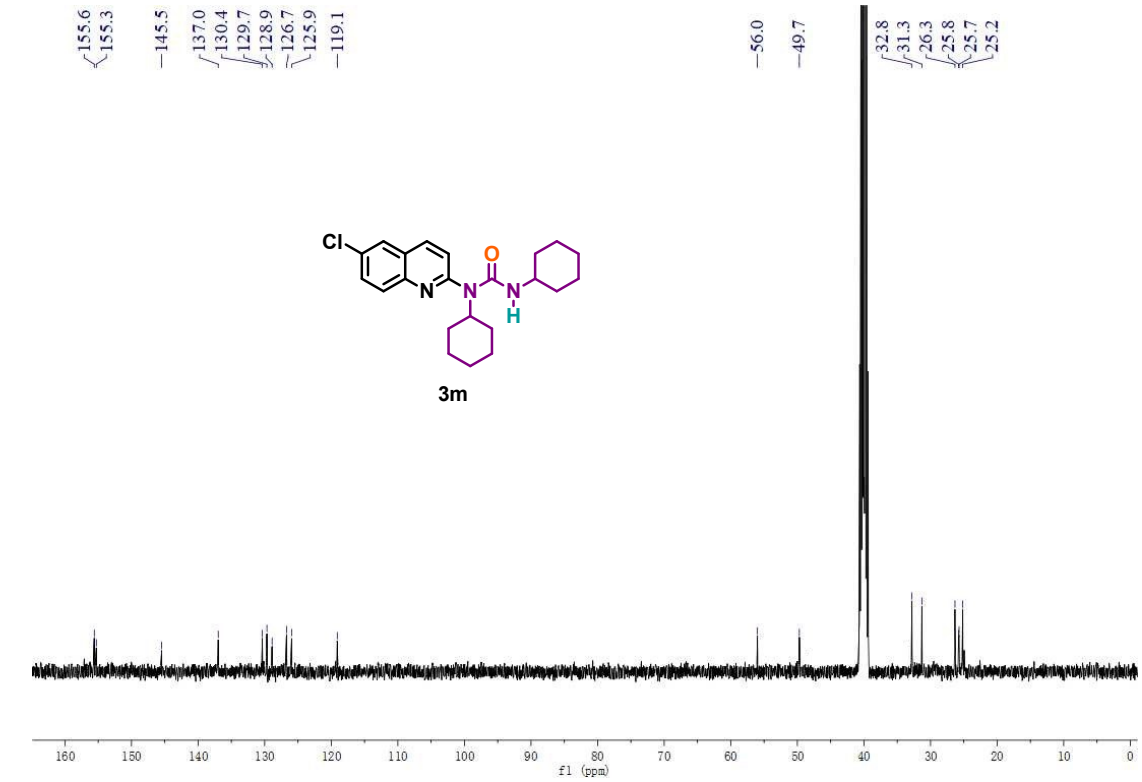

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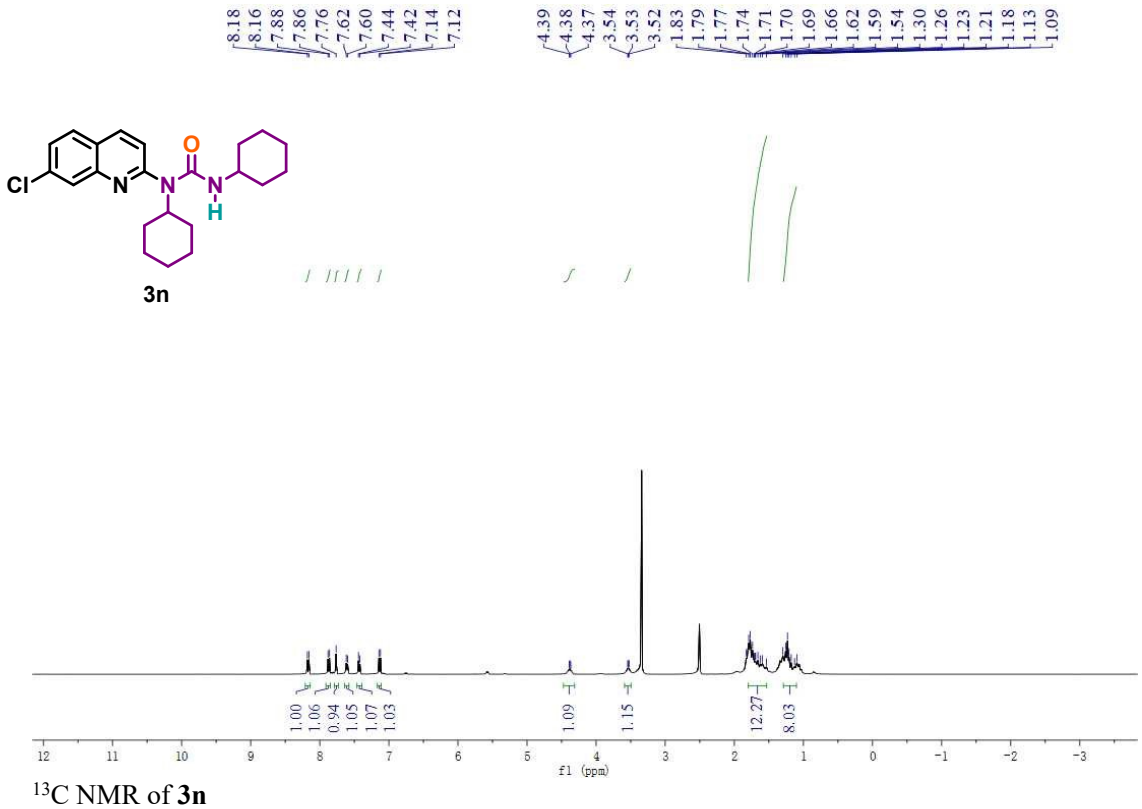

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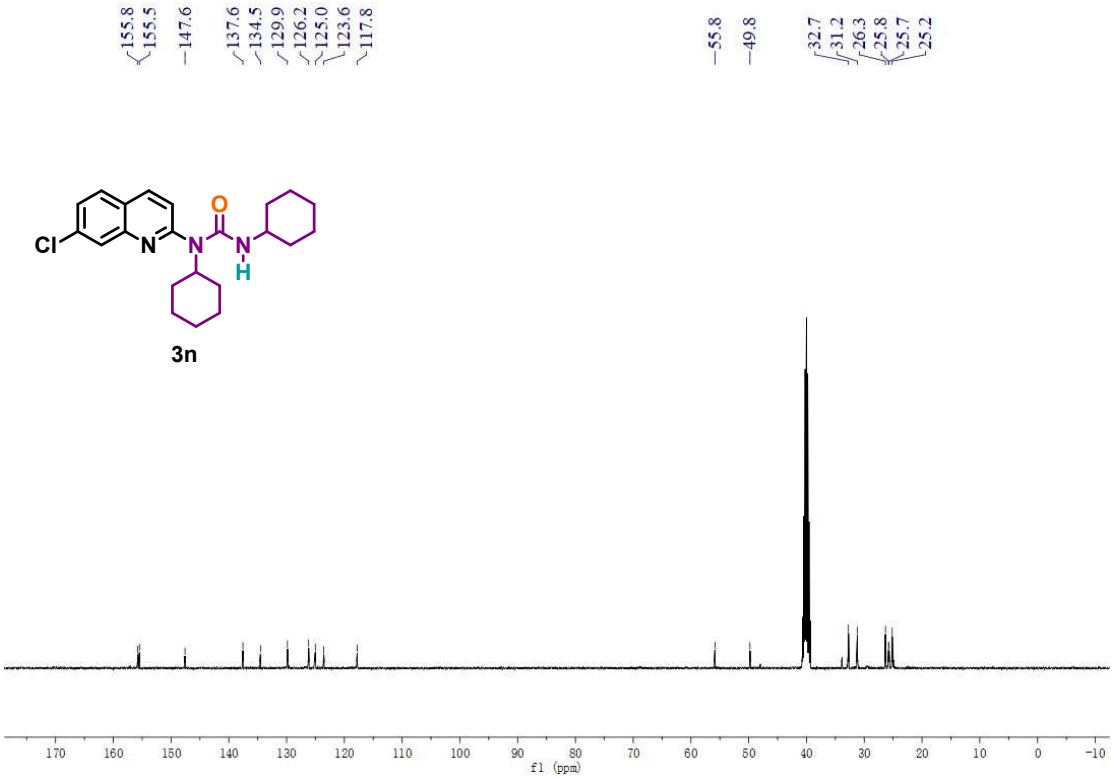

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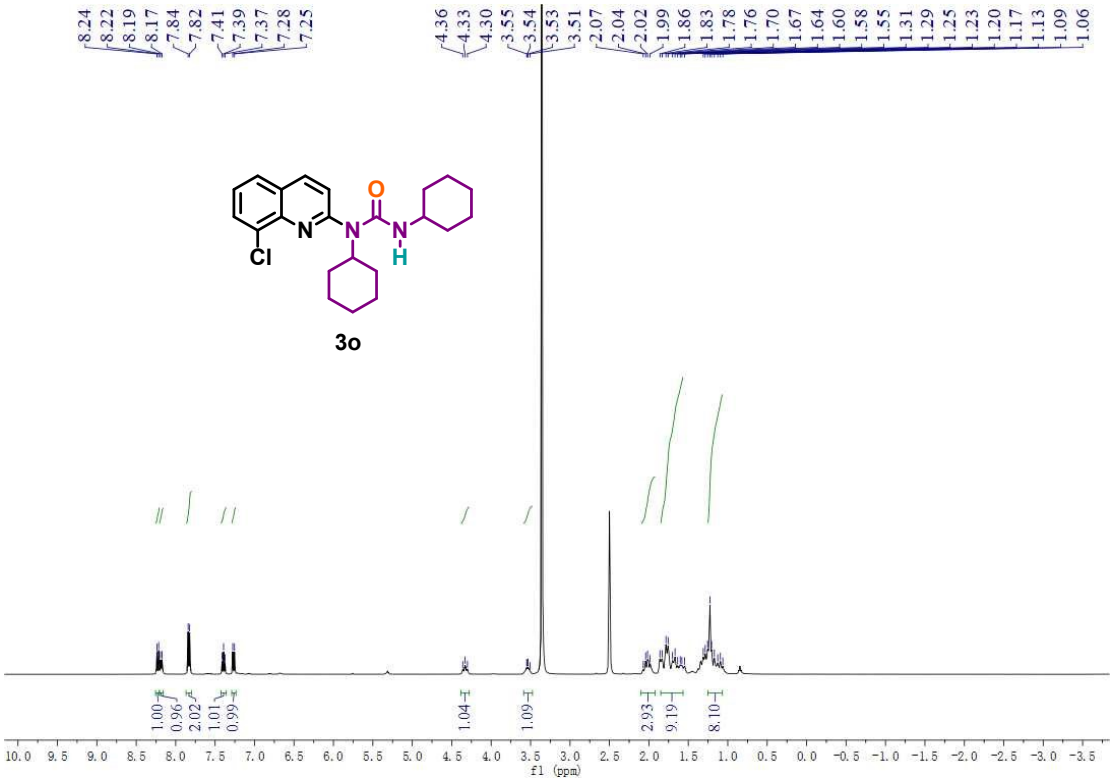

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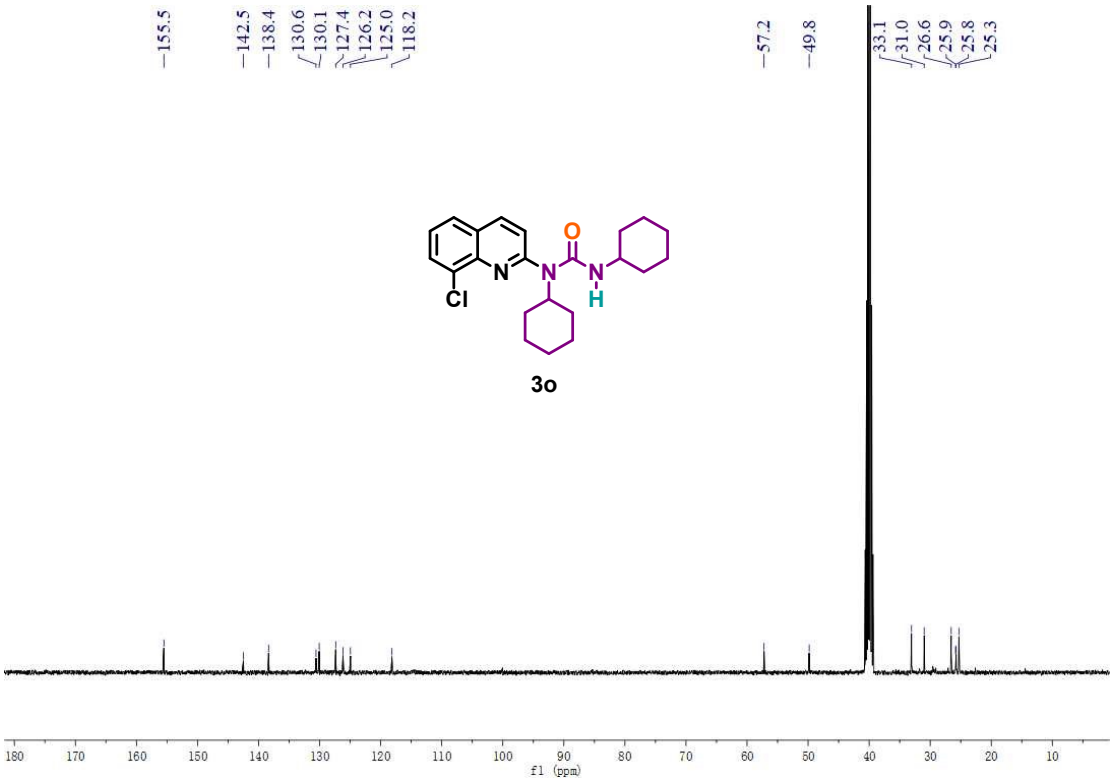

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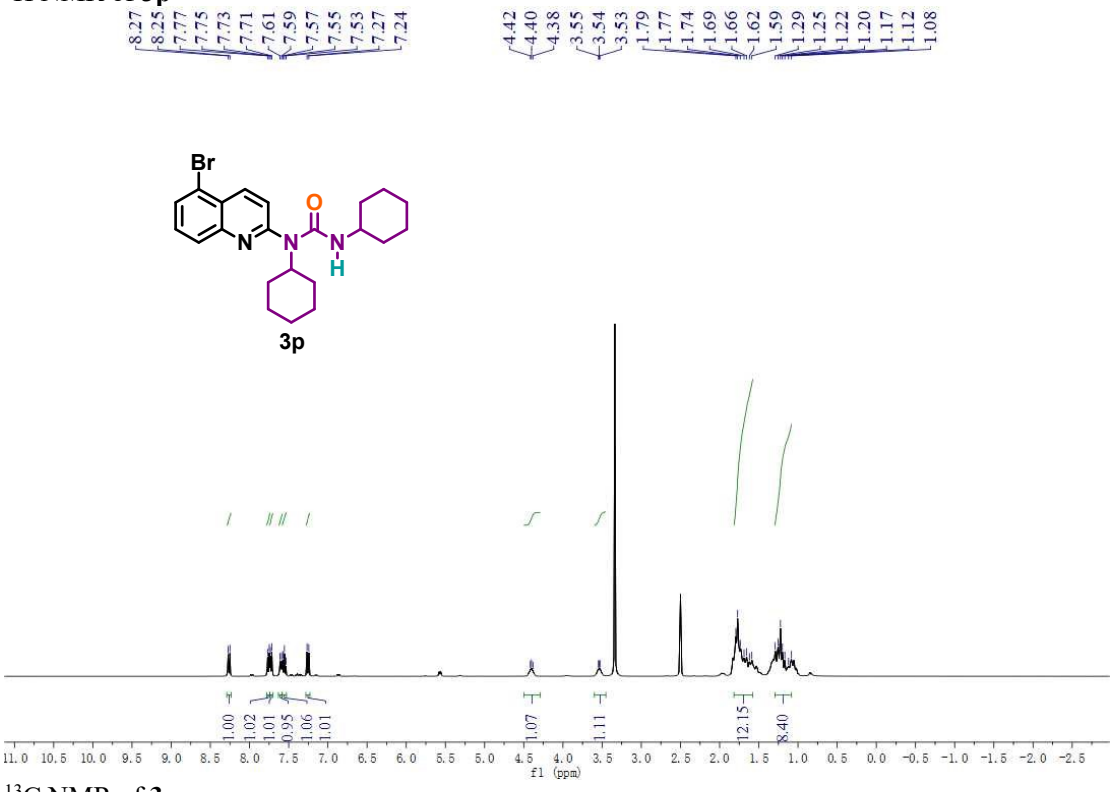
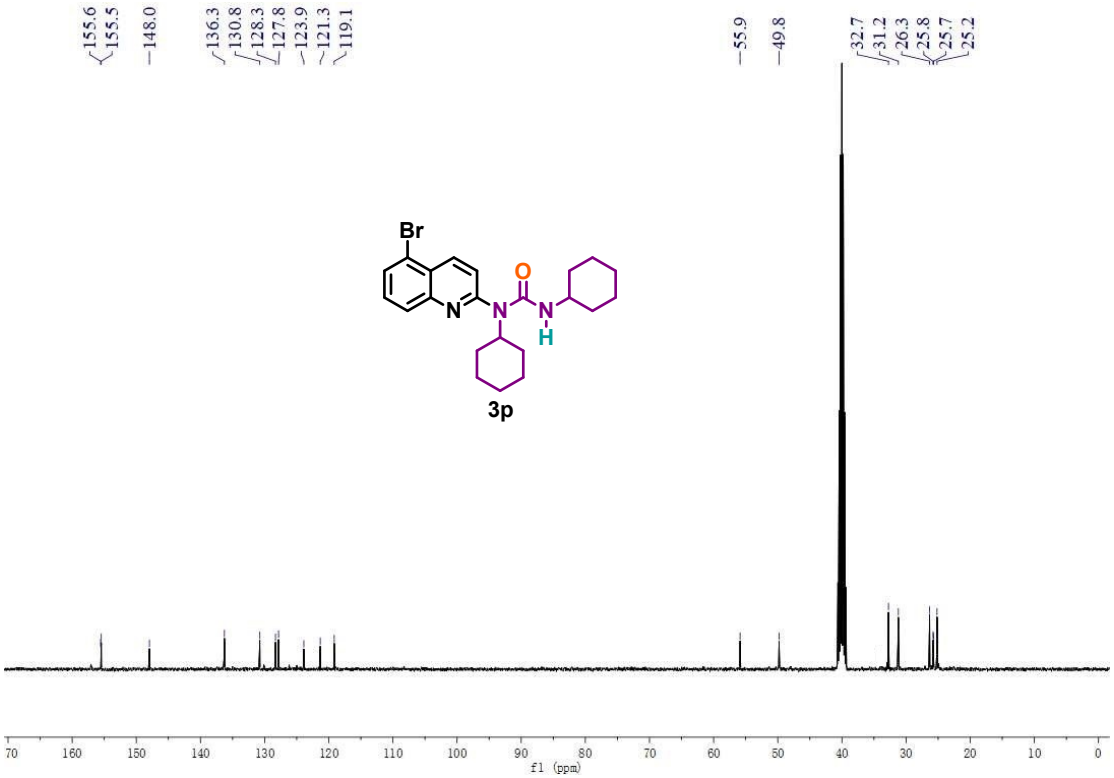
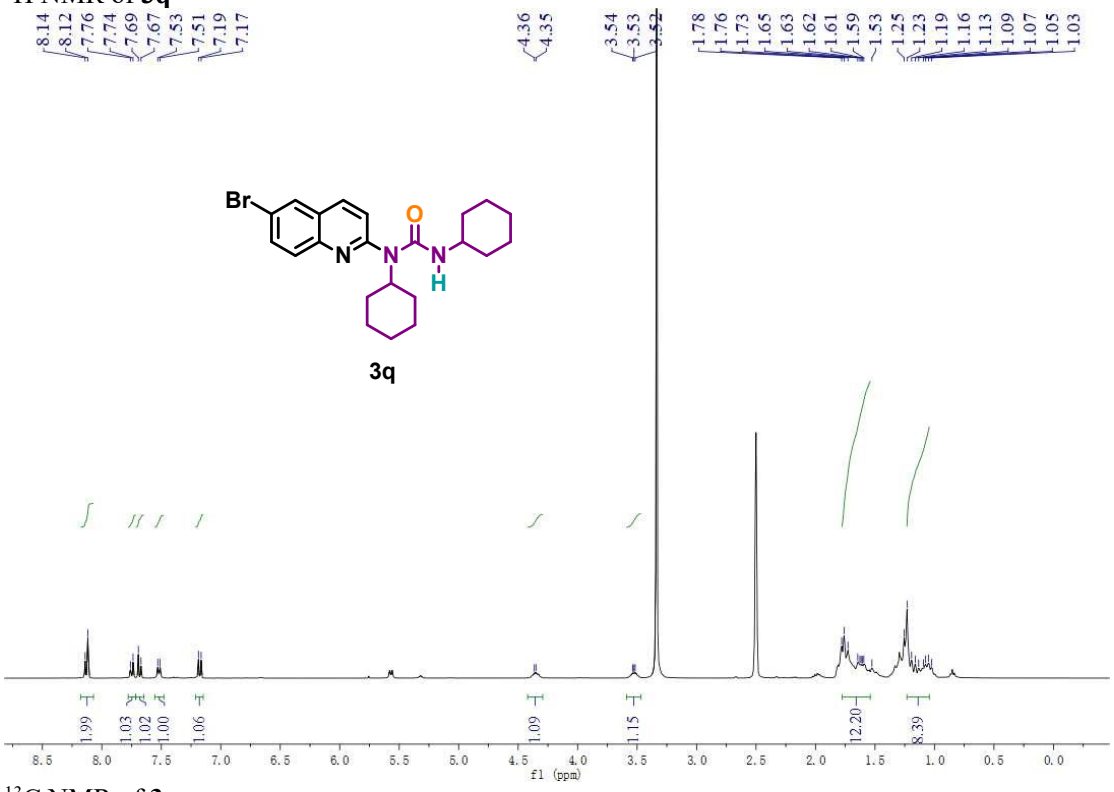


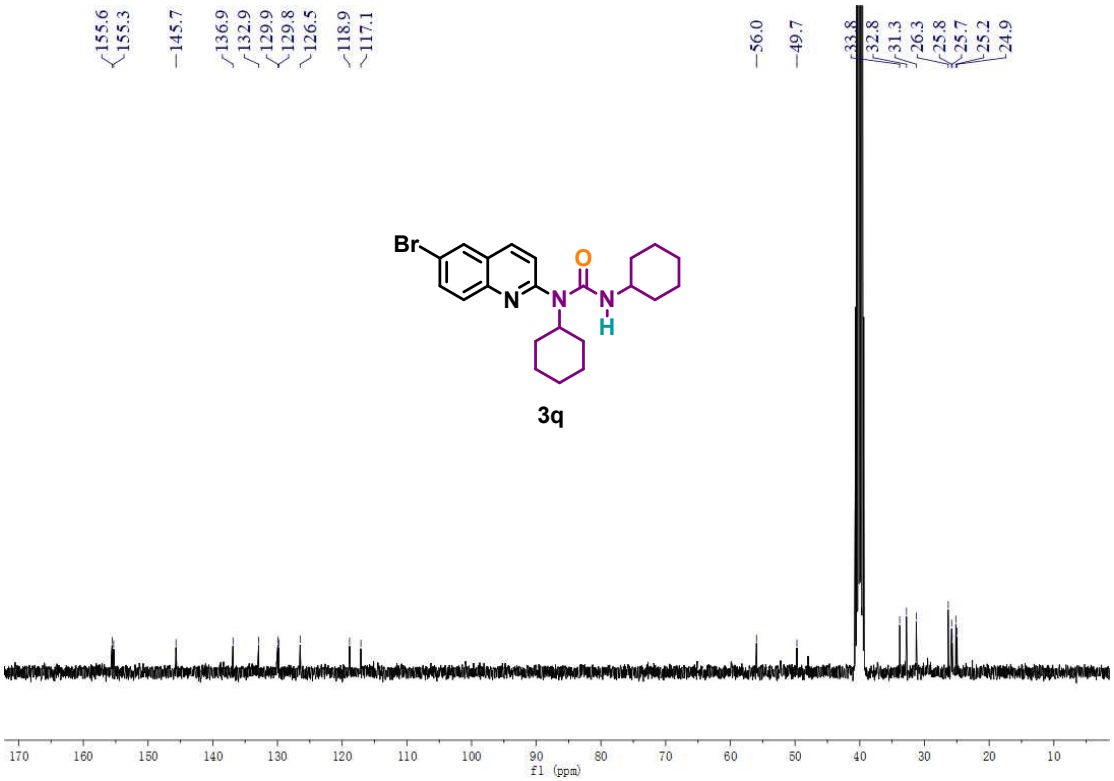
^{13}C NMR of **3p**



^{1}H NMR of **3q**



^{13}C NMR of **3q**



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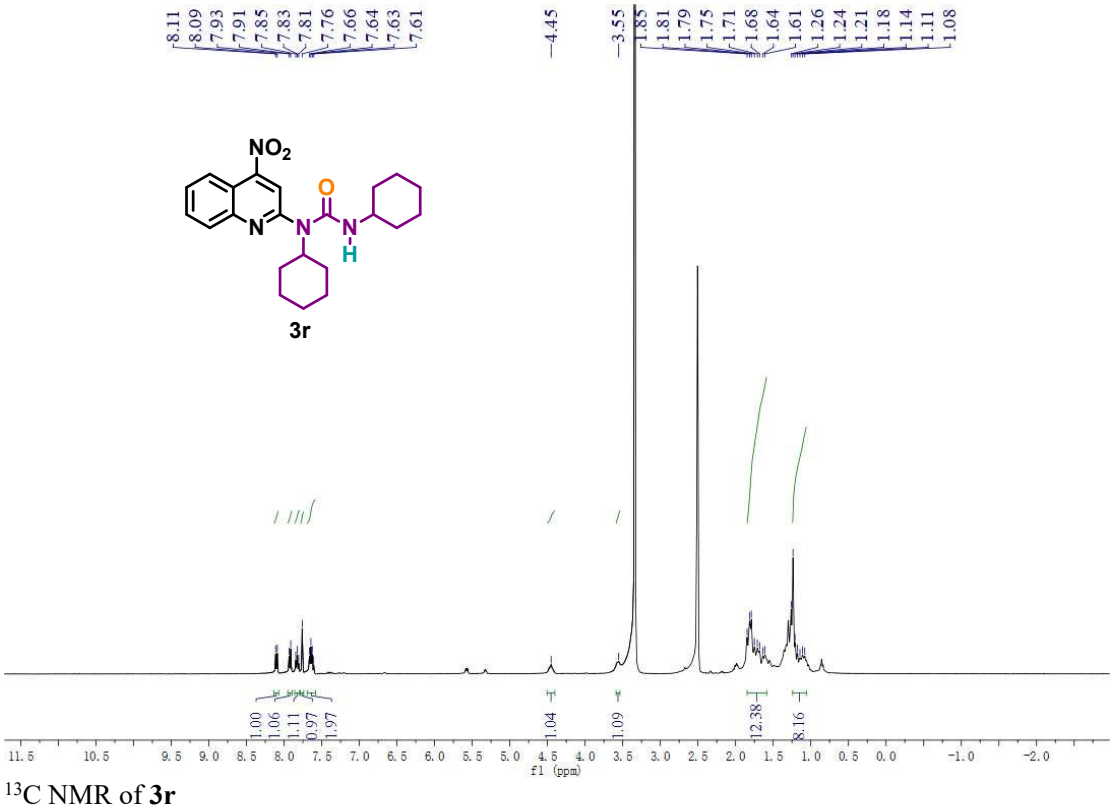

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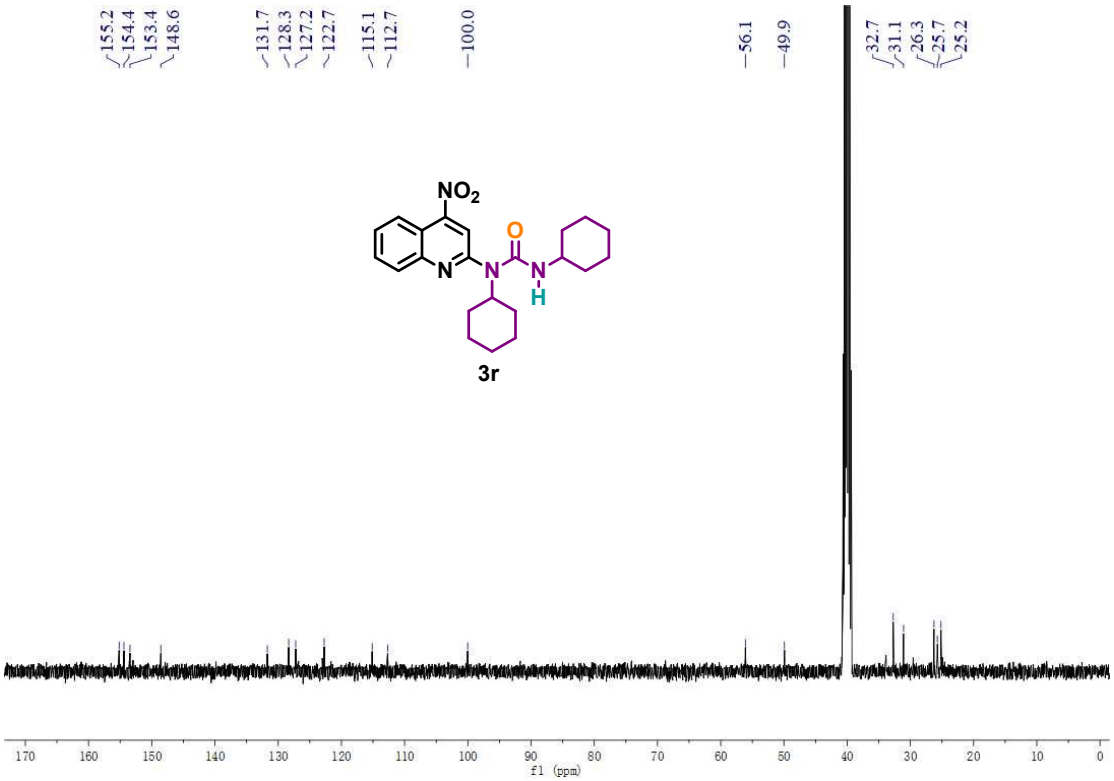
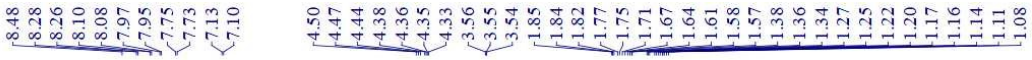
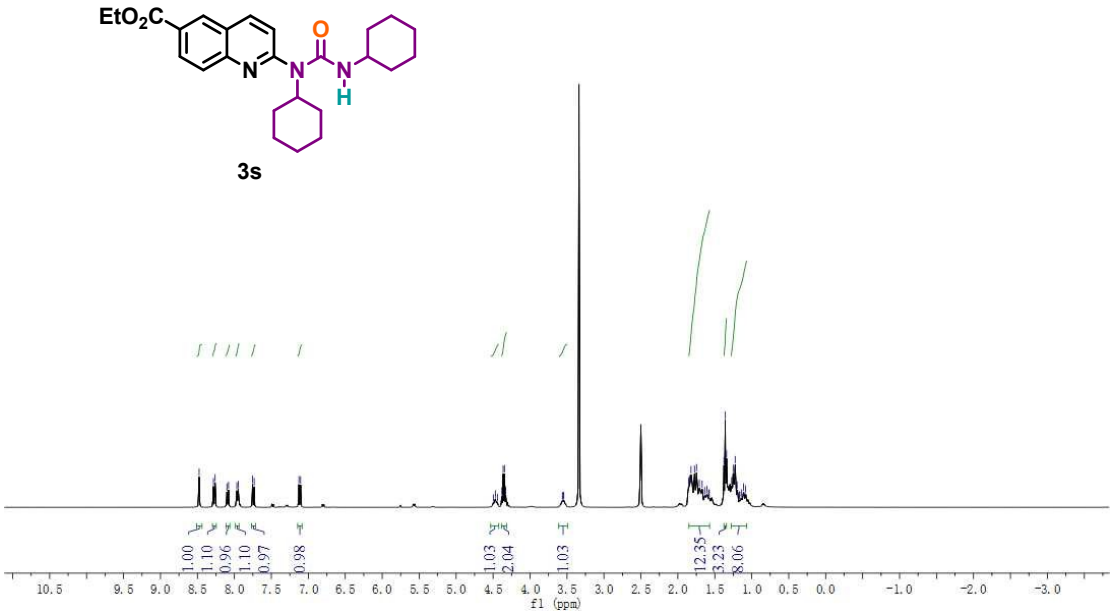


^{1}H NMR of **3s**





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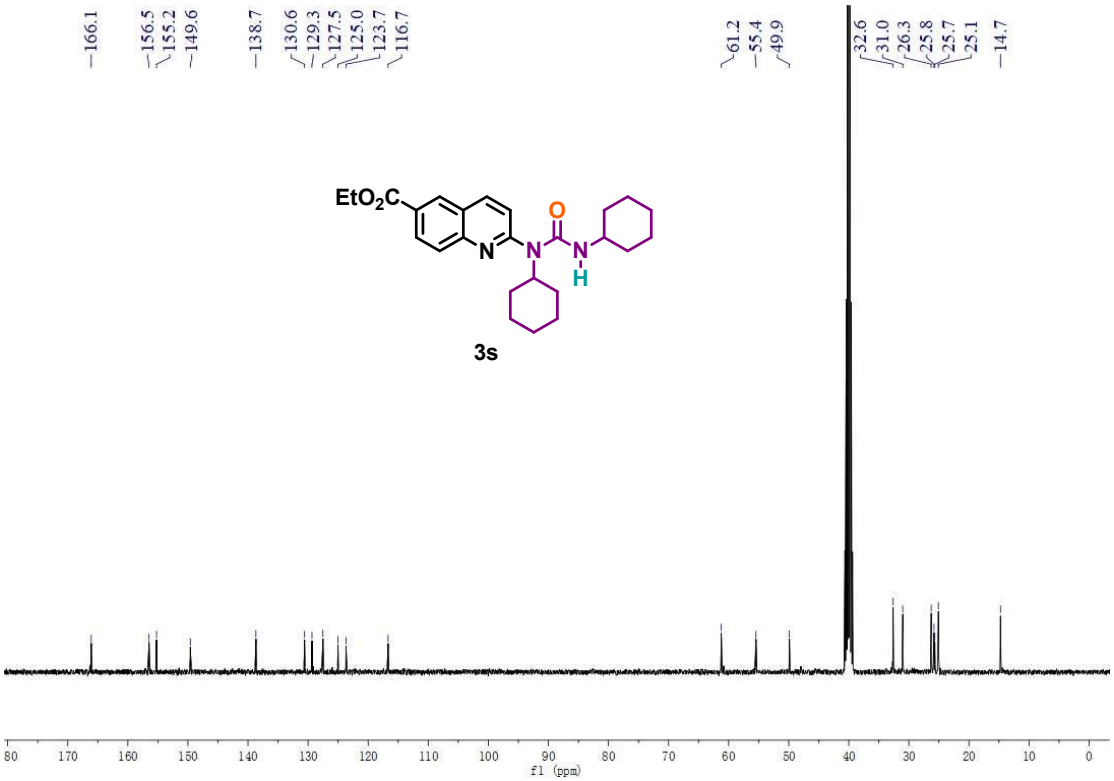
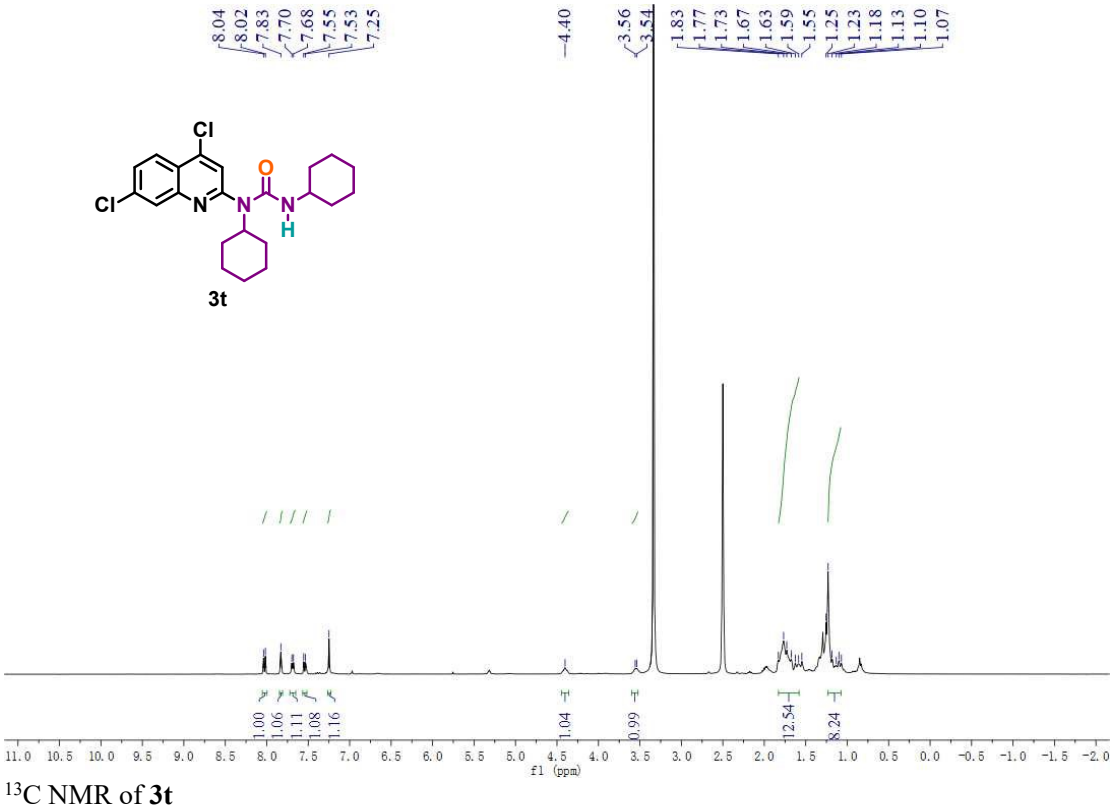
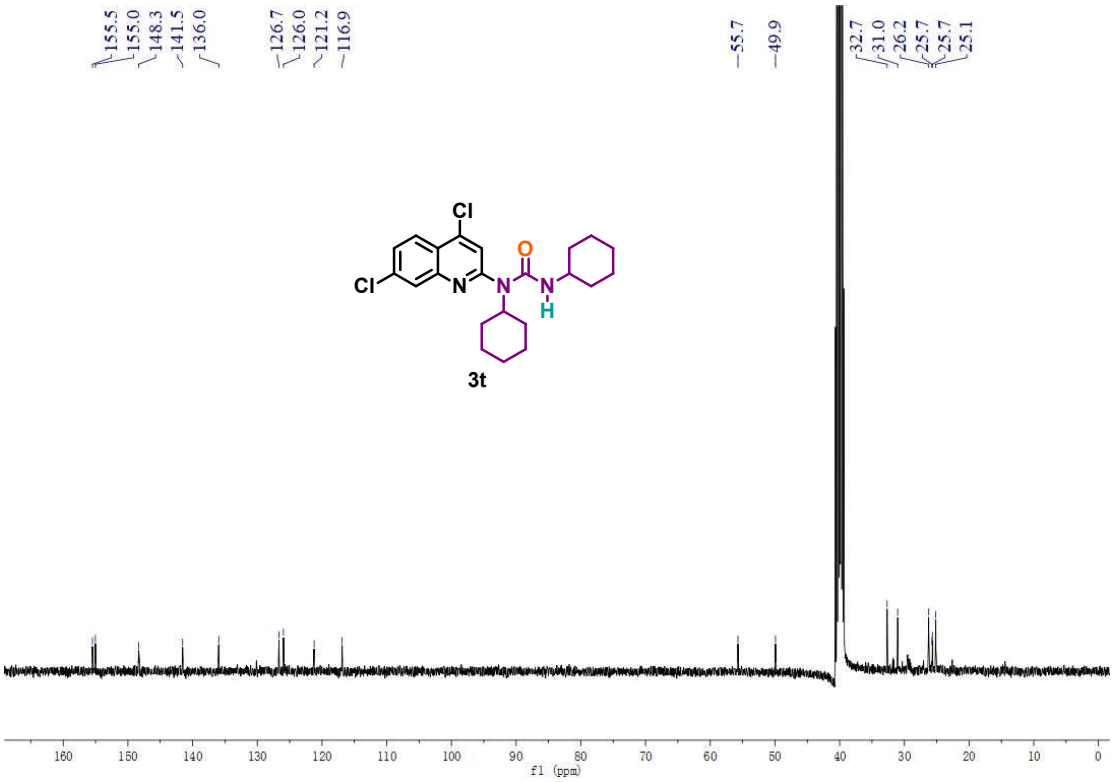


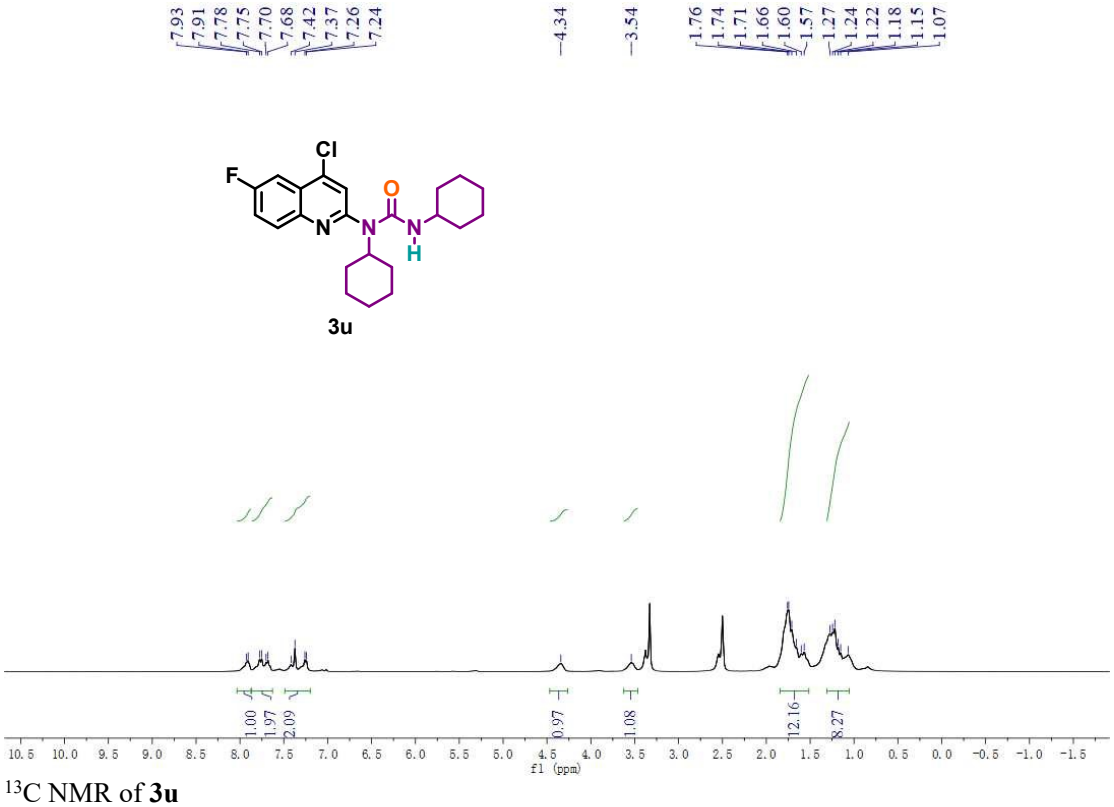
^{1}H NMR of **3t**



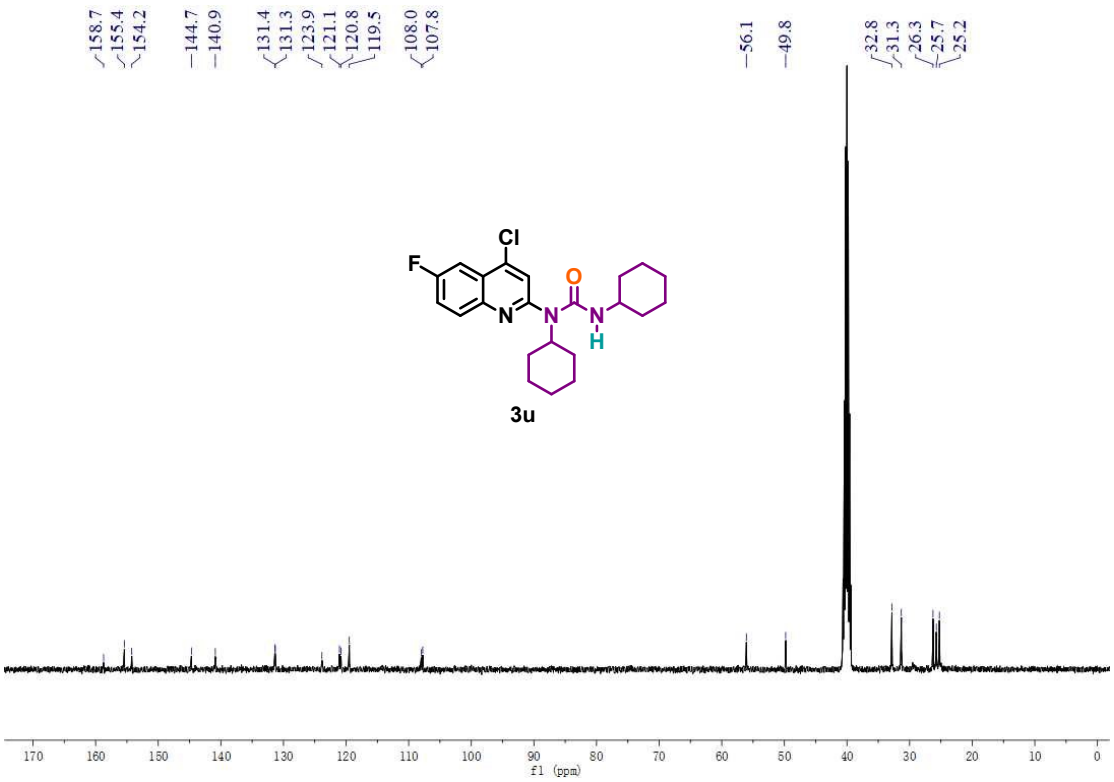
^{13}C NMR of **3t**



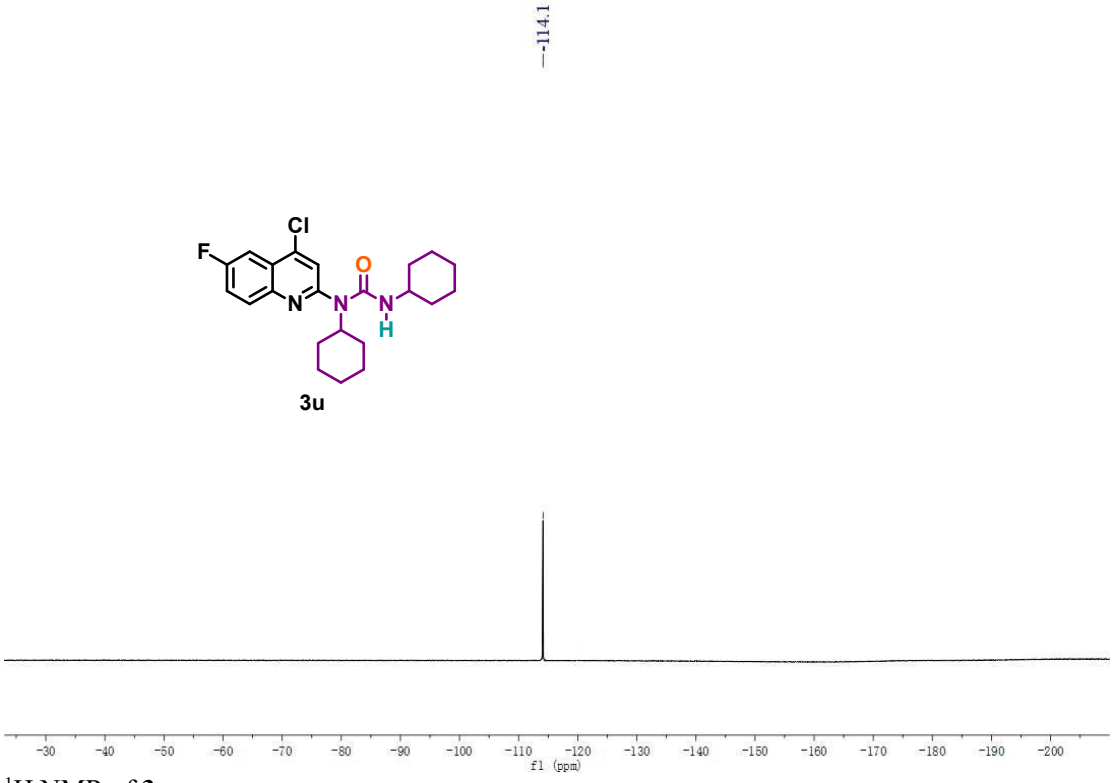
^{1}H NMR of **3u**



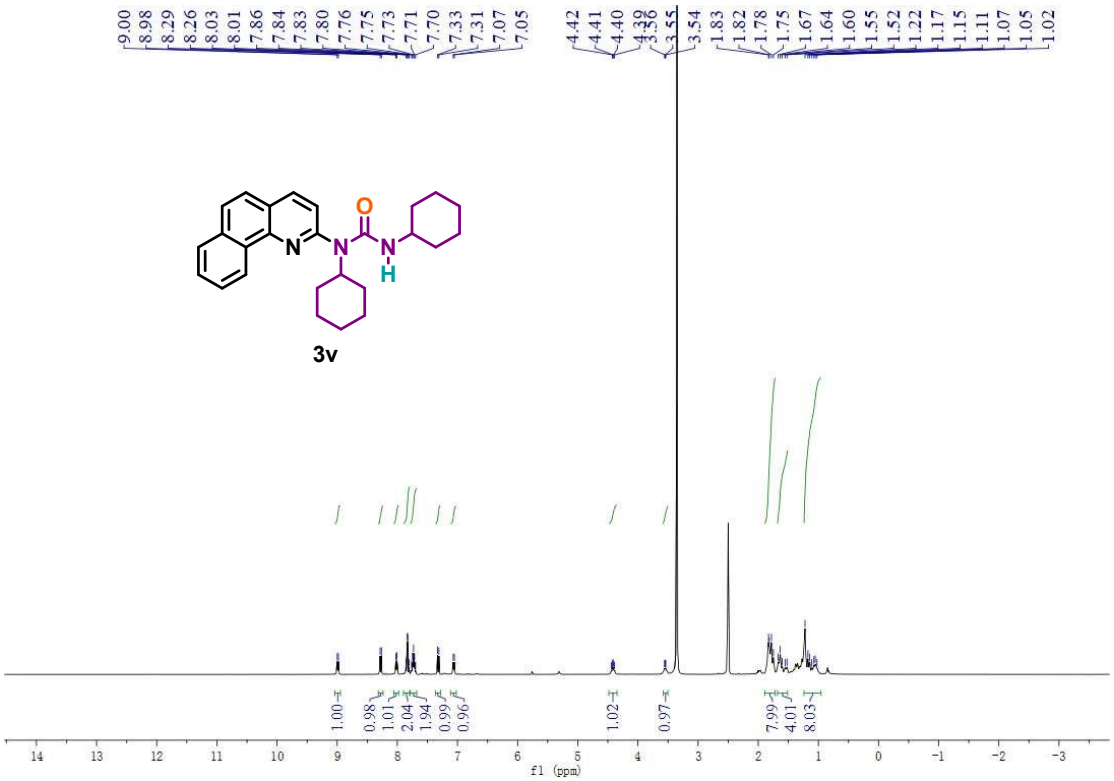
^{13}C NMR of **3u**



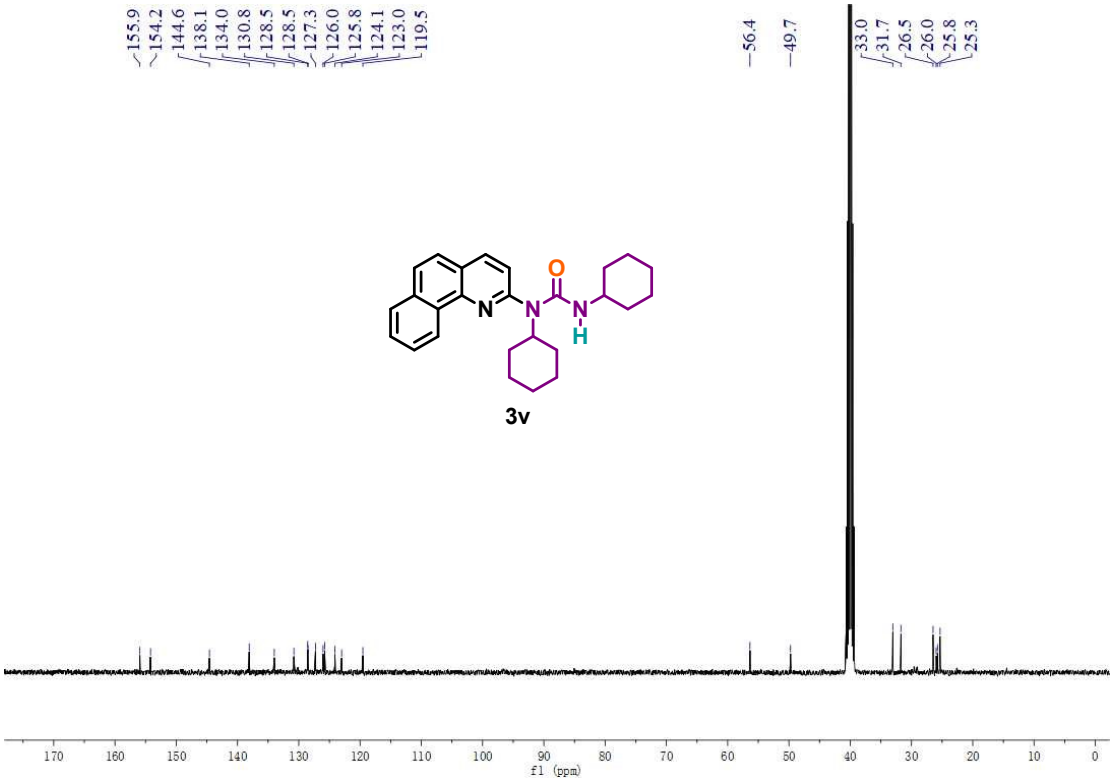
^{19}F NMR of **3u**



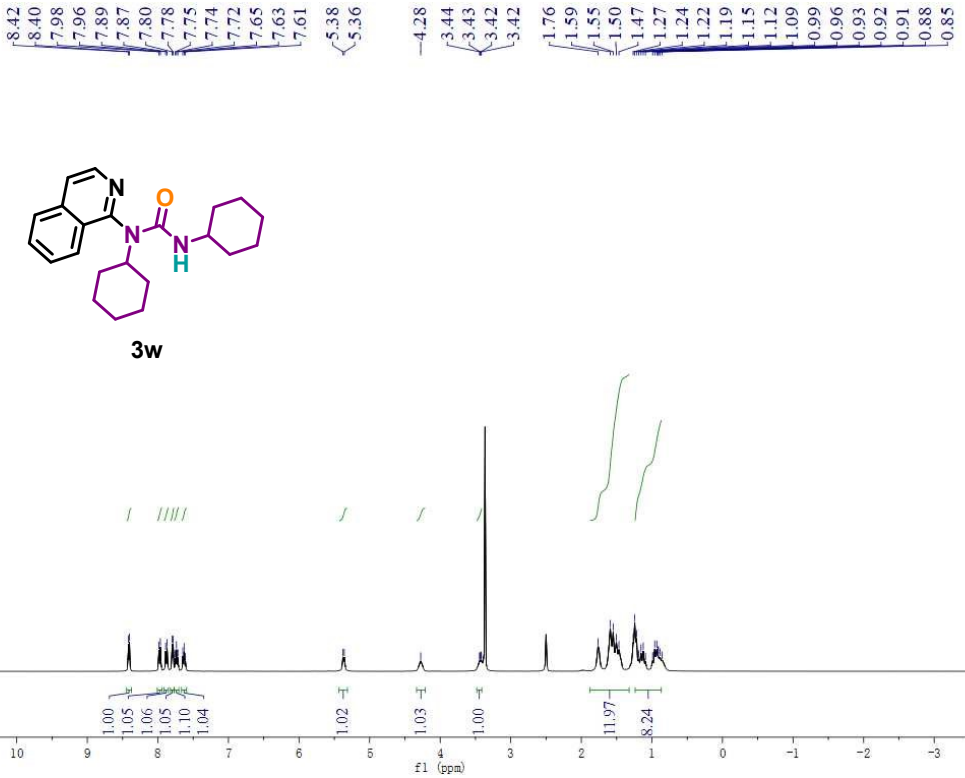
^{1}H NMR of **3v**



^{13}C NMR of **3v**

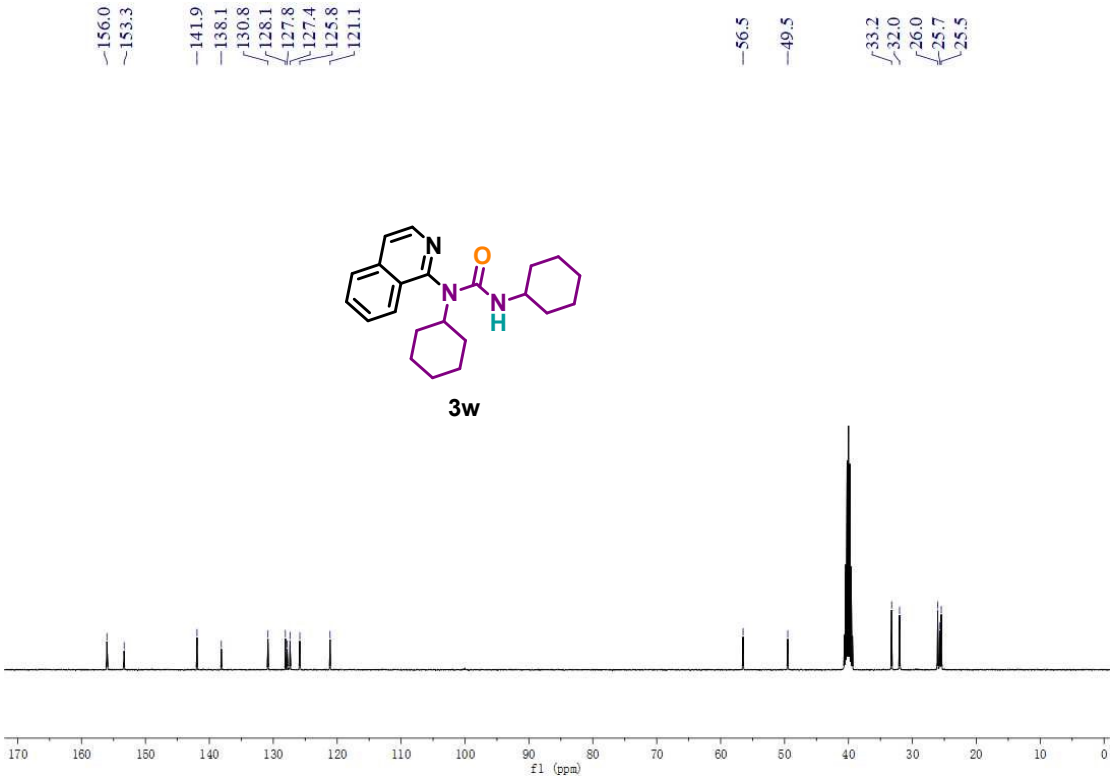


^{1}H NMR of **3w**



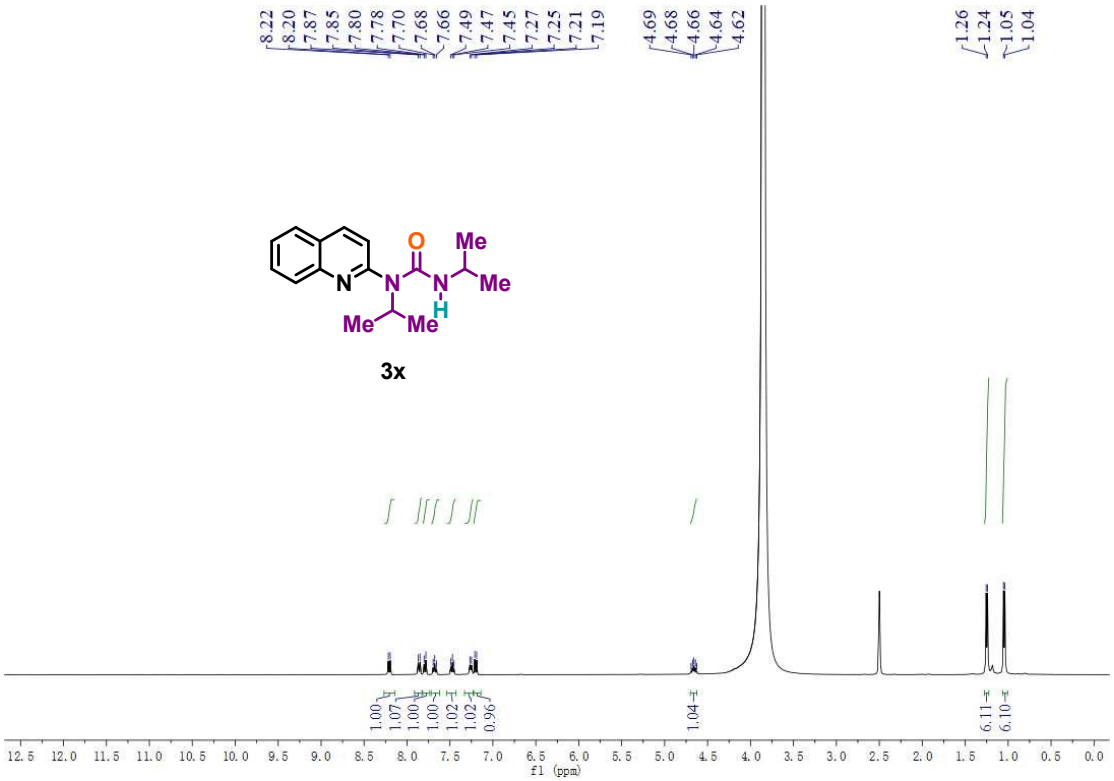
3w

^{13}C NMR of **3w**



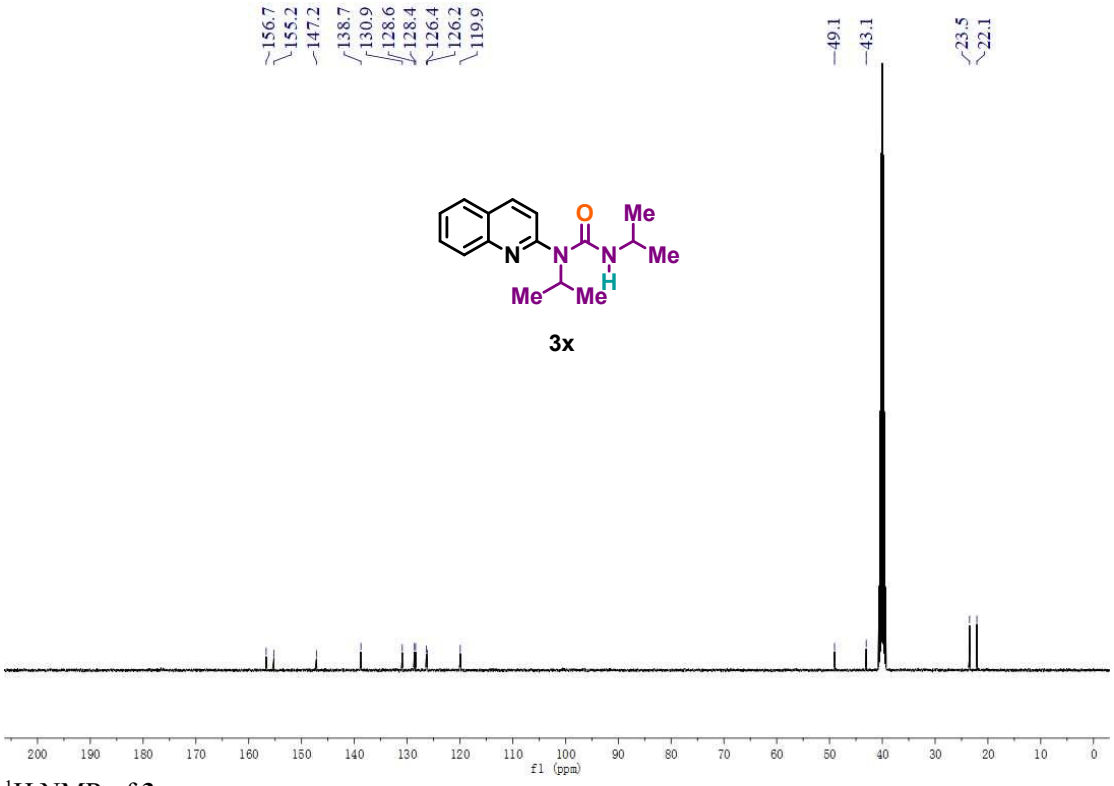
3w

^{1}H NMR of **3x**



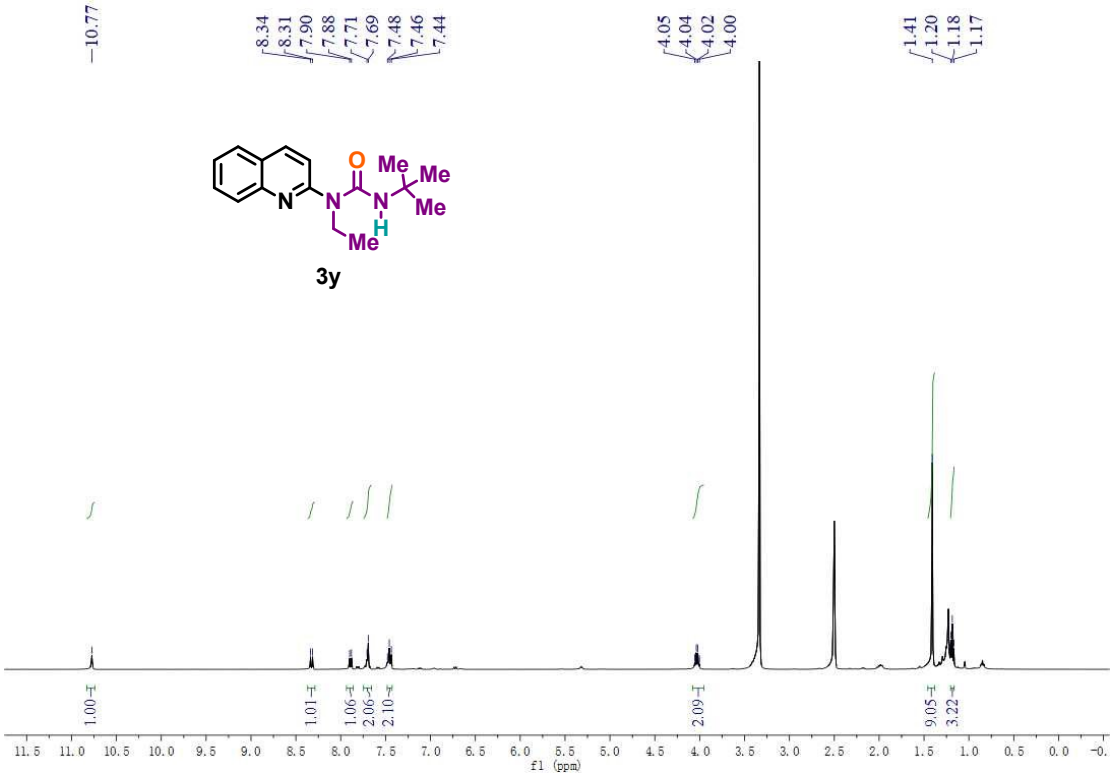
3x

^{13}C NMR of **3x**



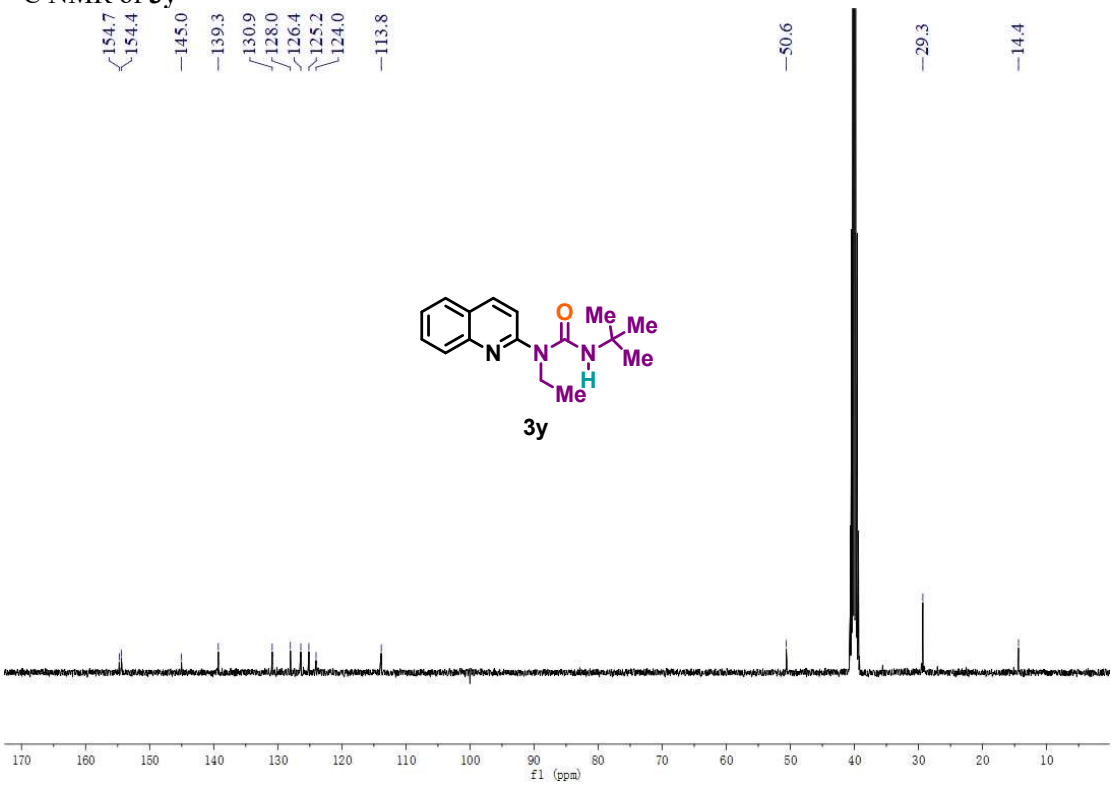
3x

^{1}H NMR of **3y**



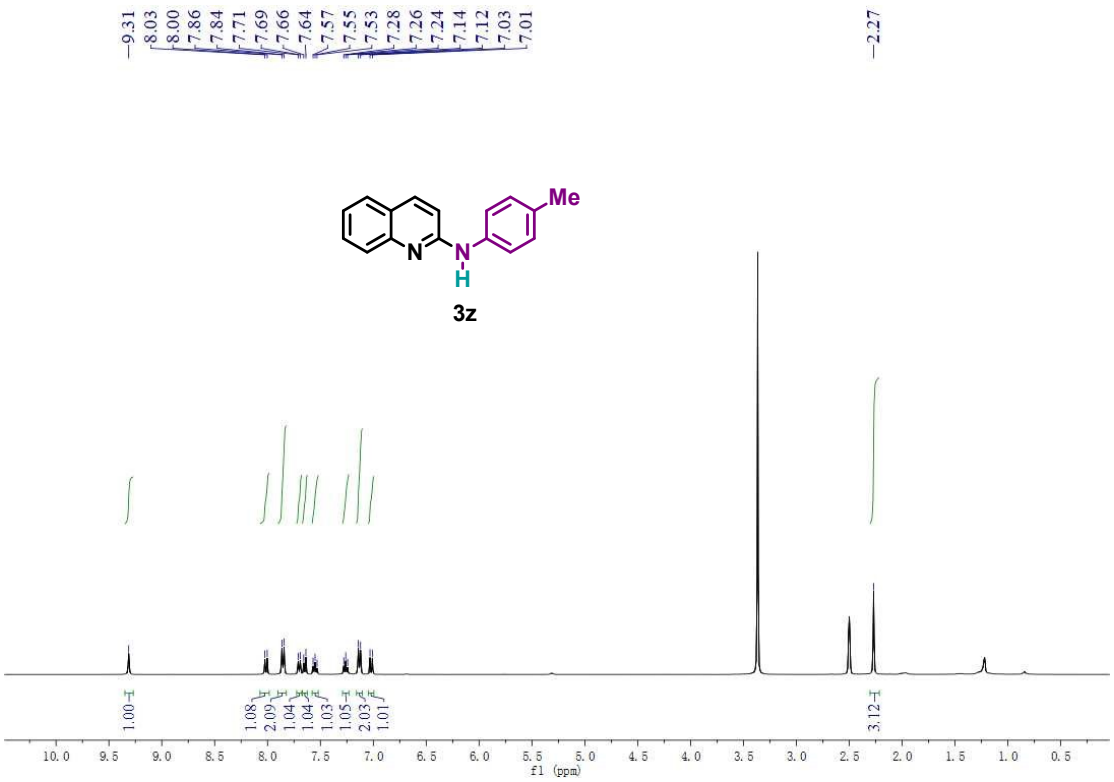
3y

^{13}C NMR of **3y**

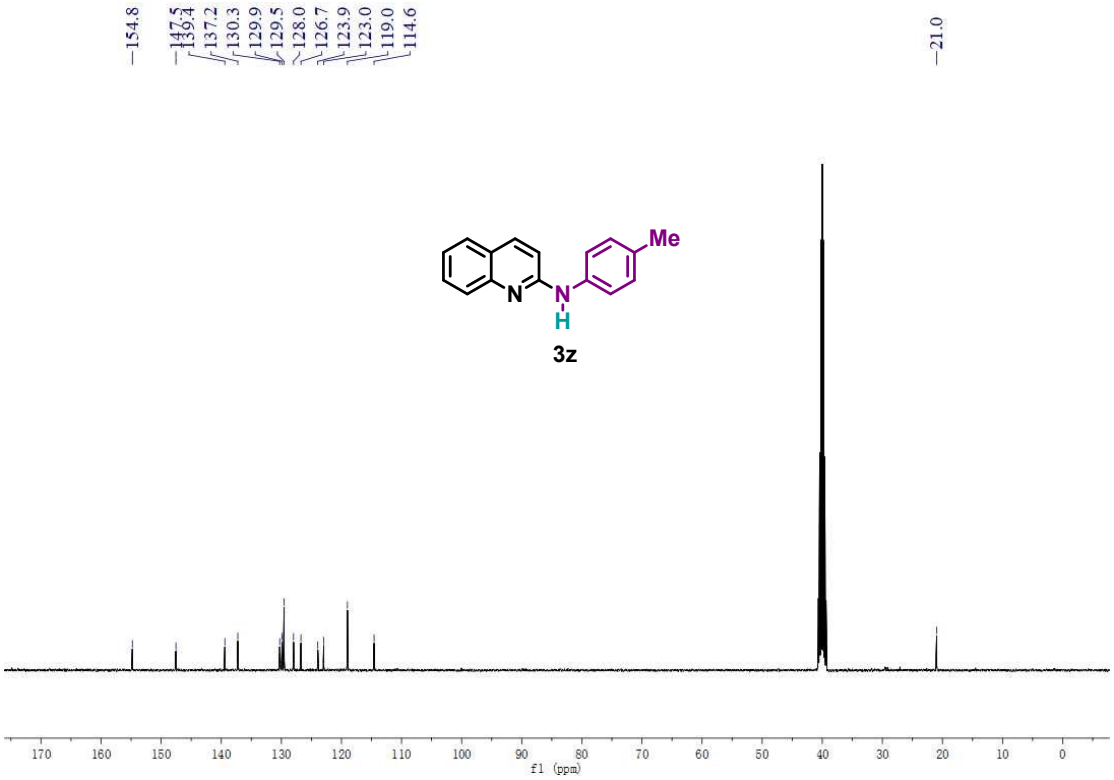


3y

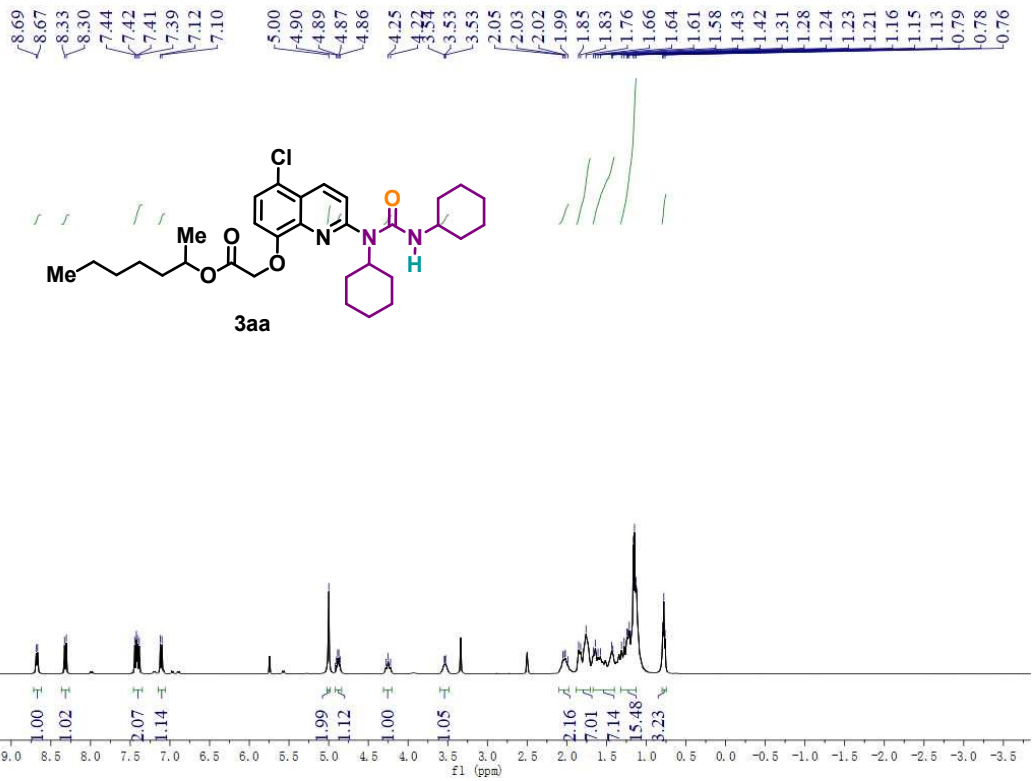
^{1}H NMR of **3z**



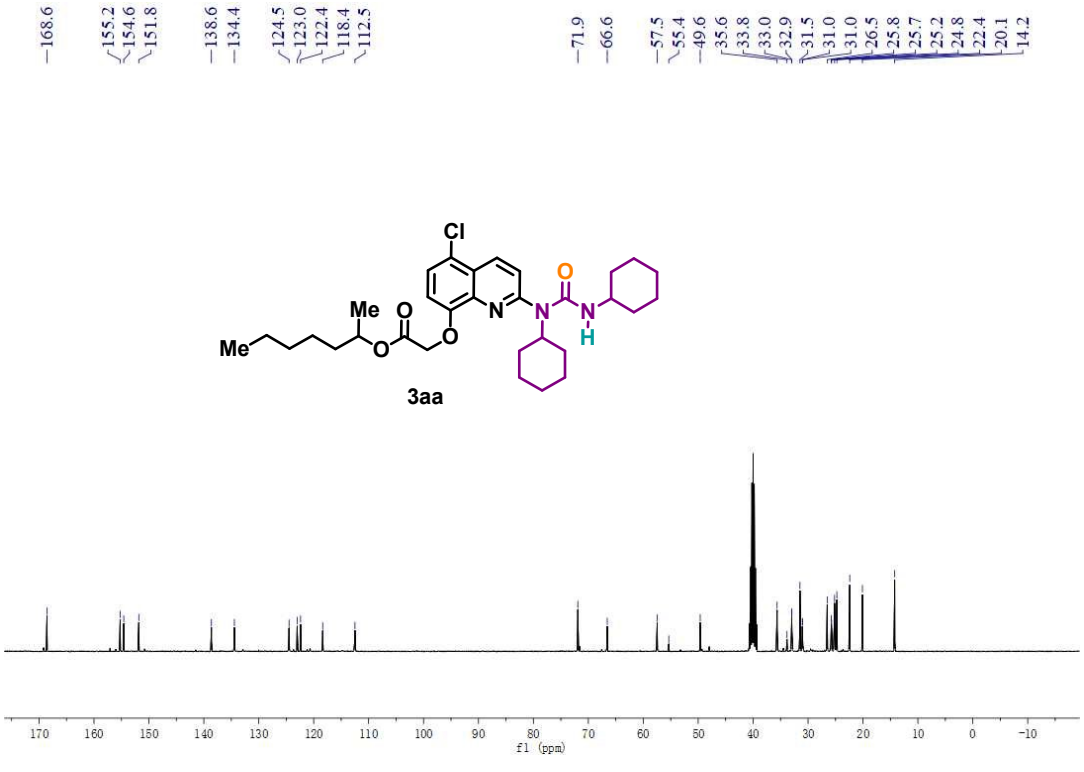
^{13}C NMR of **3z**



^{1}H NMR of **3aa**



^{13}C NMR of **3aa**



8. References

1. H. G. R. Monestel, I. S. Amiinu, A. A. González, Z. Pu, B. Mousavi and S. Mu, *Chinese Journal of Catalysis*, 2020, **41**, 839-846.
2. M. Frisch, G. Trucks, H. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, G. Petersson and H. Nakatsuji, *Gaussian Inc. Wallingford CT*, 2016, **1**, 572.
3. P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *The Journal of physical chemistry*, 1994, **98**, 11623-11627.
4. A. D. Becke, *The Journal of chemical physics*, 1993, **98**, 5648-5652.
5. W. J. Hehre, R. Ditchfield and J. A. Pople, *The Journal of Chemical Physics*, 1972, **56**, 2257-2261.
6. P. J. Hay and W. R. Wadt, *The Journal of chemical physics*, 1985, **82**, 270-283.
7. W. R. Wadt and P. J. Hay, *The Journal of chemical physics*, 1985, **82**, 284-298.
8. P. J. Hay and W. R. Wadt, *The Journal of chemical physics*, 1985, **82**, 299-310.
9. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *The Journal of chemical physics*, 2010, **132**.
10. E. R. Johnson and A. D. Becke, *The Journal of chemical physics*, 2006, **124**.
11. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
12. A. McLean and G. Chandler, *The Journal of chemical physics*, 1980, **72**, 5639-5648.
13. R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *The Journal of chemical physics*, 1980, **72**, 650-654.
14. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.
15. L.-Y. Xie, S. Peng, F. Liu, Y.-F. Liu, M. Sun, Z.-L. Tang, S. Jiang, Z. Cao and W.-M. He, *ACS Sustainable Chemistry & Engineering*, 2019, **7**, 7193-7199.
16. D. Kim, P. Ghosh, N. Y. Kwon, S. H. Han, S. Han, N. K. Mishra, S. Kim and I. S. Kim, *The Journal of Organic Chemistry*, 2020, **85**, 2476-2485.