

## *Supporting Information*

### **Visible light-triggered synthesis of oxime ethers using tetrabromomethane as mediate**

Meng Tu<sup>a</sup>, Bo-Jiang Chen<sup>a</sup>, Rukhsana<sup>a</sup>, Wen-Ying Cui<sup>a</sup>, Wen-Tao Fu<sup>a</sup>, Cheng-Shuo Shen<sup>a\*</sup>, Yong-Miao Shen<sup>a,b\*</sup>

<sup>a</sup> Department of Chemistry, Zhejiang Sci-Tech University, Hangzhou, Zhejiang 310018, PR China, E-mail: [shenym@zstu.edu.cn](mailto:shenym@zstu.edu.cn)

<sup>b</sup> Key Laboratory of Excited-State Materials of Zhejiang Province, Zhejiang University, Hangzhou 310027, PR China

### **Table of Contents**

1. General Information .....	S2
2. General Steps in the Synthesis of Ketoximes .....	S3
3. General Procedure for Synthesis of Products .....	S3
4. Gram-scale reaction.....	S4
5. Photoredox Transfer Hydrogenation under Solar Irradiation .....	S4
6. UV Spectral of Benzophenone oxime, CBr <sub>4</sub> and Reaction System . .....	S4
7. Control experiments with LED light on/off.....	S5
8. Kinetic Isotope Effect Experiments .....	S5
9. Theoretical Calculations .....	S6
10 Quantitative NMR .....	S10
11. Characterization Data .....	S12
12. <sup>1</sup> H NMR and <sup>13</sup> C NMR Spectra .....	S28
13. Reference .....	S64

## 1. General Information

**General Remarks.** Catalytic reactions were performed using pre-dried glassware. Analytical TLC was performed with silica gel GF254 plates. For column chromatography, a 200–300 mesh silica gel was employed. Organic solutions were concentrated under reduced pressure using a rotary evaporator. Room temperature (r.t.) is 23–25 °C.

**Instrumentation.**  $^1\text{H}$  NMR spectra were recorded on Bruker AVANCE III 400 and INOVA instruments with 400 MHz frequencies, and  $^{13}\text{C}$  NMR spectra were recorded on Bruker AVANCE III 400 with 101 MHz frequencies.  $^{19}\text{F}$  NMR spectra were recorded on a Bruker AVANCE III 400 spectrometer with a  $^{19}\text{F}$  operating frequency of 376 MHz were reported in ppm relative to the residual solvent signal ( $\text{CDCl}_3$   $\delta = 7.26$  for  $^1\text{H}$  NMR and  $\delta = 77.0$  for  $^{13}\text{C}$  NMR). Chemical shifts (ppm) were recorded with tetramethylsilane (TMS) as the internal reference standard. Multiplicities are given as s (singlet), d (doublet), t (triplet), dd (doublet of doublets), td (triplet of doublets) or m (multiplet). HRMS was obtained using a Q-TOF instrument equipped with an ESI source.

**Materials.** All chemicals were obtained from commercial sources and were used as received unless otherwise noted. Commercial reagents and analytical grade or anhydrous solvent were used without further purification. The ketoximes used are prepared from the corresponding ketones, except for benzophenone oxime.

**Light source in detail.** The light source used for photochemical experiments was a household 3 W fluorescent bulb (Figure S1), purchased from taobao.COM. The reaction vessel is borosilicate glass test tube and no filters were applied. The distance from the light source to the irradiation vessel is 2–3cm.



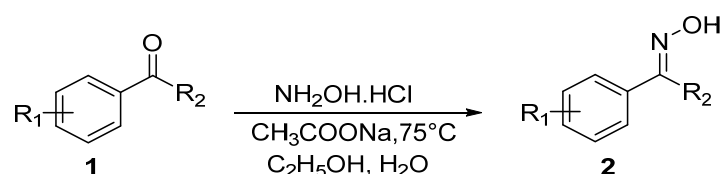
**Figure S1. Reaction device**

LED fixed lamp (Figure S2), 15–40 W ( $\lambda = 470 \pm 15$  nm). Product model: PLS-LED 100 Manufacturer: Beijing Perfect light Technology Co., Ltd. (China). The reaction vessel is borosilicate glass test tube and no filters were applied. The distance from the light source to the irradiation vessel is 4–5 cm.



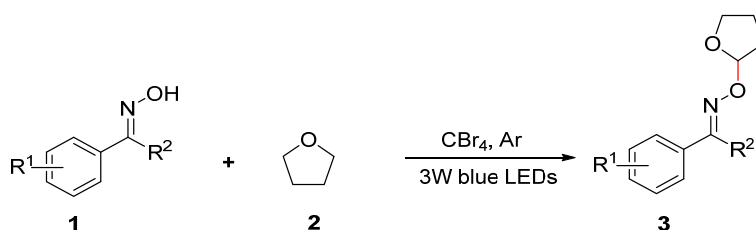
Figure S2. Photoreaction setup for scale-up reaction.

## 2. General Steps in the Synthesis of Ketoximes



To a 100 mL round bottom flask was added **1** (10 mmol), hydroxylamine hydrochloride (15.0 mmol, 1.5 equiv.), sodium acetate (15 mmol, 1.5 equiv.), ethanol (15 mL) and water (15 mL). The reaction was heated to 75 °C and monitored by thin layer chromatography spectroscopy (TLC). After complete conversion of the reactants, the mixture was cooled to room temperature and the solvent was removed by distillation under reduced pressure. The resulting residue mixture was dissolved with ethyl acetate, washed with water and saturated brine, dried with anhydrous magnesium sulphate and concentrated by rotary evaporation to give crude product **2**. If impurities are present, they are separated by column chromatography and applied to the next step.

## 3. General Procedure for Synthesis of Products



To 4 mL vials respectively equipped with a Teflon septum and magnetic stir bar were added 2 ml Anhydrous n-butyl acetate, **1** (0.1 mmol), THF (5 mmol), molecular sieves (4Å) (0.1 g), and CBr<sub>4</sub> (0.18 mmol). After aeration under argon for 15 min, the solution was irradiated under a blue LED (2 × 3 W) for 5 h. After the reaction, the molecular sieves were removed by centrifugation, and the supernatant was concentrated in vacuo. The crude mixture was directly purified by column chromatography on silica gel (ethyl acetate/petroleum ether 1:30 to 1:15) to give the desired products **3**.

## 4. Gram-scale reaction

To four 100 ml aubergine flasks with rubber flip-top stoppers and magnetic stirring bars was added 1.000 g of 1c, 1d, 1p and 1z, each with 50 ml of n-butyl acetate anhydrous, THF (50 equiv.), molecular sieve (4Å) (1.000 g) and carbon tetrabromide (1.8 equiv.), respectively. After aeration under argon for 30 min, the solution was irradiated under a blue LED (30 W) for 24 h. After the reaction, the molecular sieves were removed by centrifugation, and the supernatant was concentrated in vacuo. The crude mixture was directly purified by column chromatography on silica gel (ethyl acetate/petroleum ether 1:30 to 1:15) to give the desired products **3c**, **3d**, **3p**, **3z**.

## 5. Photoredox Transfer Hydrogenation under Solar Irradiation

This experiment was carried out on a clear day (Jan. 15, 2022) on a balcony at Zhejiang Sci-Tech University (30°31' north latitude and 120°35' east longitude, 11 meters above the sea level). It was found that the reaction proceeded swiftly under solar irradiation and it took only 3 hours (from 13.00 p.m to 16.00 p.m., local time) to reach a completion to give the product **3p** in 82% yield.

## 6. UV Spectral of Benzophenone oxime, CBr<sub>4</sub> and Reaction System

UV spectroscopy experiments were carried out on a Shimadzu Instruments UV-2600 UV-Visible spectrophotometer. Weigh an appropriate amount of carbon tetrabromide, benzophenone oxime, a mixture of carbon tetrabromide and benzophenone oxime, respectively, dissolve and dilute the solution with anhydrous n-butyl acetate to a concentration of 0.005 mol/L. Wherein the concentration of carbon tetrabromide in condition (1) is the concentration of the reaction system.

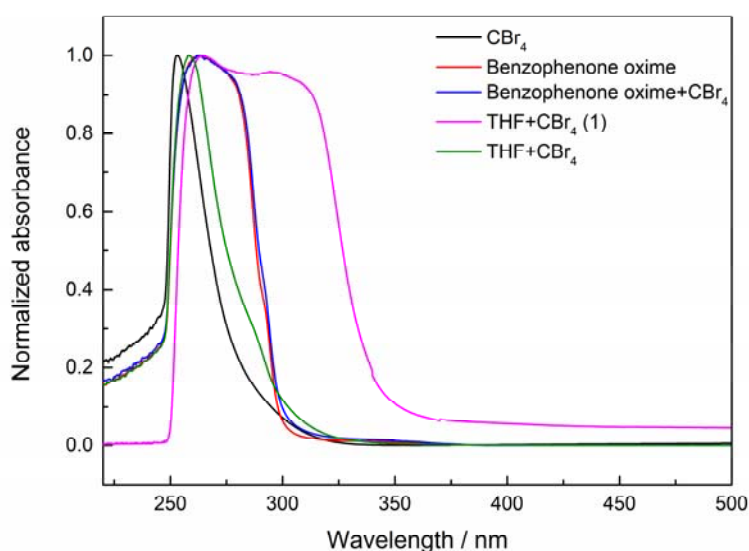


Figure S3. UV spectra of benzophenone oxime, CBr<sub>4</sub> and reaction systems.

## 7. Control experiments with LED light on/off

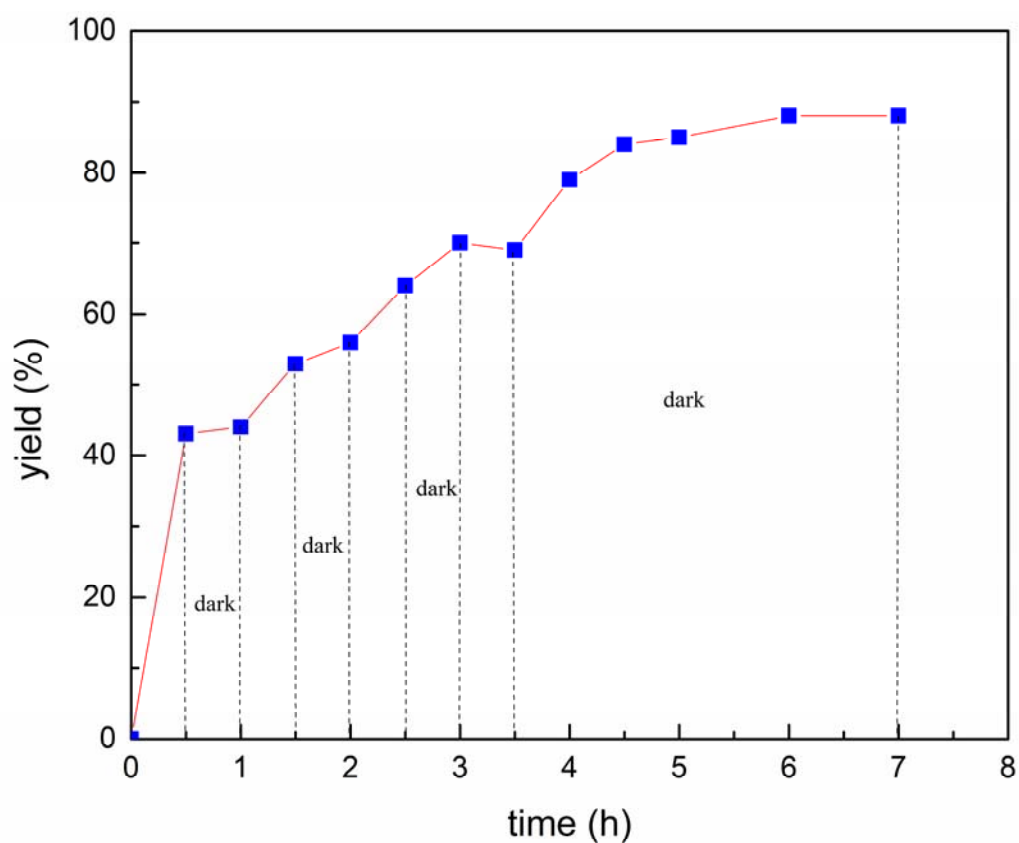
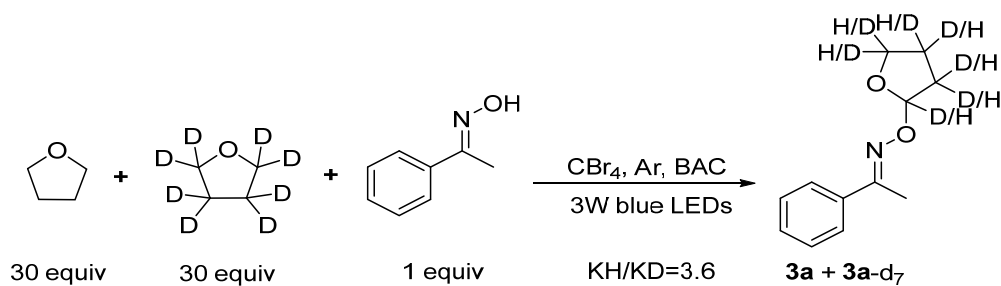


Figure S4. On/Off Experiments.

## 8. Kinetic isotope effect experiments



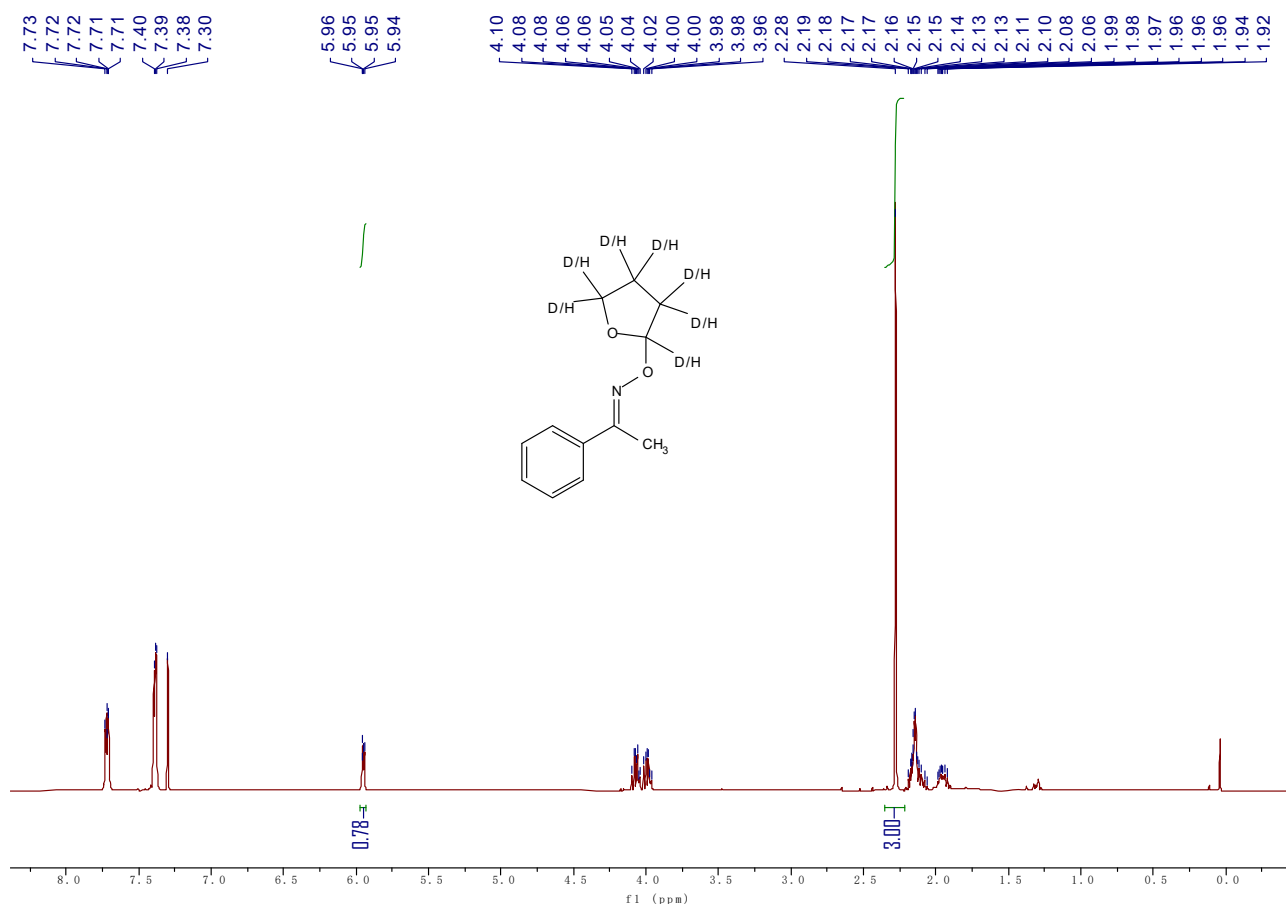


Figure S5. Crude <sup>1</sup>H-NMR spectrum for mixtures of 3a + 3a-d<sub>7</sub>.

## 9. Theoretical calculations

### 9.1 General information

Density functional theory (DFT) calculations were carried out using Gaussian 09 program.<sup>1</sup> Geometrical optimization calculations were carried out at the M06-2X-D32,3/def2-TZVPPD4,5 level with the SMD continuum solvent model<sup>6</sup> for butylethanoate without any symmetry assumptions unless otherwise stated. Harmonic vibration frequency calculations were performed at the same level for verifying the resulting geometries as local minima (with all the frequencies real) or saddle points (with only one imaginary frequency). The assignment of the saddle points was performed using the intrinsic reaction coordinate (IRC) calculations. Free energy of tetrahydrofuran, oxime H, Br • and CBr<sub>3</sub> • are set as 0 kcal mol<sup>-1</sup>. Time-dependent density functional theory (TD-DFT) calculations were performed at the PBE0-D3(BJ)/def2-TZVPPD level with the SMD continuum solvent model for butylethanoate on the optimized geometries. Absorption spectra were simulated via TD-DFT calculations of the lowest 100 vertical singlet electronic excitations with Gaussian broadening for the oscillator strength *f*, and half-width at half-height was set at 0.2 eV. No special shift or scaling was applied unless otherwise mentioned. The isosurfaces of molecular orbitals (MOs) were drawn using IQmol 2.15 program with the isovalue set to 0.1 Å<sup>3</sup>.

### 9.2 Energies of Stationary Points

Supplementary Table 1. Electronic energies ( $E$ ), zero-point energy corrected energies ( $E + ZPE$ ), electronic and thermal enthalpies ( $H$ ), Gibbs free energies ( $G$ ) of the stationary points calculated at the M06-2X-D3/def2-TZVPPD level of theory with the SMD continuum solvent model for butylethanoate.

	$E$ (Hartree)	$E + ZPE$ (Hartree)	$H$ (Hartree)	$G$ (Hartree)
<b>A</b>	-10334.859603	-10334.852291	-10334.844644	-10334.887298
<b>B</b>	-7760.621610	-7760.615985	-7760.609890	-7760.649158
<b>C</b>	-2574.154654	-2574.154654	-2574.152294	-2574.171484
<b>D</b>	-232.441126	-232.323493	-232.317686	-232.351547
<b>E</b>	-7993.048906	-7992.929967	-7992.918656	-7992.971015
<b>F</b>	-231.783667	-231.679677	-231.673936	-231.707815
<b>G</b>	-231.634966	-231.528526	-231.523067	-231.555798
<b>H</b>	-440.188458	-440.032854	-440.022824	-440.067617
<b>I</b>	-671.444546	-671.190845	-671.176117	-671.233882
CHBr <sub>3</sub>	-7761.280324	-7761.261879	-7761.255870	-7761.294327
Br <sup>-</sup>	-2574.348996	-2574.348996	-2574.346635	-2574.365171
HBr	-2574.795996	-2574.789925	-2574.786620	-2574.809147

### 9.3 Calculated UV-vis spectra

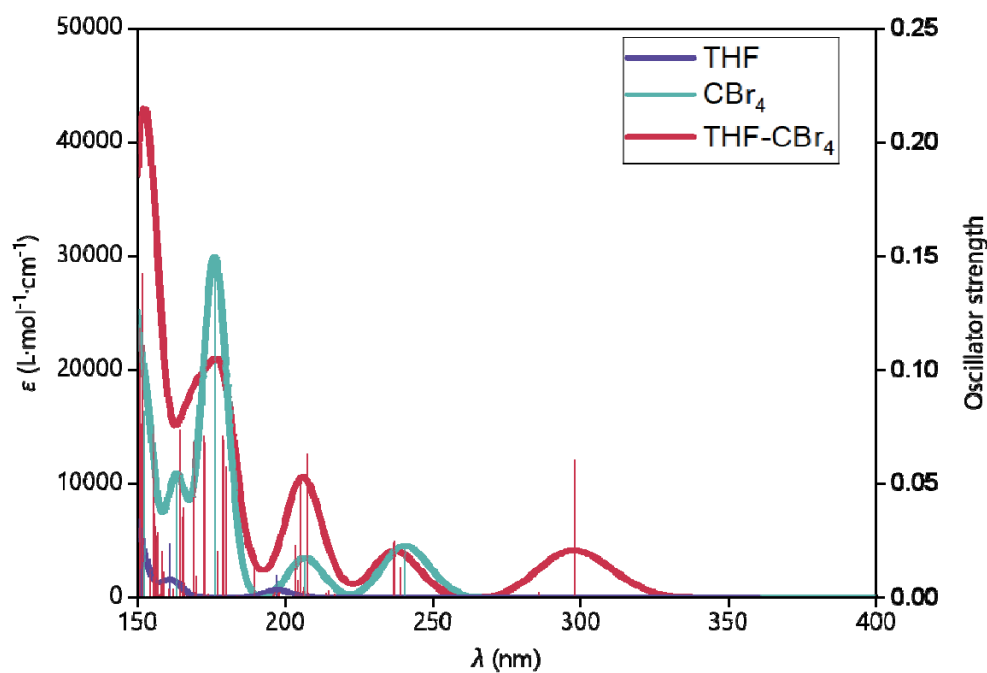
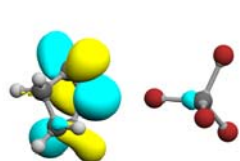


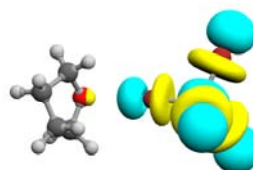
Figure S6. The calculated UV-vis spectra of THF, CBr<sub>4</sub> and THF-CBr<sub>4</sub> complex.

Excitation	$E$ (eV)	$\lambda$ (nm)	$f$	occ no.	unocc no.	%
1	4.16	298	0.0603	HOMO	LUMO	96.8



**HOMO**

-2.39 eV



**LUMO**

-7.27 eV

#### 9.4 Cartesian coordinates of the optimized geometries

**A**

$\text{CBr}_4$

C	0.000000	0.000235	-0.000356	Br	-1.583134	-0.735661	-0.843601	Br	-0.000003	1.928882	-0.196563
Br	1.583145	-0.735655	-0.843586	Br	-0.000008	-0.457607	1.883812				

**B**

$\cdot\text{CBr}_3$

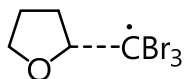
C	-0.000123	0.000065	0.256150	Br	0.842663	1.641585	-0.014637
Br	-1.843496	-0.091302	-0.014639	Br	1.000854	-1.550294	-0.014635

**D**



O	0.000043	-1.243875	0.000027	H	1.946706	-0.818176	-0.508509	C	-1.160986	-0.423477	-0.136254
C	1.160983	-0.423438	0.136209	H	1.340116	1.751608	0.235616	H	-1.509676	-0.463800	-1.173068
C	0.726141	0.987224	-0.236681	H	0.769345	1.123520	-1.318572	H	-1.946628	-0.818334	0.508463
C	-0.726187	0.987163	0.236722	H	-0.769633	1.123564	1.318584				
H	1.509798	-0.463719	1.173018	H	-1.340078	1.751506	-0.235730				

**E**



O	-2.468251	1.077029	-1.169842	H	-3.436979	-1.041095	1.091142	H	-0.665782	-0.021294	-0.793887
C	-3.121113	0.863171	0.085569	H	-4.534358	-0.740345	-0.254924	C	0.537739	0.000788	-0.024978
C	-3.510910	-0.616017	0.092675	H	-1.850102	-1.976170	-0.423389	Br	1.769849	-1.097738	-1.002158
C	-2.521188	-1.261983	-0.900457	H	-3.042111	-1.785965	-1.701726	Br	1.060999	1.840973	0.041043
H	-2.418200	1.099286	0.889981	C	-1.762331	-0.066946	-1.453951	Br	0.122454	-0.718336	1.707151
H	-3.964194	1.547117	0.140731	H	-1.441030	-0.083319	-2.493623				

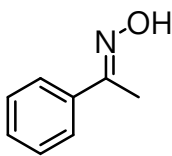


**F**

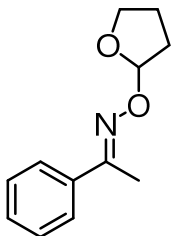
C	0.545307	-1.110664	-0.046371	C	1.246630	0.210194	-0.138972	H	0.197379	2.147647	-0.299896
O	-0.799082	-0.951112	0.124165	H	0.947618	-2.014872	0.386721	H	0.110048	1.380701	1.293978
C	-1.120419	0.412262	-0.180604	H	-1.316813	0.497404	-1.253310	H	1.616287	0.399813	-1.151646
C	0.121155	1.195304	0.219861	H	-2.019023	0.675102	0.372340	H	2.101119	0.280527	0.535009

**G**

C	1.102664	-0.452366	0.049066	C	0.783480	0.966149	-0.102081	H	-1.242058	1.677517	-0.533439
O	0.117036	-1.217151	0.062976	H	2.087100	-0.906233	0.124993	H	-0.941943	1.283273	1.166055
C	-1.152453	-0.443371	-0.111955	H	-1.459950	-0.655604	-1.132546	H	1.071740	1.225639	-1.130887
C	-0.731972	0.995673	0.139186	H	-1.852268	-0.867960	0.598763	H	1.390776	1.584062	0.557950

**H**

C	2.401677	1.049673	-0.240261	H	0.565131	2.141225	-0.342820	H	-1.242961	2.102044	1.023769
C	1.019118	1.170927	-0.189726	H	0.212874	-2.056146	0.419507	H	-2.086970	2.071516	-0.528532
C	0.217568	0.053273	0.037538	H	2.668496	-2.272535	0.339999	N	-1.923475	-0.857646	-0.234591
C	0.828479	-1.188030	0.228007	H	4.077396	-0.281725	-0.085331	O	-3.294890	-0.650845	-0.211083
C	2.207746	-1.305864	0.183730	C	-1.260841	0.189533	0.060068	H	-3.652957	-1.513977	-0.440357
C	2.999939	-0.187577	-0.052635	C	-1.893824	1.507905	0.387157				
H	3.009789	1.925183	-0.426267	H	-2.846535	1.355663	0.887557				

**I**

C	4.438088	0.562246	0.013030	H	2.985037	2.132055	0.022628	H	1.104417	2.397050	1.298351
C	3.141798	1.061363	0.026336	H	1.434665	-1.857099	0.044839	H	0.532409	2.847559	-0.309770
C	2.049052	0.196027	0.027673	H	3.735947	-2.747069	0.031792	N	-0.233825	-0.036226	-0.443096
C	2.279041	-1.181748	0.029542	H	5.666690	-1.196810	0.008656	O	-1.489471	0.537264	-0.463392
C	3.572033	-1.677390	0.022882	C	0.666577	0.739079	0.017740	C	-2.459722	-0.447079	-0.792084
C	4.657183	-0.807183	0.012432	C	0.407599	2.131968	0.506297	O	-2.659731	-1.335216	0.263459
H	5.275957	1.247035	0.004155	H	-0.610302	2.221687	0.874682	C	-3.778649	0.276805	-0.979966

H	-2.098714	-1.013219	-1.649575	H	-4.447430	-0.365380	-1.553166	H	-3.356084	-0.725290	2.112631
C	-3.732474	-0.875731	1.101104	H	-3.660556	1.223300	-1.501107	H	-5.337713	0.500734	0.552205
C	-4.257194	0.412613	0.466412	H	-4.493145	-1.657921	1.123722	H	-3.800782	1.284759	0.932706

#### CHBr<sub>3</sub>

Br	1.388310	1.210828	-0.045352	Br	-1.743174	0.596373	-0.045368	H	-0.000089	0.000107	1.607112
Br	0.354916	-1.807252	-0.045339	C	-0.000287	0.000280	0.525826				

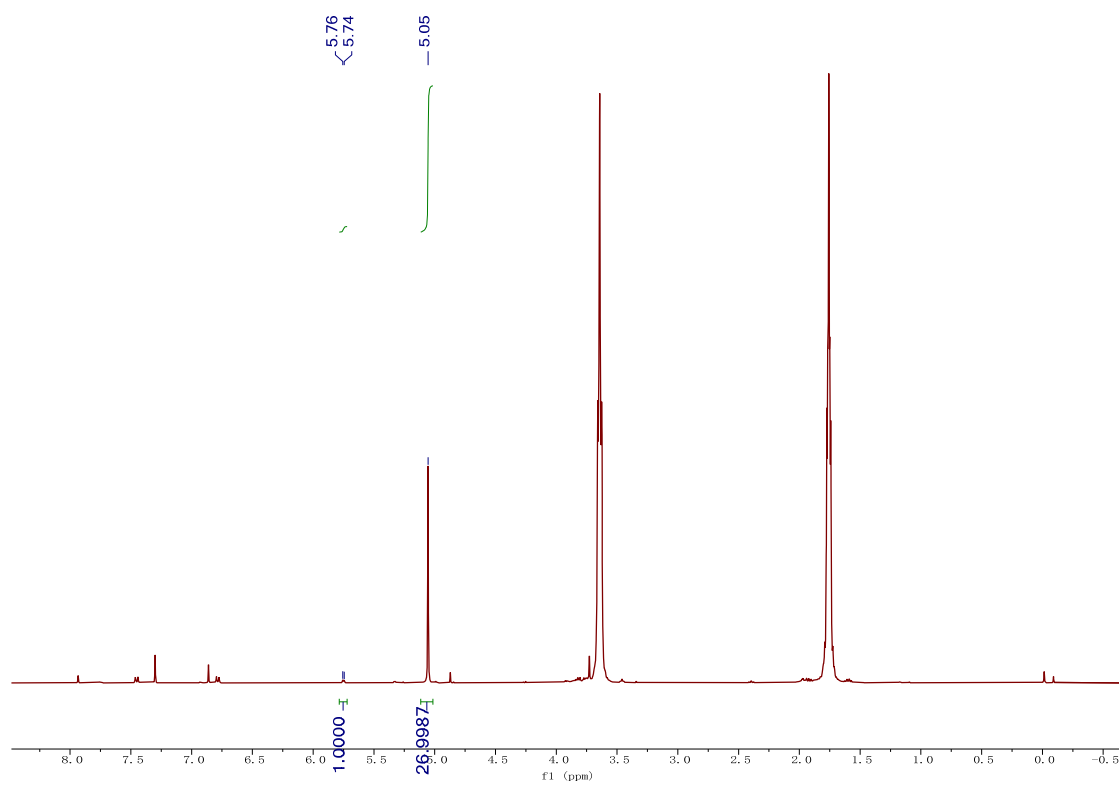
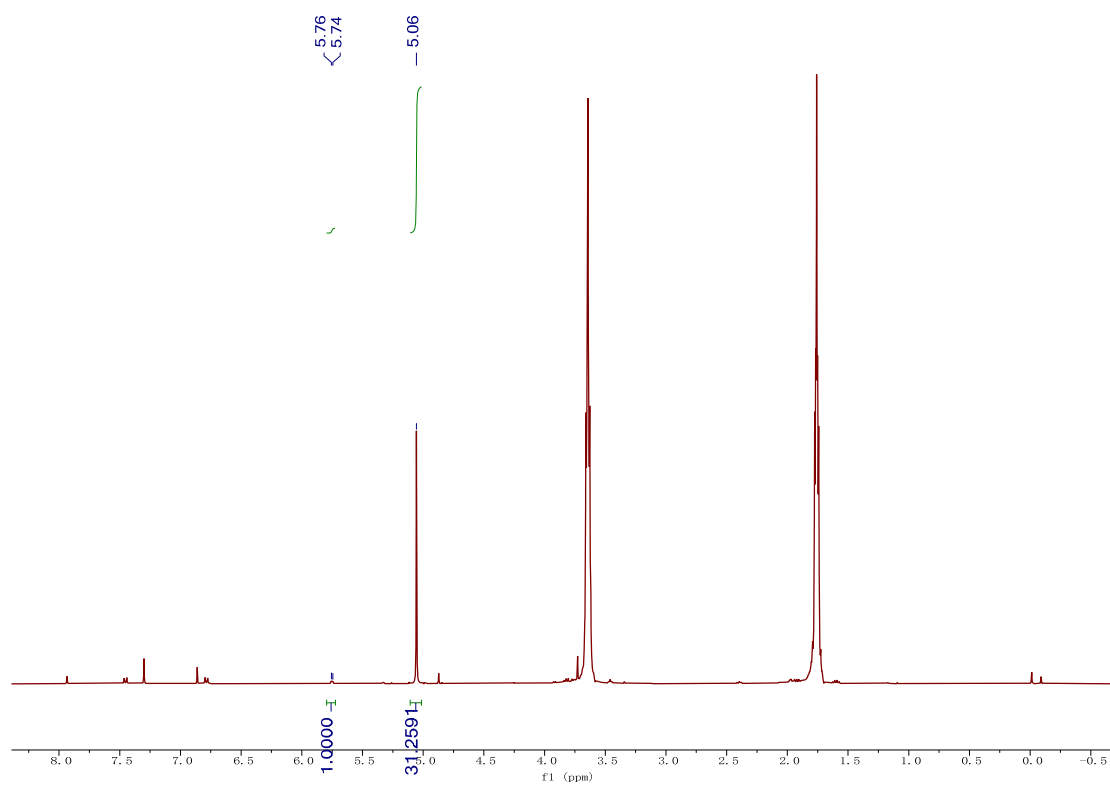
#### HBr

Br	0.000000	0.000000	0.039505	H	0.000000	0.000000	-1.382675
----	----------	----------	----------	---	----------	----------	-----------

## 10. Quantitative NMR



A 4 mL clear vial was weighed after adding the magnets to 4.3164 g. To the vial was added 0.0152 g of **1j**, 0.0601 g, 0.3612 g of THF and 0.1004 g of 4Å molecular sieves, dissolved in 2 mL of CDCl<sub>3</sub> and reacted under 2 × 3 W blue light for 5 hours. The weight was weighed at the end of the reaction as 7.5760 g. Take two clean NMR tubes, numbered A, B. 0.8163 g and 0.9305 g of the reaction solution were added to NMR tubes A and B respectively, and 0.0100 g of trioxane was added to both tubes as an internal standard. After the internal standard was completely dissolved, NMR quantification was carried out separately.



Quantitative NMR calculation of **3j** mass:

$$W_x = W_s \times (A_x/A_s) \times (E/E_s)$$

$$W_{xA}=0.0100 \times (1/31.2591) \times (221.11 \times 6/90.08) \times [(7.5760-4.3164)/0.8149] \times 100\% = 0.0188\text{g}$$

$$W_{xB}=0.0100 \times (1/26.9987) \times (221.11 \times 6/90.08) \times [(7.5760-4.3164)/0.9305] \times 100\% = 0.0191\text{g}$$

theoretical mass of **3j**:

$$W=0.0152/151.06 \times 221.11 \times 100\% = 0.0222\text{g}$$

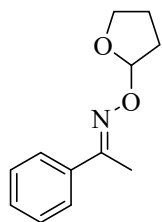
Yield of 3p:

$$Y_A=0.0188/0.0222 \times 100\% = 85\%$$

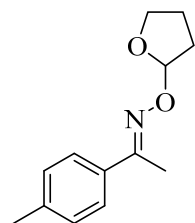
$$Y_B=0.0191/0.0222 \times 100\% = 86\%$$

$$Y_{3p}=(85\%+86\%)/2 \times 100\% = 86\%$$

## 11. Characterization Data

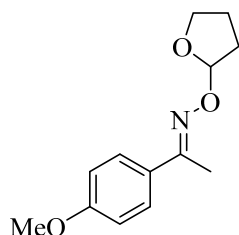


**(E)-1-phenylethan-1-one O-tetrahydrofuran-2-yl oxime (3a):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (75%, 15.4 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 7.68 (dd, J = 6.7, 3.0 Hz, 2H), 7.37 – 7.33 (m, 3H), 6.08 – 5.81 (m, 1H), 3.99 (ddd, J = 13.5, 11.5, 6.8 Hz, 2H), 2.24 (s, 3H), 2.15 – 2.03 (m, 3H), 1.96 – 1.85 (m, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 155.9, 136.6, 129.1, 128.3, 126.3, 106.5, 68.0, 30.9, 24.0, 13.0.

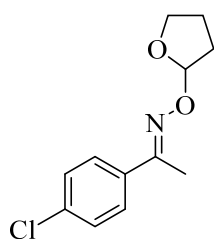


**(E)-1-(p-tolyl)ethan-1-one O-tetrahydrofuran-2-yl oxime (3b):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (84%, 18.4 mg). The

compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.57 (d,  $J = 8.2$  Hz, 2H), 7.15 (d,  $J = 8.0$  Hz, 2H), 5.95–5.85 (m, 1H), 3.99 (ddd,  $J = 13.4, 11.4, 6.4$  Hz, 2H), 2.35 (s, 3H), 2.22 (s, 3H), 2.15–2.01 (m, 3H), 1.98–1.83 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  155.8, 139.1, 133.7, 129.0, 126.2, 106.4, 67.9, 30.9, 24.0, 21.3, 12.9.

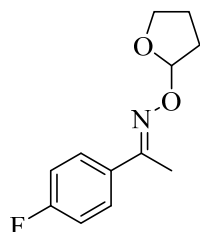


**(E)-1-(4-methoxyphenyl)ethan-1-one O-tetrahydrofuran-2-yl oxime (3c):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (88%, 20.7mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.66 – 7.59 (m, 2H), 6.89 – 6.84 (m, 2H), 5.90 – 5.87 (m, 1H), 4.06 – 3.90 (m, 2H), 3.81 (s, 3H), 2.20 (s, 3H), 2.16 – 1.99 (m, 3H), 1.96 – 1.82 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.5, 155.4, 129.1, 127.6, 113.7, 106.4, 68.0, 55.3, 30.9, 24.0, 12.8.

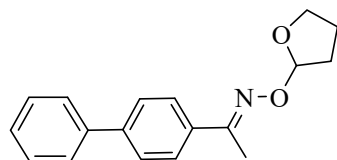


**(E)-1-(4-chlorophenyl)ethan-1-one O-tetrahydrofuran-2-yl oxime (3d):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (91%, 21.8mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.61 (d,  $J = 7.3$  Hz, 2H), 7.31 (d,  $J = 7.3$  Hz, 2H), 5.89 (d,  $J = 2.0$  Hz, 1H), 4.07 – 3.86 (m, 2H), 2.20 (s, 3H), 2.15 – 2.00

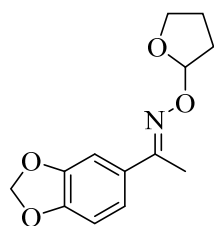
(m, 3H), 1.97 – 1.84 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  154.7, 135.0 (d,  $J = 16.1$  Hz), 128.5, 127.5, 106.6, 68.0, 30.9, 24.0, 12.8.



**(E)-1-(4-fluorophenyl)ethan-1-one O-tetrahydrofuran-2-yl oxime (3e):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (83%, 18.5mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (dd,  $J = 8.7, 5.4$  Hz, 2H), 7.03 (t,  $J = 8.6$  Hz, 2H), 5.89 (dd,  $J = 4.4, 2.5$  Hz, 1H), 3.99 (ddd,  $J = 13.4, 11.4, 6.6$  Hz, 2H), 2.22 (s, 3H), 2.17 – 2.00 (m, 3H), 1.97 – 1.84 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  164.7, 162.2, 154.8, 132.6, 128.1 (d,  $J = 8.3$  Hz), 115.3, 115.1, 106.5, 68.0, 30.9, 24.0, 12.9.  $^{19}\text{F}$  NMR (377 MHz,  $\text{CDCl}_3$ )  $\delta$  -112.22 – -112.49 (m).

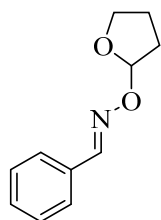


**(E)-1-([1,1'-biphenyl]-4-yl)ethan-1-one O-tetrahydrofuran-2-yl oxime (3f):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (70%, 19.7 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 8.5$  Hz, 2H), 7.62 – 7.55 (m, 4H), 7.43 (t,  $J = 7.5$  Hz, 2H), 7.34 (t,  $J = 7.3$  Hz, 1H), 5.93 (t,  $J = 3.5$  Hz, 1H), 4.00 (ddd,  $J = 13.5, 11.6, 6.8$  Hz, 2H), 2.26 (s, 3H), 2.11 (dd,  $J = 6.4, 3.2$  Hz, 3H), 1.96 – 1.85 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  155.0, 141.3, 140.0, 134.9, 128.3, 127.0, 126.5 (d,  $J = 8.9$  Hz), 126.2, 106.1, 67.5, 30.4, 23.5, 12.4. HRMS (ESI-TOF) for  $\text{C}_{18}\text{H}_{20}\text{NO}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 282.1494; found: 282.1498. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3142, 1664, 1592, 1500, 1401, 1084, 967.

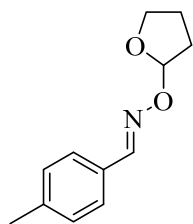


**(E)-1-(benzo[d][1,3]dioxol-5-yl)ethan-1-one O-tetrahydrofuran-2-yl oxime (3g):**

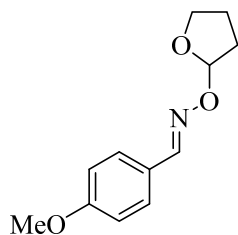
The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (92%, 22.9 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.26 (d,  $J = 1.3$  Hz, 1H), 7.12 (dd,  $J = 8.2, 1.7$  Hz, 1H), 6.77 (d,  $J = 8.2$  Hz, 1H), 5.95 (s, 2H), 5.87 (dd,  $J = 4.1, 2.7$  Hz, 1H), 3.98 (ddd,  $J = 13.3, 11.4, 6.7$  Hz, 2H), 2.18 (s, 3H), 2.14 – 2.01 (m, 3H), 1.98 – 1.83 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  155.2, 148.5, 147.8, 130.8, 107.8, 106.5 (d,  $J = 3.8$  Hz), 101.2, 67.9, 30.9, 24.0, 12.9.



**(E)-benzaldehyde O-tetrahydrofuran-2-yl oxime (3h):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (63%, 12.1 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.08 (s, 1H), 7.67 – 7.54 (m, 2H), 7.43 – 7.30 (m, 3H), 5.88 (dd,  $J = 4.9, 1.6$  Hz, 1H), 3.99 (ddd,  $J = 13.0, 11.3, 6.5$  Hz, 2H), 2.08 (dt,  $J = 12.3, 6.3$  Hz, 3H), 1.92 (d,  $J = 6.5$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.0, 132.1, 130.0, 128.6, 127.3, 106.7, 68.0, 30.8, 23.8.

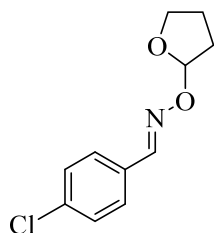


**(E)-4-methylbenzaldehyde O-tetrahydrofuran-2-yl oxime (3i):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (88%, 18.1 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.05 (s, 1H), 7.50 (d,  $J = 8.1$  Hz, 2H), 7.16 (d,  $J = 8.0$  Hz, 2H), 5.90 – 5.84 (m, 1H), 3.99 (dd,  $J = 31.1, 5.5$  Hz, 2H), 2.35 (s, 3H), 2.15 – 2.01 (m, 3H), 1.98 – 1.85 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  150.1, 140.2, 129.3, 127.3, 106.6, 67.9 (d,  $J = 9.7$  Hz), 30.8, 23.9, 21.5. HRMS (ESI-TOF) for  $\text{C}_{12}\text{H}_{16}\text{NO}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 206.1181; found: 206.1185. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3149, 3003, 1595, 1472, 1400, 1182, 1079, 950, 811.

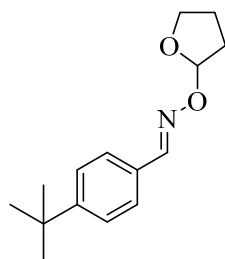


**(E)-4-methoxybenzaldehyde O-tetrahydrofuran-2-yl oxime (3j):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (66%, 14.6 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (s, 1H), 7.55 (d,  $J = 8.8$  Hz, 2H), 6.88 (d,  $J = 8.8$  Hz, 2H), 5.88 – 5.83 (m, 1H), 3.99 (ddd,  $J = 13.0, 11.1, 6.4$  Hz, 2H), 3.82 (s, 3H), 2.15 – 2.02 (m, 3H), 1.97 – 1.86 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  161.1, 149.7, 128.8, 124.8, 114.1, 106.5, 67.9, 55.3, 30.8, 23.9. HRMS (ESI-TOF) for  $\text{C}_{12}\text{H}_{16}\text{NO}_3$  ( $[\text{M}+\text{H}]^+$ ): calcd. 222.1130; found: 222.1137. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3142, 1601, 1472, 1401, 1253, 1177, 1034, 950, 829.

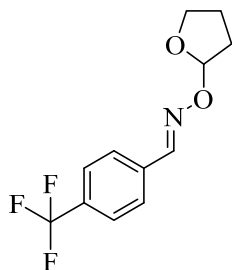




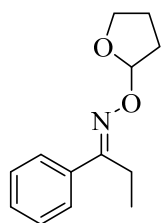
**(E)-4-chlorobenzaldehyde O-tetrahydrofuran-2-yl oxime (3k):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (73%, 16.5 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.04 (s, 1H), 7.55 (d,  $J = 8.5$  Hz, 2H), 7.33 (d,  $J = 8.5$  Hz, 2H), 5.89 – 5.85 (m, 1H), 3.99 (ddd,  $J = 13.0, 8.6, 6.0$  Hz, 2H), 2.18 – 1.99 (m, 3H), 1.93 (dd,  $J = 11.3, 4.8$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.8, 135.9, 130.7, 128.9, 128.5, 106.8, 68.1, 30.8, 23.8.



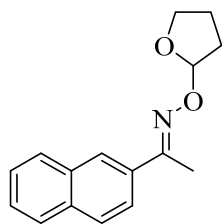
**(E)-4-(tert-butyl)benzaldehyde O-tetrahydrofuran-2-yl oxime (3l):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (70%, 17.3 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (s, 1H), 7.54 (d,  $J = 8.4$  Hz, 2H), 7.38 (d,  $J = 8.4$  Hz, 2H), 5.92 – 5.81 (m, 1H), 4.10 – 3.85 (m, 2H), 2.16 – 2.01 (m, 3H), 1.91 (ddd,  $J = 14.1, 6.6, 2.3$  Hz, 1H), 1.31 (s, 9H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  153.3, 149.9, 129.3, 127.0, 125.5, 106.5, 67.9, 34.8, 31.2, 30.8, 23.8. HRMS (ESI-TOF) for  $\text{C}_{15}\text{H}_{22}\text{NO}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 248.1651; found: 248.1658. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3149, 1597, 1474, 1401, 1079, 950, 835.



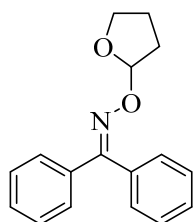
**(E)-4-(trifluoromethyl)benzaldehyde O-tetrahydrofuran-2-yl oxime (3m):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (90%, 23.3 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.11 (s, 1H), 7.72 (d,  $J = 8.2$  Hz, 2H), 7.61 (d,  $J = 8.3$  Hz, 2H), 5.90 (dd,  $J = 5.0, 1.5$  Hz, 1H), 4.07 – 3.93 (m, 2H), 2.18 – 2.02 (m, 3H), 1.93 (dt,  $J = 9.5, 4.6$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  148.5 (s), 135.6 (s), 131.6 (q,  $J = 32.6$  Hz), 125.6 (q,  $J = 3.7$  Hz), 123.9 (q,  $J = 273.2$  Hz), 107.0 (s), 68.1 (s), 30.8 (s), 23.8 (s).  $^{19}\text{F}$  NMR (377 MHz,  $\text{CDCl}_3$ )  $\delta$  -62.78 (d,  $J = 23.4$  Hz). HRMS (ESI-TOF) for  $\text{C}_{12}\text{H}_{13}\text{F}_3\text{NO}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 260.0898; found: 260.0901. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3141, 2994, 1594, 1535, 1445, 1398, 1327, 1167, 1126, 1073, 961.



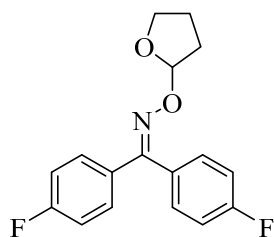
**(E)-1-phenylpropan-1-one O-tetrahydrofuran-2-yl oxime (3n):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (83%, 18.2 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.67 (dd,  $J = 6.8, 3.0$  Hz, 2H), 7.35 (dd,  $J = 5.0, 1.8$  Hz, 3H), 5.97 – 5.80 (m, 1H), 3.99 (ddd,  $J = 13.4, 11.6, 6.8$  Hz, 2H), 2.75 (qd,  $J = 7.6, 3.3$  Hz, 2H), 2.18 – 2.01 (m, 3H), 1.93 (d,  $J = 1.2$  Hz, 1H), 1.14 (t,  $J = 7.6$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  160.8, 135.6, 129.1, 128.34, 126.5, 106.4, 67.9, 30.9, 23.9, 20.4, 11.2.



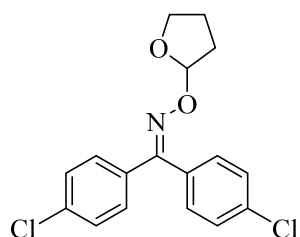
**(E)-1-(naphthalen-2-yl)ethan-1-one O-tetrahydrofuran-2-yl oxime (3o):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (84%, 21.4 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.03 (s, 1H), 7.96 (dd,  $J = 8.7, 1.7$  Hz, 1H), 7.82 (ddd,  $J = 16.9, 9.8, 6.1$  Hz, 3H), 7.53 – 7.42 (m, 2H), 5.96 (t,  $J = 3.5$  Hz, 1H), 4.02 (ddd,  $J = 13.5, 11.6, 6.7$  Hz, 2H), 2.34 (s, 3H), 2.21 – 2.04 (m, 3H), 1.92 (dt,  $J = 11.7, 6.4$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  155.6 (s), 133.9 (d,  $J = 18.2$  Hz), 133.1, 128.5, 127.9, 127.7, 126.6, 126.2, 126.0, 123.8, 106.7, 68.0, 31.0, 24.0, 12.8.



**Diphenylmethanone O-tetrahydrofuran-2-yl oxime (3p):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (87%, 23.3 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.56 – 7.46 (m, 2H), 7.44 – 7.37 (m, 3H), 7.37 – 7.31 (m, 4H), 7.30 (s, 1H), 5.91 (dd,  $J = 5.3, 1.3$  Hz, 1H), 4.05 – 3.87 (m, 2H), 2.11 – 1.75 (m, 4H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  158.2, 136.5, 133.6, 129.4 (d,  $J = 7.4$  Hz), 128.7, 128.2 (d,  $J = 7.2$  Hz), 127.9, 106.7, 68.0, 30.7, 23.9.

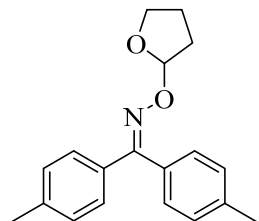


**Bis(4-fluorophenyl)methanone O-tetrahydrofuran-2-yl oxime (3q):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (85%, 25.8 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.47 (dd,  $J = 8.6, 5.5$  Hz, 2H), 7.33 (dd,  $J = 8.4, 5.5$  Hz, 2H), 7.10 (t,  $J = 8.6$  Hz, 2H), 7.00 (t,  $J = 8.6$  Hz, 2H), 5.89 (d,  $J = 4.7$  Hz, 1H), 3.94 (t,  $J = 6.6$  Hz, 2H), 2.11 – 1.99 (m, 1H), 1.99 – 1.81 (m, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  164.5 (d,  $J = 91.30$  Hz), 162.0 (d,  $J = 90.50$  Hz), 156.2, 132.5 (d,  $J = 3.0$  Hz), 131.4 (d,  $J = 8.2$  Hz), 130.0 (d,  $J = 8.3$  Hz), 129.1 (d,  $J = 3.4$  Hz), 115.2 (q,  $J = 11.00$  Hz), 106.8, 77.4, 77.1, 76.8, 68.0, 30.7, 23.9.  $^{19}\text{F}$  NMR (377 MHz,  $\text{CDCl}_3$ )  $\delta$  -111.32 – -111.80 (m). HRMS (ESI-TOF) for  $\text{C}_{17}\text{H}_{16}\text{F}_2\text{NO}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 304.1149; found: 304.1157. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3136, 2989, 1605, 1504, 1405, 1277, 1157, 1079, 961, 837.

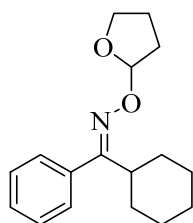


**Bis(4-chlorophenyl)methanone O-tetrahydrofuran-2-yl oxime (3r):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (79%, 26.6 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.45 – 7.42 (m, 1H), 7.41 (q,  $J = 1.9$  Hz, 2H), 7.40 – 7.37 (m, 1H), 7.31 – 7.29 (m, 1H), 7.27 (q,  $J = 1.9$  Hz, 2H), 7.26 – 7.24 (m, 1H), 5.89 (dd,  $J = 5.4, 1.2$  Hz, 1H), 3.94 (t,  $J = 6.7$  Hz, 2H), 2.11 – 1.99 (m, 1H), 1.98 – 1.84 (m, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  156.0, 135.7, 134.9, 134.5, 131.3, 130.7, 129.3, 128.5 (d,  $J = 8.7$  Hz), 107.0, 77.4, 77.1, 76.8, 68.1, 30.7, 23.9. HRMS (ESI-TOF) for

C<sub>17</sub>H<sub>16</sub>Cl<sub>2</sub>NO<sub>2</sub> ([M+H]<sup>+</sup>): calcd. 336.0558; found: 336.0568. IR (neat):  $\nu_{\max}$  (cm<sup>-1</sup>) 3142, 1600, 1484, 1444, 1405, 1092, 961.

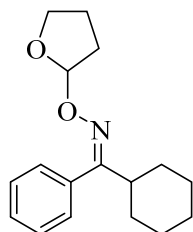


**Di-p-tolylmethanone O-tetrahydrofuran-2-yl oxime (3s):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (70%, 20.7 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.38 (d,  $J$  = 8.2 Hz, 2H), 7.24 – 7.16 (m, 4H), 7.10 (d,  $J$  = 8.0 Hz, 2H), 5.89 (dd,  $J$  = 5.2, 1.5 Hz, 1H), 4.02 – 3.88 (m, 2H), 2.39 (s, 3H), 2.34 (s, 3H), 2.08 – 1.78 (m, 4H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  158.2, 139.3, 138.5, 134.0, 130.7, 106.6, 68.0, 30.7, 24.0, 21.4 (d,  $J$  = 13.8 Hz). HRMS (ESI-TOF) for C<sub>19</sub>H<sub>22</sub>NO<sub>2</sub> ([M+H]<sup>+</sup>): calcd. 296.1651; found: 296.1659. IR (neat):  $\nu_{\max}$  (cm<sup>-1</sup>) 3136, 1600, 1485, 1438, 1398, 1080, 961.

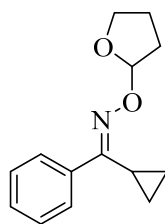


**(E)-cyclohexyl(phenyl)methanone O-tetrahydrofuran-2-yl oxime (3t):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 50/1). Colorless oil (29%, 7.9 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  7.39 (dd,  $J$  = 3.9, 2.5 Hz, 2H), 7.36 – 7.30 (m, 3H), 5.83 (t,  $J$  = 3.3 Hz, 1H), 3.98 (ddd,  $J$  = 13.4, 11.5, 6.7 Hz, 2H), 3.14 (tt,  $J$  = 12.3, 3.1 Hz, 1H), 2.13 – 2.00 (m, 3H), 1.99 – 1.85 (m, 1H), 1.72 (dd,  $J$  = 28.7, 11.1 Hz, 6H), 1.59 – 1.45 (m, 2H), 1.36 – 1.26 (m, 2H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  164.8, 136.3, 128.4, 128.01 (d,  $J$  = 8.6 Hz), 106.3, 67.8, 39.6, 31.0, 29.4 (d,  $J$  = 13.5 Hz), 26.4 (d,  $J$  = 3.7

Hz), 26.1, 23.9. HRMS (ESI-TOF) for  $C_{17}H_{24}NO_2$  ( $[M+H]^+$ ): calcd. 274.1807; found: 274.1809. IR (neat):  $\nu_{max}$  ( $cm^{-1}$ ) 3142, 1664, 1608, 1530, 1450, 1405, 1061, 961.

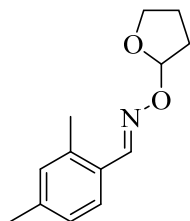


**(Z)-cyclohexyl(phenyl)methanone O-tetrahydrofuran-2-yl oxime (3t)** : The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 50/1). Colorless oil (55%, 15.1 mg).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.36 (t,  $J$  = 4.1 Hz, 1H), 7.34 – 7.28 (m, 2H), 7.20 – 7.16 (m, 2H), 5.76 – 5.72 (m, 1H), 3.90 – 3.80 (m, 2H), 2.50 (tt,  $J$  = 11.3, 3.2 Hz, 1H), 2.00 – 1.89 (m, 1H), 1.89 – 1.59 (m, 9H), 1.39 – 1.22 (m, 4H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  163.9, 134.7, 127.8 (d,  $J$  = 10.5 Hz), 127.5, 105.9, 67.7, 44.3, 30.5 (t,  $J$  = 14.7 Hz), 26.2 (d,  $J$  = 4.85 Hz), 26.0, 23.9. HRMS (ESI-TOF) for  $C_{17}H_{24}NO_2$  ( $[M+H]^+$ ): calcd. 274.1807; found: 274.1809. IR (neat):  $\nu_{max}$  ( $cm^{-1}$ ) 3142, 2923, 1605, 1485, 1444, 1398, 1074, 968.

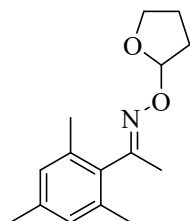


**(E)-cyclopropyl(phenyl)methanone O-tetrahydrofuran-2-yl oxime (3u)**: The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Colorless oil (60%, 13.9 mg).  $^1H$  NMR (400 MHz,  $CDCl_3$ )  $\delta$  7.45 – 7.39 (m, 2H), 7.35 – 7.29 (m, 3H), 5.86 (t,  $J$  = 3.4 Hz, 1H), 4.00 (ddd,  $J$  = 13.5, 11.5, 6.7 Hz, 2H), 2.22 (tt,  $J$  = 8.6, 5.5 Hz, 1H), 2.16 – 2.01 (m, 3H), 1.97 – 1.86 (m, 1H), 0.89 (dt,  $J$  = 8.5, 4.3 Hz, 2H), 0.71 – 0.59 (m, 2H).  $^{13}C$  NMR (101 MHz,  $CDCl_3$ )  $\delta$  162.0, 134.3, 128.6 (d,  $J$  = 12.2 Hz), 128.0, 106.5, 67.9, 31.0, 23.9, 10.0, 5.8 (d,  $J$  = 1.5 Hz). HRMS (ESI-TOF) for  $C_{14}H_{18}NO_2$

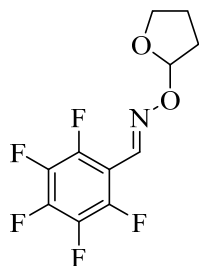
([M+H]<sup>+</sup>): calcd. 232.1338; found: 232.1337. IR (neat):  $\nu_{\max}$  (cm<sup>-1</sup>) 3142, 1599, 1493, 1446, 1405, 1186, 1079, 961.



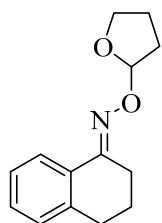
**(E)-2,4-dimethylbenzaldehyde O-tetrahydrofuran-2-yl oxime (3v):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Yellow oil (93%, 20.4 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.32 (s, 1H), 7.64 (d, *J* = 7.8 Hz, 1H), 6.99 (d, *J* = 9.6 Hz, 2H), 5.92 – 5.86 (m, 1H), 4.08 – 3.91 (m, 2H), 2.38 (s, 3H), 2.31 (s, 3H), 2.16 – 2.00 (m, 3H), 1.97 – 1.86 (m, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  148.9, 139.8, 136.8, 131.5, 127.5, 127.1, 127.0 (d, *J* = 20.8 Hz), 106.6, 68.0, 30.9, 23.9, 21.3, 19.7. HRMS (ESI-TOF) for C<sub>13</sub>H<sub>18</sub>NO<sub>2</sub> ([M+H]<sup>+</sup>): calcd. 220.1338; found: 220.1345. IR (neat):  $\nu_{\max}$  (cm<sup>-1</sup>) 3137, 2948, 1595, 1473, 1401, 1096, 957, 822.



**(E)-1-mesitylethan-1-one O-tetrahydrofuran-2-yl oxime (3w):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Colorless oil (81%, 20.1 mg). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  6.84 (s, 2H), 5.89 – 5.77 (m, 1H), 3.97 (ddd, *J* = 13.4, 11.6, 6.6 Hz, 2H), 2.26 (s, 3H), 2.21 (s, 6H), 2.08 (s, 6H), 1.93 – 1.84 (m, 1H). <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  158.1, 137.7, 135.6, 134.5, 128.3, 106.1, 67.7, 31.0, 23.8, 21.0, 19.5, 16.7. HRMS (ESI-TOF) for C<sub>15</sub>H<sub>22</sub>NO<sub>2</sub> ([M+H]<sup>+</sup>): calcd. 248.1651; found: 248.1655. IR (neat):  $\nu_{\max}$  (cm<sup>-1</sup>) 3149, 1603, 1473, 1401, 1182, 1072, 969, 896, 853.

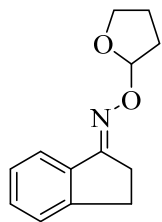


**(E)-2,3,4,5,6-pentafluorobenzaldehyde O-tetrahydrofuran-2-yl oxime (3x):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Yellow oil (50%, 14.1 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.16 (s, 1H), 5.91 (dd,  $J = 4.6, 2.1$  Hz, 1H), 4.01 (ddd,  $J = 13.7, 11.6, 6.9$  Hz, 2H), 2.18 – 2.02 (m, 3H), 1.94 (ddd,  $J = 13.7, 6.2, 2.3$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  138.7, 107.5, 68.5, 30.9, 23.7.  $^{19}\text{F}$  NMR (377 MHz,  $\text{CDCl}_3$ )  $\delta$  -139.68 (dd,  $J = 20.4, 6.1$  Hz), -151.72, -151.77, -151.83, -161.72 (dt,  $J = 19.5, 6.2$  Hz). HRMS (ESI-TOF) for  $\text{C}_{11}\text{H}_9\text{F}_5\text{NO}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 282.0553; found: 282.0557. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3147, 1600, 1522, 1493, 1398, 1274, 1133, 1085, 950.

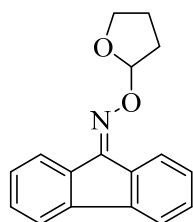


**(E)-3,4-dihydronaphthalen-1(2H)-one O-tetrahydrofuran-2-yl oxime (3y):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Colorless oil (74%, 17.1 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 7.0$  Hz, 1H), 7.30 – 7.26 (m, 1H), 7.21 (t,  $J = 6.9$  Hz, 1H), 7.15 (d,  $J = 7.5$  Hz, 1H), 5.94 (dd,  $J = 4.2, 2.7$  Hz, 1H), 4.03 (ddd,  $J = 13.4, 11.5, 6.7$  Hz, 2H), 2.78 (dd,  $J = 12.1, 6.4$  Hz, 4H), 2.21 – 2.08 (m, 3H), 2.01 – 1.92 (m, 1H), 1.93 – 1.82 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  155.3, 139.6, 130.7, 129.1, 128.4, 126.3, 124.7, 106.5, 68.0, 31.0, 29.8, 24.7, 24.0, 21.5.

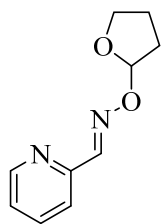




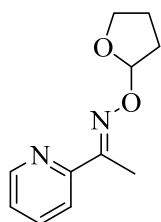
**(E)-2,3-dihydro-1H-inden-1-one O-tetrahydrofuran-2-yl oxime (3z):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (73%, 15.9 mg). The compound data was in agreement with the literature (Ref: *RSC Adv.* 2016, **6**, 16516–16519).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.75 (d,  $J = 7.7$  Hz, 1H), 7.35 – 7.26 (m, 2H), 7.23 (t,  $J = 7.2$  Hz, 1H), 5.88 (dd,  $J = 4.9, 1.9$  Hz, 1H), 3.99 (ddd,  $J = 12.9, 11.4, 6.2$  Hz, 2H), 3.06 – 2.98 (m, 2H), 2.91 – 2.84 (m, 2H), 2.18 – 2.00 (m, 3H), 1.98 – 1.83 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  164.2, 148.3, 136.1, 130.4, 126.8, 125.4, 122.1, 106.4, 67.8, 30.9, 28.5, 26.7, 24.0.



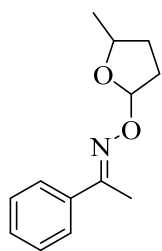
**9H-fluoren-9-one O-tetrahydrofuran-2-yl oxime (3ab):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 20/1). Yellow oil (70%, 18.6 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.22 (d,  $J = 7.6$  Hz, 1H), 7.82 (d,  $J = 7.5$  Hz, 1H), 7.61 (dd,  $J = 17.9, 7.5$  Hz, 2H), 7.38 (dt,  $J = 22.3, 7.5$  Hz, 2H), 7.28 (dd,  $J = 9.7, 5.3$  Hz, 1H), 7.24 (d,  $J = 4.5$  Hz, 1H), 6.09 – 6.01 (m, 1H), 4.14 – 3.97 (m, 2H), 2.21 (ddt,  $J = 16.0, 14.3, 6.7$  Hz, 3H), 2.07 – 1.93 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  153.3, 141.6, 140.3, 135.6, 131.1, 130.7, 130.0, 129.2, 128.0 (d,  $J = 19.6$  Hz), 122.2, 119.8 (d,  $J = 9.9$  Hz), 107.8, 68.2, 31.2, 23.9. HRMS (ESI-TOF) for  $\text{C}_{17}\text{H}_{16}\text{NO}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 220.1338; found: 220.1345. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3142, 1670, 1595, 1474, 1401, 1079, 957.



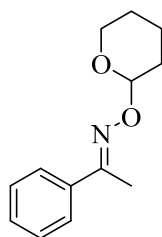
**(E)-picolinaldehyde O-tetrahydrofuran-2-yl oxime (3ac):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Colorless oil (23%, 4.4 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.60 (d,  $J = 4.5$  Hz, 1H), 8.20 (s, 1H), 7.92 (d,  $J = 8.0$  Hz, 1H), 7.71 (t,  $J = 7.8$  Hz, 1H), 7.28 (d,  $J = 6.1$  Hz, 1H), 5.95 – 5.89 (m, 1H), 4.01 (ddd,  $J = 13.4$ , 11.4, 6.5 Hz, 2H), 2.17 – 2.03 (m, 3H), 1.93 (dt,  $J = 13.2$ , 6.6 Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  151.6, 150.5, 149.3, 136.6, 124.2, 121.1, 107.1, 68.1, 30.8, 23.7. HRMS (ESI-TOF) for  $\text{C}_{10}\text{H}_{13}\text{N}_2\text{O}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 193.0977; found: 193.0980. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3136, 1664, 1591, 1499, 1400, 1185, 1085, 961.



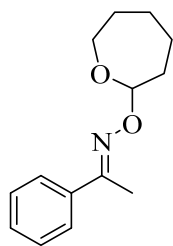
**(E)-1-(pyridin-2-yl)ethan-1-one O-tetrahydrofuran-2-yl oxime (3ad):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Colorless oil (20%, 4.1 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.60 (d,  $J = 4.8$  Hz, 1H), 7.99 (d,  $J = 8.0$  Hz, 1H), 7.67 (td,  $J = 7.9$ , 1.7 Hz, 1H), 7.26 – 7.23 (m, 1H), 5.93 (t,  $J = 3.4$  Hz, 1H), 4.00 (ddd,  $J = 13.5$ , 11.6, 6.7 Hz, 2H), 2.35 (s, 3H), 2.18 – 2.03 (m, 3H), 1.93 (dt,  $J = 11.7$ , 6.4 Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  156.9, 154.1, 148.5, 136.3, 123.7, 121.0, 106.8, 77.4, 77.1, 76.7, 68.0, 30.9, 23.9, 11.5. HRMS (ESI-TOF) for  $\text{C}_{11}\text{H}_{15}\text{N}_2\text{O}_2$  ( $[\text{M}+\text{H}]^+$ ): calcd. 207.1134; found: 207.1129. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3142, 1668, 1593, 1472, 1400, 1147, 1055, 617.



**(E)-1-phenylethan-1-one O-(5-methyltetrahydrofuran-2-yl) oxime (3ae):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Yellow oil (10%, 2.2 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (dd,  $J = 6.8, 3.0$  Hz, 2H), 7.35 (dd,  $J = 5.0, 1.8$  Hz, 3H), 5.85 (d,  $J = 4.4$  Hz, 1H), 4.27 (dd,  $J = 10.4, 4.2$  Hz, 1H), 2.24 (s, 3H), 2.21 – 2.04 (m, 3H), 1.79 – 1.67 (m, 1H), 1.34 (d,  $J = 6.2$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  155.4, 136.7, 129.1, 128.3, 126.3, 106.8, 32.3, 31.4, 22.7, 13.0. HRMS (ESI-TOF) for  $\text{C}_{13}\text{H}_{17}\text{NNaO}_2$  ( $[\text{M}+\text{Na}]^+$ ): calcd. 242.1157; found: 242.1156. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3141, 1599, 1486, 1441, 1404, 1044.



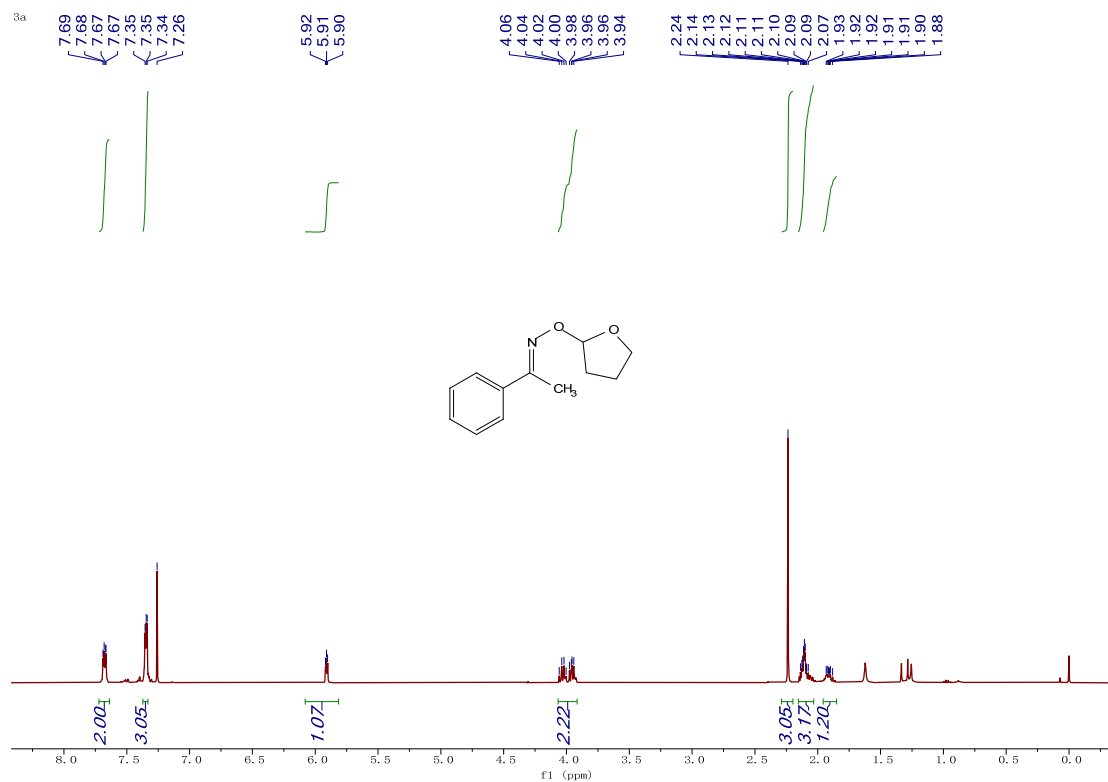
**(E)-1-phenylethan-1-one O-tetrahydro-2H-pyran-2-yl oxime (3af):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Yellow oil (29%, 6.4 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.70 – 7.66 (m, 2H), 7.37 – 7.33 (m, 3H), 5.41 (dd,  $J = 4.9, 2.6$  Hz, 1H), 3.94 (ddd,  $J = 10.8, 7.7, 3.0$  Hz, 1H), 3.68 – 3.60 (m, 1H), 2.31 (s, 3H), 1.94 – 1.76 (m, 3H), 1.62 (dd,  $J = 8.7, 3.3$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  156.4, 136.5, 129.2, 128.3, 126.4, 101.1, 63.2, 29.2, 25.3, 20.1, 13.1. HRMS (ESI-TOF) for  $\text{C}_{13}\text{H}_{17}\text{NNaO}_2$  ( $[\text{M}+\text{Na}]^+$ ): calcd. 242.1157; found: 242.1166. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3142, 2966, 1592, 1473, 1401, 1286, 1116, 975, 932.



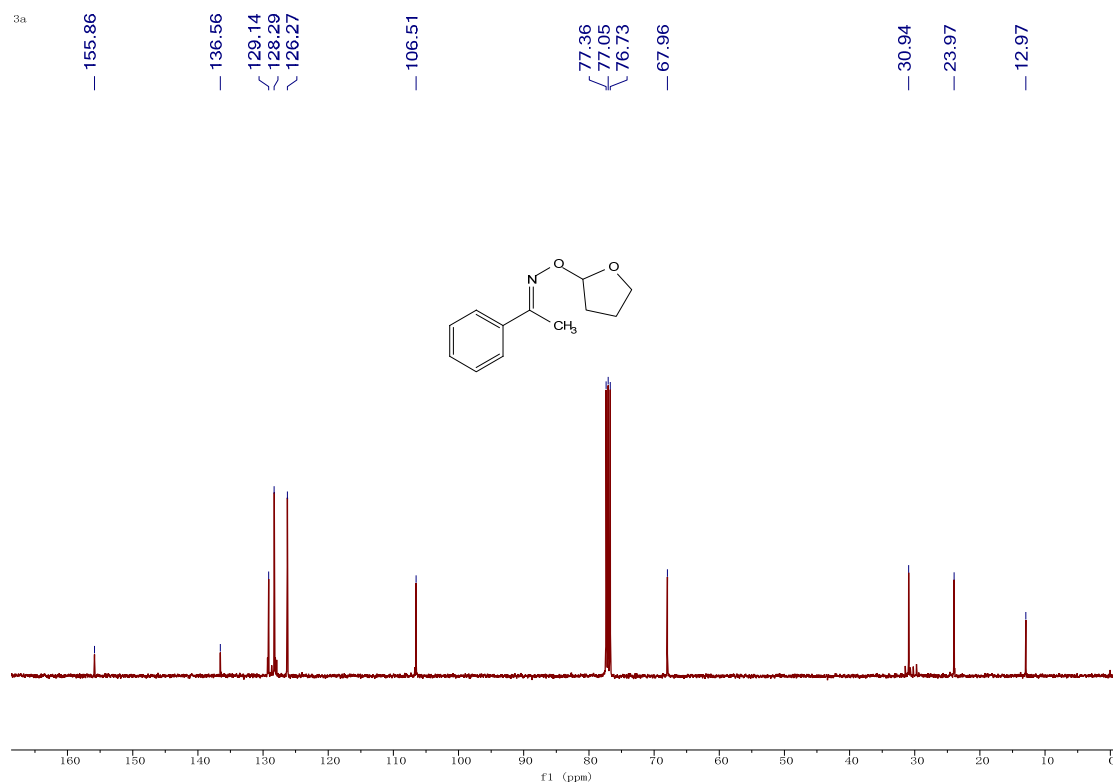
**(E)-1-phenylethan-1-one O-oxepan-2-yl oxime (3ag):** The product was purified by silica gel column chromatography with petroleum ether/ethyl acetate (eluent: petroleum ether/ethyl acetate = 30/1). Yellow oil (38%, 8.9 mg).  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  7.68 (dd,  $J = 6.5, 2.9$  Hz, 2H), 7.37 – 7.32 (m, 3H), 5.54 (dd,  $J = 9.2, 5.2$  Hz, 1H), 3.94 – 3.84 (m, 1H), 3.66 (d,  $J = 12.6$  Hz, 1H), 2.27 (s, 3H), 1.91 – 1.81 (m, 2H), 1.81 – 1.35 (m, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  156.0, 136.56, 129.2, 128.3, 126.3, 104.6, 62.8, 32.9, 30.8, 29.4, 22.9, 13.1. IR (neat):  $\nu_{\text{max}}$  ( $\text{cm}^{-1}$ ) 3137, 2936, 1664, 1594, 1501, 1402, 1131, 1020, 987.

## 12. $^1\text{H}$ NMR and $^{13}\text{C}$ NMR Spectra

### $^1\text{H}$ NMR-spectrum (400MHz, $\text{CDCl}_3$ ) of 3a



**<sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3a**

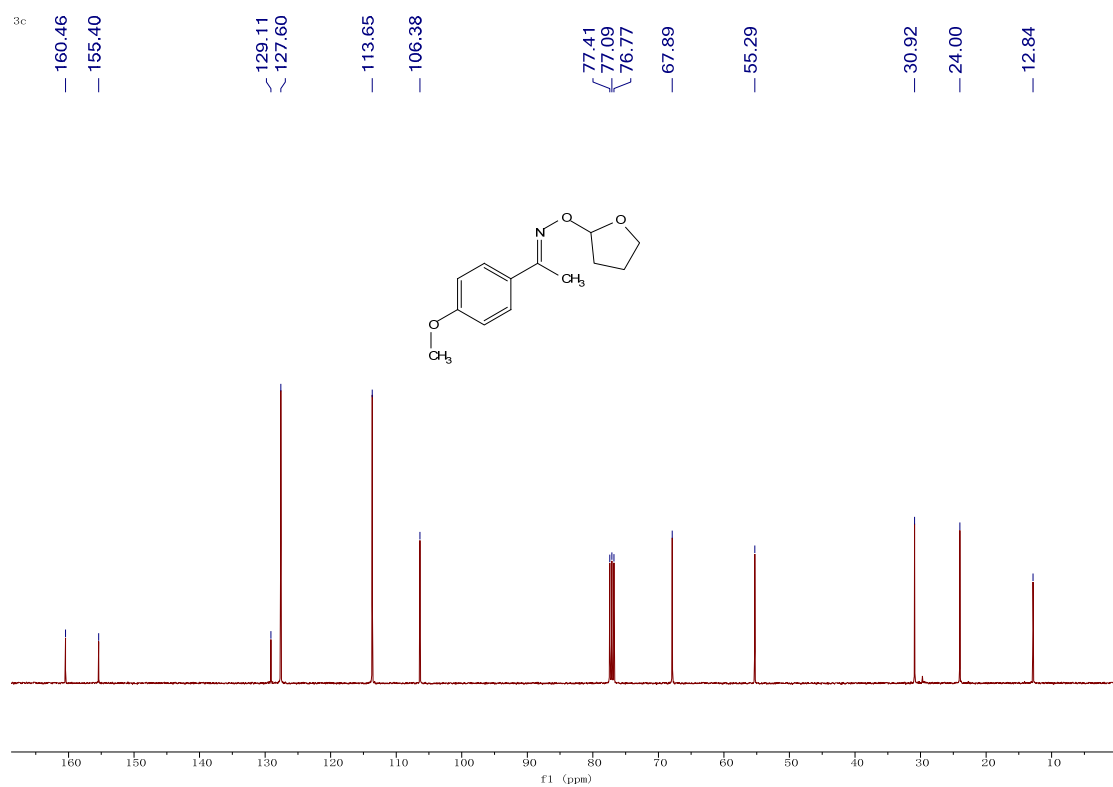


**<sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3b**

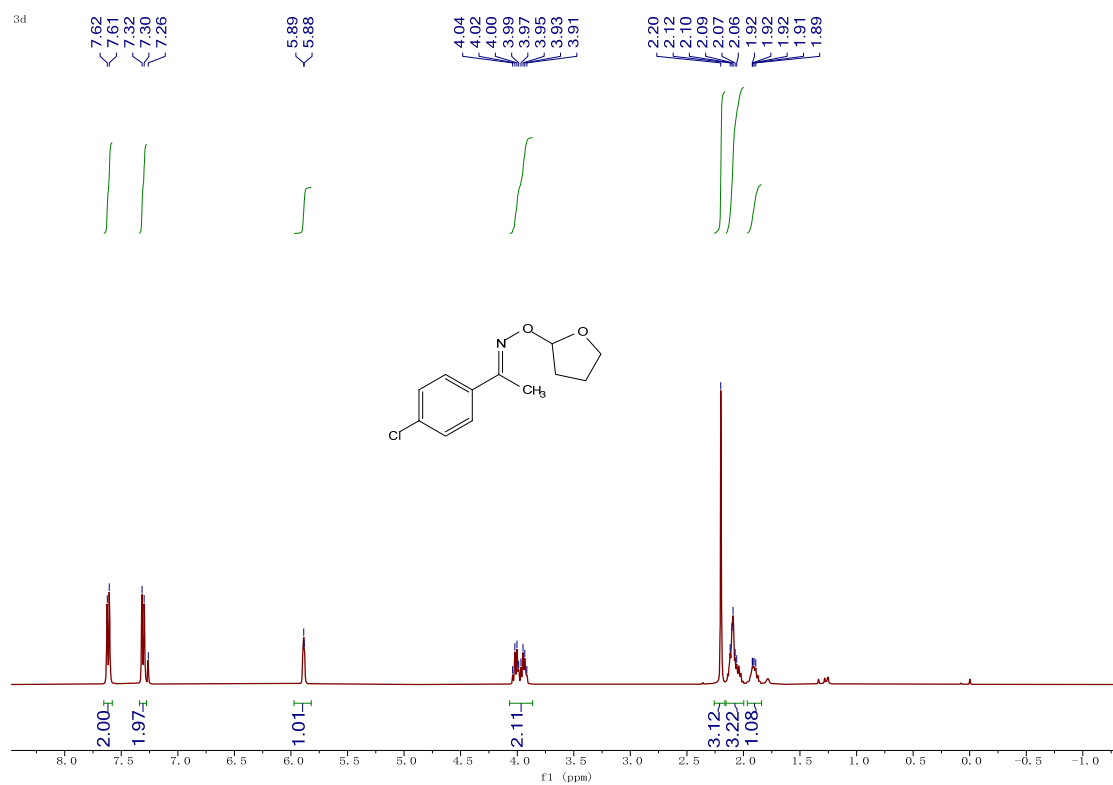




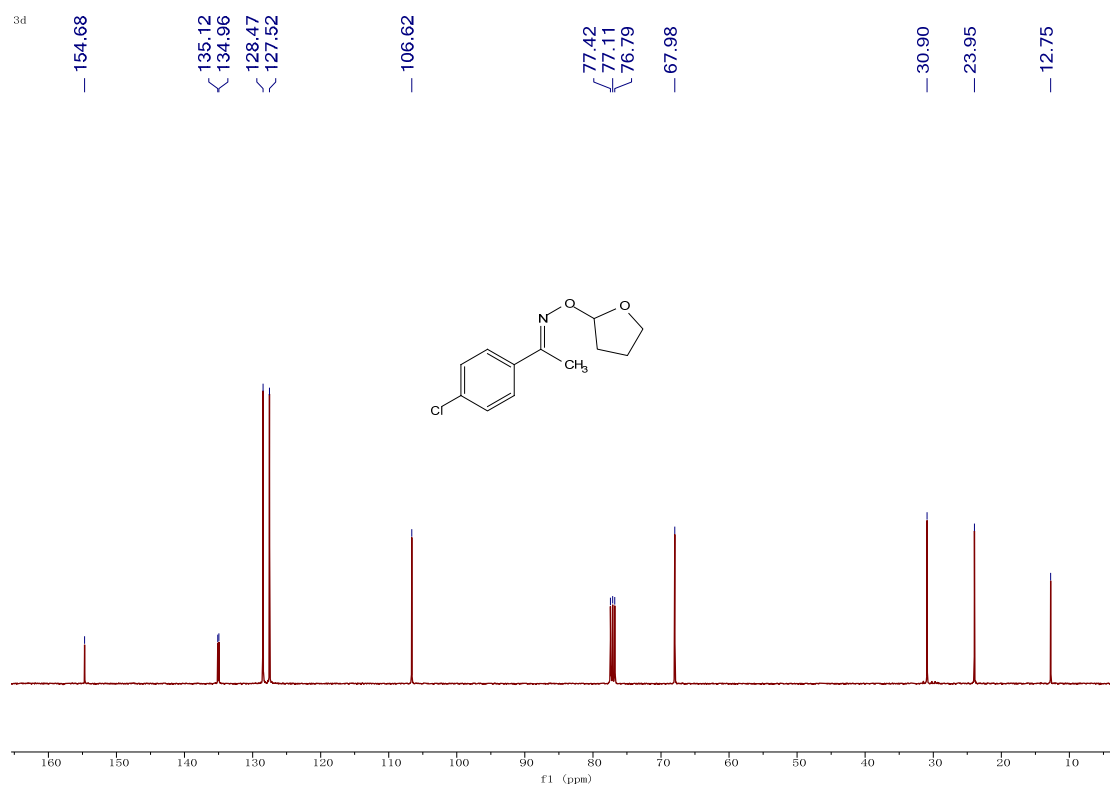
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3c



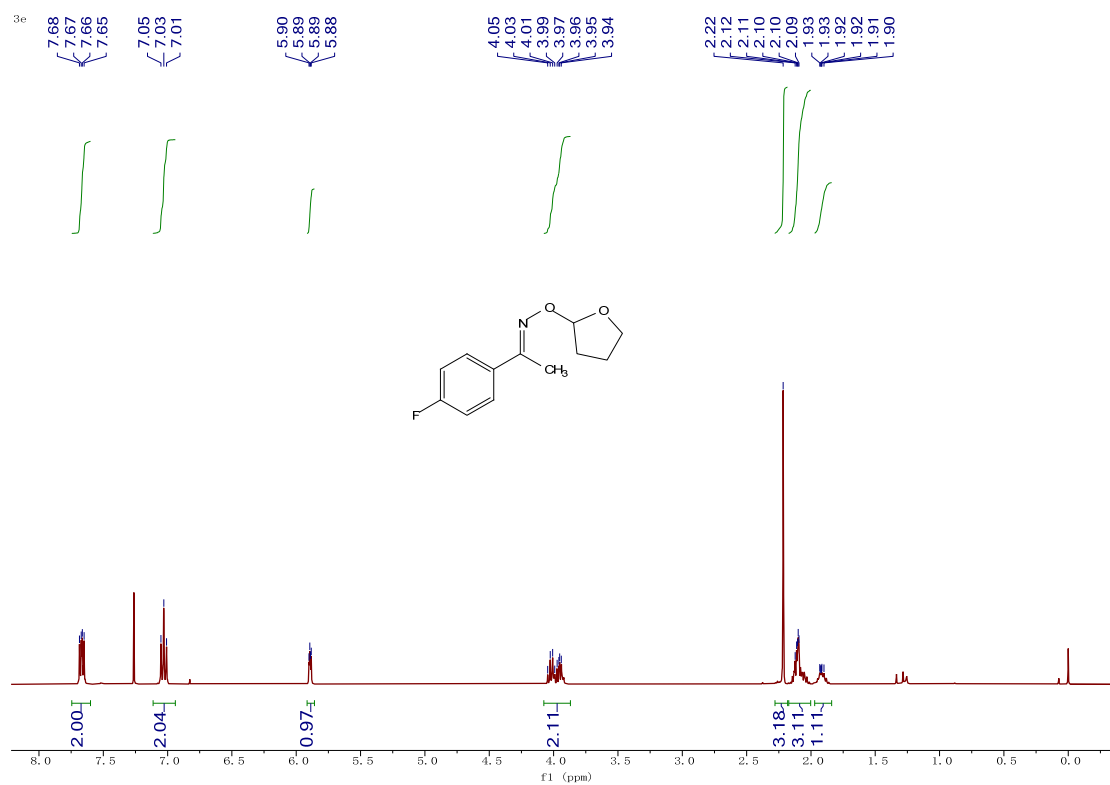
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3d



### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3d

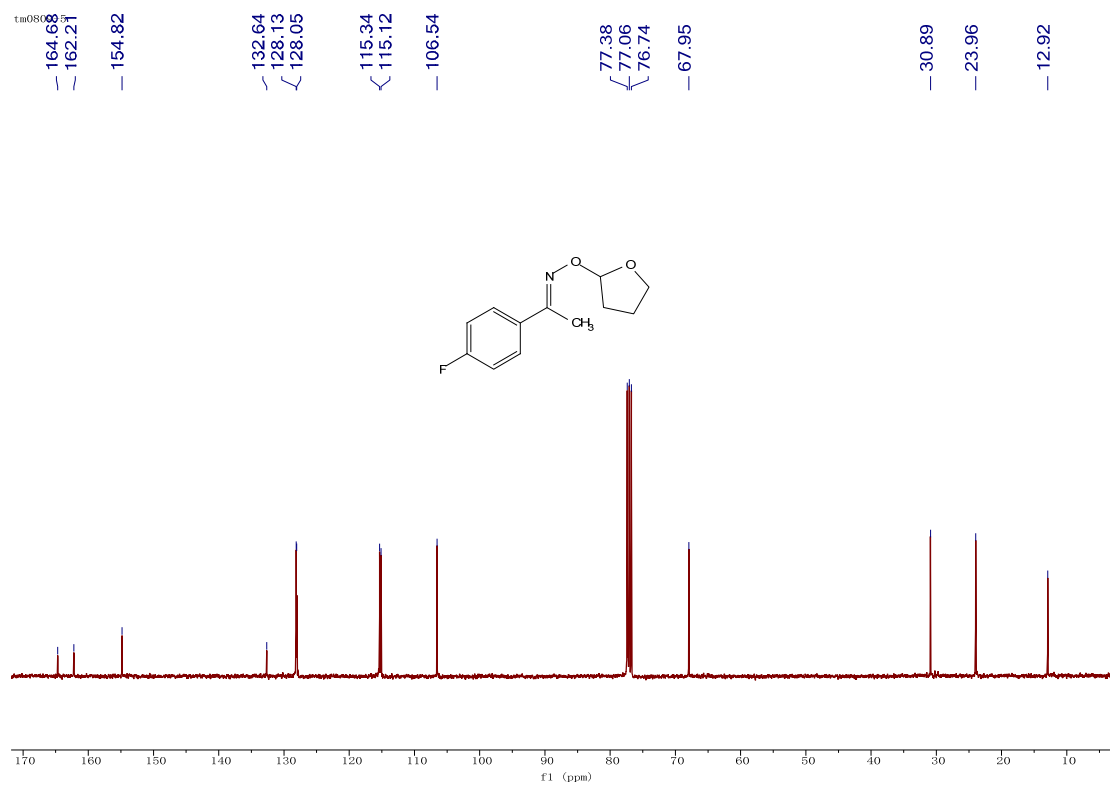


### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3e

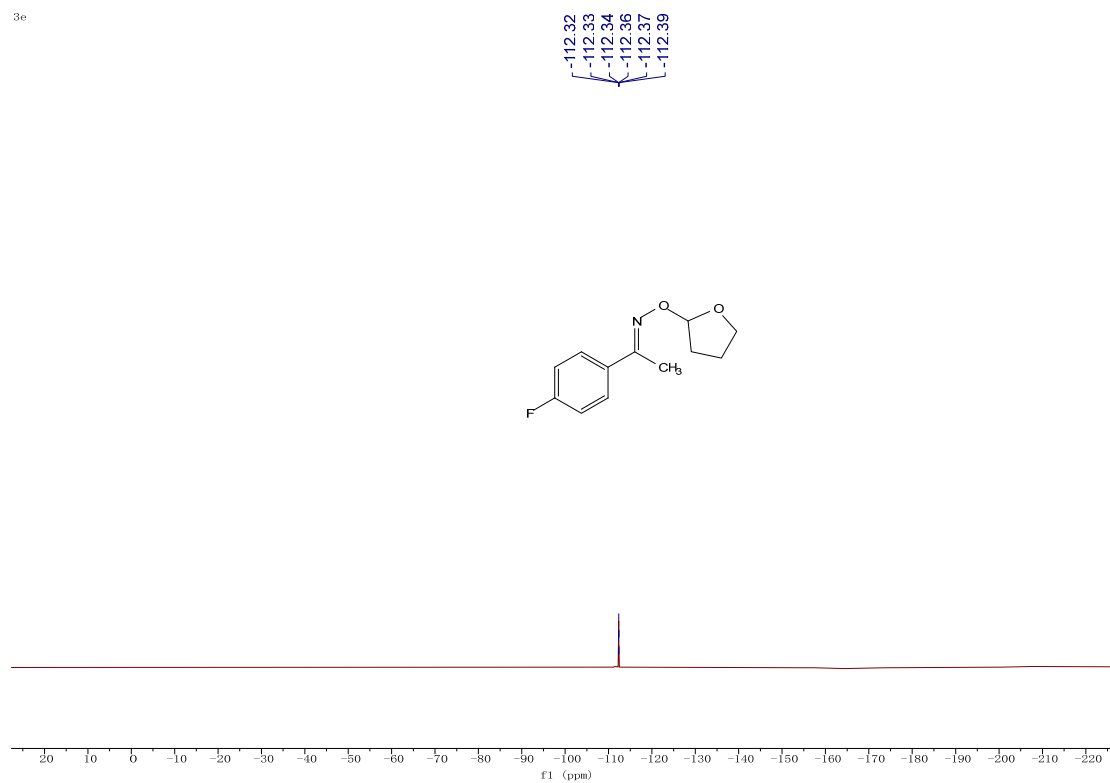




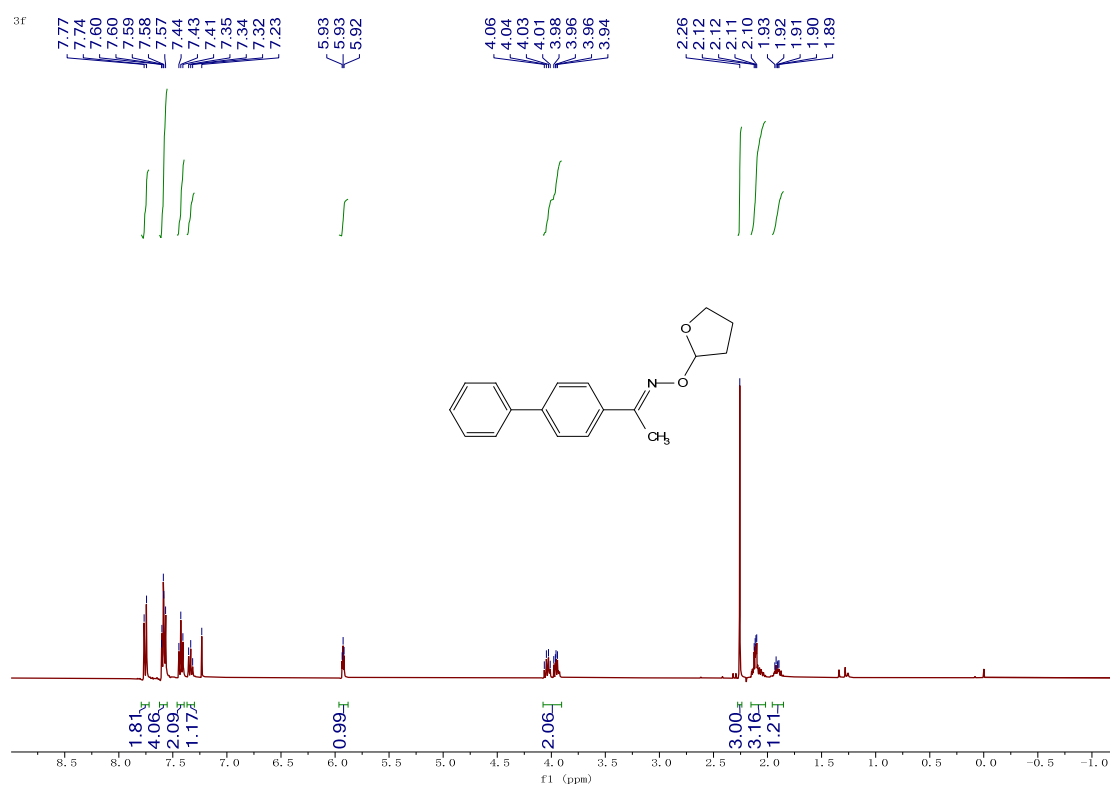
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3e



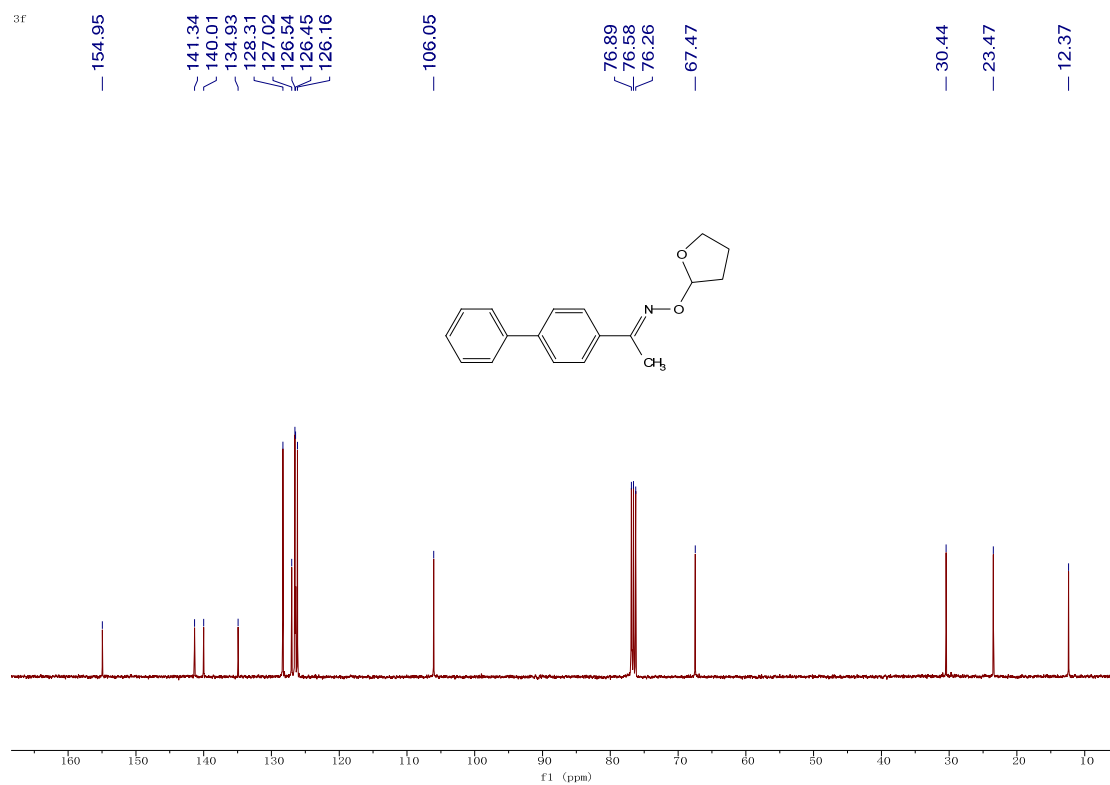
### <sup>19</sup>F NMR-spectrum (376MHz, CDCl<sub>3</sub>) of 3e



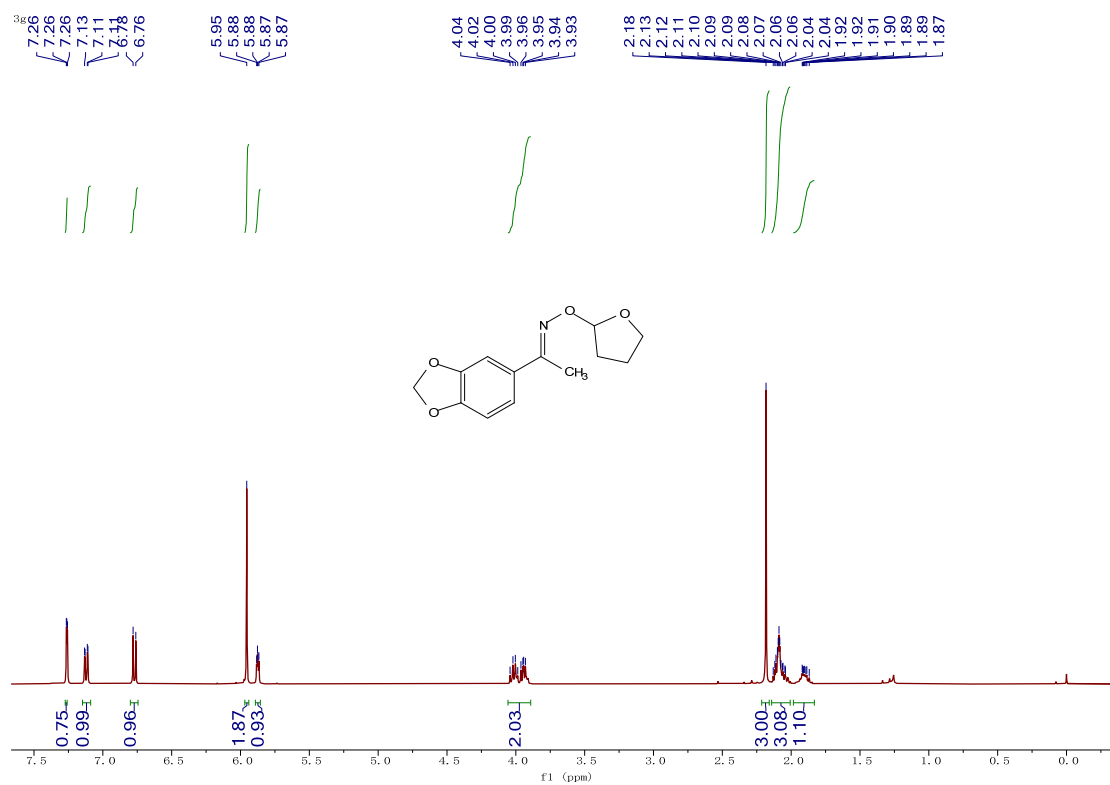
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3f



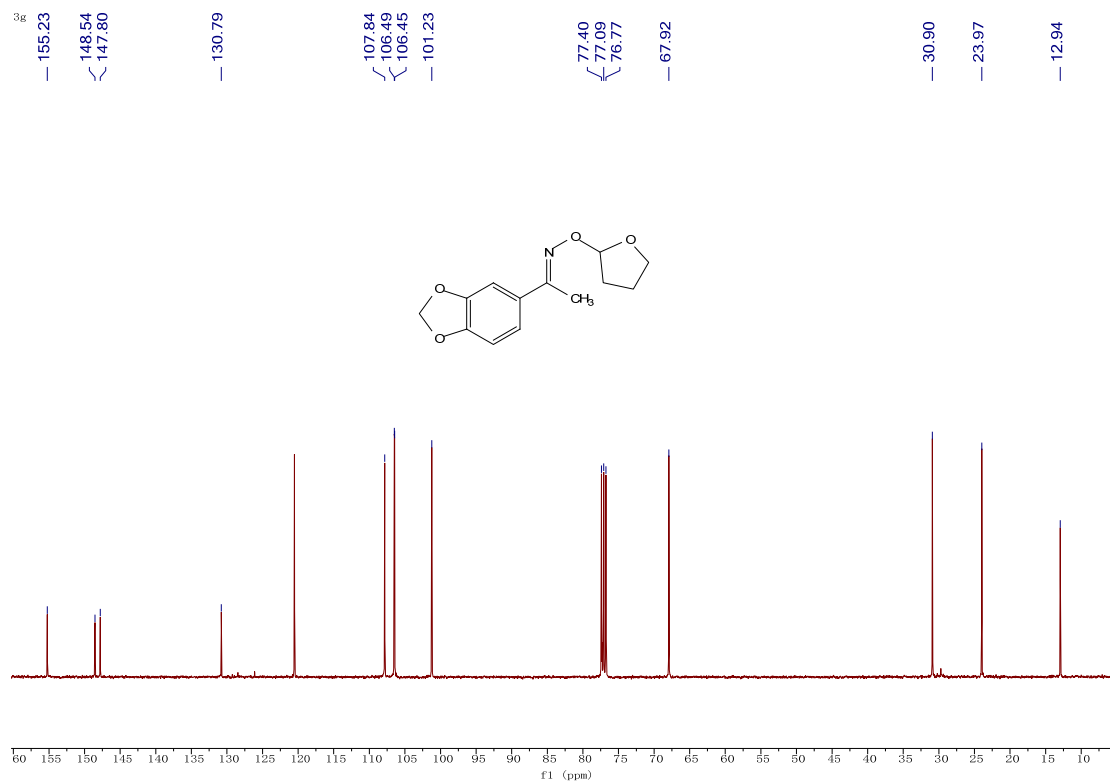
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3f



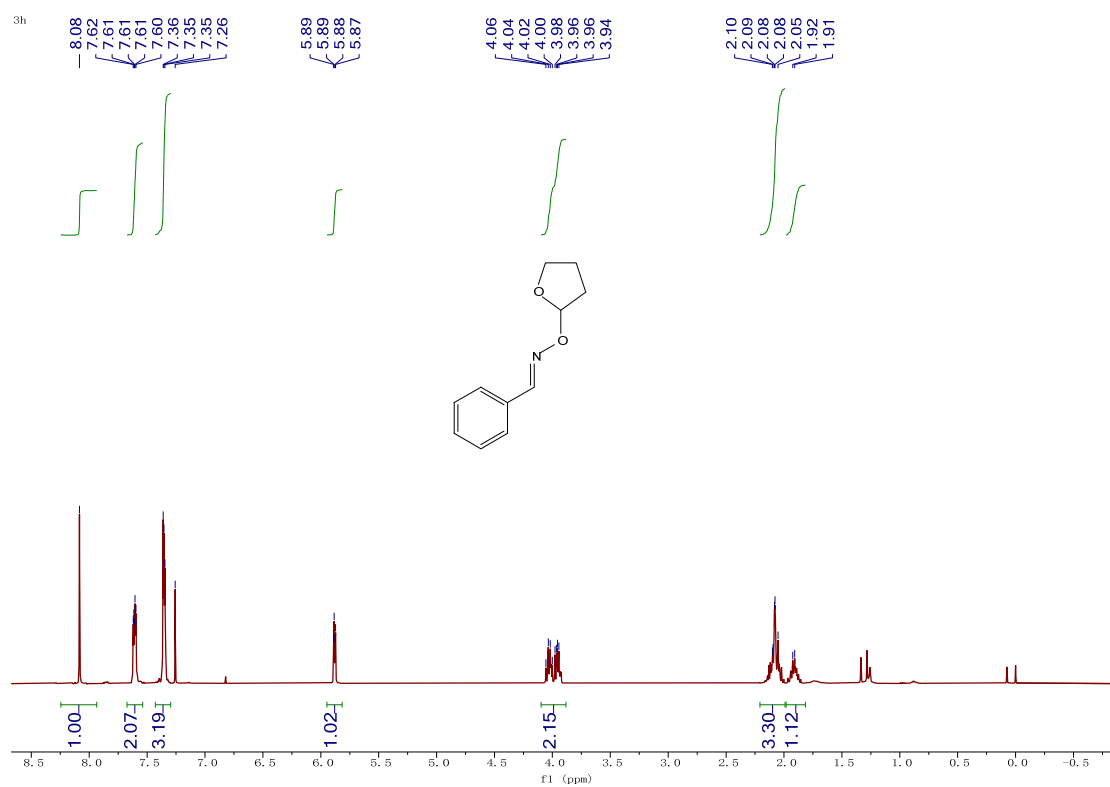
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3g



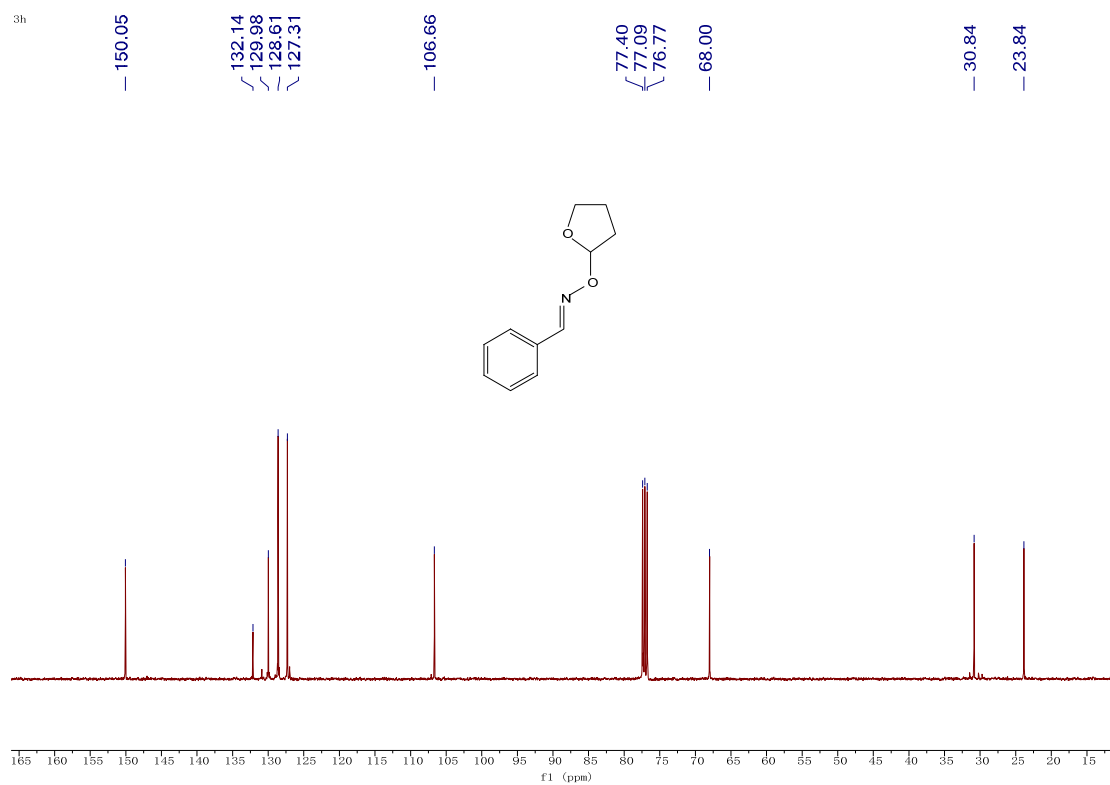
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3g



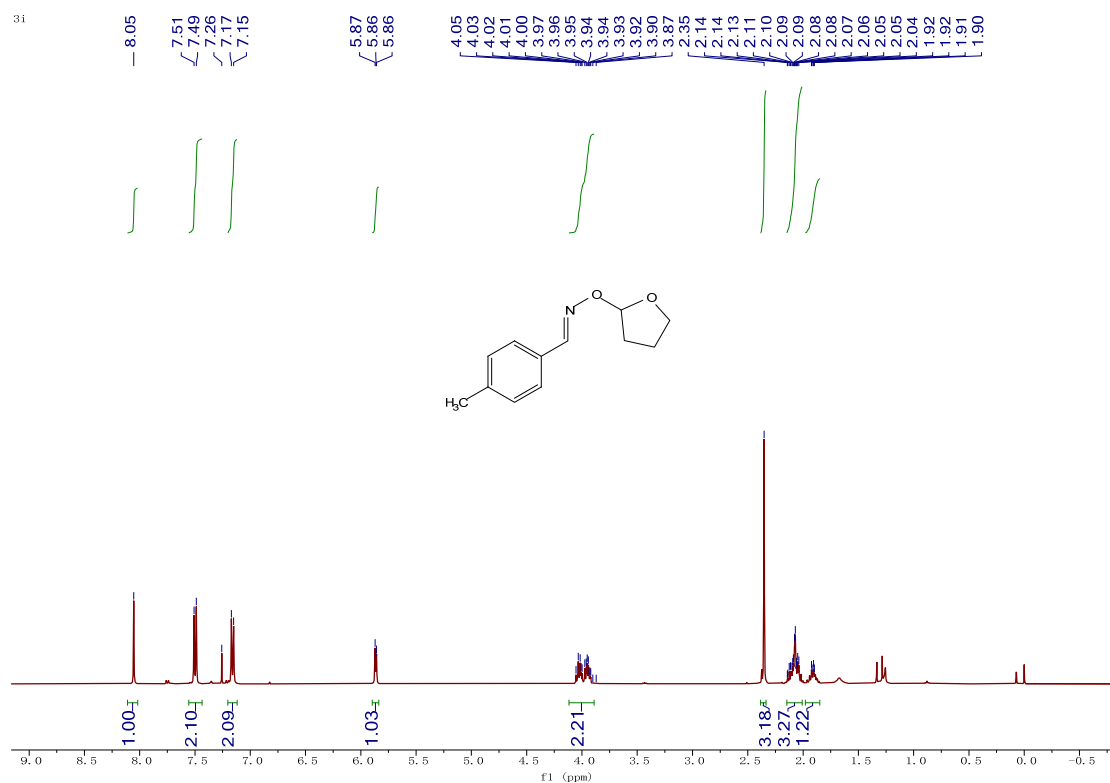
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3h



### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3h



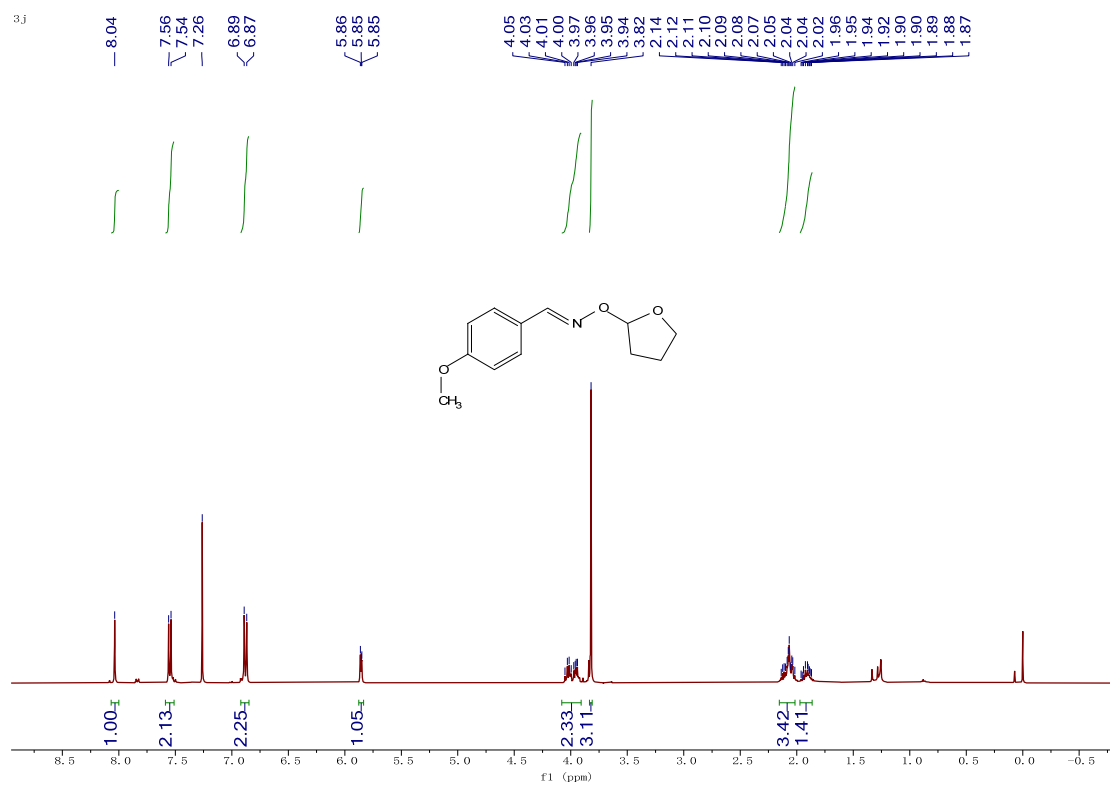
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3i



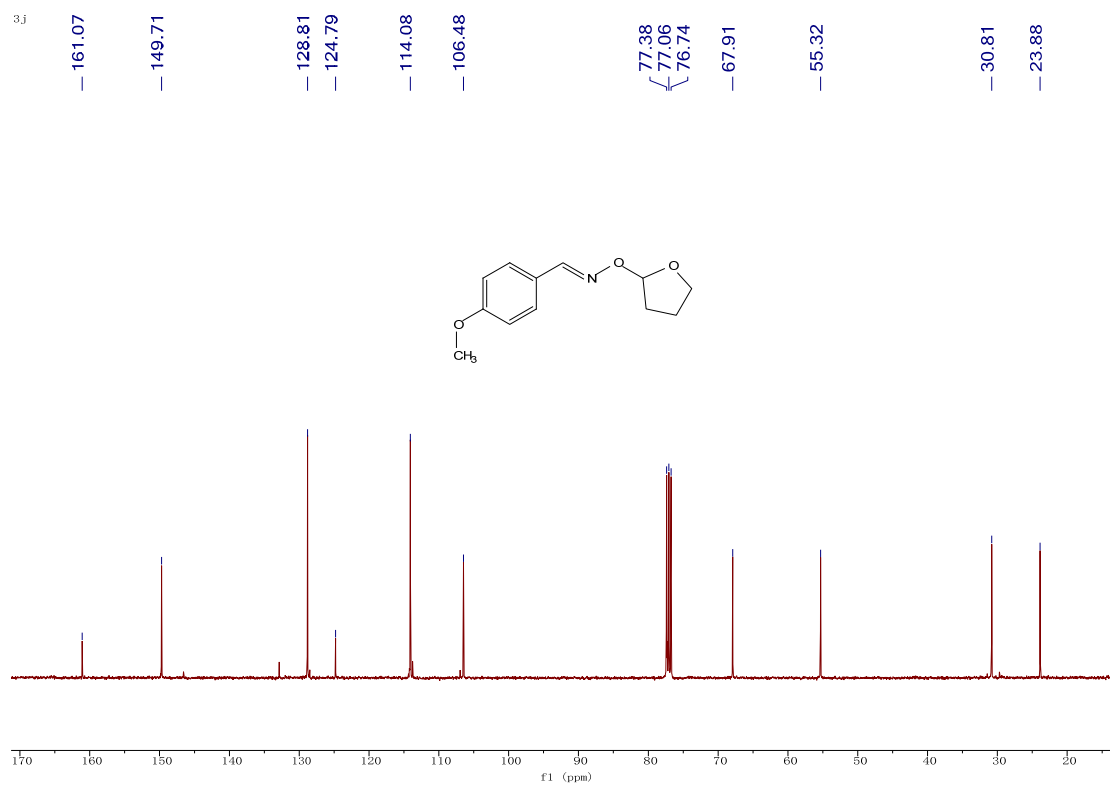
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3i



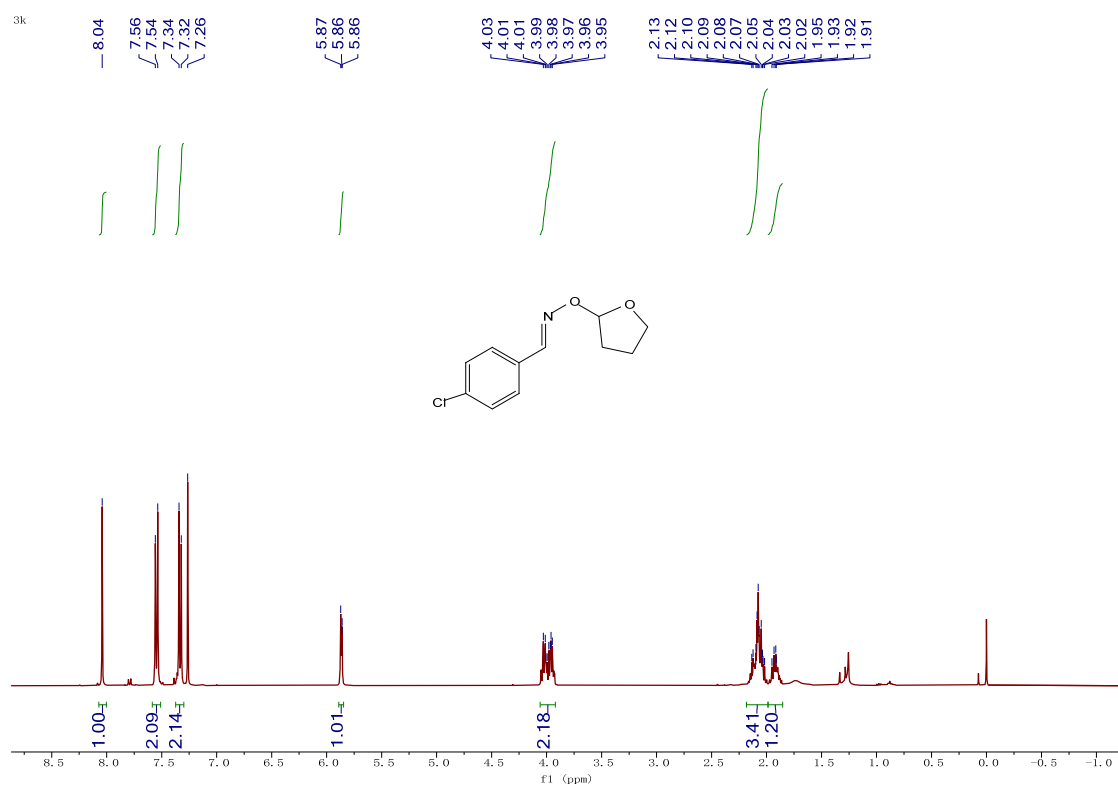
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3j



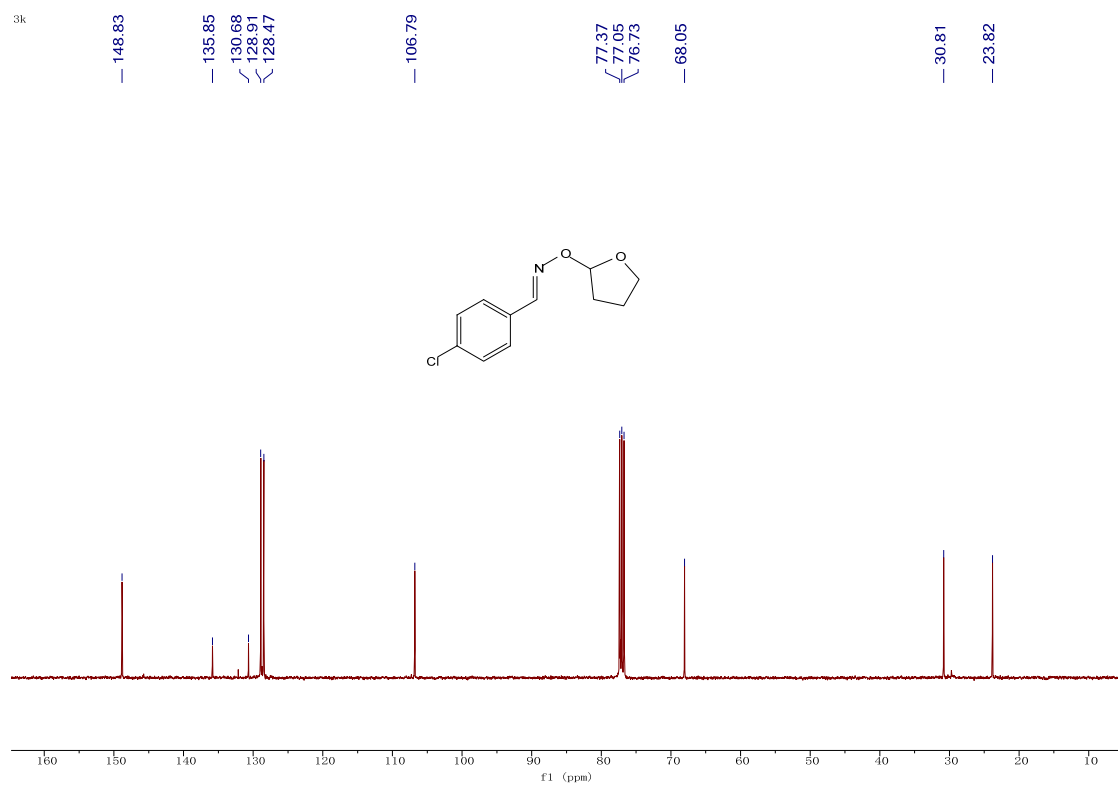
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3j



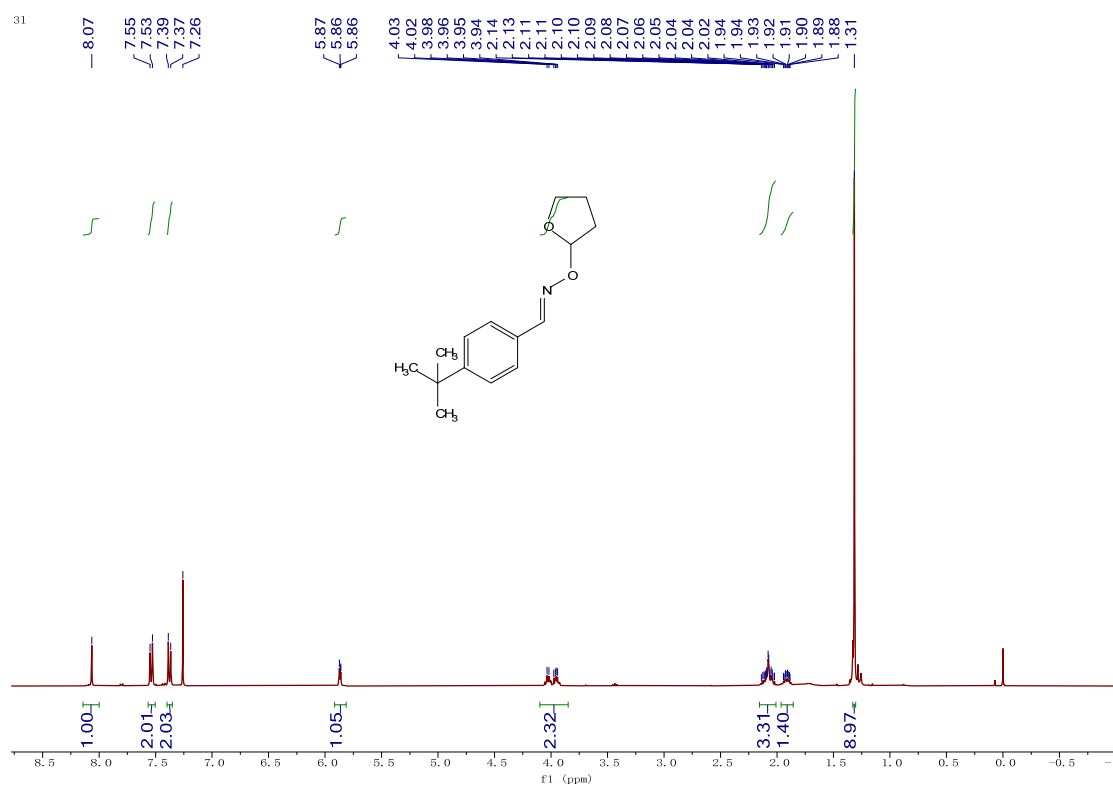
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3k



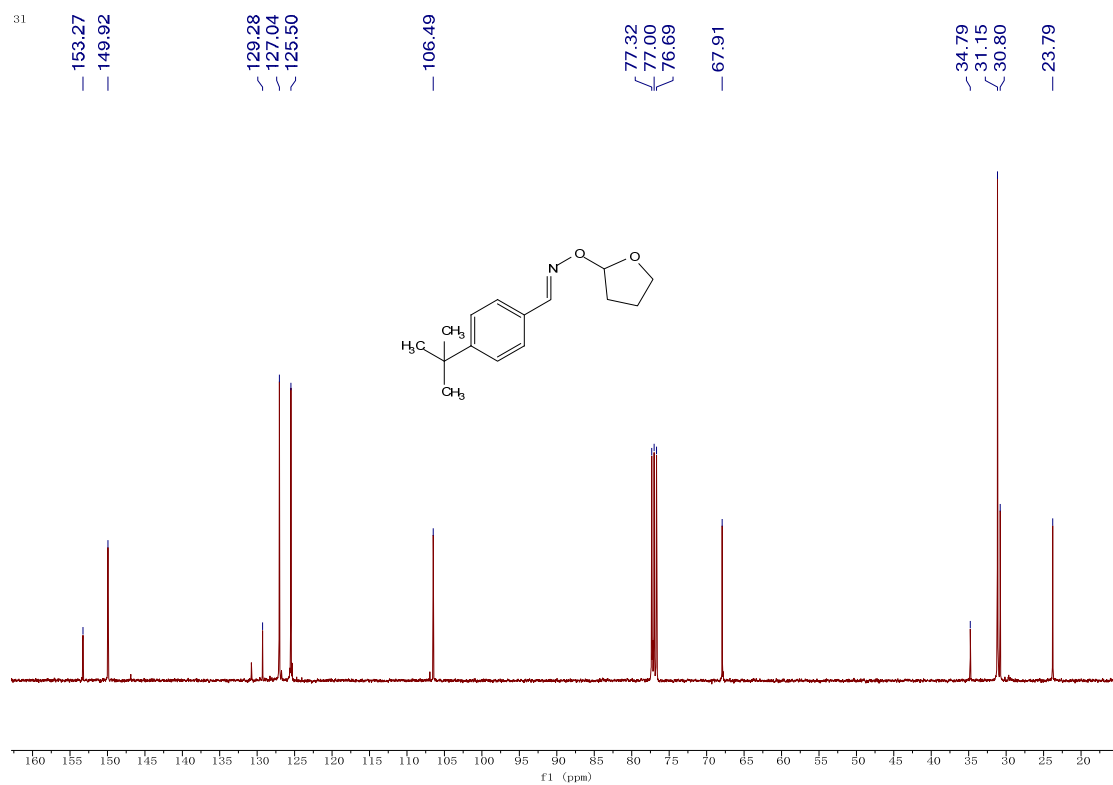
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3k



**<sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 31**

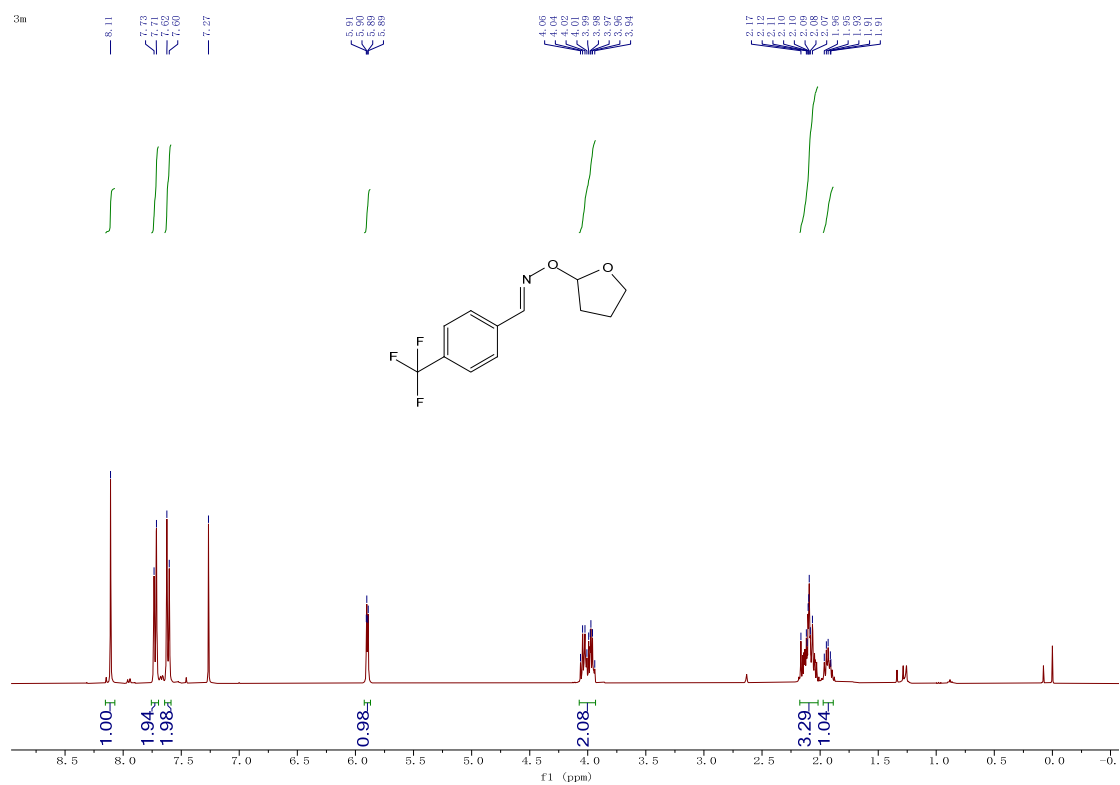


**<sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 31**

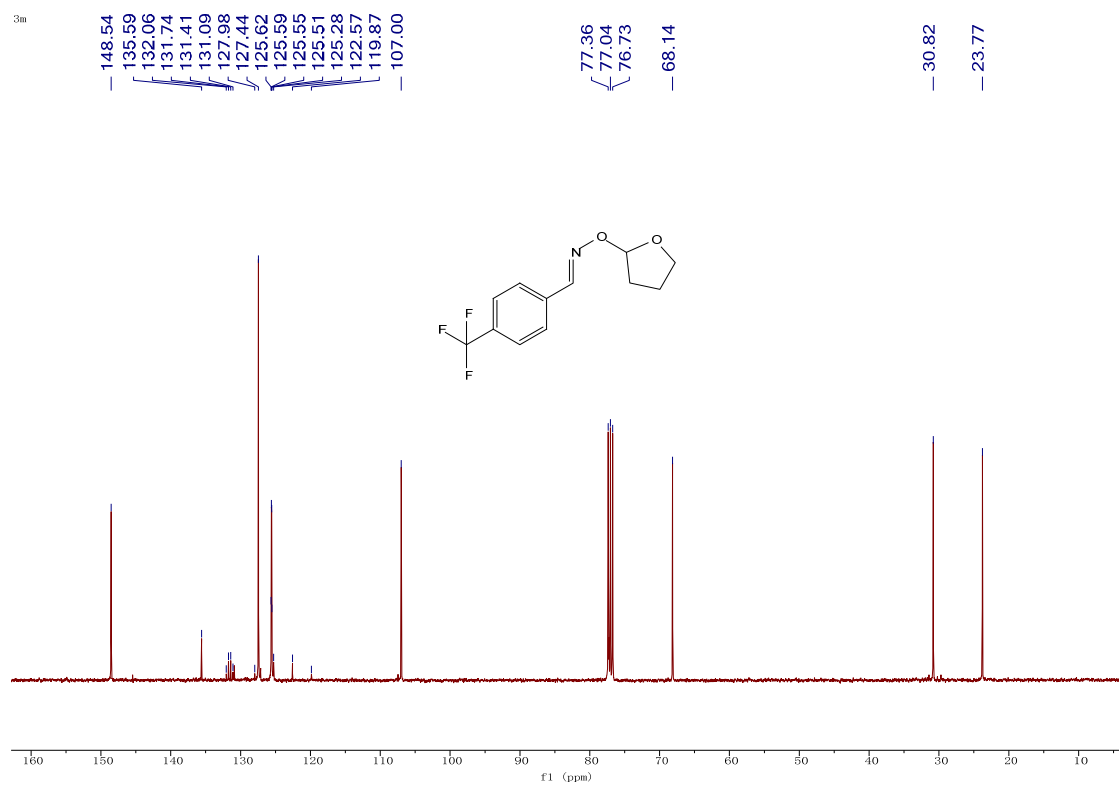




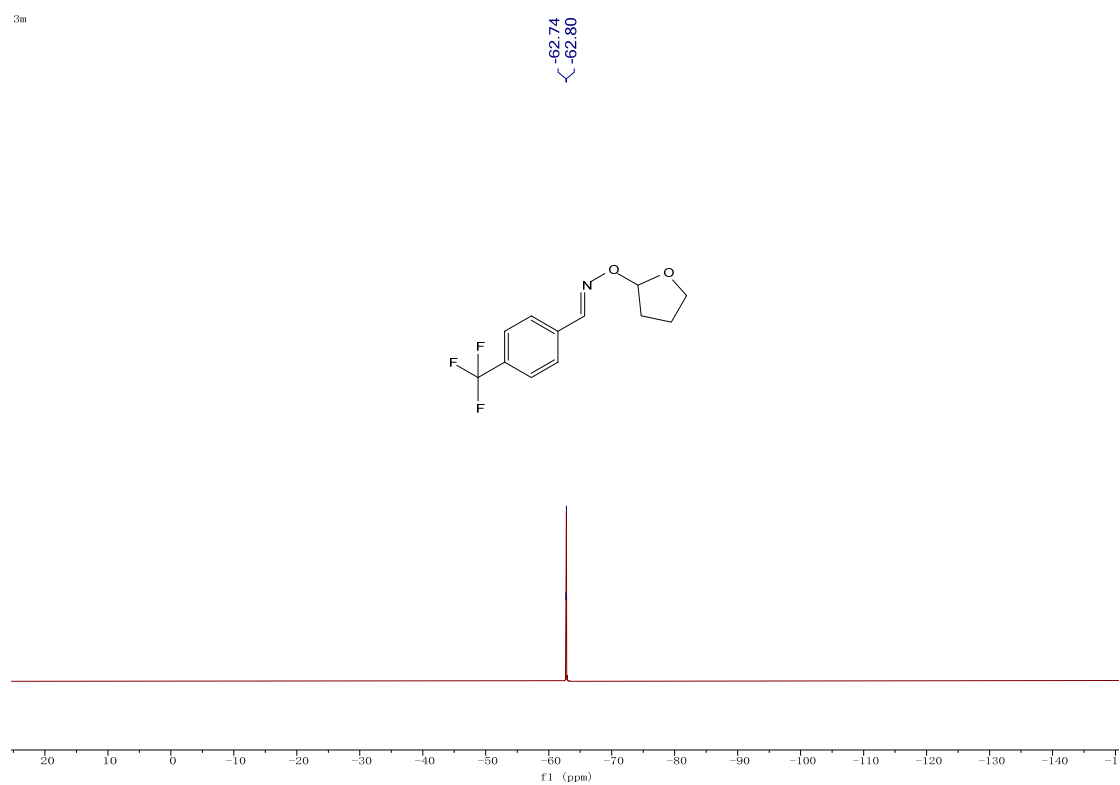
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3m



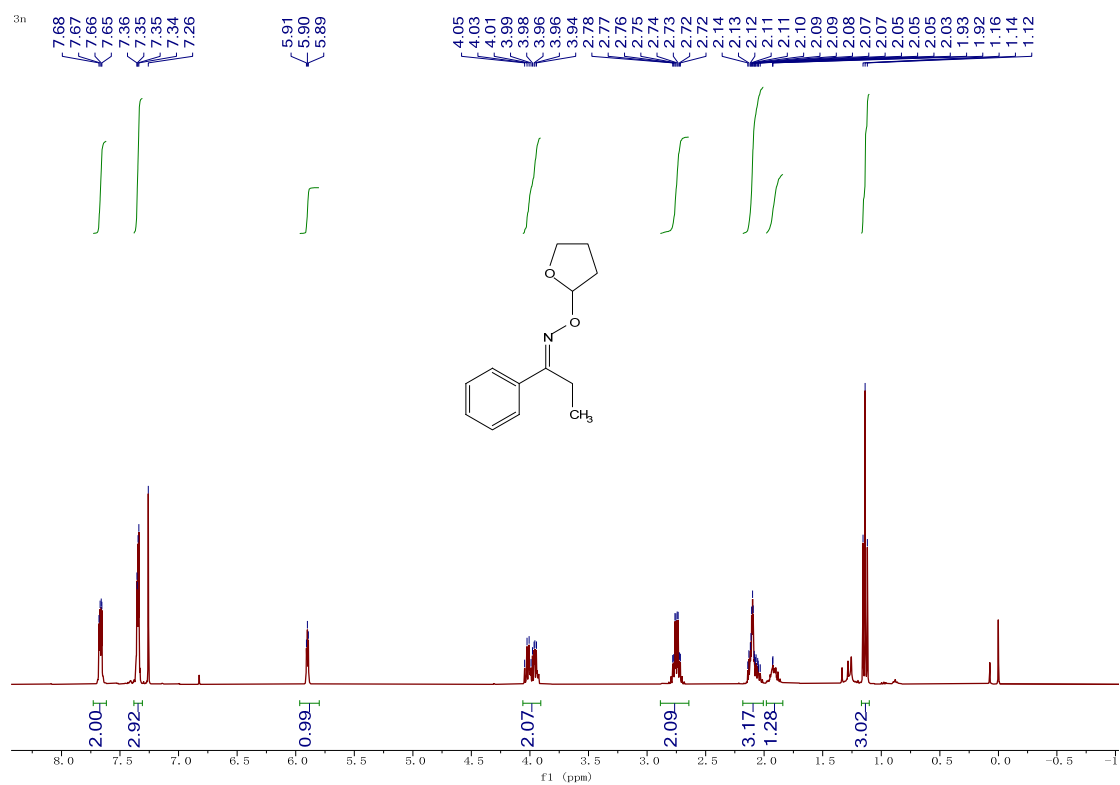
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3m



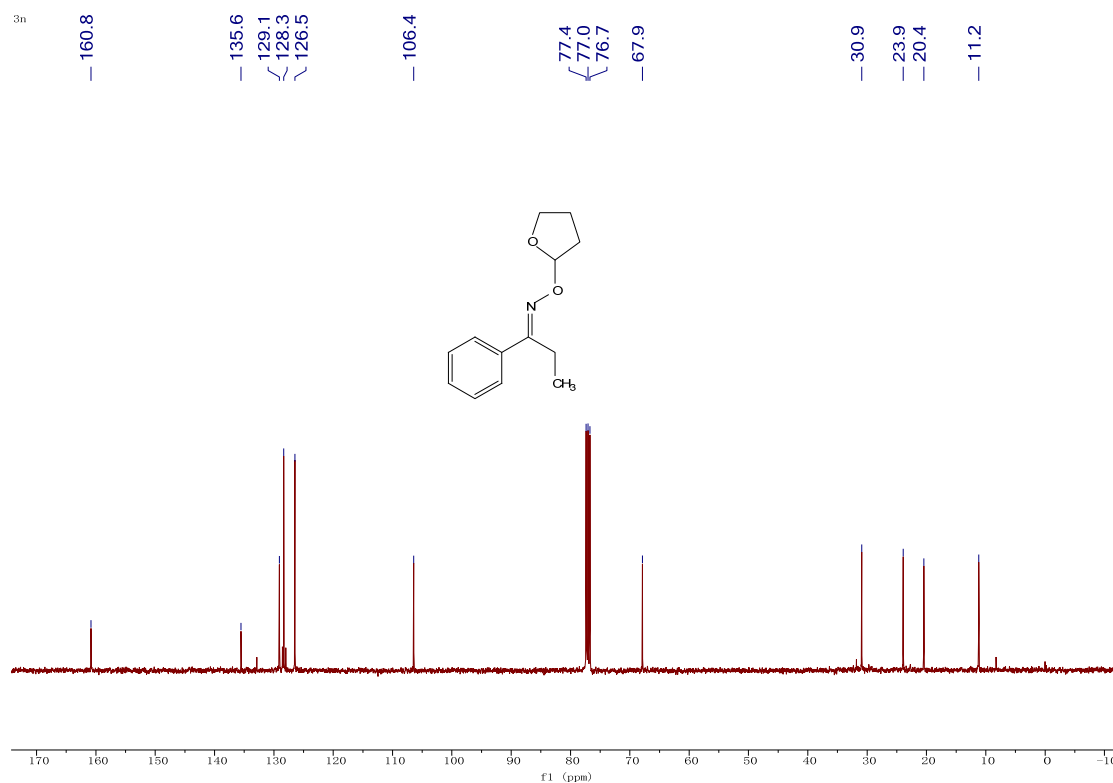
# <sup>19</sup>F NMR-spectrum (376MHz, CDCl<sub>3</sub>) of 3m



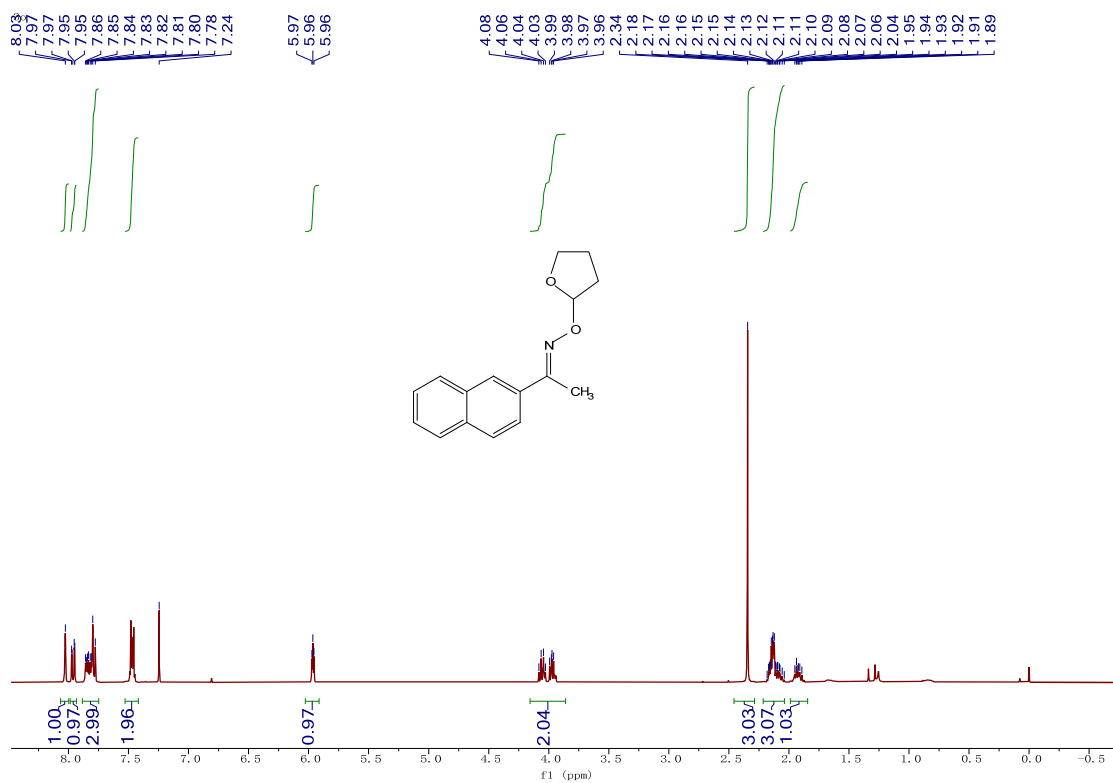
# <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3n



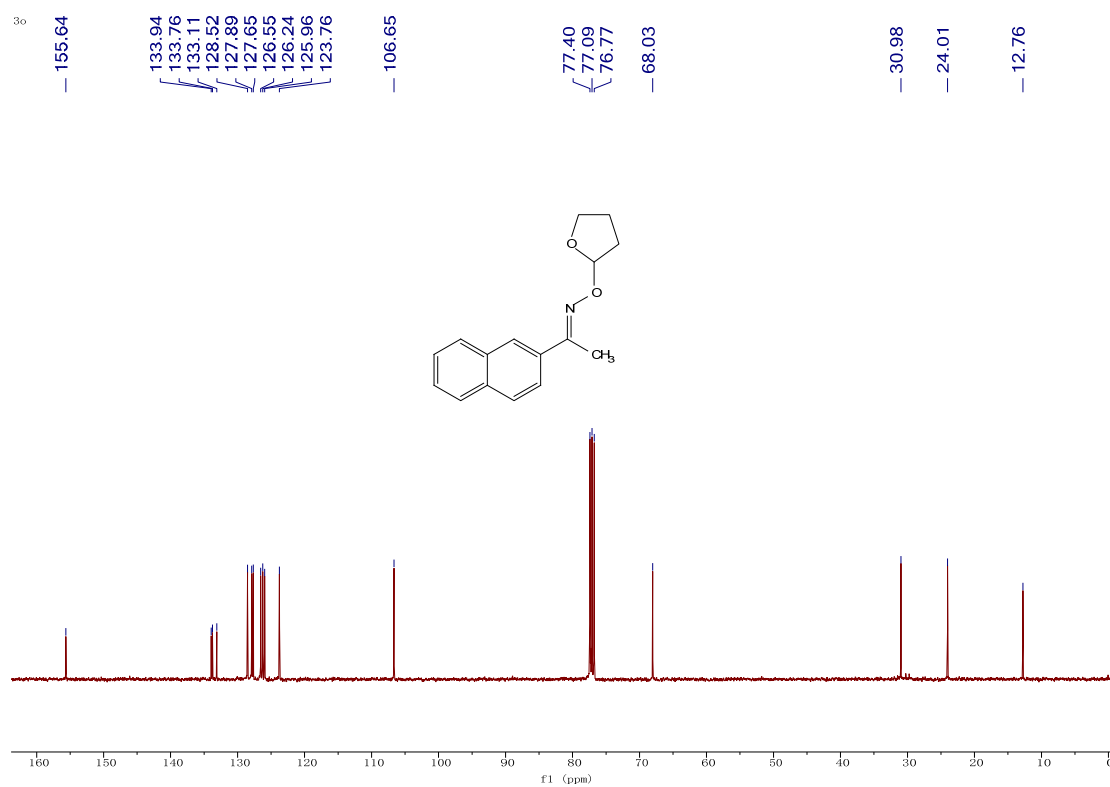
**<sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3n**



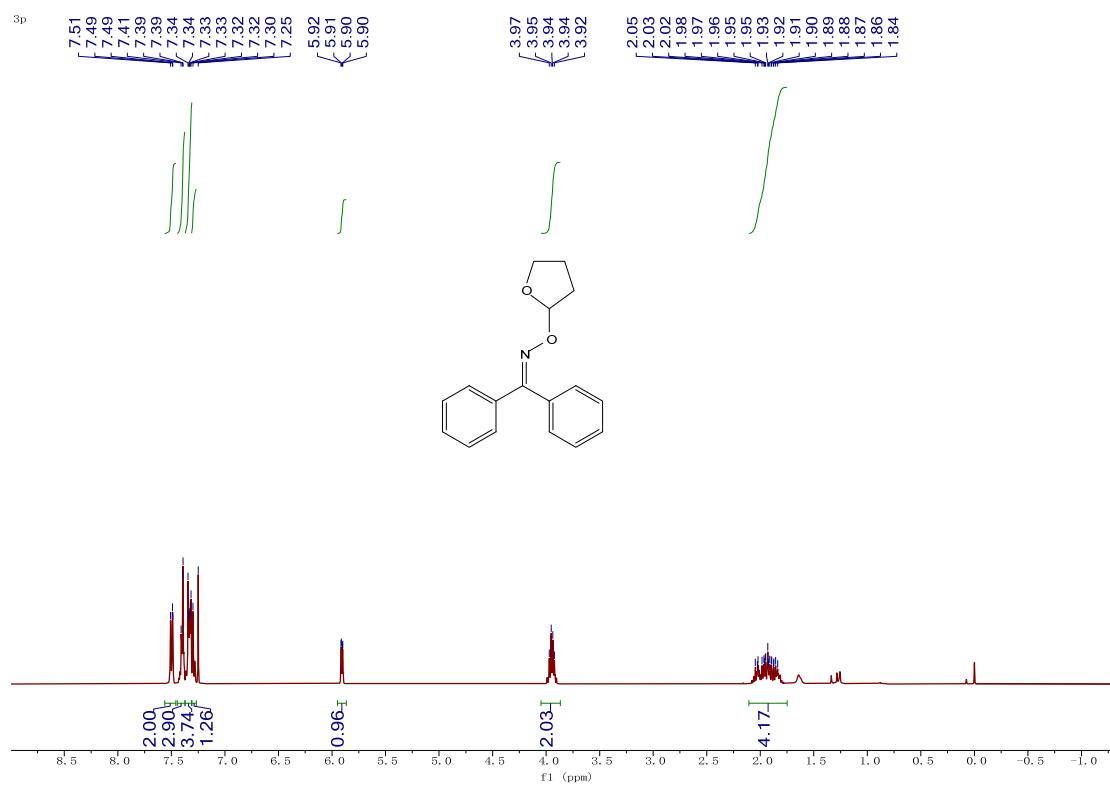
**<sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3o**



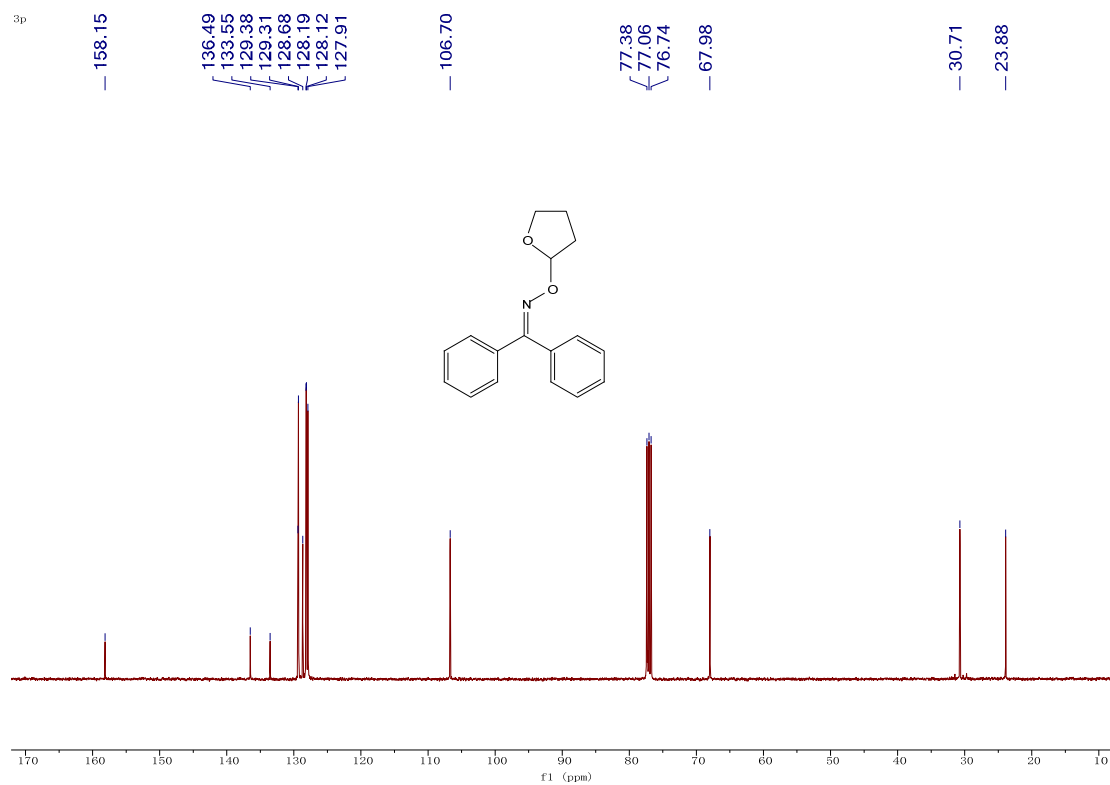
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3o



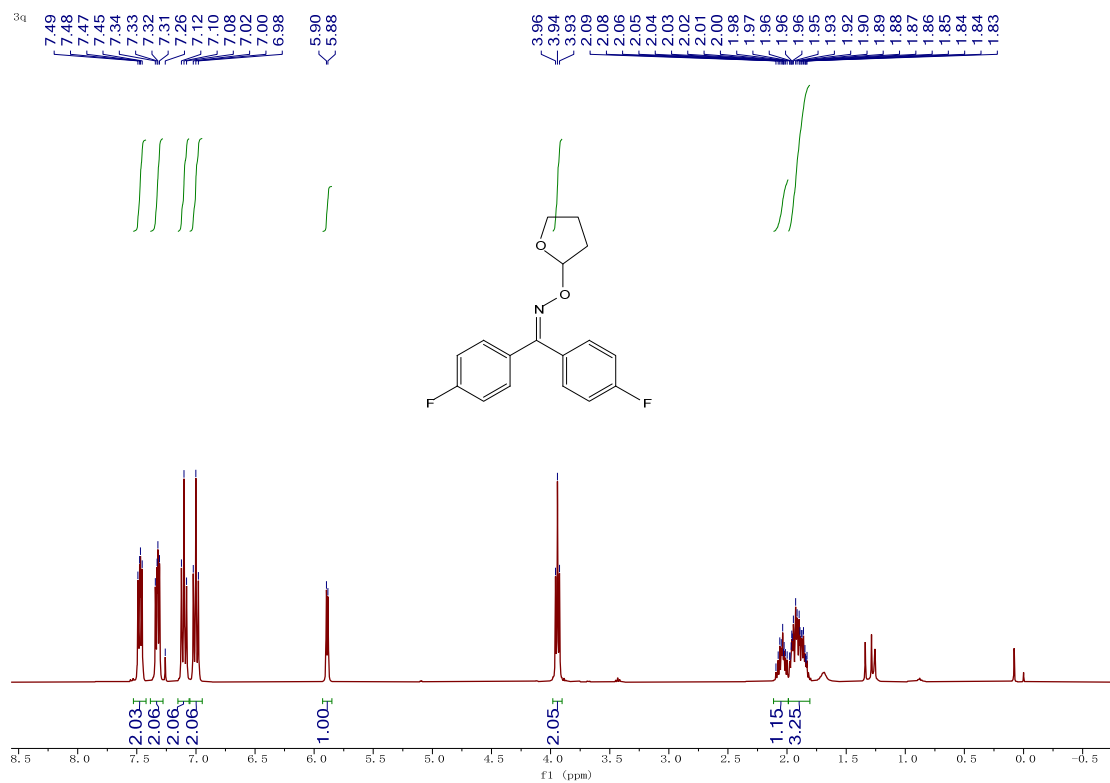
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3p



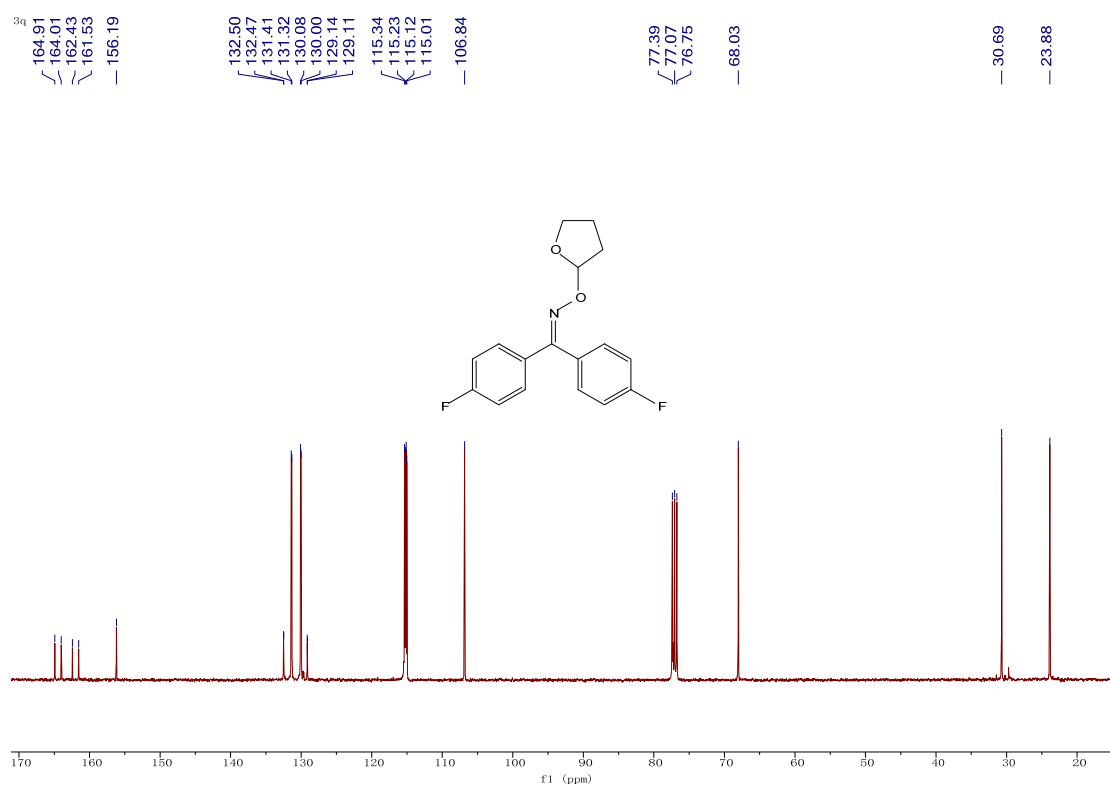
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3p



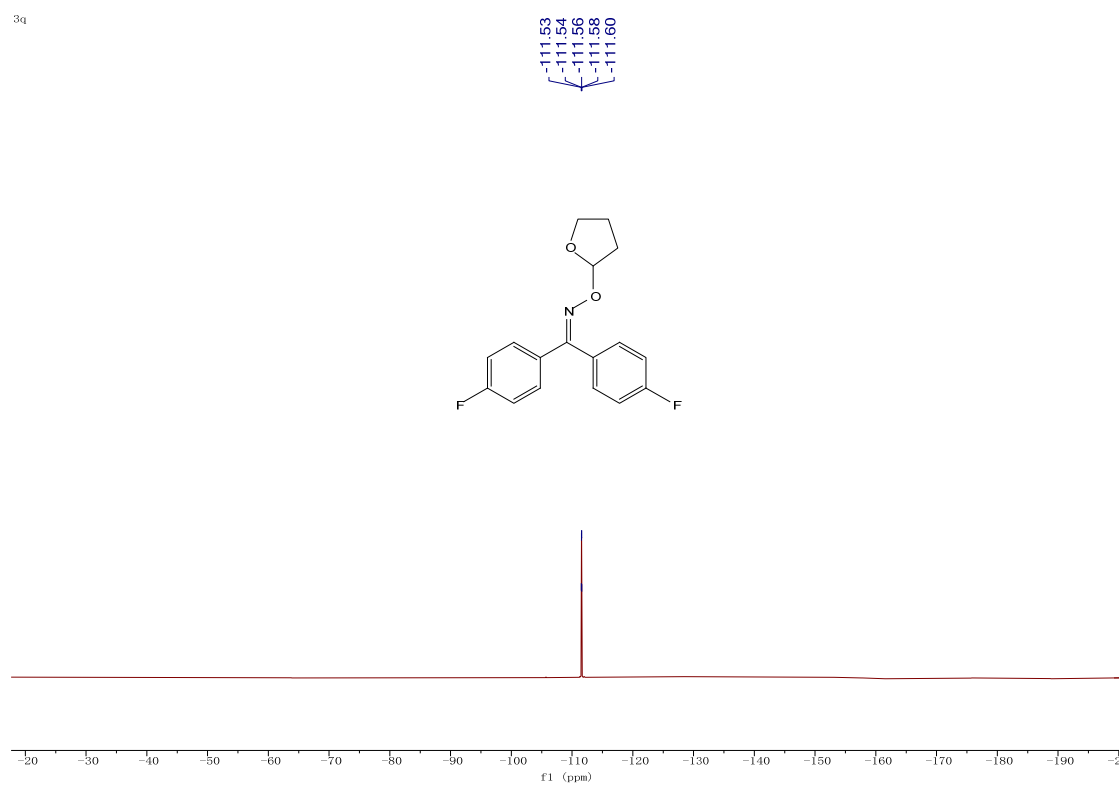
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3q



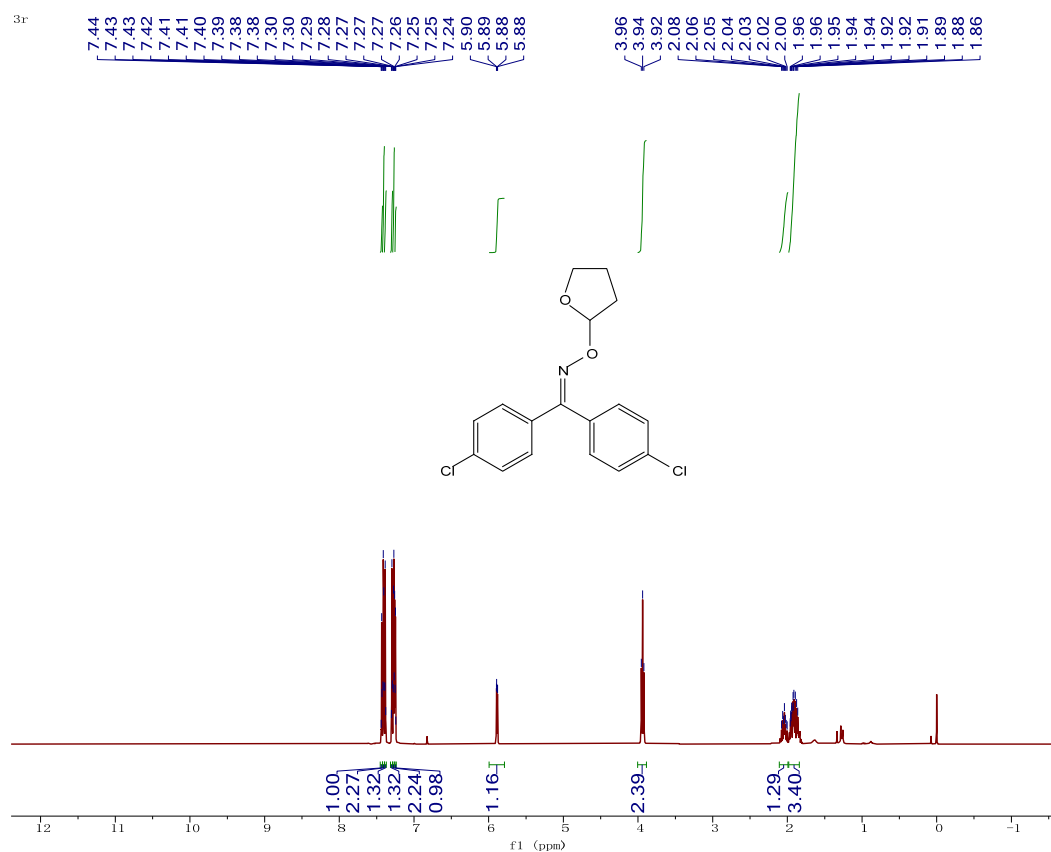
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3q



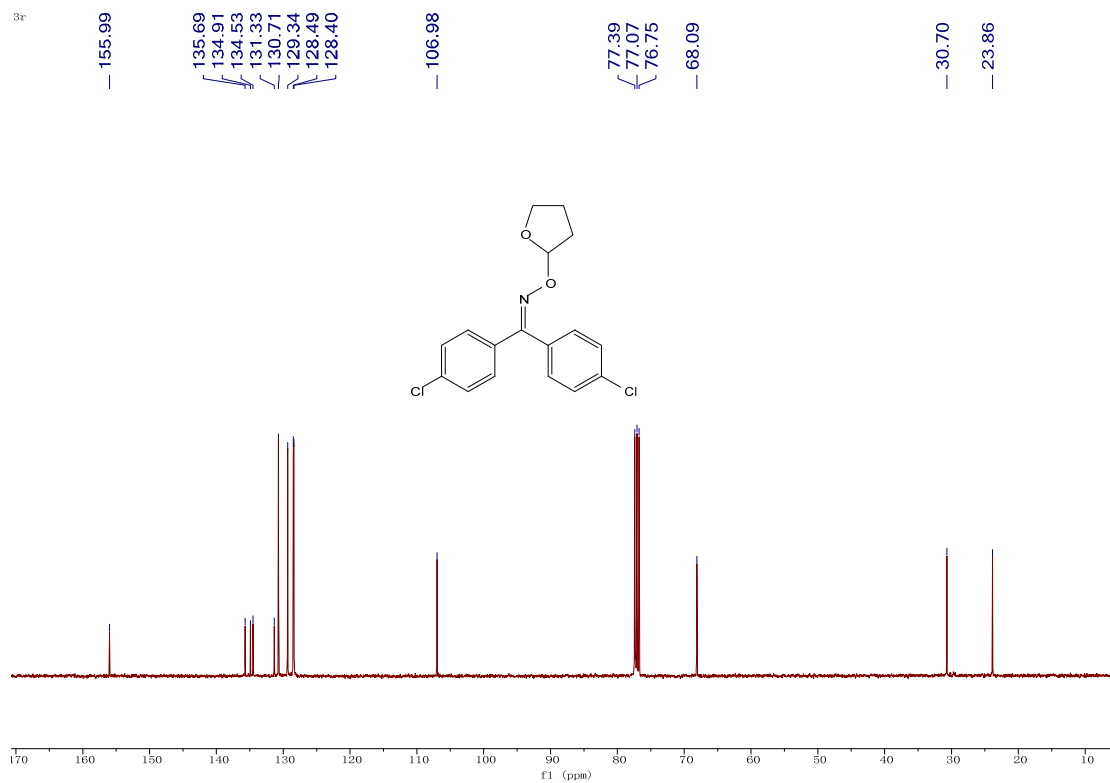
### <sup>19</sup>F NMR-spectrum (376MHz, CDCl<sub>3</sub>) of 3q



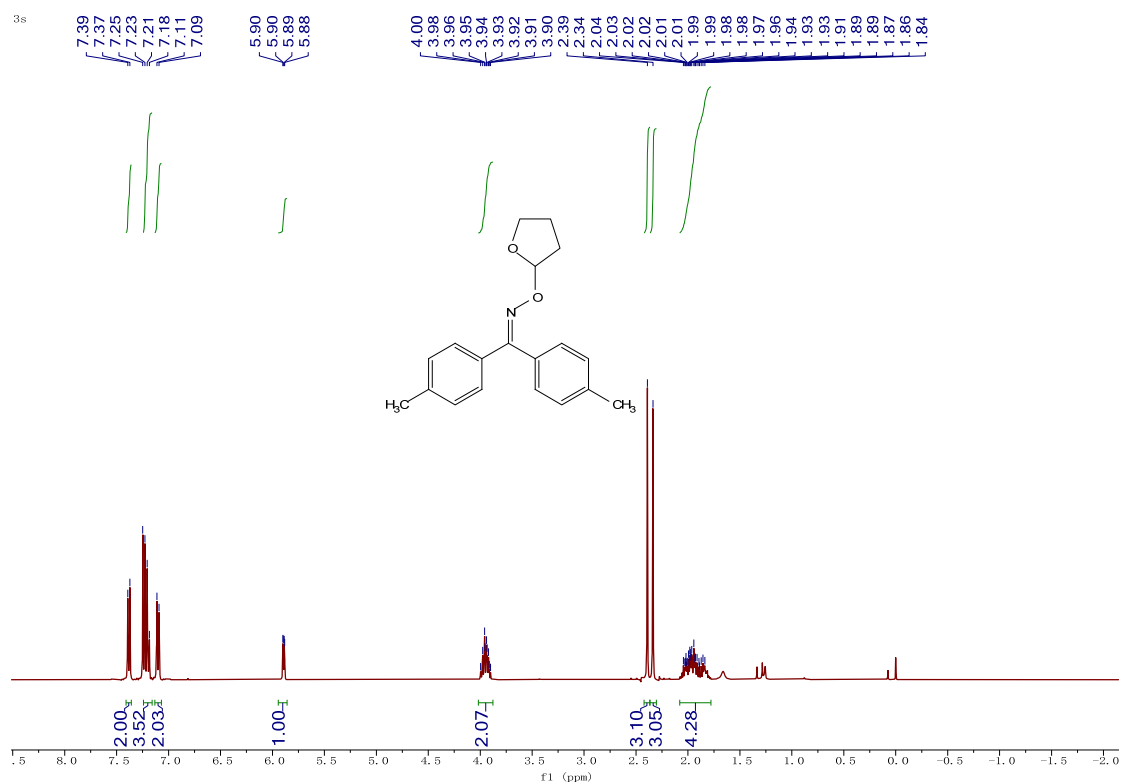
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3r



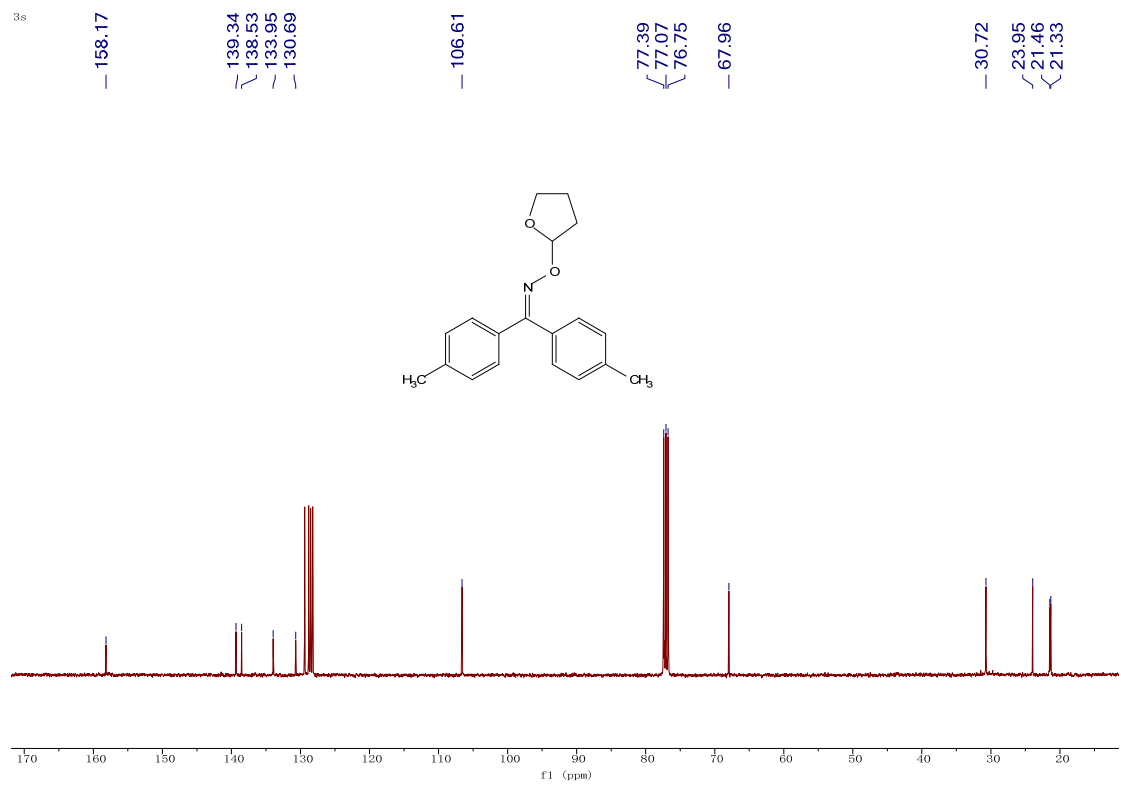
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3r



### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3s

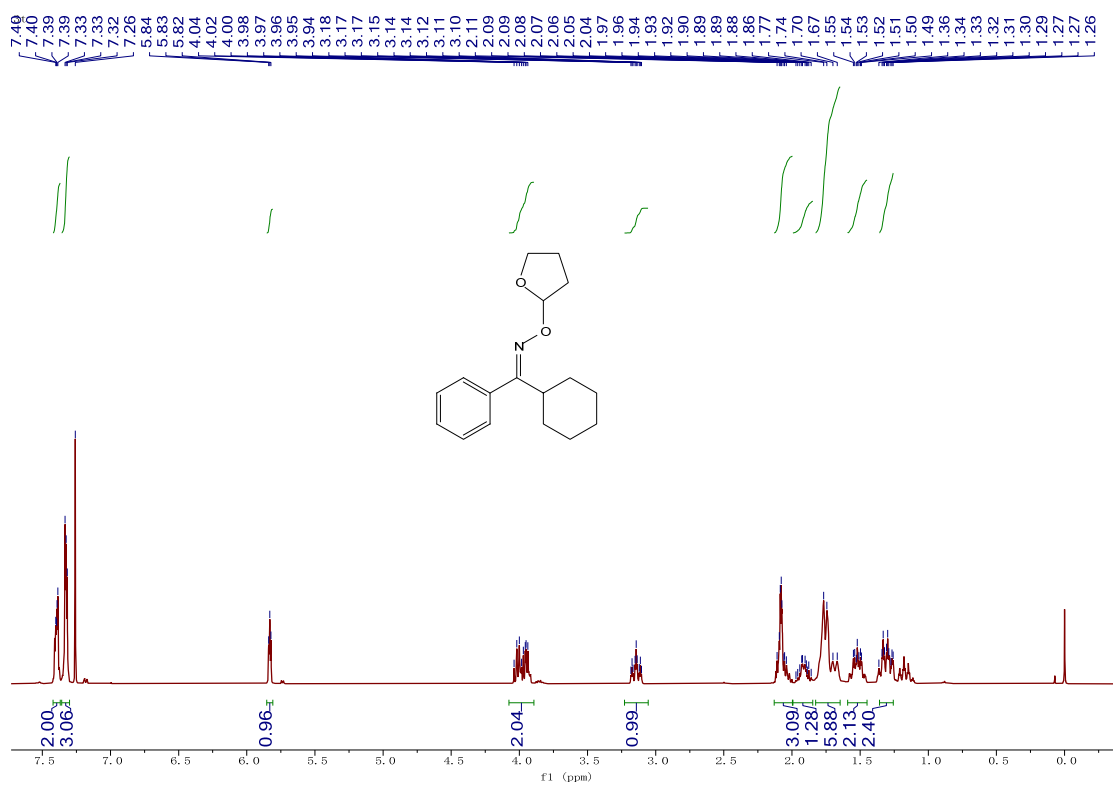


### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3s

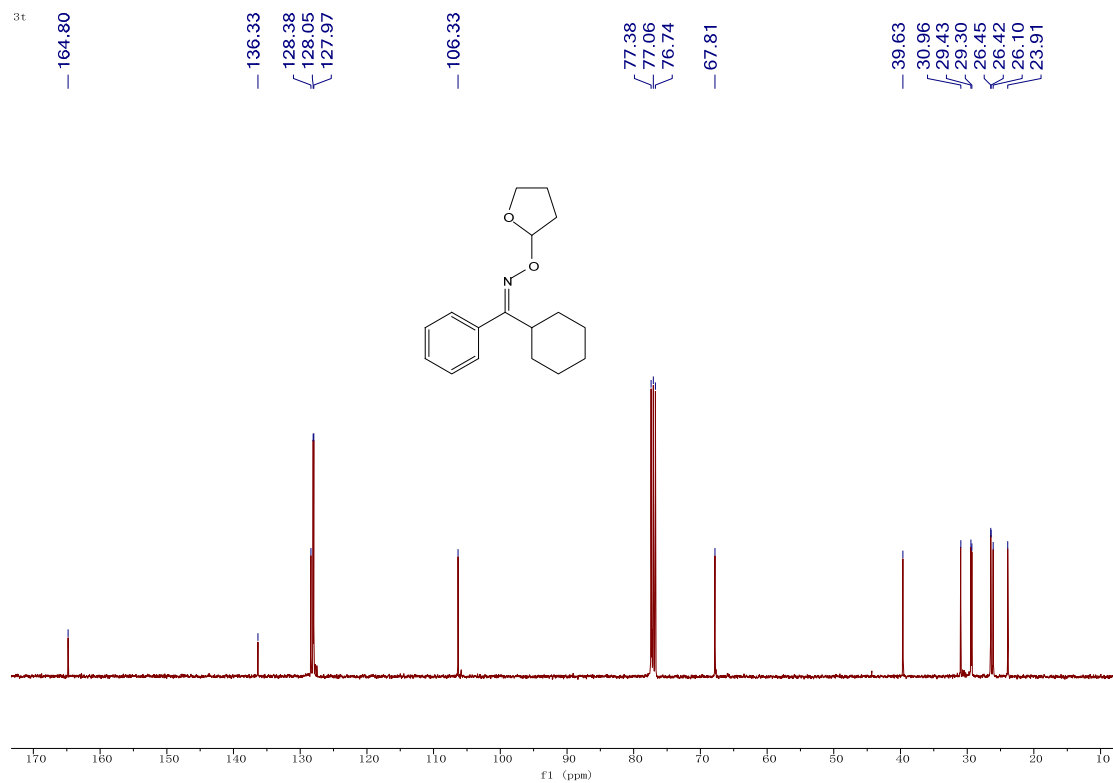




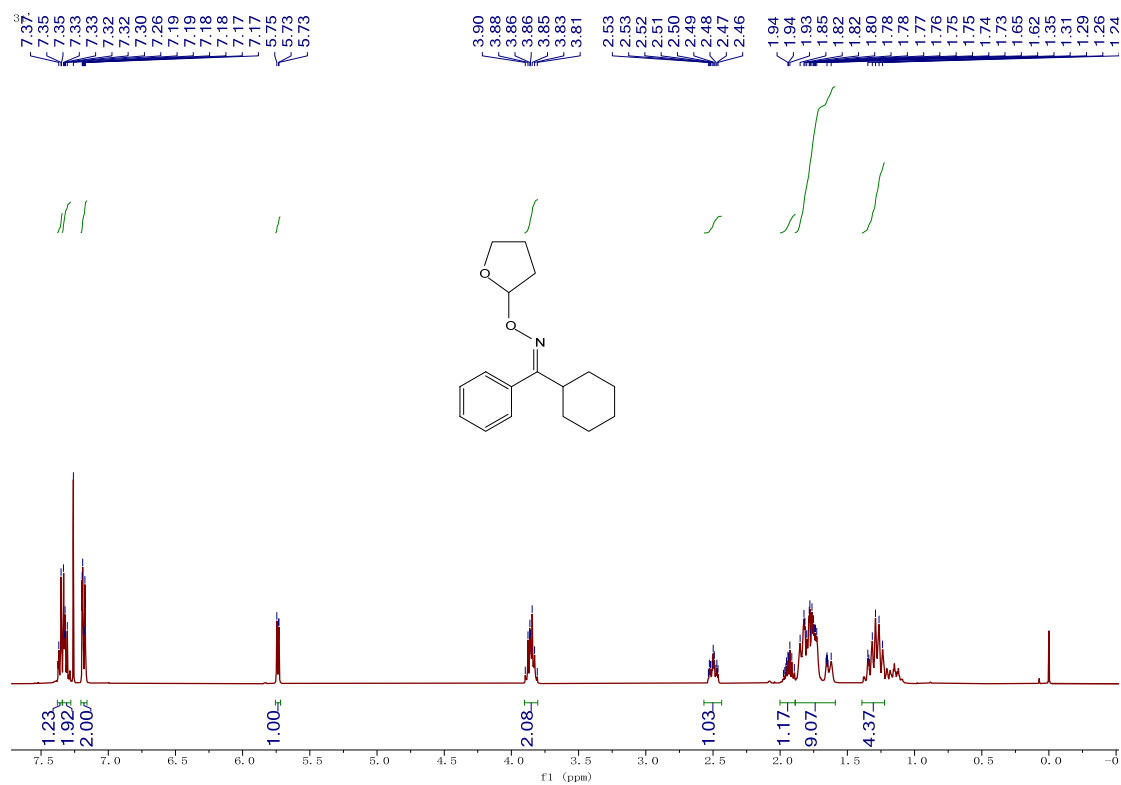
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3t



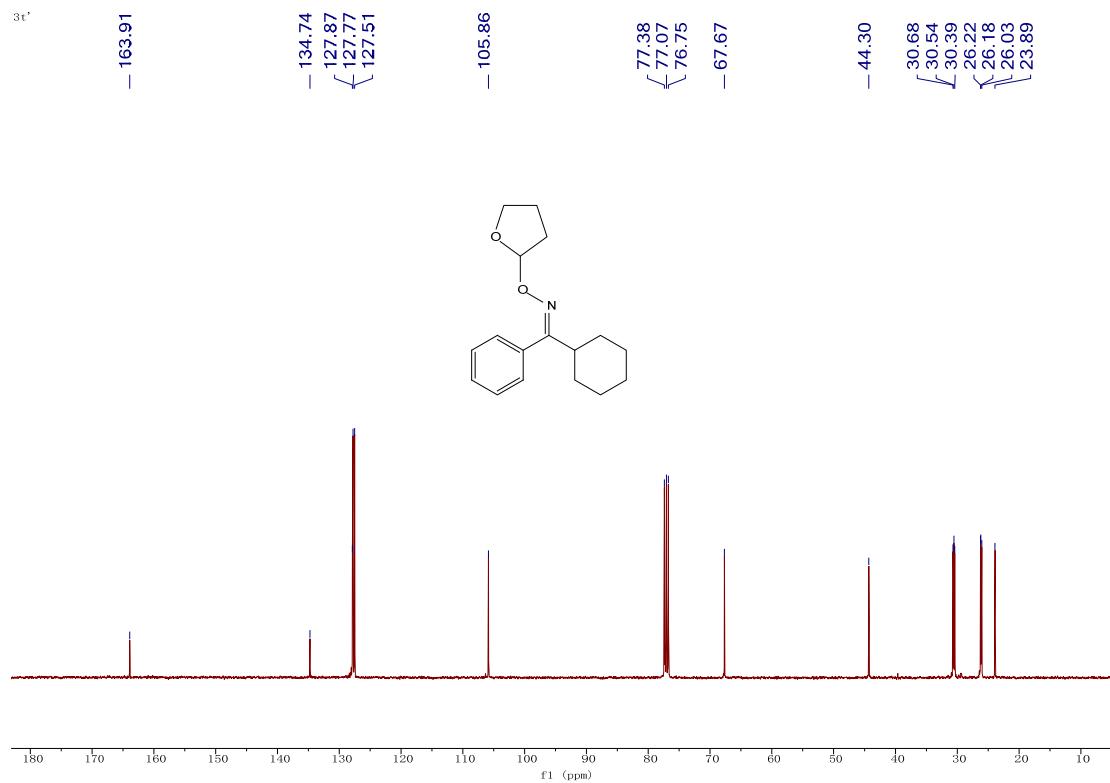
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3t



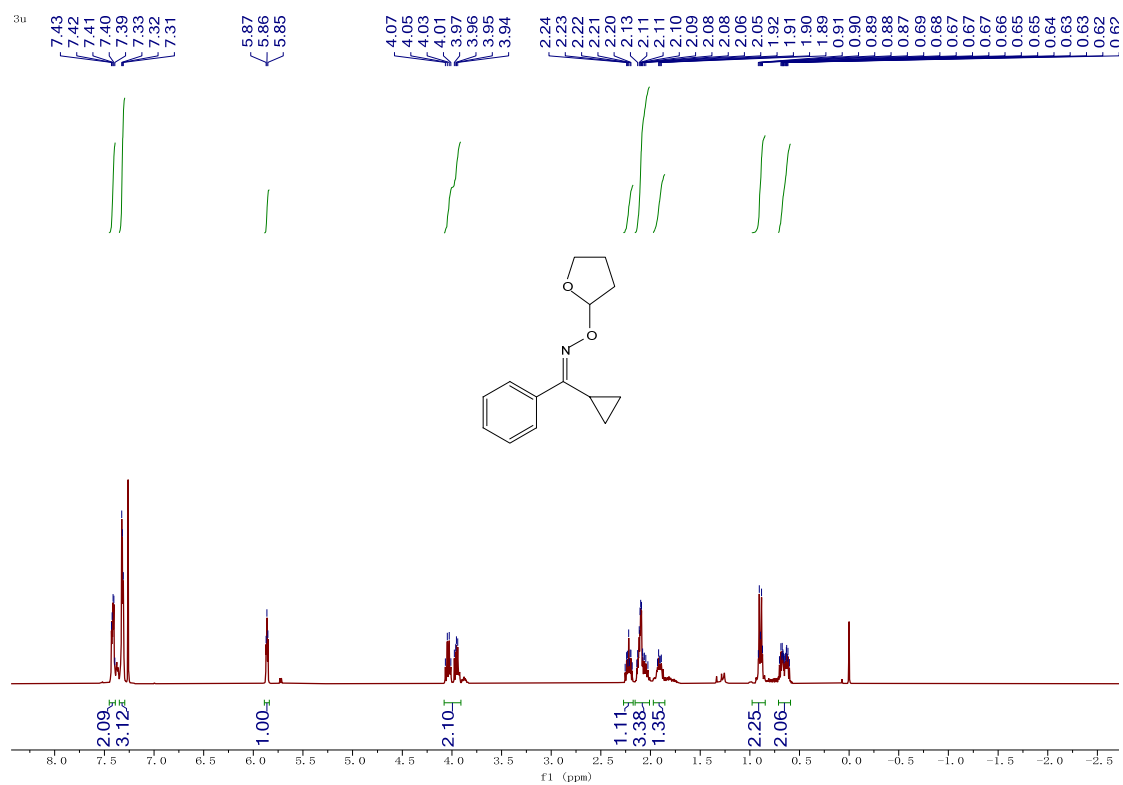
**<sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3t'**



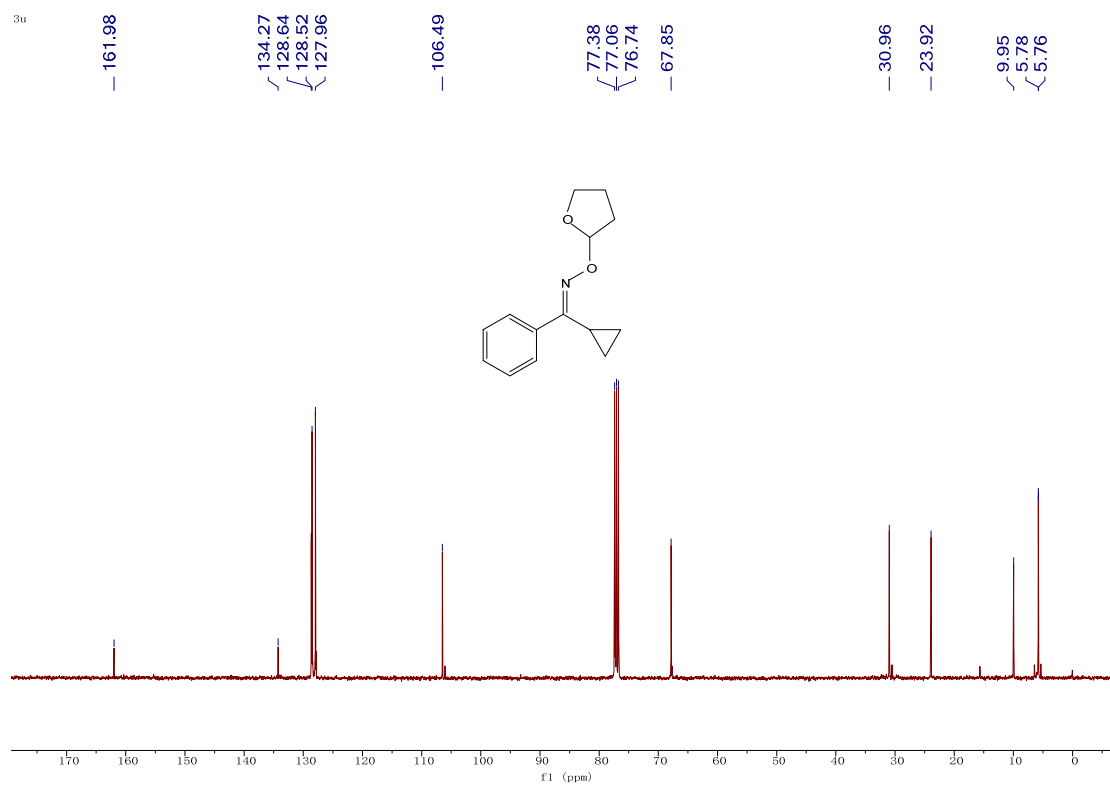
**<sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3t'**



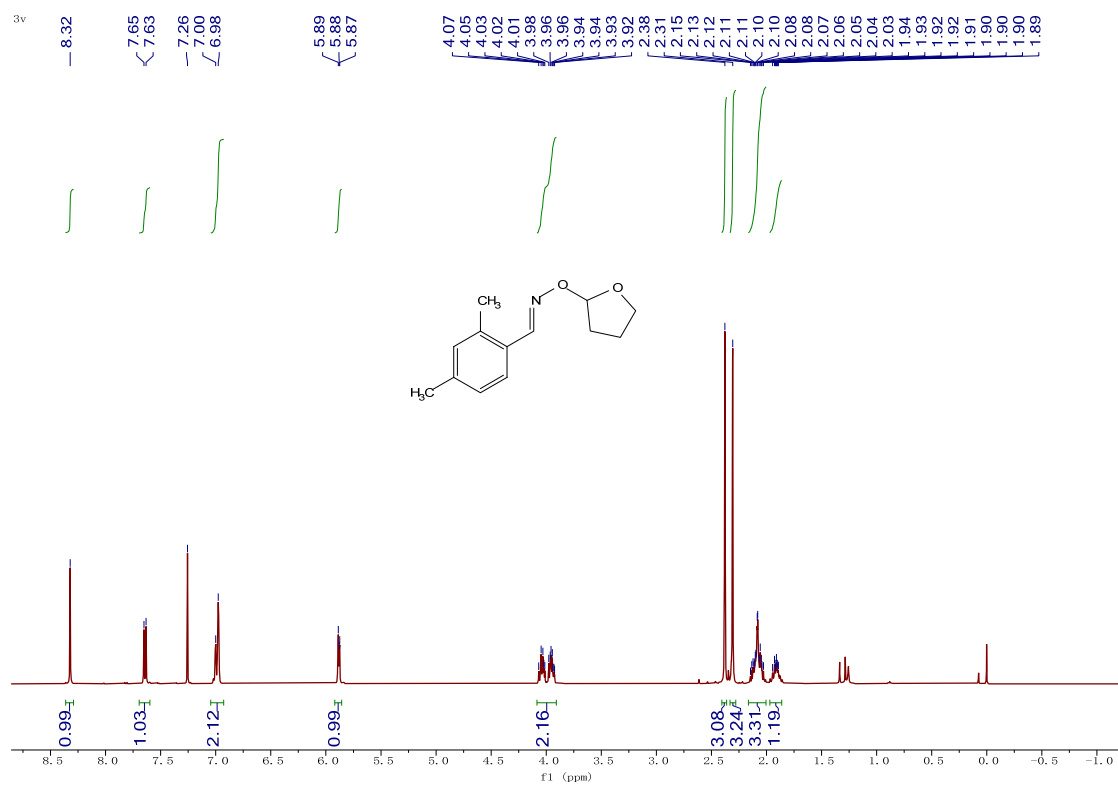
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3u



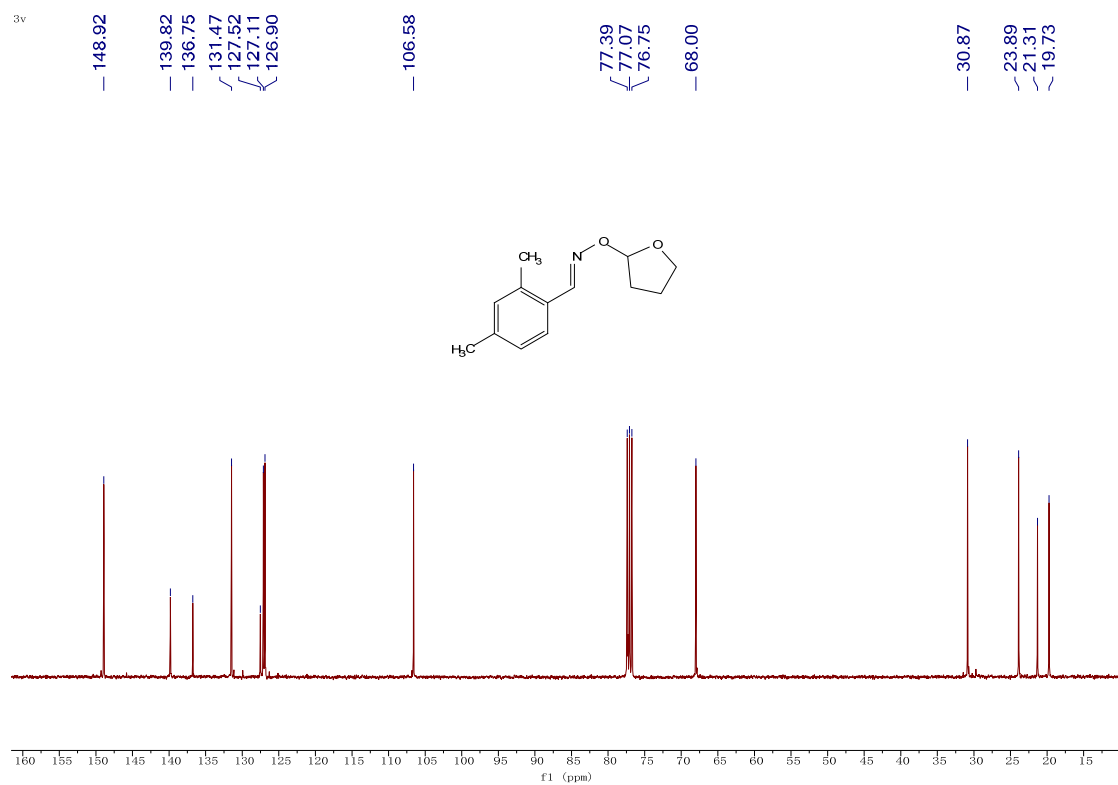
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3u



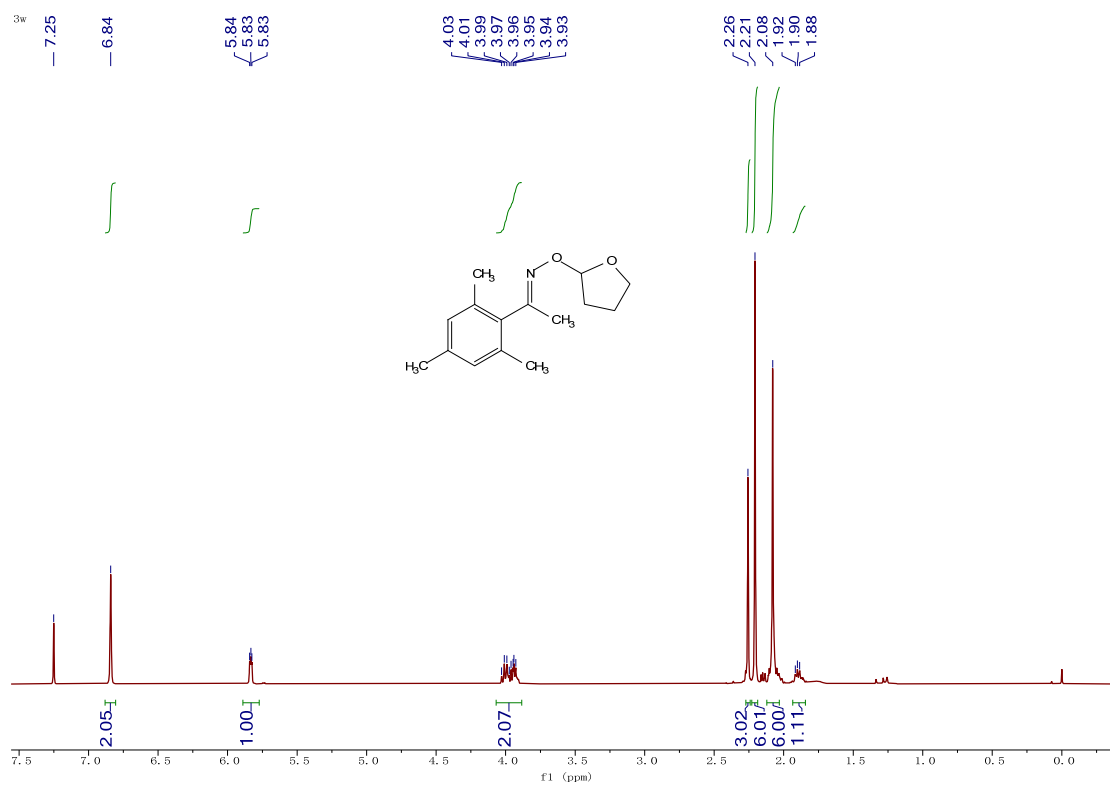
**<sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3v**



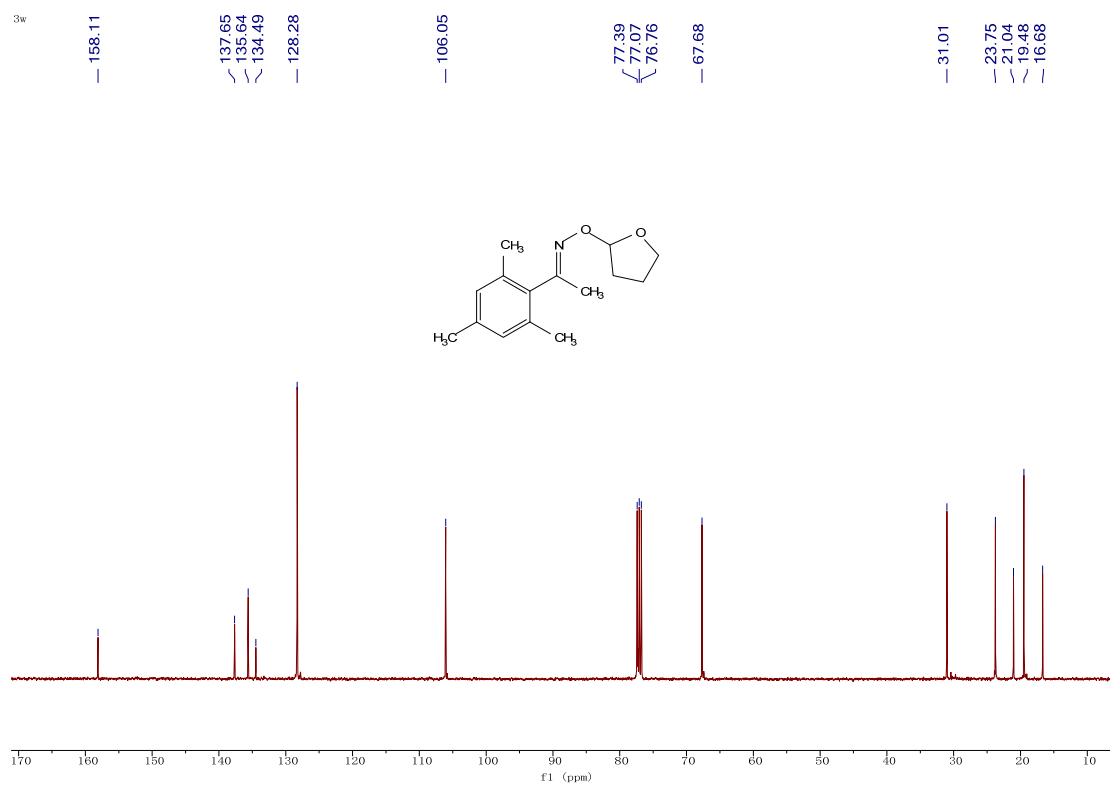
**<sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3v**



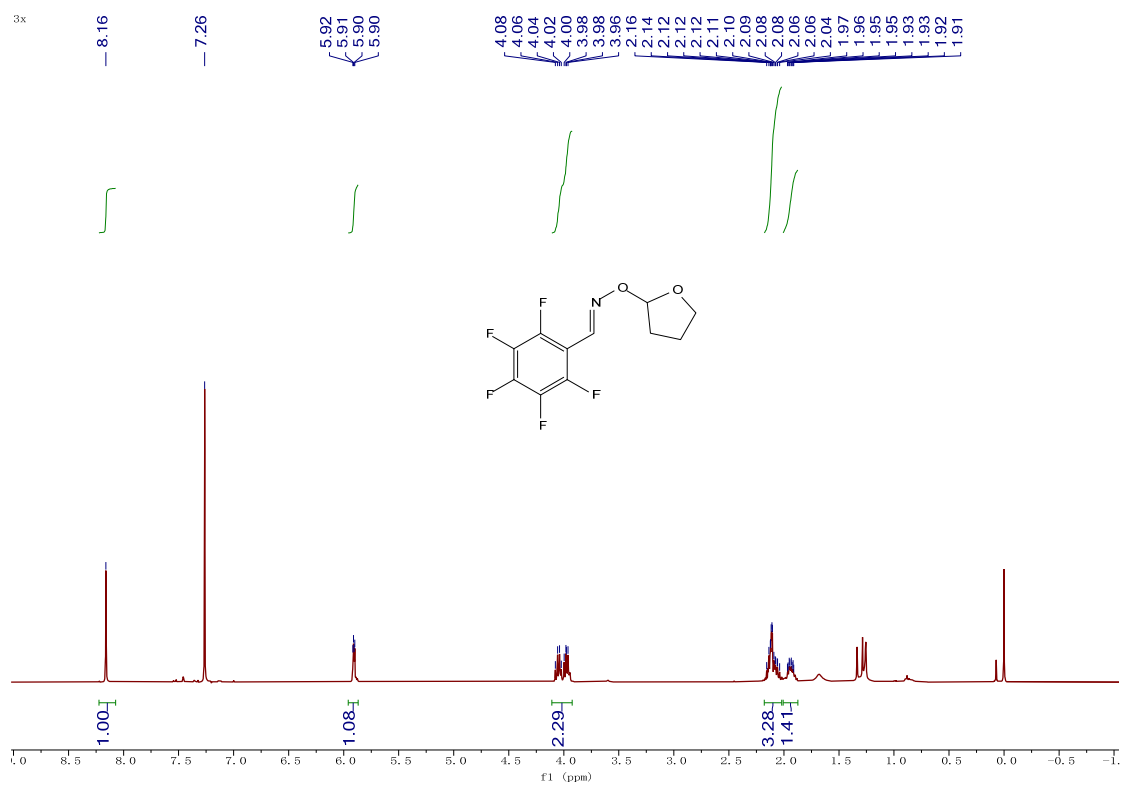
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3w



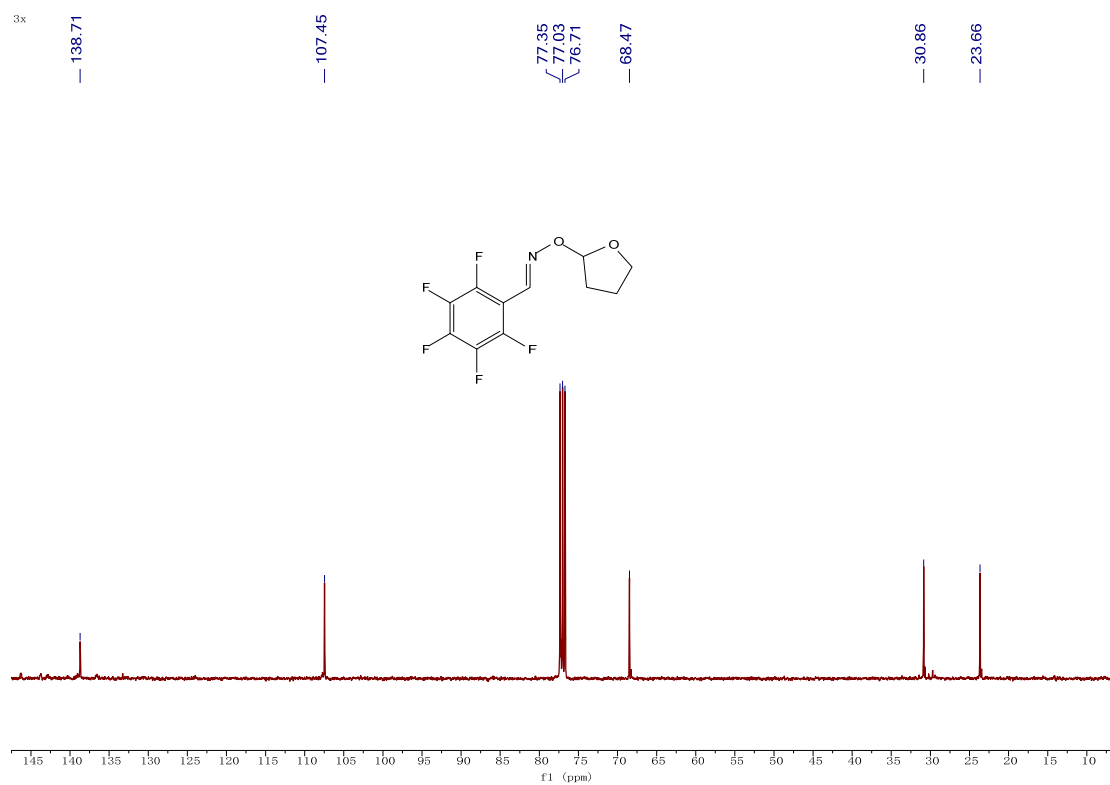
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3w



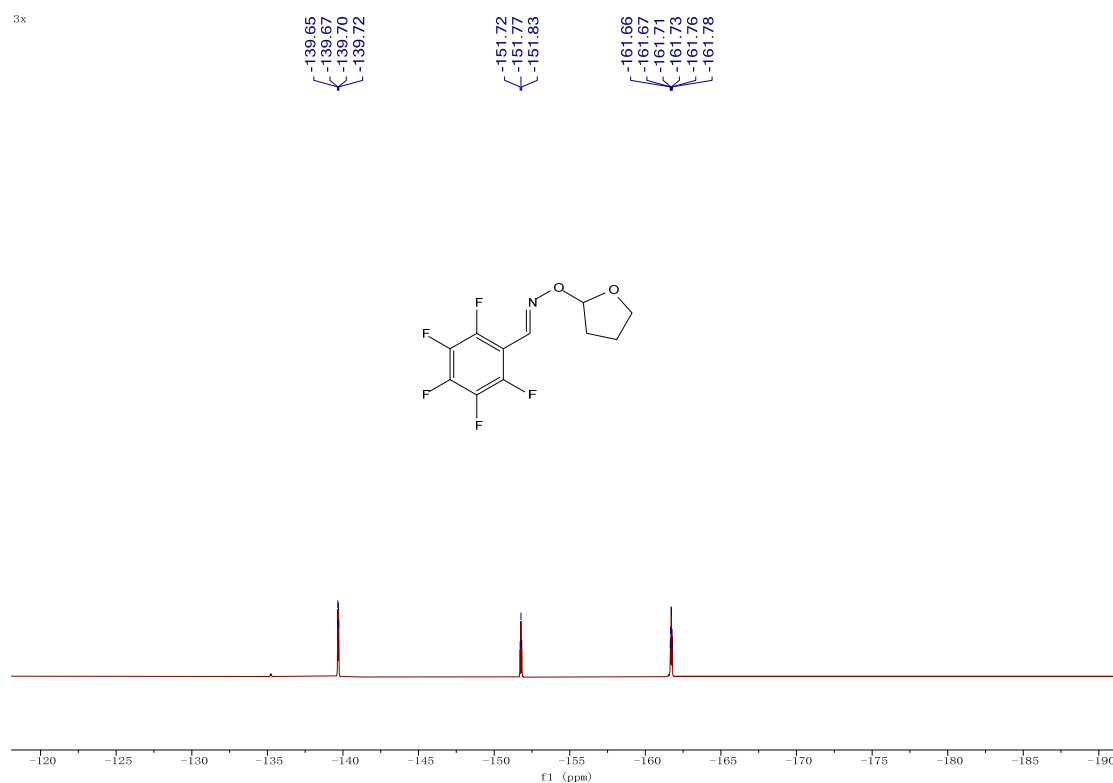
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3x



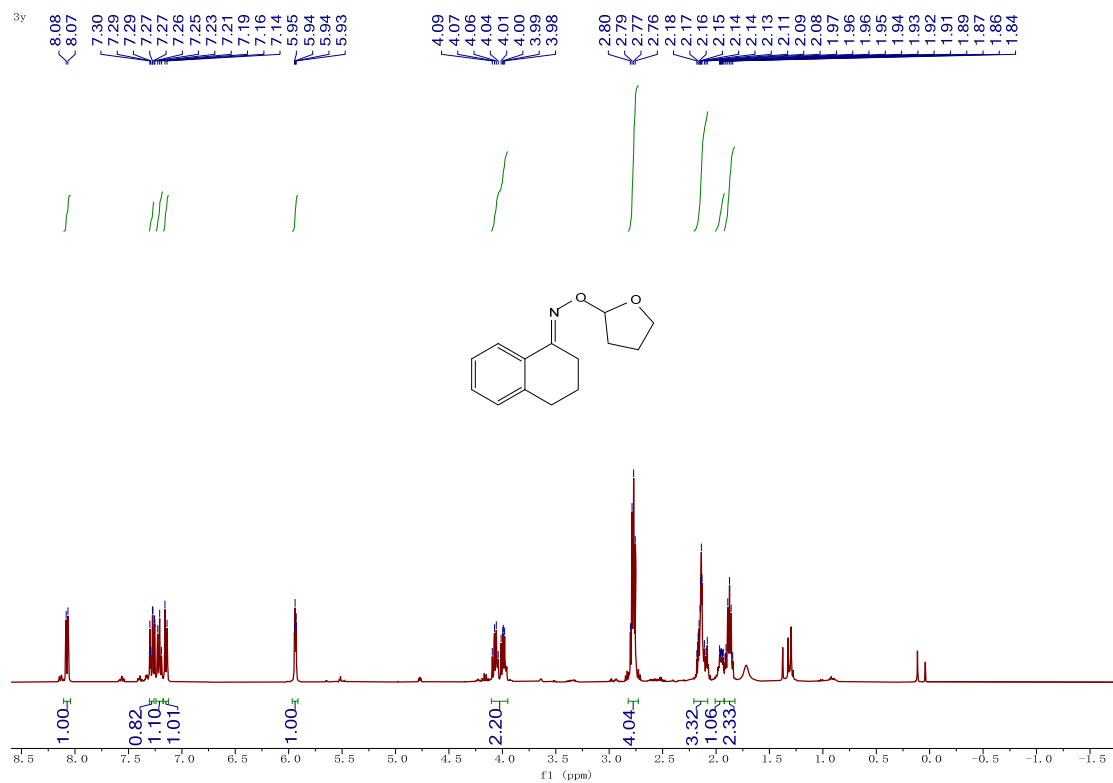
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3x



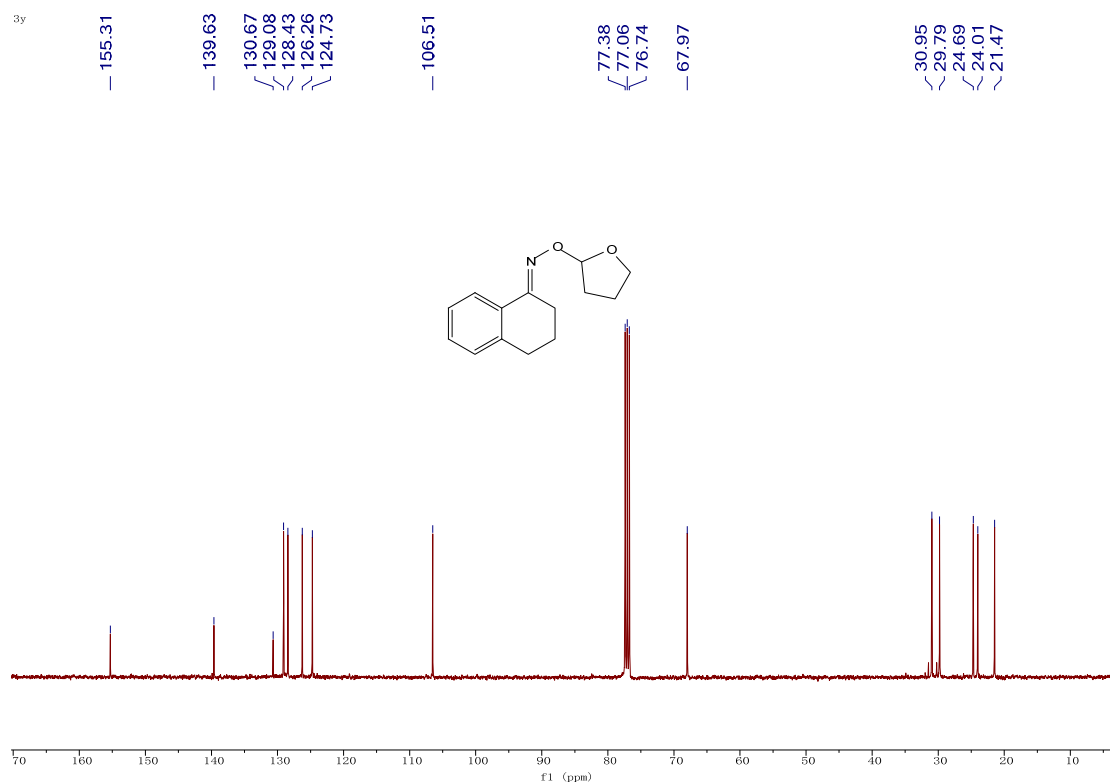
**<sup>19</sup>F NMR-spectrum (376MHz, CDCl<sub>3</sub>) of 3x**



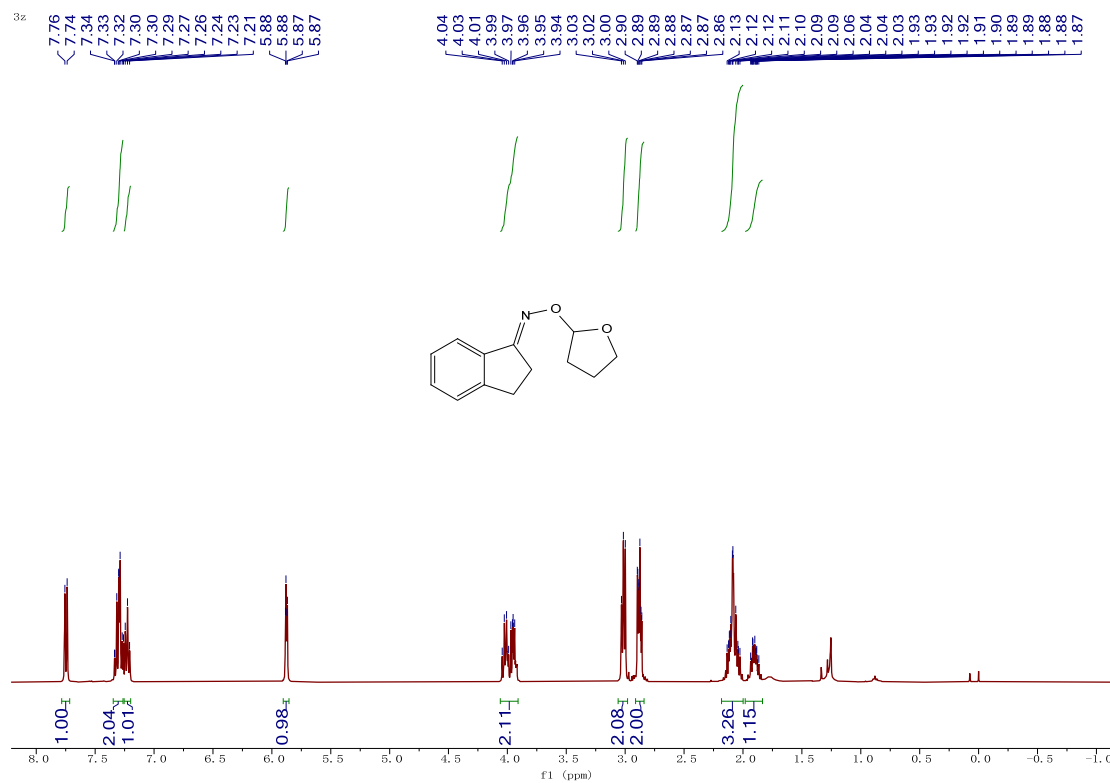
**<sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3y**



**<sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3y**

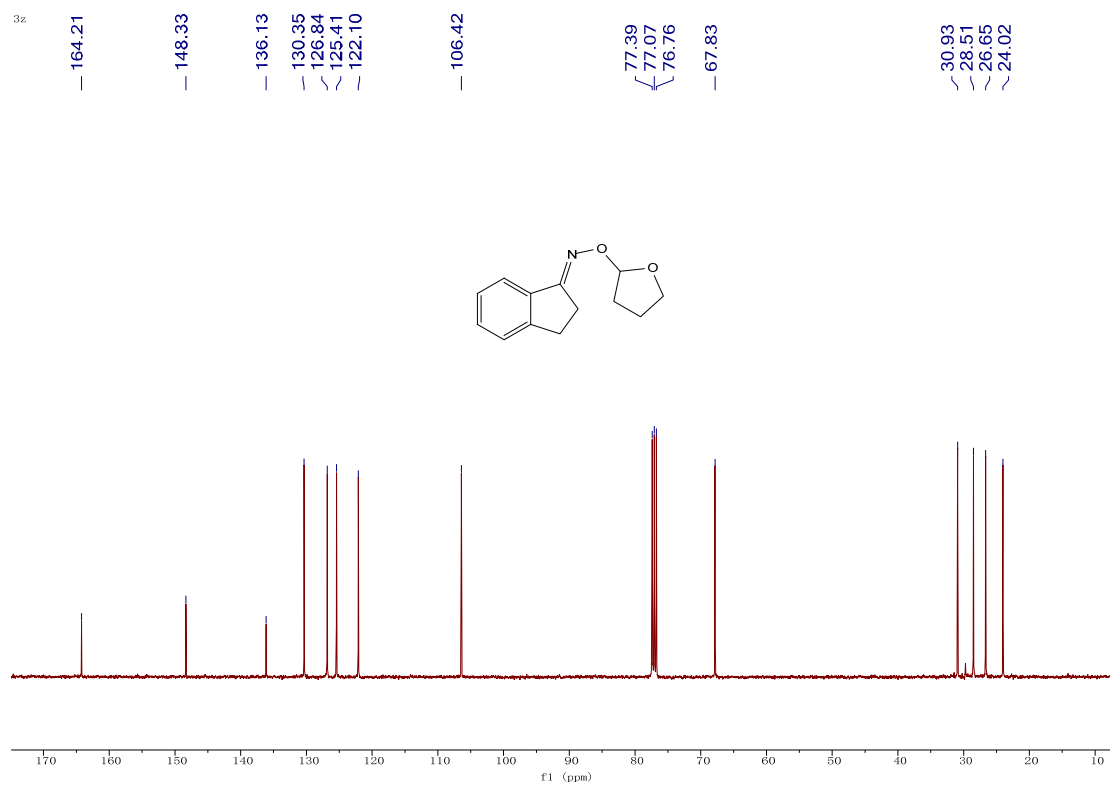


**<sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3z**

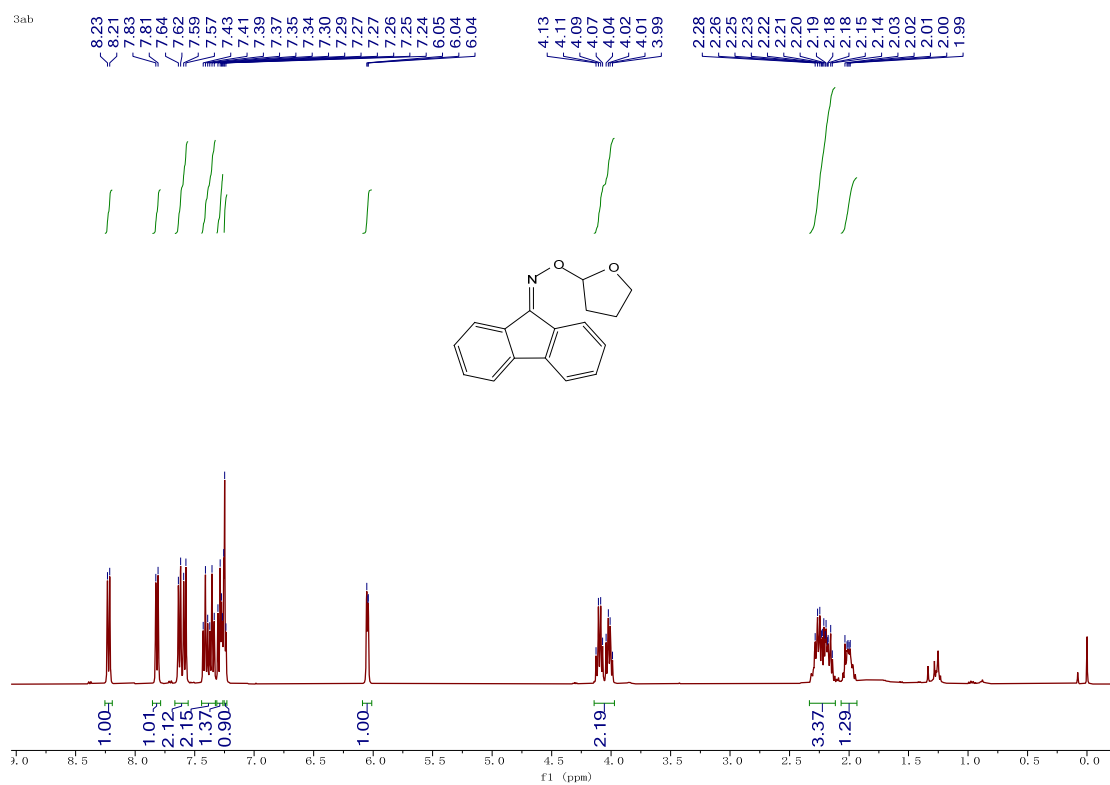




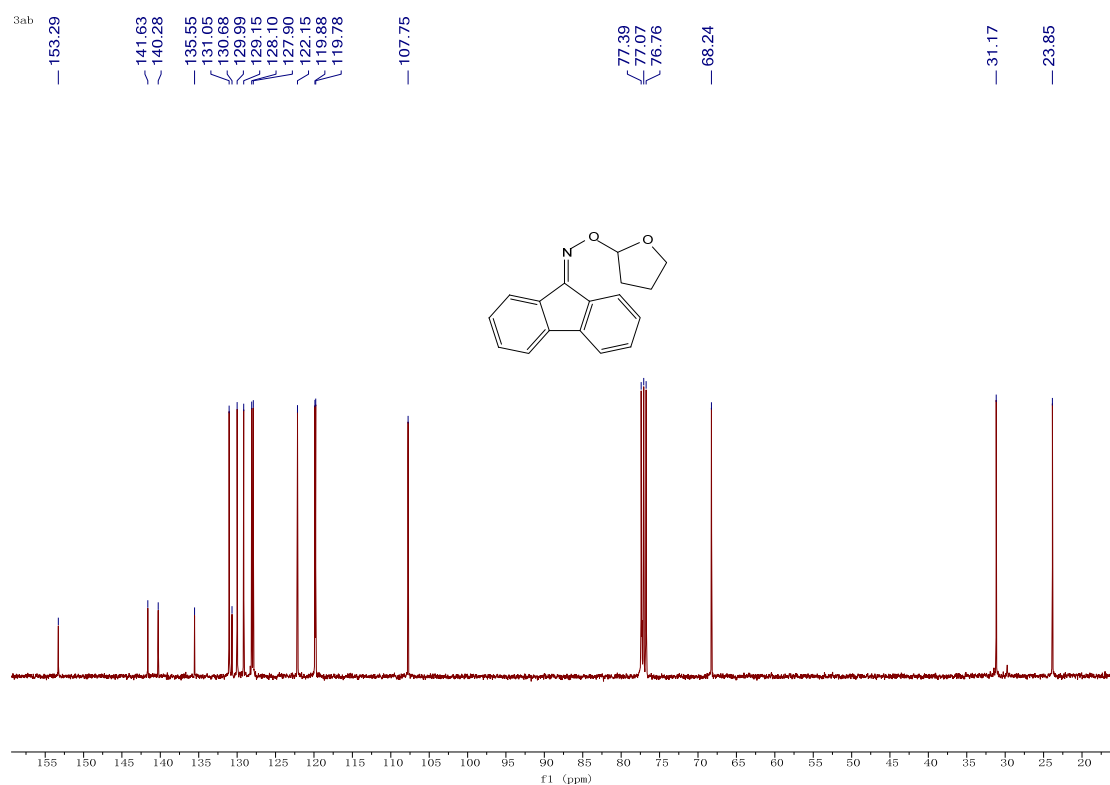
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3z



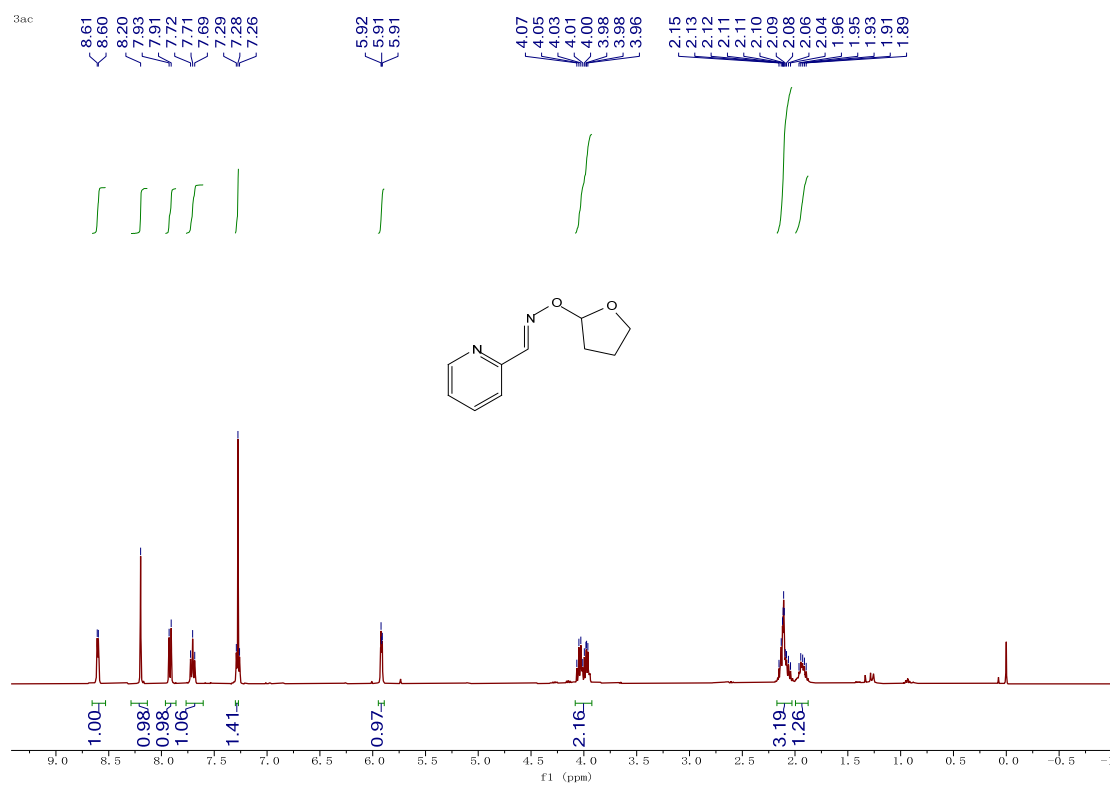
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3ab



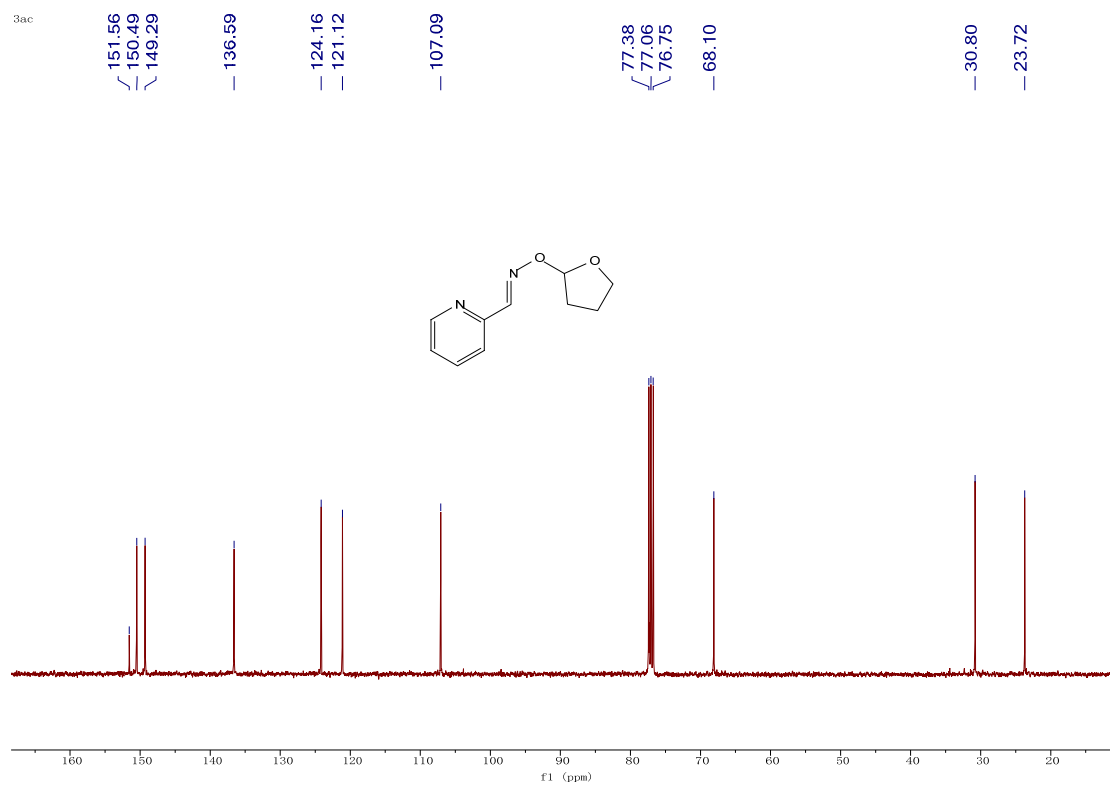
**<sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3ab**



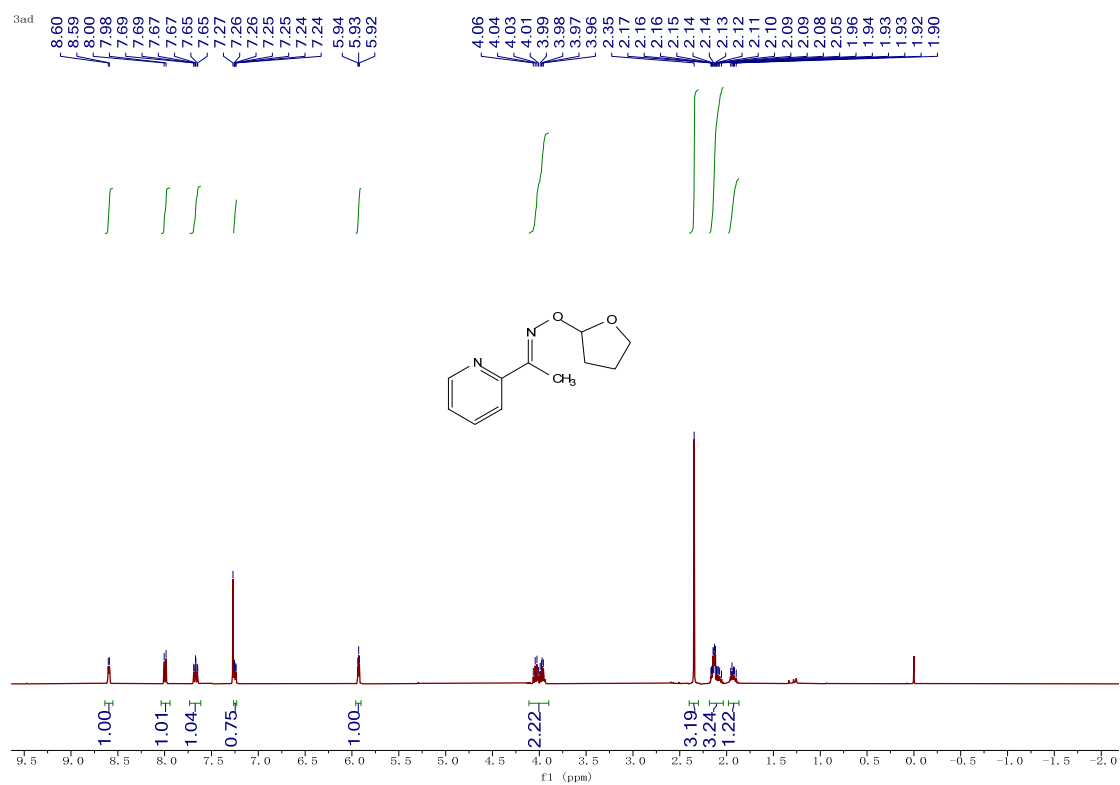
**<sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3ac**



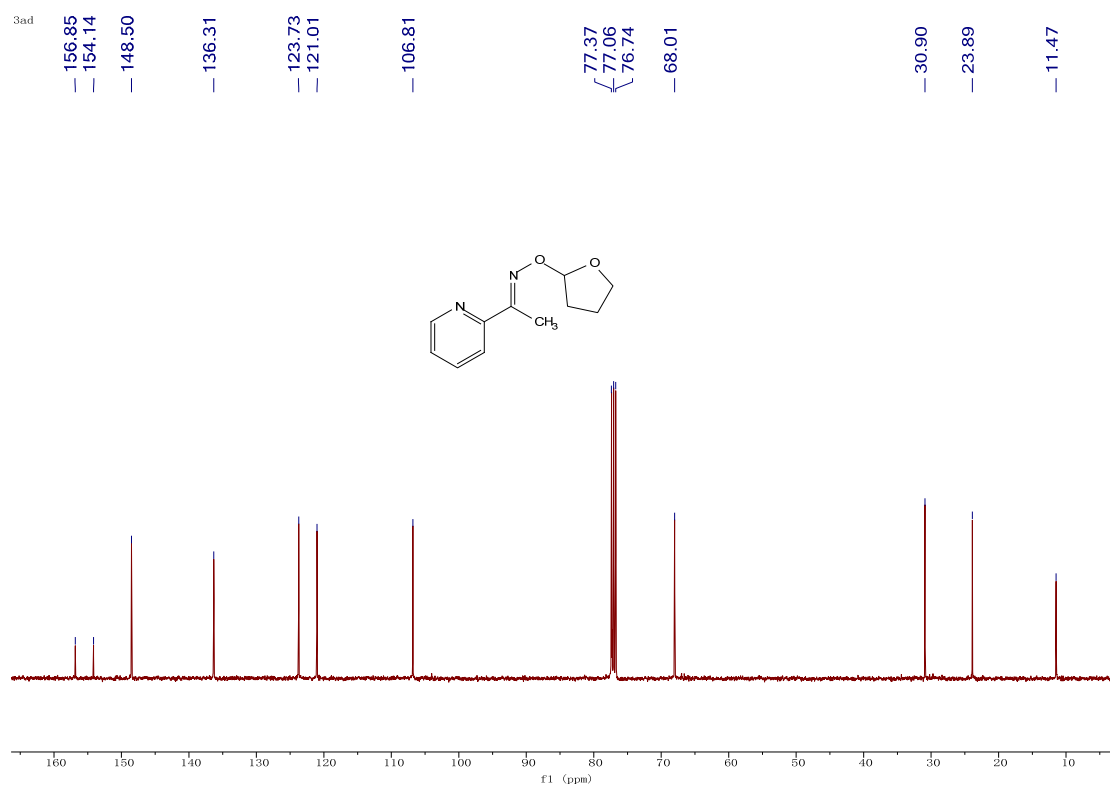
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3ac



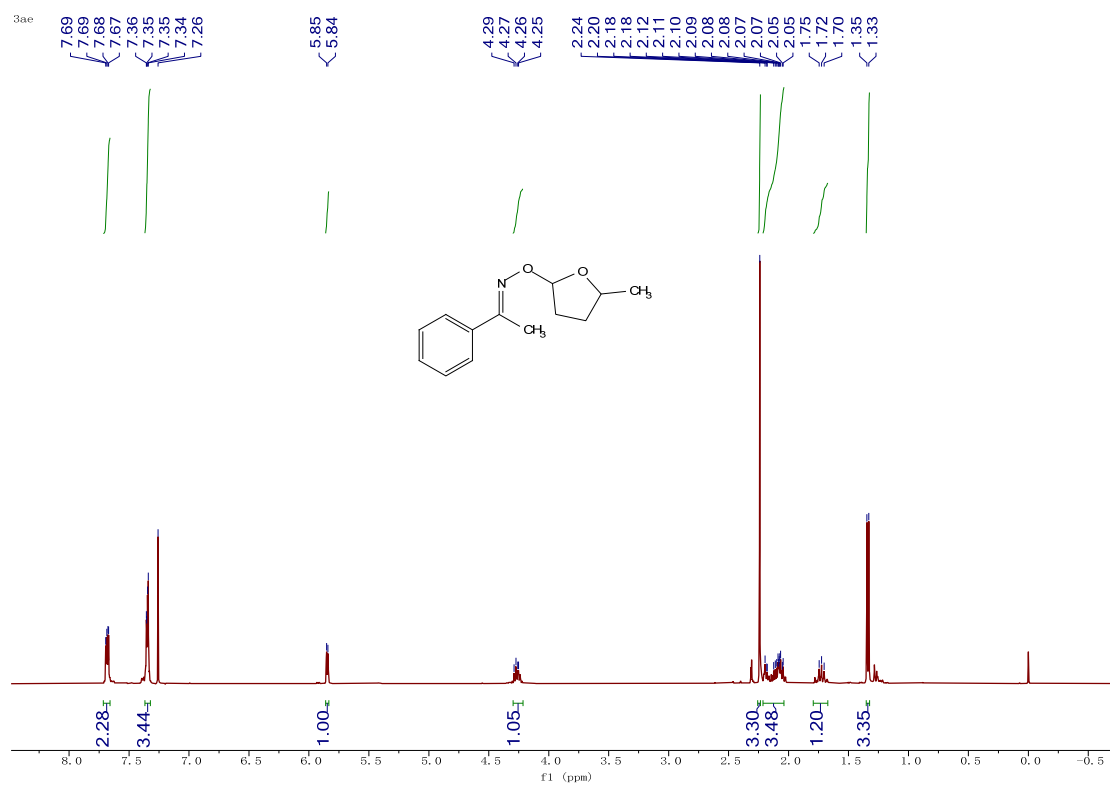
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3ad



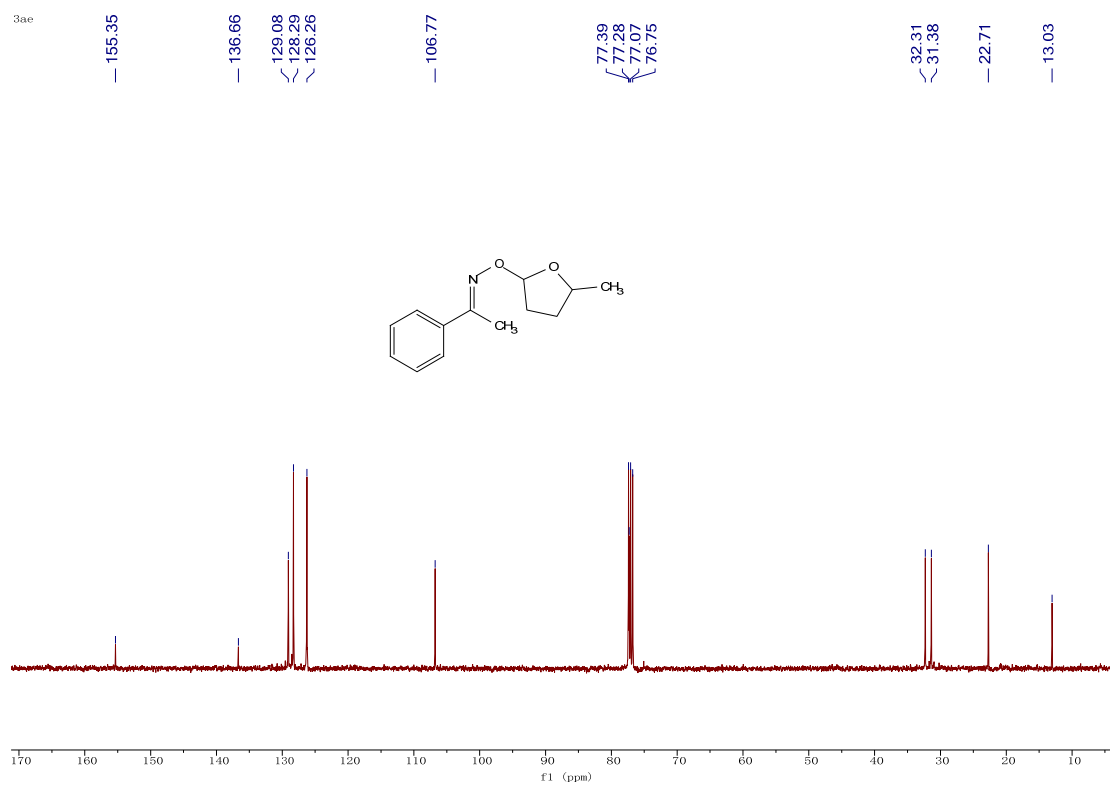
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3ad



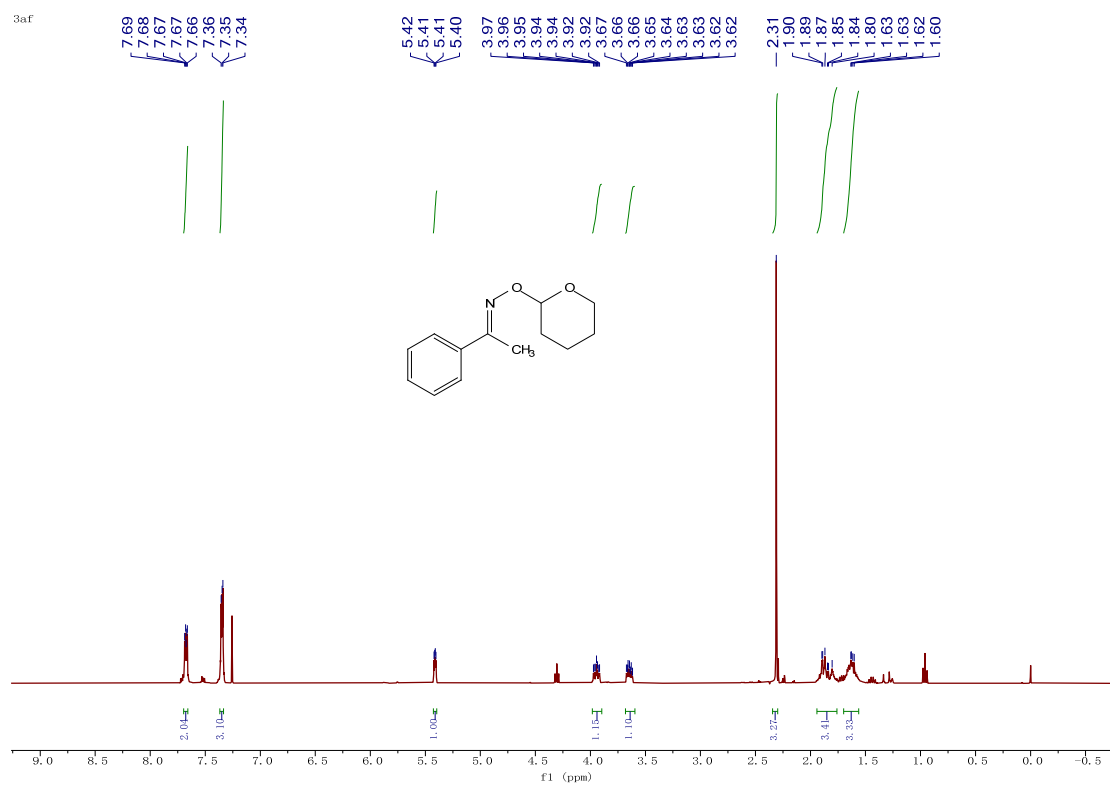
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3ae



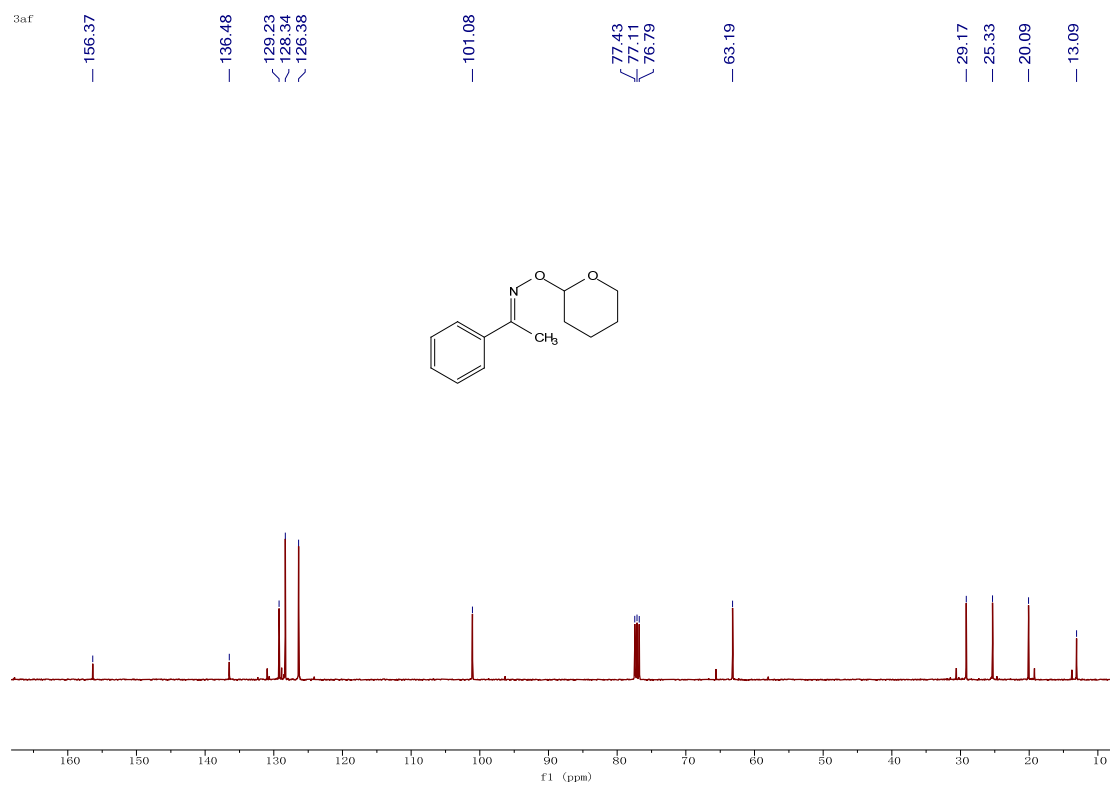
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3ae



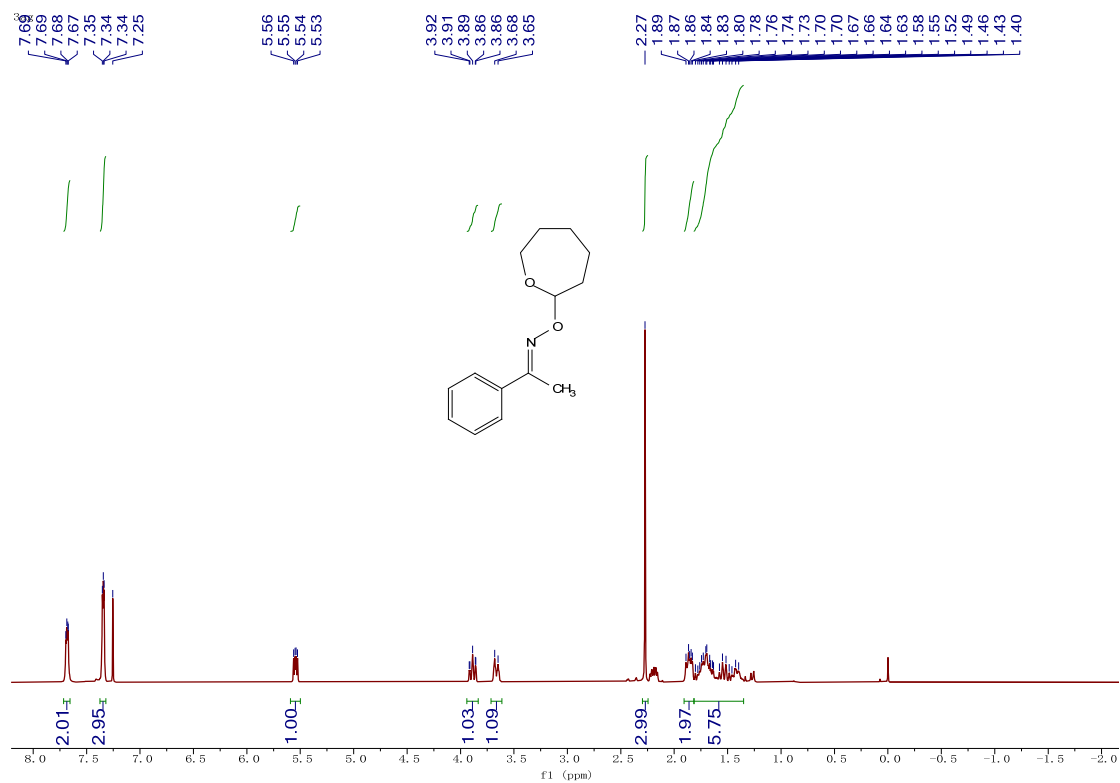
### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3af



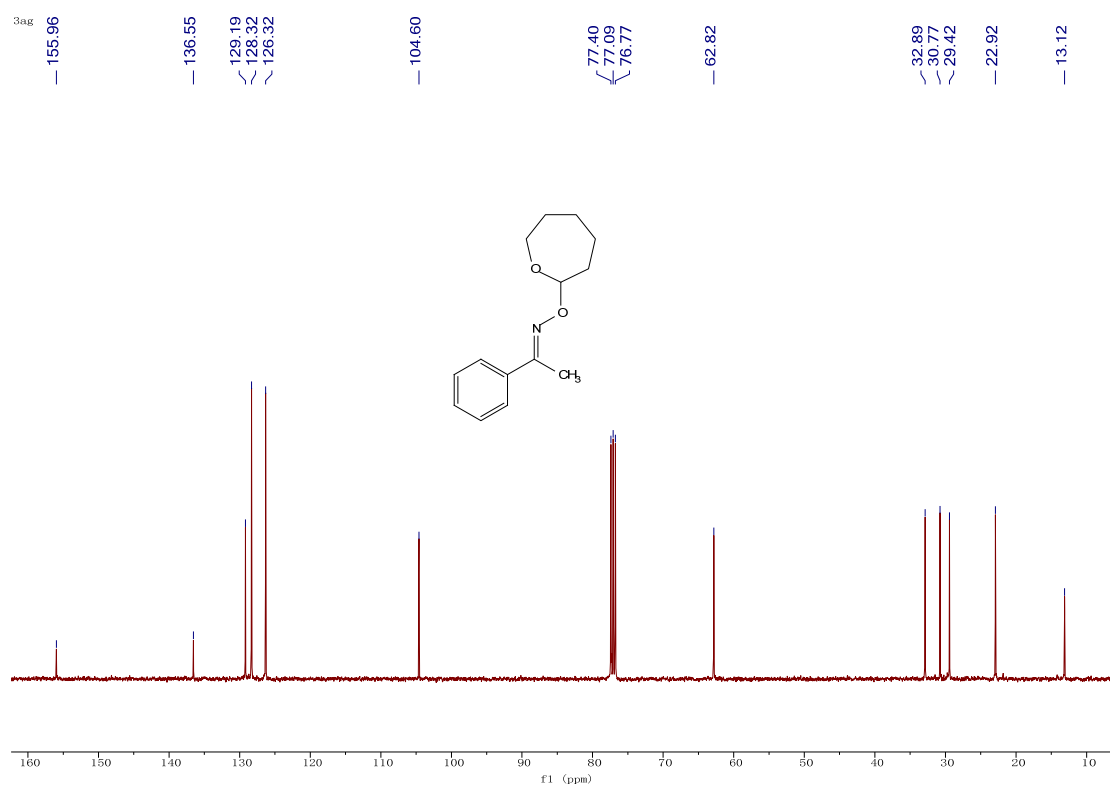
### <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3af



### <sup>1</sup>H NMR-spectrum (400MHz, CDCl<sub>3</sub>) of 3ag



# <sup>13</sup>C NMR-spectrum (101MHz, CDCl<sub>3</sub>) of 3ag



## Reference

- 1 M. J. Frisch; G. W. Trucks; H. B. Schlegel; G. E. Scuseria; M. A. Robb; J. R. Cheeseman; G. Scalmani; V. Barone; B. Mennucci; G. A. Petersson; H. Nakatsuji; M. Caricato; X. Li; H. P. Hratchian; A. F. Izmaylov; J. Bloino; G. Zheng; J. L. Sonnenberg; M. Hada; M. Ehara; K. Toyota; R. Fukuda; J. Hasegawa; M. Ishida; T. Nakajima; Y. Honda; O. Kitao; H. Nakai; T. Vreven; J. A., Jr. Montgomery; J. E. Peralta; F. Ogliaro; M. Bearpark; J. J. Heyd; E. Brothers; K. N. Kudin; V. N. Staroverov; R. Kobayashi; J. Normand; K. Raghavachari; A. Rendell; J. C. Burant; S. S. Iyengar; J. Tomasi; M. Cossi; N. Rega; N. J. Millam; M. Klene; J. E. Knox; J. B. Cross; V. Bakken; C. Adamo; J. Jaramillo; R. Gomperts; R. E. Stratmann; O. Yazyev; A. J. Austin; R. Cammi; C. Pomelli; J. W. Ochterski; R. L. Martin; K. Morokuma; V. G. Zakrzewski; G. A. Voth; P. Salvador; J. J. Dannenberg; S. Dapprich; A. D. Daniels; Ö. Farkas; J. B. Foresman; J. V. Ortiz; J. Cioslowski; D. J. Fox. Gaussian, Inc., Gaussian 09, Revision E.01. Wallingford CT, **2013**.
- 2 Y. Zhao; D. G. Truhlar. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.*, **2008**, *120*, 215–241.
- 3 S. Grimme; J. Antony; S. Ehrlich; H. Krieg. A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.*, **2010**, *132*, 154104.
- 4 F. Weigend; R. Ahlrichs. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.*, **2005**, *7*, 3297–3305.
- 5 D. Rappoport; F. Furche. Property-optimized Gaussian basis sets for molecular response calculations. *J. Chem. Phys.*, **2010**, *133*, 134105.
- 6 A. V. Marenich; C. J. Cramer; D. G. Truhlar. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B*, **2009**, *113*, 6378–6396.