Supporting Information

Cobalt-catalyzed 2-(1-methylhydrazinyl)pyridine-assisted C−H alkylation/annulation: mechanistic insights and rapid access to cyclopenta[*c*]isoquinolinone derivatives

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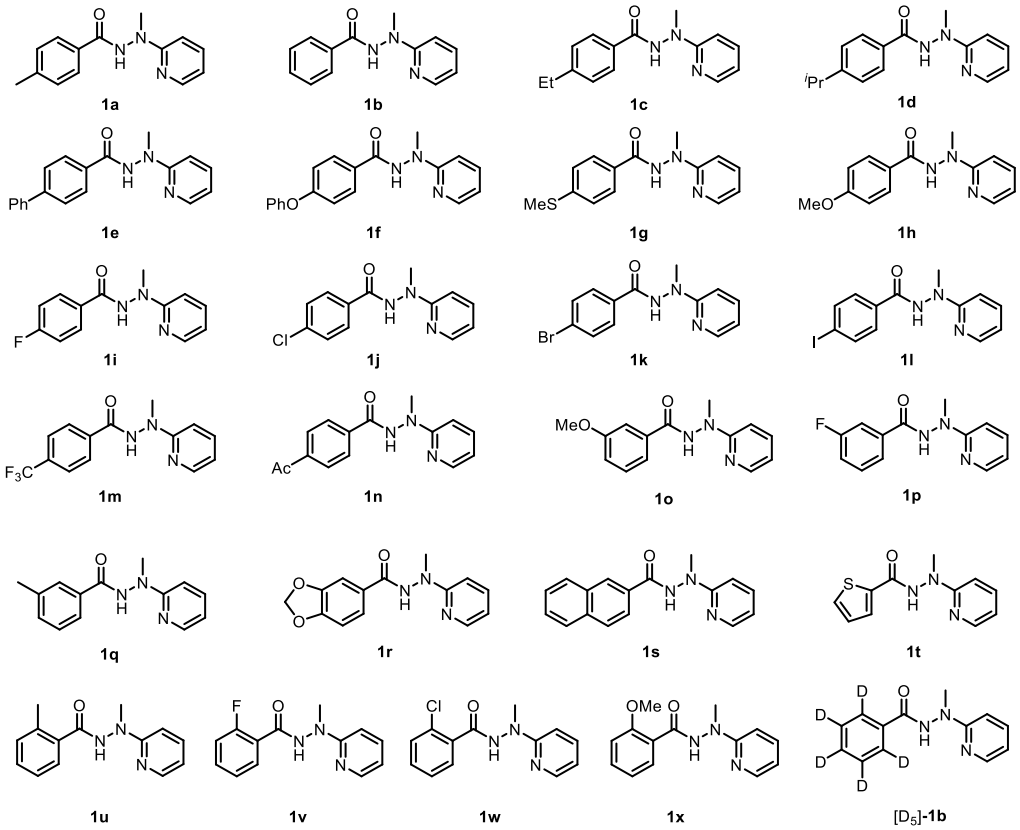
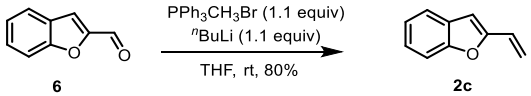
1 Starting Materials and Preparation.



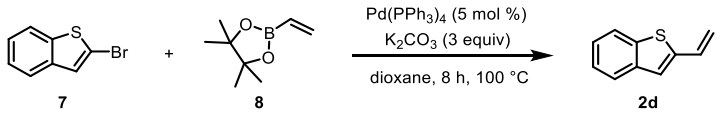
Hydrazides **1a-1c**, **1e-1o**, **1q-1x**, [D_5]-**1b** were known compounds and the spectral data matched those reported in the literature.[1]

Compounds **2c, 2d** were prepared according to known literature procedures and the spectral data matched those reported in the literature.[2]



To a solution of methyltriphenylphosphonium bromide (2.36 g, 6.6 mmol) in fresh ditilled THF (80 mL) was slowly added *n*-butyllithiurm (2.5 M solution in hexanes, 2.64 mL, 6.6 mmol) at room temperature. The resulting yellow suspension was stirred for 2 h at room temperature. A solution of aldehyde (0.87 g, 5.9 mmol) in dry THF (20 mL) was added dropwise to the suspension and the reaction mixture was stirred for 2 h at room temperature. The reaction mixture was quenched with water, and the aqueous portion was extracted with diethyl ether. The combined organic layers were washed

with brine, dried over anhydrous magnesium sulfate, filtered, and concentrated under reduced pressure. The crude mixture was purified by column chromatography to afford **2c** (0.67 g, 80%) as a colorless oil.

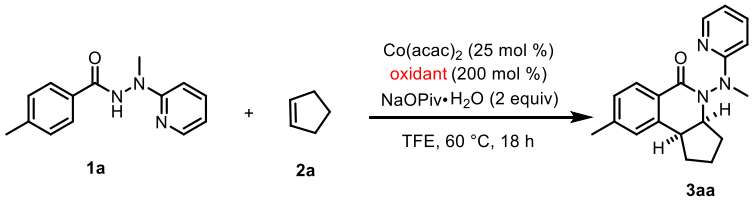


7 8 2d

A Schlenk tube was charged with 2-bromobenzothiophene (1.07 g, 5 mmol), vinylboronic acid pinacol ester (1.16 g, 7.5 mmol), $Pd(PPh_3)_4$ (289 mg, 0.25 mmol), aqueous K_2CO_3 (14.7 mL, 1.1 M) and dioxane (50 mL). The resulting solution was heated at 100 °C for 8 h. After cooling to room temperature, the reaction mixture was diluted with diethyl ether and water. The organic layer was separated and the aqueous phase was extracted with diethyl ether (×3). The combined organic extracts were dried with Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel, eluting with hexanes to give 2-vinylbenzo[*b*]thiophene (**2d**) (0.72 g, 90%) as a colorless oil.

2 Details of Optimization Studies

2.1 Table S1. Optimization Studies to Find Suitable Oxidant.[a]

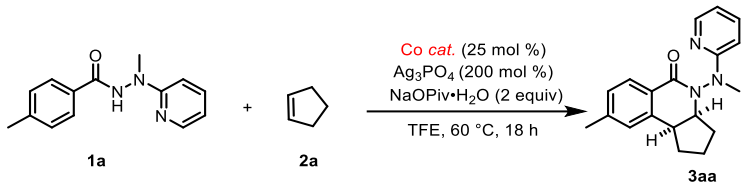


1a 2a 3aa

entry	oxidant	yield
1	Ag_3PO_4	95%
2	Ag_2CO_3	decomposed
3	$AgNO_3$	32%
4	AgOAc	<10%[b]
5	$Mn(OAc)_3{\cdot}2H_2O$	<10%[b]
6	$Mn(OAc)_2$	5%[b]
7	O_2	4%[b]
8	air	<10%[b]
9	Ar	NR.

[a] Reaction conditions: **1a** (0.2 mmol), **2** (0.4 mmol). $Co(acac)_2$ (25 mol %), oxidant (200 mol %), NaOPiv•H_2O (2 equiv), TFE (2 mL), Ar, 60 ℃, 18 h, sealed tube. Isolated yield. [b] NMR yields by employing 1,3,5-trimethoxybenzene as an internal standard. NR = no reaction.

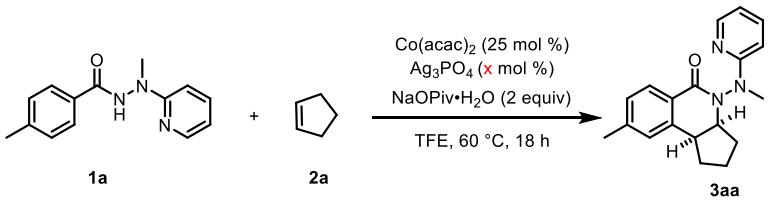
2.2 Table S2. Optimization Studies to Find Suitable Co Catalyst.[a]



entry	Co *cat.*	yield
1	$Co(acac)_2$	95%[b]
2	$Co(OAc)_2·4H_2O$	decomposed
3	$Co(OAc)_2$	trace
4	$CoCl_2$	9%[b]
5	$CoBr_2$	11%[b]
6	CoI_2	12%[b]

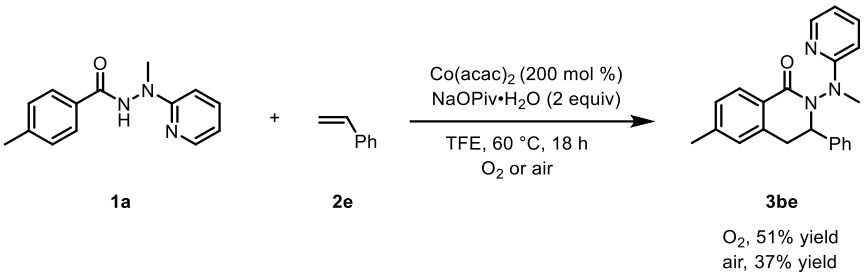
[a] Reaction conditions: **1a** (0.2 mmol), **2** (0.4 mmol). $Co(acac)_2$ (25 mol %), Ag_3PO_4 (200 mol %), NaOPiv•H_2O (2 equiv), TFE (2 mL), Ar, 60 ℃, 18 h, sealed tube. Isolated yield. [b] NMR yields by employing 1,3,5-trimethoxybenzene as an internal standard.

2.3 Table S3. Optimization Studies to Reduce the Oxidant.[a]



entry	$Co(acac)_2$	oxidant	yield
1	25 mol %	Ag_3PO_4 (200 mol %)	95%
2	25 mol %	Ag_3PO_4 (150 mol %)	95%
3	25 mol %	Ag_3PO_4 (120 mol %)	88%
4	25 mol %	Ag_3PO_4 (100 mol %)	72%
5	25 mol %	Ag_3PO_4 (67 mol %)	71%
6[b]	25 mol %	Ag_3PO_4 (67 mol %) + O_2	75%
7	25 mol %	Ag_3PO_4 (33 mol %)	50%
8[b]	25 mol %	Ag_3PO_4 (33 mol %) + O_2	67%
9[b]	**2 equiv**	**O_2**	**93%**
10[c]	2 equiv	air	75%
11[b]	1 equiv	O_2	58%
12[c]	1 equiv	air	21%

[a] Reaction conditions: **1a** (0.2 mmol), **2** (0.4 mmol). $Co(acac)_2$ (25 mol %), oxidant (200 mol %), NaOPiv•H_2O (2 equiv), TFE (2 mL), Ar, 60 ℃, 18 h, sealed tube. Isolated yield. [b] O_2 atmosphere instead of Ar. [c] Air instead of Ar.



1a **2e** **3be**

O_2, 51% yield
air, 37% yield

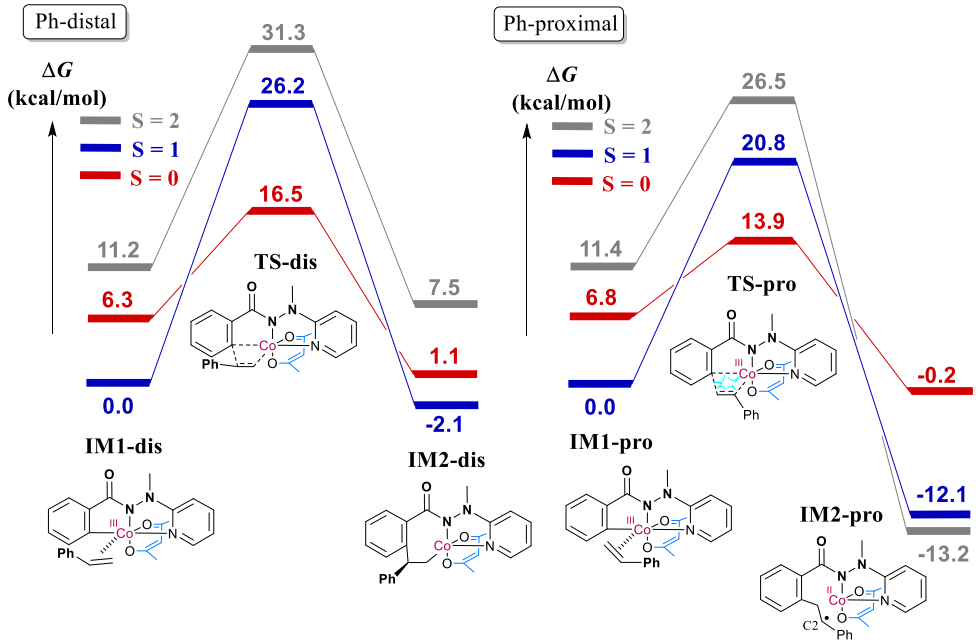
3 Computational Details

All molecular geometries were optimized in gas phase at the PBE0[3] level in combination with D3 dispersion corrections with Becke-Johnson damping scheme (D3BJ).[4,5] For the geometry optimizations the cobalt was described with SDD pseudopotential,[6] while on the other atoms the def2-SVP basis set was used.[7] All intermediates (no imaginary frequencies) and transition states (only one imaginary frequency) were checked by analytical frequency calculations, analytical frequency calculations were carried out at the same level of theory. The thermal correction to the Gibbs free energy in gas-phase was calculated in these harmonic vibrational analyses at the corresponding experimental temperatures in 333.15 K. Geometry optimization and thermal corrections were performed by using Gaussian 09, Revision D.01 package.[8]

To refine the calculated electronic energy, single-point calculations with larger basis set def2-TZVP basis set were then done on the optimized geometries, by using PW6B95[9] functional in combination with RIJCOSX approximations and dispersion corrections (D3BJ). Solvent effect was also included implicitly through the use of the SMD continuum solvation model.[10] The experimental solvent corresponds to 2,2,2-trifluoroethanol (TFE) in each calculation. This energetic refinement was performed by using the ORCA program package version 4.2.1.[11] Energies reported are based on gas-phase Gibbs free energies with def2-SVP basis set for which the electronic energies were corrected to PW6B95-D3BJ with def2-TZVP basis set and solvent effects.

The migratory insertion step starts from a triplet state (S = 1) intermediate **IM1-dis/pro.** However, the singlet state (S = 0) transition state is calculated to be much more stable than the triplet state. Thus, a spin-crossover occurs during the insertion process. The triplet state is found to be more stable than the singlet state again for the intermediate **IM2-dis/pro**. Overall, the energy barriers for the regiocontrol step are 13.1 kcal/mol for Ph-distal species and 11.0 kcal/mol for Ph-proximal species respectively. We also carried out the above calculation by removing the dispersion corrections and reoptimized the reaction species, the energy profiles shown similar tendency of spin-crossover behavior and barrier difference. The calculated barriers for **TS-dis** and **TS-pro** are 16.5 and 13.9 kcal/mol, respectively (Scheme S1). This indicates that the dispersion interaction stabilizes both transition states to similar extents, and is not the major factor for the preference of the **TS-pro**. Although the target model contains a lot of adjacent π-electron rich groups, especially for the singlet state pathway. However, the dispersion correction does not change the sequence for electron spin states of

transition state, and the barrier for Ph-proximal species is more favorable than Ph-distal species also. Hence, the dispersion correction makes no difference to this regiocontrol step but reduces the reaction energies for all species.



Scheme S1. DFT calculated energy profiles without D3BJ dispersion correction for migratory insertion step of Ph-distal and Ph-proximal species.

Comparing the electron states and geometry structures of **IM2** species, for the triplet intermediate **IM2**, the Mulliken spin density for **IM2-dis** is 2.3271 for Co and -0.4180 for C1, in **IM2-pro** the Mulliken spin density for Co is 2.7405, for C2 is -0.8120. From C1 in **IM2-dis** to C2 in **IM2-pro**, the C atom in styrene who is close to Co, its spin density increases and it indicates that the radical properties for C2 is enhanced. The electron spin density differences also reflect in the **IM2** geometries. The electron spin on C2 atom of **IM2-pro** keeps the C2 is more likely a sp^2 hybrid carbon than sp^3 hybrid carbon. Thus, C2 in **IM2-pro** structure is tend to be as a plane with C1 and Ph-group of styrene, so that the electron spin on C2 could easily to forming a conjugated structure with the rest of π-electron rich groups, and which is contribute to reduce the system energy. The Co with high spin state obtained an electron from the broken C3-Co bond, and the Co^{III} in **IM1-pro** was reduced to Co^{II} in high spin state **IM2-pro**.

In Figure S1 for **IM2-pro** structure, the bond length for Co and C2 atom is 3.010 Å, it is much longer than Co-C1 bond length 2.009 Å in **IM2-dis** structure, the **IM2-dis** is a seven-membered ringlike intermediate. However, the **IM2-pro** is a linear intermediate and not a seven-membered ringlike intermediate. The electron state has

effect on the **IM2** species, and the non-ringlike **IM2** leads to a lower energy intermediate **IM2-pro**, which is 10.5 kcal/mol lower than **IM2-dis**, the migratory insertion step for Ph-proximal is an exothermic reaction pathway and a preferred lower barrier pathway for regioselectivity. Therefore, the regioselectivity was controlled by the steric effect and election state.

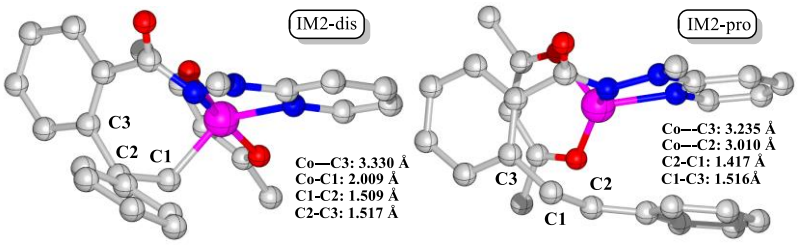
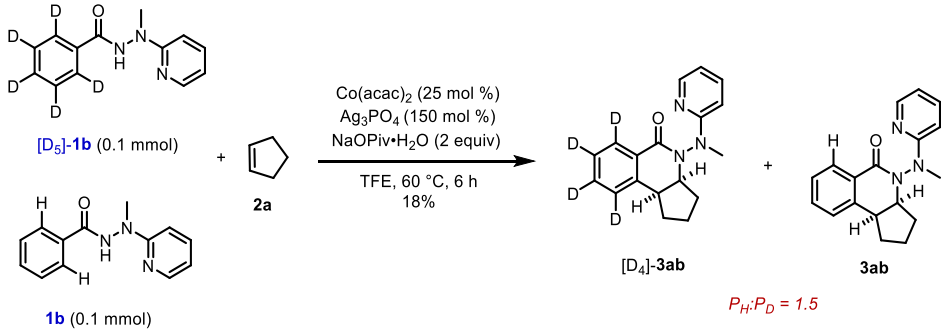
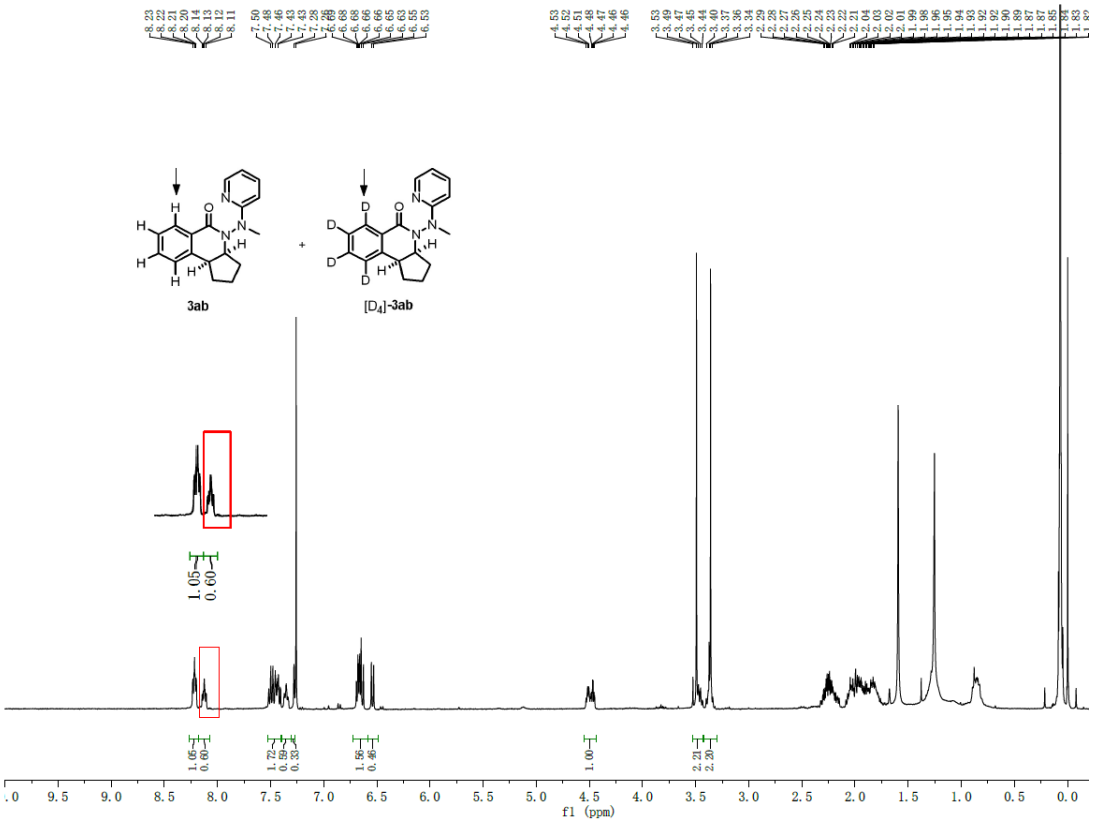


Figure S1. Optimized triplet state **IM2** geometry structures, the bond length was shown in the figure, C atoms in gray, N atoms in blue, O atoms in red and Co atom in magenta, the H atoms were omitted for clarity.

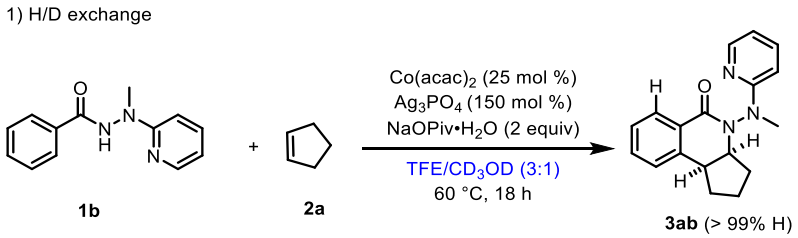
4 Preliminary Mechanistic Experiments

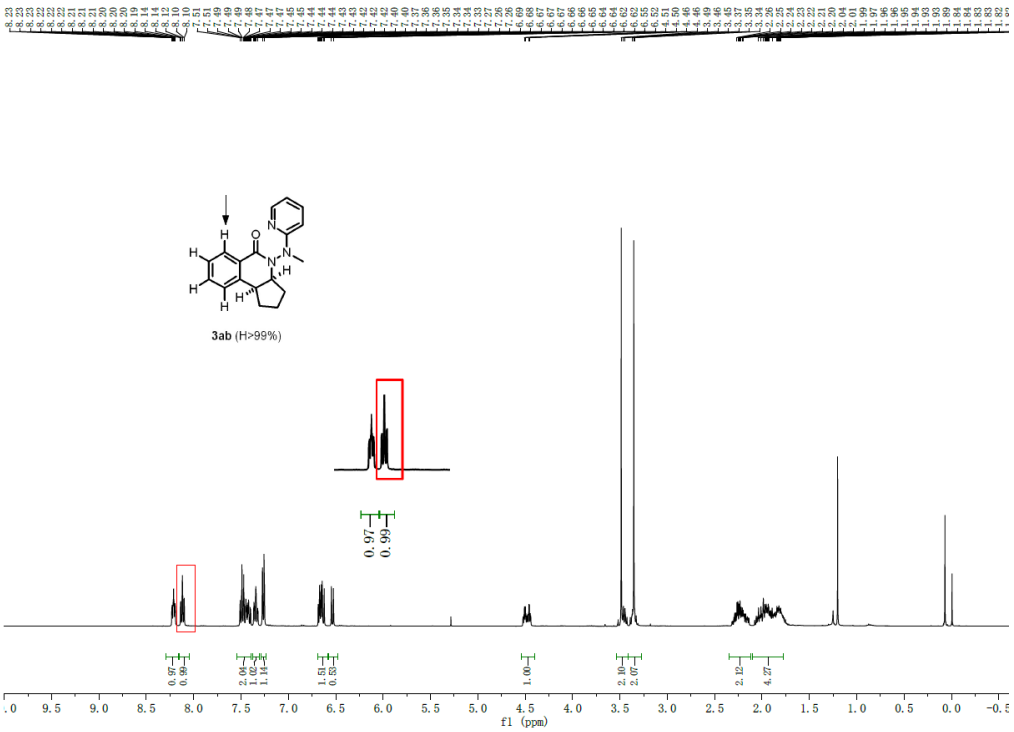
4.1 KIE Experiments:



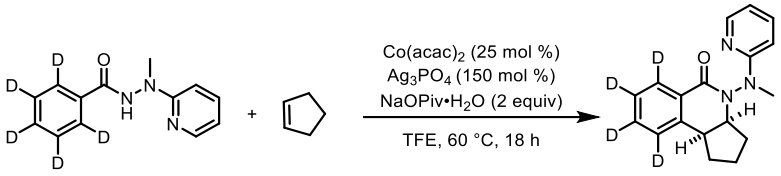


4.2 Deuterium Labeling Experiments:

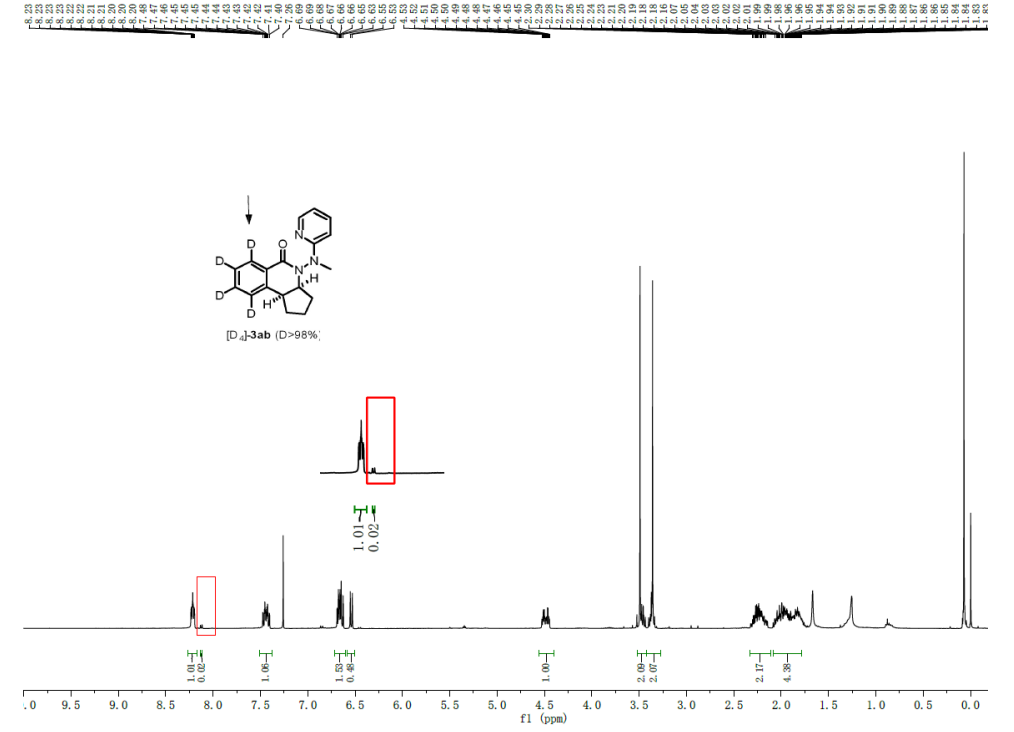




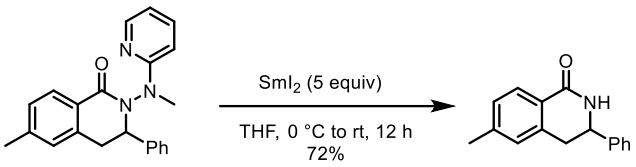
2) D/H exchange



[D_5]-**1b** **2a** [D_4]-**3ab** (> 98% D)



5 Removal of the Directing Group for 3be



3be **5**

An oven-dried 25 mL two-neck round bottom flask was charged with **3be** (0.175 mmol, 60 mg). After purging with Ar three times, 5 mL fresh distilled THF was added, then SmI_2 (0.1 M in THF, 5 equiv) was added dropwise at 0 °C. After 5 minutes, the mixture was warmed to rt and stirred for 12 h. After that the mixture was quenched with 5 mL saturated aqueous $Na_2S_2O_3$ and extracted with DCM, dried over Na_2SO_4, filtered, and concentrated under reduced pressure and **5** was obtained in 72% yield via column chromatography.

After cleavage of the MHP, we found that the doubled peaks in ^{1}H NMR and ^{13}C{^{1}H} NMR of **3be** was the atropisomer caused by restricted rotation of the MHP. Both the ^{1}H and ^{13}C{^{1}H} NMR of the cleavage product **5** indicate only one product was obtained.

6-Methyl-3-phenyl-3,4-dihydroisoquinolin-1(2*H*)-one (5): Purified by flash column chromatography on silica gel (eluting with *n*-hexane/EtOAc = 2:1), white solid (30 mg, 72%), mp 144.6–146.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 7.9 Hz, 1H), 7.46 – 7.29 (m, 5H), 7.17 (d, J = 7.8 Hz, 1H), 6.98 (s, 1H), 6.14 (s, 1H), 4.83 (dd, J = 10.6, 4.9 Hz, 1H), 3.11 (qd, J = 15.7, 7.9 Hz, 2H), 2.37 (s, 3H). ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 166.5, 143.1, 141.0, 137.5, 128.9, 128.3, 128.0, 127.9, 126.4, 125.7, 56.1, 37.4, 21.6. HRMS (ESI) m/z: [M + H$^+$] calcd for $C_{16}H_{15}NO$ 238.1226; found 238.1229.

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7 ^{1}H, ^{13}C{^{1}H} and ^{19}F NMR Spectra

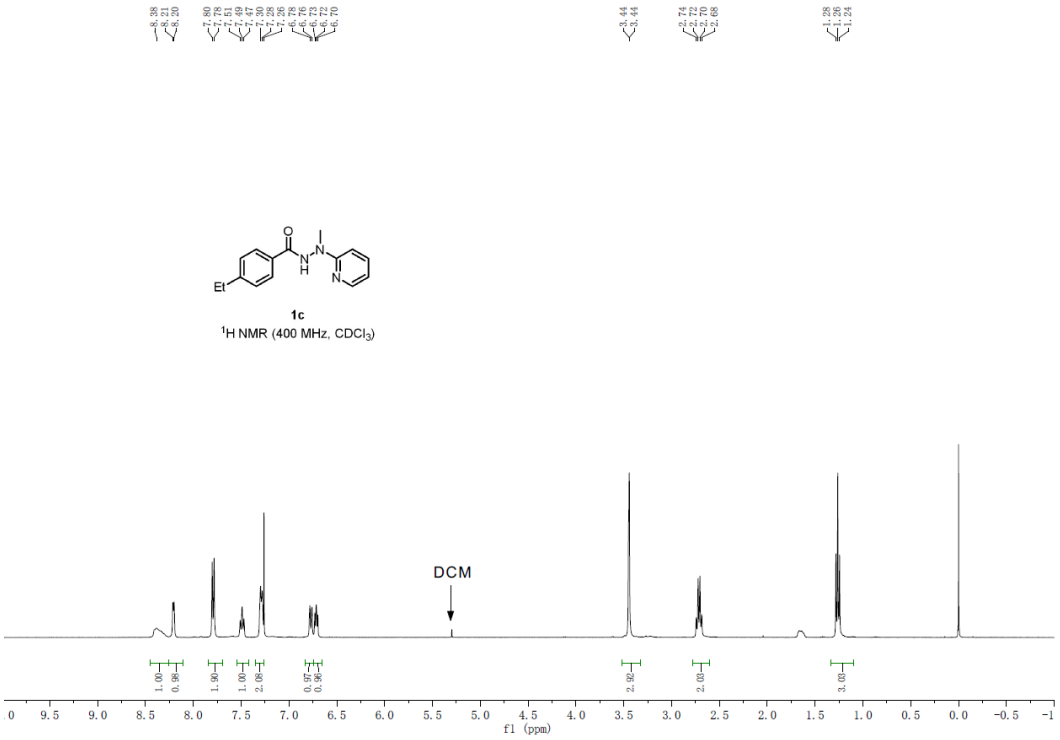


Figure S2. ^{1}H NMR Spectrum of **1c**

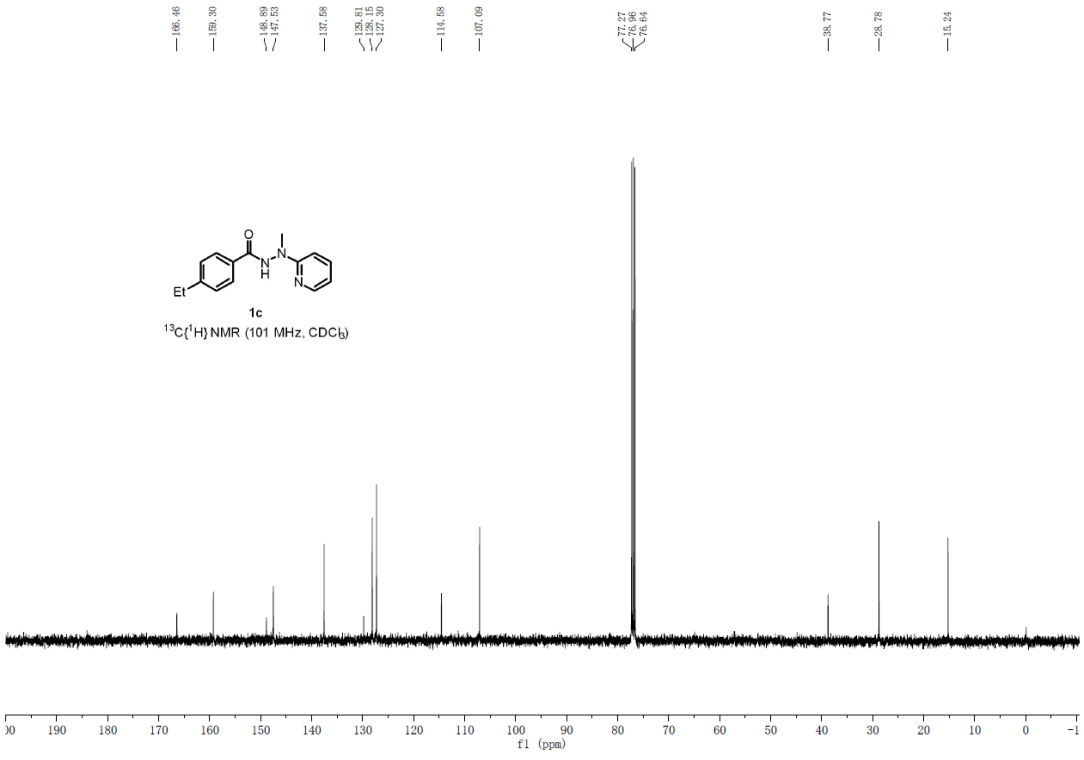


Figure S3. ^{13}C{^{1}H} NMR Spectrum of **1c**

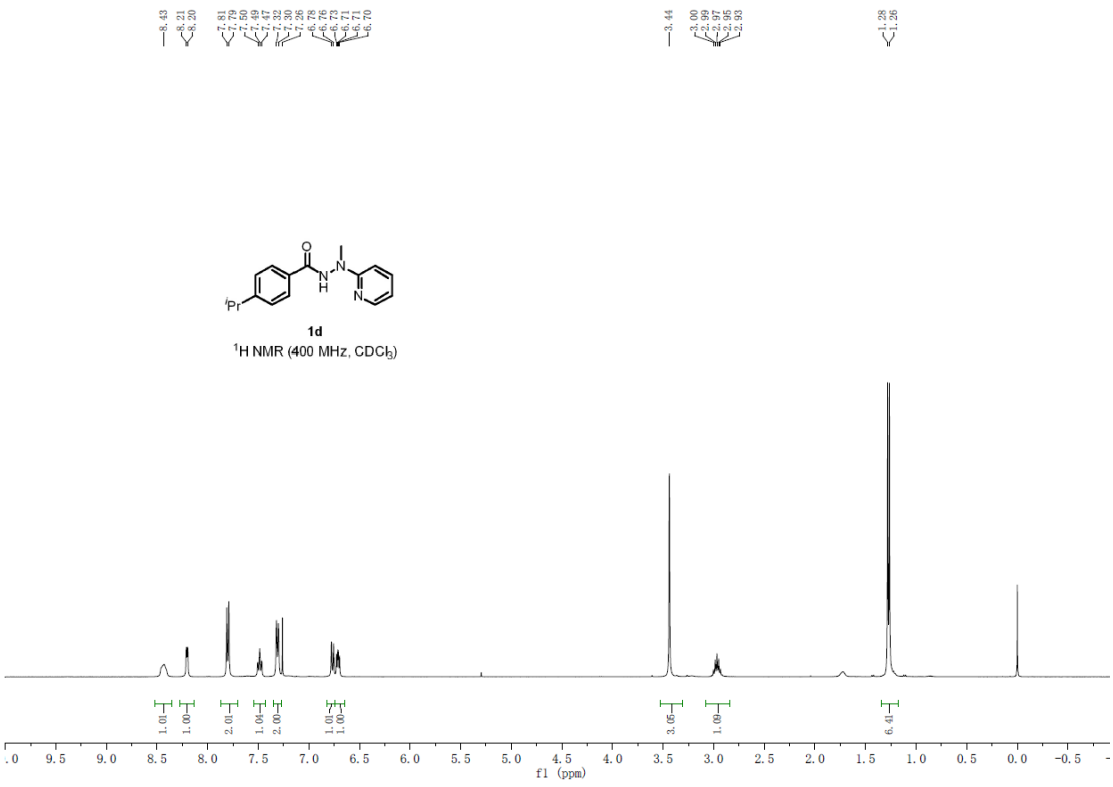


Figure S4. ^{1}H NMR Spectrum of **1d**

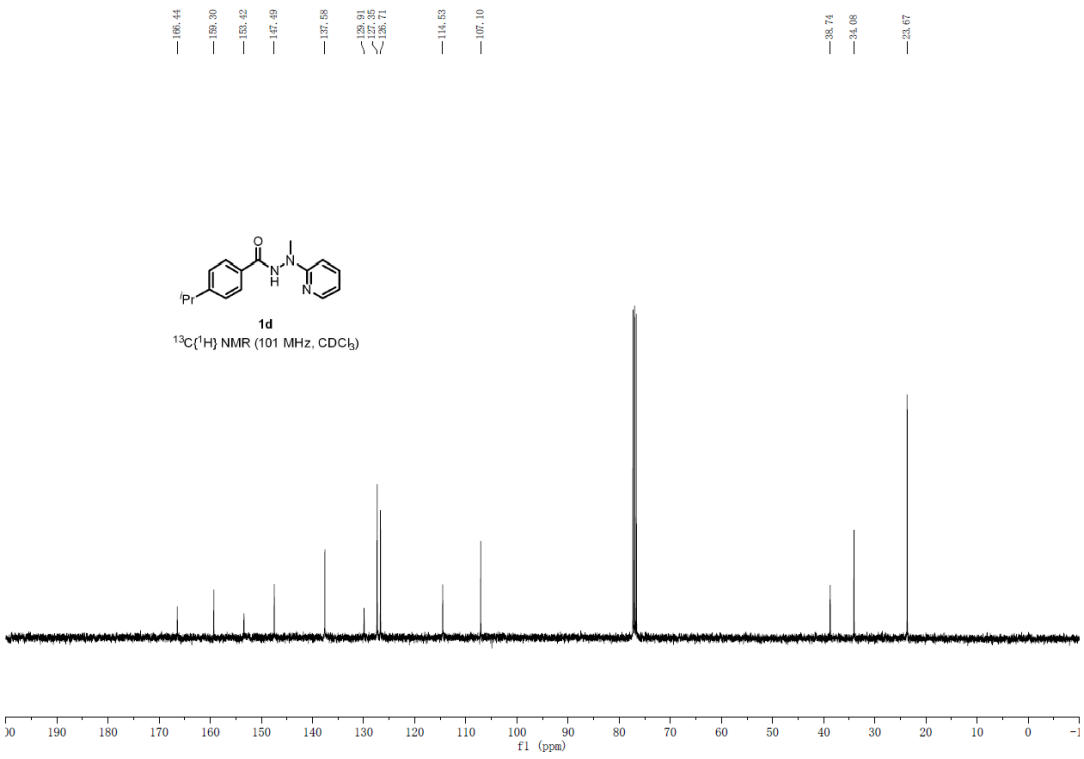


Figure S5. ^{13}C{^{1}H} NMR Spectrum of **1d**

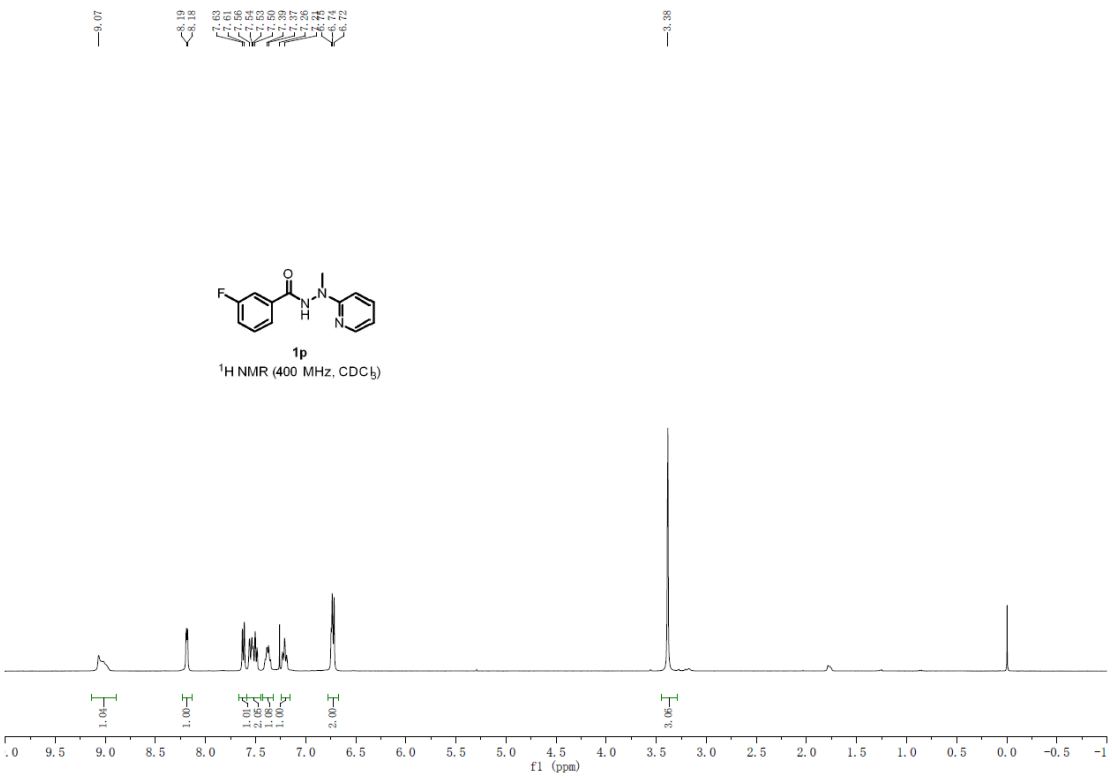


Figure S6. ^{1}H NMR Spectrum of **1p**

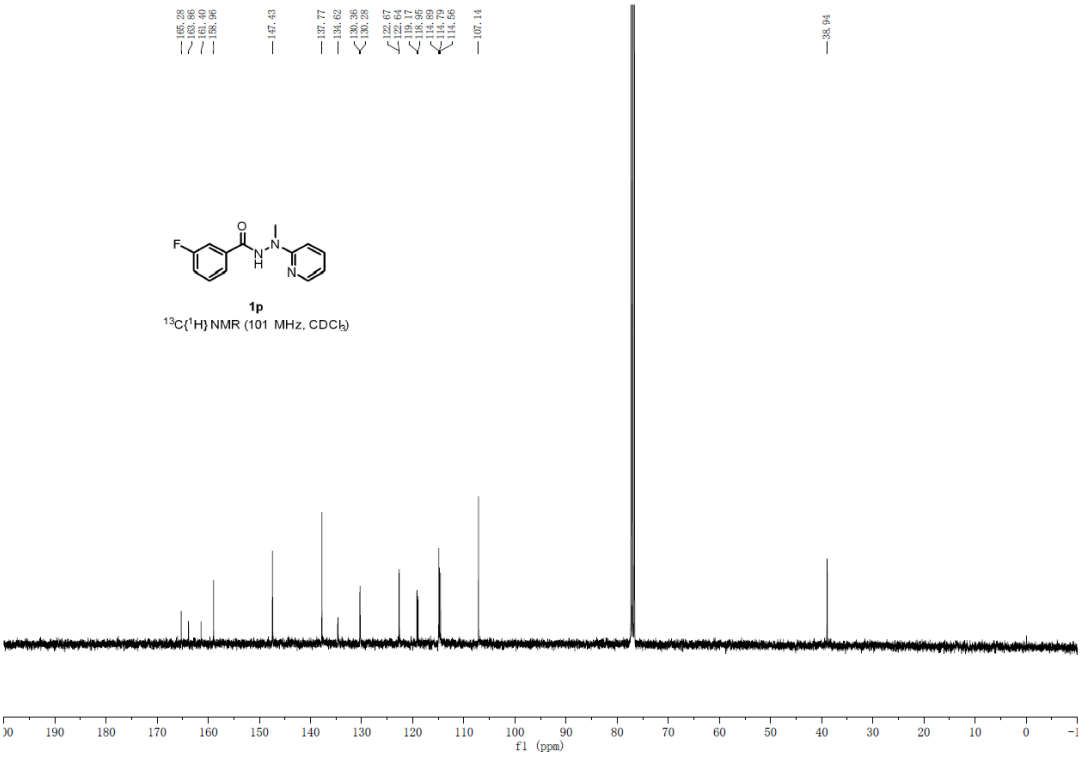


Figure S7. ^{13}C{^{1}H} NMR Spectrum of **1p**

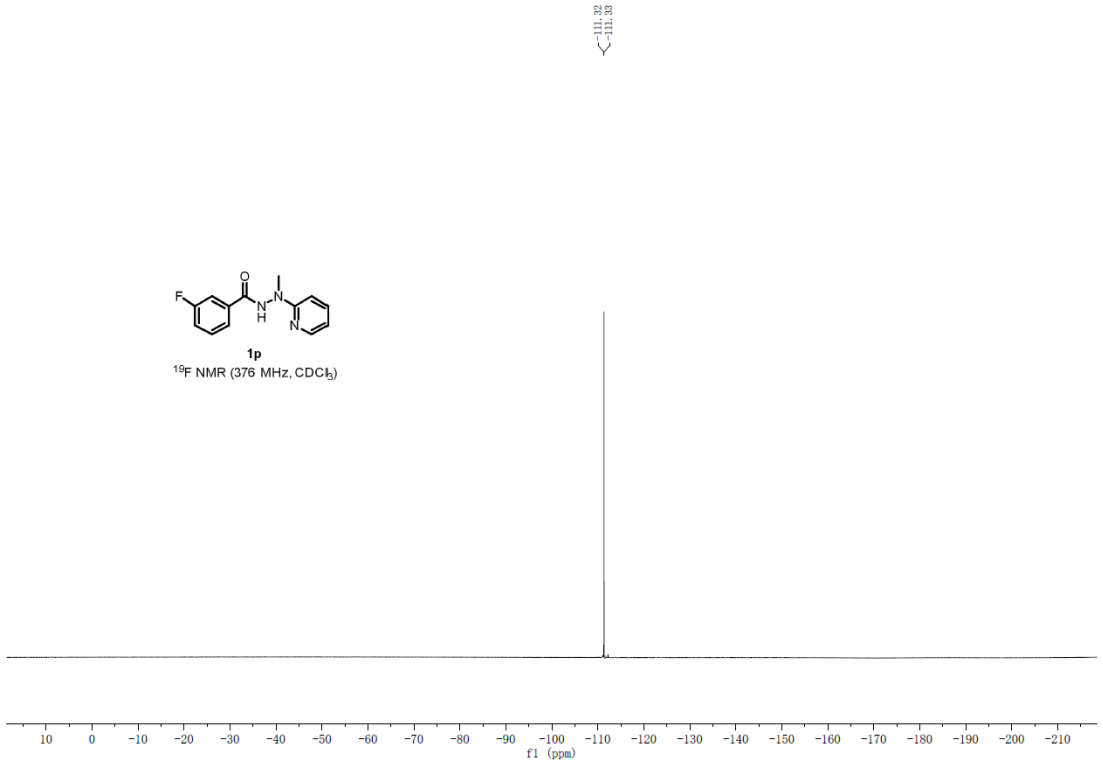


Figure S8. ^{19}F NMR Spectrum of **1p**

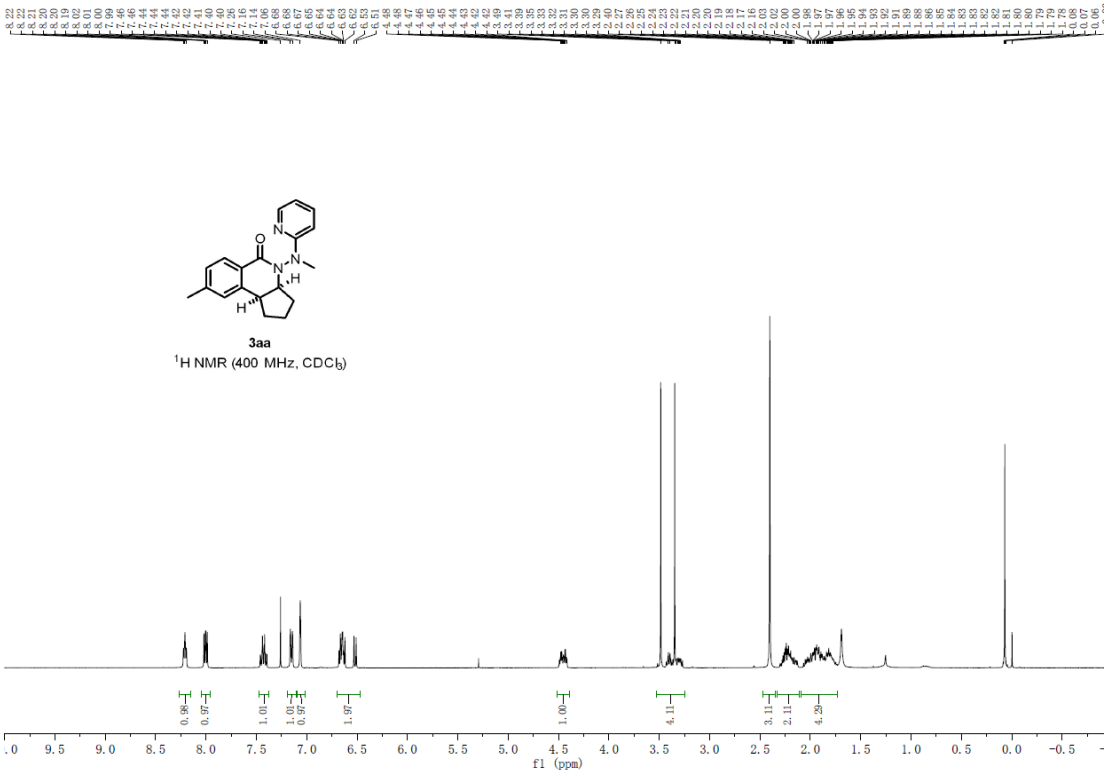


Figure S9. ^{1}H NMR Spectrum of **3aa**

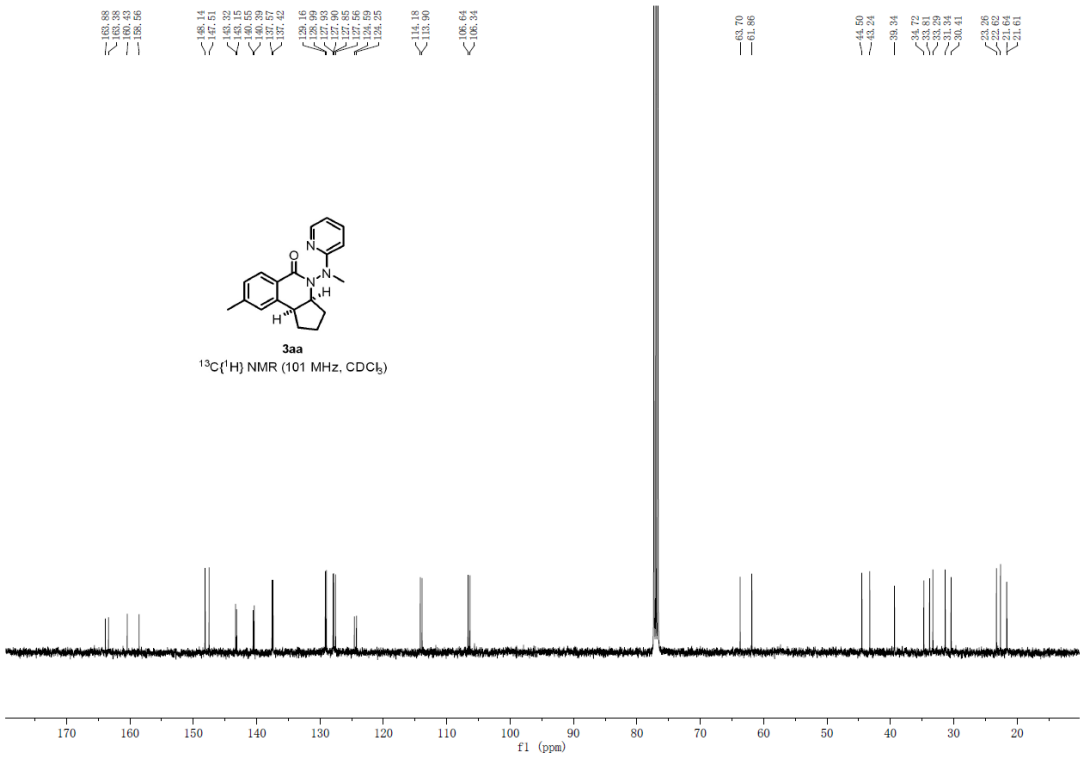


Figure S10. $^{13}C\{^{1}H\}$ NMR Spectrum of **3aa**

***** The doubled carbon peaks in $^{13}C\{^{1}H\}$ NMR of annulation products proven to be the atropisomer caused by restricted rotation of the 2-(1-methylhydrazinyl)pyridine (MHP), cleavage of the MHP by SmI_2 gave a single compound **4**. Both ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR of **4** indicate only one product was obtained (see **Figure S14** and **Figure S15**).

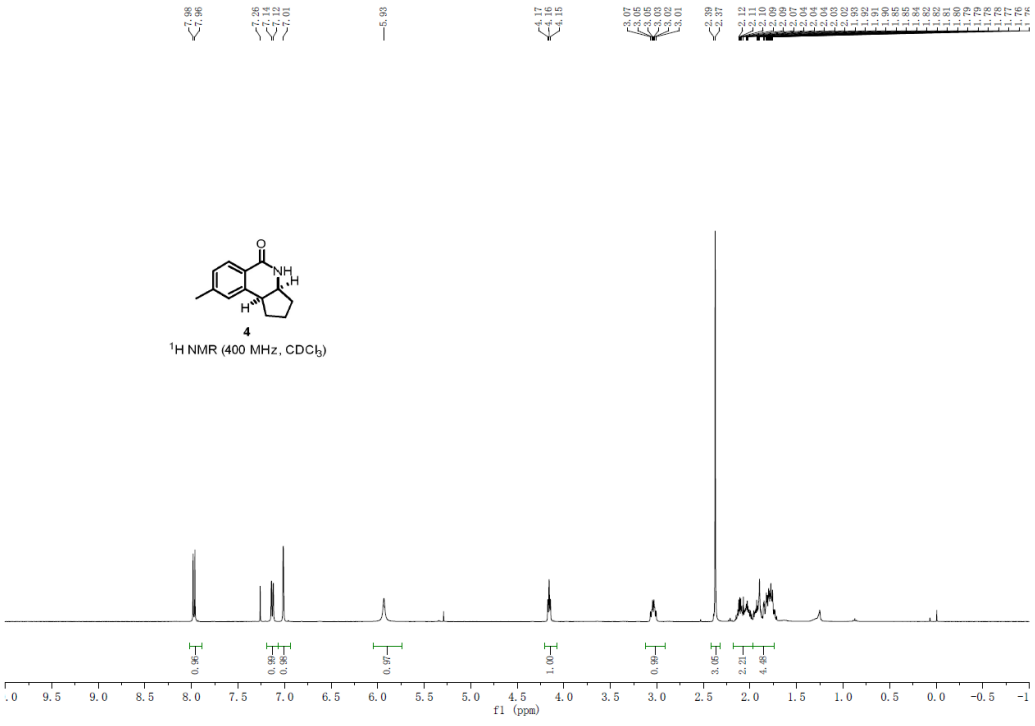


Figure S11. ^{1}H NMR Spectrum of **4**

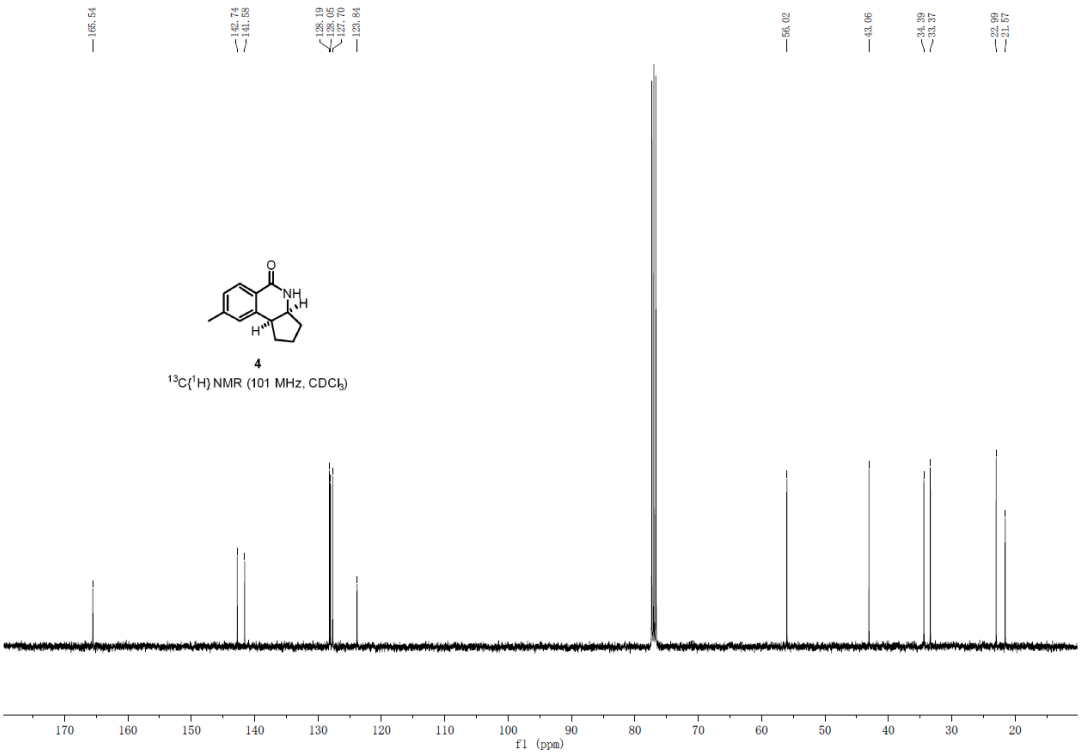


Figure S12. $^{13}C\{^{1}H\}$ NMR Spectrum of **4**

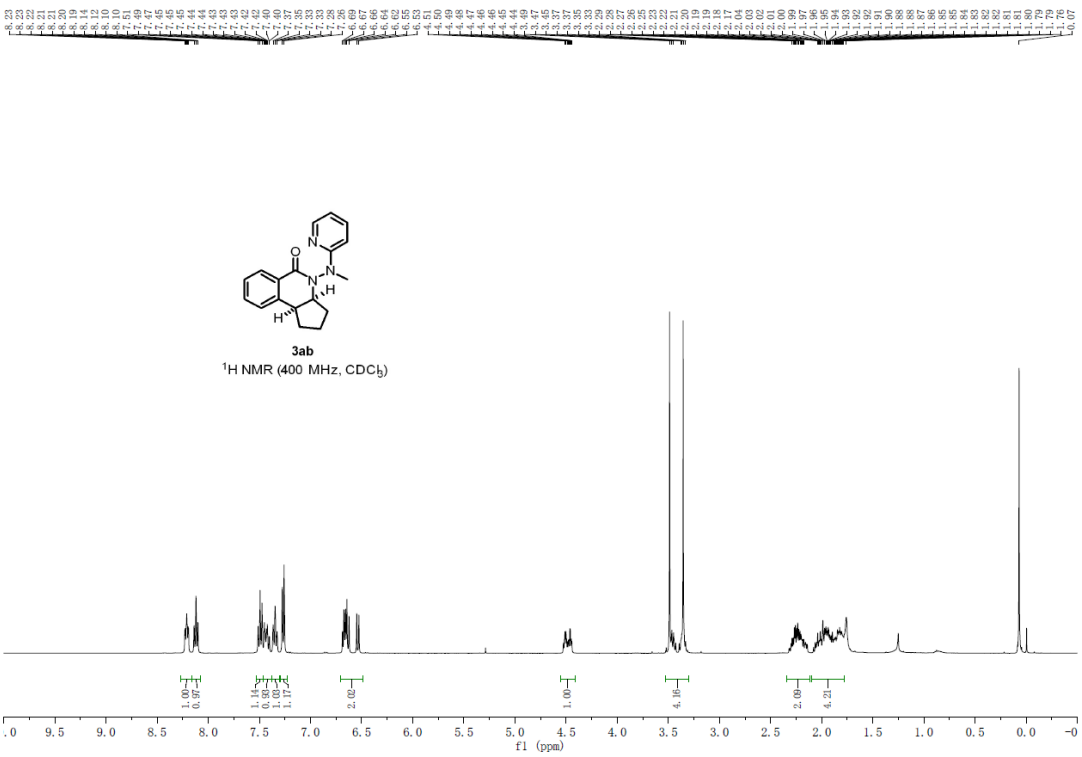


Figure S13. ^{1}H NMR Spectrum of **3ab**

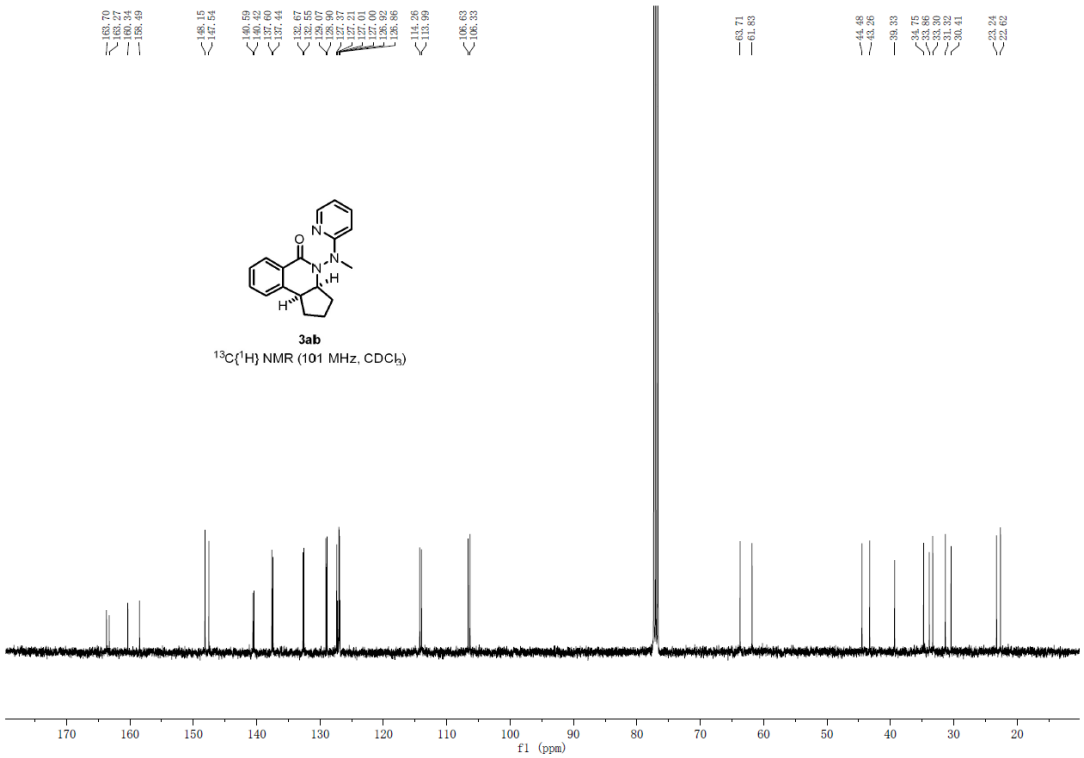


Figure S14. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ab**

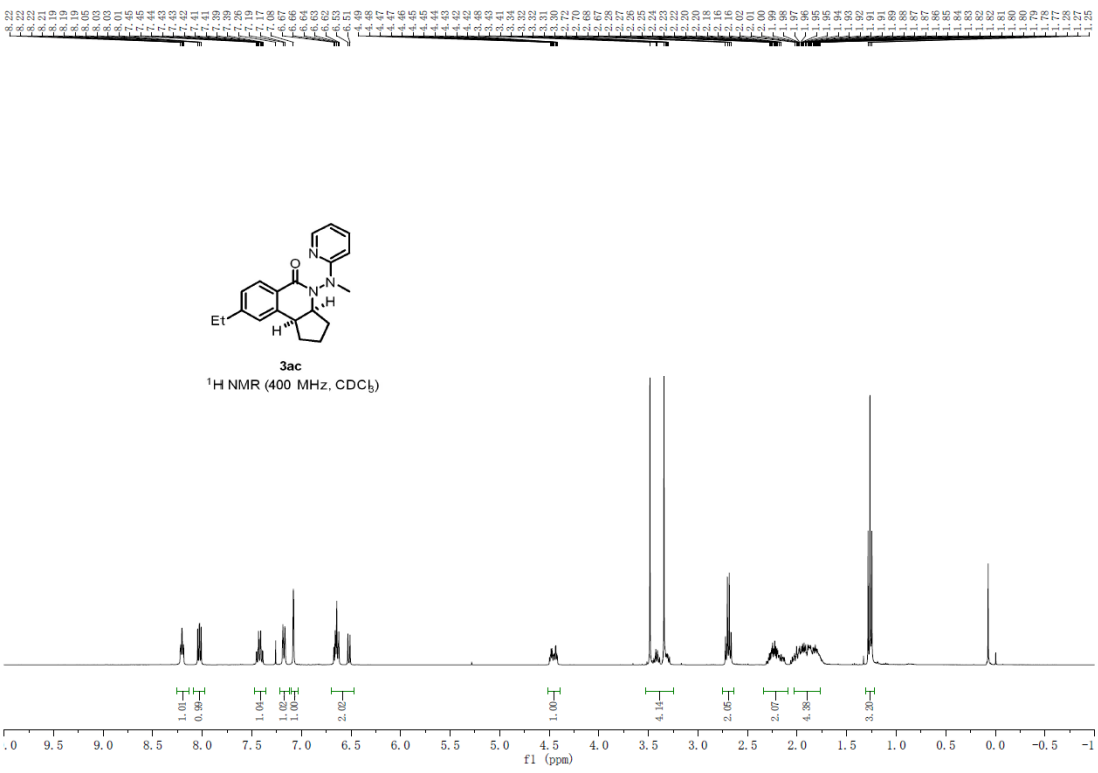


Figure S15. ^{1}H NMR Spectrum of **3ac**

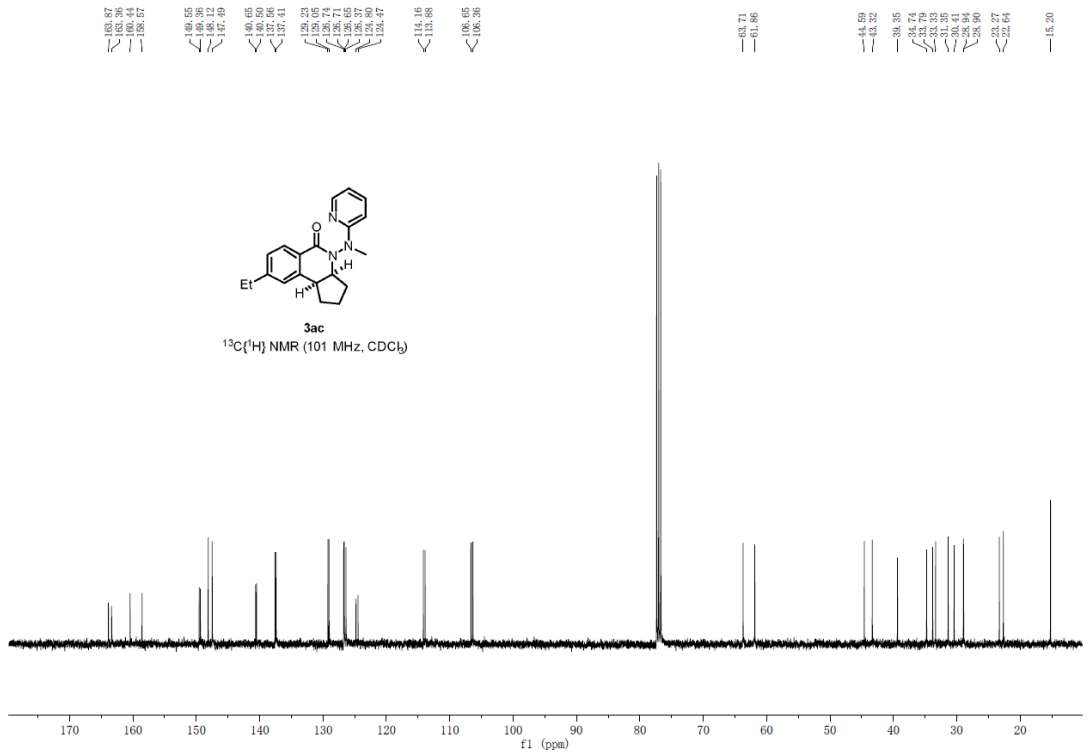


Figure S16. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ac**

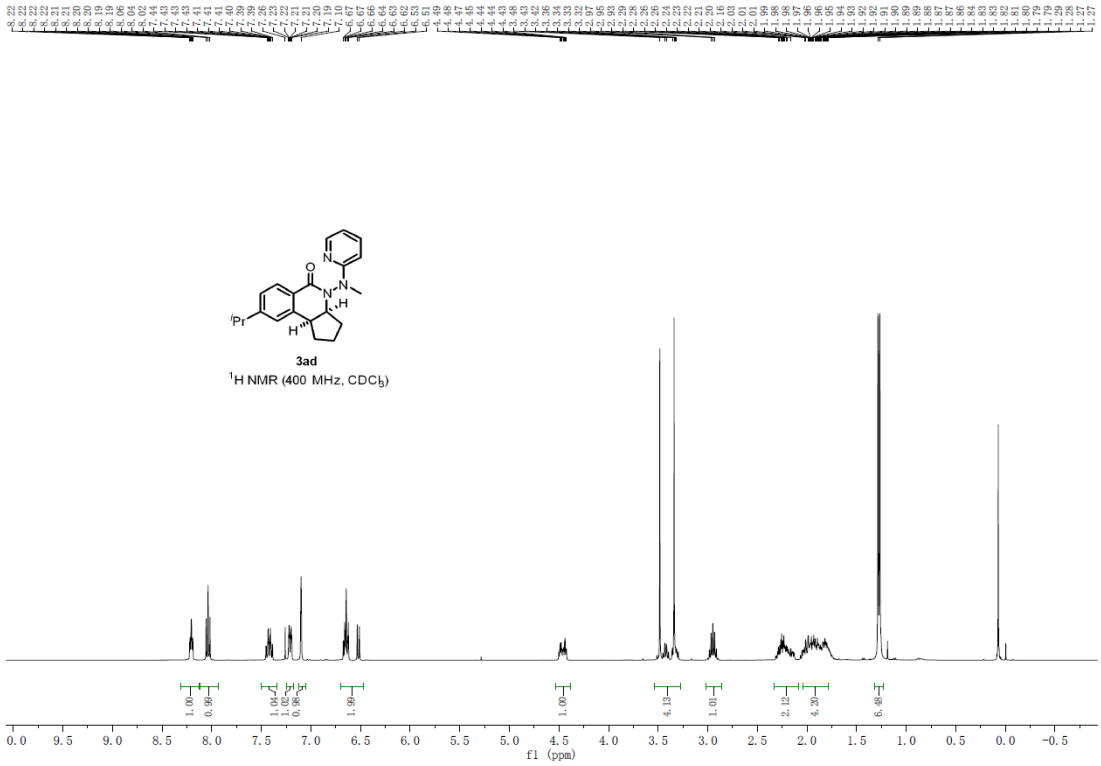


Figure S17. ^{1}H NMR Spectrum of **3ad**

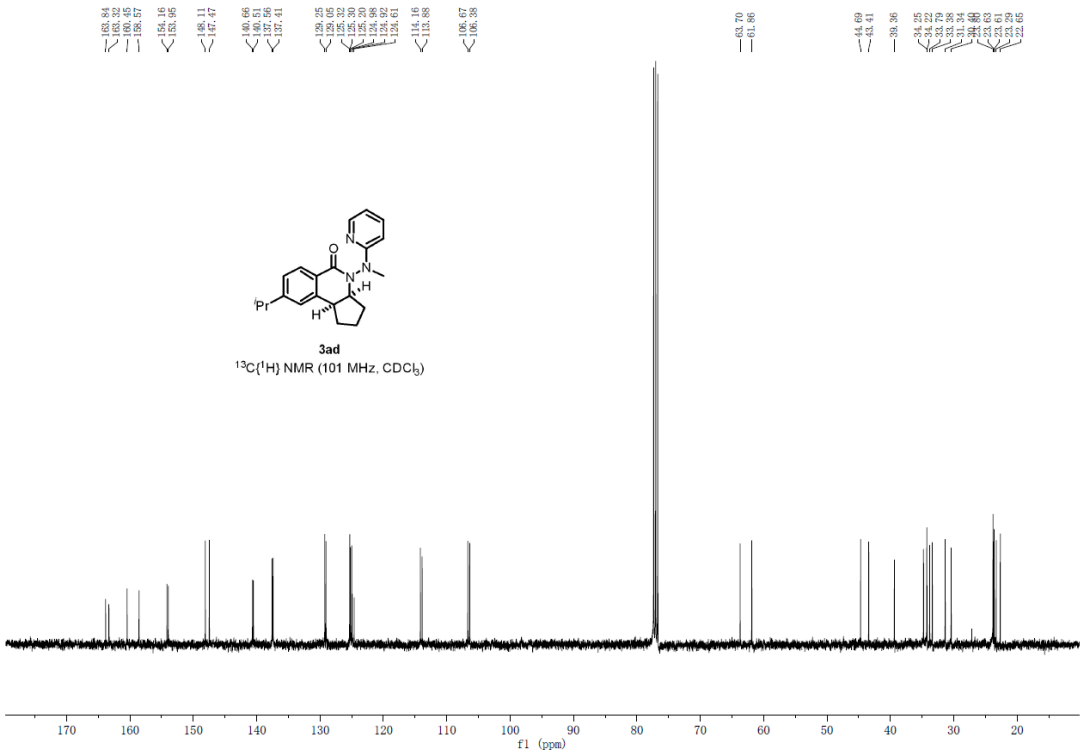


Figure S18. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ad**

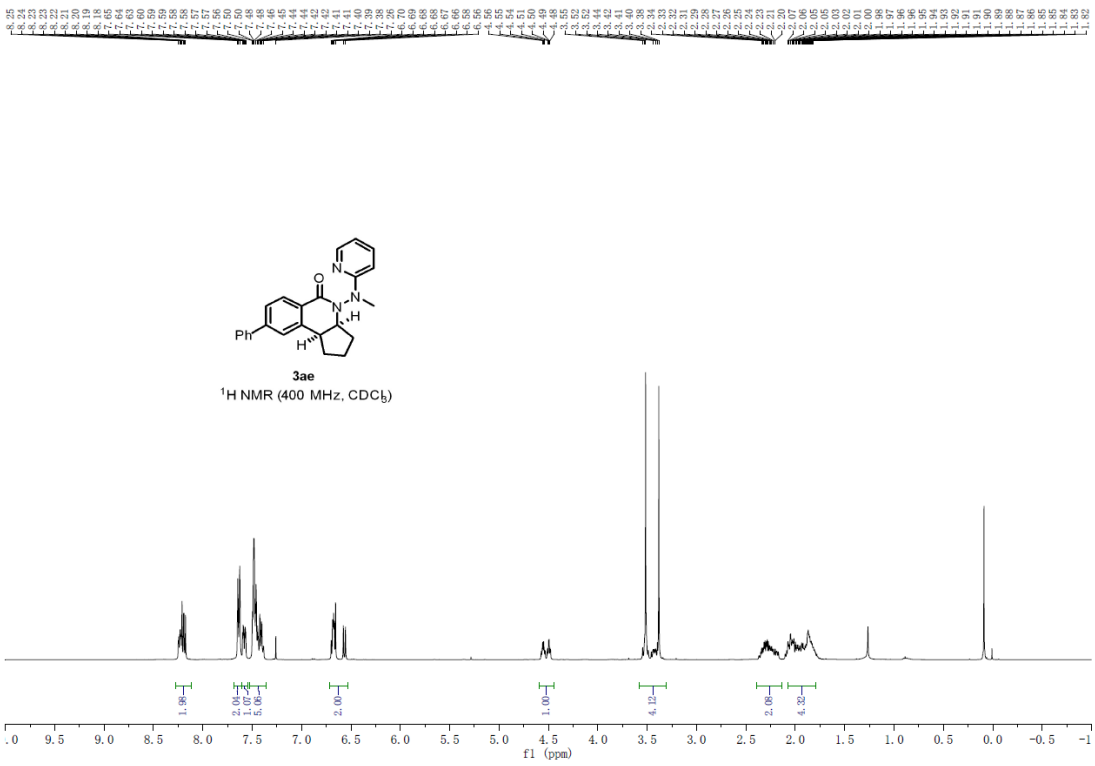


Figure S19. ^{1}H NMR Spectrum of **3ae**

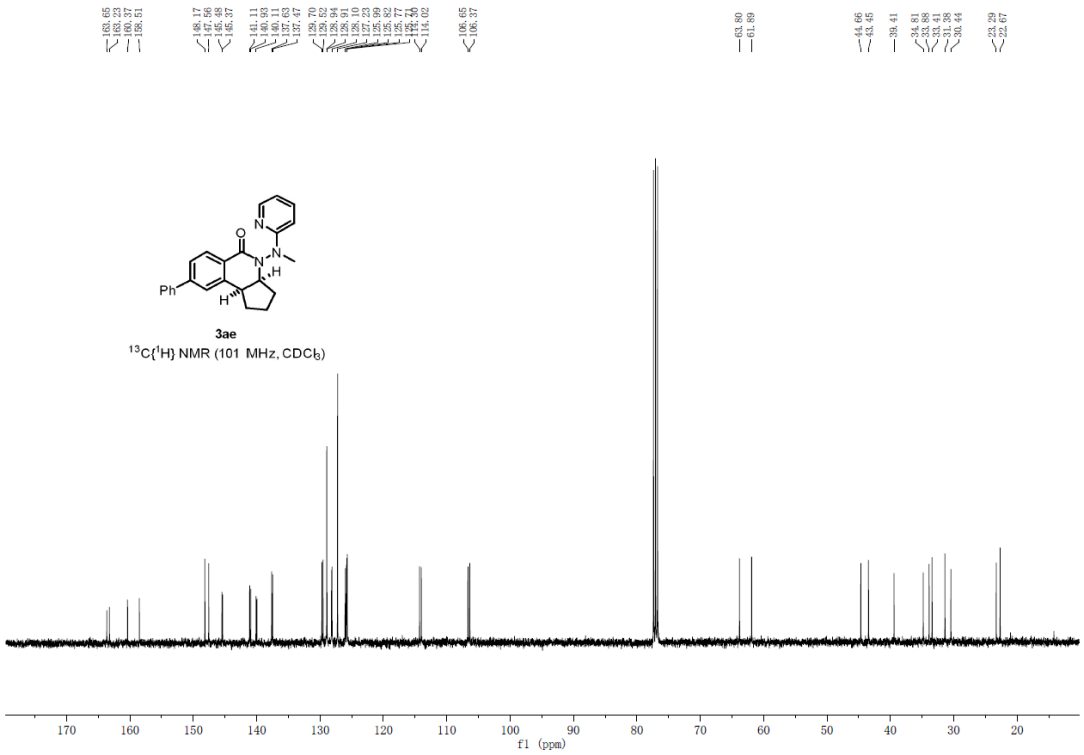


Figure S20. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ae**

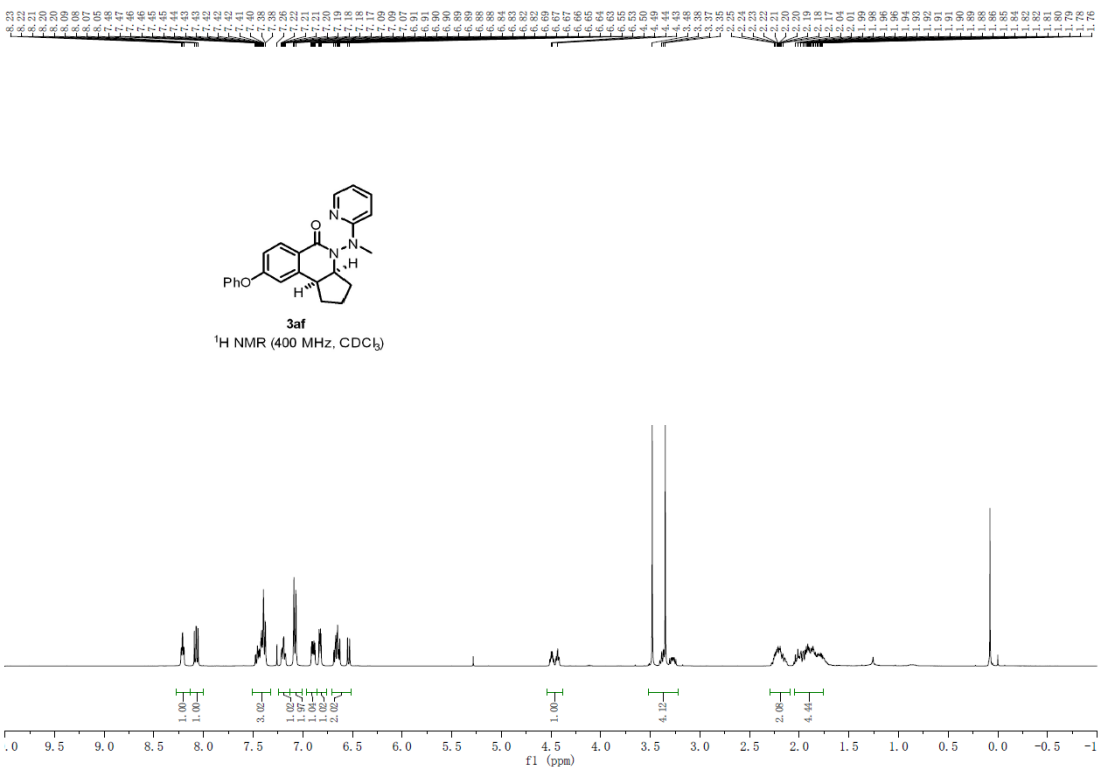


Figure S21. ^{1}H NMR Spectrum of **3af**

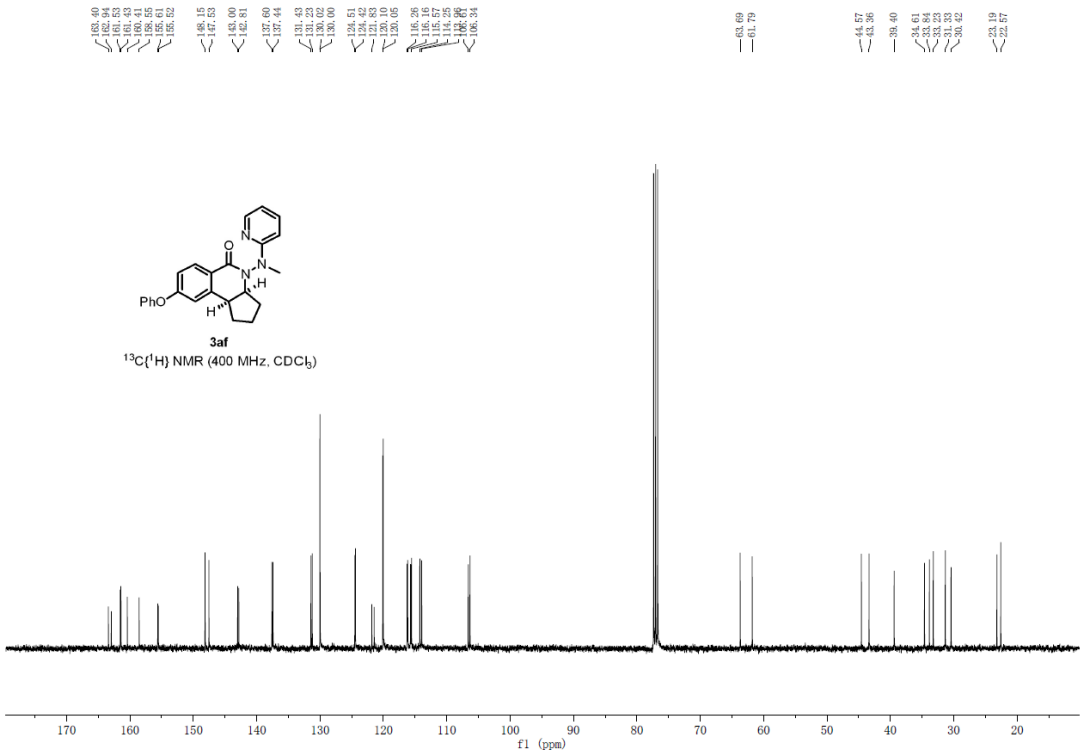


Figure S22. $^{13}C\{^{1}H\}$ NMR Spectrum of **3af**

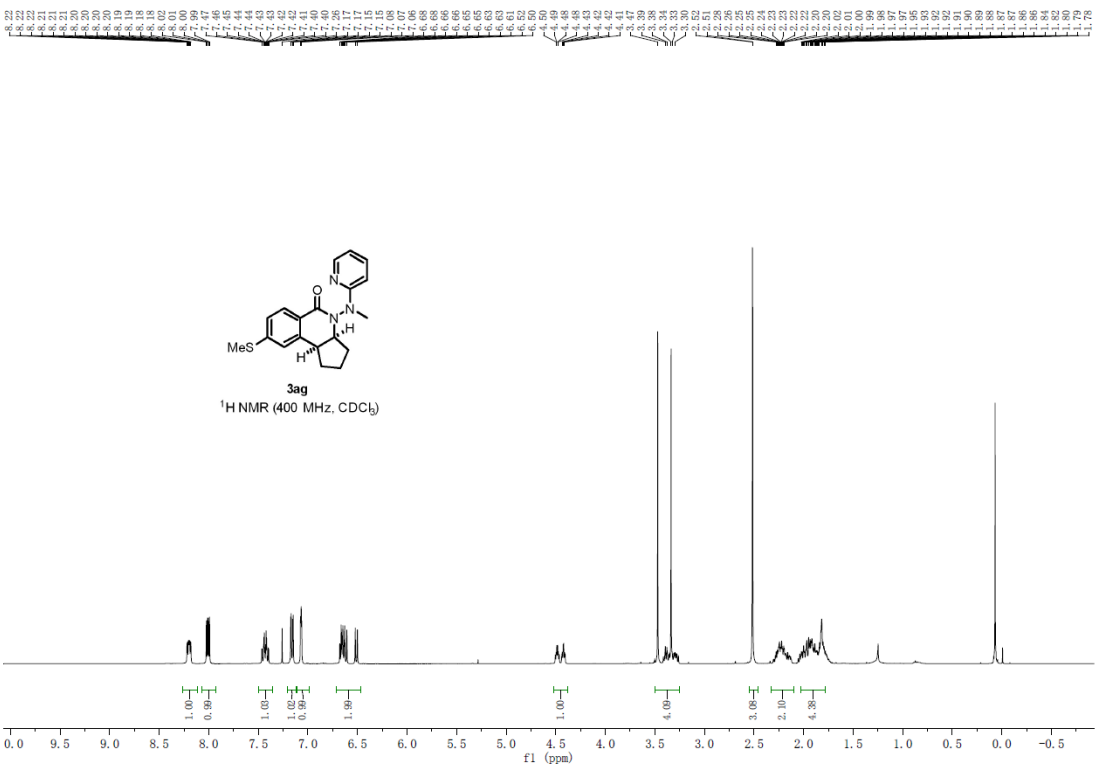


Figure S23. ^{1}H NMR Spectrum of **3ag**

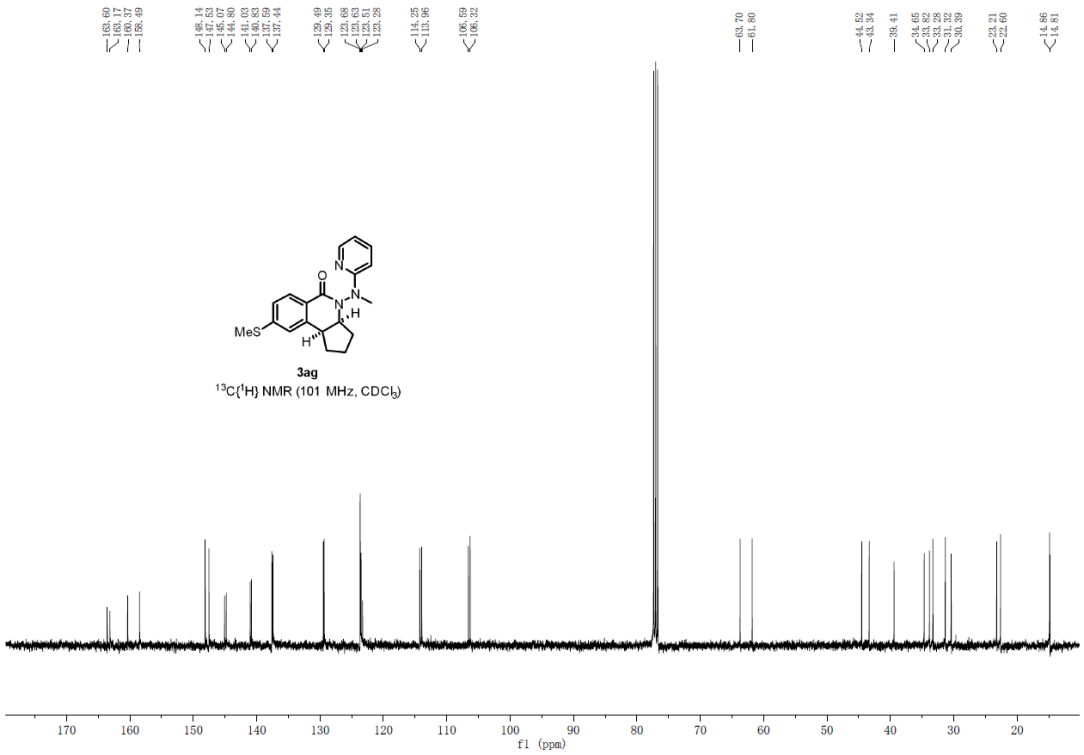


Figure S24. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ag**

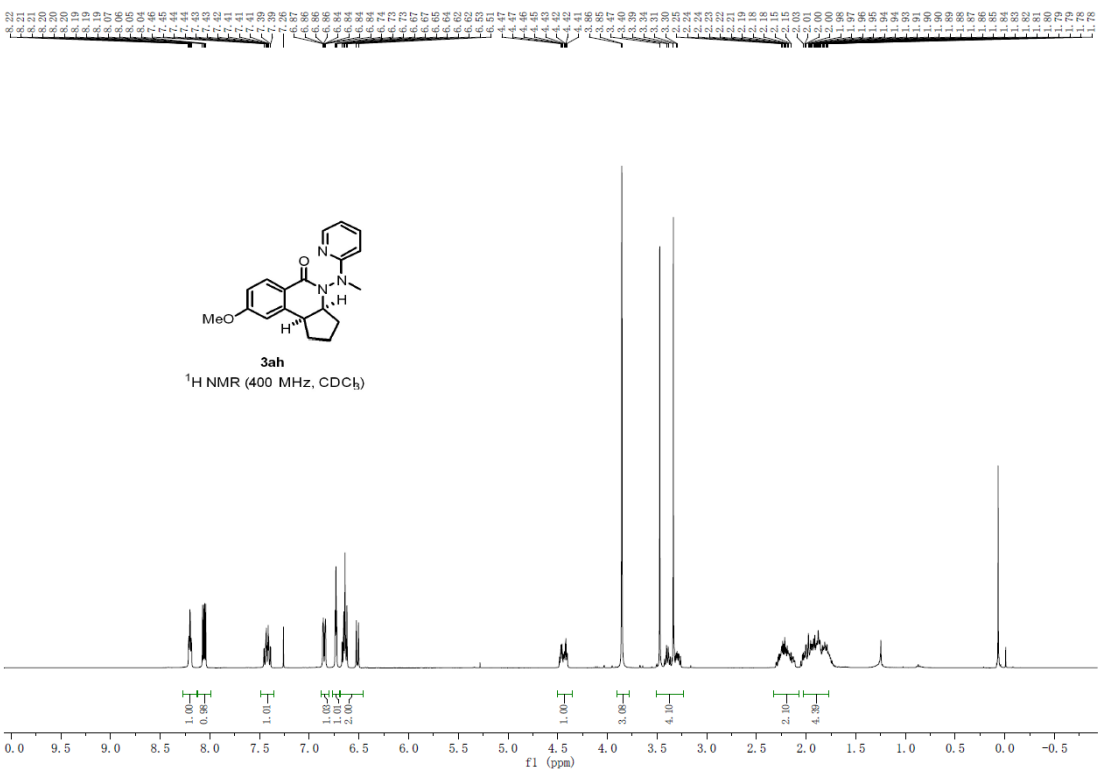


Figure S25. ^{1}H NMR Spectrum of **3ah**

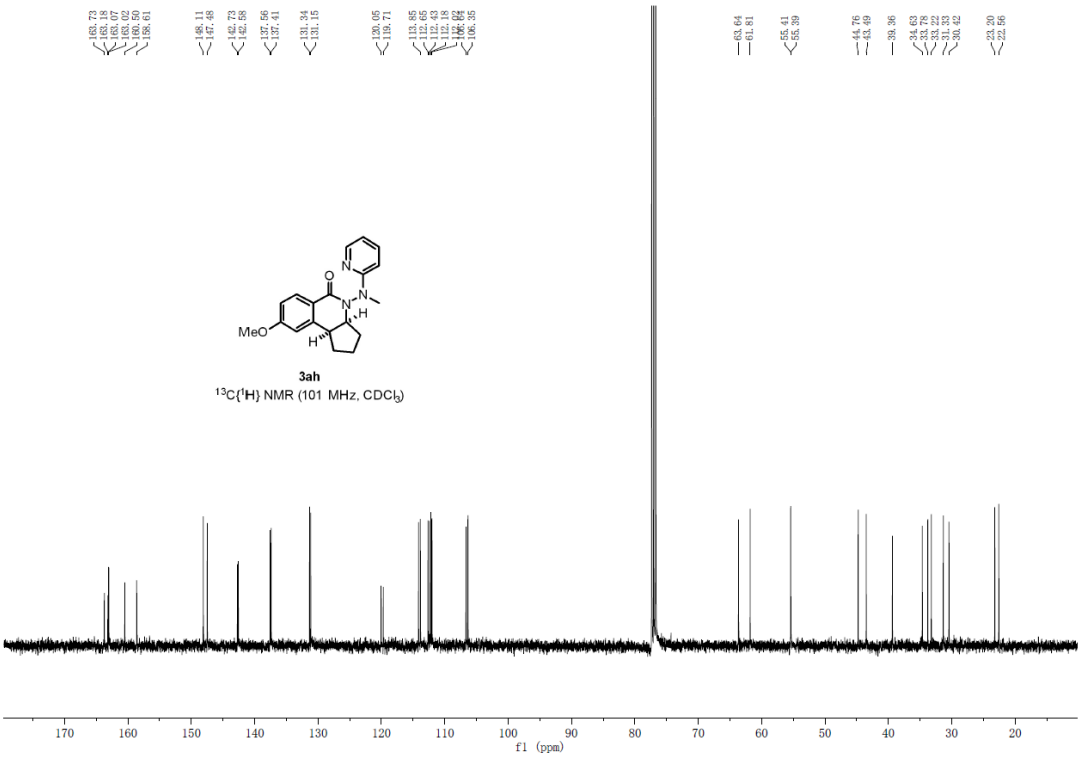


Figure S26. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ah**

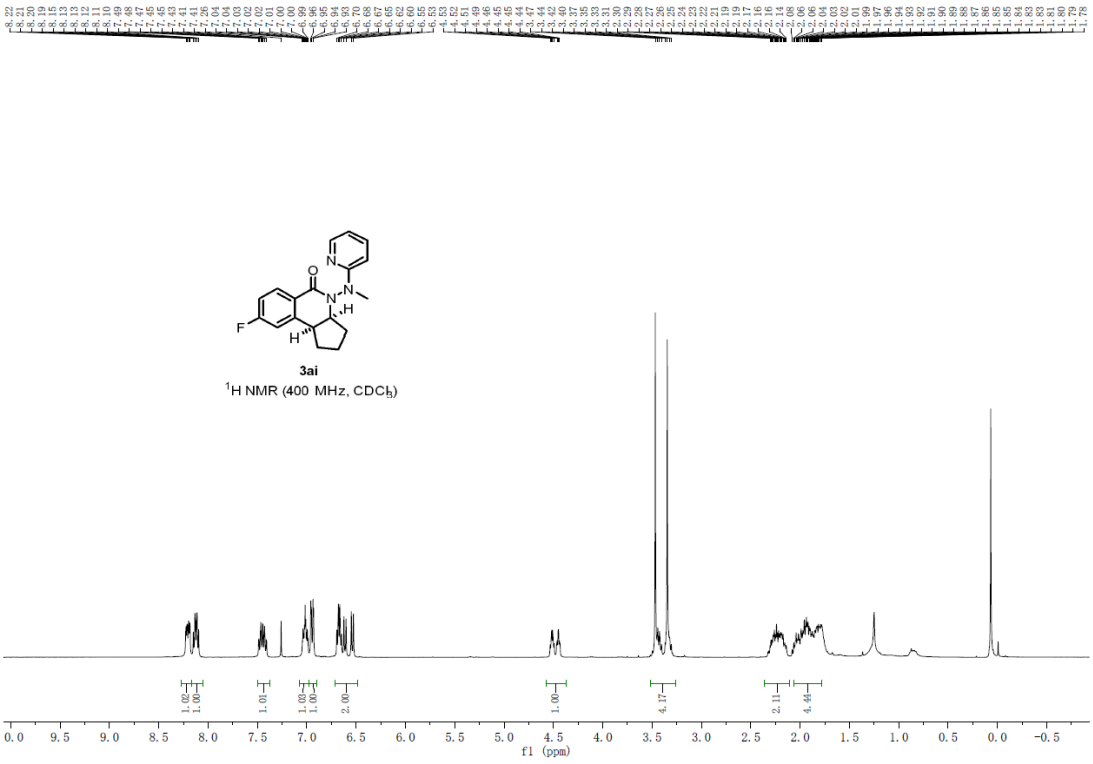


Figure S27. ^{1}H NMR Spectrum of **3ai**

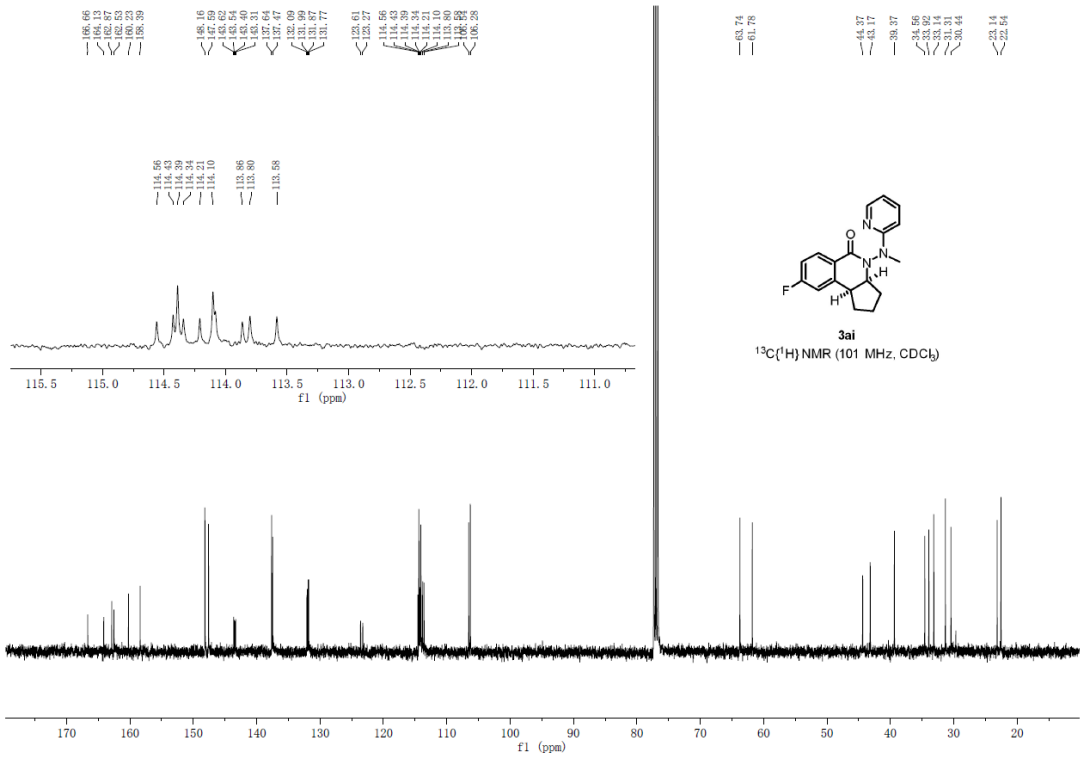


Figure S28. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ai**

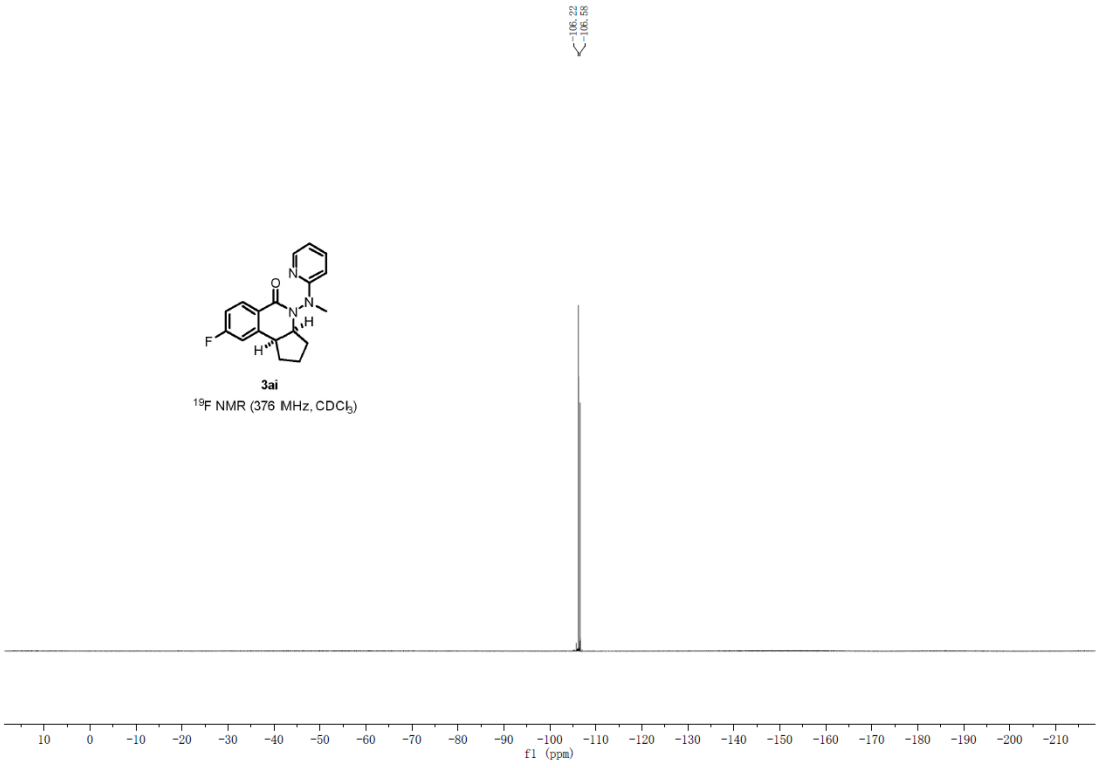


Figure S29. ^{19}F NMR Spectrum of **3ai**

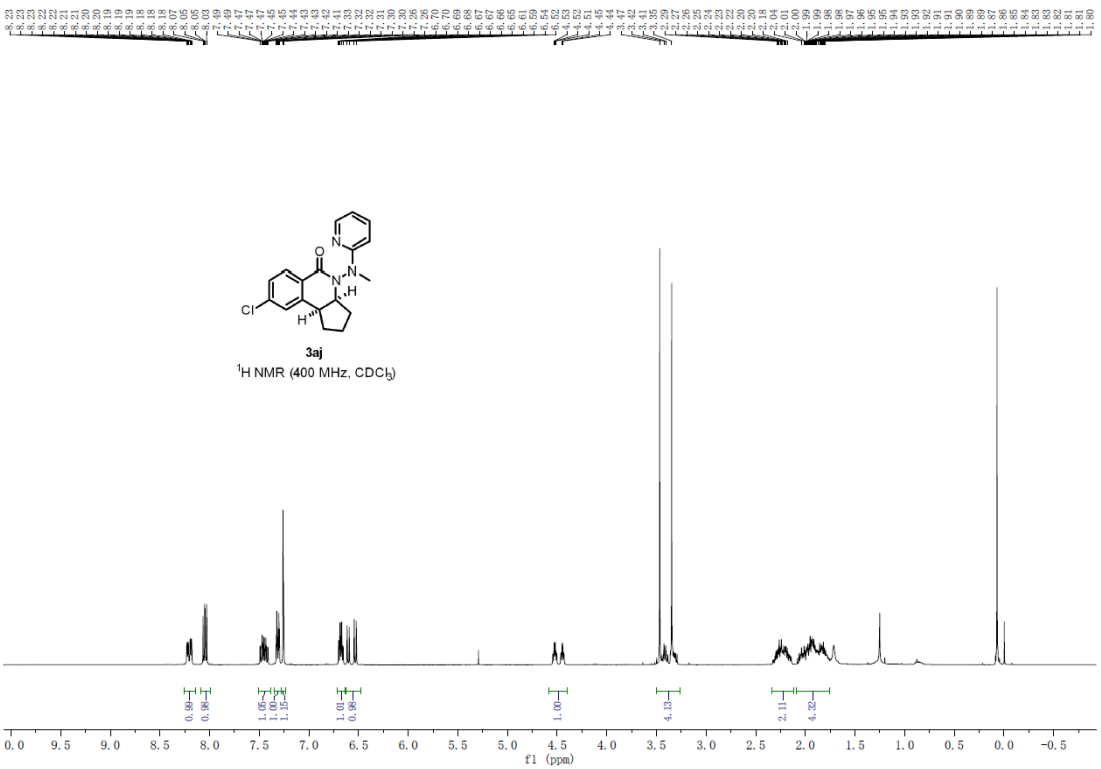


Figure S30. ^{1}H NMR Spectrum of **3aj**

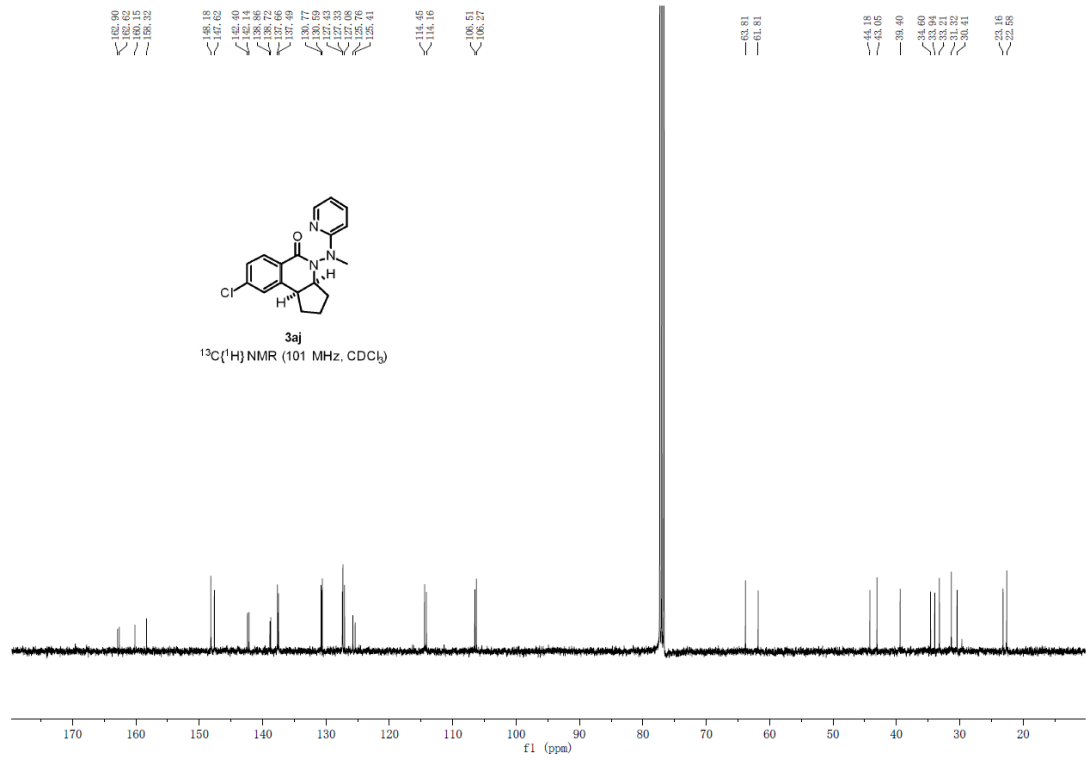


Figure S31. ^{13}C{^{1}H} NMR Spectrum of **3aj**

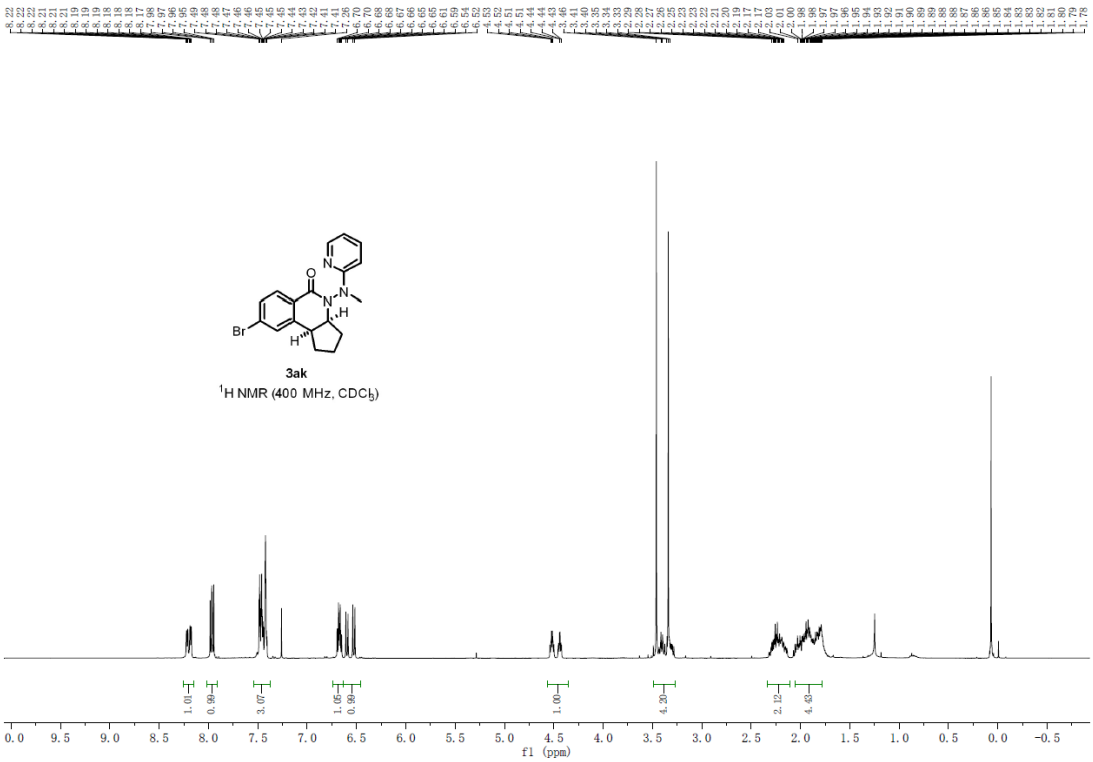


Figure S32. ^{1}H NMR Spectrum of **3ak**

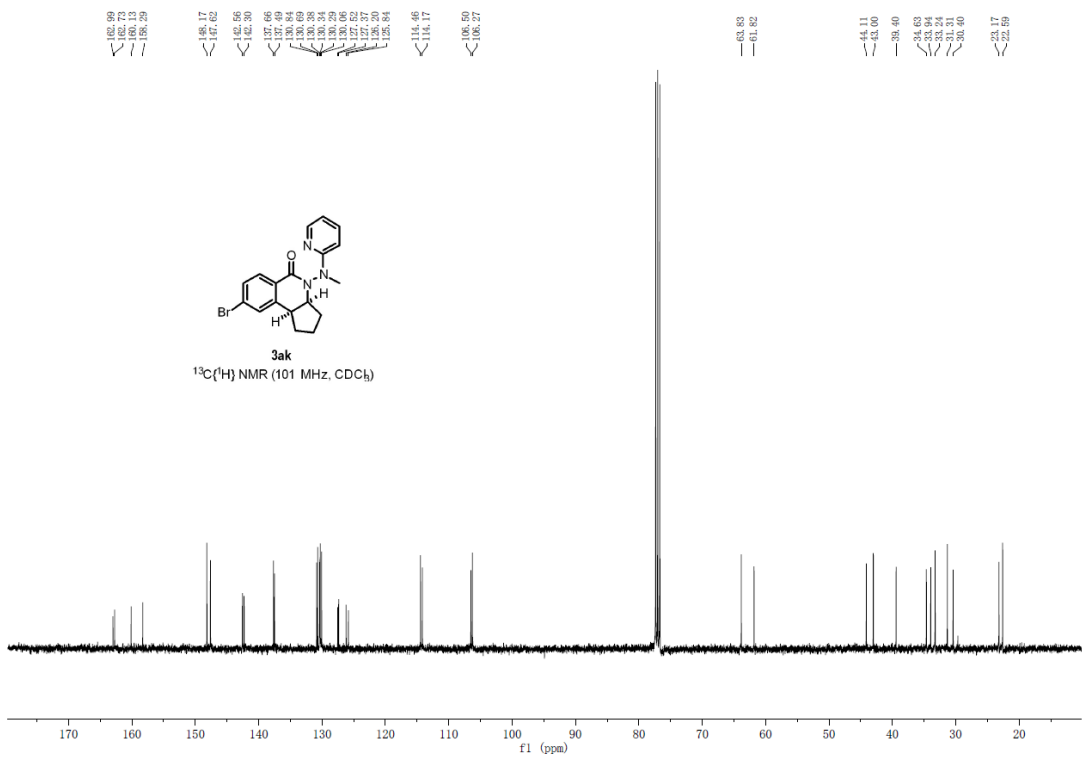


Figure S33. ^{13}C{^{1}H} NMR Spectrum of **3ak**

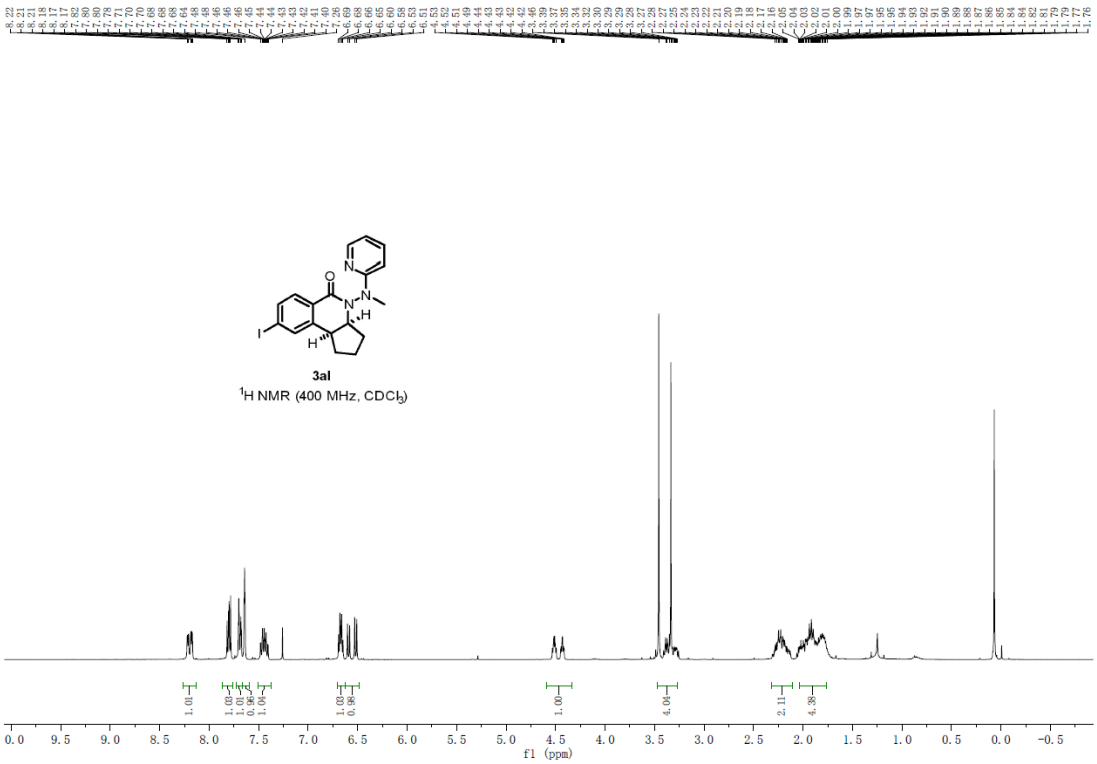


Figure S34. ^{1}H NMR Spectrum of **3al**

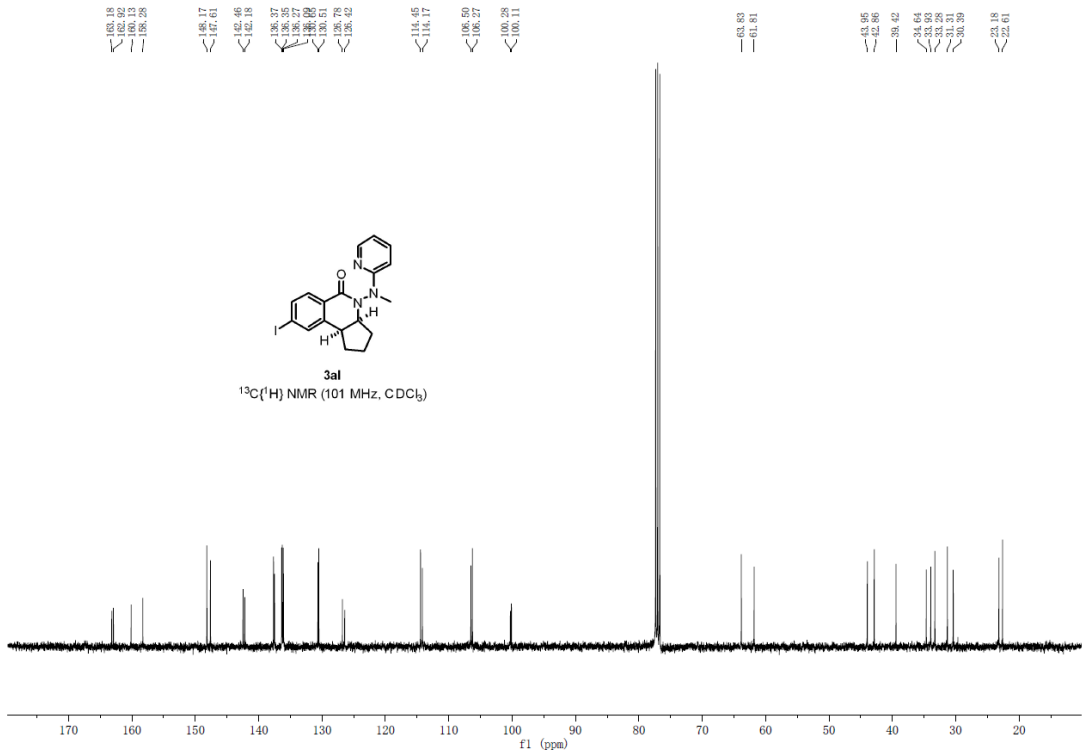


Figure S35. ^{13}C{^{1}H} NMR Spectrum of **3al**

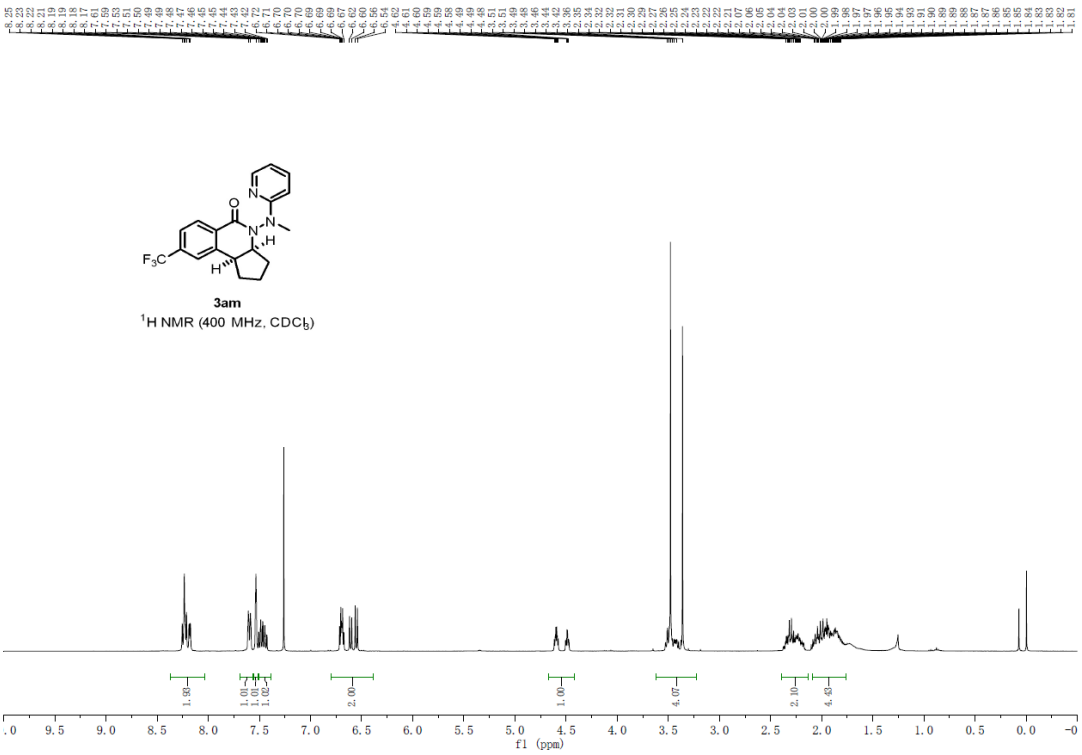


Figure S36. ^{1}H NMR Spectrum of **3am**

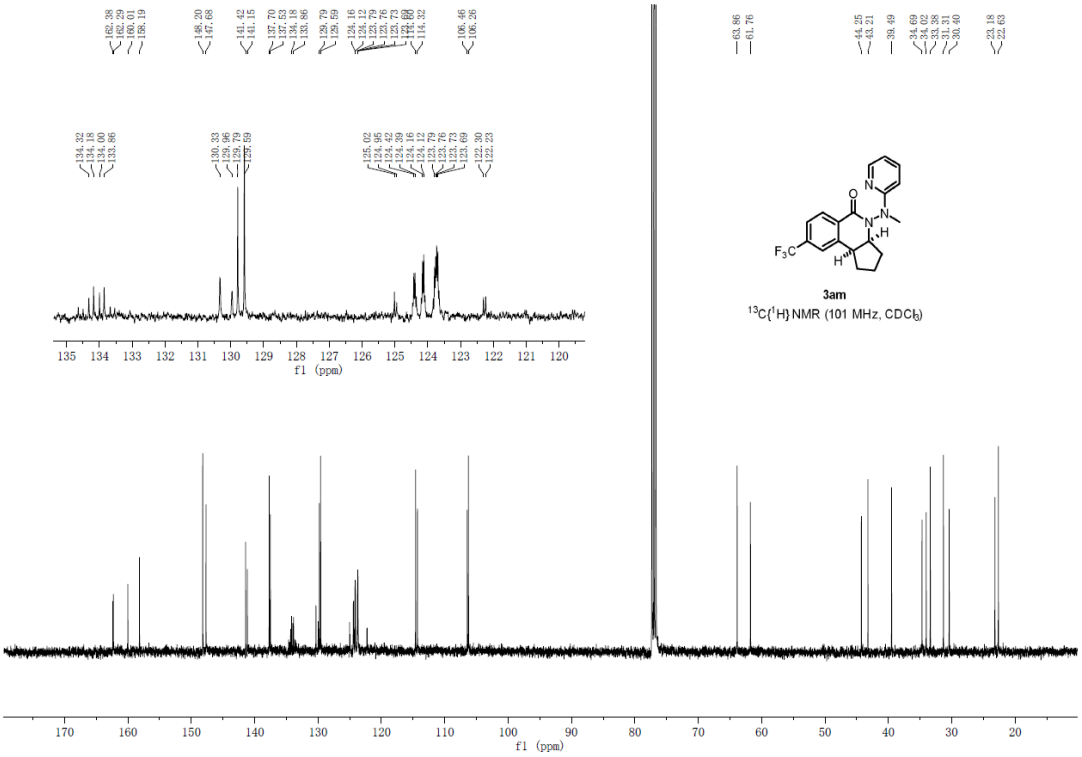


Figure S37. ^{13}C{^{1}H} NMR Spectrum of **3am**

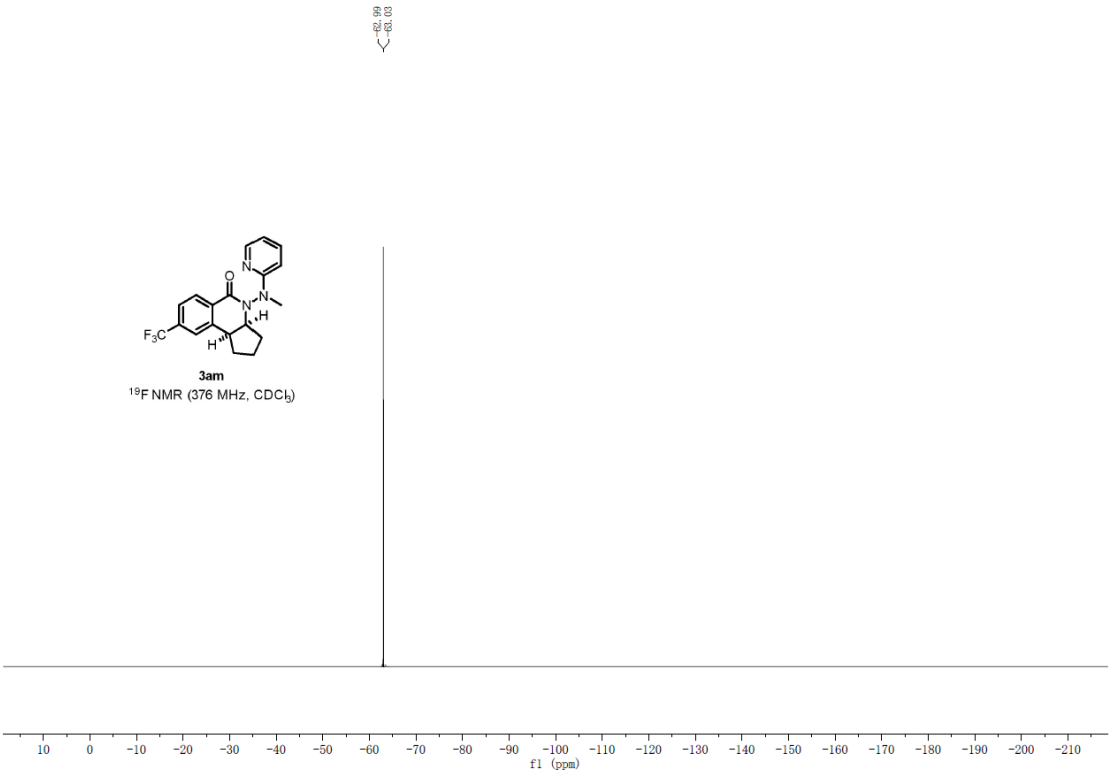


Figure S38. ^{19}F NMR Spectrum of **3am**

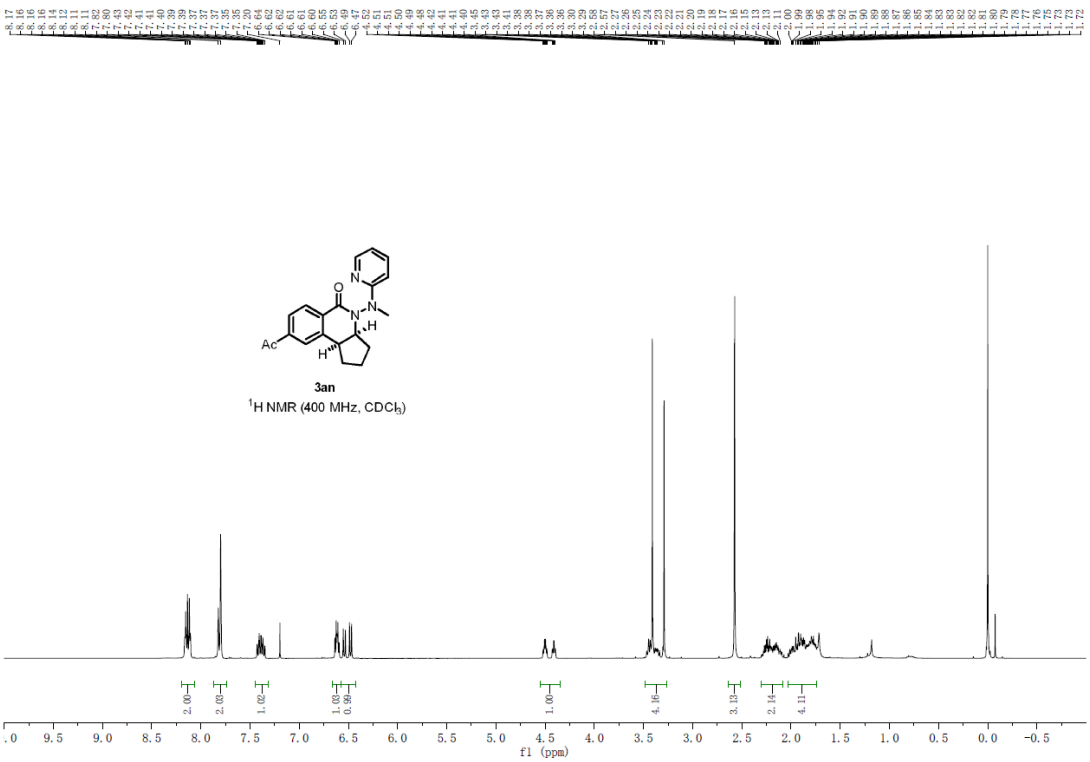


Figure S39. ^{1}H NMR Spectrum of **3an**

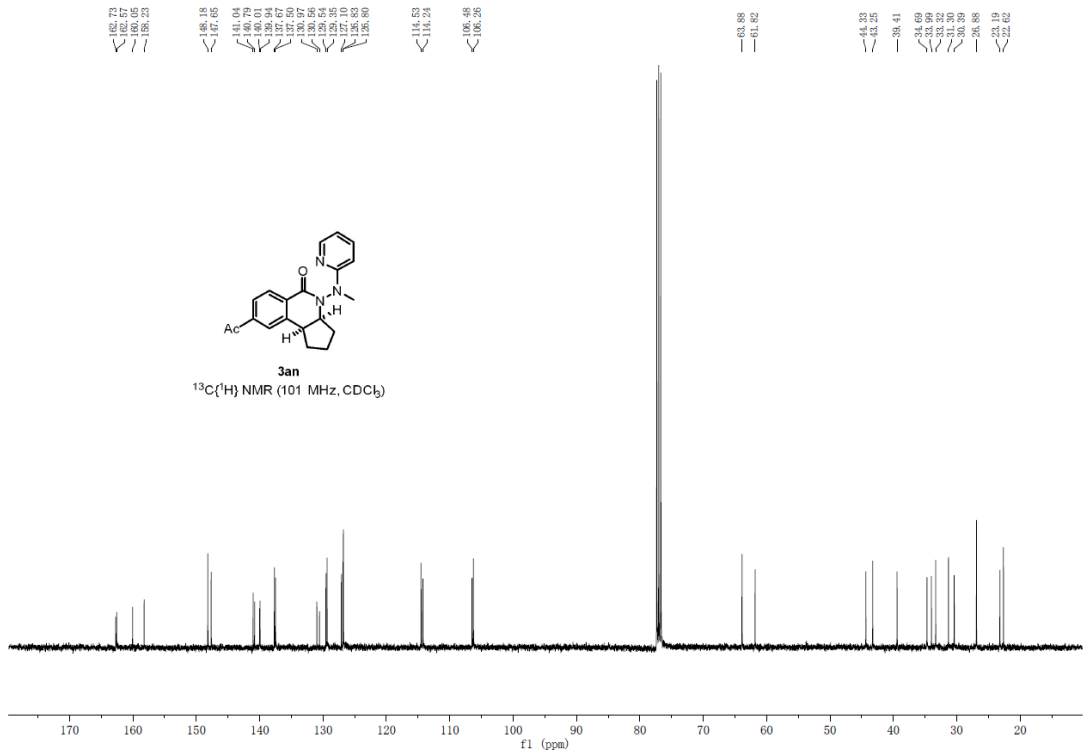


Figure S40. $^{13}C\{^{1}H\}$ NMR Spectrum of **3an**

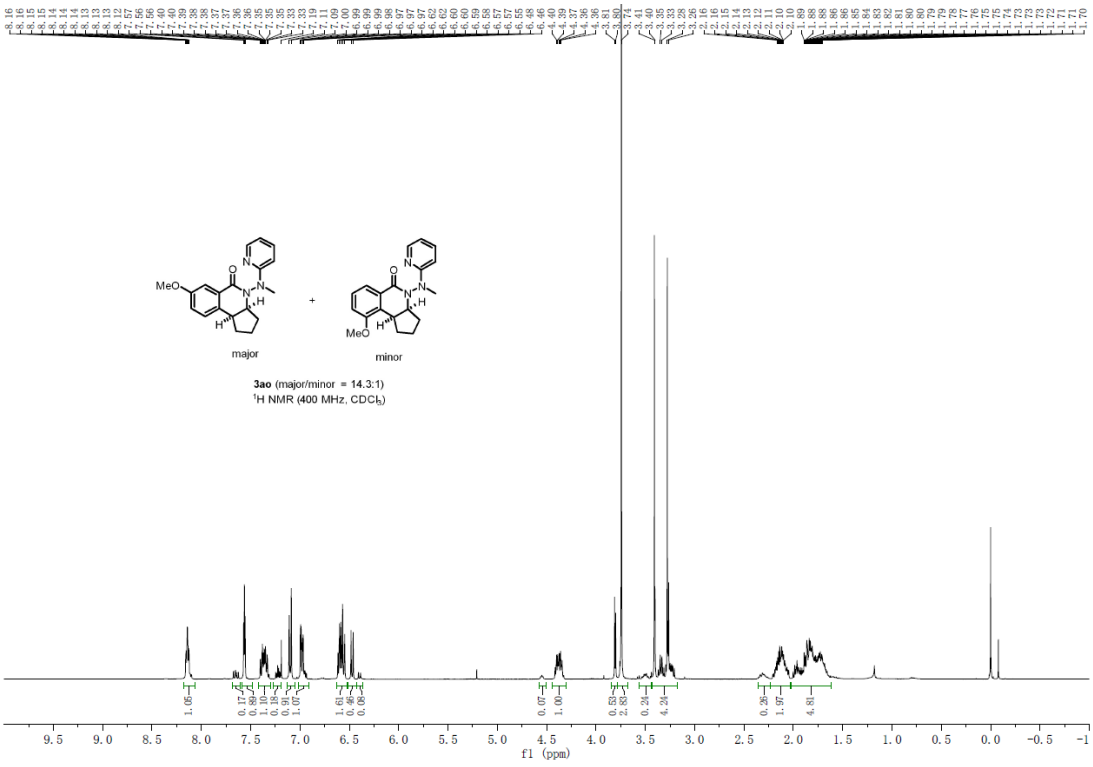


Figure S41. ^{1}H NMR Spectrum of **3ao**

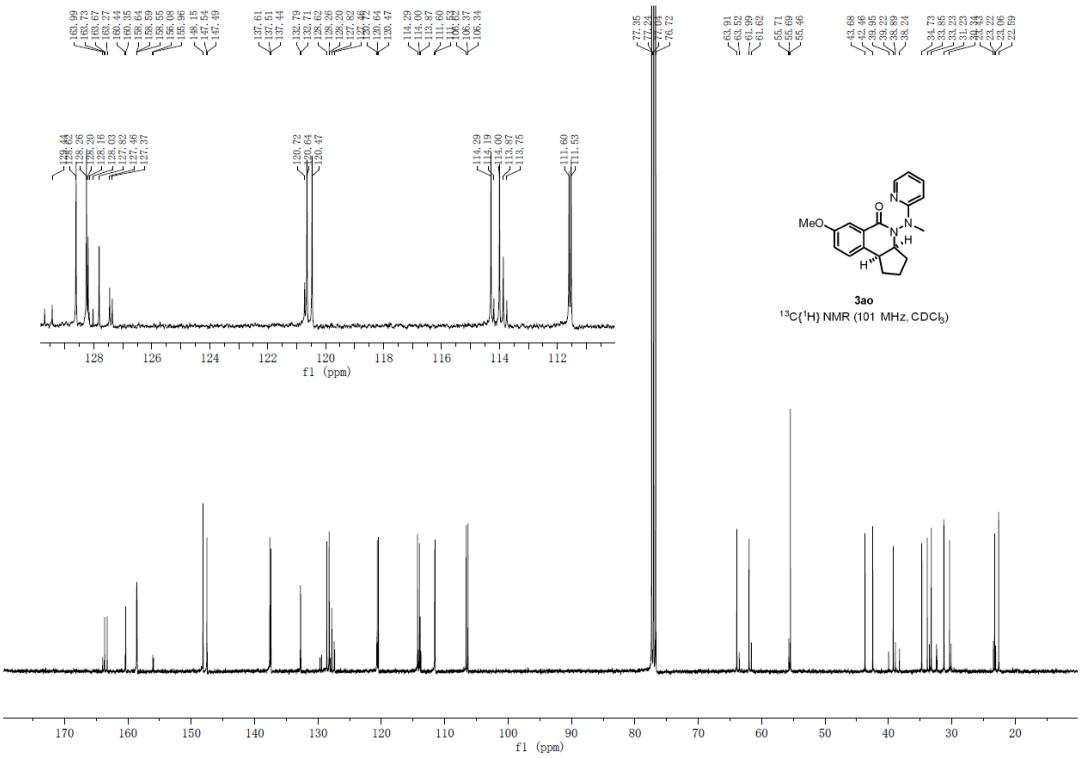


Figure S42. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ao**

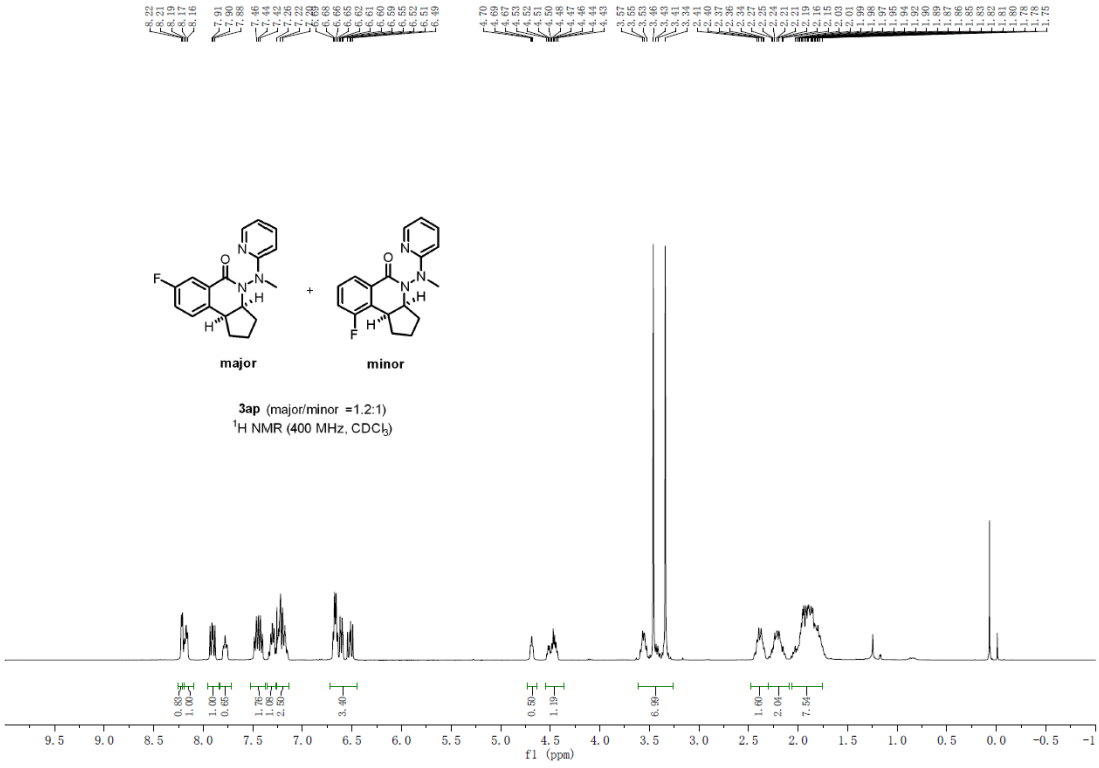


Figure S43. ^{1}H NMR Spectrum of **3ap**

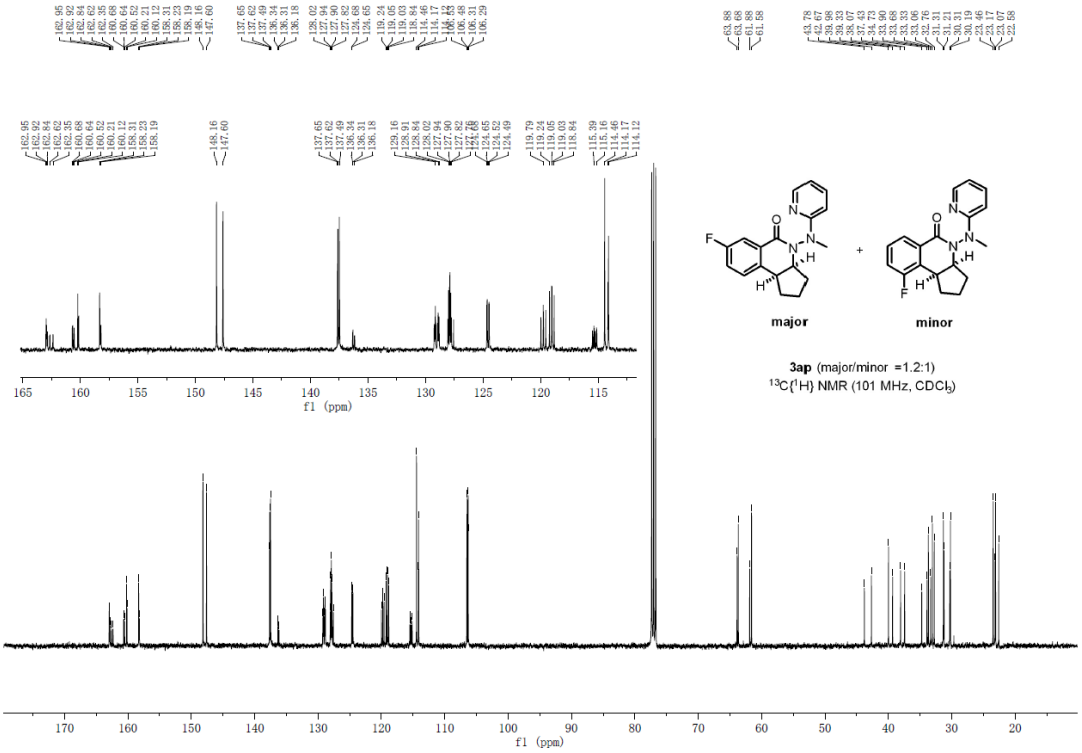


Figure S44. $^{13}C\{^{1}H\}$ NMR Spectrum of **3ap**

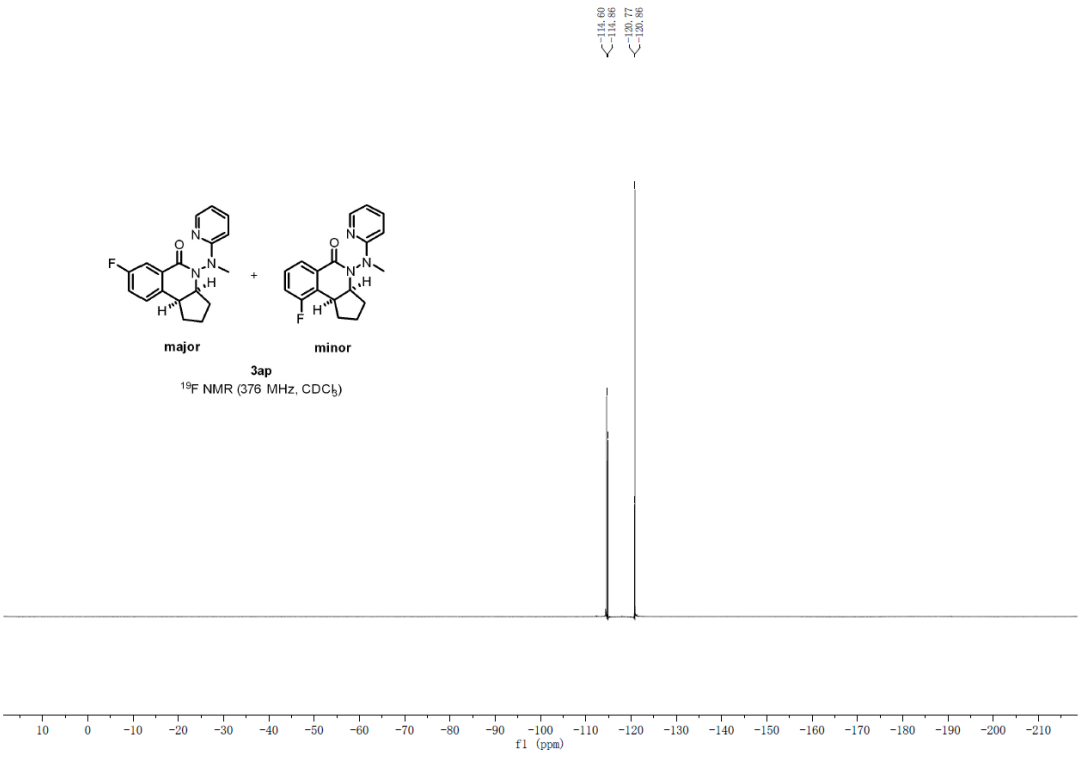


Figure S45. ^{19}F NMR Spectrum of **3ap**

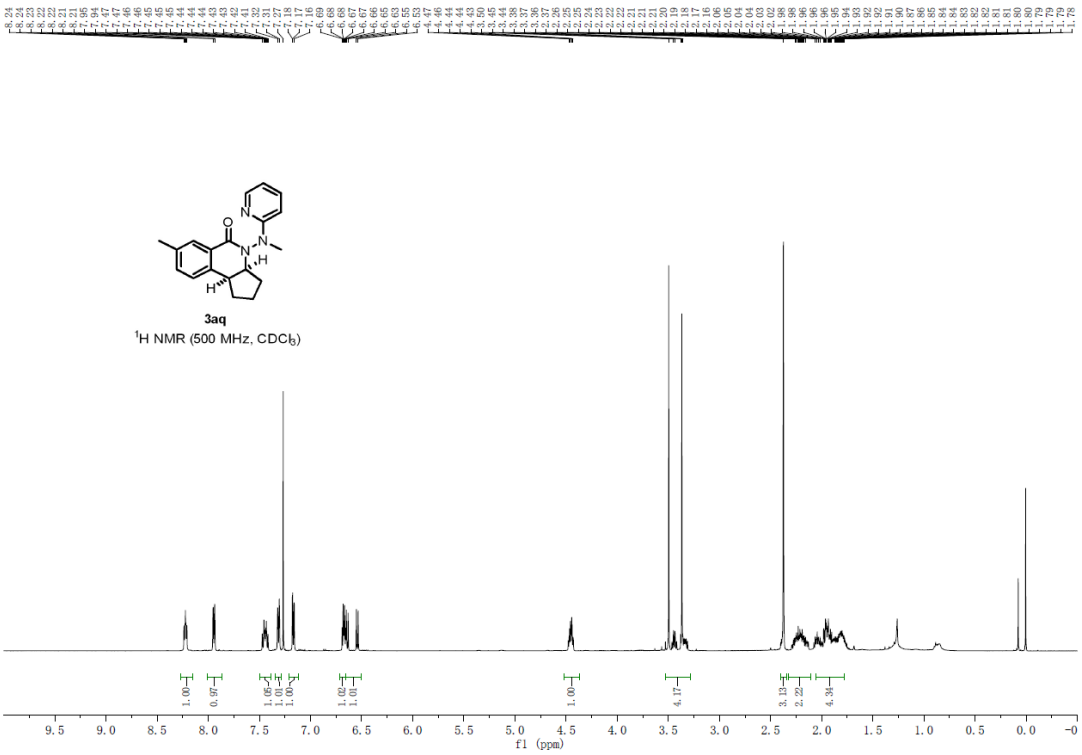


Figure S46. ^{1}H NMR Spectrum of **3aq**

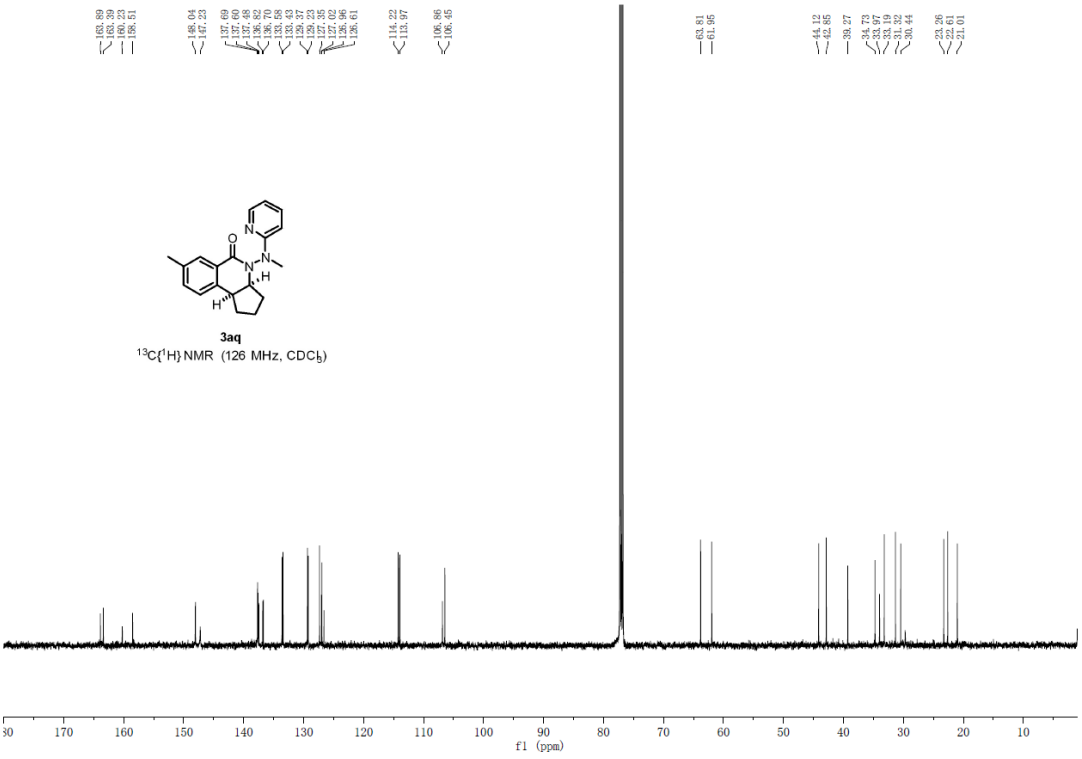


Figure S47. ^{13}C{^{1}H} NMR Spectrum of **3aq**

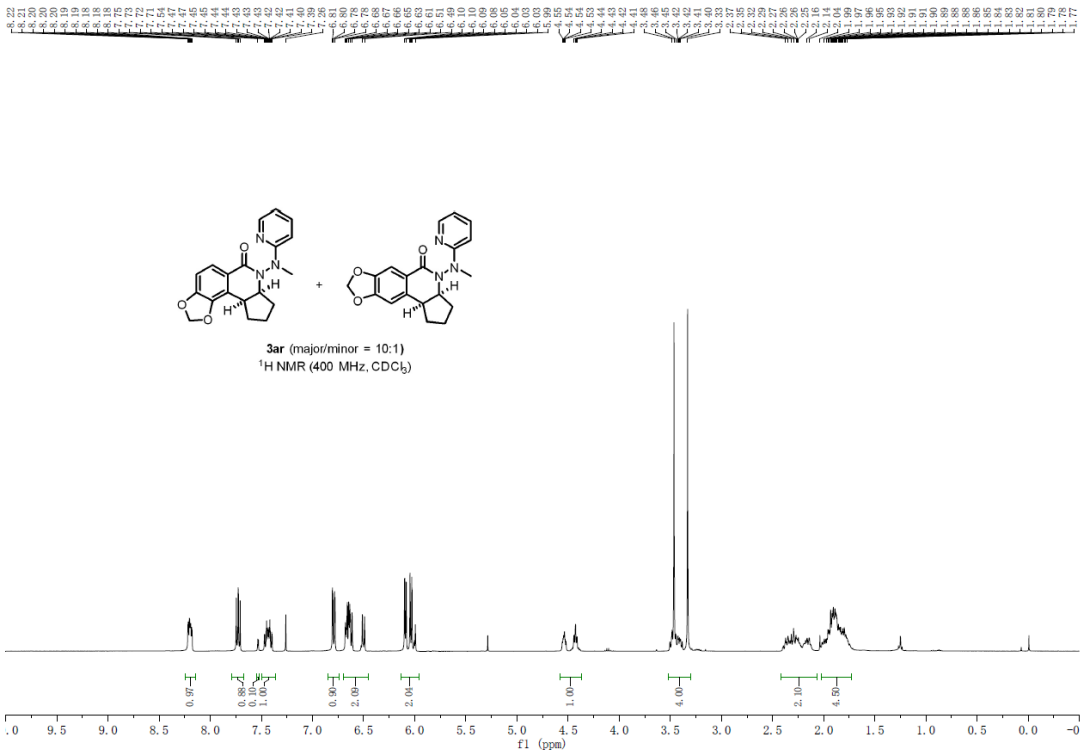


Figure S48. ^{1}H NMR Spectrum of **3ar**

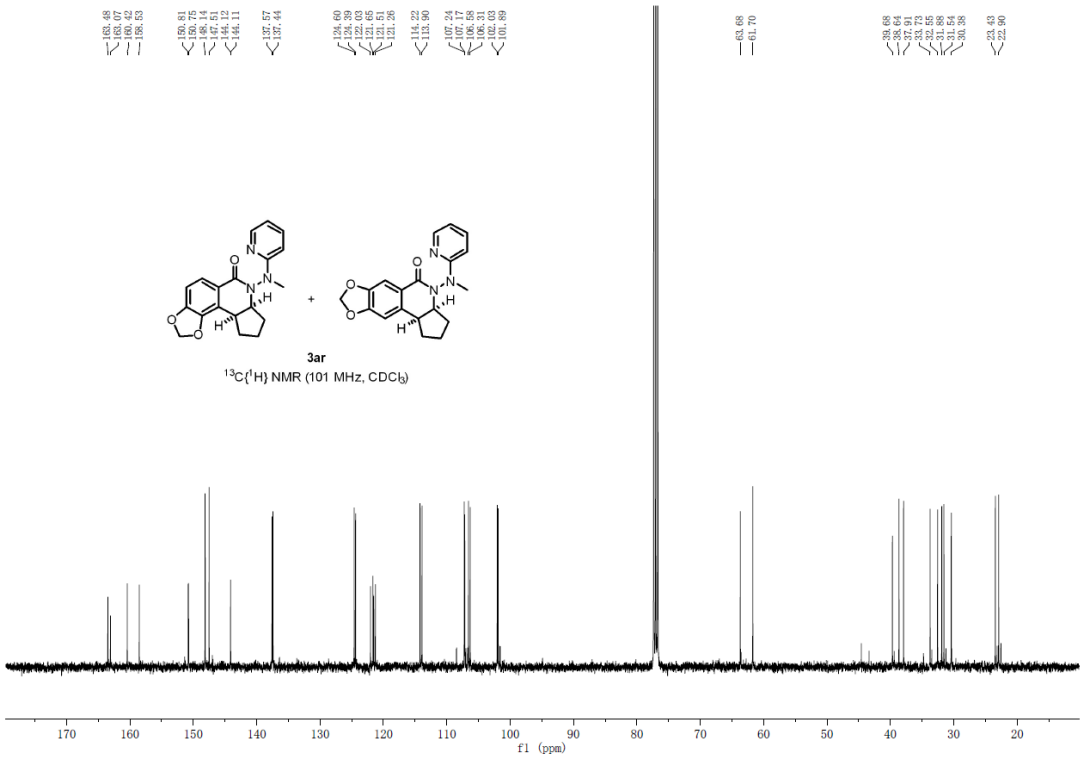


Figure S49. ^{13}C{^{1}H} NMR Spectrum of **3ar**

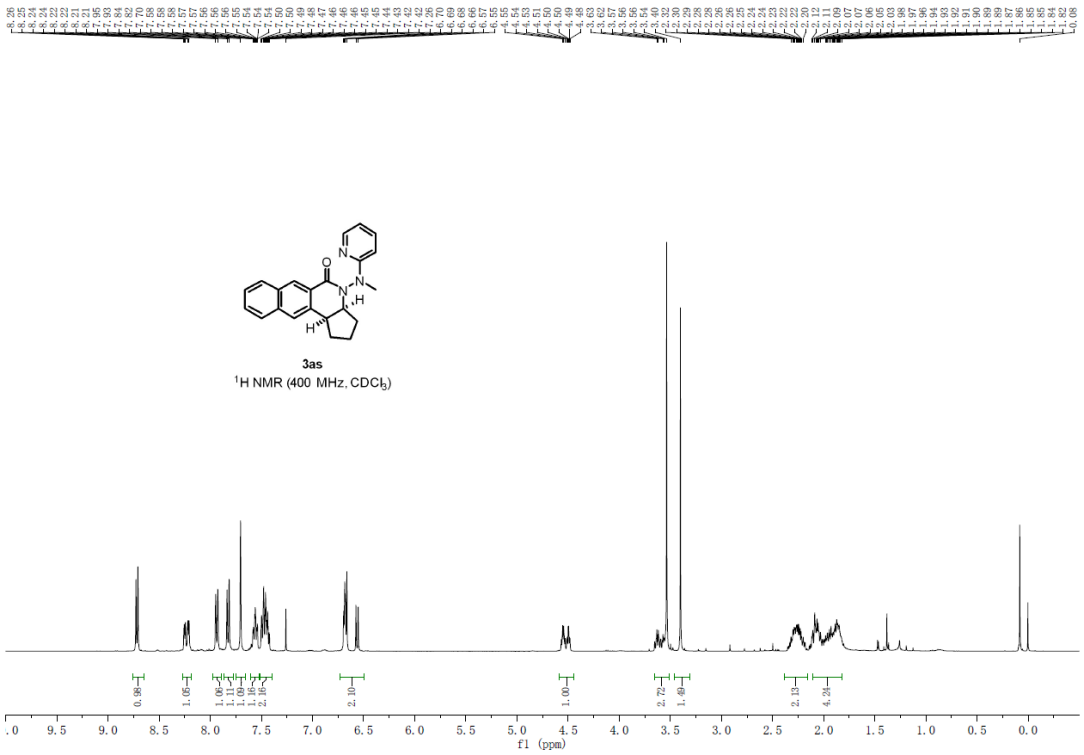


Figure S50. ^{1}H NMR Spectrum of **3as**

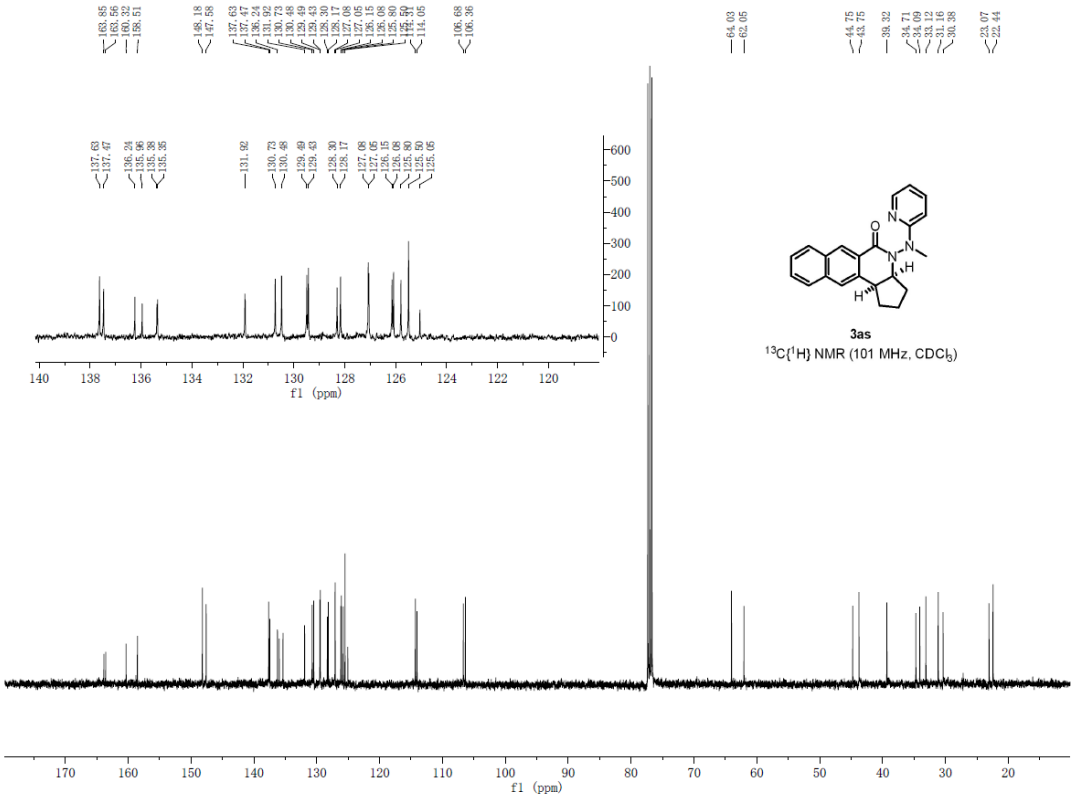


Figure S51. ^{13}C{^{1}H} NMR Spectrum of **3as**

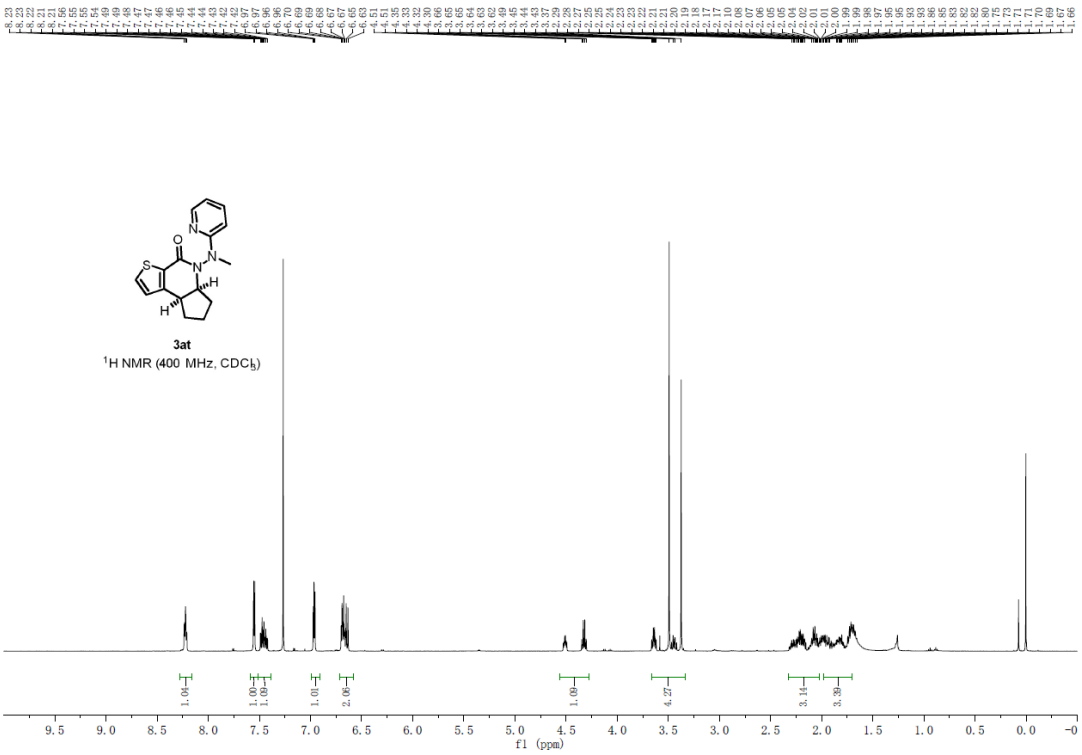


Figure S52. ^{1}H NMR Spectrum of **3at**

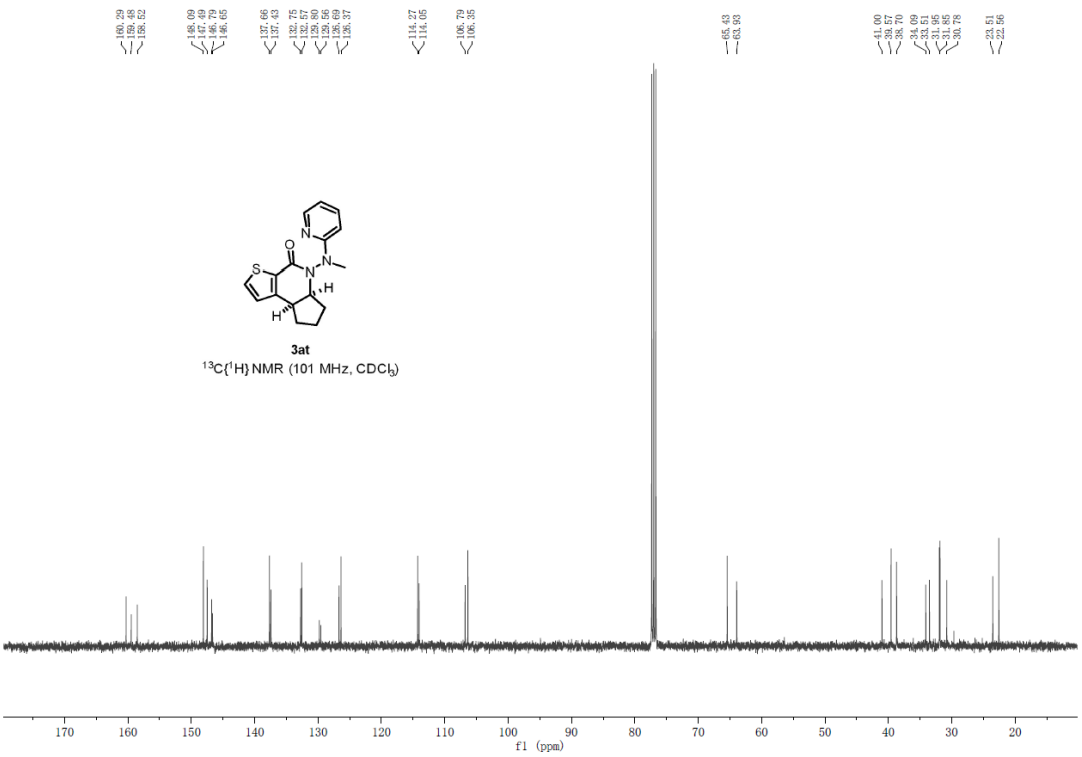


Figure S53. ^{13}C{^{1}H} NMR Spectrum of **3at**

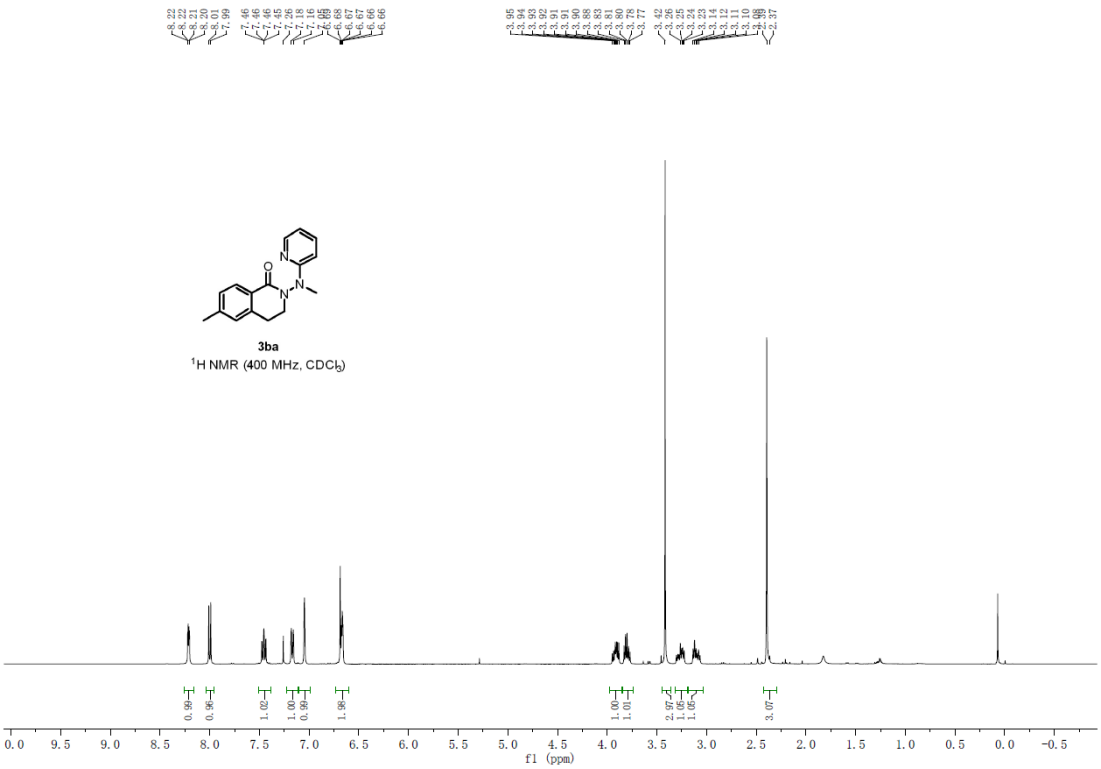


Figure S54. ^{1}H NMR Spectrum of **3ba**

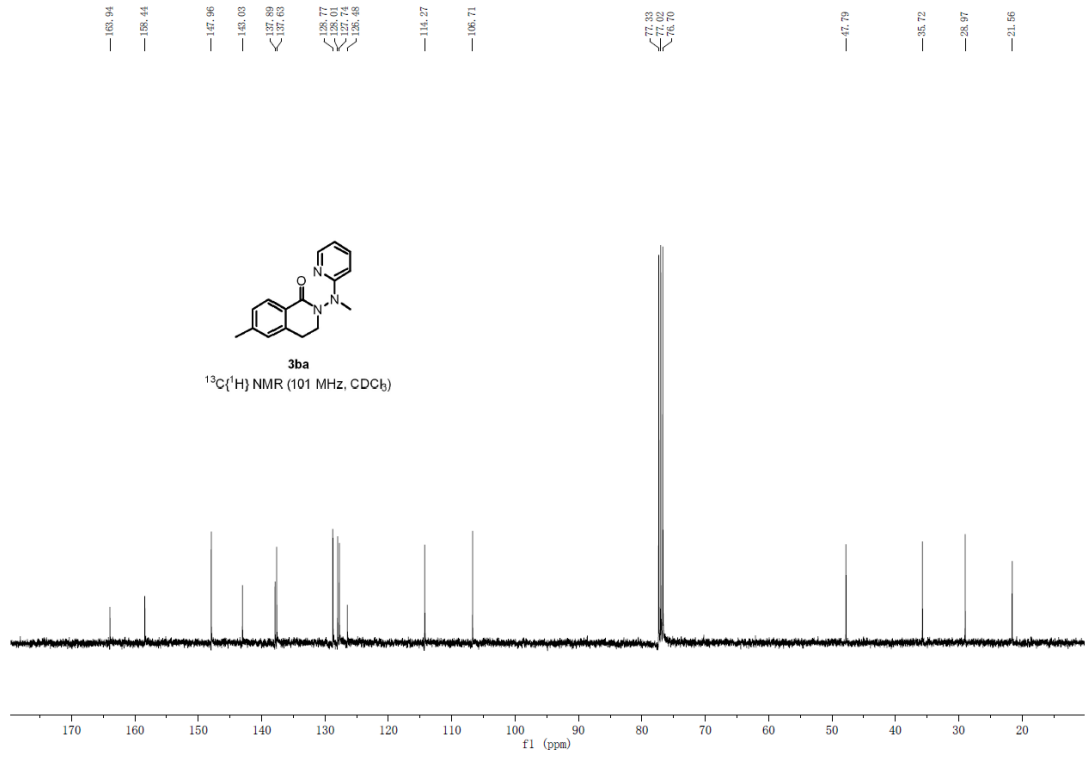


Figure S55. ^{13}C{^{1}H} NMR Spectrum of **3ba**

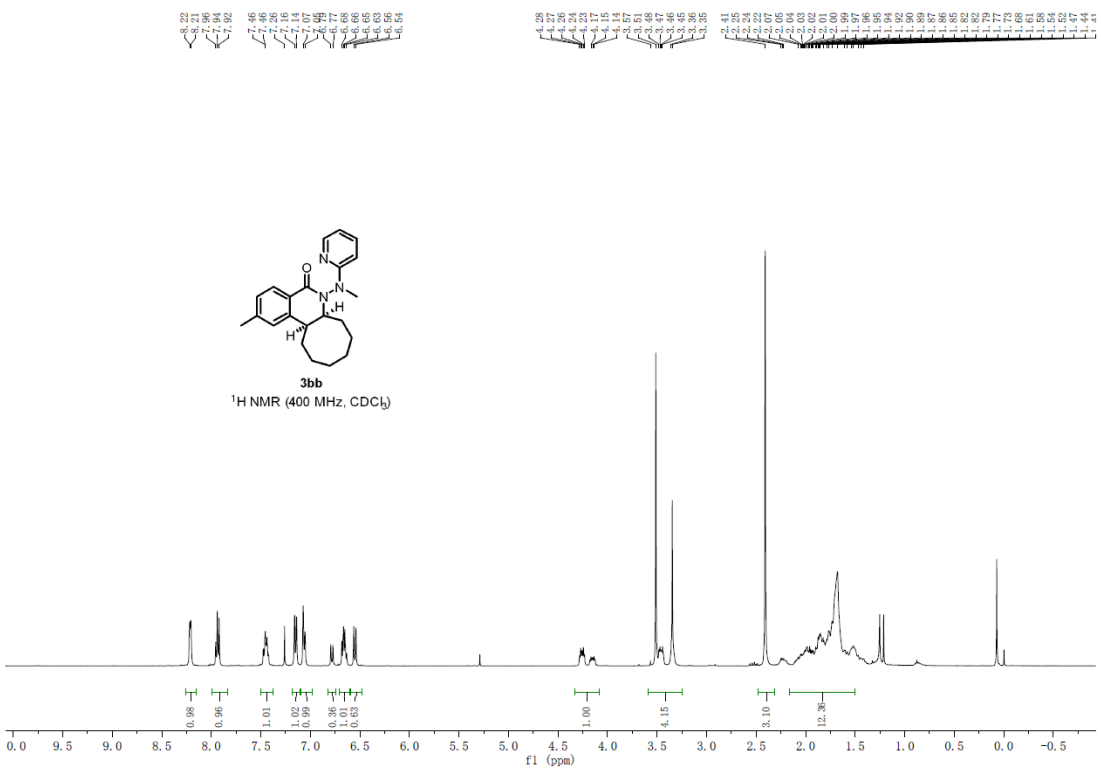


Figure S56. ^{1}H NMR Spectrum of **3bb**

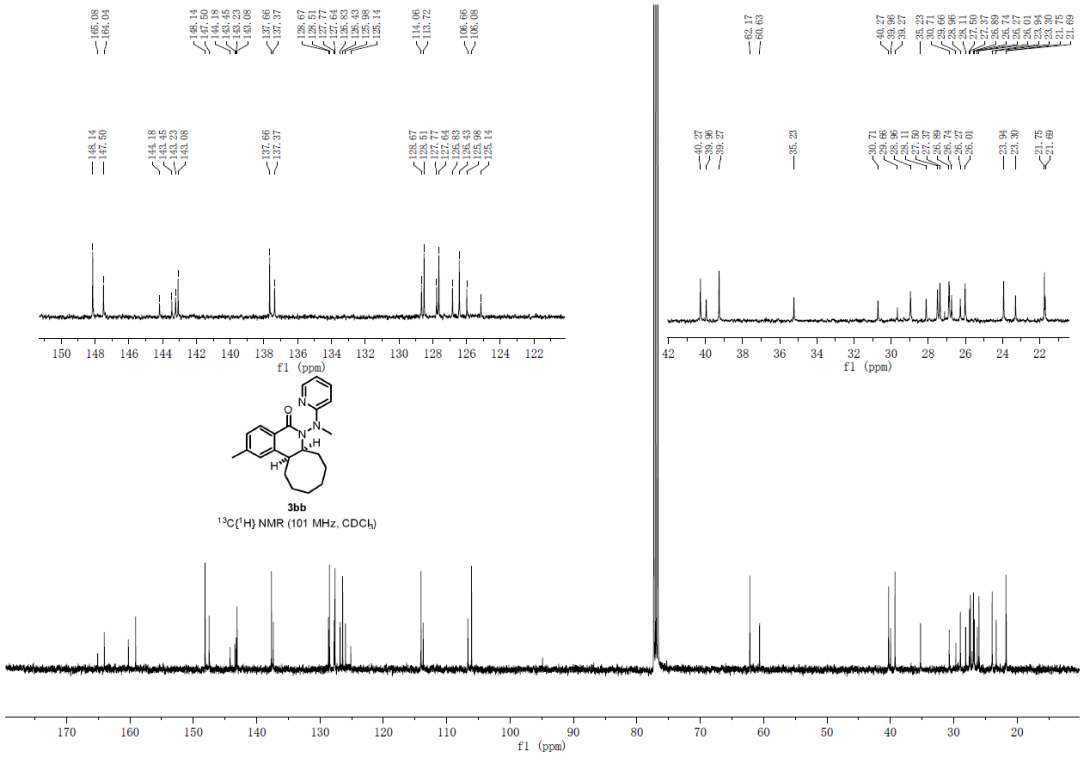
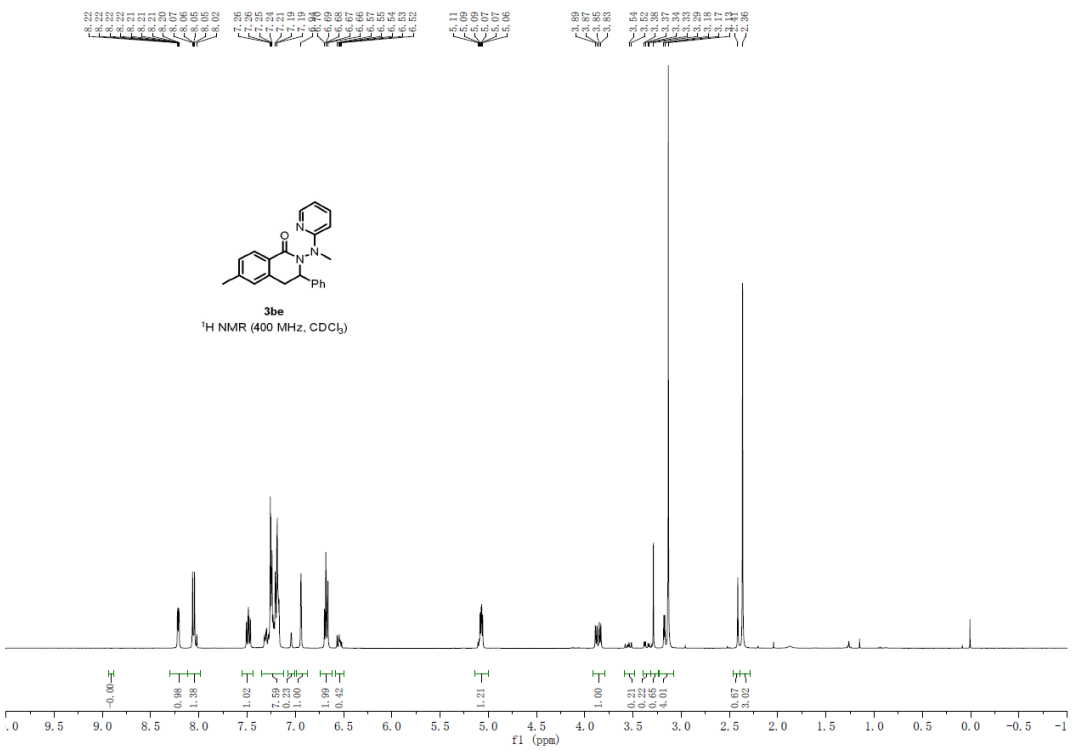


Figure S57. ^{13}C{^{1}H} NMR Spectrum of **3bb**



***** The doubled peaks in ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR of **3be-3bi** was proven to be atropisomer rised by restricted rotation of the MHP, which were confirmed by HSQC and HMBC. (see Figure S61 and Figure S62). And cleavage of the MHP gave a single compound **5**. Both ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR of **5** indicate only one product was obtained (see Figure S63 and Figure S64).

Figure S58. ^{1}H NMR Spectrum of **3be**

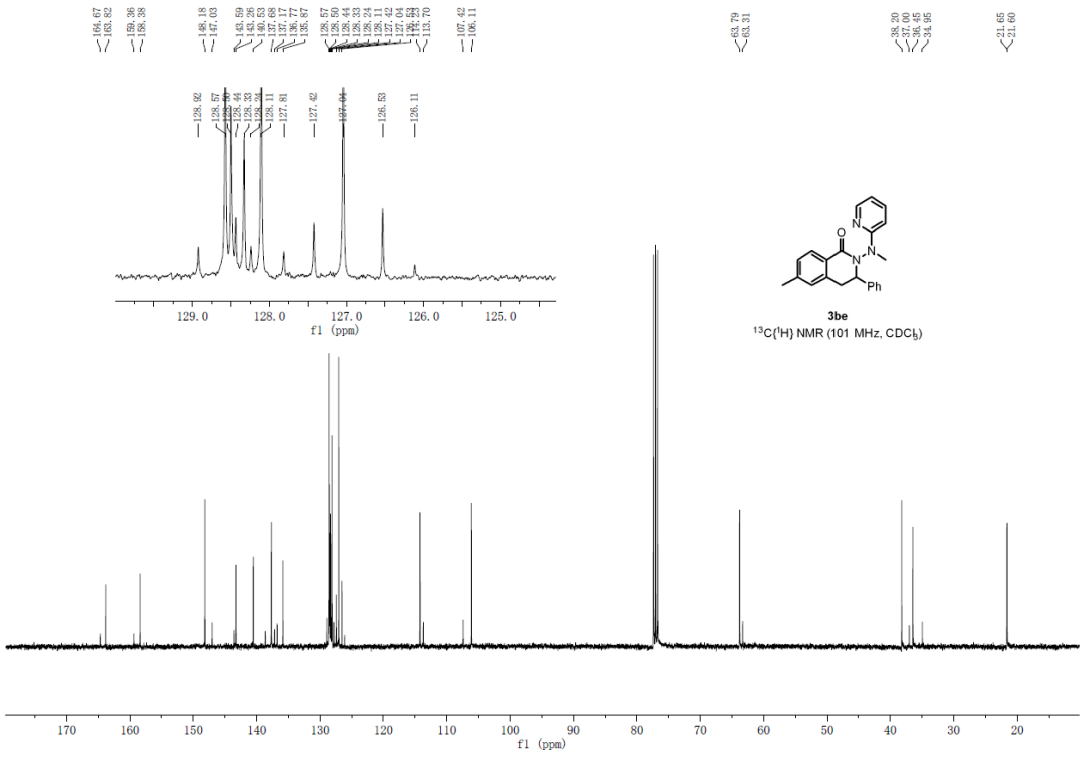


Figure S59. $^{13}C\{^{1}H\}$ NMR Spectrum of **3be**

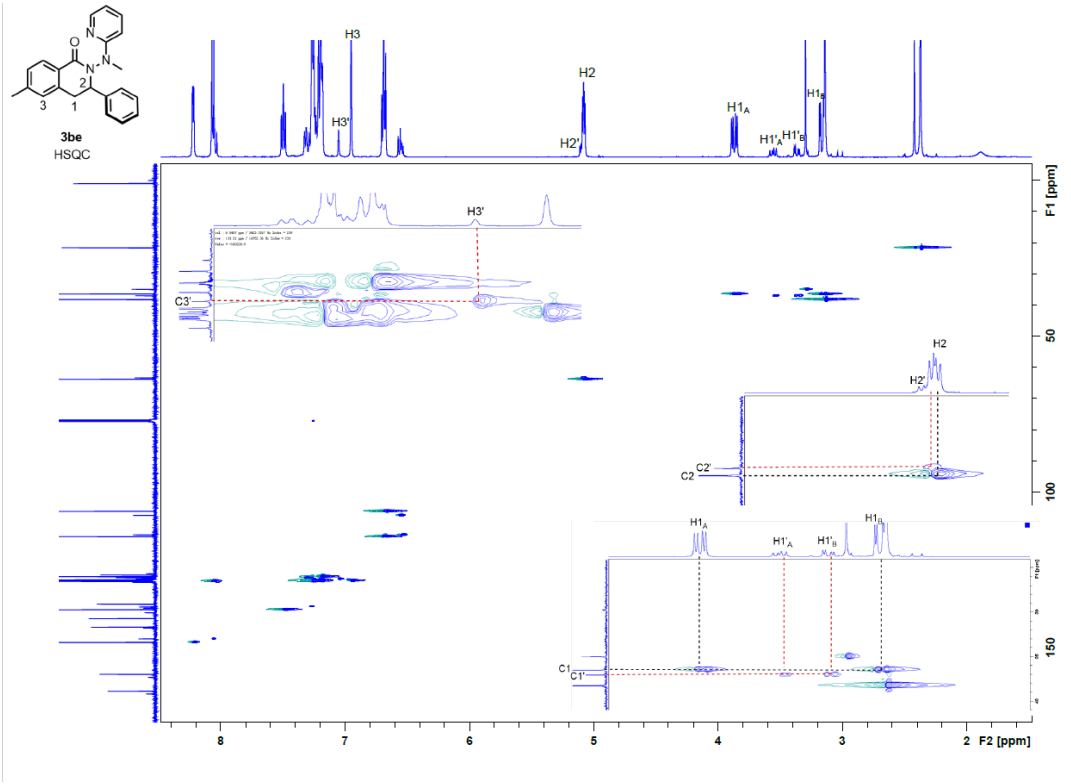


Figure S60. Heteronuclear Single Quantum Coherence (HSQC) Spectrum of **3be**

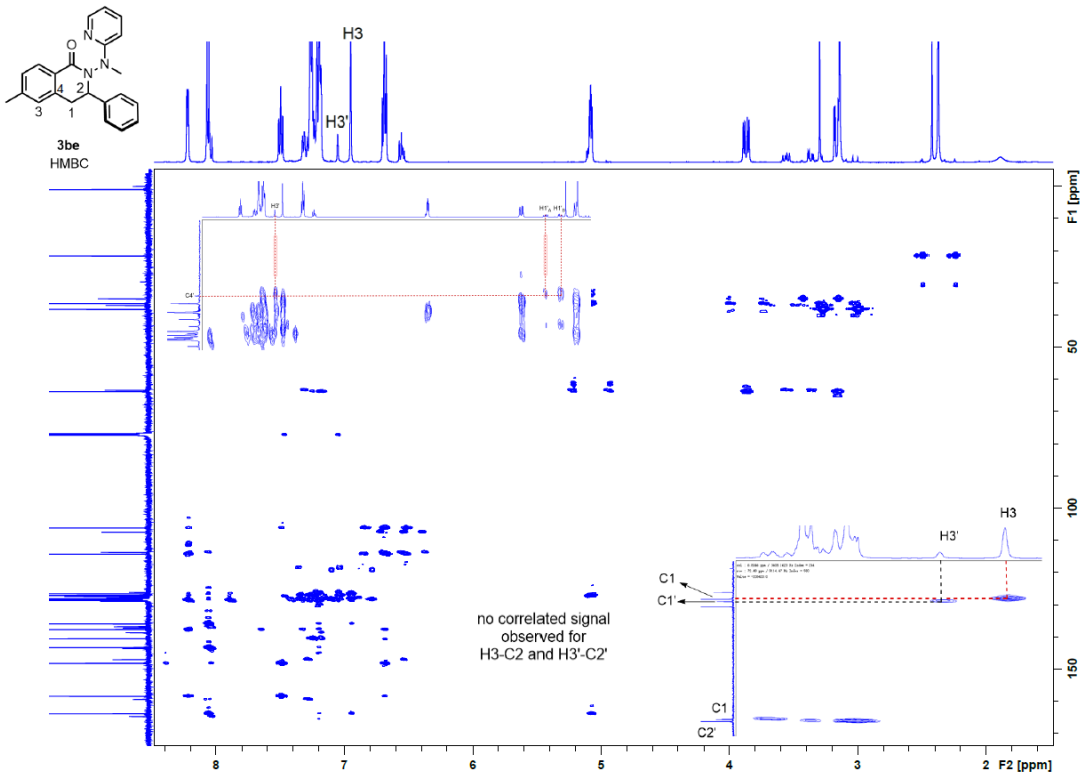


Figure S61. Heteronuclear Multiple Quantum Coherence (HMBC) Spectrum of **3be**

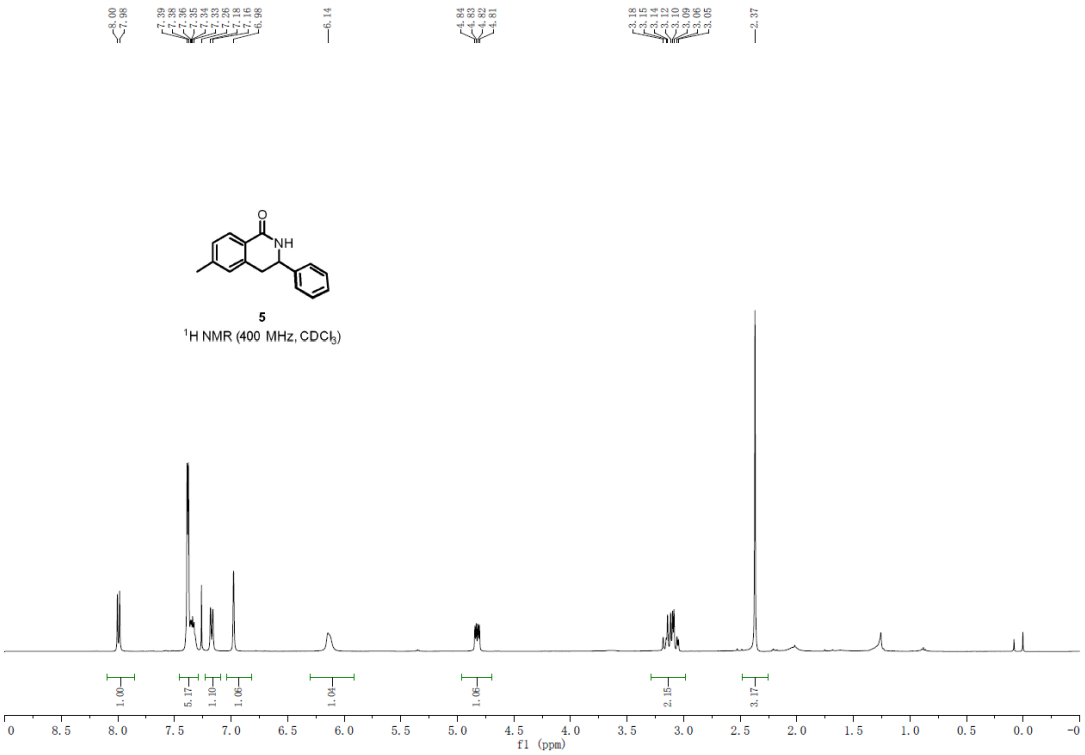


Figure S62. ^{1}H NMR Spectrum of **5**

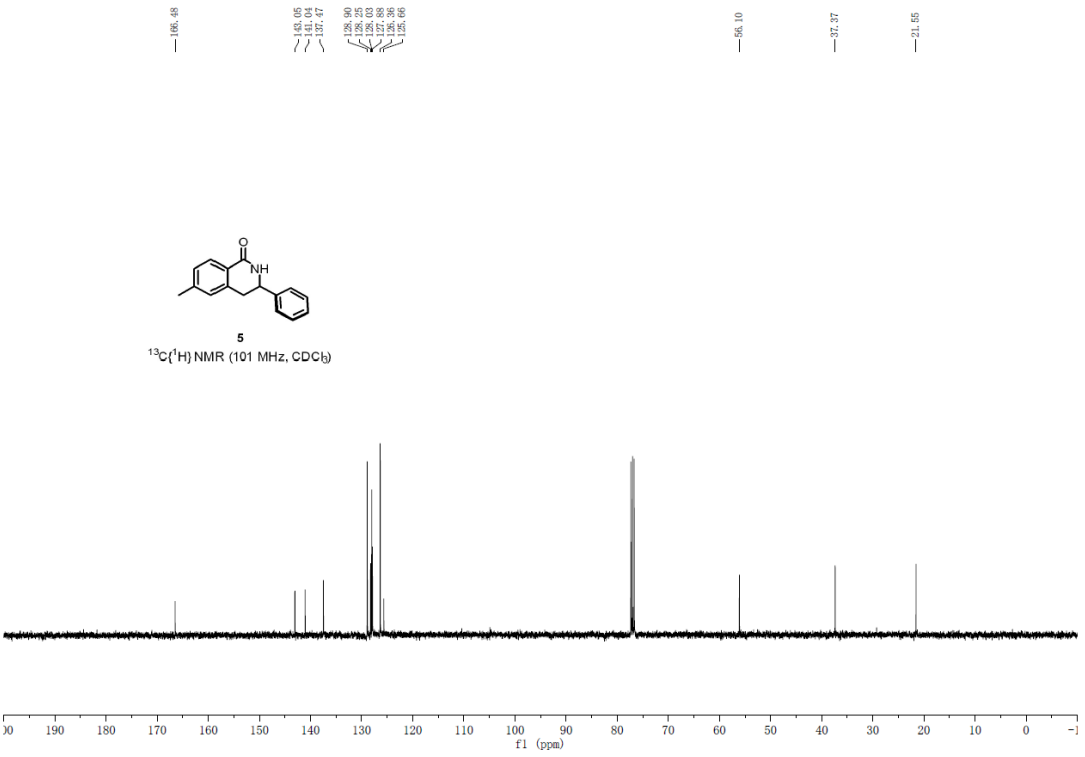


Figure S63. ^{13}C{^{1}H} NMR Spectrum of **5**

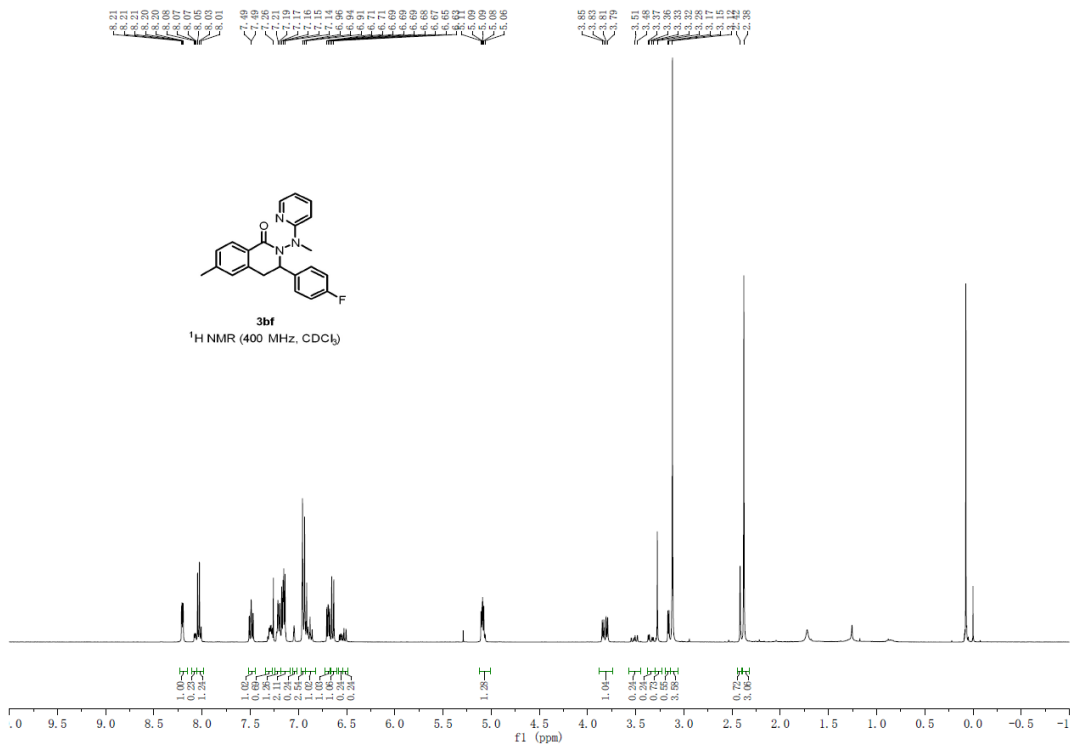


Figure S64. ^{1}H NMR Spectrum of **3bf**

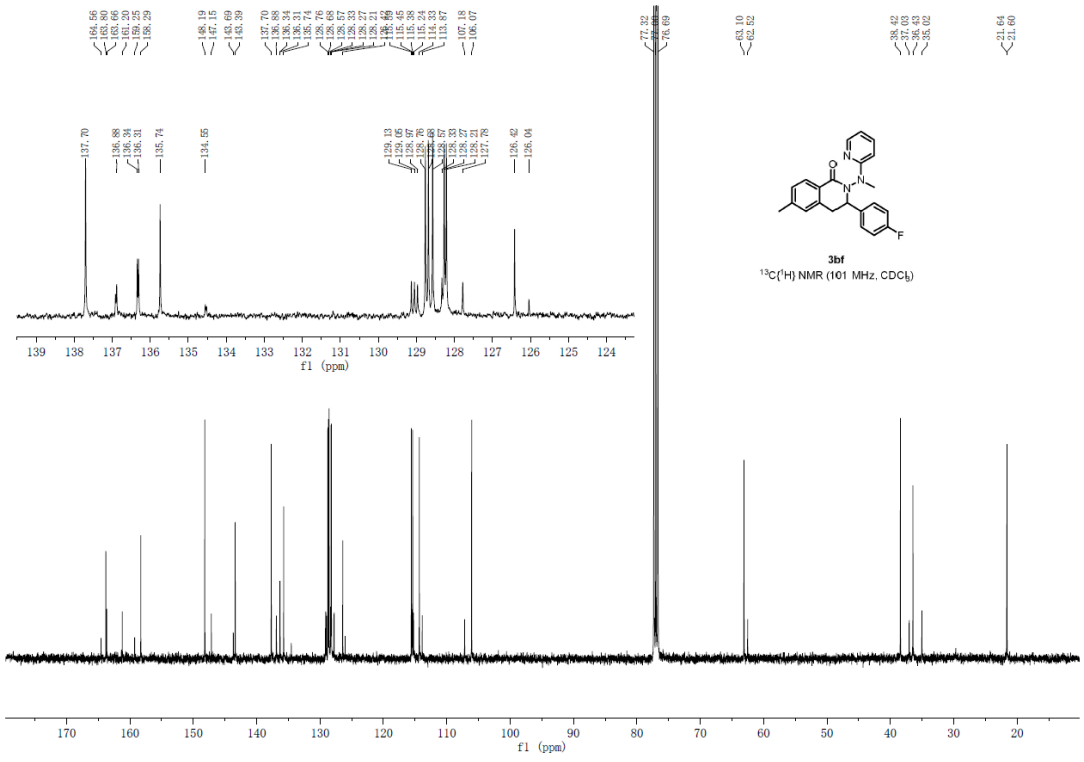


Figure S65. ^{13}C{^{1}H} NMR Spectrum of **3bf**

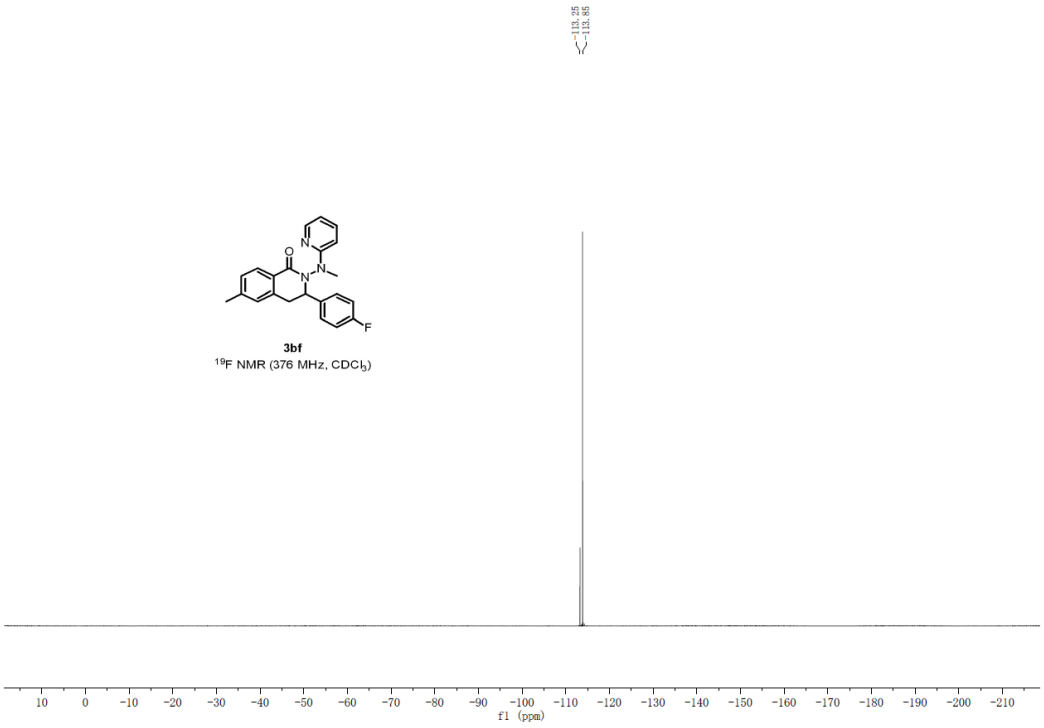


Figure S66. ^{19}F NMR Spectrum of **3bf**

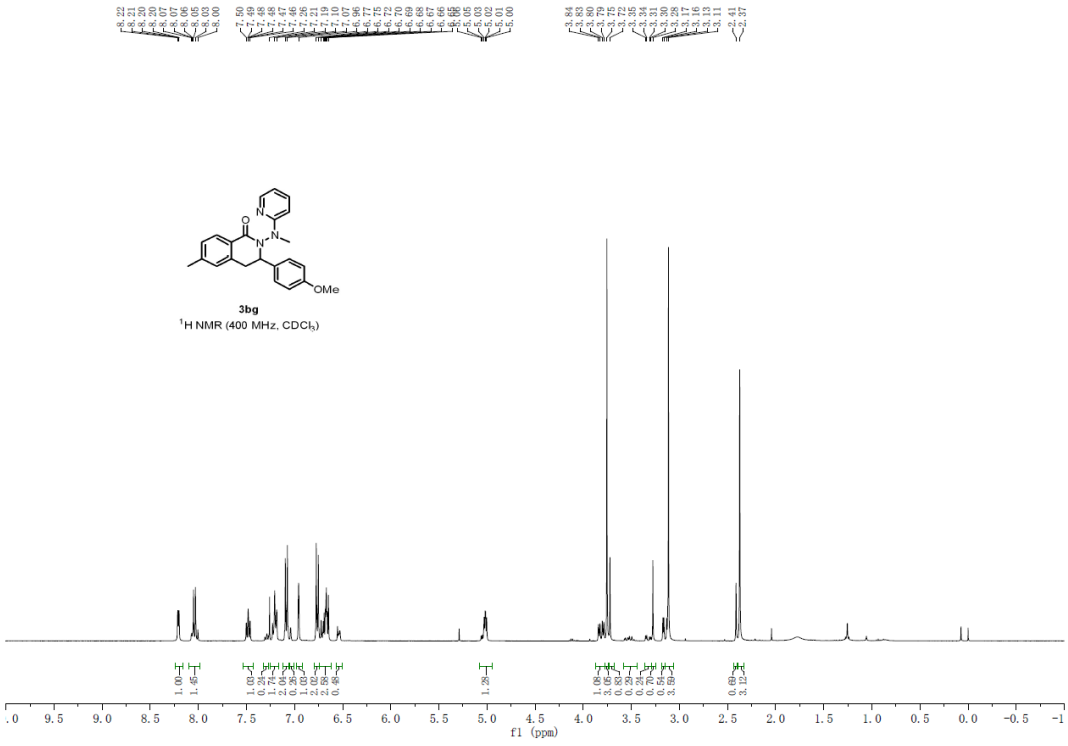


Figure S67. ^{1}H NMR Spectrum of **3bg**

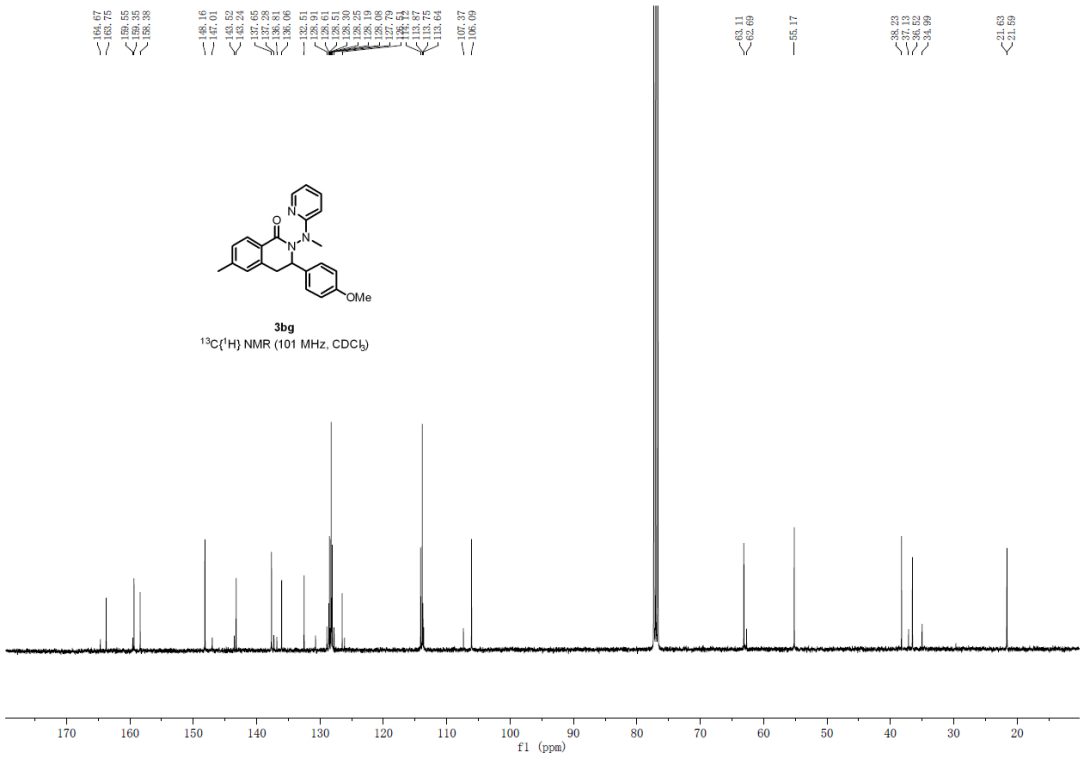


Figure S68. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bg**

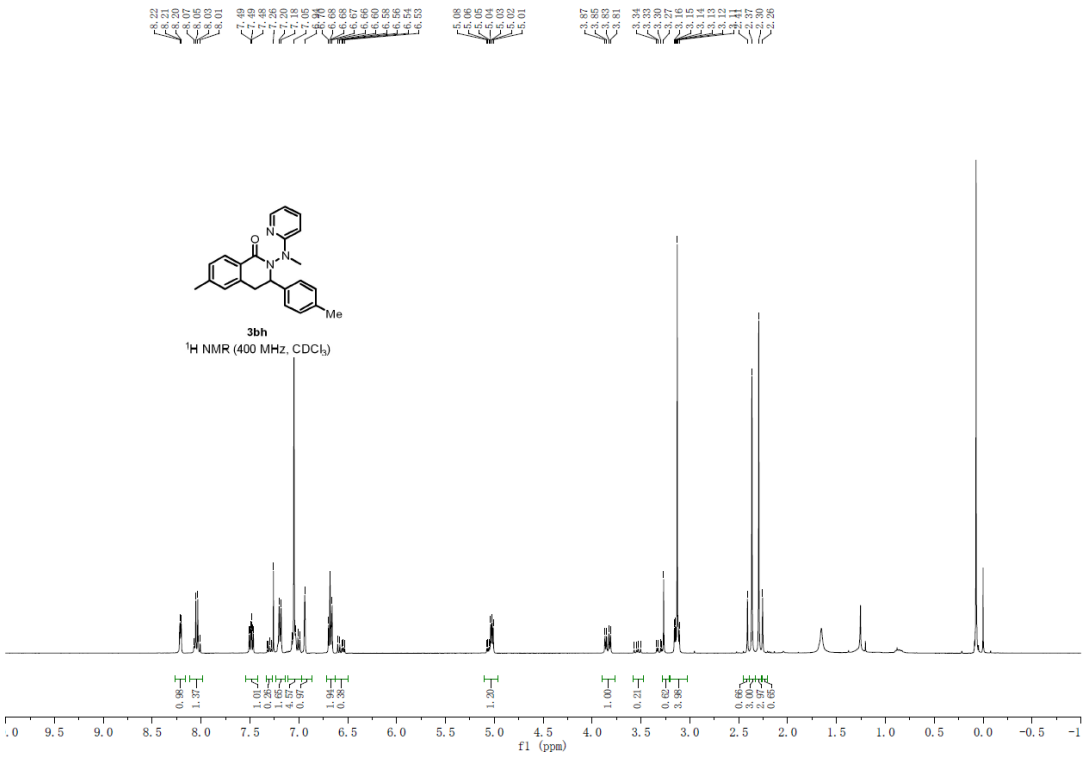


Figure S69. ^{1}H NMR Spectrum of **3bh**

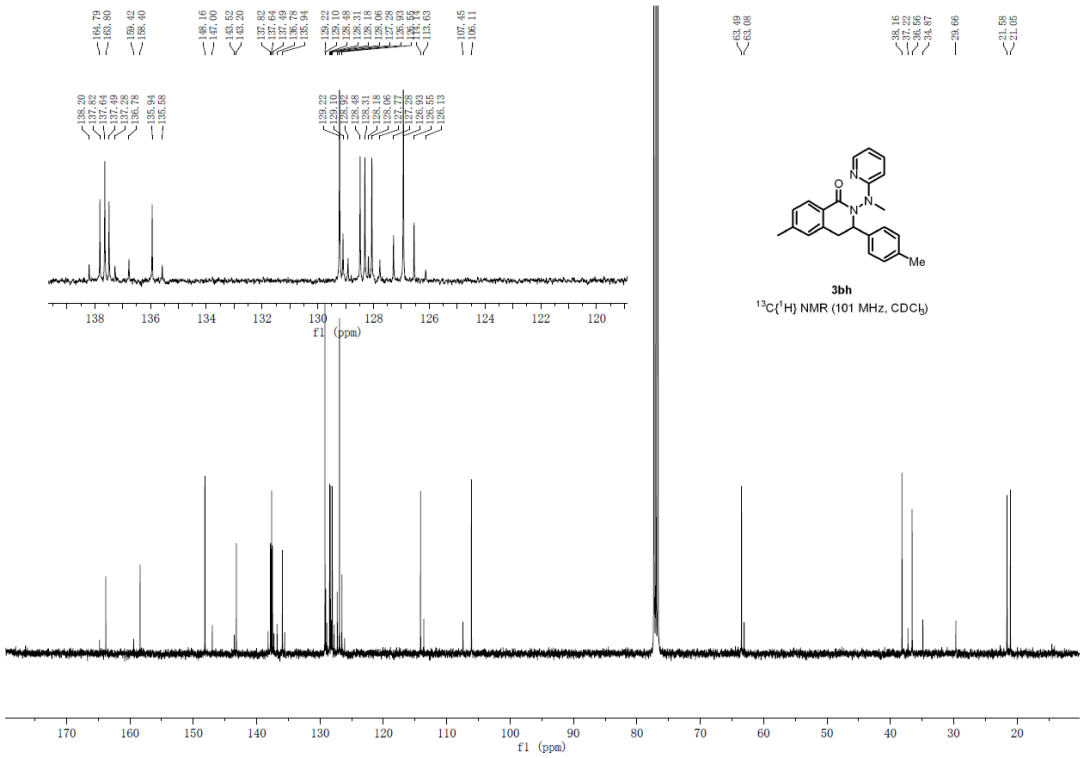


Figure S70. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bh**

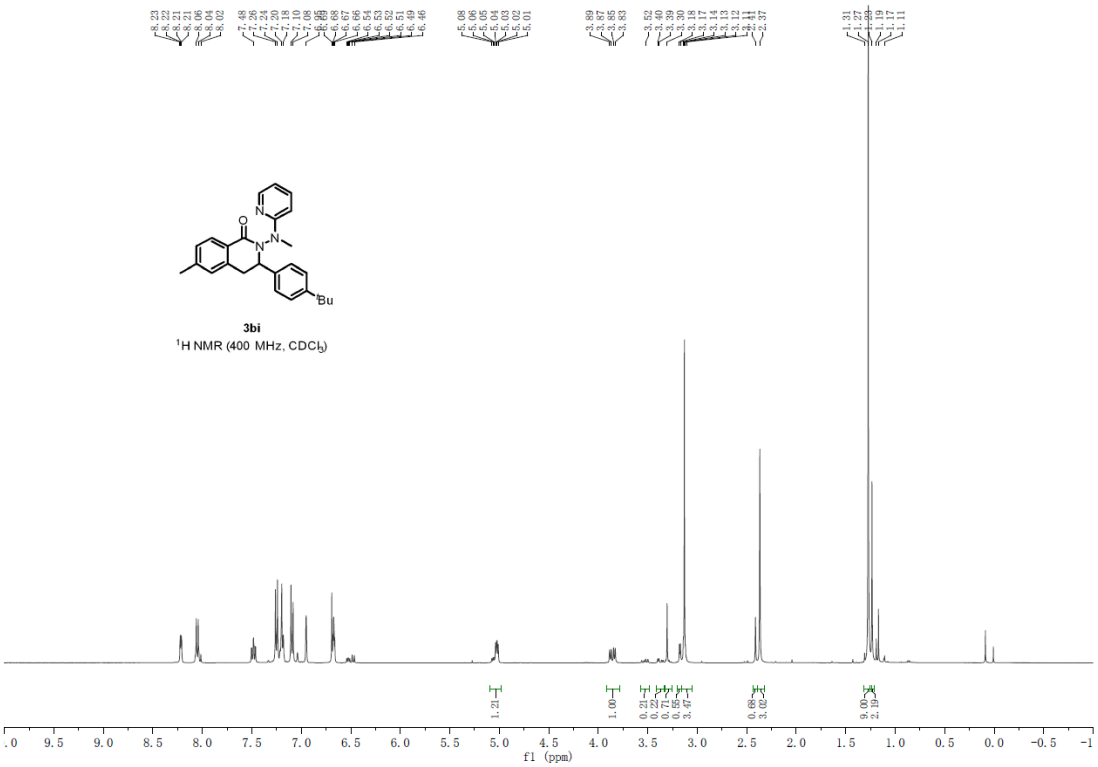


Figure S71. ^{1}H NMR Spectrum of **3bi**

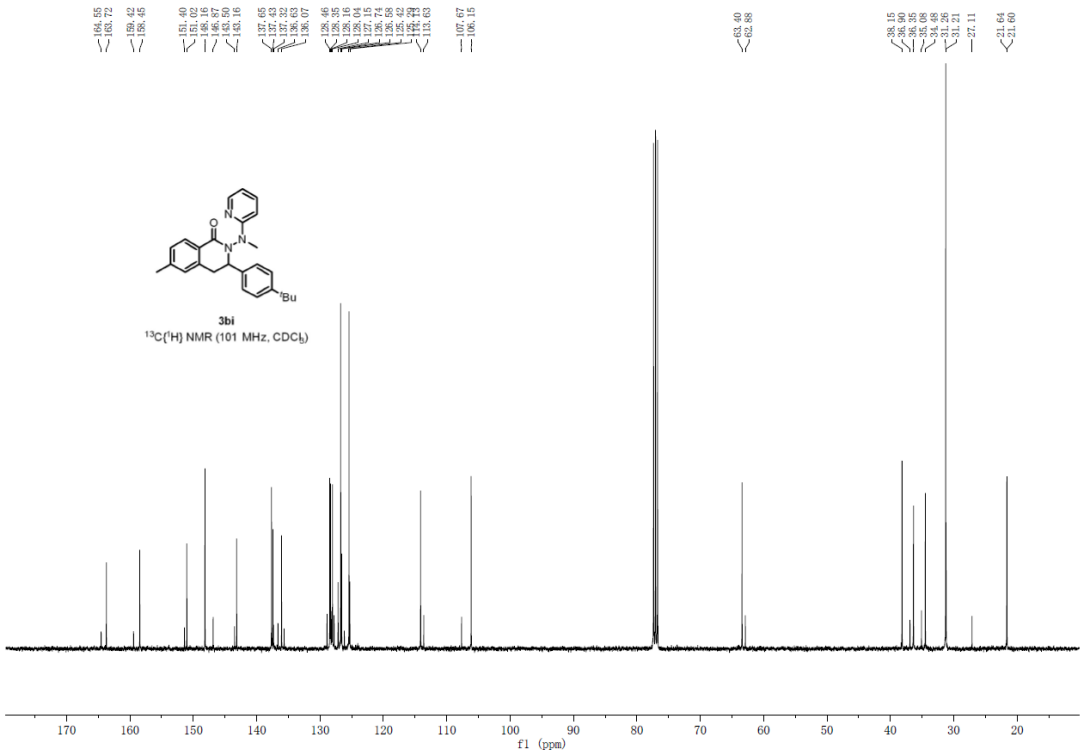


Figure S72. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bi**

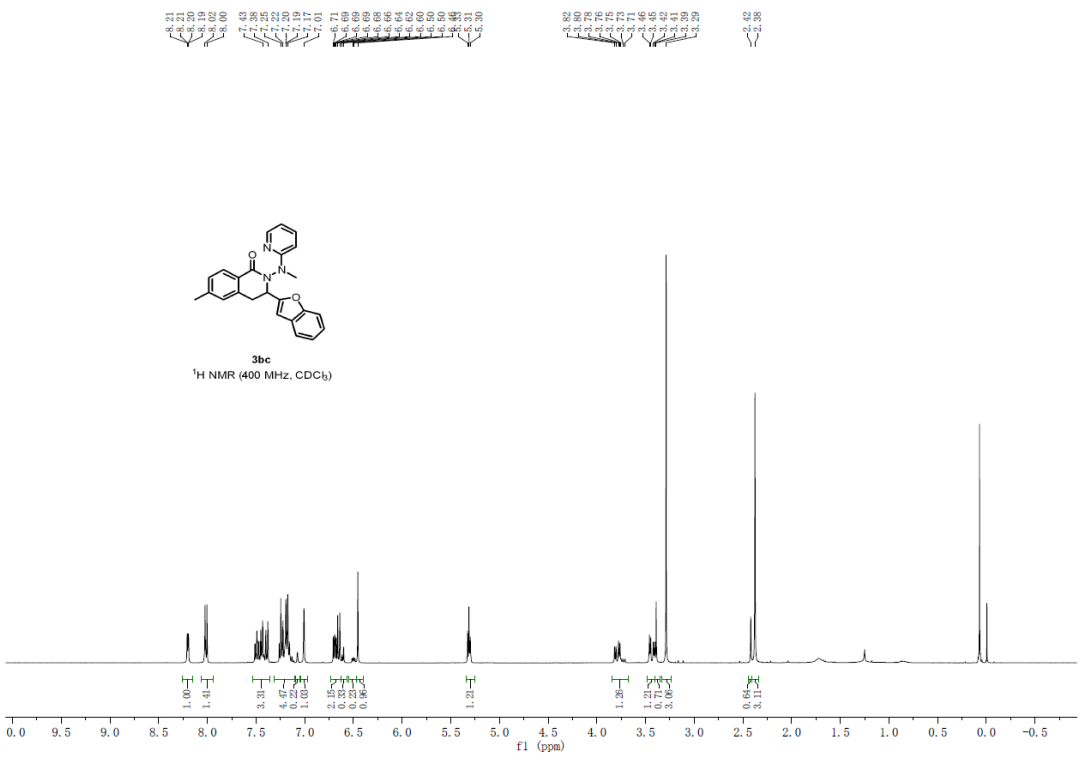


Figure S73. ^{1}H NMR Spectrum of **3bc**

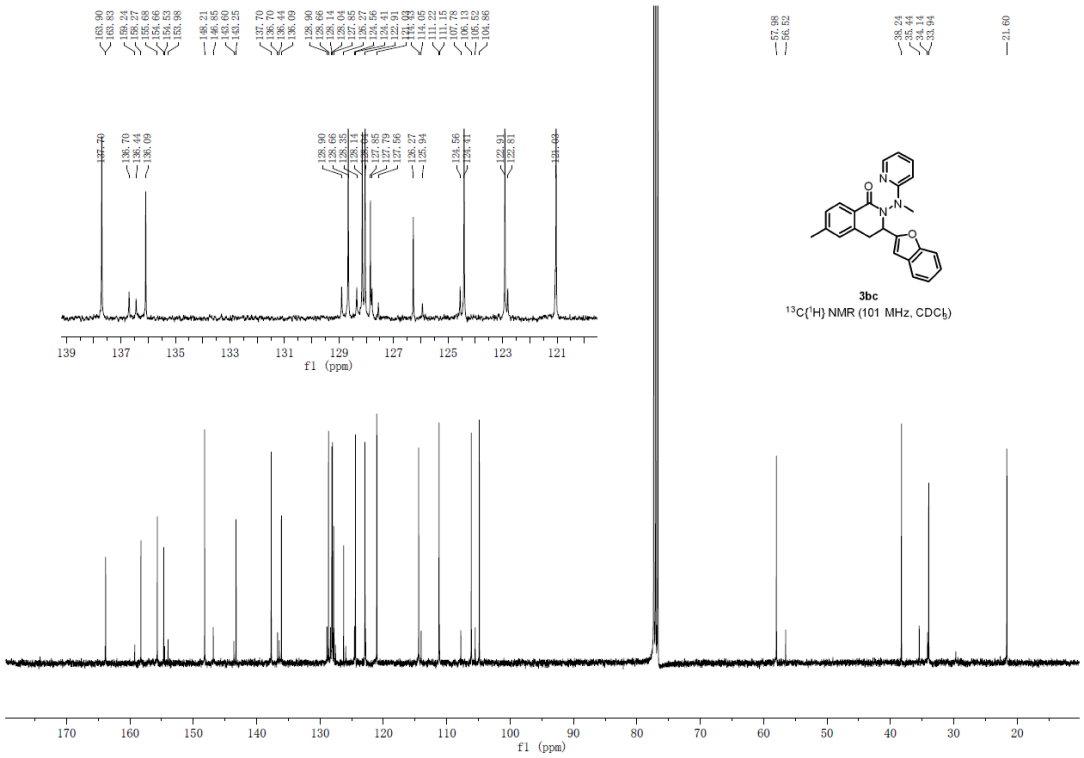


Figure S74. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bc**

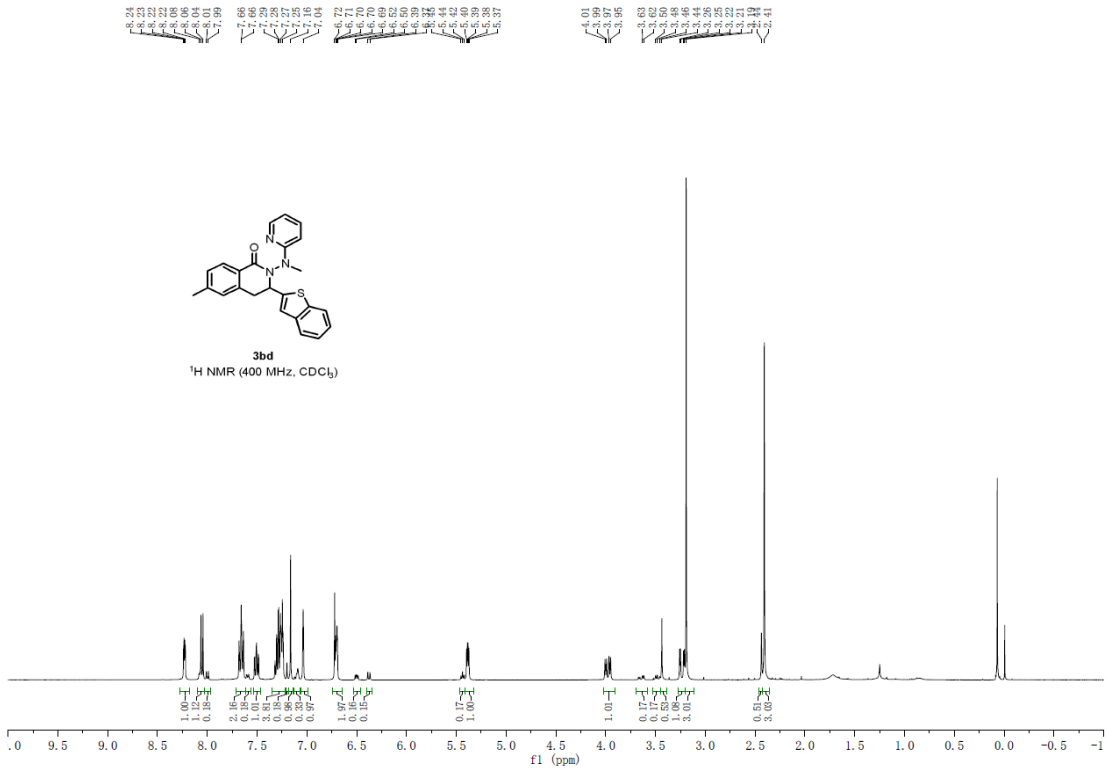


Figure S75. ^{1}H NMR Spectrum of **3bd**

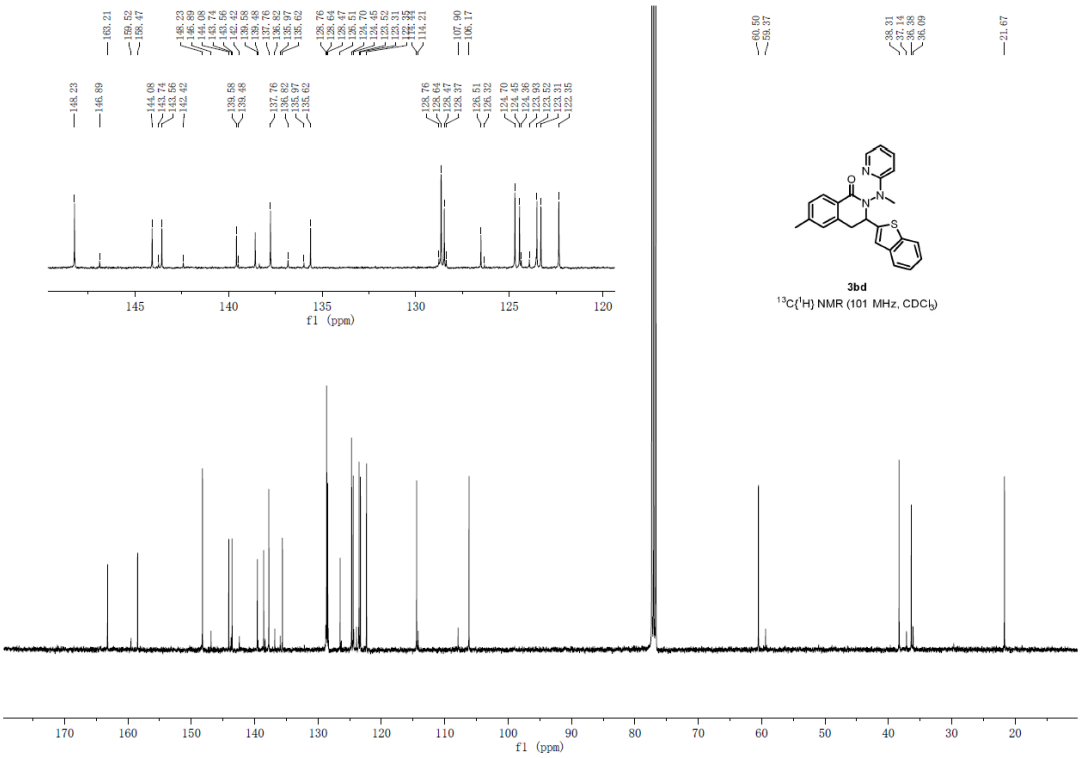


Figure S76. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bd**

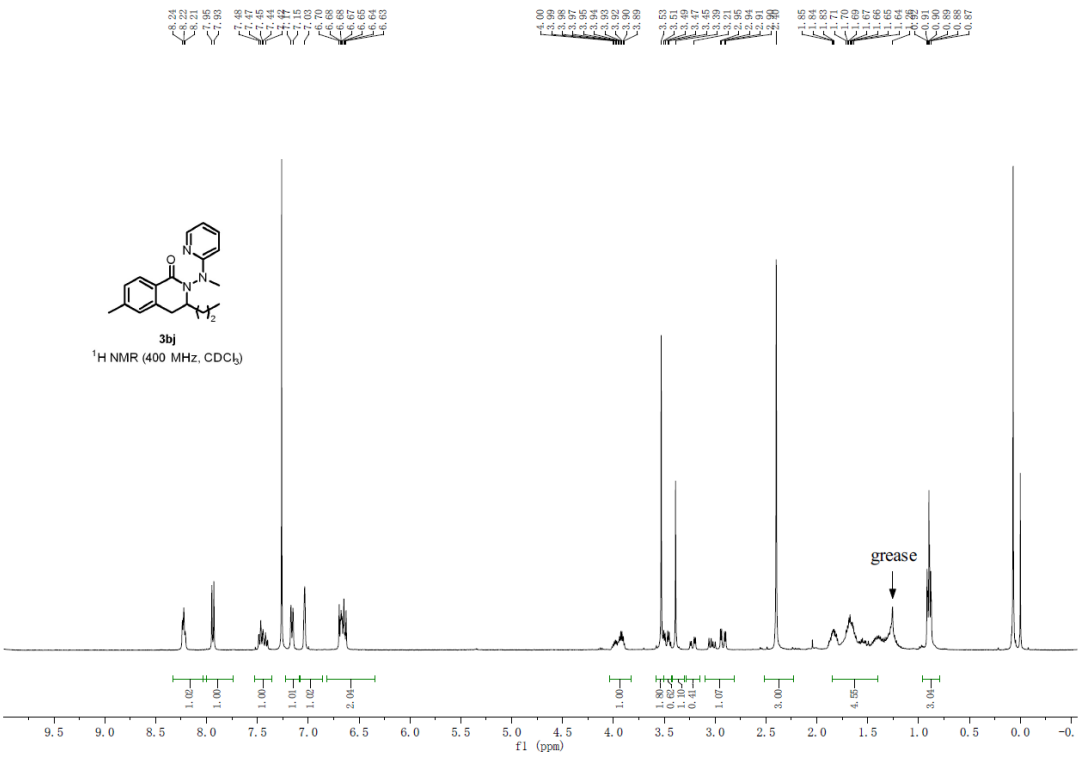


Figure S77. ^{1}H NMR Spectrum of **3bj**

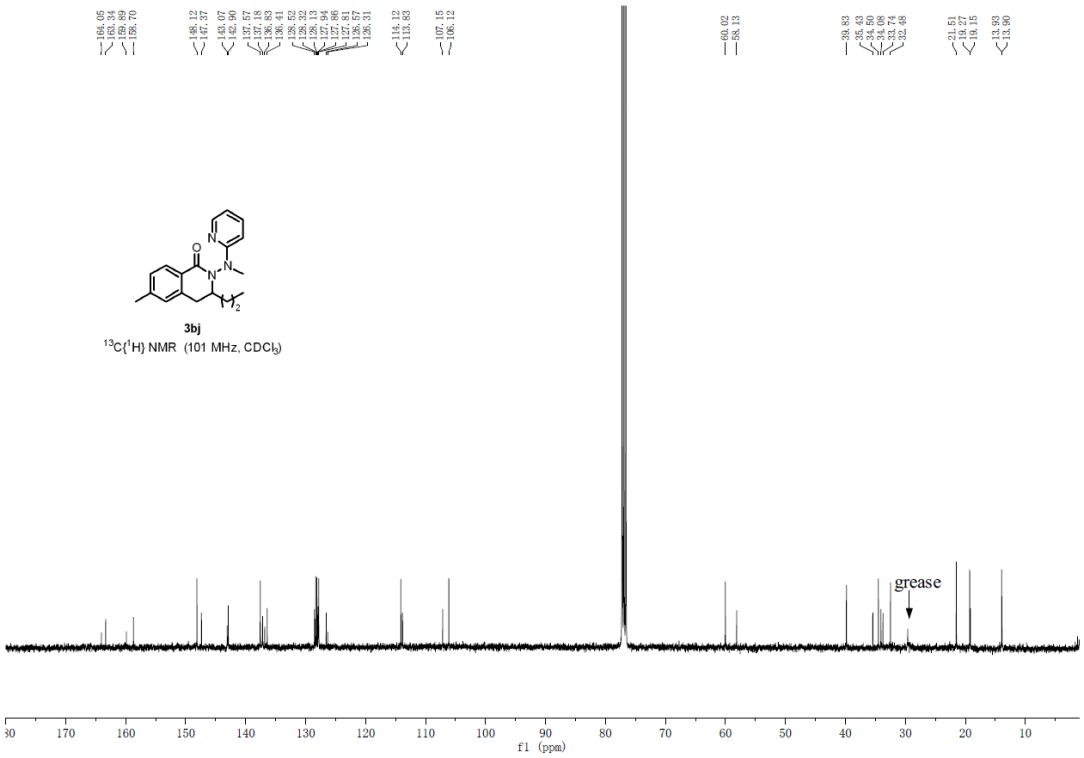


Figure S78. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bj**

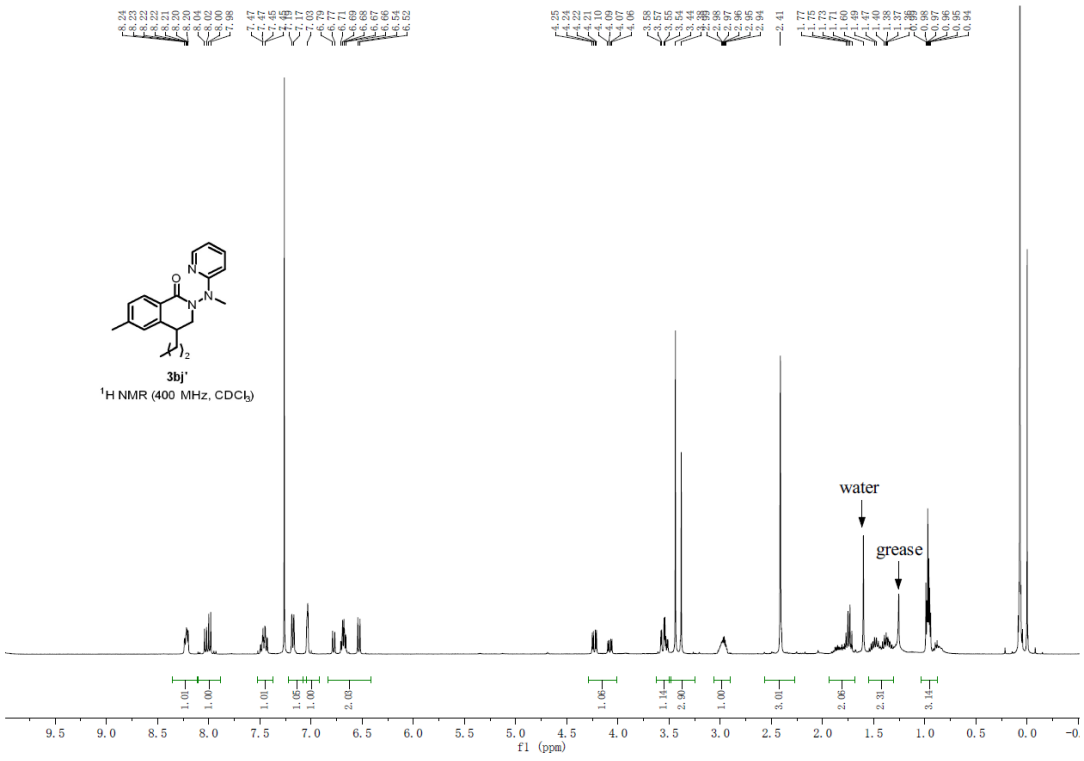


Figure S79. ^{1}H NMR Spectrum of **3bj'**

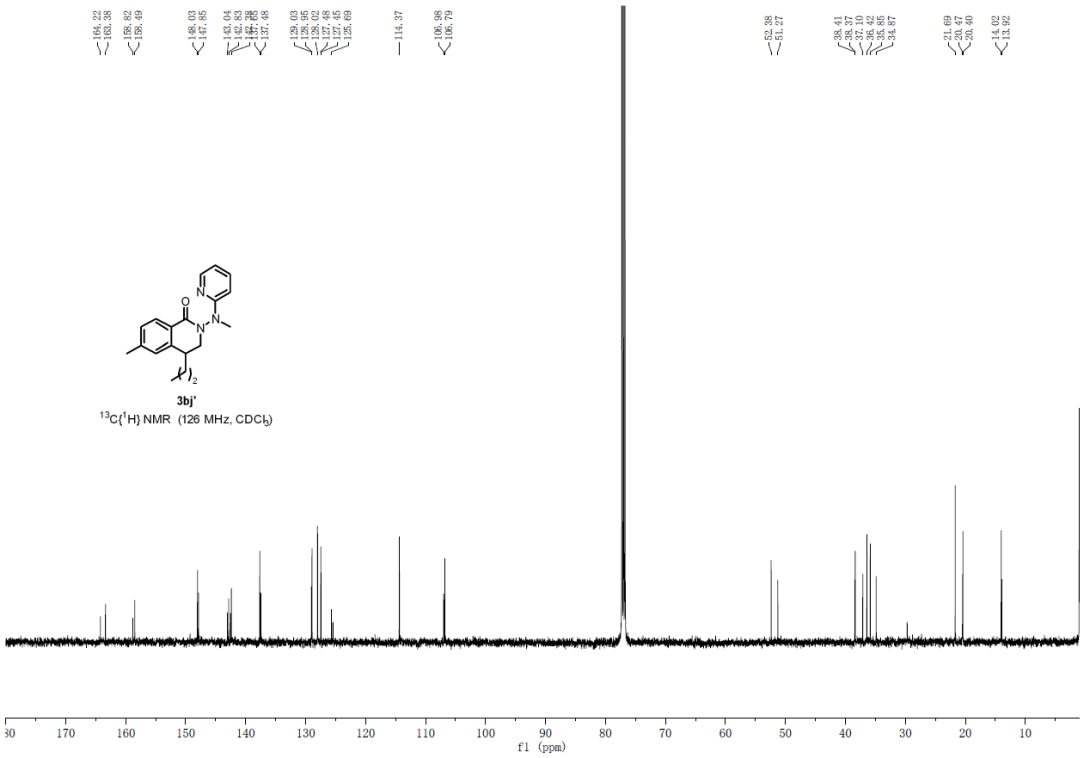


Figure S80. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bj'**

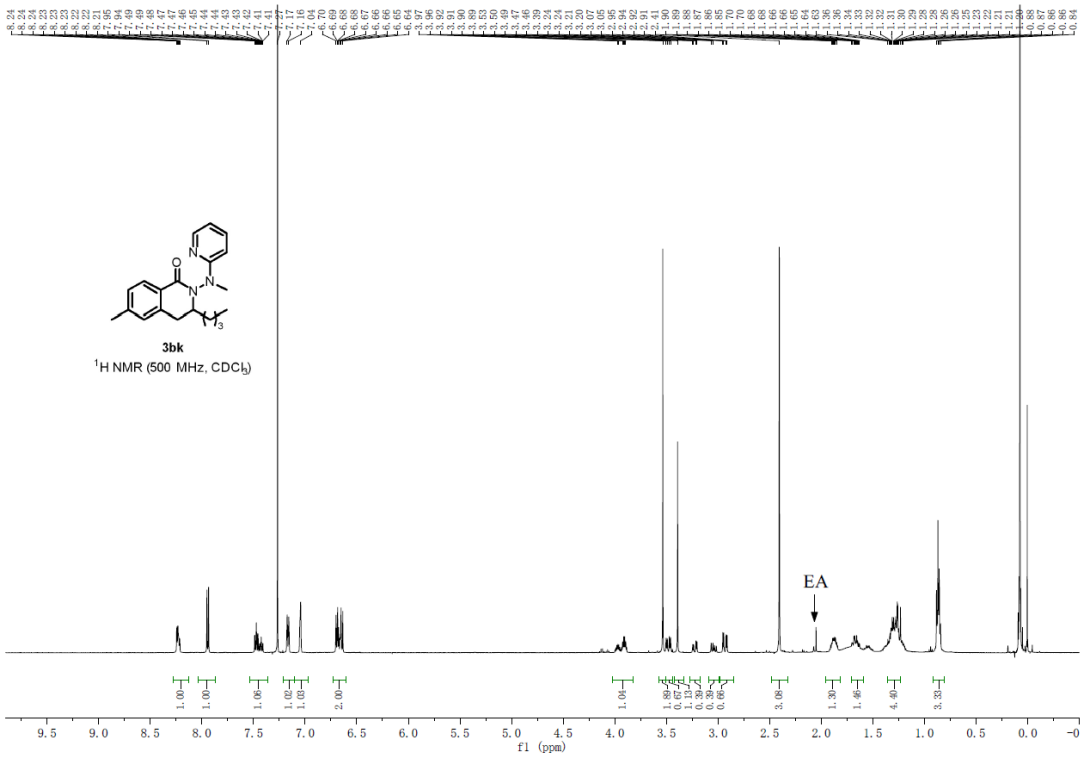


Figure S81. ^{1}H NMR Spectrum of **3bk**

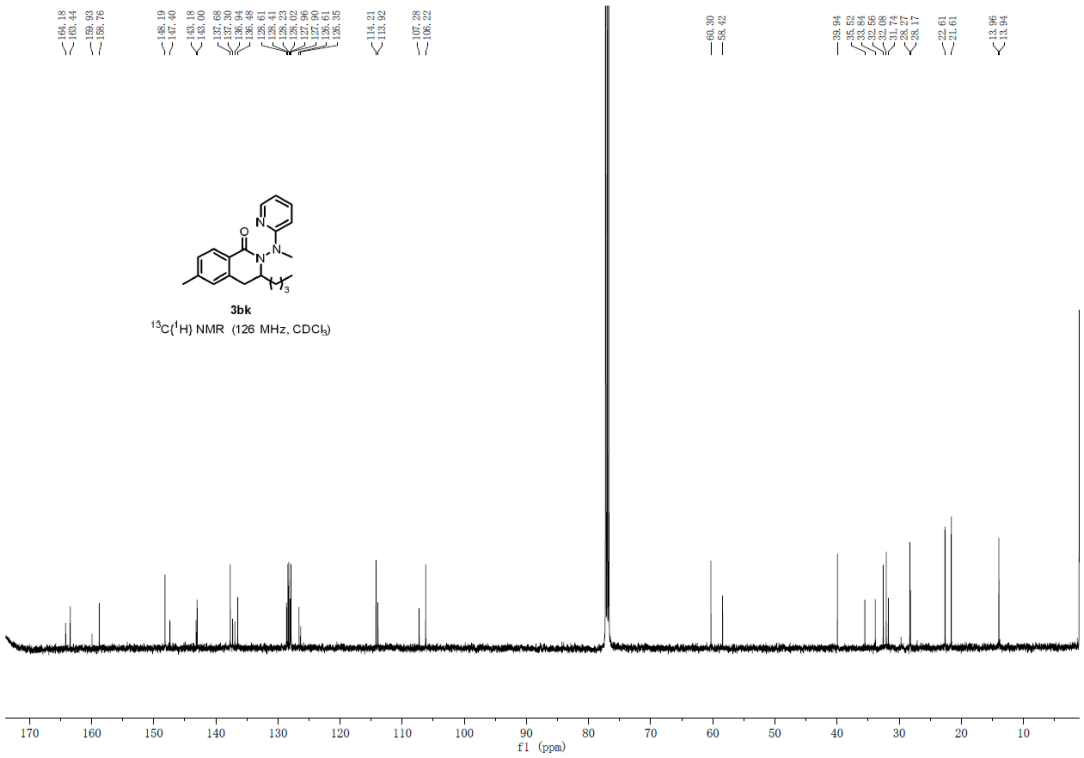


Figure S82. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bk**

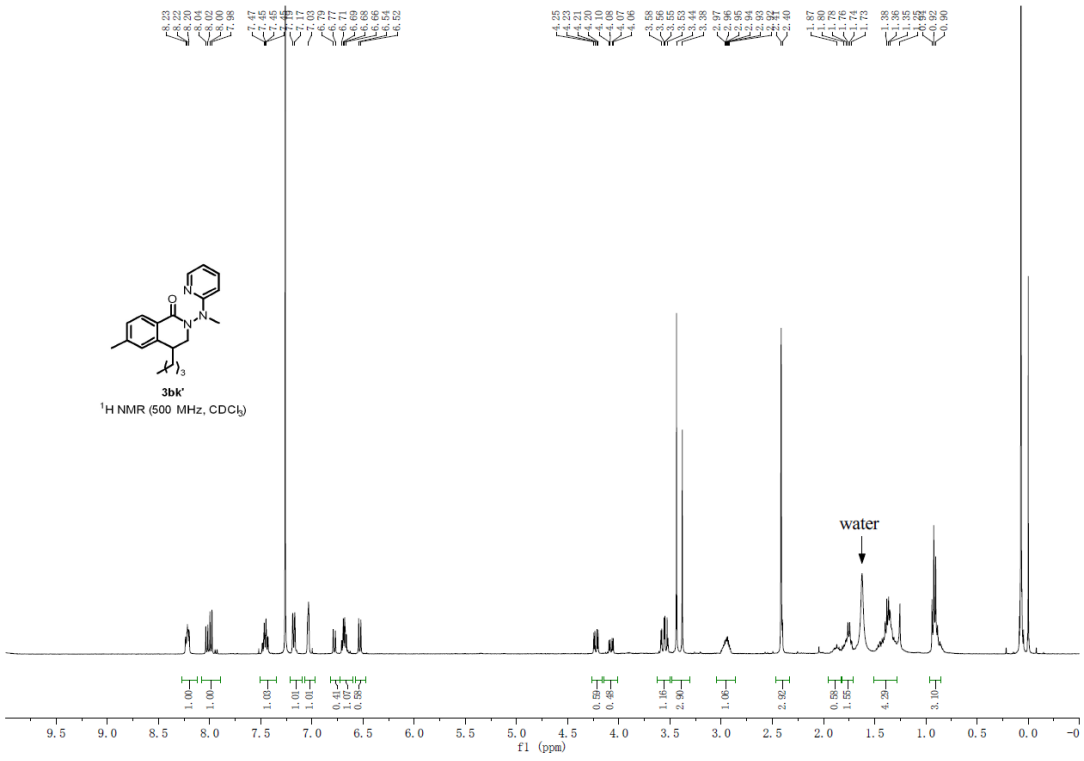


Figure S83. ^{1}H NMR Spectrum of **3bk'**

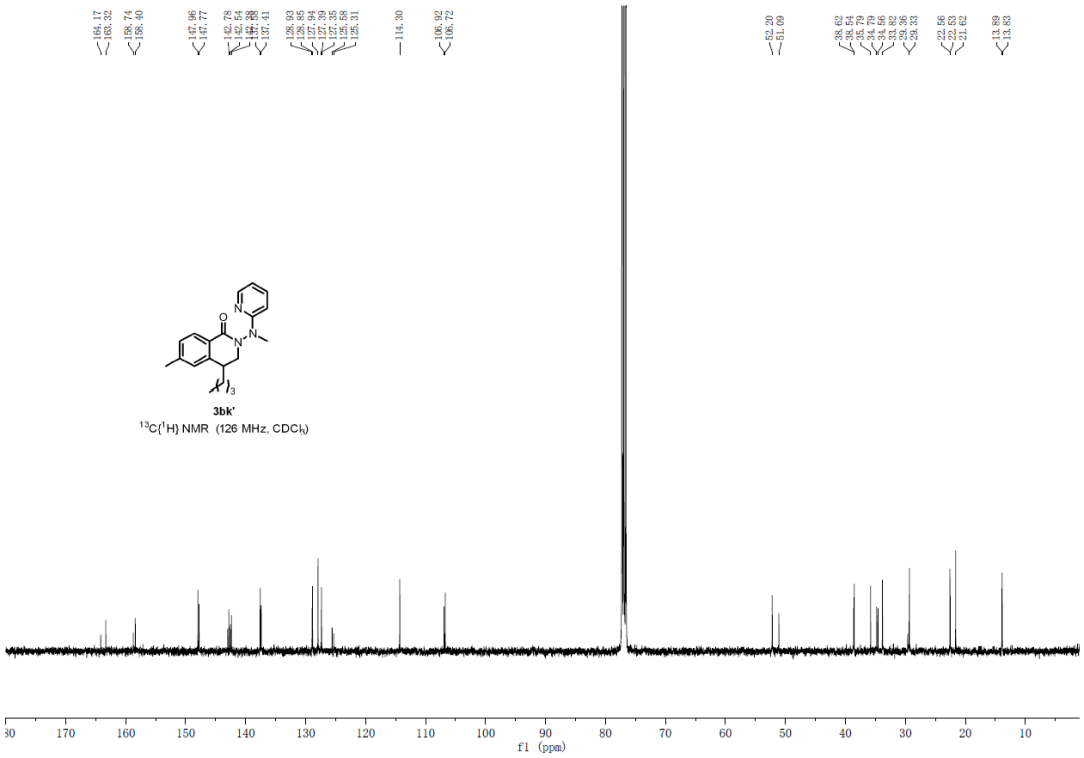


Figure S84. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bk'**

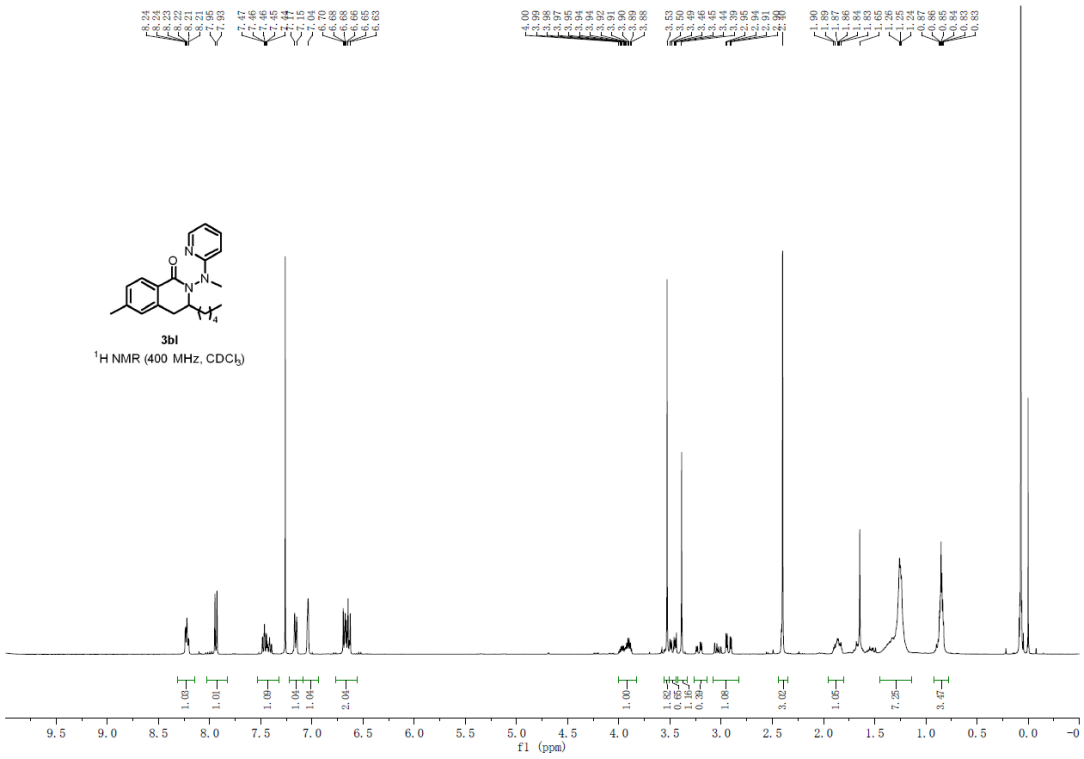


Figure S85. ^{1}H NMR Spectrum of **3bl**

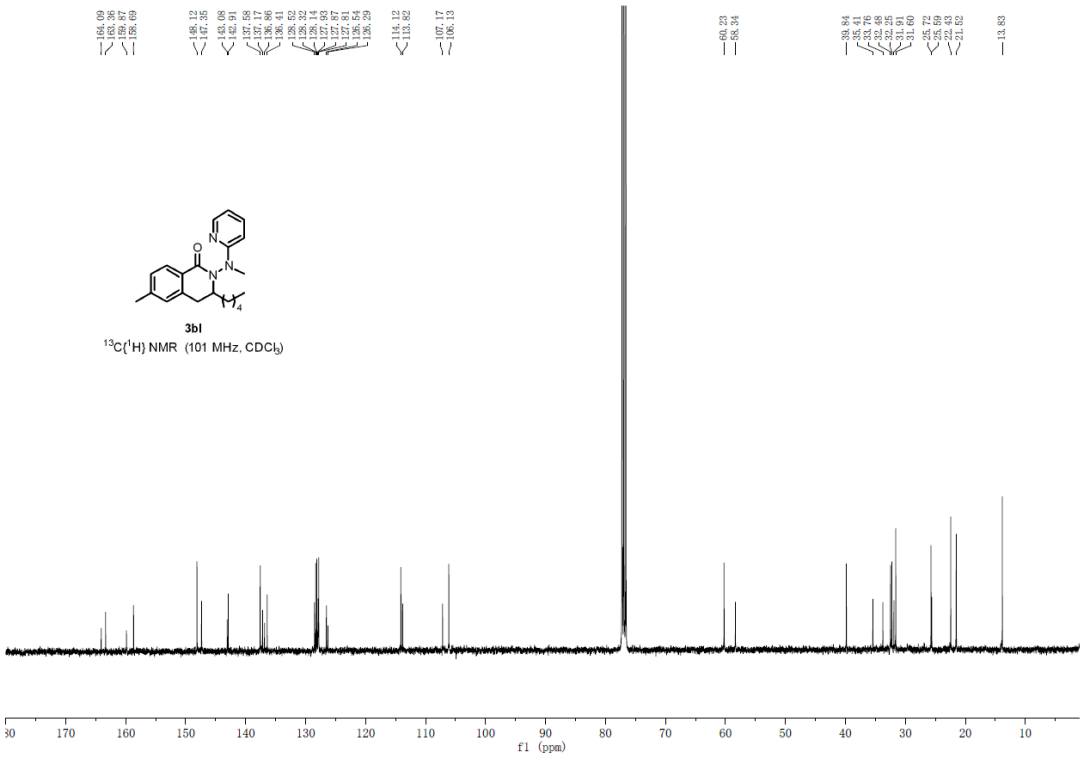


Figure S86. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bl**

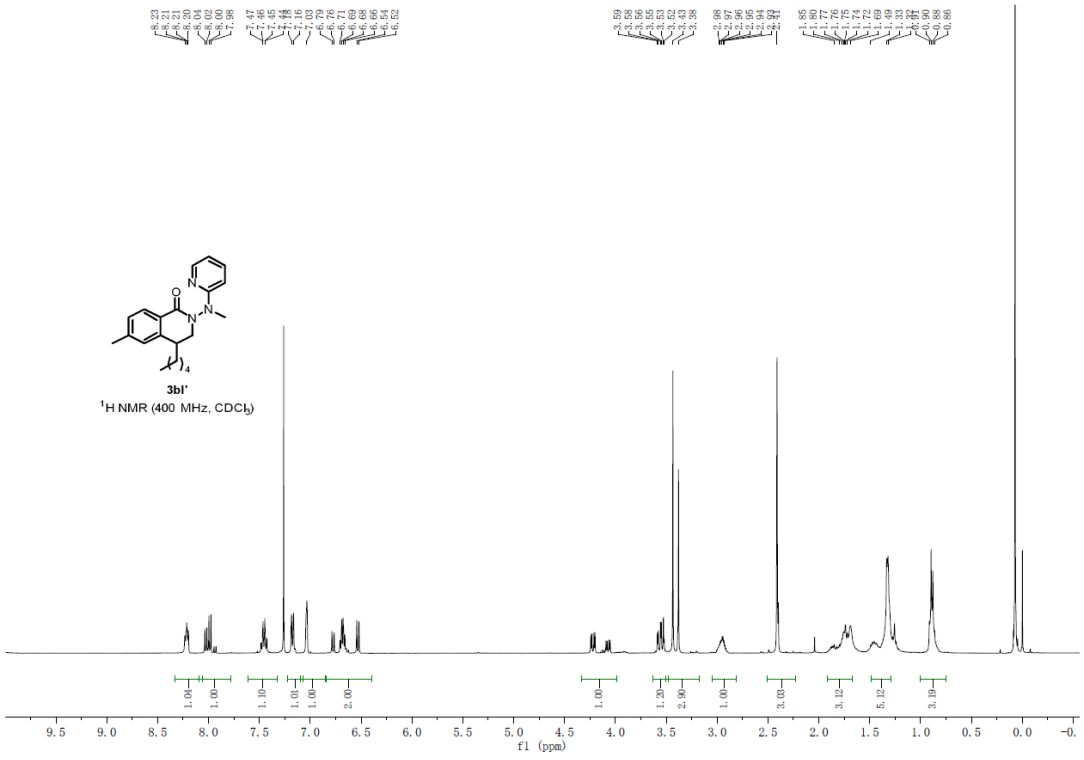


Figure S87. ^{1}H NMR Spectrum of **3bl'**

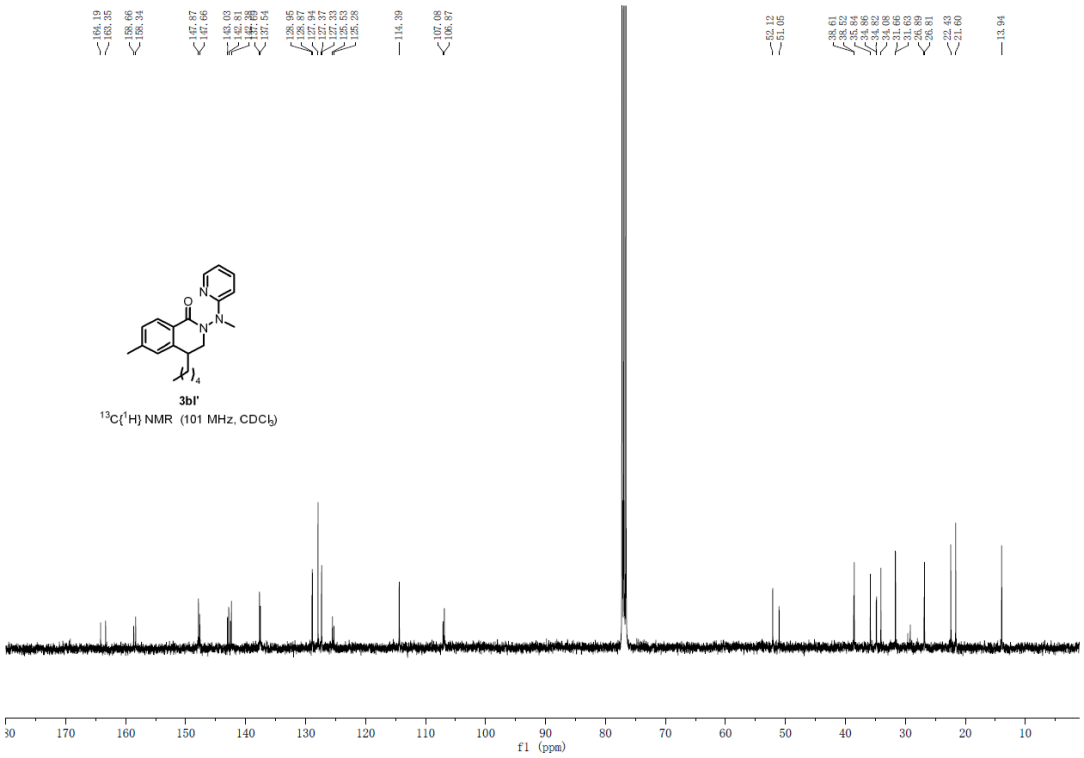


Figure S88. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bl'**

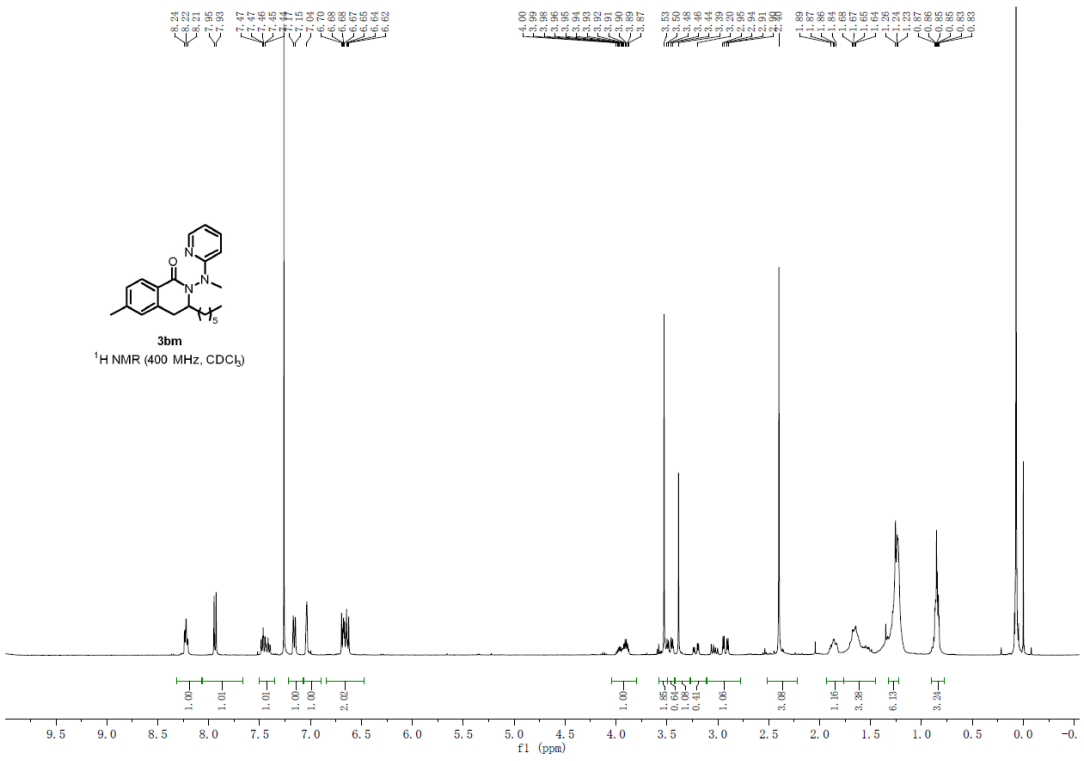


Figure S89. ^{1}H NMR Spectrum of **3bm**

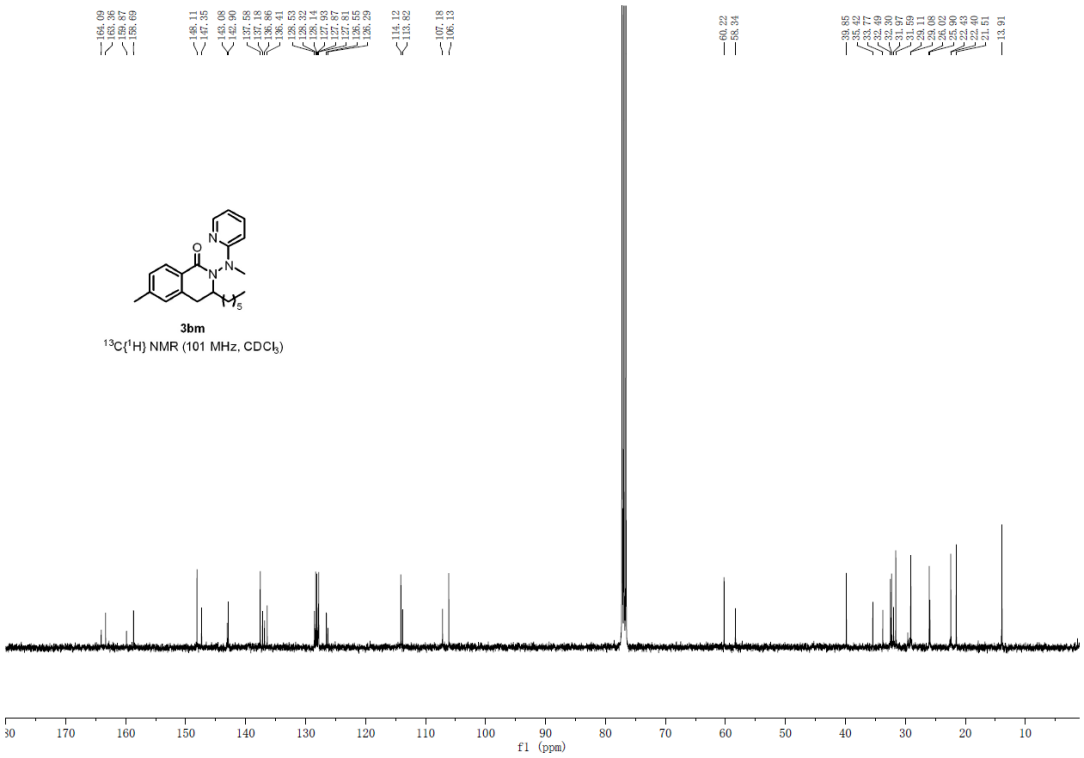


Figure S90. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bm**

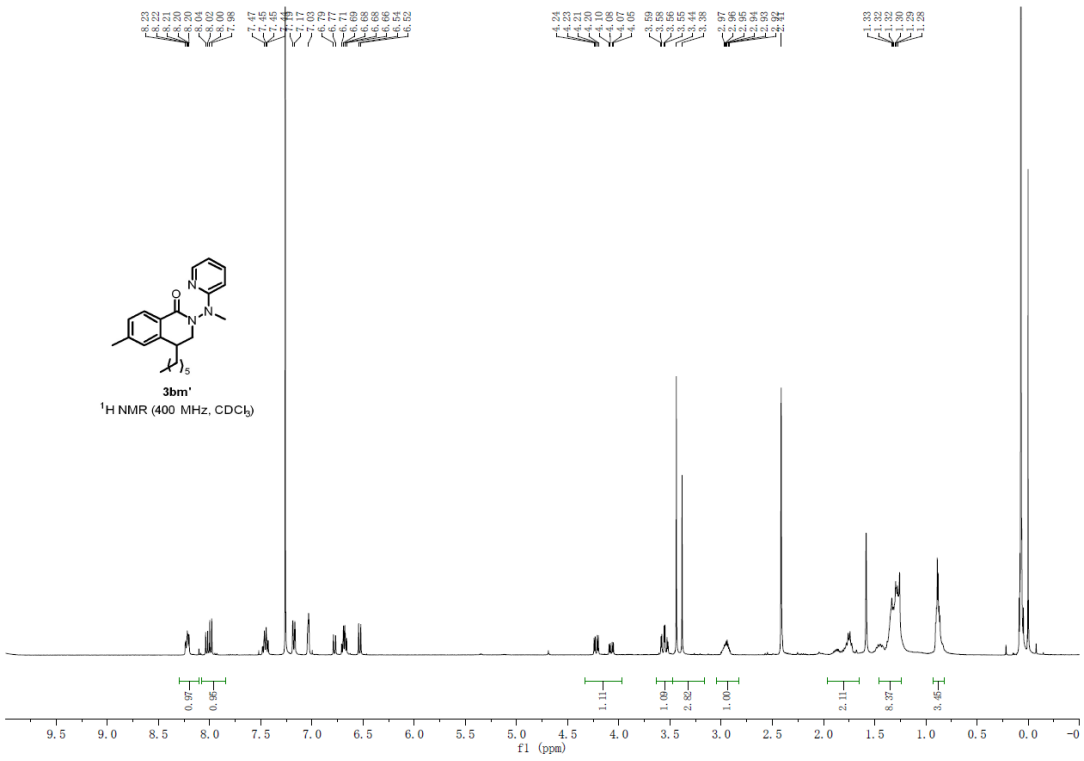


Figure S91. ^{1}H NMR Spectrum of **3bm'**

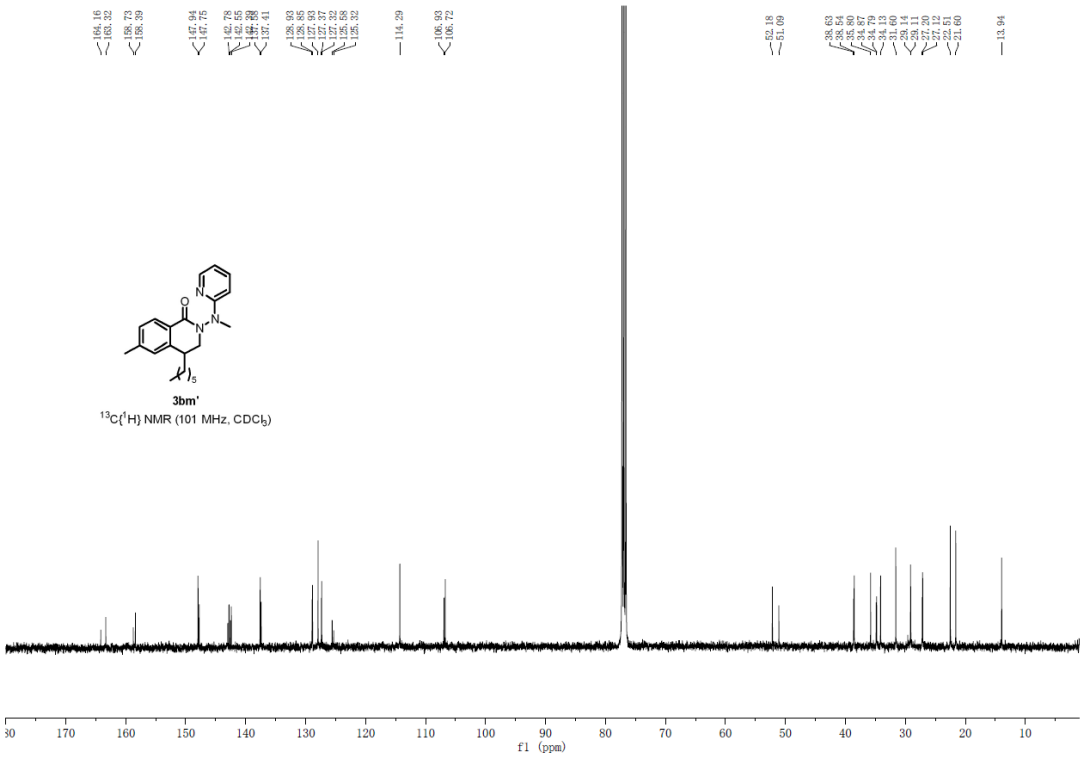


Figure S92. $^{13}C\{^{1}H\}$ NMR Spectrum of **3bm'**

8. DFT Calculation Data

8.1 Calculated election energies

Table S4. DFT calculated Gibbs free energies at the PBE0-D3BJ/def2-SVP/SDD and PW6B95-GD3BJ/def2-TZVP/SMD(THF) level of theory, the Gibbs free energies with and without dispersion corrections for all structures in this work (all in Hartree).

Spin-state	Structures	Gibbs free energy	Gibbs free energy without dispersion
S = 0	IM1-dis	-2781.895381	-2781.838453
	TS-dis	-2781.878388	-2781.822236
	IM2-dis	-2781.904198	-2781.846783
	IM1-pro	-2781.895305	-2781.838104
	TS-pro	-2781.883137	-2781.826771
	IM2-pro	-2781.906478	-2781.849176
S = 1	IM1-dis	-2781.899291	-2781.848482
	TS-dis	-2781.859544	-2781.806699
	IM2-dis	-2781.905187	-2781.851798
	IM1-pro	-2781.900631	-2781.848896
	TS-pro	-2781.870226	-2781.815686
	IM2-pro	-2781.922058	-2781.868226
S = 2	IM1-dis	-2781.884046	-2781.830672
	TS-dis	-2781.849728	-2781.798619
	IM2-dis	-2781.889067	-2781.836541
	IM1-pro	-2781.882217	-2781.830756
	TS-pro	-2781.858341	-2781.806688
	IM2-pro	-2781.923389	-2781.869981

8.2 Cartesian coordinates of the optimized structures:

IM1-dis

Charge 0, S = 0

Co	0.415307	0.123578	-0.319593	O	0.641571	-2.626183	2.494879
C	-1.127746	0.025760	0.811001	N	0.902670	-1.489808	0.487016
C	-2.246249	0.849960	0.886697	O	-0.093138	1.719101	-1.233411
C	-3.200484	0.634280	1.888177	O	1.217430	1.033778	1.129048
C	-3.037300	-0.393400	2.819098	H	-1.732855	-2.013725	3.478983
C	-1.907433	-1.208484	2.760896	H	-3.790908	-0.552392	3.594396
C	-0.964872	-0.994120	1.758710	H	-4.082355	1.279489	1.941883
C	0.280533	-1.806087	1.657111	H	-2.396730	1.657936	0.165024

C	2.883650	-1.134257	-0.645698
C	4.187611	-1.438910	-1.113040
C	2.858023	0.816597	-1.930078
C	4.803194	-0.556023	-1.975888
H	4.694186	-2.344668	-0.784707
C	4.143163	0.609888	-2.397338
H	2.261887	1.682563	-2.231644
H	5.813229	-0.773312	-2.332212
H	4.610129	1.322619	-3.076773
N	2.247439	-0.027638	-1.098313
N	2.198474	-1.907003	0.221865
C	2.606723	-3.266582	0.508650
H	1.956979	-3.642965	1.305526
H	2.542897	-3.907169	-0.389892
H	3.639913	-3.278097	0.883907
C	-1.310617	-0.977155	-1.639481
H	-1.970761	-0.113444	-1.757767
C	-0.075532	-0.908114	-2.217841
H	0.173441	-0.062672	-2.858318
H	0.578830	-1.779852	-2.267422
C	-1.913000	-2.148643	-1.000567
C	-1.204301	-3.341463	-0.793314
C	-3.238052	-2.064965	-0.548678
C	-1.795301	-4.404673	-0.121185
H	-0.173649	-3.428053	-1.137521
C	-3.833464	-3.131977	0.112922
H	-3.790162	-1.133312	-0.690222
C	-3.108724	-4.301738	0.337797
H	-1.224551	-5.319092	0.054607
H	-4.860600	-3.043347	0.473167
H	-3.566703	-5.135882	0.874631
C	-0.046463	2.885907	-0.736119
C	0.501080	3.208387	0.509280
H	0.476568	4.248892	0.829696
C	1.112957	2.269207	1.359167
C	1.699939	2.714871	2.666254
H	1.087882	2.294712	3.479804
H	2.710492	2.295934	2.774605
H	1.733159	3.806670	2.764534
C	-0.637628	3.967514	-1.595030
H	-0.504767	4.968482	-1.167180
H	-0.181539	3.930640	-2.595716
H	-1.713235	3.771359	-1.727759

Charge 0, S = 1

Co	0.628448	0.217068	-0.057323
C	-0.964002	0.032426	1.015939
C	-2.064657	0.876270	1.096969
C	-3.095212	0.567734	1.993568
C	-3.023440	-0.565766	2.805382
C	-1.917636	-1.410051	2.724989
C	-0.898300	-1.105554	1.826405
C	0.301347	-1.967177	1.661421
O	0.570189	-2.937175	2.353056
N	1.019183	-1.483223	0.594396
O	0.090904	1.757747	-1.085503
O	1.383629	1.458217	1.384603
H	-1.825372	-2.309863	3.338223
H	-3.836359	-0.790679	3.500023
H	-3.966033	1.226460	2.058302
H	-2.138414	1.772198	0.477088
C	2.931424	-1.266717	-0.658379
C	4.152480	-1.669114	-1.252282
C	3.053197	0.800840	-1.738271
C	4.806783	-0.777649	-2.076347
H	4.569524	-2.653733	-1.048740
C	4.262516	0.493351	-2.329174
H	2.546689	1.755507	-1.902996
H	5.756032	-1.068082	-2.533092
H	4.762919	1.212589	-2.977419
N	2.402261	-0.054504	-0.942424
N	2.212321	-2.045735	0.181851
C	2.451606	-3.473096	0.266550
H	1.787834	-3.879057	1.035960
H	2.275421	-3.969368	-0.704258
H	3.488318	-3.659493	0.581110
C	-1.328624	-1.063589	-1.907681
H	-1.955984	-0.169167	-1.982673
C	-0.117289	-1.029192	-2.489119
H	0.211706	-0.140503	-3.029408
H	0.563180	-1.884190	-2.474348
C	-1.911720	-2.168391	-1.142560
C	-1.210674	-3.352889	-0.868461
C	-3.199012	-2.018991	-0.608580
C	-1.768625	-4.340349	-0.066441
H	-0.204684	-3.491757	-1.267798
C	-3.764158	-3.010852	0.186417
H	-3.748790	-1.094132	-0.798901

C	-3.047558	-4.172226	0.466812
H	-1.197352	-5.243933	0.157692
H	-4.762186	-2.866568	0.606199
H	-3.480227	-4.945231	1.106097
C	-0.045587	2.957018	-0.670732
C	0.387933	3.441241	0.562545
H	0.197985	4.489348	0.792039
C	1.086620	2.667113	1.524501
C	1.502115	3.313098	2.817620
H	0.853137	2.924913	3.619106
H	2.530800	3.013006	3.061963
H	1.422859	4.407305	2.795472
C	-0.735530	3.879994	-1.635791
H	-0.792207	4.912759	-1.270602
H	-0.206048	3.860359	-2.600526
H	-1.753442	3.504351	-1.825845

Charge 0, S = 2

Co	0.015698	0.618738	0.309518
C	-1.764455	0.328358	1.244581
C	-2.941976	1.085827	1.164766
C	-4.040755	0.825549	1.986823
C	-3.994877	-0.208783	2.928478
C	-2.845449	-0.980888	3.039511
C	-1.753699	-0.708001	2.203631
C	-0.564965	-1.588070	2.289270
O	-0.451146	-2.524488	3.065378
N	0.373202	-1.210691	1.321322
O	-0.016034	2.229792	-0.884654
O	1.364233	1.529768	1.522315
H	-2.774567	-1.801392	3.758054
H	-4.857276	-0.407359	3.569666
H	-4.946159	1.433829	1.898378
H	-3.008351	1.906034	0.441089
C	2.002645	-1.514787	-0.235010
C	3.109119	-2.177671	-0.789467
C	1.974595	0.025996	-1.957194
C	3.625538	-1.697323	-1.983102
H	3.546158	-3.048191	-0.305146
C	3.052802	-0.578077	-2.591299
H	1.481328	0.916904	-2.355868
H	4.481579	-2.198553	-2.440634
H	3.437940	-0.176749	-3.529248
N	1.465112	-0.436722	-0.817269
N	1.383109	-1.951801	0.932236
C	1.876059	-3.148976	1.600624
H	1.228658	-3.342942	2.459697
H	1.840031	-3.999870	0.906505
H	2.910881	-2.979849	1.935396
C	-1.781957	-0.984075	-1.924376
H	-2.579269	-0.588844	-1.287447
C	-1.350381	-0.228261	-2.942211
H	-1.778162	0.759809	-3.121640
H	-0.555318	-0.552386	-3.619836
C	-1.282816	-2.307394	-1.530921
C	-0.232391	-2.961490	-2.195002
C	-1.859941	-2.942739	-0.420238
C	0.221481	-4.202706	-1.762573
H	0.241843	-2.491017	-3.059481
C	-1.401220	-4.181283	0.020536
H	-2.668334	-2.440062	0.116079
C	-0.359893	-4.819096	-0.651817
H	1.037849	-4.695103	-2.297218
H	-1.854771	-4.643672	0.899963
H	-0.003039	-5.795357	-0.313974
C	0.466798	3.370824	-0.613670
C	1.270607	3.673016	0.496085
H	1.621529	4.700172	0.596222
C	1.681041	2.748147	1.481624
C	2.577914	3.227681	2.593615
H	2.057672	3.085581	3.553475
H	3.480374	2.598641	2.624418
H	2.868010	4.280868	2.490876
C	0.133455	4.463456	-1.595165
H	0.596043	5.425658	-1.342195
H	0.454314	4.157485	-2.602967
H	-0.960181	4.585452	-1.633888

TS-dis

Charge 0, S = 0

C	-1.239047	-3.069708	1.253123
C	-0.078876	-2.595413	1.875942
C	0.760930	-3.512879	2.521109
C	0.455140	-4.868715	2.540140
C	-0.693118	-5.333736	1.898777
C	-1.537046	-4.429739	1.256703
Co	0.513103	0.294355	0.151157
C	1.692509	-1.303224	0.457941
C	2.941511	-1.355830	1.081306
C	3.907245	-2.265226	0.650869
C	3.634064	-3.132518	-0.409245
C	2.408634	-3.058942	-1.069861
C	1.449864	-2.143490	-0.648948
C	0.214557	-1.931629	-1.459884
O	-0.096827	-2.624319	-2.424440
N	-0.442074	-0.859694	-0.958591
O	1.466286	1.482988	1.310418
O	1.689140	0.692753	-1.372202
H	2.174485	-3.682275	-1.936308
H	4.387732	-3.855604	-0.730599
H	4.877961	-2.302778	1.152055
H	3.156057	-0.700969	1.930581
H	1.677885	-3.154188	2.995762
H	1.121753	-5.568966	3.048880
H	-0.929527	-6.400384	1.899829
H	-2.438067	-4.785800	0.751964
H	-1.903110	-2.373277	0.741335
C	-1.674418	1.038581	-1.328253
C	-2.751227	1.821668	-1.809231
C	-0.840869	2.873177	-0.141075
C	-2.813046	3.152411	-1.449521
H	-3.506980	1.379811	-2.456278
C	-1.840541	3.708925	-0.604570
H	-0.064681	3.212414	0.548660
H	-3.632214	3.770581	-1.825030
H	-1.869415	4.756256	-0.304925
N	-0.762865	1.586834	-0.487246
N	-1.491744	-0.263560	-1.630344
C	-2.530007	-1.066856	-2.238676
H	-2.086365	-2.034947	-2.495757
H	-3.392366	-1.197203	-1.559757
H	-2.873050	-0.594008	-3.169540
C	-0.666565	-0.121400	1.658591
H	-0.607441	0.761891	2.297653
C	0.292622	-1.153584	1.881169
H	-1.672093	-0.396661	1.334119
H	1.046653	-0.908313	2.633127
C	2.599339	2.007923	1.063191
C	3.294829	1.922268	-0.143101
H	4.267968	2.407494	-0.207981
C	2.796850	1.276414	-1.297673
C	3.195273	2.776412	2.210358
H	2.480884	3.543699	2.545599
H	3.349473	2.094229	3.061067
H	4.148428	3.253575	1.952077
C	3.632439	1.251154	-2.546662
H	3.988355	0.219776	-2.699364
H	3.004257	1.506138	-3.411834
H	4.496542	1.925212	-2.496211

Charge 0, S = 1

C	-1.258664	-2.994327	1.336511
C	-0.057035	-2.585689	1.927135
C	0.784997	-3.557581	2.484497
C	0.440809	-4.903589	2.445079
C	-0.749254	-5.302394	1.835937
C	-1.596312	-4.343573	1.283791
Co	0.564640	0.364505	0.079157
C	1.696281	-1.332482	0.392712
C	2.974701	-1.365347	0.948339
C	3.906418	-2.297957	0.490290
C	3.556729	-3.202816	-0.513790
C	2.292746	-3.141911	-1.098530
C	1.365316	-2.196029	-0.668726
C	0.089630	-2.024210	-1.436390
O	-0.274846	-2.819870	-2.299045
N	-0.482564	-0.861875	-1.051483
O	1.540803	1.723744	1.294031
O	1.896814	0.832109	-1.333917
H	1.999326	-3.796096	-1.923405
H	4.281623	-3.945881	-0.854882
H	4.906362	-2.324082	0.930883
H	3.244132	-0.676513	1.752910
H	1.733836	-3.249339	2.931221
H	1.110310	-5.648376	2.881553
H	-1.015103	-6.361022	1.790409
H	-2.528355	-4.648322	0.802695
H	-1.926008	-2.256214	0.890410

C	-1.804437	0.988979	-1.348684
C	-2.943481	1.705035	-1.796816
C	-1.032085	2.889049	-0.225017
C	-3.069799	3.033514	-1.450026
H	-3.699710	1.214351	-2.406741
C	-2.097081	3.658257	-0.651401
H	-0.240899	3.285364	0.417697
H	-3.938430	3.597470	-1.798915
H	-2.174359	4.707540	-0.366735
N	-0.888848	1.602076	-0.558901
N	-1.585241	-0.314161	-1.652790
C	-2.598415	-1.118082	-2.306883
H	-2.151277	-2.094729	-2.522504
H	-3.493615	-1.233120	-1.670164
H	-2.894688	-0.654618	-3.259227
C	-0.540932	-0.096825	1.765661
H	-0.372148	0.837203	2.304137
C	0.368329	-1.165336	1.954927
H	-1.562294	-0.298225	1.440038
H	1.180486	-0.956222	2.654994
C	2.717304	2.162769	1.132134
C	3.496908	1.981509	-0.019312
H	4.505712	2.393461	-0.026149
C	3.036652	1.344858	-1.190826
C	3.290564	2.934033	2.292775
H	2.629140	3.783349	2.523368
H	3.300570	2.289363	3.185614
H	4.305076	3.306223	2.102598
C	3.951723	1.239345	-2.379902
H	4.207345	0.177543	-2.524209
H	3.414788	1.565665	-3.282365
H	4.875000	1.820605	-2.263374

Charge 0, S = 2

C	-1.481048	-2.826249	1.595622
C	-0.173623	-2.694445	2.079896
C	0.598824	-3.855701	2.227518
C	0.088931	-5.104217	1.889294
C	-1.209022	-5.218206	1.392391
C	-1.992122	-4.073788	1.251530
Co	0.668625	0.875450	-0.422308
C	1.889759	-1.376317	0.674800
C	3.183146	-1.350444	1.164109
C	4.194415	-1.954775	0.410116
C	3.878035	-2.594678	-0.789987
C	2.567395	-2.597470	-1.261402
C	1.550431	-1.957679	-0.541672
C	0.190622	-1.864211	-1.175374
O	-0.215758	-2.711547	-1.960039
N	-0.428524	-0.713607	-0.803750
O	1.498996	1.979287	0.967851
O	2.252083	1.004424	-1.583245
H	2.295292	-3.077382	-2.204925
H	4.663203	-3.090990	-1.365670
H	5.226424	-1.938915	0.771139
H	3.418959	-0.882461	2.124824
H	1.626873	-3.767001	2.588950
H	0.712353	-5.994114	2.003456
H	-1.608980	-6.196203	1.115296
H	-3.012060	-4.153232	0.867293
H	-2.107719	-1.940457	1.485428
C	-1.995070	0.879576	-1.418301
C	-3.287933	1.333610	-1.791453
C	-1.272145	3.090354	-1.193803
C	-3.516673	2.689248	-1.875539
H	-4.080464	0.621807	-2.013872
C	-2.492644	3.605551	-1.578470
H	-0.436001	3.742430	-0.925485
H	-4.505448	3.048317	-2.171663
H	-2.649644	4.682584	-1.634803
N	-1.025096	1.775087	-1.109107
N	-1.677140	-0.431047	-1.329528
C	-2.705162	-1.448416	-1.402770
H	-2.219837	-2.427224	-1.369102
H	-3.433786	-1.345791	-0.579035
H	-3.237382	-1.380371	-2.362562
C	-0.256693	-0.191956	2.399990
H	0.212534	0.718650	2.773836
C	0.417117	-1.383466	2.414498
H	-1.241117	-0.090682	1.938944
H	1.329301	-1.434553	3.015074
C	2.745017	2.224106	1.046176
C	3.694207	1.926709	0.059517
H	4.732976	2.183061	0.265976
C	3.405049	1.339933	-1.191159
C	3.188733	2.881629	2.323162
H	2.590249	3.789633	2.490936
H	2.978959	2.202577	3.164993

H	4.255124	3.138796	2.325127	H	4.642373	-0.021641	-2.241515
C	4.525500	1.070226	-2.154099	H	4.249624	1.447182	-3.149500
H	5.479153	1.510116	-1.837206				

IM2-dis

Charge 0, S = 0

Co	1.152411	0.496788	0.028831	C	-1.301443	-2.005668	-0.738036
C	-1.974797	-0.167572	0.896177	C	-0.504454	-2.478056	-1.788211
C	-3.199081	0.492435	1.050513	C	-1.982692	-2.951987	0.040318
C	-3.694742	0.847120	2.303542	C	-0.386060	-3.842800	-2.047372
C	-2.966254	0.524101	3.446311	H	0.039301	-1.775665	-2.421414
C	-1.750032	-0.135977	3.313025	C	-1.869455	-4.316135	-0.217539
C	-1.231459	-0.464266	2.056755	H	-2.610465	-2.612915	0.866982
C	0.050788	-1.249373	2.072856	C	-1.069502	-4.771549	-1.264471
O	0.278510	-1.988544	3.028393	H	0.249999	-4.178962	-2.870151
N	0.837929	-1.101418	0.975400	H	-2.410865	-5.028688	0.409561
O	1.760339	2.014930	-0.921114	H	-0.978952	-5.841179	-1.468033
O	0.407841	1.573891	1.372167	C	1.363185	3.212487	-0.775866
H	-1.163936	-0.423848	4.187766	C	0.519884	3.648053	0.251790
H	-3.347440	0.779608	4.437970	H	0.232760	4.698111	0.285540
H	-4.656989	1.358812	2.384273	C	0.134420	2.806666	1.310226
H	-3.787285	0.719858	0.156722	C	1.882258	4.188104	-1.792062
C	2.382166	-1.872548	-0.526706	H	2.982714	4.169625	-1.781409
C	3.169014	-2.832031	-1.216490	H	1.563779	3.868882	-2.796474
C	2.822945	-0.287922	-2.196485	H	1.534729	5.212288	-1.610127
C	3.772880	-2.466859	-2.396755	C	-0.634266	3.355239	2.473418
H	3.270815	-3.841605	-0.825329	H	-0.815290	4.433704	2.390045
C	3.604501	-1.167201	-2.912628	H	-1.592298	2.817504	2.544326
H	2.642930	0.740308	-2.514831	H	-0.084165	3.142378	3.402125
H	4.377324	-3.198526	-2.938398				
H	4.071037	-0.855357	-3.846876				
N	2.230414	-0.625558	-1.038266				
N	1.727277	-2.113819	0.620963				
C	1.581706	-3.481869	1.084989				
H	1.129481	-3.461143	2.079646				
H	0.955662	-4.066642	0.391920				
H	2.577627	-3.937565	1.164705				
C	-1.529511	-0.518517	-0.512164				
H	-2.406589	-0.283236	-1.149989				
C	-0.439726	0.418163	-1.010866				
H	-0.806744	1.455915	-0.977608				
H	-0.130446	0.190447	-2.041043				

Charge 0, S = 1

Co	0.952882	0.349051	-0.227099
C	-2.070779	-0.223450	1.044584
C	-3.148946	0.566021	1.459723
C	-3.331791	0.913370	2.795602
C	-2.433108	0.451326	3.755268
C	-1.365546	-0.346381	3.361402
C	-1.157729	-0.671657	2.016885
C	0.016101	-1.569891	1.752628
O	0.338478	-2.415974	2.575865
N	0.669597	-1.366559	0.574188
O	1.375141	1.883412	-1.408697

O	0.702294	1.656239	1.268878
H	-0.658819	-0.744603	4.091567
H	-2.569435	0.704222	4.809374
H	-4.184157	1.532438	3.086122
H	-3.867869	0.909209	0.710110
C	2.729384	-1.857333	-0.375488
C	3.832007	-2.685234	-0.710032
C	3.768299	-0.018989	-1.373903
C	4.893765	-2.121111	-1.382164
H	3.848288	-3.731116	-0.407316
C	4.877516	-0.757647	-1.730349
H	3.663089	1.040729	-1.621089
H	5.758228	-2.740423	-1.634486
H	5.706316	-0.293727	-2.265185
N	2.723098	-0.549890	-0.722722
N	1.634273	-2.305932	0.266278
C	1.327099	-3.717241	0.371091
H	0.240963	-3.830749	0.447049
H	1.663065	-4.236483	-0.538421
H	1.779765	-4.167237	1.265933
C	-1.921256	-0.514416	-0.436555
H	-2.881850	-0.194177	-0.892354
C	-0.886537	0.408483	-1.033380
H	-1.134985	1.463085	-0.847520
H	-0.671170	0.247054	-2.098308
C	-1.806987	-1.988600	-0.787555
C	-1.102699	-2.435940	-1.911565
C	-2.492160	-2.938839	-0.020372
C	-1.080816	-3.785747	-2.256004
H	-0.548551	-1.727183	-2.529052
C	-2.467115	-4.290962	-0.358259
H	-3.045387	-2.614706	0.864162
C	-1.761656	-4.722555	-1.479968
H	-0.520071	-4.107550	-3.137290
H	-3.004346	-5.011487	0.263200
H	-1.741043	-5.781791	-1.746713
C	0.971786	3.075008	-1.247186
C	0.398181	3.579212	-0.069385
H	0.070167	4.618385	-0.063955
C	0.330047	2.854136	1.139585
C	1.153376	3.984683	-2.431046
H	2.217201	4.000491	-2.713516
H	0.601492	3.573311	-3.290244
H	0.814949	5.009872	-2.236412
C	-0.205248	3.514138	2.377778
H	-0.495546	4.559916	2.217549
H	-1.073942	2.934328	2.727375
H	0.554386	3.457878	3.171941

Charge 0, S = 2

Co	0.890744	0.443064	-0.305963
C	-2.142309	-0.229824	0.860679
C	-3.255667	0.566577	1.158276
C	-3.517263	1.021114	2.447391
C	-2.665415	0.660296	3.489505
C	-1.561890	-0.138368	3.217094
C	-1.270714	-0.567131	1.916645
C	-0.055001	-1.443086	1.800799
O	0.244020	-2.208788	2.707104
N	0.650741	-1.285492	0.645479
O	1.385875	2.102171	-1.356942
O	0.782839	1.573168	1.306314
H	-0.885587	-0.456753	4.012555
H	-2.865550	0.992362	4.511053
H	-4.396213	1.641788	2.638057
H	-3.943019	0.826773	0.348094
C	2.588080	-1.853536	-0.465125
C	3.644468	-2.708376	-0.875381
C	3.475344	-0.109554	-1.748348
C	4.602374	-2.209974	-1.729534
H	3.708420	-3.727059	-0.497345
C	4.529905	-0.881527	-2.187810
H	3.337391	0.930428	-2.055788
H	5.427562	-2.854193	-2.043085
H	5.279083	-0.465822	-2.861575
N	2.532377	-0.577133	-0.913975
N	1.599029	-2.238483	0.366677
C	1.369394	-3.635877	0.682558
H	0.295342	-3.793488	0.819132
H	1.695443	-4.257171	-0.161949
H	1.880697	-3.934864	1.607853
C	-1.951382	-0.644347	-0.592833
H	-2.942504	-0.471308	-1.063623
C	-0.987758	0.294199	-1.279746
H	-1.266610	1.350760	-1.141358
H	-0.781174	0.084779	-2.337941
C	-1.704186	-2.128196	-0.800947
C	-0.866790	-2.612334	-1.812489

C	-2.400514	-3.060948	-0.021094
C	-0.735524	-3.980417	-2.043658
H	-0.293806	-1.914263	-2.424638
C	-2.266083	-4.429891	-0.244620
H	-3.053719	-2.706063	0.780045
C	-1.435077	-4.897918	-1.261725
H	-0.073984	-4.330463	-2.840381
H	-2.817211	-5.135446	0.381937
H	-1.330680	-5.970683	-1.440448
C	1.062561	3.286388	-1.040905
C	0.580187	3.671609	0.220758

IM1-pro

Charge 0, S = 0

C	-3.084065	1.293294	1.551327
C	-2.226827	0.183480	1.563257
C	-2.788660	-1.097839	1.454888
C	-4.164888	-1.257914	1.341412
C	-5.007256	-0.144194	1.329757
C	-4.461457	1.133727	1.433365
Co	0.453549	0.173796	-0.157534
C	1.604014	-1.356085	0.034575
C	2.867648	-1.469869	0.607078
C	3.591869	-2.658123	0.460261
C	3.061602	-3.732906	-0.256416
C	1.800639	-3.620519	-0.839568
C	1.080676	-2.436789	-0.687118
C	-0.230272	-2.218245	-1.361108
O	-0.720852	-2.997915	-2.171029
N	-0.757403	-1.042678	-0.917296
H	1.357946	-4.427470	-1.429327
H	3.638125	-4.654894	-0.364312
H	4.584802	-2.743434	0.911059
H	3.302131	-0.640728	1.173184
H	-2.141880	-1.976055	1.441538
H	-4.585420	-2.262799	1.257350
H	-6.088251	-0.275168	1.239657
H	-5.110738	2.012098	1.420922
H	-2.657816	2.297055	1.626169
C	-1.875427	0.900419	-1.481431
C	-2.931047	1.683169	-2.016960
C	-0.839701	2.828324	-0.661458
C	-2.884153	3.051444	-1.861863
H	0.321510	4.719150	0.372726
C	0.502161	2.807273	1.329797
C	1.236357	4.323369	-2.115732
H	2.292836	4.345487	-2.424977
H	0.651390	4.026662	-2.999748
H	0.932357	5.327590	-1.795482
C	0.069346	3.343280	2.663113
H	-0.123873	4.422943	2.649683
H	-0.840278	2.804735	2.972038
H	0.843640	3.113229	3.410347
H	-3.758341	1.206896	-2.539151
C	-1.817417	3.658748	-1.177100
H	0.012814	3.214591	-0.095718
H	-3.689099	3.664072	-2.275588
H	-1.756570	4.738890	-1.045832
N	-0.873034	1.502272	-0.797180
N	-1.813981	-0.438451	-1.586566
C	-2.947663	-1.207065	-2.059002
H	-2.640286	-2.255311	-2.109616
H	-3.818253	-1.079875	-1.394280
H	-3.214496	-0.891057	-3.078423
C	-0.784262	0.409804	1.725762
H	-0.493455	1.446784	1.914851
C	0.174078	-0.552010	1.902297
H	-0.074166	-1.613662	1.903131
H	1.142640	-0.275963	2.314784
C	2.809042	0.735608	-3.548819
H	3.661659	1.383393	-3.785964
H	1.983593	0.927304	-4.249056
H	3.104333	-0.317371	-3.679413
C	2.319743	0.914110	-2.141580
C	3.064325	1.689151	-1.233125
C	2.670900	1.928410	0.086145
C	3.507012	2.815023	0.964894
H	3.880222	2.226359	1.817478
H	4.357362	3.257760	0.432553
H	2.877070	3.615232	1.381870
O	1.239005	0.321254	-1.879834
O	1.630650	1.453853	0.638738
H	3.985218	2.149736	-1.587579

Charge 0, S = 1

C	-2.979811	1.398069	1.852701
C	-2.222544	0.219603	1.769203
C	-2.876738	-0.965626	1.394097
C	-4.239470	-0.964784	1.118332
C	-4.980920	0.215000	1.210670
C	-4.344650	1.398392	1.580575
Co	0.605255	0.129481	-0.710024
C	1.694791	-1.433297	-0.406773
C	3.045392	-1.502976	-0.087752
C	3.620361	-2.754979	0.161347
C	2.853215	-3.921030	0.103667
C	1.499077	-3.849711	-0.218331
C	0.933558	-2.604192	-0.483707
C	-0.501591	-2.427323	-0.830920
O	-1.351754	-3.305085	-0.776556
N	-0.685486	-1.119821	-1.202413
H	0.866420	-4.739600	-0.271555
H	3.317752	-4.888419	0.309073
H	4.683837	-2.818675	0.408372
H	3.661492	-0.601570	-0.037738
H	-2.316008	-1.895318	1.279560
H	-4.725599	-1.897217	0.820753
H	-6.051613	0.210418	0.992095
H	-4.912436	2.329388	1.649618
H	-2.479666	2.330432	2.127838
C	-2.034467	0.719014	-1.463637
C	-3.193070	1.440422	-1.837936
C	-0.973891	2.695566	-0.817062
C	-3.200548	2.806594	-1.659551
H	-4.063207	0.922001	-2.235195
C	-2.077187	3.464071	-1.129169
H	-0.054028	3.127774	-0.414852
H	-4.092595	3.376854	-1.929642
H	-2.061858	4.543725	-0.980335
N	-0.945872	1.370132	-0.993835
N	-1.925041	-0.624110	-1.557004
C	-2.861069	-1.407247	-2.334195
H	-2.628263	-2.464899	-2.182502
H	-3.880649	-1.234096	-1.960576
H	-2.810407	-1.147040	-3.405676
C	-0.782393	0.284505	2.042941
H	-0.375276	1.294946	2.156388
C	0.066707	-0.747065	2.164751
H	-0.254908	-1.787885	2.078441
H	1.124721	-0.575050	2.367594
C	3.376526	1.390483	-3.766284
H	4.209148	2.104866	-3.778963
H	2.640388	1.658432	-4.537693
H	3.758468	0.388990	-4.020392
C	2.688872	1.312660	-2.430493
C	3.282320	1.953565	-1.313903
C	2.736714	1.958639	-0.028553
C	3.441679	2.688817	1.079707
H	3.748607	1.960123	1.846510
H	4.322893	3.241602	0.731795
H	2.738712	3.382951	1.564411
O	1.617929	0.661593	-2.393964
O	1.656639	1.378769	0.317029
H	4.217077	2.490803	-1.471228

Charge 0, S = 2

C	-3.334241	0.632841	1.532717
C	-2.105057	0.068145	1.905174
C	-1.908732	-1.304012	1.674584
C	-2.902378	-2.075304	1.082602
C	-4.119772	-1.497973	0.714547
C	-4.332938	-0.139363	0.943336
Co	0.821924	0.281676	-0.540429
C	1.262236	-1.597689	0.099858
C	2.299092	-2.029669	0.939616
C	2.550323	-3.385735	1.161872
C	1.766998	-4.364346	0.540517
C	0.732706	-3.977445	-0.302490
C	0.492938	-2.612437	-0.511506
C	-0.652981	-2.222703	-1.366013
O	-1.400412	-3.012349	-1.922973
N	-0.771437	-0.828566	-1.392468
H	0.096853	-4.712627	-0.802233
H	1.967570	-5.423882	0.717711
H	3.366384	-3.689076	1.824842
H	2.936252	-1.289085	1.436395
H	-0.962414	-1.772295	1.950337
H	-2.720816	-3.136114	0.896544
H	-4.899407	-2.110232	0.254745
H	-5.283762	0.322749	0.665256
H	-3.500851	1.700552	1.702301
C	-1.859148	1.167658	-1.448799
C	-2.914930	2.018000	-1.813480

C	-0.796339	2.864655	-0.295667
C	-2.878770	3.329743	-1.365619
H	-3.744074	1.661189	-2.420781
C	-1.807843	3.771643	-0.585662
H	0.085490	3.133794	0.292526
H	-3.691122	4.011517	-1.627542
H	-1.752573	4.796874	-0.218280
N	-0.828599	1.601308	-0.714465
N	-1.833514	-0.178723	-1.802956
C	-2.935474	-0.739869	-2.572902
H	-2.749138	-1.810423	-2.690586
H	-3.879907	-0.582738	-2.034307
H	-2.978857	-0.250241	-3.557899
C	-1.071367	0.929937	2.490000
H	-1.400457	1.951309	2.715044
C	0.204803	0.603181	2.730751

TS-pro

Charge 0, S = 0

C	-2.924256	0.997949	1.562628
C	-2.012731	-0.069278	1.562214
C	-2.529712	-1.374758	1.566740
C	-3.901957	-1.600477	1.577330
C	-4.795523	-0.528043	1.572579
C	-4.298389	0.774047	1.562257
Co	0.441484	0.223769	-0.176035
C	1.559882	-1.383475	0.189606
C	2.883879	-1.455232	0.625941
C	3.685802	-2.539086	0.266667
C	3.172457	-3.565194	-0.529594
C	1.861322	-3.488594	-0.994739
C	1.062811	-2.401214	-0.646650
C	-0.265485	-2.208374	-1.301154
O	-0.776571	-3.032821	-2.054646
N	-0.747130	-0.999107	-0.937772
H	1.432669	-4.242440	-1.659995
H	3.802704	-4.416270	-0.798615
H	4.720364	-2.583820	0.616861
H	3.293666	-0.670644	1.267912
H	-1.852114	-2.230017	1.552474
H	-4.278068	-2.626395	1.583638
H	-5.873068	-0.708280	1.579117
H	-4.984648	1.624304	1.556710
H	0.610956	-0.385704	2.503741
H	0.901411	1.337453	3.139612
C	2.972161	1.276841	-4.142414
H	3.854812	1.895338	-4.348016
H	2.129644	1.621974	-4.760722
H	3.179088	0.236708	-4.437939
C	2.558779	1.295533	-2.693387
C	3.337004	2.036144	-1.776337
C	3.060009	2.178594	-0.408120
C	3.971770	3.027289	0.438372
H	4.395586	2.403439	1.240567
H	4.788203	3.485068	-0.134022
H	3.381653	3.817073	0.928500
O	1.524142	0.634401	-2.412012
O	2.081347	1.653060	0.204014
H	4.212711	2.554579	-2.1669
H	-2.543128	2.022859	1.556419
C	-1.874560	0.924850	-1.471743
C	-2.948603	1.716587	-1.949110
C	-0.768844	2.842944	-0.716513
C	-2.876998	3.084749	-1.802090
H	-3.811146	1.245533	-2.416173
C	-1.766966	3.679852	-1.178641
H	0.115153	3.216904	-0.194753
H	-3.697069	3.706209	-2.170189
H	-1.688389	4.759135	-1.050246
N	-0.822387	1.516384	-0.854917
N	-1.832354	-0.416682	-1.562817
C	-3.001256	-1.191115	-1.928604
H	-2.692665	-2.238547	-2.000255
H	-3.805737	-1.067318	-1.185049
H	-3.359484	-0.877074	-2.919778
C	-0.569990	0.228426	1.582930
H	-0.323769	1.240025	1.916266
C	0.445909	-0.744813	1.747236
H	0.153329	-1.784123	1.907190
H	1.328149	-0.435095	2.307726
C	3.092142	0.505891	-3.446846
H	3.989185	1.104779	-3.646822
H	2.338811	0.682993	-4.227519
H	3.354060	-0.563254	-3.488491
C	2.489996	0.787819	-2.099716
C	3.203597	1.575402	-1.169926
C	2.725507	1.907057	0.097633

C	3.536986	2.807979	0.986266
H	3.803129	2.264188	1.906191
H	4.452414	3.168157	0.501513
H	2.922291	3.667833	1.293209
O	1.362852	0.274587	-1.894556
O	1.626476	1.512833	0.604539
H	4.171536	1.972773	-1.472335

Charge 0, S = 1

C	-2.860118	0.862702	1.617457
C	-1.869515	-0.136150	1.665279
C	-2.281467	-1.482618	1.646578
C	-3.626911	-1.811916	1.566827
C	-4.597767	-0.807856	1.518252
C	-4.208310	0.531463	1.547996
Co	0.511687	0.323317	-0.455841
C	1.476250	-1.417873	0.101014
C	2.839635	-1.538105	0.371246
C	3.498073	-2.728115	0.062756
C	2.792047	-3.803855	-0.483559
C	1.434612	-3.675087	-0.767660
C	0.776185	-2.472535	-0.507073
C	-0.635285	-2.275995	-0.967295
O	-1.392315	-3.223833	-1.178880
N	-0.842040	-0.949984	-1.122320
H	0.857148	-4.482286	-1.225550
H	3.309990	-4.740787	-0.702039
H	4.568130	-2.820963	0.265834
H	3.389714	-0.710954	0.827442
H	-1.542707	-2.285202	1.662855
H	-3.920508	-2.863091	1.529750
H	-5.656247	-1.071489	1.455392
H	-4.959316	1.323629	1.505921
H	-2.555704	1.912726	1.617759
C	-2.070386	0.957858	-1.474648
C	-3.201768	1.707120	-1.891283
C	-0.970550	2.926336	-0.861828
C	-3.173157	3.077353	-1.757739
H	-4.077681	1.203967	-2.295396
C	-2.040154	3.719682	-1.225929
H	-0.048822	3.341943	-0.444917
H	-4.040899	3.664341	-2.069078
H	-1.993106	4.802869	-1.113689
N	-0.976904	1.593977	-0.988673
N	-2.027407	-0.392191	-1.530227
C	-3.129546	-1.149017	-2.090751
H	-2.883445	-2.211254	-1.993824
H	-4.053710	-0.942609	-1.528602
H	-3.281260	-0.891474	-3.152283
C	-0.472336	0.259116	1.704649
H	-0.268956	1.331674	1.770606
C	0.623975	-0.607816	1.823483
H	0.449884	-1.635543	2.144876
H	1.559603	-0.162273	2.162617
C	3.675649	0.614991	-3.352639
H	3.922788	-0.458404	-3.334114
H	4.602455	1.196366	-3.436428
H	3.045939	0.783785	-4.238112
C	2.886386	0.939897	-2.113036
C	3.473284	1.756961	-1.121004
C	2.833156	2.144549	0.064173
C	3.543082	3.077197	1.010969
H	3.635634	2.592962	1.995671
H	4.538490	3.373630	0.657310
H	2.927710	3.978230	1.158401
O	1.737206	0.435524	-2.048575
O	1.677554	1.772906	0.427584
H	4.477603	2.137481	-1.306200

Charge 0, S = 2

C	-2.947853	0.907777	1.680860
C	-1.954426	-0.082964	1.778143
C	-2.353841	-1.431202	1.727553
C	-3.690915	-1.770277	1.574520
C	-4.666507	-0.773908	1.485036
C	-4.288885	0.567610	1.541174
Co	0.612991	0.411681	-0.836722
C	1.534662	-1.440921	0.151949
C	2.882709	-1.565377	0.452928
C	3.545367	-2.732008	0.059246
C	2.840091	-3.759228	-0.572480
C	1.481640	-3.618179	-0.849297
C	0.817114	-2.436642	-0.506030
C	-0.621731	-2.232310	-0.892376
O	-1.413639	-3.172920	-0.920164
N	-0.812733	-0.931639	-1.193160
H	0.910726	-4.405559	-1.348423
H	3.358481	-4.679363	-0.852961

H	4.612569	-2.846600	0.267756	H	-3.211447	-0.949432	-3.170042
H	3.423071	-0.778860	0.987179	C	-0.562906	0.323160	1.889143
H	-1.609170	-2.227172	1.770065	H	-0.371305	1.397191	1.801377
H	-3.972066	-2.823494	1.508913	C	0.516166	-0.491297	2.074738
H	-5.718406	-1.044966	1.366004	H	0.399474	-1.546800	2.325696
H	-5.042462	1.354839	1.463203	H	1.489949	-0.040615	2.263774
H	-2.651754	1.960182	1.700960	C	3.836367	0.809859	-3.570672
C	-2.147102	0.934354	-1.416576	H	4.839027	1.252160	-3.521825
C	-3.331992	1.640502	-1.753605	H	3.292918	1.213230	-4.437846
C	-1.087795	2.942172	-0.870389	H	3.925824	-0.276656	-3.726704
C	-3.354196	3.008114	-1.597300	C	3.026899	1.048703	-2.327398
H	-4.211300	1.106010	-2.106780	C	3.629764	1.676752	-1.219069
C	-2.216418	3.692299	-1.131284	C	2.955179	1.999137	-0.030279
H	-0.153661	3.397592	-0.528385	C	3.682930	2.756078	1.047781
H	-4.265892	3.560344	-1.838757	H	3.137679	3.687540	1.264201
H	-2.210158	4.774156	-0.998199	H	3.673267	2.161846	1.975001
N	-1.045913	1.611484	-1.016695	H	4.719540	2.995591	0.780333
N	-2.056042	-0.413460	-1.481515	O	1.825652	0.660409	-2.372800
C	-3.106361	-1.198003	-2.099645	O	1.749958	1.704736	0.224846
H	-2.849322	-2.254178	-1.974246	H	4.672574	1.978948	-1.3120
H	-4.060820	-1.015151	-1.585161				

IM2-pro

Charge 0, S = 0

C	-2.272310	1.069125	1.894947	H	4.609988	-2.952032	-1.572945
C	-1.732400	-0.177298	1.529047	H	4.962159	-1.840661	0.632954
C	-2.639469	-1.212429	1.250456	H	3.011281	-1.250139	2.042539
C	-4.015755	-1.005725	1.314936	H	-2.266876	-2.196426	0.960004
C	-4.529177	0.245092	1.653441	H	-4.694884	-1.834598	1.097244
C	-3.644875	1.283252	1.947619	H	-5.608678	0.407047	1.698346
Co	0.509633	0.023572	-0.359905	H	-4.028703	2.268386	2.224637
C	1.537506	-1.904145	0.609846	H	-1.587055	1.888047	2.130059
C	2.857316	-1.683563	1.050707	C	-1.880499	0.508490	-1.517502
C	3.949538	-2.030347	0.270074	C	-3.048863	1.216312	-1.882312
C	3.750742	-2.650775	-0.968563	C	-0.894703	2.487791	-0.739220
C	2.463042	-2.863106	-1.437068	C	-3.084890	2.579210	-1.680072
C	1.355316	-2.457530	-0.682903	H	-3.901839	0.683945	-2.298501
C	0.015915	-2.474319	-1.375319	C	-1.987616	3.245578	-1.110614
O	-0.363287	-3.386025	-2.104338	H	-0.015460	2.914765	-0.253920
N	-0.572464	-1.300869	-1.093172	H	-3.981889	3.138057	-1.957112
H	2.276316	-3.316430	-2.412768	H	-1.991310	4.322598	-0.945443

N	-0.845127	1.166163	-0.933950
N	-1.710096	-0.815657	-1.692518
C	-2.759855	-1.682368	-2.179684
H	-2.320570	-2.674219	-2.332954
H	-3.597098	-1.734748	-1.463085
H	-3.129394	-1.309765	-3.146246
C	-0.264338	-0.311817	1.396133
H	0.244857	0.456579	1.992436
C	0.372926	-1.679309	1.574067
H	-0.360025	-2.478489	1.403675
H	0.752420	-1.808537	2.601125
C	3.279014	0.452425	-3.607744
H	4.163910	1.081474	-3.766034
H	2.547359	0.626200	-4.409946
H	3.574041	-0.607324	-3.666106
C	2.620626	0.685725	-2.275256
C	3.264387	1.508278	-1.322204
C	2.747674	1.784916	-0.056927
C	3.508295	2.688645	0.873545
H	3.787839	2.120392	1.774562
H	4.412733	3.107159	0.415317
H	2.852522	3.507668	1.205973
O	1.523785	0.106299	-2.093838
O	1.656708	1.335026	0.423778
H	4.216332	1.962216	-1.595505

Charge 0, S = 1

C	-1.711350	1.227742	1.844284
C	-1.454653	-0.166371	1.718807
C	-2.579833	-1.028227	1.631238
C	-3.871253	-0.523138	1.661670
C	-4.097487	0.853097	1.768607
C	-3.004122	1.722790	1.860400
Co	0.459956	0.495586	-1.075051
C	1.524929	-2.125317	0.494451
C	2.822538	-2.072390	1.018104
C	3.939741	-2.201433	0.198096
C	3.776198	-2.421951	-1.169073
C	2.494740	-2.482857	-1.705845
C	1.370244	-2.299679	-0.894582
C	0.006835	-2.310003	-1.546616
O	-0.397111	-3.280503	-2.177743
N	-0.609774	-1.130139	-1.309968
H	2.342712	-2.655350	-2.773731
H	4.648626	-2.547968	-1.814808
H	4.941713	-2.149639	0.630814
H	2.953749	-1.944057	2.096666
H	-2.427011	-2.105608	1.543774
H	-4.719809	-1.209787	1.600396
H	-5.116849	1.244809	1.781259
H	-3.169929	2.799952	1.938803
H	-0.858006	1.908785	1.900043
C	-2.295121	0.407522	-1.697026
C	-3.643673	0.812333	-1.877486
C	-1.643811	2.641754	-1.487707
C	-3.940744	2.156268	-1.870356
H	-4.429320	0.071234	-2.005696
C	-2.926536	3.110348	-1.677208
H	-0.807446	3.324099	-1.311094
H	-4.976741	2.476130	-2.006441
H	-3.136155	4.179791	-1.664861
N	-1.330908	1.338178	-1.493526
N	-1.914705	-0.890543	-1.705764
C	-2.900749	-1.950011	-1.767696
H	-2.367164	-2.899272	-1.874972
H	-3.538617	-1.956068	-0.868236
H	-3.531945	-1.818617	-2.658472
C	-0.114634	-0.622645	1.659781
H	0.667931	0.125633	1.808653
C	0.334034	-2.026385	1.427241
H	-0.488990	-2.640898	1.036741
H	0.626318	-2.484289	2.392160
C	3.984710	0.774949	-3.407407
H	4.992363	1.163578	-3.215600
H	3.562517	1.253961	-4.302818
H	4.048212	-0.303928	-3.619851
C	3.048110	0.974011	-2.250380
C	3.553758	1.462416	-1.028685
C	2.783244	1.713285	0.113984
C	3.447345	2.248482	1.350440
H	3.404284	1.474563	2.133831
H	4.494480	2.530699	1.186172
H	2.881786	3.115153	1.723091
O	1.838751	0.675892	-2.466315
O	1.529033	1.517238	0.214207
H	4.620266	1.678577	-0.974906

Charge 0, S = 2

C	-1.351922	1.269267	2.019606
C	-1.240163	-0.129789	1.782194
C	-2.440666	-0.839195	1.507839
C	-3.660379	-0.184952	1.450205
C	-3.741143	1.196501	1.659010
C	-2.575858	1.914078	1.950506
Co	0.341775	0.487667	-0.973034
C	1.518872	-2.247686	0.458155
C	2.823944	-2.267145	0.968436
C	3.928966	-2.397046	0.133864
C	3.745014	-2.546369	-1.240779
C	2.457688	-2.537915	-1.763880
C	1.344763	-2.352396	-0.935466
C	-0.006558	-2.300828	-1.605928
O	-0.372059	-3.185564	-2.371088
N	-0.672911	-1.175642	-1.250402
H	2.286520	-2.660815	-2.835551
H	4.605946	-2.675283	-1.901299
H	4.935470	-2.403759	0.559105
H	2.968982	-2.196300	2.050553
H	-2.400210	-1.916236	1.337155
H	-4.568776	-0.754361	1.236341
H	-4.703908	1.707969	1.596392
H	-2.628559	2.993035	2.115769
H	-0.439035	1.836060	2.213362
C	-2.373983	0.322181	-1.746361
C	-3.717493	0.694021	-2.016166
C	-1.790738	2.572142	-1.510973
C	-4.045130	2.030749	-2.042106
H	-4.474936	-0.066085	-2.194696
C	-3.068827	3.009250	-1.787412
H	-0.984388	3.275058	-1.283317
H	-5.076041	2.325461	-2.253332
H	-3.303781	4.073425	-1.794621
N	-1.446876	1.276545	-1.490858
N	-1.962278	-0.965110	-1.717587
C	-2.920800	-2.048453	-1.772925
H	-2.367439	-2.988946	-1.845019
H	-3.584145	-2.045645	-0.891121
H	-3.531292	-1.962629	-2.683142
C	0.037312	-0.742272	1.798113
H	0.883424	-0.110292	2.080362
C	0.354379	-2.151523	1.425671
H	-0.523959	-2.653221	1.000570
H	0.630640	-2.719811	2.334399
C	3.918605	0.775474	-3.234924
H	4.913481	1.190654	-3.032433
H	3.505108	1.224888	-4.149711
H	4.008074	-0.306236	-3.419899
C	2.954145	0.983315	-2.102758
C	3.415622	1.542634	-0.894069
C	2.609692	1.815194	0.219014
C	3.222248	2.444991	1.438291
H	3.143274	1.739372	2.280713
H	4.275437	2.716720	1.296817
H	2.643896	3.339402	1.714568
O	1.760992	0.631413	-2.327135
O	1.363102	1.572700	0.303925
H	4.471557	1.803123	-0.829149