

Supplementary Information

High-throughput screening and machine learning prediction of Rh-catalyzed *ortho*-C(sp²)-H amidation of arylaldehyde hydrazones

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Table of Contents

1. General Information	S2
2. General Procedure for the Preparation of Starting Materials	S3
3. General Experimental Procedure.....	S6
4. HTE for Substrate Scope	S11
5. HTE for 400 Unknown Reactions	S17
6. Development of Machine Learning Model	S20
7. X-ray Crystallographic Data of 3	S26
8. Reaction Mechanism	S27
9. Characterization Data for the Products.....	S31
10. Characterization Data for Hydrazones and Dioxazolones.....	S62
11. References	S74
12. NMR Spectral Data for Isolated Products and Starting Materials.....	S76

1. General Information

Materials. Reactions were carried out under a nitrogen atmosphere in oven-dried Schlenk tubes unless otherwise specified. The heat source is IKA magnetic stirrer with RCT Basic. Reagents were purchased from commercial suppliers (Energy, Bidepharm, Macklin, Alfa Aesar, Sigma-Aldrich, and J&K Scientific) and used with no further purification. Catalysts and additives were stored in glovebox. Anhydrous solvents in sure-seal bottle were purchased from Energy and used with no further purification. All reactions were set up inside Vigor glovebox with constant N₂ purge (oxygen typically < 5 ppm). Organic solutions were concentrated under reduced pressure on a Heidolph rotary evaporator using a water bath.

Instruments. ¹H and ¹³C NMR spectra were recorded at 600 MHz (¹³C at 150 MHz) on Bruker Avance III 600 MHz spectrometer as indicated. NMR spectra run in solutions of deuterated chloroform (CDCl₃) with residual chloroform as internal standard (7.256 ppm for ¹H and 77.00 ppm for ¹³C), and chemical shifts were reported in parts per million (ppm). ¹⁹F NMR spectra were recorded on a Bruker Avance III 600 MHz (¹⁹F at 564 MHz), and were reported unreferenced. Abbreviations for signal multiplicity are as follow: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, etc. Coupling constants (*J* values) were calculated directly from the spectra. Flash column chromatography was performed on silica gel (300–400 mesh) with the solvents given in the procedures. Thin layer chromatographic (TLC) analysis was performed with glass-backed silica gel plates, visualizing with UV light (254 nm). The high resolution mass spectra (HRMS) were measured on a Waters Xevo G2-XS using electrospray ionization time-of-flight (ESI-TOF). The single-crystal X-ray diffraction was conducted on a XtaLAB Synergy-Custom X-ray single-crystal diffractometer.

Standard Workflow

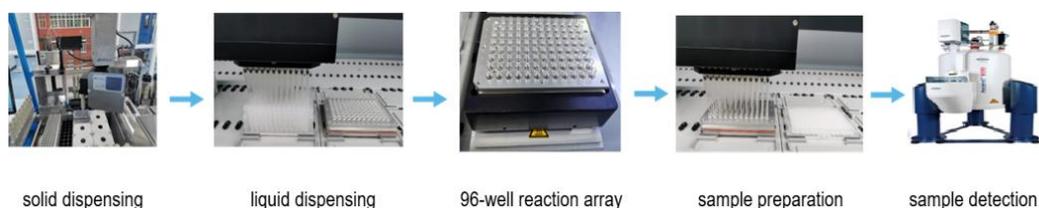


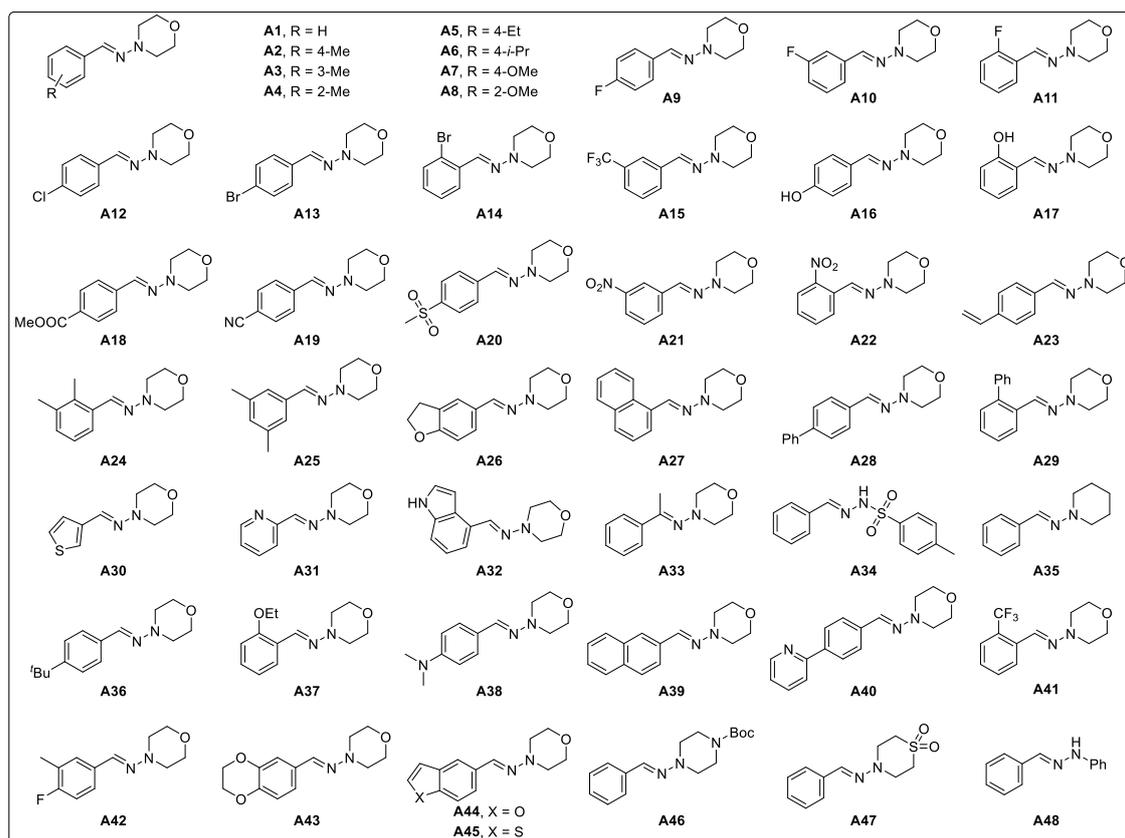
Figure S1. A 900 μ L-glass tube equipped with a magnetic stir bar (C3*5 mm) was charged with catalyst (5 mol %), additive (20 mol %), arylaldehyde hydrazone (0.005 mmol, 1.0 equiv), and dioxazolone (0.0075 mmol, 1.5 equiv); then DCE (100 μ L) was added. The plate was sealed and stirred (820 r/min in IKA RCT basic) at 100 °C for 20 h

under N₂ atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature, the plate was opened and add internal standard to each well (100 μL of 1.0 M 1,3,5-trimethoxybenzene solution in MeOH). The Opentrons 8-channels pipetting device was used to add 200 μL MeOH to each well, mixed dissolution. Then, the Opentrons 8-channels pipetting device was used to transfer 200 μL of reaction liquor to a deep well plate (each well, 2 mL). At that point, organic solutions for 2 mL deep well plate were concentrated under reduced pressure on a miniVac at 37 °C for 4 h under 10 mbar. Finally, pipette was used to add 300 μL CDCl₃ to each well, mixed dissolution, were sampled into 3 mm NMR tube and analyzed by ¹H NMR.

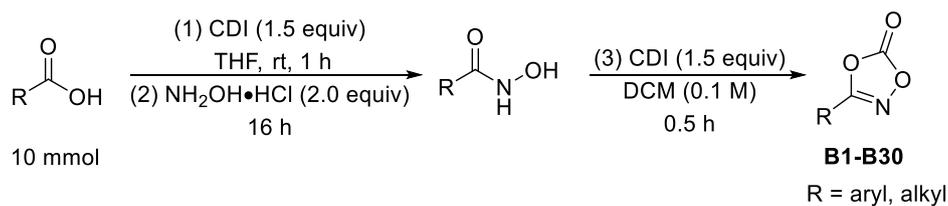
2. General Procedure for the Preparation of Starting Materials

A) Synthesis of Hydrazones

The following hydrazones were used in this study and were prepared according to the previous literature.¹⁻⁵ All new compounds have been characterized by ¹H NMR and ¹³C NMR.



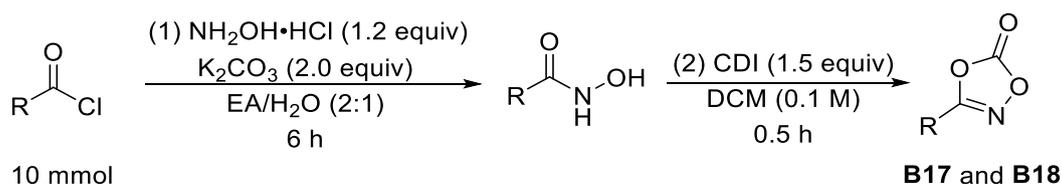
a) Synthesis of dioxazolones from carboxylic acids⁶⁻⁸



Carboxylic acid (10 mmol, 1.0 equiv) was dissolved in anhydrous THF (20 mL) in a 100 mL round bottom flask with a magnetic stir bar. Then, 1,1'-carbonyldiimidazole (CDI, 15 mmol, 1.5 equiv) was added to the solution at room temperature, and the resulting mixture was stirred at room temperature for 1 h. $\text{NH}_2\text{OH}\cdot\text{HCl}$ (1.39 g, 20 mmol) was added and the resulting mixture was stirred overnight. The mixture was diluted with 5% aq. KHSO_4 (30 mL) and extracted with ethyl acetate (2×30 mL). The combined organic phase was washed with brine (50 mL) and dried over anhydrous Na_2SO_4 . The extract was filtered and concentrated in vacuo. The crude product was used in the next step without any further purification.

Crude hydroxamic acid was dissolved in DCM (0.1 M solution), followed by the addition of CDI (1.5 equiv). The mixture was then stirred at room temperature for 0.5 h and then quenched with 1 M HCl (20 mL), followed by extraction with DCM (20 mL \times 3). The combined organic layers were dried over anhydrous Na_2SO_4 , and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to give the desired dioxazolones.

b) Synthesis of dioxazolones from acyl chlorides⁹⁻¹¹



A 250 mL round bottom flask was charged with K_2CO_3 (2.0 equiv, 20.0 mmol), ethyl acetate (80 mL) and water (40 mL). At 0 °C, $\text{NH}_2\text{OH}\cdot\text{HCl}$ (1.2 equiv, 12 mmol) was added, then acyl chloride (10.0 mmol) was dropwised slowly. The resulting solution was stirred at room temperature for 6 h. The organic phase was separated and the aqueous phase was extracted with ethyl acetate (2×40 mL). The combined organic layers were dried over anhydrous Na_2SO_4 , filtered and concentrated in vacuo. The crude products were used in the next step without any further purification.

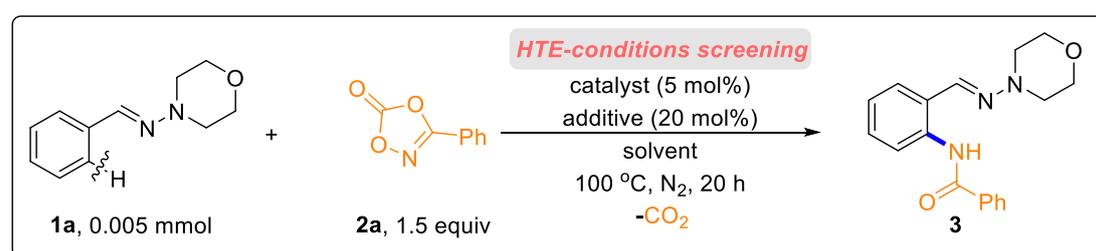
Crude hydroxamic acid was dissolved in DCM (0.1 M solution), followed by the addition of CDI (1.5 equiv).

The mixture was then stirred at room temperature for 0.5 h and then quenched with 1 M HCl (20 mL), followed by extraction with DCM (20 mL × 3). The combined organic layers were dried over anhydrous Na₂SO₄, and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to give the desired dioxazolones.

3. General Experimental Procedure

A) Reaction Optimization

Table S1. HTE screening of conditions for C–H amidation of **1a** and **2a**^a

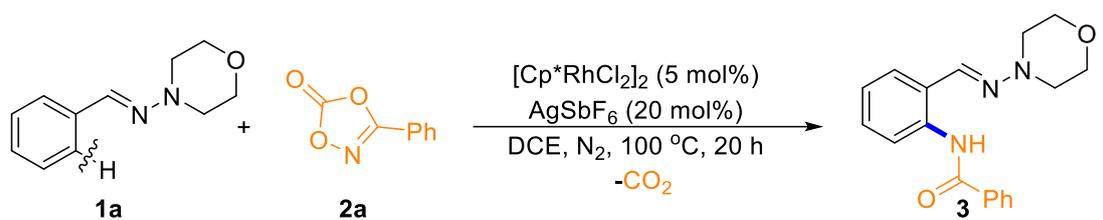


	[Cp*RhCl ₂] ₂	[Rh(COD)Cl] ₂	Rh(PPh ₃) ₃ Cl	[Ru(p-cymene)Cl ₂] ₂	[Cp*IrCl ₂] ₂	Pd(OAc) ₂	Mn(CO) ₅ Br	Cp*Co(CO) ₂	Cu(OTf) ₂	Cu(OAc) ₂	Fe(OAc) ₃	Zn(OAc) ₂	
AgSbF ₆	86	0	0	16	5	0	0	0	0	0	0	0	DCE
AgOTf	24	0	0	0	0	0	0	0	0	0	0	0	
AgBF ₄	60	0	0	0	0	0	0	0	0	0	0	0	
AgNTf ₂	38	2	0	0	0	0	0	0	0	0	0	0	
AgSbF ₆	12	0	0	0	0	0	0	0	0	0	0	0	CH ₃ CN
AgOTf	8	0	0	0	3	0	0	0	0	0	0	0	
AgBF ₄	3	0	0	0	2	0	0	0	0	0	0	0	
AgNTf ₂	6	0	0	0	0	0	0	0	0	0	0	0	
AgSbF ₆	22	0	0	3	0	0	0	0	0	0	0	0	1,4-dioxane
AgOTf	14	3	0	0	0	0	0	0	0	0	0	0	
AgBF ₄	7	0	0	0	0	0	0	0	0	0	0	0	
AgNTf ₂	16	2	0	0	2	0	0	0	0	0	0	0	
AgSbF ₆	6	0	0	2	0	0	0	0	0	0	0	0	THF
AgOTf	10	0	0	0	0	0	0	0	0	0	0	0	
AgBF ₄	2	0	0	0	0	0	0	0	0	0	0	0	
AgNTf ₂	36	2	0	2	0	0	0	0	0	0	0	0	

numbers indicated yield (%) of **3**

^aReaction conditions: **1a** (0.005 mmol), **2a** (0.0075 mmol), catalyst (5 mol%), additive (20 mol%) in solvent (100 μL) at 100°C for 20 h under N₂ atmosphere. Yields were determined by ¹H NMR using 1,3,5-trimethoxybenzene as internal standard.

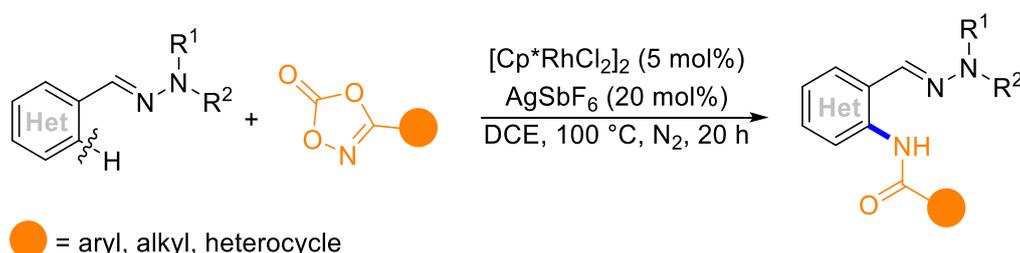
Table S2. Screening of temperature for Rh-catalyzed C–H amidation of **1a and **2a**^a**



entry	catalyst	additive	temp (°C)	3 (%) ^b
1	[Cp*RhCl ₂] ₂	AgSbF ₆	100	88
2	-	AgSbF ₆	100	0
3	[Cp*RhCl ₂] ₂	-	100	0
4	[Cp*RhCl ₂] ₂	AgSbF ₆	80	86
5	[Cp*RhCl ₂] ₂	AgSbF ₆	120	81
6 ^c	[Cp*RhCl ₂] ₂	AgSbF ₆	100	79

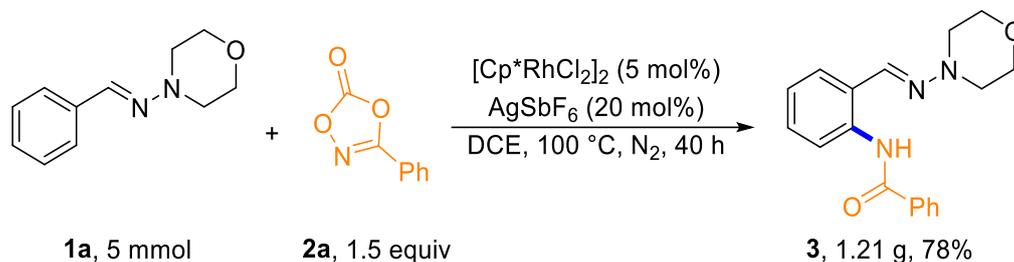
^aReaction conditions: **1a** (0.10 mmol), **2a** (0.15 mmol), [Cp*RhCl₂]₂ (5 mol%), and AgSbF₆ (20 mol%), in DCE (1.0 mL) at 100 °C for 20 h under N₂ atmosphere. ^bYields were determined by ¹H NMR using 1,3,5-trimethoxybenzene as internal standard. ^cair.

B) General Experimental Procedure for Rh-Catalyzed *ortho*-C(sp²)-H Amidation of Arylaldehyde Hydrazones with Dioxazolones



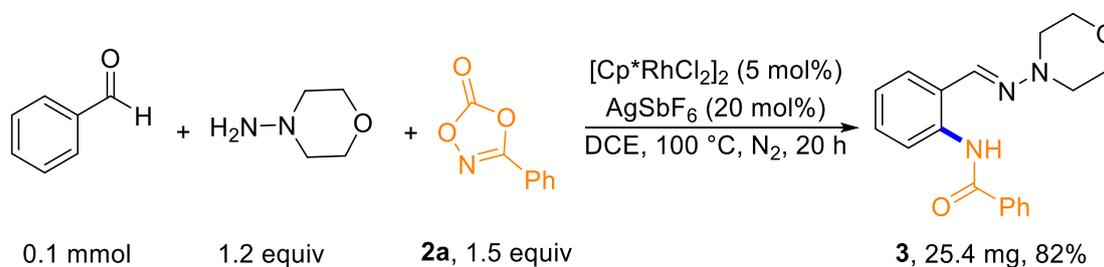
An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with [Cp*RhCl₂]₂ (3.0 mg, 0.005 mmol, 5 mol%), AgSbF₆ (5.0 mg, 0.02 mmol, 20 mol%), arylaldehyde hydrazones (0.1 mmol, 1.0 equiv), and dioxazolones (0.15 mmol, 1.5 equiv); then DCE (1.0 mL) was added. The reaction mixture was stirred (820 r/min in IKA RCT basic) at 100 °C for 20 h under N₂ atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature. The crude product was extracted with ethyl acetate (3 × 3.0 mL), and the solution was washed with saturated solution of NH₄Cl (3.0 mL), and the organic layer was dried over anhydrous Na₂SO₄ and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to give the desired products.

C) Gram-Scale Synthesis of **3**



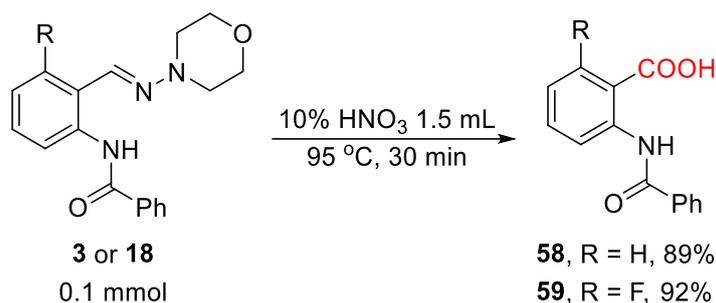
An oven dried Schlenk tube of 100 mL equipped with a magnetic stir bar was charged with $[\text{Cp}^*\text{RhCl}_2]_2$ (154.5 mg, 0.25 mmol, 5 mol%), AgSbF_6 (249.9 mg, 1.0 mmol, 20 mol%), arylaldehyde hydrazone (**1a**, 5.0 mmol, 1.0 equiv), and dioxazolone (**2a**, 7.5 mmol, 1.5 equiv); then DCE (40 mL) was added. The reaction mixture was stirred (820 r/min in IKA RCT basic) at 100 °C for 40 h under N_2 atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature. The crude product was extracted with ethyl acetate (3×15 mL), and the solution was washed with saturated solution of NH_4Cl (25 mL), and the organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to afford the corresponding product **3** in 78% yield (1.210 g).

D) One-Pot Synthesis of **3**



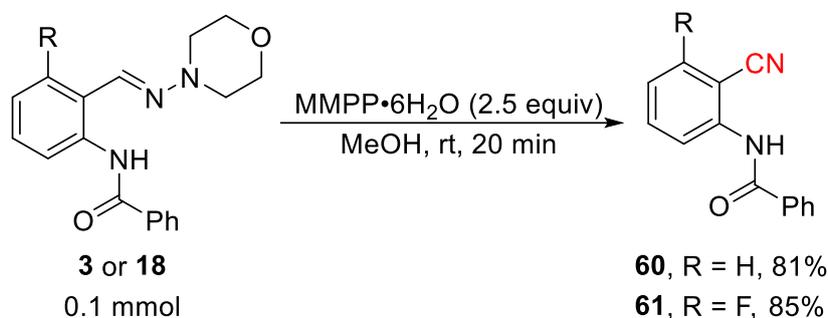
An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with $[\text{Cp}^*\text{RhCl}_2]_2$ (3.0 mg, 0.005 mmol, 5 mol%), AgSbF_6 (5.0 mg, 0.02 mmol, 20 mol%), benzaldehyde (0.1 mmol, 1.0 equiv), morpholin-4-amine (0.12 mmol, 1.2 equiv), and dioxazolone (**2a**, 0.15 mmol, 1.5 equiv); then DCE (1.0 mL) was added. The reaction mixture was stirred (820 r/min in IKA RCT basic) at 100 °C for 20 h under N_2 atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature. The crude product was extracted with ethyl acetate (3×3.0 mL), and the solution was washed with saturated solution of NH_4Cl (3.0 mL), and the organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to afford the corresponding product **3** in 82% yield (25.4 mg).

E) Synthesis of 2-Benzamidobenzoic Acids



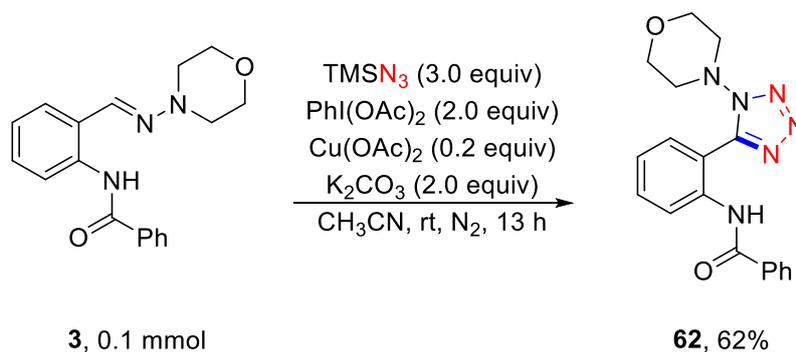
The preparation of this compound was performed according to a literature reference.¹² An oven dried Schlenk tube of 25 mL was equipped with 1.5 mL of 10% HNO₃ and **3** or **18** (0.1 mmol, 30.9 mg) and heated to 95 °C and stirred for 30 min. After completion of the reaction detected by TLC, the reaction mixture was cooled to room temperature and extracted with dichloromethane (2 × 5 mL), the organic layers were combined and dried over anhydrous Na₂SO₄. The organic layer was dried, filtered and precipitated by vacuum evaporation to give a white solid. The crude product was purified by flash column chromatography on silica gel to afford 2-benzamidobenzoic acid **58** in 89% yield (21.4 mg) or 2-benzamido-6-fluorobenzoic acid **59** in 92% yield (23.8 mg).

F) Synthesis of *N*-(2-Cyanophenyl)benzamides



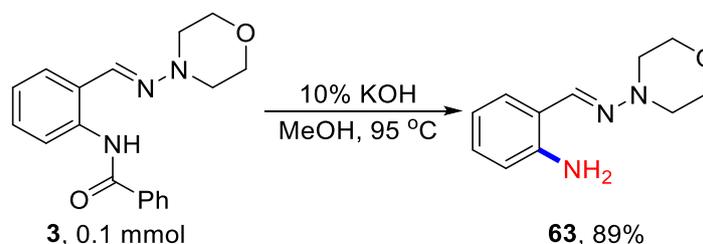
The preparation of this compound was performed according to a literature reference.¹³ An oven dried Schlenk tube of 25 mL was charged with a suspension of **3** or **18** (0.1 mmol, 30.9 mg) in MeOH (0.5 mL), then a solution of magnesium monoperoxyphthalate hexahydrate (MMPP·6H₂O, 0.25 mmol, 124 mg) in MeOH (0.5 mL) was added dropwise. After consumption of the starting material (20 min, TLC monitoring), dichloromethane (15 mL) and water (15 mL) were added. The organic layer was washed with brine (2 × 10 mL), dried over Na₂SO₄, and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to afford *N*-(2-cyanophenyl)benzamide **60** in 81% yield (18.0 mg) or *N*-(2-cyano-3-fluorophenyl)benzamide **61** in 85% yield (20.4 mg).

G) Synthesis of *N*-(2-(1-Morpholino-1*H*-tetrazol-5-yl)phenyl)benzamide **62**



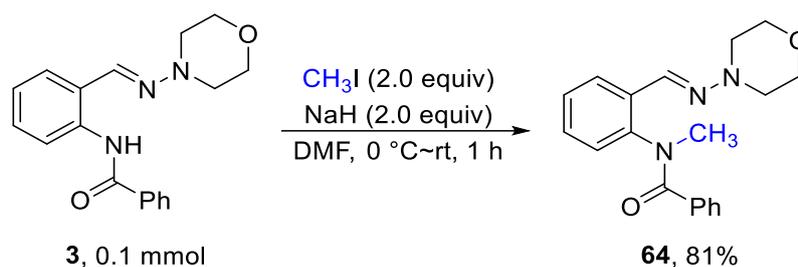
The preparation of this compound was performed according to a literature reference.¹⁴ An oven-dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with **3** (0.1 mmol, 30.9 mg), TMSN₃ (3.0 equiv, 0.3 mmol, 34.5 mg), PhI(OAc)₂ (2.0 equiv, 0.2 mmol, 64.4 mg), Cu(OAc)₂ (0.2 equiv, 0.02 mmol, 3.6 mg), and K₂CO₃ (2.0 equiv, 0.2 mmol, 27.6 mg). The flask was evacuated and backfilled with N₂ for 3 times; then CH₃CN (2.0 mL) was added with syringe under N₂. The reaction mixture was stirred at room temperature and monitored by TLC. After completion of the reaction, the reaction mixture was concentrated under vacuum to remove CH₃CN, and the residue was purified by chromatography on silica gel to afford the **62** in 62% yield (21.7 mg).

H) Synthesis of (*E*)-2-((Morpholinoimino)methyl)aniline **63**



The preparation of this compound was performed according to a literature reference.¹⁵ An oven-dried Schlenk tube of 25 mL charged with **3** (0.1 mmol, 30.9 mg) was added 10% KOH aqueous solution (2.0 mL) in MeOH (1.0 mL) solution. The reaction mixture was stirred at 95 °C for 8 h. The mixture was extracted with EtOAc (3 × 5 mL), and the combined organic phases were washed with water, dried over anhydrous Na₂SO₄ and concentrated in vacuo. The residue was purified by flash column chromatography (PE/EA = 10:1) to afford yellow solid **63** in 89% yield (18.2 mg).

D) Synthesis of (*E*)-*N*-methyl-*N*-(2-((morpholinoimino)methyl)phenyl)benzamide



The preparation of this compound was performed according to a literature reference.¹⁶ An oven-dried Schlenk tube of 25 mL charged with NaH (5.0 mg, 0.2 mmol, 2.0 equiv.) was suspended in 1.0 mL DMF. A solution of **3** (0.1 mmol, 30.9 mg) in 1.0 mL DMF was added dropwise under vigorous stirring. Subsequently, methyl iodide (13 μL , 0.2 mmol, 2.0 equiv.) was added dropwise and the reaction mixture was stirred at room temperature for one hour. The reaction was then quenched by addition of ice-cold water and extracted twice with Et₂O. The combined organic phases were washed with water, dried over anhydrous Na₂SO₄ and concentrated in vacuo. Purification by flash chromatography (PE/EA= 10:1) gave the product **64** as a colorless oil in 81% yield (26.2 mg).

4. HTE for Substrate Scope

a) Reaction Setup

A 900 μL -glass tube equipped with a magnetic stir bar (C3*5 mm) was charged with catalyst (5 mol%), additive (20 mol %), hydrazone (0.005 mmol, 1.0 equiv), and dioxazolone (0.0075 mmol, 1.5 equiv); then DCE (100 μL) was added. The plate was sealed and stirred (820 r/min in IKA RCT basic) at 100 °C for 20 h under N₂ atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature, the plate was opened and add internal standard to each well (100 μL of 1.0 M 1,3,5-trimethoxybenzene solution in MeOH). The Opentrons 8-channels pipetting device was used to add 200 μL MeOH to each well, mixed dissolution. Then, the Opentrons 8-channels pipetting device was used to transfer 200 μL of reaction liquor to a deep well plate (each well, 2 mL). At that point, organic solutions for 2 mL deep well plate were concentrated under reduced pressure on a miniVac at 37 °C for 4 h under 10 mbar. Finally, pipette was used to add 300 μL CDCl₃ to each well, mixed dissolution, were sampled into 3 mm NMR tube and analyzed by ¹H NMR.

b) Plate Layout

Under optimal conditions, below is a summary (**Figure S2**) of other 30 arylaldehyde hydrazones and 20 dioxazolones used in this work, furnishing 600 scattered of micromolar reactions via HTE.

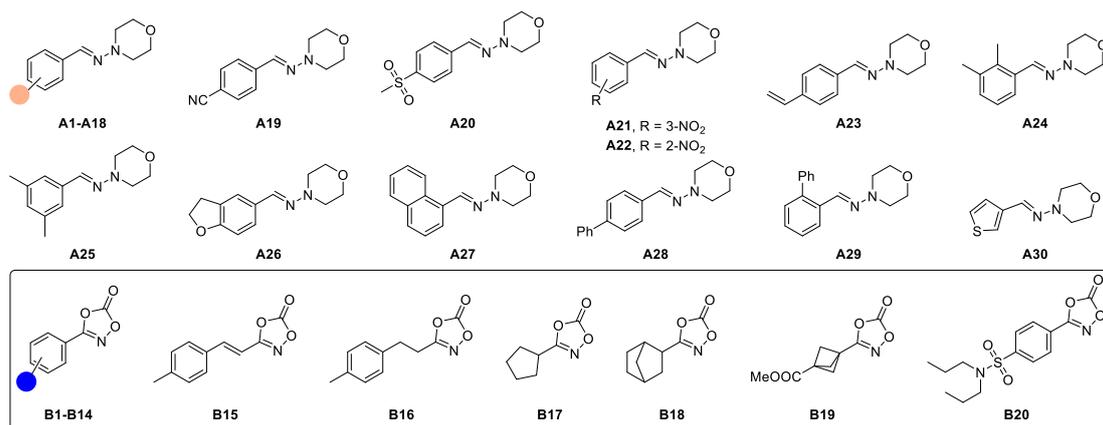


Figure S2. All reaction components for 600 scattered of micromolar reactions.

Table S3–S9 describe the components of each well for each plate.

Table S3. Layout of plate 1.

	1	2	3	4	5	6	7	8
A	A1B1	A2B1	A3B1	A4B1	A5B1	A6B1	A7B1	A8B1
B	A9B1	A10B1	A11B1	A12B1	A13B1	A14B1	A15B1	A16B1
C	A17B1	A18B1	A19B1	A20B1	A21B1	A22B1	A23B1	A24B1
D	A25B1	A26B1	A27B1	A28B1	A29B1	A30B1	A1B2	A2B2
E	A3B2	A4B2	A5B2	A6B2	A7B2	A8B2	A9B2	A10B2
F	A11B2	A12B2	A13B2	A14B2	A15B2	A16B2	A17B2	A18B2
G	A19B2	A20B2	A21B2	A22B2	A23B2	A24B2	A25B2	A26B2
H	A27B2	A28B2	A29B2	A30B2	A1B3	A2B3	A3B3	A4B3
I	A5B3	A6B3	A7B3	A8B3	A9B3	A10B3	A11B3	A12B3
J	A13B3	A14B3	A15B3	A16B3	A17B3	A18B3	A19B3	A20B3
K	A21B3	A22B3	A23B3	A24B3	A25B3	A26B3	A27B3	A28B3
L	A29B3	A30B3						

Table S4. Layout of plate 2.

	1	2	3	4	5	6	7	8
A	A1B4	A2B4	A3B4	A4B4	A5B4	A6B4	A7B4	A8B4
B	A9B4	A10B4	A11B4	A12B4	A13B4	A14B4	A15B4	A16B4
C	A17B4	A18B4	A19B4	A20B4	A21B4	A22B4	A23B4	A24B4
D	A25B4	A26B4	A27B4	A28B4	A29B4	A30B4	A1B5	A2B5
E	A3B5	A4B5	A5B5	A6B5	A7B5	A8B5	A9B5	A10B5

F	A11B5	A12B5	A13B5	A14B5	A15B5	A16B5	A17B5	A18B5
G	A19B5	A20B5	A21B5	A22B5	A23B5	A24B5	A25B5	A26B5
H	A27B5	A28B5	A29B5	A30B5	A1B6	A2B6	A3B6	A4B6
I	A5B6	A6B6	A7B6	A8B6	A9B6	A10B6	A11B6	A12B6
J	A13B6	A14B6	A15B6	A16B6	A17B6	A18B6	A19B6	A20B6
K	A21B6	A22B6	A23B6	A24B6	A25B6	A26B6	A27B6	A28B6
L	A29B6	A30B6						

Table S5. Layout of plate 3.

	1	2	3	4	5	6	7	8
A	A1B7	A2B7	A3B7	A4B7	A5B7	A6B7	A7B7	A8B7
B	A9B7	A10B7	A11B7	A12B7	A13B7	A14B7	A15B7	A16B7
C	A17B7	A18B7	A19B7	A20B7	A21B7	A22B7	A23B7	A24B7
D	A25B7	A26B7	A27B7	A28B7	A29B7	A30B7	A1B8	A2B8
E	A3B8	A4B8	A5B8	A6B8	A7B8	A8B8	A9B8	A10B8
F	A11B8	A12B8	A13B8	A14B8	A15B8	A16B8	A17B8	A18B8
G	A19B8	A20B8	A21B8	A22B8	A23B8	A24B8	A25B8	A26B8
H	A27B8	A28B8	A29B8	A30B8	A1B9	A2B9	A3B9	A4B9
I	A5B9	A6B9	A7B9	A8B9	A9B9	A10B9	A11B9	A12B9
J	A13B9	A14B9	A15B9	A16B9	A17B9	A18B9	A19B9	A20B9
K	A21B9	A22B9	A23B9	A24B9	A25B9	A26B9	A27B9	A28B9
L	A29B9	A30B9						

Table S6. Layout of plate 4.

	1	2	3	4	5	6	7	8
A	A1B10	A2B10	A3B10	A4B10	A5B10	A6B10	A7B10	A8B10
B	A9B10	A10B10	A11B10	A12B10	A13B10	A14B10	A15B10	A16B10
C	A17B10	A18B10	A19B10	A20B10	A21B10	A22B10	A23B10	A24B10
D	A25B10	A26B10	A27B10	A28B10	A29B10	A30B10	A1B11	A2B11
E	A3B11	A4B11	A5B11	A6B11	A7B11	A8B11	A9B11	A10B11
F	A11B11	A12B11	A13B11	A14B11	A15B11	A16B11	A17B11	A18B11
G	A19B11	A20B11	A21B11	A22B11	A23B11	A24B11	A25B11	A26B11
H	A27B11	A28B11	A29B11	A30B11	A1B12	A2B12	A3B12	A4B12

I	A5B12	A6B12	A7B12	A8B12	A9B12	A10B12	A11B12	A12B12
J	A13B12	A14B12	A15B12	A16B12	A17B12	A18B12	A19B12	A20B12
K	A21B12	A22B12	A23B12	A24B12	A25B12	A26B12	A27B12	A28B12
L	A29B12	A30B12						

Table S7. Layout of plate 5.

	1	2	3	4	5	6	7	8
A	A1B13	A2B13	A3B13	A4B13	A5B13	A6B13	A7B13	A8B13
B	A9B13	A10B13	A11B13	A12B13	A13B13	A14B13	A15B13	A16B13
C	A17B13	A18B13	A19B13	A20B13	A21B13	A22B13	A23B13	A24B13
D	A25B13	A26B13	A27B13	A28B13	A29B13	A30B13	A1B14	A2B14
E	A3B14	A4B14	A5B14	A6B14	A7B14	A8B14	A9B14	A10B14
F	A11B14	A12B14	A13B14	A14B14	A15B14	A16B14	A17B14	A18B14
G	A19B14	A20B14	A21B14	A22B14	A23B14	A24B14	A25B14	A26B14
H	A27B14	A28B14	A29B14	A30B14	A1B15	A2B15	A3B15	A4B15
I	A5B15	A6B15	A7B15	A8B15	A9B15	A10B15	A11B15	A12B15
J	A13B15	A14B15	A15B15	A16B15	A17B15	A18B15	A19B15	A20B15
K	A21B15	A22B15	A23B15	A24B15	A25B15	A26B15	A27B15	A28B15
L	A29B15	A30B15						

Table S8. Layout of plate 6.

	1	2	3	4	5	6	7	8
A	A1B16	A2B16	A3B16	A4B16	A5B16	A6B16	A7B16	A8B16
B	A9B16	A10B16	A11B16	A12B16	A13B16	A14B16	A15B16	A16B16
C	A17B16	A18B16	A19B16	A20B16	A21B16	A22B16	A23B16	A24B16
D	A25B16	A26B16	A27B16	A28B16	A29B16	A30B16	A1B17	A2B17
E	A3B17	A4B17	A5B17	A6B17	A7B17	A8B17	A9B17	A10B17
F	A11B17	A12B17	A13B17	A14B17	A15B17	A16B17	A17B17	A18B17
G	A19B17	A20B17	A21B17	A22B17	A23B17	A24B17	A25B17	A26B17
H	A27B17	A28B17	A29B17	A30B17	A1B18	A2B18	A3B18	A4B18
I	A5B18	A6B18	A7B18	A8B18	A9B18	A10B18	A11B18	A12B18
J	A13B18	A14B18	A15B18	A16B18	A17B18	A18B18	A19B18	A20B18
K	A21B18	A22B18	A23B18	A24B18	A25B18	A26B18	A27B18	A28B18
L	A29B18	A30B18						

Table S9. Layout of plate 7.

	1	2	3	4	5	6	7	8
A	A1B19	A2B19	A3B19	A4B19	A5B19	A6B19	A7B19	A8B19
B	A9B19	A10B19	A11B19	A12B19	A13B19	A14B19	A15B19	A16B19
C	A17B19	A18B19	A19B19	A20B19	A21B19	A22B19	A23B19	A24B19
D	A25B19	A26B19	A27B19	A28B19	A29B19	A30B19	A1B20	A2B20
E	A3B20	A4B20	A5B20	A6B20	A7B20	A8B20	A9B20	A10B20
F	A11B20	A12B20	A13B20	A14B20	A15B20	A16B20	A17B20	A18B20
G	A19B20	A20B20	A21B20	A22B20	A23B20	A24B20	A25B20	A26B20
H	A27B20	A28B20	A29B20	A30B20				
I								
J								
K								
L								

c) Yield Determination

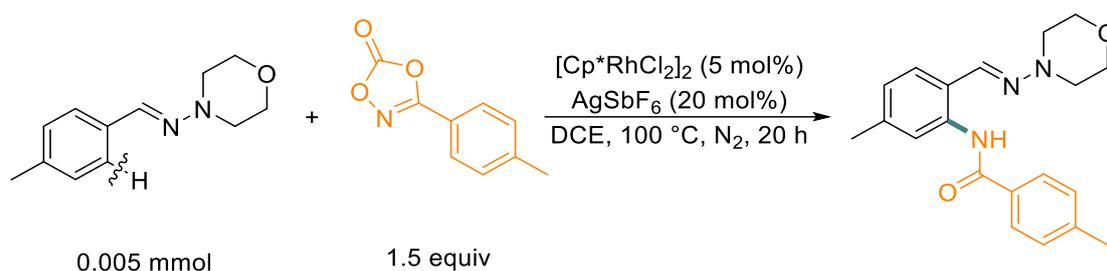


Figure S3. Reaction summary for plate 1, row 1, column 2.

In light of the unique ^1H NMR shift of the $\text{C}(\text{sp}^2)\text{-H}$ of $\text{C}=\text{N}$ bond, we were able to identify the reaction yield by ^1H NMR analysis. The reaction above (**Figure S3**) was set up in 96-well plate 1 (90 reactions) following the HTE protocol described in the general section. After 20 h, the reaction was analyzed by ^1H NMR (CDCl_3) and the yield determined using 1,3,5-trimethoxybenzene as an internal standard (**Figure S4**).

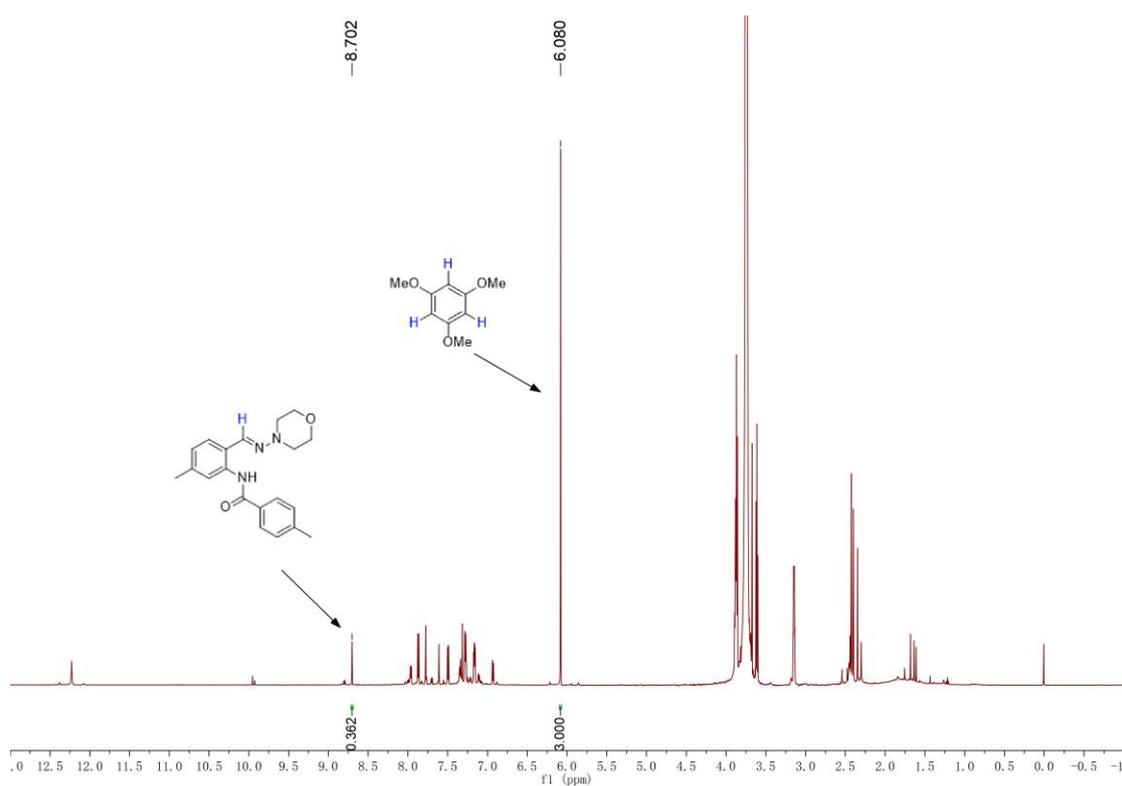


Figure S4. Crude ^1H NMR spectra for plate 1, row 1, column 2.

Table S10. Chemical shifts of characteristic peaks of product and internal standard (^1H NMR).

entry	characteristic peak	chemical shift	results
product	$\text{C}(\text{sp}^2)\text{-H}$ of $\text{C}=\text{N}$ (s, 1H)	8.702 ppm	0.36, 36% yield
internal standard	$\text{C}(\text{sp}^2)\text{-H}$ (s, 3H)	6.080 ppm	3.00

5. HTE for 400 Unknown Reactions

a) Plate Layout

Under optimal conditions, we performed the 400 reactions for external dataset prediction via HTE, which were randomly designed by experimenters. As shown in **Figure S5**, those new reactions included some unseen substrates, such as arylaldehyde hydrazones (**A31–A40**) and dioxazolones (**B21–B25**).

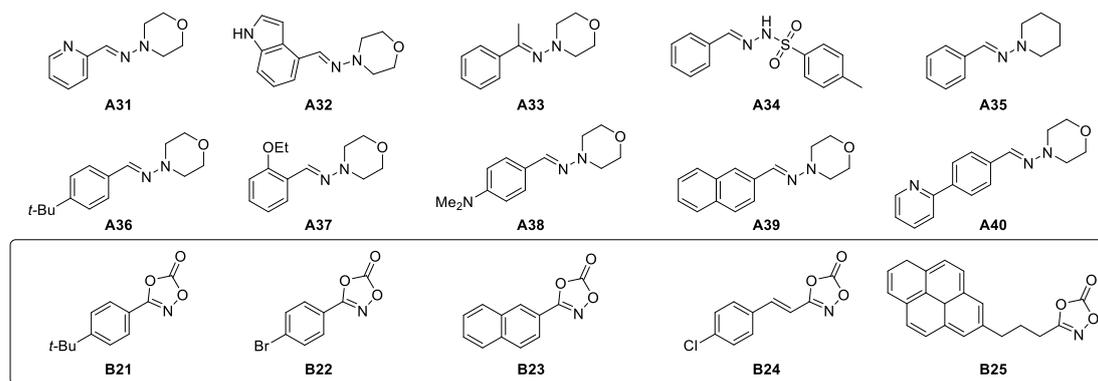


Figure S5. Unseen substrates.

Table S11–S15 describe the components of each well for each plate (10 arylaldehyde hydrazones and 5 dioxazolones).

Table S11. Layout of plate 8.

	1	2	3	4	5	6	7	8
A	A1B24	A2B24	A3B24	A4B24	A5B24	A6B24	A7B24	A8B24
B	A9B24	A10B24	A11B24	A12B24	A13B24	A14B24	A15B24	A16B24
C	A17B24	A18B24	A19B24	A20B24	A21B24	A22B24	A23B24	A24B24
D	A25B24	A26B24	A27B24	A28B24	A29B24	A30B24	A1B25	A2B25
E	A3B25	A4B25	A5B25	A6B25	A7B25	A8B25	A9B25	A10B25
F	A11B25	A12B25	A13B25	A14B25	A15B25	A16B25	A17B25	A18B25
G	A19B25	A20B25	A21B25	A22B25	A23B25	A24B25	A25B25	A26B25
H	A27B25	A28B25	A29B25	A30B25	A31B1	A32B1	A33B1	A34B1
I	A35B1	A36B1	A37B1	A38B1	A39B1	A40B1	A31B2	A32B2
J	A33B2	A34B2	A35B2	A36B2	A37B2	A38B2	A39B2	A40B2
K	A31B3	A32B3	A33B3	A34B3	A35B3	A36B3	A37B3	A38B3
L	A39B3	A40B3						

Table S12. Layout of plate 9.

	1	2	3	4	5	6	7	8
A	A31B4	A32B4	A33B4	A34B4	A35B4	A36B4	A37B4	A38B4
B	A39B4	A40B4	A31B5	A32B5	A33B5	A34B5	A35B5	A36B5
C	A37B5	A38B5	A39B5	A40B5	A31B6	A32B6	A33B6	A34B6
D	A35B6	A36B6	A37B6	A38B6	A39B6	A40B6	A31B7	A32B7
E	A33B7	A34B7	A35B7	A36B7	A37B7	A38B7	A39B7	A40B7
F	A31B8	A32B8	A33B8	A34B8	A35B8	A36B8	A37B8	A38B8
G	A39B8	A40B8	A31B9	A32B9	A33B9	A34B9	A35B9	A36B9
H	A37B9	A38B9	A39B9	A40B9	A31B10	A32B10	A33B10	A34B10
I	A35B10	A36B10	A37B10	A38B10	A39B10	A40B10	A31B11	A32B11
J	A33B11	A34B11	A35B11	A36B11	A37B11	A38B11	A39B11	A40B11
K	A31B12	A32B12	A33B12	A34B12	A35B12	A36B12	A37B12	A38B12
L	A39B12	A40B12						

Table S13. Layout of plate 10.

	1	2	3	4	5	6	7	8
A	A31B4	A32B4	A33B4	A34B4	A35B4	A36B4	A37B4	A38B4
B	A39B4	A40B4	A31B5	A32B5	A33B5	A34B5	A35B5	A36B5
C	A37B5	A38B5	A39B5	A40B5	A31B6	A32B6	A33B6	A34B6
D	A35B6	A36B6	A37B6	A38B6	A39B6	A40B6	A31B7	A32B7
E	A33B7	A34B7	A35B7	A36B7	A37B7	A38B7	A39B7	A40B7
F	A31B8	A32B8	A33B8	A34B8	A35B8	A36B8	A37B8	A38B8
G	A39B8	A40B8	A31B9	A32B9	A33B9	A34B9	A35B9	A36B9
H	A37B9	A38B9	A39B9	A40B9	A31B10	A32B10	A33B10	A34B10
I	A35B10	A36B10	A37B10	A38B10	A39B10	A40B10	A31B11	A32B11
J	A33B11	A34B11	A35B11	A36B11	A37B11	A38B11	A39B11	A40B11
K	A31B12	A32B12	A33B12	A34B12	A35B12	A36B12	A37B12	A38B12
L	A39B12	A40B12						

Table S14. Layout of plate 11.

	1	2	3	4	5	6	7	8
A	A31B13	A32B13	A33B13	A34B13	A35B13	A36B13	A37B13	A38B13
B	A39B13	A40B13	A31B14	A32B14	A33B14	A34B14	A35B14	A36B14
C	A37B14	A38B14	A39B14	A40B14	A31B15	A32B15	A33B15	A34B15
D	A35B15	A36B15	A37B15	A38B15	A39B15	A40B15	A31B16	A32B16
E	A33B16	A34B16	A35B16	A36B16	A37B16	A38B16	A39B16	A40B16
F	A31B17	A32B17	A33B17	A34B17	A35B17	A36B17	A37B17	A38B17
G	A39B17	A40B17	A31B18	A32B18	A33B18	A34B18	A35B18	A36B18
H	A37B18	A38B18	A39B18	A40B18	A31B19	A32B19	A33B19	A34B19
I	A35B19	A36B19	A37B19	A38B19	A39B19	A40B19	A31B20	A32B20
J	A33B20	A34B20	A35B20	A36B20	A37B20	A38B20	A39B20	A40B20
K								
L								

Table S15. Layout of plate 12.

	1	2	3	4	5	6	7	8
A	A31B21	A32B21	A33B21	A34B21	A35B21	A36B21	A37B21	A38B21
B	A39B21	A40B21	A31B22	A32B22	A33B22	A34B22	A35B22	A36B22
C	A37B22	A38B22	A39B22	A40B22	A31B23	A32B23	A33B23	A34B23
D	A35B23	A36B23	A37B23	A38B23	A39B23	A40B23	A31B24	A32B24
E	A33B24	A34B24	A35B24	A36B24	A37B24	A38B24	A39B24	A40B24
F	A31B25	A32B25	A33B25	A34B25	A35B25	A36B25	A37B25	A38B25
G	A39B25	A40B25						
H								
I								
J								
K								
L								

6. Development of Machine Learning Model

a) Preparation

All codes were executed in KNIME (the Konstanz Information Miner), which is a free and open-source data analytics platform and can be easily used by chemists without programming background. All workflows for modelling were provided in https://hub.knime.com/theliaogroup/spaces/C-H_Amidation.

b) Date Set

In our study, two datasets were used, one dataset for modelling and one dataset for external validation. The SMILES of arylaldehyde hydrazones, dioxazolones, and products, as well as the corresponding yields were included in datasets.

(1) Data set A (600 reactions data) was split as 80/20, 480 reactions data were used as training set, 120 reactions data were used as test set for modeling.

(2) Data set B (400 unknown reactions data) included 10 unseen hydrazones and 5 unseen dioxazolones, which were used as an external validation set for the model built from dataset. We used dataset A to build model, and then used dataset B as an external validation for the model built from dataset A.

(3) As shown in the **Figure S6**, dataset A was split as 80/20 at the work unit (named X-Partitioner), 480 reactions data were inputted the work unit [named XGBoost Tree Ensemble Learner (Regression) (deprecated)] as training set and the model_set will be divided into two parts, training set and test set, automatically by this work unit. But we cannot know how this unit divides the dataset. At the same time, remaining dataset A (evaluate set, including 120 reactions data) will be input to the work unit [named XGBoost Predictor (Regression)]. This unit is used to confirm if the hyper-parameters are best for models by the results (R^2 , MAE, and RMSE).

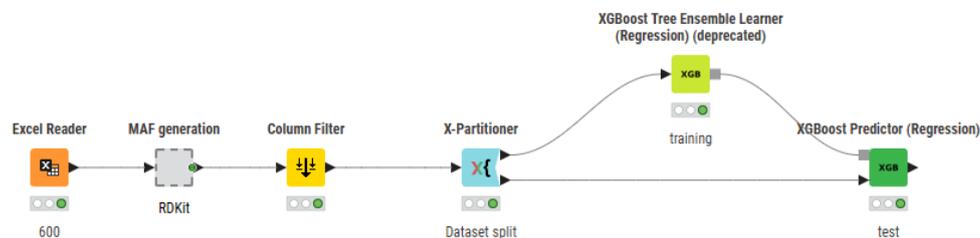


Figure S6. Part of the workflow of KNIME (one of the workflows).

c) Molecular additive fingerprints (MAF)

We provided a representation, molecular additive fingerprints (MAF) as inputs, that show the capacity of

reaction prediction in good practices. The example for MAF development in this reaction were shown in **Figure S7**.

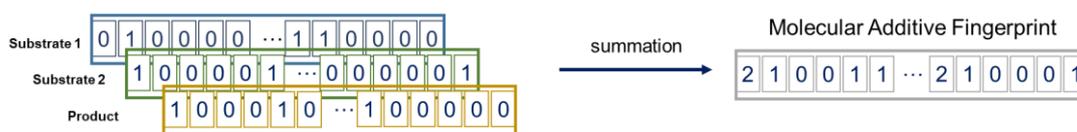


Figure S7. Example of the generation of MAF fingerprints in this reaction.

d) RDKit descriptors

RDKit descriptor generation was conducted in a KNIME workflow. In total, 119 descriptors were calculated for each reaction component using “RDKit Descriptors Calculation” node. The descriptors we used are as following: *SlogP*, *SMR*, *LabuteASA*, *TPSA*, *AMW*, *ExactMW*, *NumLipinskiHBA*, *NumLipinskiHBD*, *NumRotatableBonds*, *NumHBD*, *NumHBA*, *NumAmideBonds*, *NumHeteroAtoms*, *NumHeavyAtoms*, *NumAtoms*, *NumStereocenters*, *NumUnspecifiedStereocenters*, *NumRings*, *NumAromaticRings*, *NumSaturatedRings*, *NumAliphaticRings*, *NumAromaticHeterocycles*, *NumSaturatedHeterocycles*, *NumAliphaticHeterocycles*, *NumAromaticCarbocycles*, *NumSaturatedCarbocycles*, *NumAliphaticCarbocycles*, *FractionCSP3*, *Chi0v*, *Chi1v*, *Chi2v*, *Chi3v*, *Chi4v*, *Chi1n*, *Chi2n*, *Chi3n*, *Chi4n*, *HallKierAlpha*, *kappa1*, *kappa2*, *kappa3*, *slogp_VSA1*, *slogp_VSA2*, *slogp_VSA3*, *slogp_VSA4*, *slogp_VSA5*, *slogp_VSA6*, *slogp_VSA7*, *slogp_VSA8*, *slogp_VSA9*, *slogp_VSA10*, *slogp_VSA11*, *slogp_VSA12*, *smr_VSA1*, *smr_VSA2*, *smr_VSA3*, *smr_VSA4*, *smr_VSA5*, *smr_VSA6*, *smr_VSA7*, *smr_VSA8*, *smr_VSA9*, *smr_VSA10*, *peoe_VSA1*, *peoe_VSA2*, *peoe_VSA3*, *peoe_VSA4*, *peoe_VSA5*, *peoe_VSA6*, *peoe_VSA7*, *peoe_VSA8*, *peoe_VSA9*, *peoe_VSA10*, *peoe_VSA11*, *peoe_VSA12*, *peoe_VSA13*, *peoe_VSA14*, *MQN1*, *MQN2*, *MQN3*, *MQN4*, *MQN5*, *MQN6*, *MQN7*, *MQN8*, *MQN9*, *MQN10*, *MQN11*, *MQN12*, *MQN13*, *MQN14*, *MQN15*, *MQN16*, *MQN17*, *MQN18*, *MQN19*, *MQN20*, *MQN21*, *MQN22*, *MQN23*, *MQN24*, *MQN25*, *MQN26*, *MQN27*, *MQN28*, *MQN29*, *MQN30*, *MQN31*, *MQN32*, *MQN33*, *MQN34*, *MQN35*, *MQN36*, *MQN37*, *MQN38*, *MQN39*, *MQN40*, *MQN41*, *MQN42*.

e) One-hot encoding

A one-hot encoding based on all available reaction substrates was generated. The bit value ‘0’ or ‘1’ corresponds to the absence or presence for specific reaction component. The creation of one-hot descriptor was done via a KNIME workflow and an array of one-hot encodings of substrates and products was calculated in “One to Many” node. As shown in **Figure S8**, the generation of one-hot encoding in substrate exploration, respectively.

	Substrate1	Substrate2
One-hot encoding (total length m = 89)	$A_1 A_2 A_3 \dots A_{80}$	$B_1 B_2 B_3 \dots B_9$
	[0 1 0 ... 0	1 0 0 ... 0]

Figure S8. The generation of one-hot encoding in substrate exploration.

f) Machine Learning Methods

Four commonly used ML methods were proceeded for modelling, including eXtreme Gradient Boosting (XGB), Gradient Boosted Trees (GBT), Random Forest Regression (RF), and Support Vector Regression (SVR). 60% of the dataset (600 reactions) were used to train our regression model and the remaining 40% were used as test set (400 reactions). The model performance was then evaluated by coefficient of determination (R^2), mean absolute error (MAE), and root mean squared error (RMSE).

Table S16. The hyper-parameters of 4 models.

Model	Hyper-parameters
Random Forest	Enable Hilighting (#patterns to store) = 2000, tree depth = 10, Minimum node size = 5, number of models = 100, Use static random seed = 68909
Gradient Boosting Tree	Limit number of levels = 6, number of models (n_estimators) = 100, learning rate = 0.5, alpha = 0.95
XGBoost	Boosting rounds = 100, Use static random seed = 68909, Manual numbers of threads = 4, Objective = 'squarederror', Booster = 'tree', Eta = 0.1, Gamma = 0, Maximum depth = 5, Minimum child weight = 5. Maximum delta step = 0, Subsampling rate = 0.8
SVR	Type of SVR = 'nu-SVR', Kernal = 'linear', Cost = 1.5, nu = 0.5, Cachesize = 3163, Epsilon = 0.001

Table S17. The hyper-parameters of XGB model for grid search.

Hyper-parameters	Considered values
booster	tree
eta	{0.05, 0.1 , 0.15, 0.2}
min child weight	{ 5 , 6, 7}
max depth	{ 5 , 7, 9}
boosting rounds	{50, 100 , 150}

As shown in **Figure S9**, we can get the following page by open the work unit of model, and where we can change all kinds of hype-parameters of four models.

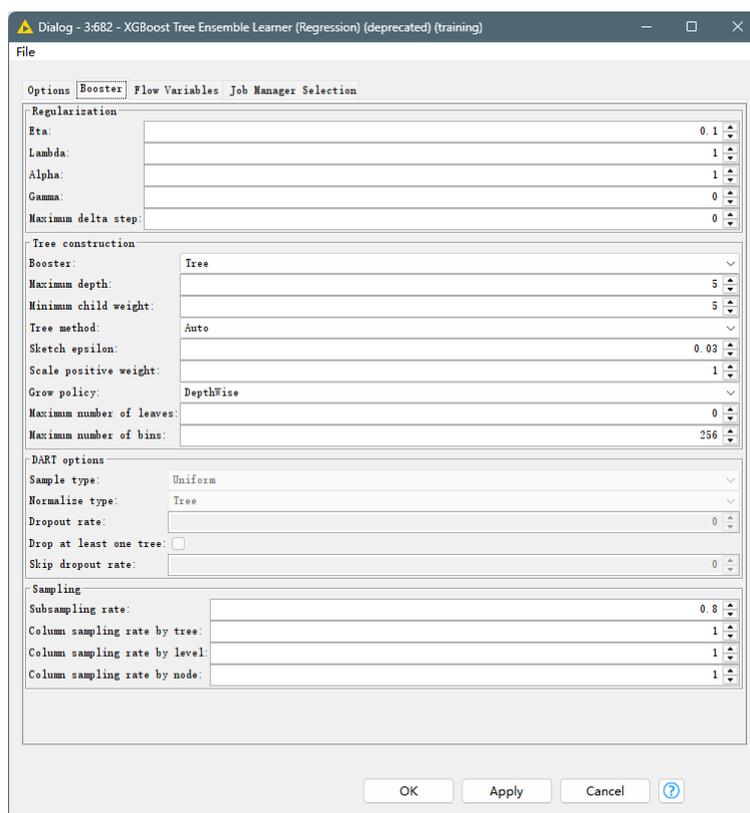


Figure S9. The page of changing hype-parameters.

g) The Development of ML-Based Models using MAF, RDKit, and One-hot

As shown in **Table S18**, three types of descriptors were applied for model building and 12 models were obtained in total.

Table S18. The development of ML-based models using MAF, RDKit and One-hot.

entry	model	R ²	MAE (%)	RMSE (%)
1	GBT-MAF	0.77	8.0	11.0
2	RF-MAF	0.56	12.2	15.1
3	XGB-MAF	0.79	7.7	10.4
4	SVR-MAF	0.70	10.1	12.5
5	GBT-RDKit	0.80	6.8	10.0
6	RF-RDKit	0.73	8.3	11.7
7	XGB-RDKit	0.84	6.2	9.0
8	SVR-RDKit	0.64	10.5	13.8
9	GBT-one hot	0.52	10.7	15.8
10	RF-one hot	0.20	17.7	20.4
11	XGB-one hot	0.54	10.9	15.6
12	SVR-one hot	0.49	12.9	16.3

h) Performance of XGB-RDKit Model

As shown in **Figure S10**, XGB-RDKit model deliver the best performance overall, with a result of R^2 value of 0.84, MAE of 6.2%, and RMSE of 9.0%.

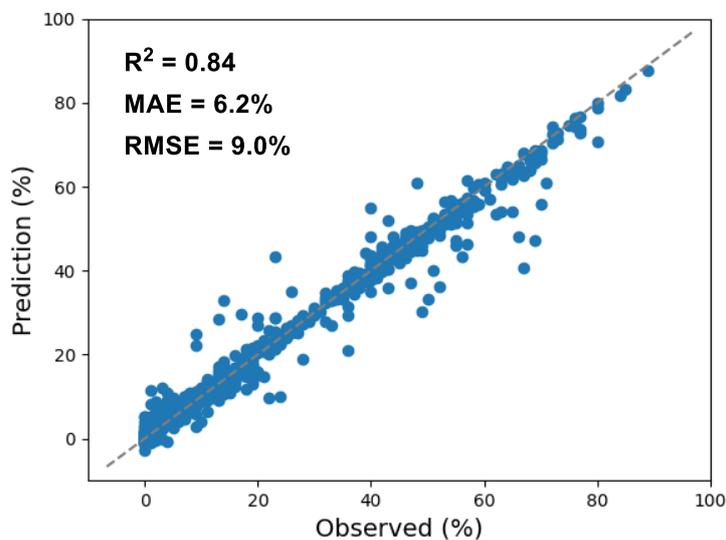


Figure S10. Prediction results on validation set for XGB-RDKit model.

Under the obtained best model (XGB-RDKit), we also evaluated 10 random splits of the entire data set (600 reaction data). These results are shown in **Table S19**, with a best result of R^2 value of 0.85, MAE of 6.1%, and RMSE of 8.8%.

Table S19. Results for 10 random splits of 600 reaction data.

splits	R^2	MAE(%)	RMSE(%)
splits 01	0.85	6.0	8.7
splits 02	0.86	5.9	8.5
splits 03	0.84	6.4	9.2
splits 04	0.86	5.9	8.6
splits 05	0.85	6.1	8.9
splits 06	0.85	6.1	8.7
splits 07	0.86	6.0	8.6
splits 08	0.84	6.2	9.0
splits 09	0.85	6.1	8.8
splits 10	0.85	6.1	8.9
average	0.85	6.1	8.8

i) Performance of External Dataset

Our best model in yield prediction (XGB-MFF model, as shown in **Figure S10**) was then evaluated on external dataset. The performance of external test is shown in **Figure S11**, with a result of R^2 value of 0.78, MAE of 5.2%, and RMSE of 7.1%.

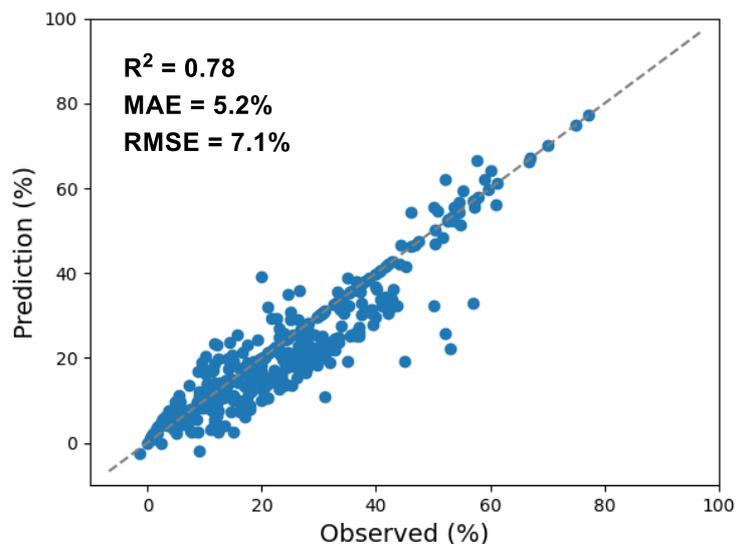


Figure S11. Regression plot for external dataset (400 scattered reactions).

j) SHAP Analysis and Feature Importance

To investigate feature importance in the XGB-RDKit-based yield prediction model, we computed SHAP values for all features. Figure S12 shows the top 10 features ranked by mean absolute SHAP value, with Chi3n, NumRotatableBonds, and smr_VSA5 identified as the three most important variables.

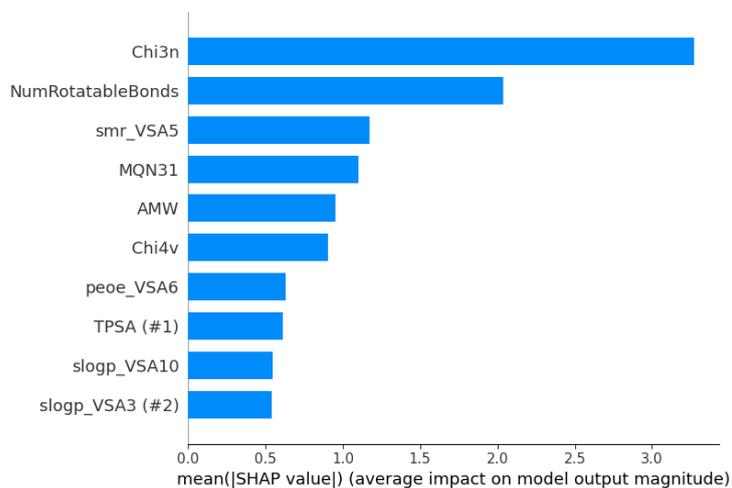


Figure S12. SHAP important features bar chart.

7. X-ray Crystallographic Data of 3

The preparation of crystal **3**: 11.0 mg of **3** was dissolved in dichloromethane (1.0 mL), it was filtered through a plug of silica gel. The filtrate was transferred to a tube (diameter, 0.6 cm), and 2.0 mL of petroleum ether was slowly added. Clear light orange crystals were grown from standing it for two weeks.

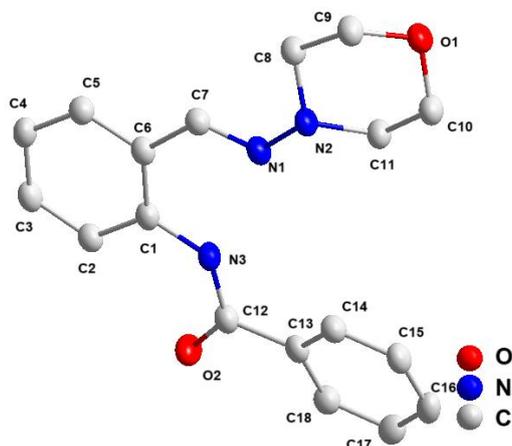


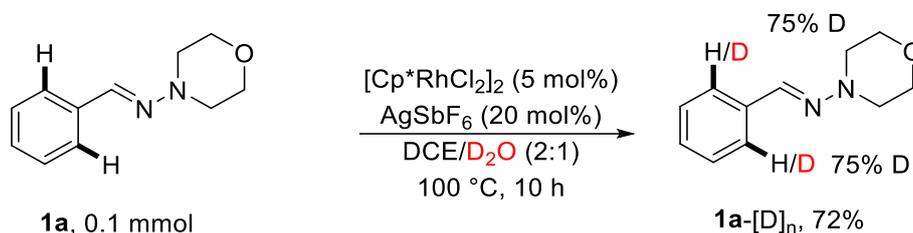
Figure S13. Molecular structure of compound **3** (CCDC number: 2405539). Thermal ellipsoids are drawn at 50% probability. H atoms are omitted for clarity.

Table S20. Summary of X-ray crystallographic data for compound 3

formula	C ₁₈ H ₁₉ N ₃ O ₂
Fw.	309.36
T/K	100.01(10)
crystal system	monoclinic
space group	P21/c
<i>a</i> /Å	10.3021(4)
<i>b</i> /Å	15.5649(4)
<i>c</i> /Å	10.7040(4)
<i>a</i> /deg	90.00
<i>β</i> /deg	116.829(4)
<i>γ</i> /deg	90.00
<i>V</i> /Å ³	1531.64(10)
<i>Z</i>	4
<i>D</i> /g cm ⁻³	1.342
cryst size/mm	0.2×0.15×0.1
reflns collected	20849
ind reflns, <i>R</i> _{int}	2917, 0.0506
goodness-of-fit on <i>F</i> ²	1.069
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.0489, 0.1048
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0583, 0.1426

8. Reaction Mechanism

A) *H/D* Exchange Experiment



An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with $[\text{Cp}^*\text{RhCl}_2]_2$ (3.0 mg, 0.005 mmol, 5 mol %), AgSbF_6 (5.0 mg, 0.02 mmol, 20 mol %), and arylaldehyde hydrazone (**1a**, 0.1 mmol, 1.0 equiv); then DCE (0.66 mL) and D_2O (0.33 mL) were added. The reaction mixture was stirred (820 r/min in IKA RCT basic) at 100 °C for 10 h under N_2 atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature, filtered through a pad of celite and then the celite pad was washed with CH_2Cl_2 (5 mL \times 2). The solvent was removed under reduced pressure and the crude residue was purified by flash column chromatography on silica gel to give the desired product **1a**- $[\text{D}]_n$ in 72% yield (13.7 mg) and the extents of deuterium incorporation was measured by ^1H NMR analysis (**Figure S14**).

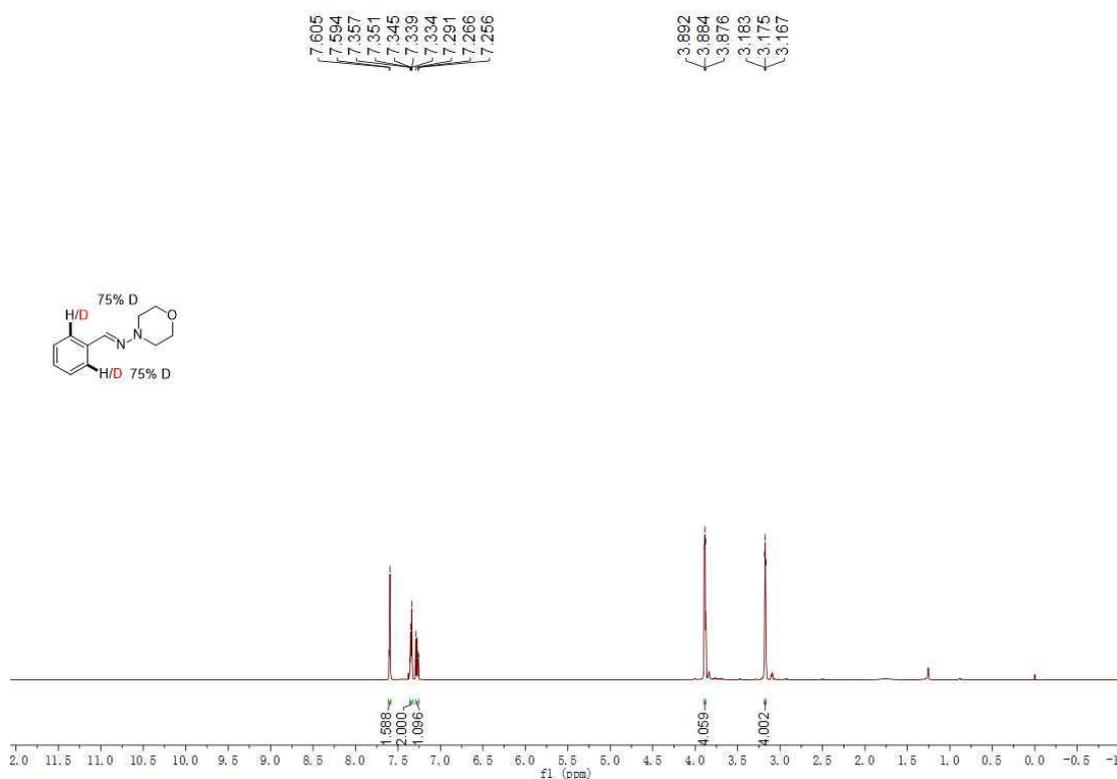
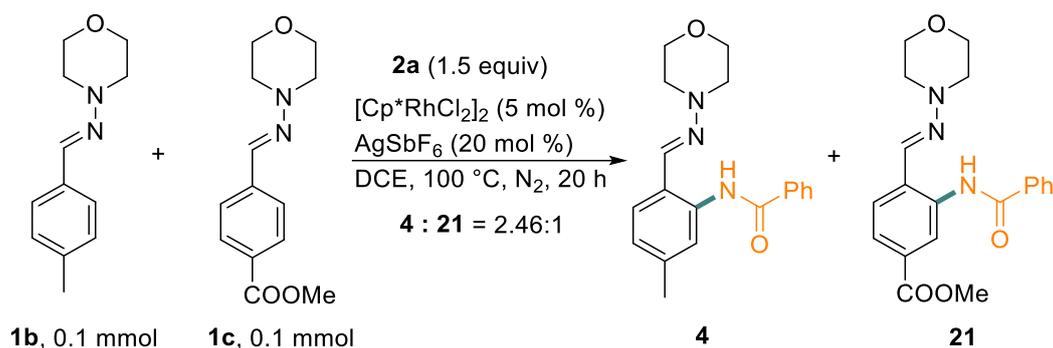


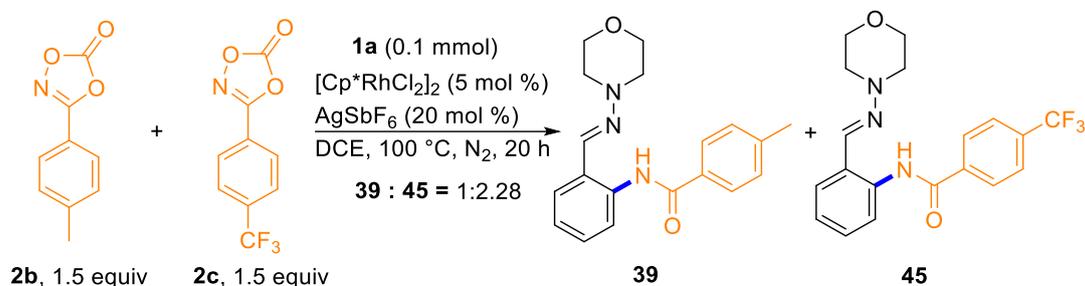
Figure S14. ^1H NMR (600 MHz, CDCl_3) Spectrum of *H/D* exchange reaction.

B) Intermolecular Competitive Experiments between Hydrazones



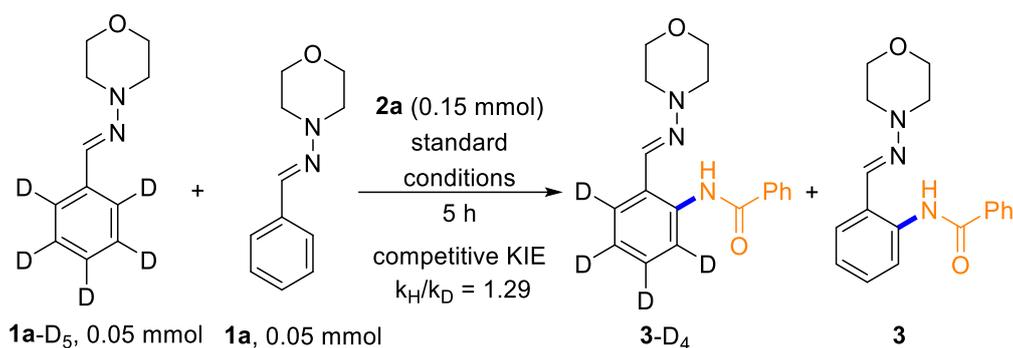
An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with $[\text{Cp}^*\text{RhCl}_2]_2$ (3.0 mg, 0.005 mmol, 5 mol %), AgSbF_6 (5 mg, 0.02 mmol, 20 mol %), arylaldehyde hydrazone **1b** (0.1 mmol, 1.0 equiv), **1c** (0.1 mmol, 1.0 equiv), and dioxazolone (**2a**, 0.15 mmol, 1.5 equiv); then DCE (1.0 mL) was added. The reaction mixture was stirred (820 r/min in IKA RCT basic) at 100 °C for 20 h under N_2 atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature. The crude product was extracted with ethyl acetate (3×5 mL), and the solution was washed with saturated solution of NH_4Cl (5 mL), and the organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to afford the corresponding products (**4** and **21**) in 86% and 35% yields, respectively.

C) Intermolecular Competitive Experiments between Dioxazolones



An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with $[\text{Cp}^*\text{RhCl}_2]_2$ (3.0 mg, 0.005 mmol, 5 mol %), AgSbF_6 (5 mg, 0.02 mmol, 20 mol %), arylaldehyde hydrazone **1a** (0.1 mmol, 1.0 equiv), dioxazolone **2b** (0.15 mmol, 1.5 equiv) and dioxazolone **2c** (0.15 mmol, 1.5 equiv); then DCE (1.0 mL) was added. The reaction mixture was stirred (820 r/min in IKA RCT basic) at 100 °C for 20 h under N_2 atmosphere. After completion of the reaction, the reaction mixture was cooled to room temperature. The crude product was extracted with ethyl acetate (3×5 mL), and the solution was washed with saturated solution of NH_4Cl (5 mL), and the organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel to afford the corresponding products (**39** and **45**) in 14% and 33% yields, respectively.

D) Competitive Kinetic Isotope Experiment



An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with [Cp*RhCl₂]₂ (3.0 mg, 0.005 mmol, 5 mol %), AgSbF₆ (5.0 mg, 0.02 mmol, 20 mol %), dioxazolones (0.15 mmol, 1.5 equiv) and DCE (1.0 mL) was added; then arylaldehyde hydrazone (**1a**, 0.05 mmol, 0.5 equiv) and deuterated arylaldehyde hydrazone (**1a-D₅**, 0.05 mmol, 0.5 equiv) were added. The reaction mixture was stirred (820 r/min in IKA RCT basic) at 100 °C for 5 h under N₂ atmosphere. After completion, the reaction mixture was cooled to room temperature. The crude product was extracted with ethyl acetate (3 × 3.0 mL), and the solution was washed with saturated solution of NH₄Cl (3.0 mL), and the organic layer was dried over anhydrous Na₂SO₄ and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel (PE/EA = 5/1) to afford the mixture of **3** and **3-D₄** in 40.5% yield ($k_H/k_D = 0.228/(0.405-0.228) = 1.29$, 12.6 mg). KIE was determined by ¹H NMR analysis using 1,3,5-trimethoxybenzene as internal standard (**Figure S15**).

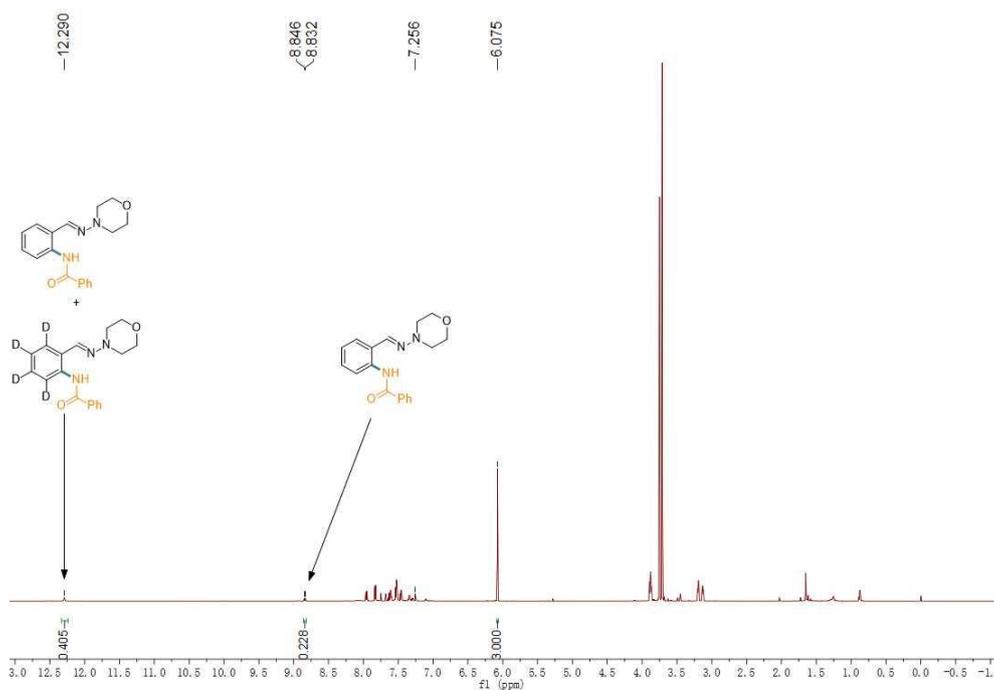
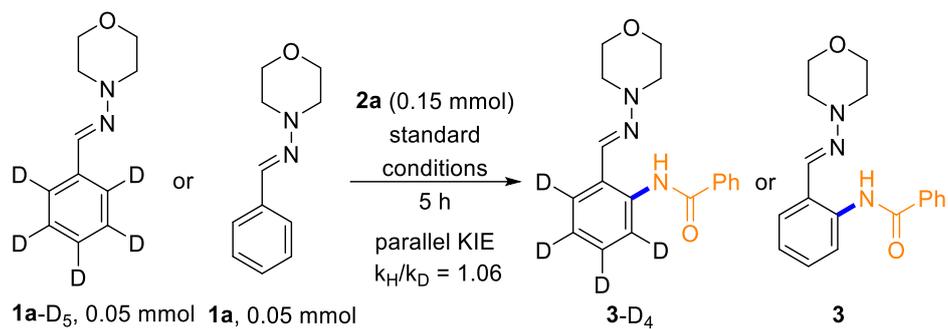


Figure S15. ¹H NMR (600 MHz, CDCl₃) Spectrum of kinetic isotope experiment.

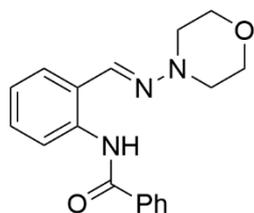
E) Parallel Kinetic Isotopic Experiment



An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with $[\text{Cp}^*\text{RhCl}_2]_2$ (3.0 mg, 0.005 mmol, 5 mol %), AgSbF_6 (5.0 mg, 0.02 mmol, 20 mol %), dioxazolones (0.15 mmol, 1.5 equiv) and DCE (1.0 mL) was added; then arylaldehyde hydrazone (**1a**, 0.05 mmol, 0.5 equiv) or deuterated arylaldehyde hydrazone (**1a-D₅**, 0.05 mmol, 0.5 equiv) were added. The reaction mixture was stirred (820 r/min in IKA RCT basic) at 100 °C for 5 h under N_2 atmosphere. After completion, the reaction mixture was cooled to room temperature. The crude product was extracted with ethyl acetate (3×3.0 mL), and the solution was washed with saturated solution of NH_4Cl (3.0 mL), and the organic layer was dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 5/1) to afford the mixture of **3** in 45.2% yield and **3-D₄** in 42.5% yield ($k_{\text{H}}/k_{\text{D}} = 0.452/0.425=1.06$). KIE was determined by ^1H NMR analysis using 1,3,5-trimethoxybenzene as internal standard.

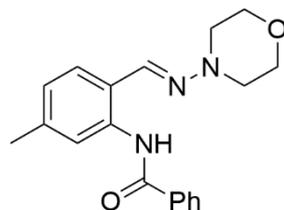
9. Characterization Data for the Products

(*E*)-*N*-(2-((morpholinoimino)methyl)phenyl)benzamide (3)



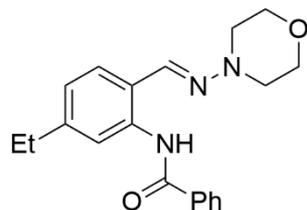
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 88% yield (27.2 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.29 (s, 1H), 8.88–8.85 (m, 1H), 7.96 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.72 (s, 1H), 7.54–7.49 (m, 1H), 7.47–7.42 (m, 2H), 7.33 (td, *J* = 8.6, 8.1, 1.5 Hz, 1H), 7.23 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.08 (td, *J* = 7.5, 1.2 Hz, 1H), 3.87–3.84 (m, 4H), 3.14–3.09 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.5, 140.9, 137.7, 135.9, 131.6, 131.3, 129.3, 128.4, 127.6, 122.9, 121.1, 119.9, 66.1, 51.6. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₂₀N₃O₂[M+H]⁺, 310.1550, found 310.1548.

(*E*)-*N*-(5-methyl-2-((morpholinoimino)methyl)phenyl)benzamide (4)



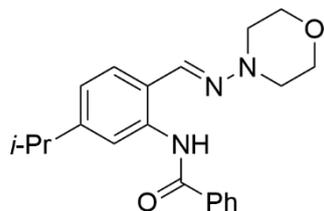
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 83% yield (26.8 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.28 (s, 1H), 8.72 (s, 1H), 7.97 (dt, *J* = 8.4, 1.7 Hz, 2H), 7.76 (s, 1H), 7.55–7.50 (m, 1H), 7.49–7.43 (m, 1H), 7.14 (d, *J* = 7.8 Hz, 1H), 6.92 (ddd, *J* = 7.8, 1.6, 0.6 Hz, 2H), 3.90–3.86 (m, 4H), 3.12 (dd, *J* = 5.6, 4.1 Hz, 4H), 2.40 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.5, 141.8, 140.1, 137.7, 136.1, 131.6, 131.4, 128.4, 127.6, 123.9, 120.5, 118.7, 66.2, 51.9, 21.8. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₂[M+H]⁺, 324.1707, found 324.1740.

(E)-N-(5-ethyl-2-((morpholinoimino)methyl)phenyl)benzamide (5)



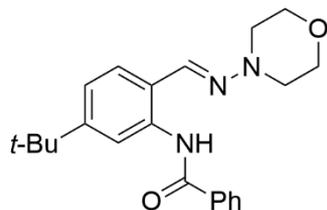
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 70% yield (23.6 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.30 (s, 1H), 8.76 (s, 1H), 8.00–7.93 (m, 3H), 7.75 (s, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 7.8 Hz, 1H), 6.97–6.92 (m, 1H), 3.90–3.79 (m, 4H), 3.15–3.07 (m, 4H), 2.70 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.5, 146.3, 141.7, 137.8, 136.1, 131.6, 131.4, 128.4, 127.6, 122.6, 119.4, 118.8, 66.2, 51.9, 29.1, 15.3. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₄N₃O₂[M+H]⁺, 338.1863, found 338.1866.

(E)-N-(5-isopropyl-2-((morpholinoimino)methyl)phenyl)benzamide (6)



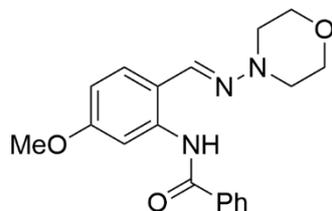
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 72% yield (25.3 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.30 (s, 1H), 8.81 (d, *J* = 1.4 Hz, 1H), 8.00–7.95 (m, 2H), 7.76 (s, 1H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 7.9 Hz, 1H), 6.98 (dd, *J* = 7.9, 1.6 Hz, 1H), 3.90–3.81 (m, 4H), 3.14–3.07 (m, 4H), 2.99–2.87 (m, 1H), 1.29 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (150 MHz, CDCl₃): δ 166.5, 150.9, 141.7, 137.9, 136.1, 131.6, 131.5, 128.4, 127.6, 121.1, 118.9, 118.2, 66.2, 51.9, 34.3, 23.7. HRMS (ESI-TOF) *m/z* calcd. for C₂₁H₂₆N₃O₂[M+H]⁺, 352.2020, found 352.2033.

(E)-N-(5-(tert-butyl)-2-((morpholinoimino)methyl)phenyl)benzamide (7)



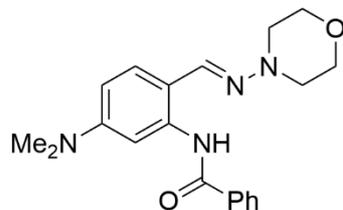
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 60% yield (21.9 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.28 (s, 1H), 9.00 (d, *J* = 1.8 Hz, 1H), 8.00–7.96 (m, 2H), 7.77 (s, 1H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.19 (d, *J* = 8.1 Hz, 1H), 7.14 (dd, *J* = 8.1, 1.9 Hz, 1H), 3.92–3.84 (m, 4H), 3.15–3.09 (m, 4H), 1.38 (s, 9H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 153.2, 141.6, 137.7, 136.1, 131.6, 131.1, 128.4, 127.6, 120.1, 118.6, 117.3, 66.2, 51.9, 35.1, 31.2. HRMS (ESI-TOF) *m/z* calcd. for C₂₂H₂₈N₃O₂[M+H]⁺, 366.2176, found 366.2194.

(E)-N-(5-methoxy-2-((morpholinoimino)methyl)phenyl)benzamide (8)



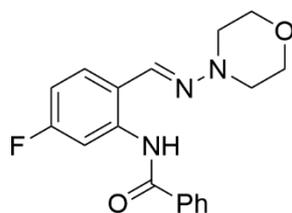
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 83% yield (28.2 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.45 (s, 1H), 8.58 (d, *J* = 2.6 Hz, 1H), 7.99–7.93 (m, 2H), 7.74 (s, 1H), 7.52 (s, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.13 (d, *J* = 8.6 Hz, 1H), 6.64 (dd, *J* = 8.5, 2.6 Hz, 1H), 3.87 (d, *J* = 4.8 Hz, 7H), 3.13–2.99 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.7, 160.6, 142.4, 139.4, 135.9, 132.6, 131.7, 128.4, 127.6, 114.3, 109.8, 104.5, 66.2, 55.4, 52.2. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₄[M+H]⁺, 340.1656, found 340.1663.

(E)-N-(5-(dimethylamino)-2-((morpholinoimino)methyl)phenyl)benzamide (9)



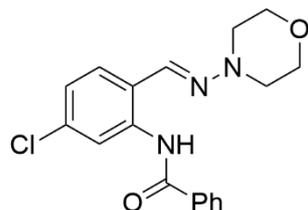
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 71% yield (25.0 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.45 (s, 1H), 8.40 (d, *J* = 2.6 Hz, 1H), 8.01–7.99 (m, 2H), 7.80 (s, 1H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.08 (d, *J* = 8.6 Hz, 1H), 6.41 (dd, *J* = 8.6, 2.6 Hz, 1H), 3.87–3.85 (m, 4H), 3.07–3.05 (m, 4H), 3.04 (s, 6H). ¹³C NMR (150 MHz, CDCl₃): δ 166.7, 151.3, 145.2, 139.4, 136.1, 132.9, 131.5, 128.3, 127.6, 109.9, 106.5, 103.0, 66.3, 52.9, 40.1. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₅N₄O₂[M+H]⁺, 353.1972, found 353.1999.

(E)-N-(5-fluoro-2-((morpholinoimino)methyl)phenyl)benzamide (10)



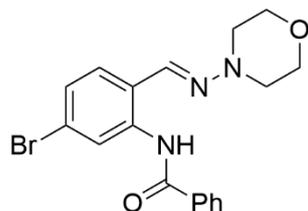
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 51% yield (16.7 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.45 (s, 1H), 8.68 (dd, *J* = 12.0, 2.6 Hz, 1H), 7.96–7.93 (m, 2H), 7.72 (s, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.7 Hz, 2H), 7.19 (dd, *J* = 8.5, 6.3 Hz, 1H), 6.78 (td, *J* = 8.3, 2.6 Hz, 1H), 3.89–3.87 (m, 4H), 3.13–3.11 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.7, 162.9 (d, *J* = 247.6 Hz), 140.6, 139.4 (d, *J* = 12.0 Hz), 135.6, 132.7 (d, *J* = 10.1 Hz), 131.9, 128.5, 127.6, 117.6 (d, *J* = 2.9 Hz), 109.9 (d, *J* = 22.7 Hz), 107.4 (d, *J* = 28.6 Hz), 66.1, 51.8. ¹⁹F NMR (564 MHz, CDCl₃): δ -108.9. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₁₉FN₃O₂[M+H]⁺, 328.1456, found 328.1463.

(E)-N-(5-chloro-2-((morpholinoimino)methyl)phenyl)benzamide (11)



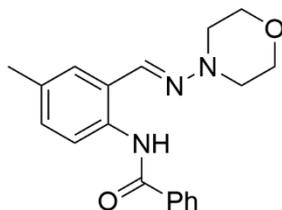
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 74% yield (25.4 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.34 (s, 1H), 8.94 (d, *J* = 2.1 Hz, 1H), 7.94 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.69 (s, 1H), 7.57–7.52 (m, 1H), 7.48–7.44 (m, 2H), 7.14 (d, *J* = 8.3 Hz, 1H), 7.06 (dd, *J* = 8.2, 2.1 Hz, 1H), 3.88 (dd, *J* = 5.7, 4.1 Hz, 4H), 3.15–3.11 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.7, 139.8, 138.5, 135.6, 135.1, 132.1, 131.9, 128.5, 127.6, 123.1, 119.9, 119.7, 66.1, 51.6. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₁₉ClN₃O₂[M+H]⁺, 344.1160, found 344.1173.

(E)-N-(5-bromo-2-((morpholinoimino)methyl)phenyl)benzamide (12)



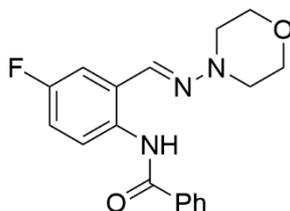
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 95% yield (36.8 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.31 (s, 1H), 9.10 (d, *J* = 2.0 Hz, 1H), 7.94 (dt, *J* = 8.4, 1.6 Hz, 2H), 7.67 (s, 1H), 7.57–7.52 (m, 1H), 7.49–7.44 (m, 2H), 7.22 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.08 (d, *J* = 8.3 Hz, 1H), 3.88 (dd, *J* = 5.7, 4.1 Hz, 4H), 3.19–3.03 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 139.8, 138.6, 135.7, 132.3, 131.9, 128.5, 127.6, 126.1, 123.4, 122.9, 120.0, 66.1, 51.6. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₁₉BrN₃O₂[M+H]⁺, 388.0655, found 388.0663.

(E)-N-(4-methyl-2-((morpholinoimino)methyl)phenyl)benzamide (13)



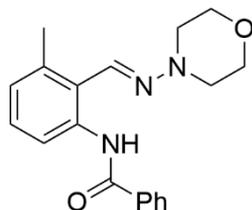
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 82% yield (26.5 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.18 (s, 1H), 8.74 (d, *J* = 8.4 Hz, 1H), 7.97–7.93 (m, 2H), 7.70 (s, 1H), 7.54–7.48 (m, 1H), 7.44 (t, *J* = 7.5 Hz, 2H), 7.15 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.04 (d, *J* = 1.5 Hz, 1H), 3.97–3.77 (m, 4H), 3.16–3.08 (m, 4H), 2.32 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.3, 141.3, 136.1, 135.3, 132.4, 131.8, 131.5, 130.0, 128.4, 127.5, 121.0, 119.9, 66.1, 51.7, 20.6. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₂[M+H]⁺, 324.1707, found 324.1746.

(E)-N-(4-fluoro-2-((morpholinoimino)methyl)phenyl)benzamide (14)



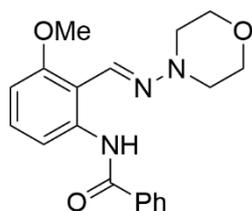
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 70% yield (22.9 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.13 (s, 1H), 8.85 (dd, *J* = 9.2, 5.3 Hz, 1H), 7.96–7.92 (m, 2H), 7.65 (s, 1H), 7.54 (tt, *J* = 6.7, 1.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.05 (ddd, *J* = 9.1, 7.9, 3.0 Hz, 1H), 6.96 (dd, *J* = 9.1, 3.0 Hz, 1H), 3.90–3.87 (m, 4H), 3.17–3.14 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.4, 158.2 (d, *J* = 242.1 Hz), 139.0 (d, *J* = 2.6 Hz), 136.0, 134.0 (d, *J* = 2.5 Hz), 131.7, 128.5, 127.6, 122.8 (d, *J* = 6.9 Hz), 121.8 (d, *J* = 7.4 Hz), 117.0 (d, *J* = 23.5 Hz), 115.8 (d, *J* = 21.7 Hz), 66.1, 51.5. ¹⁹F NMR (564 MHz, CDCl₃): δ -119.9. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₁₉N₃O₂[M+H]⁺, 328.1456, found 328.1483.

(E)-N-(3-methyl-2-((morpholinoimino)methyl)phenyl)benzamide (15)



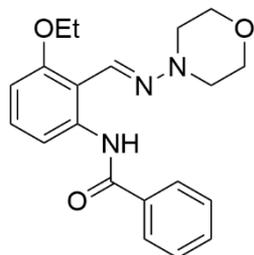
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 91% yield (29.4 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.50 (s, 1H), 8.70 (d, *J* = 8.3 Hz, 1H), 8.01 (s, 1H), 7.96–7.94 (m, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.24 (t, *J* = 7.9 Hz, 1H), 6.92 (d, *J* = 7.5 Hz, 1H), 3.89–3.87 (m, 4H), 3.13–3.11 (m, 4H), 2.43 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.5, 138.2, 138.0, 137.2, 136.3, 131.5, 129.3, 128.4, 127.6, 125.6, 119.2, 118.5, 66.1, 51.8, 20.5. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₂[M+H]⁺, 324.1707, found 324.1717.

(E)-N-(3-methoxy-2-((morpholinoimino)methyl)phenyl)benzamide (16)



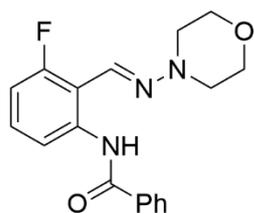
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 72% yield (24.4 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.62 (s, 1H), 8.47 (d, *J* = 8.4 Hz, 1H), 8.31 (s, 1H), 7.97–7.94 (m, 2H), 7.53–7.50 (m, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 8.4 Hz, 1H), 6.64 (d, *J* = 8.1 Hz, 1H), 3.88–3.86 (m, 4H), 3.85 (s, 3H), 3.13–3.10 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.7, 157.9, 139.0, 136.9, 136.2, 131.6, 130.4, 128.4, 127.7, 112.8, 110.1, 105.3, 66.2, 55.8, 52.0. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₃[M+H]⁺, 340.1656, found 340.1692.

(E)-N-(3-ethoxy-2-((morpholinoimino)methyl)phenyl)benzamide (17)



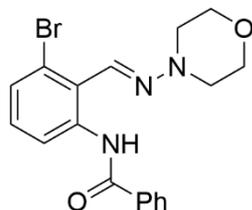
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 82% yield (29.0 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.60 (s, 1H), 8.46 (d, *J* = 8.3 Hz, 1H), 8.35 (s, 1H), 7.97–7.95 (m, 2H), 7.53–7.50 (m, 1H), 7.46–7.43 (m, 2H), 7.27 (t, *J* = 8.5 Hz, 1H), 6.64–6.62 (m, 1H), 4.07 (q, *J* = 7.0 Hz, 2H), 3.87 (dd, *J* = 5.7, 4.1 Hz, 4H), 3.12–3.10 (m, 4H), 1.42 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (150 MHz, CDCl₃): ¹³C NMR (151 MHz, Chloroform-*d*) δ 166.6, 157.4, 139.0, 137.3, 136.2, 131.5, 130.3, 128.3, 127.7, 112.6, 110.1, 106.4, 66.2, 64.2, 51.9, 14.8. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₄N₃O₃[M+H]⁺, 354.1812, found 352.1804.

(E)-N-(3-fluoro-2-((morpholinoimino)methyl)phenyl)benzamide (18)



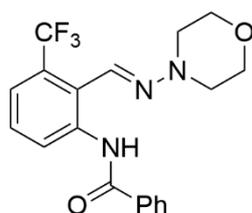
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 81% yield (26.5 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.36 (s, 1H), 8.64 (d, *J* = 8.5 Hz, 1H), 8.01 (s, 1H), 7.95–7.93 (m, 2H), 7.54–7.52 (m, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.30–7.26 (m, 1H), 6.82–6.78 (m, 1H), 3.88–3.86 (m, 4H), 3.15–3.13 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 161.3 (d, *J* = 248.4 Hz), 139.0 (d, *J* = 3.4 Hz), 135.8, 132.8 (d, *J* = 10.7 Hz), 131.8, 130.3 (d, *J* = 10.5 Hz), 128.4, 127.6, 115.6 (d, *J* = 3.4 Hz), 109.9 (d, *J* = 10.4 Hz), 109.5 (d, *J* = 22.1 Hz), 66.0, 51.5. ¹⁹F NMR (564 MHz, CDCl₃): δ -120.0. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₁₉N₃O₂[M+H]⁺, 328.1436, found 328.1429.

(E)-N-(3-bromo-2-((morpholinoimino)methyl)phenyl)benzamide (19)



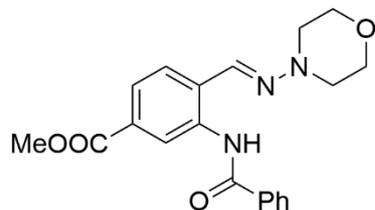
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 83% yield (32.1 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.51 (s, 1H), 8.81 (d, $J = 8.3$ Hz, 1H), 8.22 (s, 1H), 7.94–7.91 (m, 2H), 7.53 (t, $J = 7.4$ Hz, 1H), 7.45 (t, $J = 7.6$ Hz, 2H), 7.34–7.31 (m, 1H), 7.15 (t, $J = 8.2$ Hz, 1H), 3.88–3.86 (m, 4H), 3.16–3.14 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 166.5, 139.7, 139.1, 135.9, 131.8, 129.9, 128.4, 127.9, 127.6, 125.3, 119.6, 119.4, 66.0, 51.4. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{18}\text{H}_{19}\text{BrN}_3\text{O}_2[\text{M}+\text{H}]^+$, 388.0655, found 388.0668.

(E)-N-(2-((morpholinoimino)methyl)-3-(trifluoromethyl)phenyl)benzamide (20)



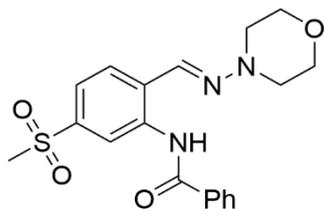
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 25% yield (9.4 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.41 (s, 1H), 8.98 (d, $J = 8.7$ Hz, 1H), 7.97–7.94 (m, 2H), 7.74 (s, 1H), 7.58–7.54 (m, 2H), 7.51–7.47 (m, 3H), 3.91–3.89 (m, 4H), 3.18–3.16 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 166.9, 140.4, 139.0, 135.6, 132.1, 128.6, 128.0 (q, $J = 3.8$ Hz), 127.7, 126.0 (q, $J = 3.6$ Hz), 124.9 (d, $J = 32.9$ Hz), 124.0 (d, $J = 271.5$ Hz), 121.2, 120.1, 66.1, 51.5. ^{19}F NMR (564 MHz, CDCl_3): δ -62.2. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{19}\text{H}_{19}\text{F}_3\text{N}_3\text{O}_2[\text{M}+\text{H}]^+$, 378.1424, found 378.1426.

methyl (*E*)-3-benzamido-4-((morpholinoimino)methyl)benzoate (21)



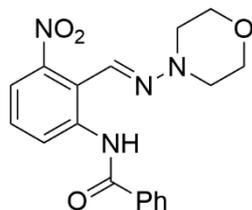
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 70% yield (25.7 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.24 (s, 1H), 9.48 (d, *J* = 1.3 Hz, 1H), 7.96 (d, *J* = 7.3 Hz, 2H), 7.78–7.76 (m, 1H), 7.72 (s, 1H), 7.54 (t, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 1H), 3.93 (s, 3H), 3.90–3.88 (m, 4H), 3.19–3.17 (m, 4H). ¹³C NMR (150 MHz, CDCl₃) δ 166.7, 166.6, 138.9, 137.5, 135.8, 131.9, 131.0, 130.3, 128.5, 127.6, 124.9, 124.2, 121.0, 66.1, 52.3, 51.4. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₂N₃O₄[M+H]⁺, 368.1605, found 368.1639.

(*E*)-*N*-(5-(methylsulfonyl)-2-((morpholinoimino)methyl)phenyl)benzamide (22)



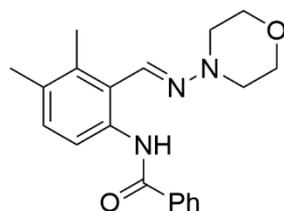
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (1/1) to afford a yellow solid in 22% yield (8.5 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.34 (s, 1H), 9.44 (d, *J* = 1.9 Hz, 1H), 7.94 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.72 (s, 1H), 7.65 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.56 (ddd, *J* = 7.4, 5.6, 1.2 Hz, 1H), 7.49–7.46 (m, 2H), 7.39 (d, *J* = 8.1 Hz, 1H), 3.91–3.89 (m, 4H), 3.22–3.21 (m, 4H), 3.12 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.7, 140.2, 138.1, 137.5, 135.4, 132.1, 131.4, 128.6, 127.6, 125.5, 121.2, 118.8, 66.0, 51.2, 44.1. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₄S[M+H]⁺, 388.1326, found 388.1341.

(E)-N-(2-((morpholinoimino)methyl)-3-nitrophenyl)benzamide (23)



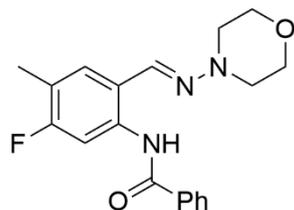
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 73% yield (25.9 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.46 (s, 1H), 9.03 (d, *J* = 8.4 Hz, 1H), 7.93–7.90 (m, 3H), 7.57–7.52 (m, 2H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.41 (t, *J* = 8.3 Hz, 1H), 3.87–3.85 (m, 4H), 3.18–3.16 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.7, 150.4, 138.7, 135.4, 132.9, 132.2, 128.8, 128.6, 127.6, 124.5, 118.8, 114.8, 65.9, 51.1. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₁₉N₄O₄[M+H]⁺, 355.1401, found 355.1426.

(E)-N-(3,4-dimethyl-2-((morpholinoimino)methyl)phenyl)benzamide (24)



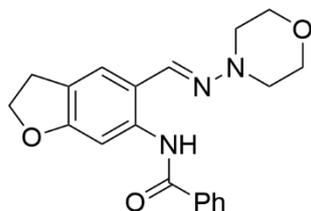
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 88% yield (29.7 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.39 (s, 1H), 8.56 (d, *J* = 8.5 Hz, 1H), 8.06 (s, 1H), 7.95–7.92 (m, 2H), 7.52–7.49 (m, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 7.15 (d, *J* = 8.5 Hz, 1H), 3.88–3.86 (m, 4H), 3.12–3.10 (m, 4H), 2.30 (s, 3H), 2.28 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.2, 138.9, 136.3, 135.9, 135.5, 131.6, 131.4, 131.0, 128.3, 127.5, 119.5, 117.9, 66.1, 51.9, 20.5, 15.7. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₄N₃O₂[M+H]⁺, 338.1863, found 338.1891.

(E)-N-(5-fluoro-4-methyl-2-((morpholinoimino)methyl)phenyl)benzamide (25)



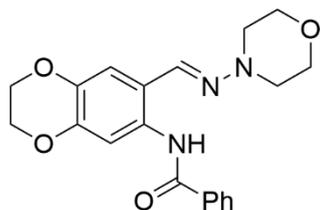
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a white solid in 56% yield (19.1 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.33 (s, 1H), 8.62 (d, *J* = 12.6 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 2H), 7.71 (s, 1H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.04 (d, *J* = 8.2 Hz, 1H), 3.90–3.87 (m, 4H), 3.13–3.11 (m, 4H), 2.24 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.5, 161.2 (d, *J* = 247.0 Hz), 140.9, 137.1 (d, *J* = 11.8 Hz), 135.8, 133.9 (d, *J* = 7.1 Hz), 131.8, 128.5, 127.6, 119.2 (d, *J* = 18.7 Hz), 117.3 (d, *J* = 3.2 Hz), 107.3 (d, *J* = 29.6 Hz), 66.2, 51.9, 14.0. ¹⁹F NMR (564 MHz, CDCl₃): δ -112.9. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₁N₃O₂[M+H]⁺, 342.1612, found 342.1647.

(E)-N-(5-((morpholinoimino)methyl)-2,3-dihydrobenzofuran-6-yl)benzamide (26)



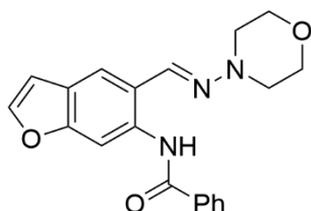
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with dichloromethane/ethyl acetate (5/1) to afford a white solid in 70% yield (24.6 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.47 (s, 1H), 8.40 (s, 1H), 7.96 (d, *J* = 7.3 Hz, 2H), 7.77 (s, 1H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.05 (s, 1H), 4.62 (t, *J* = 8.6 Hz, 2H), 3.89–3.86 (m, 4H), 3.18 (t, *J* = 8.6 Hz, 2H), 3.10–3.07 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 161.7, 143.5, 138.9, 136.1, 131.6, 128.4, 127.8, 127.7, 121.6, 114.2, 101.6, 71.9, 66.3, 52.4, 29.0. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₂N₃O₃[M+H]⁺, 352.1656, found 352.1658.

(E)-N-(7-((morpholinoimino)methyl)-2,3-dihydrobenzo[b][1,4]dioxin-6-yl)benzamide (27)



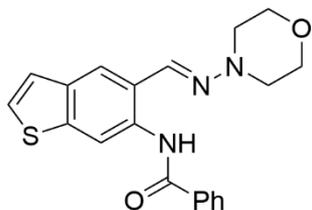
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 31% yield (11.4 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.16 (s, 1H), 8.47 (s, 1H), 7.94 (d, *J* = 7.8 Hz, 2H), 7.66 (s, 1H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.5 Hz, 2H), 6.75 (s, 1H), 4.29 (d, *J* = 3.5 Hz, 2H), 4.25 (d, *J* = 3.6 Hz, 2H), 3.88–3.86 (m, 4H), 3.11–3.09 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.1, 144.2, 141.5, 139.0, 136.1, 132.4, 131.5, 128.4, 127.6, 119.4, 115.5, 109.5, 66.2, 64.6, 64.3, 52.1. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₂N₃O₄[M+H]⁺, 368.1605, found 368.1606.

(E)-N-(5-((morpholinoimino)methyl)benzofuran-6-yl)benzamide (28)



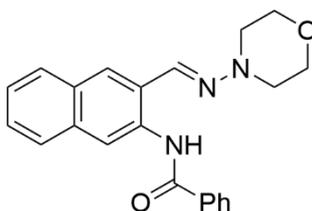
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a white solid in 55% yield (19.2 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.51 (s, 1H), 9.12 (s, 1H), 7.97 (d, *J* = 7.7 Hz, 2H), 7.83 (s, 1H), 7.59 (s, 1H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 2H), 7.41 (s, 1H), 6.67 (s, 1H), 3.88–3.86 (m, 4H), 3.12–3.10 (m, 4H). ¹³C NMR (150MHz, CDCl₃): δ 166.4, 155.3, 145.6, 142.3, 136.0, 135.3, 131.6, 128.4, 127.6, 124.1, 122.7, 118.0, 106.1, 103.3, 66.2, 51.9. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₀N₃O₃[M+H]⁺, 350.1499, found 350.1504.

(E)-N-(5-((morpholinoimino)methyl)benzo[b]thiophen-6-yl)benzamide (29)



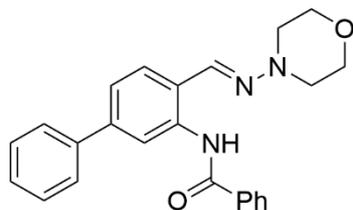
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 36% yield (13.1 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.45 (s, 1H), 9.49 (s, 1H), 8.00–7.98 (m, 2H), 7.89 (s, 1H), 7.68 (s, 1H), 7.56–7.53 (m, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.38 (d, *J* = 5.4 Hz, 1H), 7.26 (s, 1H), 3.92–3.90 (m, 4H), 3.18–3.16 (m, 4H). ¹³C NMR (150 MHz, CDCl₃) δ 166.6, 141.8, 141.3, 136.2, 135.1, 134.5, 131.6, 128.5, 127.7, 126.4, 126.4, 123.2, 119.6, 113.2, 66.2, 51.9. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₀N₃O₂[M+H]⁺, 366.1271, found 366.1292.

(E)-N-(3-((morpholinoimino)methyl)naphthalen-2-yl)benzamide (30)



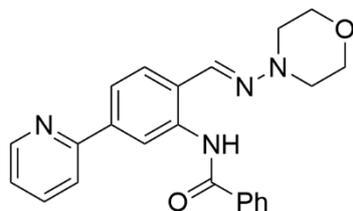
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 97% yield (34.8 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.38 (s, 1H), 9.33 (s, 1H), 8.00 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.91 (s, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.74–7.71 (m, 2H), 7.56–7.53 (m, 1H), 7.49–7.46 (m, 3H), 7.40–7.37 (m, 1H), 3.90 (dd, *J* = 5.7, 4.1 Hz, 4H), 3.19–3.17 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 141.0, 136.2, 134.9, 133.7, 131.8, 131.6, 129.5, 128.5, 127.8, 127.6, 127.4, 127.3, 125.2, 122.2, 117.1, 66.2, 51.7. HRMS (ESI-TOF) *m/z* calcd. for C₂₂H₂₂N₃O₂[M+H]⁺, 360.1707, found 360.1744.

(E)-N-(4-((morpholinoimino)methyl)-[1,1'-biphenyl]-3-yl)benzamide (31)



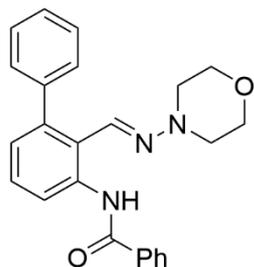
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 79% yield (30.4 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.34 (s, 1H), 9.24 (d, *J* = 1.7 Hz, 1H), 8.01–7.98 (m, 2H), 7.76 (s, 1H), 7.73–7.71 (m, 2H), 7.56–7.53 (m, 1H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.37–7.35 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 3.89–3.87 (m, 4H), 3.15–3.13 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 141.9, 140.7, 140.1, 138.1, 136.0, 131.7, 131.7, 128.7, 128.4, 127.7, 127.6, 127.1, 121.5, 120.2, 118.5, 66.1, 51.7. HRMS (ESI-TOF) *m/z* calcd. for C₂₄H₂₄N₃O₂[M+H]⁺, 386.1863, found 386.1858.

(E)-N-(2-((morpholinoimino)methyl)-5-(pyridin-2-yl)phenyl)benzamide (32)



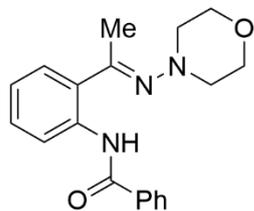
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 81% yield (31.3 mg). ¹H NMR (600 MHz, CDCl₃): δ 13.55 (s, 1H), 8.94 (d, *J* = 1.6 Hz, 1H), 8.63–8.61 (m, 1H), 8.05–8.03 (m, 2H), 7.78 (dt, *J* = 7.5, 1.3 Hz, 2H), 7.70 (d, *J* = 8.3 Hz, 1H), 7.64 (s, 1H), 7.58 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.52–7.47 (m, 3H), 7.23 (ddd, *J* = 6.8, 4.9, 2.0 Hz, 1H), 3.89–3.87 (m, 4H), 3.22–3.20 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 165.5, 157.8, 147.0, 138.4, 137.7, 137.7, 135.6, 135.2, 131.4, 128.8, 128.5, 127.3, 124.4, 122.6, 121.7, 120.5, 119.8, 66.3, 51.6. HRMS (ESI-TOF) *m/z* calcd. for C₂₃H₂₃N₄O₂[M+H]⁺, 387.1816, found 387.1829.

(E)-N-(2-((morpholinoimino)methyl)-[1,1'-biphenyl]-3-yl)benzamide (33)



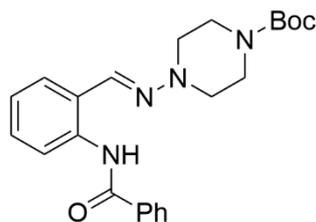
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 82% yield (31.6 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.56 (s, 1H), 8.87 (d, *J* = 8.3 Hz, 1H), 7.99–7.96 (m, 2H), 7.73 (s, 1H), 7.53 (t, *J* = 7.3 Hz, 1H), 7.48–7.38 (m, 6H), 7.34–7.32 (m, 2H), 7.05–7.02 (m, 1H), 3.79–3.76 (m, 4H), 2.94–2.91 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 143.6, 140.4, 140.2, 138.0, 136.2, 131.6, 129.7, 129.0, 128.4, 128.2, 127.6, 127.5, 125.2, 119.5, 118.7, 66.0, 51.5. HRMS (ESI-TOF) *m/z* calcd. for C₂₄H₂₄N₃O₂[M+H]⁺, 386.1863, found 386.1874.

(E)-N-(2-(1-(morpholinoimino)ethyl)phenyl)benzamide (34)



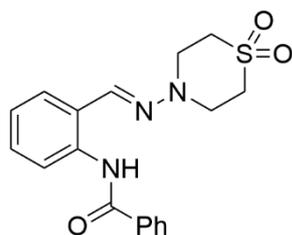
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 21% yield (6.8 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.89 (s, 1H), 8.77 (dd, *J* = 8.4, 1.0 Hz, 1H), 7.98–7.95 (m, 2H), 7.60 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.53 (td, *J* = 6.3, 5.3, 3.1 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 2H), 7.44–7.41 (m, 1H), 7.15–7.12 (m, 1H), 3.84–3.82 (m, 4H), 2.84–2.82 (m, 4H), 2.51 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 167.8, 166.7, 138.6, 136.0, 131.7, 130.5, 129.3, 128.4, 127.7, 123.7, 122.8, 121.2, 66.2, 55.4, 16.6. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₂[M+H]⁺, 324.1707, found 324.1704.

tert-butyl (E)-4-((2-benzamidobenzylidene)amino)piperazine-1-carboxylate (35)



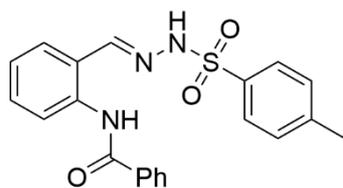
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a white solid in 40% yield (16.3 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.27 (s, 1H), 8.86 (d, $J = 8.3$ Hz, 1H), 7.96 (d, $J = 7.8$ Hz, 2H), 7.77 (s, 1H), 7.54 (t, $J = 7.3$ Hz, 1H), 7.47 (t, $J = 7.5$ Hz, 2H), 7.35 (t, $J = 7.8$ Hz, 1H), 7.25 (d, $J = 8.4$ Hz, 1H), 7.11 (t, $J = 7.5$ Hz, 1H), 3.64–3.60 (m, 4H), 3.13–3.09 (m, 4H), 1.47 (s, 9H). ^{13}C NMR (150 MHz, CDCl_3): δ 166.6, 154.4, 141.9, 137.8, 136.1, 131.7, 131.4, 129.5, 128.5, 127.6, 123.0, 121.1, 120.0, 80.3, 51.0, 28.3. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{23}\text{H}_{29}\text{N}_4\text{O}_3[\text{M}+\text{H}]^+$, 409.2234, found 409.2271.

(E)-N-(2-(((1,1-dioxidothiomorpholino)imino)methyl)phenyl)benzamide (36)



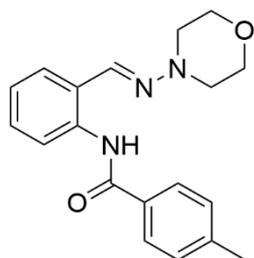
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a colorless oil in 24% yield (8.6 mg). ^1H NMR (600 MHz, CDCl_3): δ 11.90 (s, 1H), 8.82 (d, $J = 8.3$ Hz, 1H), 7.92–7.89 (m, 2H), 7.81 (s, 1H), 7.57–7.54 (m, 1H), 7.48 (t, $J = 7.6$ Hz, 2H), 7.44–7.41 (m, 1H), 7.27 (dd, $J = 7.7, 1.4$ Hz, 1H), 7.15 (td, $J = 7.6, 1.0$ Hz, 1H), 3.88–3.85 (m, 4H), 3.02–2.99 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 166.5, 145.3, 137.9, 136.2, 131.9, 131.7, 130.5, 128.6, 127.3, 123.3, 120.4, 48.8, 48.3. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{18}\text{H}_{20}\text{N}_3\text{O}_3\text{S}[\text{M}+\text{H}]^+$, 358.1220, found 358.1224.

(E)-N-(2-((2-tosylhydrazineylidene)methyl)phenyl)benzamide (38)



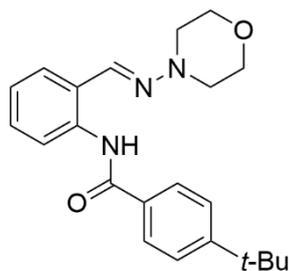
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 30% yield (11.8 mg). ¹H NMR (600 MHz, CDCl₃): δ 11.31 (s, 1H), 8.81–8.79 (m, 1H), 8.14–8.11 (m, 2H), 7.96 (s, 1H), 7.60 (q, *J* = 3.6 Hz, 3H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.38–7.35 (m, 1H), 7.12 (d, *J* = 7.3 Hz, 1H), 7.05–7.02 (m, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 2.26 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.8, 151.9, 144.4, 138.3, 134.6, 134.5, 132.8, 132.2, 131.5, 129.8, 129.0, 127.9, 127.4, 123.2, 120.5, 119.3, 21.4. HRMS (ESI-TOF) *m/z* calcd. for C₂₁H₂₀N₃O₃S[M+H]⁺, 394.1220, found 394.1245.

(*E*)-4-methyl-*N*-(2-((morpholinoimino)methyl)phenyl)benzamide (39)



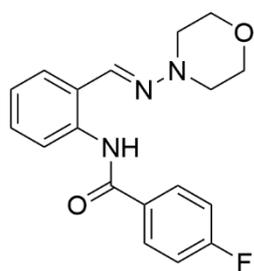
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 79% yield (25.5 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.22 (s, 1H), 8.87 (d, *J* = 8.3 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 2H), 7.74 (s, 1H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.26–7.21 (m, 3H), 7.08 (t, *J* = 7.4 Hz, 1H), 3.90–3.88 (m, 4H), 3.15–3.13 (m, 4H), 2.41 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.4, 142.1, 141.2, 137.9, 133.1, 131.3, 129.4, 129.0, 127.6, 122.8, 121.1, 119.9, 66.1, 51.7, 21.4. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₂[M+H]⁺, 324.1707, found 324.1740.

(*E*)-4-(*tert*-butyl)-*N*-(2-((morpholinoimino)methyl)phenyl)benzamide (40)



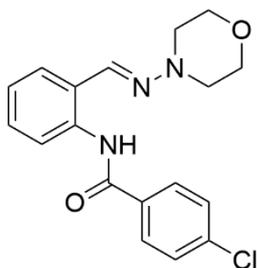
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 76% yield (27.8 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.22 (s, 1H), 8.87 (d, $J = 8.3$ Hz, 1H), 7.91 (d, $J = 8.4$ Hz, 2H), 7.75 (s, 1H), 7.47 (d, $J = 8.4$ Hz, 2H), 7.35–7.32 (m, 1H), 7.24–7.22 (m, 1H), 7.08 (t, $J = 7.4$ Hz, 1H), 3.89–3.87 (m, 4H), 3.16–3.14 (m, 4H), 1.35 (s, 9H). ^{13}C NMR (150 MHz, CDCl_3): δ 166.4, 155.1, 141.3, 137.9, 133.1, 131.3, 129.3, 127.4, 125.3, 122.8, 121.1, 120.0, 66.1, 51.8, 34.9, 31.1. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{22}\text{H}_{28}\text{N}_3\text{O}_2[\text{M}+\text{H}]^+$, 366.2176, found 366.2211.

(E)-4-fluoro-N-(2-((morpholinoimino)methyl)phenyl)benzamide (41)



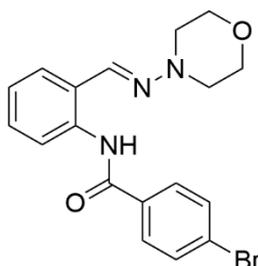
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 89% yield (29.1 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.24 (s, 1H), 8.82–8.80 (m, 1H), 7.98–7.95 (m, 2H), 7.75 (s, 1H), 7.36–7.33 (m, 1H), 7.24 (dd, $J = 7.7, 1.5$ Hz, 1H), 7.15–7.09 (m, 3H), 3.90–3.88 (m, 4H), 3.13–3.11 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 165.4, 164.8 (d, $J = 252.3$ Hz), 141.3, 137.7, 132.3 (d, $J = 3.1$ Hz), 131.4, 129.9 (d, $J = 8.9$ Hz), 129.5, 123.1, 121.1, 120.0, 115.5 (d, $J = 21.8$ Hz), 66.1, 51.8. ^{19}F NMR (564 MHz, CDCl_3): δ -107.8. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{18}\text{H}_{19}\text{FN}_3\text{O}_2[\text{M}+\text{H}]^+$, 328.1456, found 328.1467.

(E)-4-chloro-N-(2-((morpholinoimino)methyl)phenyl)benzamide (42)



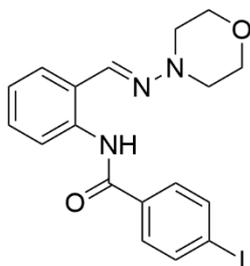
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 91% yield (31.2 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.25 (s, 1H), 8.81 (d, $J = 8.3$ Hz, 1H), 7.91–7.88 (m, 2H), 7.74 (s, 1H), 7.42 (dd, $J = 8.8, 1.9$ Hz, 2H), 7.36–7.32 (m, 1H), 7.24 (dd, $J = 7.7, 1.2$ Hz, 1H), 7.12–7.09 (m, 1H), 3.90–3.88 (m, 4H), 3.13–3.11 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 165.3, 141.2, 137.8, 137.6, 134.4, 131.4, 129.4, 129.0, 128.7, 123.2, 121.1, 120.0, 66.1, 51.8. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{18}\text{H}_{19}\text{ClN}_3\text{O}_2[\text{M}+\text{H}]^+$, 344.1160, found 344.1152.

(E)-4-bromo-N-(2-((morpholinoimino)methyl)phenyl)benzamide (43)



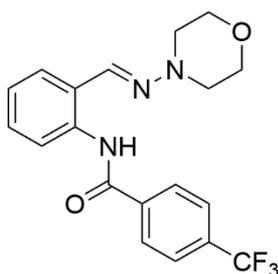
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 92% yield (35.6 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.24 (s, 1H), 8.82–8.80 (m, 1H), 7.83–7.80 (m, 2H), 7.72 (s, 1H), 7.59–7.57 (m, 2H), 7.33 (td, $J = 8.6, 8.1, 1.5$ Hz, 1H), 7.23 (dd, $J = 7.7, 1.5$ Hz, 1H), 7.09 (td, $J = 7.5, 1.2$ Hz, 1H), 3.89–3.87 (m, 4H), 3.12–3.10 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 165.3, 141.2, 137.5, 134.8, 131.6, 131.3, 129.4, 129.2, 126.3, 123.2, 121.1, 119.9, 66.1, 51.7. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{18}\text{H}_{19}\text{BrN}_3\text{O}_2[\text{M}+\text{H}]^+$, 388.0655, found 388.0692.

(E)-4-iodo-N-(2-((morpholinoimino)methyl)phenyl)benzamide (44)



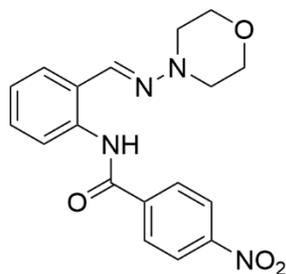
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 98% yield (42.6 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.26 (s, 1H), 8.83–8.81 (m, 1H), 7.83–7.80 (m, 2H), 7.76 (s, 1H), 7.71–7.68 (m, 2H), 7.35 (td, $J = 8.6, 8.1, 1.5$ Hz, 1H), 7.26–7.25 (m, 1H), 7.12 (td, $J = 7.5, 1.1$ Hz, 1H), 3.92–3.90 (m, 4H), 3.15–3.13 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 165.6, 141.4, 137.7, 137.6, 135.4, 131.4, 129.5, 129.2, 123.3, 121.1, 120.1, 98.7, 66.2, 51.8. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{18}\text{H}_{19}\text{IN}_3\text{O}_2[\text{M}+\text{H}]^+$, 436.0516, found 436.0522.

(E)-N-(2-((morpholinoimino)methyl)phenyl)-4-(trifluoromethyl)benzamide (45)



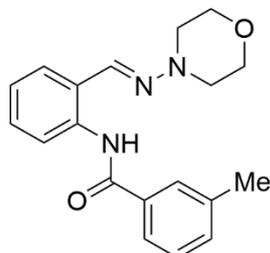
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 98% yield (37.0 mg). ^1H NMR (600 MHz, CDCl_3): δ 12.35 (s, 1H), 8.84–8.81 (m, 1H), 8.06 (d, $J = 8.1$ Hz, 2H), 7.74–7.70 (m, 3H), 7.36–7.33 (m, 1H), 7.24 (dd, $J = 7.7, 1.4$ Hz, 1H), 7.12 (td, $J = 7.5, 1.1$ Hz, 1H), 3.88 (dd, $J = 5.7, 4.1$ Hz, 4H), 3.12–3.10 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 164.9, 141.1, 139.2, 137.3, 133.2 (q, $J = 32.6$ Hz), 131.4, 129.4, 128.0, 125.4 (q, $J = 3.6$ Hz), 123.6 (d, $J = 272.6$ Hz), 123.4, 121.2, 120.0, 66.1, 51.7. ^{19}F NMR (564 MHz, CDCl_3): δ -62.8. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{19}\text{H}_{19}\text{F}_3\text{N}_3\text{O}_2[\text{M}+\text{H}]^+$, 378.1424, found 378.1425.

(E)-N-(2-((morpholinoimino)methyl)phenyl)-4-nitrobenzamide (46)



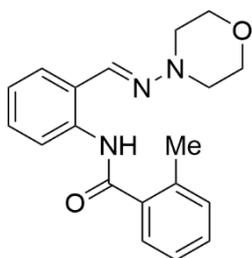
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 93% yield (32.9 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.43 (s, 1H), 8.82–8.80 (m, 1H), 8.33–8.30 (m, 2H), 8.13–8.10 (m, 2H), 7.77 (s, 1H), 7.39–7.35 (m, 1H), 7.28 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.16 (td, *J* = 7.5, 1.2 Hz, 1H), 3.91–3.89 (m, 4H), 3.14–3.11 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 164.2, 149.6, 141.6, 141.2, 137.2, 131.5, 129.6, 128.7, 123.8, 123.7, 121.3, 120.1, 66.1, 51.8. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₁₉N₄O₄[M+H]⁺, 355.1401, found 355.1409.

(E)-3-methyl-N-(2-((morpholinoimino)methyl)phenyl)benzamide (47)



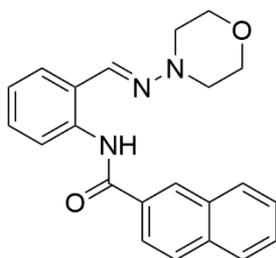
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 85% yield (27.5 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.28 (s, 1H), 8.88–8.86 (m, 1H), 7.77–7.75 (m, 2H), 7.72 (s, 1H), 7.35–7.32 (m, 3H), 7.23 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.08 (td, *J* = 7.5, 1.2 Hz, 1H), 3.88–3.85 (m, 4H), 3.12 (dd, *J* = 5.6, 4.1 Hz, 4H), 2.40 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 166.7, 140.9, 138.1, 137.8, 136.0, 132.3, 131.3, 129.3, 128.3, 128.1, 124.8, 122.9, 121.1, 119.9, 66.1, 51.7, 21.2. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₂[M+H]⁺, 324.1707, found 324.1700.

(E)-2-methyl-N-(2-((morpholinoimino)methyl)phenyl)benzamide (48)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 36% yield (11.6 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.12 (s, 1H), 8.87 (d, *J* = 8.2 Hz, 1H), 7.70 (s, 1H), 7.58 (d, *J* = 7.4 Hz, 1H), 7.37–7.33 (m, 2H), 7.27 (d, *J* = 4.2 Hz, 1H), 7.24 (t, *J* = 7.4 Hz, 2H), 7.13–7.10 (m, 1H), 3.82–3.79 (m, 4H), 2.99–2.96 (m, 4H), 2.55 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 168.6, 140.2, 137.8, 137.1, 137.0, 131.2, 131.1, 130.1, 129.3, 127.2, 125.4, 123.0, 120.9, 119.8, 66.1, 51.5, 20.1. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₂[M+H]⁺, 324.1707, found 324.1746.

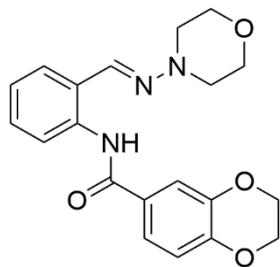
(*E*)-*N*-(2-((morpholinoimino)methyl)phenyl)-2-naphthamide (49)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 38% yield (13.6 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.52 (s, 1H), 8.93 (d, *J* = 8.2 Hz, 1H), 8.46 (s, 1H), 8.05 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.93–7.89 (m, 3H), 7.77 (s, 1H), 7.59–7.56 (m, 1H), 7.56–7.53 (m, 1H), 7.39–7.36 (m, 1H), 7.26 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.12 (td, *J* = 7.5, 1.0 Hz, 1H), 3.87–3.85 (m, 4H), 3.16–3.14 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 141.0, 137.9, 134.8, 133.5, 132.5, 131.3, 129.5, 128.5, 128.4, 127.9, 127.9, 127.7, 126.8, 124.4, 123.0, 121.1, 120.0, 66.2, 51.8. HRMS (ESI-TOF) *m/z* calcd. for C₂₂H₂₂N₃O₂[M+H]⁺, 360.1707, found 360.1715.

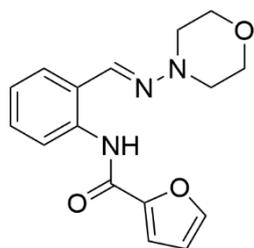
(*E*)-*N*-(2-((morpholinoimino)methyl)phenyl)-2,3-dihydrobenzo[*b*][1,4]dioxine-6-carboxamide

(50)



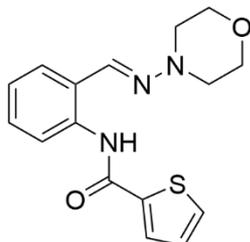
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 43% yield (15.8 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.18 (s, 1H), 8.83 (d, *J* = 8.2 Hz, 1H), 7.74 (s, 1H), 7.53 (d, *J* = 2.1 Hz, 1H), 7.49 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.34–7.31 (m, 1H), 7.22 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.07 (td, *J* = 7.5, 1.0 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 4.30 (dd, *J* = 5.6, 2.3 Hz, 2H), 4.26 (dd, *J* = 5.6, 2.3 Hz, 2H), 3.90–3.88 (m, 4H), 3.19–3.17 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 165.7, 146.6, 143.3, 141.1, 137.9, 131.3, 129.4, 129.2, 122.7, 121.3, 121.1, 119.8, 117.1, 117.0, 66.2, 64.5, 64.1, 51.8. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₂N₃O₄[M+H]⁺, 368.1605, found 368.1641.

(*E*)-*N*-(2-((morpholinoimino)methyl)phenyl)furan-2-carboxamide (51)



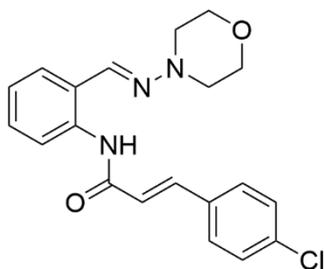
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 78% yield (23.3 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.49 (s, 1H), 8.81 (d, *J* = 8.3 Hz, 1H), 7.71 (s, 1H), 7.45–7.43 (m, 1H), 7.32–7.28 (m, 1H), 7.23–7.20 (m, 2H), 7.08 (td, *J* = 7.6, 0.9 Hz, 1H), 6.54 (dd, *J* = 3.4, 1.7 Hz, 1H), 3.93–3.90 (m, 4H), 3.26–3.24 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 156.9, 148.9, 143.6, 140.1, 137.1, 131.1, 129.1, 123.0, 121.3, 120.2, 115.0, 112.5, 66.2, 51.5. HRMS (ESI-TOF) *m/z* calcd. for C₁₆H₁₈N₃O₃[M+H]⁺, 300.1343, found 300.1370.

(E)-N-(2-((morpholinoimino)methyl)phenyl)thiophene-2-carboxamide (52)



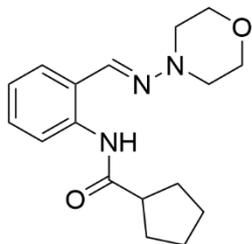
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 71% yield (22.4 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.09 (s, 1H), 8.74 (d, *J* = 8.3 Hz, 1H), 7.74 (s, 1H), 7.68 (d, *J* = 3.4 Hz, 1H), 7.52 (d, *J* = 4.8 Hz, 1H), 7.31 (t, *J* = 7.8 Hz, 1H), 7.22 (d, *J* = 7.1 Hz, 1H), 7.11–7.07 (m, 2H), 3.91–3.89 (m, 4H), 3.19–3.17 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 160.7, 141.4, 140.7, 137.4, 131.4, 130.5, 129.3, 128.6, 127.4, 123.0, 121.0, 120.1, 66.2, 51.8. HRMS (ESI-TOF) *m/z* calcd. for C₁₆H₁₈N₃O₂S[M+H]⁺, 316.1114, found 316.1139.

(E)-3-(4-chlorophenyl)-N-(2-((E)-(morpholinoimino)methyl)phenyl)acrylamide (53)



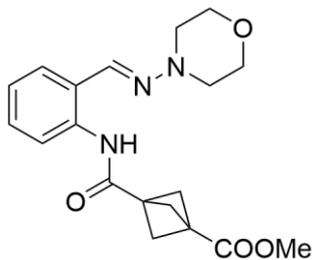
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a white solid in 59% yield (21.8 mg). ¹H NMR (600 MHz, CDCl₃): δ 11.95 (s, 1H), 8.78 (d, *J* = 8.3 Hz, 1H), 7.72 (s, 1H), 7.64 (d, *J* = 15.6 Hz, 1H), 7.43–7.41 (m, 2H), 7.36–7.33 (m, 2H), 7.33–7.30 (m, 1H), 7.21 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.08 (td, *J* = 7.5, 1.1 Hz, 1H), 6.44 (d, *J* = 15.6 Hz, 1H), 3.94–3.91 (m, 4H), 3.20–3.18 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 164.2, 140.9, 139.8, 137.7, 135.5, 133.2, 131.2, 129.3, 129.1, 128.8, 123.0, 122.8, 120.7, 120.1, 66.1, 51.9. HRMS (ESI-TOF) *m/z* calcd. for C₂₀H₂₁ClN₃O₂[M+H]⁺, 370.1317, found 370.1352.

(E)-N-(2-((morpholinoimino)methyl)phenyl)cyclopentanecarboxamide (54)



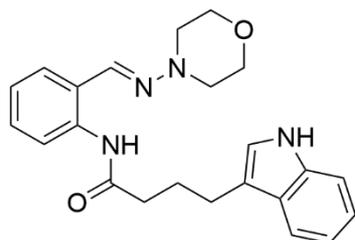
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 37% yield (11.1 mg). ¹H NMR (600 MHz, CDCl₃): δ 11.60 (s, 1H), 8.68 (d, *J* = 8.1 Hz, 1H), 7.72 (s, 1H), 7.29–7.26 (m, 1H), 7.19 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.04 (td, *J* = 7.5, 1.2 Hz, 1H), 3.93–3.91 (m, 4H), 3.16 (dd, *J* = 5.7, 4.1 Hz, 4H), 2.71 (p, *J* = 8.1 Hz, 1H), 1.96–1.92 (m, 4H), 1.77 (dt, *J* = 9.7, 4.5 Hz, 2H), 1.63–1.59 (m, 2H). ¹³C NMR (150 MHz, CDCl₃): δ 175.3, 141.2, 137.9, 131.2, 129.4, 122.5, 120.4, 119.8, 66.2, 51.9, 47.6, 30.5, 26.0. HRMS (ESI-TOF) *m/z* calcd. for C₁₇H₂₄N₃O₂[M+H]⁺, 302.1863, found 302.1902.

methyl(E)-3-((2-((morpholinoimino)methyl)phenyl)carbamoyl)bicyclo[1.1.1]pentane-1-carboxylate (55)



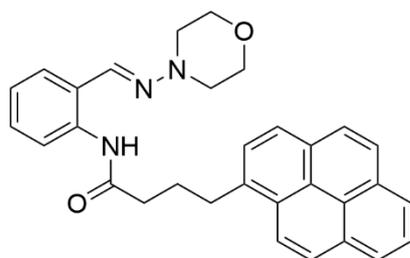
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 31% yield (11.1 mg). ¹H NMR (600 MHz, CDCl₃): δ 11.30 (s, 1H), 8.69 (d, *J* = 8.3 Hz, 1H), 7.73 (s, 1H), 7.31–7.27 (m, 1H), 7.22–7.19 (m, 1H), 7.08 (t, *J* = 7.2 Hz, 1H), 3.93–3.91 (m, 4H), 3.71 (s, 3H), 3.18–3.16 (m, 4H), 2.39 (s, 6H). ¹³C NMR (150 MHz, CDCl₃): δ 169.9, 168.2, 142.1, 137.0, 131.5, 129.5, 123.2, 120.9, 120.2, 66.3, 53.4, 52.5, 52.1, 51.8, 29.6. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₄N₃O₄[M+H]⁺, 358.1761, found 358.1752.

(E)-4-(1H-indol-3-yl)-N-(2-((morpholinoimino)methyl)phenyl)butanamide (56)



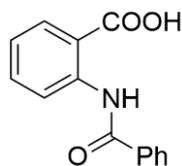
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a white solid in 71% yield (27.7 mg). ¹H NMR (600 MHz, CDCl₃): δ 11.67 (s, 1H), 8.74 (d, *J* = 8.3 Hz, 1H), 8.32 (s, 1H), 7.65 (s, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.35–7.33 (m, 1H), 7.32–7.29 (m, 1H), 7.18 (qd, *J* = 7.9, 1.3 Hz, 2H), 7.11–7.06 (m, 2H), 6.97 (d, *J* = 2.2 Hz, 1H), 3.78 (dd, *J* = 5.7, 4.1 Hz, 4H), 2.97–2.95 (m, 4H), 2.88 (t, *J* = 7.2 Hz, 2H), 2.47–2.44 (m, 2H), 2.22–2.17 (m, 2H). ¹³C NMR (150 MHz, CDCl₃): δ 172.1, 140.5, 137.5, 136.3, 131.1, 129.2, 127.4, 122.7, 121.7, 121.7, 120.5, 119.8, 119.0, 118.7, 115.3, 111.1, 66.0, 51.5, 38.1, 26.1, 24.4. HRMS (ESI-TOF) *m/z* calcd. for C₂₃H₂₇N₄O₂[M+H]⁺, 391.2129, found 391.2140.

(E)-N-(2-((morpholinoimino)methyl)phenyl)-4-(pyren-1-yl)butanamide (57)



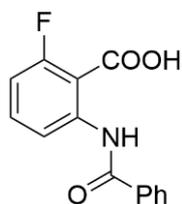
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (3/1) to afford a yellow solid in 72% yield (34.2 mg). ¹H NMR (600 MHz, CDCl₃): δ 11.55 (s, 1H), 8.77 (d, *J* = 8.3 Hz, 1H), 8.25 (d, *J* = 9.2 Hz, 1H), 8.13 (dd, *J* = 12.8, 7.5 Hz, 2H), 8.06 (d, *J* = 7.7 Hz, 1H), 8.00–7.96 (m, 4H), 7.84 (d, *J* = 7.7 Hz, 1H), 7.42 (s, 1H), 7.34–7.31 (m, 1H), 7.11 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.06 (td, *J* = 7.5, 1.1 Hz, 1H), 3.46–3.41 (m, 6H), 2.63–2.60 (m, 4H), 2.42–2.39 (m, 2H), 2.35 (p, *J* = 6.8 Hz, 2H). ¹³C NMR (150 MHz, CDCl₃): δ 171.5, 139.9, 137.4, 135.6, 131.2, 130.9, 130.7, 129.7, 129.1, 128.7, 127.3, 127.3, 127.2, 126.6, 125.7, 124.8, 124.8, 124.8, 124.6, 124.6, 123.2, 122.6, 120.4, 119.7, 65.6, 51.1, 37.5, 32.1, 27.1. HRMS (ESI-TOF) *m/z* calcd. for C₃₁H₃₀N₃O₂[M+H]⁺, 476.2333, found 476.2479.

2-benzamidobenzoic acid (58)¹⁸



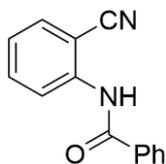
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a yellow solid in 89% yield (21.5 mg). ¹H NMR (600 MHz, DMSO-*d*₆): δ 12.21 (s, 1H), 8.73–8.70 (m, 1H), 8.06 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.98–7.95 (m, 2H), 7.69–7.63 (m, 2H), 7.62–7.57 (m, 2H), 7.21 (td, *J* = 8.0, 1.1 Hz, 1H). ¹³C NMR (150 MHz, DMSO-*d*₆): δ 170.0, 164.7, 141.1, 134.5, 134.3, 132.2, 131.3, 129.0, 127.0, 123.0, 119.9, 116.6.

2-benzamido-6-fluorobenzoic acid (59)¹⁹



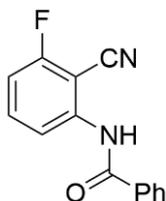
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 92% yield (23.8 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.06 (s, 1H), 10.33 (s, 1H), 8.48 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 7.5 Hz, 2H), 7.80 (q, *J* = 7.7 Hz, 1H), 7.69 (t, *J* = 7.3 Hz, 1H), 7.63 (t, *J* = 7.3 Hz, 2H), 7.16 (t, *J* = 9.6 Hz, 1H). ¹³C NMR (150 MHz, CDCl₃): δ 191.2 (d, *J* = 11.7 Hz), 166.1 (d, *J* = 258.5 Hz), 166.2, 142.5 (d, *J* = 2.4 Hz), 138.3 (d, *J* = 11.4 Hz), 134.0, 132.4, 128.9, 127.5, 115.8 (d, *J* = 3.7 Hz), 110.9 (d, *J* = 8.4 Hz), 109.6 (d, *J* = 20.8 Hz). ¹⁹F NMR (564 MHz, CDCl₃): δ -120.0.

N-(2-cyanophenyl)benzamide (60)²⁰



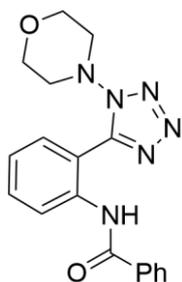
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a yellow solid in 81% yield (18.0 mg). ^1H NMR (600 MHz, CDCl_3): δ 8.57 (d, $J = 8.5$ Hz, 1H), 8.43 (s, 1H), 7.93 (d, $J = 7.4$ Hz, 2H), 7.61 (td, $J = 15.9, 15.2, 7.5$ Hz, 3H), 7.51 (t, $J = 7.7$ Hz, 2H), 7.20 (t, $J = 7.6$ Hz, 1H). ^{13}C NMR (150 MHz, CDCl_3): δ 165.4, 140.6, 134.3, 133.6, 132.6, 132.1, 129.0, 127.2, 124.2, 121.2, 116.4, 102.2.

***N*-(2-cyano-3-fluorophenyl)benzamide (61)**²¹



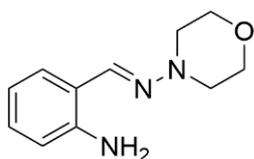
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 85% yield (20.4 mg). ^1H NMR (600 MHz, CDCl_3): δ 8.42 (d, $J = 8.4$ Hz, 2H), 7.92 (d, $J = 7.5$ Hz, 2H), 7.65–7.58 (m, 2H), 7.53 (t, $J = 7.7$ Hz, 2H), 6.96 (t, $J = 8.4$ Hz, 1H). ^{13}C NMR (150 MHz, CDCl_3): δ 165.4, 162.9 (d, $J = 258.3$ Hz), 141.8, 135.7 (d, $J = 9.5$ Hz), 133.3, 132.9, 129.1, 127.2, 116.4 (d, $J = 3.4$ Hz), 112.0, 111.0 (d, $J = 18.8$ Hz), 92.0 (d, $J = 18.6$ Hz). ^{19}F NMR (564 MHz, CDCl_3): δ -104.9.

***N*-(2-(1-morpholino-1*H*-tetrazol-5-yl)phenyl)benzamide (62)**



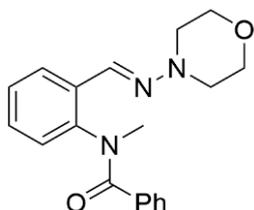
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a yellow solid in 62% yield (21.7 mg). ¹H NMR (600 MHz, CDCl₃): δ 11.68 (s, 1H), 8.86 (d, *J* = 8.4 Hz, 1H), 8.37 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.12–8.09 (m, 2H), 7.62–7.59 (m, 1H), 7.55 (dd, *J* = 14.1, 7.4 Hz, 3H), 7.27 (t, *J* = 7.6 Hz, 1H), 3.95 (t, *J* = 4.6 Hz, 4H), 3.48–3.41 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 165.7, 148.3, 138.4, 134.3, 132.7, 132.1, 128.8, 128.3, 127.4, 123.2, 122.1, 110.8, 66.4, 55.8. HRMS (ESI-TOF) *m/z* calcd. for C₁₈H₁₉N₆O₂[M+H]⁺, 351.1564, found 351.1569.

(*E*)-2-((morpholinoimino)methyl)aniline (63)



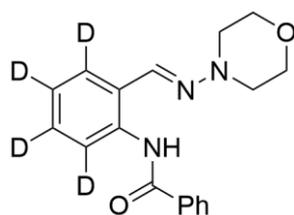
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 89% yield (18.2 mg). ¹H NMR (600 MHz, CDCl₃): δ 7.80 (s, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.71–6.64 (m, 2H), 5.84 (s, 2H), 3.91–3.87 (m, 4H), 3.14–3.10 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 146.1, 142.7, 131.6, 129.0, 117.4, 116.5, 115.7, 52.4. HRMS (ESI-TOF) *m/z* calcd. for C₁₁H₁₆N₃O[M+H]⁺, 206.1288, found 206.1293.

(*E*)-*N*-methyl-*N*-(2-((morpholinoimino)methyl)phenyl)benzamide (64)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid in 81% yield (26.2 mg). ¹H NMR (600 MHz, CDCl₃): δ 7.79–7.76 (m, 1H), 7.60 (s, 1H), 7.26 (d, *J* = 7.3 Hz, 2H), 7.19 (q, *J* = 7.2 Hz, 2H), 7.15–7.10 (m, 3H), 7.00 (d, *J* = 7.7 Hz, 1H), 3.90–3.88 (m, 4H), 3.40 (s, 3H), 3.21–3.18 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 170.9, 142.1, 135.4, 132.4, 130.4, 129.7, 128.8, 128.7, 128.2, 127.7, 127.5, 126.4, 66.2, 51.4, 38.2. HRMS (ESI-TOF) *m/z* calcd. for C₁₉H₂₂N₃O₂[M+H]⁺, 324.1707, found 324.1705.

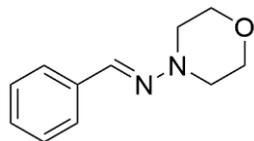
(*E*)-*N*-(2-((morpholinoimino)methyl)phenyl-3,4,5,6-*d*₄)benzamide (3-*D*₄)



The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 95% yield (29.7 mg). ¹H NMR (600 MHz, CDCl₃): δ 12.31 (s, 1H), 7.99–7.97 (m, 2H), 7.76 (s, 1H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 3.90–3.88 (m, 4H), 3.15–3.13 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 166.6, 141.1, 141.1, 137.6, 137.6, 136.0, 131.6, 131.2, 128.4, 127.6, 121.1, 121.1, 119.5, 51.7.

10. Characterization Data for Hydrazones and Dioxazolones

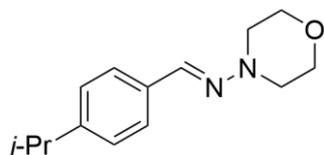
(*E*)-*N*-morpholino-1-phenylmethanimine (A1)¹



The title compound was prepared according to the general procedure to afford a white solid in 96% yield (1.83 g).

¹H NMR (600 MHz, CDCl₃): δ 7.61–7.58 (m, 3H), 7.34 (td, *J* = 7.0, 1.5 Hz, 2H), 7.29–7.26 (m, 1H), 3.90–3.88 (m, 4H), 3.19–3.17 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 136.3, 135.9, 128.5, 128.4, 126.2, 66.5, 51.9.

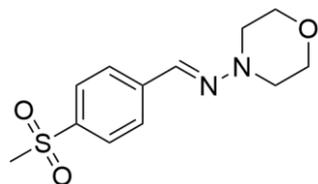
(*E*)-1-(4-isopropylphenyl)-*N*-morpholinomethanimine (A6)



The title compound was prepared according to the general procedure to afford a white solid in 93% yield (2.16 g).

¹H NMR (600 MHz, CDCl₃): δ 7.60 (s, 1H), 7.53 (d, *J* = 7.9 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 3.90–3.87 (m, 4H), 3.17–3.14 (m, 4H), 2.90 (hept, *J* = 6.2 Hz, 1H), 1.25 (d, *J* = 6.9 Hz, 6H). ¹³C NMR (150 MHz, CDCl₃): δ 149.4, 136.8, 133.5, 126.6, 126.3, 66.5, 52.0, 33.9, 23.9. HRMS (ESI-TOF) *m/z* calcd. for C₁₄H₂₁N₂O [M+H]⁺, 233.1648, found 233.1645.

(*E*)-1-(4-(methylsulfonyl)phenyl)-*N*-morpholinomethanimine (A20)



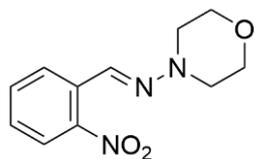
The title compound was prepared according to the general procedure to afford a yellow solid in 95% yield (2.55 g).

¹H NMR (600 MHz, CDCl₃): δ 7.89 (d, *J* = 8.5 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.53 (s, 1H), 3.90–3.88 (m, 4H),

3.25–3.23 (m, 4H), 3.05 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3): δ 141.4, 139.1, 132.3, 127.7, 126.5, 66.3, 51.3, 44.6.

HRMS (ESI-TOF) m/z calcd. for $\text{C}_{12}\text{H}_{17}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$, 269.0954, found 269.0950.

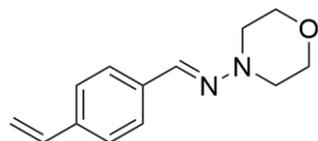
(*E*)-*N*-morpholino-1-(2-nitrophenyl)methanimine (A22)



The title compound was prepared according to the general procedure to afford a yellow solid in 94% yield (2.21 g).

^1H NMR (600 MHz, CDCl_3): δ 8.10 (dd, $J = 8.0, 1.3$ Hz, 1H), 8.07 (s, 1H), 7.95 (dd, $J = 8.2, 1.2$ Hz, 1H), 7.58–7.55 (m, 1H), 7.38 (ddd, $J = 8.4, 7.4, 1.4$ Hz, 1H), 3.90–3.88 (m, 4H), 3.27–3.25 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 147.4, 133.0, 131.0, 130.1, 128.1, 127.6, 124.7, 66.3, 51.4. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{11}\text{H}_{14}\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$, 236.1030, found 236.1037.

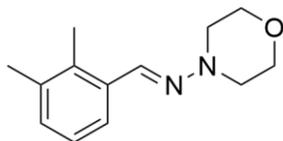
(*E*)-*N*-morpholino-1-(4-vinylphenyl)methanimine (A23)



The title compound was prepared according to the general procedure to afford a yellow solid in 97% yield (2.10 g).

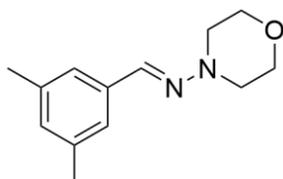
^1H NMR (600 MHz, CDCl_3): δ 7.58–7.54 (m, 3H), 7.39 (d, $J = 7.9$ Hz, 2H), 6.70 (dd, $J = 17.6, 10.9$ Hz, 1H), 5.76 (d, $J = 17.6$ Hz, 1H), 5.25 (d, $J = 10.9$ Hz, 1H), 3.90–3.87 (m, 4H), 3.21–3.16 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 137.5, 136.5, 135.9, 135.4, 126.4, 126.3, 113.9, 66.5, 51.8. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{13}\text{H}_{17}\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$, 217.1335, found 217.1336.

(*E*)-1-(2,3-dimethylphenyl)-*N*-morpholinomethanimine (A24)



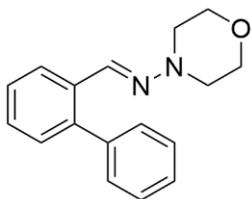
The title compound was prepared according to the general procedure to afford a white solid in 96% yield (2.09 g). ¹H NMR (600 MHz, CDCl₃): δ 7.91 (s, 1H), 7.63 (dd, *J* = 6.6, 2.6 Hz, 1H), 7.11–7.08 (m, 2H), 3.91–3.89 (m, 4H), 3.19–3.17 (m, 4H), 2.31 (s, 3H), 2.30 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 136.9, 136.0, 134.1, 133.9, 130.0, 125.6, 123.8, 66.5, 52.1, 20.5, 14.8. HRMS (ESI-TOF) *m/z* calcd. for C₁₃H₁₉N₂O [M+H]⁺, 219.1492, found 219.1498.

(*E*)-1-(3,5-dimethylphenyl)-*N*-morpholinomethanimine (A25)



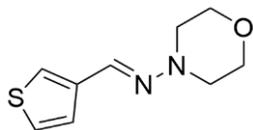
The title compound was prepared according to the general procedure to afford a white solid in 98% yield (2.14 g). ¹H NMR (600 MHz, CDCl₃): δ 7.55 (s, 1H), 7.22 (s, 2H), 6.93 (s, 1H), 3.89–3.87 (m, 4H), 3.17–3.15 (m, 4H), 2.32 (s, 6H). ¹³C NMR (150 MHz, CDCl₃): δ 138.1, 137.0, 135.7, 130.2, 124.1, 66.5, 51.9, 21.2. HRMS (ESI-TOF) *m/z* calcd. for C₁₃H₁₉N₂O [M+H]⁺, 219.1492, found 219.1496.

(*E*)-1-([1,1'-biphenyl]-2-yl)-*N*-morpholinomethanimine (A29)



The title compound was prepared according to the general procedure to afford a yellow solid in 94% yield (2.50 g). ¹H NMR (600 MHz, CDCl₃): δ 8.01–7.98 (m, 1H), 7.55 (s, 1H), 7.38–7.35 (m, 2H), 7.33–7.26 (m, 5H), 7.24–7.22 (m, 1H), 3.74–3.72 (m, 4H), 3.00–2.97 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 140.7, 139.9, 135.3, 132.9, 129.8, 129.4, 127.9, 127.8, 127.3, 127.0, 125.1, 66.0, 51.5. HRMS (ESI-TOF) *m/z* calcd. for C₁₇H₁₉N₂O [M+H]⁺, 267.1492, found 267.1493.

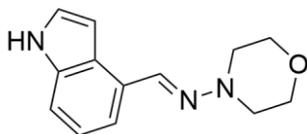
(E)-N-morpholino-1-(thiophen-3-yl)methanimine (A30)



The title compound was prepared according to the general procedure to afford a yellow solid in 95% yield (1.86 g).

^1H NMR (600 MHz, CDCl_3): δ 7.67 (s, 1H), 7.43 (d, $J = 5.0$ Hz, 1H), 7.34–7.31 (m, 1H), 7.28 (dd, $J = 5.0, 3.0$ Hz, 1H), 3.89–3.86 (m, 4H), 3.13–3.11 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 139.2, 132.3, 126.1, 125.1, 123.2, 66.5, 51.9. HRMS (ESI-TOF) m/z calcd. for $\text{C}_9\text{H}_{13}\text{N}_2\text{OS}$ $[\text{M}+\text{H}]^+$, 197.0743, found 197.0745.

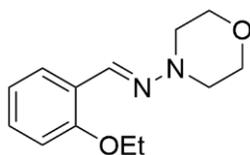
(E)-1-(1H-indol-4-yl)-N-morpholinomethanimine (A32)



The title compound was prepared according to the general procedure to afford a yellow solid in 93% yield (2.13 g).

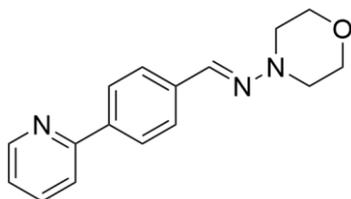
^1H NMR (600 MHz, CDCl_3): δ 8.29 (s, 1H), 7.96 (s, 1H), 7.35 (d, $J = 8.0$ Hz, 1H), 7.28–7.26 (m, 1H), 7.24 (s, 1H), 7.22–7.17 (m, 2H), 3.94–3.92 (m, 4H), 3.27–3.25 (m, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 137.9, 136.3, 127.7, 124.7, 124.5, 121.8, 120.2, 111.4, 103.2, 66.5, 52.1. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{13}\text{H}_{16}\text{N}_3\text{O}$ $[\text{M}+\text{H}]^+$, 230.1228, found 230.1231.

(E)-1-(2-ethoxyphenyl)-N-morpholinomethanimine (A37)



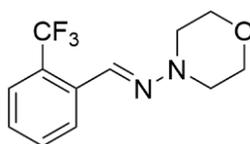
The title compound was prepared according to the general procedure to afford a yellow solid in 97% yield (2.27 g). ¹H NMR (600 MHz, CDCl₃): δ 8.01 (s, 1H), 7.86 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.22 (ddd, *J* = 8.4, 7.4, 1.8 Hz, 1H), 6.93 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 8.0 Hz, 1H), 4.06 (q, *J* = 7.0 Hz, 2H), 3.88 (dd, *J* = 5.7, 4.1 Hz, 4H), 3.17 (dd, *J* = 5.7, 4.1 Hz, 4H), 1.42 (t, *J* = 7.0 Hz, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 156.4, 132.7, 129.3, 125.4, 124.5, 120.7, 111.9, 66.4, 63.8, 52.0, 14.8. HRMS (ESI-TOF) *m/z* calcd. for C₁₄H₁₉N₂O₂ [M+H]⁺, 235.1441, found 235.1446.

(*E*)-*N*-morpholino-1-(4-(pyridin-2-yl)phenyl)methanimine (A40)



The title compound was prepared according to the general procedure to afford a yellow solid in 95% yield (1.86 g). ¹H NMR (600 MHz, CDCl₃): δ 8.69 (d, *J* = 4.7 Hz, 1H), 8.00 (d, *J* = 8.3 Hz, 2H), 7.74 (d, *J* = 3.5 Hz, 2H), 7.70 (d, *J* = 8.3 Hz, 2H), 7.63 (s, 1H), 7.22 (h, *J* = 4.4 Hz, 1H), 3.91–3.89 (m, 4H), 3.22–3.20 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 156.9, 149.7, 139.1, 136.7, 136.5, 135.5, 127.0, 126.5, 122.1, 120.4, 66.5, 51.8. HRMS (ESI-TOF) *m/z* calcd. for C₁₆H₁₈N₃O [M+H]⁺, 268.1444, found 268.1448.

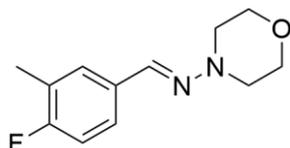
(*E*)-4-((morpholinoimino)methyl)phenol (A41)



The title compound was prepared according to the general procedure to afford a yellow solid in 94% yield (2.43 g). ¹H NMR (600 MHz, CDCl₃): δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.85–7.82 (m, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.48 (t, *J* = 7.7 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 3.86–3.84 (m, 4H), 3.22–3.19 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 134.2–

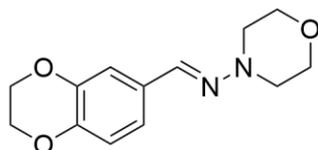
134.1 (m), 131.6, 130.9 (d, $J = 1.8$ Hz), 127.4, 126.7 (d, $J = 30.4$ Hz), 126.2, 125.4 (q, $J = 5.7$ Hz), 124.4 (d, $J = 273.9$ Hz), 66.1, 51.4. ^{19}F NMR (564 MHz, CDCl_3): δ -58.4. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{12}\text{H}_{14}\text{F}_3\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$, 233.1648, found 233.1645.

(E)-1-(4-fluoro-3-methylphenyl)-N-morpholinomethanimine (A42)



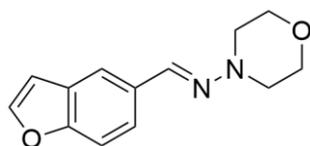
The title compound was prepared according to the general procedure to afford a yellow solid in 98% yield (2.18 g). ^1H NMR (600 MHz, CDCl_3): δ 7.53 (s, 1H), 7.46 (d, $J = 7.4$ Hz, 1H), 7.35 (s, 1H), 6.97 (t, $J = 8.9$ Hz, 1H), 3.88 (s, 4H), 3.15 (s, 4H), 2.27 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3): δ 161.5 (d, $J = 246.8$ Hz), 135.9–135.1 (m), 131.7, 128.9 (d, $J = 5.2$ Hz), 125.4 (d, $J = 8.1$ Hz), 125.0 (d, $J = 17.8$ Hz), 115.1 (d, $J = 22.9$ Hz), 66.4, 51.9, 14.5. ^{19}F NMR (564 MHz, CDCl_3): δ -117.3. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{12}\text{H}_{16}\text{FN}_2\text{O}$ $[\text{M}+\text{H}]^+$, 223.1241, found 223.1645.

(E)-1-(2,3-dihydrobenzo[*b*][1,4]dioxin-6-yl)-N-morpholinomethanimine (A43)



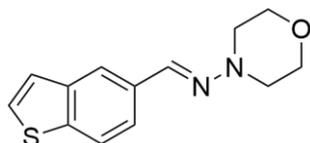
The title compound was prepared according to the general procedure to afford a yellow solid in 96% yield (2.38 g). ^1H NMR (600 MHz, CDCl_3): δ 7.50 (s, 1H), 7.14 (s, 1H), 7.08 (d, $J = 8.3$ Hz, 1H), 6.83 (d, $J = 8.3$ Hz, 1H), 4.25 (s, 4H), 3.87 (s, 4H), 3.13 (s, 4H). ^{13}C NMR (150 MHz, CDCl_3): δ 144.0, 143.6, 136.3, 129.8, 119.8, 117.3, 114.8, 66.5, 64.4, 64.3, 52.0. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{13}\text{H}_{17}\text{N}_2\text{O}_3$ $[\text{M}+\text{H}]^+$, 249.1234, found 249.1235.

(E)-1-(benzofuran-5-yl)-N-morpholinomethanimine (A44)



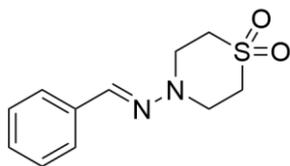
The title compound was prepared according to the general procedure to afford a yellow solid in 93% yield (2.14 g). ¹H NMR (600 MHz, CDCl₃): δ 7.80 (s, 1H), 7.71 (s, 1H), 7.62 (d, *J* = 11.3 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 1H), 6.76 (s, 1H), 3.90 (s, 4H), 3.18 (s, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 155.2, 145.5, 137.0, 131.1, 127.7, 122.7, 119.2, 111.5, 106.7, 66.5, 52.1. HRMS (ESI-TOF) *m/z* calcd. for C₁₃H₁₅N₂O₂ [M+H]⁺, 231.1128, found 231.1124.

(*E*)-1-(benzo[*b*]thiophen-5-yl)-*N*-morpholinomethanimine (A45)



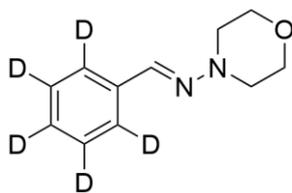
The title compound was prepared according to the general procedure to afford a yellow solid in 94% yield (2.31 g). ¹H NMR (600 MHz, CDCl₃): δ 7.96 (s, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.72–7.69 (m, 2H), 7.44 (d, *J* = 5.4 Hz, 1H), 7.33 (d, *J* = 5.4 Hz, 1H), 3.92–3.90 (m, 4H), 3.21–3.20 (m, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 139.8, 139.7, 136.6, 132.5, 126.9, 124.0, 122.6, 122.1, 121.8, 66.5, 52.0. HRMS (ESI-TOF) *m/z* calcd. for C₁₃H₁₅N₂OS [M+H]⁺, 247.0900, found 247.0904.

(*E*)-4-(benzylideneamino)thiomorpholine 1,1-dioxide (A47)



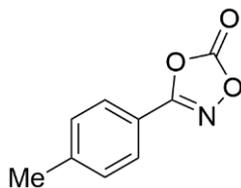
The title compound was prepared according to the general procedure to afford a yellow solid in 95% yield (2.26 g). ¹H NMR (600 MHz, CDCl₃): δ 7.60 (d, *J* = 8.8 Hz, 3H), 7.38 (t, *J* = 7.3 Hz, 2H), 7.35–7.31 (m, 1H), 3.92 (s, 4H), 3.10 (s, 4H). ¹³C NMR (150 MHz, CDCl₃): δ 140.0, 134.9, 129.2, 128.7, 126.3, 48.7, 48.4. HRMS (ESI-TOF) *m/z* calcd. for C₁₁H₁₅N₂O₂S [M+H]⁺, 239.0849, found 239.0847.

(*E*)-*N*-morpholino-1-(phenyl-*d*₅)methanimine (A1-D₅)



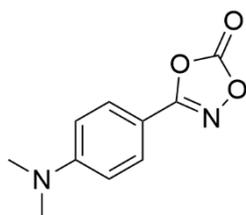
The title compound was prepared according to the general procedure to afford a white solid in 97% yield (1.89 g). ^1H NMR (600 MHz, CDCl_3): δ 7.60 (s, 1H), 3.91–3.86 (m, 2H), 3.20–3.16 (m, 2H). ^{13}C NMR (150 MHz, CDCl_3): δ 136.3, 135.7, 128.2, 127.9 (d, $J = 24.8$ Hz), 125.8 (t), 66.5, 51.9. HRMS (ESI-TOF) m/z calcd. for $\text{C}_{11}\text{H}_{10}\text{D}_5\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$, 196.1493, found 196.1497.

3-(*p*-tolyl)-1,4,2-dioxazol-5-one (B1)⁶



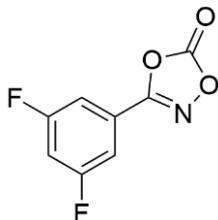
The title compound was prepared according to the general procedure to afford a white solid in 82% yield (1.45 g). ^1H NMR (600 MHz, CDCl_3): δ 7.73 (d, $J = 8.3$ Hz, 2H), 7.34 (d, $J = 8.0$ Hz, 2H), 2.45 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3): δ 163.6, 154.0, 144.8, 130.1, 126.6, 117.2, 21.8.

3-(4-(dimethylamino)phenyl)-1,4,2-dioxazol-5-one (B10)⁹



The title compound was prepared according to the general procedure to afford a white solid in 72% yield (1.48 g). ^1H NMR (600 MHz, CDCl_3): δ 7.64 (d, $J = 9.0$ Hz, 2H), 6.70 (d, $J = 9.0$ Hz, 2H), 3.07 (s, 6H). ^{13}C NMR (150 MHz, CDCl_3): δ 164.0, 154.5, 153.4, 128.1, 111.4, 105.7, 40.0.

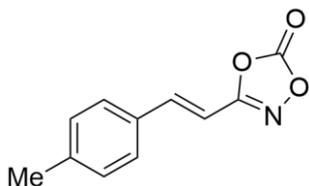
3-(3,5-difluorophenyl)-1,4,2-dioxazol-5-one (B13)⁶



The title compound was prepared according to the general procedure to afford a white solid in 57% yield (1.13 g).

¹H NMR (600 MHz, CDCl₃): δ 7.43–7.38 (m, 2H), 7.11 (tt, *J* = 8.5, 2.3 Hz, 1H). ¹³C NMR (150 MHz, CDCl₃): δ 163.3 (dd, *J* = 252.9, 12.3 Hz), 161.9 (t, *J* = 3.8 Hz), 153.0, 122.8 (t, *J* = 10.7 Hz), 110.0 (dd, *J* = 22.1, 6.7 Hz), 109.4 (t, *J* = 25.0 Hz). ¹⁹F NMR (564 MHz, CDCl₃): δ -105.3.

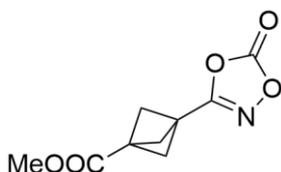
(*E*)-3-(4-methylstyryl)-1,4,2-dioxazol-5-one (B15)



The title compound was prepared according to the general procedure to afford a white solid in 85% yield (1.72 g).

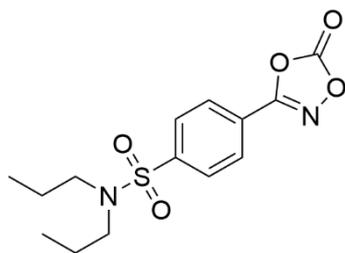
¹H NMR (600 MHz, CDCl₃): δ 7.44 (d, *J* = 3.7 Hz, 2H), 7.42 (d, *J* = 4.4 Hz, 2H), 6.59 (d, *J* = 16.4 Hz, 1H), 2.40 (s, 3H). ¹³C NMR (150 MHz, CDCl₃): δ 163.5, 153.5, 143.0, 141.9, 130.7, 129.9, 128.0, 104.6, 21.5. HRMS (ESI-TOF) *m/z* calcd. for C₁₁H₁₀NO₃[M+H]⁺, 204.0655, found 204.0650.

methyl 3-(5-oxo-1,4,2-dioxazol-3-yl)bicyclo[1.1.1]pentane-1-carboxylate (B19)⁶



The title compound was prepared according to the general procedure to afford a yellow oil in 68% yield (1.43 g). ^1H NMR (600 MHz, CDCl_3): δ 3.72 (s, 3H), 2.50 (s, 6H). ^{13}C NMR (150 MHz, CDCl_3): δ 168.2, 162.9, 153.7, 53.2, 52.1, 39.9.

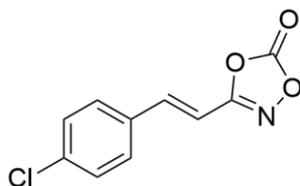
4-(5-oxo-1,4,2-dioxazol-3-yl)-*N,N*-dipropylbenzenesulfonamide (B20)¹¹



The title compound was prepared according to the general procedure to afford a yellow solid in 54% yield (1.76 g).

¹H NMR (600 MHz, CDCl₃): δ 8.01–7.95 (m, 4H), 3.12 (dd, *J* = 8.6, 6.8 Hz, 4H), 1.57–1.53 (m, 4H), 0.87 (t, *J* = 7.4 Hz, 6H). ¹³C NMR (150 MHz, CDCl₃): δ 162.4, 153.2, 145.4, 127.9, 127.3, 123.4, 49.9, 21.9, 11.1.

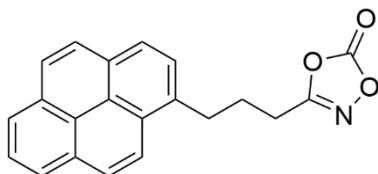
(*E*)-3-(4-chlorostyryl)-1,4,2-dioxazol-5-one (B24)⁷



The title compound was prepared according to the general procedure to afford a yellow solid in 78% yield (1.74 g).

¹H NMR (600 MHz, CDCl₃): δ 7.48 (d, *J* = 7.7 Hz, 2H), 7.45–7.39 (m, 3H), 6.62 (d, *J* = 16.4 Hz, 1H). ¹³C NMR (150 MHz, CDCl₃): δ 163.1, 153.3, 141.6, 137.3, 131.9, 129.5, 129.2, 106.4.

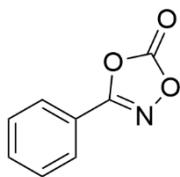
3-(3-(pyren-1-yl)propyl)-1,4,2-dioxazol-5-one (B25)⁶



The title compound was prepared according to the general procedure to afford a yellow solid in 64% yield (2.11 g).

¹H NMR (600 MHz, CDCl₃): δ 8.22–8.17 (m, 3H), 8.13 (dd, *J* = 8.4, 6.7 Hz, 2H), 8.05 (s, 2H), 8.01 (t, *J* = 7.6 Hz, 1H), 7.84 (d, *J* = 7.8 Hz, 1H), 3.47 (t, *J* = 7.5 Hz, 2H), 2.71 (t, *J* = 7.4 Hz, 2H), 2.30 (p, *J* = 7.5 Hz, 2H). ¹³C NMR (150 MHz, CDCl₃): δ 166.4, 133.8, 131.4, 130.8, 130.3, 128.7, 127.8, 127.4, 127.3, 127.1, 126.0, 125.2, 125.2, 125.0, 124.9, 124.9, 122.7, 32.1, 26.0, 24.4.

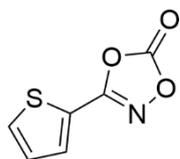
3-phenyl-1,4,2-dioxazol-5-one (B26)⁶



The title compound was prepared according to the general procedure to afford a white solid in 82% yield (1.34 g).

¹H NMR (600 MHz, CDCl₃): δ 7.87–7.84 (m, 2H), 7.65 (t, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 2H). ¹³C NMR (150 MHz, CDCl₃): δ 163.5, 153.8, 133.8, 129.4, 120.1.

3-(thiophen-2-yl)-1,4,2-dioxazol-5-one (B29)¹⁰



The title compound was prepared according to the general procedure to afford a yellow solid in 56% yield (0.95 g).

¹H NMR (600 MHz, CDCl₃): δ 7.73 (d, *J* = 3.8 Hz, 1H), 7.71–7.68 (m, 1H), 7.23–7.21 (m, 1H). ¹³C NMR (150 MHz, CDCl₃): δ 160.2, 153.3, 132.7, 132.3, 128.5, 120.3.

11. References

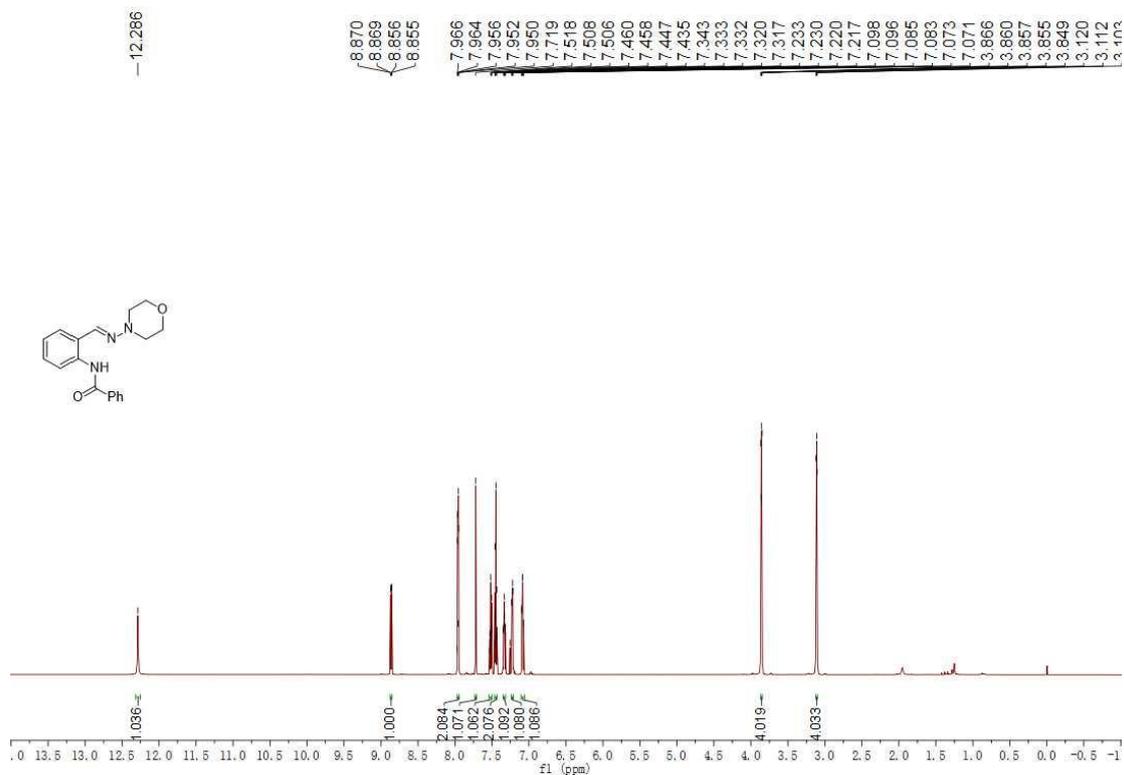
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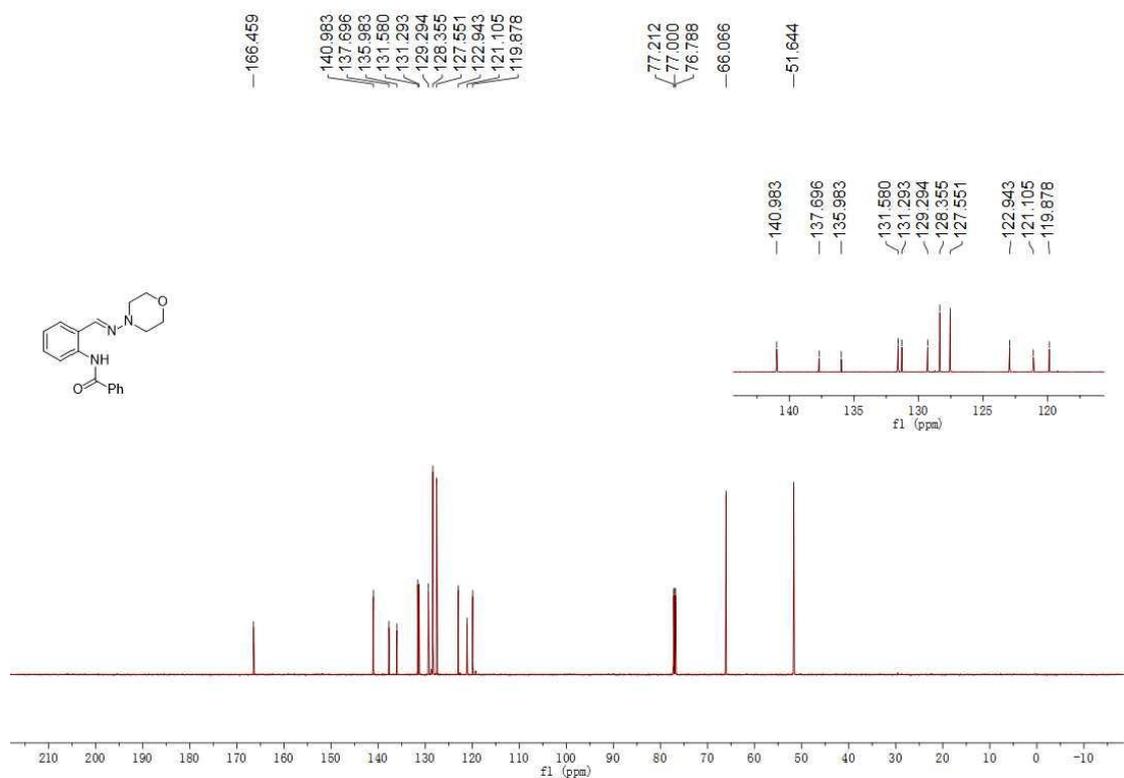
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12. NMR Spectral Data for Isolated Products and Starting Materials

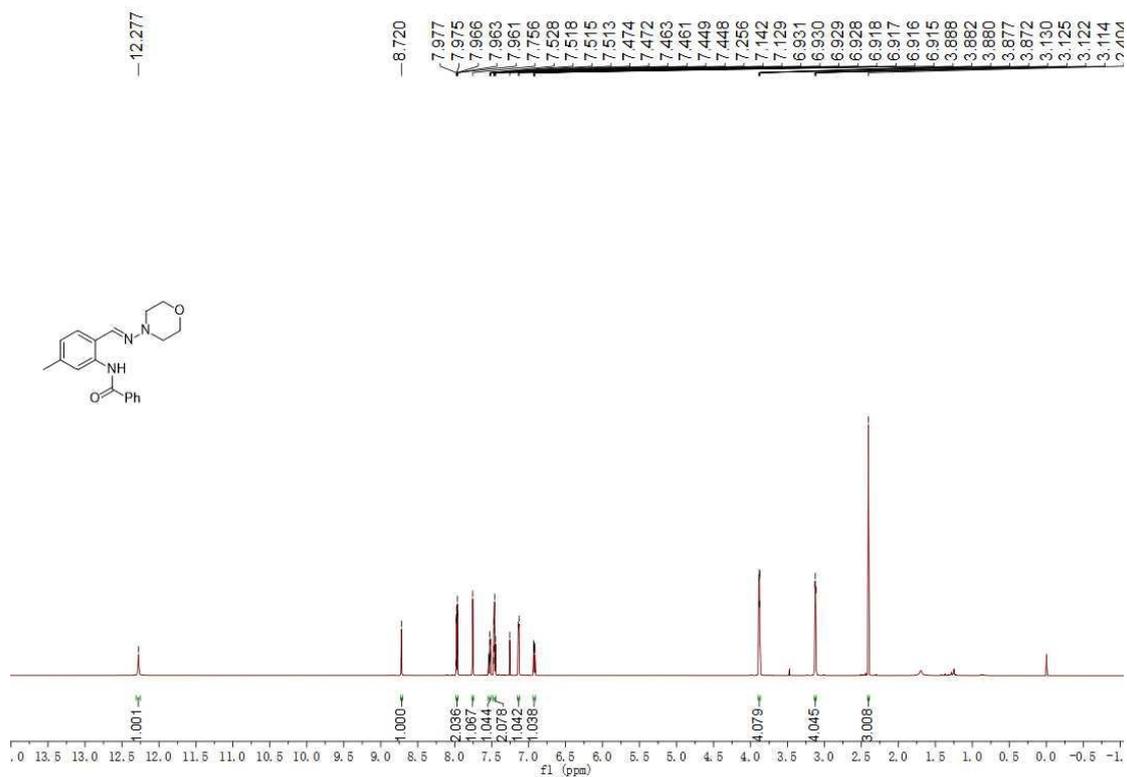
¹H NMR (600 MHz, CDCl₃) Spectrum of **3**



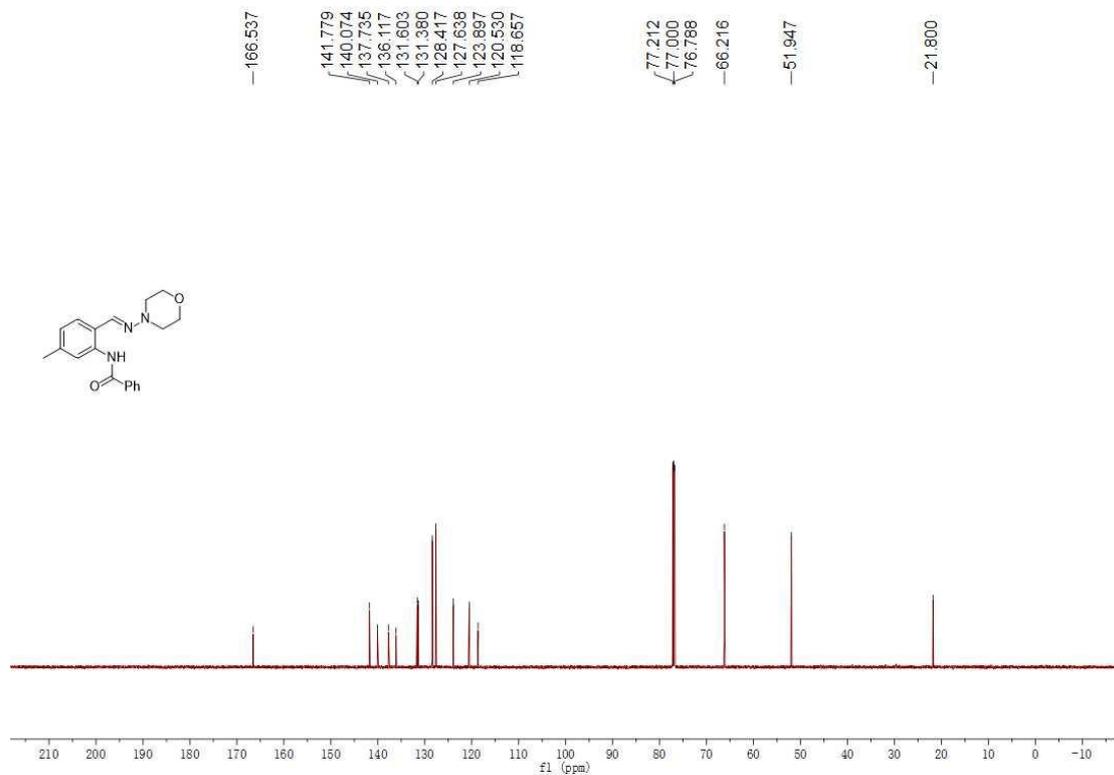
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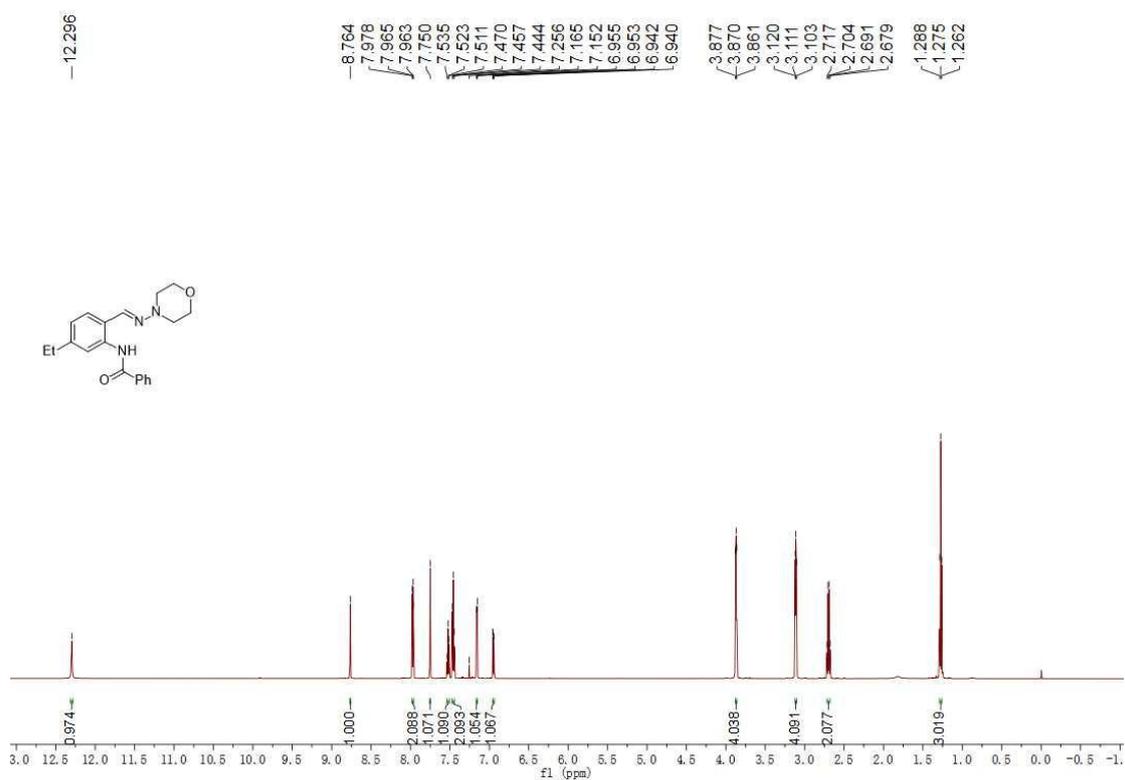
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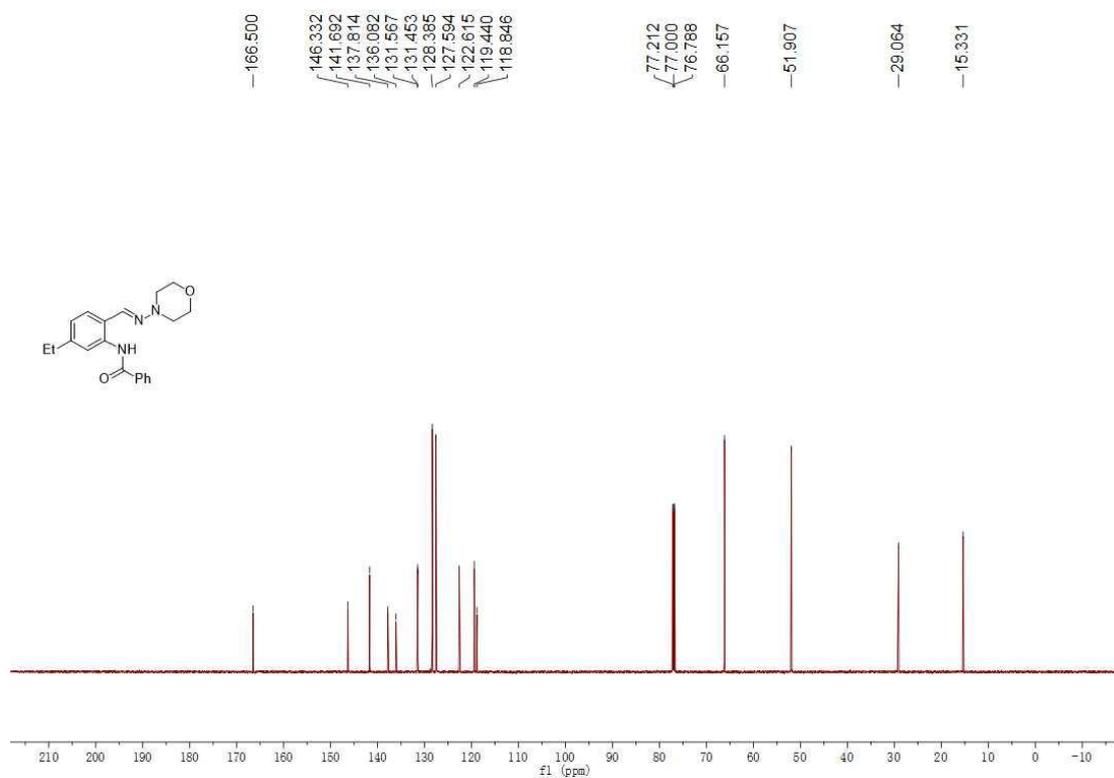
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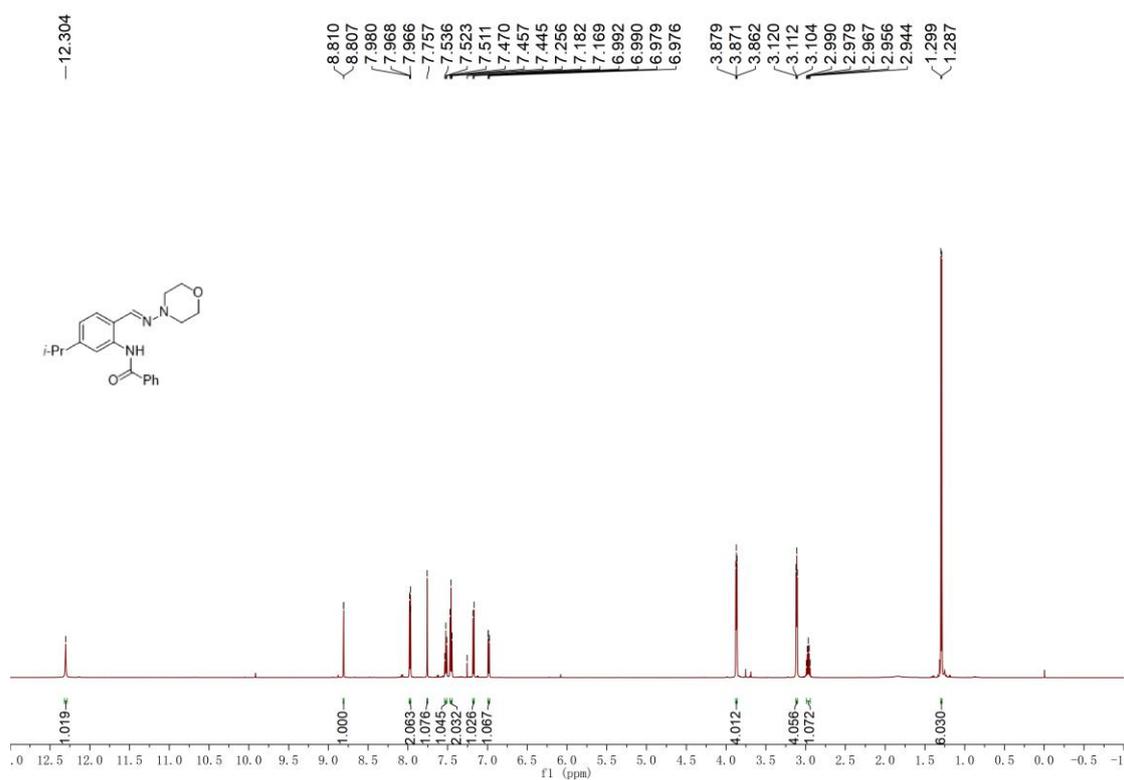
¹H NMR (600 MHz, CDCl₃) Spectrum of **5**



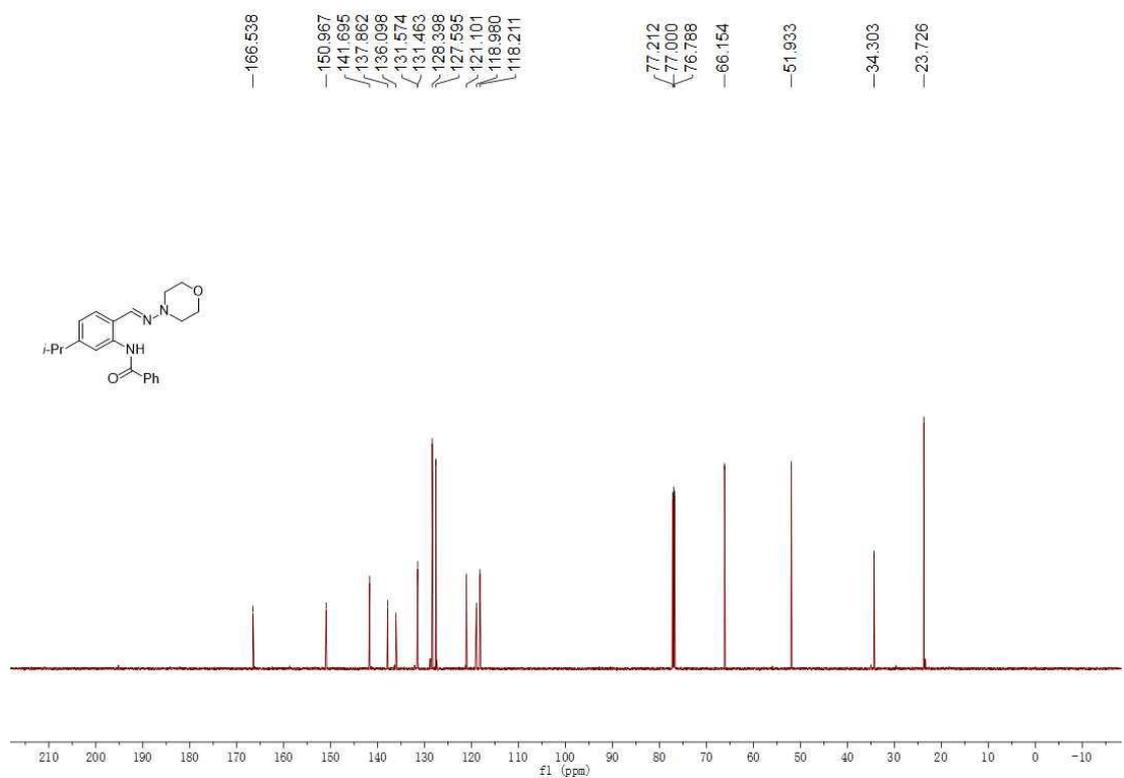
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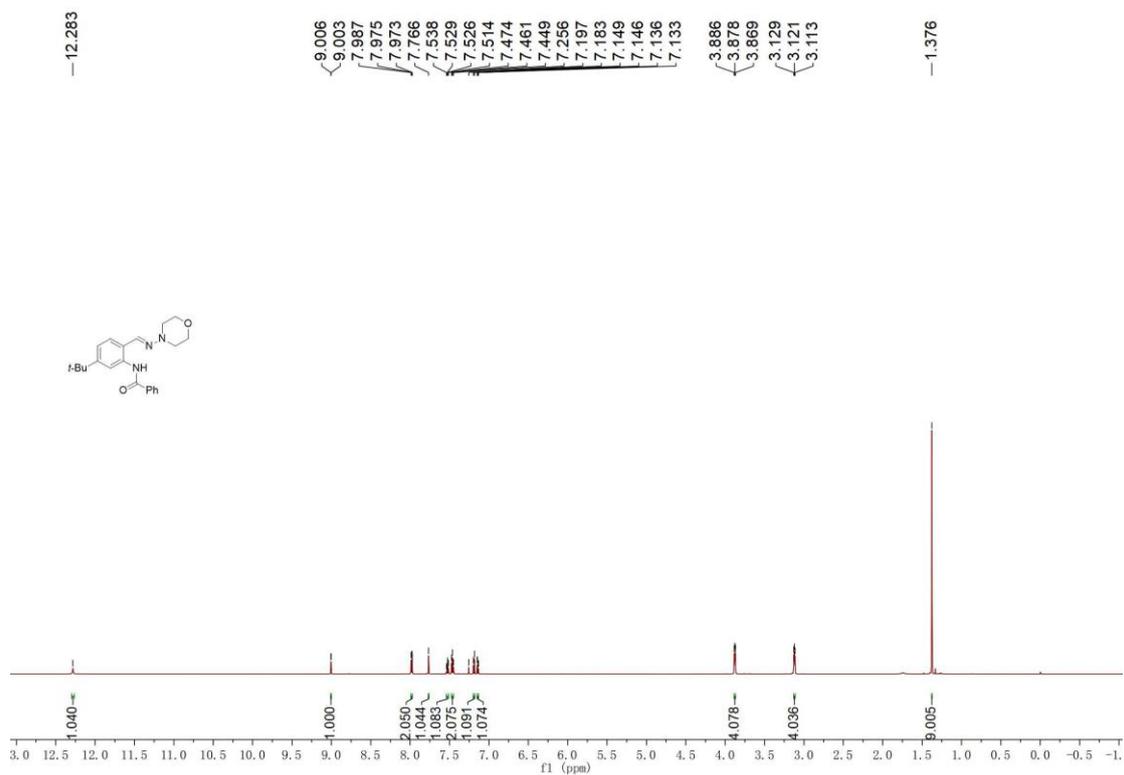
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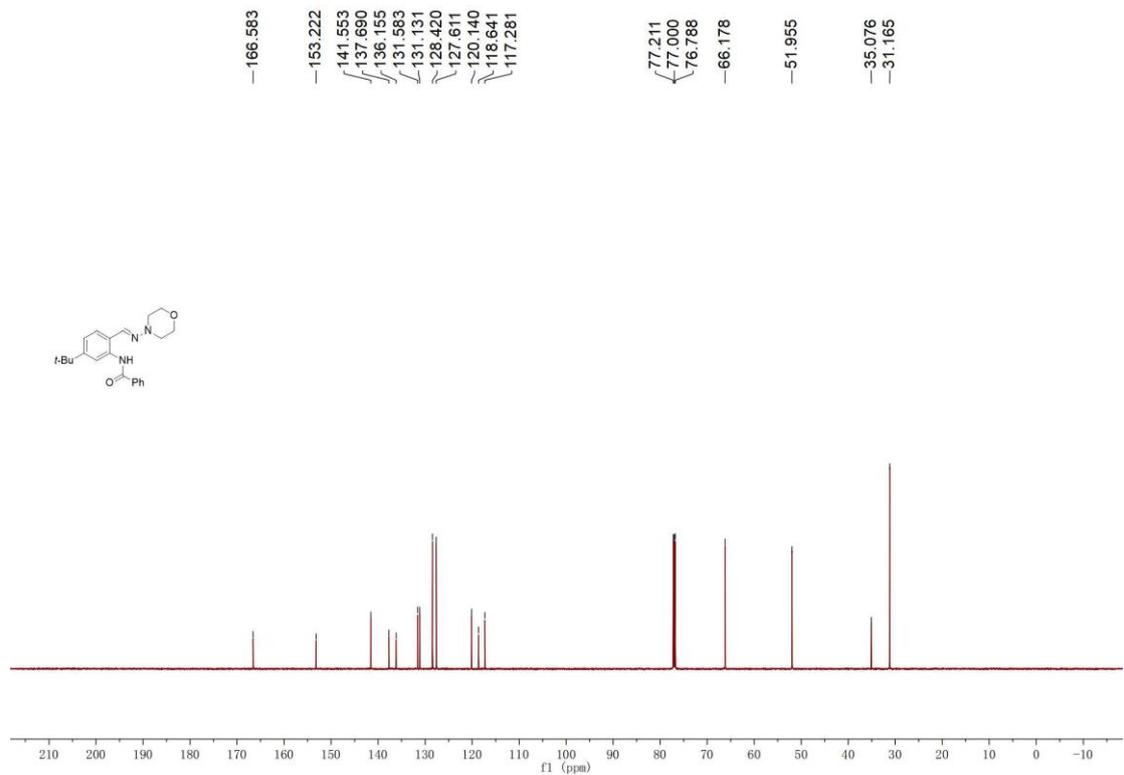
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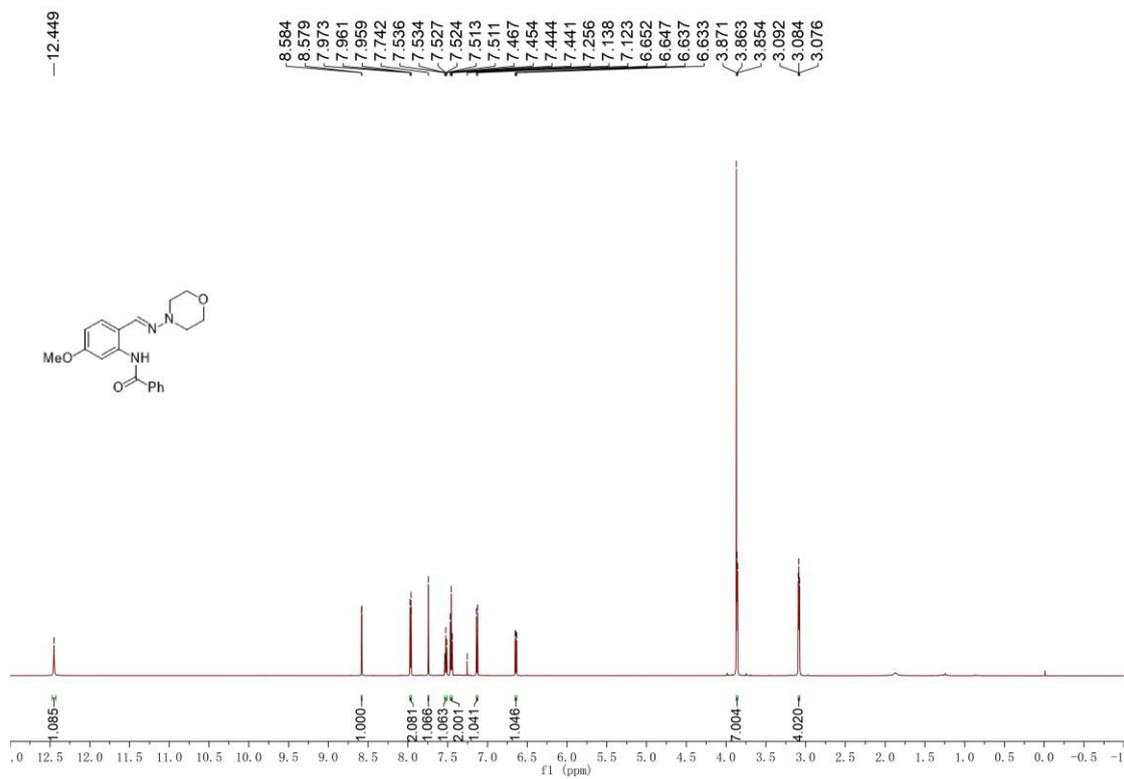
¹H NMR (600 MHz, CDCl₃) Spectrum of 7



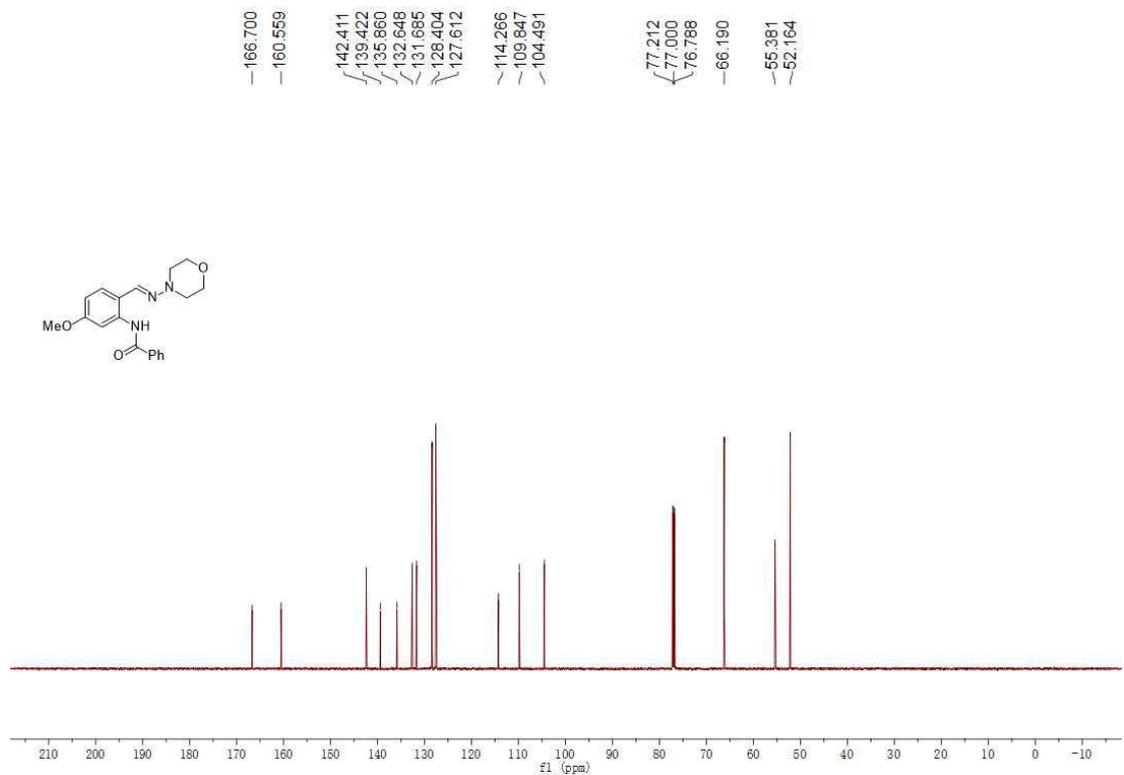
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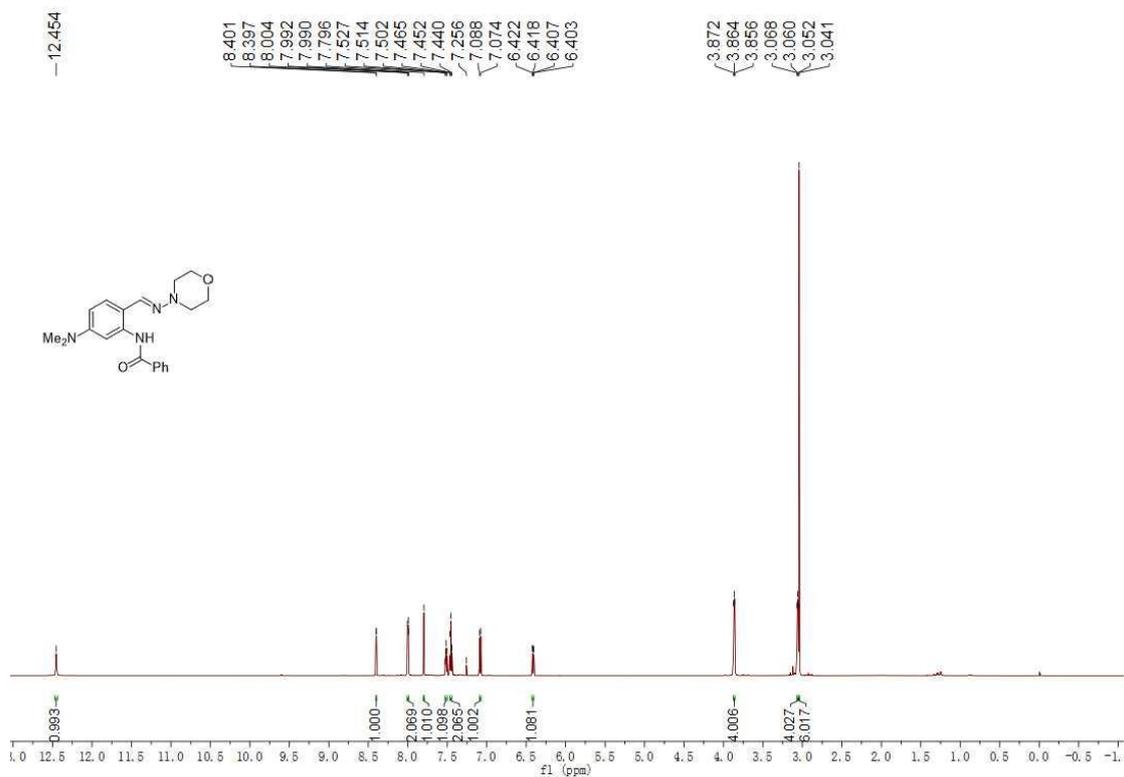
¹H NMR (600 MHz, CDCl₃) Spectrum of **8**



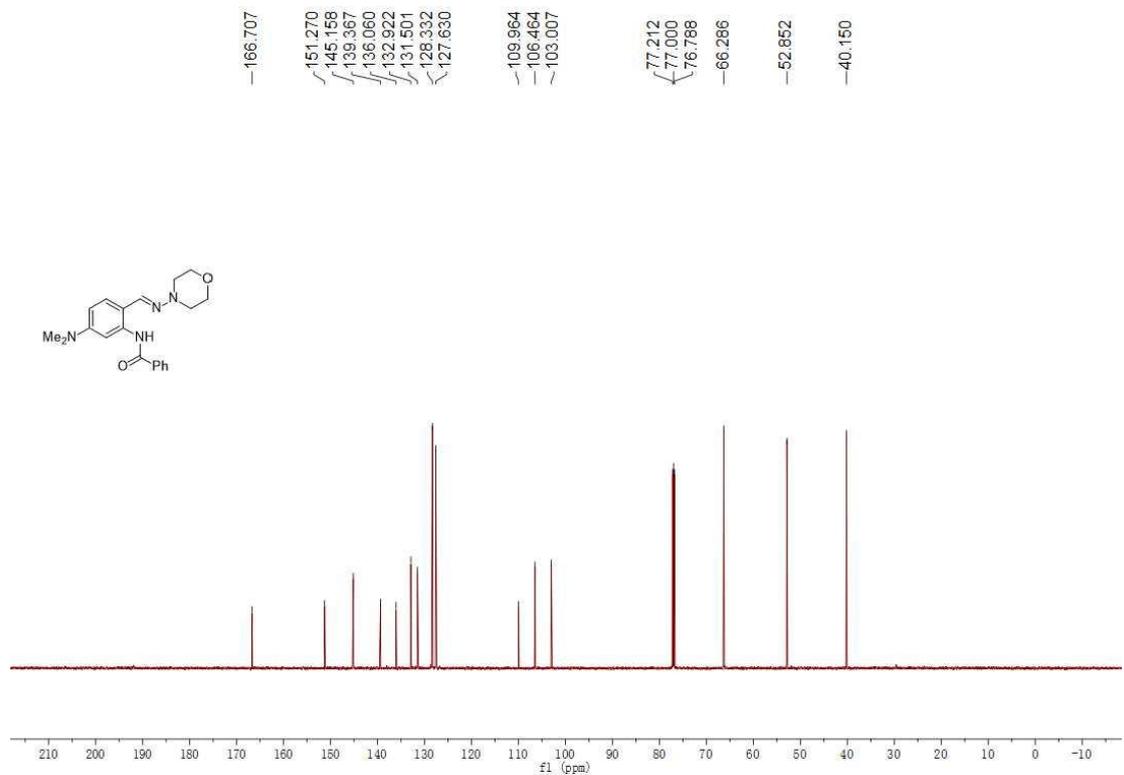
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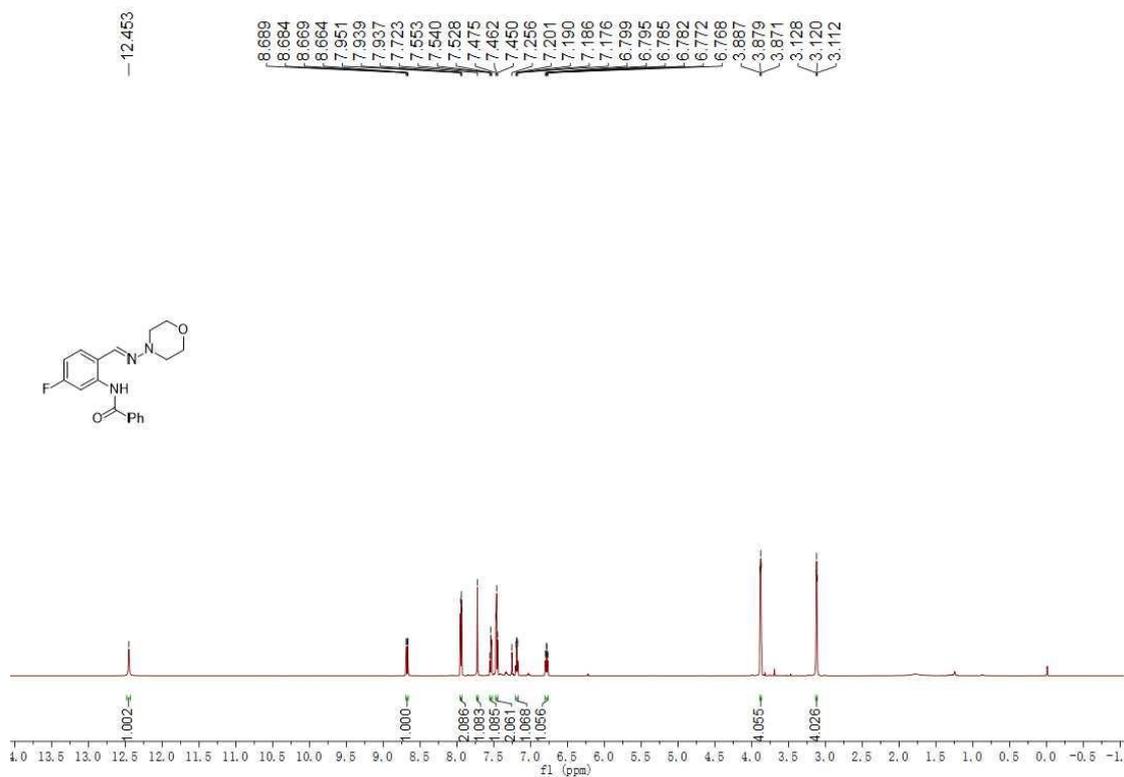
¹H NMR (600 MHz, CDCl₃) Spectrum of **9**



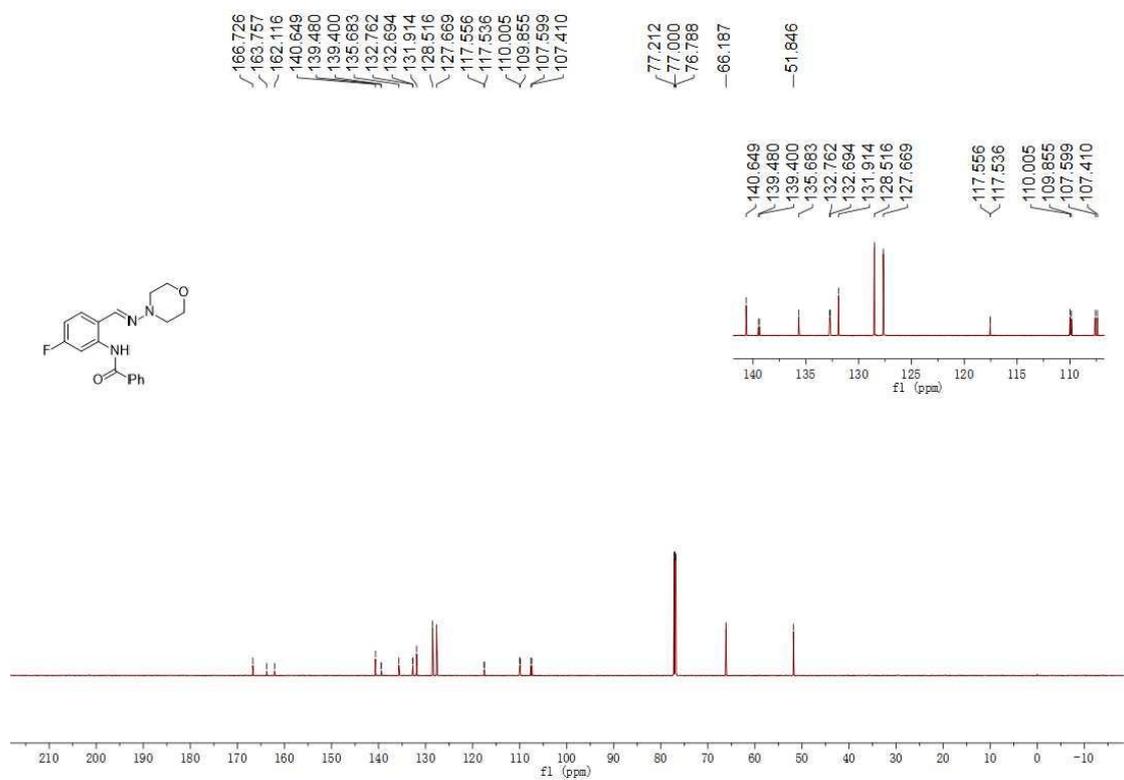
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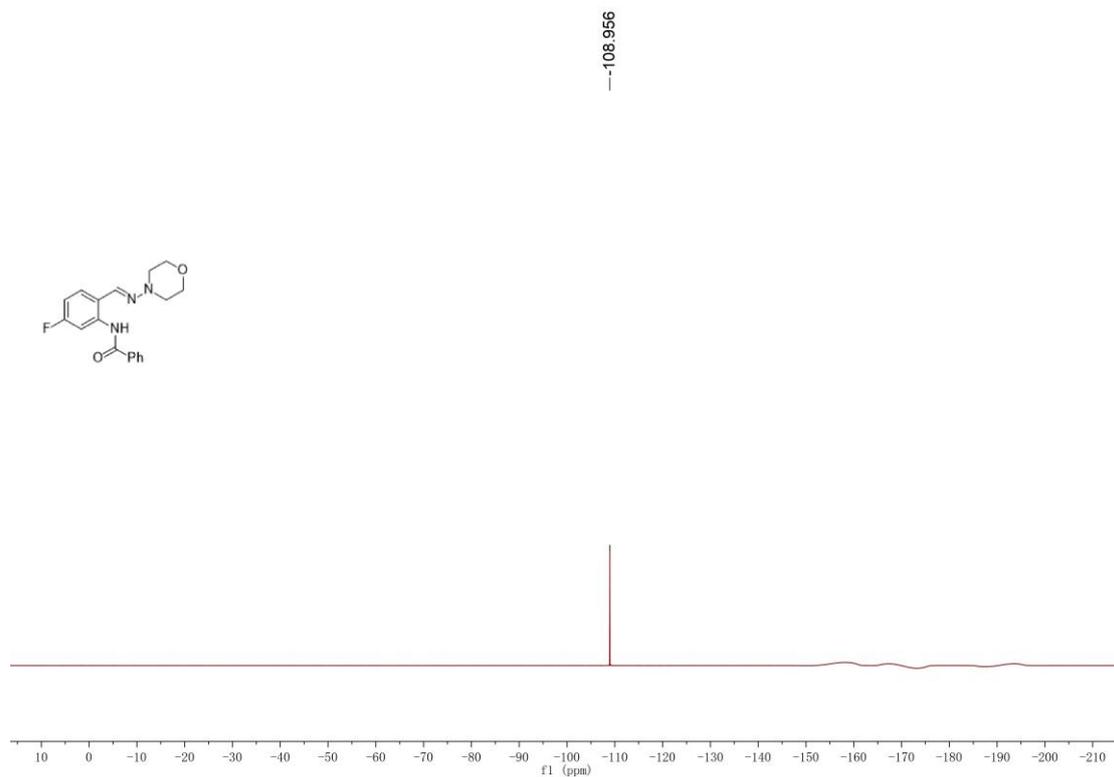
¹H NMR (600 MHz, CDCl₃) Spectrum of **10**



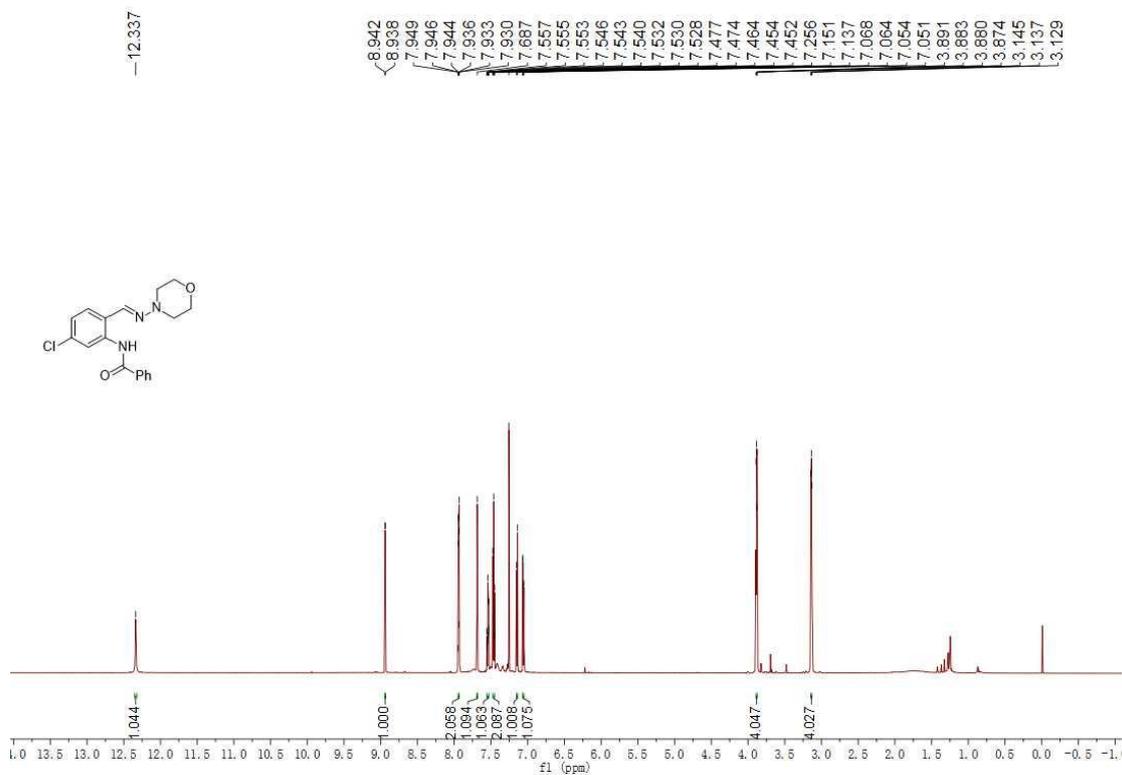
¹³C NMR (150 MHz, CDCl₃) Spectrum of **10**



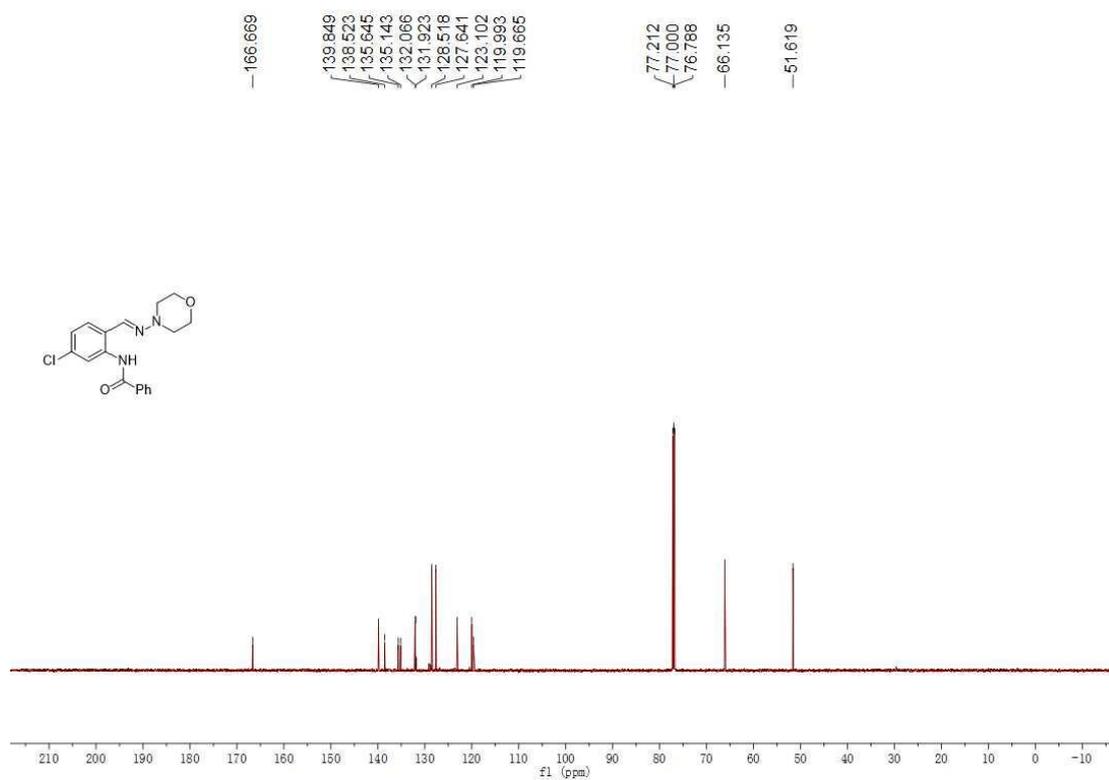
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **10**



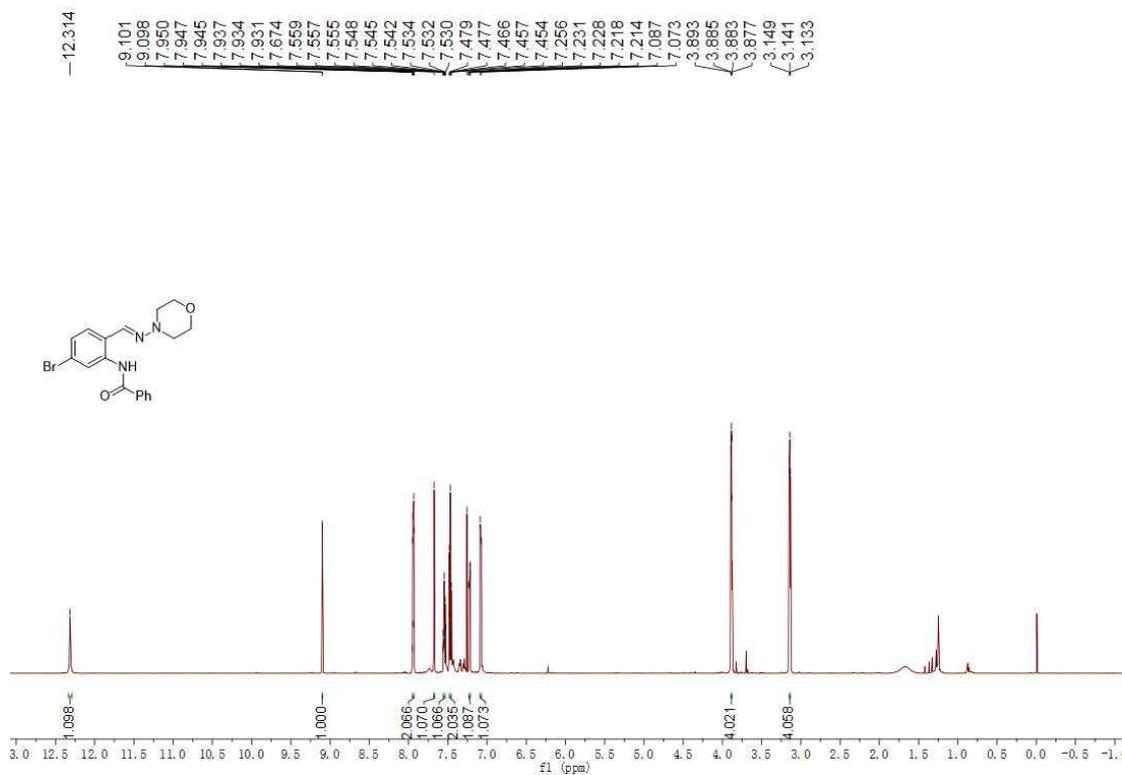
¹H NMR (600 MHz, CDCl₃) Spectrum of **11**



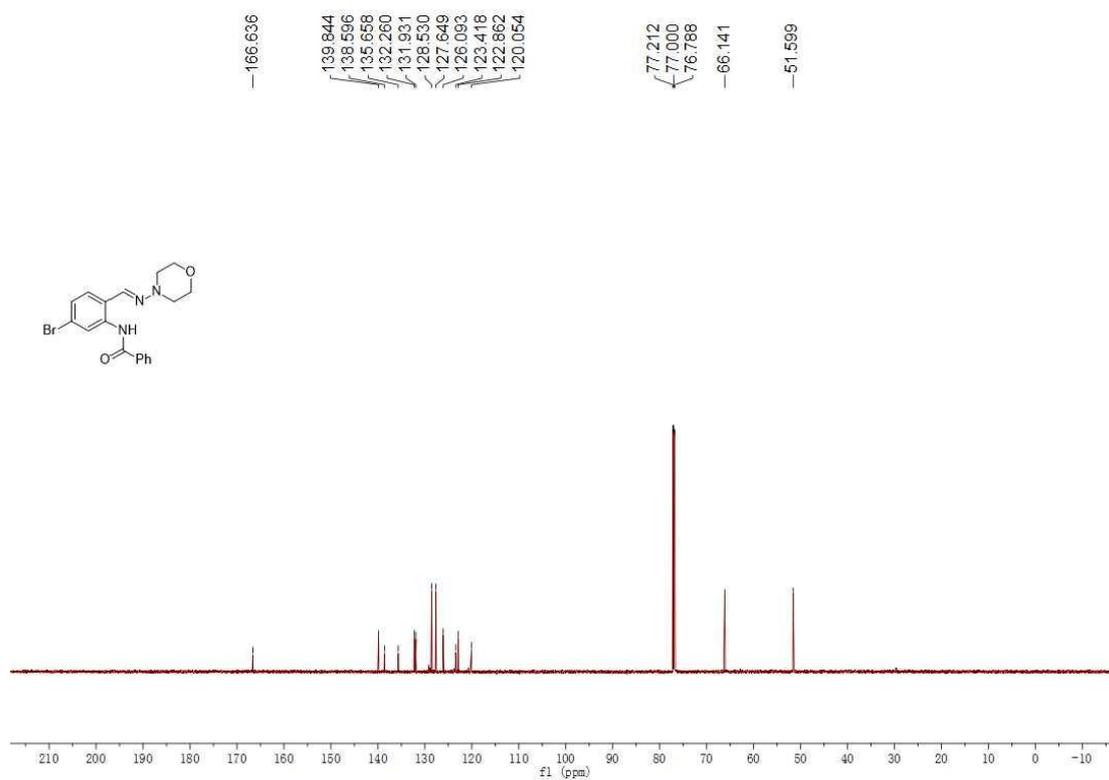
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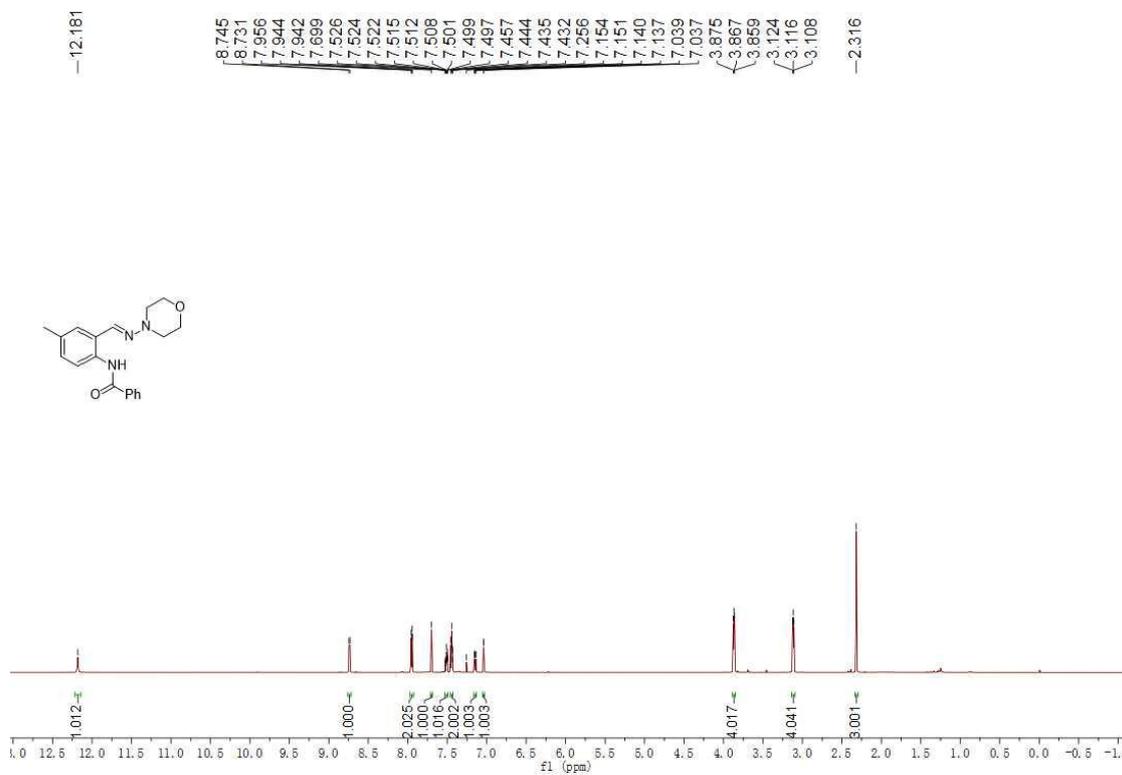
¹H NMR (600 MHz, CDCl₃) Spectrum of **12**



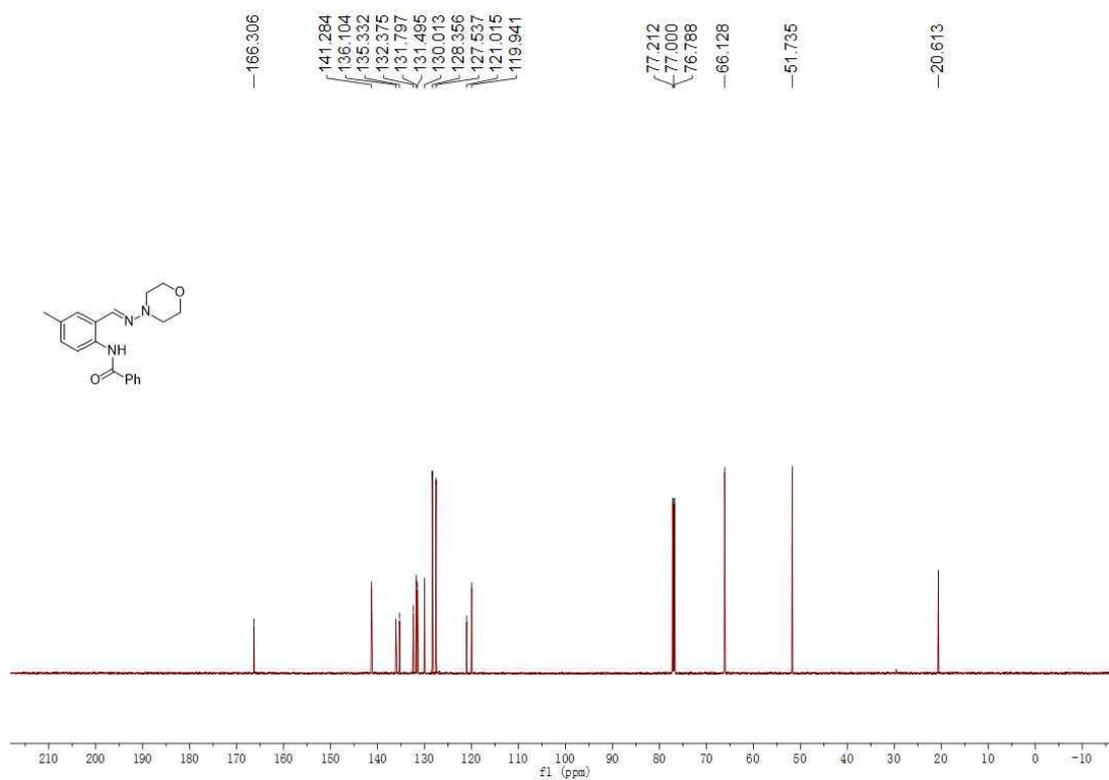
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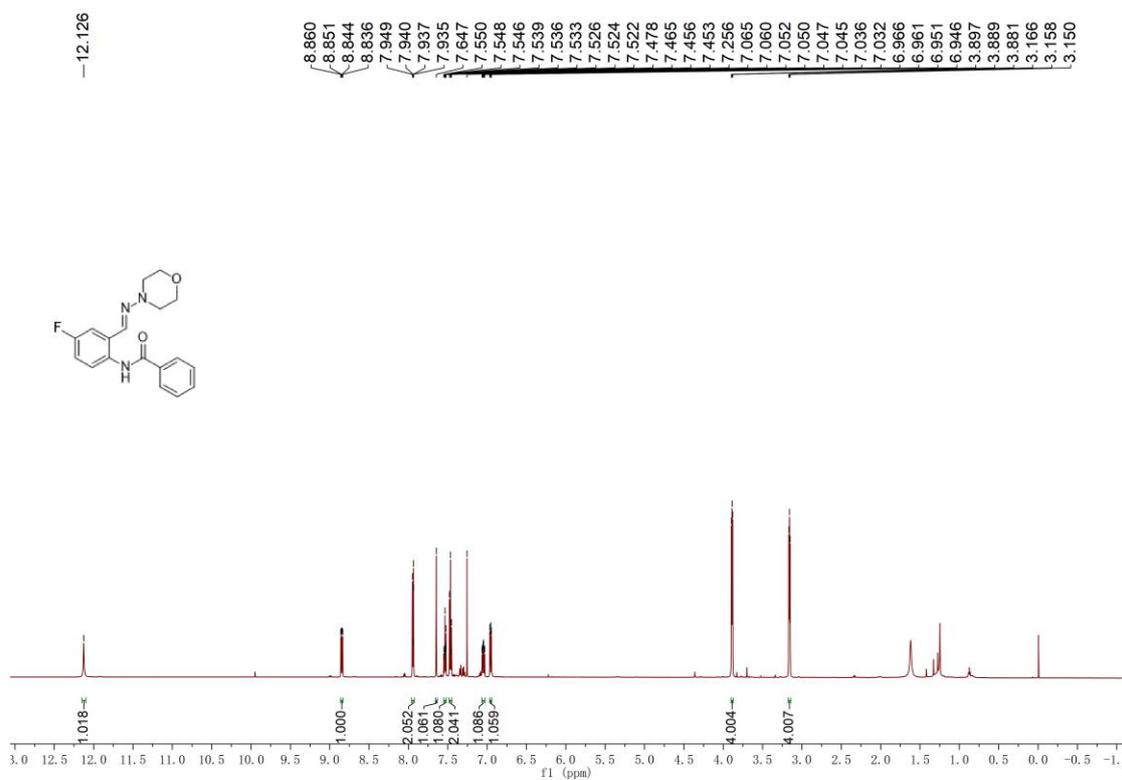
¹H NMR (600 MHz, CDCl₃) Spectrum of **13**



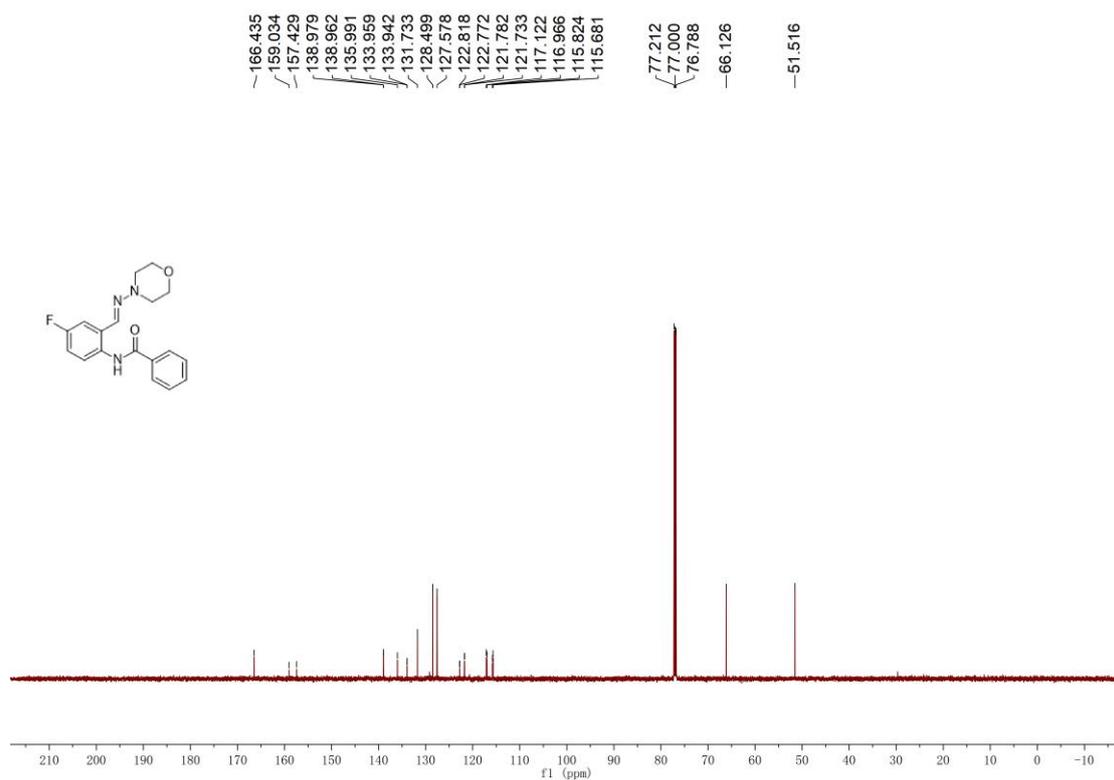
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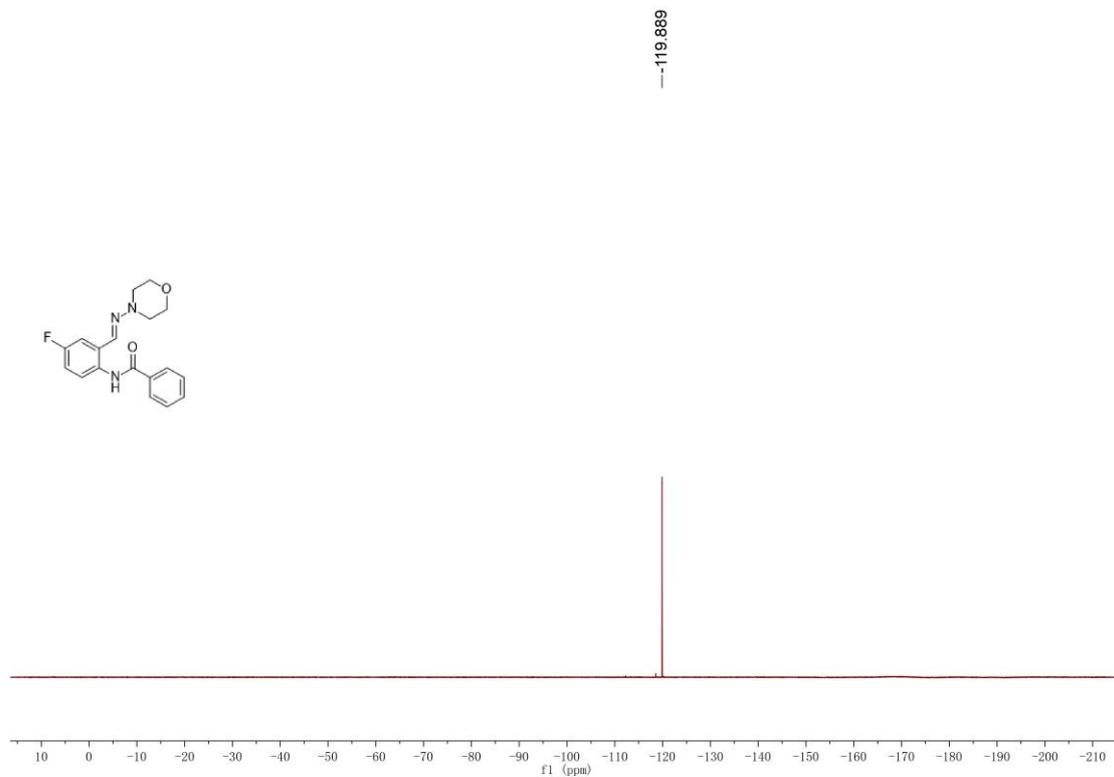
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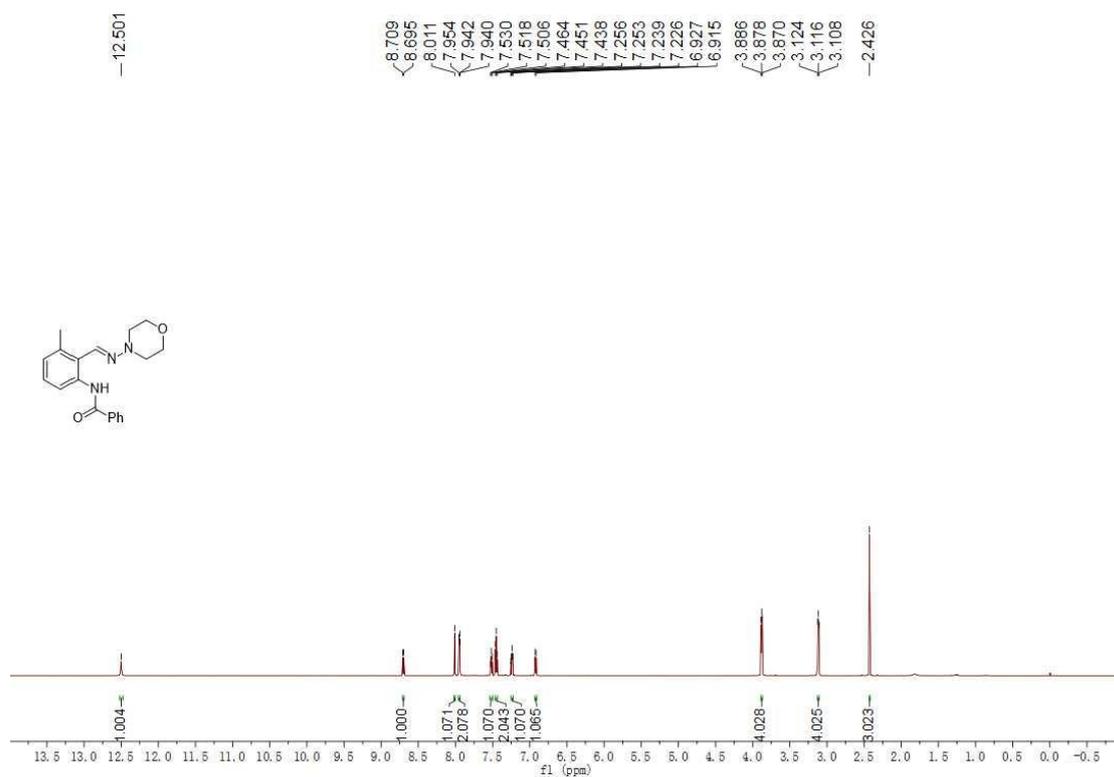
¹³C NMR (150 MHz, CDCl₃) Spectrum of **14**



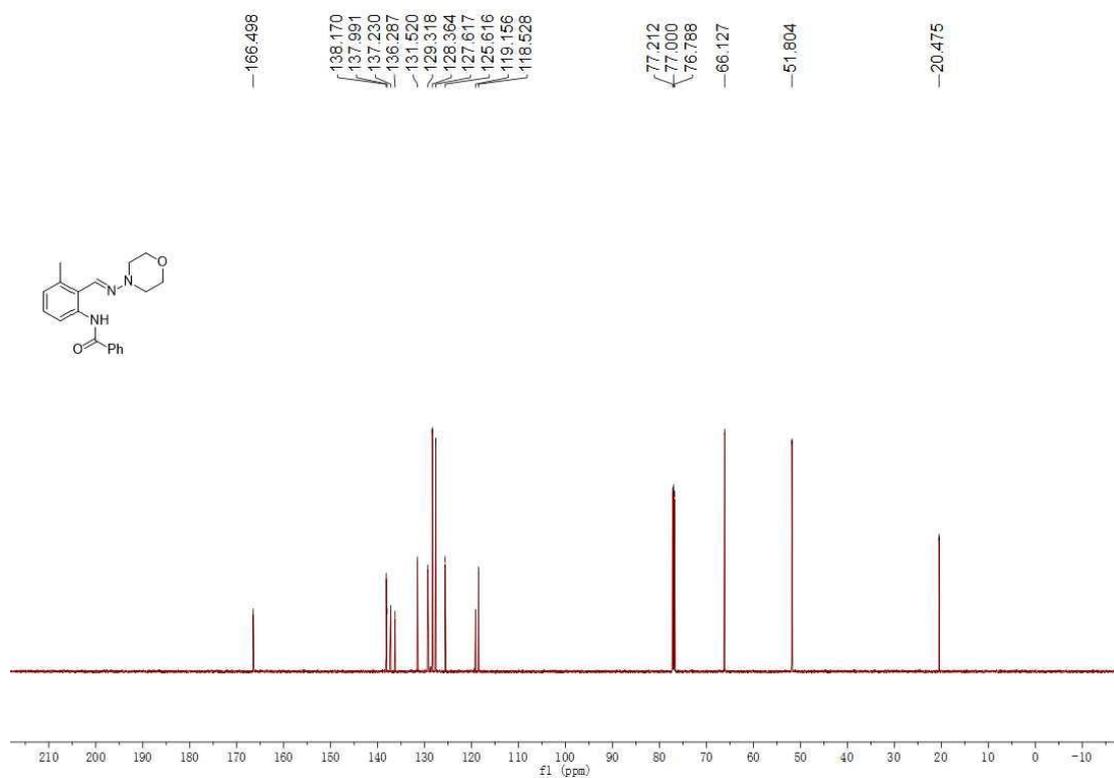
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **14**



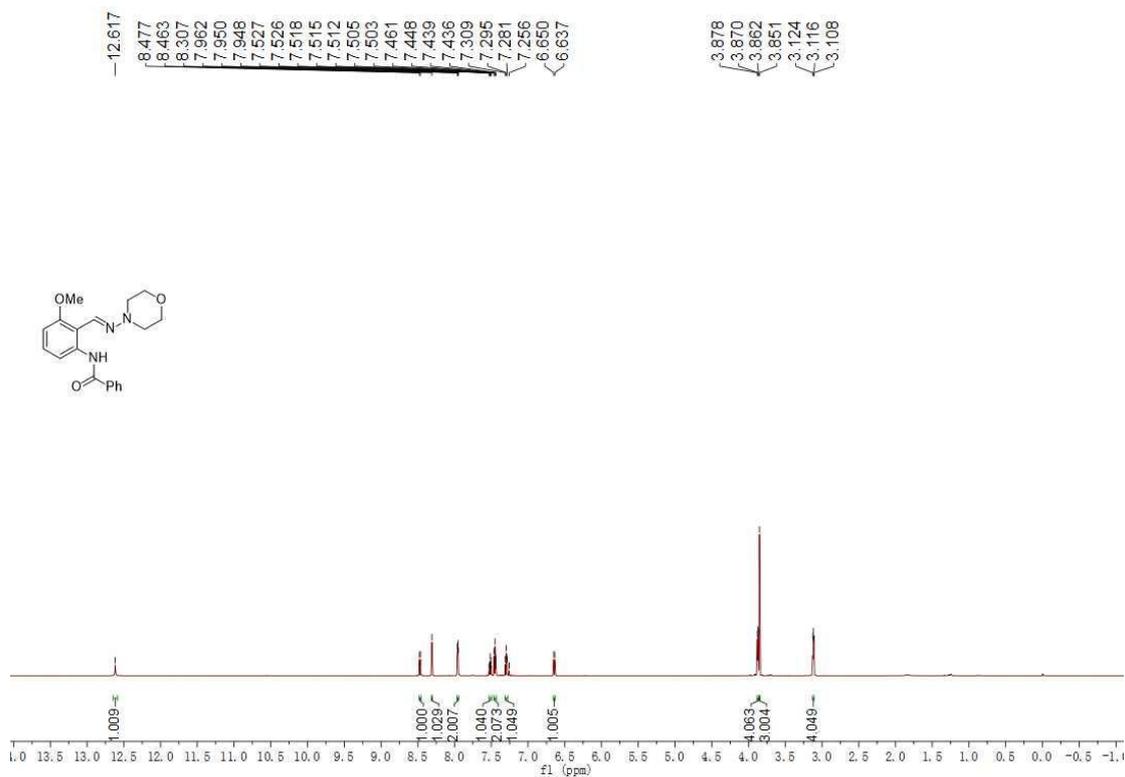
¹H NMR (600 MHz, CDCl₃) Spectrum of **15**



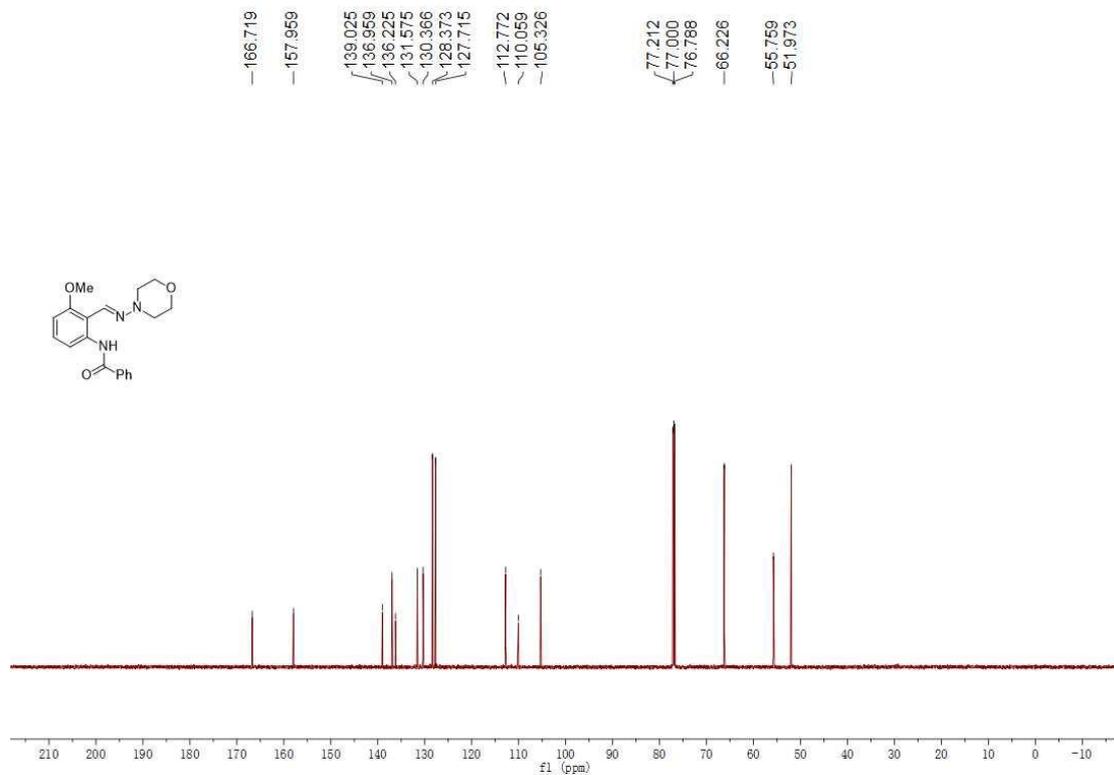
¹³C NMR (150 MHz, CDCl₃) Spectrum of **15**



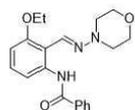
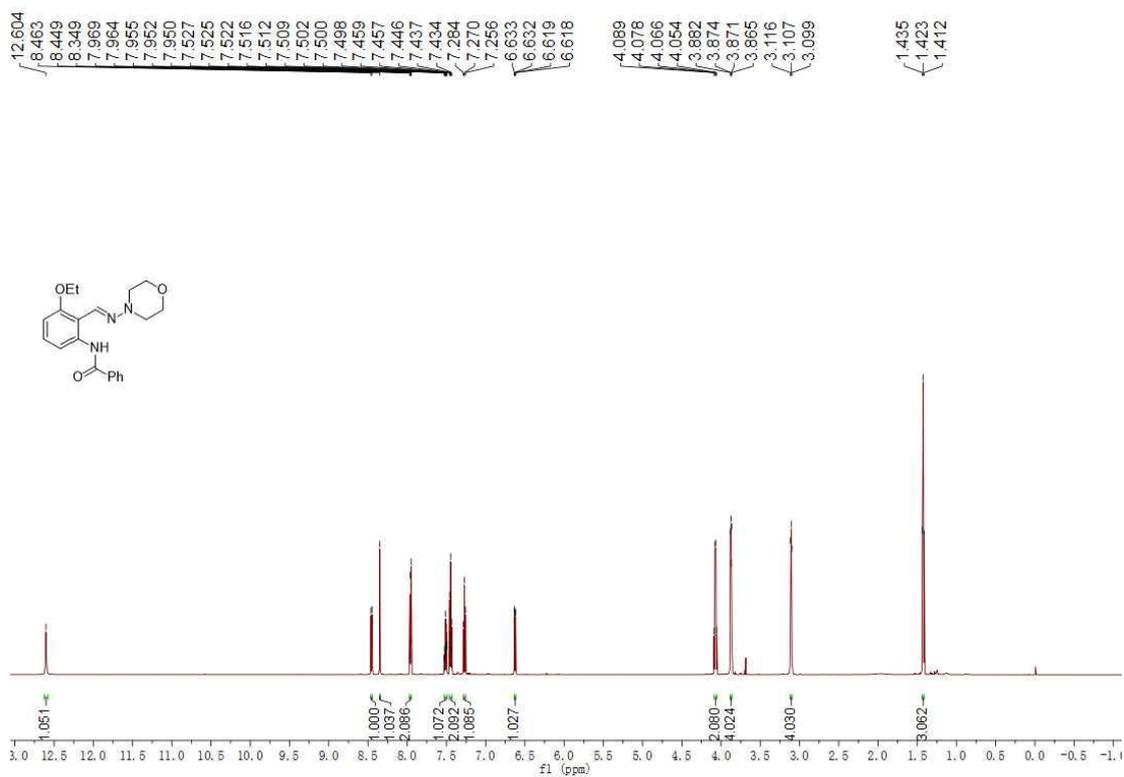
¹H NMR (600 MHz, CDCl₃) Spectrum of **16**



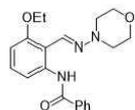
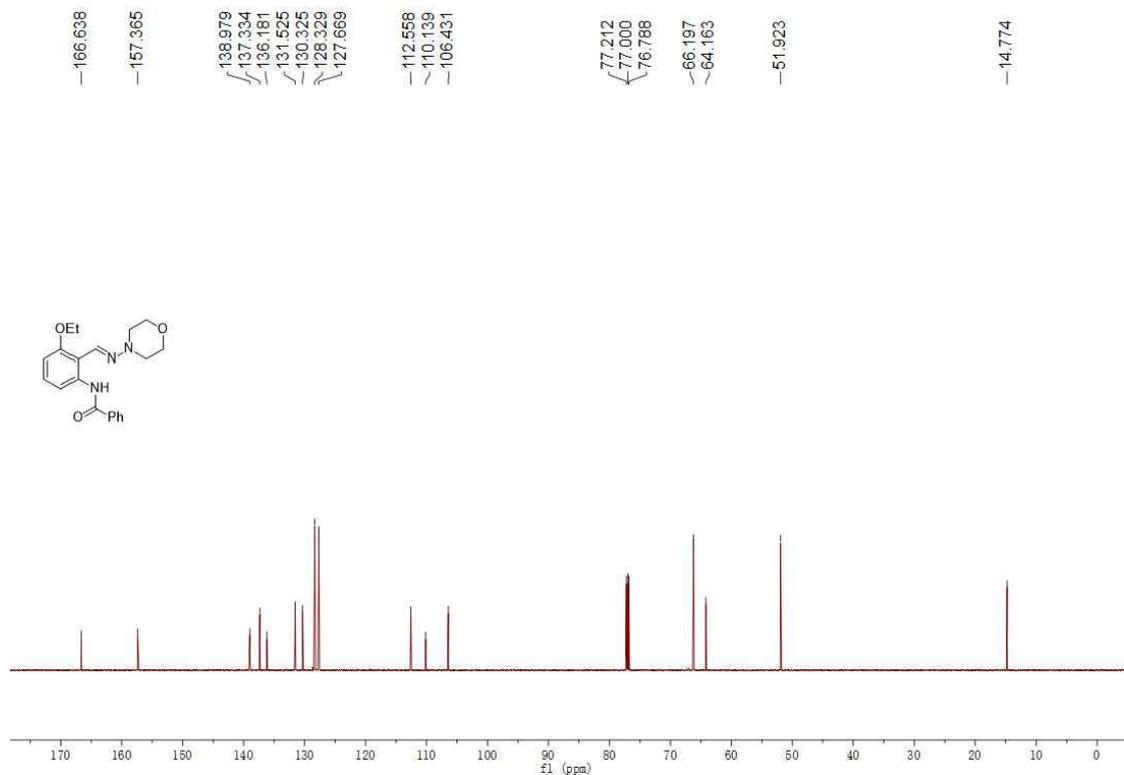
¹³C NMR (150 MHz, CDCl₃) Spectrum of **16**



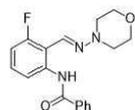
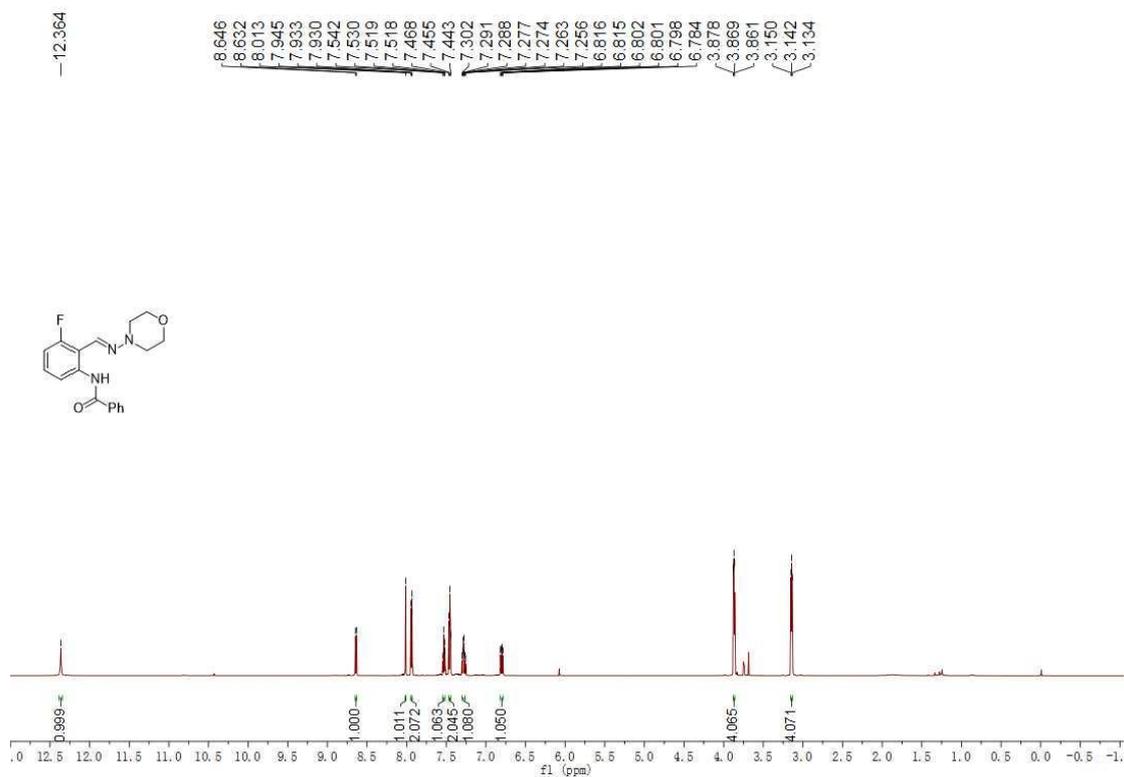
¹H NMR (600 MHz, CDCl₃) Spectrum of 17



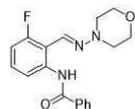
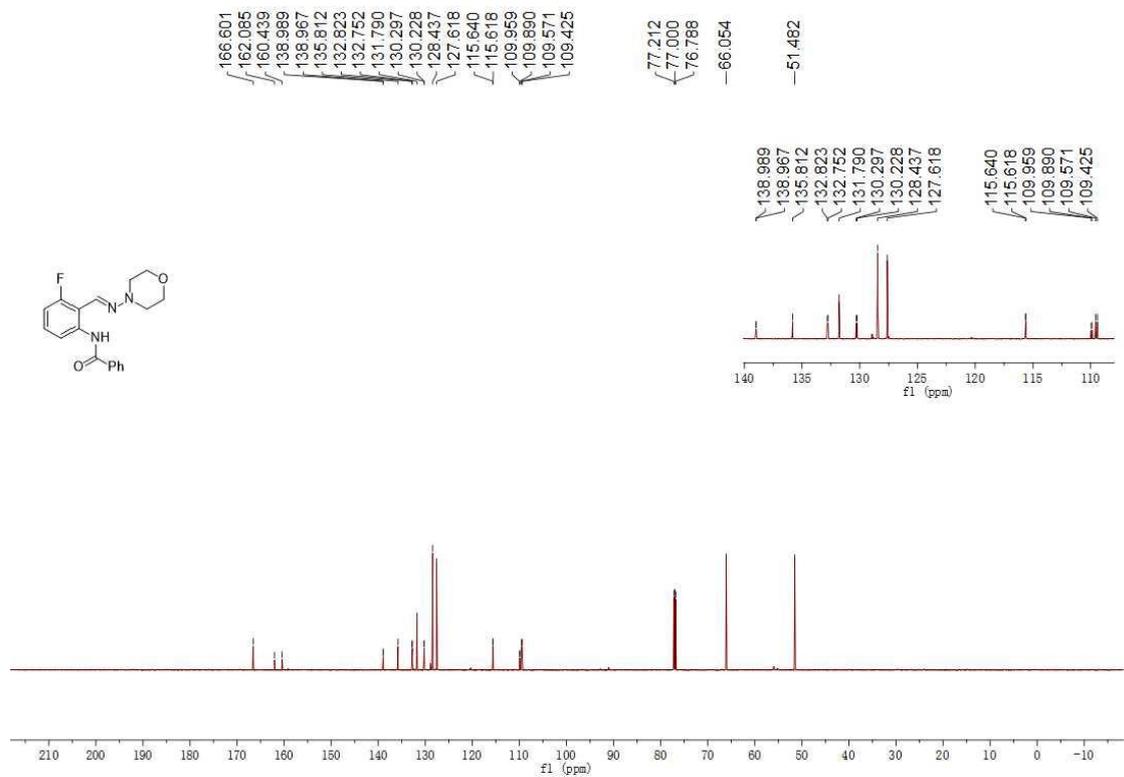
¹³C NMR (150 MHz, CDCl₃) Spectrum of 17



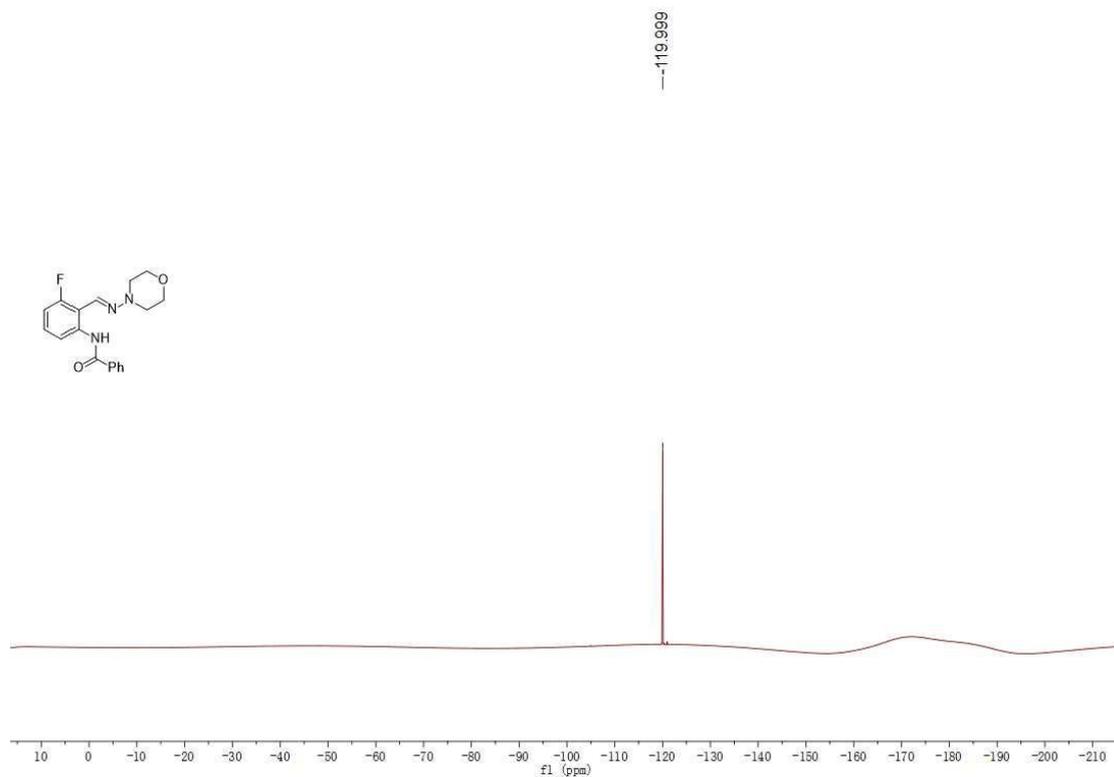
¹H NMR (600 MHz, CDCl₃) Spectrum of **18**



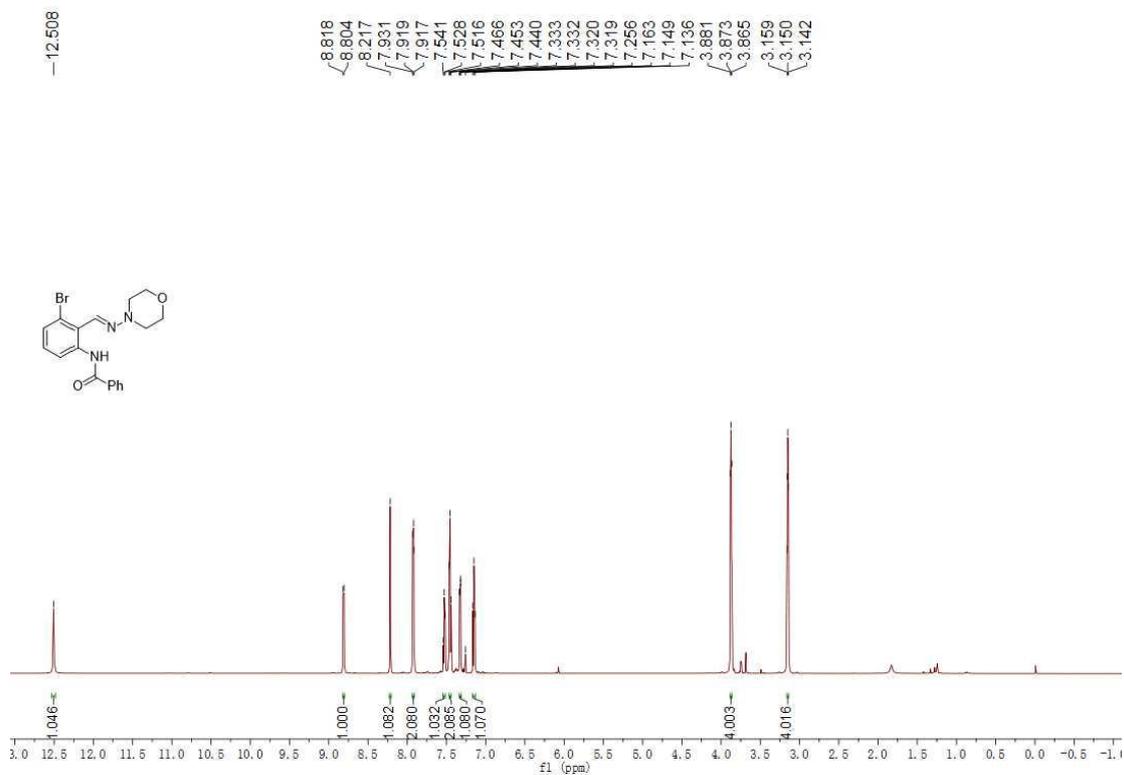
¹³C NMR (150 MHz, CDCl₃) Spectrum of **18**



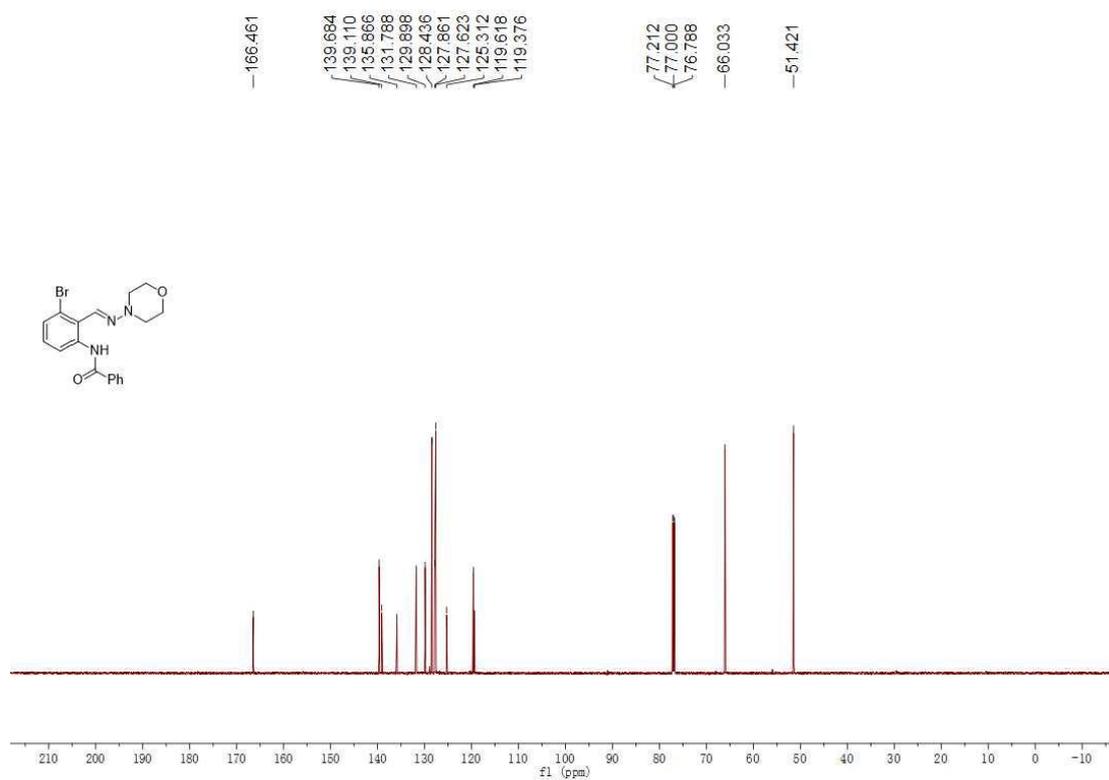
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **18**



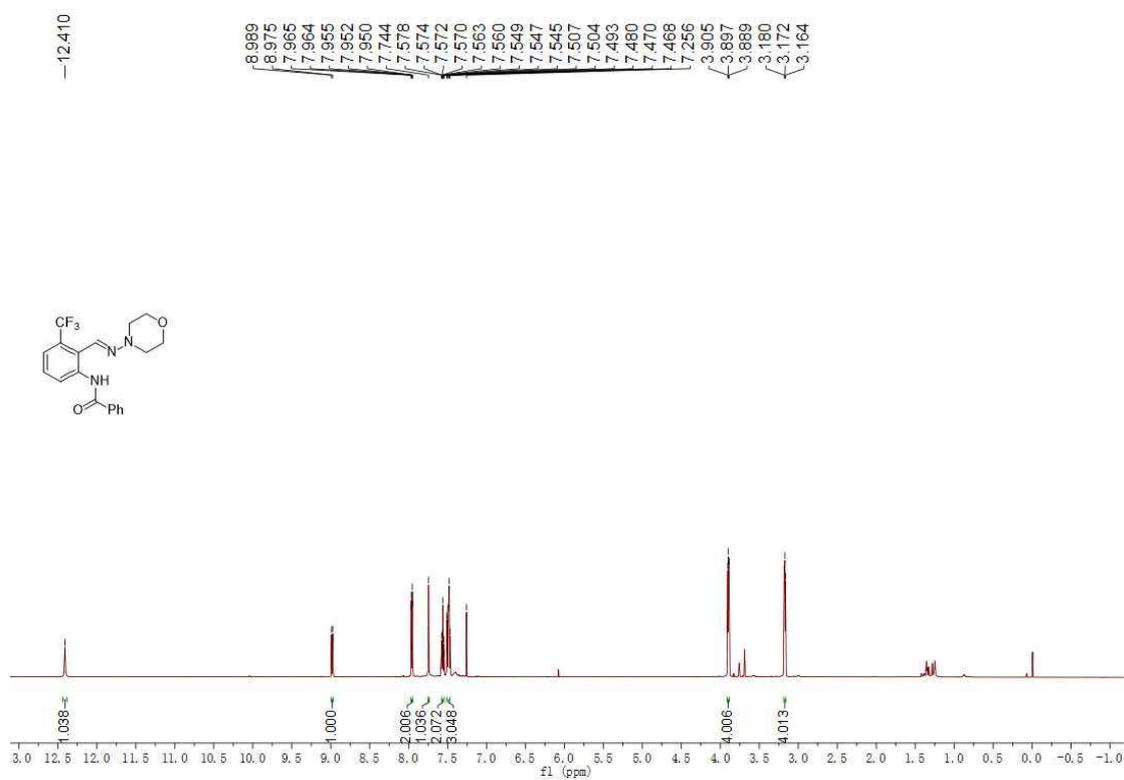
¹H NMR (600 MHz, CDCl₃) Spectrum of **19**



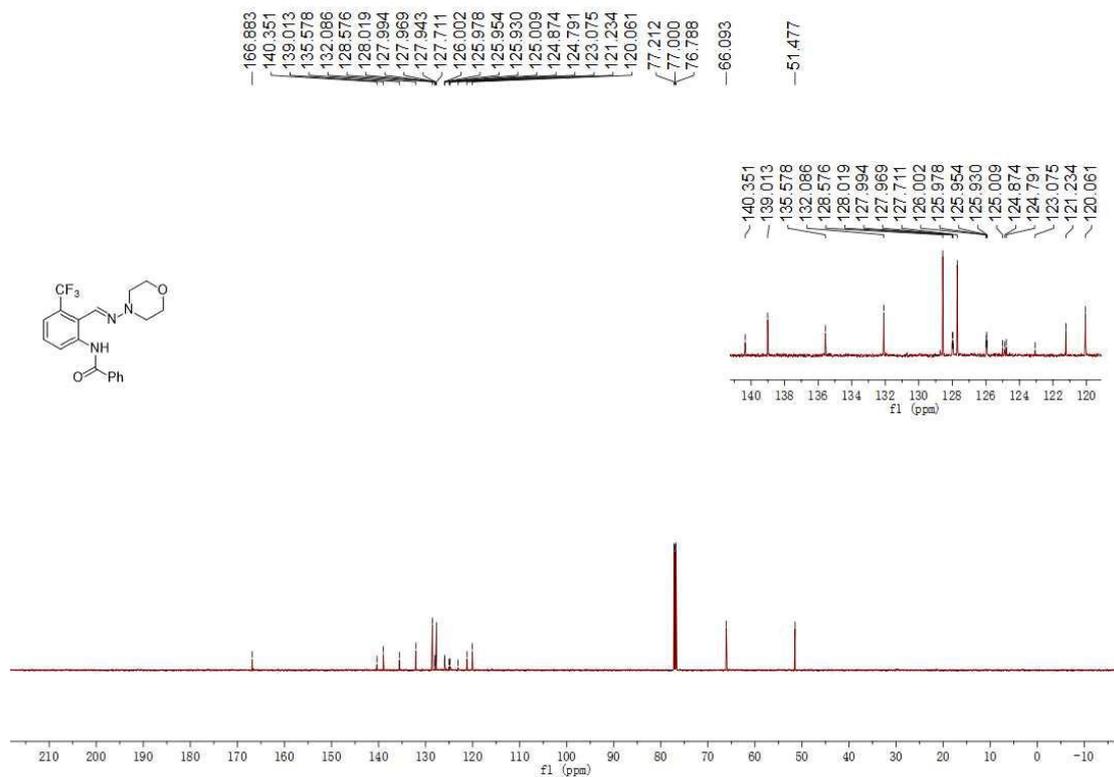
¹³C NMR (150 MHz, CDCl₃) Spectrum of **19**



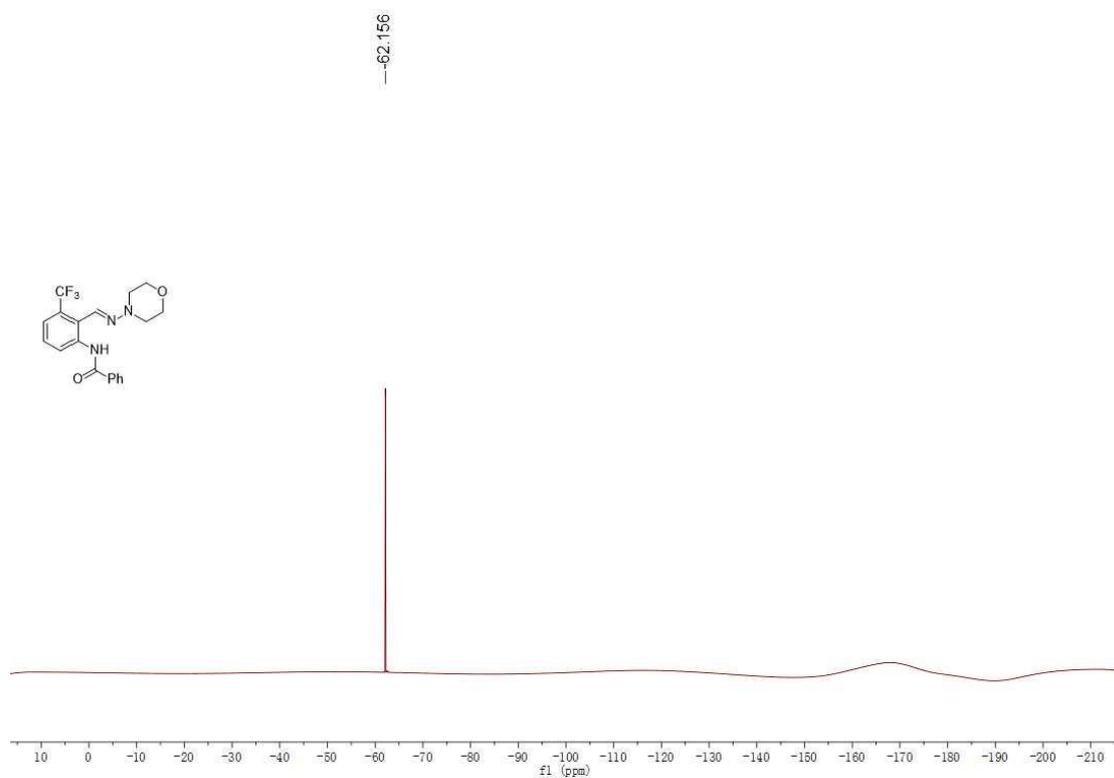
¹H NMR (600 MHz, CDCl₃) Spectrum of **20**



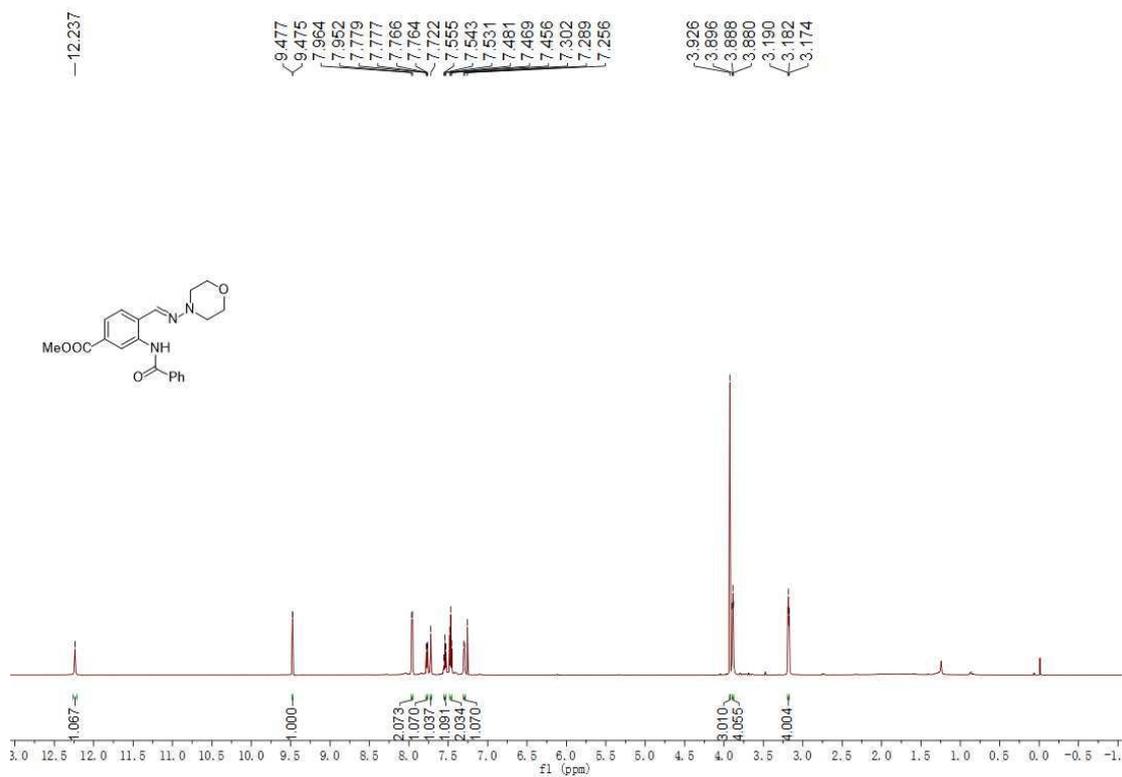
¹³C NMR (150 MHz, CDCl₃) Spectrum of **20**



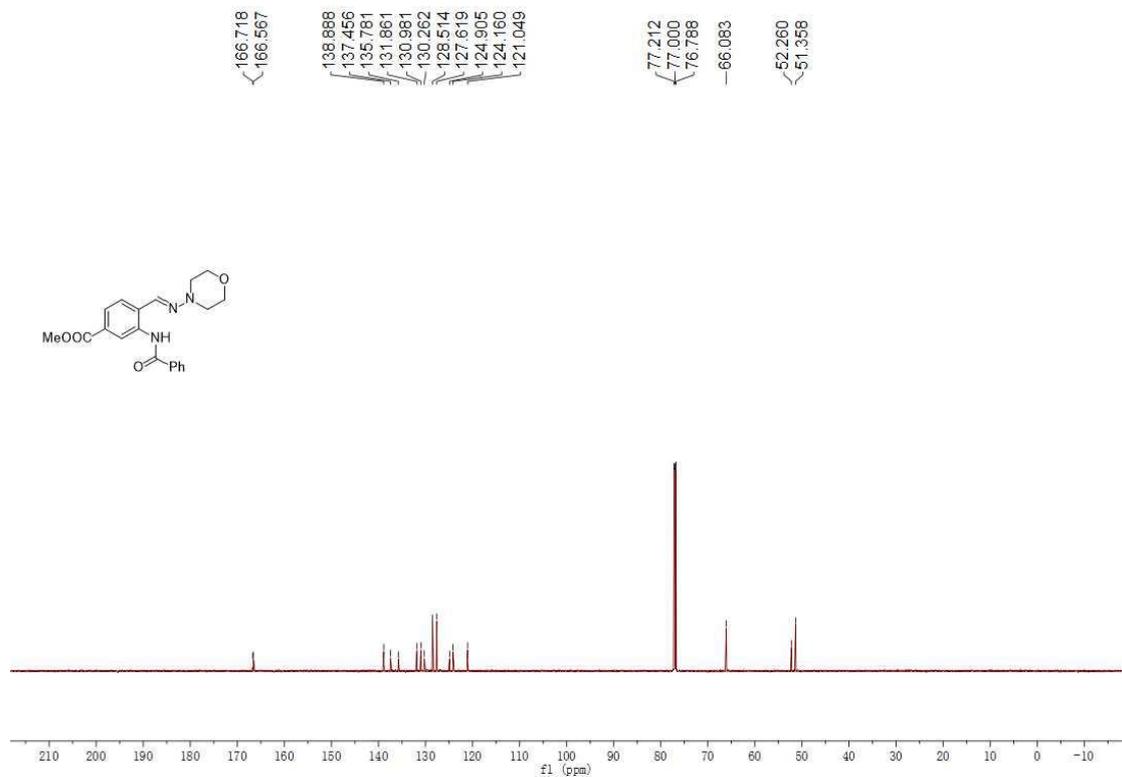
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **20**



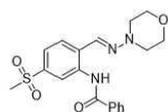
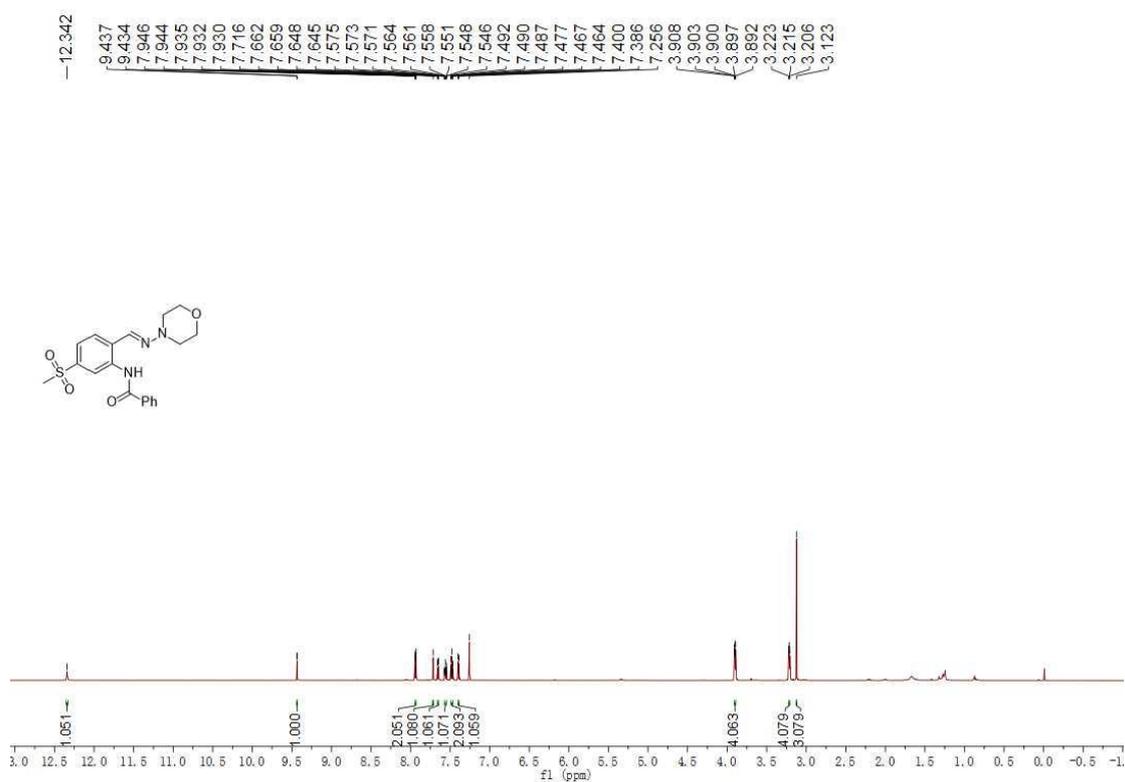
¹H NMR (600 MHz, CDCl₃) Spectrum of **21**



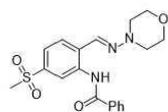
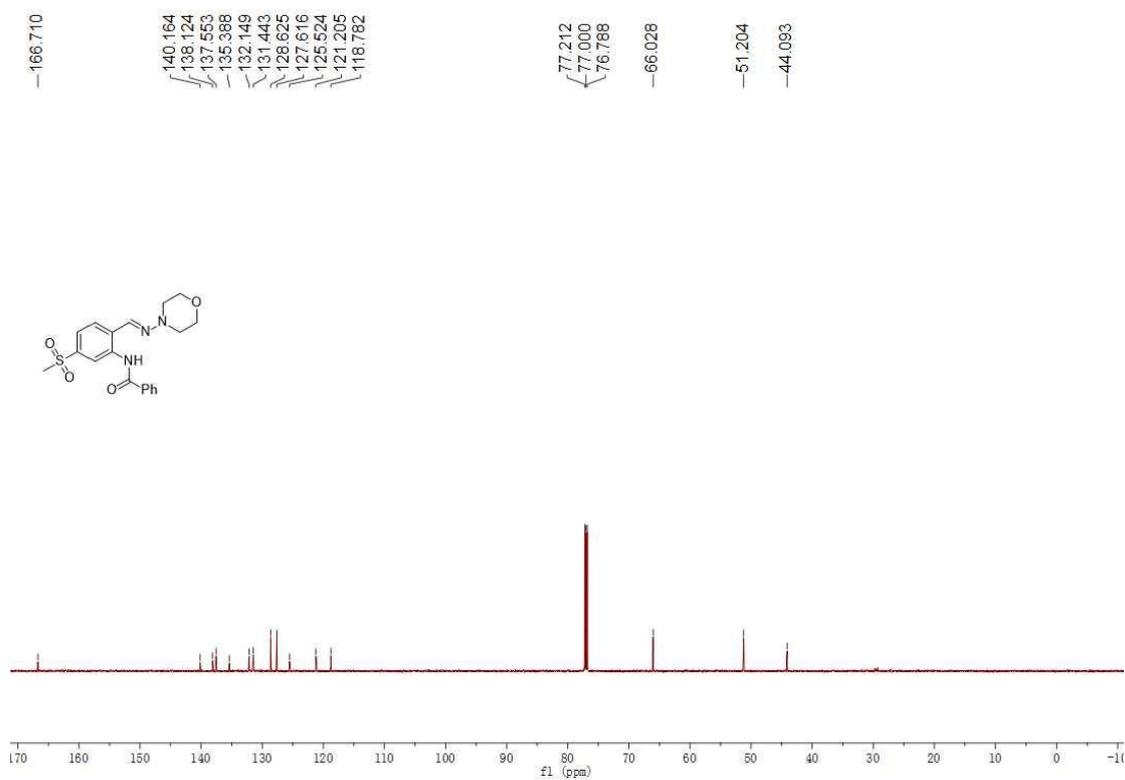
¹³C NMR (150 MHz, CDCl₃) Spectrum of **21**



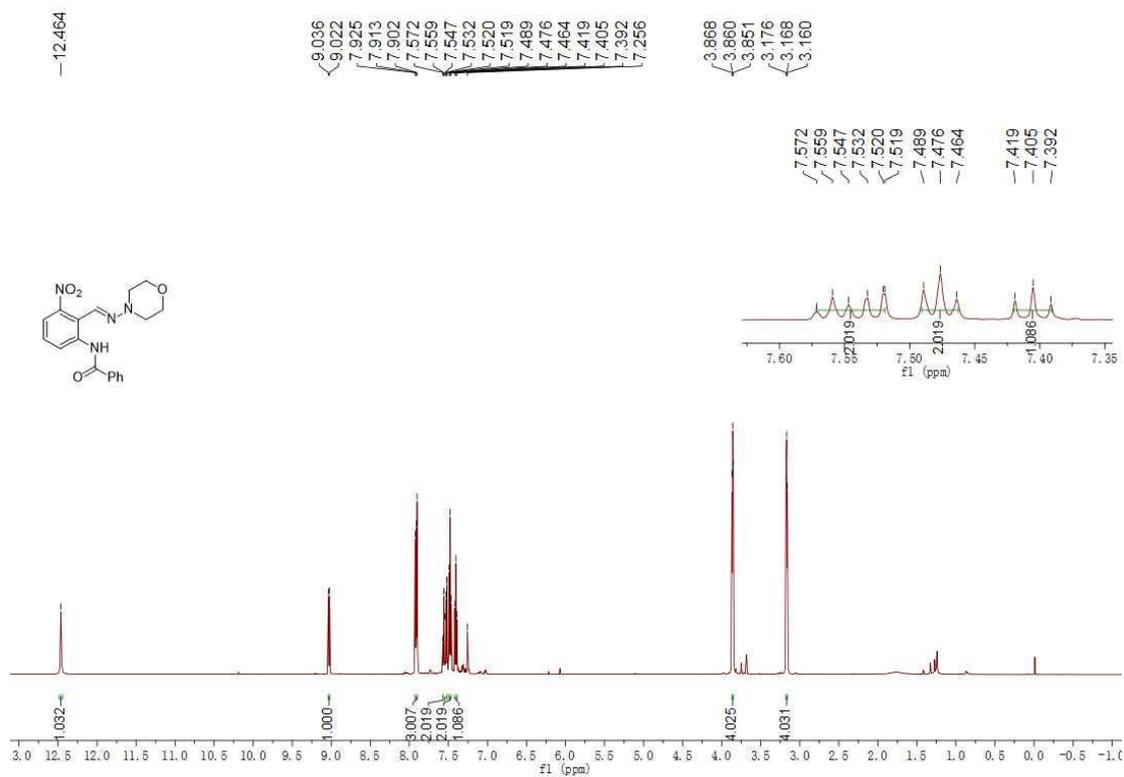
¹H NMR (600 MHz, CDCl₃) Spectrum of **22**



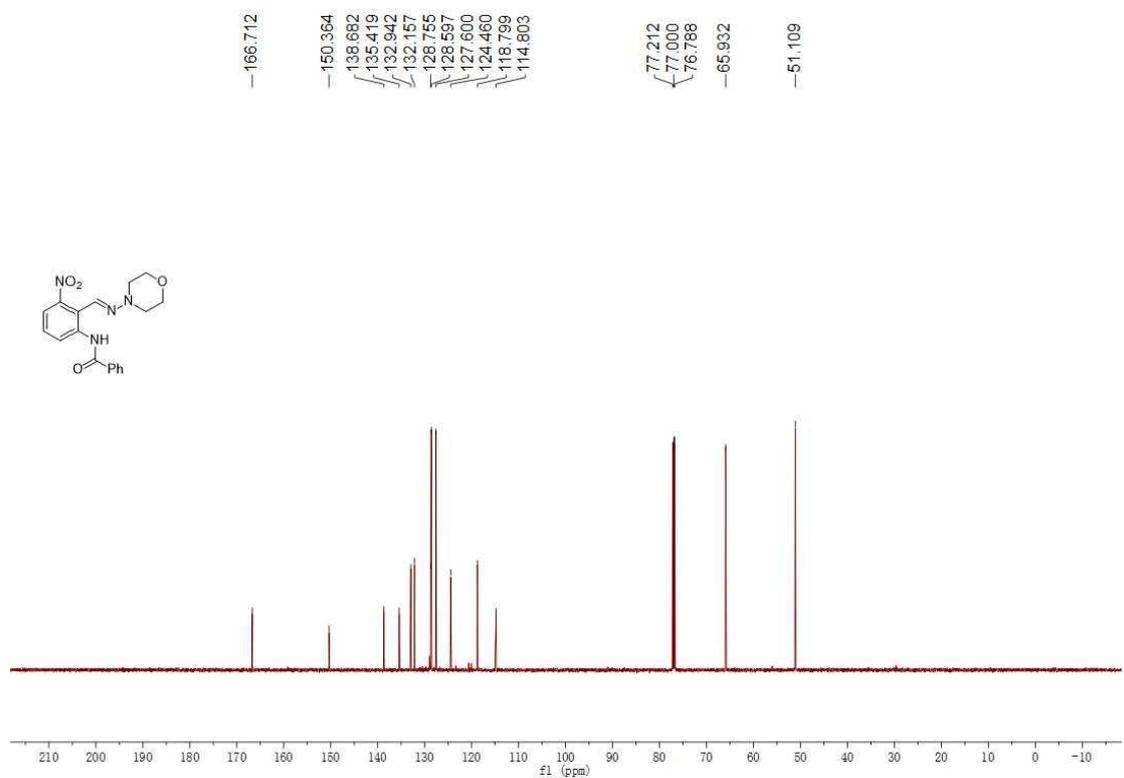
¹³C NMR (150 MHz, CDCl₃) Spectrum of **22**



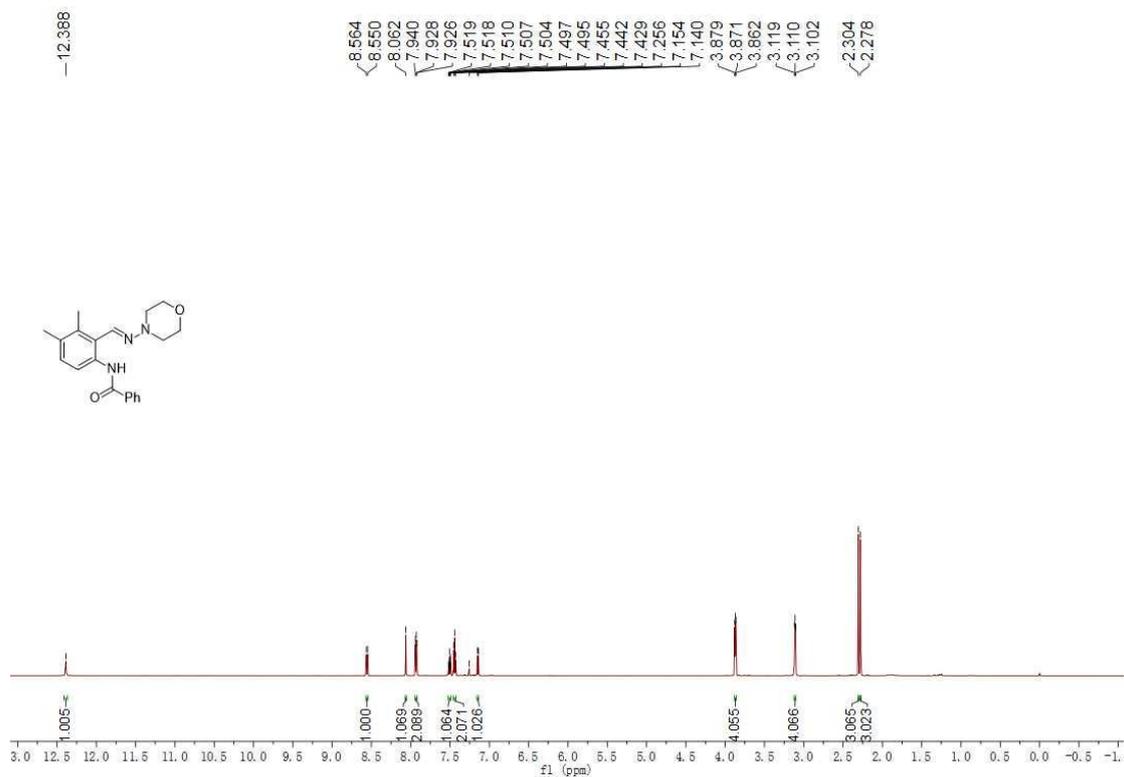
¹H NMR (600 MHz, CDCl₃) Spectrum of **23**



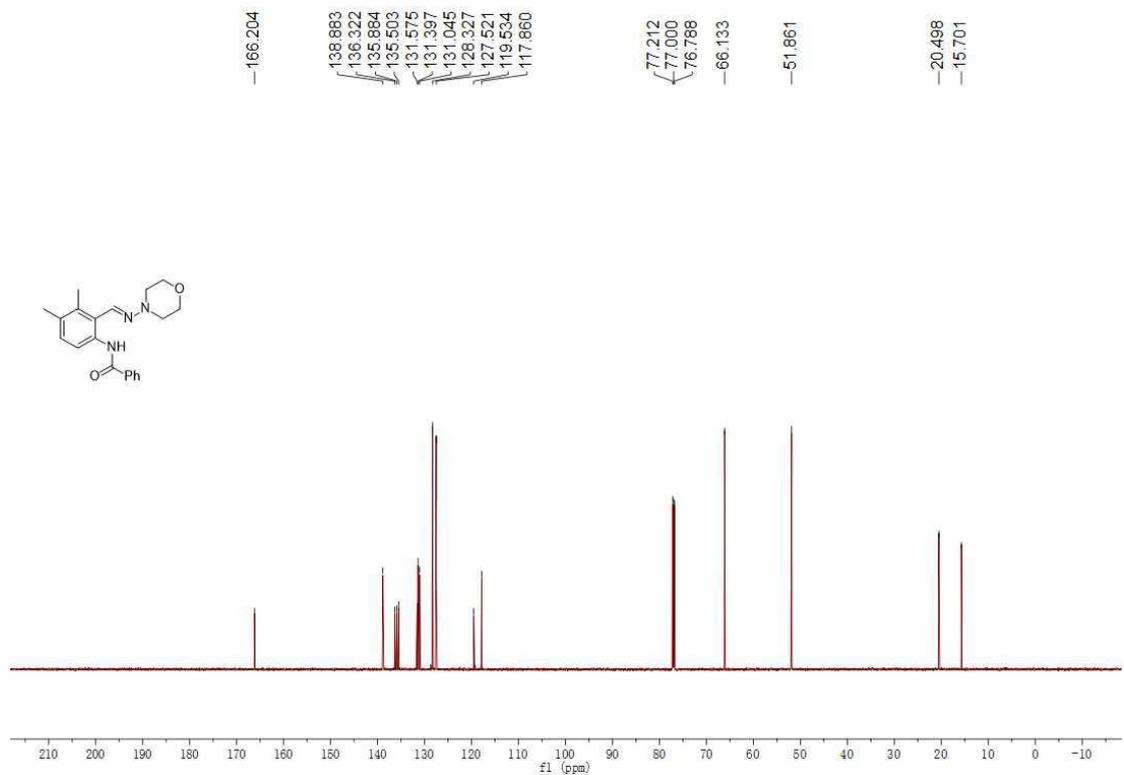
¹³C NMR (150 MHz, CDCl₃) Spectrum of **23**



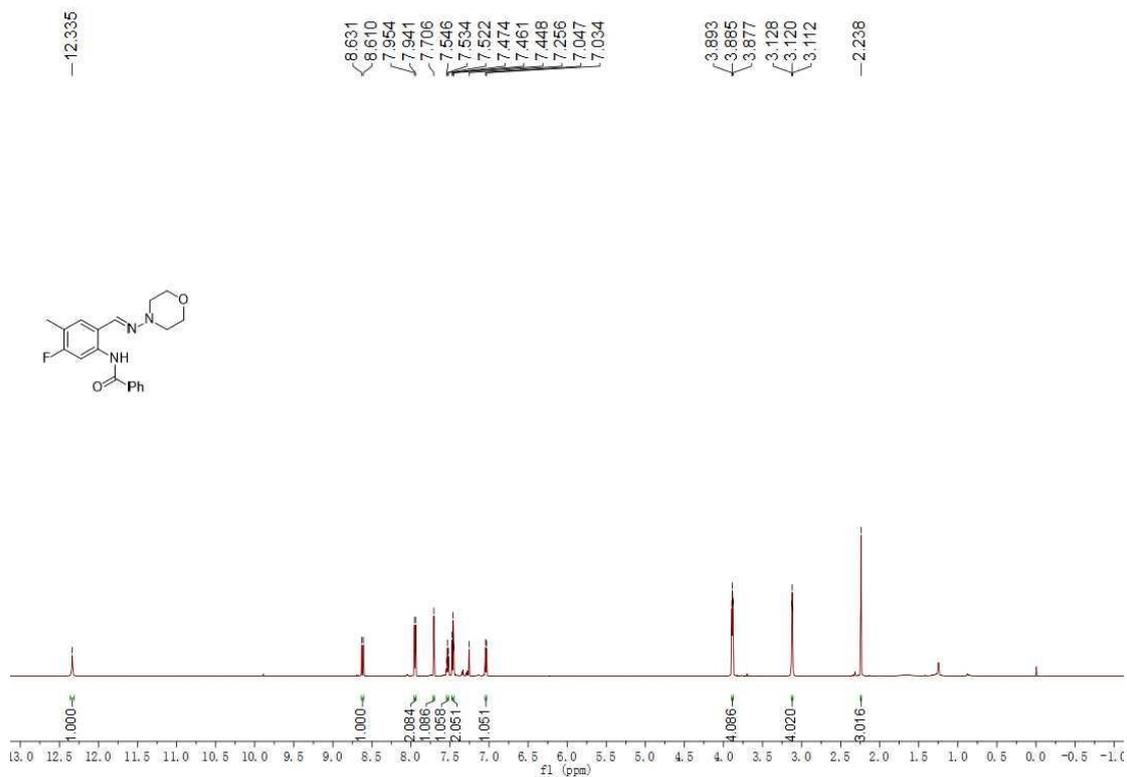
¹H NMR (600 MHz, CDCl₃) Spectrum of **24**



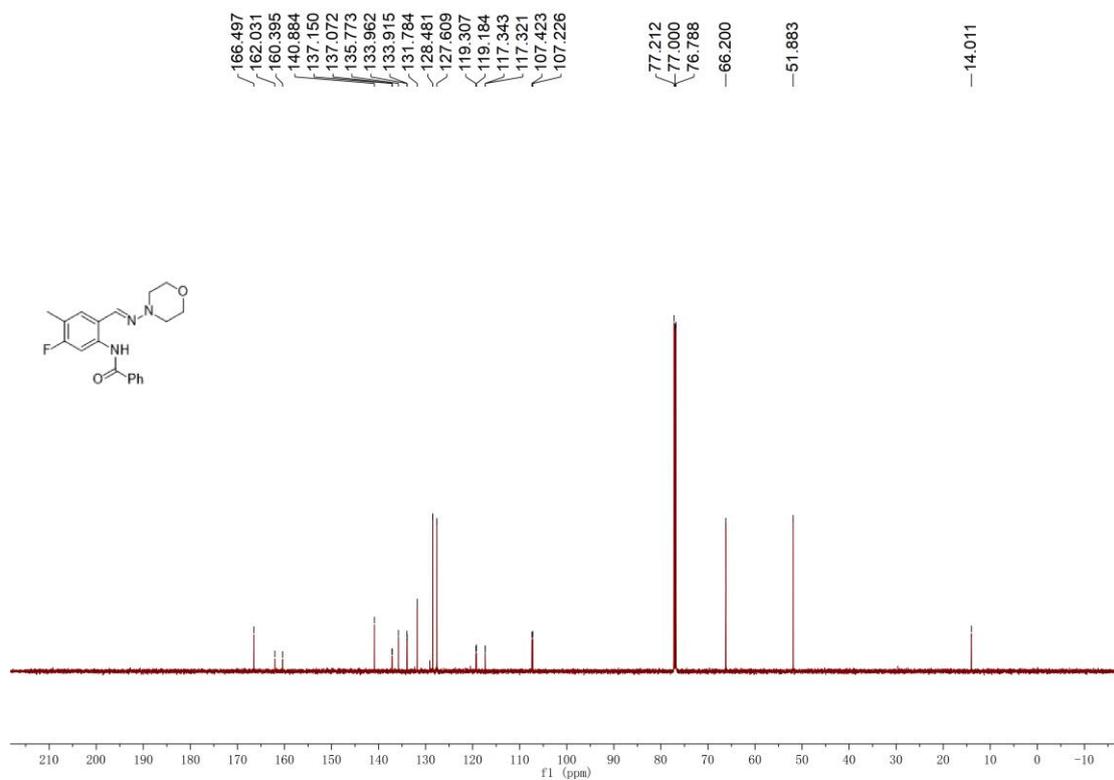
¹³C NMR (150 MHz, CDCl₃) Spectrum of **24**



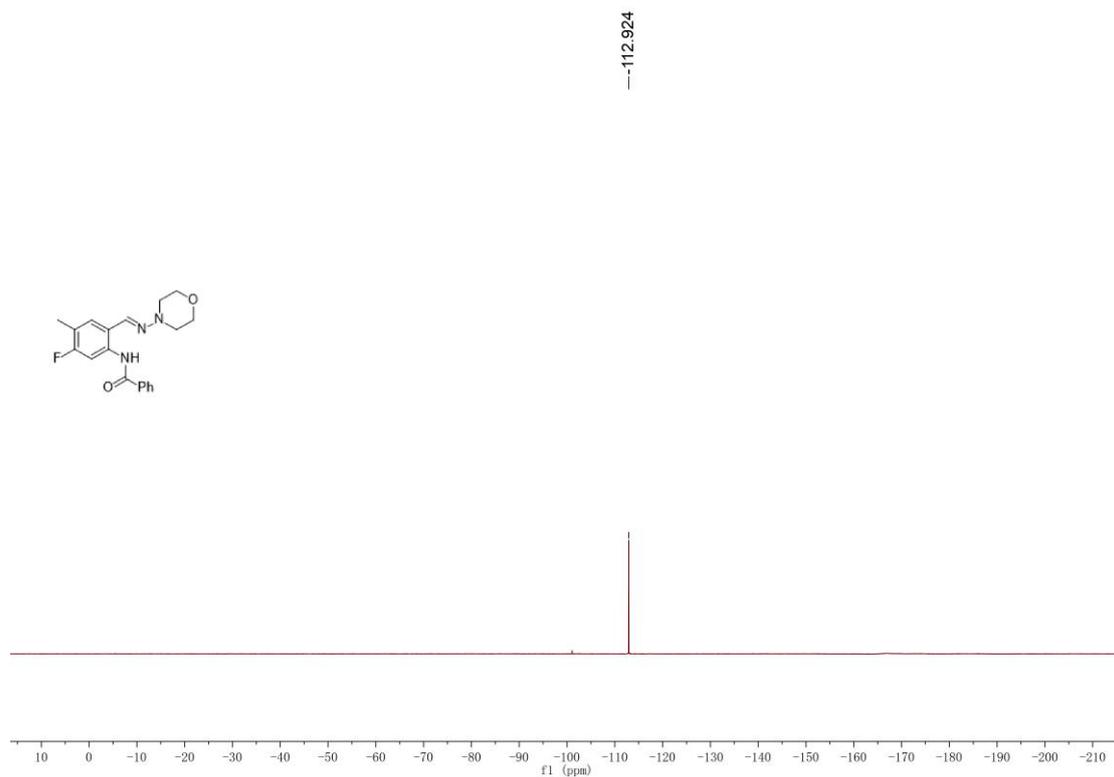
¹H NMR (600 MHz, CDCl₃) Spectrum of **25**



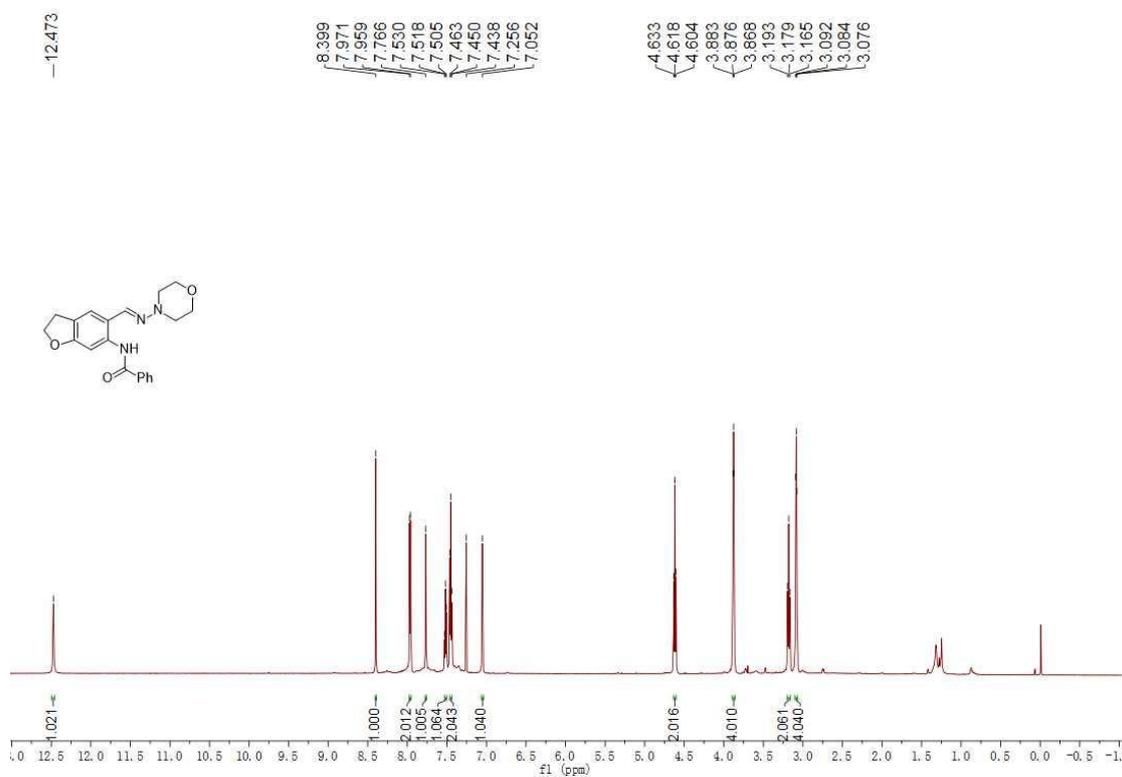
¹³C NMR (150 MHz, CDCl₃) Spectrum of **25**



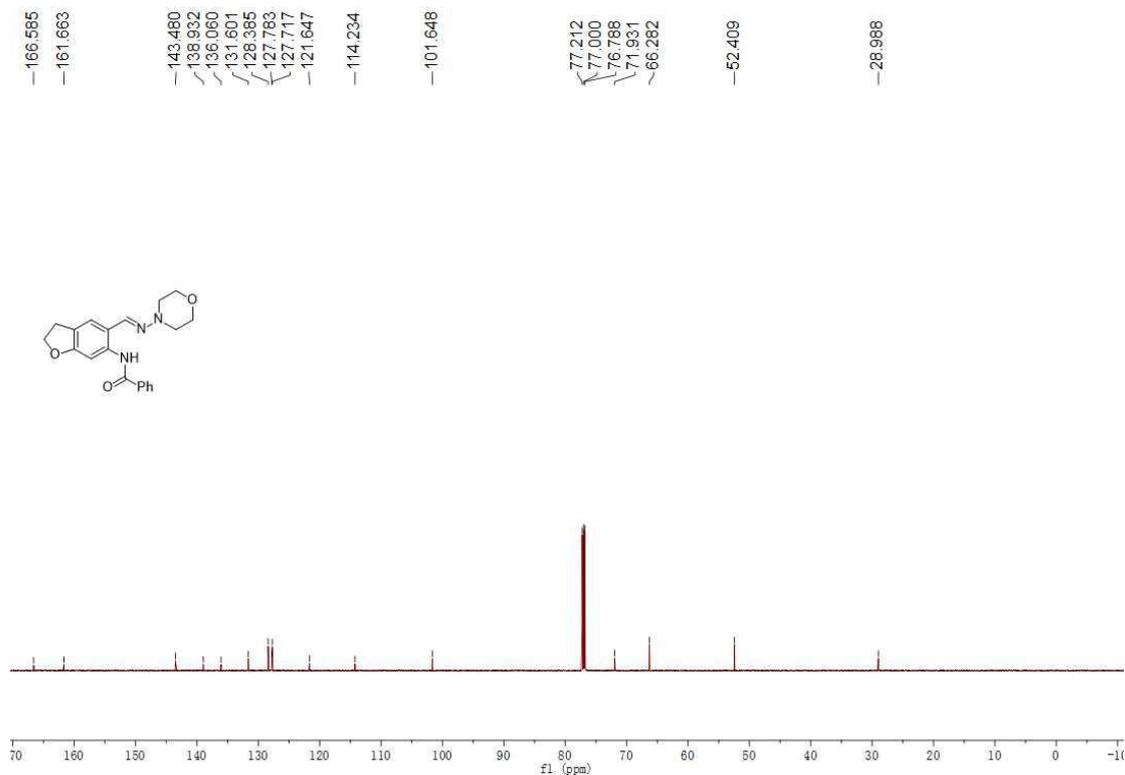
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **25**



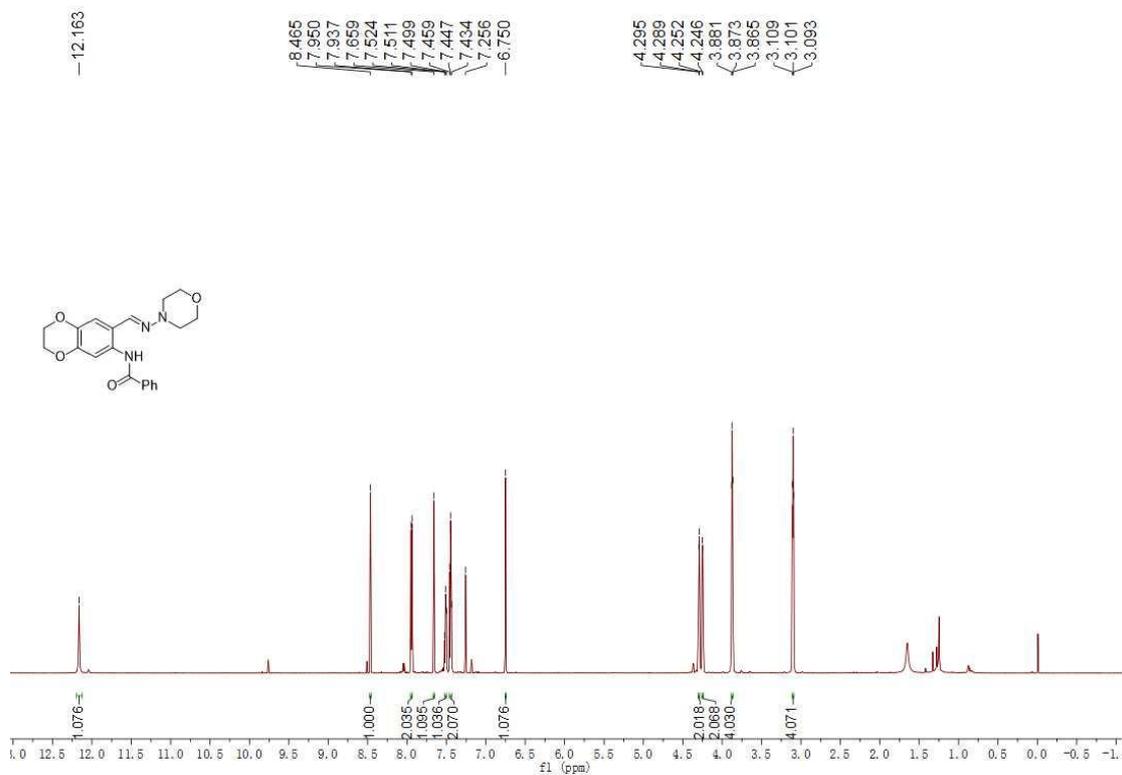
¹H NMR (600 MHz, CDCl₃) Spectrum of **26**



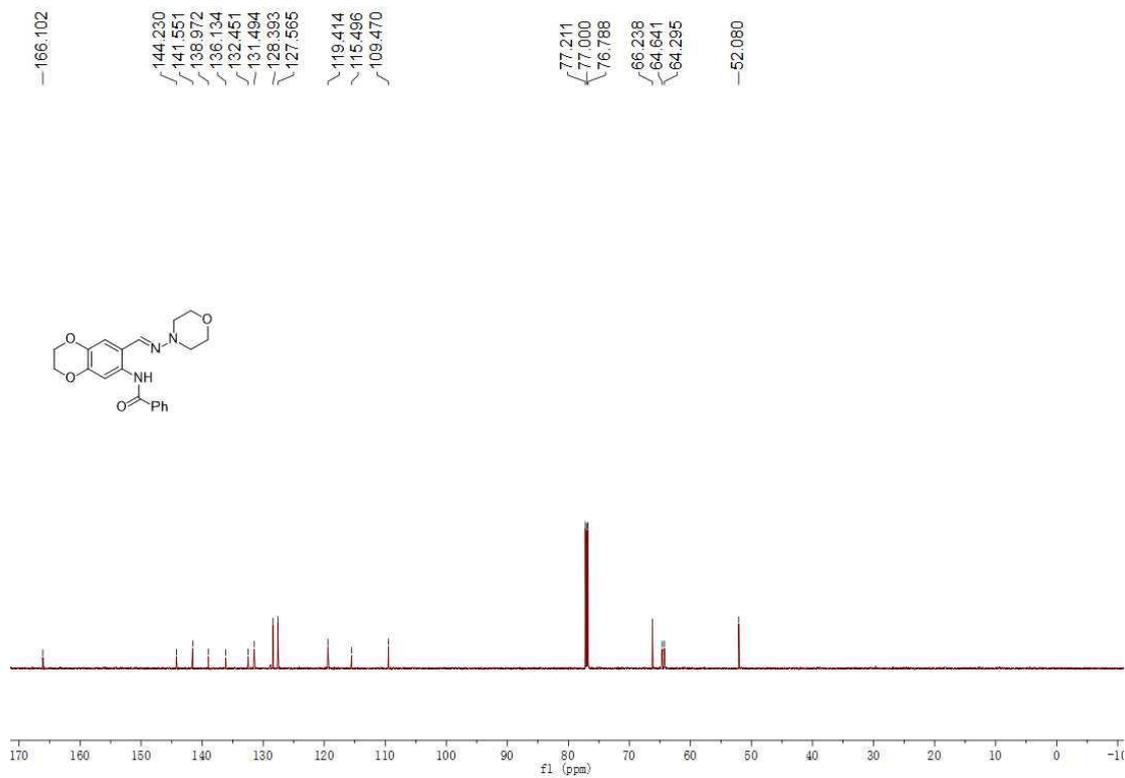
¹³C NMR (150 MHz, CDCl₃) Spectrum of 26



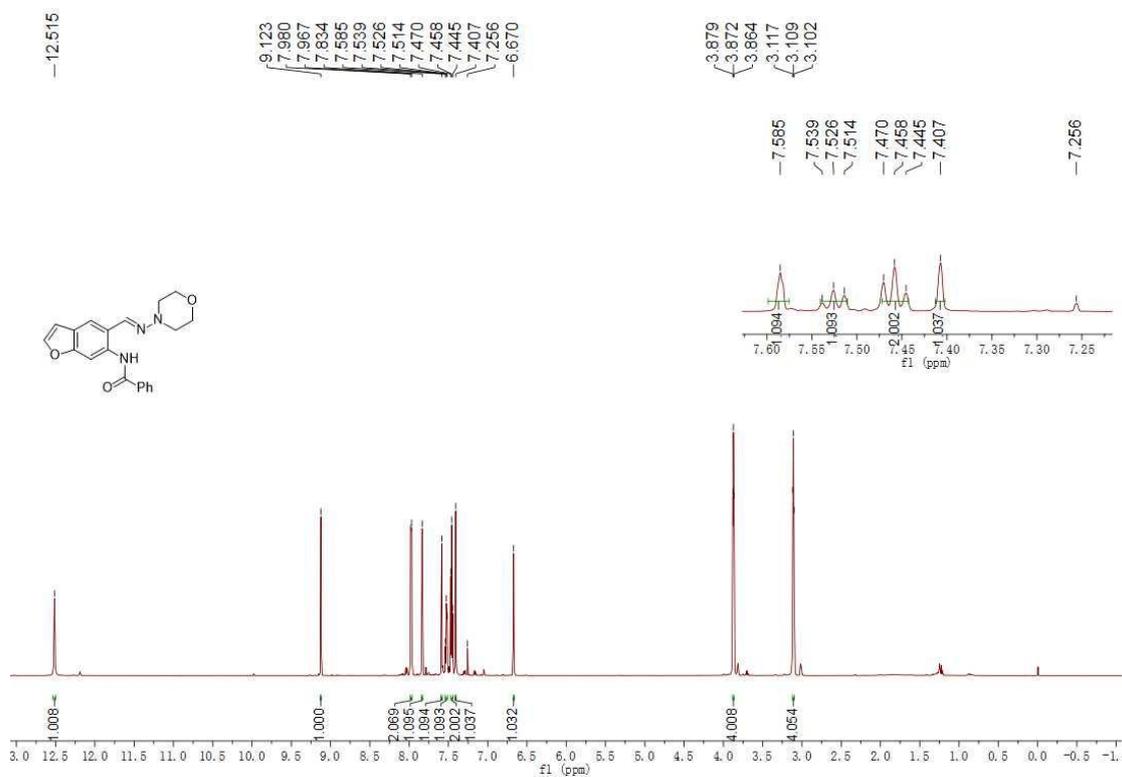
¹H NMR (600 MHz, CDCl₃) Spectrum of 27



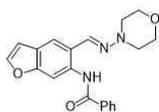
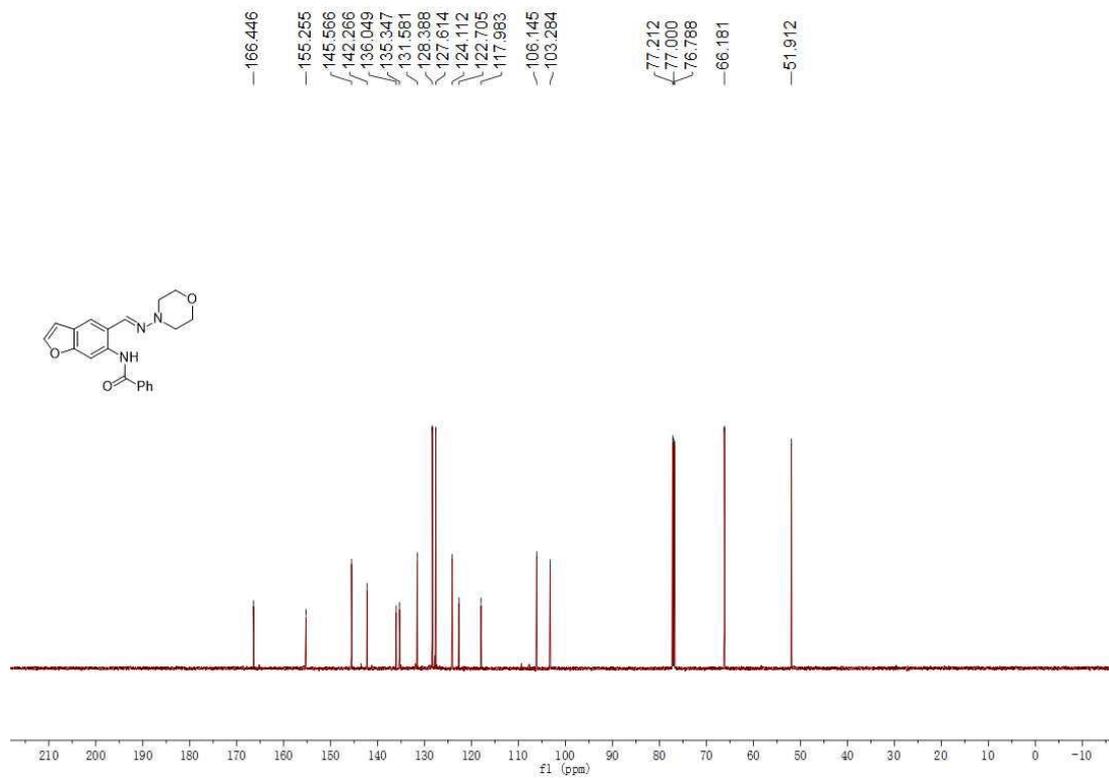
¹³C NMR (150 MHz, CDCl₃) Spectrum of **27**



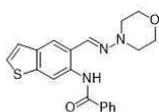
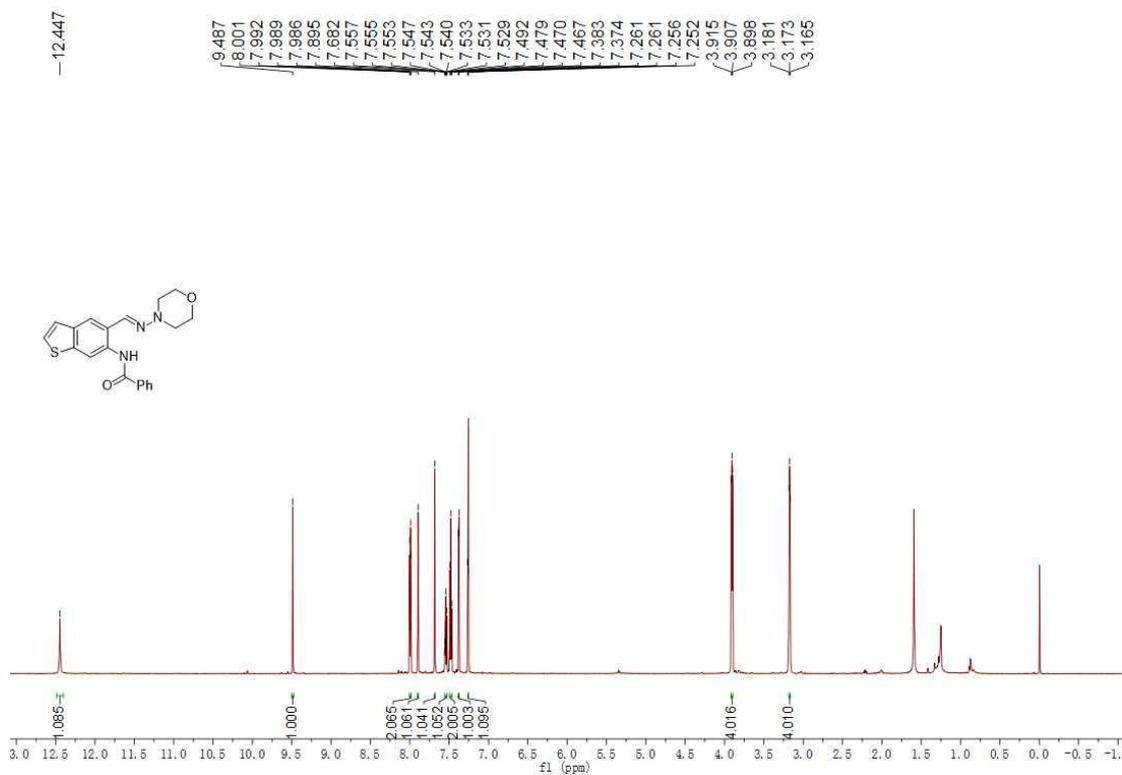
¹H NMR (600 MHz, CDCl₃) Spectrum of **28**



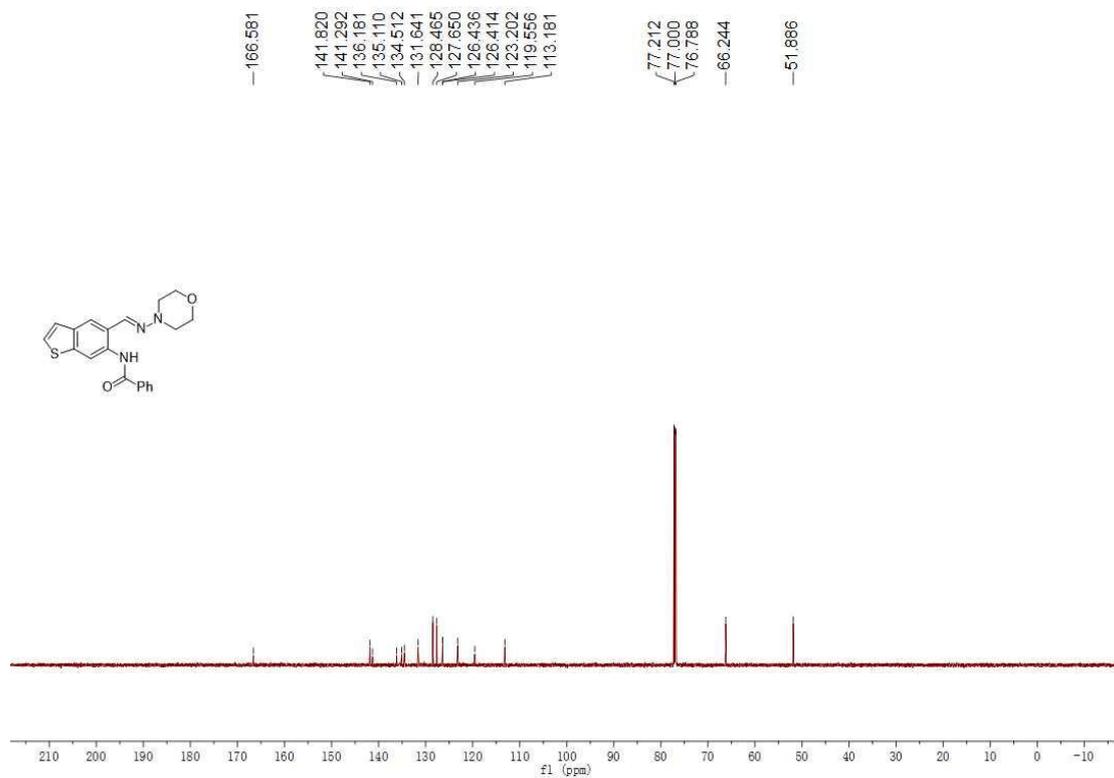
¹³C NMR (150 MHz, CDCl₃) Spectrum of **28**



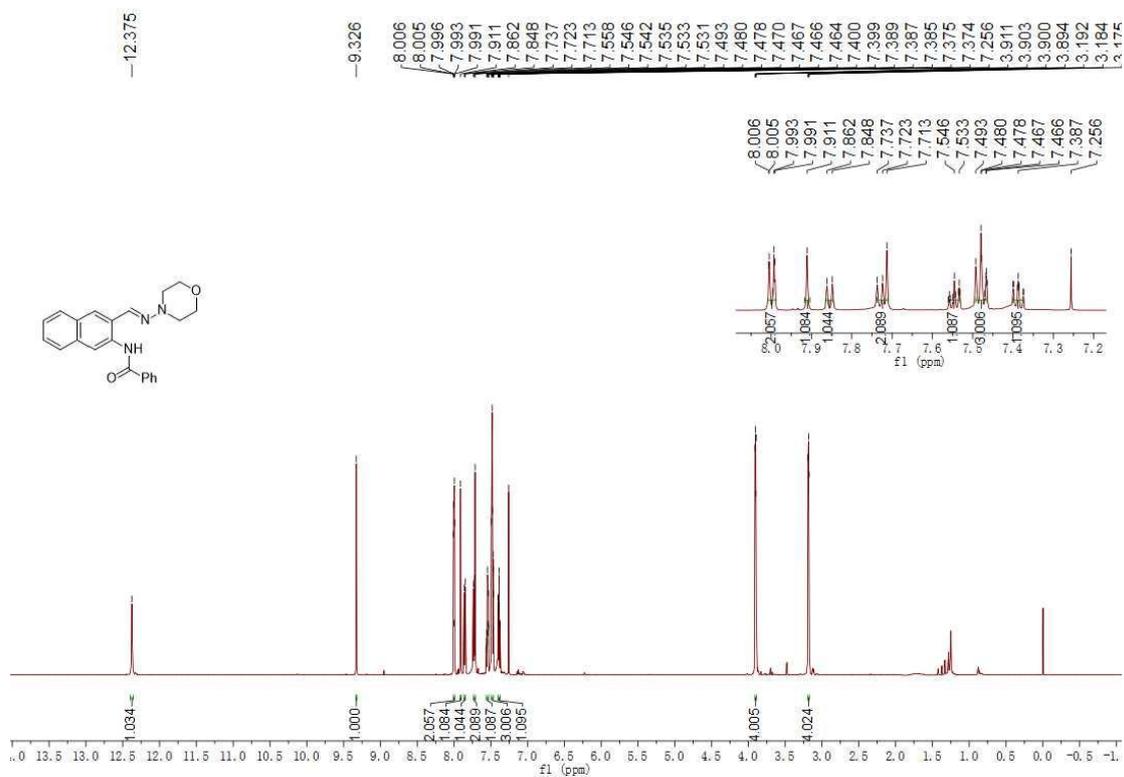
¹H NMR (600 MHz, CDCl₃) Spectrum of **29**



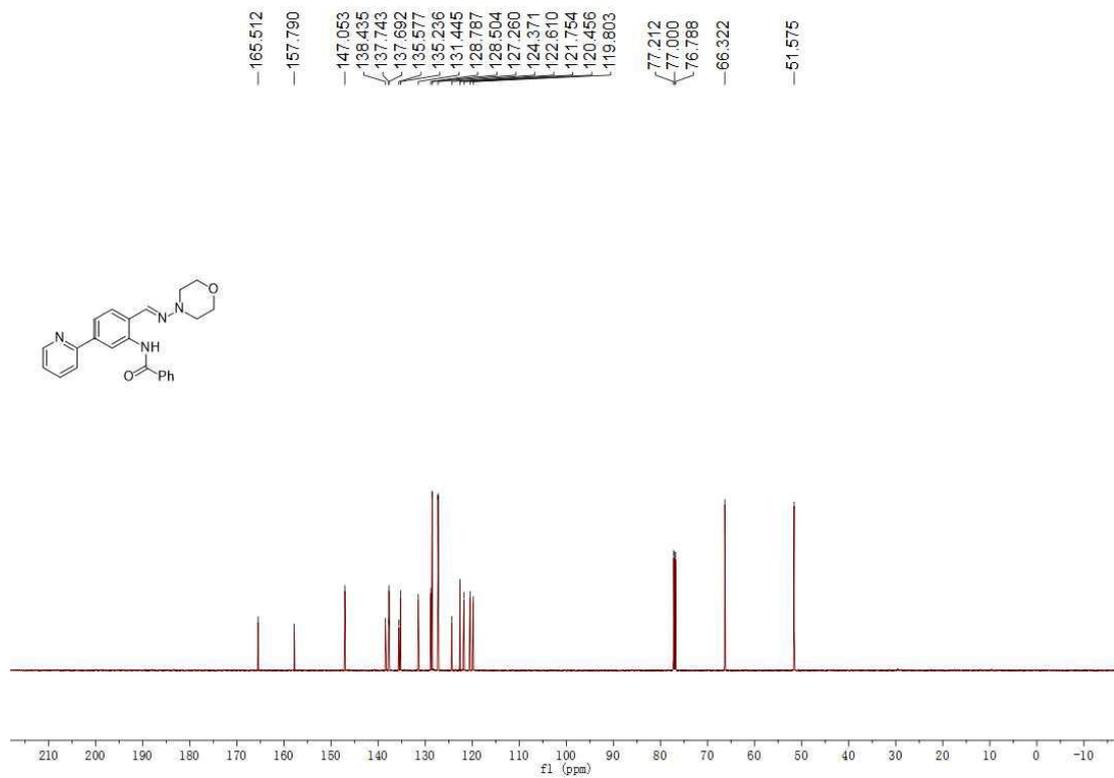
¹³C NMR (150 MHz, CDCl₃) Spectrum of **29**



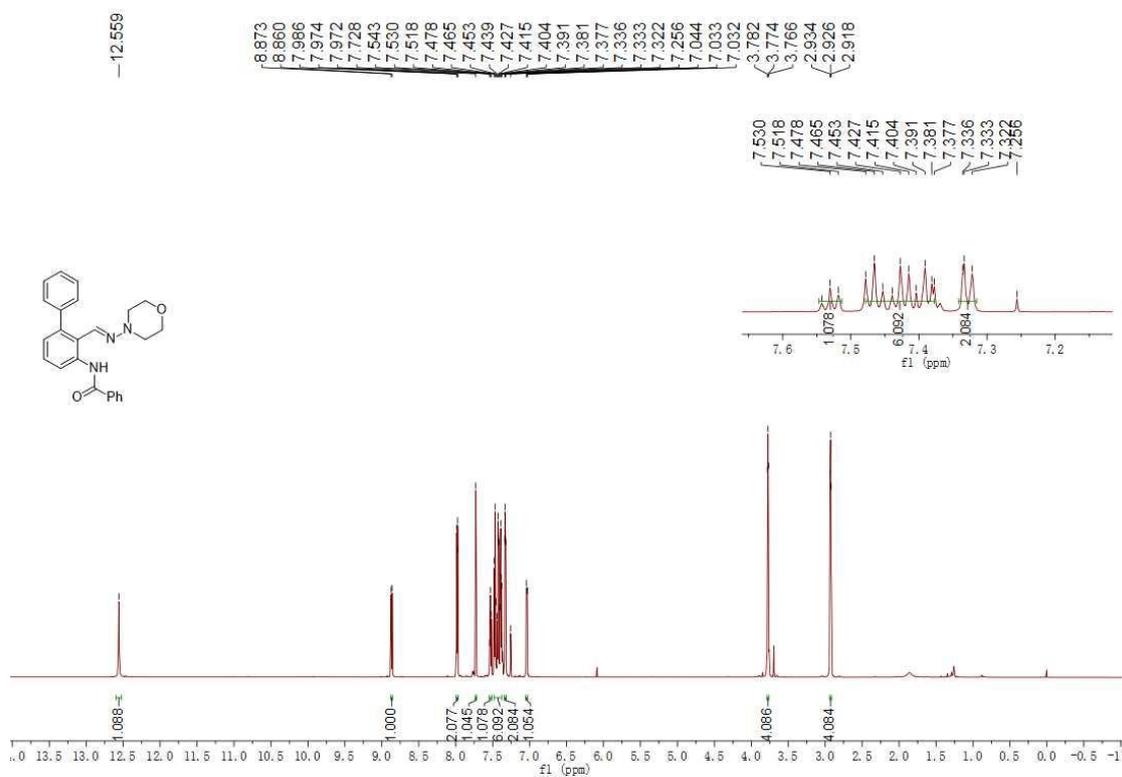
¹H NMR (600 MHz, CDCl₃) Spectrum of **30**



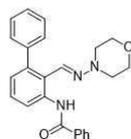
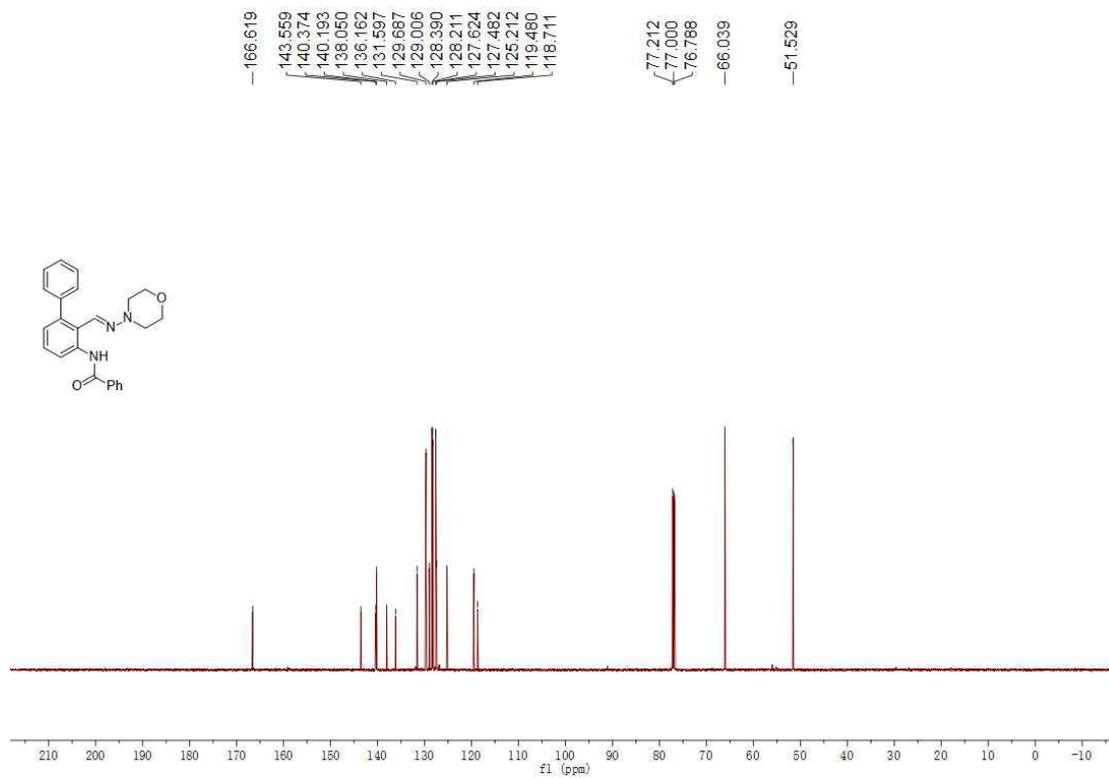
¹³C NMR (150 MHz, CDCl₃) Spectrum of **32**



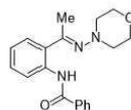
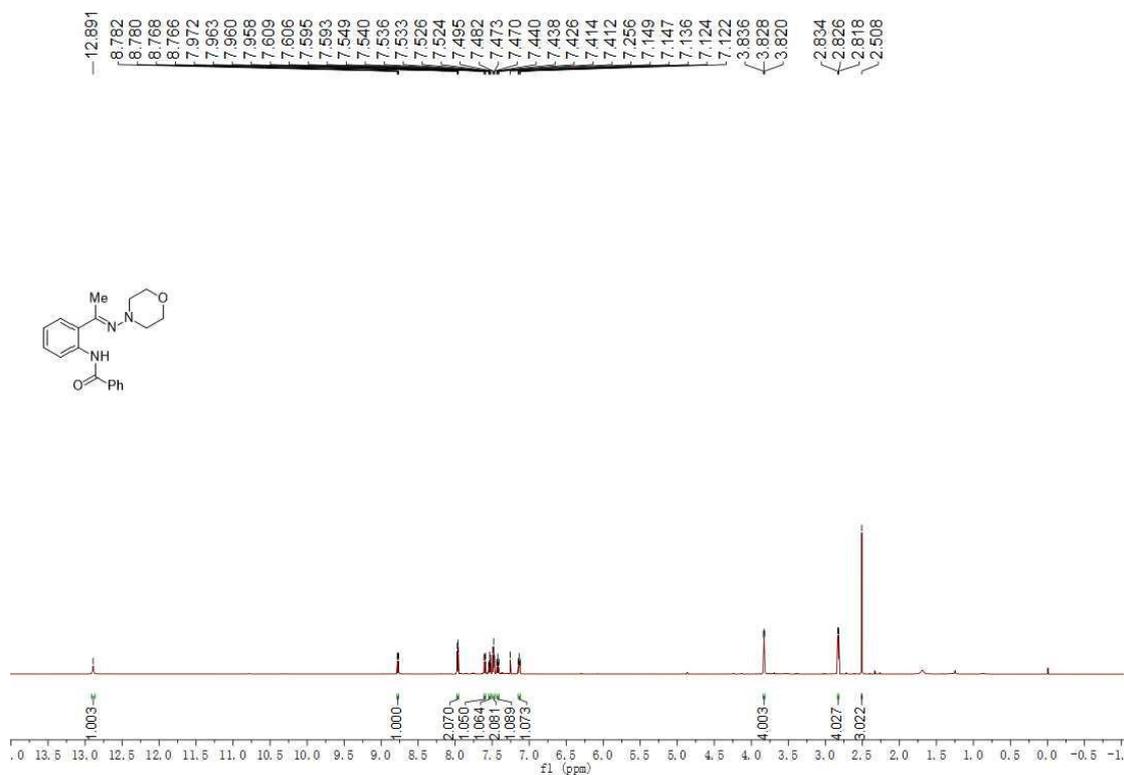
¹H NMR (600 MHz, CDCl₃) Spectrum of **33**



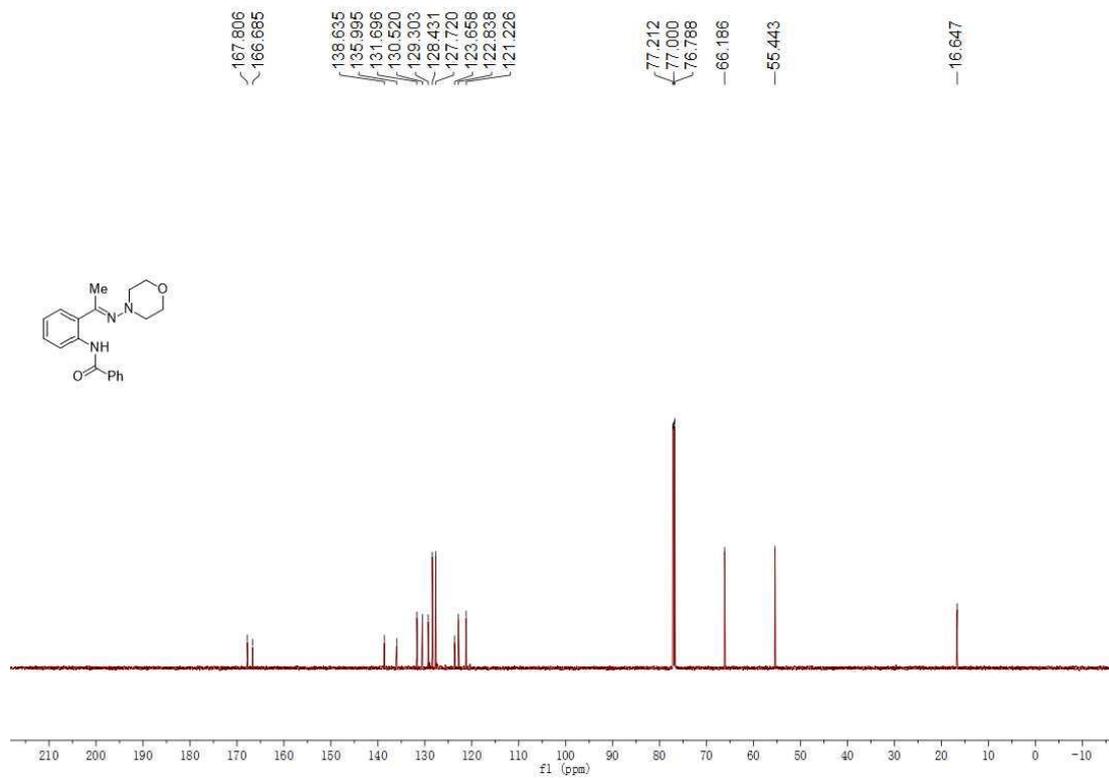
¹³C NMR (150 MHz, CDCl₃) Spectrum of **33**



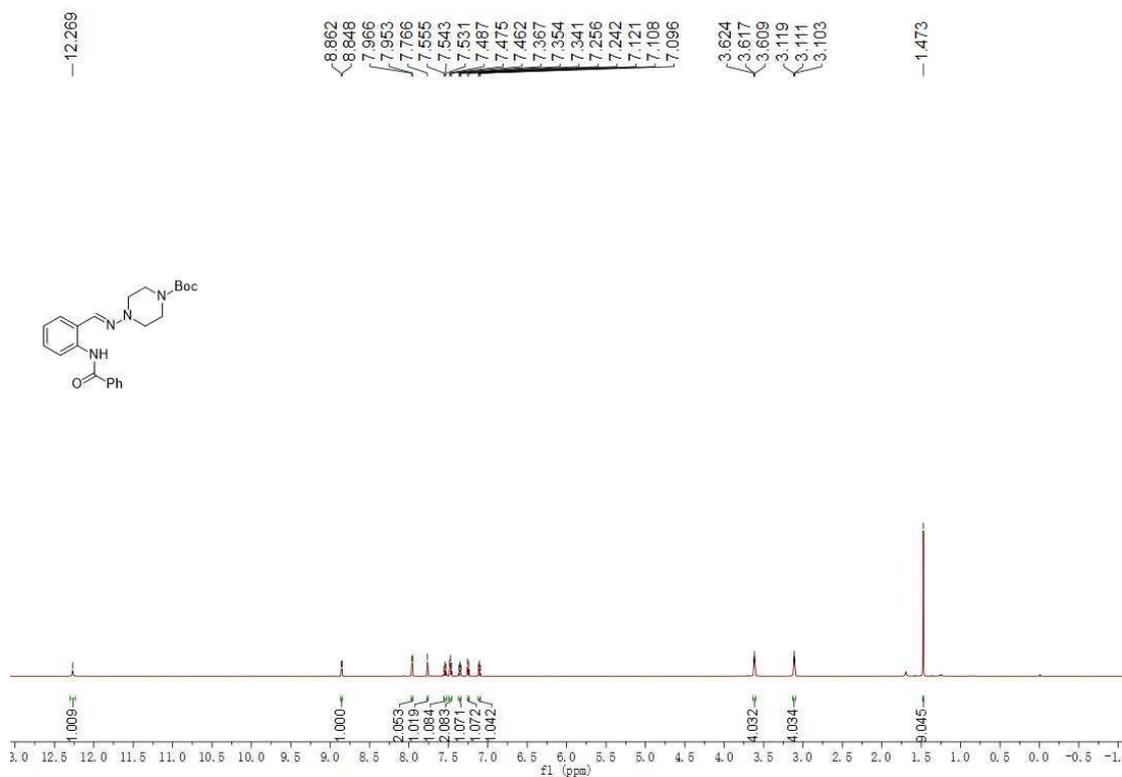
¹H NMR (600 MHz, CDCl₃) Spectrum of **34**



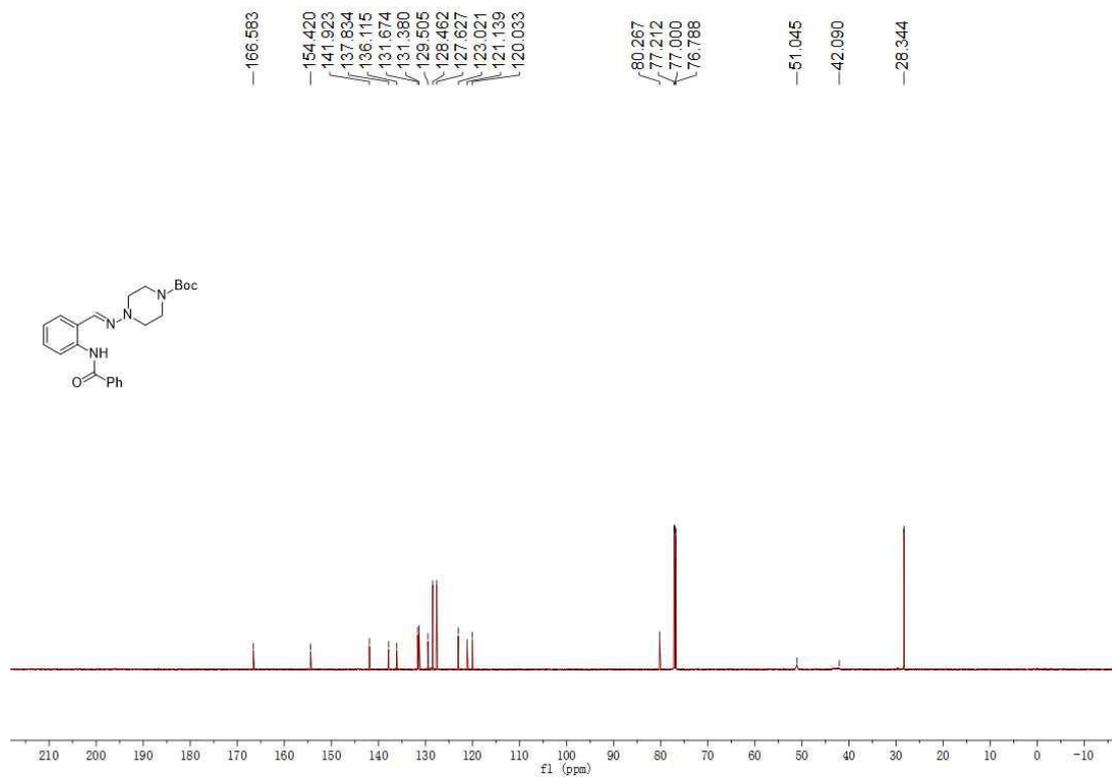
¹³C NMR (150 MHz, CDCl₃) Spectrum of **34**



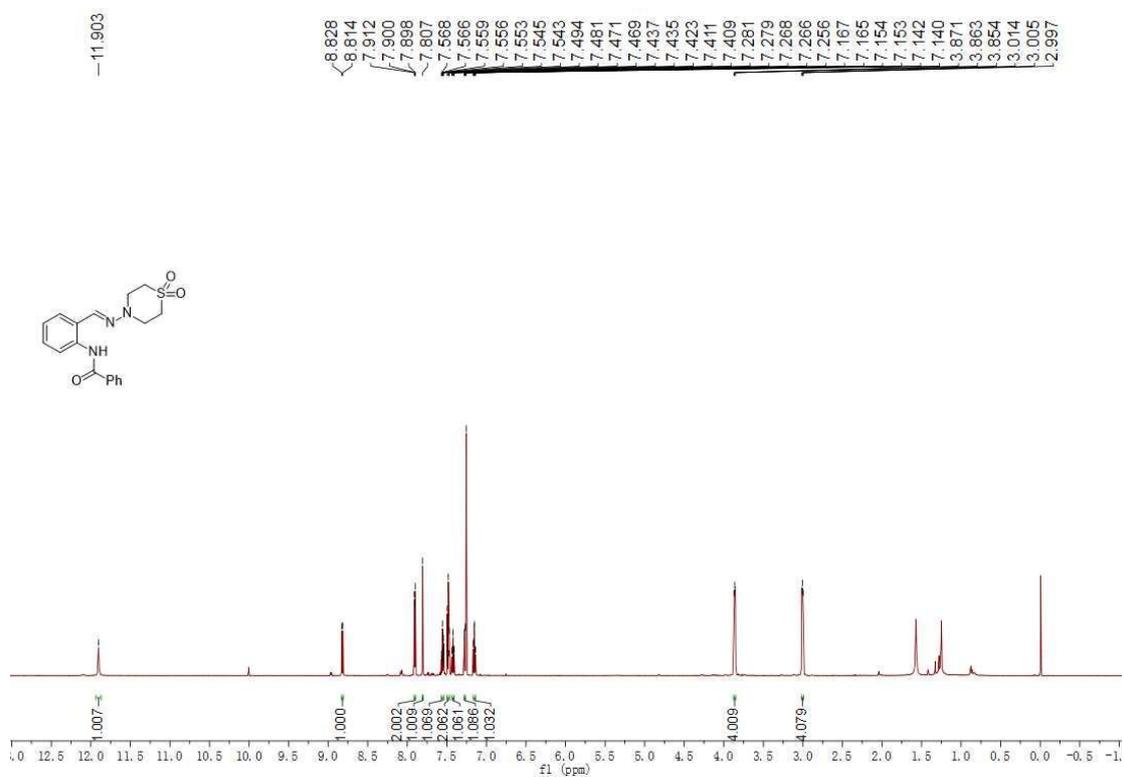
¹H NMR (600 MHz, CDCl₃) Spectrum of **35**



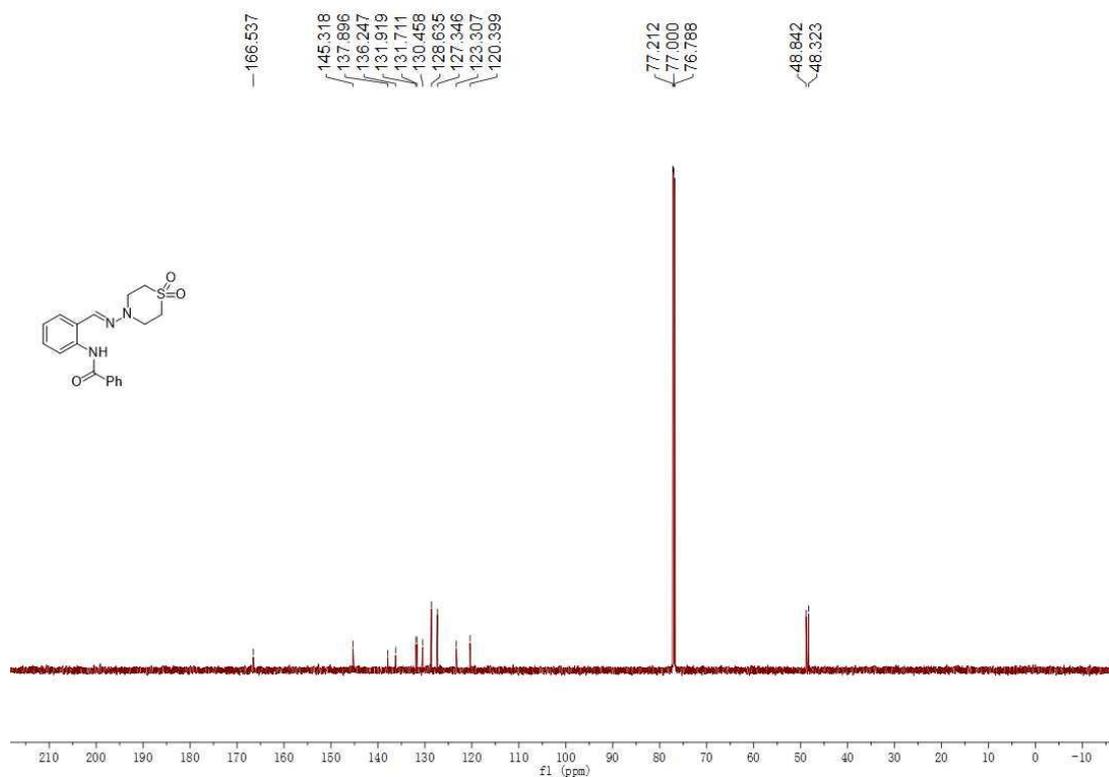
¹³C NMR (150 MHz, CDCl₃) Spectrum of **35**



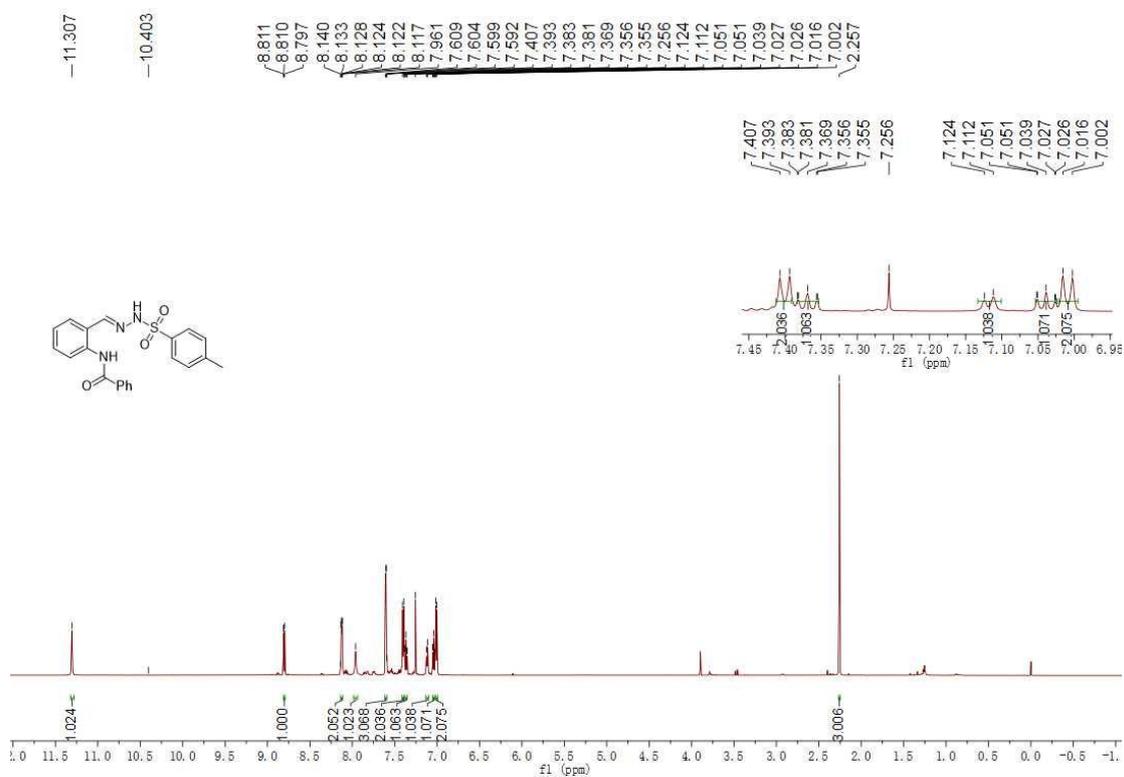
¹H NMR (600 MHz, CDCl₃) Spectrum of **36**



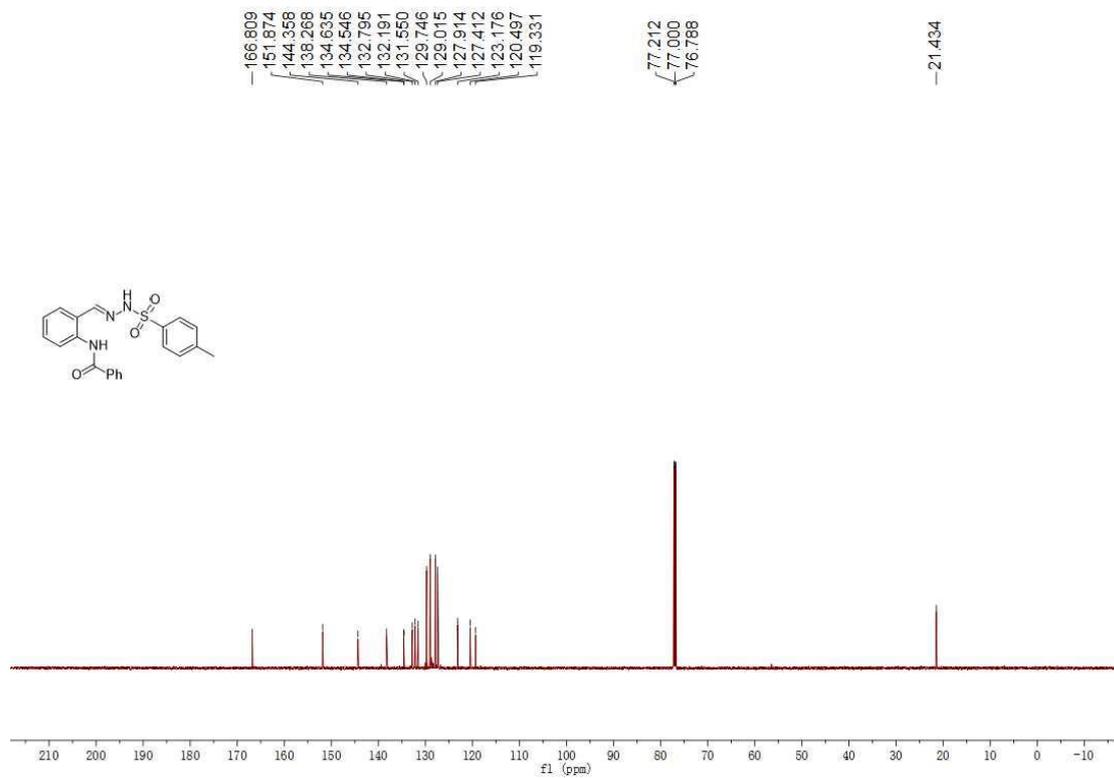
¹³C NMR (150 MHz, CDCl₃) Spectrum of **36**



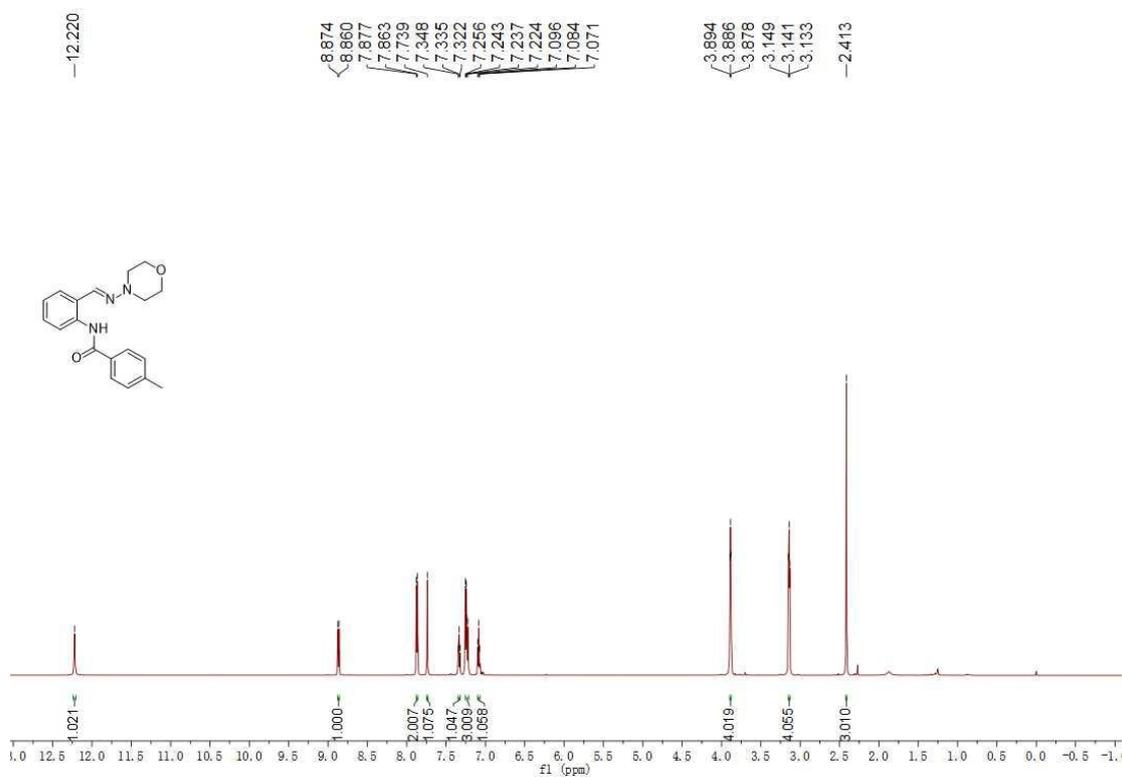
¹H NMR (600 MHz, CDCl₃) Spectrum of **38**



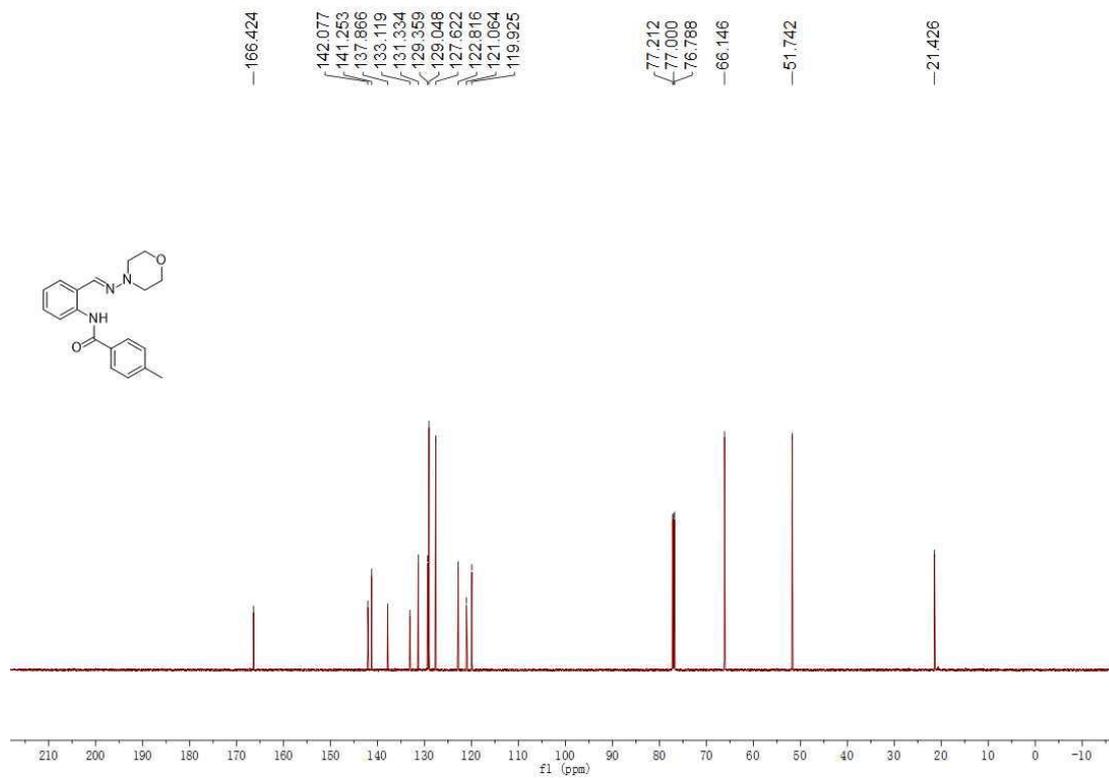
¹³C NMR (150 MHz, CDCl₃) Spectrum of **38**



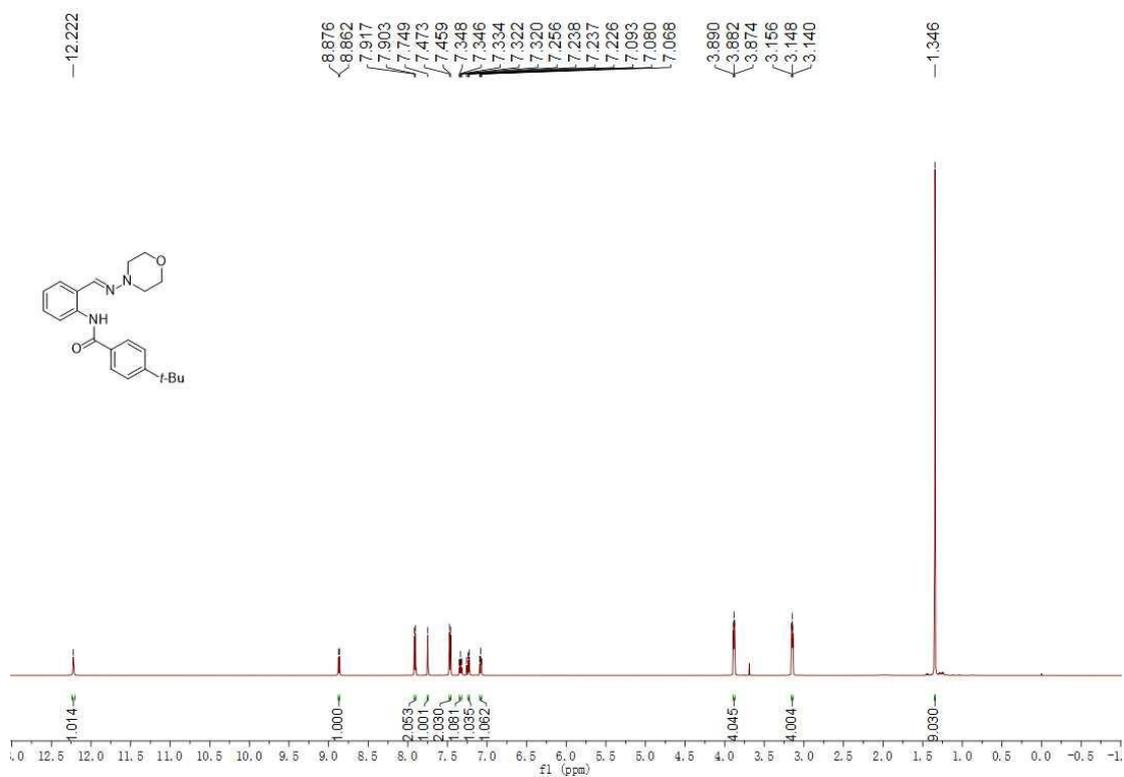
¹H NMR (600 MHz, CDCl₃) Spectrum of **39**



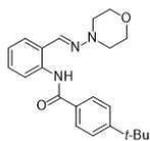
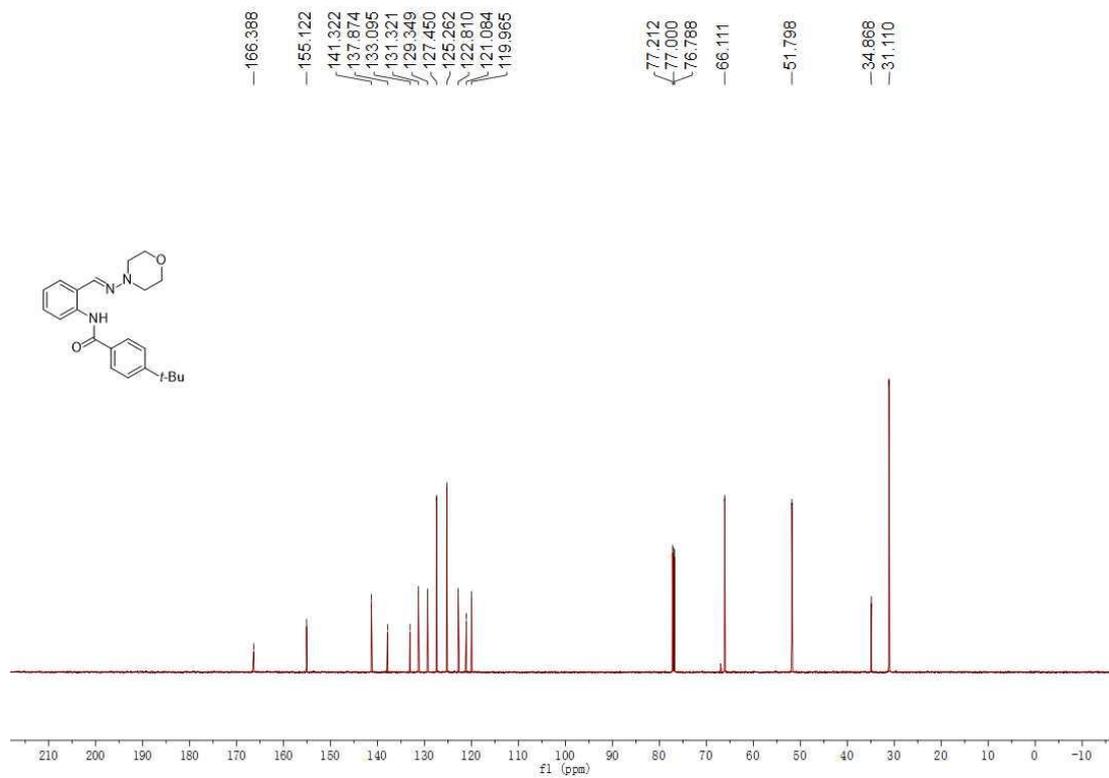
¹³C NMR (150 MHz, CDCl₃) Spectrum of **39**



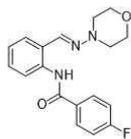
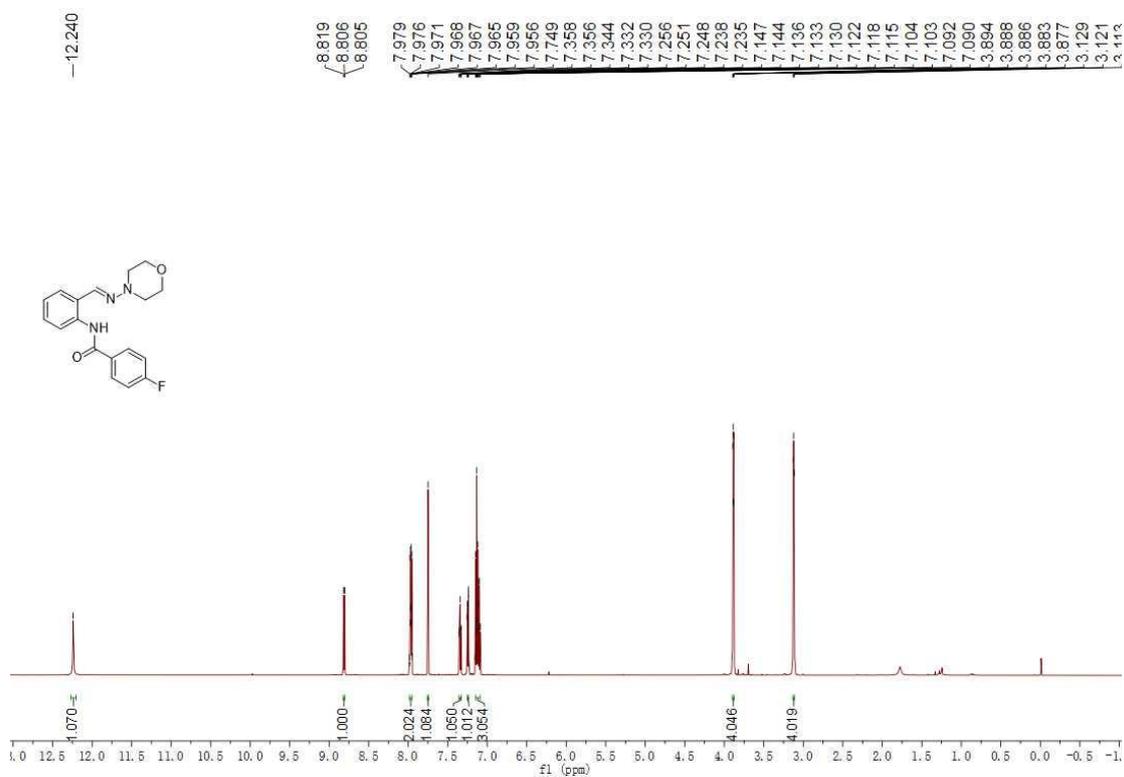
¹H NMR (600 MHz, CDCl₃) Spectrum of **40**



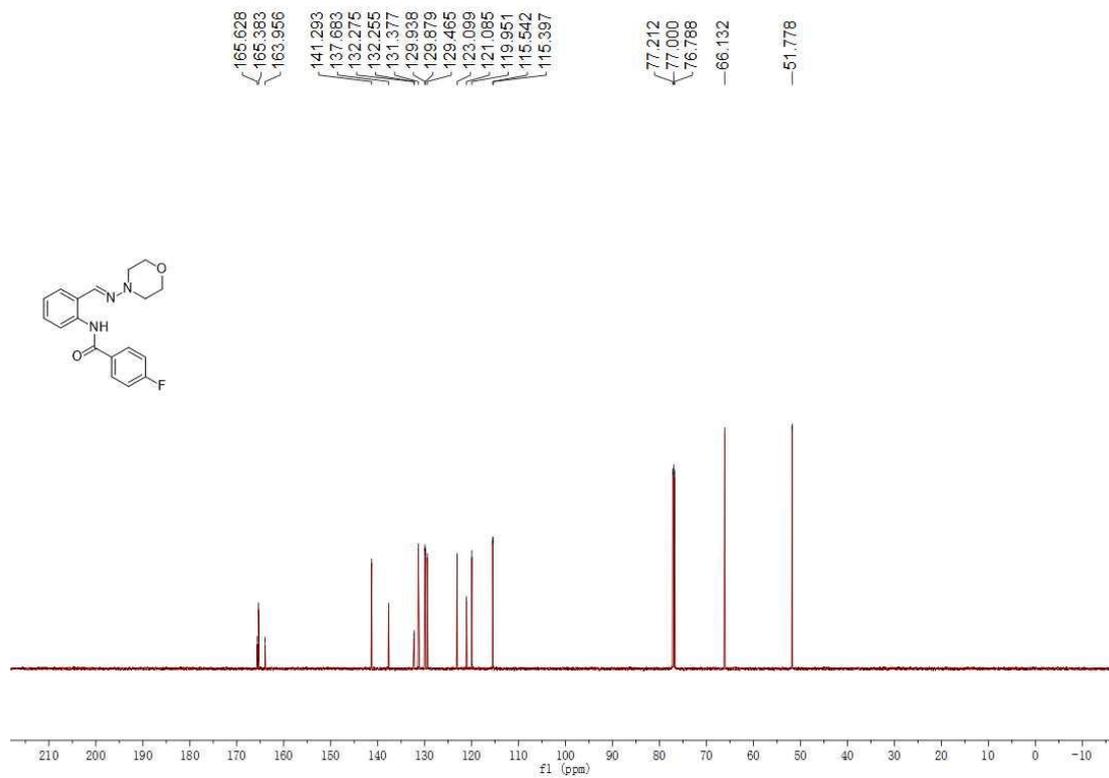
¹³C NMR (150 MHz, CDCl₃) Spectrum of **40**



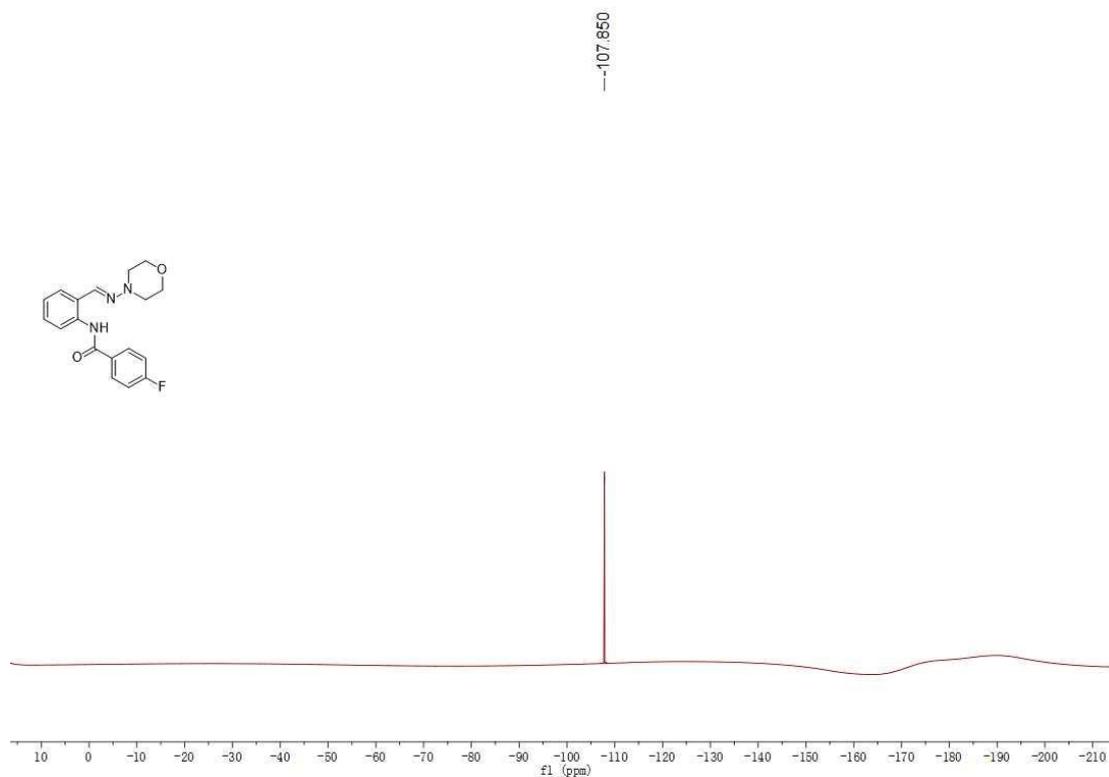
¹H NMR (600 MHz, CDCl₃) Spectrum of **41**



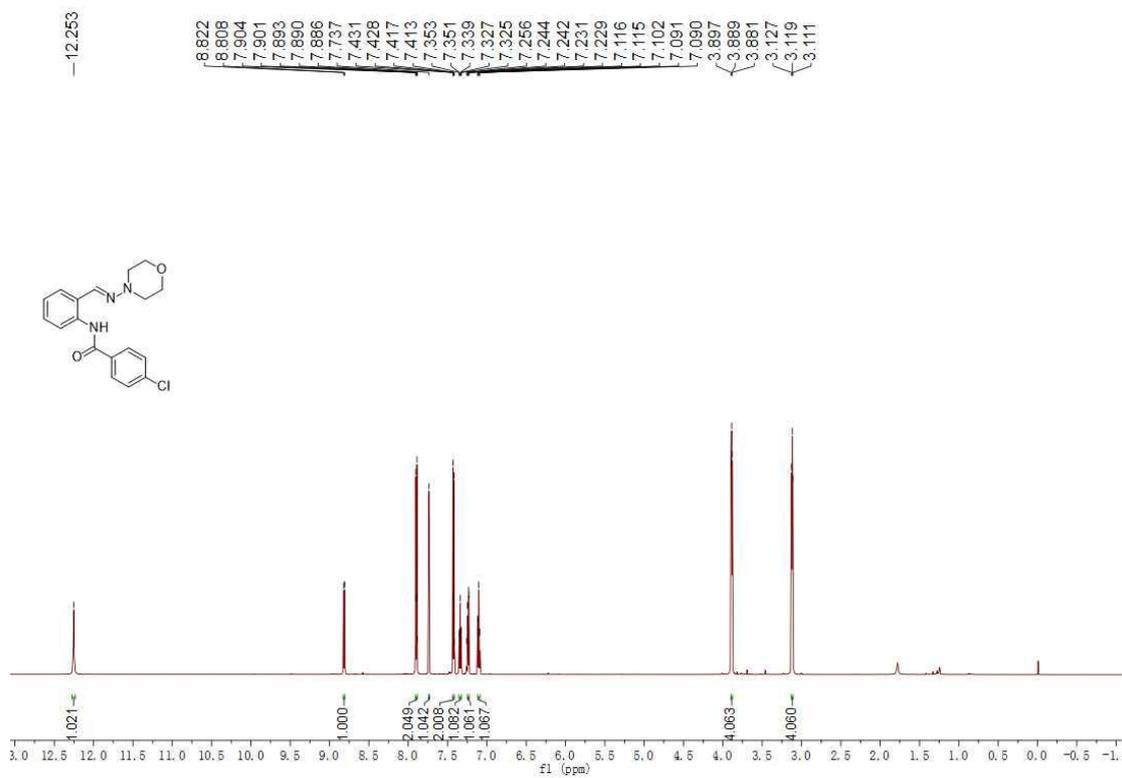
¹³C NMR (150 MHz, CDCl₃) Spectrum of **41**



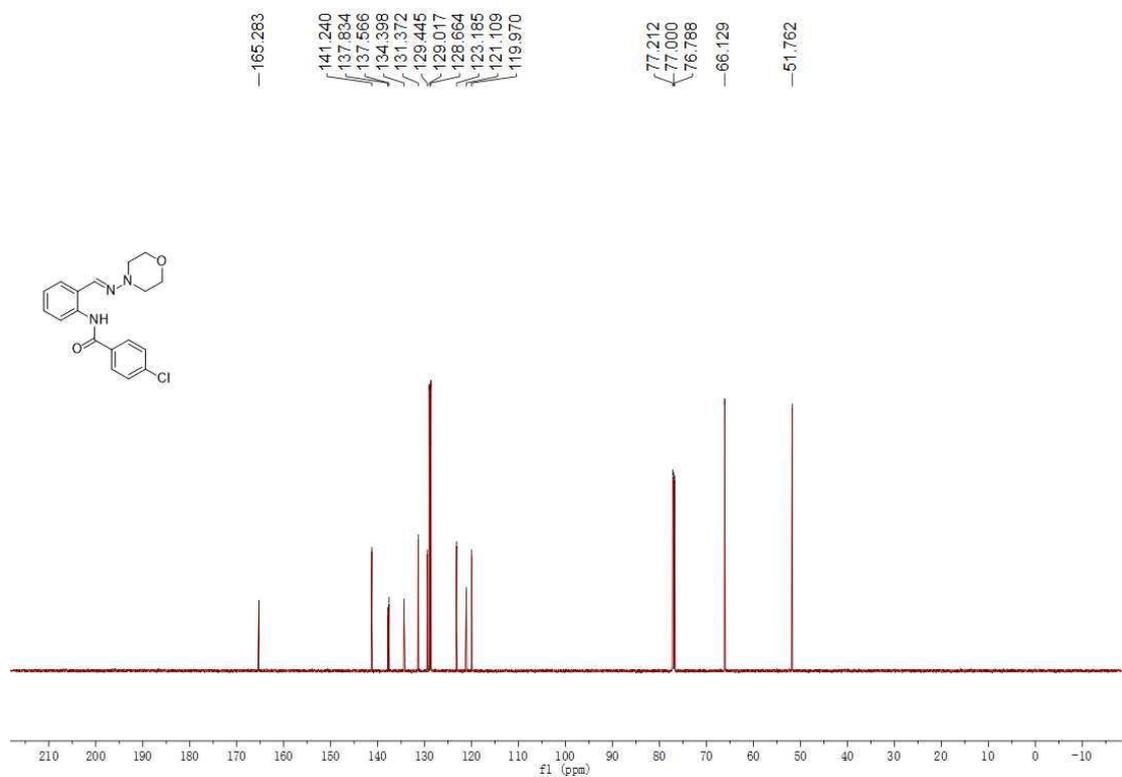
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **41**



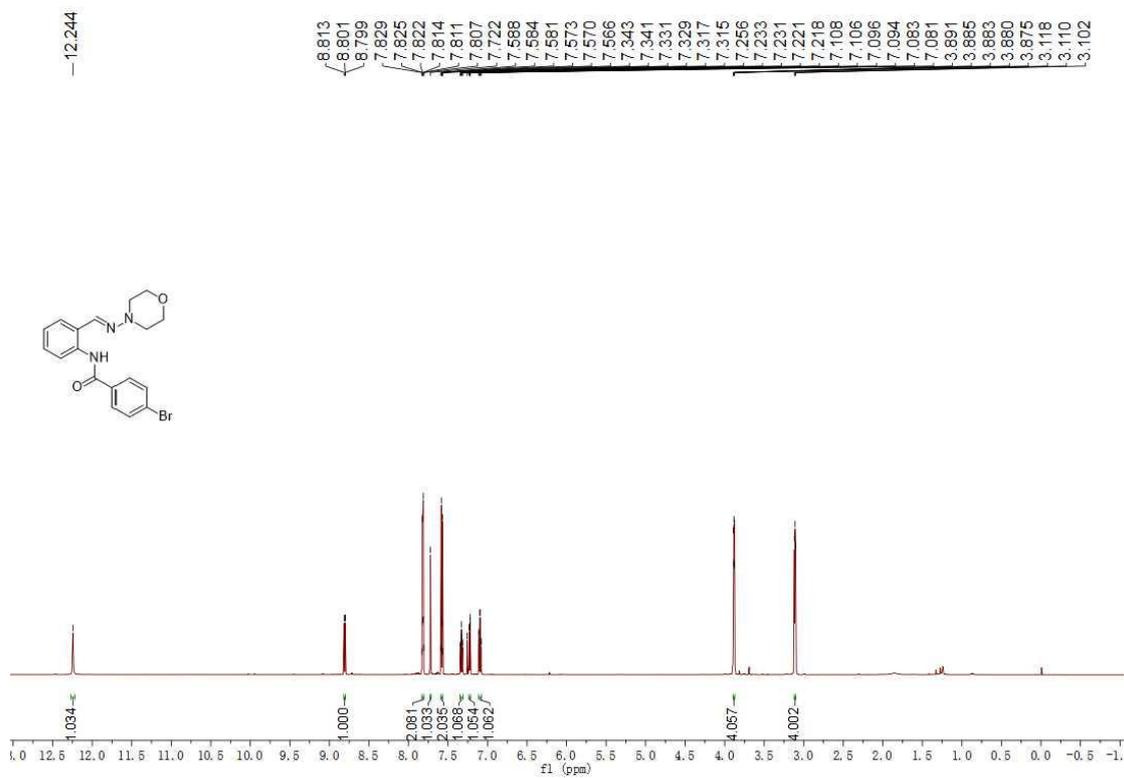
¹H NMR (600 MHz, CDCl₃) Spectrum of **42**



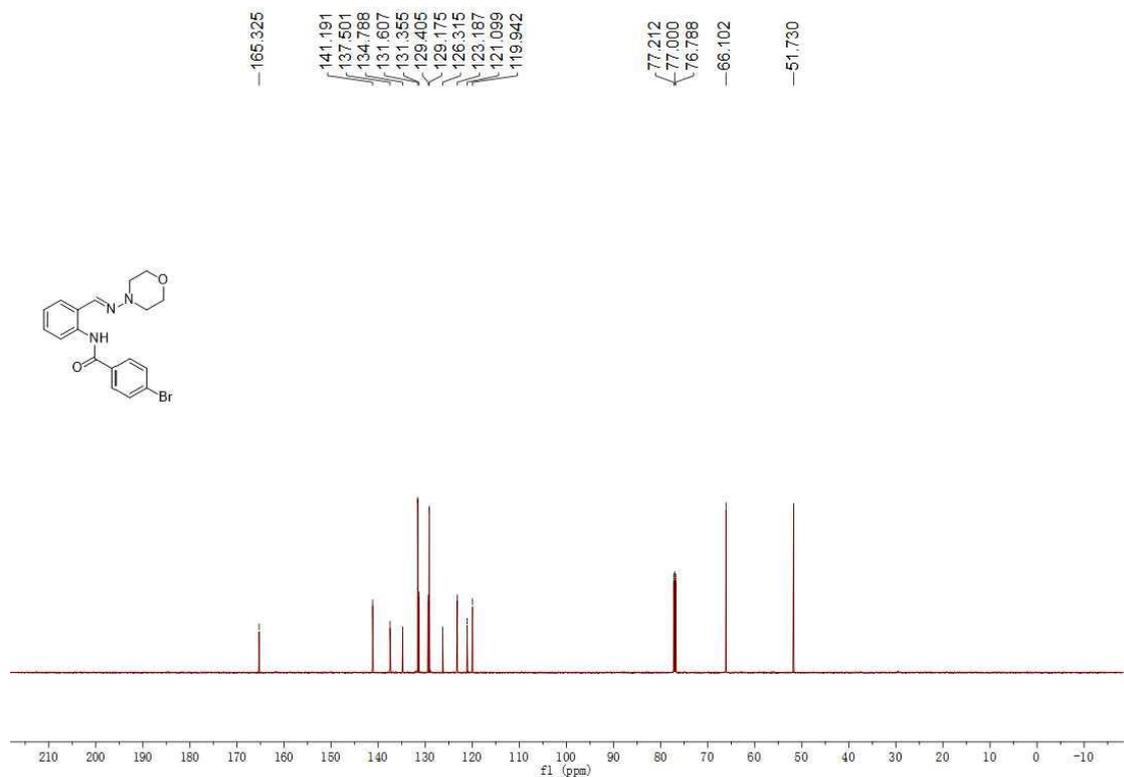
¹³C NMR (150 MHz, CDCl₃) Spectrum of **42**



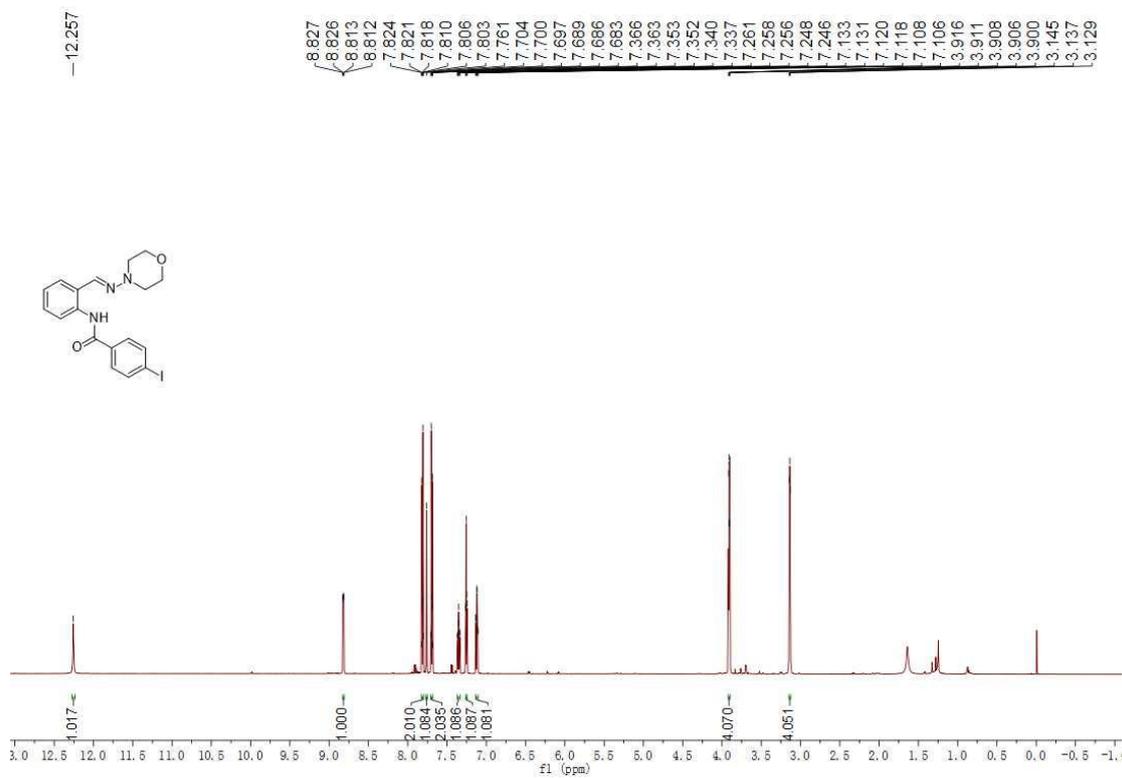
¹H NMR (600 MHz, CDCl₃) Spectrum of **43**



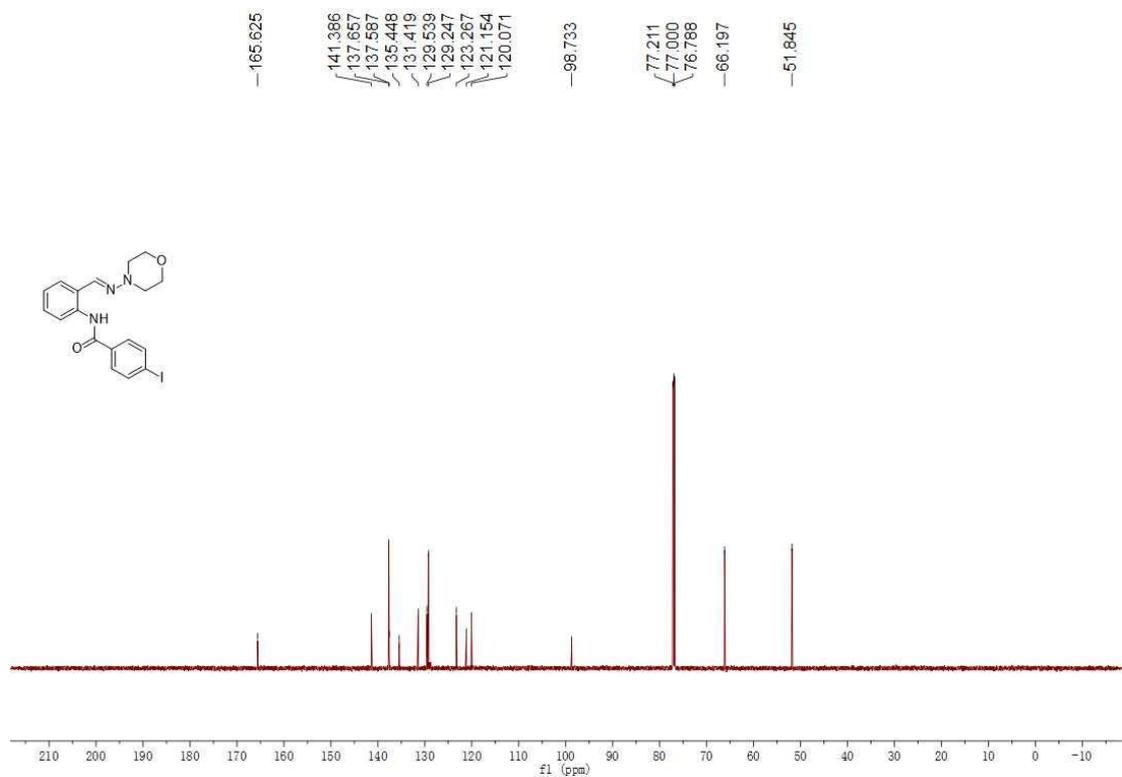
¹³C NMR (150 MHz, CDCl₃) Spectrum of **43**



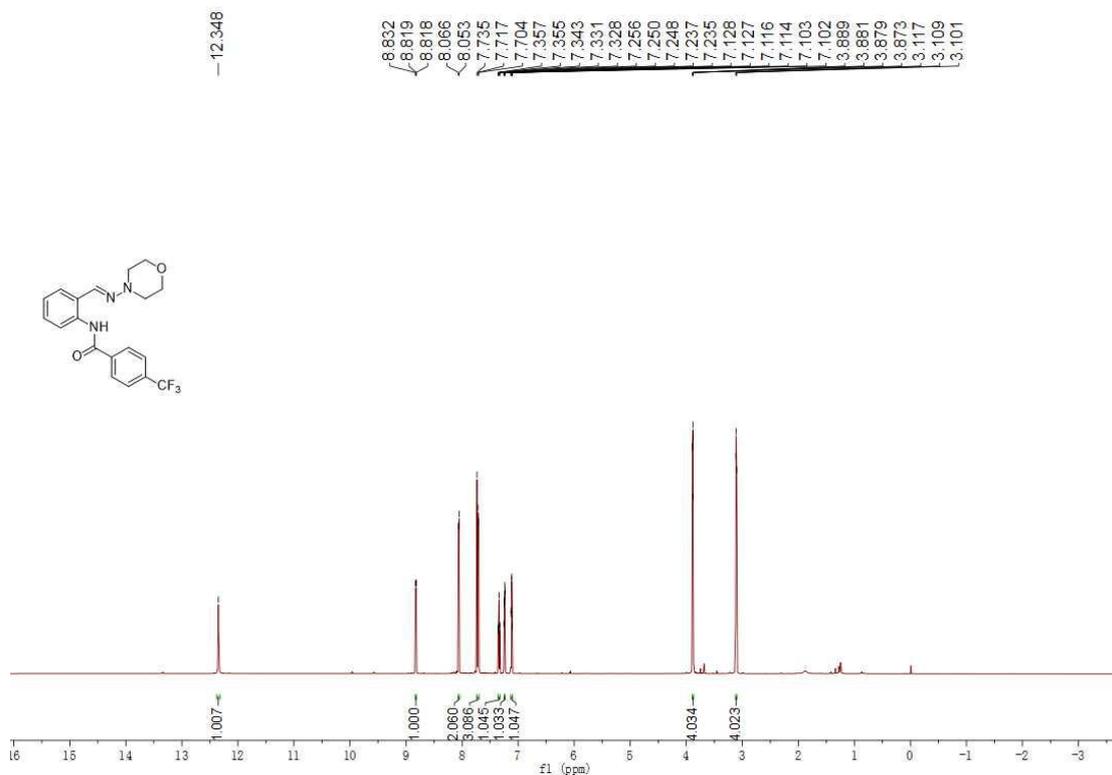
¹H NMR (600 MHz, CDCl₃) Spectrum of **44**



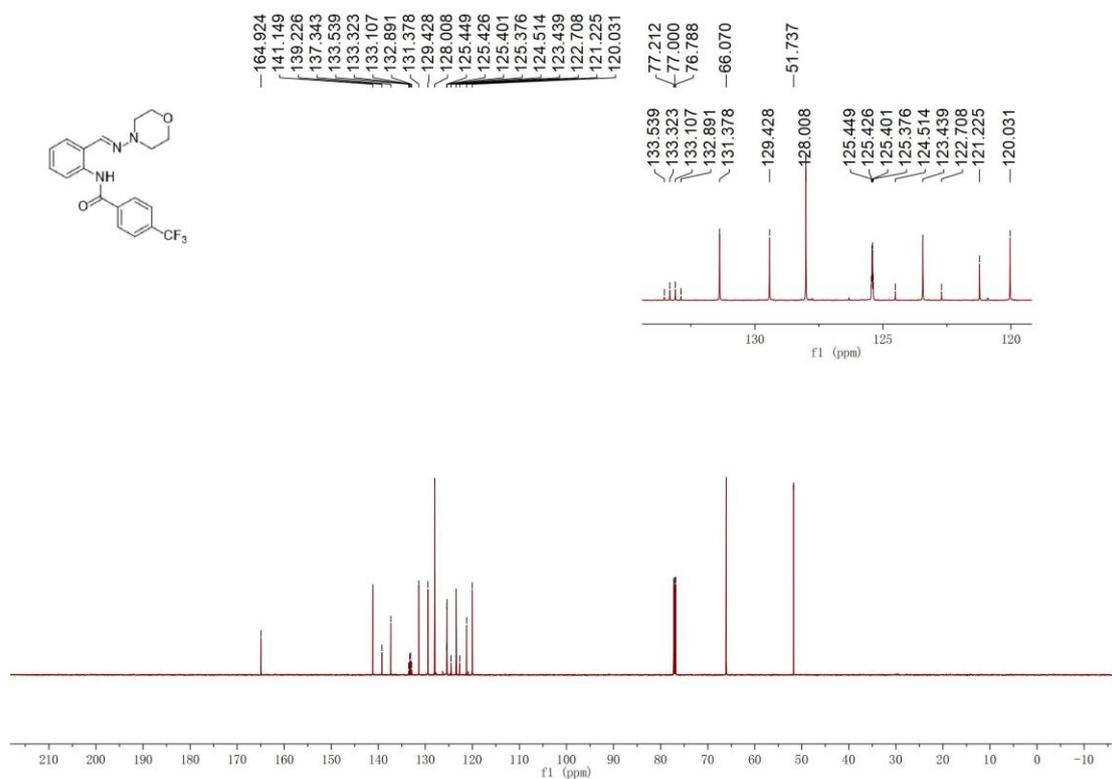
¹³C NMR (150 MHz, CDCl₃) Spectrum of **44**



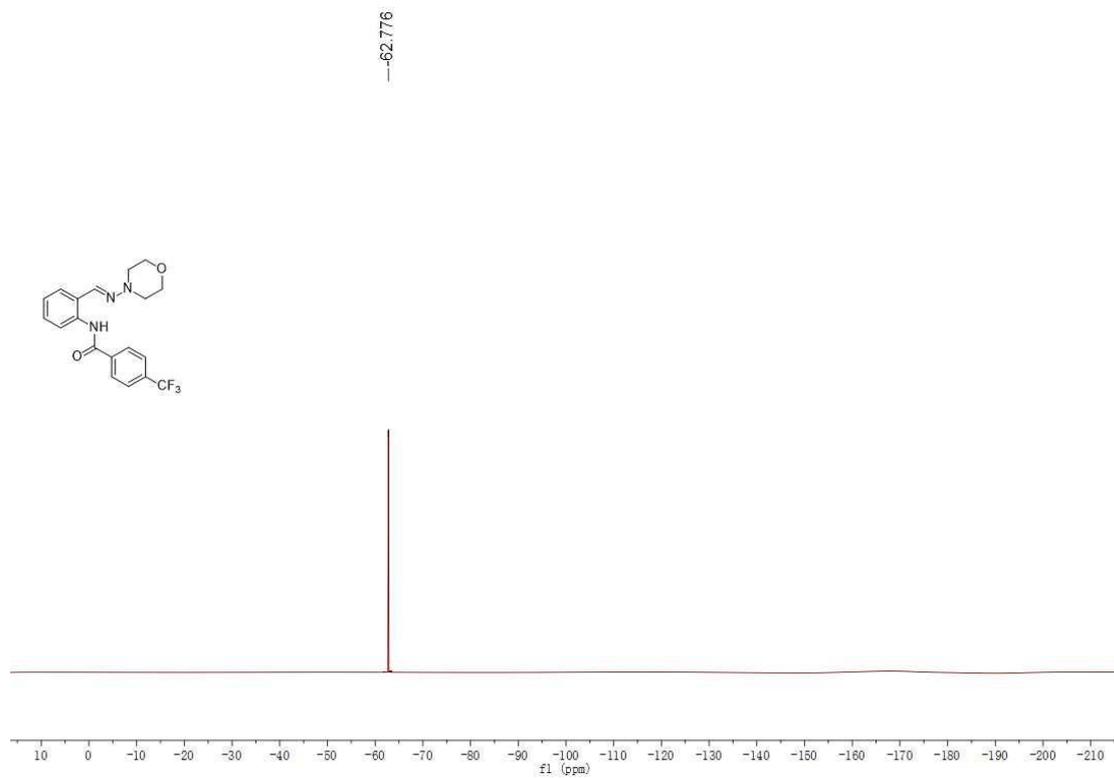
¹H NMR (600 MHz, CDCl₃) Spectrum of **45**



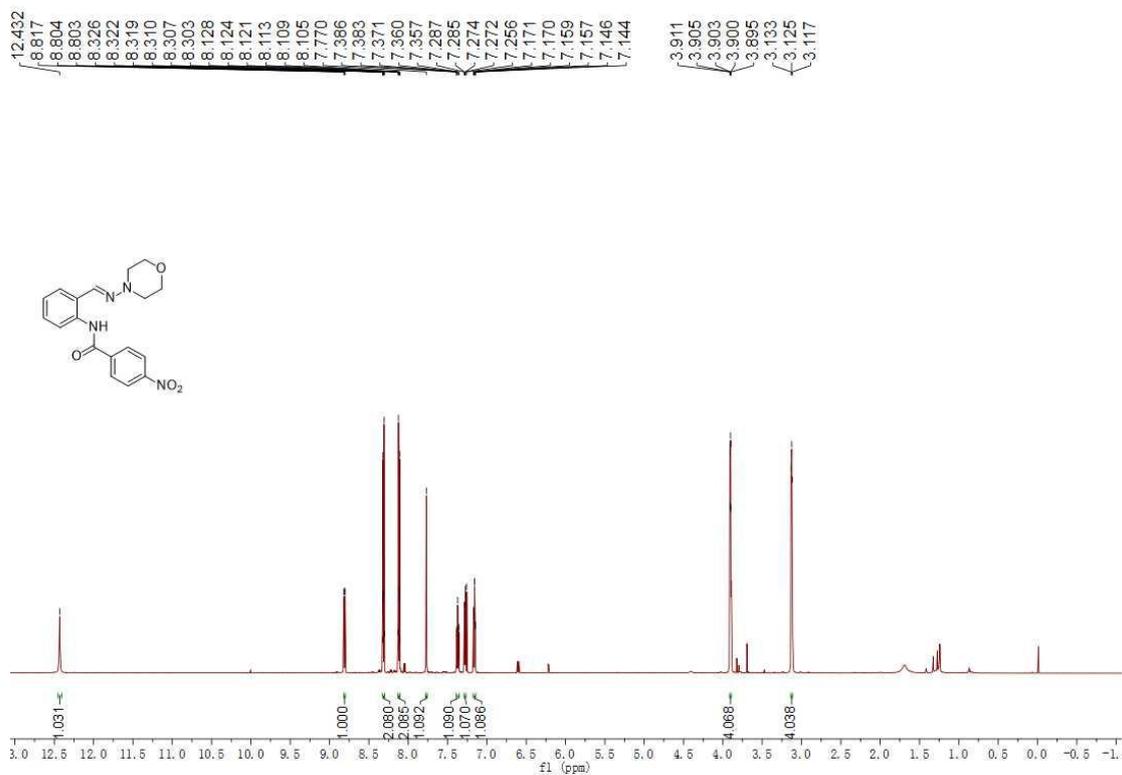
¹³C NMR (150 MHz, CDCl₃) Spectrum of **45**



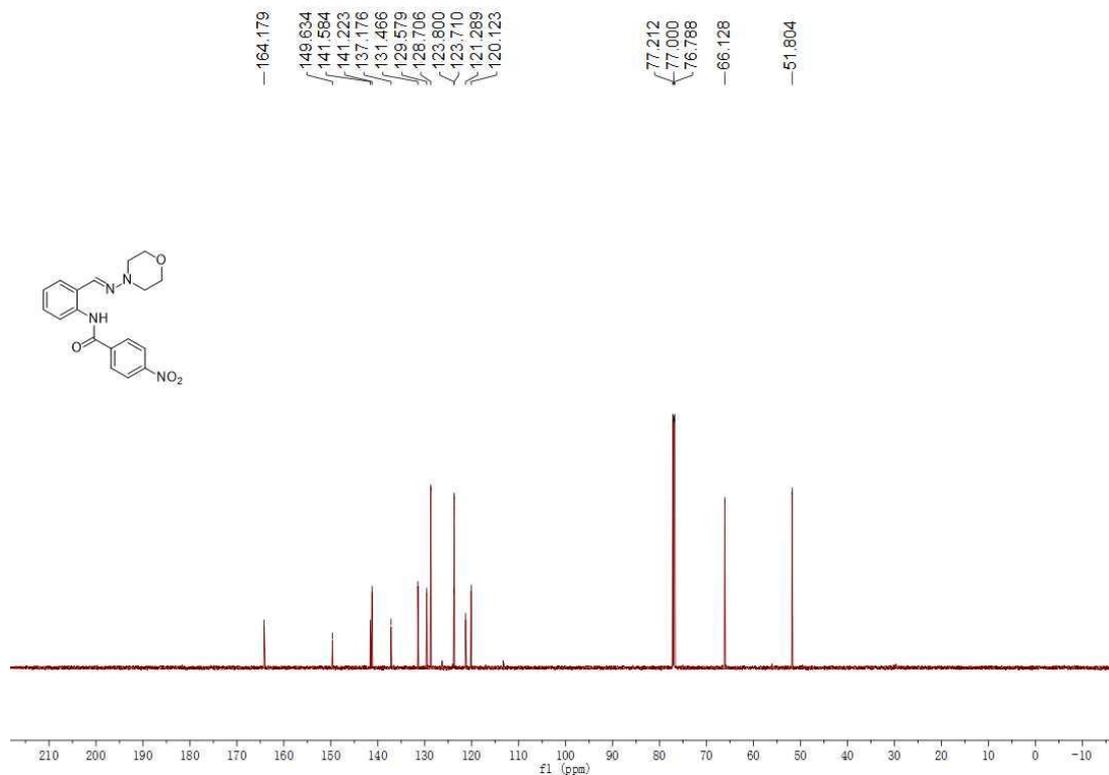
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **45**



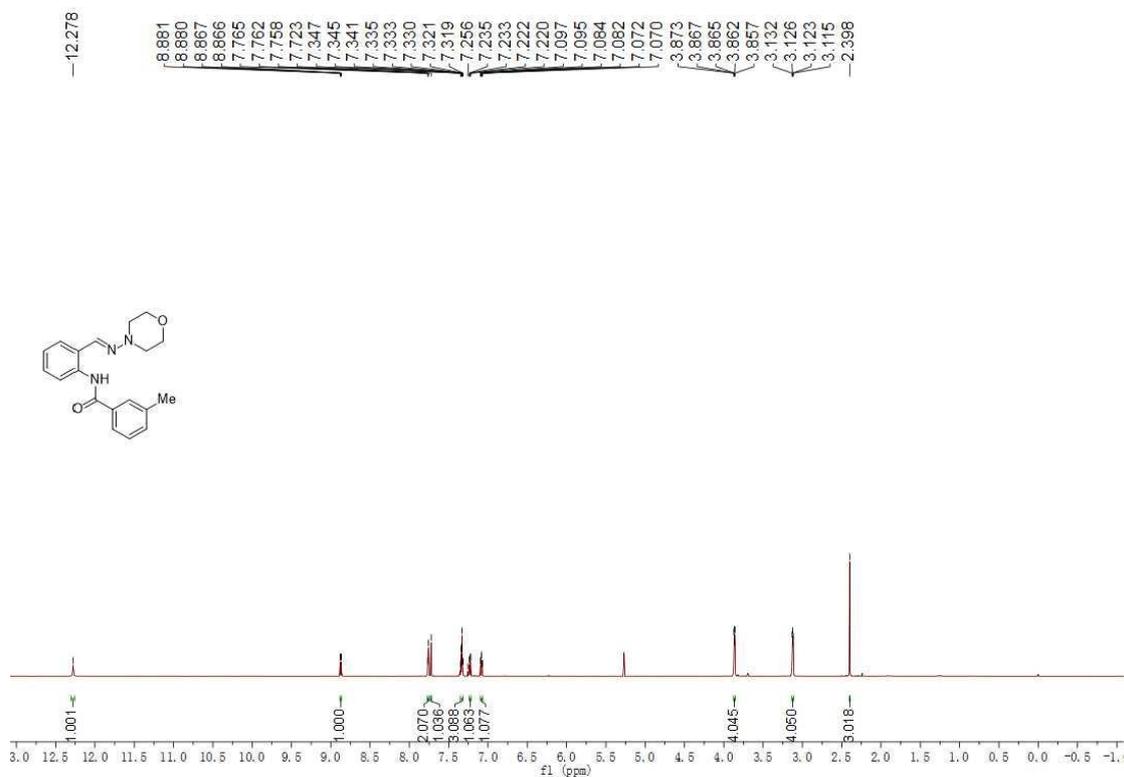
¹H NMR (600 MHz, CDCl₃) Spectrum of **46**



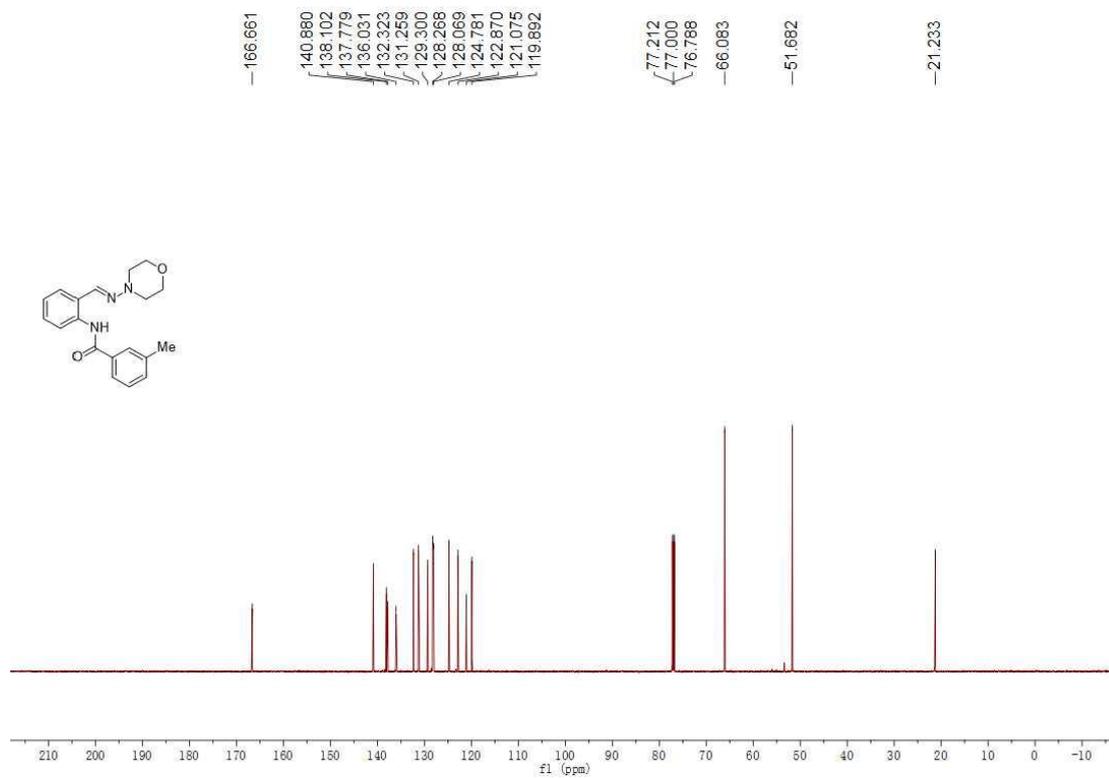
¹³C NMR (150 MHz, CDCl₃) Spectrum of **46**



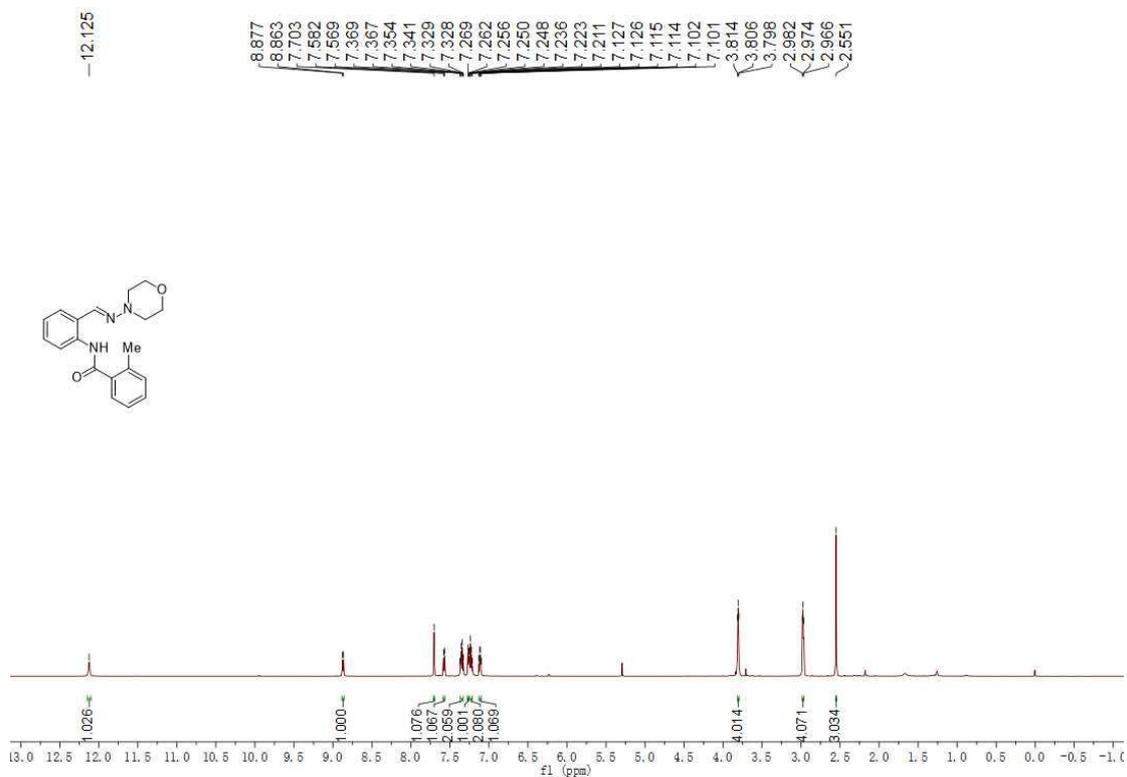
¹H NMR (600 MHz, CDCl₃) Spectrum of **47**



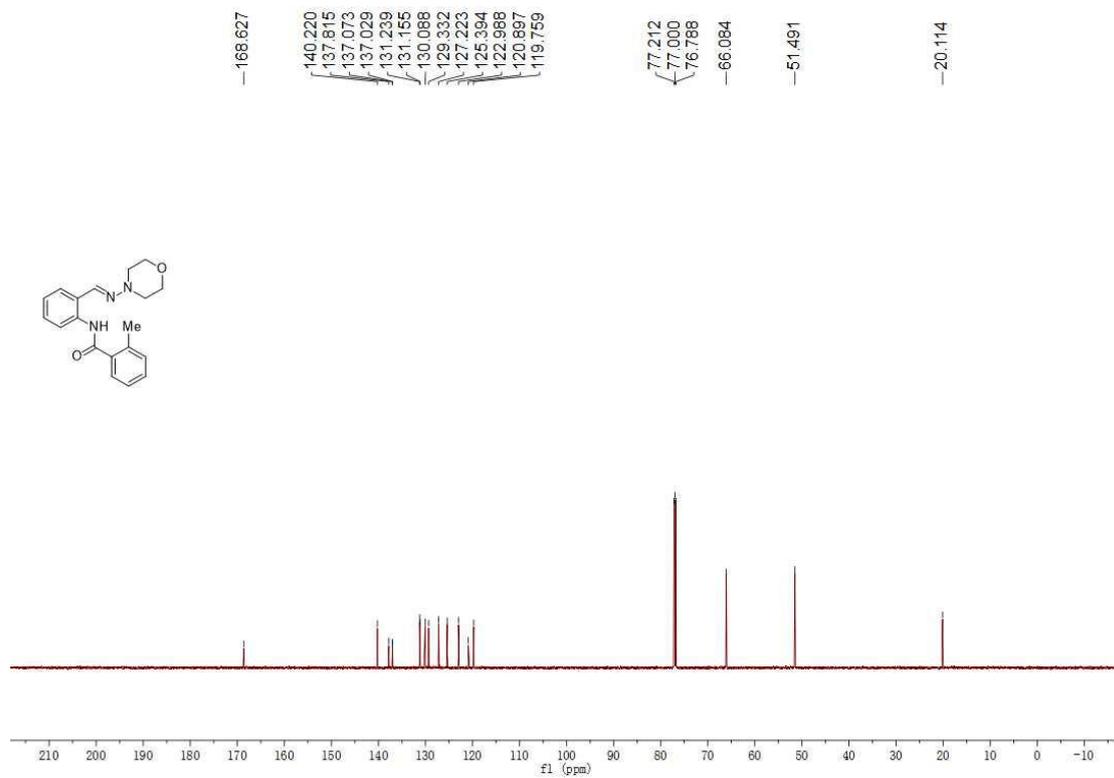
¹³C NMR (150 MHz, CDCl₃) Spectrum of **47**



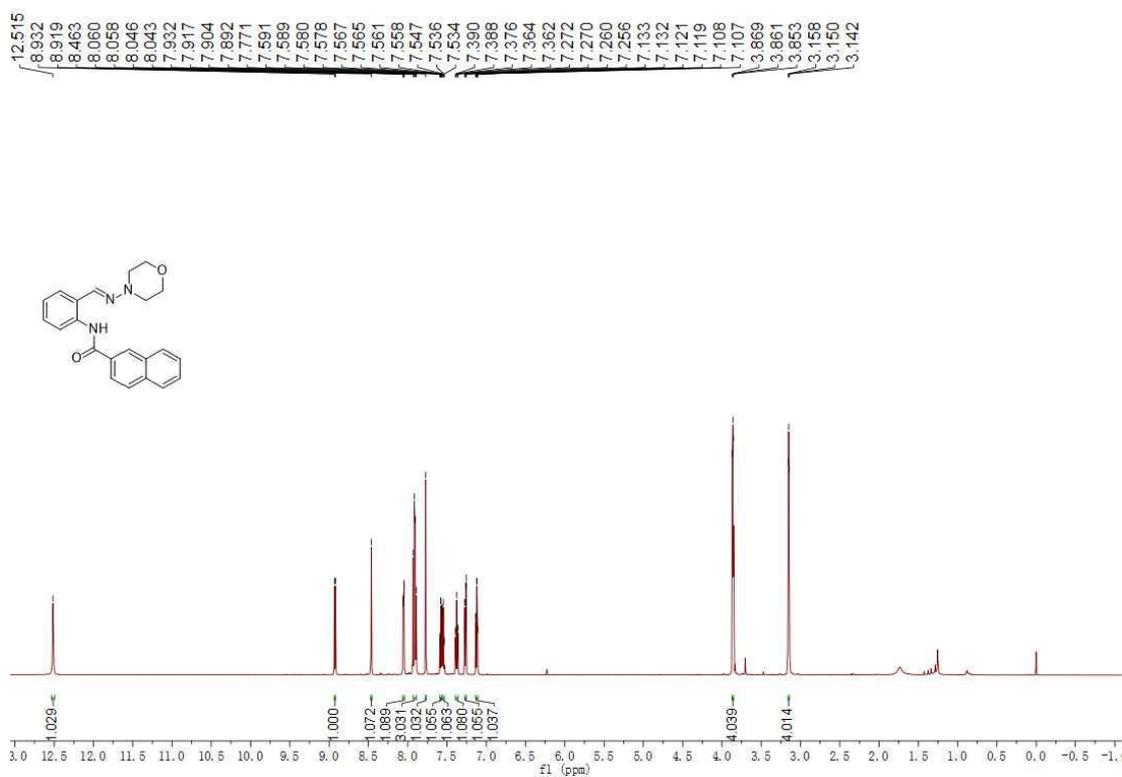
¹H NMR (600 MHz, CDCl₃) Spectrum of **48**



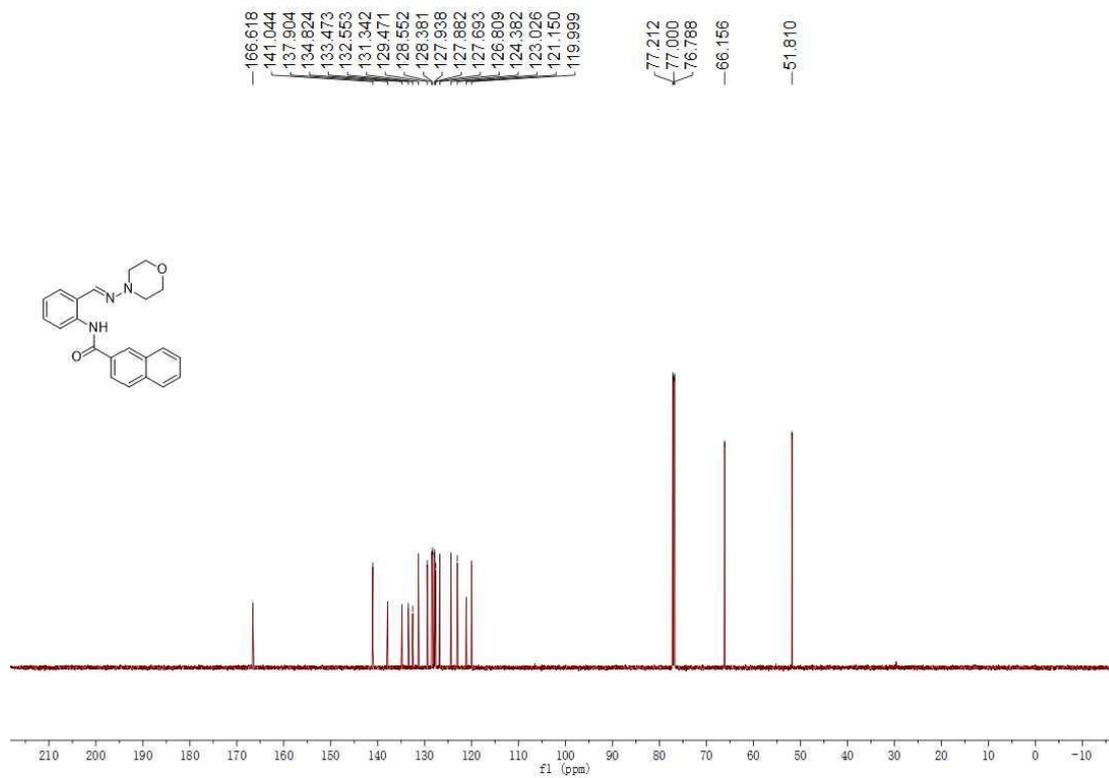
¹³C NMR (150 MHz, CDCl₃) Spectrum of **48**



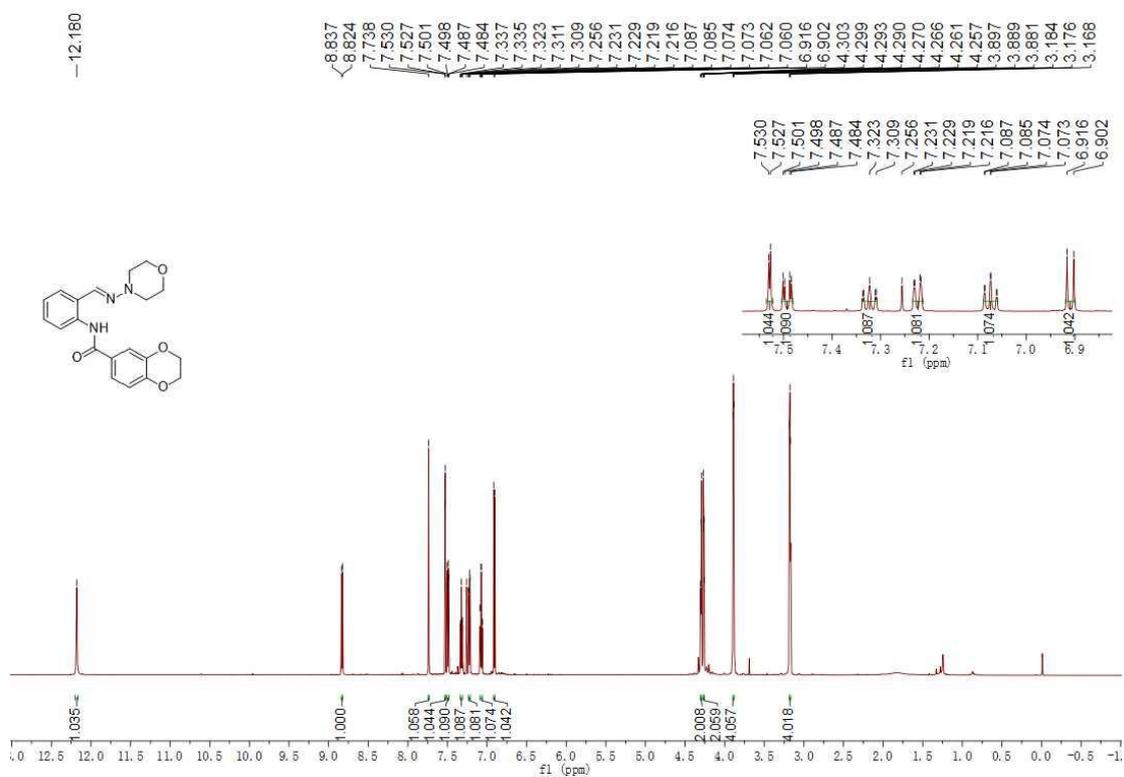
¹H NMR (600 MHz, CDCl₃) Spectrum of **49**



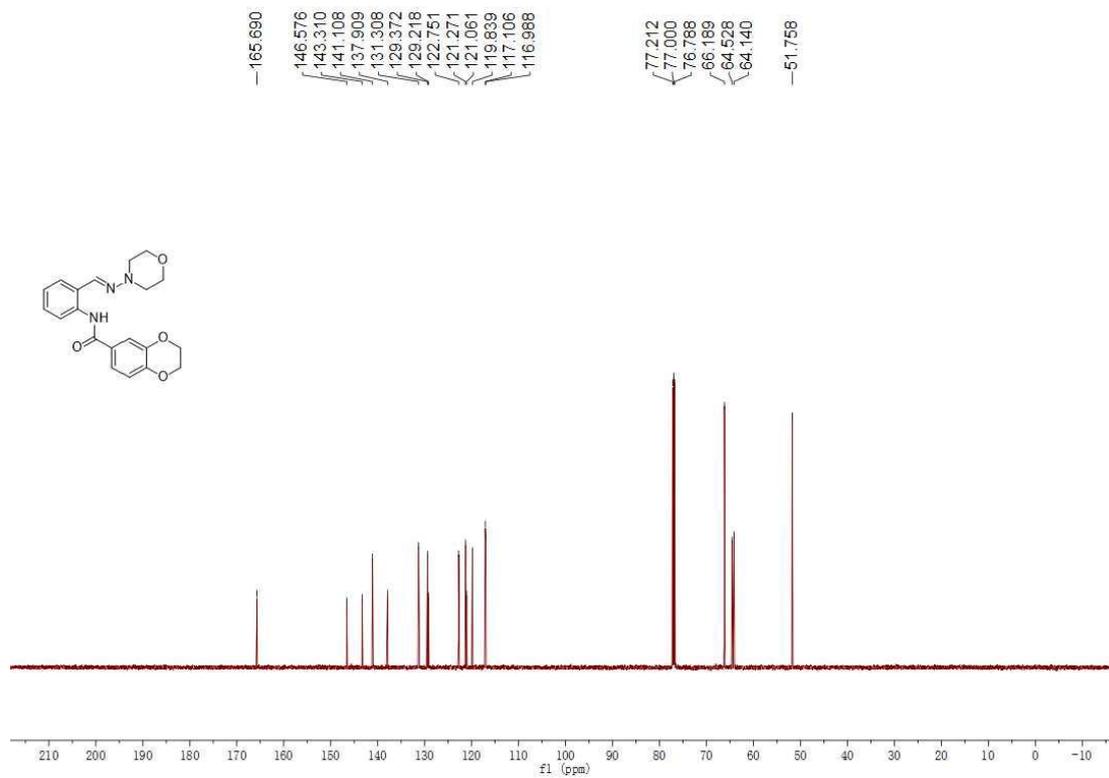
¹³C NMR (150 MHz, CDCl₃) Spectrum of **49**



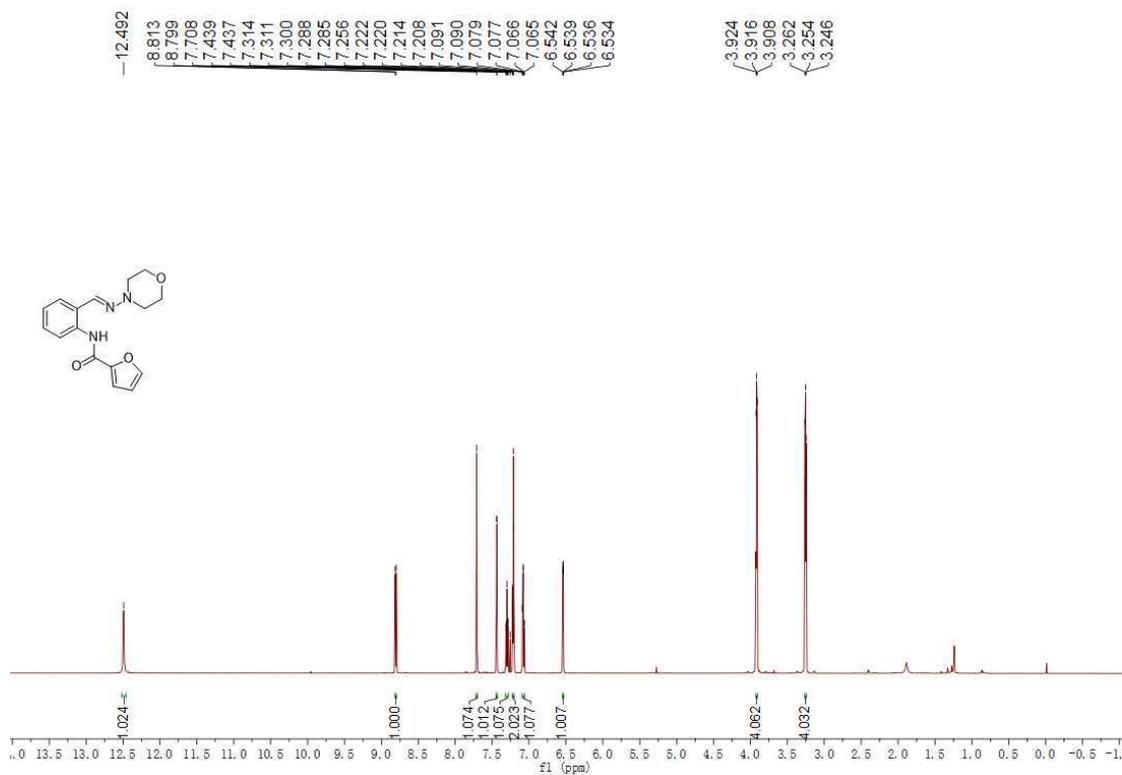
¹H NMR (600 MHz, CDCl₃) Spectrum of **50**



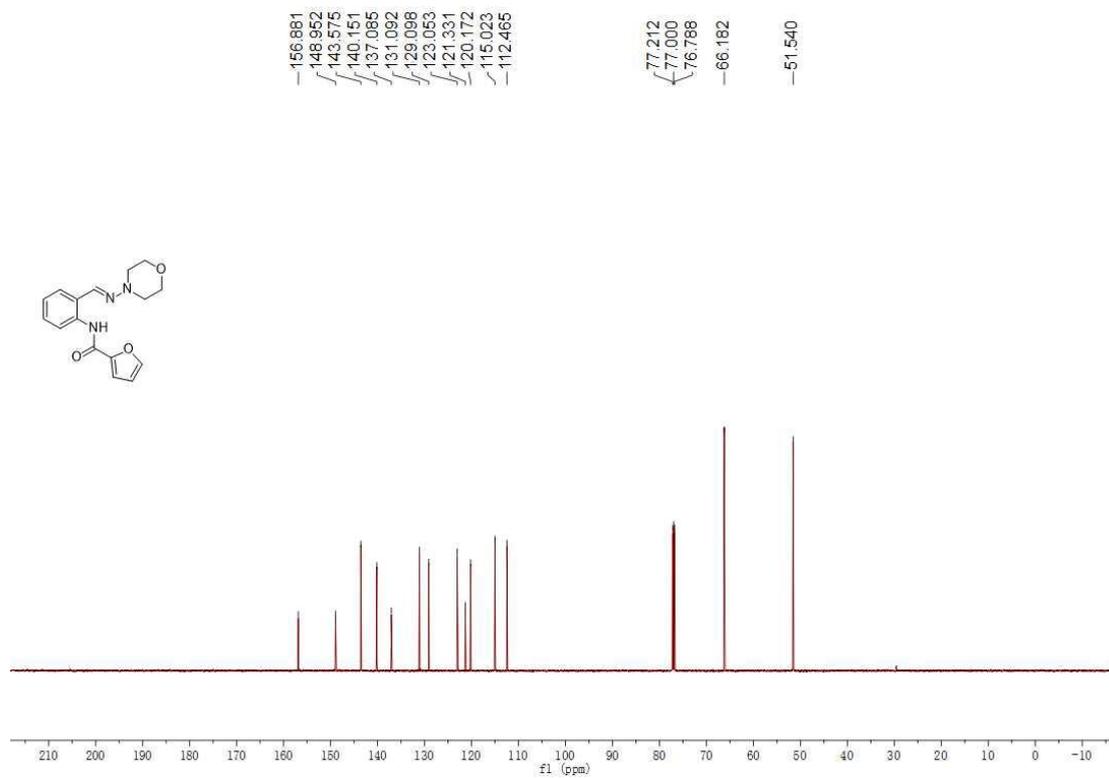
¹³C NMR (150 MHz, CDCl₃) Spectrum of **50**



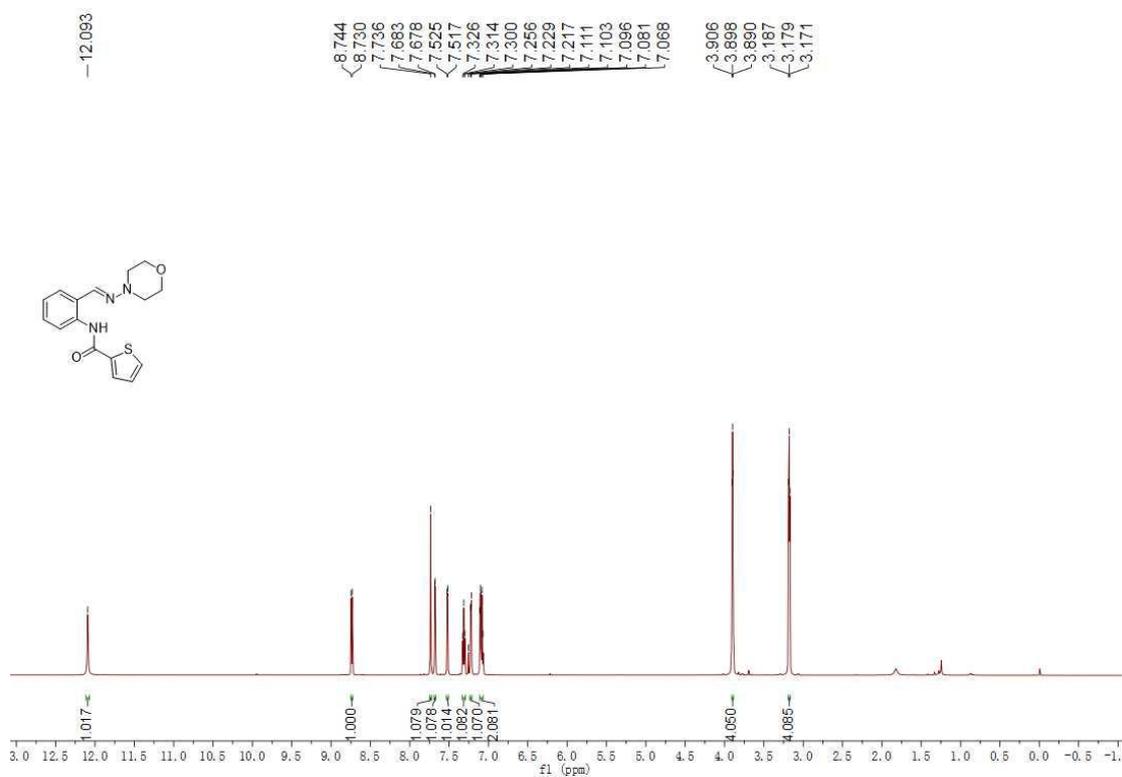
¹H NMR (600 MHz, CDCl₃) Spectrum of **51**



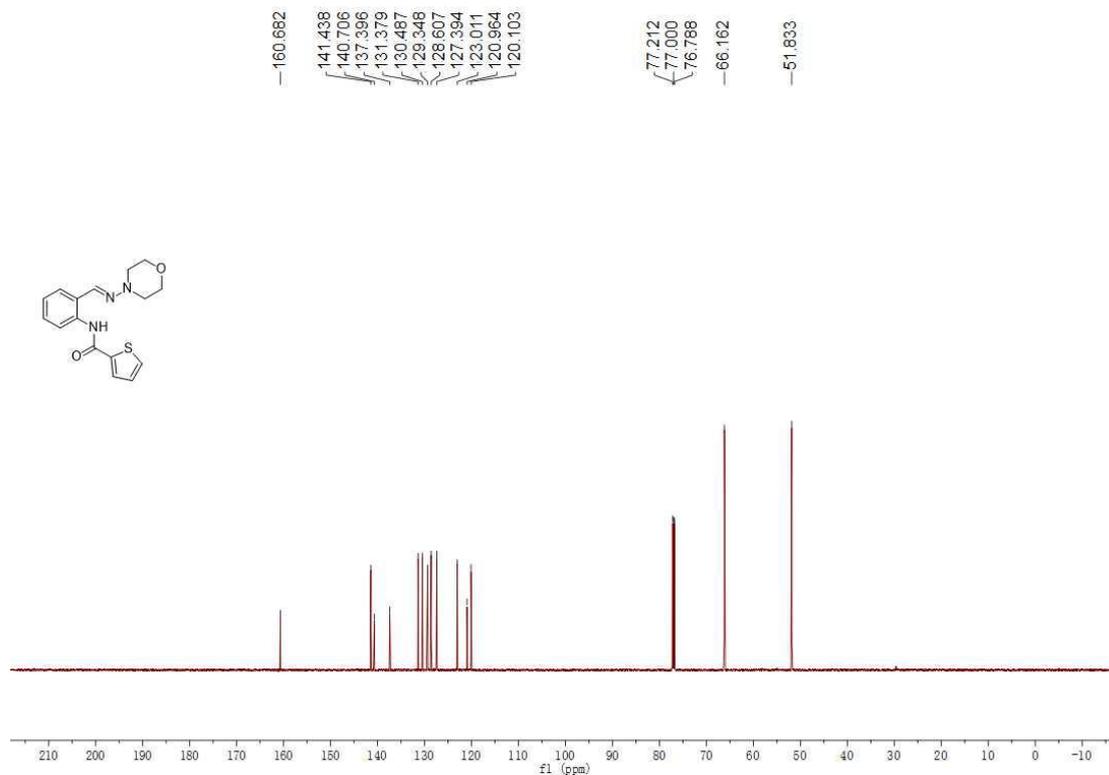
¹³C NMR (150 MHz, CDCl₃) Spectrum of **51**



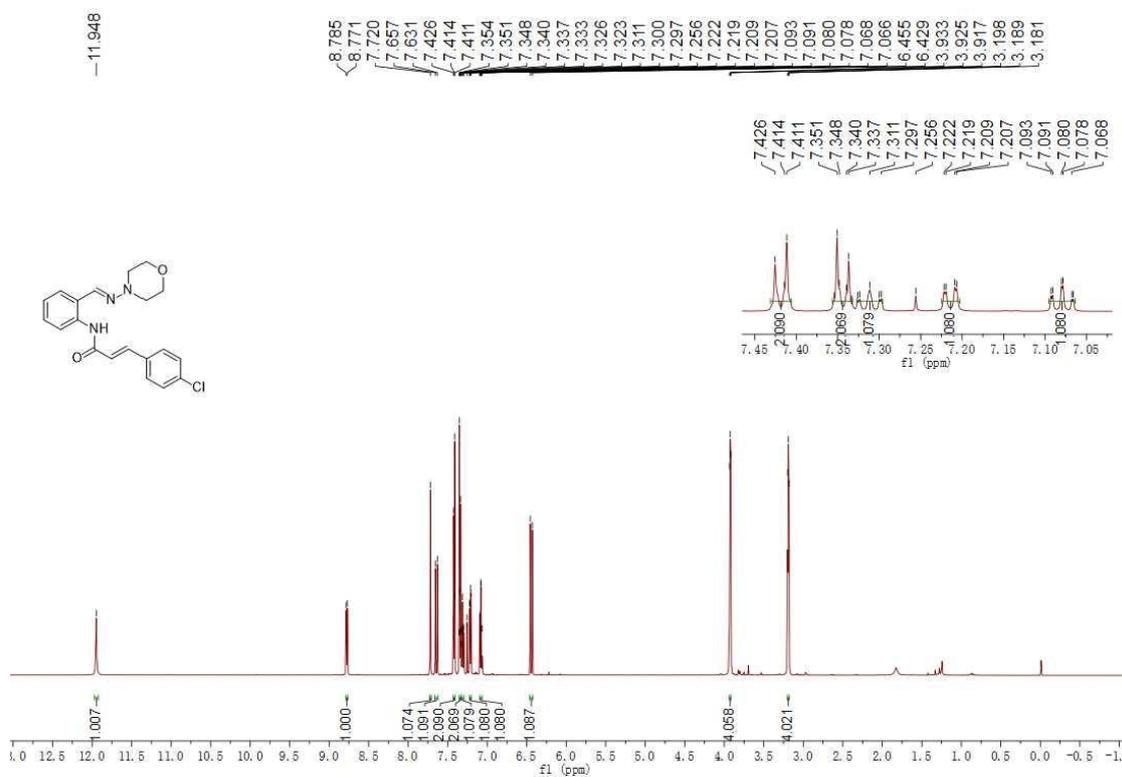
¹H NMR (600 MHz, CDCl₃) Spectrum of **52**



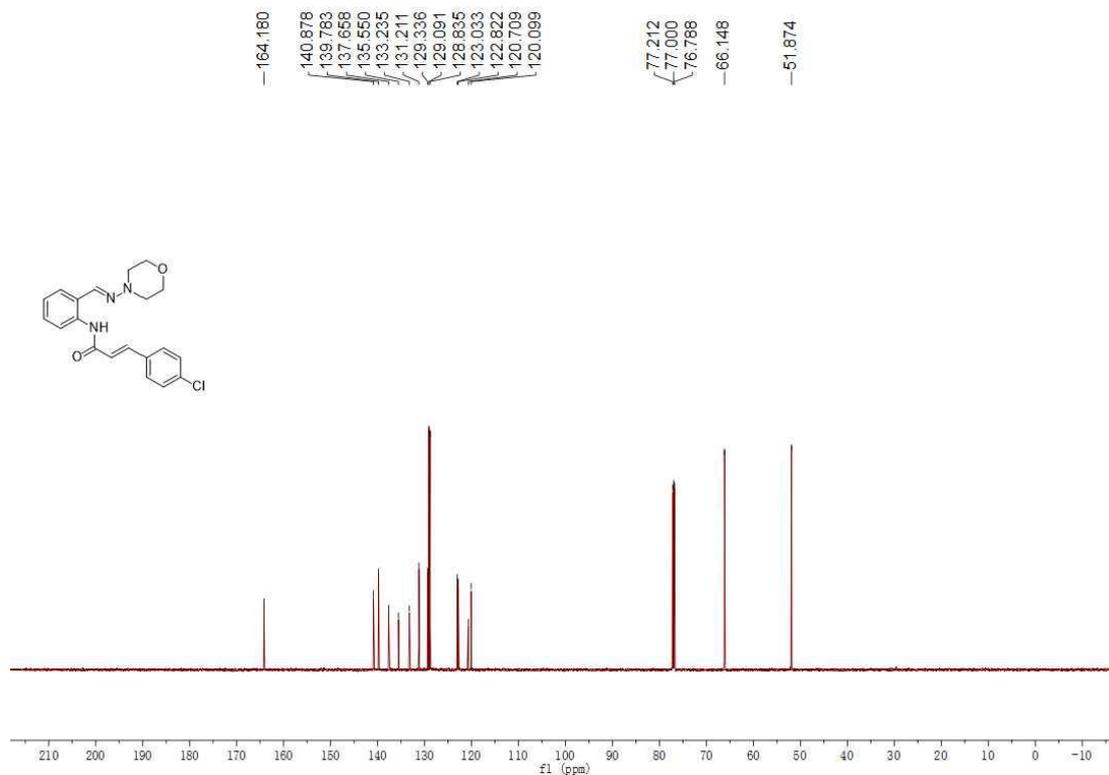
¹³C NMR (150 MHz, CDCl₃) Spectrum of **52**



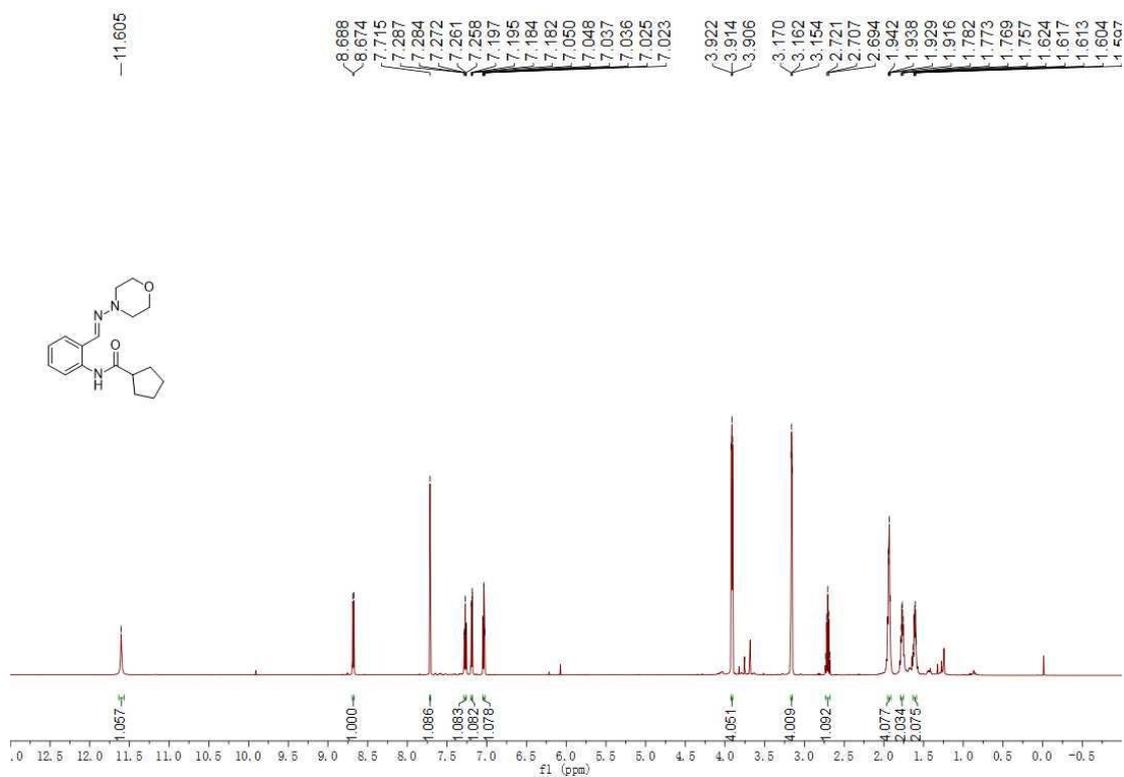
¹H NMR (600 MHz, CDCl₃) Spectrum of **53**



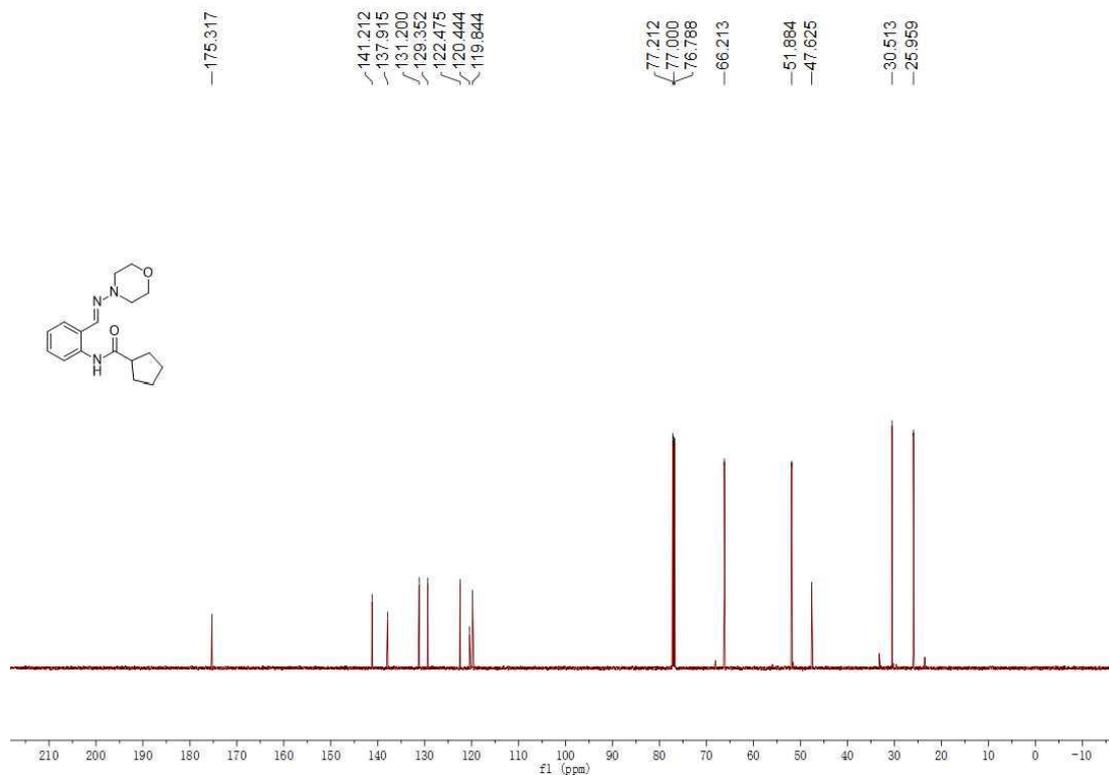
¹³C NMR (150 MHz, CDCl₃) Spectrum of **53**



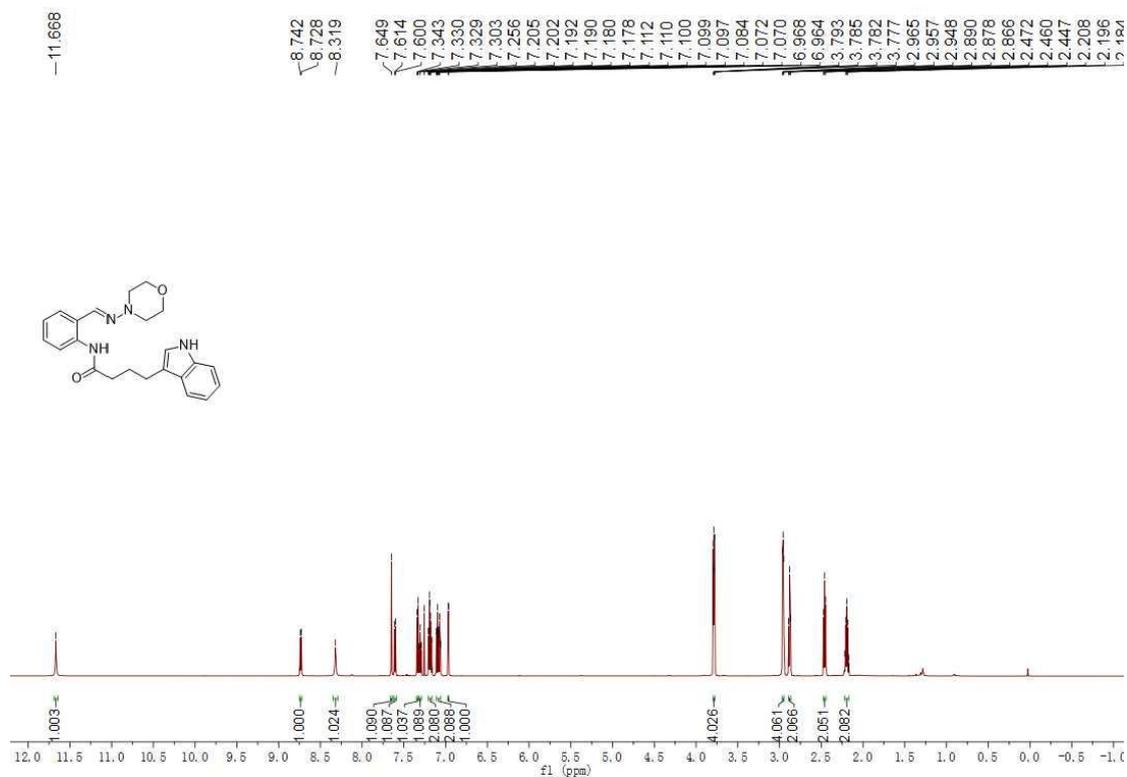
¹H NMR (600 MHz, CDCl₃) Spectrum of **54**



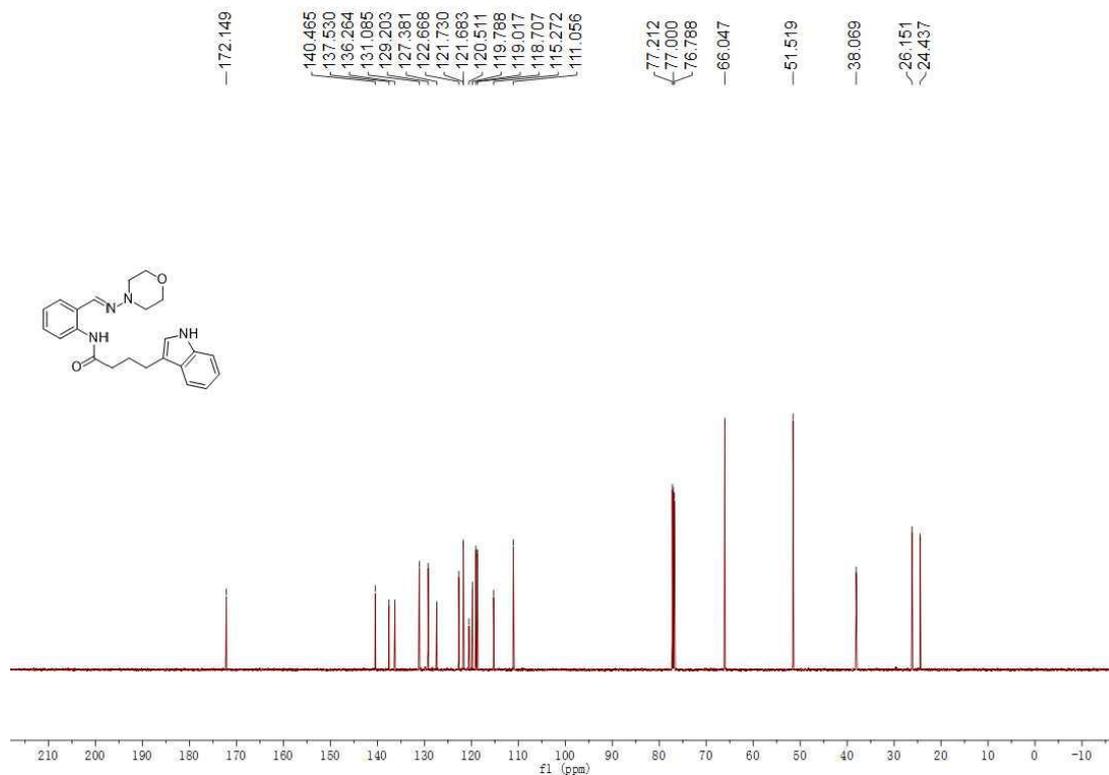
¹³C NMR (150 MHz, CDCl₃) Spectrum of **54**



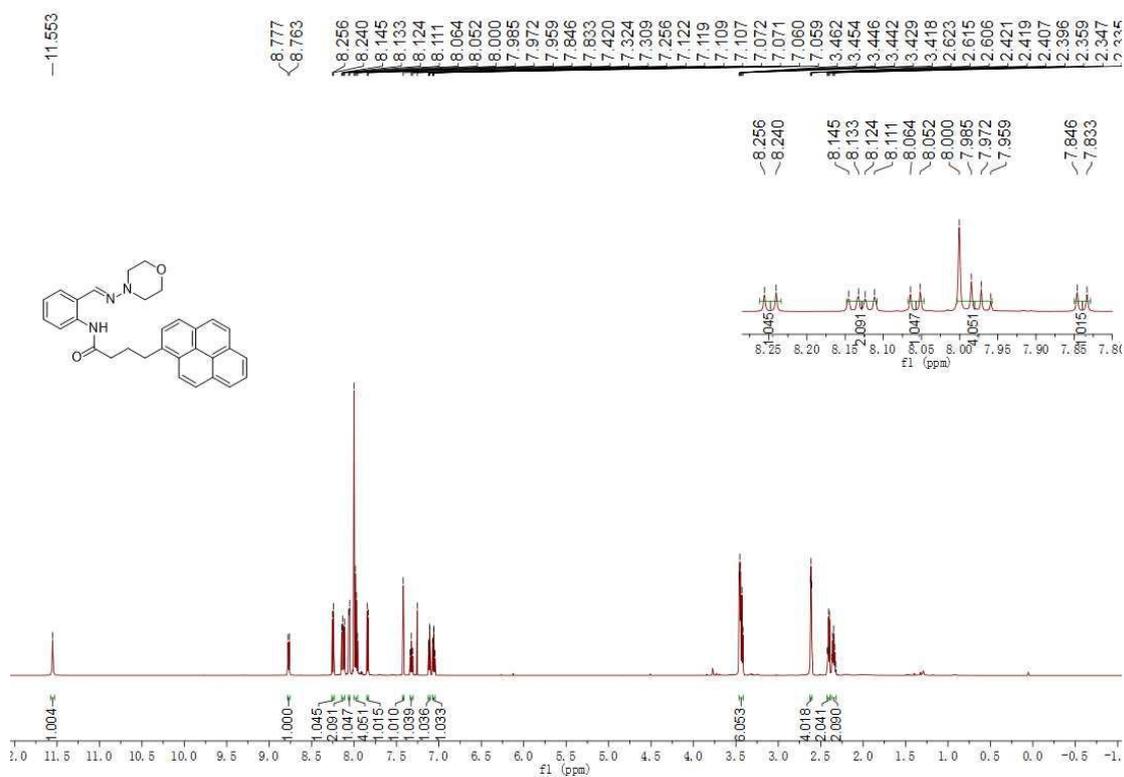
¹H NMR (600 MHz, CDCl₃) Spectrum of **56**



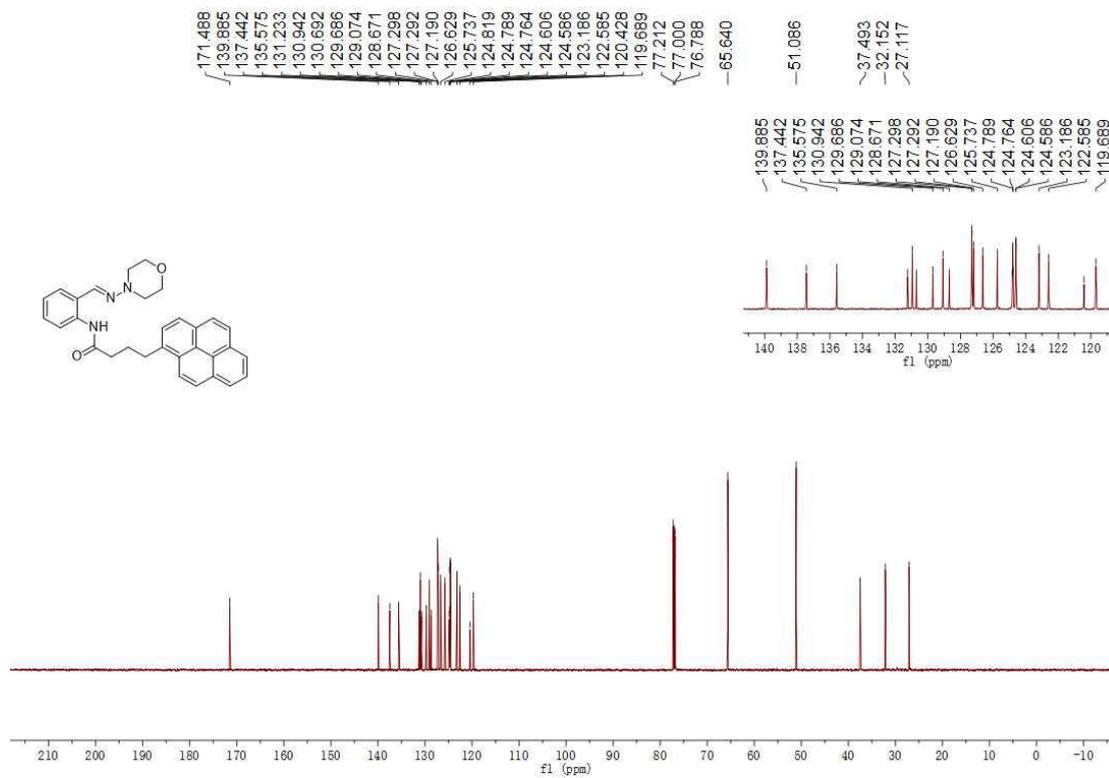
¹³C NMR (150 MHz, CDCl₃) Spectrum of **56**



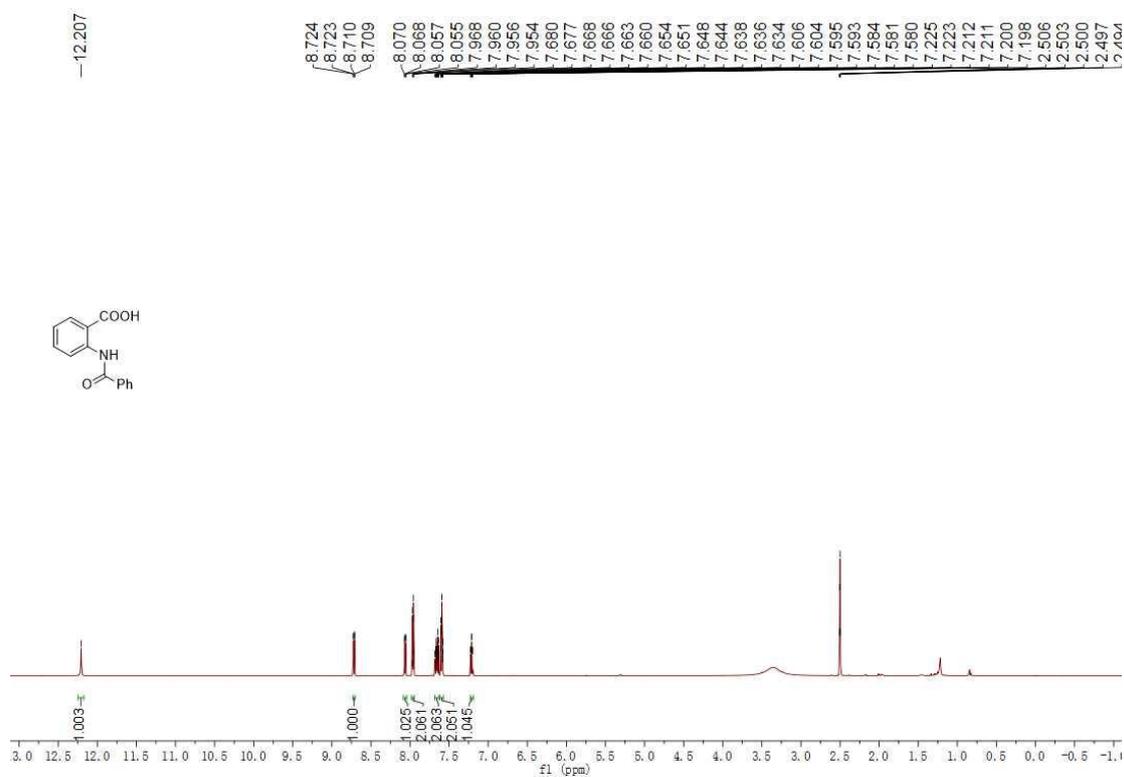
¹H NMR (600 MHz, CDCl₃) Spectrum of **57**



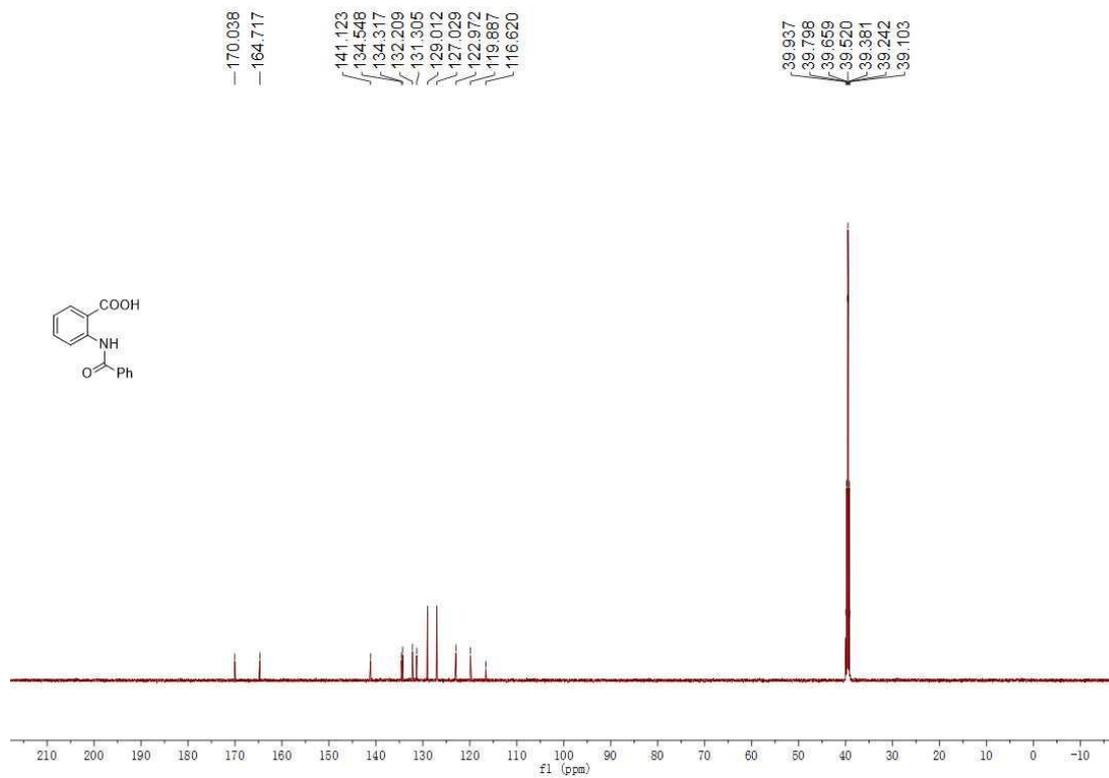
¹³C NMR (150 MHz, CDCl₃) Spectrum of **57**



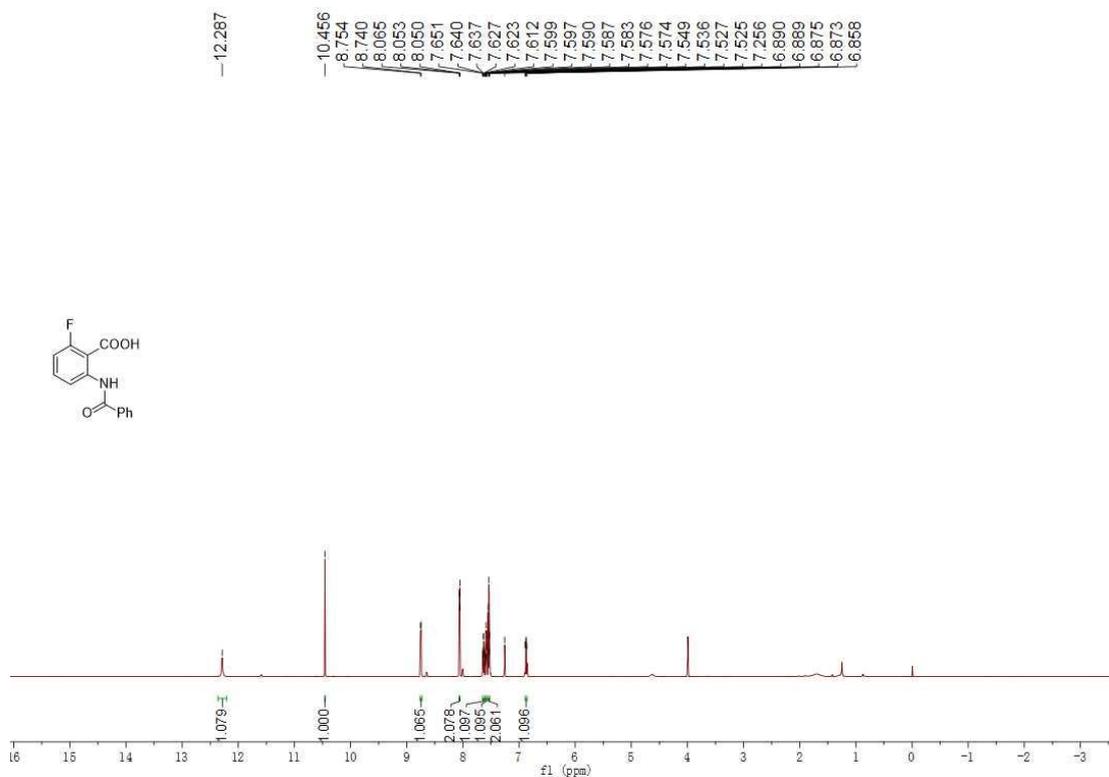
¹H NMR (600 MHz, DMSO-*d*₆) Spectrum of **58**



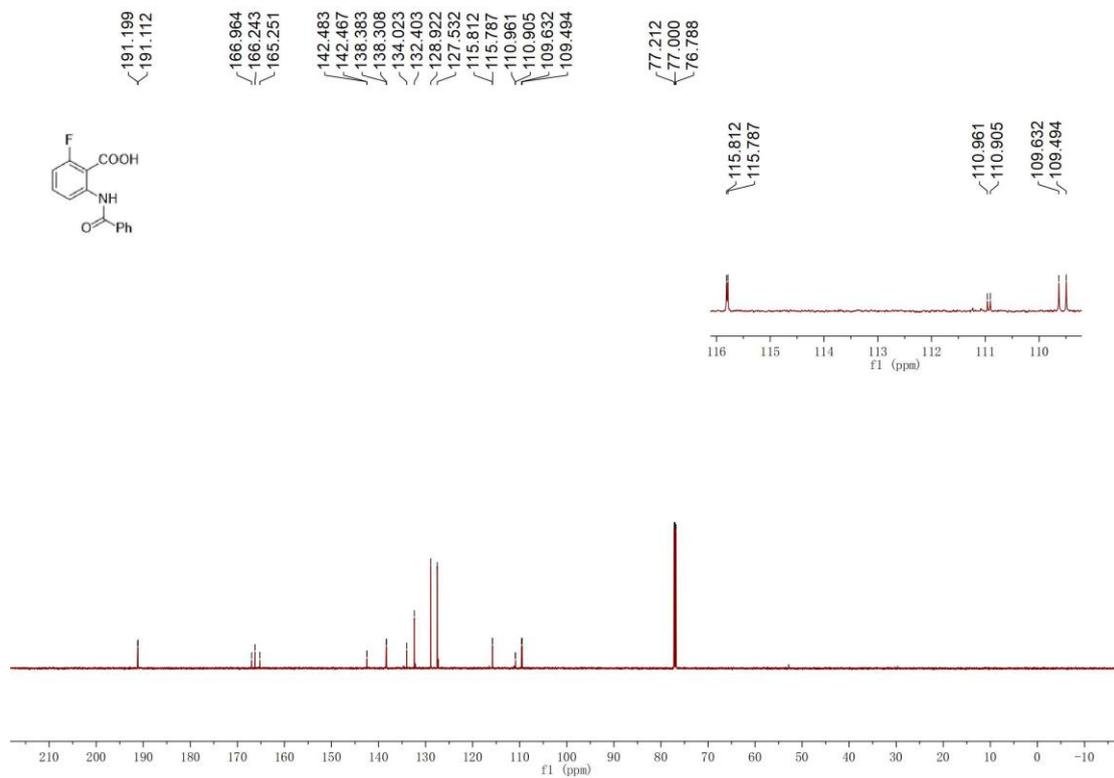
¹³C NMR (150 MHz, DMSO-*d*₆) Spectrum of **58**



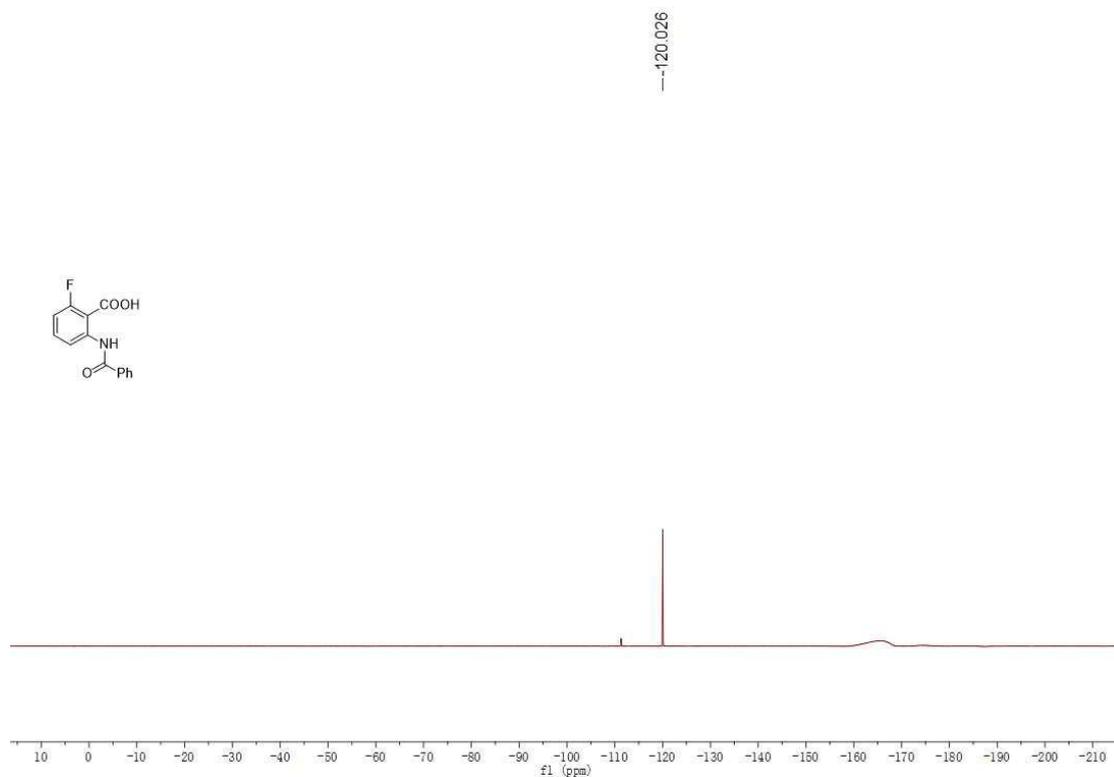
¹H NMR (600 MHz, CDCl₃) Spectrum of **59**



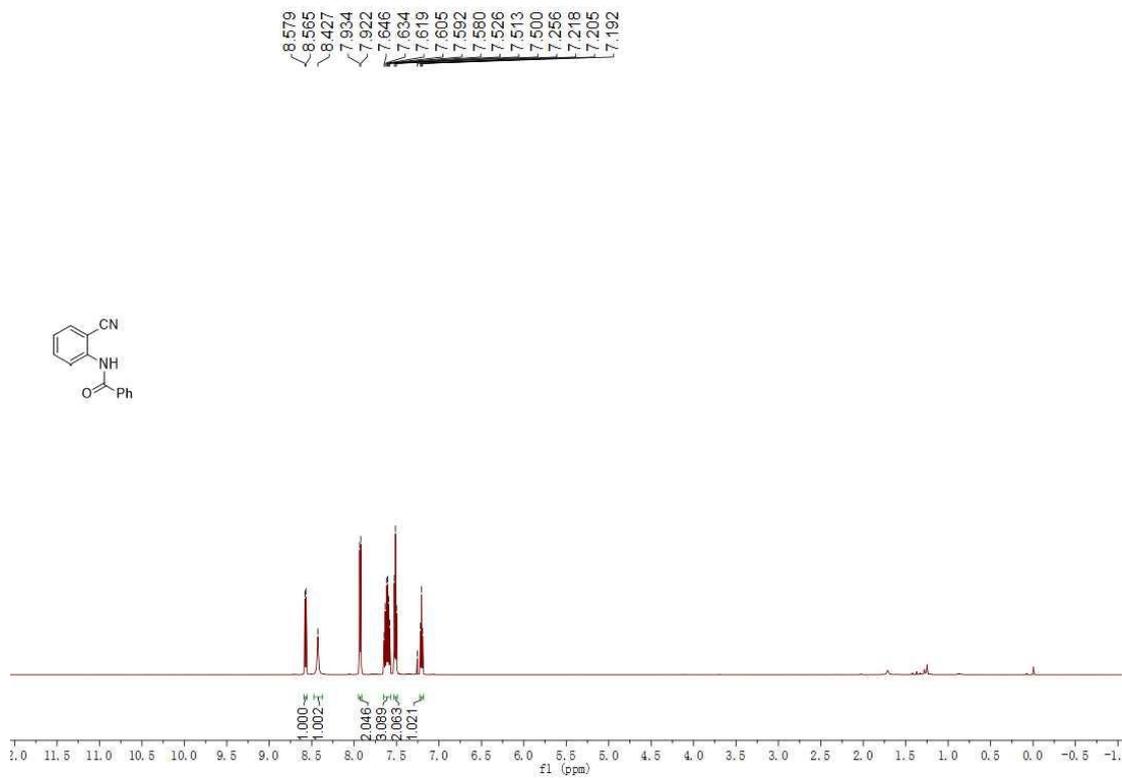
¹³C NMR (150 MHz, CDCl₃) Spectrum of **59**



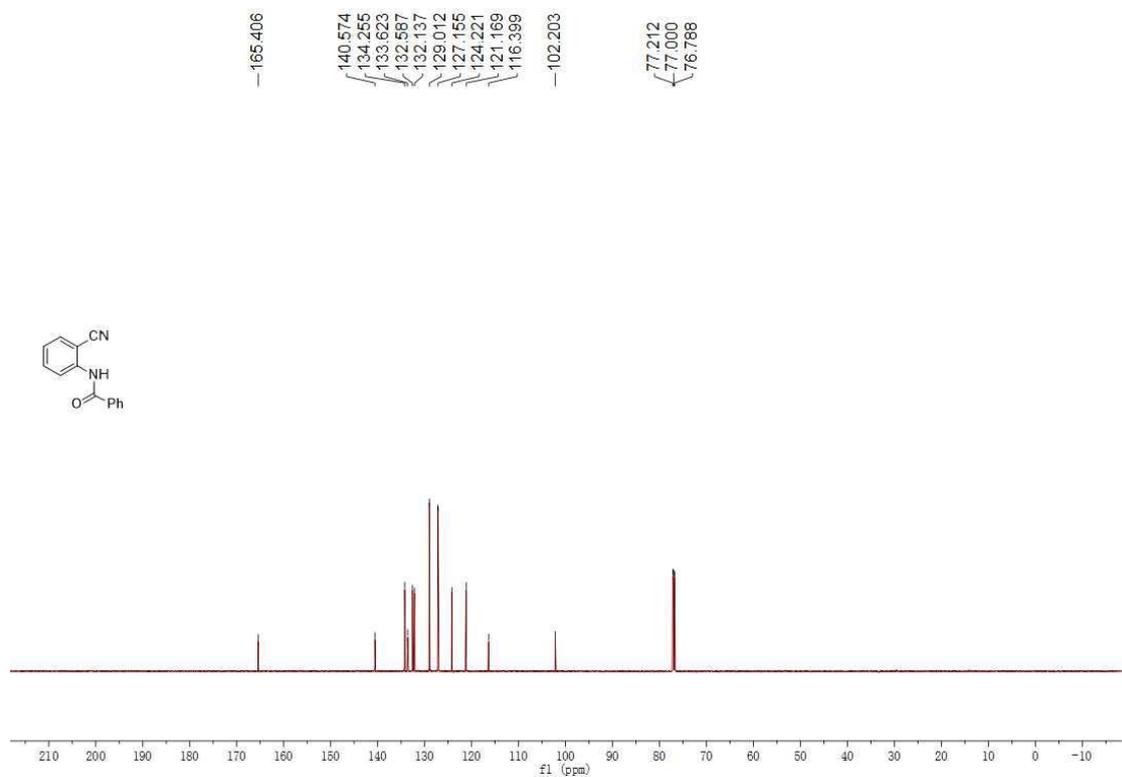
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **59**



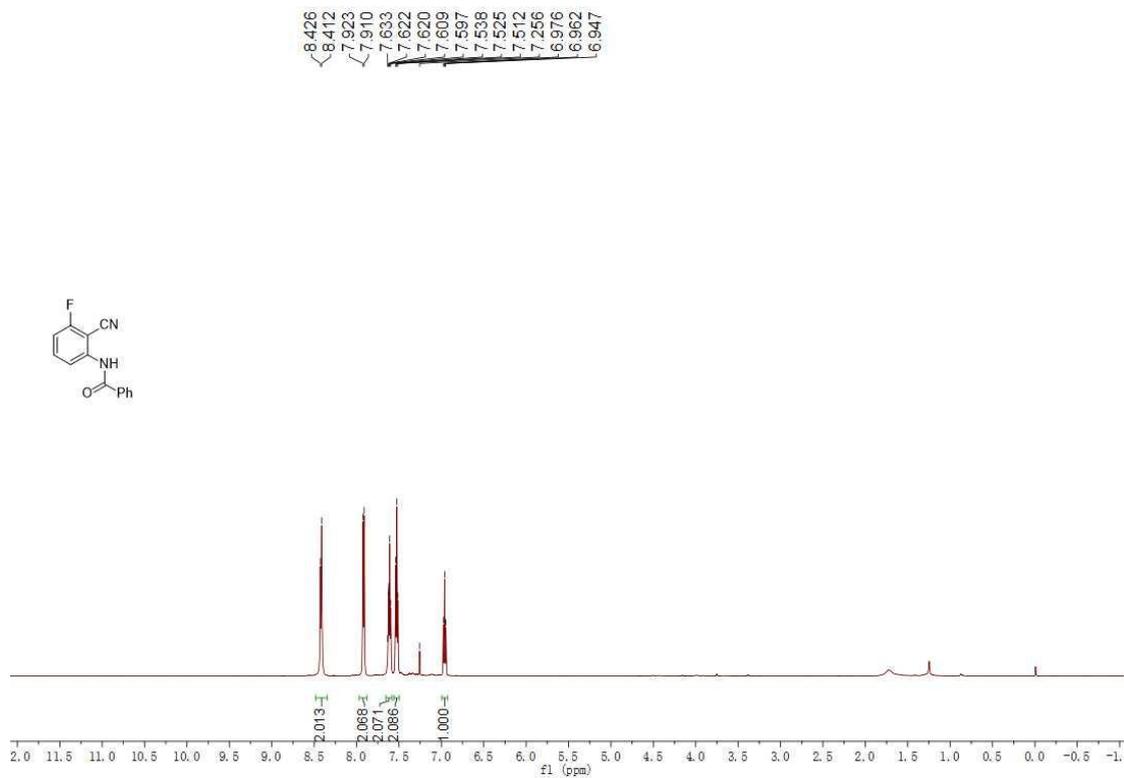
¹H NMR (600 MHz, CDCl₃) Spectrum of **60**



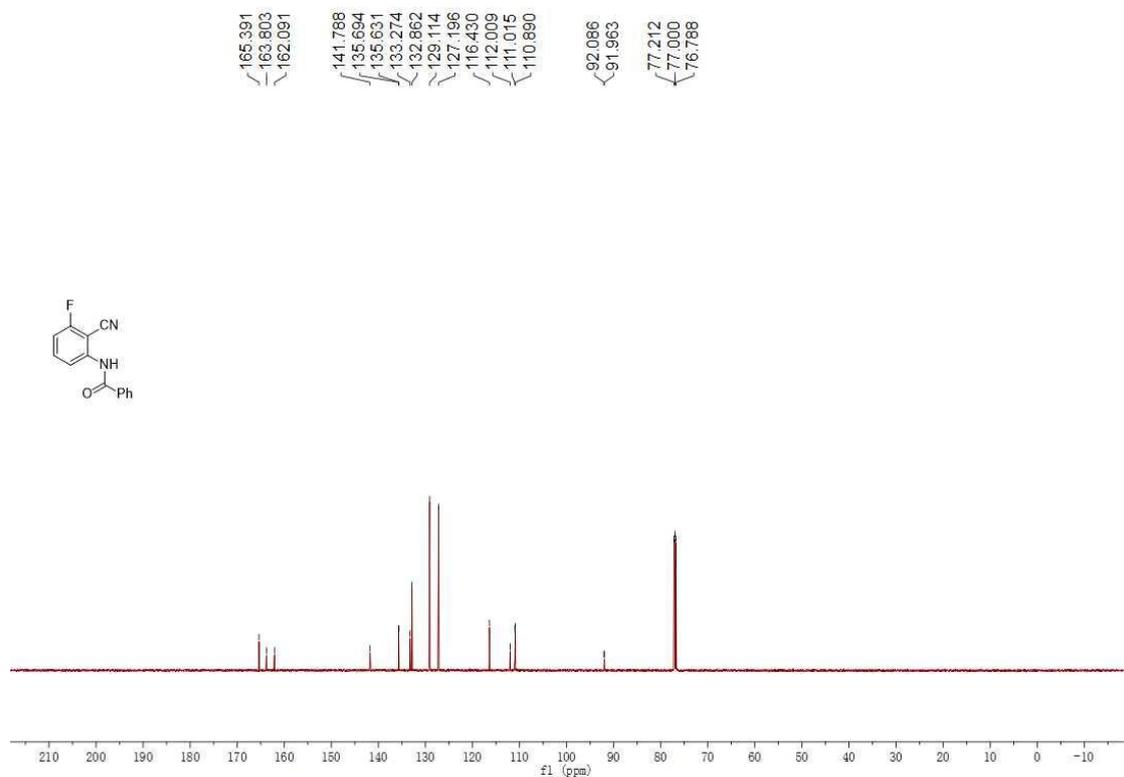
¹³C NMR (150 MHz, CDCl₃) Spectrum of **60**



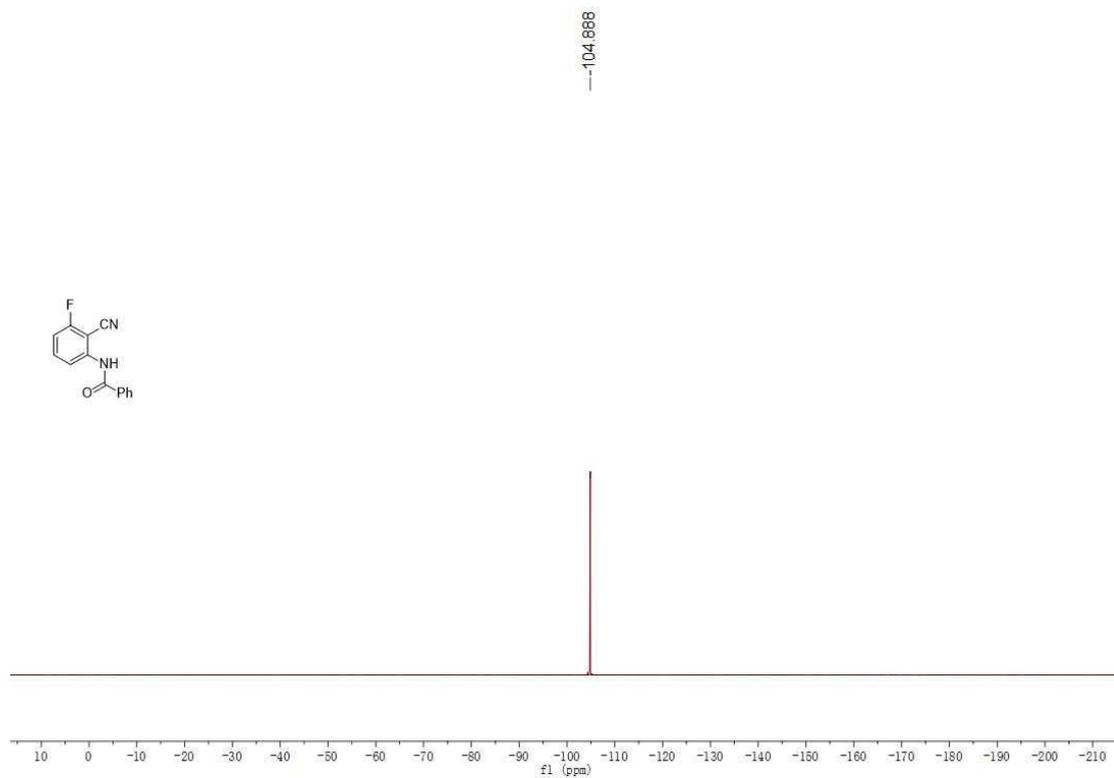
¹H NMR (600 MHz, CDCl₃) Spectrum of **61**



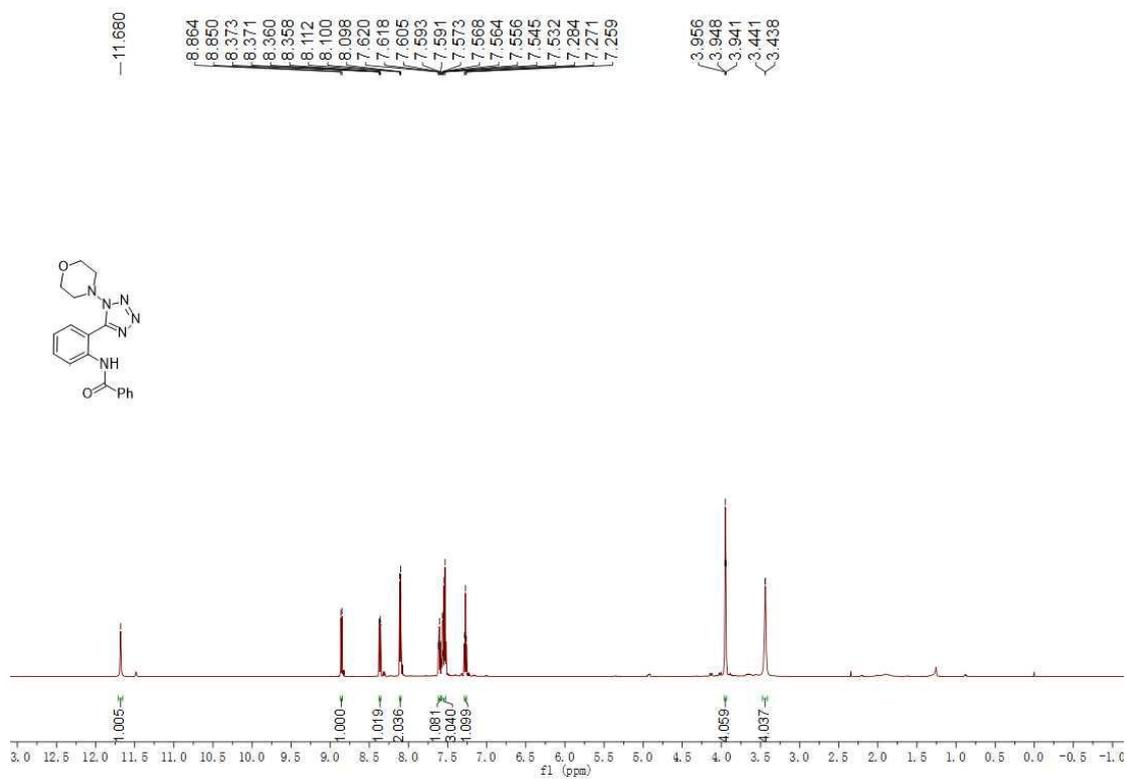
¹³C NMR (150 MHz, CDCl₃) Spectrum of **61**



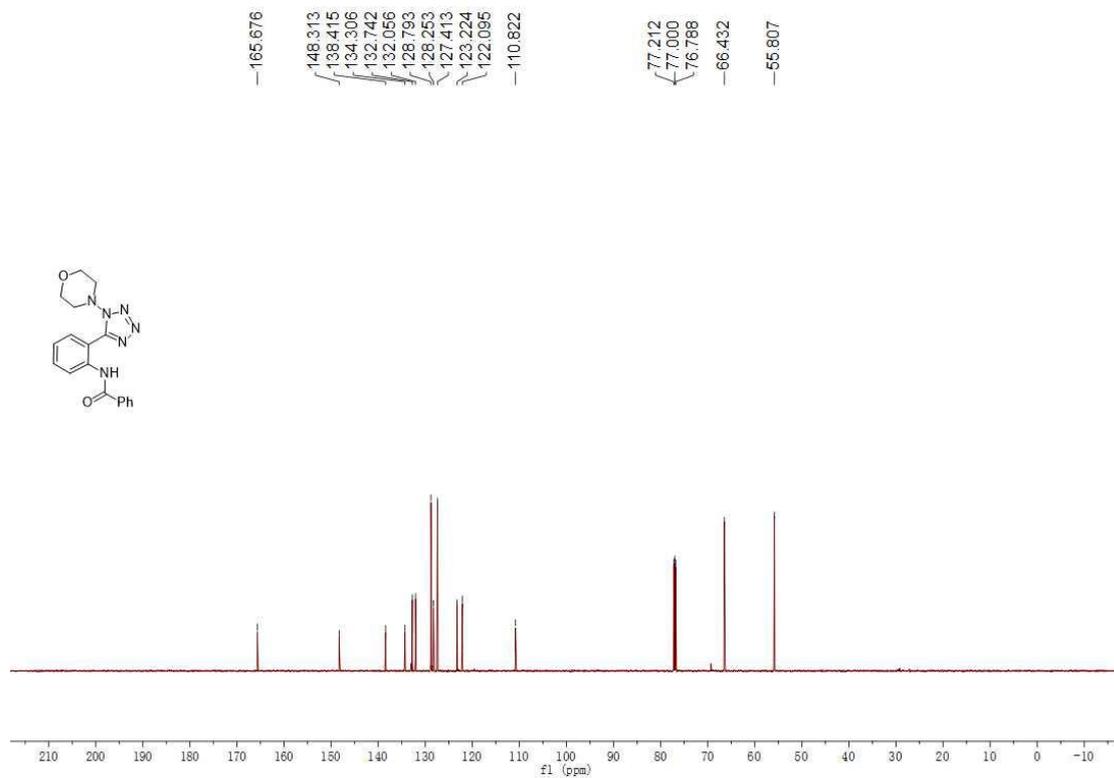
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of **61**



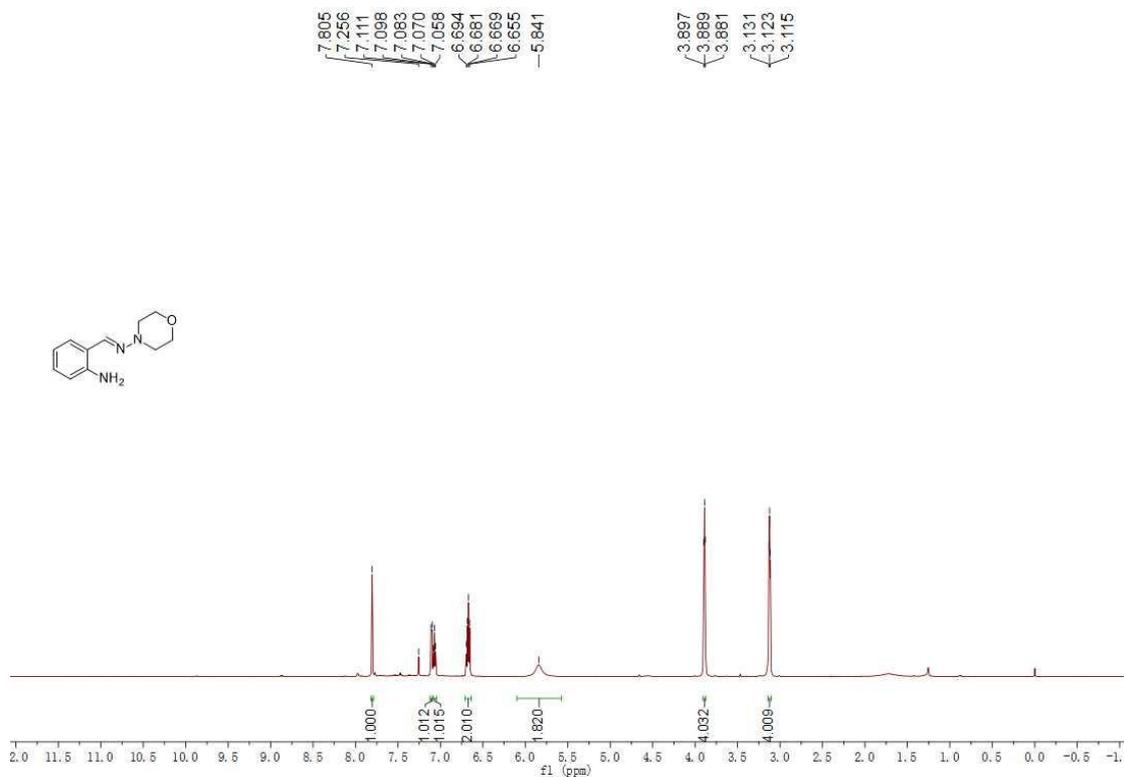
¹H NMR (600 MHz, CDCl₃) Spectrum of **62**



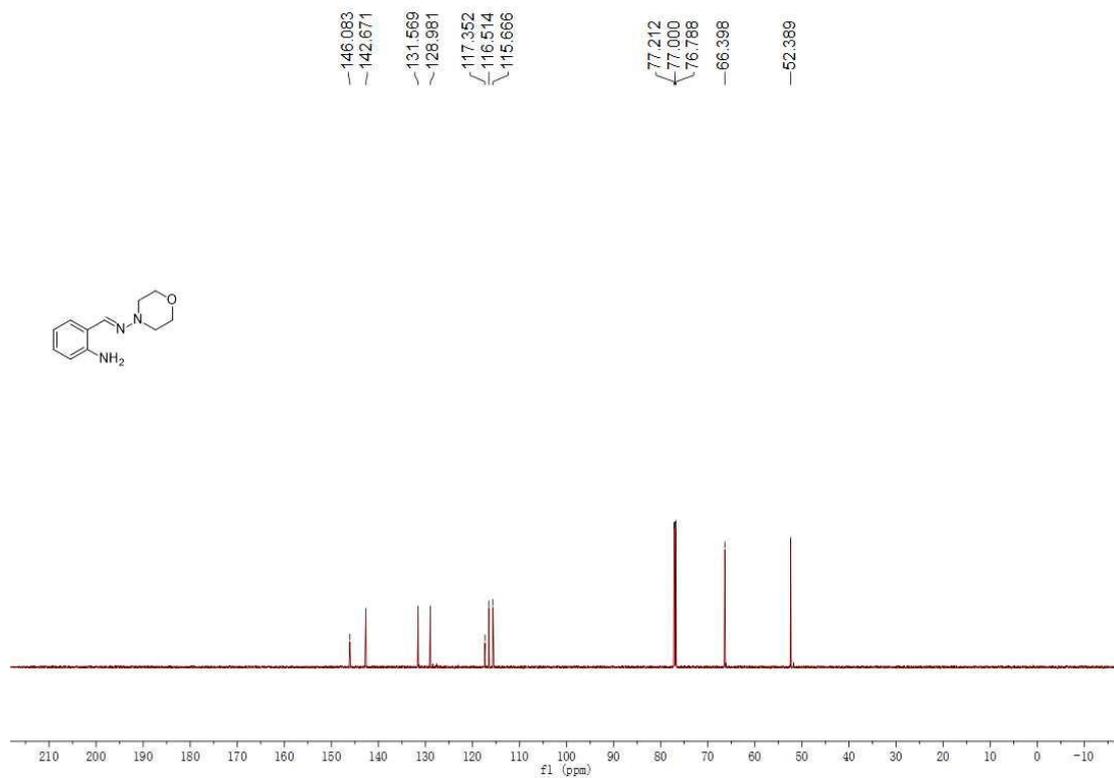
¹³C NMR (150 MHz, CDCl₃) Spectrum of **62**



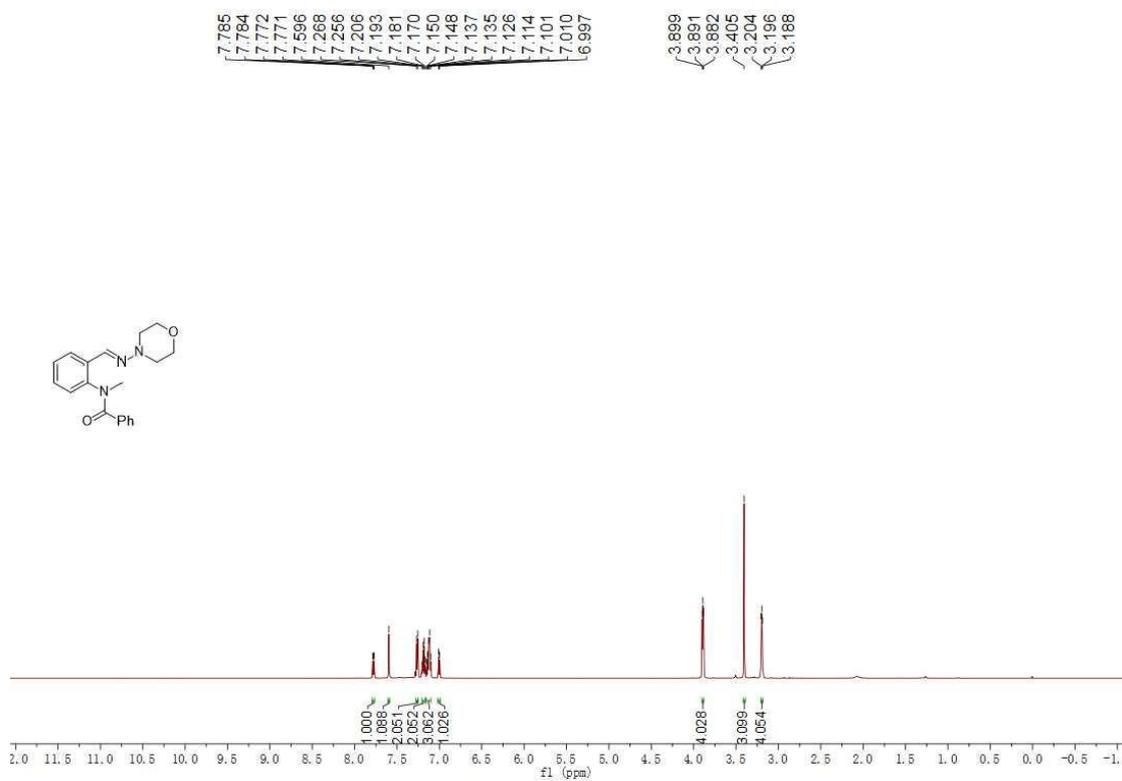
¹H NMR (600 MHz, CDCl₃) Spectrum of **63**



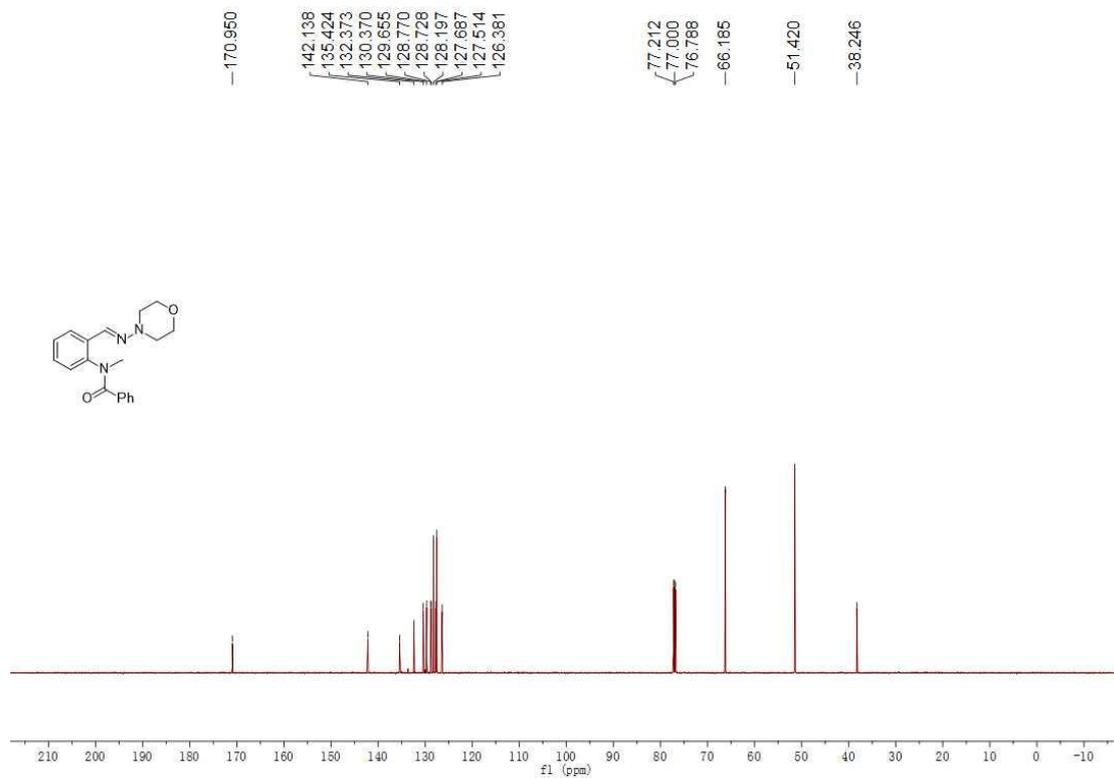
¹³C NMR (150 MHz, CDCl₃) Spectrum of **63**



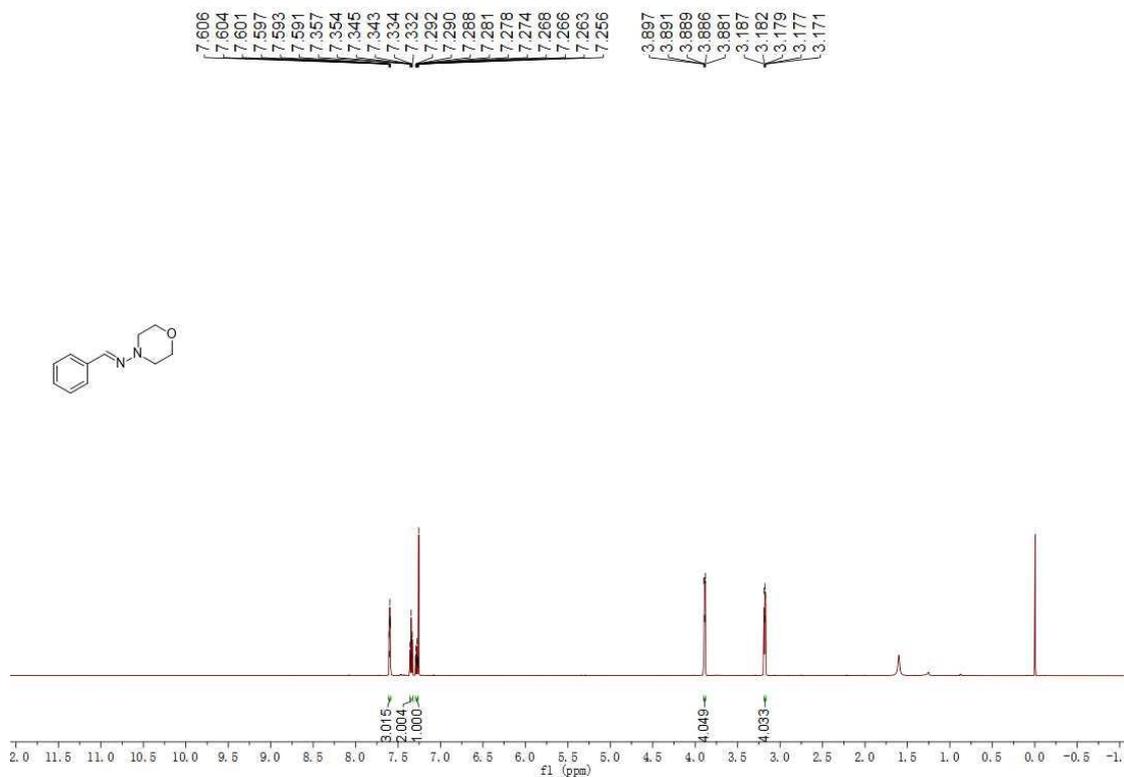
¹H NMR (600 MHz, CDCl₃) Spectrum of **64**



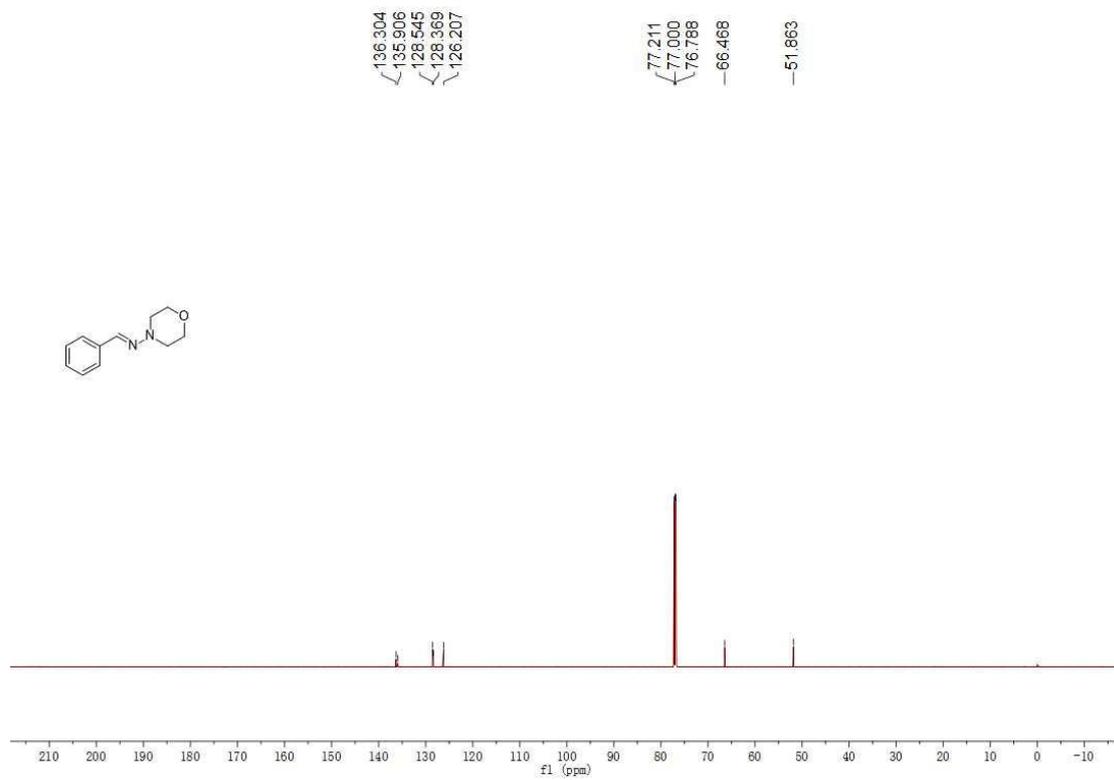
¹³C NMR (150 MHz, CDCl₃) Spectrum of **64**



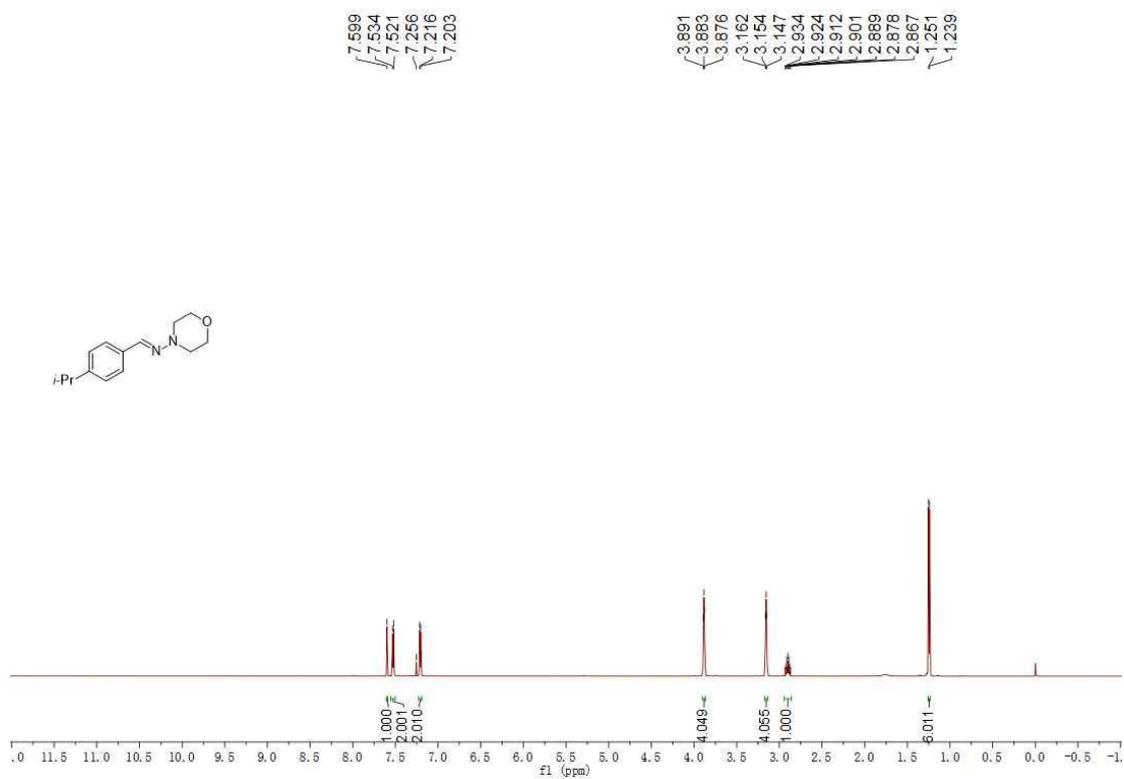
¹H NMR (600 MHz, CDCl₃) Spectrum of **A1**



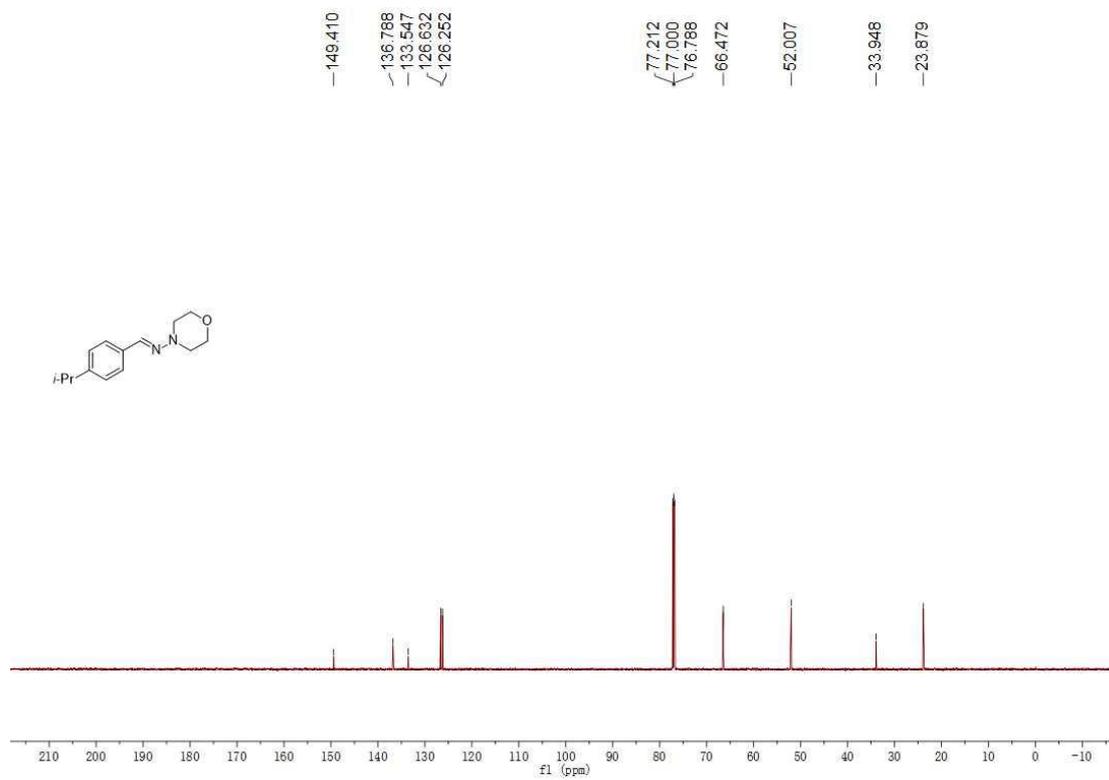
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A1**



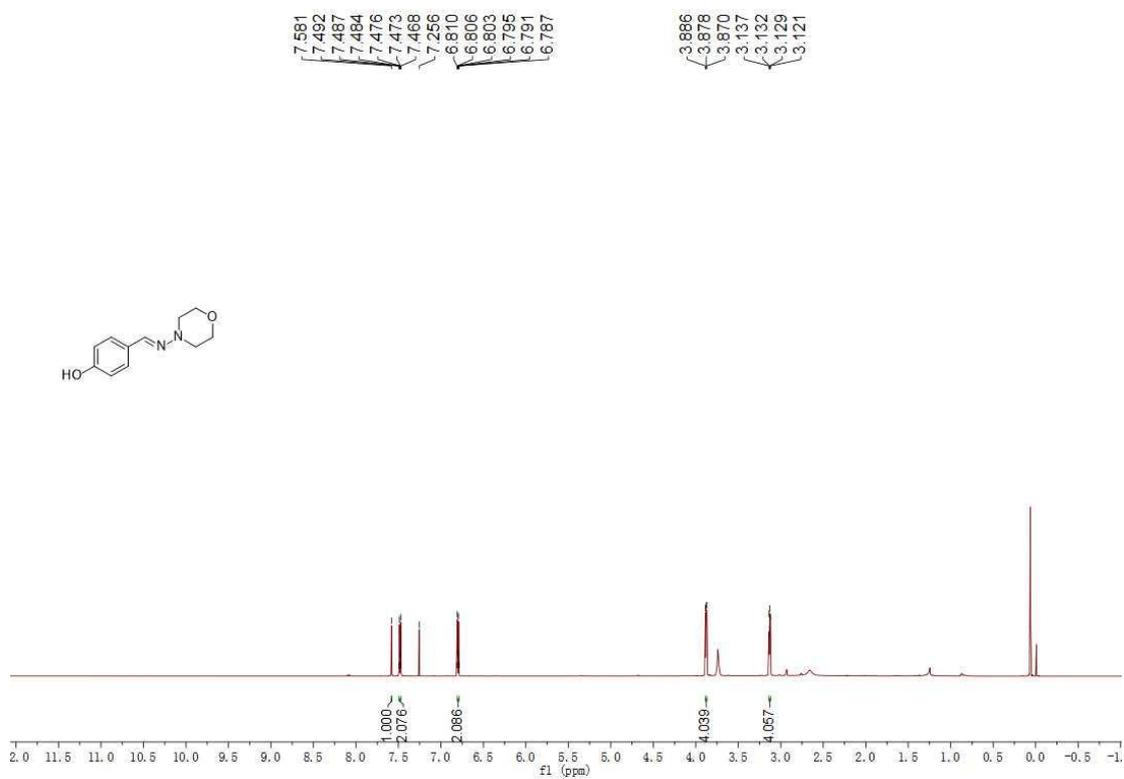
¹H NMR (600 MHz, CDCl₃) Spectrum of **A6**



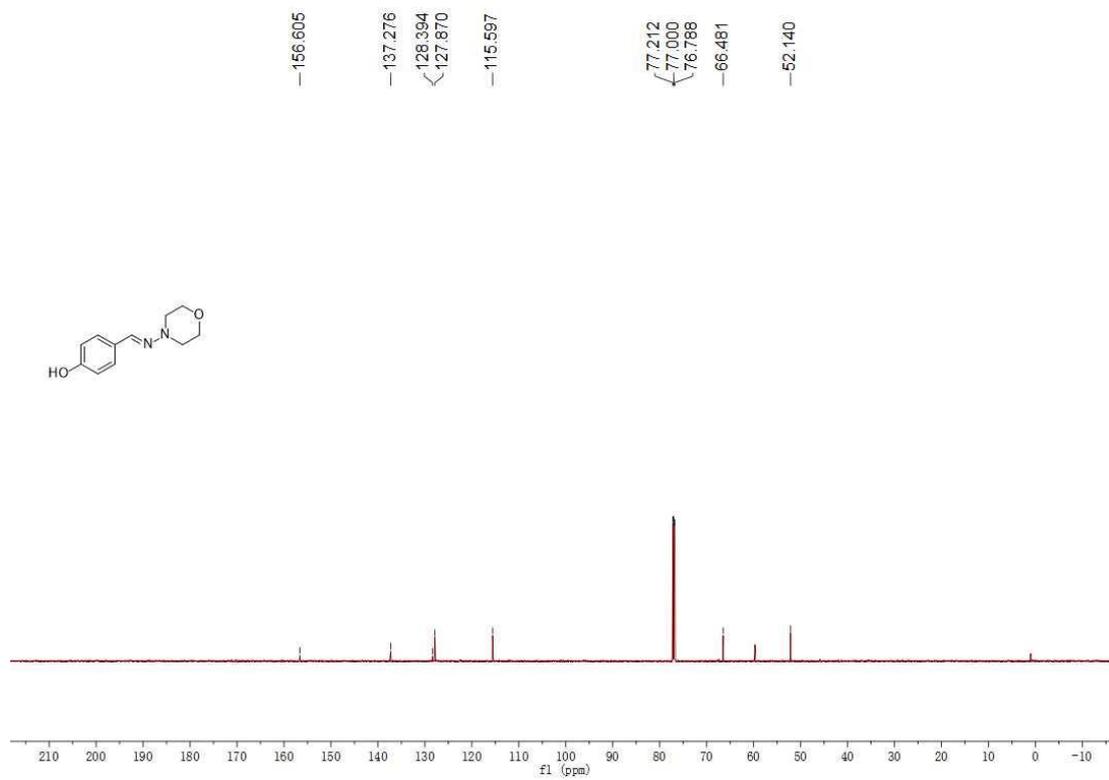
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A6**



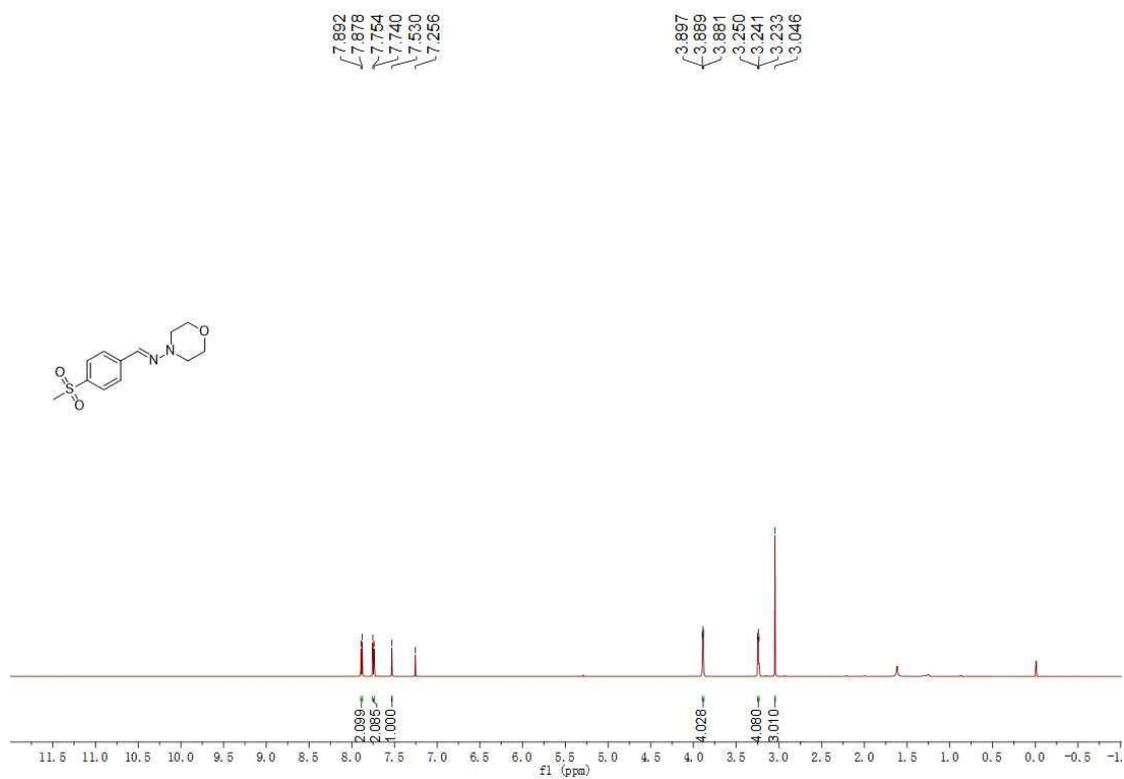
¹H NMR (600 MHz, CDCl₃) Spectrum of **A16**



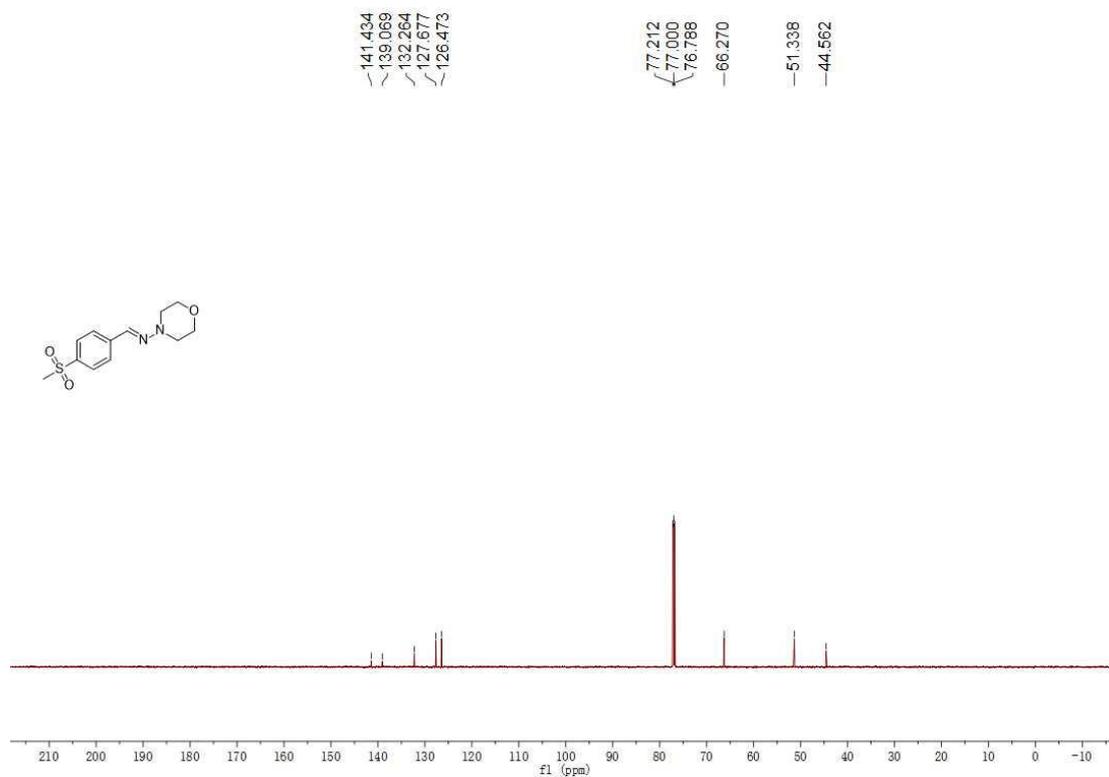
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A16**



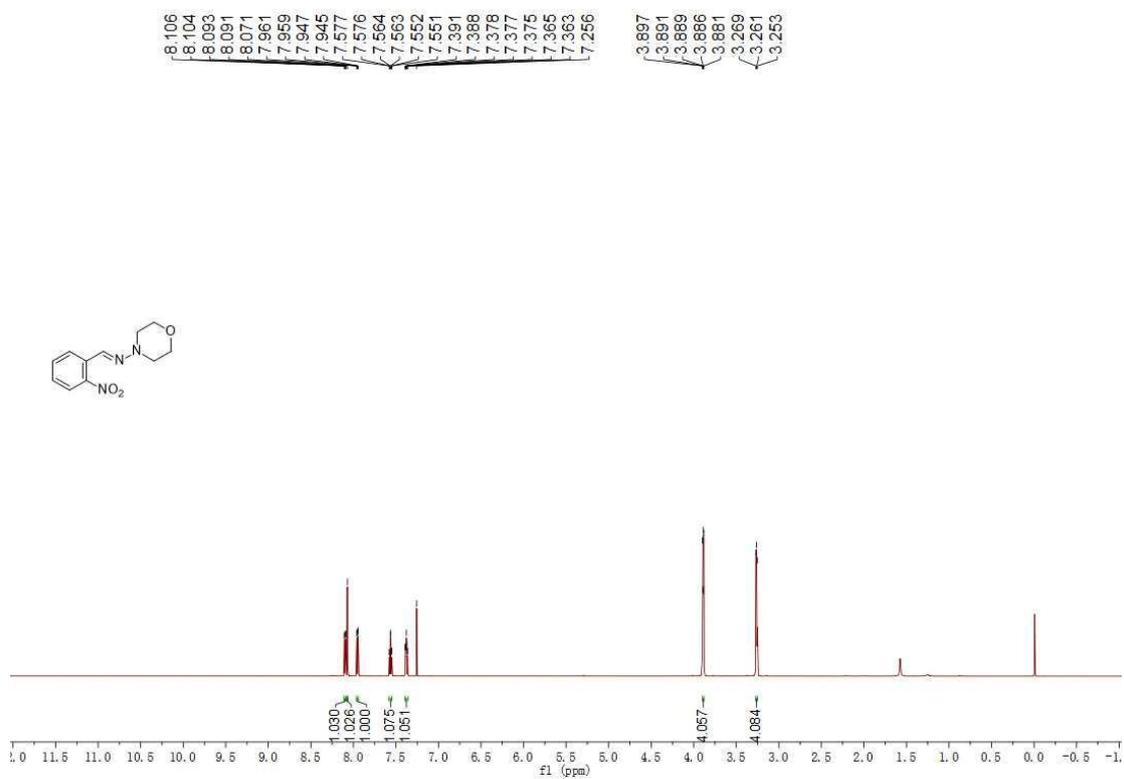
¹H NMR (600 MHz, CDCl₃) Spectrum of **A20**



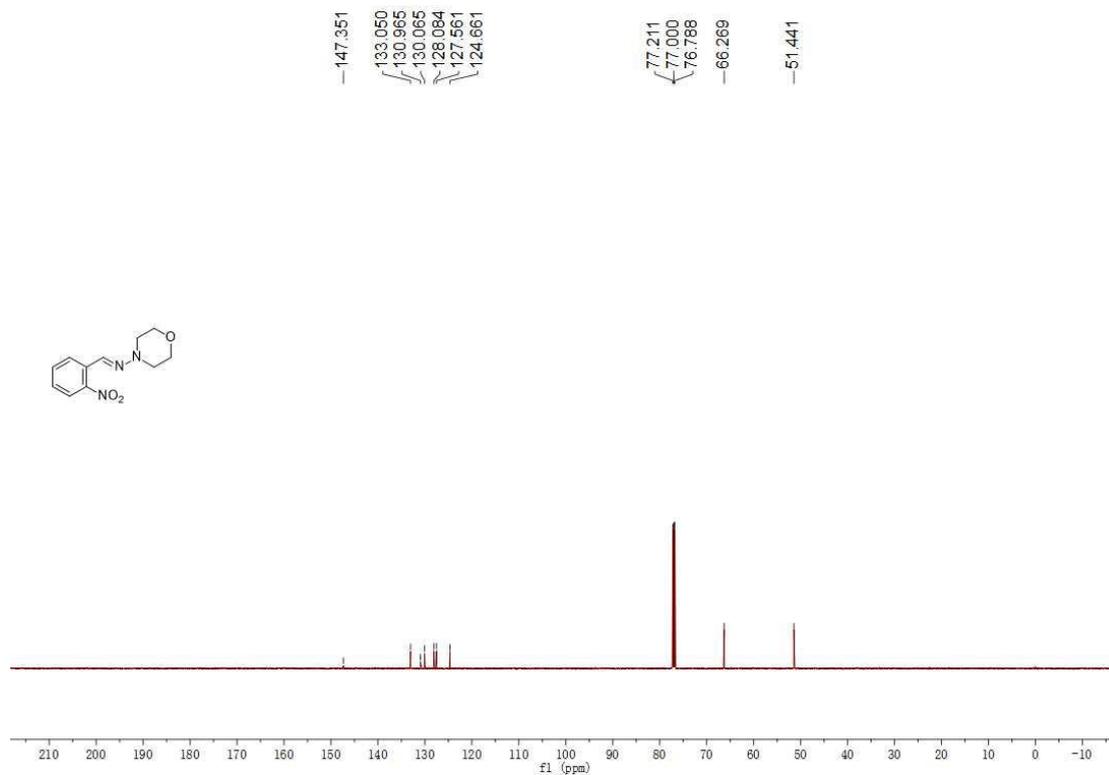
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A20**



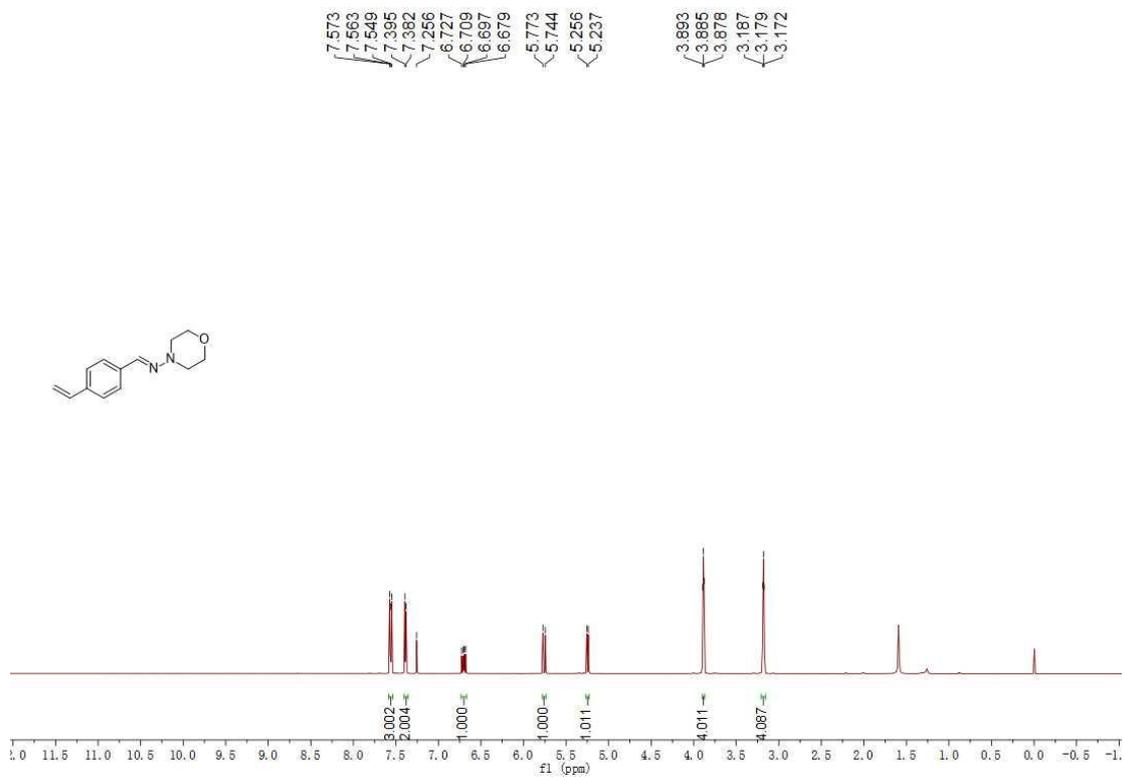
¹H NMR (600 MHz, CDCl₃) Spectrum of **A22**



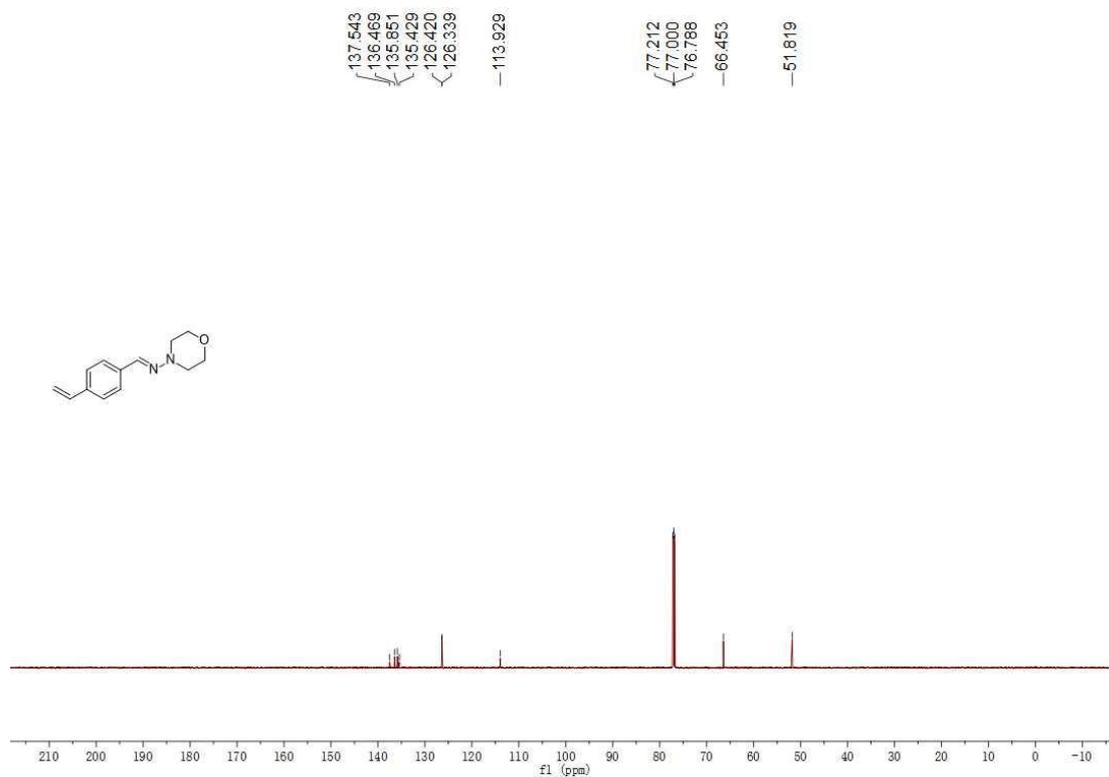
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A22**



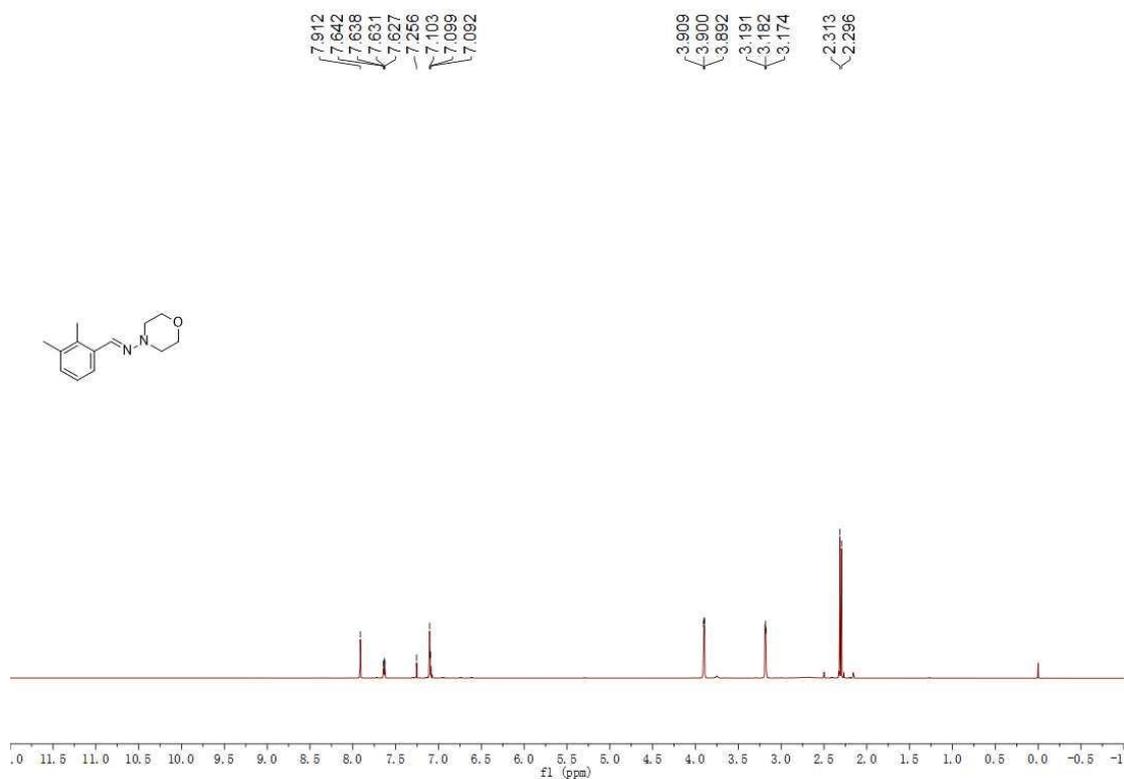
¹H NMR (600 MHz, CDCl₃) Spectrum of **A23**



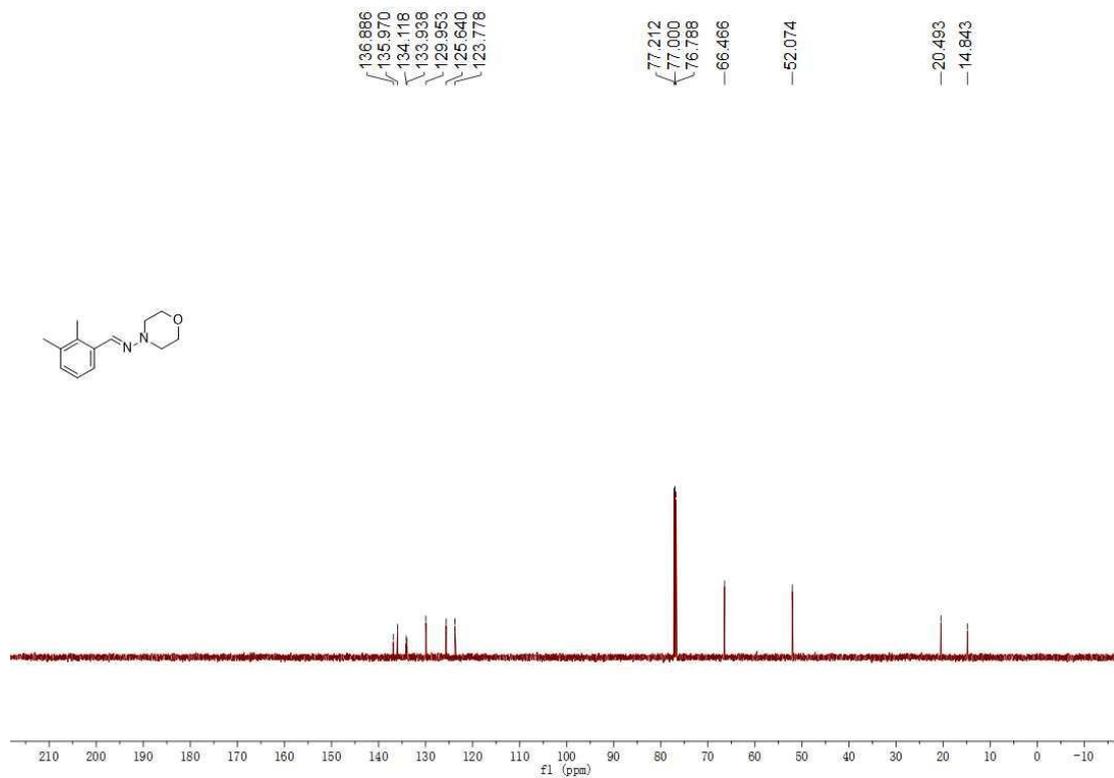
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A23**



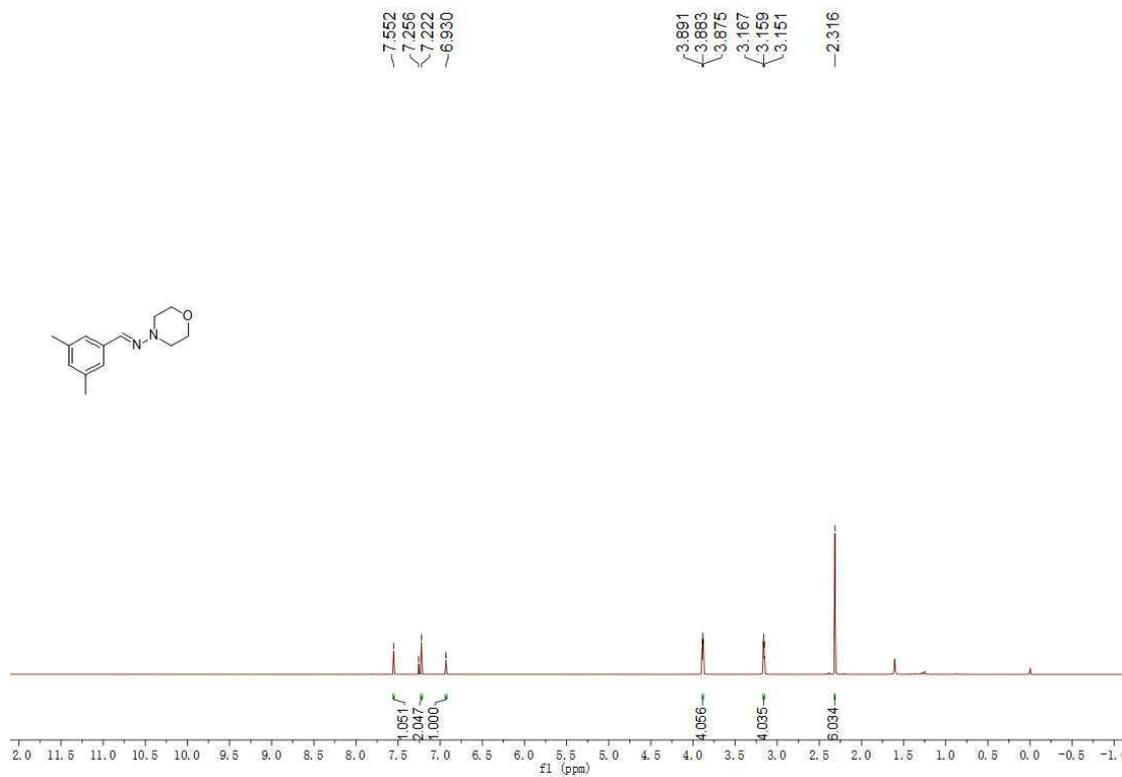
¹H NMR (600 MHz, CDCl₃) Spectrum of **A24**



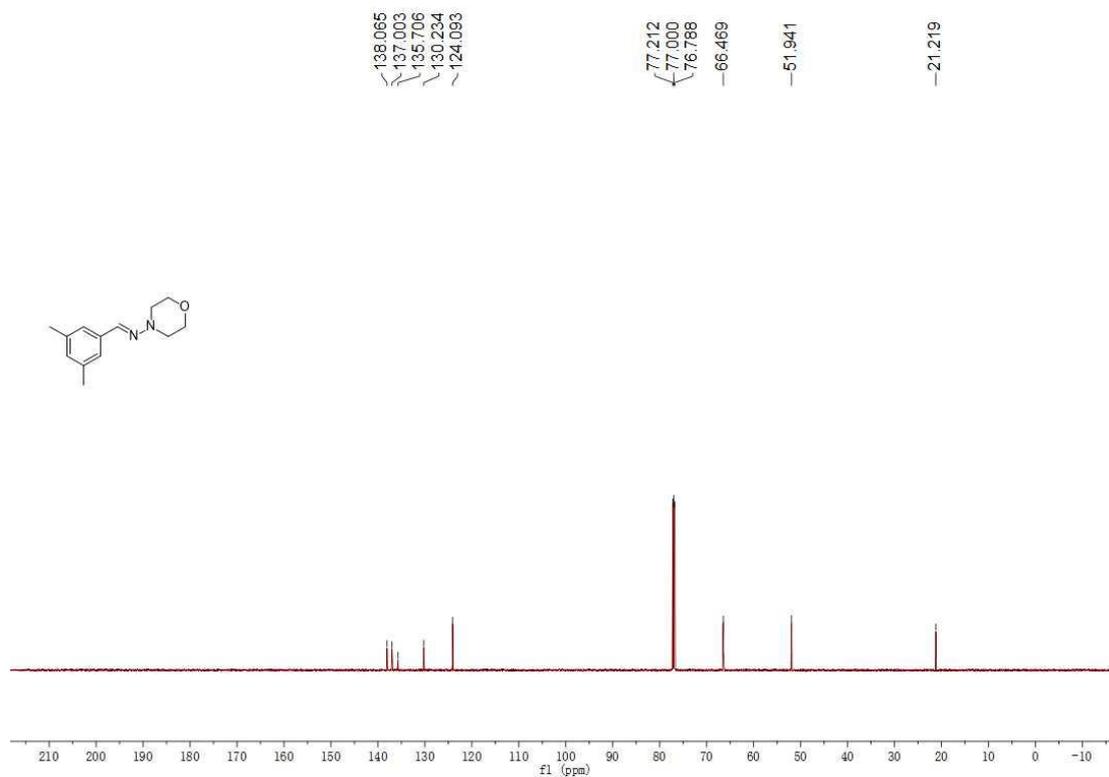
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A24**



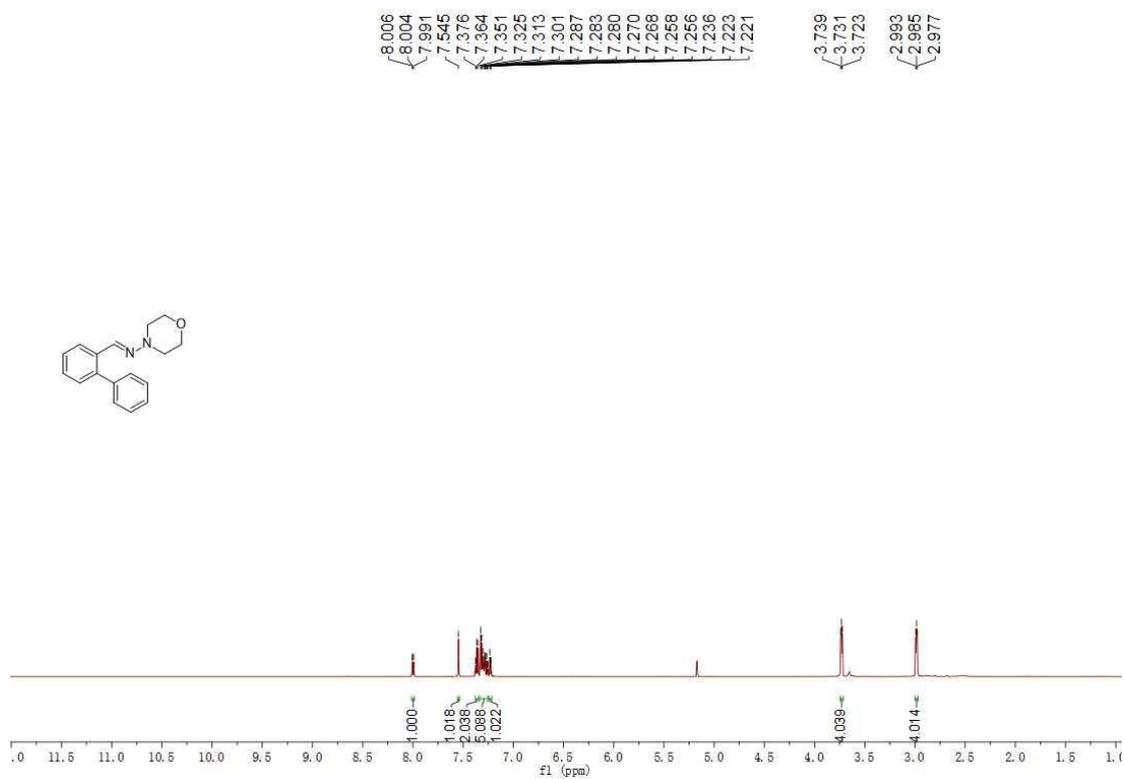
¹H NMR (600 MHz, CDCl₃) Spectrum of **A25**



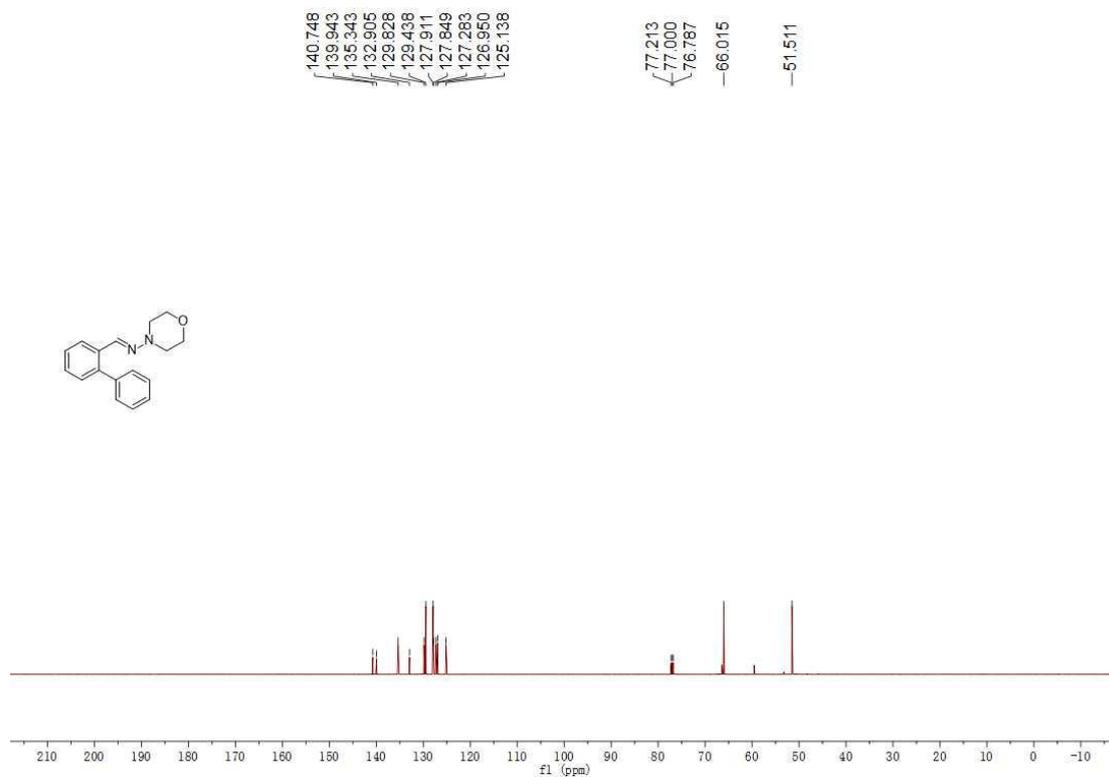
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A25**



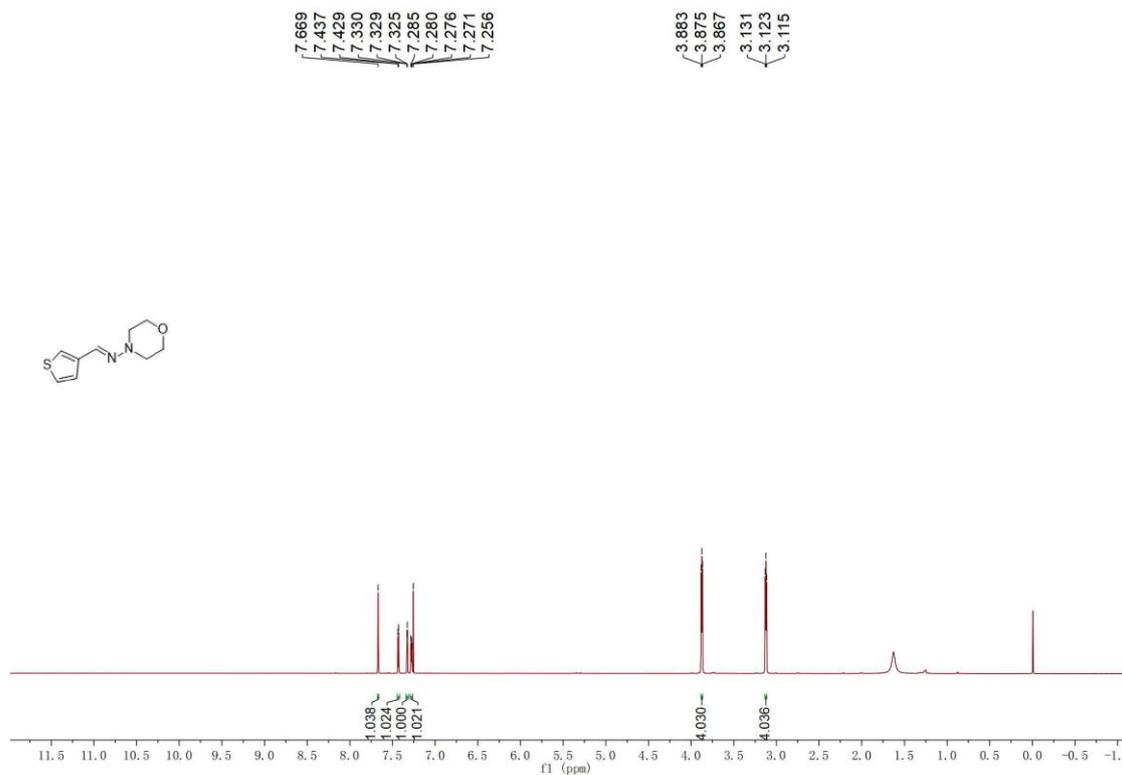
¹H NMR (600 MHz, CDCl₃) Spectrum of **A29**



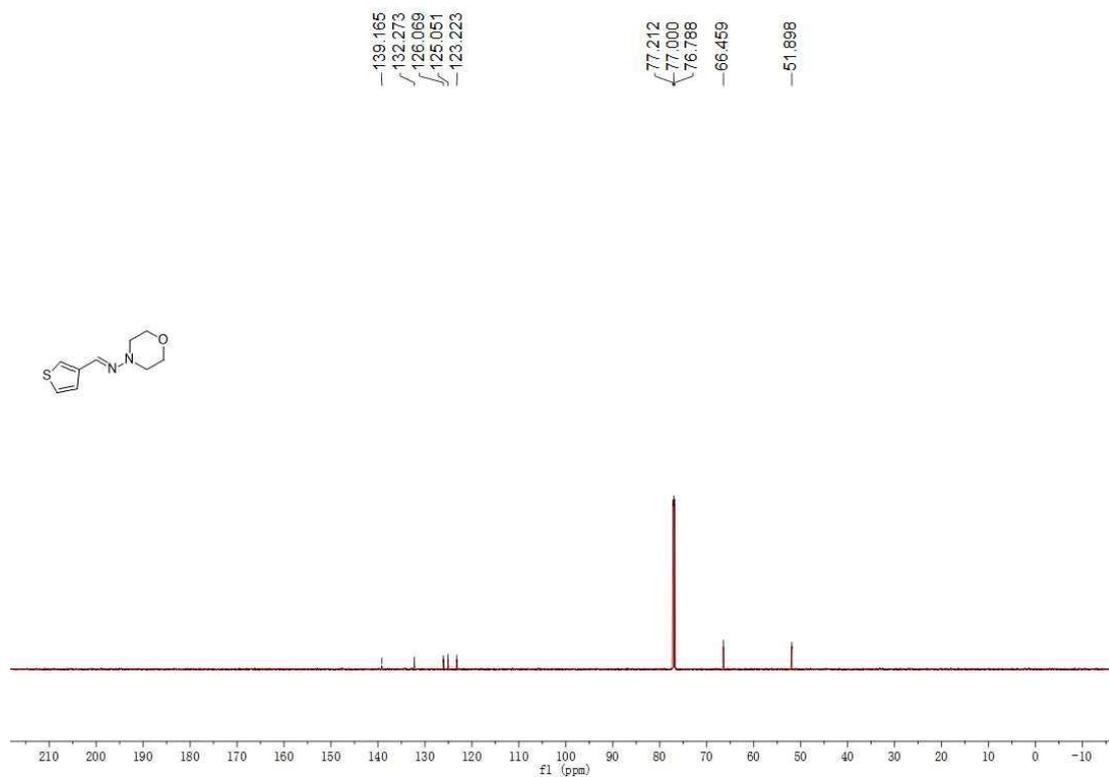
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A29**



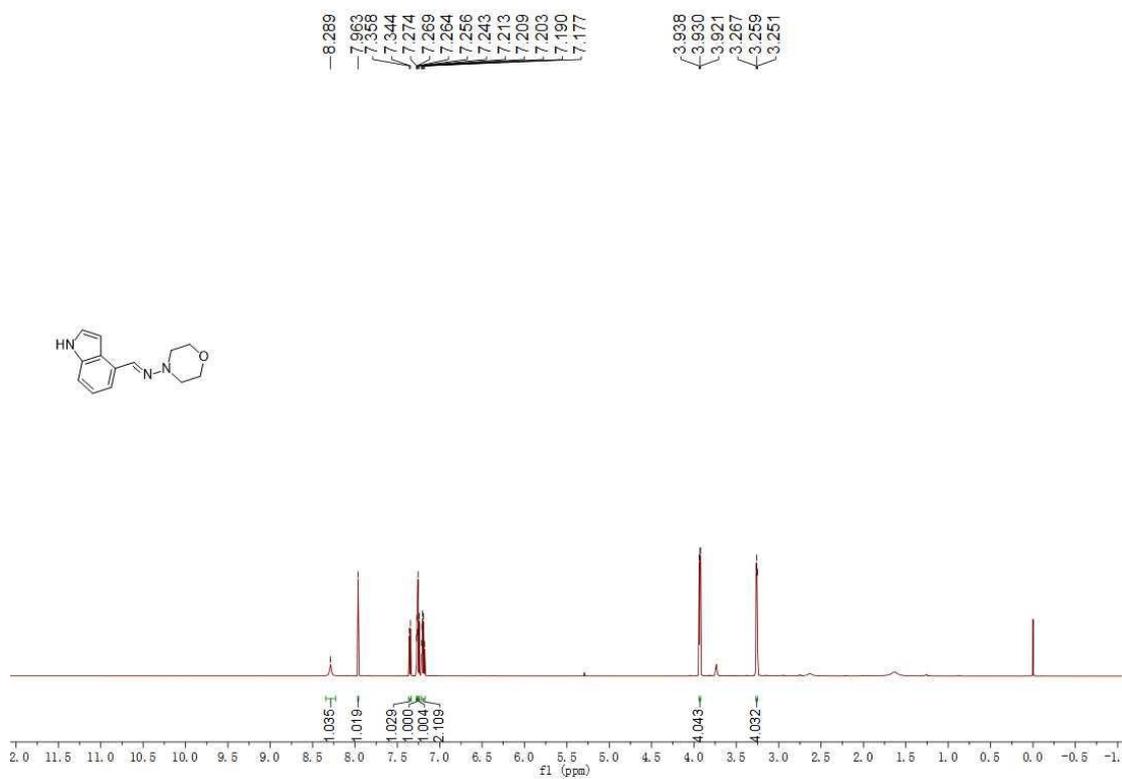
¹H NMR (600 MHz, CDCl₃) Spectrum of **A30**



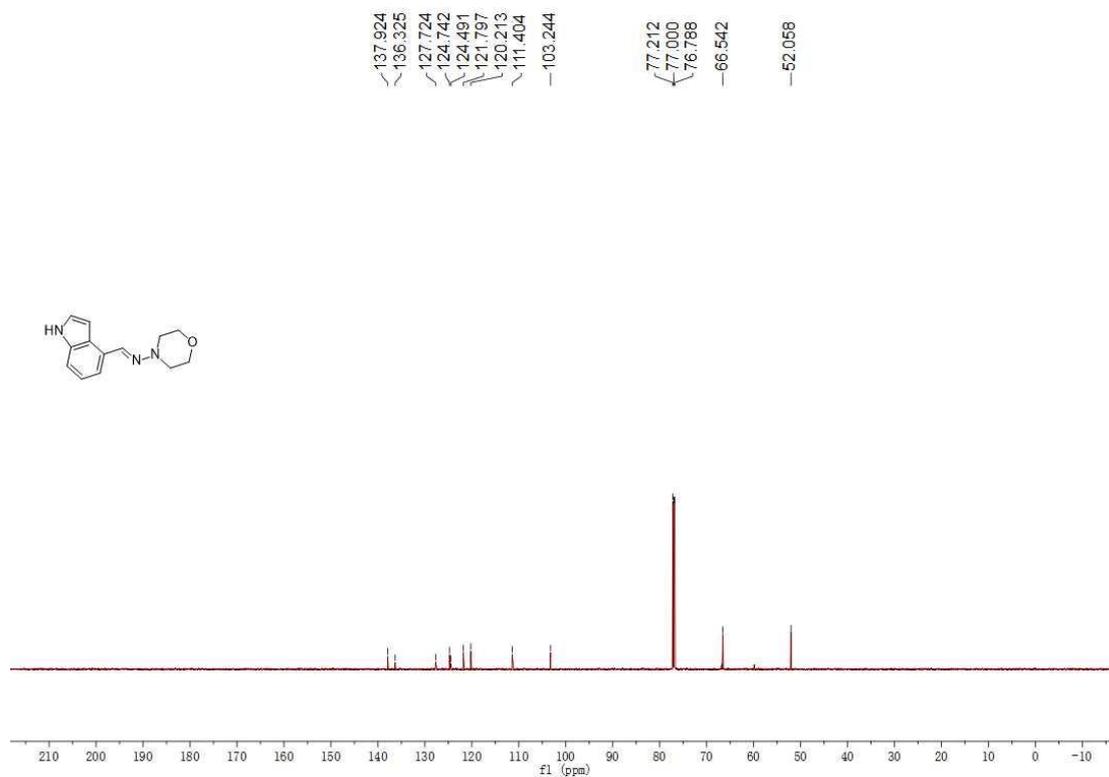
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A30**



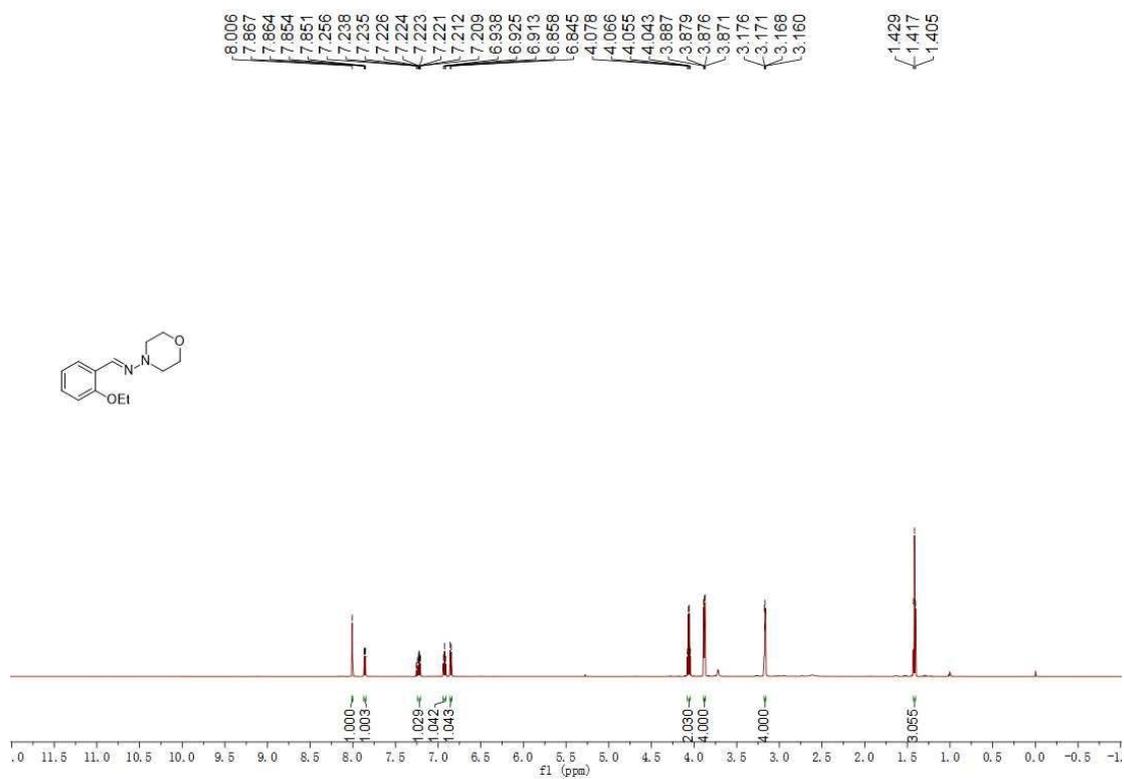
¹H NMR (600 MHz, CDCl₃) Spectrum of **A32**



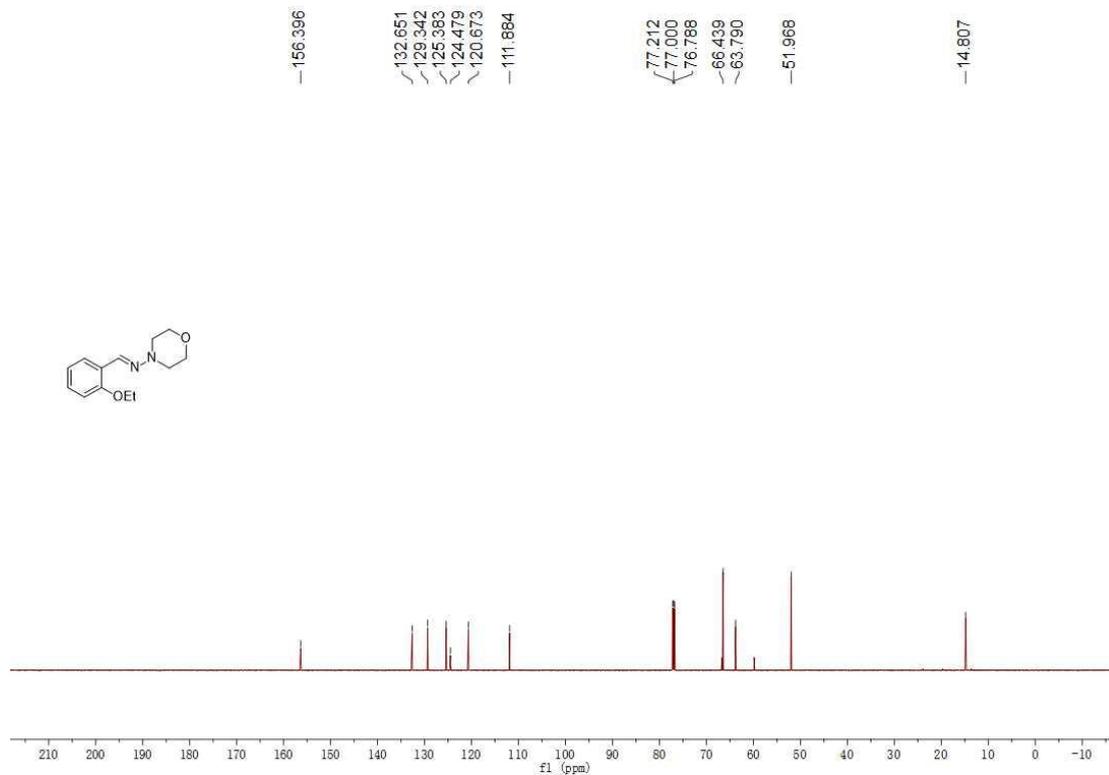
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A32**



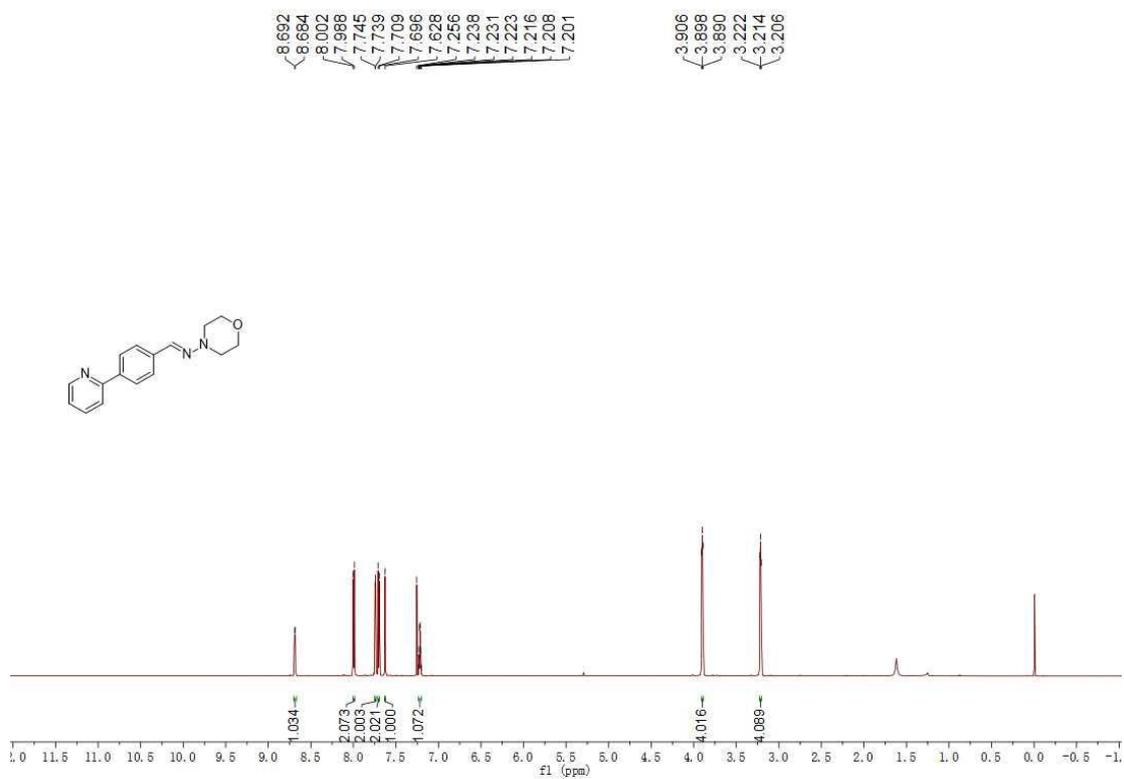
¹H NMR (600 MHz, CDCl₃) Spectrum of **A37**



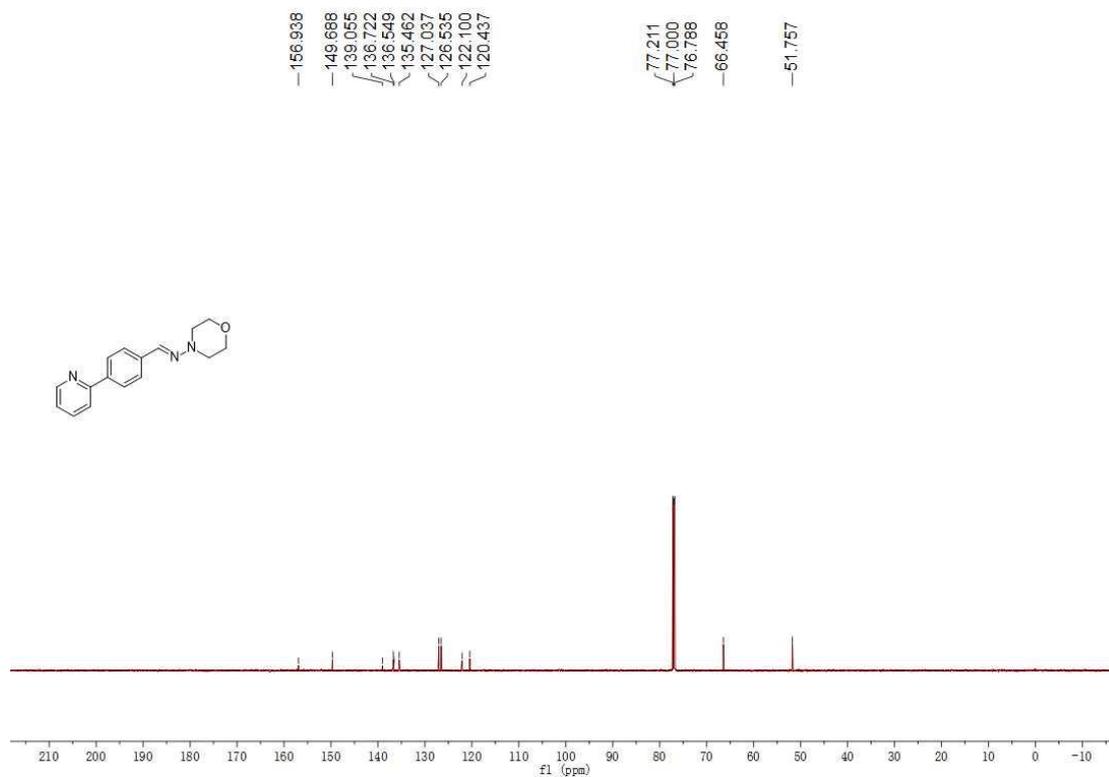
¹³C NMR (150 MHz, CDCl₃) Spectrum of A37



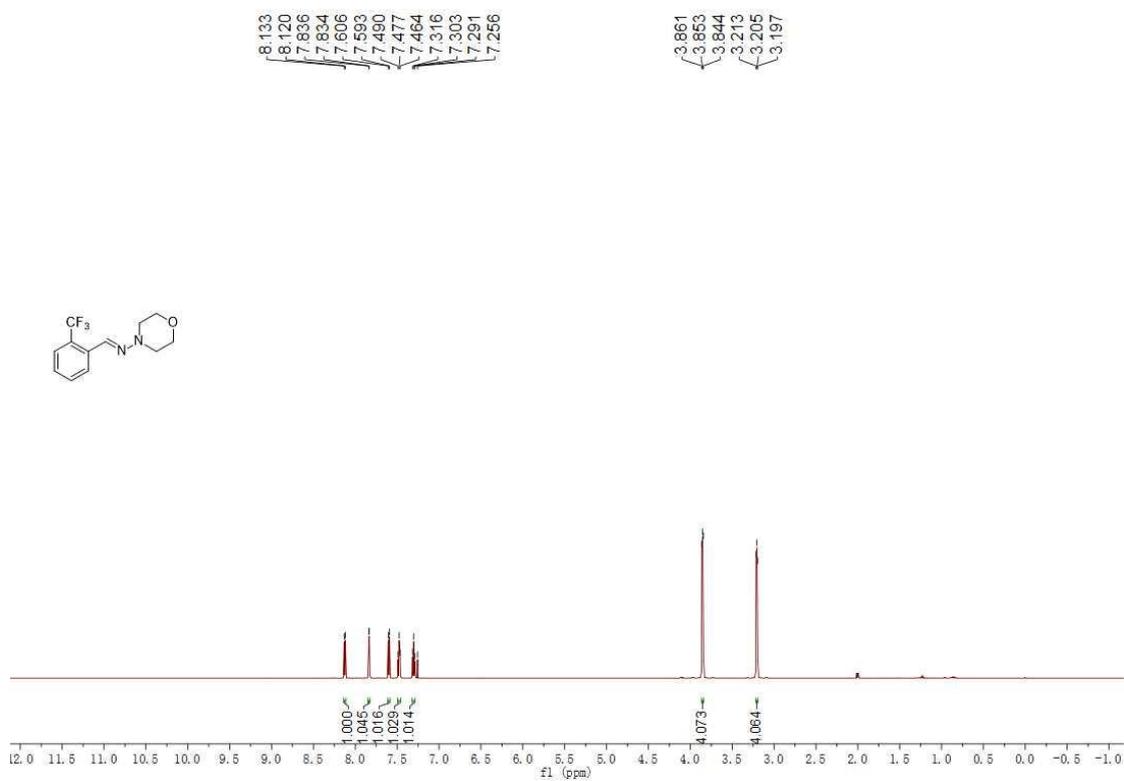
¹H NMR (600 MHz, CDCl₃) Spectrum of A40



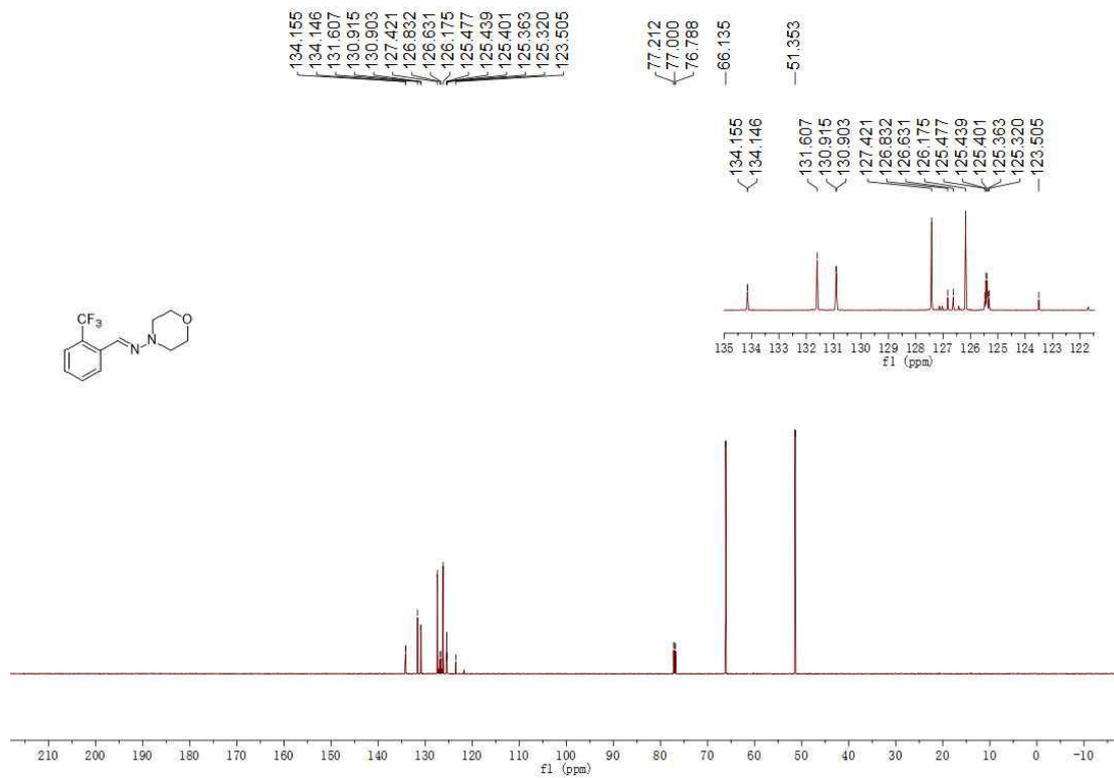
¹³C NMR (150 MHz, CDCl₃) Spectrum of A40



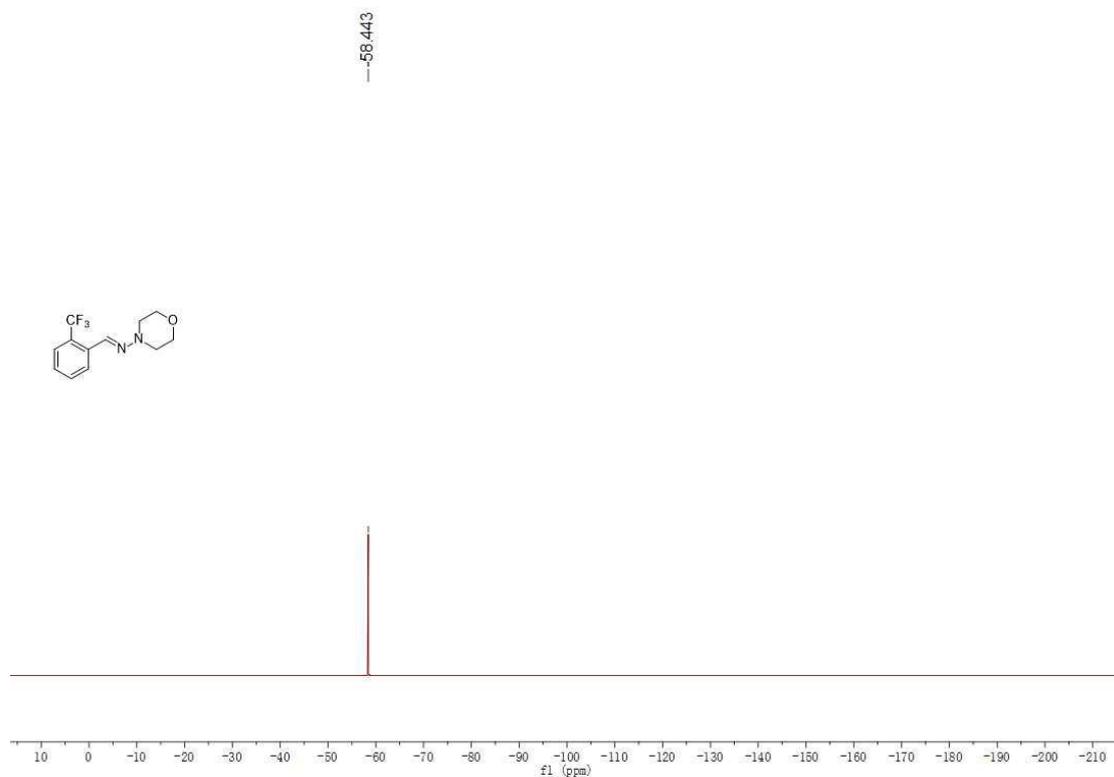
¹H NMR (600 MHz, CDCl₃) Spectrum of A41



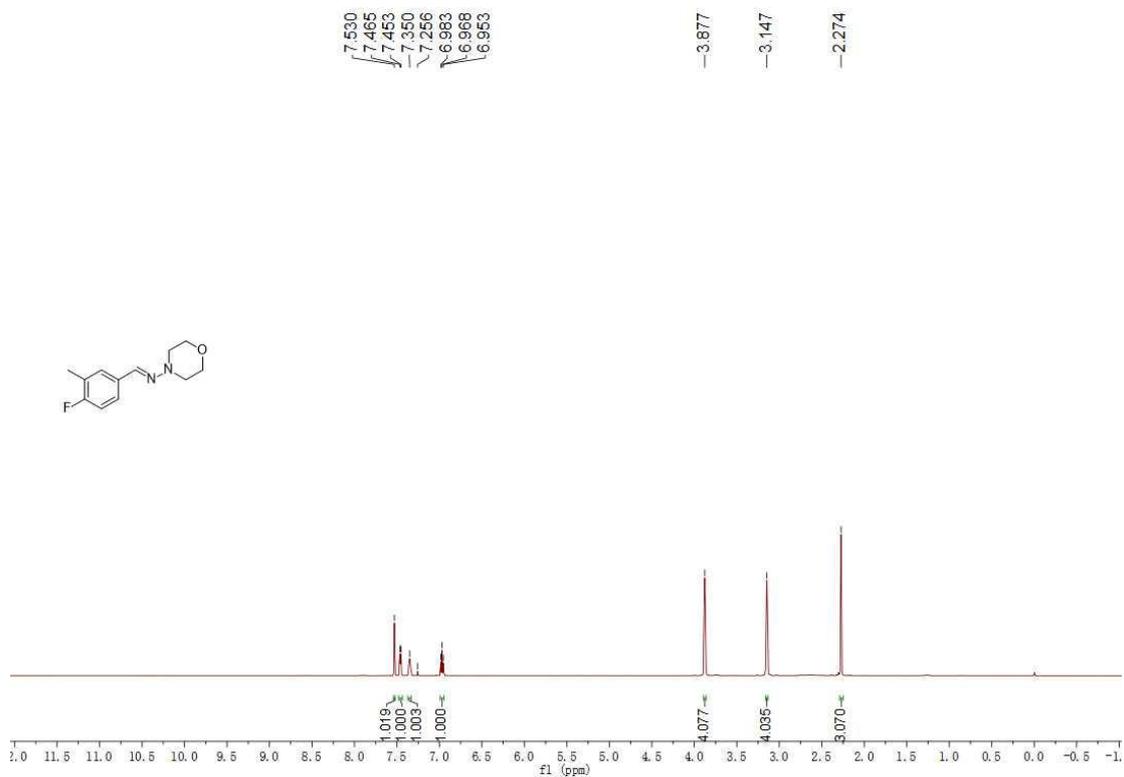
¹³C NMR (150 MHz, CDCl₃) Spectrum of A41



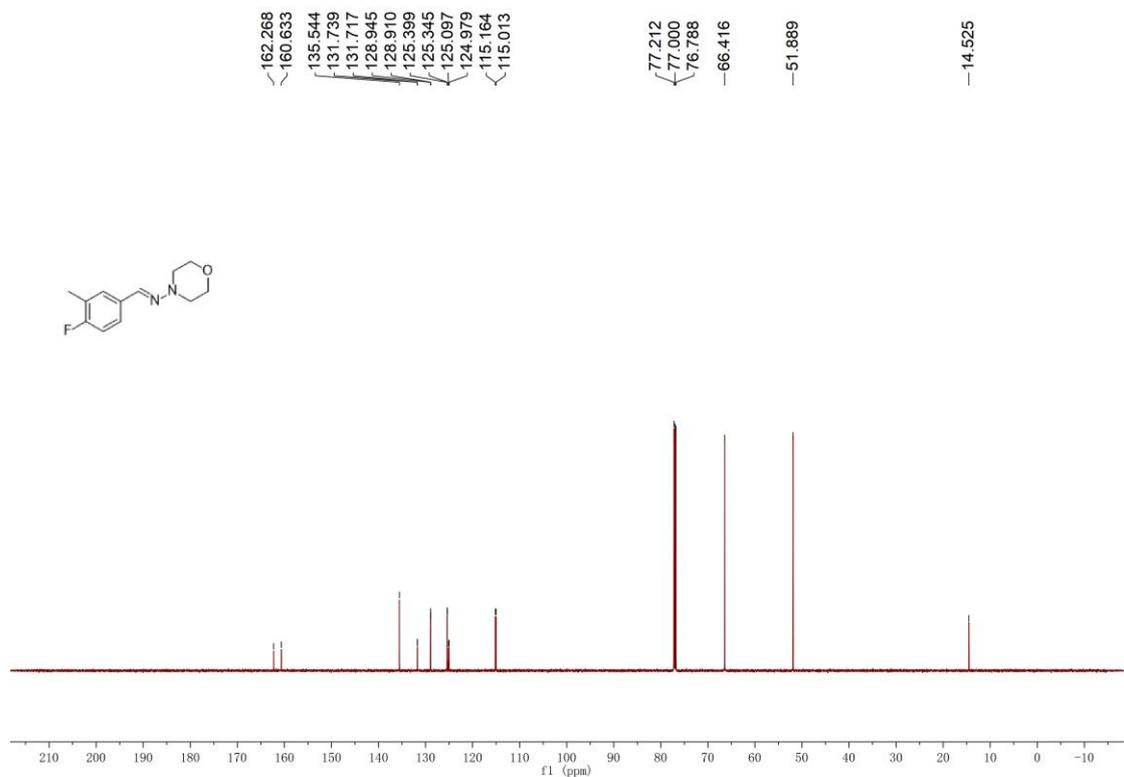
¹⁹F NMR (564 MHz, CDCl₃) Spectrum of A41



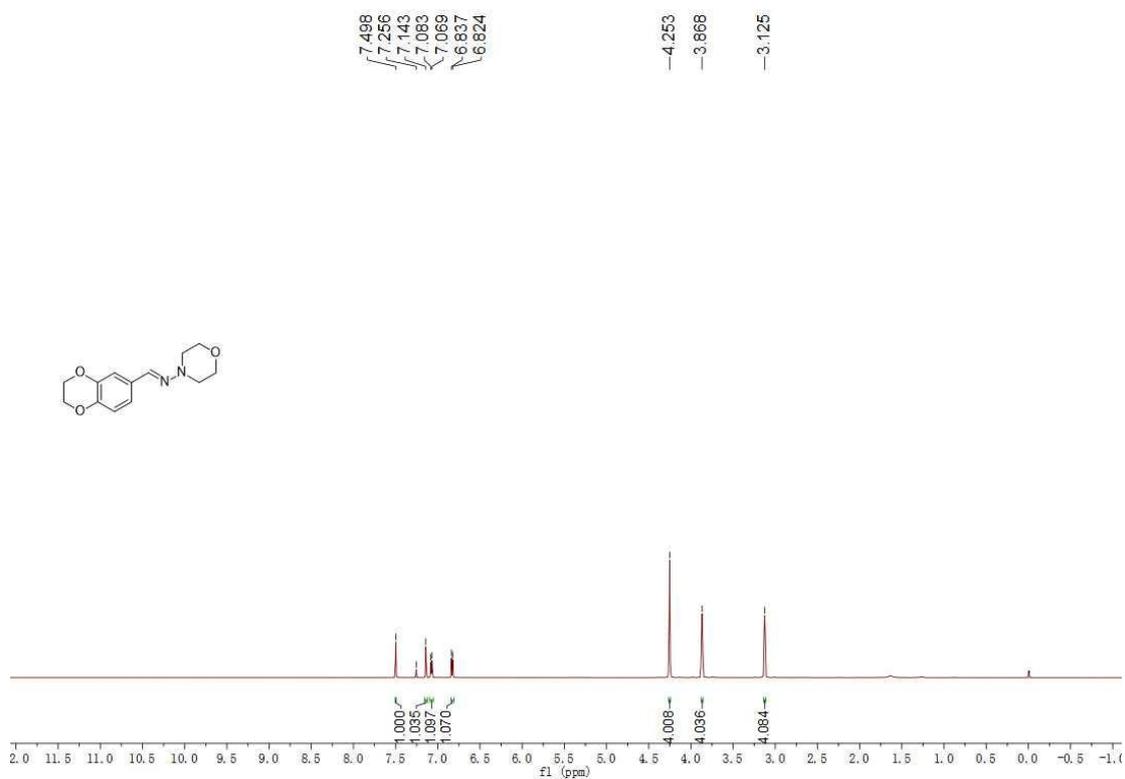
¹H NMR (600 MHz, CDCl₃) Spectrum of **A42**



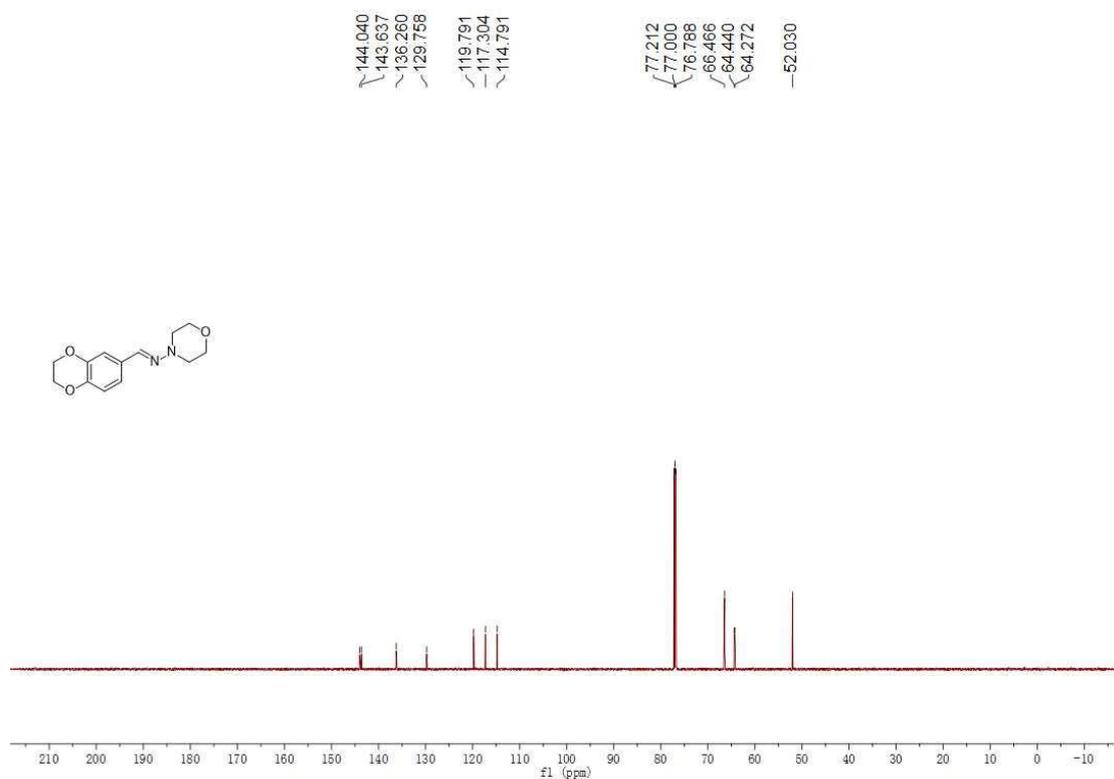
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A42**



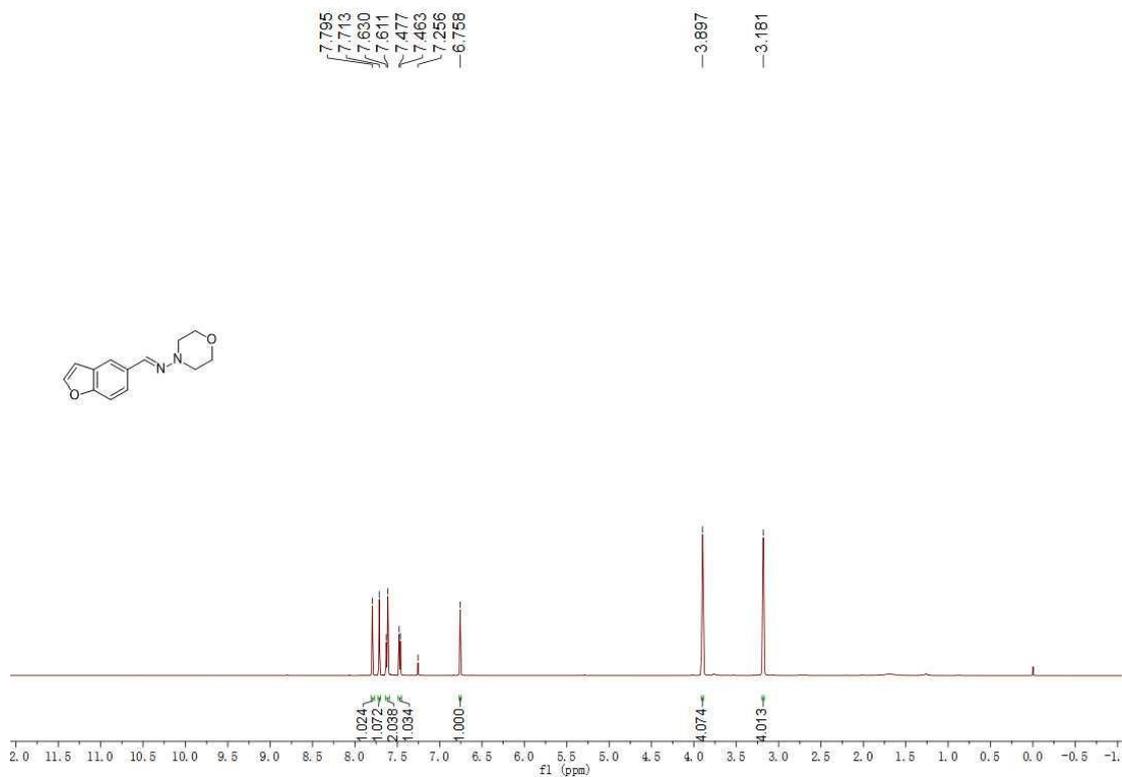
¹H NMR (600 MHz, CDCl₃) Spectrum of **A43**



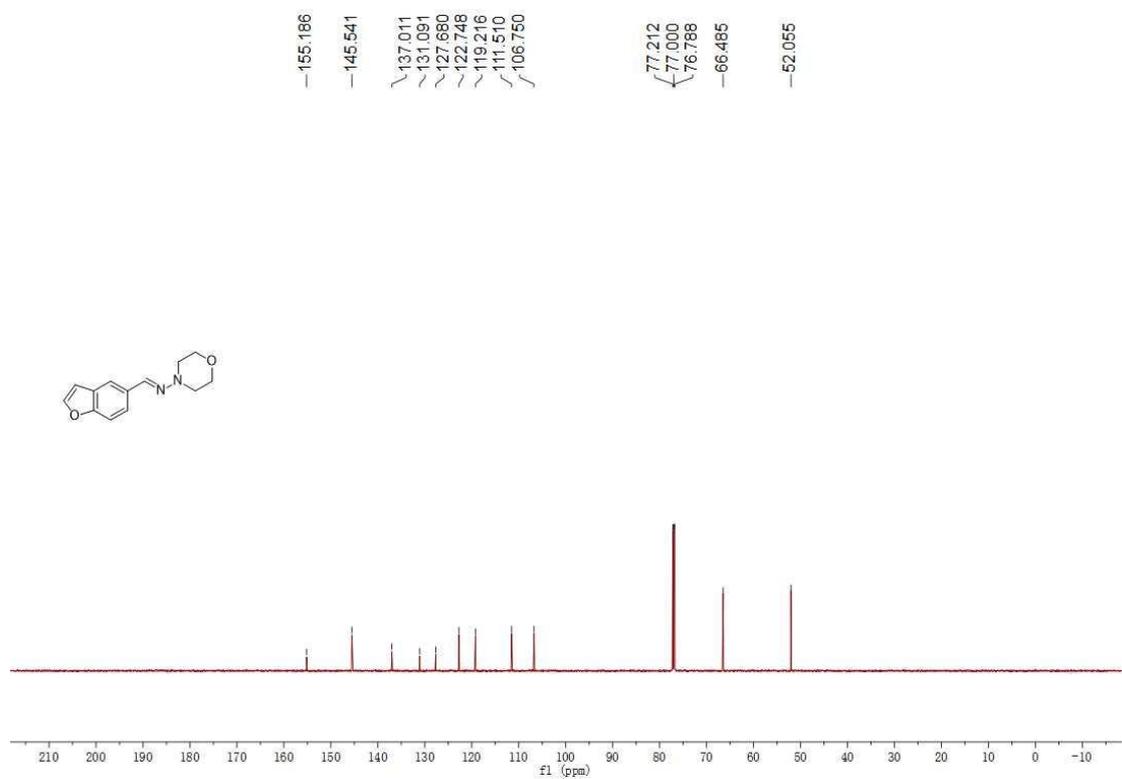
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A43**



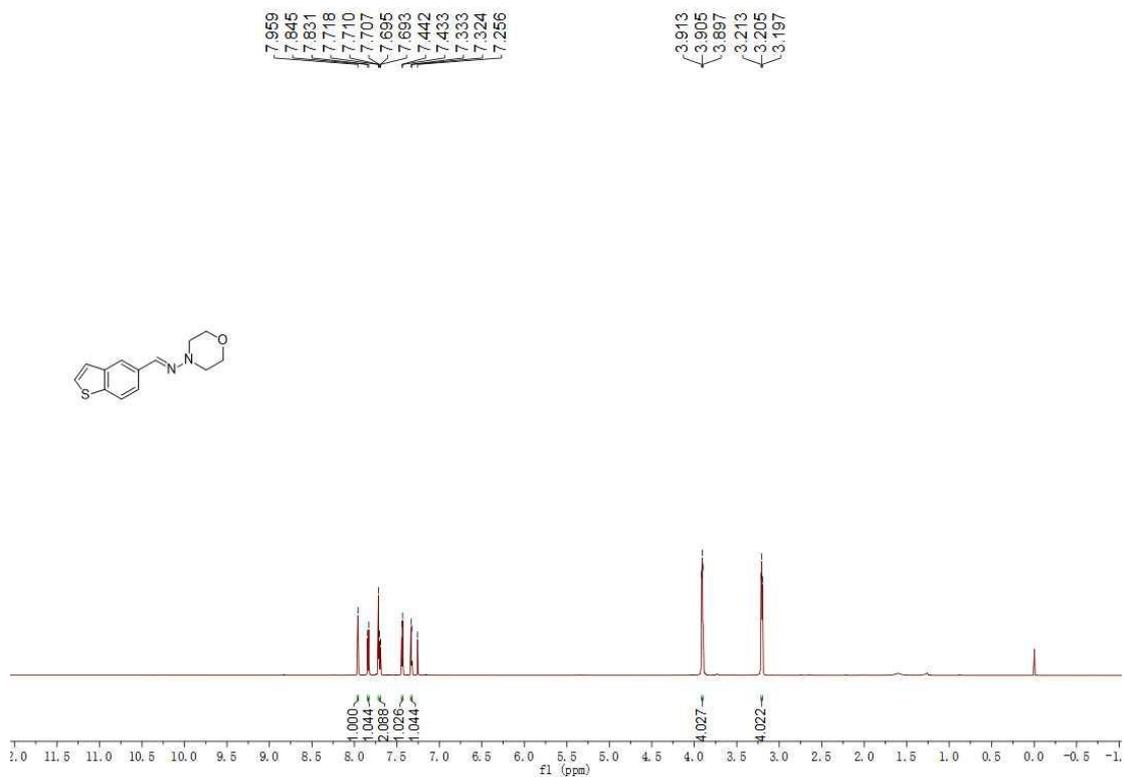
¹H NMR (600 MHz, CDCl₃) Spectrum of **A44**



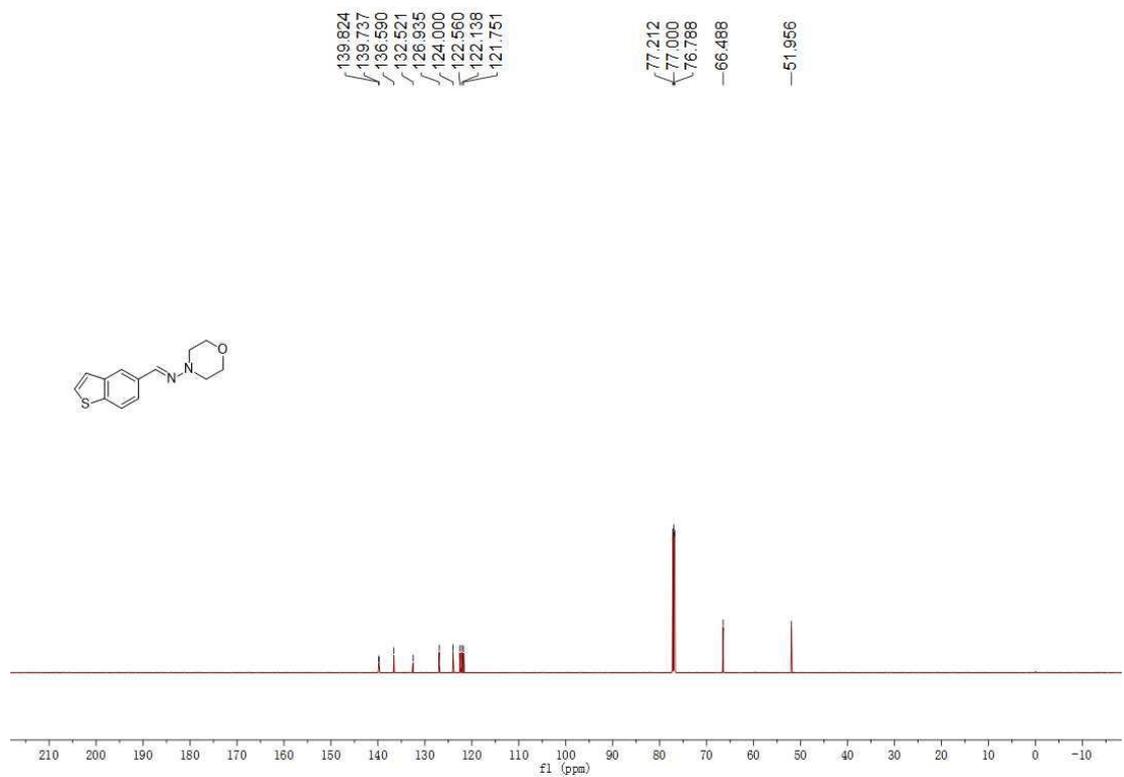
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A44**



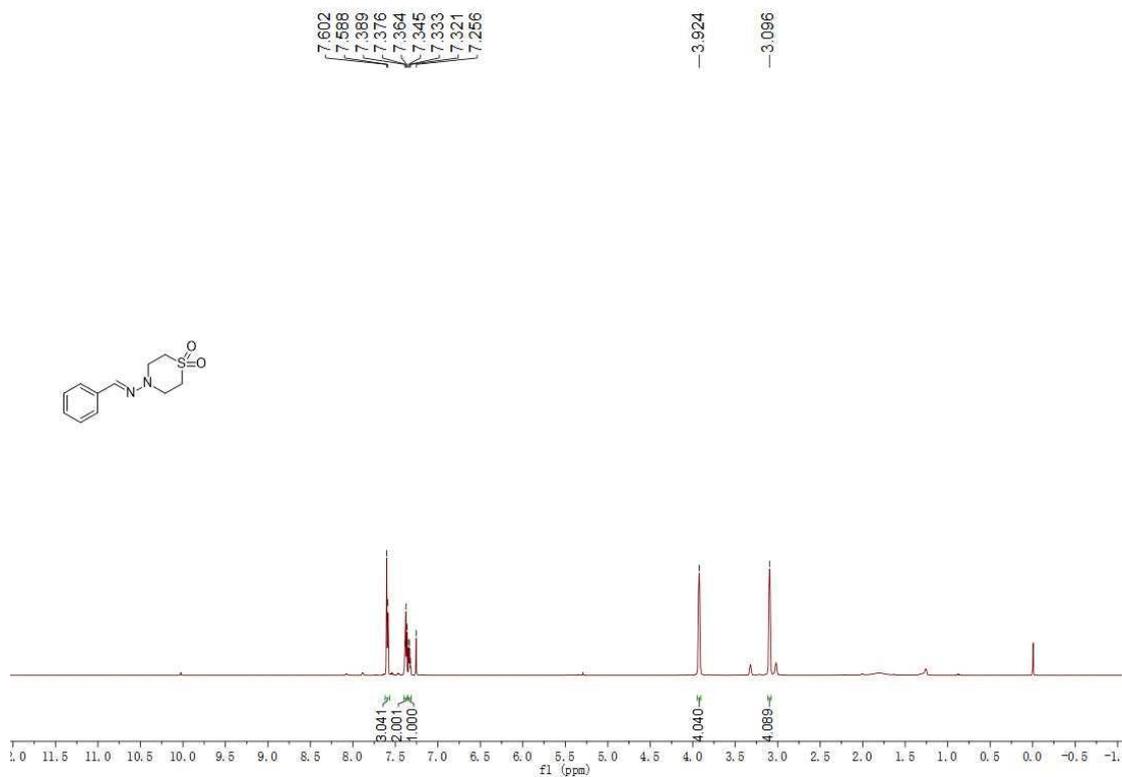
¹H NMR (600 MHz, CDCl₃) Spectrum of **A45**



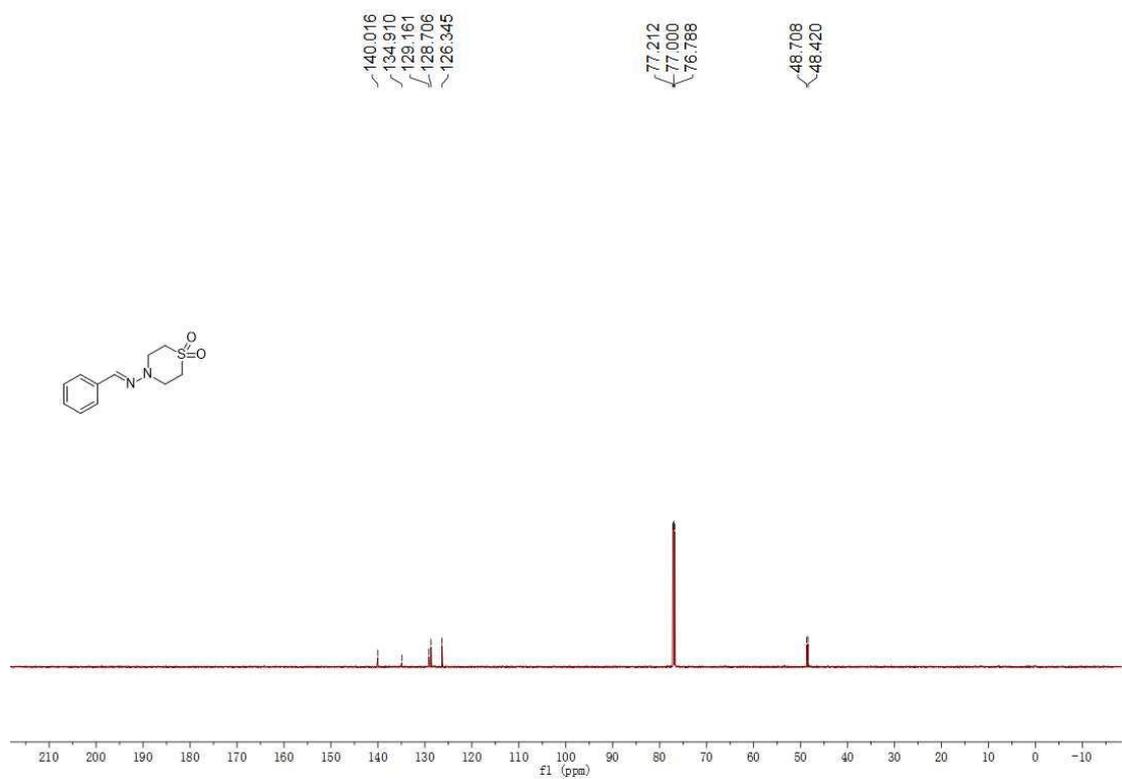
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A45**



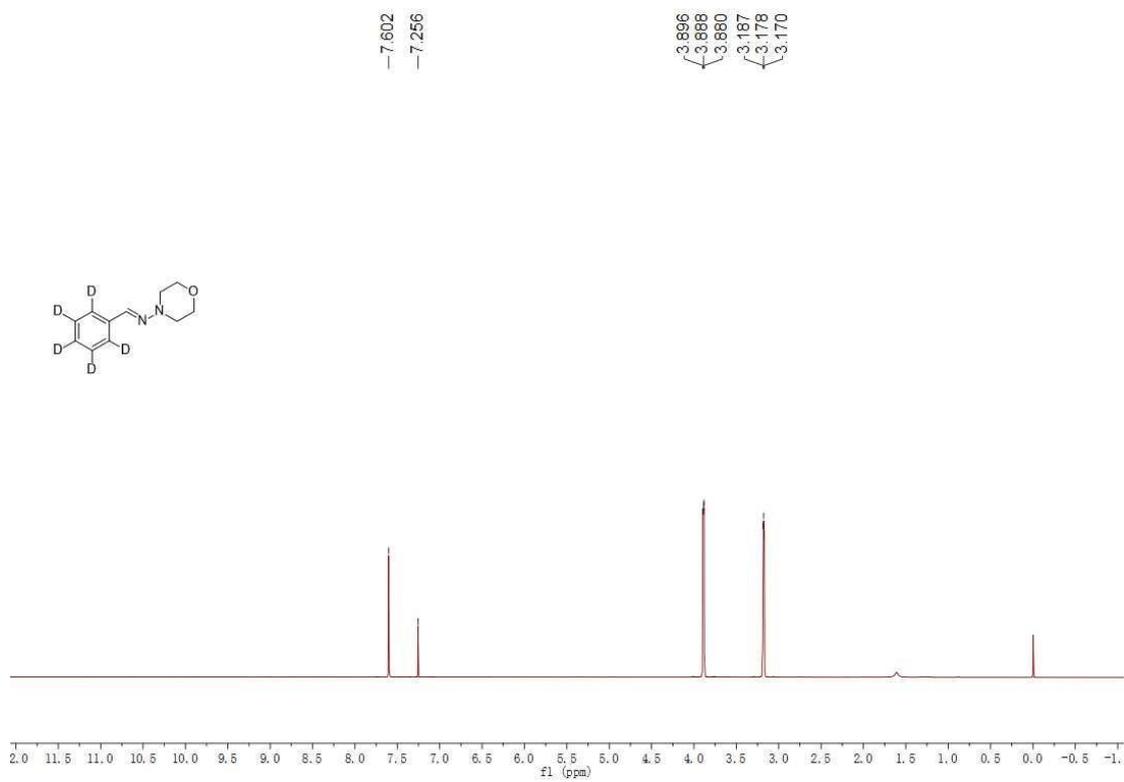
¹H NMR (600 MHz, CDCl₃) Spectrum of A47



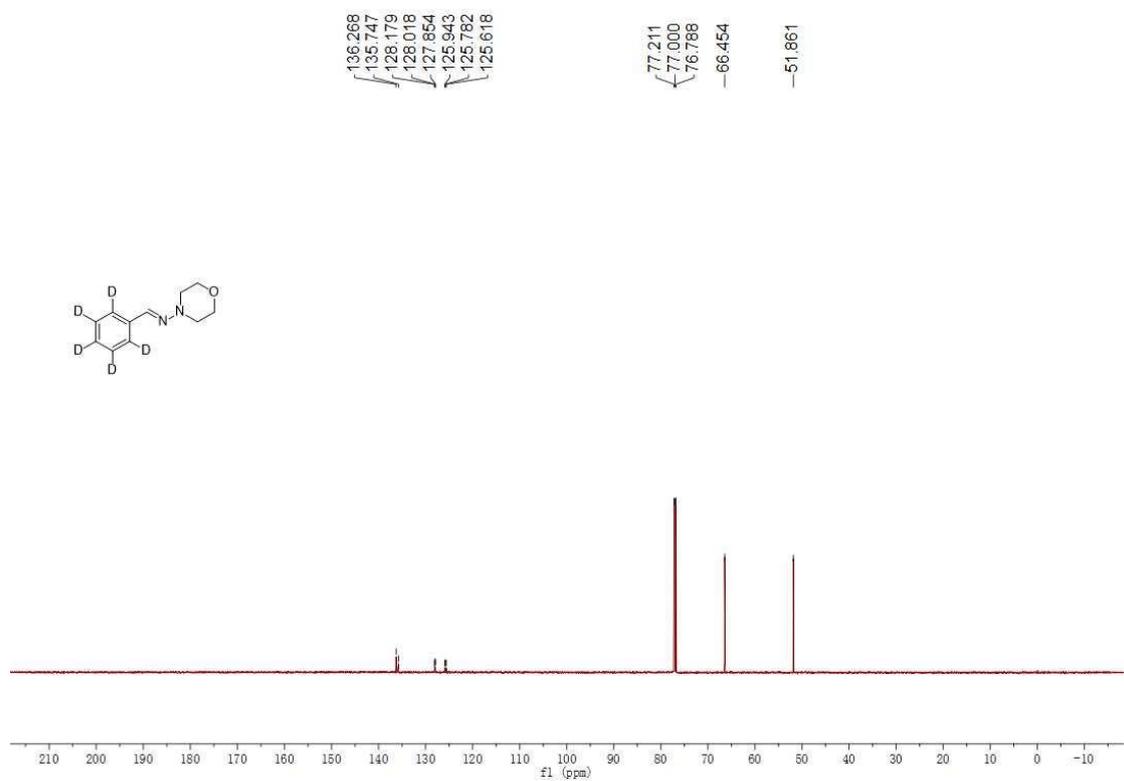
¹³C NMR (150 MHz, CDCl₃) Spectrum of A46



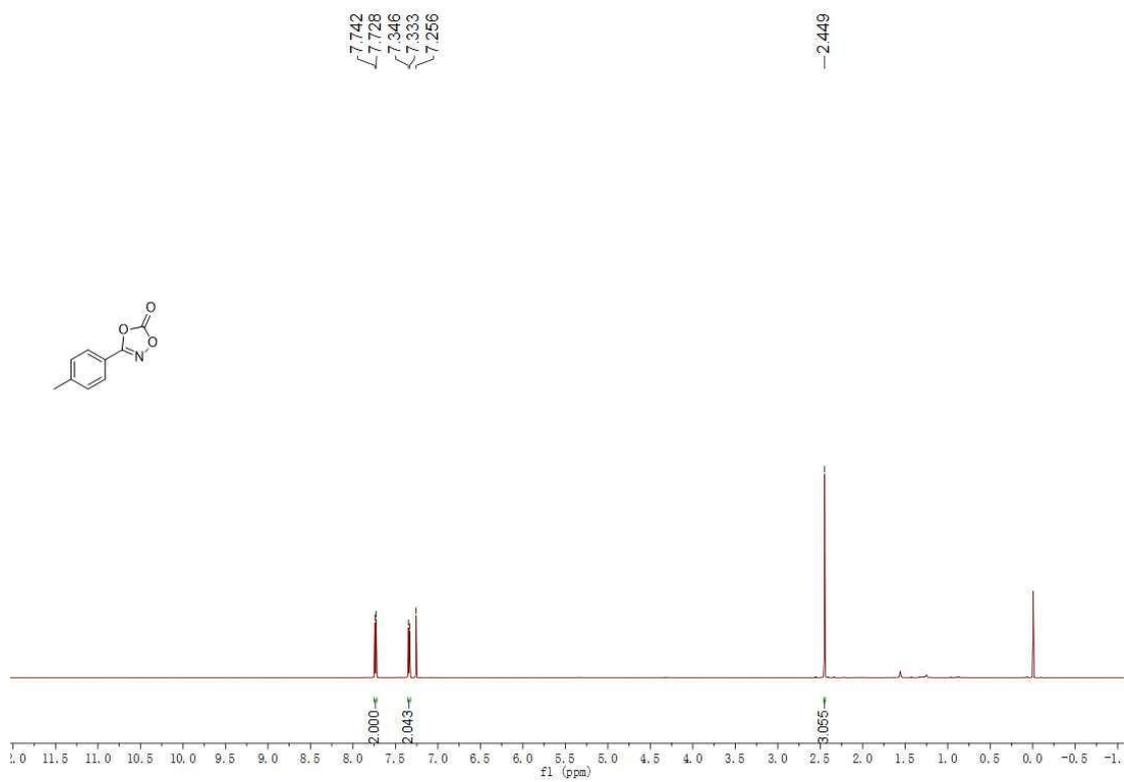
¹H NMR (600 MHz, CDCl₃) Spectrum of **A1-D5**



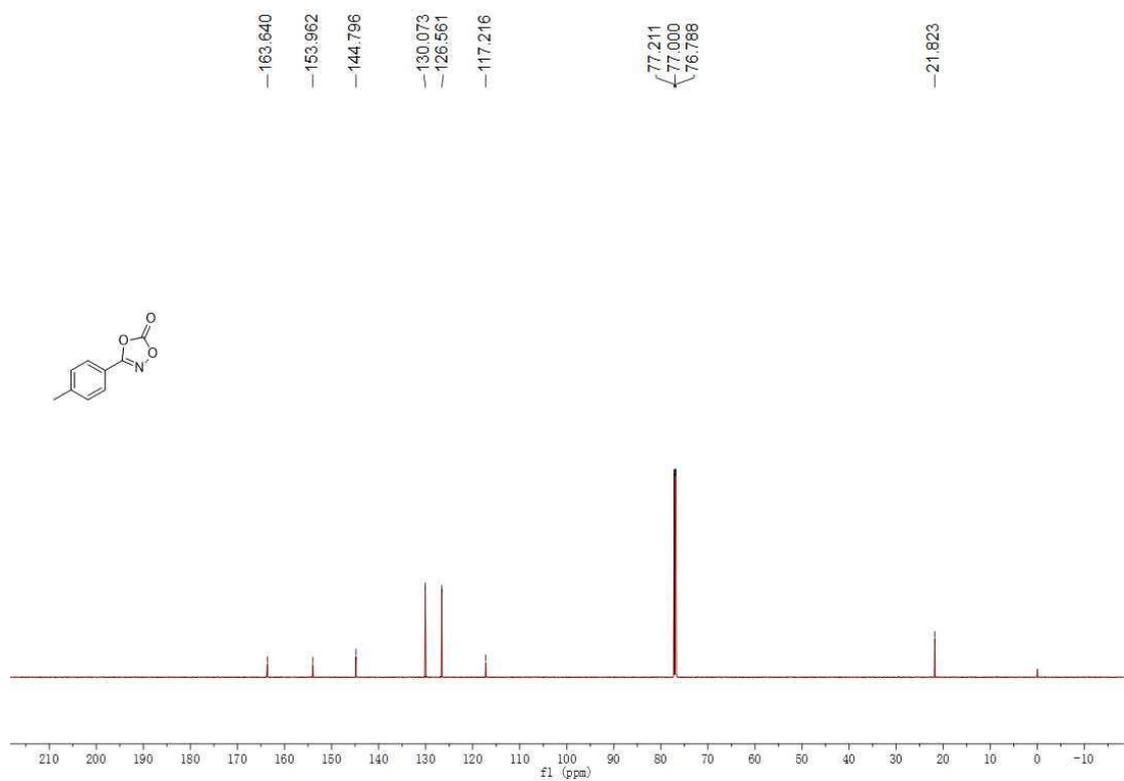
¹³C NMR (150 MHz, CDCl₃) Spectrum of **A1-D5**



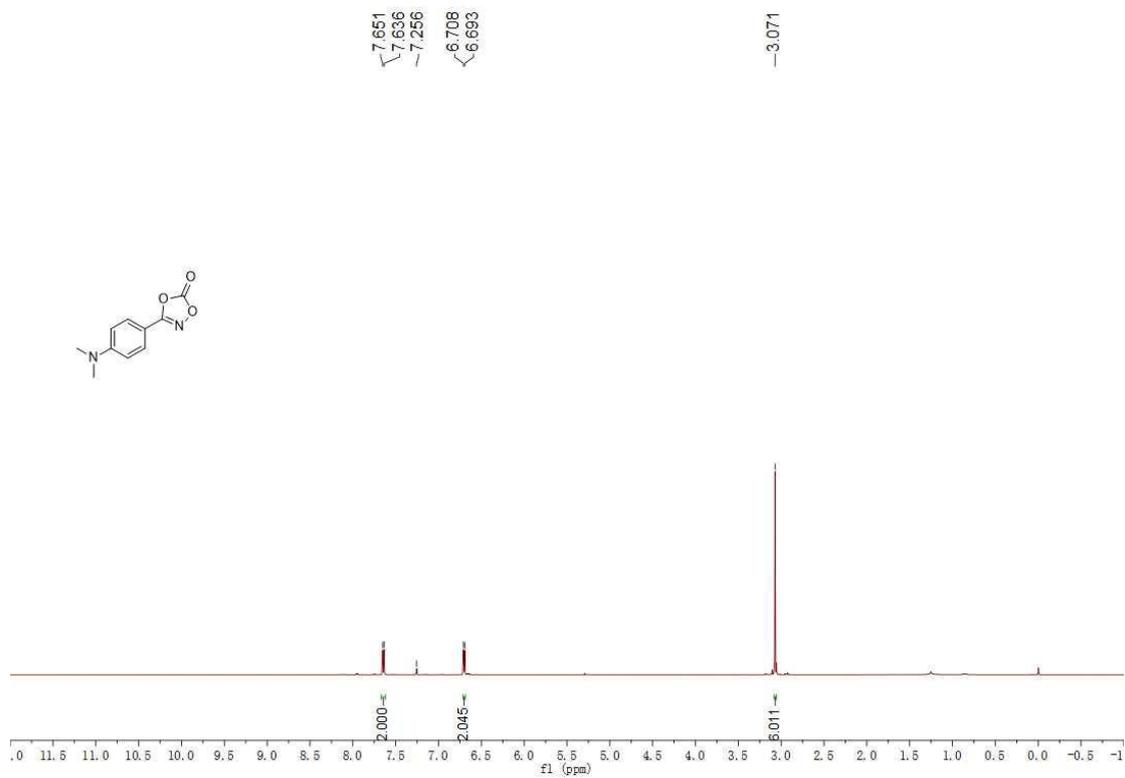
¹H NMR (600 MHz, CDCl₃) Spectrum of **B1**



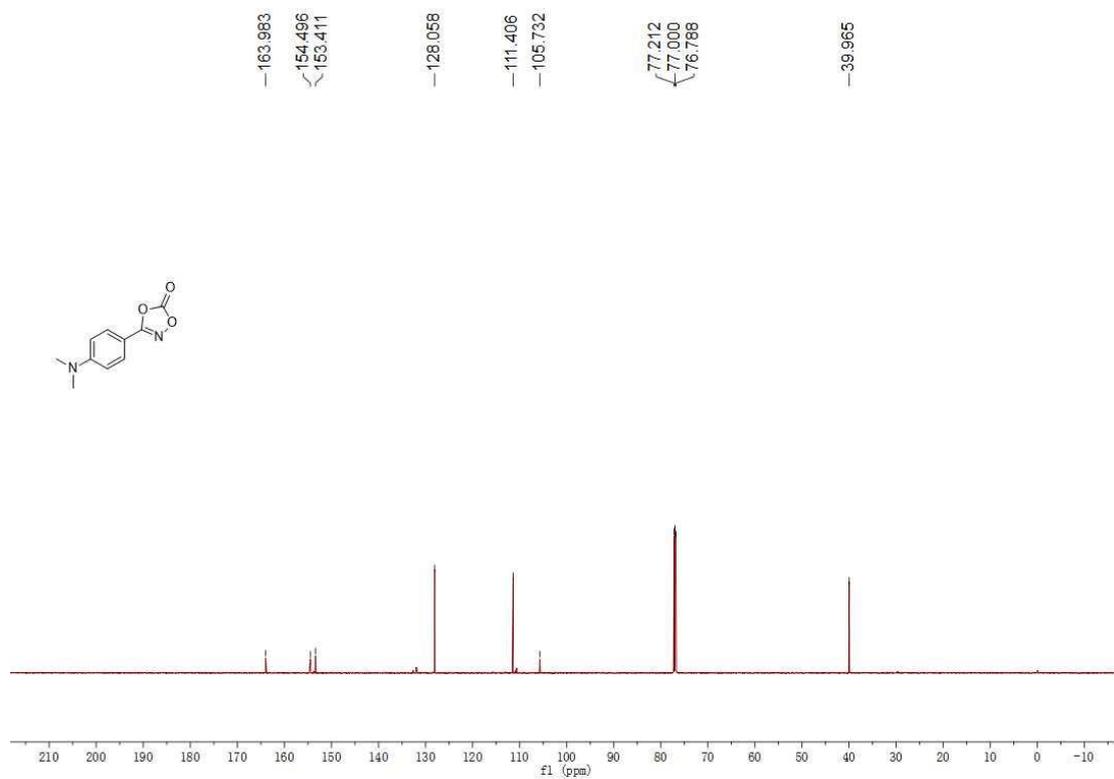
¹³C NMR (150 MHz, CDCl₃) Spectrum of **B1**



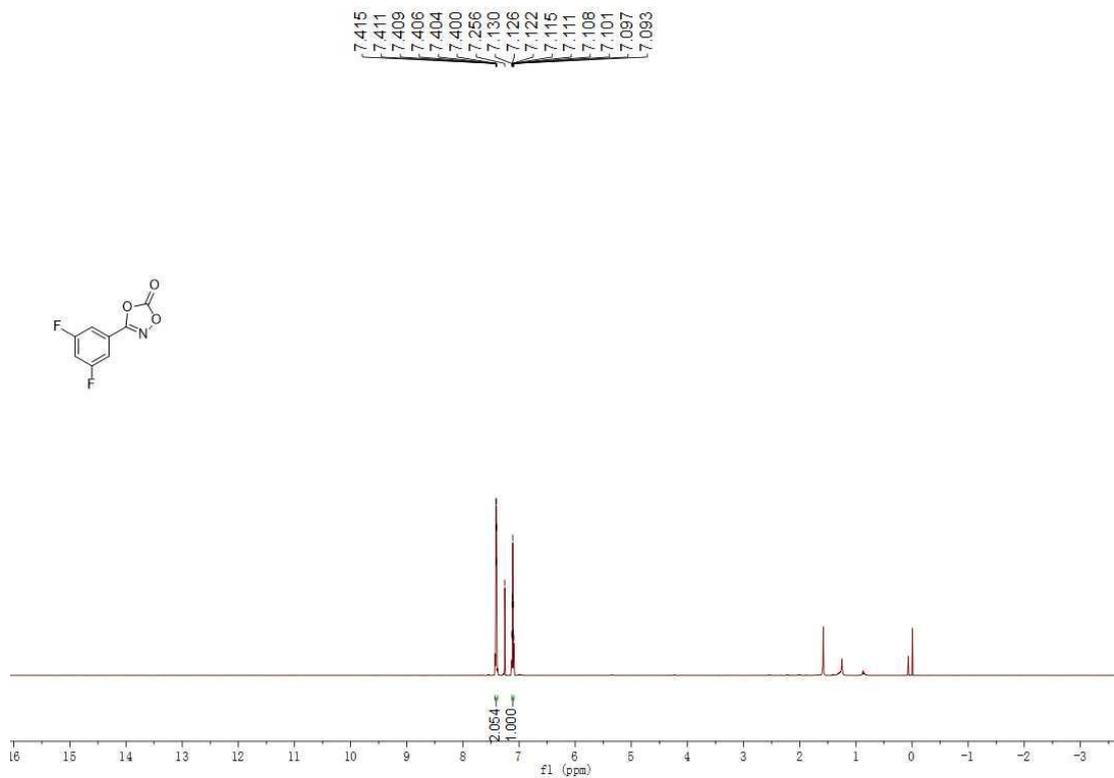
¹H NMR (600 MHz, CDCl₃) Spectrum of **B10**



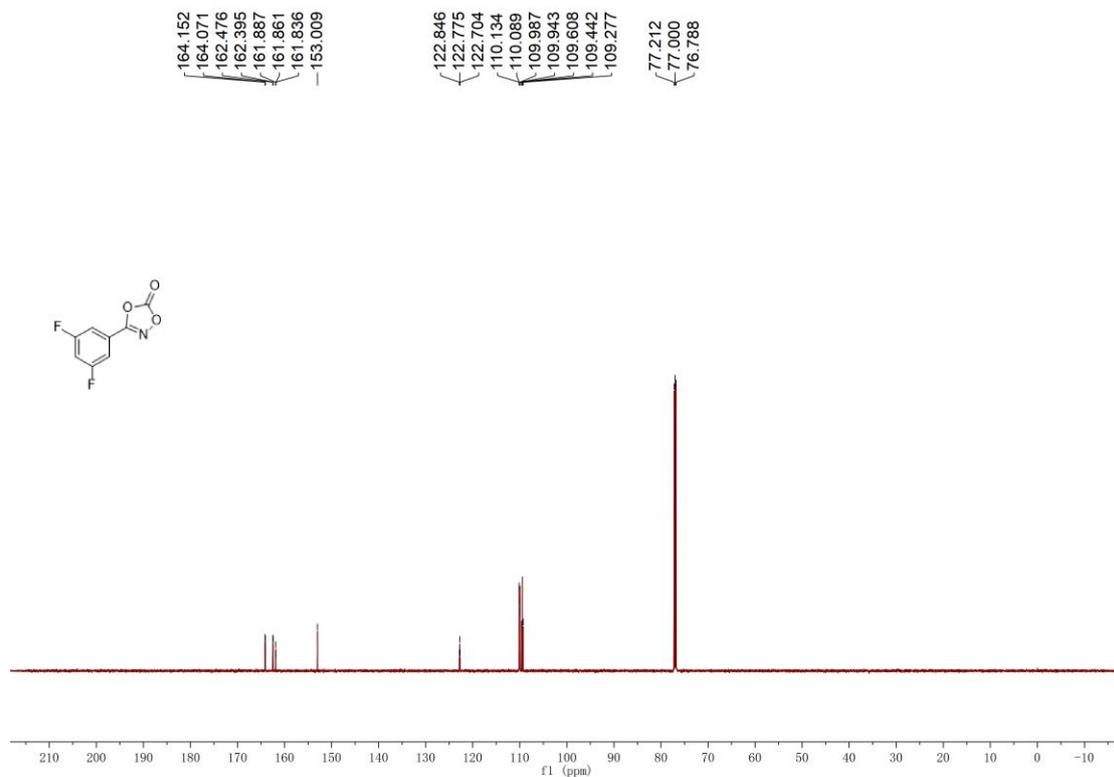
¹³C NMR (150 MHz, CDCl₃) Spectrum of **B10**



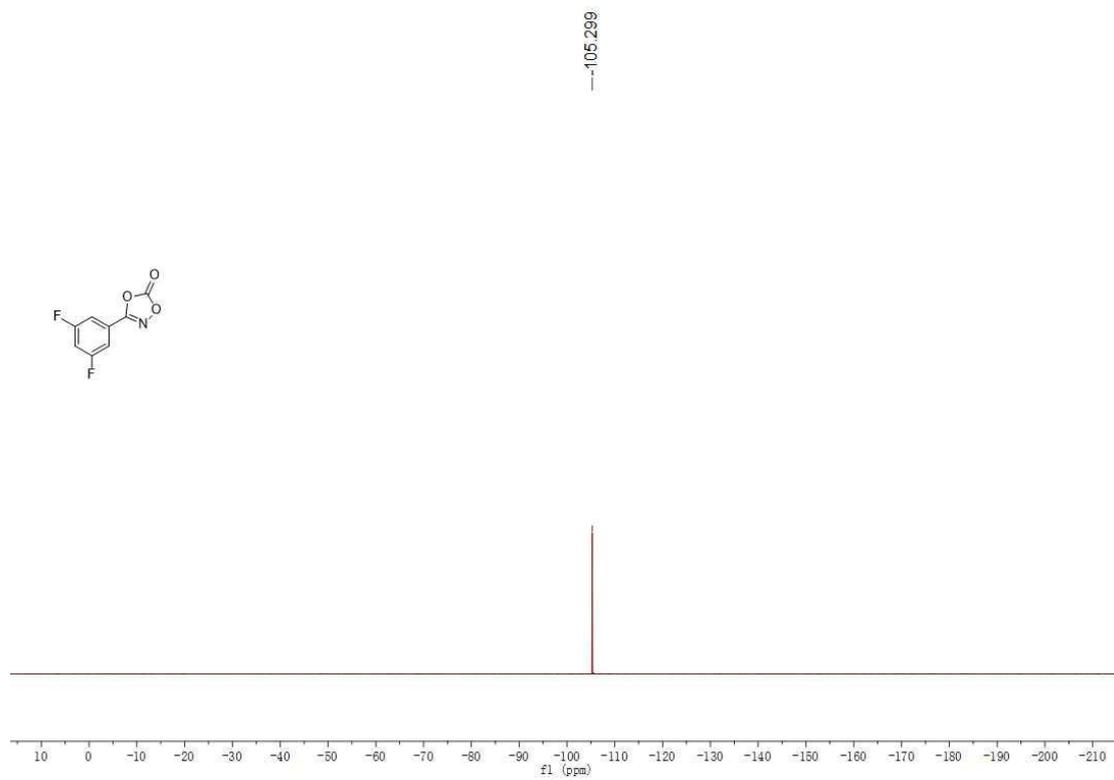
¹H NMR (600 MHz, CDCl₃) Spectrum of **B13**



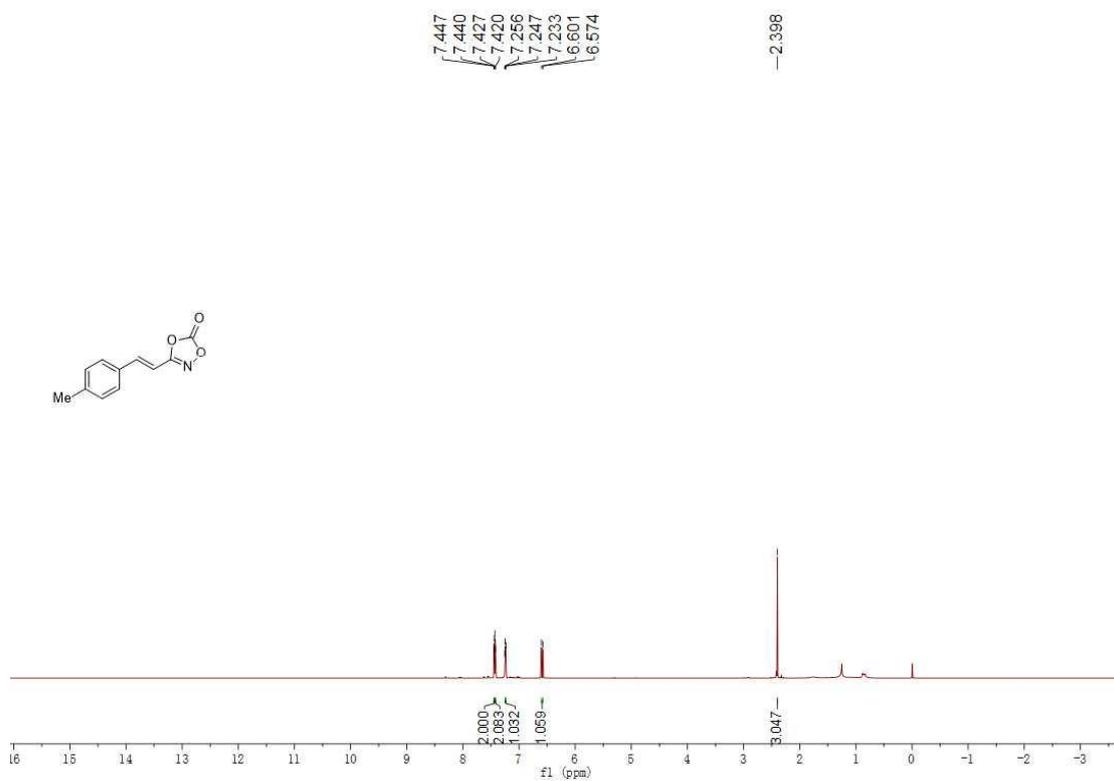
¹³C NMR (150 MHz, CDCl₃) Spectrum of **B13**



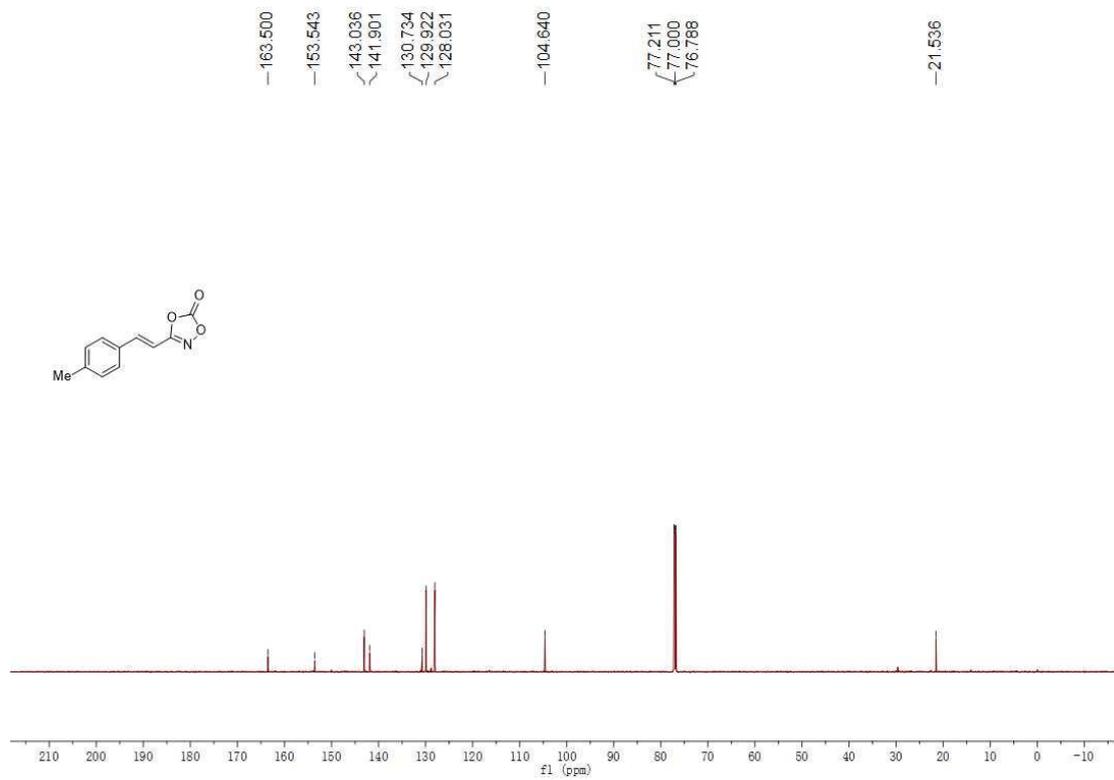
^{19}F NMR (564 MHz, CDCl_3) Spectrum of **B13**



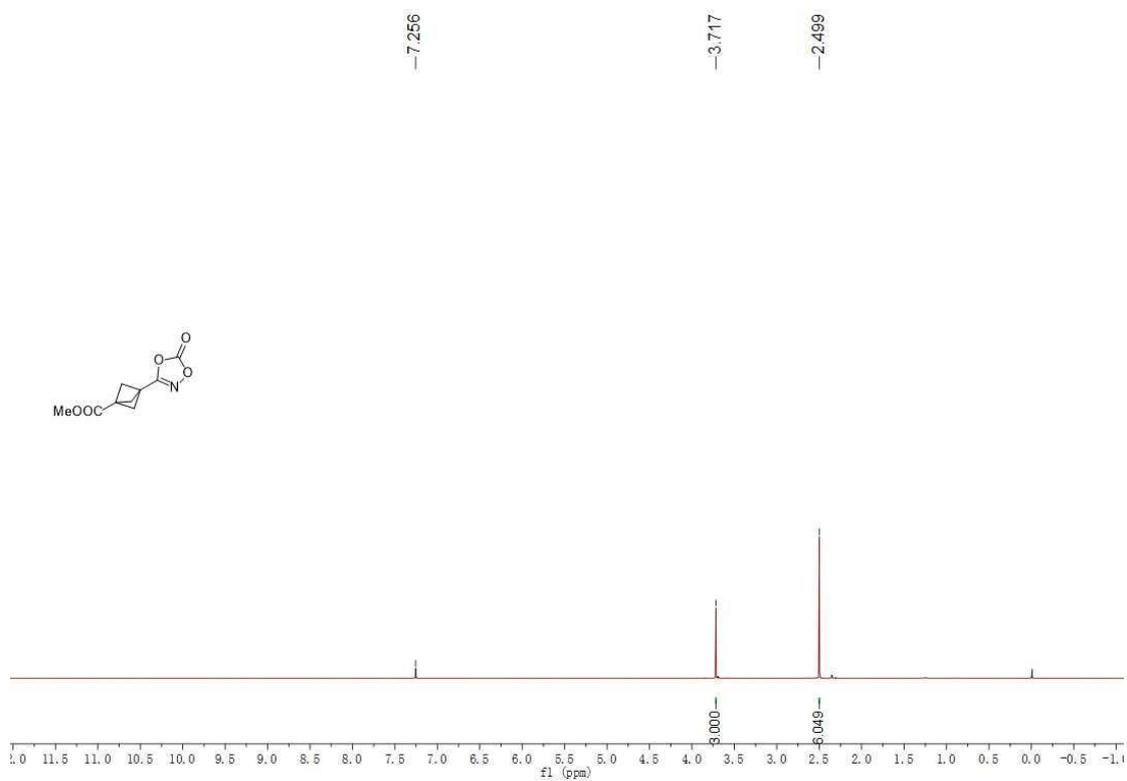
^1H NMR (600 MHz, CDCl_3) Spectrum of **B15**



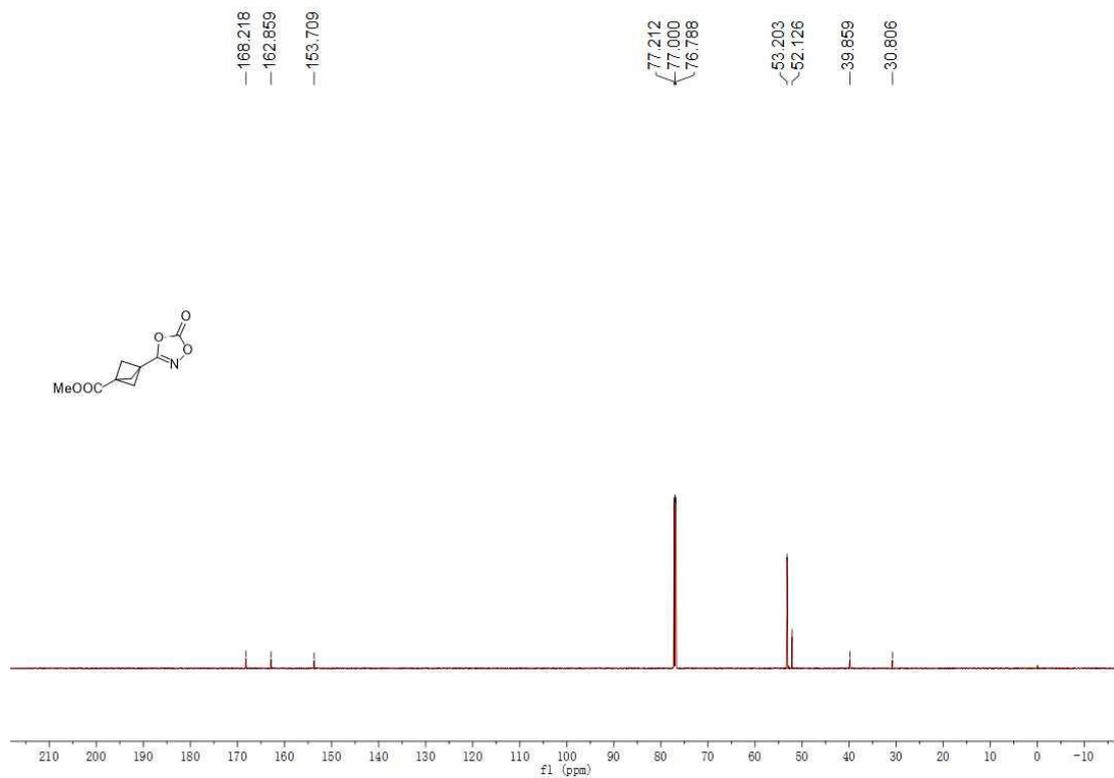
¹³C NMR (150 MHz, CDCl₃) Spectrum of **B15**



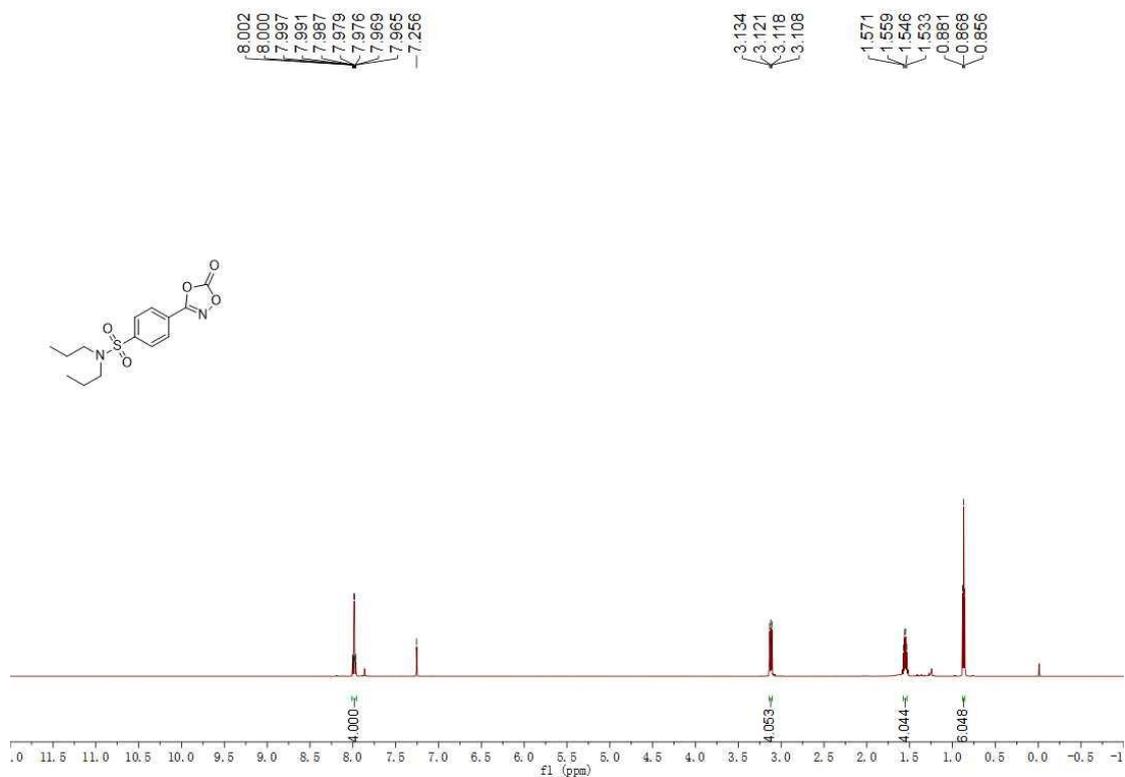
¹H NMR (600 MHz, CDCl₃) Spectrum of **B19**



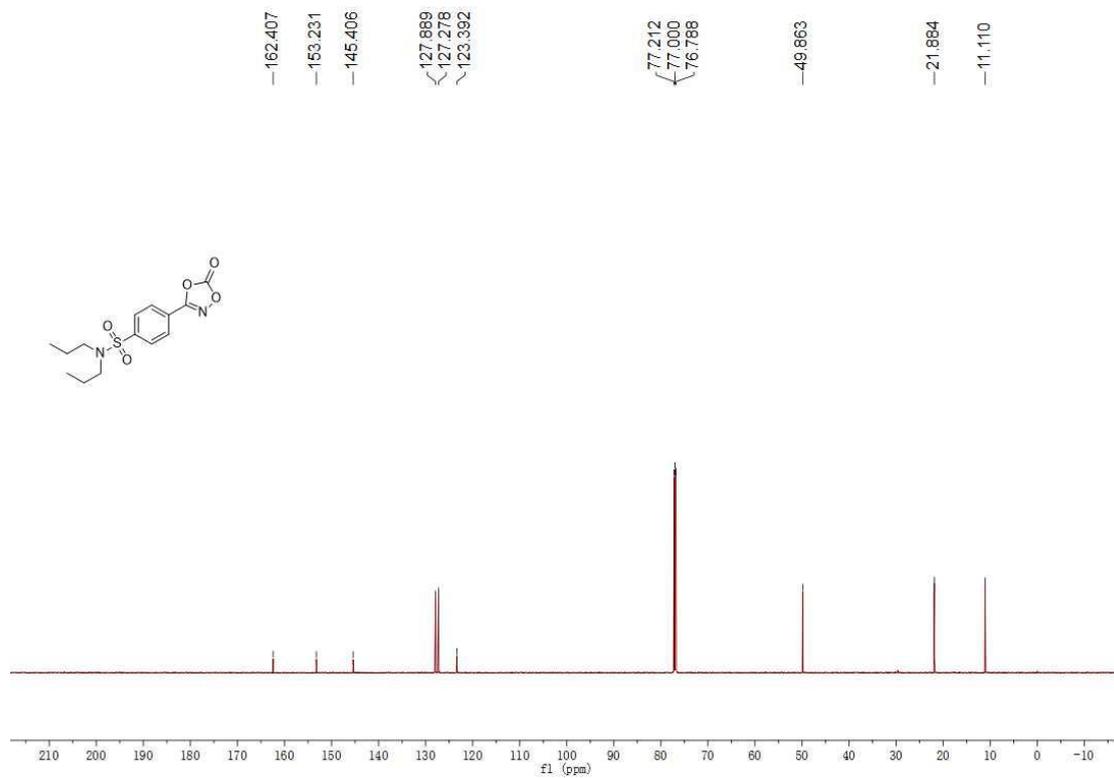
¹³C NMR (150 MHz, CDCl₃) Spectrum of **B19**



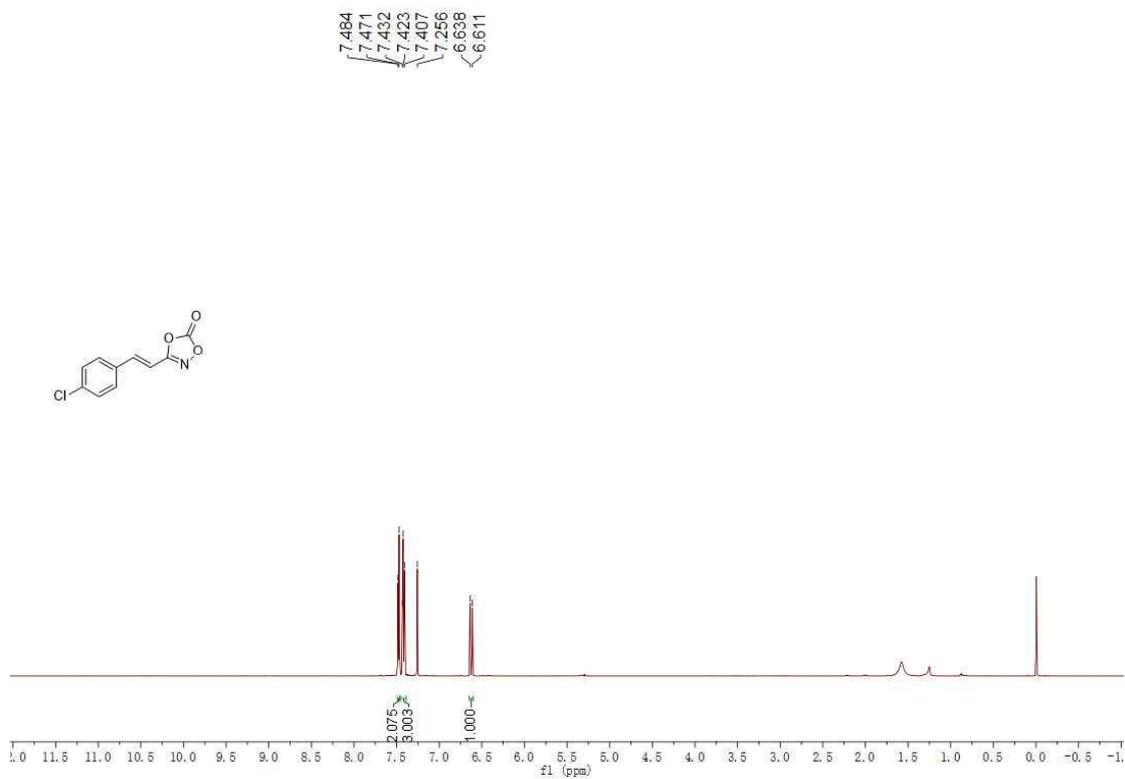
¹H NMR (600 MHz, CDCl₃) Spectrum of **B20**



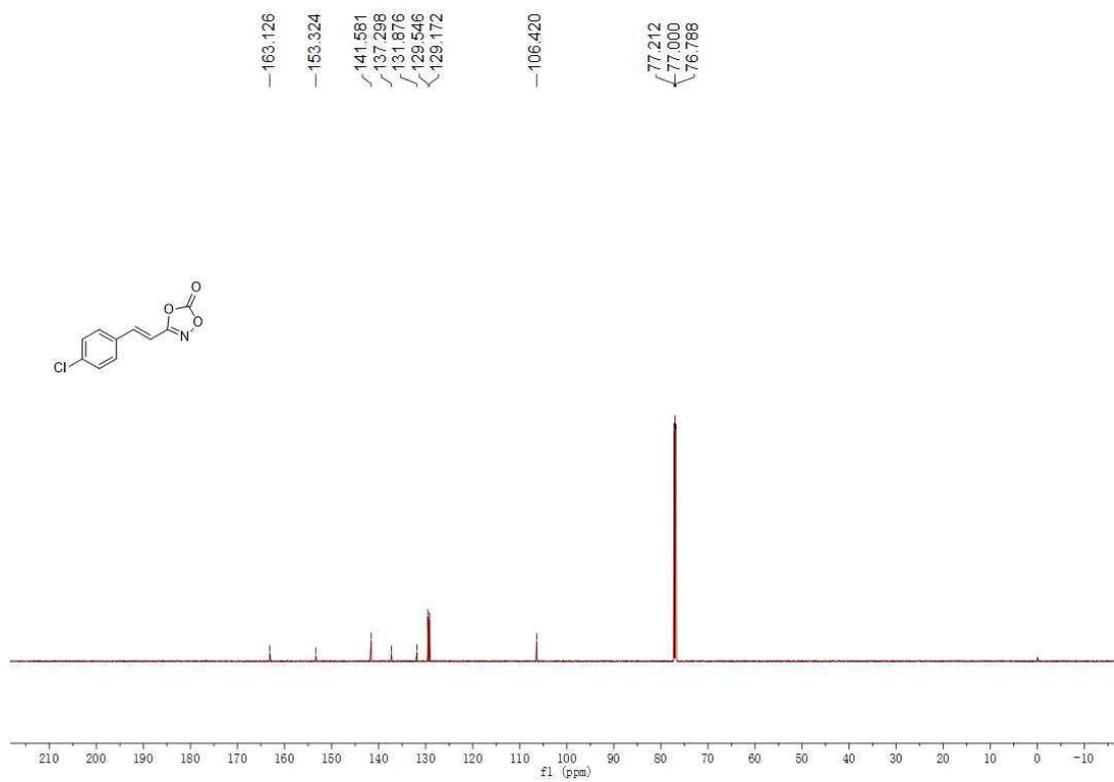
¹³C NMR (150 MHz, CDCl₃) Spectrum of **B20**



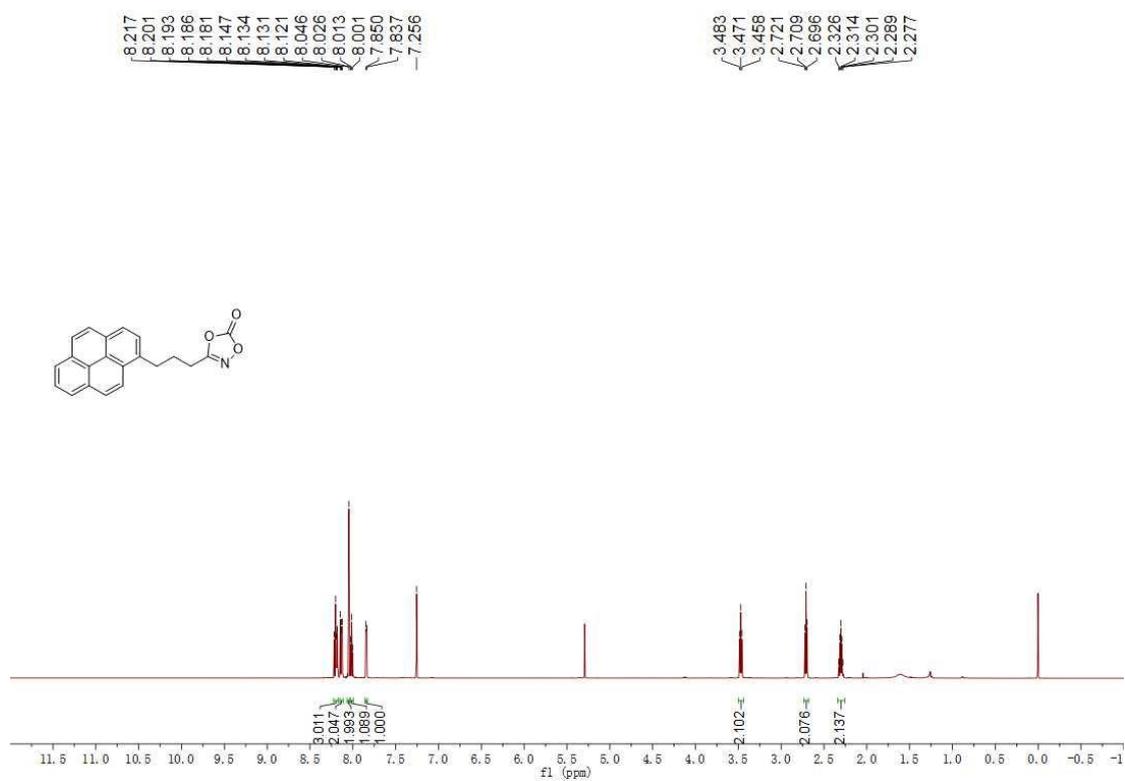
¹H NMR (600 MHz, CDCl₃) Spectrum of **B24**



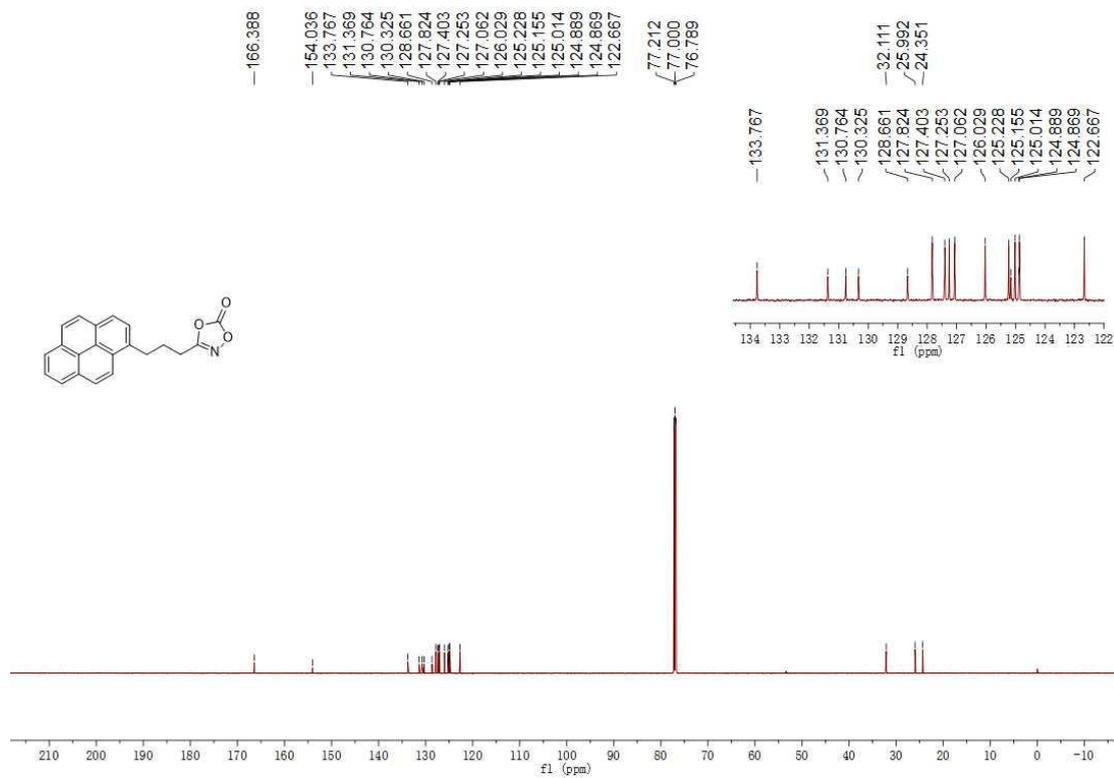
¹³C NMR (150 MHz, CDCl₃) Spectrum of **B24**



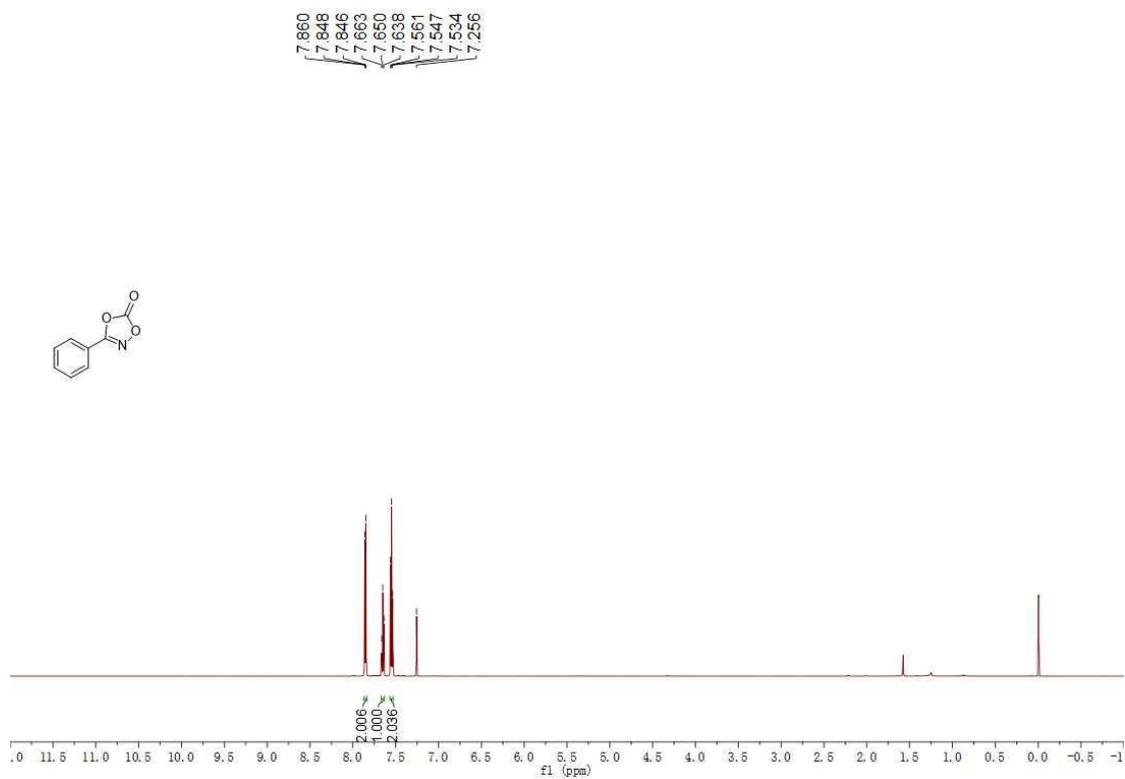
¹H NMR (600 MHz, CDCl₃) Spectrum of **B25**



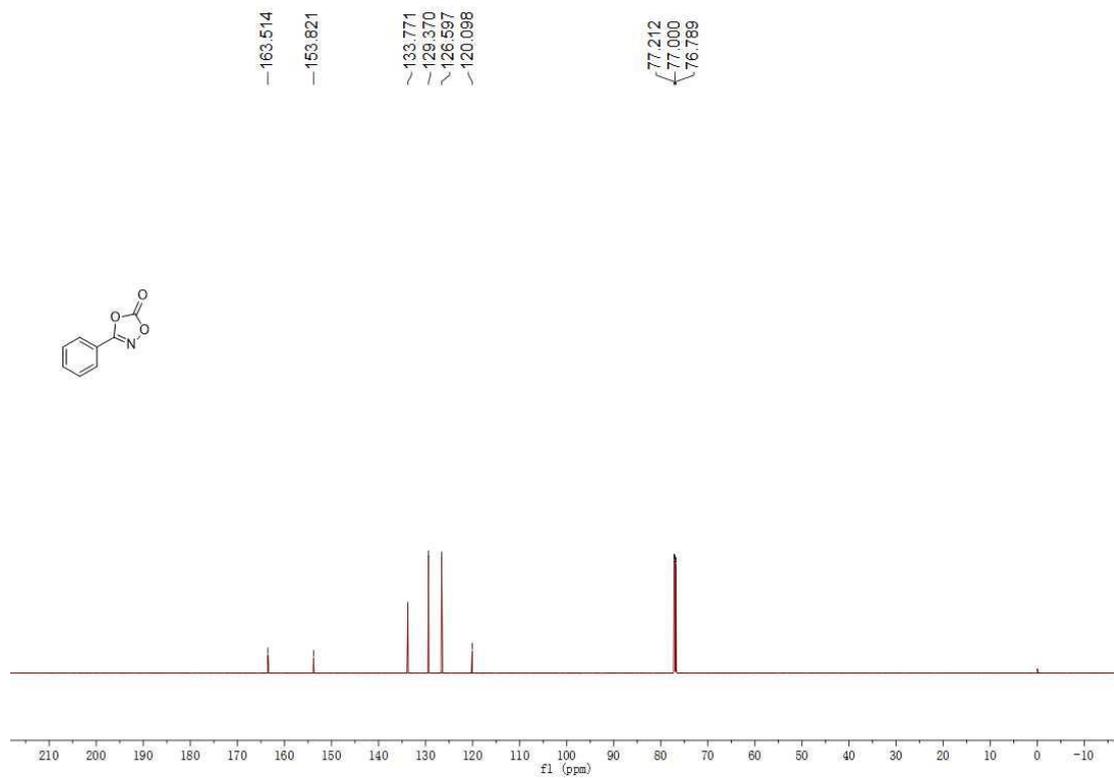
¹³C NMR (150 MHz, CDCl₃) Spectrum of **B25**



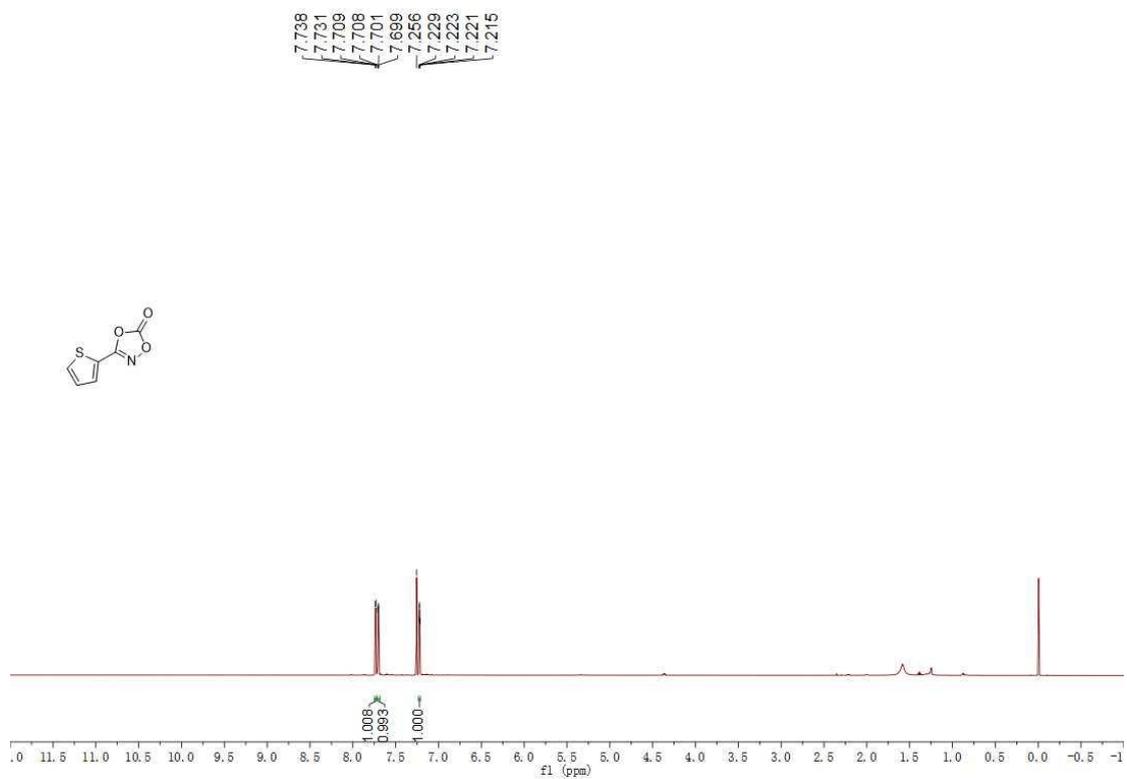
¹H NMR (600 MHz, CDCl₃) Spectrum of **B26**



¹³C NMR (150 MHz, CDCl₃) Spectrum of **B26**



¹H NMR (600 MHz, CDCl₃) Spectrum of **B29**



¹³C NMR (150 MHz, CDCl₃) Spectrum of **B29**

