Photocatalytic oxidative cleavage of aryl alkenes C=C bonds *via* uranyl cation

Supporting information

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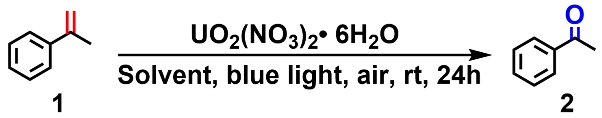
1) General Information

Commercial reagents and solvents were used without further purification and all the reactions were carried out in air if without special instruction. High efficiency silicone plates (0.2 mm ± 0.03 mm, 20 cm*20 cm) containing a fluorescent indicator F_{254} from Shanghai Heqi Classware Co., Ltd. were used for reaction monitoring, retardation factor determination and 200-300 mesh silica gel was used for isolation. Rotary evaporator (AnkeYq®, N-1200B) with DL-400 was used for solvent remove. ^1H and ^{13}C spectra were collected on 400 MHz NMR spectrometers with deuterated solvent (AVIII400 HD, Bruker, $CDCl_3$ = δ 7.26, DMSO-d_6 = δ 2.50, Acetonnitrile-d_3 = δ 1.94 for H and $CDCl_3$ = δ 77.0, DMSO-d_6 = δ 39.52 for carbon). Electron paramagnetic resonance spectrometer data (EPR) was collected on EPR-A300-9.5/12, Bruker. Fluorescence Quenching Experiments were measured and data was collected on a F96 pro fluorescence spectrophotometer, Lengguang Technology. UV-visible absorption spectra were collected on UV 3600i plus, SHIMADZU. Inductively coupled plasma emission spectroscopy (ICP) were carried on OPTIMA 8000, PerkinElmer.

2) Condition optimization

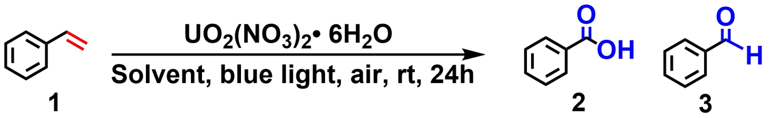
Table S1. Oxidative cleavage of 2-phenyl-1-propene in different solvents. [a]



Entry	Solvent	Yield[b] (%)
1	MeCN	86
2	Acetone	32
3	THF	13
4	MeOH	82
5	EtOH	67
6	Acetone : H_2O = 10:1	34

[a]Detailed condition: **1** (0.2 mmol), uranyl nitrate (2 mol%), solvent (2 mL), blue light, air, 24 h; [b]Isolated yields.

Table S2. Oxidative cleavage of styrene in different solvents. [a]



Entry	Solvent	Yield of 2[b] (%)	Yield of 3[b] (%)
1	MeCN	trace	61
2	MeCN : H_2O = 9 : 1	70	6
3	MeCN : H_2O = 5 : 5	27	39
4	MeOH	6	67
5	MeOH : H_2O = 9 : 1	17	44
6	MeOH : H_2O = 5 : 5	9	51

3) General Procedures

Paralleled and Scale-up experiments

Figure S1. Paralleled photo-reactor at resting state and on work (top); Photo-reaction under sunlight and scale-up experiment under sunlight (bottom).

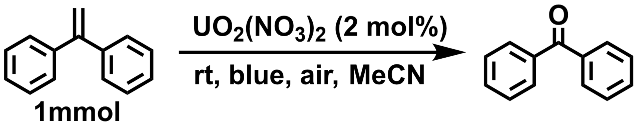
Catalyst, solvent and substrate were added into reaction tube if without specific indication. When using N_2 or O_2 atmosphere, the reaction vessel was purged with corresponding gas for 3 times first. Solvent was removed after reaction completed and the product was separated and purified by TLC or column chromatography.

Recycling experiments and recovery of catalyst

Substrate (1,1-diphenylethene **3a**, 1mmol, 180 mg), uranyl nitrate hexahydrate (0.02 mmol, 10 mg), and solvent (MeCN, 5 mL) were added into a reaction tube with a magnetic stirrer and irradiated under blue light for specialized time. After reaction was completed, the yield of product was analyzed by GC (using dodecane as internal standard). Firstly, solvent was removed by rotary evaporation, then the residue was dissolved by 5 mL ethyl acetate and the catalyst was extracted with H_2O, at last the catalyst was then used for next run after removing H_2O.

Condition of Table 5, entry 6: catalyst uranyl nitrate hexahydrate (200 mg), solvent (MeCN, 60 mL) and substrate (3a, 20 mmol, 3.6 g) were added into a two-necked flask, purged with O_2 for 3 times and filled with O_2. After reaction was completed, the mixture was concentrated by rotary evaporation. Then 50 mL ethyl acetate was added to the mixture and was extracted by water with 20 × 3 mL. Then the aqueous mixture (60 mL) was collected and 30 uL of it was taken out following by nitric acid digestion (4 M, 2 mL) for 2h at 50 °C. Then the solution was diluted to 10 mL (about 10 ppm) and was quantitatively analyzed by ICP using the standard curve method.

Table S3. Recycling of catalyst.



Recycle	Yield/%	Rate/mmol*h^{-1}
1	26.1	0.01088
2	26.7	0.01113
3(42h)	46.7	0.01095
4(48h)	55.6	0.01159

Table S4. Recovery of catalyst.

Sample	Concentration of U/ppm	Intensity
Standard 1	1	6438.8
Standard 2	2	175231.7
Standard 3	5	435794.9
Standard 4	10	850924.3
Table 5, entry 6	4.69	383849.5

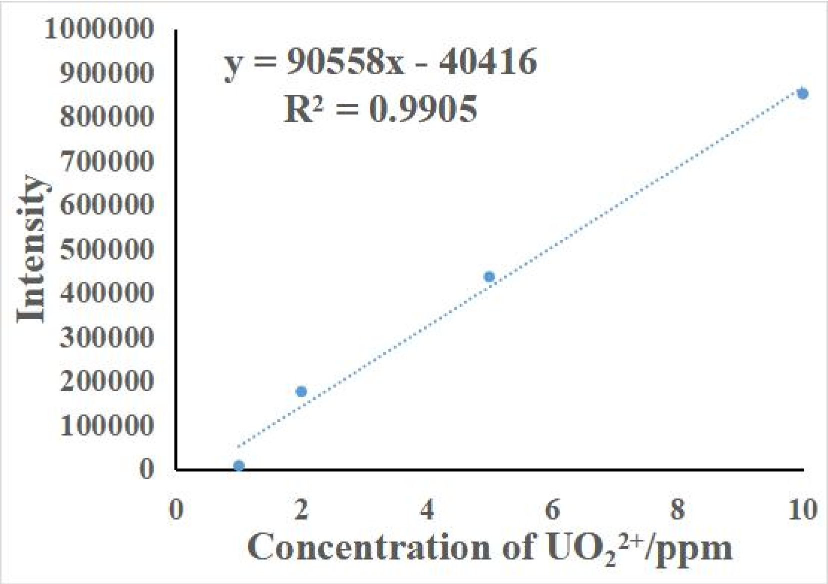


Figure S2. Internal standard curve about uranium.

The recovery of UO_2^{2+} $= \frac{4.69\text{ppm} * 0.01\text{L} * 60000\text{uL} * 502}{30\text{ul} * 238 * 200\text{mg}} * 100\% = 98.9\%$.

Among them, 4.69 ppm was the concentrate of uranium; 0.01 L was the volume of the tested uranium containing liquid; 60000 uL/30 uL was the dilution ration between origin liquid and the tested one; 502 was the mole weight of uranyl nitrate hexahydrate and 238 was that of uranium; 200 mg was the mass of the catalyst.

4) Mechanism study

Isotope labelling experiments.

Deuterated solvent experiments were performed in NMR tube. Styrene (0.2 mmol) and $UO_2(NO_3)_2{\cdot}6H_2O$ (2 mg, 2 mol%) were dissolved in 1 mL deuterated solvent and were analyzed by ^{1}H NMR after reacting for 24 h under blue light without stirring.

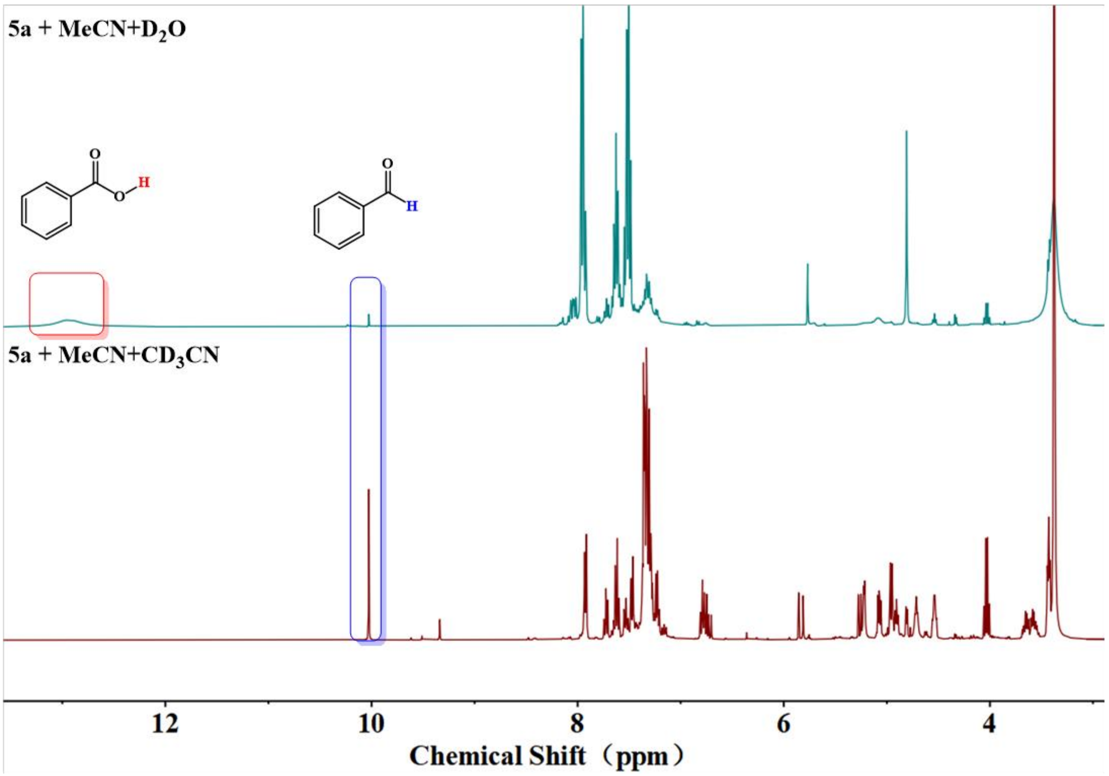


Figure S3. Oxidation of styrene in different deuterated solvents.

Isotope labelling experiment was performed under standard condition with mixed solvent of MeCN/$H_2{}^{18}O$ and the residue was analyzed by MS spectra.

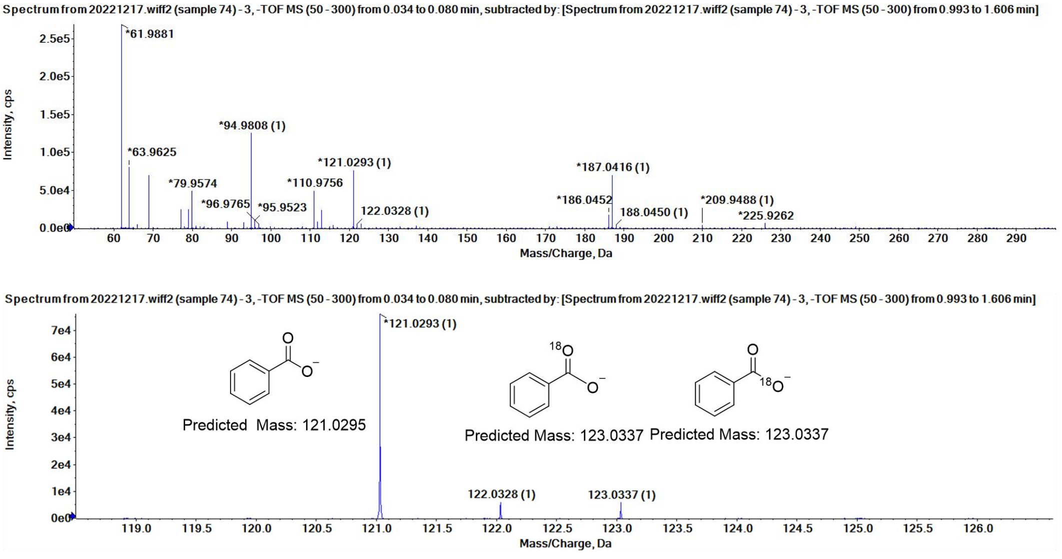


Figure S4. MS spectra after $H_2{}^{18}O$ Isotope labelling experiment.

Isotope labelling experiment was performed under standard condition with $^{18}O_2$ and the residue was analyzed by MS spectra.

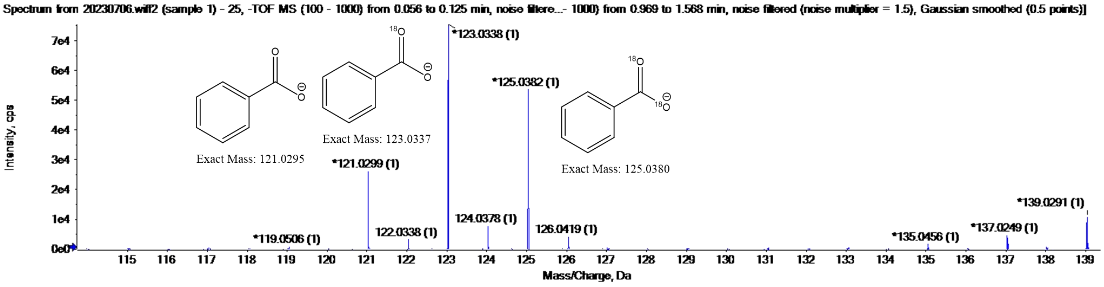


Figure S5. MS spectra after $^{18}O_2$ Isotope labelling experiment.

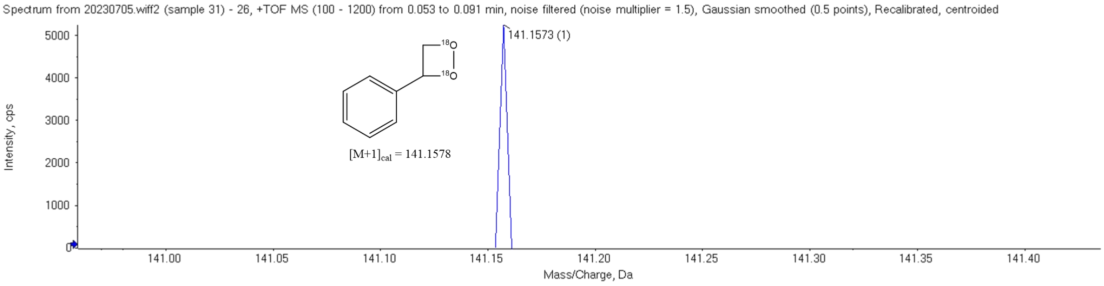


Figure S6. Captured mass of ^{18}O labeled 3-phenyl-1,2-dioxetane (D).

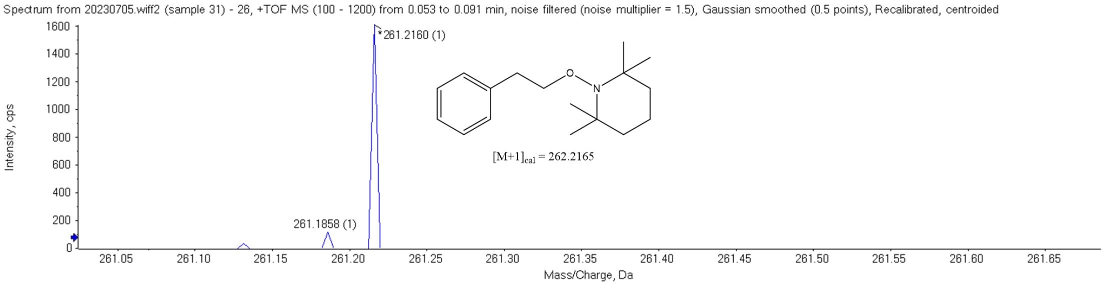
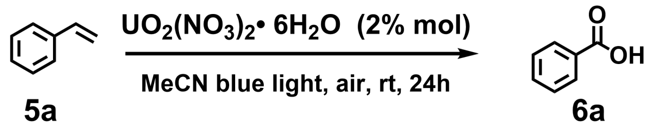
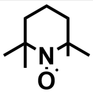
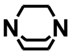
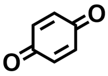


Figure S7. Captured mass of TEMPO-styrene complex.

Radical quenching experiments

Table S5. Standard reaction of 5a with different quenchers[a].



Entry	Reagent	Yield (%)
1	 Tempo	ND
2	 Dabco	ND
3	 Benzoquinone	Trace

[a]Detailed reaction conditions: substrate (0.5 mmol), uranyl nitrate (2 mol%), quencher (1 mmol),

solvent (3 mL), blue light, air, 24 h, the result was detected by GC-MS. ND means no detected.

The quenching result of Tempo and Dabco shows that the $^1O_2$ may participate in the reaction. The result of Benzoquinone shows that peroxy radical may participate in the reaction.

Detailed information of EPR testing.

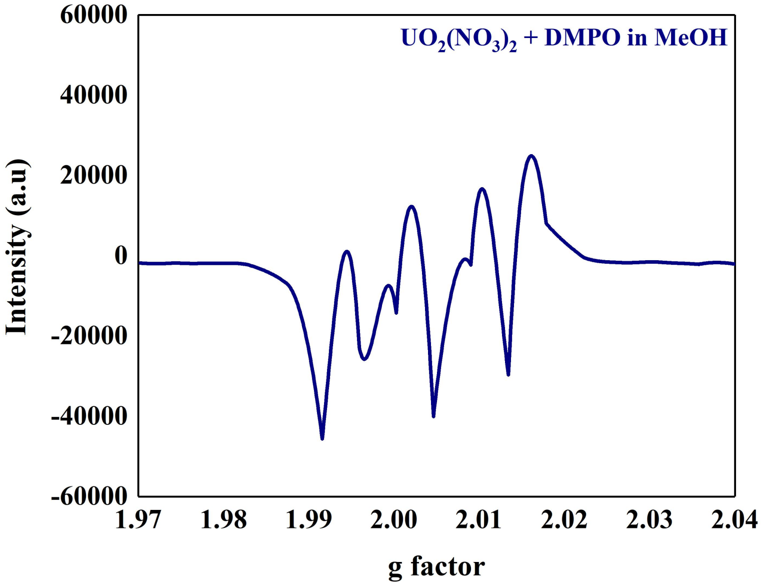


Figure S8. EPR spectra of $UO_2(NO_3)_2{\cdot}6H_2O$ + DMPO in MeOH.

$UO_2(NO_3)_2{\cdot}6H_2O$ (0.004 mmol) was dissolved in 2 mL MeOH followed by irradiation of blue light about 30 min. Then DMPO (0.5 mmol) was added to the mixture, followed by testing after another 10 minutes irradiation.

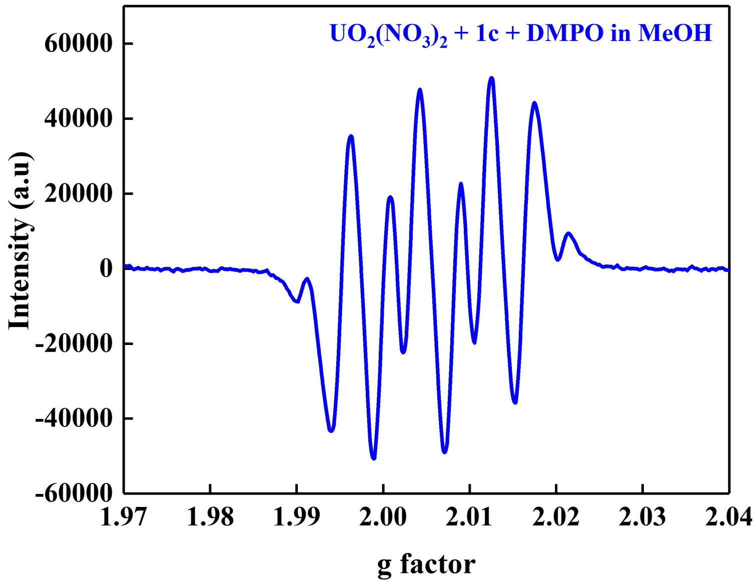


Figure S9. EPR spectra of $UO_2(NO_3)_2 \cdot 6H_2O$ + **1c** + DMPO in MeOH.

Combined $UO_2(NO_3)_2 \cdot 6H_2O$ (0.004 mmol) with **1c** (0.1 mmol) in 2 mL MeOH followed by irradiation of blue light for 30 min. Then DMPO (0.5 mmol) was added to the mixture, followed by testing after another 10-minute irradiation.

Figure S8 and S9 indicated that this reaction was radical process and the alkyl peroxy radical (ROO·) or superoxide radical anion was participated.

UV-visible absorption experiments

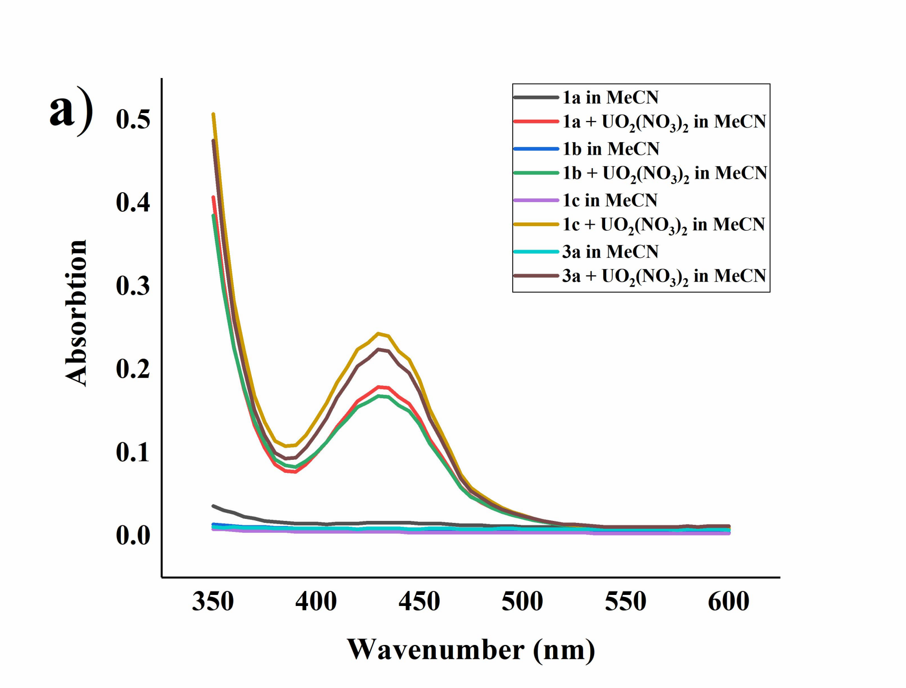


Figure S10. UV-visible absorption spectra of $UO_2(NO_3)_2 \cdot 6H_2O$ and several substrates.

In each experiment, the varying samples were combined with MeCN in screw-top 1.0 cm quartz cuvettes. The concentration of $UO_2(NO_3)_2 \cdot 6H_2O$ was about 5.0×10^{-4} M, and the concentration of substrates was 0.1 M, respectively. And the UV-visible absorption data showed that $UO_2(NO_3)_2 \cdot 6H_2O$ played the role of photo-catalyst.

Fluorescence Quenching Experiments

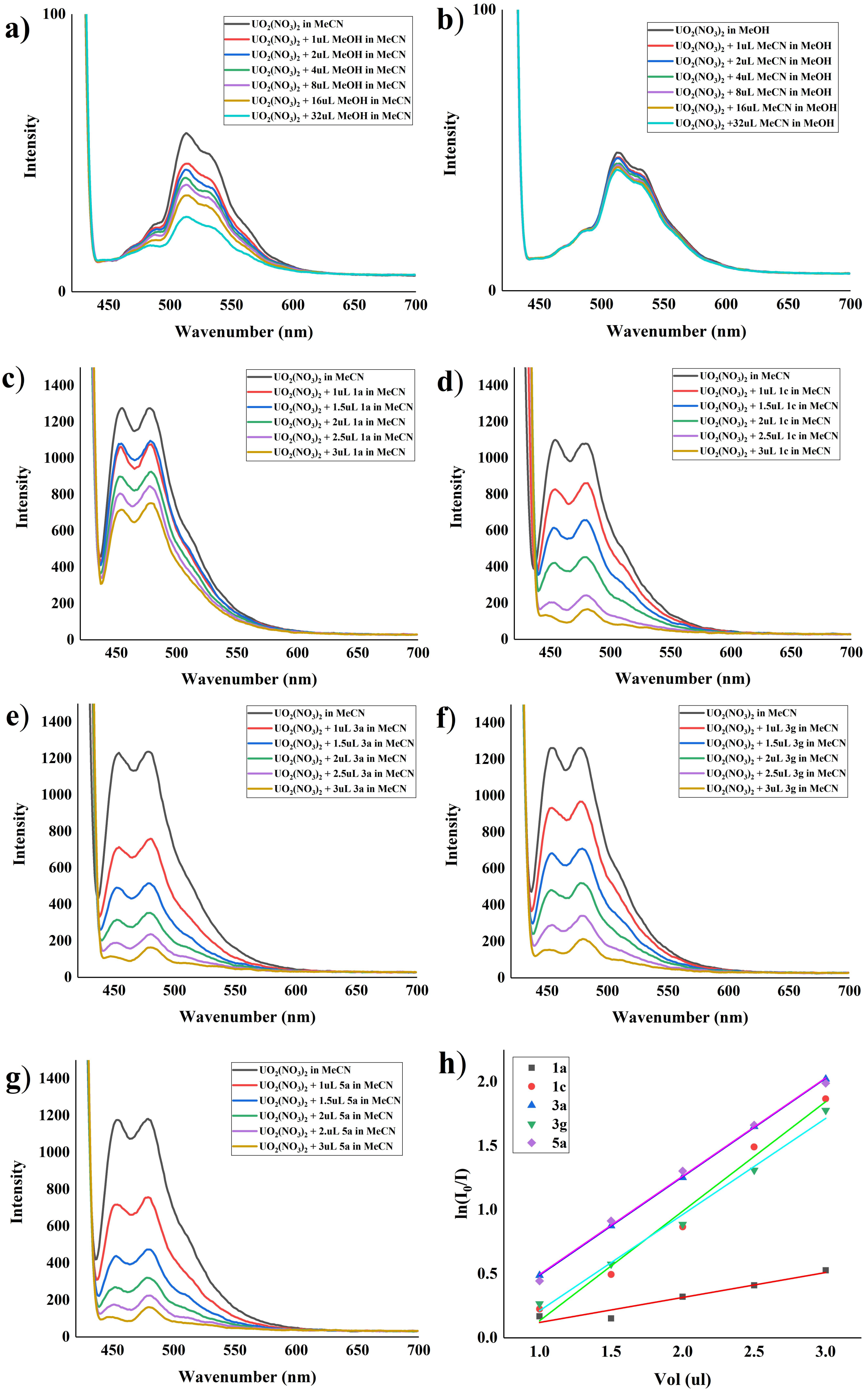


Figure S11. Fluorescence spectrum of $UO_2(NO_3)_2{\cdot}6H_2O$ with different quenchers.

a-g): the varying samples were combined with MeCN in screw-top 1.0 cm quartz cuvettes. The concentration of $UO_2(NO_3)_2{\cdot}6H_2O$ was about 5.0×10^{-4} M with different volumes of component; h) Stern–Volmer analysis between several substrates and $UO_2(NO_3)_2{\cdot}6H_2O$. The results showed that excited states of $UO_2(NO_3)_2{\cdot}6H_2O$ could be efficiently quenched by MeOH or substrates at room temperature.

Detailed information of Kinetic experiments.

Each experiment was performed with dodecane as internal standard. Substrate (2 mmol) and $UO_2(NO_3)_2{\cdot}6H_2O$ (2 mol%) were dissolved in 20 mL MeOH and were put into reaction under blue light in air. Samples were taken out every other hour and were analyzed by ^1H NMR after dissolved in $CDCl_3$ with dodecane as internal standard.

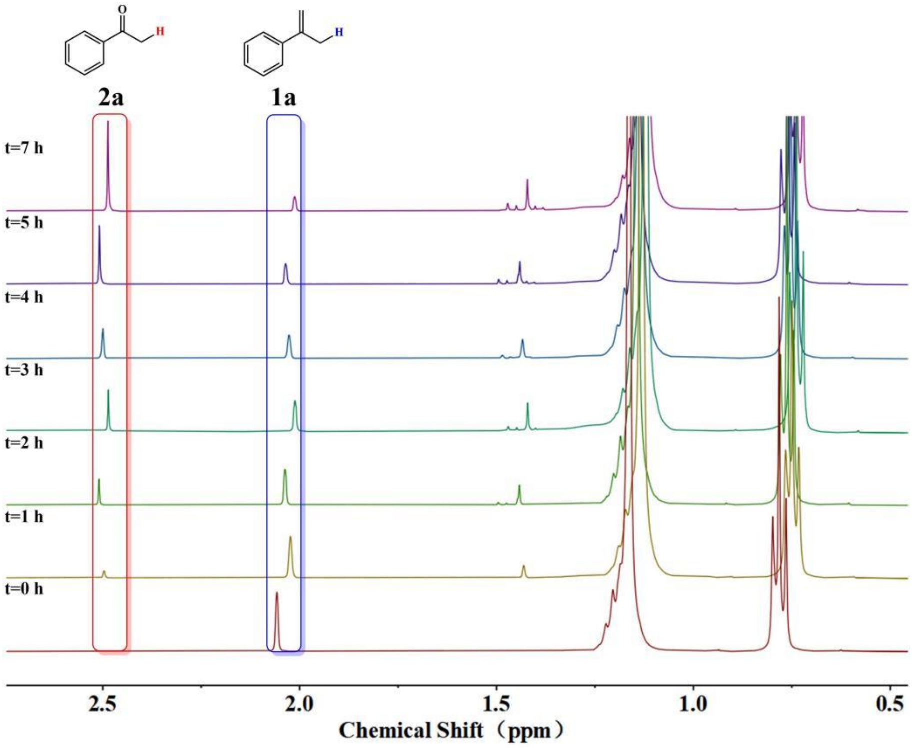


Figure S12. Kinetic experiment of **1a** to **2a**.

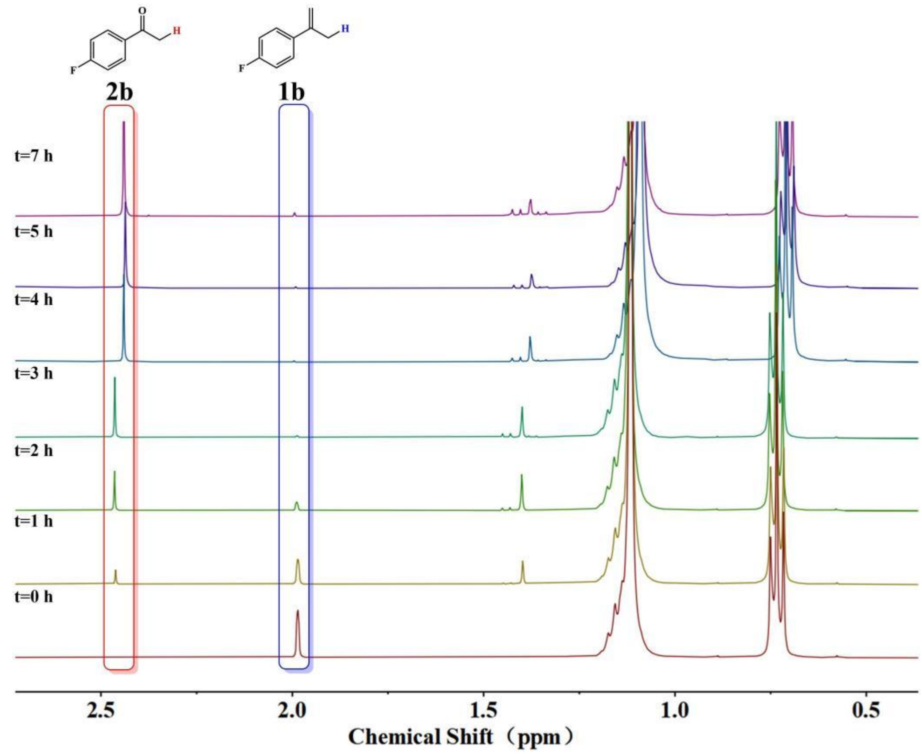


Figure S13. Kinetic experiment of **1b** to **2b**.

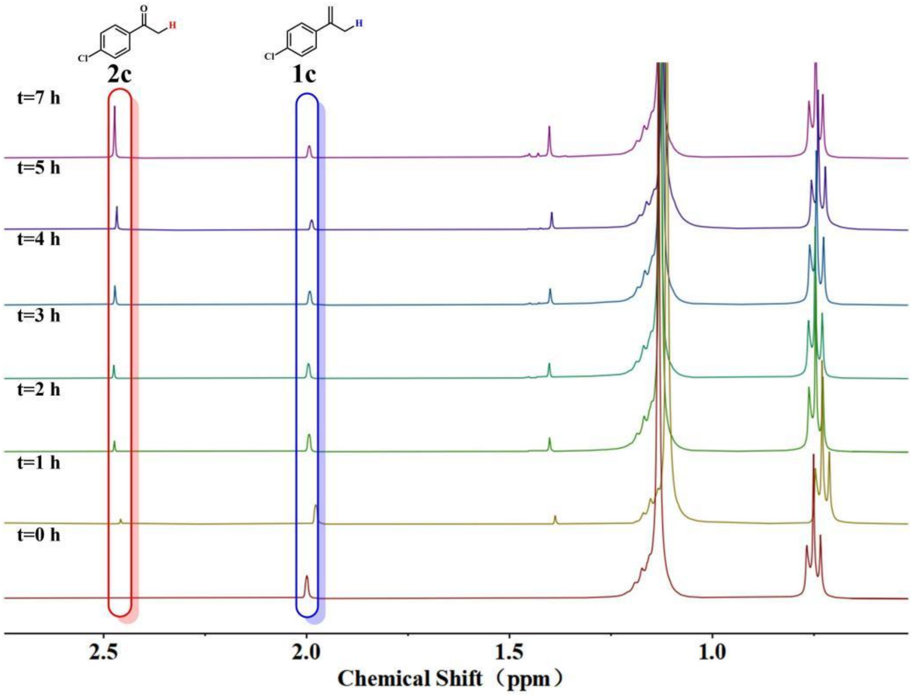


Figure S14. Kinetic experiment of **1c** to **2c**.

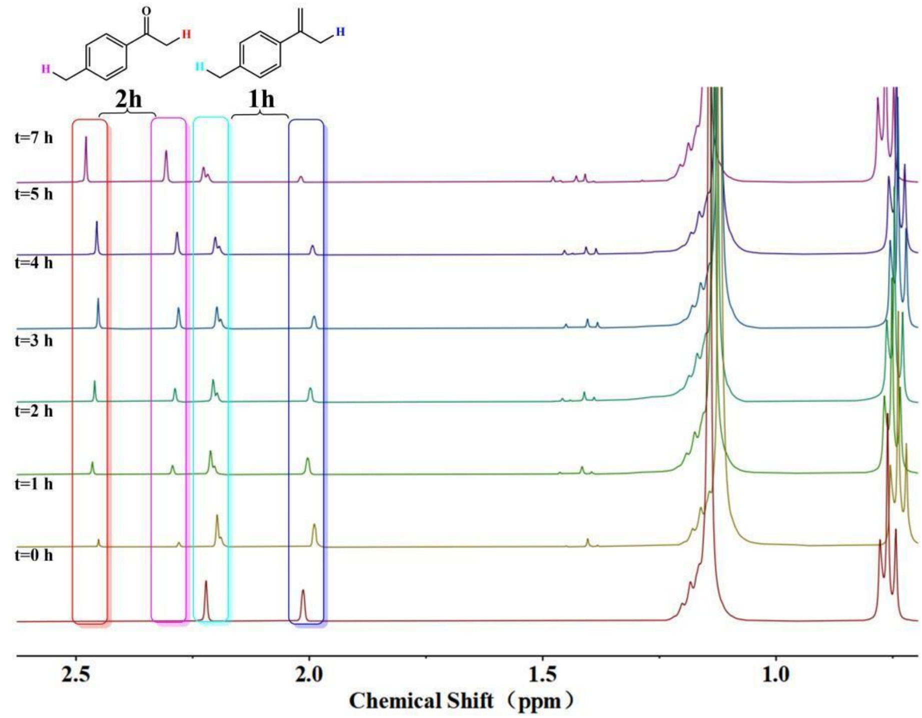


Figure S15. Kinetic experiment of **1h** to **2h**.

5) Computational details

The calculations for all species were carried out through density functional theory (DFT) [1] method with the hybrid PBE0[2] exchange-correlation functional as implemented in the Gaussian 16 program[3]. Stuttgart energy-consistent relativistic pseudopotential ECP60MWB and the corresponding ECP60MWB-SEG basis set[4] was applied to uranium and 6-31G(d,p) basis set[5] was applied for the C, H, O, and N atoms. The harmonic vibrational frequencies were calculated to verify that the optimized geometries were stationary points on the potential energy surface and to obtain the corresponding thermochemical corrections. Intrinsic reaction paths (IRPs)[6] were traced from the transition structures to ensure that no unexpected intermediates exist. For refining the electronic energy, single-point calculations by DFT/PBE0 were done for all compounds with the larger basis set 6-311G(2d,p)[7] for the non-metal elements. Solvent effects were taken into account by using the continuum solvation model IEFPCM[8] with default settings for acetonitrile.

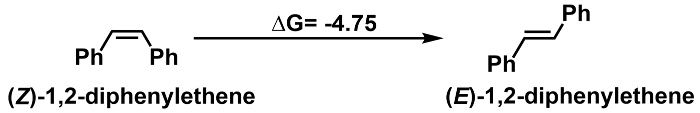


Figure S16. Calculated Gibbs free energy (in kcal/mol) of configuration transformation from (*Z*)-1,2-diphenylethene to (*E*)-1,2-diphenylethene.

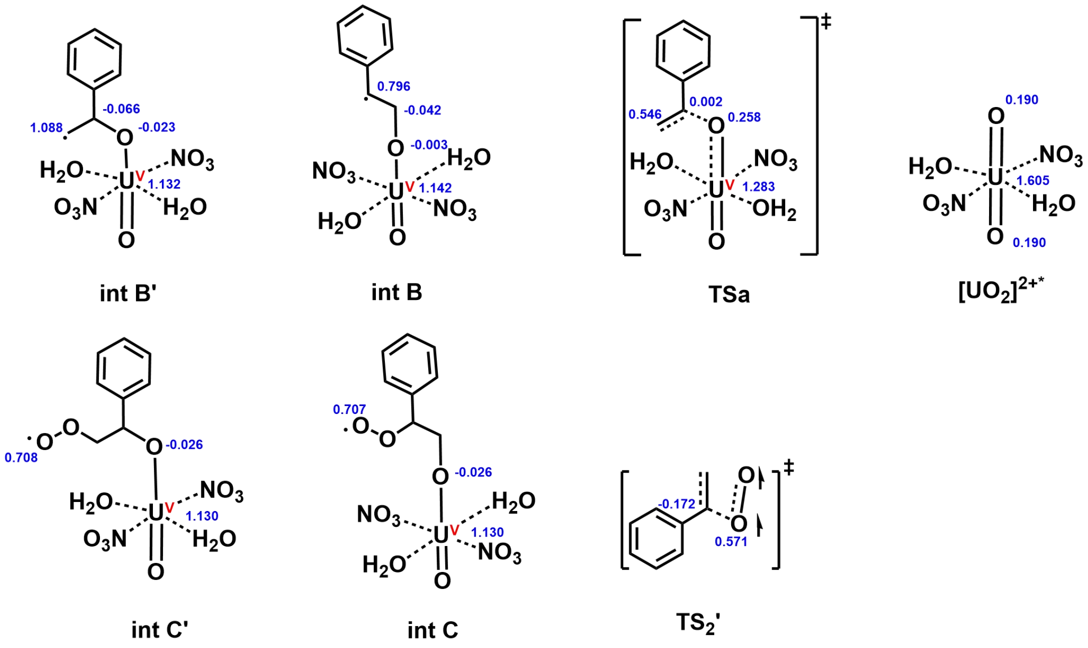


Figure S17. Spin density of the open-shell compounds in Scheme 3.

SET or HAT ?

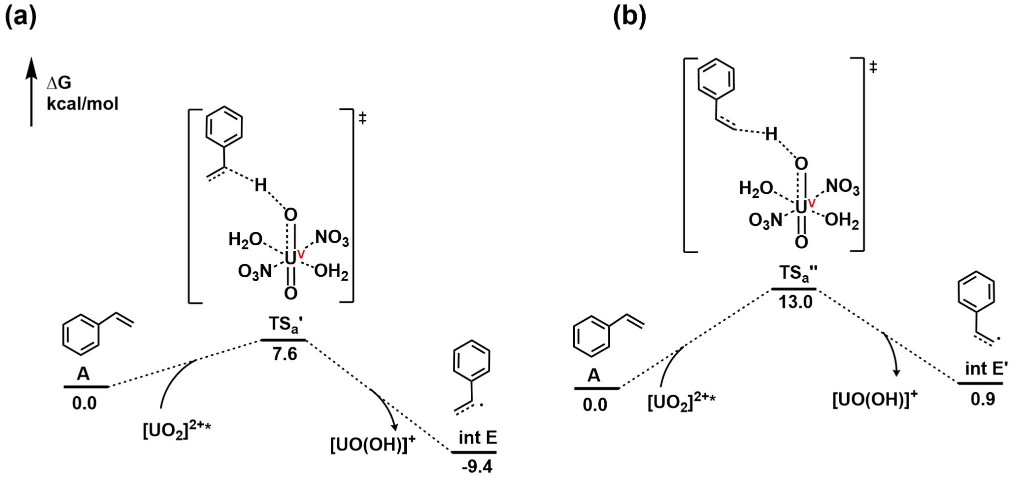


Figure S18. Free energy profiles illustrating the HAT process between styrene and excited uranyl complex based on DFT/PBE0 calculations: (a) Extract H(α-C) process; (b) Extract H (β-C) process. Relative Gibbs free energies (G) are given in kcal/mol.

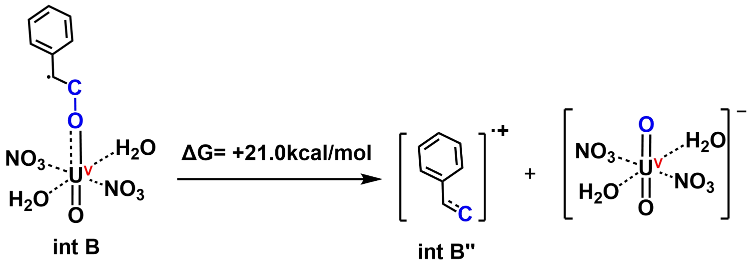


Figure S19. Calculated free energy (in kcal/mol) of formation of int B '' and pentavalent uranyl from the C-O bond cleavage of int B. This indicates that the C-O bond breakage of int B to form a two-molecule process with a free energy of 21.0 kcal/mol for the reaction is unfavorable thermodynamically and cannot proceed spontaneously. Therefore, the generation of int B process is finally considered in Scheme 3.

Thermodynamic study of the formation of uranyl-organic complex between $[UO_2]^{2+*}$ and styrene

In order to estimate the reaction barrier of forming int B from the reaction of styrene with excited uranyl nitrate $[UO_2]^{2+*}$, we carried out the potential energy surface (PES) scan along the direction of C-O_{ax} bond formation between the terminal carbon of styrene and the axial oxygen (O_{ax}) of $[UO_2]^{2+*}$ at the DFT/PBE0 level. The initial structure (**I-1**) of this scan corresponds to a stable hydrogen-bonding complex of styrene and $[UO_2]^{2+*}$, where weak hydrogen bonds are formed between NO_3 unit and $H_2C{=}CH-$ group. The C-O_{ax} distance is 3.879 Å, showing a non-bonding interaction. The scan step size was set as 0.024 Å and the potential energy curve was obtained by taking the energy of the initial structure as the reference zero. As shown in **Figure S20**, at the beginning, styrene lies between the coordinated nitric acid and water with the benzene ring below the coordinated water. When C-O_{ax} distance decreases from **I-1** to **II-1**, the configurations of styrene has little change but with the whole styrene molecule moving away from NO_3^- and to the top of $[UO_2]^{2+*}$, which breaks the hydrogen bonds between NO_3 and $H_2C{=}CH-$ and increases the steric hindrance. When the C-O_{ax} distance is further shortened, styrene is well above water molecule and UO_2 unit (structure **III-1**) but with hydrogen bonding interaction between NO_3 and benzene accompanied by an energy drop of 2.3 kcal/mol from **II-1** to **III-1**. However, the potential energy continuously declines when the C-O_{ax} distance keeps shortening until the formation of C-O_{ax} covalent bonding (**IV-1**). Overall, for terminal carbon, although there appears an energy barrier at structure **II-1** from initial **I-1** to the final **IV-1**, this does not correspond to a transition state as the C-O distance at **II-1** is 3.096 Å far without any bonding interaction. The slight energy increase, i.e., 1.6 kcal/mol, from structure **I-1** to **II-1** is caused by the change in the spatial arrangement of $[UO_2]^{2+*}$ and styrene that breaks the hydrogen bonding but not by a formation of C-O_{ax} bond. Therefore, the whole process of forming int B is demonstrated to be free of energy barrier.

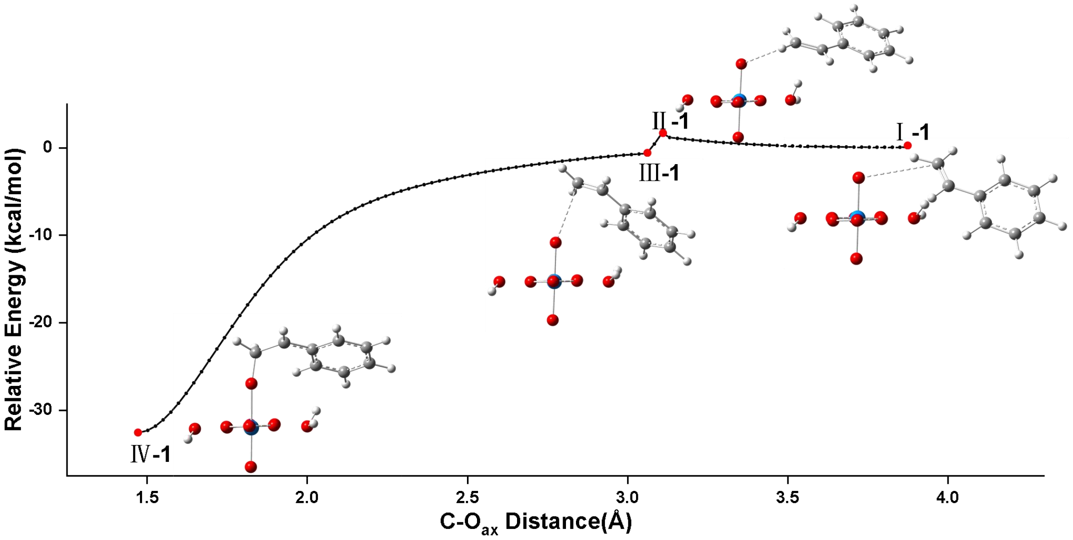
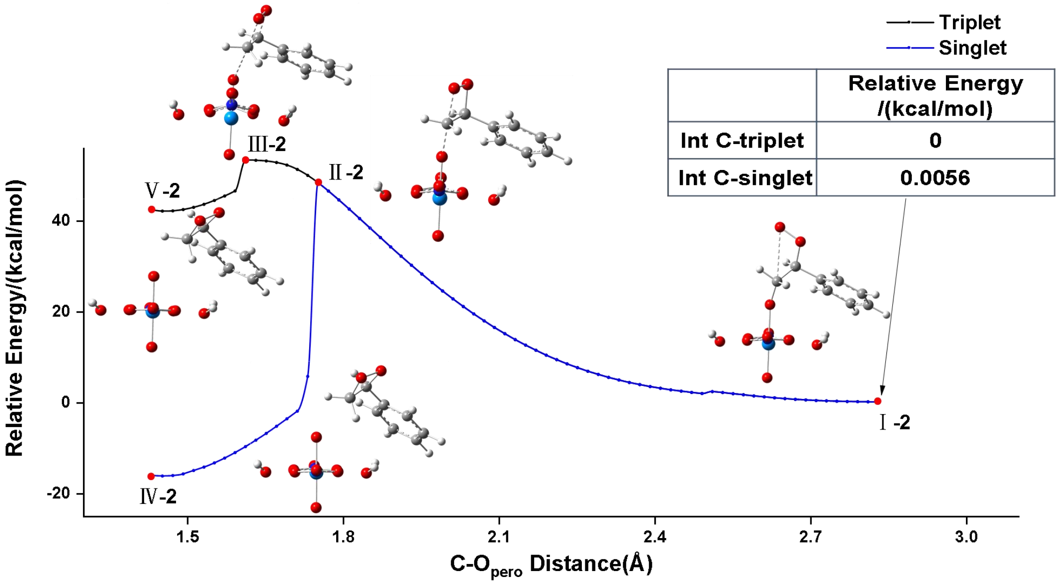


Figure S20. Potential energy surface (PES) scan illustrating energetics during the formation of uranyl-organic complex **int B** (corresponding to structure **IV-1**) from the reaction of styrene with excited uranyl $[UO_2]^{2+*}$ based on DFT/PBE0 calculations. The C-O$_{axl}$ distance is defined as the distance between the terminal ethene carbon of styrene and the axial oxygen of the $[UO_2]^{2+*}$(dot line), which is gradually decreased from 3.879 to 1.432 Å with the step size of 0.024 Å. The key structures, i.e., **I-1** to **IV-1**, on the potential curves are given, where structure **I-1** corresponds to a stable hydrogen-bonding complex of styrene and $[UO_2]^{2+*}$.

Thermodynamic study of the formation of D (1, 2-dioxetane) through the leaving of uranyl moiety and cyclization

In order to estimate the reaction barrier of forming 1, 2-dioxetane from **int C**, we carried out the PES scan along the direction of C-O$_{pero}$ bond formation between the terminal carbon of styrene and terminal oxygen (O$_{pero}$) of peroxy radical in **int C** at the DFT/PBE0 level. The initial structure **I-2** of this scan corresponds to a stable pentavalent uranyl-organic complex containing a peroxy radical (i.e., **int C**) with one unpaired electron on uranium and one unpaired electron on oxygen, respectively. These two unpaired electrons can have the same spin (i.e., +1/2) that gives a triplet state or different spins (+1/2 and – 1/2, respectively) that produces an open-shell singlet state. Due to exchange interaction between two unpaired electrons, the triplet state is usually slightly lower in energy than the singlet state. As shown in **Figure S21**, the energy difference between the singlet and triplet states is calculated to be 0.0056 kcal/mol in **int C**. The C-O$_{pero}$ distance is 2.832 Å in **int C** (i.e., structure **I-2)**, showing a non-bonding interaction. The scan step size was set as 0.020 Å and the respective triplet (black line) and singlet (blue line) potential curves were obtained by taking the triplet ground-state energy of **I-2** as the reference zero. As shown in **Figure S21**, when C-O_{pero} distance gradually decreases from **I-2** (2.832 Å) to **II-2 (**1.752 Å**)**, the singled and triplet potential curves give very similar evolutions in structure and energetics. Specifically, the whole uranyl moiety moves away slowly with little change in the configurations of **I-2**, and there is very little energy difference between singled and triplet potential curves albeit with the triplet state slightly lower in energy. When the C-O_{pero} distance is further shortened, evolution behaviors of the singled and triplet potential curves are very different. For the triplet state, the potential curve firstly goes up till the highest energy point at structure **III-2** (corresponding to C-O_{pero} distance of 1.596 Å) then goes down until the formation of C-O covalent bonding at **V-2** (corresponding to C-O_{pero} distance of 1.414 Å). In contrast, for the singlet state, the potential curve goes down continuously until the formation of C-O_{pero} covalent bond at **IV-2** with the C-O_{pero} distance of 1.415 Å. It is noted that the potential energy curve of the singlet state is always lower than that of the triplet state when C-O_{pero} distance is shorter than 1.752 Å. Overall, the PES scans show that the singlet−triplet crossing will happen during the formation of C-O_{pero} bond with the turning point at **II-2**. Herein, for the formation of the key intermediate **D** in the C1 attack path, we finally take triplet ground-state for **int C** and singlet ground states for **TS1** and **D**. By the way, in case of the C2 attack path, the same PES scan results were obtained for the formation of the key intermediate **D** from **int C'** and the details were not discussed here for the sake of briefness.



	Relative Energy /(kcal/mol)
Int C-triplet	**0**
Int C-singlet	**0.0056**

Figure S21. Potential energy surface (PES) scan illustrating the energetics during the formation of the key intermediate **D** (corresponding to **IV-2**) from **int C** (corresponding to **I-2**) based on DFT/PBE0 calculations. The C-O_{pero} distance is defined as the distance between the terminal carbon of styrene and terminal oxygen (O_{pero}) of peroxy radical, which is decreased from 2.832 to 1.415 Å with the step size of 0.020 Å. Due to the existence of two unpaired electrons in **int C** with one on uranium and one on oxygen, respectively, the respective triplet (black line) and singlet (blue line) potential curves were scanned and the relative energies were obtained by taking the triplet ground-state energy of **I-2** as the reference zero.

Energy profiles of uranyl photocatalytic oxidative cleavage of styrene: a comparison of $^3O_2$ and $^1O_2$ involved reaction pathways

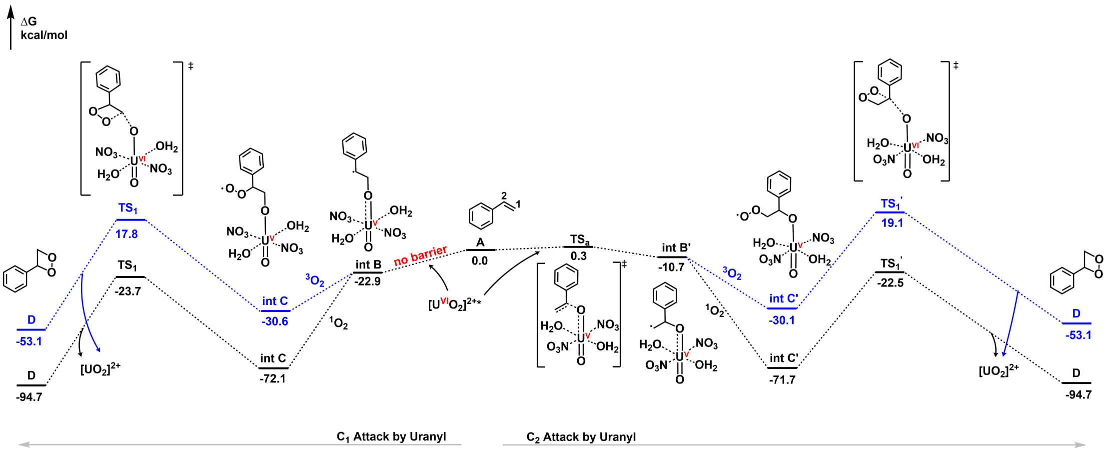
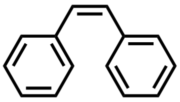


Figure S22. Energy profiles of uranyl photocatalytic oxidative cleavage of styrene with the triplet oxygen ($^3O_2$) (blue line) or singlet oxygen $^1O_2$ (black line) as the oxidant, respectively. Relative Gibbs free energies are given in kcal/mol.

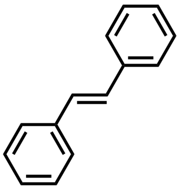
As shown in Figure S22, int B(B') reacting with triplet oxygen ($^3O_2$) to finally form intermediate D(D') is less favorable both thermodynamically and kinetically than with singlet oxygen ($^1O_2$) due to the inert nature of $^3O_2$ in reactivity. Take the reaction path of int B for example, the relative Gibbs energies of TS1 and intermediate D for $^3O_2$ involved path are much higher than those for $^1O_2$ involved path, i.e., 17.8 *vs* -23.7 kcal/mol and -53.1 *vs* -94.7 kcal/mol, respectively. The same phenomenon is also observed for the reaction path of int B'.

Table S6. Cartesian coordinates (in Å) of DFT/PBE0 optimized geometries of all compounds.



(*Z*)-1,2-diphenylethene

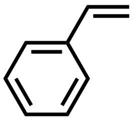
C	2.30411300	-1.42515700	0.93029300
C	3.50653600	-1.33218800	0.23301300
C	3.77186300	-0.19758200	-0.52709300
C	2.83937600	0.83108100	-0.59255800
C	1.61383000	0.73808500	0.07915000
C	1.36820900	-0.40242600	0.85487300
C	0.67182200	1.86494300	0.00575100
C	-0.67191300	1.86484600	-0.00556600
C	-1.61382100	0.73793300	-0.07912000
C	-2.83974000	0.83123000	0.59188800
C	-3.77221600	-0.19743200	0.52637700
C	-3.50650600	-1.33237600	-0.23309500
C	-2.30371600	-1.42565800	-0.92969900
C	-1.36782100	-0.40292300	-0.85422000
H	2.09792500	-2.29731800	1.54265500
H	4.23584900	-2.13346100	0.29251300
H	4.71052400	-0.10898200	-1.06466700
H	3.05747300	1.72008500	-1.17753700
H	0.44081400	-0.47988800	1.41197000
H	1.14914500	2.84298600	-0.03071300
H	-1.14936500	2.84282000	0.03107100
H	-3.05813000	1.72049900	1.17635700
H	-4.71116200	-0.10857400	1.06341000
H	-4.23579700	-2.13366500	-0.29263600
H	-2.09721900	-2.29808200	-1.54158200
H	-0.44015100	-0.48066800	-1.41081200



(*E*)-1,2-diphenylethene

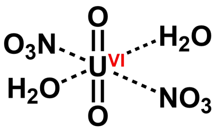
C	3.85306000	1.29575300	-0.00017700
C	4.71855900	0.20262800	-0.00024600
C	4.19262600	-1.08457000	-0.00024900
C	2.81589600	-1.27421100	-0.00018200

C	1.93117500	-0.18629100	-0.00011100
C	2.47929000	1.10614100	-0.00011000
C	0.49414000	-0.45527500	-0.00004200
C	-0.49414000	0.45527600	0.00004000
C	-1.93117500	0.18629100	0.00011000
C	-2.81589600	1.27421100	0.00019700
C	-4.19262600	1.08457000	0.00026600
C	-4.71855900	-0.20262800	0.00024800
C	-3.85306000	-1.29575300	0.00016100
C	-2.47929000	-1.10614100	0.00009300
H	4.25446600	2.30420400	-0.00017500
H	5.79264900	0.35621000	-0.00029800
H	4.85486700	-1.94437800	-0.00030300
H	2.41192200	-2.28265900	-0.00018400
H	1.82914100	1.97458100	-0.00005800
H	0.23811100	-1.51291800	-0.00005900
H	-0.23811100	1.51291800	0.00006000
H	-2.41192200	2.28265900	0.00021200
H	-4.85486700	1.94437800	0.00033400
H	-5.79264900	-0.35621000	0.00030200
H	-4.25446500	-2.30420400	0.00014600
H	-1.82914100	-1.97458100	0.00002500



A

C	-1.94826000	-0.53010400	0.00020000
C	-0.51341900	-0.22097700	0.00011600
C	-0.01110100	1.08883100	0.00016900
C	0.40560000	-1.27835200	-0.00000500
C	1.35608100	1.32645800	0.00005500
H	-0.69730300	1.93056100	0.00033300
C	1.77611300	-1.04265100	-0.00012200
H	0.03393600	-2.30036300	-0.00002100
C	2.25750200	0.26234600	-0.00010000
H	1.72368800	2.34875800	0.00010200
H	2.46814200	-1.87994100	-0.00022400
H	3.32684100	0.45211800	-0.00018400
C	-2.96570400	0.33539800	-0.00026300
H	-2.82192400	1.41206800	-0.00078600
H	-3.99272800	-0.01420900	-0.00016200
H	-2.18152600	-1.59468100	0.00064500



$[UO_2]^{2+}$

U	0.00002700	0.00004300	0.00008300
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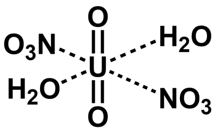
O	-0.00018000	0.12749100	1.74217600
O	0.00007700	-2.50911100	0.13014300
H	0.78271300	-2.92052900	-0.25413700
O	-0.00026900	2.50916700	-0.13027400
H	-0.78283000	2.92067800	0.25404000
H	-0.78319600	-2.92010200	-0.25331500
H	0.78312400	2.92005600	0.25306800
N	-2.90191900	-0.00011300	-0.00021100
N	2.90188900	-0.00009000	-0.00008300
O	-2.20570300	-1.06994300	0.03734600
O	-4.09820000	-0.00029900	-0.00016900
O	-2.20599100	1.06985200	-0.03763400
O	2.20597600	-1.07010700	0.03765900
O	4.09811900	0.00014800	-0.00016900
O	2.20563900	1.06980000	-0.03770500



$[UO_2]^{2+*}$

U	-0.00000200	0.00001000	0.00004900
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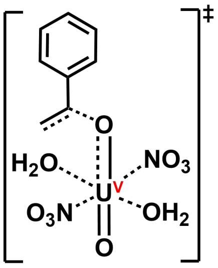
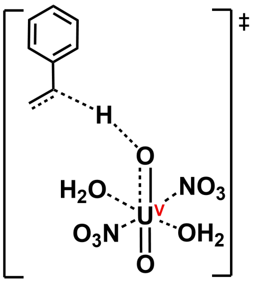
O	-0.00047600	0.15921900	1.78999700
O	-0.00014700	-2.51209700	0.15287700
H	0.78226700	-2.93032900	-0.22429000
O	-0.00005800	2.51225800	-0.15269600
H	-0.78281000	2.93011000	0.22422600
H	-0.78320500	-2.92983900	-0.22352600
H	0.78259200	2.93034500	0.22415400
N	-2.90080800	-0.00001200	-0.00019700
N	2.90089800	-0.00007900	-0.00001400
O	-2.20690300	-1.07161200	0.03002500
O	-4.09774800	-0.00003900	-0.00033000
O	-2.20692200	1.07158000	-0.03043700
O	2.20703000	-1.07161500	0.03098600
O	4.09785000	-0.00002200	-0.00048300
O	2.20696400	1.07153200	-0.03049900



TS$_a$

U	0.95029600	0.38912100	-0.13588000
O	0.03771100	-0.78143600	1.03504000
O	1.77794000	1.47125200	-1.28361500
O	1.97810800	1.56439300	1.86045900
H	2.56161700	0.97071000	2.34655400
O	-0.05301500	-0.75703200	-2.18896200
H	-0.55806200	-0.06266800	-2.63070800
H	1.31882700	1.91427300	2.46913000
H	0.70210700	-0.96666100	-2.75254000
N	-1.41332800	2.14452000	0.00947800
N	3.19977500	-1.50531400	-0.17288400
O	-0.45878700	2.22358200	0.84517300
O	-2.39609200	2.83833700	0.08117200
O	-1.26136600	1.27133500	-0.90461100
O	3.10220800	-0.57606600	0.69200400
O	4.11740700	-2.28314200	-0.18596800
O	2.24941800	-1.55379100	-1.02004700
C	-2.70414400	-1.52976900	0.56340800
C	-3.03953900	-1.96482600	-0.72873400
C	-4.08428100	-1.37180400	-1.42389500
H	-2.46806200	-2.76972500	-1.18269300
H	-4.34070600	-1.72041600	-2.41964800
H	-1.89593900	-1.47326000	3.26539500
C	-1.33787400	-2.12056300	2.59776800
H	-0.52489200	-2.69912000	3.01979500
C	-1.60278500	-2.18083900	1.24627700
H	-1.04665200	-2.90766400	0.65999200
C	-4.79183200	-0.31998000	-0.84652300
H	-5.59783800	0.15787300	-1.39537000
C	-4.45768800	0.13422500	0.43050300
H	-4.99166400	0.97224200	0.86616800
C	-3.42853100	-0.46926500	1.13415800
H	-3.15930500	-0.09168900	2.11578400



TS$_a$'

U	-1.41944600	-0.09375100	-0.16762600
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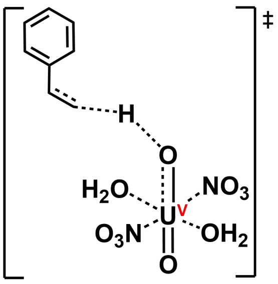
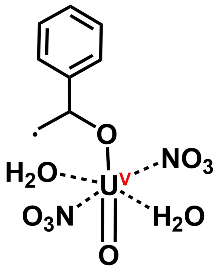
O	-3.17732100	0.05371300	-0.40711900
O	-1.69095600	-0.57998600	2.31753500
H	-1.23086000	0.07326000	2.85627300
O	-1.21972500	0.33776900	-2.68278200
H	-1.49682800	-0.49487700	-3.08777200
H	-1.34244000	-1.45135600	2.53741800
H	-1.87741400	0.99876200	-2.92727000
N	-1.45455900	-2.97606300	-0.71870800
N	-1.03598500	2.74755100	0.45030200
O	-1.55499700	-2.49928300	0.45702900
O	-1.46097800	-4.15631500	-0.94488900
O	-1.34230400	-2.10144600	-1.64005600
O	-1.32767800	1.89105600	1.34195400
O	-0.79638600	3.89877000	0.70588300
O	-0.99919600	2.29334600	-0.74379000
C	2.41102700	2.24890100	-1.00555200
C	2.65325600	1.05568500	-0.45226600
H	1.66103000	0.37392100	-0.31690100
H	1.39687600	2.63185800	-1.09839500
H	3.21230600	2.83582400	-1.45468300
C	3.86578600	0.43883600	0.01478300
C	4.00556700	-0.96307500	-0.04763400
C	4.91811600	1.20952700	0.55331100
C	5.18218500	-1.56789500	0.36357000
H	3.17778600	-1.55737200	-0.42387200
C	6.09354000	0.59838600	0.95725800
H	4.79325900	2.28475300	0.63890700
C	6.22834300	-0.78918900	0.86270900
H	5.28792100	-2.64660500	0.30310800
H	6.90718700	1.19719800	1.35523400
H	7.14789100	-1.26539100	1.19034600



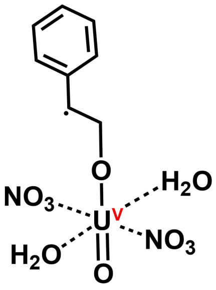
TS_a''

U	1.47604800	0.24525700	0.07394900
O	0.23333600	-0.91342200	-0.86315600
O	2.56301000	1.31749100	0.98411500
O	2.34544400	1.02482400	-2.16544200
H	1.66384800	1.40198300	-2.73227600
O	0.64817400	-0.58065000	2.32999900
H	1.36233400	-1.13733500	2.66835200
H	2.78494000	0.31295700	-2.64473000
H	0.56110200	0.16730100	2.93182800
N	3.46867700	-1.91349200	0.06906000
N	-0.68463000	2.23971600	-0.08132900
O	3.36564100	-1.07309800	-0.88118000
O	4.28867900	-2.79031700	0.07727300
O	2.62678000	-1.75099100	1.01412700
O	0.25195800	2.18983700	-0.93505300
O	-1.62309400	2.98758800	-0.18136500
O	-0.57526600	1.41774100	0.89236200
C	-2.92413400	-0.58121500	-0.38638300
C	-2.16941000	-1.43254600	-1.08840100
H	-0.91182300	-1.36148800	-0.85619400
H	-2.40478900	0.21185400	0.15749200
H	-2.43127600	-2.11722100	-1.89080200
C	-4.36766000	-0.62578000	-0.17497300
C	-5.18705600	-1.63651900	-0.70495100
C	-4.95413900	0.39657300	0.58774100
C	-6.55547200	-1.61334200	-0.48681400
H	-4.74562100	-2.44099600	-1.28594900
C	-6.32688800	0.41977400	0.79863500
H	-4.32178700	1.18177500	0.99430000
C	-7.12919600	-0.58555600	0.26460400
H	-7.18202900	-2.39725100	-0.90165800
H	-6.77101100	1.22200000	1.38003000
H	-8.20217900	-0.57115000	0.43203700



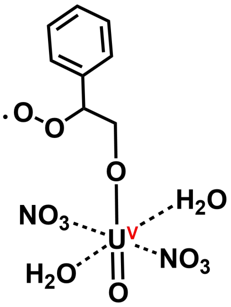
int B'

U	0.96291200	-0.05787400	-0.22154800
O	2.15610900	-0.15517300	-1.53367800
O	-0.37031900	0.03626300	1.27500200
O	2.84318800	-0.58709100	1.40091900
H	3.52078600	0.09650000	1.33472500
O	-0.93469200	0.52522400	-1.77719100
H	-1.76072200	0.06123000	-1.57324000
H	3.25058300	-1.42899100	1.16549600
H	-1.12450700	1.46976600	-1.71586300
N	0.31711400	-2.89368800	-0.35960900
N	1.51345500	2.78888900	0.13771400
O	1.28700100	-2.44030300	0.33487500
O	0.03791600	-4.05982000	-0.40039300
O	-0.33596900	-2.00452200	-0.99999400
O	2.17241500	1.87644500	0.73570400
O	1.74999000	3.95718300	0.27075300
O	0.57537400	2.35453400	-0.61047400
C	-1.62742000	-0.11533200	1.93462700
H	-1.64090000	0.65528300	2.72580400
C	-1.71761000	-1.46427900	2.54908100
H	-0.80807600	-1.97246400	2.84761400
H	-2.67687900	-1.84191100	2.88494400
C	-2.74324100	0.20493000	0.95735400
C	-3.21920400	1.51233000	0.84809500
C	-3.23913900	-0.77547200	0.09013000
C	-4.17266000	1.84239400	-0.11311500
H	-2.83445400	2.27933200	1.51613600
C	-4.19050600	-0.44578900	-0.87455300
H	-2.86449600	-1.79283700	0.16256900
C	-4.65786200	0.86478400	-0.97832800
H	-4.53585800	2.86341100	-0.18578900
H	-4.56901900	-1.21452500	-1.54219800
H	-5.40059600	1.11989900	-1.72846200



int B

U	1.05559700	0.34806100	-0.14075000
O	2.04417000	1.41650300	-1.16002800
O	-0.04622800	-0.86852000	0.98928500
O	0.14028800	-0.72638300	-2.24299600
H	0.85563600	-1.00995400	-2.82394800
O	1.96867400	1.44734700	1.94603000
H	1.32735600	1.91298100	2.49295200
H	-0.39361600	-0.08228300	-2.72430600
H	2.50736300	0.87990100	2.50778600
N	-1.17149800	2.23480500	-0.15648900
N	3.17900000	-1.64006800	-0.01076100
O	-0.98677900	1.37849000	-1.08044600
O	-2.08462000	3.01391700	-0.16279600
O	-0.30886500	2.19247100	0.78367700
O	2.30552400	-1.62251300	-0.94033400
O	4.06267600	-2.44990800	0.03543100
O	3.03177300	-0.72841700	0.87018600
C	-0.84875000	-1.89389000	1.58578400
H	-0.19008900	-2.73636700	1.81768300
H	-1.22525600	-1.48713500	2.53369800
C	-1.96477000	-2.32642500	0.70318500
H	-1.87990600	-3.29310500	0.21410300
C	-3.10018500	-1.53069200	0.42046900
C	-4.12173400	-2.02959900	-0.42946600
C	-3.26984500	-0.22575700	0.95350600
C	-5.24091700	-1.27186100	-0.72348200
H	-4.01139900	-3.02625100	-0.84958800
C	-4.38978300	0.52807600	0.64723000
H	-2.50071600	0.19507600	1.59480200
C	-5.38314500	0.01244300	-0.18954900
H	-6.01031700	-1.67637500	-1.37506600
H	-4.48638700	1.53186800	1.04973200
H	-6.25818200	0.60922600	-0.42825200



int C

U	1.22800000	-0.44100000	0.11600000
O	2.37800000	-1.43500000	1.03200000
O	-0.07500000	0.71200000	-0.89300000
O	0.18300000	0.36900000	2.27800000
H	0.83700000	0.78000000	2.85500000
O	2.22700000	-1.22100000	-2.06500000
H	1.66500000	-1.75300000	-2.63800000
H	-0.21700000	-0.36800000	2.75600000
H	2.68000000	-0.55700000	-2.59600000
N	-0.70600000	-2.61300000	0.01700000
N	3.03700000	1.83500000	0.13200000
O	-0.62400000	-1.80500000	0.99900000
O	-1.49600000	-3.51400000	-0.02100000
O	0.12100000	-2.37900000	-0.92800000
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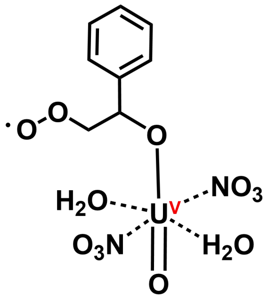

int C'

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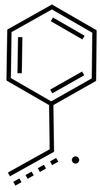

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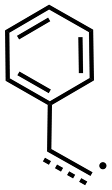

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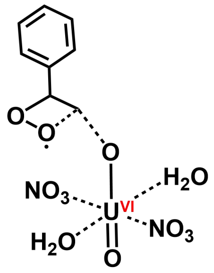

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O	1.43798700	3.92448600	-0.96713600
O	0.55264700	1.96768100	-1.32278100
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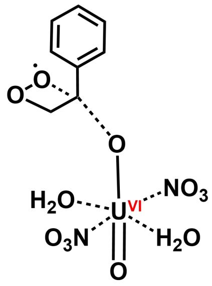

TS_1'

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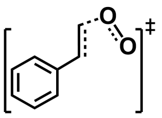 TS$_2$			
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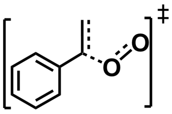 TS$_2$'			
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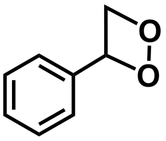 **D**			
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C	0.62795800	1.06238400	-0.00091200
C	1.97982300	1.35720100	-0.13613700
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H	-0.11531200	1.85392300	0.01646900
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C	-1.24620100	-0.58734200	0.24649400
H	-1.39565800	-1.56810400	0.71868300
C	-2.15713800	-0.37309400	-0.95544000
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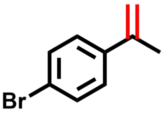
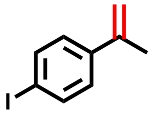
O	-2.02035700	0.42392200	0.93345300
$^1O_2$			
O	0.00000000	0.00000000	0.60205400
O	0.00000000	0.00000000	-0.60205400

6) Characterization of starting materials.

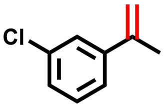
Most of starting materials were commercially available and used without purification. The following starting materials were synthesized according to the reported literature under 10 mmol scale.



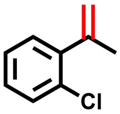
1-Bromo-4-(prop-1-en-2-yl)benzene (1d).[9] Yield: 65%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.45 (m, 2H), 7.37 – 7.33 (m, 2H), 5.38 (t, *J* = 1.1 Hz, 1H), 5.13 (p, *J* = 1.5 Hz, 1H), 2.17 - 2.13 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.2, 140.1, 131.3, 127.2, 121.3, 113.1, 21.7.



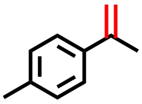
1-Iodo-4-(prop-1-en-2-yl)benzene (1e).[10] Yield: 36%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.66 (m, 2H), 7.25 – 7.21 (m, 2H), 5.40 (t, J = 1.1 Hz, 1H), 5.13 (p, J = 1.5 Hz, 1H), 2.17 - 2.13 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 140.7, 137.3, 127.4, 113.2, 92.9, 21.6.



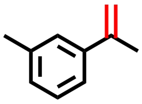
1-Chloro-3-(prop-1-en-2-yl)benzene (1f).[11] Yield: 51%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 - 7.47 (m, 1H), 7.37 - 7.36 (m, 1H), 7.29 – 7.27 (m, 2H), 5.41 (t, J = 1.1 Hz, 1H), 5.16 (p, J = 1.5 Hz, 1H), 2.20 – 2.13 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 142.1, 134.3, 129.5, 127.4, 125.8, 123.7, 113.7, 21.7.



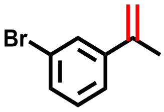
1-Chloro-2-(prop-1-en-2-yl)benzene (1g).[11] Yield: 13%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.37 (m, 1H), 7.27 – 7.20 (m, 3H), 5.28 - 5.26 (m, 1H), 5.01 – 5.00 (m, 1H). 2.17 - 2.13 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.4, 142.8, 131.8, 129.8, 129.6, 128.2, 126.6, 116.2, 23.4.



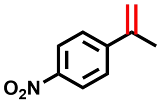
1-Methyl-4-(prop-1-en-2-yl)benzene (1h).[12] Yield: 44%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, J = 8.2 Hz, 2H), 7.22 (d, J = 7.9 Hz, 2H), 5.48 – 5.40 (m, 1H), 5.13 - 5.12 (m, 1H), 2.43 (s, 3H), 2.23 (d, J = 1.5 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 138.4, 137.2, 129.0, 125.4, 111.6, 21.9, 21.1.



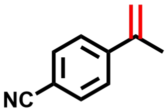
1-Methyl-3-(prop-1-en-2-yl)benzene (1i).[13] Yield: 45%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.23 (m, 3H), 7.13 – 7.10 (m, 1H), 5.38 – 5.37 (m, 1H), 5.10 - 5.09 (m, 1H), 2.39 (s, 3H), 2.18 (t, J = 1.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.4, 141.3, 137.7, 128.2, 128.1, 126.3, 122.6, 112.3, 77.3, 21.9, 21.5.



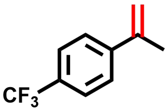
1-**Bromo-3-(prop-1-en-2-yl)benzene (1j).**[14] Yield: 24%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 (t, J = 2.0 Hz, 1H), 7.43 – 7.40 (m, 2H), 7.22 (t, J = 7.9 Hz, 1H), 5.40 (s, 1H), 5.15 (t, J = 1.6 Hz, 1H), 2.16 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.5, 142.1, 130.3, 129.8, 128.7, 124.1, 122.5, 113.7, 21.7.



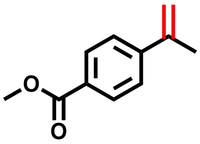
1-Nitro-4-(prop-1-en-2-yl)benzene (1k).[15] Yield: 11%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 – 8.19 (m, 2H), 7.63 – 7.60 (m, 2H), 5.55 – 5.54 (m, 1H), 5.32 – 5.31 (m, 1H), 2.23 - 2.16 (m, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 147.7, 147.0, 141.6, 126.2, 123.6, 116.4, 21.6.



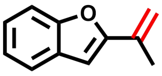
4-(Prop-1-en-2-yl)benzonitrile (1l).[16] Yield: 29%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 – 7.61 (m, 2H), 7.58 – 7.54 (m, 2H), 5.49 (t, *J* = 1.0 Hz, 1H), 5.27 - 5.26 (m, 1H), 2.18 (t, *J* = 1.1 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 145.7, 141.8, 132.1, 126.1, 119.0, 115.7, 110.9, 21.4.



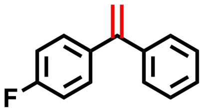
1-(Prop-1-en-2-yl)-4-(trifluoromethyl)benzene (1m).[17] Yield: 31%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 – 7.57 (m, 4H), 5.47 - 5.46 (m, 1H), 5.23 - 5.22 (m, 1H), 2.24 – 2.18 (m, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 144.8, 142.2, 129.4 (d, *J* = 16.16 Hz), 125.8, 125.2 (q, *J* = 2.02 Hz), 122.9, 114.6, 21.7.



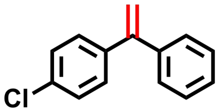
Methyl 4-(prop-1-en-2-yl)benzoate (1n).[18] Yield: 17%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.03 – 8.00 (m, 2H), 7.56 – 7.53 (m, 2H), 5.49 (m, 1H), 5.22 - 5.21 (m, 1H), 3.94 (s, 3H), 2.21 - 2.18 (m, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 167.0, 145.7, 142.5, 129.6, 129.0, 125.4, 114.6, 52.1, 21.7.



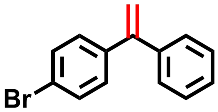
2-(Prop-1-en-2-yl)benzofuran (1s).[19] Yield: 67%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 – 7.58 (m, 1H), 7.54 - 7.51 (m, 1H), 7.35 - 7.31 (m, 1H), 7.28 – 7.24 (m, 1H), 6.69 (s, 1H), 5.88 (t, *J* = 1.1 Hz, 1H), 5.25 (q, *J* = 1.6 Hz, 1H), 2.24 – 2.14 (m, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 156.9, 154.8, 132.9, 129.0, 124.5, 122.7, 121.0, 113.2, 111.0, 102.8, 19.4.



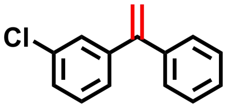
1-Fluoro-4-(1-phenylvinyl)benzene (3b).[20] Yield: 52%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.32 (m, 7H), 7.10 - 7.05 (m, 2H), 5.50 (d, *J* = 1.2 Hz, 1H), 5.48 (d, *J* = 1.2 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 163.8, 161.4, 149.2, 141.4, 137.6, 137.6, 130.0, 129.9, 128.3, 128.2, 127.9, 115.2, 115.0, 114.2.



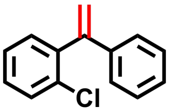
1-Chloro-4-(1-phenylvinyl)benzene (3c).[21] Yield: 46%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 7.32 (m, 9H), 5.57 (d, *J* = 1.4 Hz, 1H), 5.55 (d, *J* = 1.1 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 149.1, 141.1, 140.1, 133.7, 129.7, 128.5, 128.4, 128.3, 128.0, 114.8.



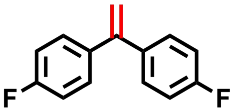
1-Bromo-4-(1-phenylvinyl)benzene (3d).[9] Yield: 68%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.51 (m, 2H), 7.43 - 7.37 (m, 5H), 7.30– 7.27 (m, 2H), 5.55 (d, *J* = 1.1 Hz, 1H), 5.53 (d, *J* = 1.1 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 149.1, 141.0, 140.5, 131.4, 130.0, 128.4, 128.3, 128.0, 121.9, 114.8.



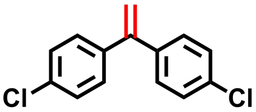
1-Chloro-3-(1-phenylvinyl)benzene (3e).[21] Yield: 56%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.28 (m, 9H), 5.58 (d, *J* = 1.1 Hz, 1H), 5.55 (d, *J* = 1.1 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 149.0, 143.5, 140.9, 134.3, 129.5, 128.4, 128.3, 128.1, 127.9, 126.6, 115.3.



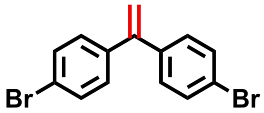
1-Chloro-2-(1-phenylvinyl)benzene (3f).[22] Yield: 26%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.49 (m, 1H), 7.47 – 7.34 (m, 8H), 5.94 (d, *J* = 1.1 Hz, 1H), 5.40 (d, *J* = 1.1 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 147.6, 140.8, 139.9, 133.4, 131.7, 129.8, 129.0, 128.4, 127.9, 126.8, 126.5, 116.3.



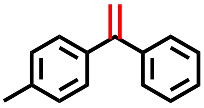
4,4'-(Ethene-1,1-diyl)bis(fluorobenzene) (3g).[16] Yield: 68%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.33 (m, 4H), 7.11 – 7.05 (m, 4H), 5.46 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 163.9, 161.4, 148.1, 137.5, 137.4, 129.9, 129.8, 115.3, 115.1, 114.1.



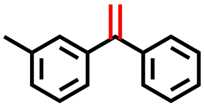
4,4'-(Ethene-1,1-diyl)bis(chlorobenzene) (3h).[16] Yield: 36%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.31 (m, 4H), 7.30 – 7.24 (m, 4H), 5.49 (s, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 148.0, 139.5, 133.9, 129.5, 128.5, 115.1.



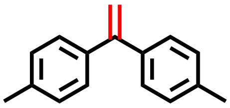
4,4'-(Ethene-1,1-diyl)bis(bromobenzene) (3i).[23] Yield: 52%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 – 7.47 (m, 4H), 7.25 – 7.19 (m, 4H), 5.49 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.0, 139.9, 131.5, 129.8, 122.1, 115.2.



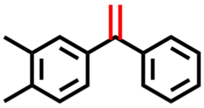
1-Methyl-4-(1-phenylvinyl)benzene (3j).[9] Yield: 47%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 - 7.37 (m,5H), 7.35 – 7.33 (m, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 5.53 (d, 1.1Hz, 1H), 5.51 (d, 1.1Hz, 1H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.1, 141.9, 138.8, 137.6, 129.0, 128.4, 128.3, 128.3, 127.8, 113.8, 21.3.



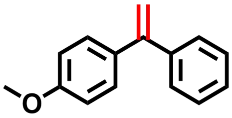
1-Methyl-3-(1-phenylvinyl)benzene (3k).[24] Yield: 27%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.50 - 7.43 (m, 5H), 7.36 – 7.25 (m, 4H), 5.59 (t, *J* = 2.3 Hz, 2H), 2.48 (d, *J* = 2.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.2, 141.7, 141.5, 137.8, 129.0, 128.5, 128.3, 128.2, 128.1, 127.7, 125.5, 114.2, 21.5.



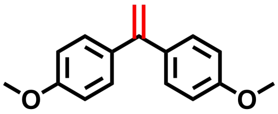
4,4'-(Ethene-1,1-diyl)bis(methylbenzene) (3l).[21] Yield: 58%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.28 (m, 4H), 7.25 - 7.18 (m, 4H), 5.43 (s, 2H), 2.42 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.8, 138.9, 137.5, 128.9, 128.2, 113.0, 21.2.



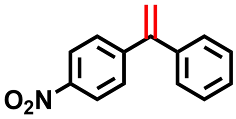
1,2-Dimethyl-4-(1-phenylvinyl)benzene (3m).[25] Yield: 60%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.43 (m, 5H), 7.28 (t, *J* = 1.9 Hz, 1H), 7.23 (d, *J* = 1.9 Hz, 2H), 5.58 - 5.54 (m, 2H), 2.46 - 2.39 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.2, 141.9, 139.3, 136.4, 136.3, 129.6, 128.4, 128.2, 127.7, 125.9, 113.7, 19.9, 19.6.



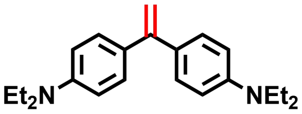
1-Methoxy-4-(1-phenylvinyl)benzene (3n).[20] Yield: 40%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.33 (m, 7H), 6.94 – 6.92 (m, 2H), 5.47 (d, *J* = 1.4 Hz, 1H), 5.43 (d, *J* = 1.4 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.4, 149.6, 141.9, 134.0, 129.5, 128.4, 128.2, 127.7, 113.6, 113.0, 55.3.



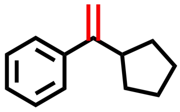
4,4'-(Ethene-1,1-diyl)bis(methoxybenzene) (3o).[21] Yield: 20%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 – 7.30 (m, 4H), 6.96 – 6.89 (m, 4H), 5.34 (d, *J* = 0.9 Hz, 2H), 3.86 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 159.3, 149.0, 134.3, 129.5, 113.5, 111.7, 55.3.



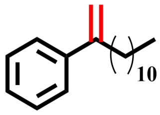
1-Nitro-4-(1-phenylvinyl)benzene (3p).[26] Yield: 15%. ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 8.24 – 8.20 (m, 2H), 7.54 – 7.51 (m, 2H), 7.41 – 7.38 (m, 3H), 7.33 – 7.31 (m, 2H), 5.64 (d, *J* = 15.9 Hz, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 148.4, 148.1, 147.3, 140.2, 129.0, 128.6, 128.4, 128.2, 123.6, 117.3.



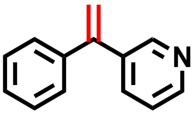
4,4'-(Ethene-1,1-diyl)bis(*N*,*N*-diethylaniline) (3q). Yield: 34%. ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.30 – 7.27 (m, 4H), 6.67 (d, *J* = 8.3 Hz, 4H), 5.19 (s, 2H), 3.40 (q, *J* = 7.1 Hz, 8H), 1.21 (t, *J* = 7.0 Hz, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 149.6, 147.3, 129.5, 129.1, 111.1, 108.1, 44.4, 12.7.



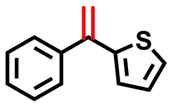
(1-Cyclopentylvinyl)benzene (3s).[27] Yield: 39%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.41 (m, 2H), 7.39 – 7.35 (m, 2H), 7.32 – 7.28 (m, 1H), 5.22 (d, *J* = 1.2 Hz, 1H), 5.13 (t, *J* = 1.5 Hz, 1H), 3.01 (m, 1H), 1.96 - 1.92 (m, 2H), 1.79 – 1.66 (m, 4H), 1.52 - 1.47 (m, 2H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 153.0, 143.2, 128.1, 127.0, 126.6, 110.1, 44.6, 32.2, 24.9.



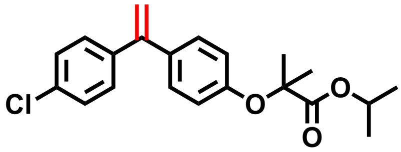
Tridec-1-en-2-ylbenzene (3t).[28] Yield: 59%. ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.50 – 7.48 (m, 2H), 7.40 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.0 Hz, 1H), 5.34 (d, *J* = 1.7 Hz, 1H), 5.13 (d, *J* = 1.8 Hz, 1H), 2.58 (t, *J* = 7.6 Hz, 2H), 1.53 (d, *J* = 6.6 Hz, 2H), 1.43 - 1.34 (m, 16H), 0.97 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 148.9, 141.6, 128.3, 127.3, 126.2, 112.0, 35.5, 32.1, 29.8, 29.8, 29.8, 29.6, 29.5, 28.4, 22.8, 14.2.



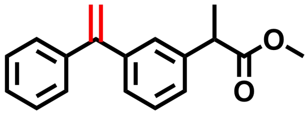
1-(1-Phenylvinyl)pyridine (3w).[22] Yield: 24%. ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 8.66 (t, *J* = 2.4 Hz, 1H), 8.58 (t, *J* = 4.8, 1.7 Hz, 1H), 7.65 - 7.62 (m, 1H), 7.40 – 7.30 (m, 5H), 7.29 - 7.26 (m, 1H), 5.59 (d, *J* = 0.9 Hz, 1H), 5.52 (d, *J* = 1.0 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 149.2, 148.9, 146.9, 140.4, 137.1, 135.6, 128.5, 128.2, 128.0, 123.1, 115.8.



2-(1-Phenylvinyl)thiophene (3x).[20] Yield: 35%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.48 (m, 2H), 7.42 – 7.38 (m, 3H), 7.28 – 7.27 (m, 1H), 7.03 - 7.01 (m, 1H), 6.96 - 6.95 (m, 1H), 5.63 (d, J = 0.9 Hz, 1H), 5.29 (d, J = 0.9 Hz, 1H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 144.8, 143.4, 141.1, 128.4, 128.2, 128.1, 127.3, 126.5, 125.1, 113.7.

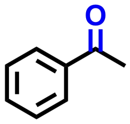


Isopropyl 2-(4-(1-(4-chlorophenyl)vinyl)phenoxy)-2-methylpropanoate (3y).[22] Yield: 70%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.25 (m, 4H), 7.23 – 7.20 (m, 2H), 6.85 – 6.82 (m, 2H), 5.41 (t, J = 1.5 Hz, 1H), 5.34 (d, J = 1.3 Hz, 1H), 5.15 - 5.09 (m, 1H), 1.65 (s, 6H), 1.25 (d, J = 6.4 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 173.6, 155.5, 148.4, 140.2, 134.5, 133.5, 129.6, 128.9, 128.3, 118.4, 113.6, 79.1, 69.0, 25.4, 21.6.

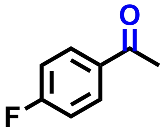


Methyl 2-(3-(1-phenylvinyl)phenyl)propanoate (3z).[29] Total yield: 28%. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.45 – 7.31 (m, 9H), 5.56 (s, 2H), 3.81 (q, J = 7.2 Hz, 1H), 3.73 (s, 3H), 1.59 (d, J = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 174.9, 149.9, 141.8, 141.4, 140.5, 128.5, 128.3, 128.2, 127.8, 127.5, 127.2, 126.8, 114.5, 52.0, 45.4, 18.7.

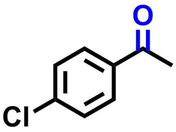
7) Characterization of products.



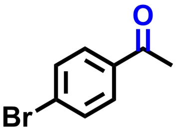
Acetophenone (2a). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.00 – 7.97 (m, 2H), 7.61 – 7.56 (m, 1H), 7.50 – 7.46 (m, 2H), 2.63 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 198.2, 137.1, 133.1, 128.6, 128.3, 26.6.



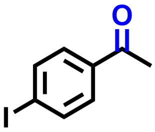
1-(4-Fluorophenyl)ethan-1-one (2b). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 – 7.99 (m, 2H), 7.17 – 7.13 (m, 2H), 2.61 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 196.5, 165.8 (d, J = 128.27 Hz) 133.6 (d, J = 1.52 Hz), 131.0 (d, J = 5.05 Hz), 115.7 (d, J = 11.11 Hz), 26.5.



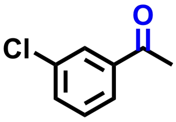
1-(4-Chlorophenyl)ethan-1-one (2c). ^{1}H NMR (400 MHz, Chloroform-d) δ 7.95 – 7.89 (m, 2H), 7.49 – 7.43 (m, 2H), 2.62 (d, J = 1.0 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 196.8, 139.6, 135.4, 129.7, 128.9, 26.6.



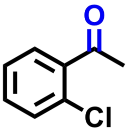
1-(4-Bromophenyl)ethan-1-one (2d). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.84 - 7.82 (m, 2H), 7.62 - 7.59 (m, 2H), 2.59 (t, *J* = 1.1 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 197.0, 135.8, 131.9, 129.8, 128.3, 26.5.



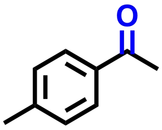
1-(4-Iodophenyl)ethan-1-one (2e). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.87– 7.83 (m, 2H), 7.70 – 7.66 (m, 2H), 2.59 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 197.3, 137.9, 136.4, 129.7, 101.1, 26.5.



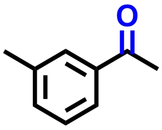
1-(3-Chlorophenyl)ethan-1-one (2f). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.91-7.88 (m, 1H), 7.82 - 7.78 (m, 1H), 7.53 - 7.48 (m, 1H), 7.41 - 7.35 (m, 1H), 2.57 (q, *J* = 2.0 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 196.7, 138.6, 134.9, 133.0, 129.9, 128.3, 126.4, 26.6.



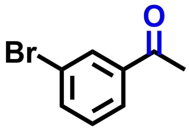
1-(2-Chlorophenyl)ethan-1-one (2g). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.56 - 7.53 (m, 1H), 7.43 - 7.33 (m, 2H), 7.32 - 7.29 (m, 1H), 2.63 (t, *J* = 1.1 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 200.4, 139.1, 132.0, 131.3, 130.6, 129.4, 126.9, 30.7.



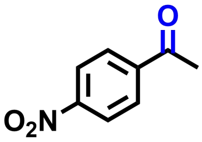
1-(*p*-Tolyl)ethan-1-one (2h). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.82 - 7.78 (m, 2H), 7.21 - 7.16 (m, 2H), 2.50 (t, *J* = 1.1 Hz, 3H), 2.34 (t, *J* = 1.1 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 197.6, 143.8, 134.7, 129.2, 128.4, 26.4, 21.5.



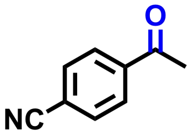
1-(*m*-Tolyl)ethan-1-one (2i). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 – 7.72 (m, 2H), 7.36 – 7.30 (m, 2H), 2.60 - 2.56 (m, 3H), 2.39 – 2.35 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.3, 138.3, 137.1, 133.8, 128.8, 128.4, 125.6, 26.6, 21.3.



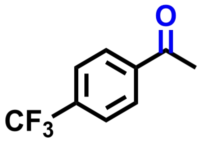
1-(3-Bromophenyl)ethan-1-one (2j). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 – 7.90 (m, 1H), 7.75 – 7.70 (m, 1H), 7.55 – 7.50 (m, 1H), 7.23 – 7.17 (m, 1H), 2.48 – 2.44 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 138.6, 135.8, 131.1, 130.2, 126.8, 122.8, 26.5.



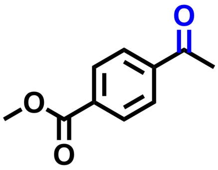
1-(4-Nitrophenyl)ethan-1-one (2k). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 – 8.31 (m, 2H), 8.15 – 8.11 (m, 2H), 2.70 (t, *J* = 1.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 150.4, 141.4, 129.3, 123.9, 27.0.



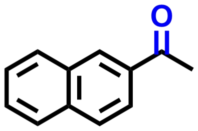
4-Acetylbenzonitrile (2l). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06– 8.03 (m, 2H), 7.82 – 7.79 (m, 2H), 2.65 (t, *J* = 1.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.6, 139.9, 132.5, 128.7, 117.9, 116.4, 26.8.



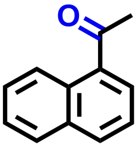
1-**(4-(Trifluoromethyl)phenyl)ethan-1-one (2m).** ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 – 8.06 (m, 2H), 7.76 – 7.73 (m, 2H), 2.66 (t, *J* = 0.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.0, 139.7, 134.4 (d, *J* = 16.16 Hz), 128.6, 125.7 (d, *J* = 2.02 Hz), 124.6 (d, *J* = 35.35 Hz), 26.8.



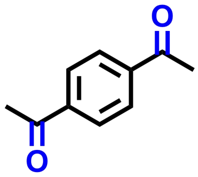
Methyl 4-acetylbenzoate (2n). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 – 8.12 (m, 2H), 8.03 – 8.00 (m, 2H), 3.96 (s, 3H), 2.65 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 197.5, 166.2, 140.2, 133.9, 129.8, 128.2, 52.5, 26.9.



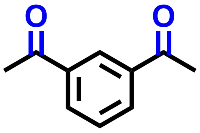
1-(Naphthalen-2-yl)ethan-1-one (2o). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.49 – 8.48 (m, 1H), 8.07 - 8.05 (m, 1H), 8.00 - 7.97 (m, 1H), 7.92 – 7.89 (m, 2H), 7.65 - 7.56 (m, 2H), 2.75 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 198.1, 135.6, 134.5, 132.5, 130.2, 129.6, 128.5, 128.4, 127.8, 126.8, 123.9, 26.7.



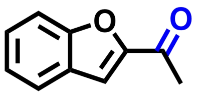
1-(Naphthalen-1-yl)ethan-1-one (2p). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.84 - 8.81 (m, 1H), 8.00 - 7.97 (m, 1H), 7.93 - 7.91 (m, 1H), 7.89 – 7.87 (m, 1H), 7.65 - 7.61 (m, 1H), 7.57 - 7.53 (m, 1H), 7.50 - 7.46 (m, 1H), 2.74 (s, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 201.8, 135.4, 134.0, 133.1, 130.2, 128.8, 128.5, 128.1, 126.5, 126.1, 124.4, 30.0.



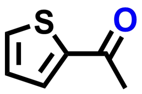
1,1'-(1,4-Phenylene)bis(ethan-1-one) (2q). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.05 (s, 4H), 2.67 (t, J = 1.1 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 197.5, 140.2, 128.5, 26.9.



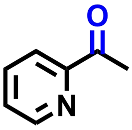
1,1'-(1,3-Phenylene)bis(ethan-1-one) (2r). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.54 - 8.53 (m, 1H), 8.18 - 8.16(m, 2H), 7.62 - 7.58 (m, 1H), 2.68 (d, J = 1.1 Hz, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 197.4, 137.4, 132.5, 129.1, 128.1, 26.7.



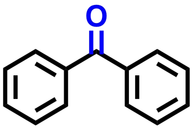
1-(Benzofuran-2-yl)ethan-1-one (2s). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.71 (m, 1H), 7.62 – 7.58 (m, 1H), 7.53 – 7.47 (m, 2H), 7.35 - 7.31 (m, 1H), 2.67 – 2.60 (m, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 188.7, 155.7, 152.7, 128.3, 127.1, 123.9, 123.3, 113.1, 112.5, 26.5.



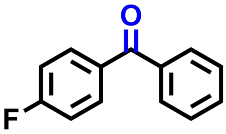
1-(Thiophen-2-yl)ethan-1-one (2t). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 - 7.64 (m, 1H), 7.61 - 7.58 (m, 1H), 7.11 – 7.06 (m, 1H), 2.53 – 2.50 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.7, 144.5, 133.8, 132.6, 128.2, 26.9.



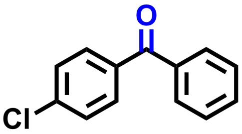
1-(Pyridin-2-yl)ethan-1-one (2u). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.62 – 8.57 (m, 1H), 7.97 – 7.91 (m, 1H), 7.77 - 7.71 (m, 1H), 7.41 – 7.35 (m, 1H), 2.65 – 2.61 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.0, 153.5, 148.9, 136.7, 127.0, 121.5, 25.7.



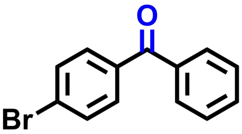
Benzophenone (4a). ^{1}H NMR (400 MHz, Chloroform-d) δ 7.92 – 7.81 (m, 4H), 7.65 – 7.59 (m, 2H), 7.53 - 7.49 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.8, 137.6, 132.4, 130.1, 128.3.



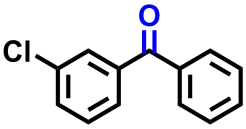
(4-Fluorophenyl)(phenyl)methanone (4b). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.89 – 7.84 (m, 2H), 7.81 – 7.78 (m, 2H), 7.64 – 7.59 (m, 1H), 7.53 – 7.49 (m, 2H), 7.21 – 7.15 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 166.7, 164.1, 137.5, 133.83, 133.80, 132.7, 132.6, 132.5, 129.9, 128.4, 115.6, 115.4.



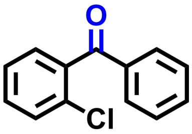
(4-Chlorophenyl)(phenyl)methanone (4c). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.76 (m, 4H), 7.65 – 7.60 (m, 1H), 7.55 – 7.47 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.5, 138.9, 137.3, 135.9, 132.7, 131.5, 129.9, 128.7, 128.4.



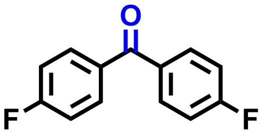
(4-Bromophenyl)(phenyl)methanone (4d). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 – 7.79 (m, 2H), 7.72 – 7.69 (m, 2H), 7.67 – 7.61 (m, 3H), 7.53 – 7.49 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.7, 137.2, 136.3, 132.7, 131.6, 131.6, 130.0, 128.4, 127.5.



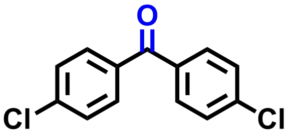
(3-Chlorophenyl)(phenyl)methanone (4e). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.80 (m, 3H), 7.70 - 7.68 (m, 1H), 7.66 – 7.62 (m, 1H), 7.61 - 7.59 (m, 1H), 7.58 – 7.50 (m, 2H), 7.45 (t, J = 7.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 139.3, 137.0, 134.6, 132.9, 132.4, 130.0, 129.9, 129.7, 128.5, 128.1.



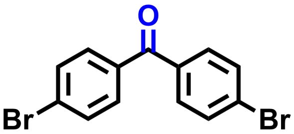
(2-Chlorophenyl)(phenyl)methanone (4f). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.86 – 7.83 (m, 2H), 7.65 – 7.60 (m, 1H), 7.51 – 7.40 (m, 4H), 7.39 – 7.37 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.3, 138.6, 136.5, 133.7, 131.3, 131.2, 130.1, 130.1, 129.1, 128.6, 126.7.



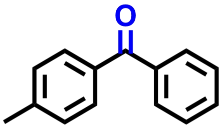
Bis(4-fluorophenyl)methanone (4g). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 – 7.80 (m, 4H), 7.21 – 7.15 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.8, 166.7, 164.1, 133.7, 133.7, 132.5, 132.5, 115.7, 115.5.



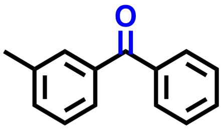
Bis(4-chlorophenyl)methanone (4h). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 – 7.68 (m, 4H), 7.53 – 7.43 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.2, 139.2, 135.5, 131.3, 128.8.



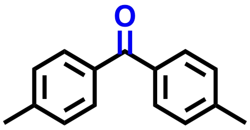
Bis(4-bromophenyl)methanone (4i). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.60 (m, 8H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.5, 135.9, 131.8, 131.4, 127.8.



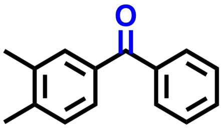
Phenyl(*p*-tolyl)methanone (4j). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.80 (m, 2H), 7.76 – 7.74 (m, 2H), 7.61 – 7.57 (m, 1H), 7.51 – 7.47 (m, 2H), 7.31 – 7.29 (m, 2H), 2.46 (d, J = 1.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.5, 143.3, 138.0, 134.9, 132.2, 130.3, 130.0, 129.0, 128.2, 21.7.



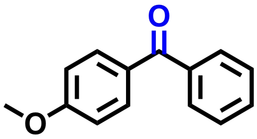
Phenyl(*m*-tolyl)methanone (4k). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 - 7.80 (m, 2H), 7.65 (d, J = 2.1 Hz, 1H), 7.61 - 7.56 (m, 2H), 7.50 - 7.41 (m, 2H), 7.40 - 7.34 (m, 2H), 2.42 (t, J = 1.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.9, 138.2, 137.8, 137.7, 133.2, 132.4, 130.5, 130.1, 128.3, 128.1, 127.4, 21.4.



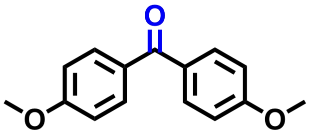
Di-*p*-tolylmethanone (4l). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.72 (m, 4H), 7.30 (d, J = 1.1 Hz, 4H), 2.45 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.3, 142.9, 135.2, 130.2, 128.9, 21.6.



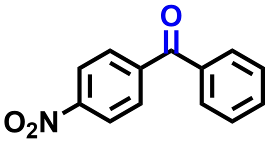
(3,4-Dimethylphenyl)(phenyl)methanone (4m). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.80 (m, 2H), 7.64 (d, J = 1.9 Hz, 1H), 7.62 – 7.52 (m, 2H), 7.50 – 7.46 (m, 2H), 7.25 (d, J = 7.8 Hz, 1H), 2.37 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.7, 142.0, 138.1, 136.8, 135.3, 132.1, 131.2, 130.0, 129.5, 128.2, 128.1, 20.0, 19.8.



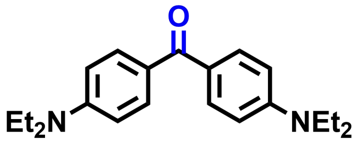
(4-Methoxyphenyl)(phenyl)methanone (4n). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 – 7.83 (m, 2H), 7.80 – 7.76 (m, 2H), 7.60 – 7.56 (m, 1H), 7.52 – 7.47 (m, 2H), 7.01 – 6.97 (m, 2H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.6, 163.3, 138.3, 132.6, 131.9, 130.2, 129.7, 128.2, 113.6, 55.5.



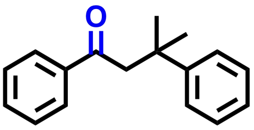
Bis(4-methoxyphenyl)methanone (4o). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.82 – 7.78 (m, 4H), 7.01 – 6.96 (m, 4H), 3.90 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.5, 162.9, 132.2, 130.8, 113.5, 55.5.



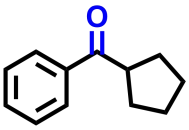
(4-Nitrophenyl)(phenyl)methanone (4p). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 - 8.34 (m, 2H), 8.03 – 7.94 (m, 2H), 7.84 - 7.81 (m, 2H), 7.70 – 7.65 (m, 1H), 7.53 (t, J = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.8, 149.8, 142.9, 136.3, 133.5, 130.7, 130.1, 128.7, 123.6.



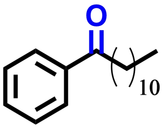
Bis(4-(diethylamino)phenyl)methanone (4q). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.80 – 7.76 (m, 4H), 6.69 – 6.66 (m, 4H), 3.45 (q, *J* = 7.1 Hz, 8H), 1.28 - 1.21 (m, 12H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 193.5, 150.3, 132.5, 125.6, 110.0, 44.5, 12.6.



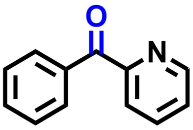
3-Methyl-1,3-diphenylbutan-1-one (4r). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.0 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 1H), 7.41 – 7.37 (m, 4H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.17 (t, *J* = 7.3 Hz, 1H), 3.32 (s, 2H), 1.52 (s, 6H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 199.1, 148.9, 138.2, 132.7, 128.4, 128.2, 128.1, 125.8, 125.5, 50.9, 37.5, 29.1.



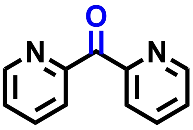
Cyclopentyl(phenyl)methanone (4s). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 – 7.93 (m, 2H), 7.49 (t, *J* = 7.0 Hz, 1H), 7.39 (d, *J* = 7.3 Hz, 2H), 3.72 – 3.62 (m, 1H), 1.91 - 1.85 (m, 4H), 1.74 – 1.57 (m, 4H). ^{13}C NMR (101 MHz, CDCl$_3$) δ 202.59, 136.9, 132.7, 128.5, 128.4, 46.3, 29.9, 26.3.



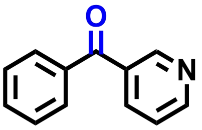
1-Phenyldodecan-1-one (4t). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.99 – 7.95 (m, 2H), 7.57 (t, *J* = 7.3 Hz, 1H), 7.49 - 7.45 (m, 2H), 2.98 (t, *J* = 7.4 Hz, 2H), 1.79 - 1.72 (m, 2H), 1.44 - 1.26 (m, 16H), 0.90 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 200.6, 137.1, 132.8, 128.5, 128.1, 38.6, 31.9, 29.6, 29.6, 29.5, 29.5, 29.4, 29.4, 24.4, 22.7, 14.1.



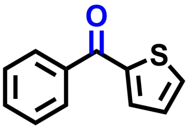
Phenyl(pyridin-2-yl)methanone (4u). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 8.71 – 8.68 (m, 1H), 8.08 – 8.00 (m, 2H), 7.89 - 7.87 (m, 1H), 7.86 - 7.83 (m, 1H), 7.59 - 7.55 (m, 1H), 7.49 – 7.43 (m, 3H). ^{13}C NMR (101 MHz, CDCl$_3$) *δ* 193.8, 155.1, 148.55, 137.07, 136.28, 132.92, 130.99, 128.16, 126.19, 124.60.



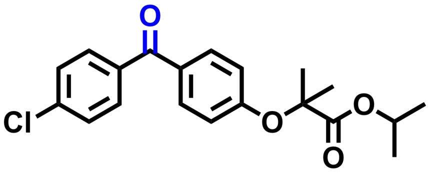
Di(pyridin-2-yl)methanone (4v). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 8.74 - 8.71 (m, 2H), 8.08 - 8.06 (m, 2H), 7.89 - 7.87 (m, 2H), 7.48 - 7.44 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 193.00, 154.31, 149.17, 136.76, 126.41, 125.24.



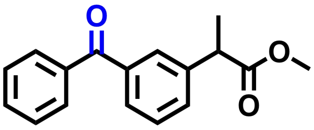
Phenyl(pyridin-3-yl)methanone (4w). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 8.92 - 8.89 (m, 1H), 8.73 – 8.69 (m, 1H), 8.05 - 7.98 (m, 1H), 7.74 – 7.69 (m, 2H), 7.57 - 7.49 (m, 1H), 7.45 – 7.32 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 194.7, 152.7, 150.8, 137.1, 136.6, 133.1, 133.0, 129.9, 128.6, 123.3.



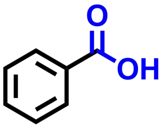
Phenyl(thiophen-2-yl)methanone (4x). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.90 – 7.87 (m, 2H), 7.76 - 7.73 (m, 1H), 7.68 - 7.66 (m, 1H), 7.63 – 7.59 (m, 1H), 7.54 – 7.49 (m, 2H), 7.28 – 7.18 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 188.3, 143.6, 138.2, 134.9, 134.3, 132.3, 129.2, 128.4, 128.0.



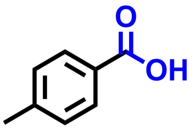
Isopropyl 2-(4-(4-chlorobenzoyl)phenoxy)-2-methylpropanoate (4y, fenofibrate). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.76 – 7.70 (m, 4H), 7.47 – 7.43 (m, 2H), 6.90 – 6.86 (m, 2H), 5.15 - 5.05 (m, 1H), 1.68 (d, *J* = 1.2 Hz, 6H), 1.27 - 1.19 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 194.3, 173.1, 159.8, 138.4, 136.4, 132.0, 131.2, 130.2, 128.5, 117.3, 79.4, 69.4, 25.4, 21.5.



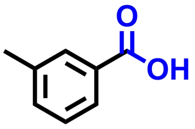
Methyl 2-(3-benzoylphenyl)propanoate (4z, ketoprofen methyl ester). ^{1}H NMR (400 MHz, Chloroform-*d*) *δ* 7.84 – 7.81 (m, 2H), 7.77 (t, *J* = 1.9 Hz, 1H), 7.71 - 7.68 (m, 1H), 7.64 – 7.59 (m, 1H), 7.58 - 7.55 (m, 1H), 7.52 – 7.44 (m, 3H), 3.83 (q, *J* = 7.2 Hz, 1H), 3.70 (s, 3H), 1.56 (d, *J* = 7.2 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 196.2, 174.4, 140.9, 137.9, 137.4, 132.5, 131.5, 130.0, 129.1, 128.9, 128.6, 128.3, 52.0, 45.2, 18.5.



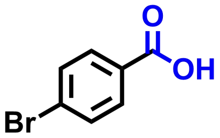
Benzoic acid (6a). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.92 (s, 1H), 7.97 – 7.94 (m, 2H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.7 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.78, 133.33, 131.22, 129.73, 129.03.



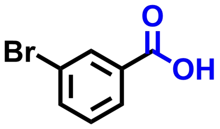
4-Methylbenzoic acid (6b). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.79 (s, 1H), 7.85 – 7.83 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.77, 143.49, 129.80, 129.59, 128.49, 21.59.



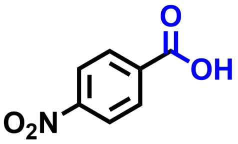
3-Methylbenzoic acid (6c). ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.89 (s, 1H), 7.77 – 7.74 (m, 2H), 7.45 - 7.35 (m, 2H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.89, 138.33, 133.88, 131.19, 130.20, 128.87, 126.92, 21.24.



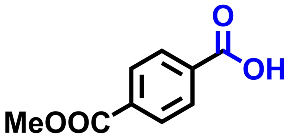
4-Bromobenzoic acid (6d). ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.15 (s, 1H), 7.89 – 7.85 (m, 2H), 7.73 – 7.70 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.08, 132.18, 131.76, 130.46, 127.35.



3-Bromobenzoic acid (6e). ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.35 (s, 1H), 8.04 (t, *J* = 1.8 Hz, 1H), 7.95 - 7.93 (m, 1H), 7.87 - 7.82 (m, 1H), 7.48 (t, *J* = 7.9 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.44, 136.06, 133.56, 132.21, 131.37, 128.74, 122.19.

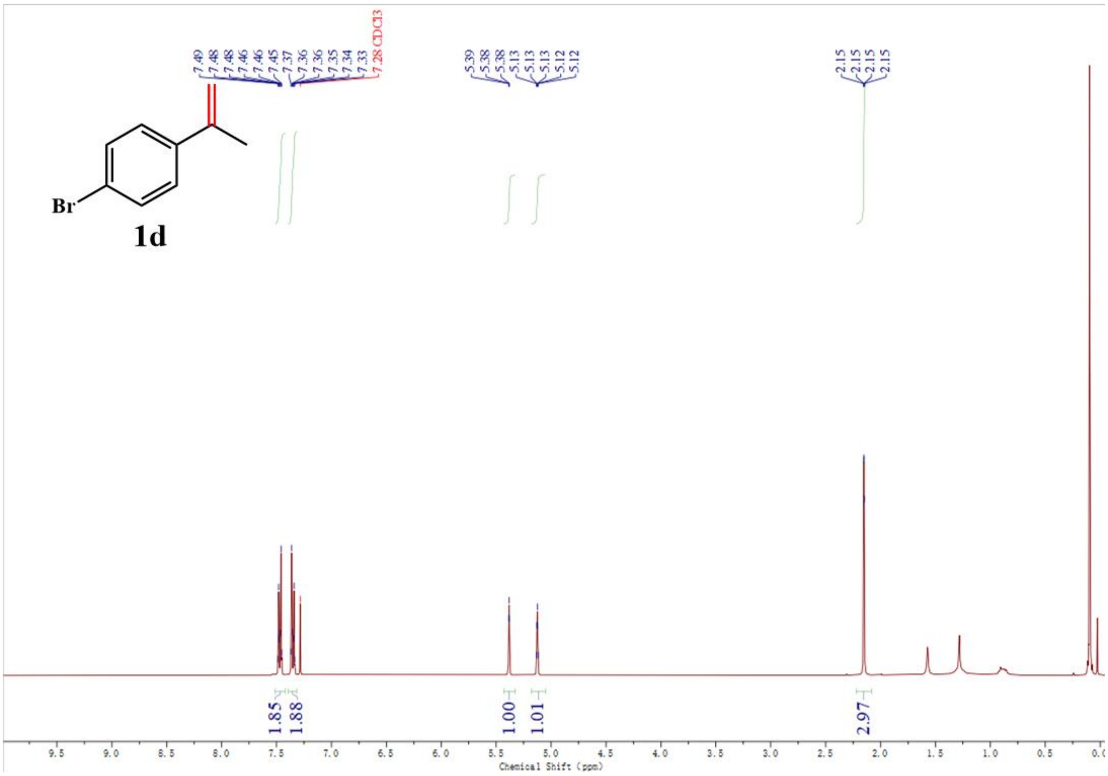


4-Nitrobenzoic acid (6f). ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.56 (s, 1H), 8.34 - 8.31 (m, 2H), 8.19 – 8.16 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.28, 150.53, 136.84, 131.18, 124.22.

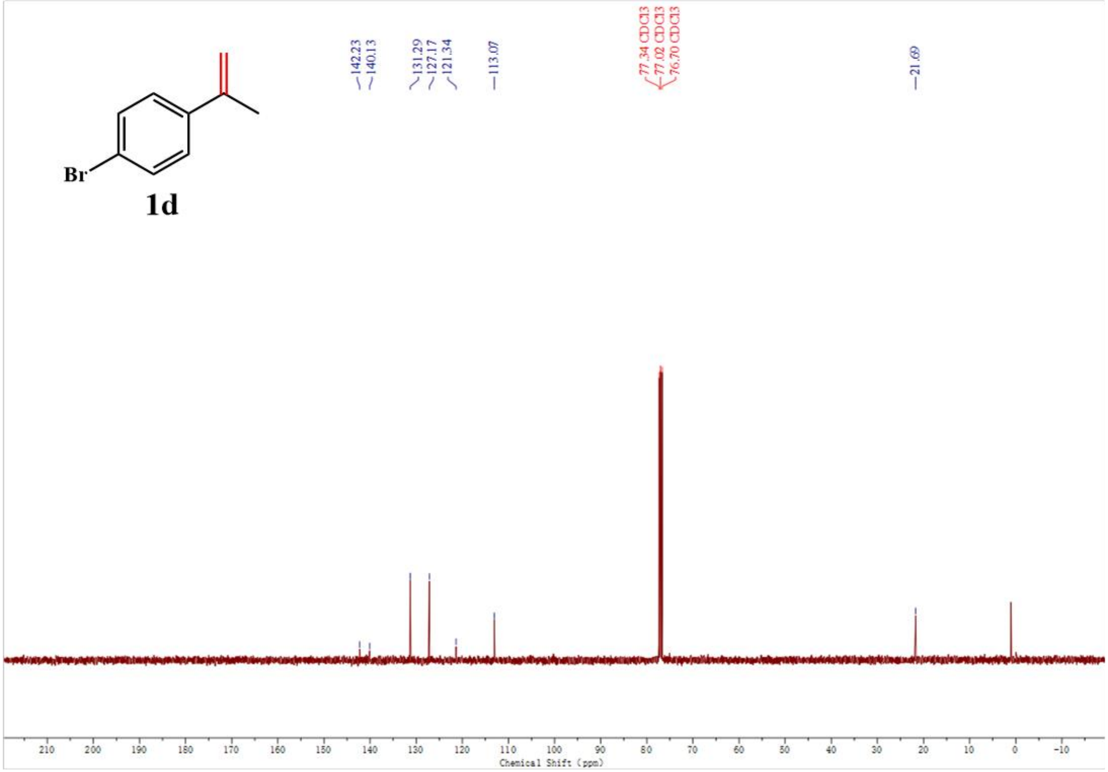


4-(Methoxycarbonyl)benzoic acid (6g). ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.31 (s, 1H), 8.06 (d, J = 9.3 Hz, 4H), 3.89 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 167.02, 166.09, 135.28, 134.91, 133.64, 130.08, 129.93, 129.83, 52.95.

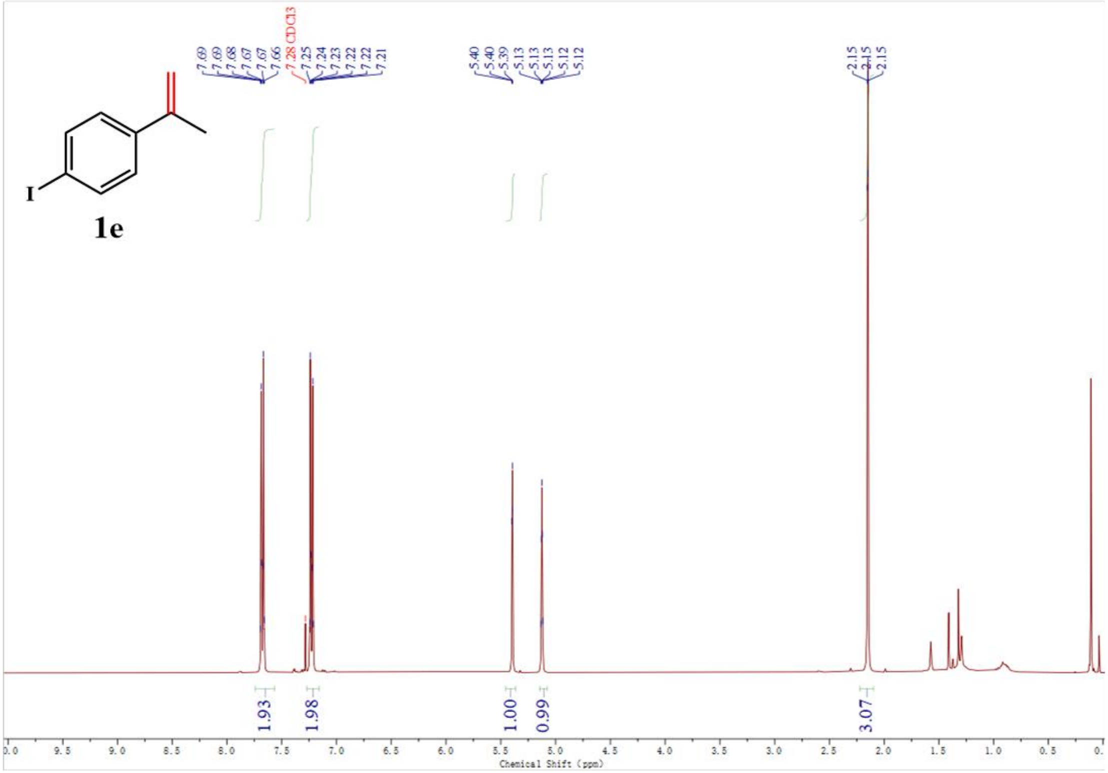
8) NMR spectra



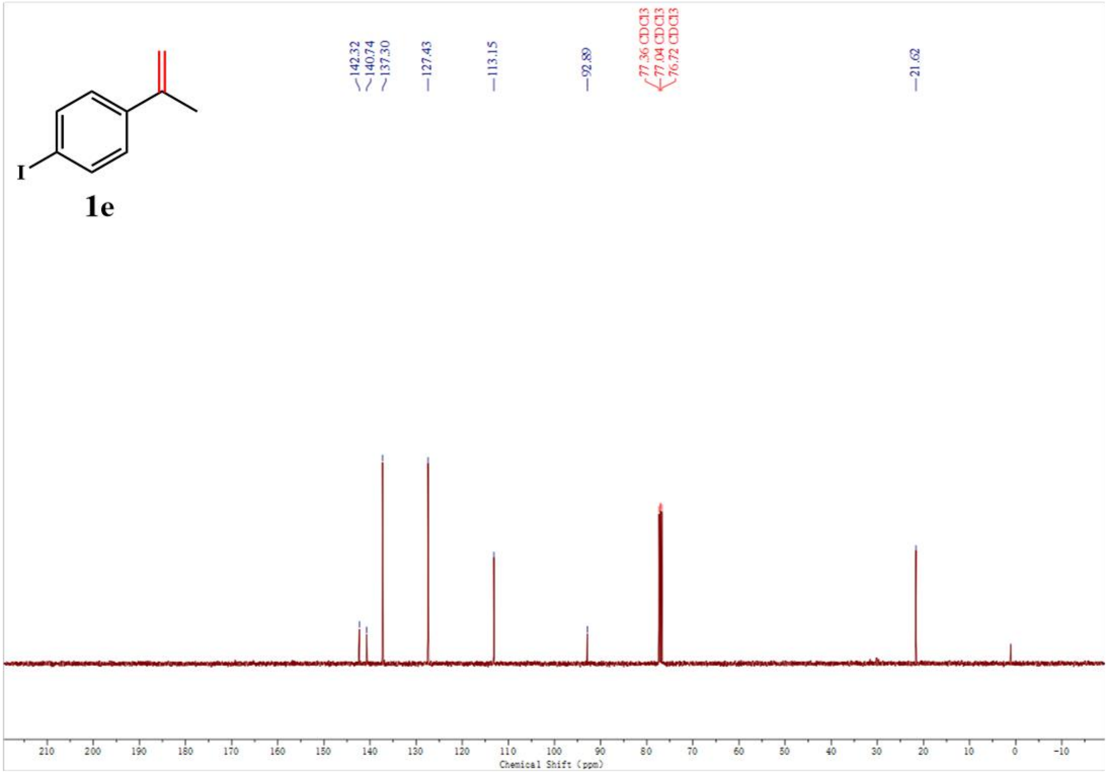
^{1}H NMR of **1d** in CDCl$_3$



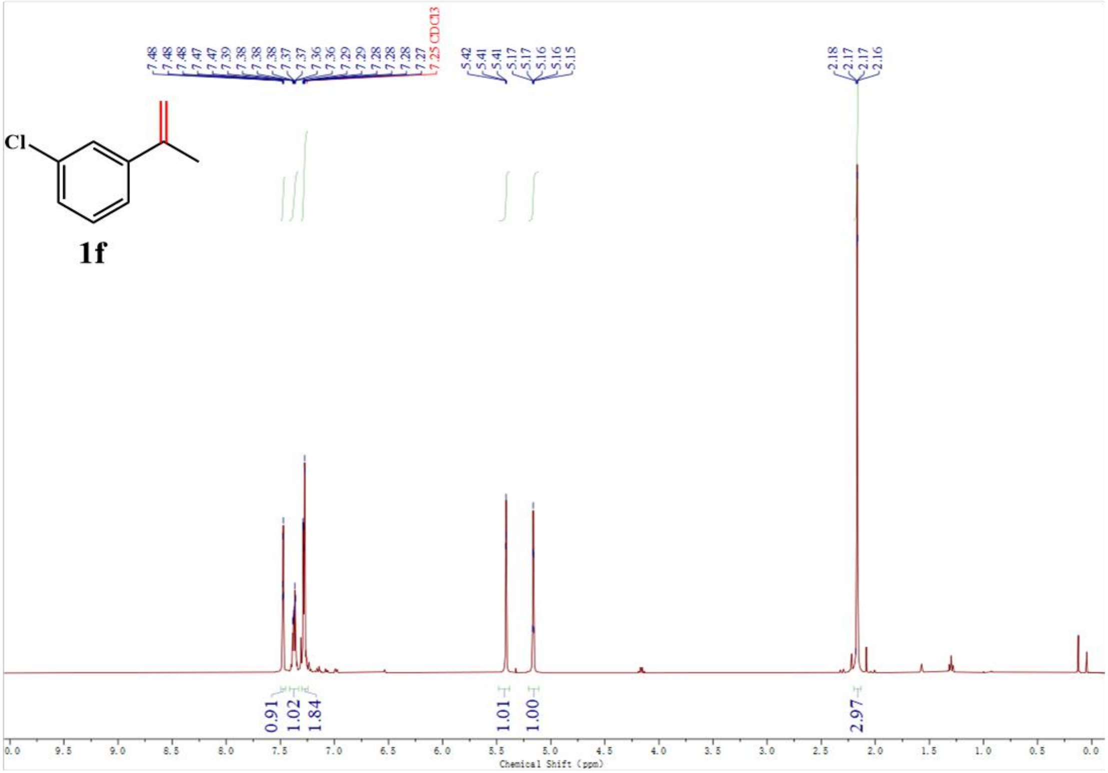
^{13}C NMR of **1d** in CDCl$_3$



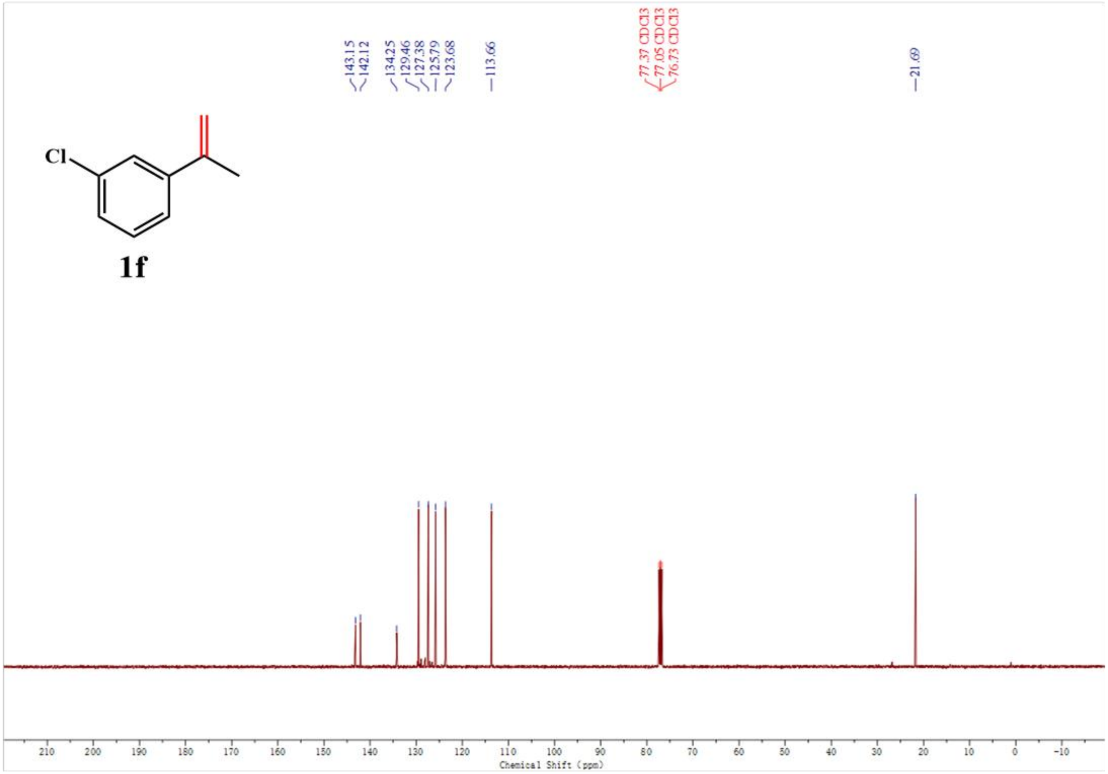
^{1}H NMR of **1e** in $CDCl_3$



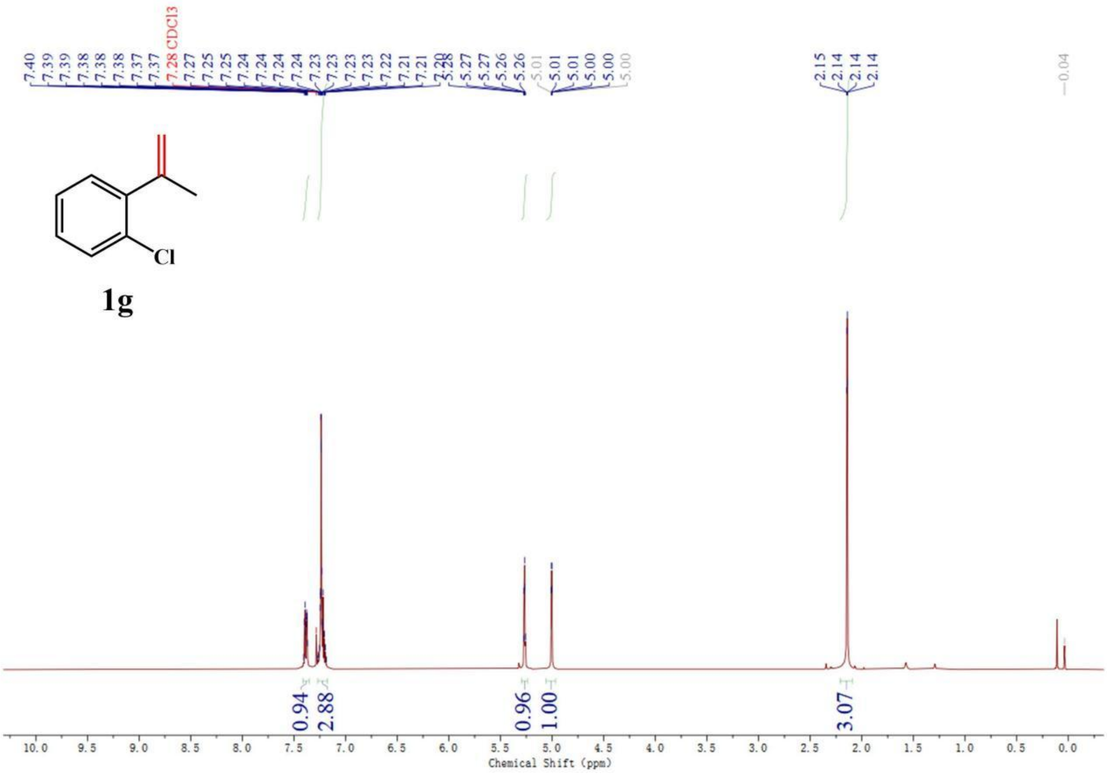
^{13}C NMR of **1e** in $CDCl_3$



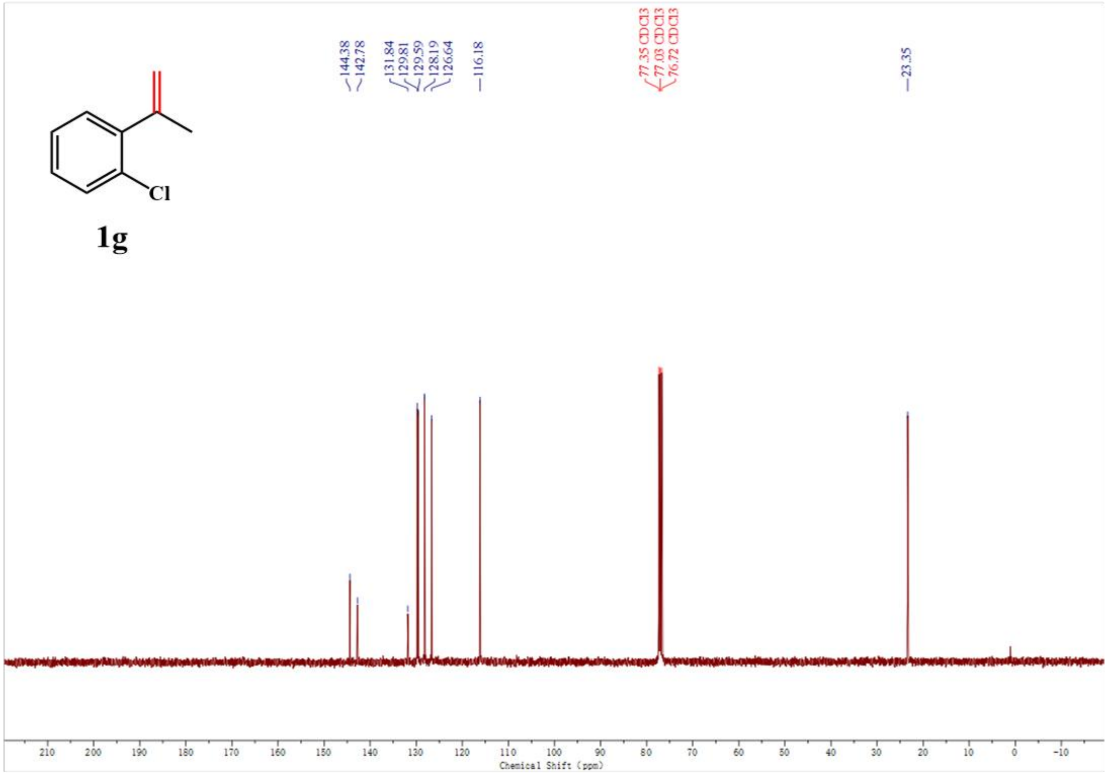
^{1}H NMR of **1f** in CDCl$_3$



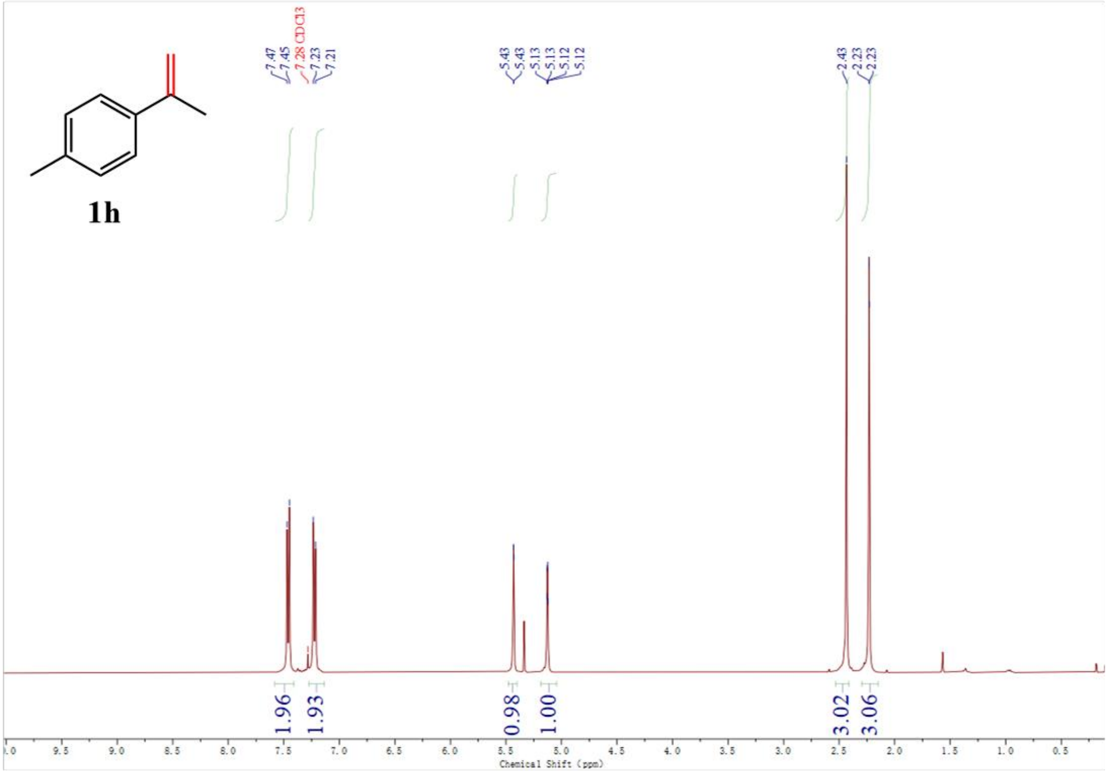
^{13}C NMR of **1f** in CDCl$_3$



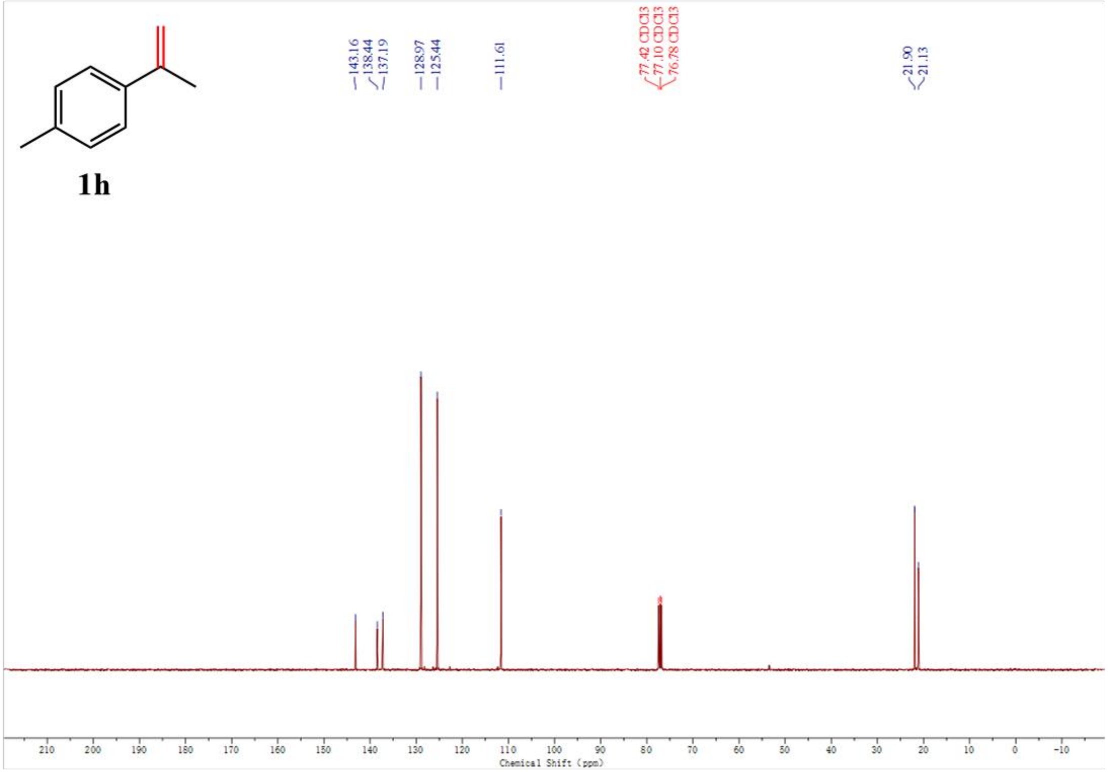
^{1}H NMR of **1g** in $CDCl_3$



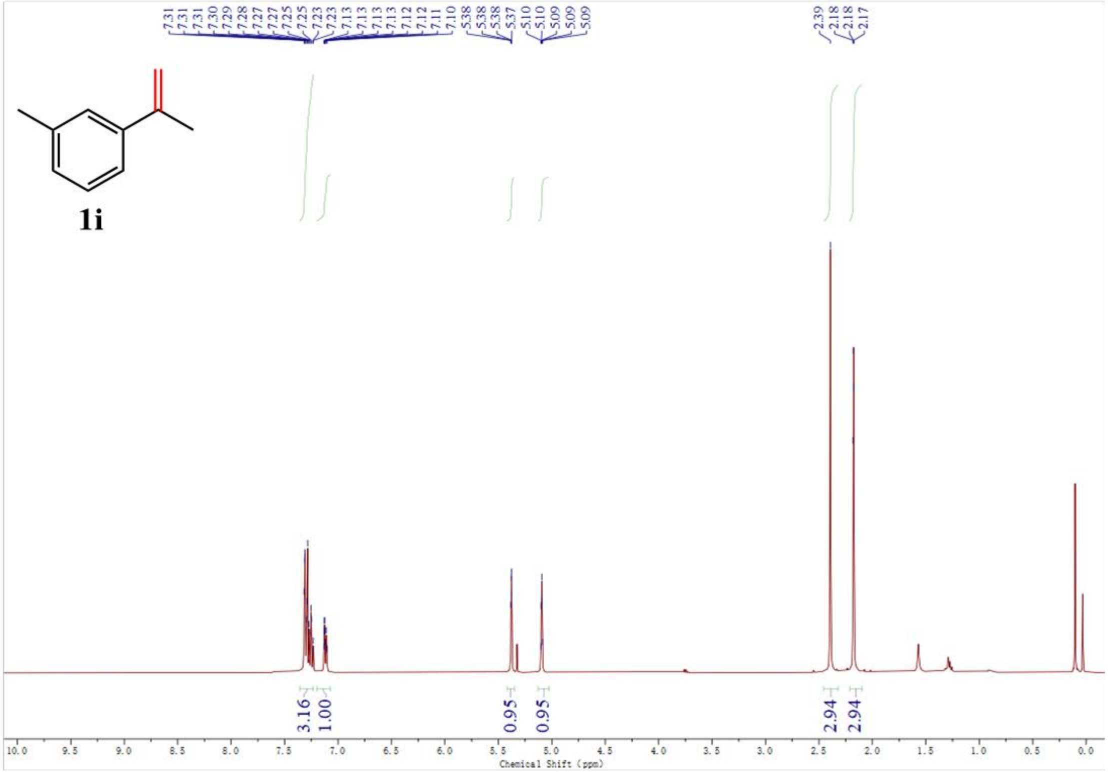
^{13}C NMR of **1g** in $CDCl_3$



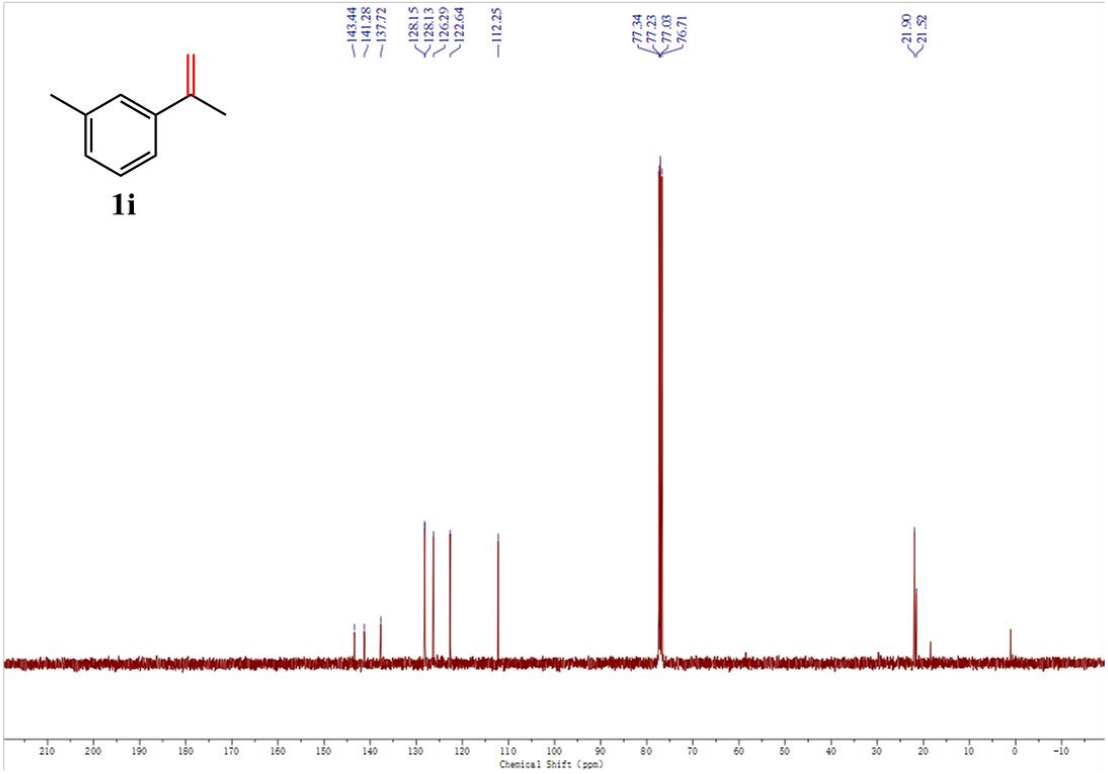
^{1}H NMR of **1h** in CDCl$_3$



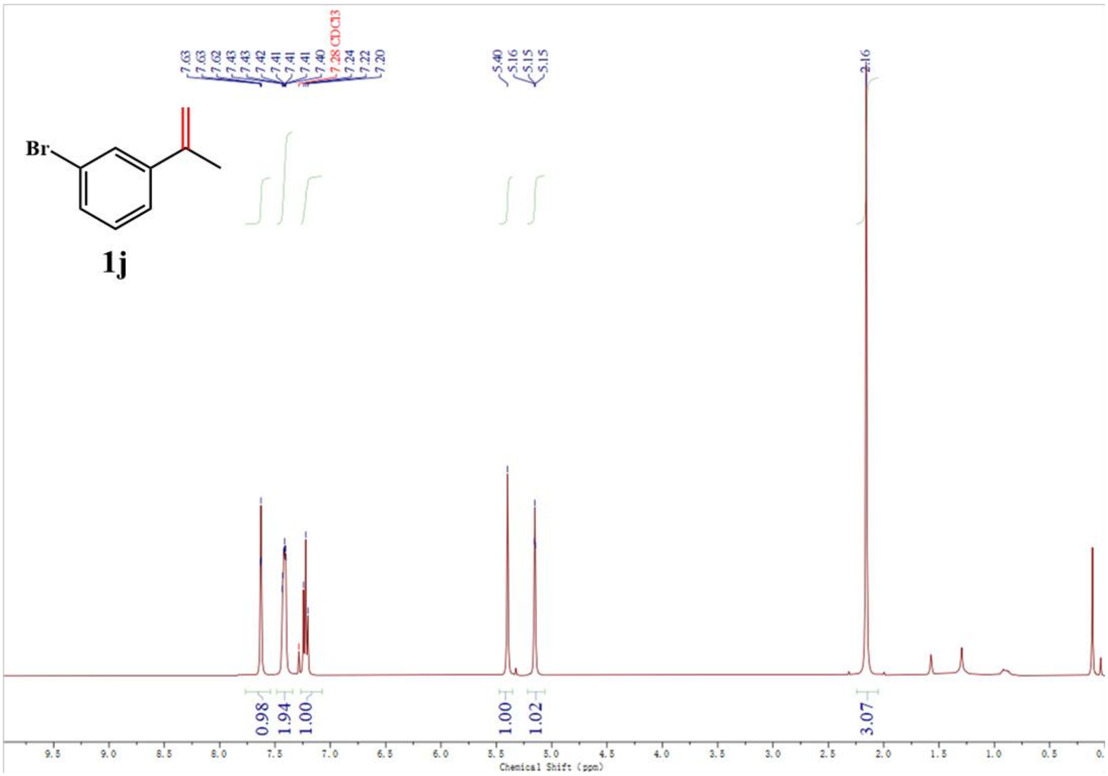
^{13}C NMR of **1h** in CDCl$_3$



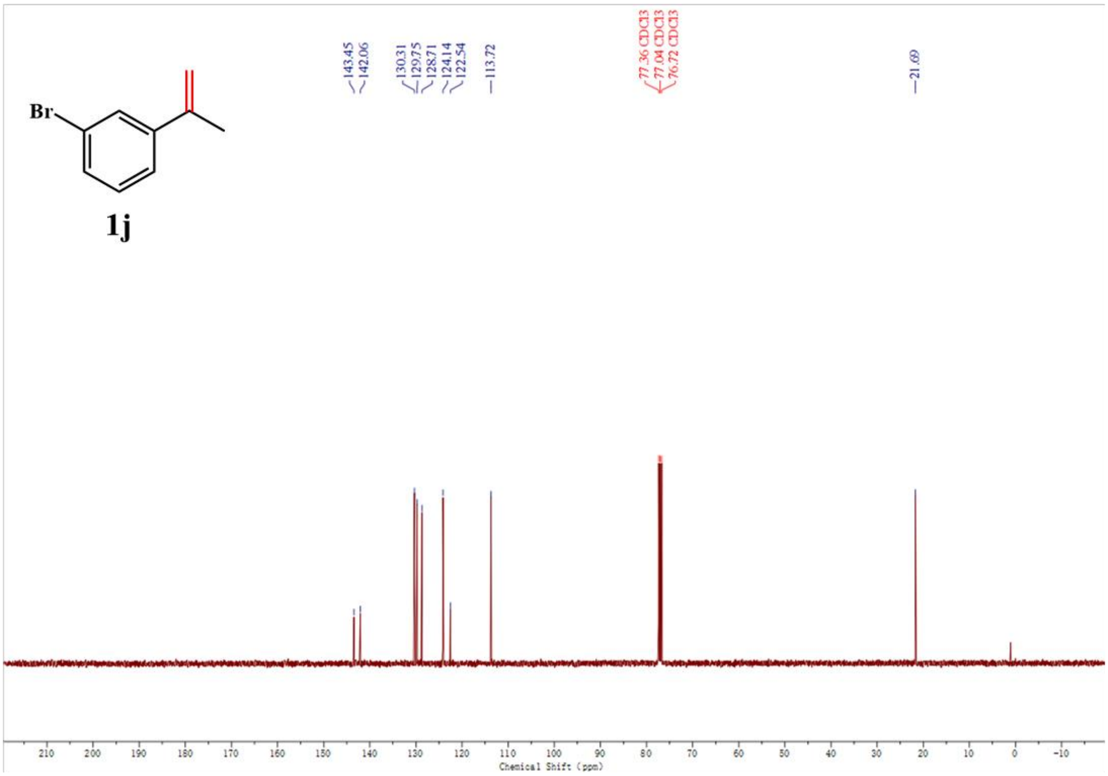
^{1}H NMR of **1i** in CDCl$_3$



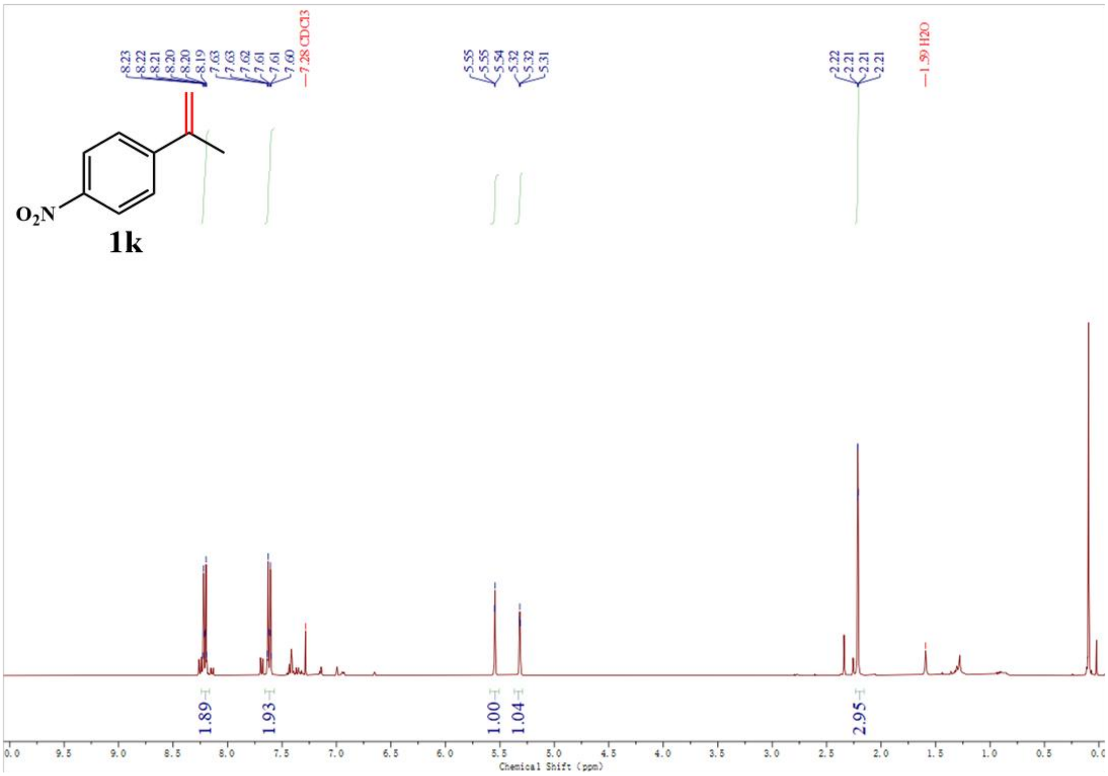
^{13}C NMR of **1i** in CDCl$_3$



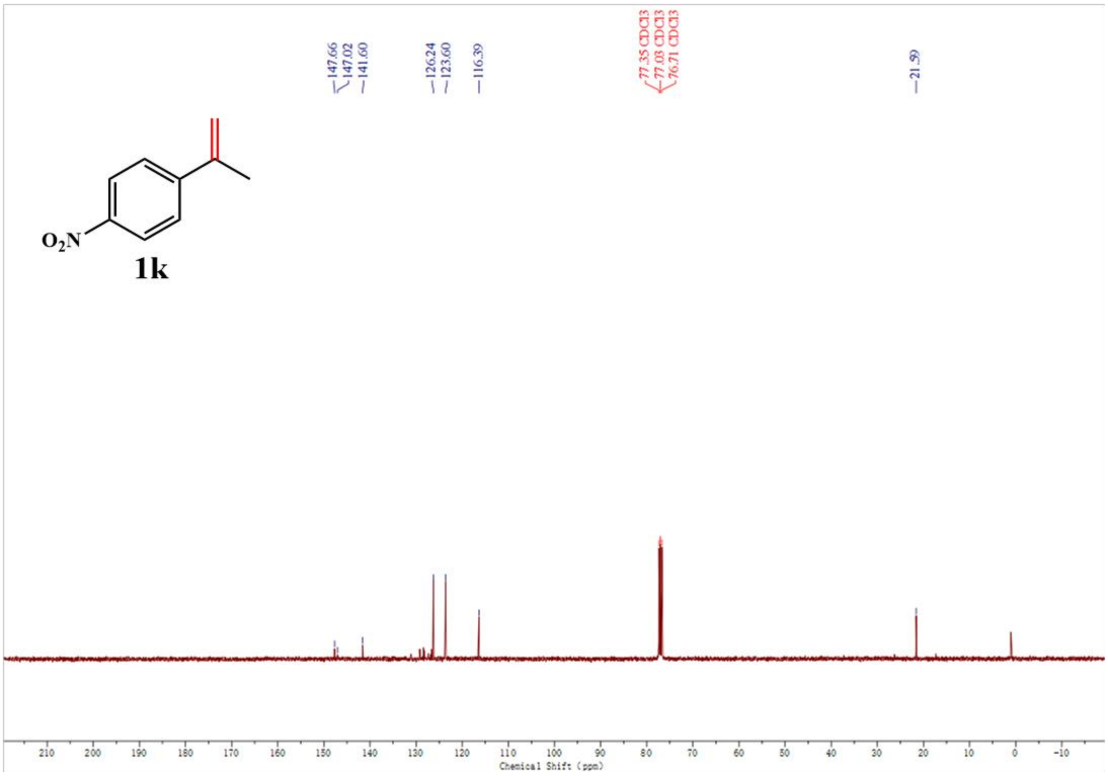
^{1}H NMR of **1j** in CDCl$_3$



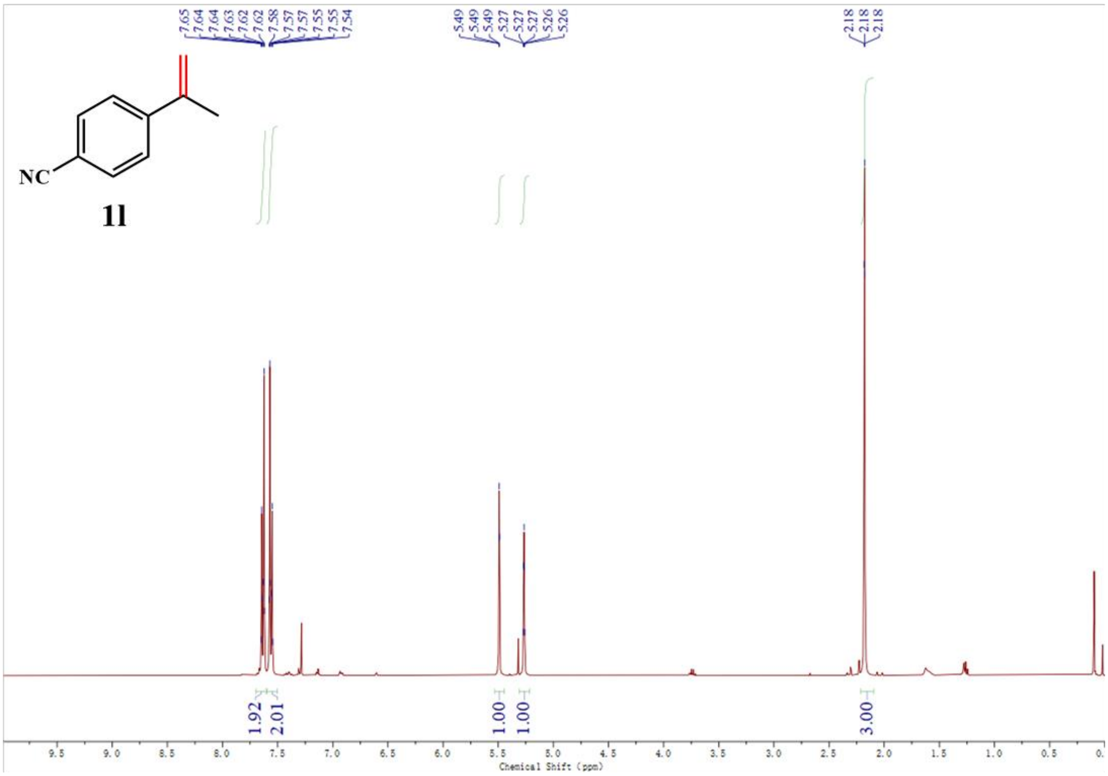
^{13}C NMR of **1j** in CDCl$_3$



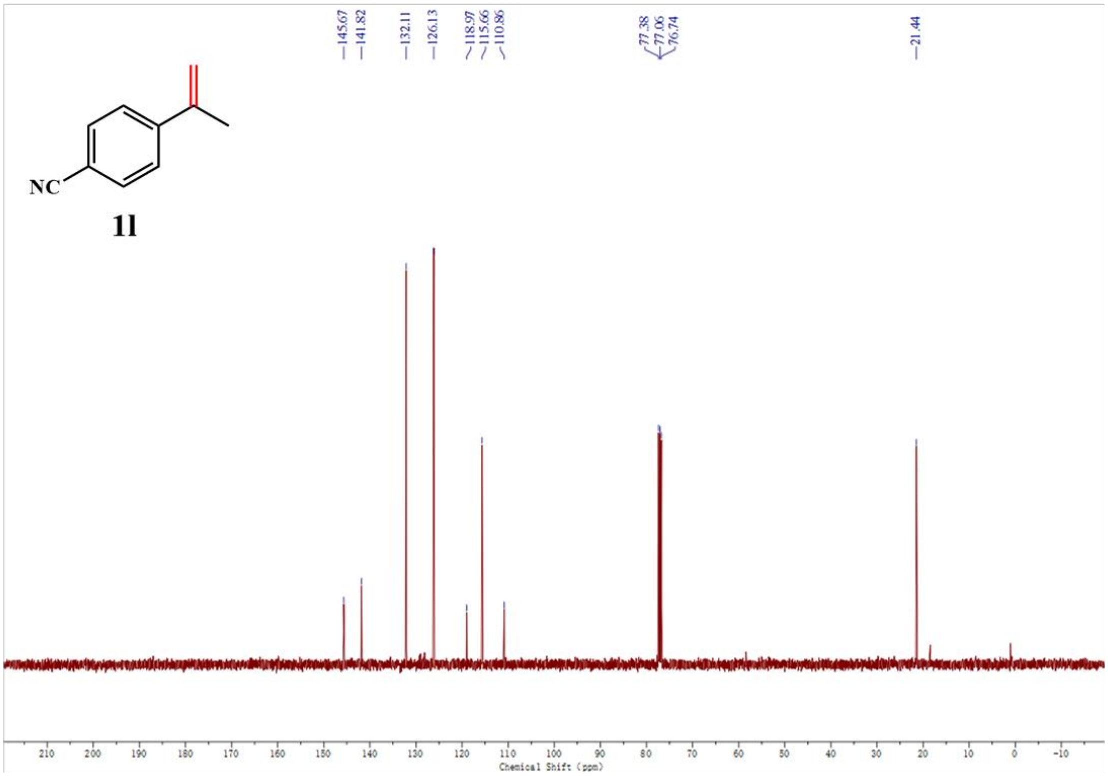
^{1}H NMR of **1k** in $CDCl_3$



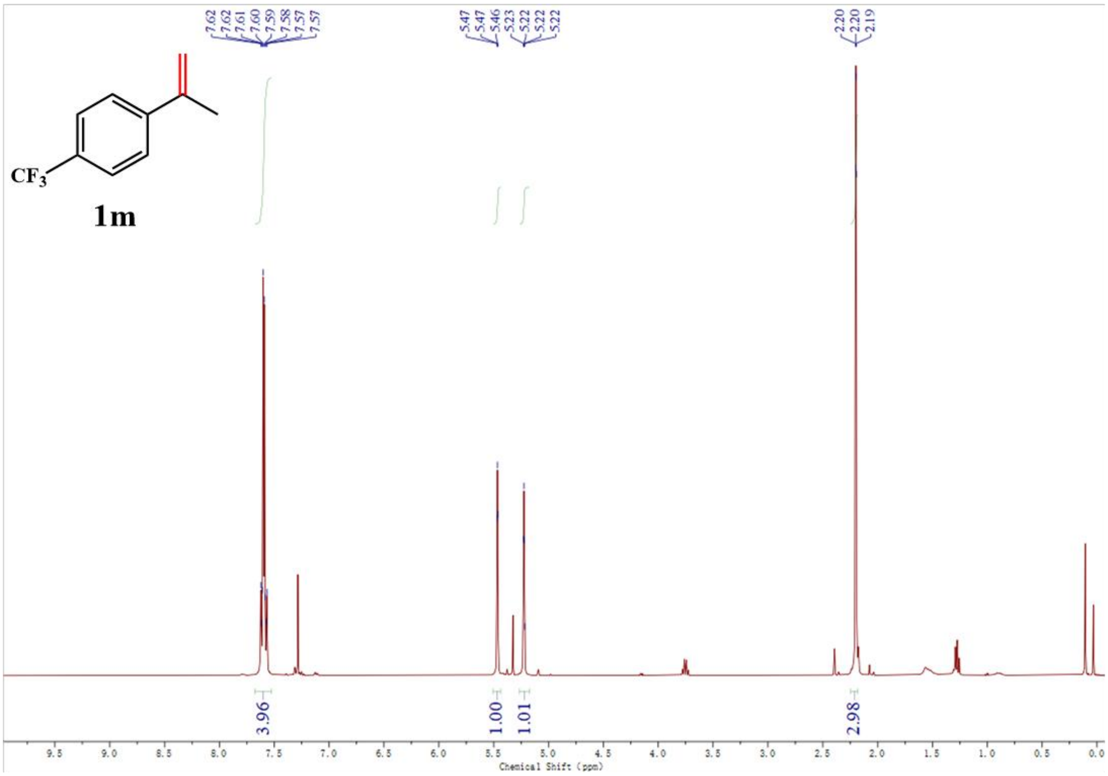
^{13}C NMR of **1k** in $CDCl_3$



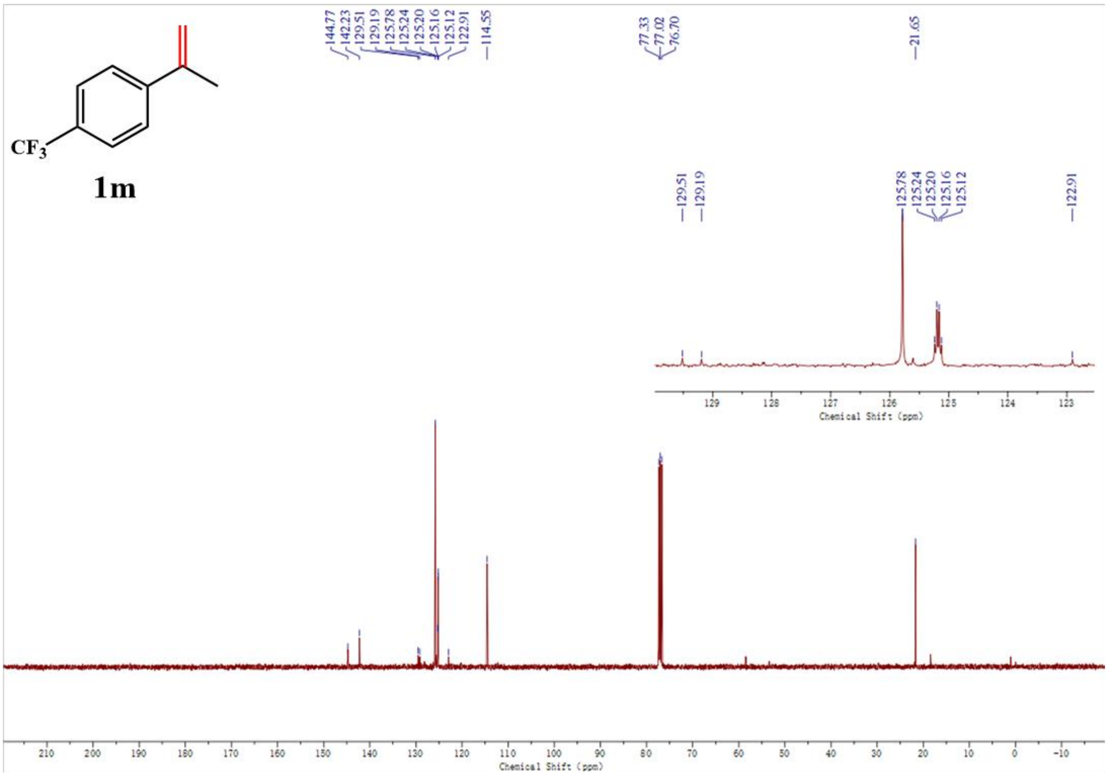
^{1}H NMR of **1l** in CDCl$_3$



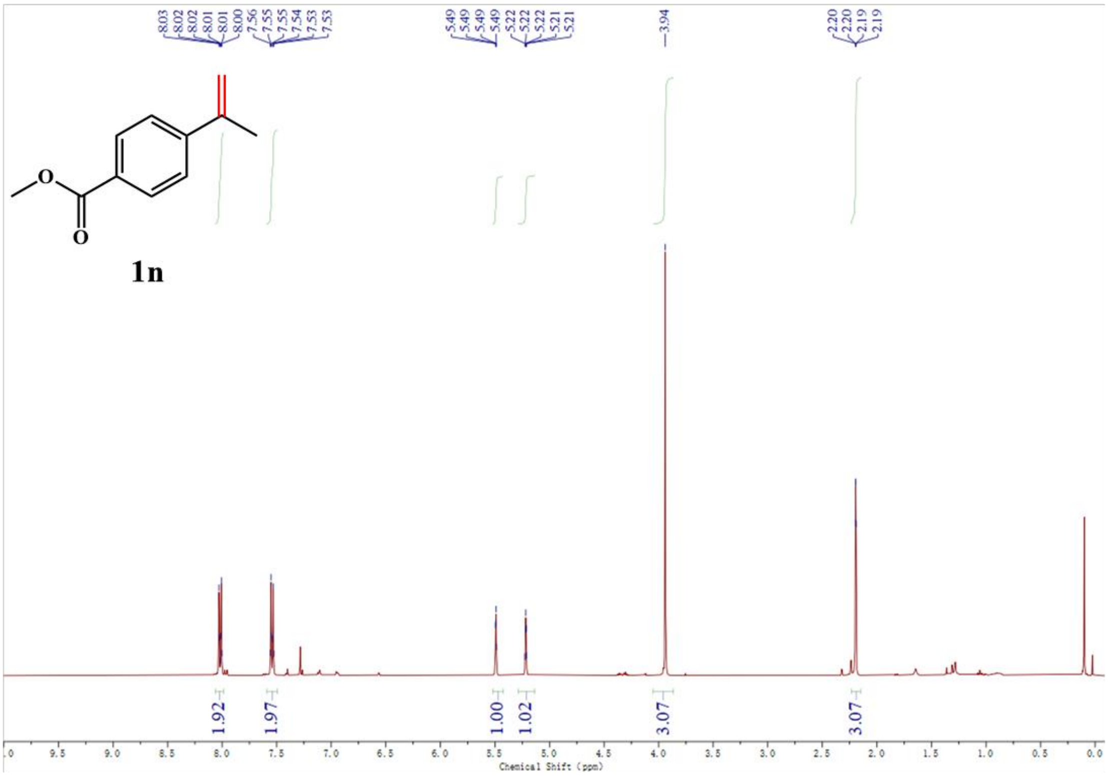
^{13}C NMR of **1l** in CDCl$_3$



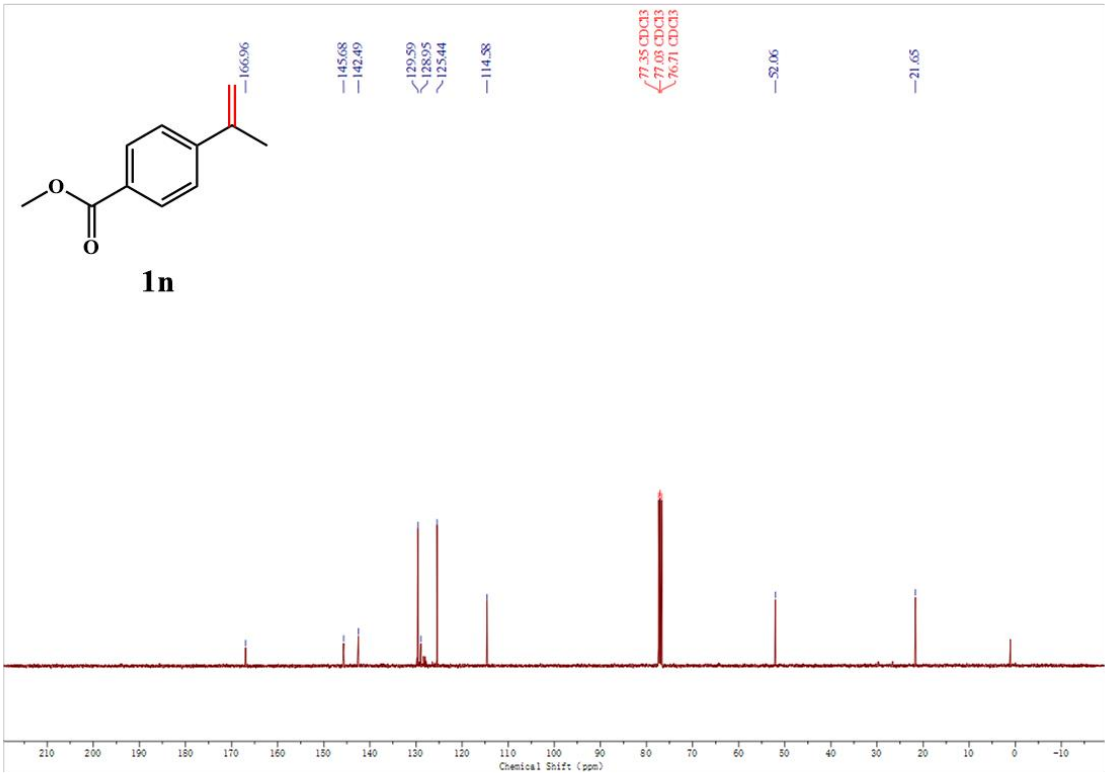
^{1}H NMR of **1m** in $CDCl_3$



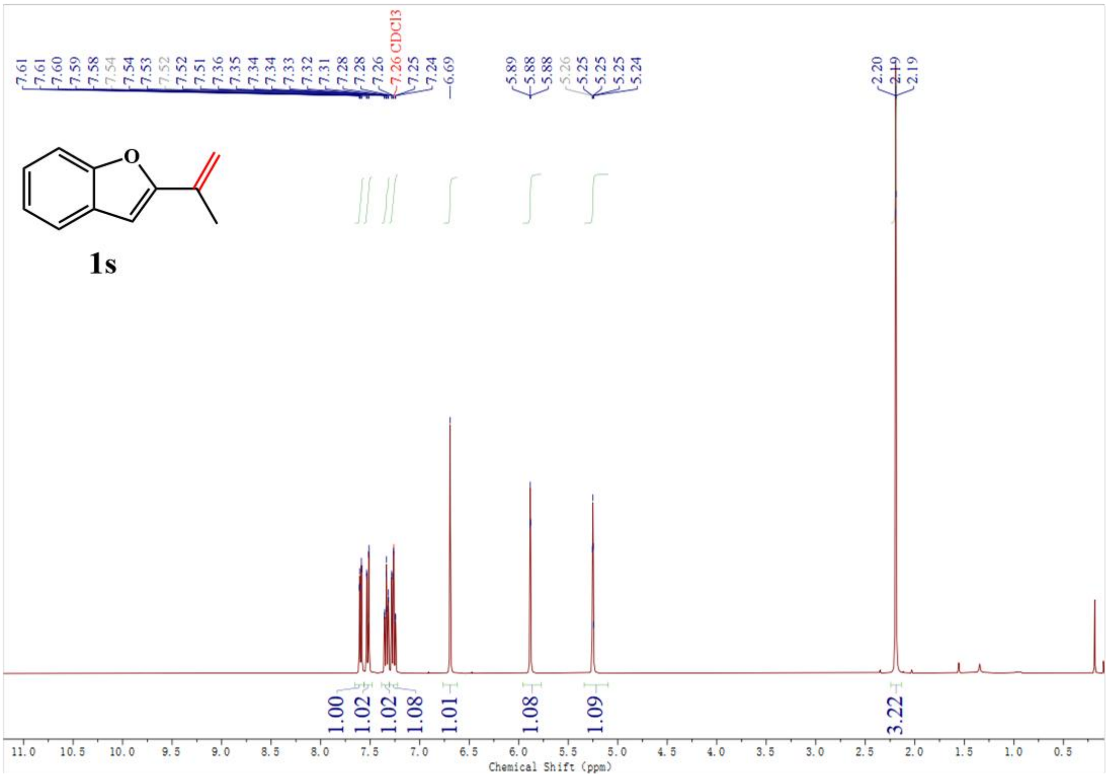
^{13}C NMR of **1m** in $CDCl_3$



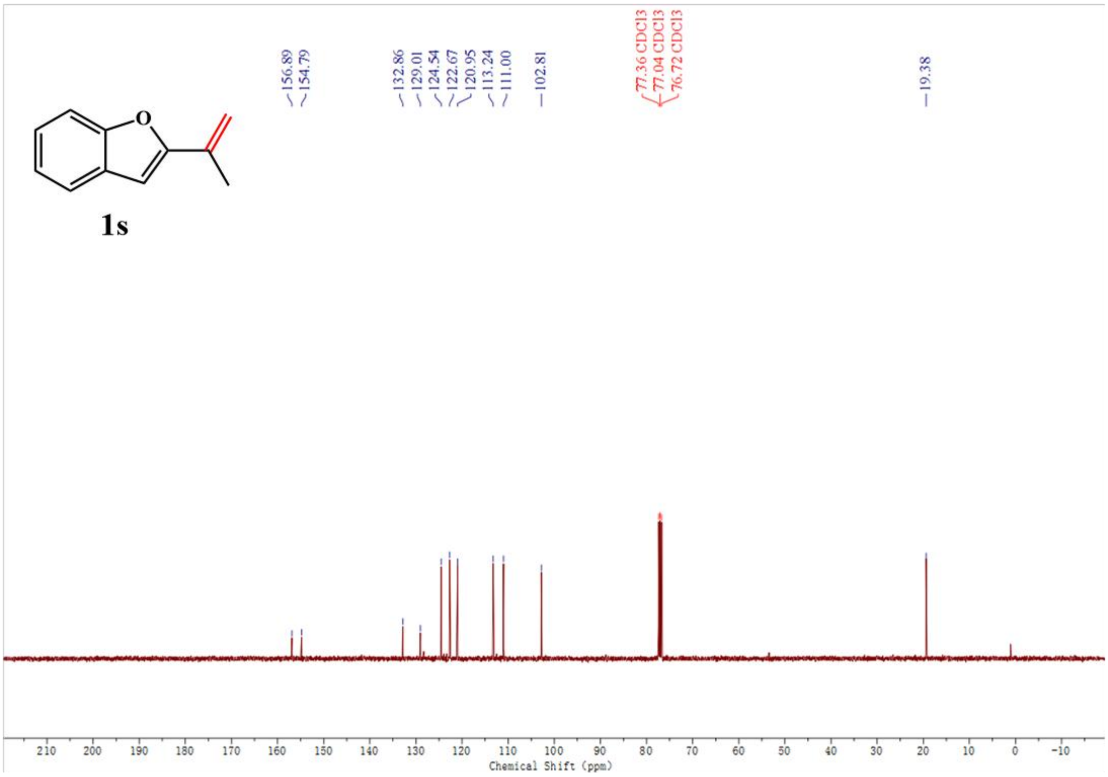
^{1}H NMR of **1n** in $CDCl_3$



^{13}C NMR of **1n** in $CDCl_3$



^{1}H NMR of **1s** in $CDCl_3$



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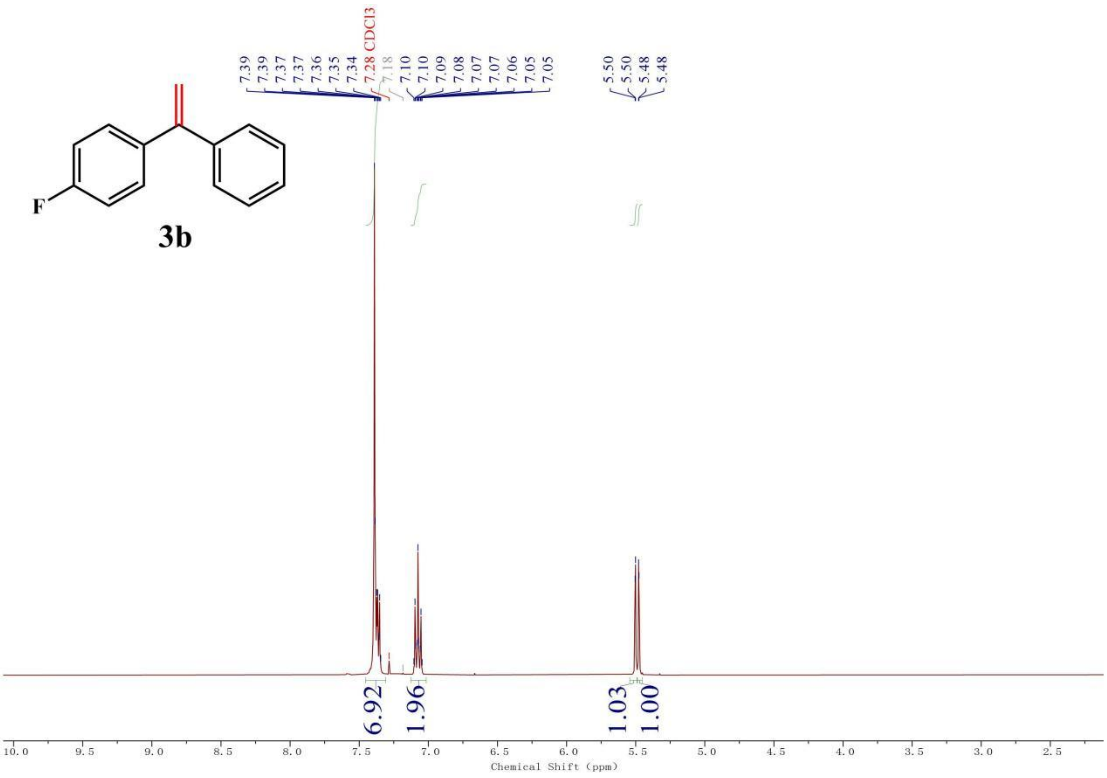
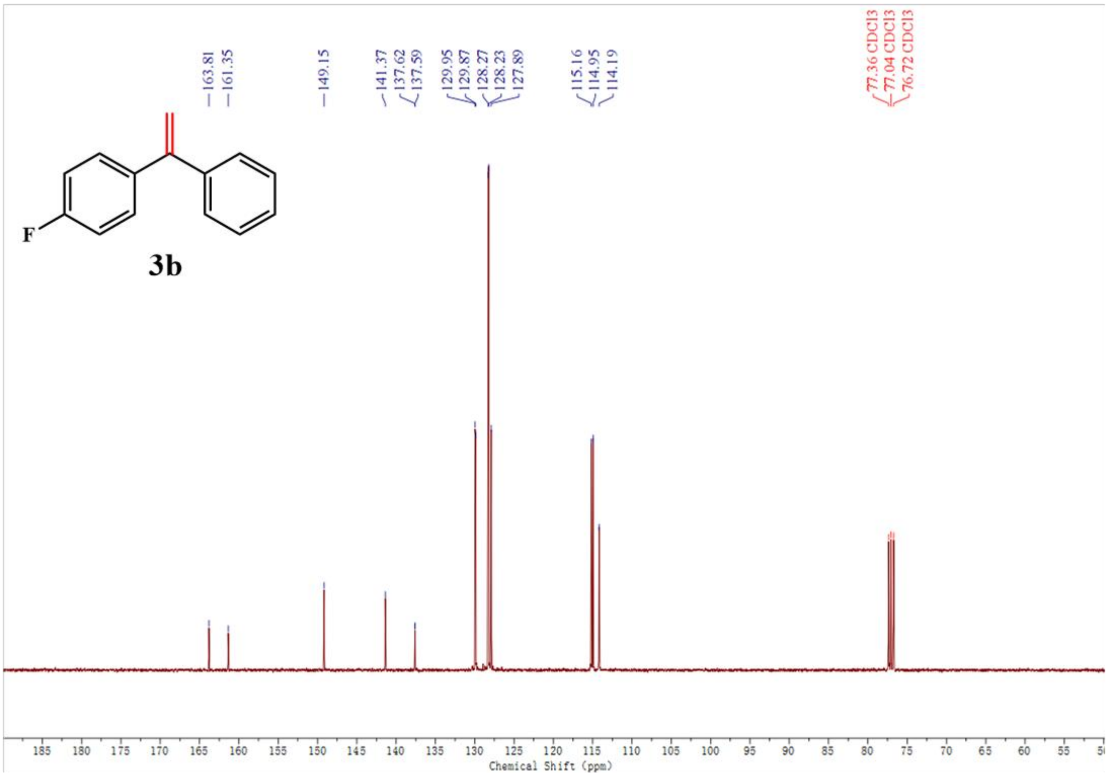
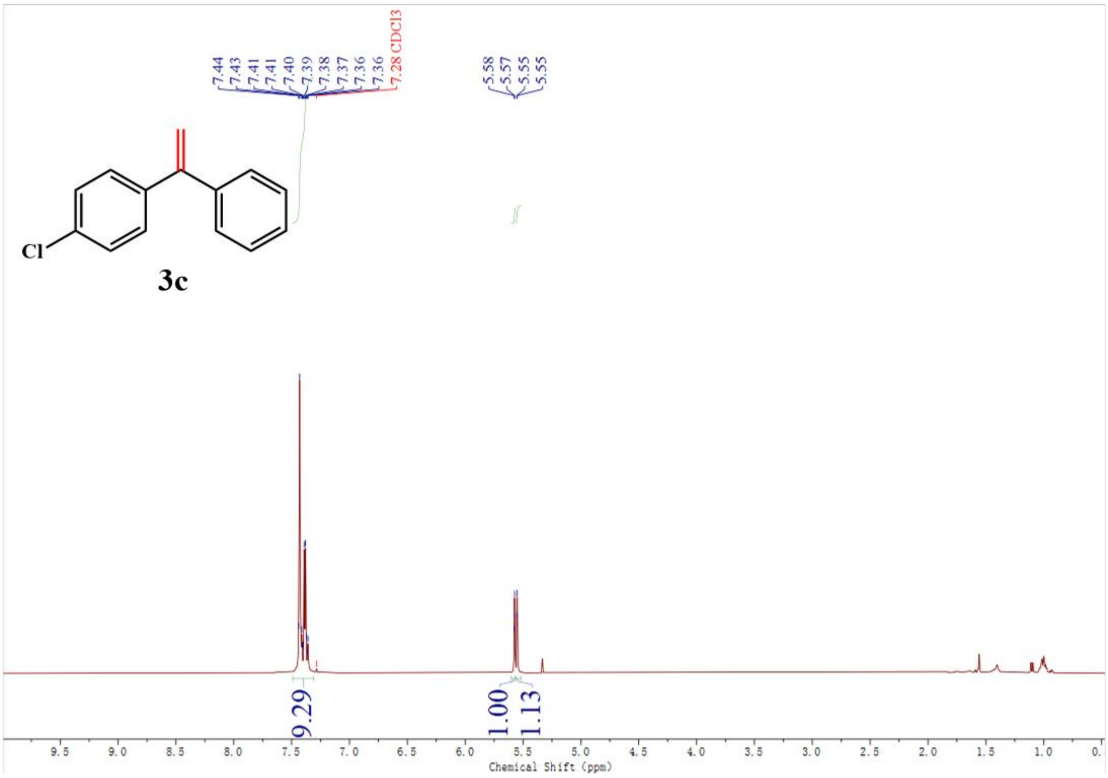


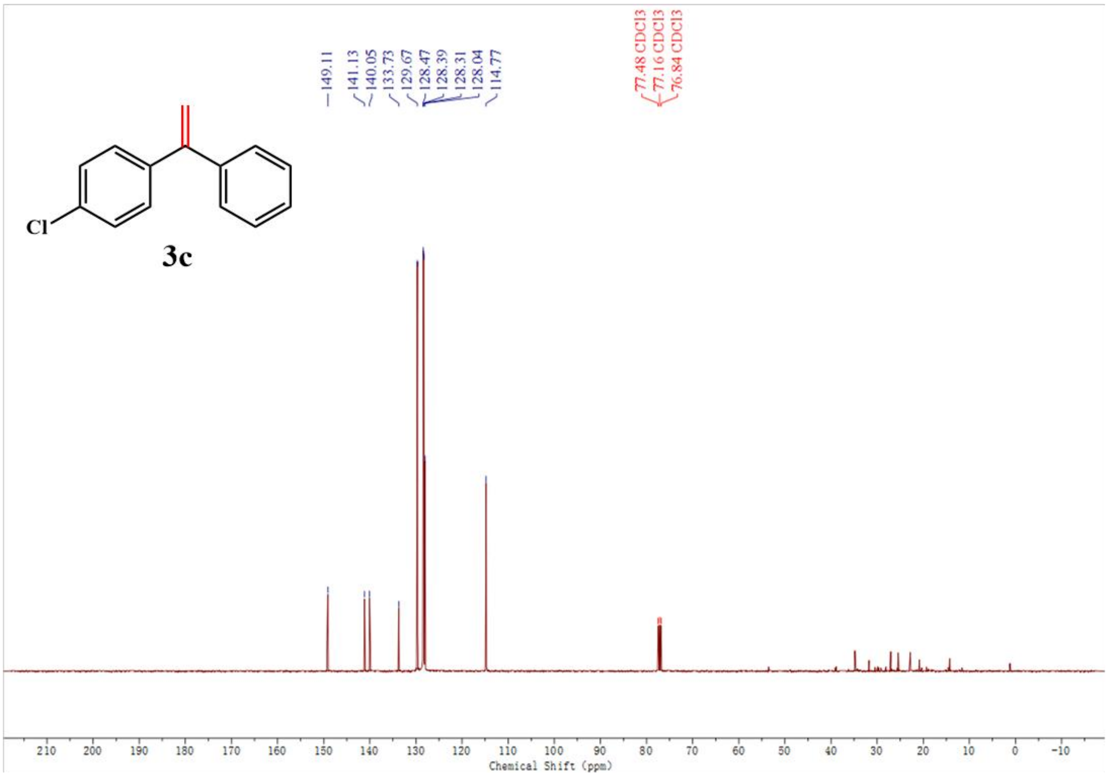
^{1}H NMR of **3b** in $CDCl_3$



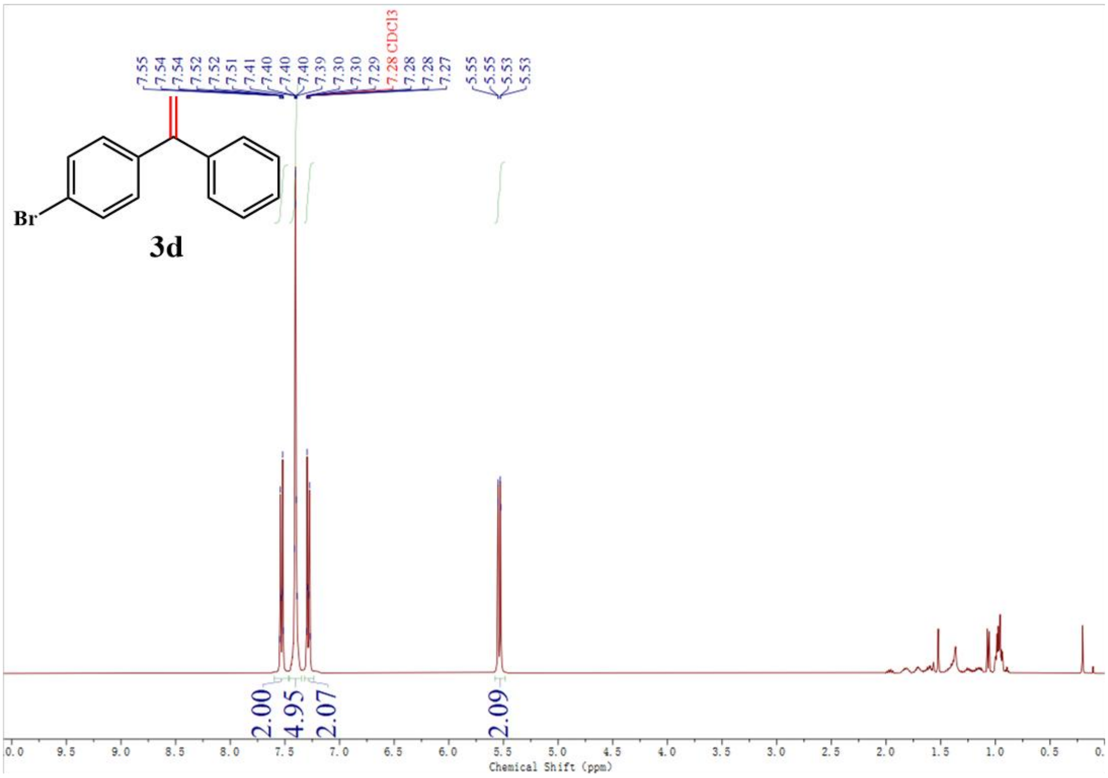
^{13}C NMR of **3b** in $CDCl_3$



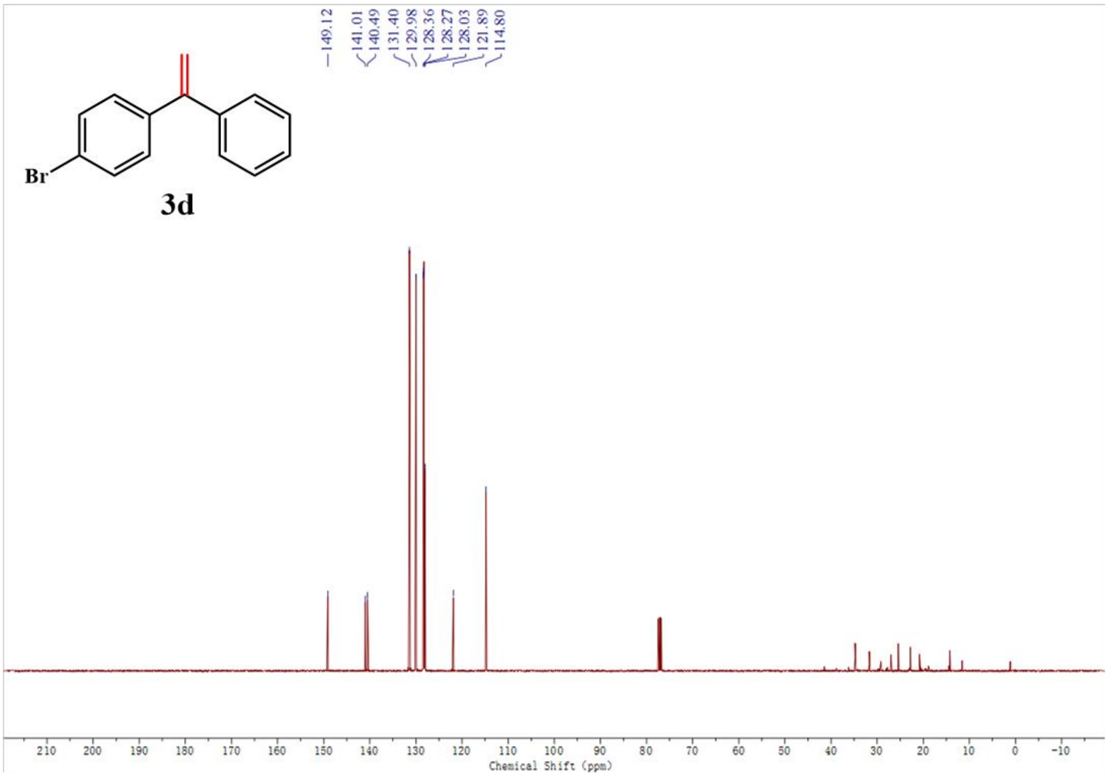
^{1}H NMR of **3c** in $CDCl_3$



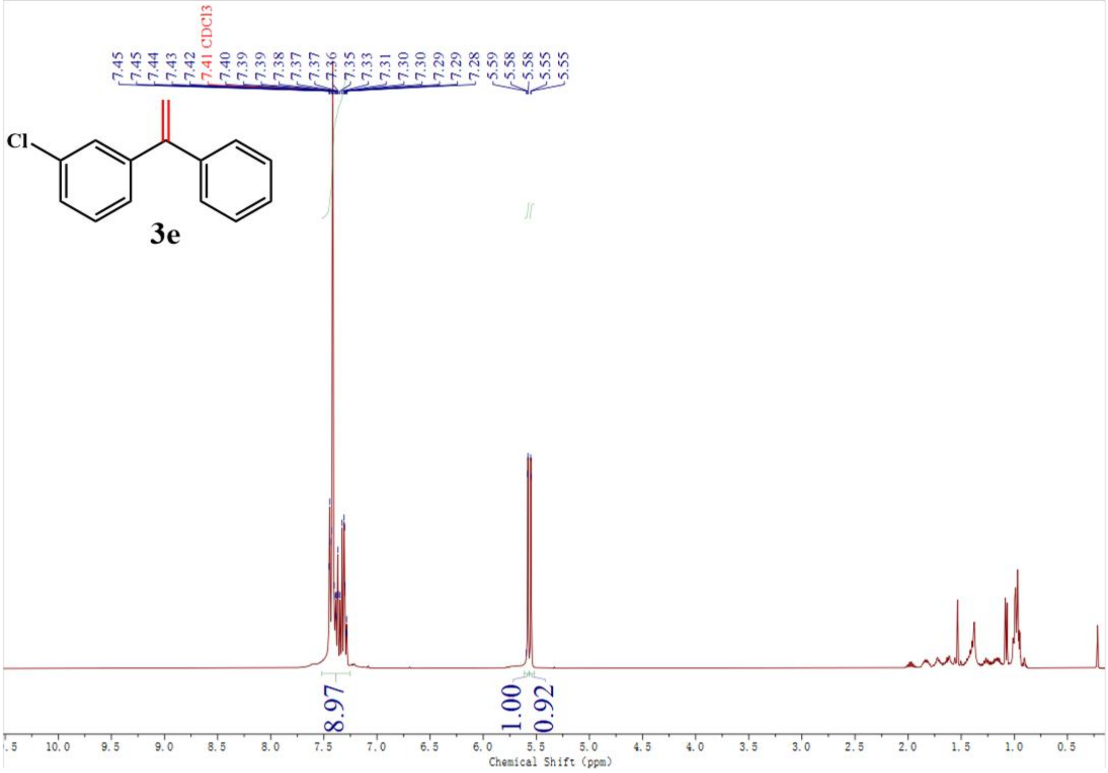
^{13}C NMR of **3c** in $CDCl_3$



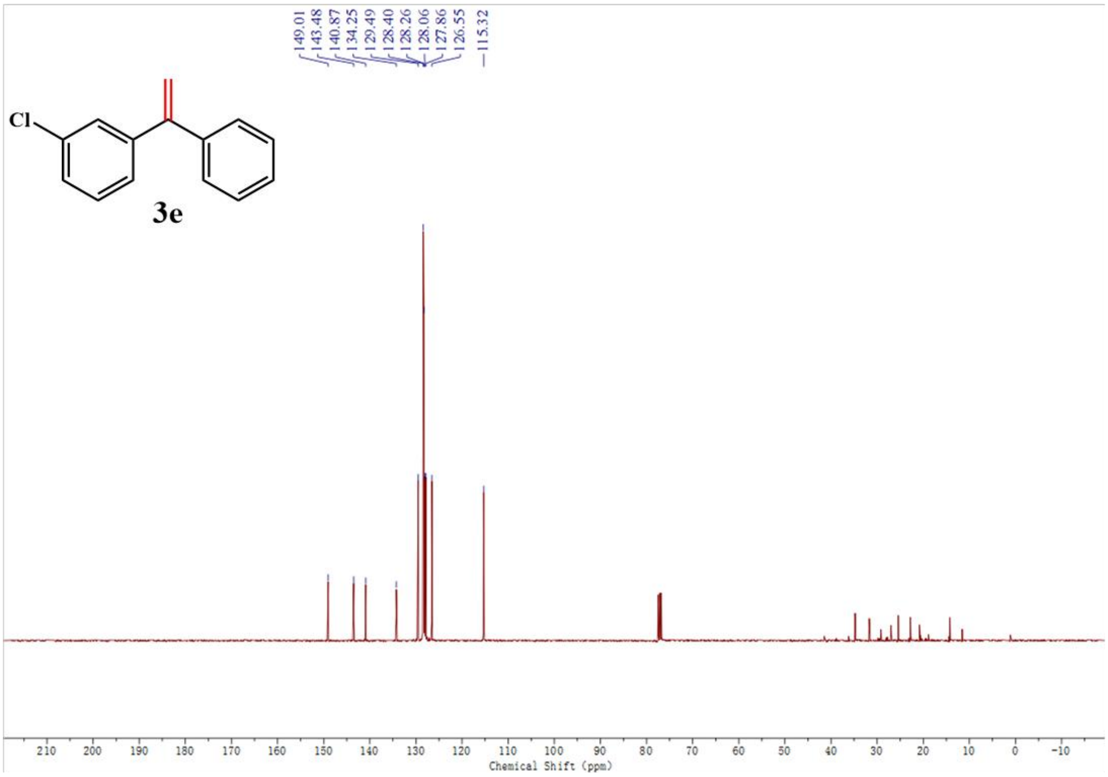
^{1}H NMR of **3d** in $CDCl_3$



^{13}C NMR of **3d** in $CDCl_3$



^{1}H NMR of **3e** in $CDCl_3$



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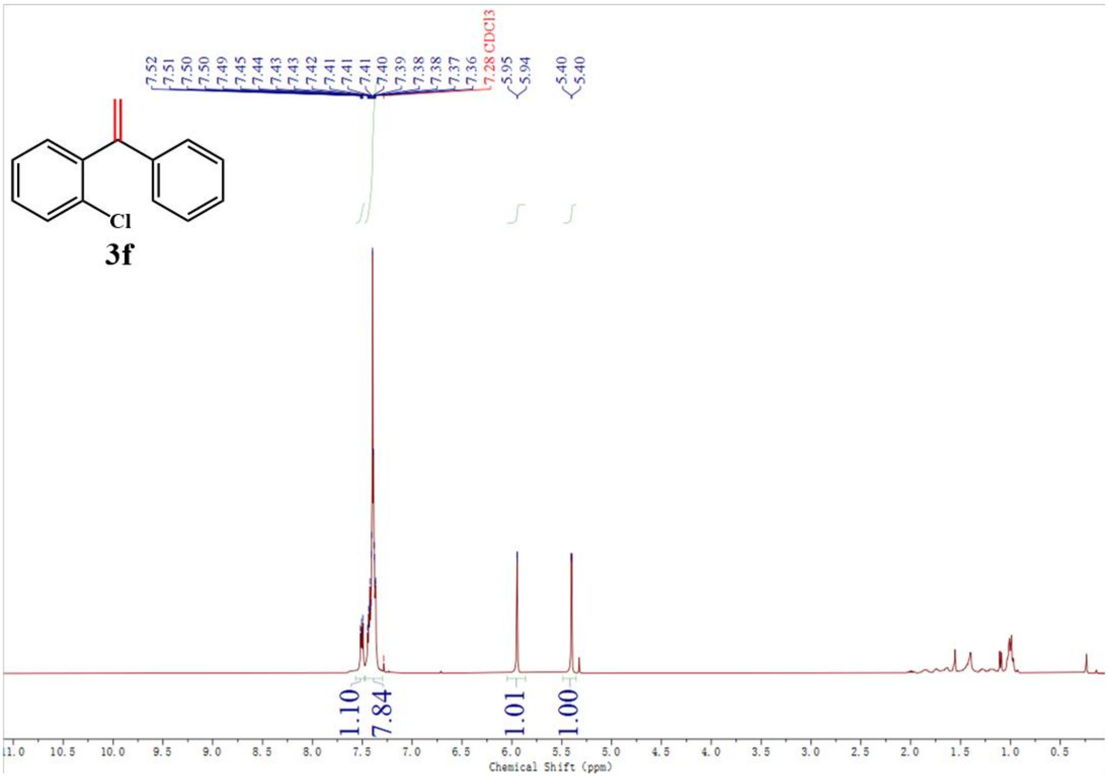
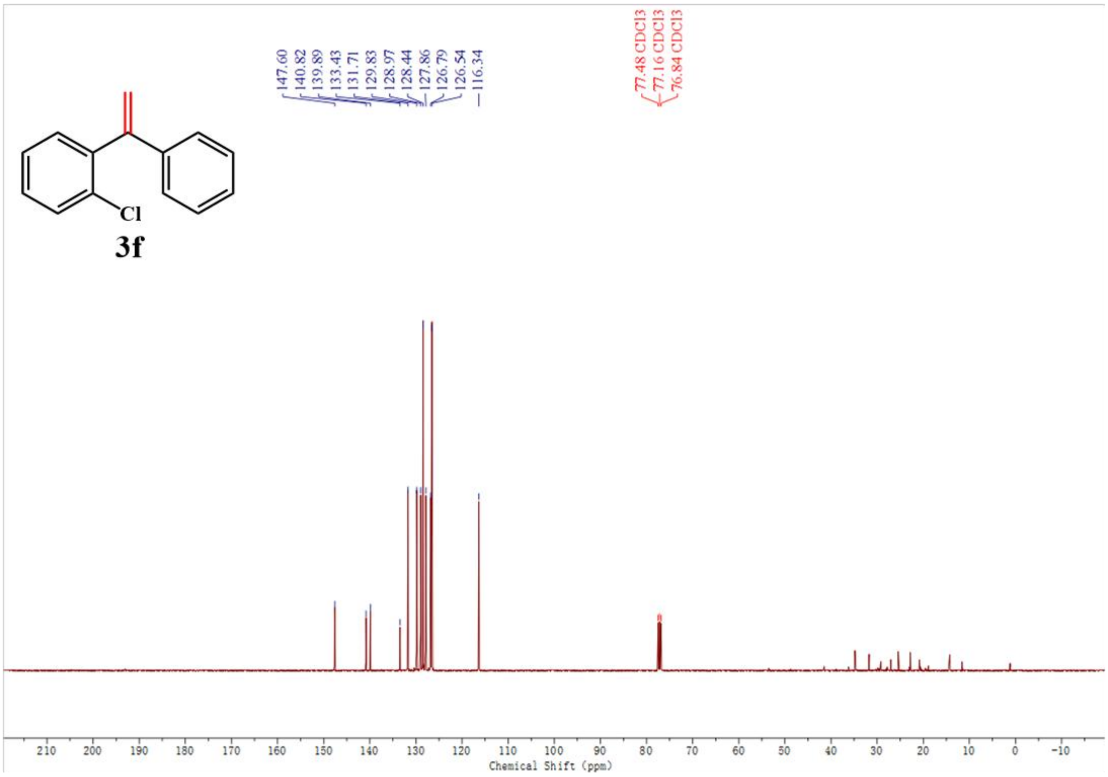


^{1}H NMR of **3f** in CDCl$_3$



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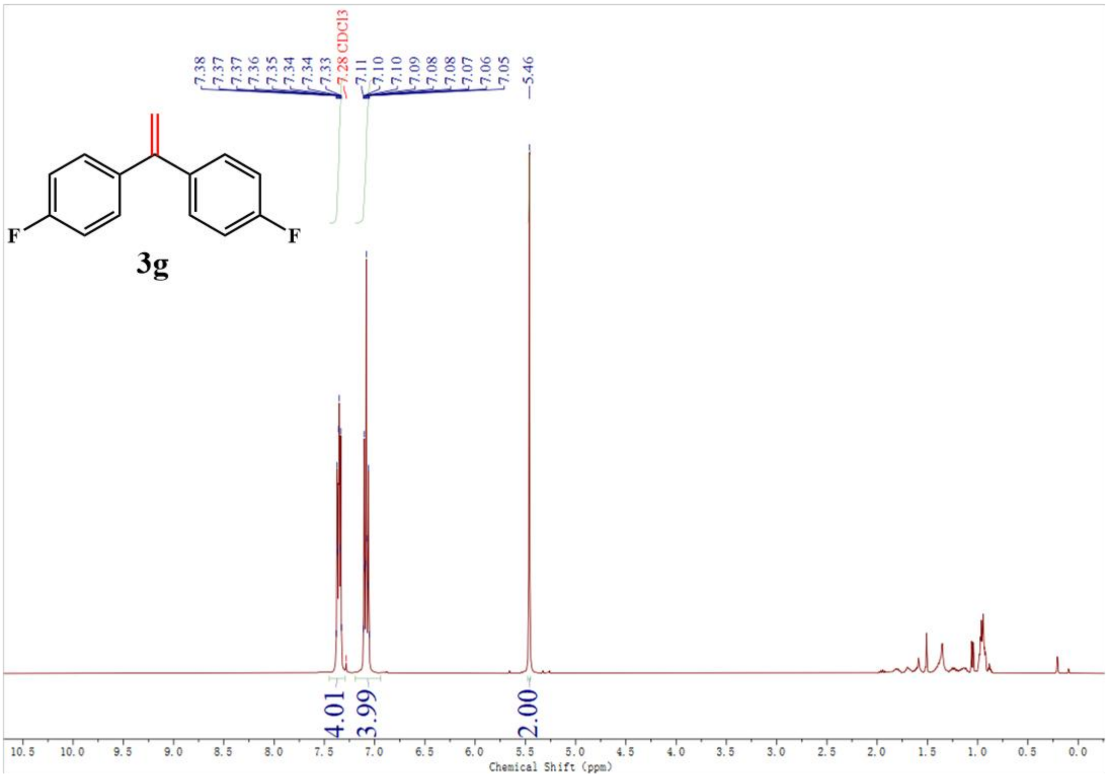

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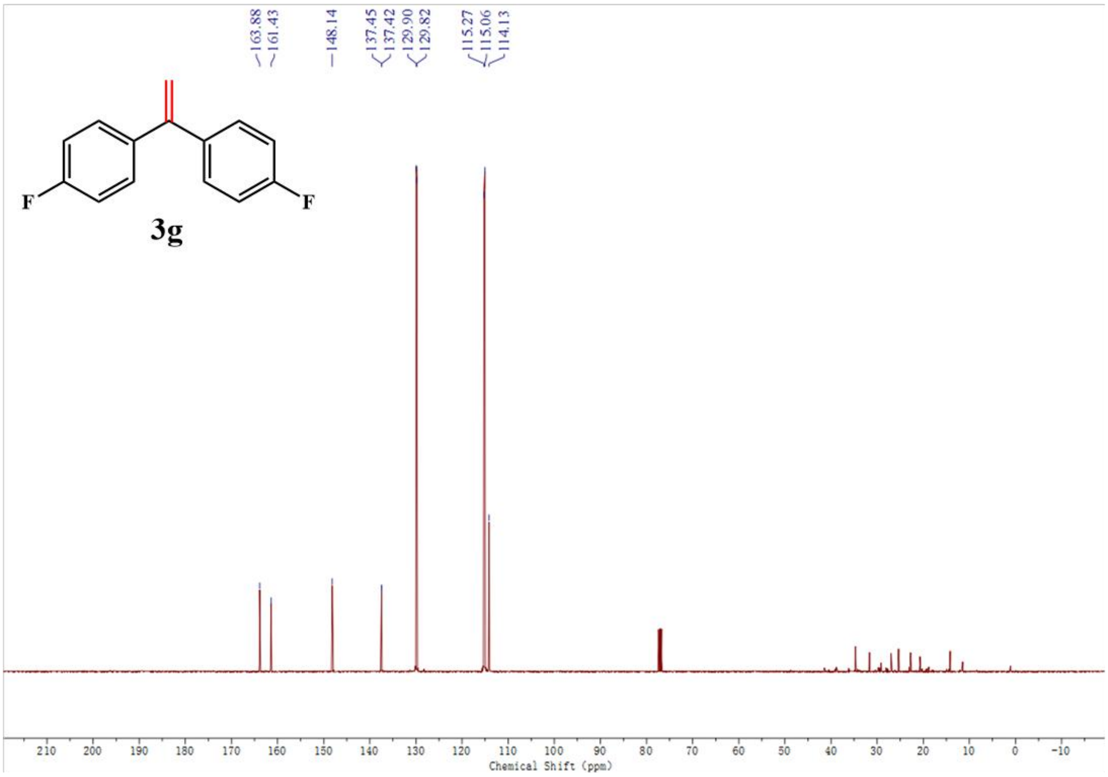
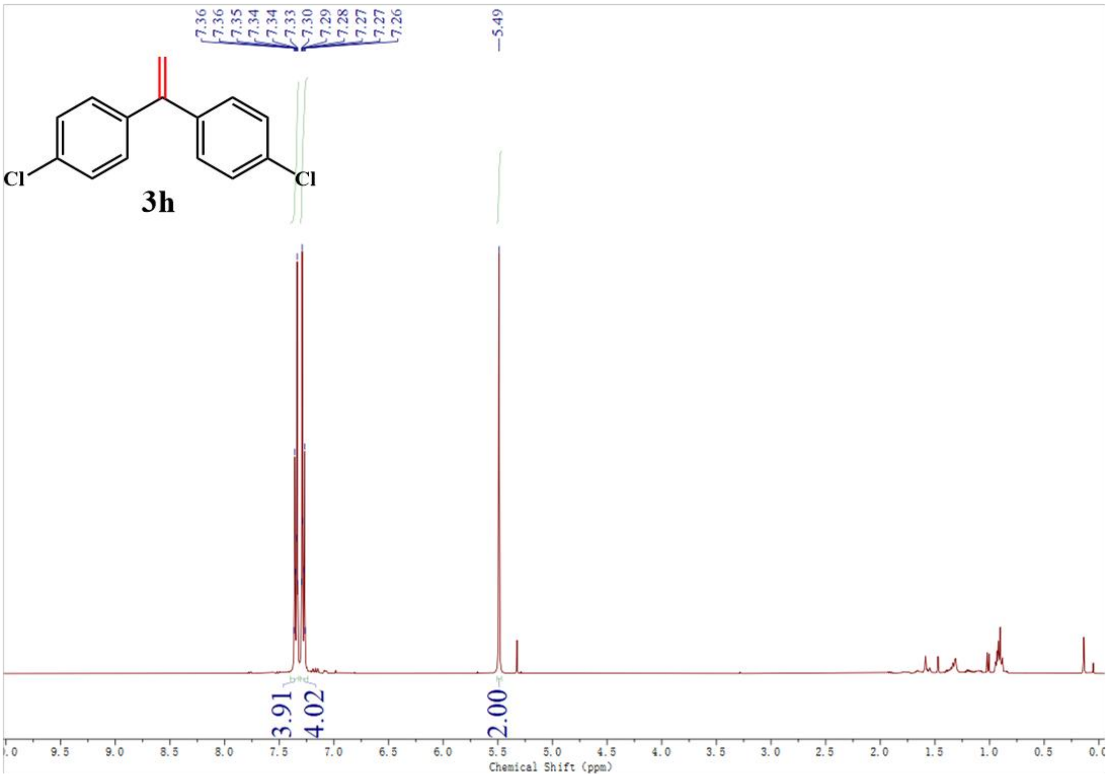
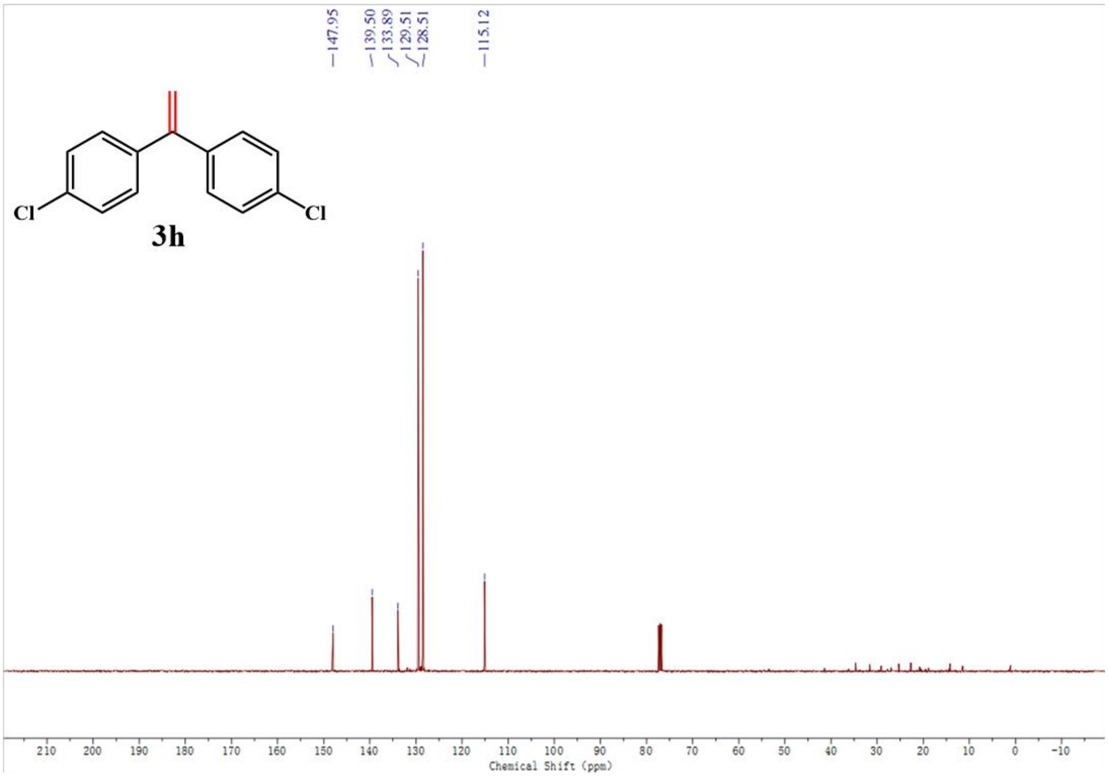


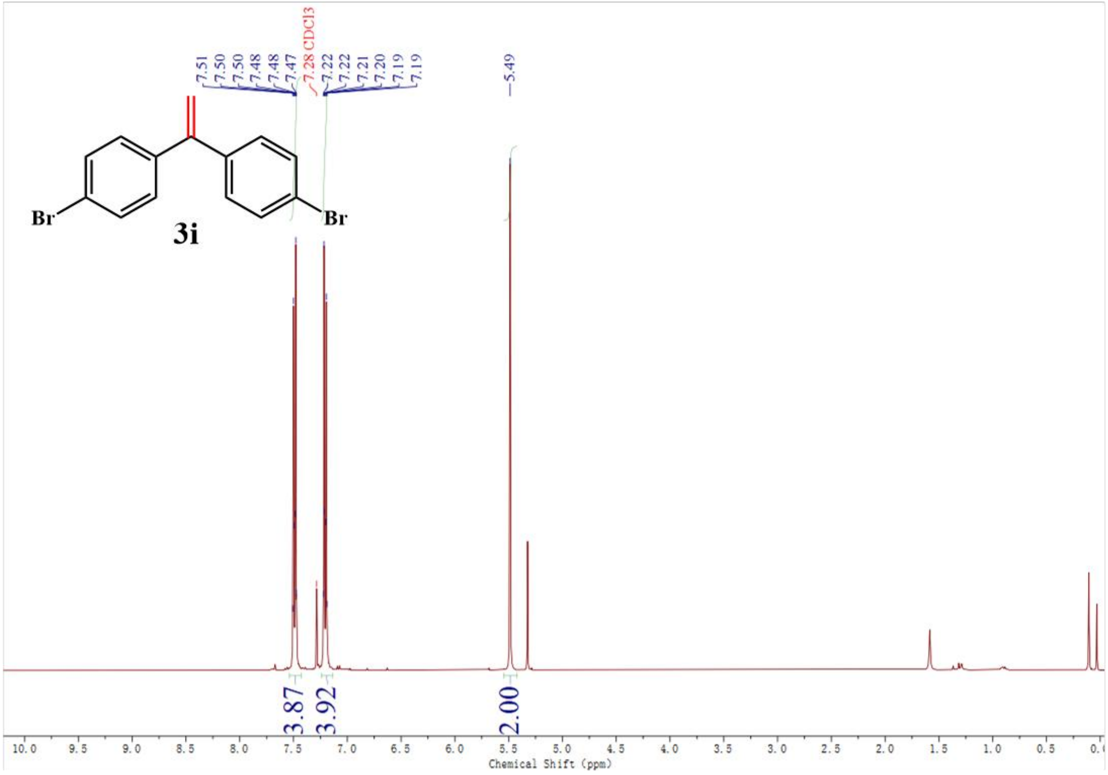
^{13}C NMR of **3g** in CDCl$_3$



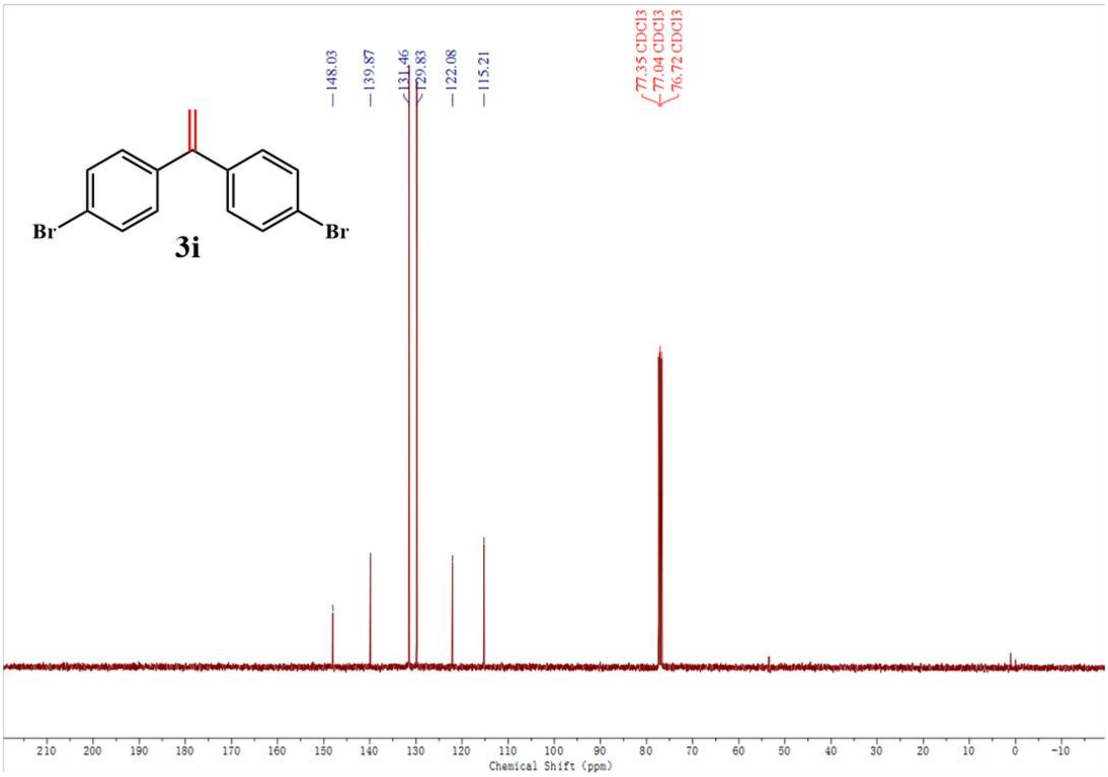
^{1}H NMR of **3h** in CDCl$_3$



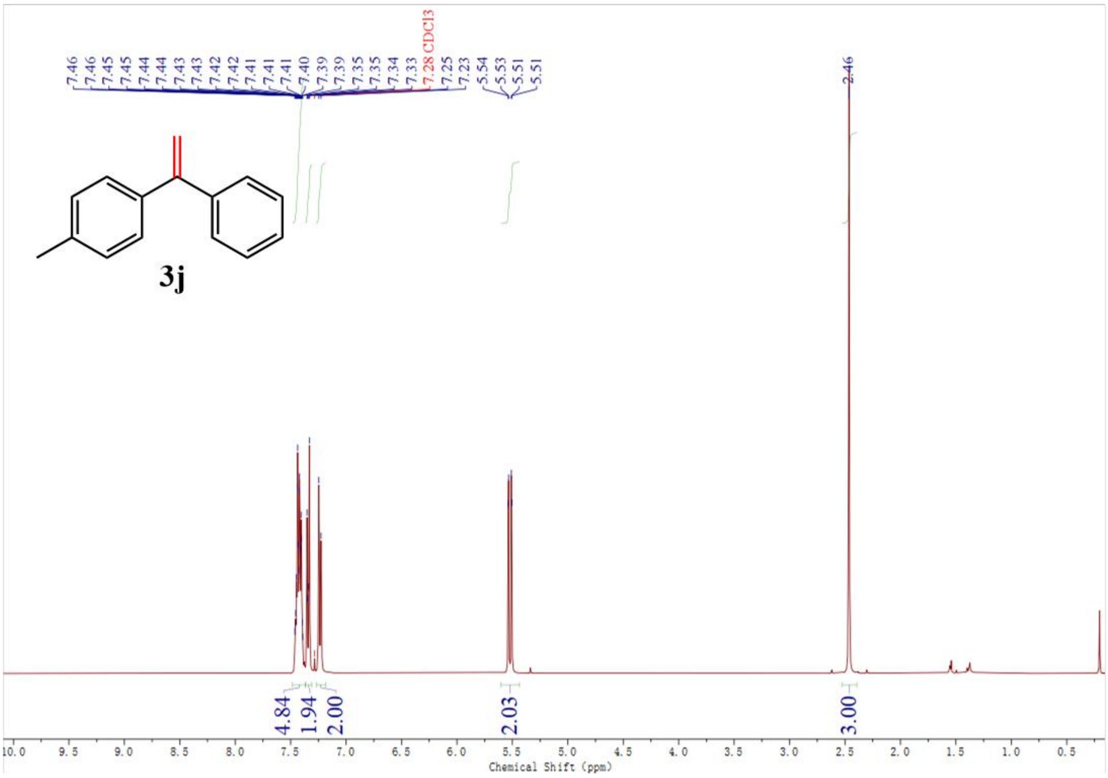
^{13}C NMR of **3h** in CDCl$_3$



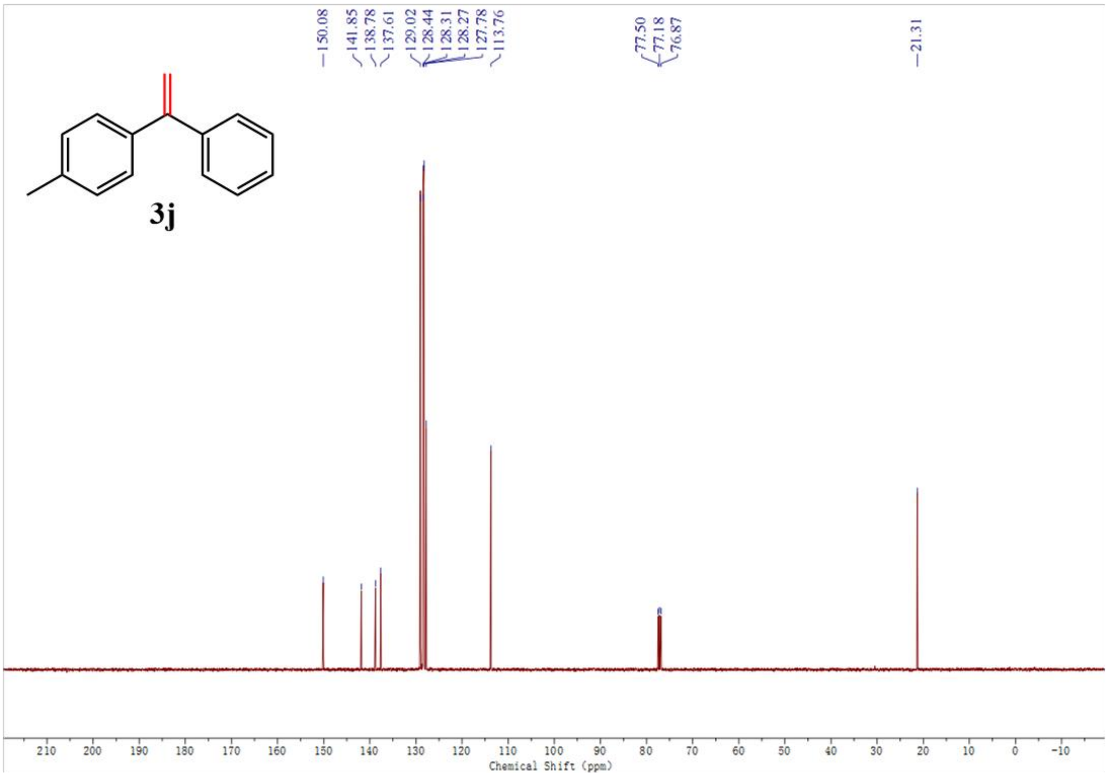
^{1}H NMR of **3i** in CDCl$_3$



^{13}C NMR of **3i** in CDCl$_3$



^{1}H NMR of **3j** in $CDCl_3$



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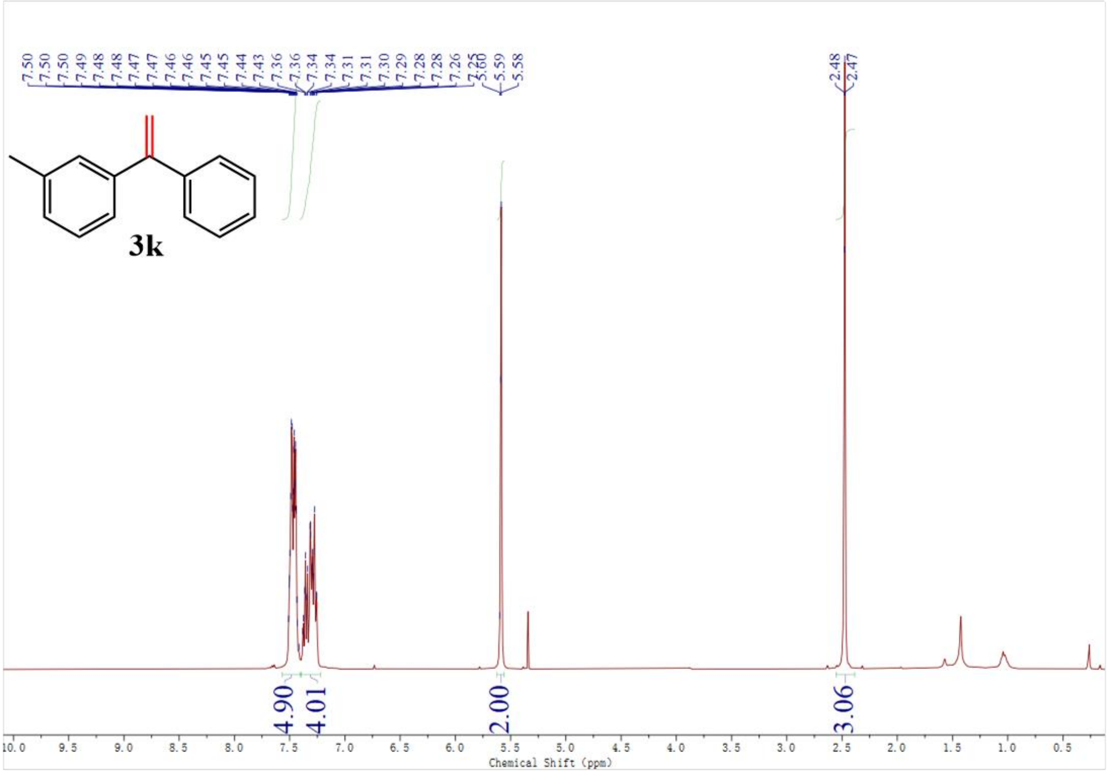
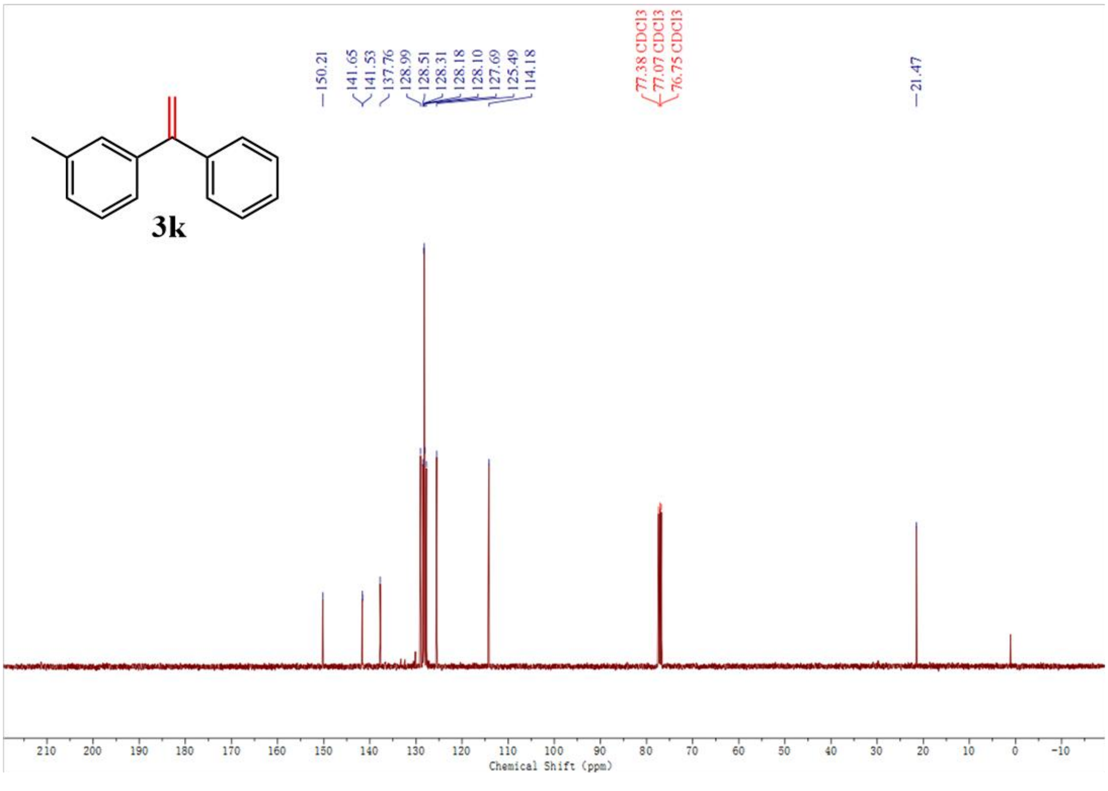


^{1}H NMR of **3k** in $CDCl_3$



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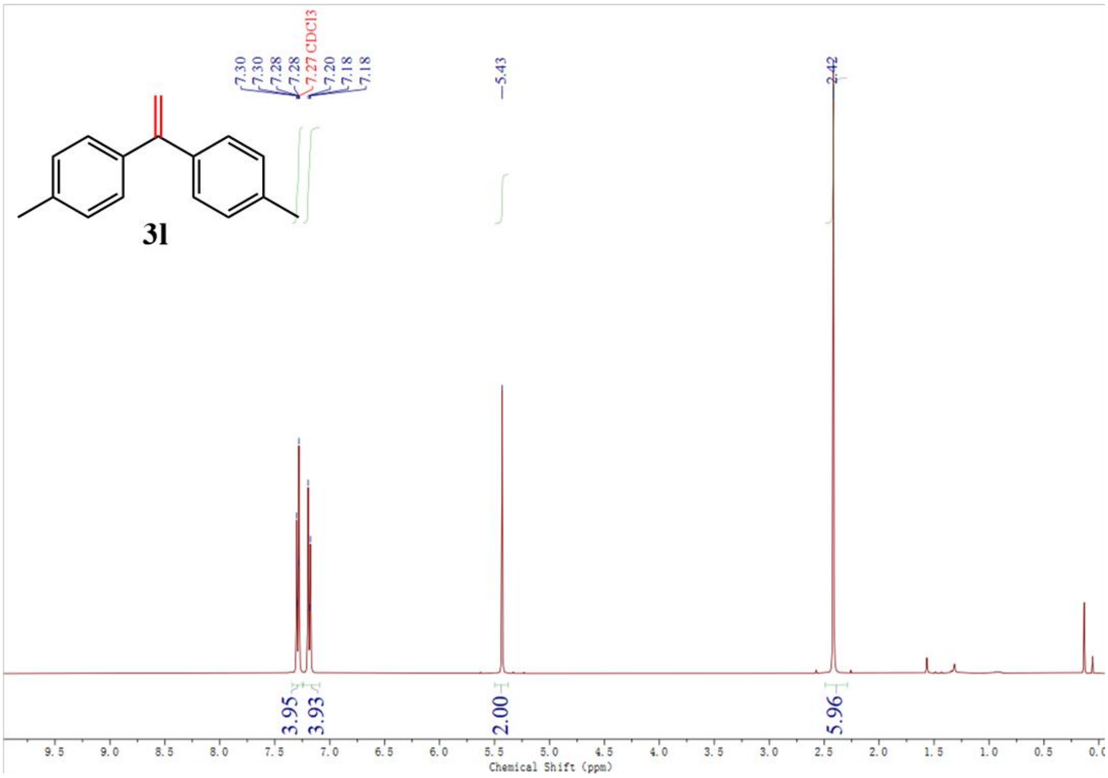

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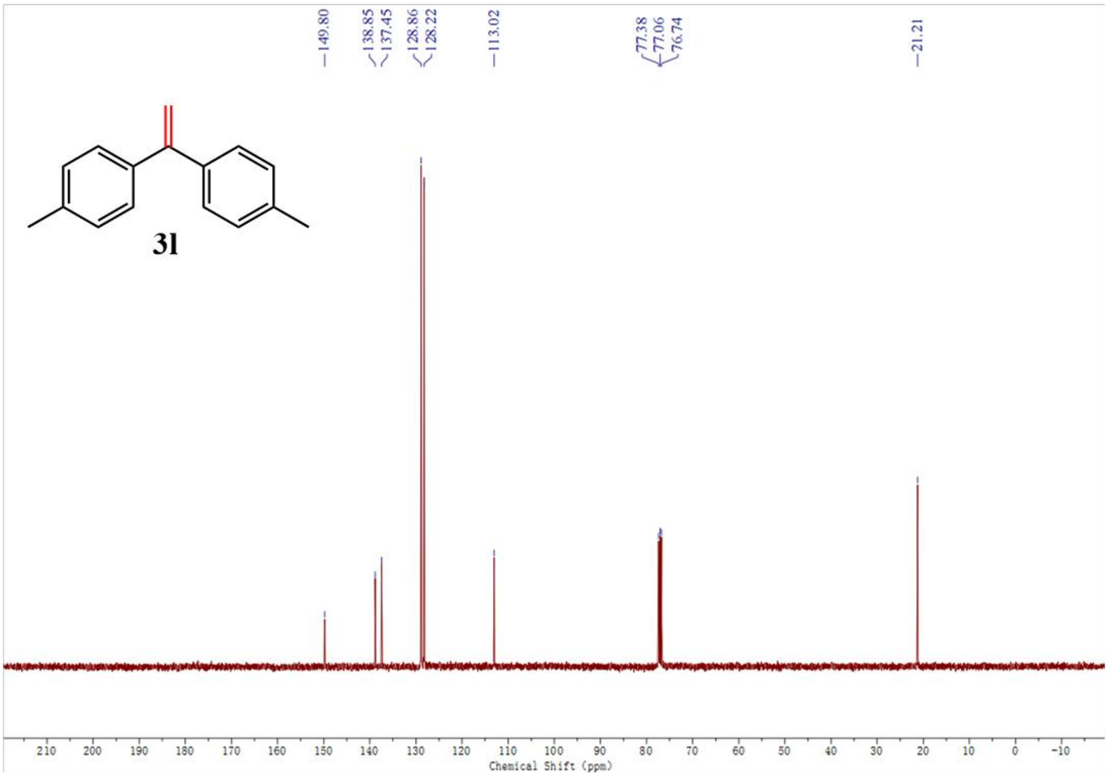
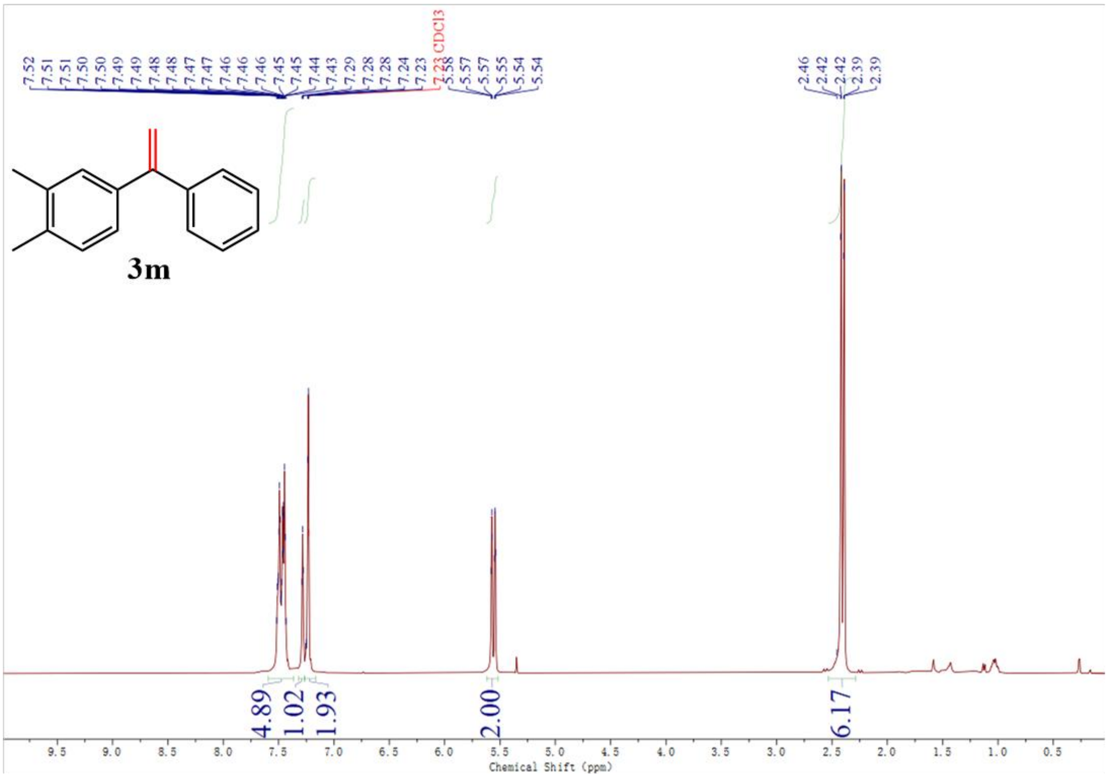


^{13}C NMR of **3l** in $CDCl_3$



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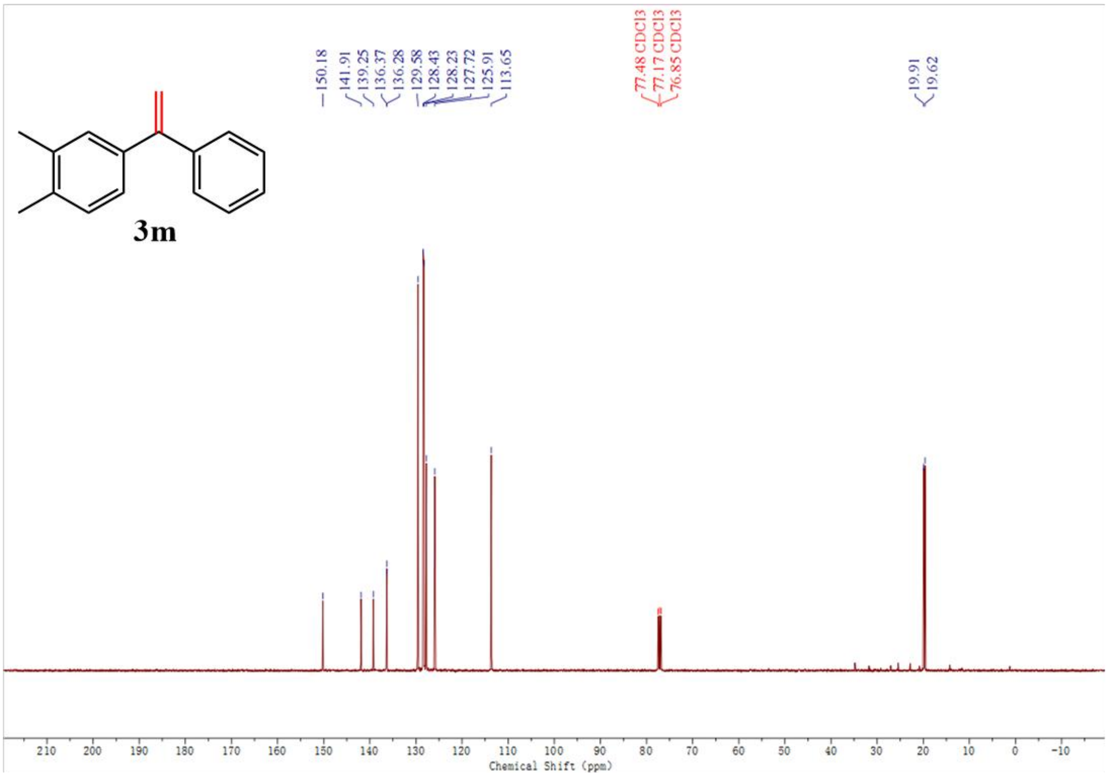

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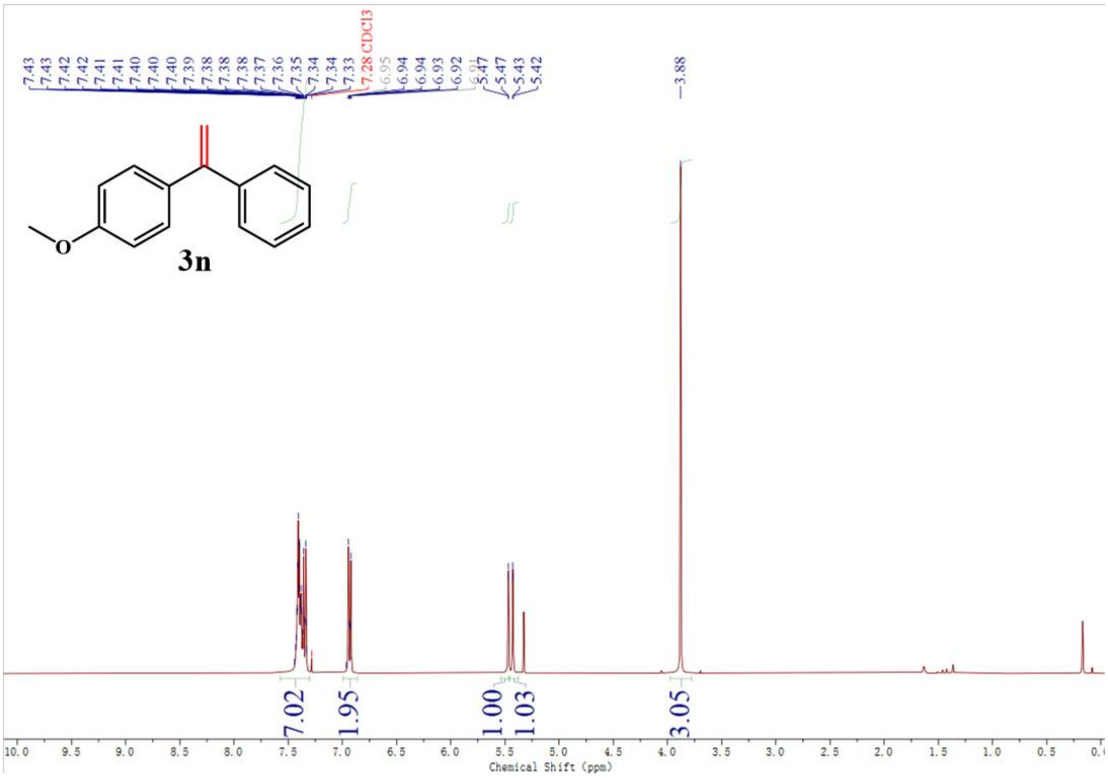

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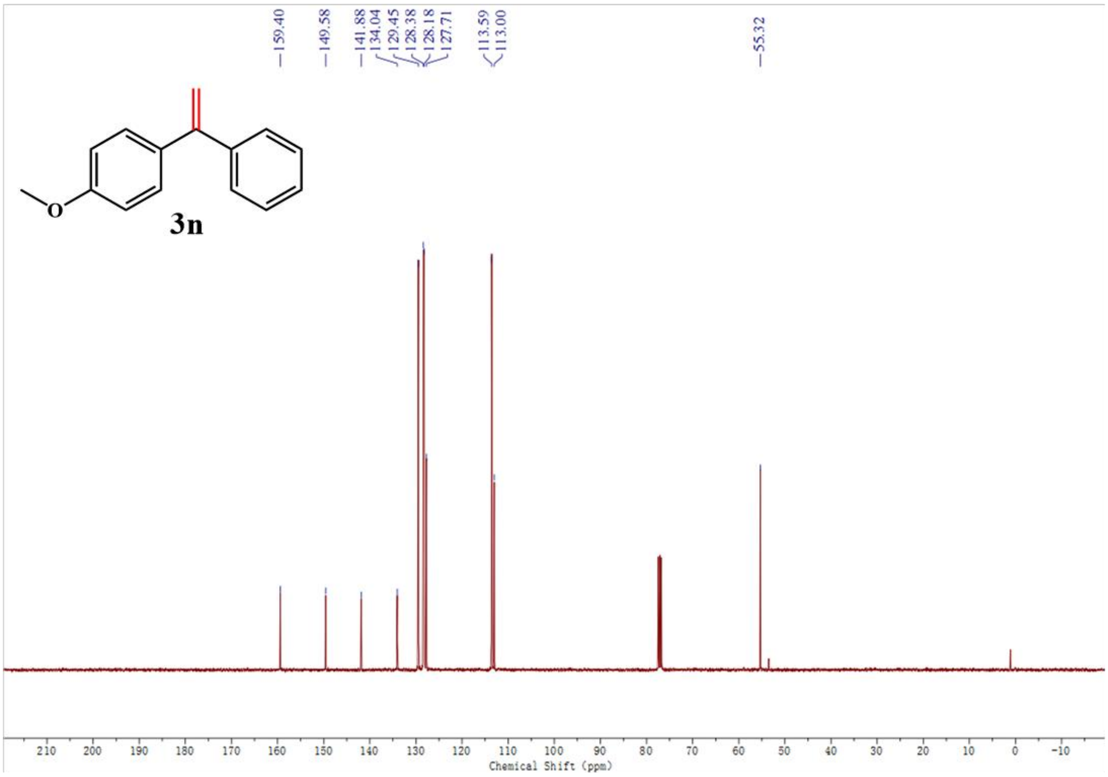

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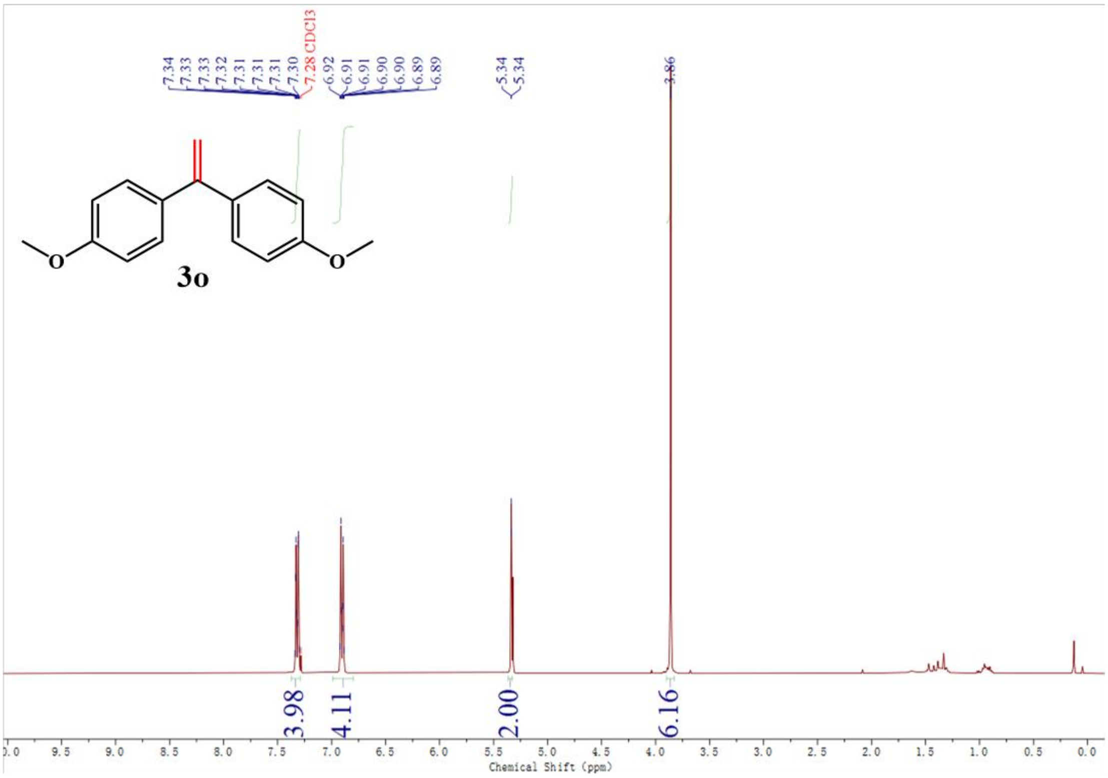

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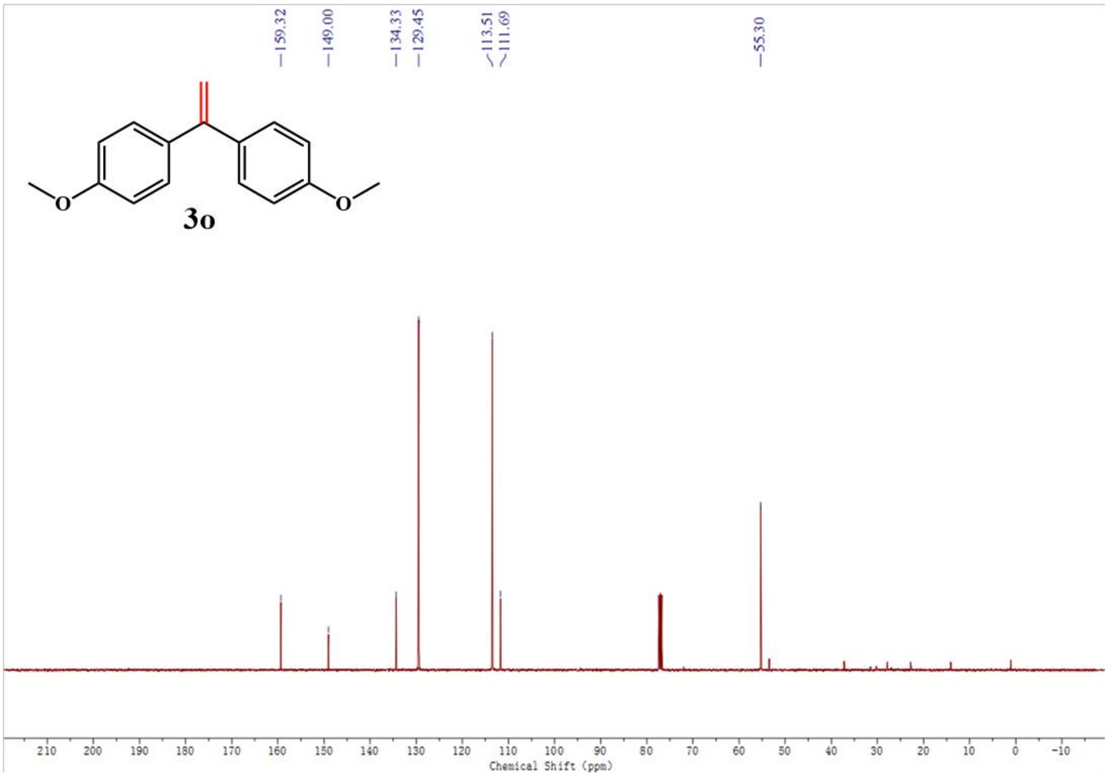

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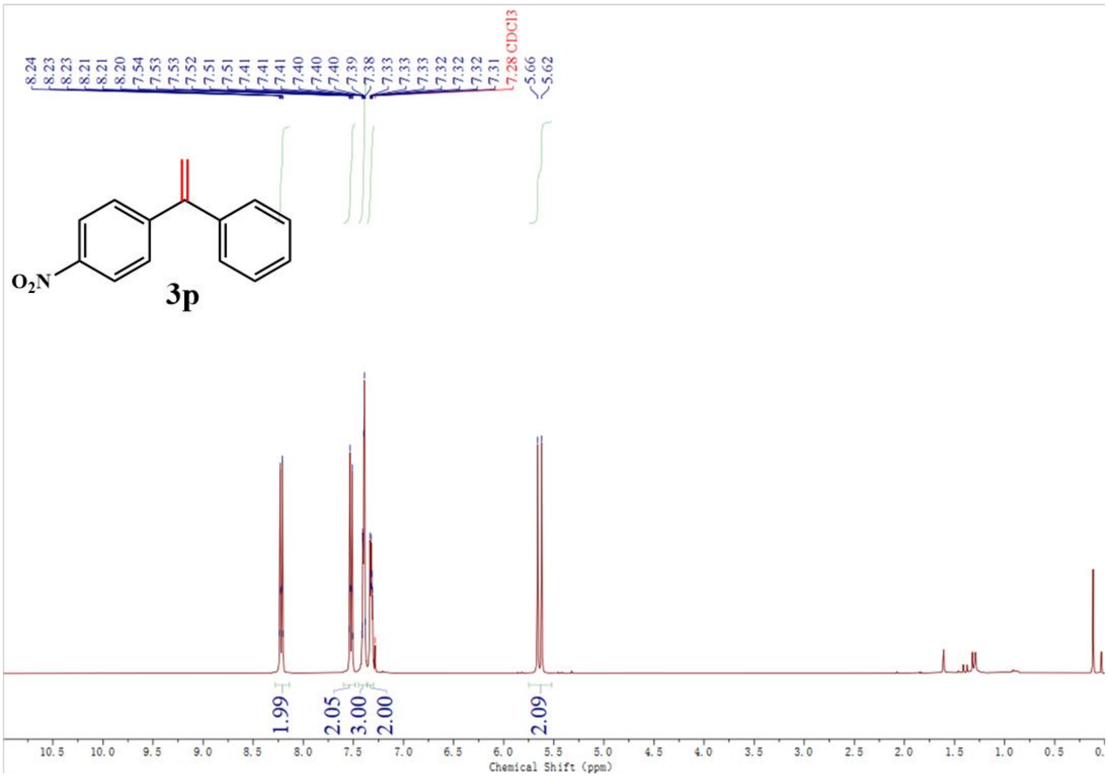

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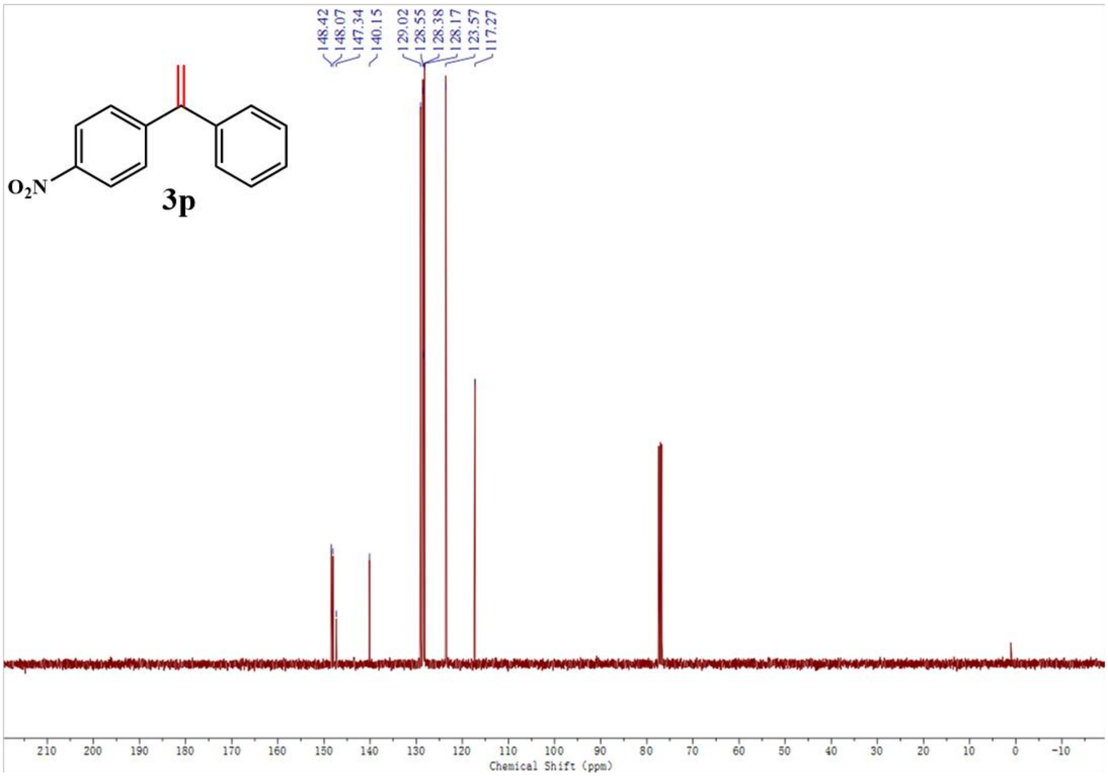

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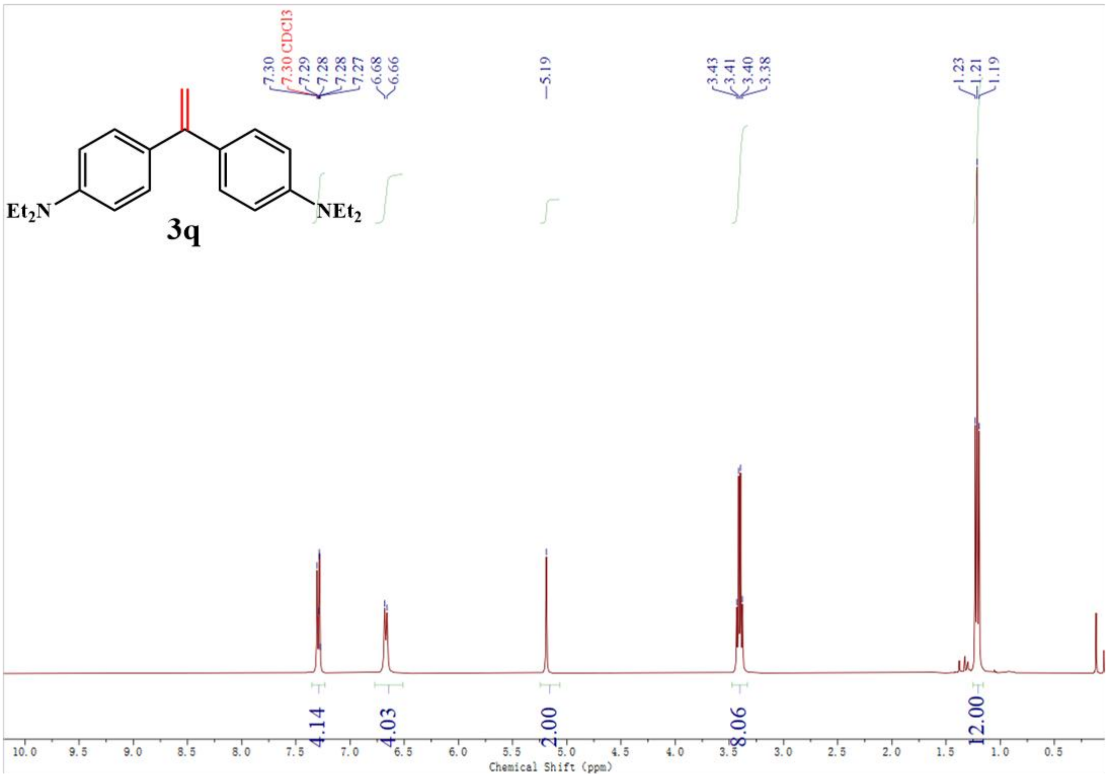

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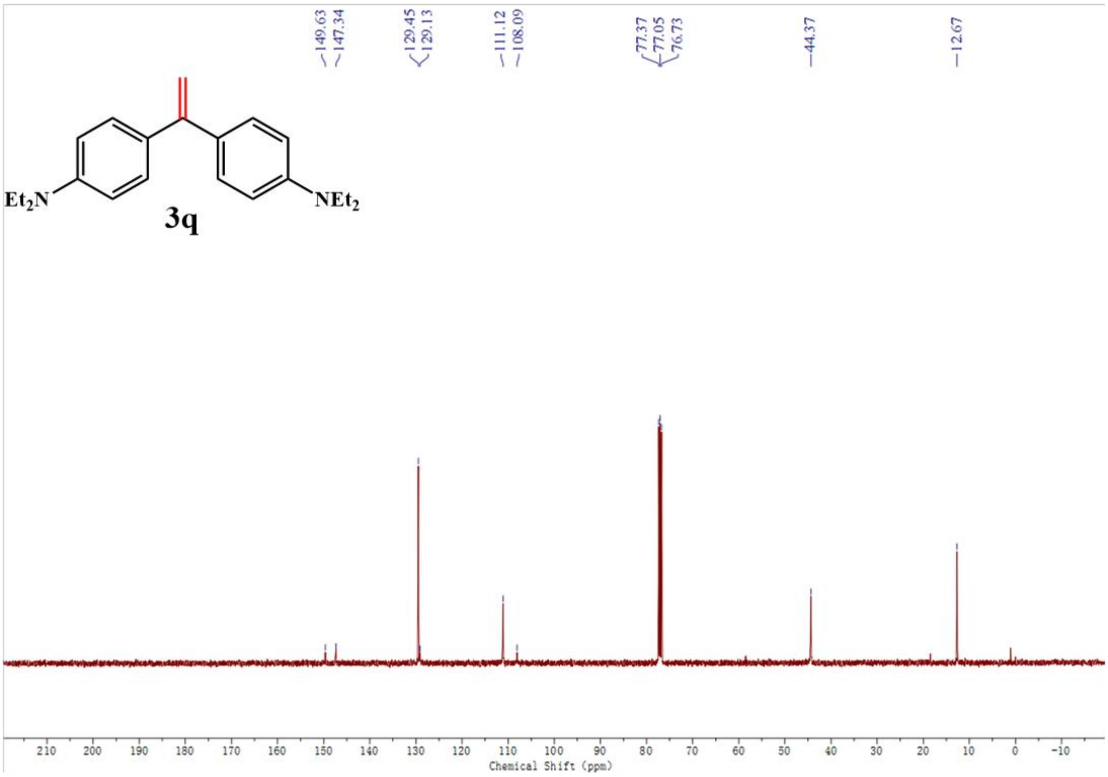

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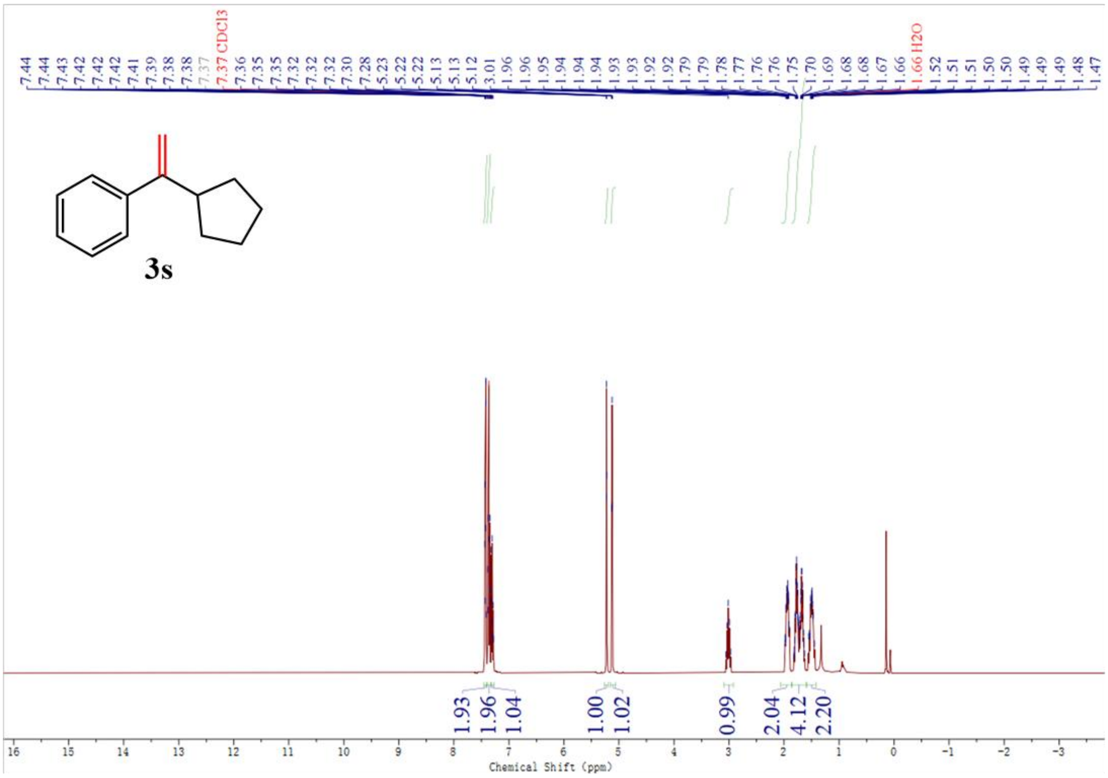

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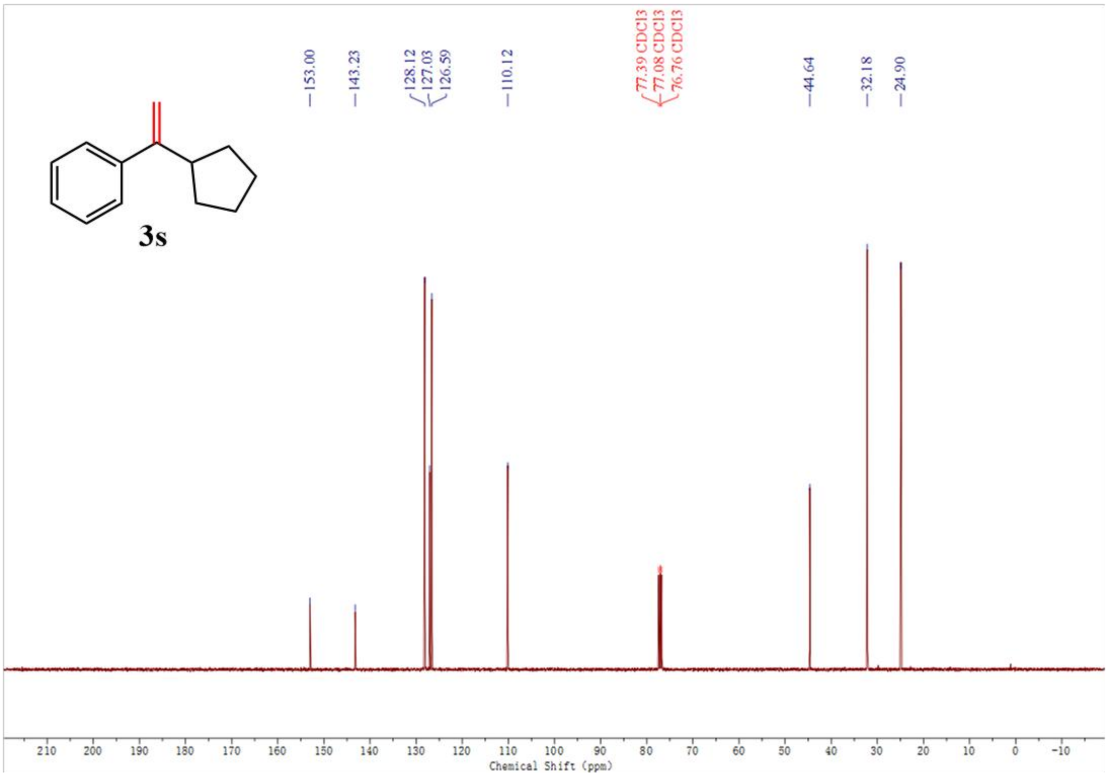

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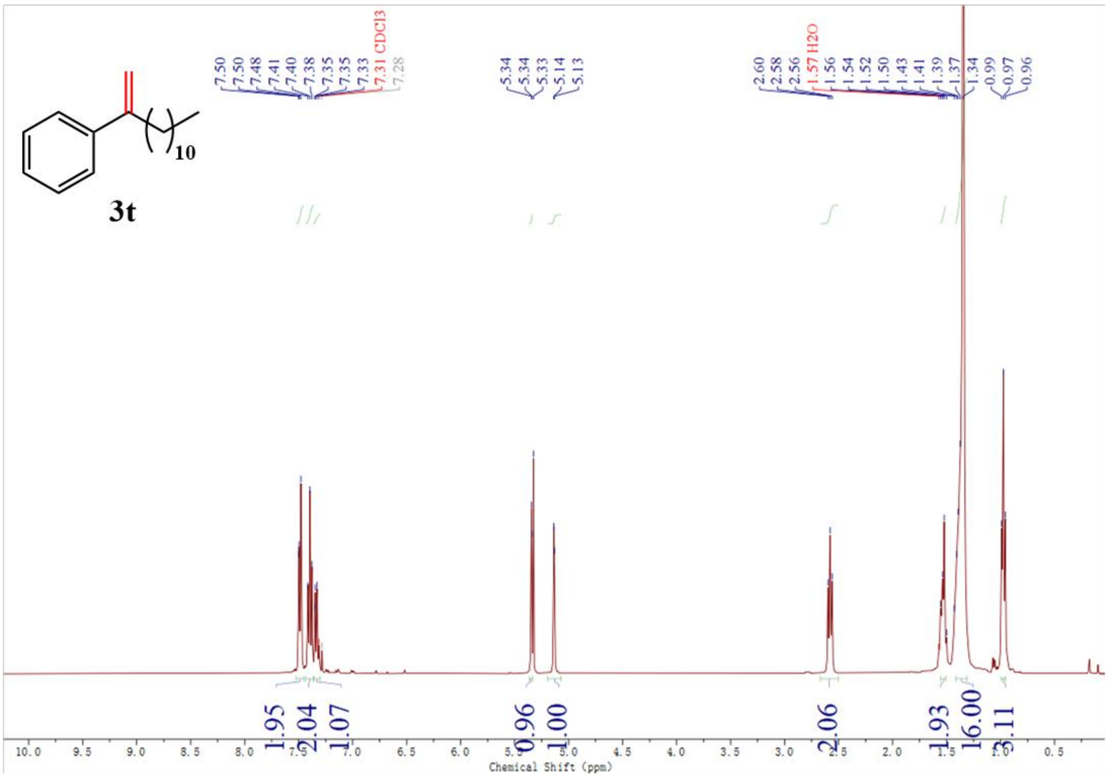

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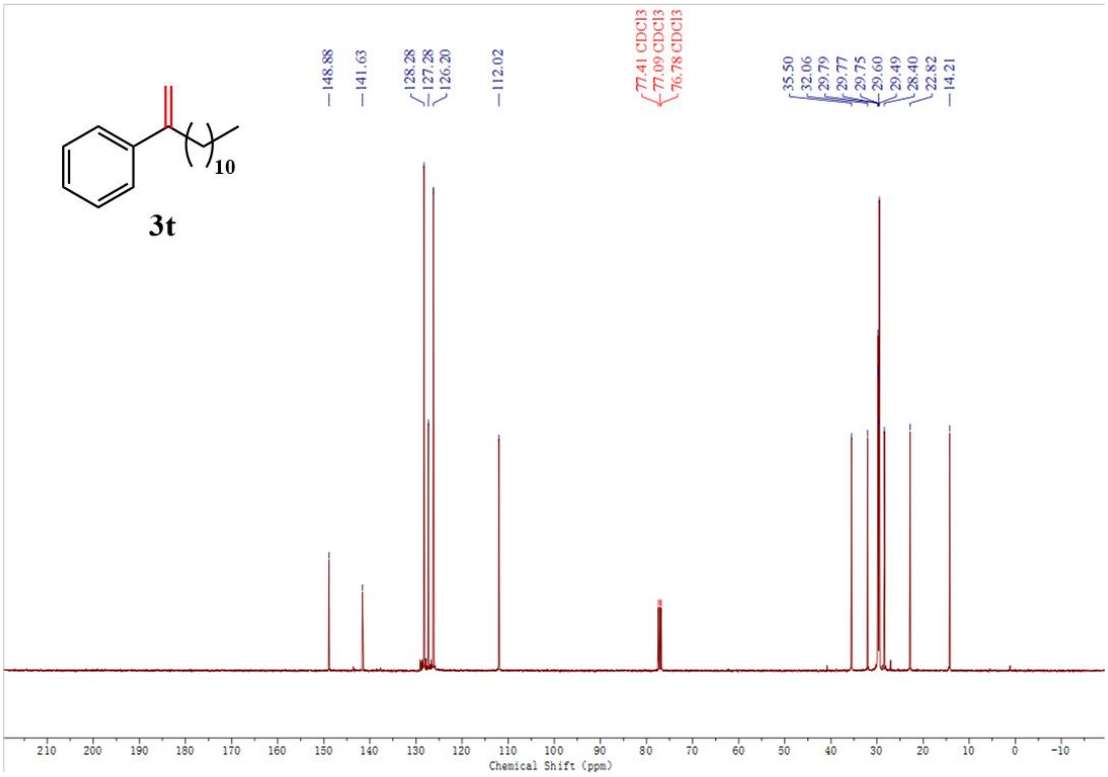
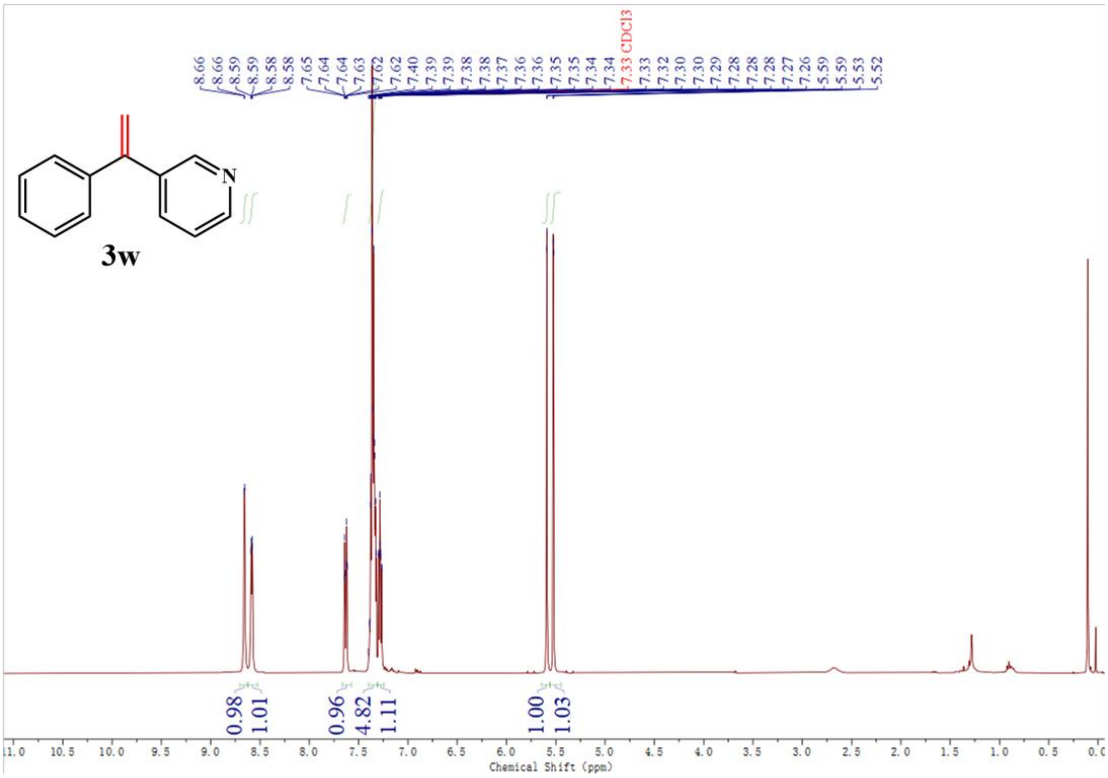
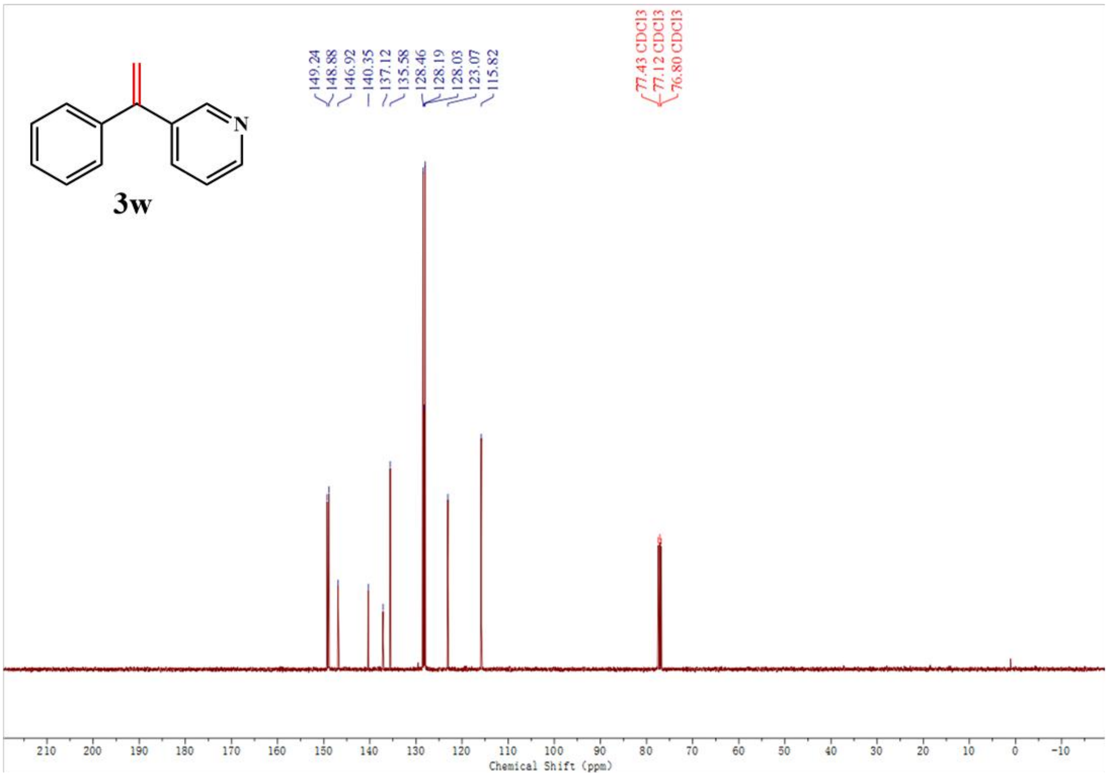


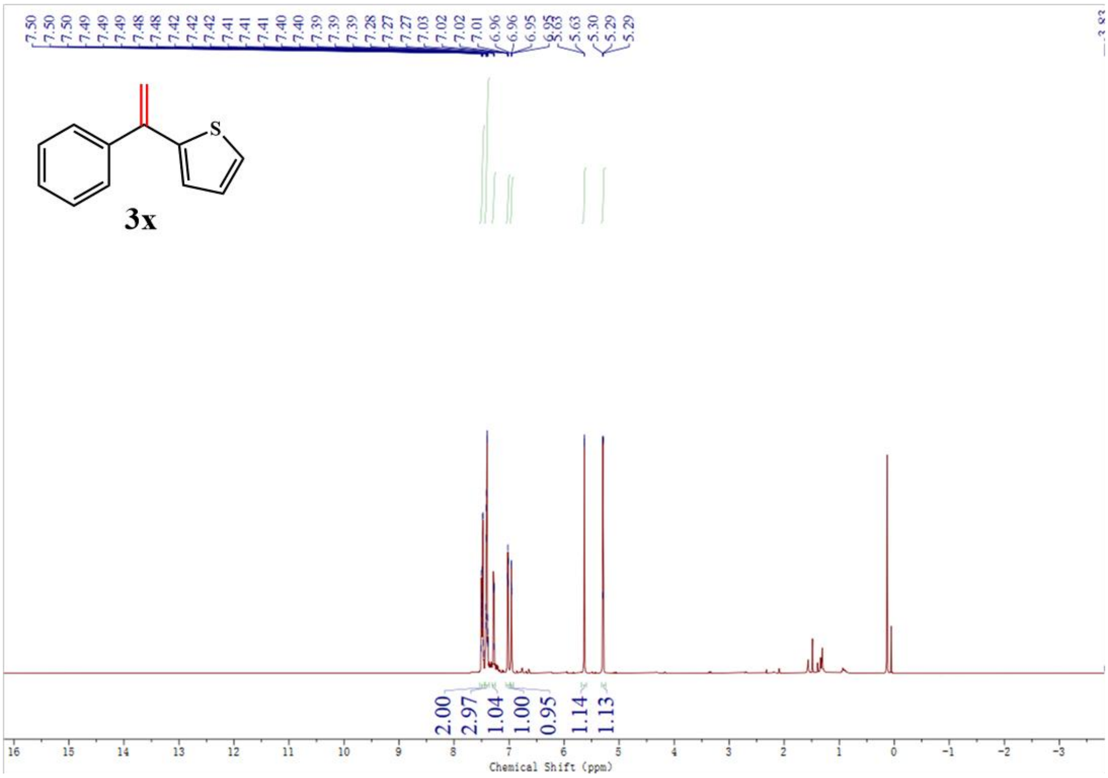
^{13}C NMR of **3t** in $CDCl_3$



^{1}H NMR of **3w** in $CDCl_3$



^{13}C NMR of **3w** in $CDCl_3$



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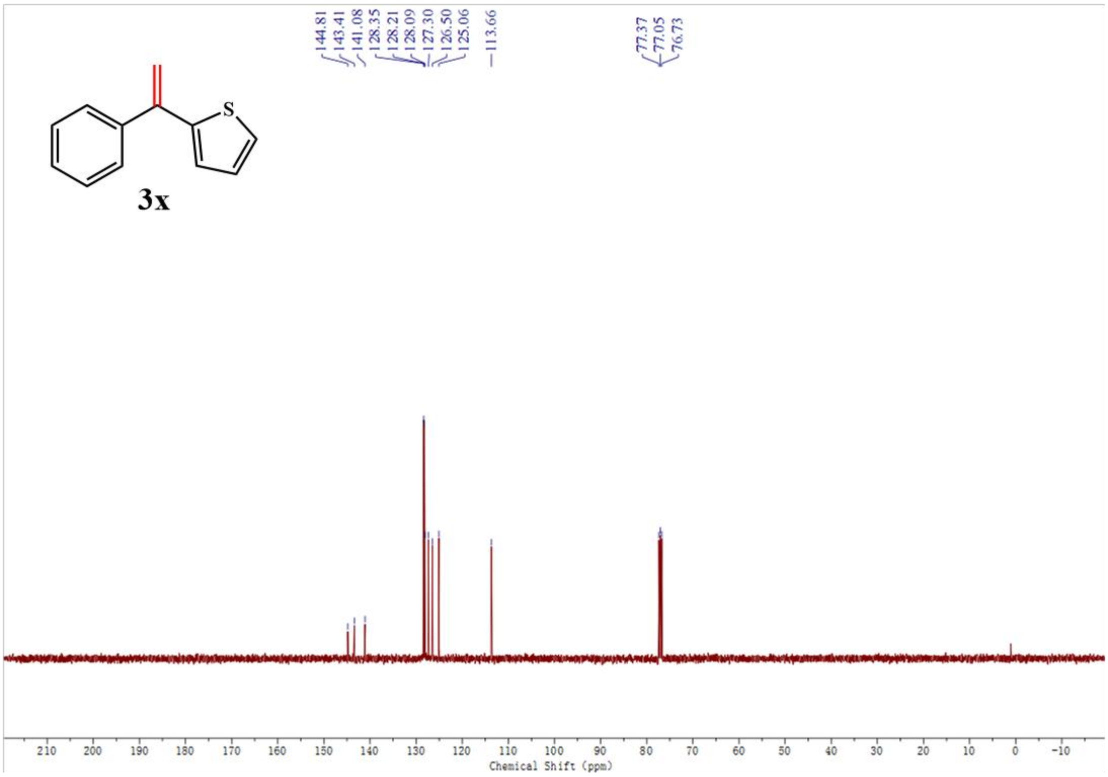
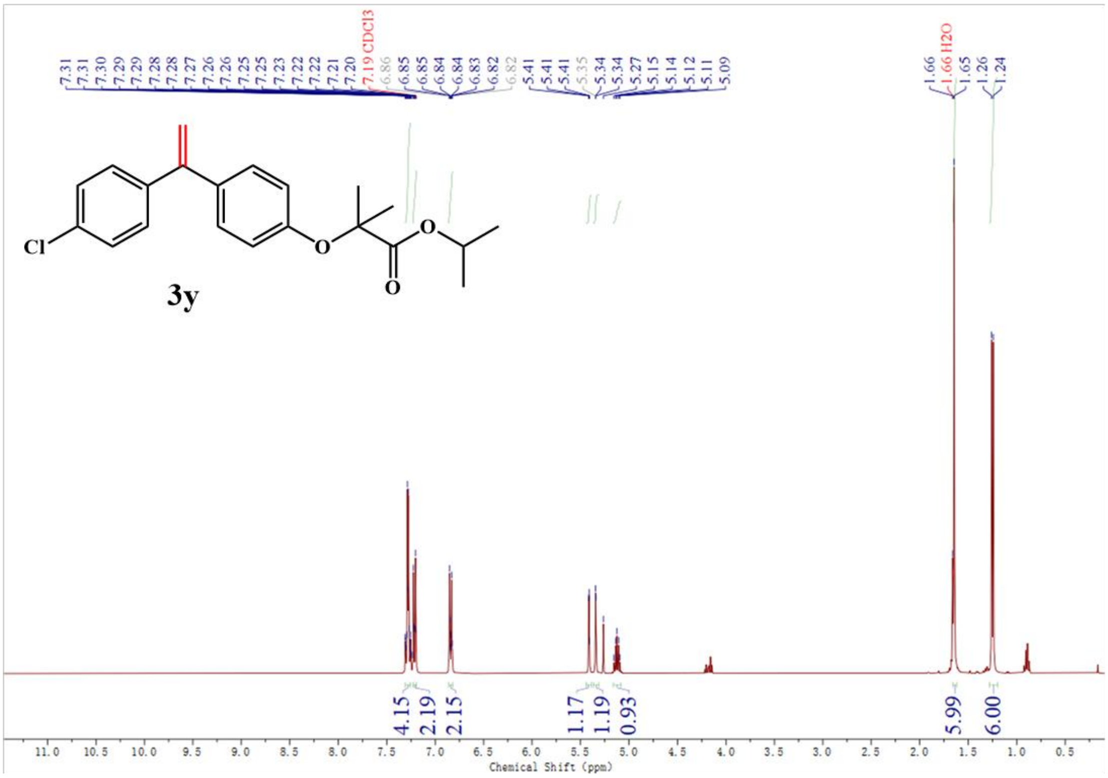


^{13}C NMR of **3x** in $CDCl_3$



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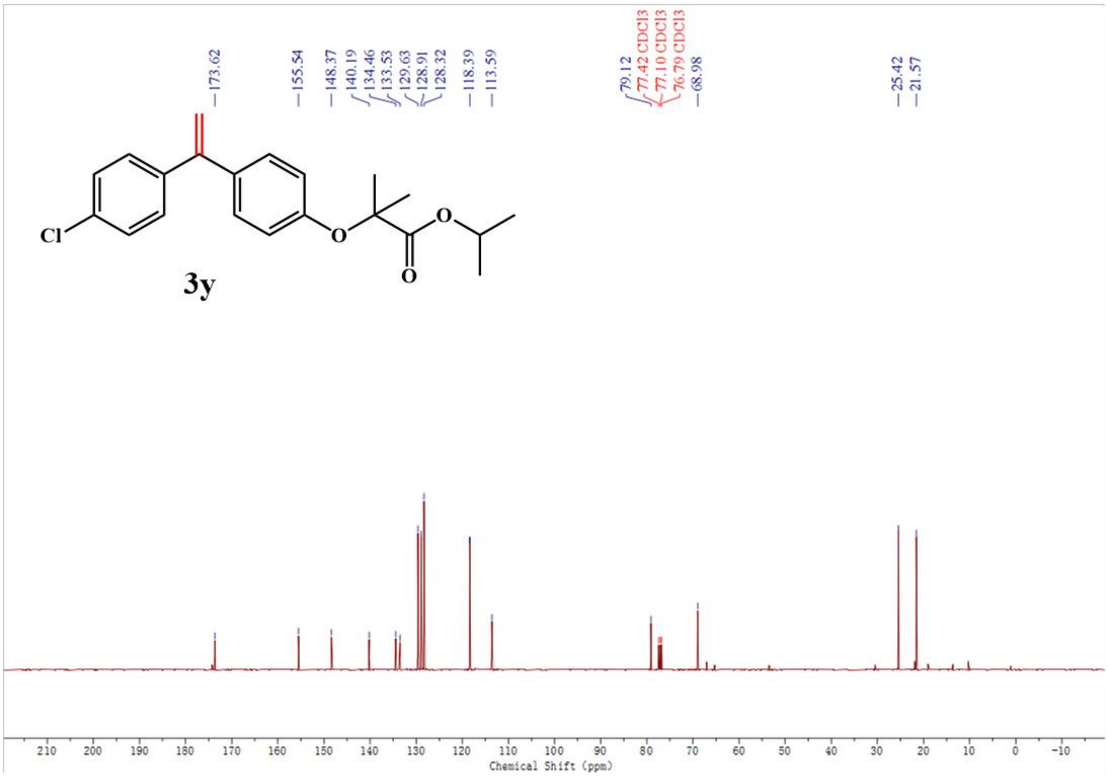

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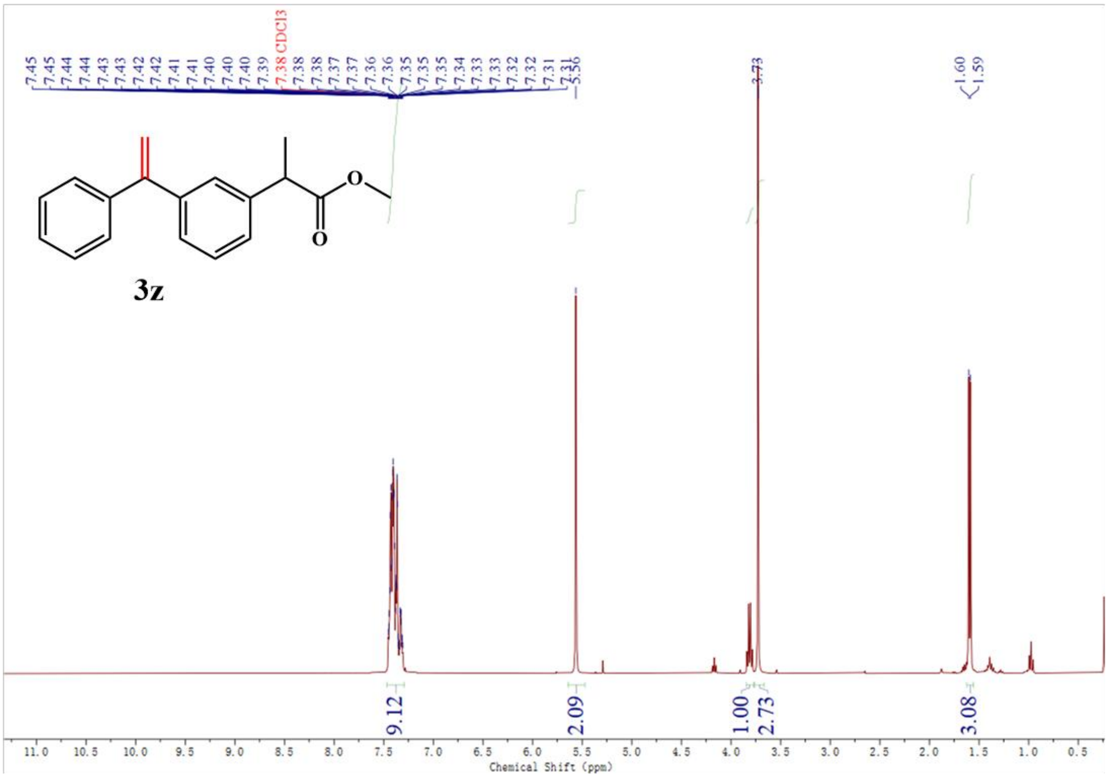

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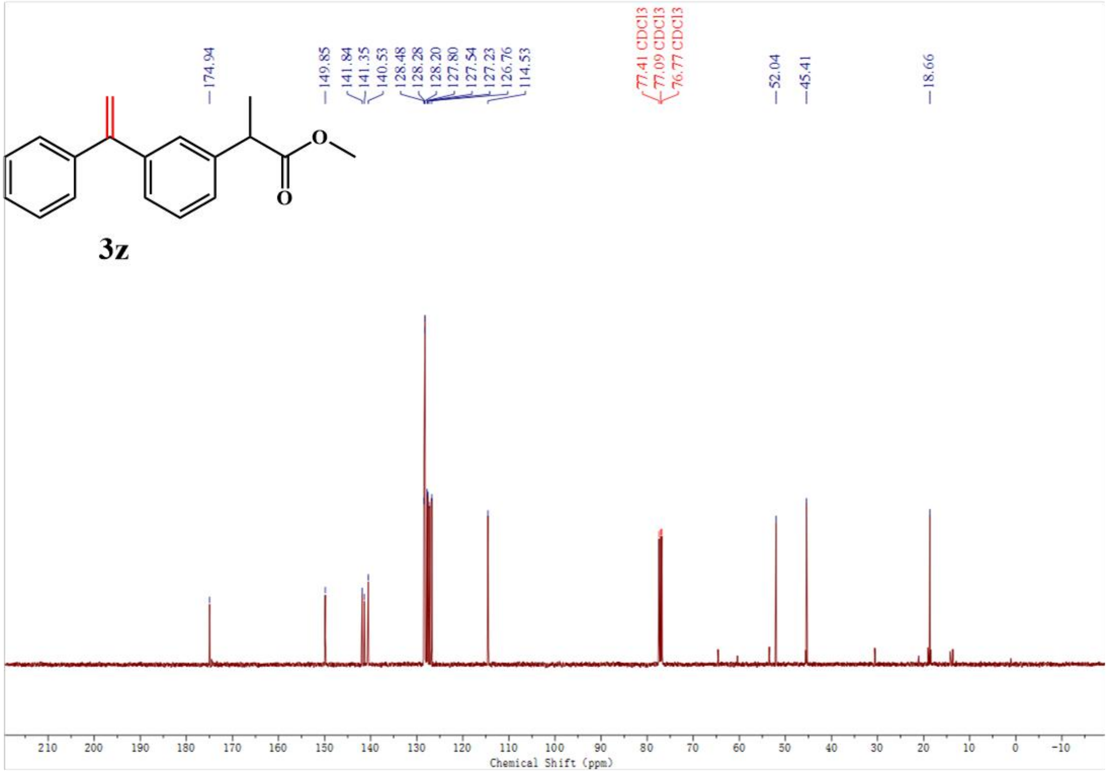

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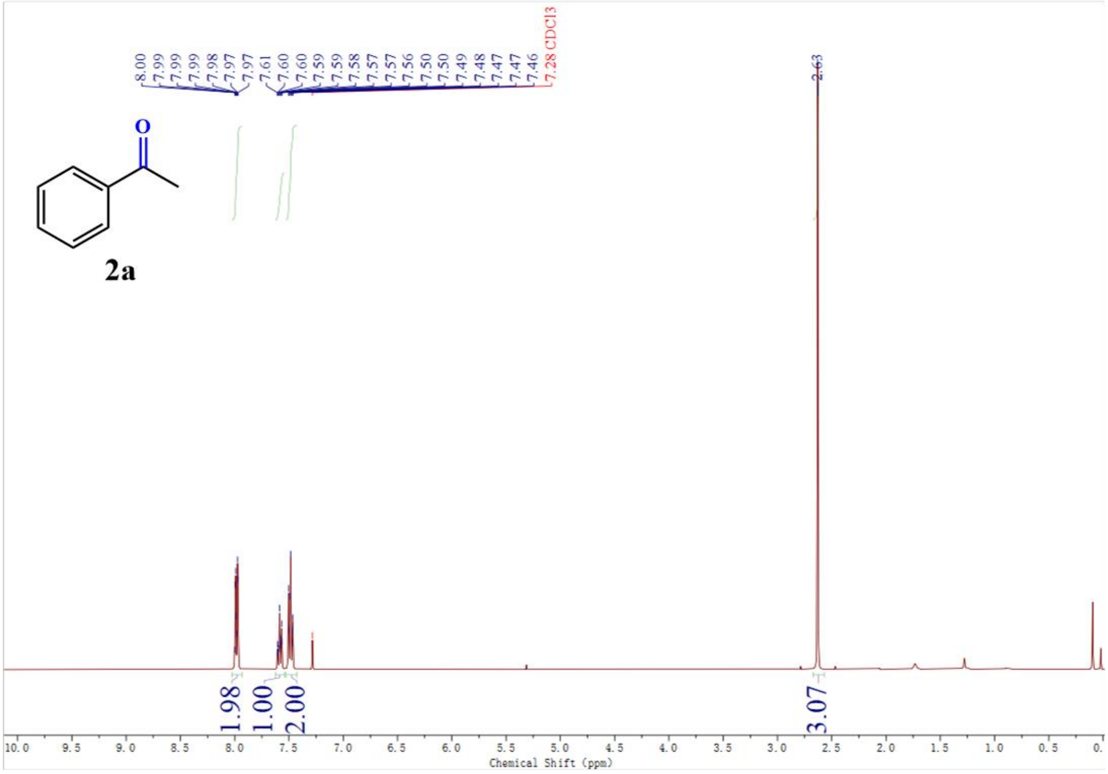

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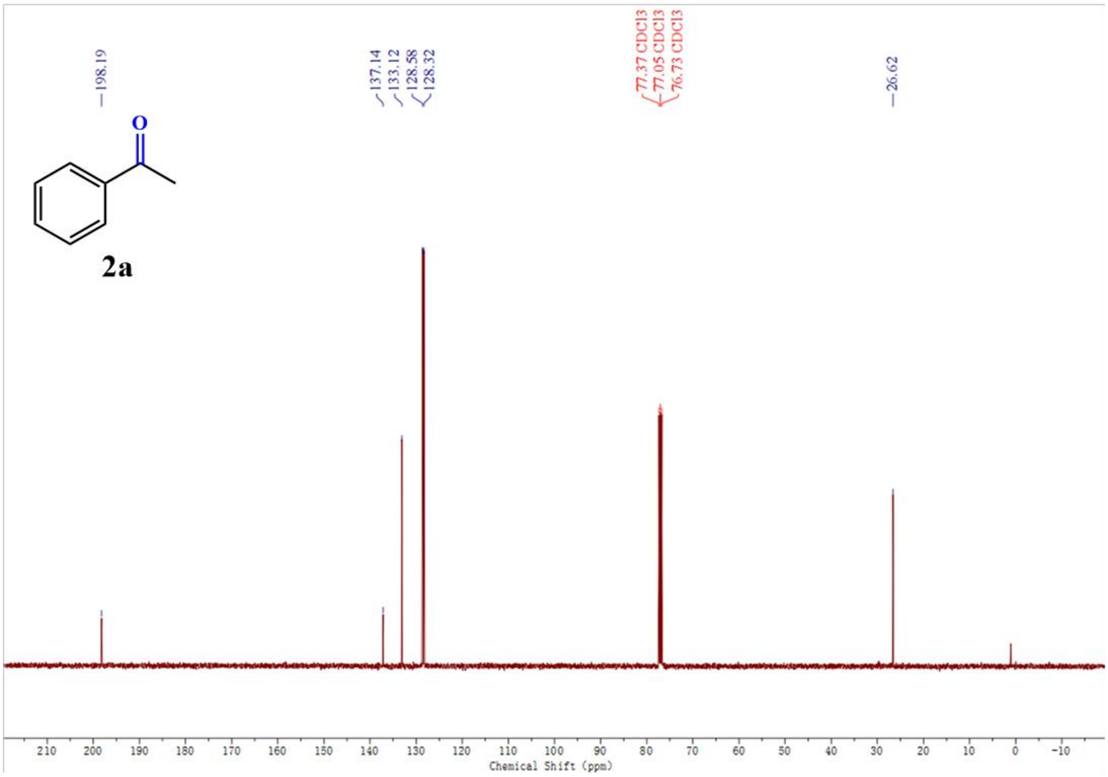
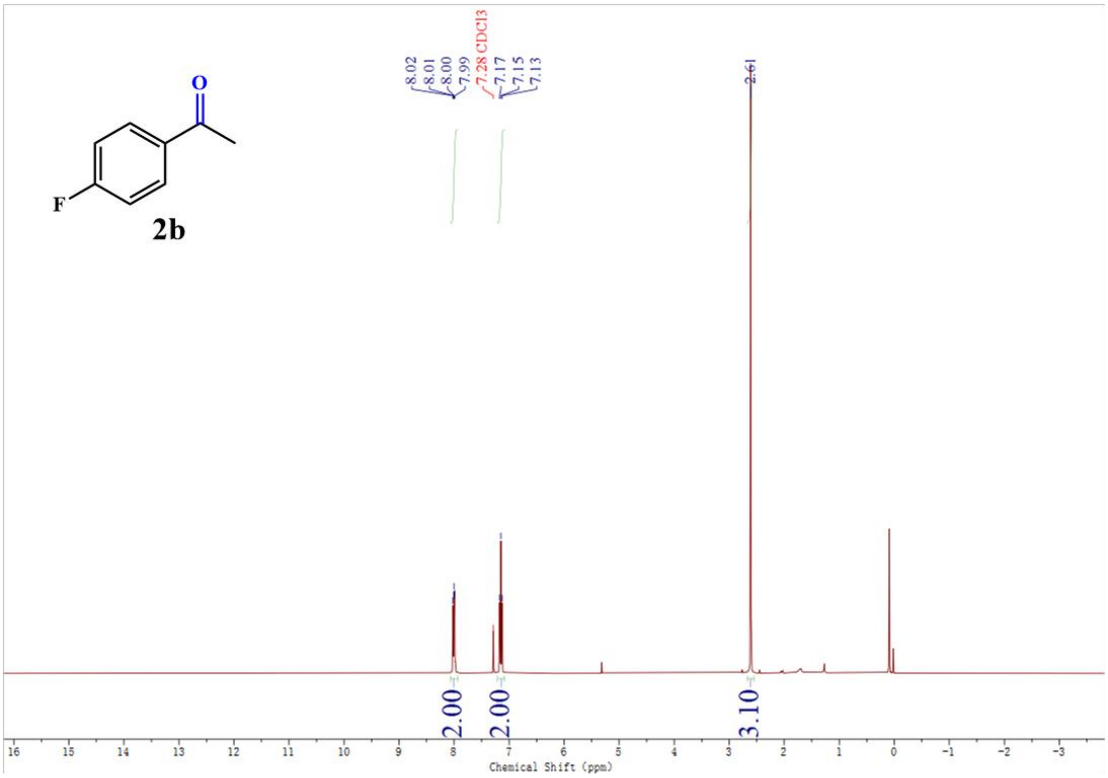


^{13}C NMR of **2a** in CDCl$_3$



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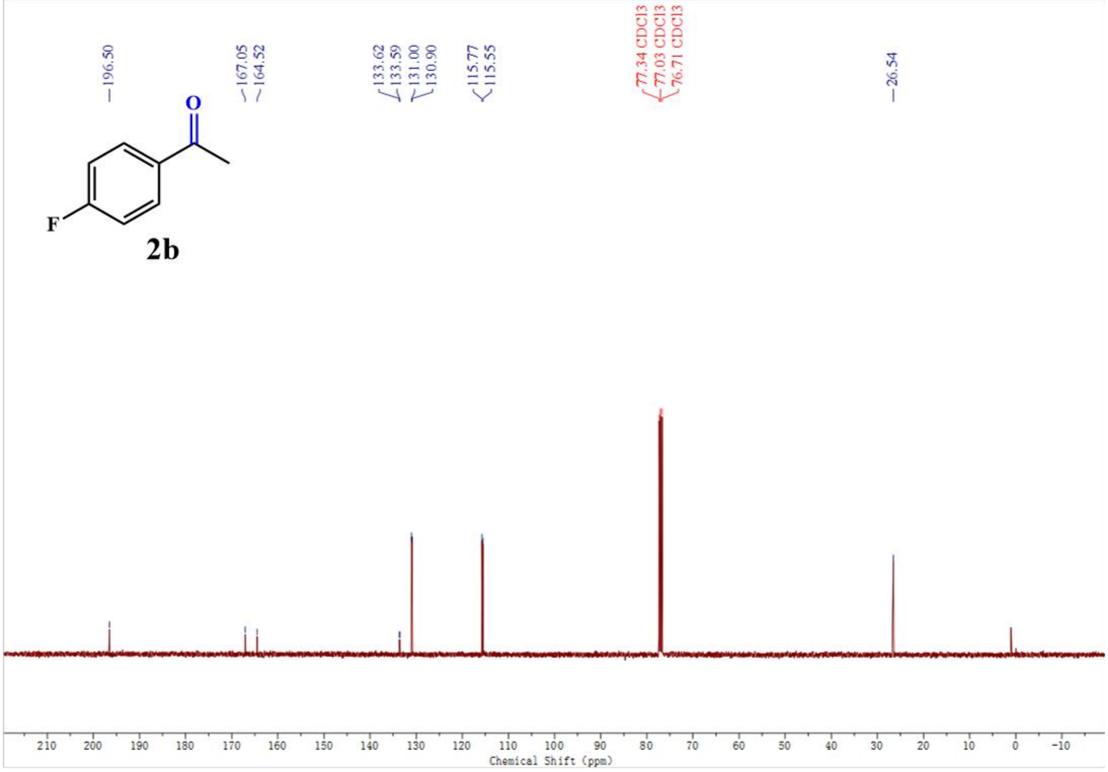

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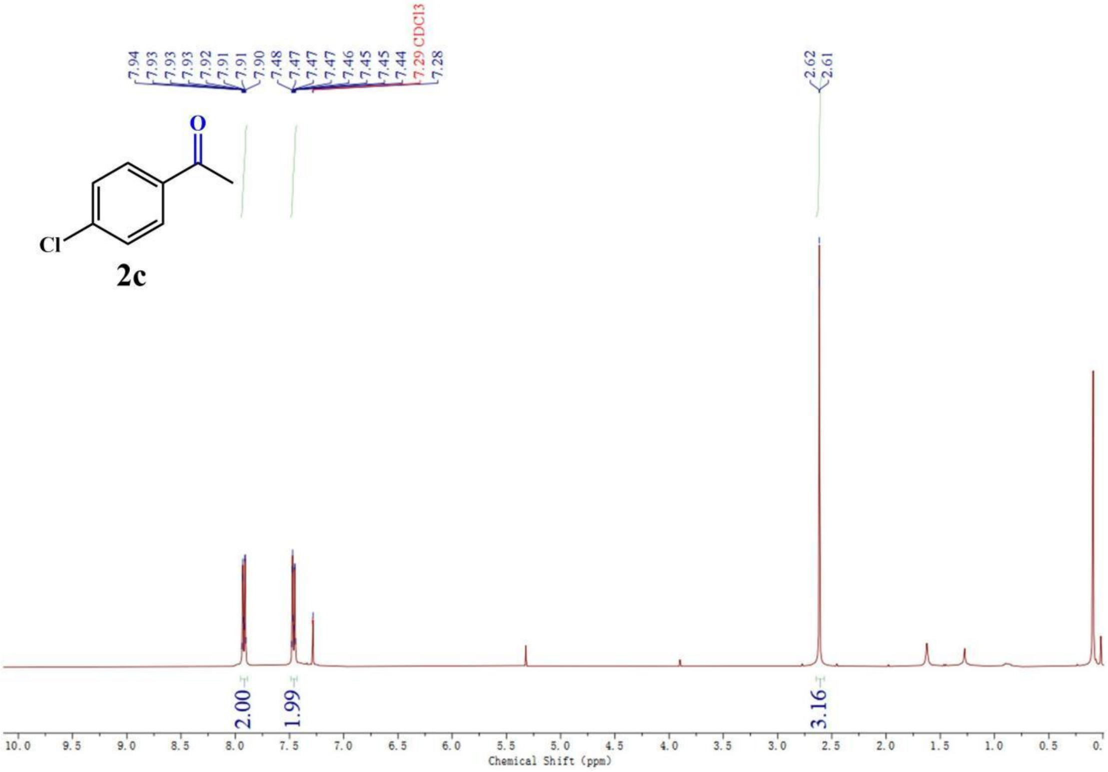

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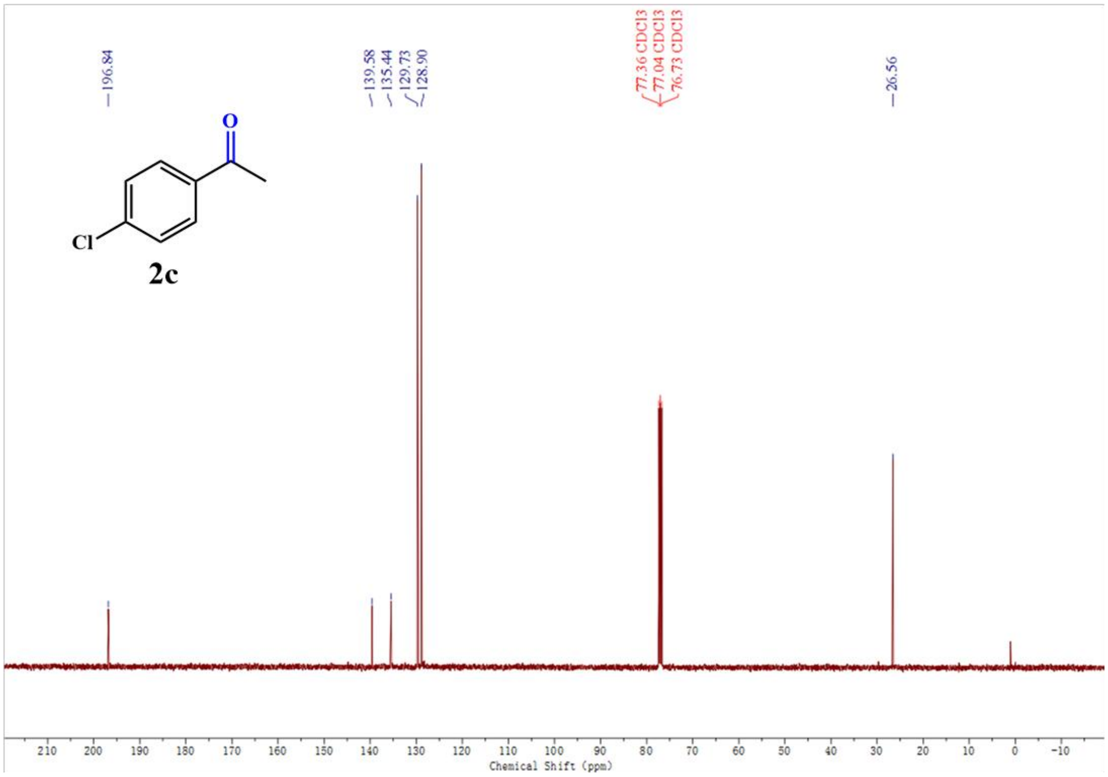

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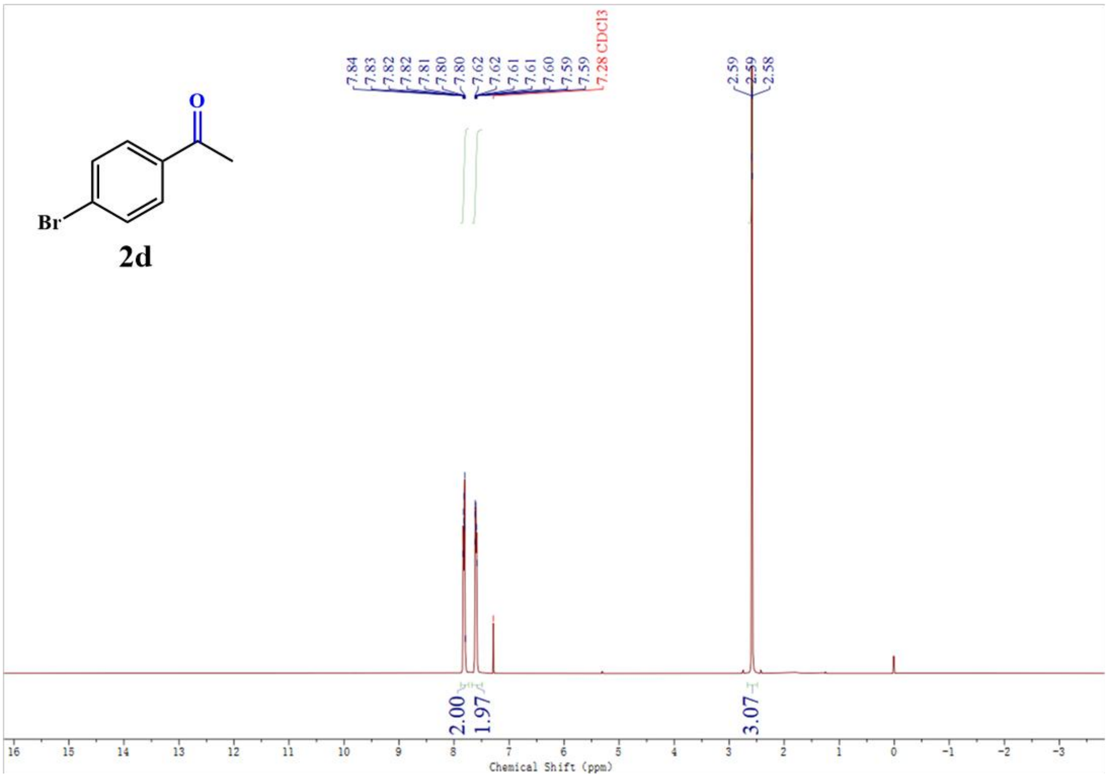

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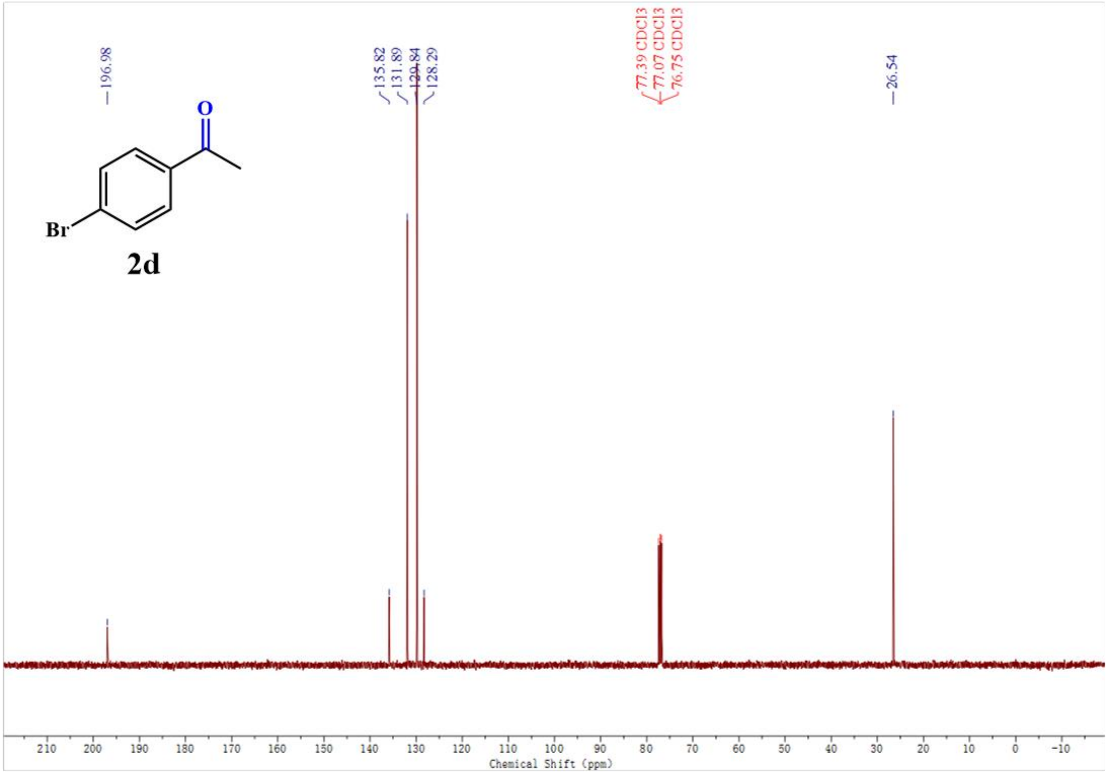

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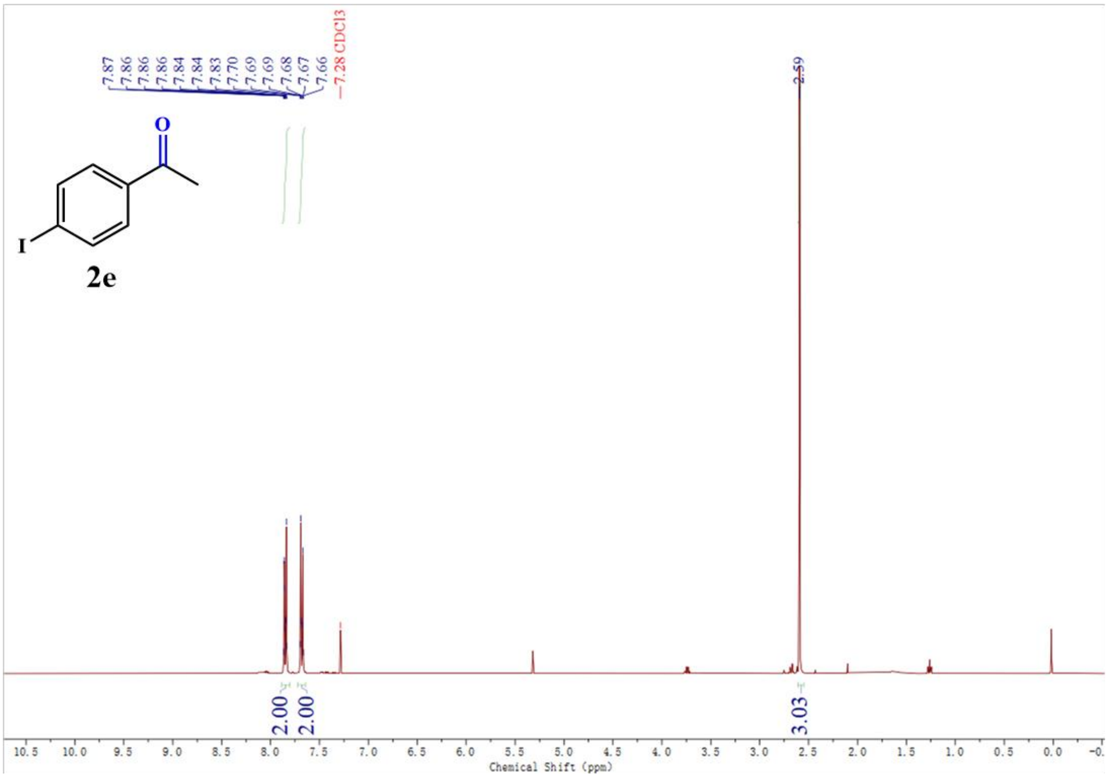

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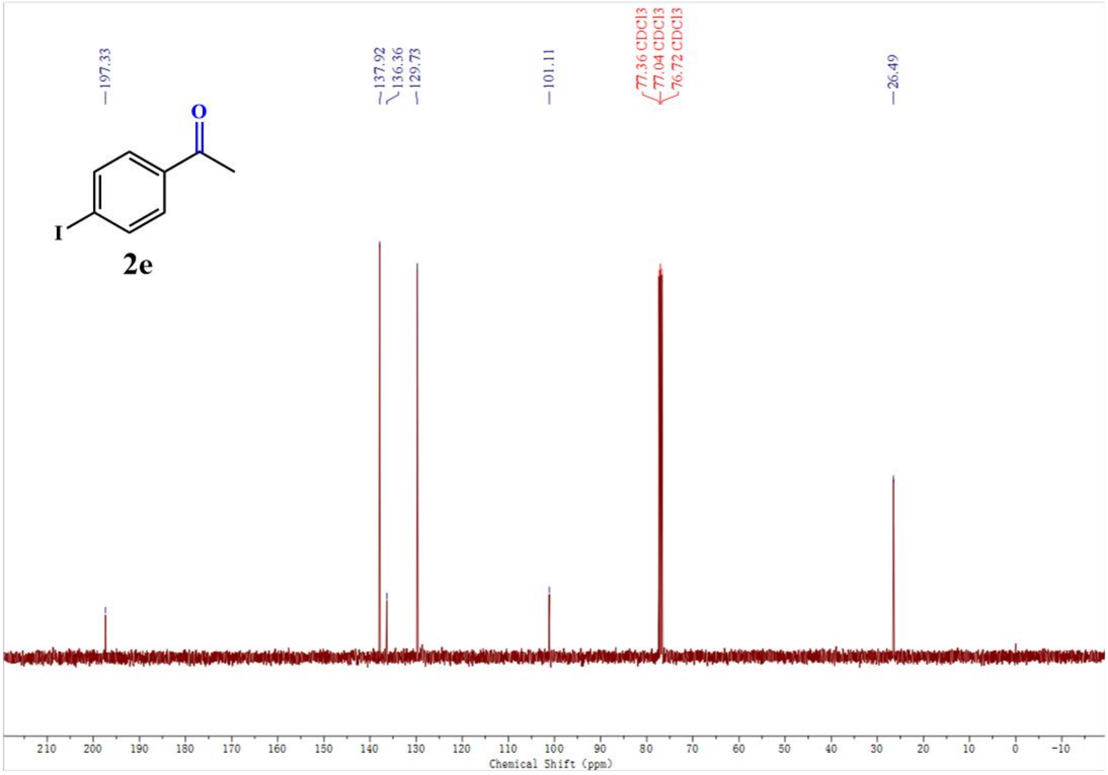

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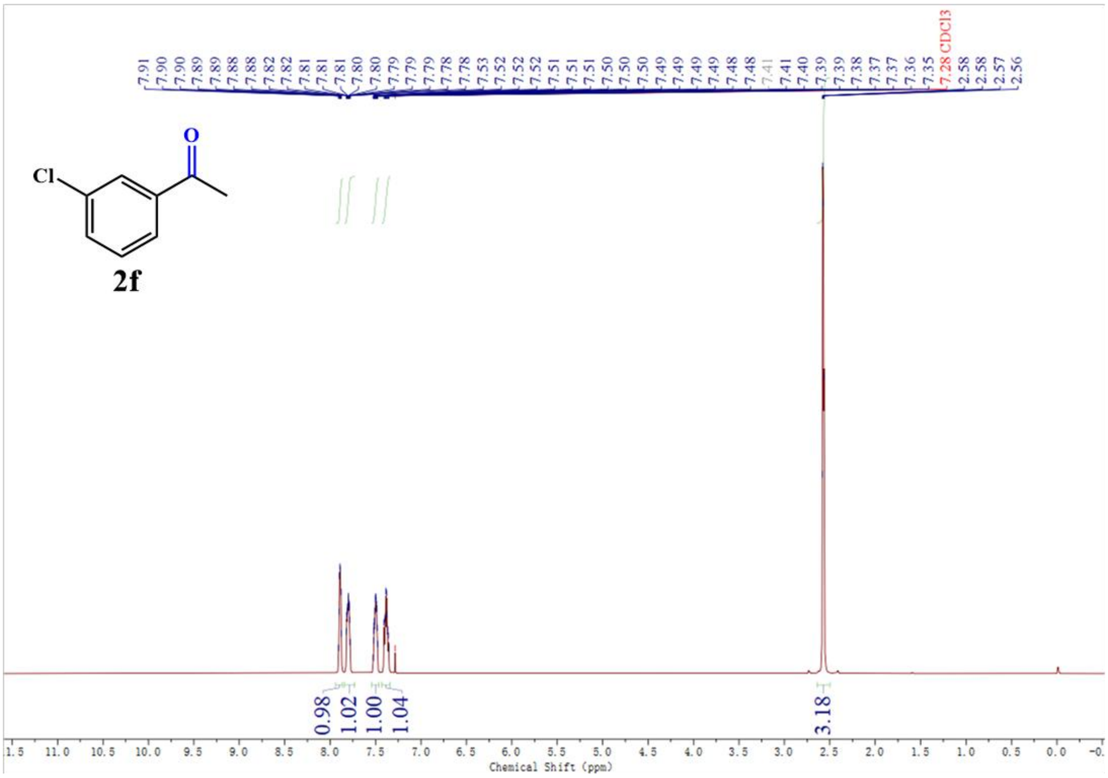

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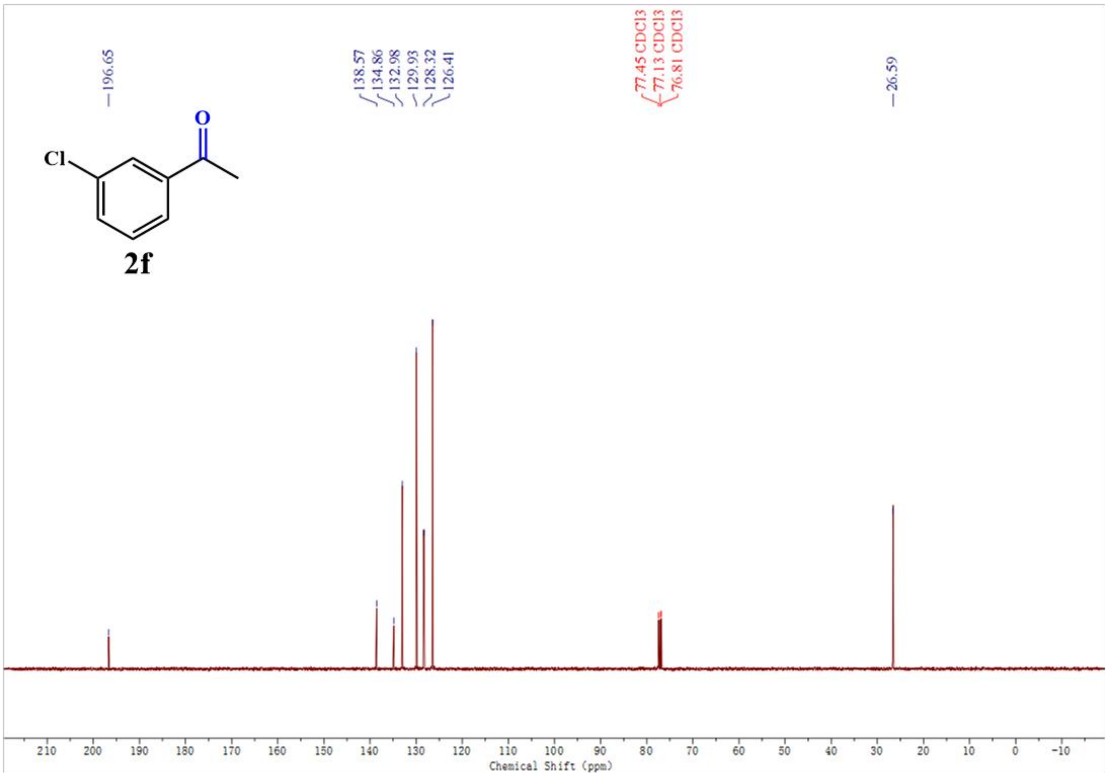

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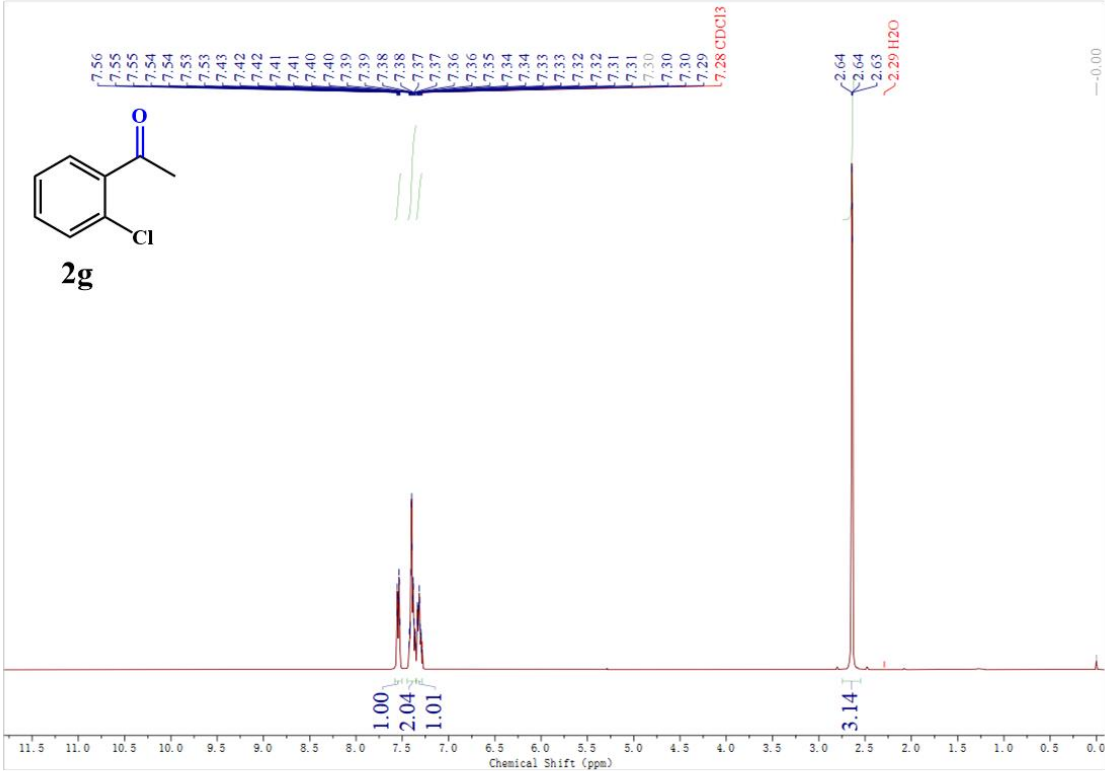

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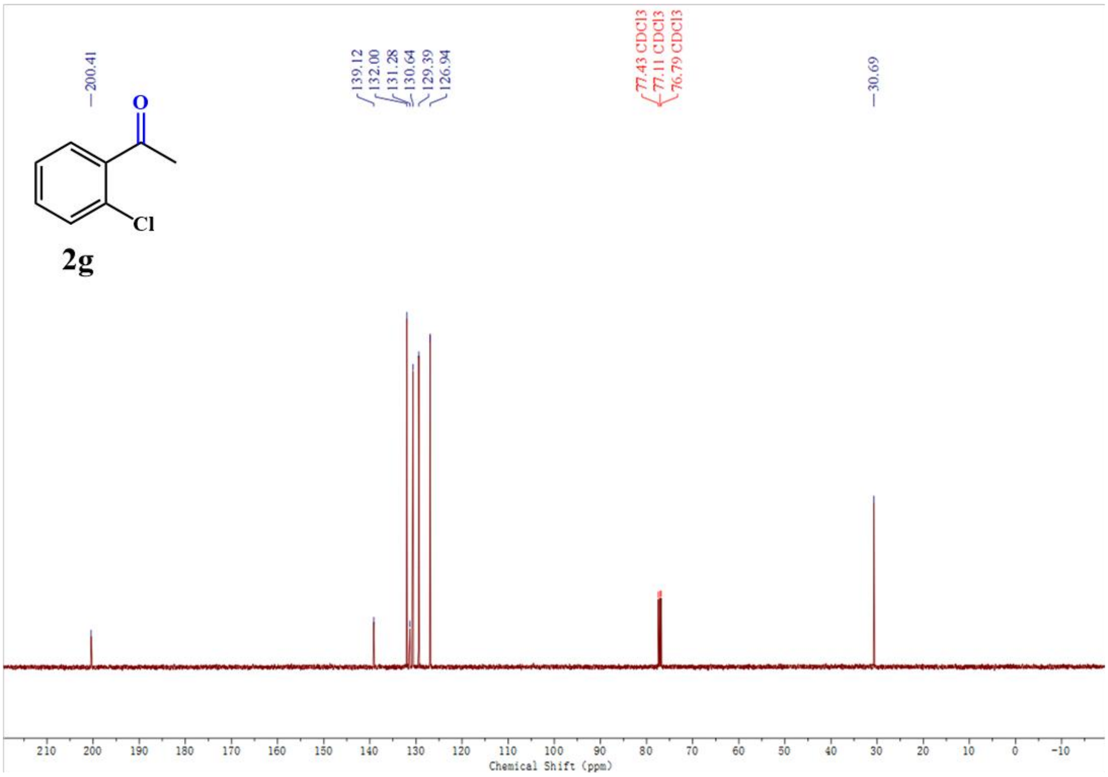

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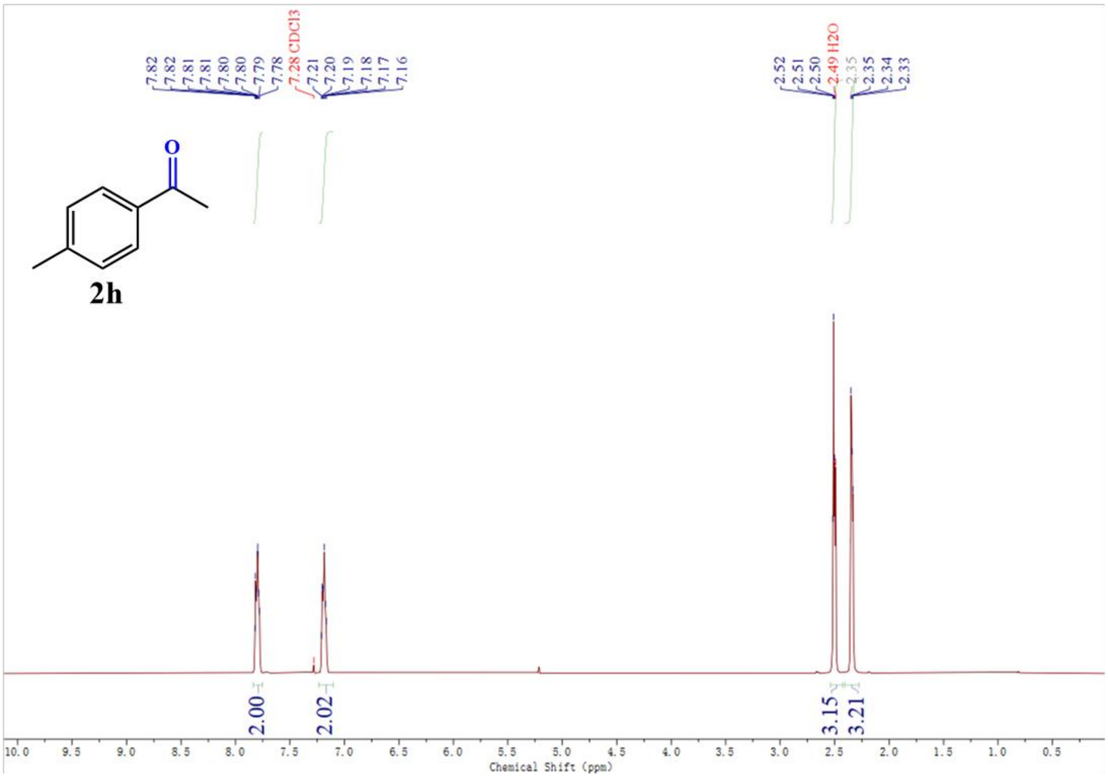

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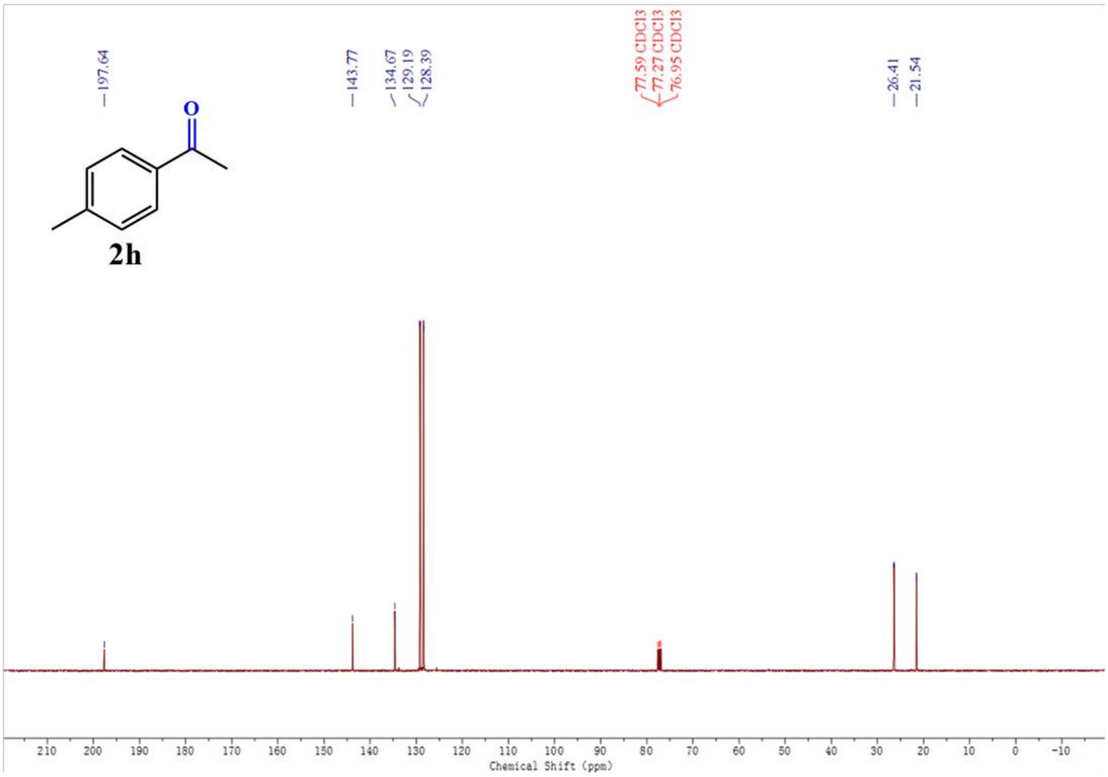

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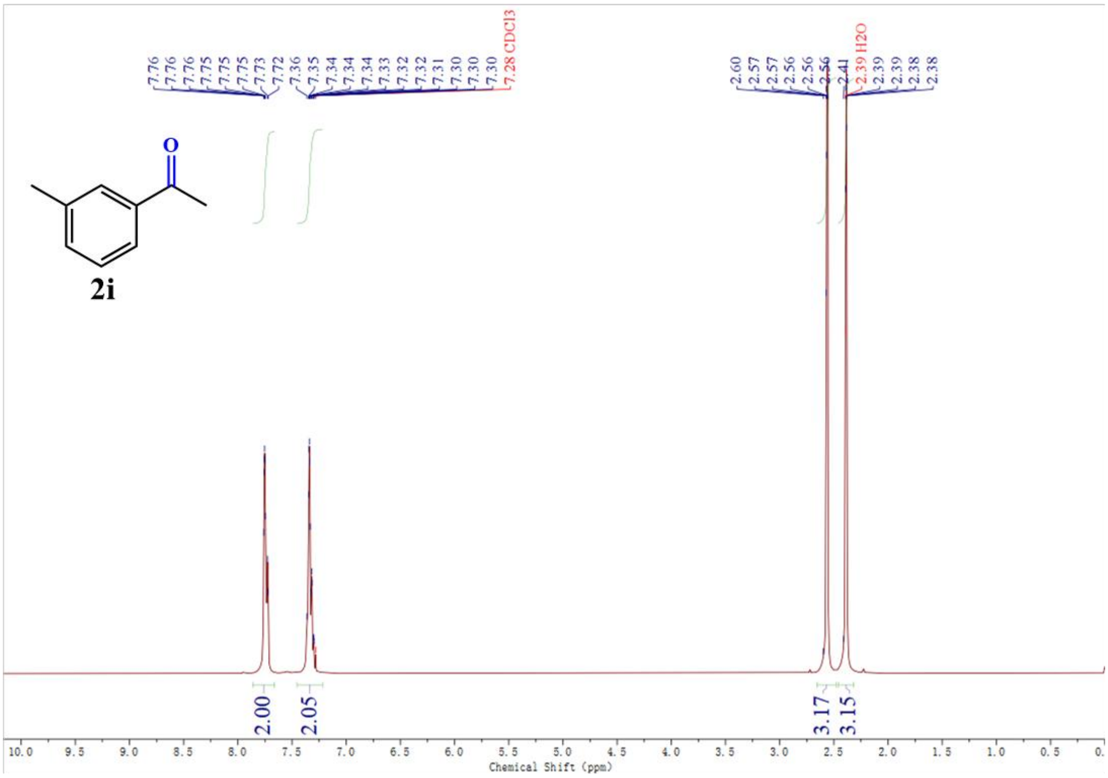

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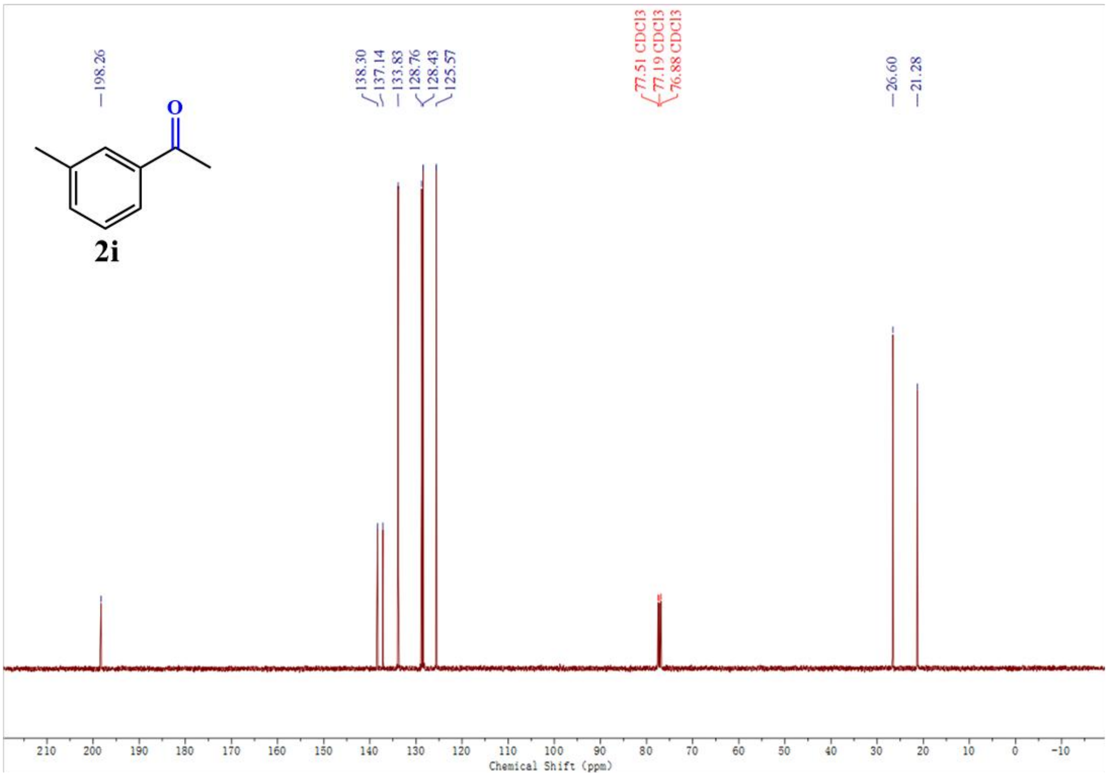
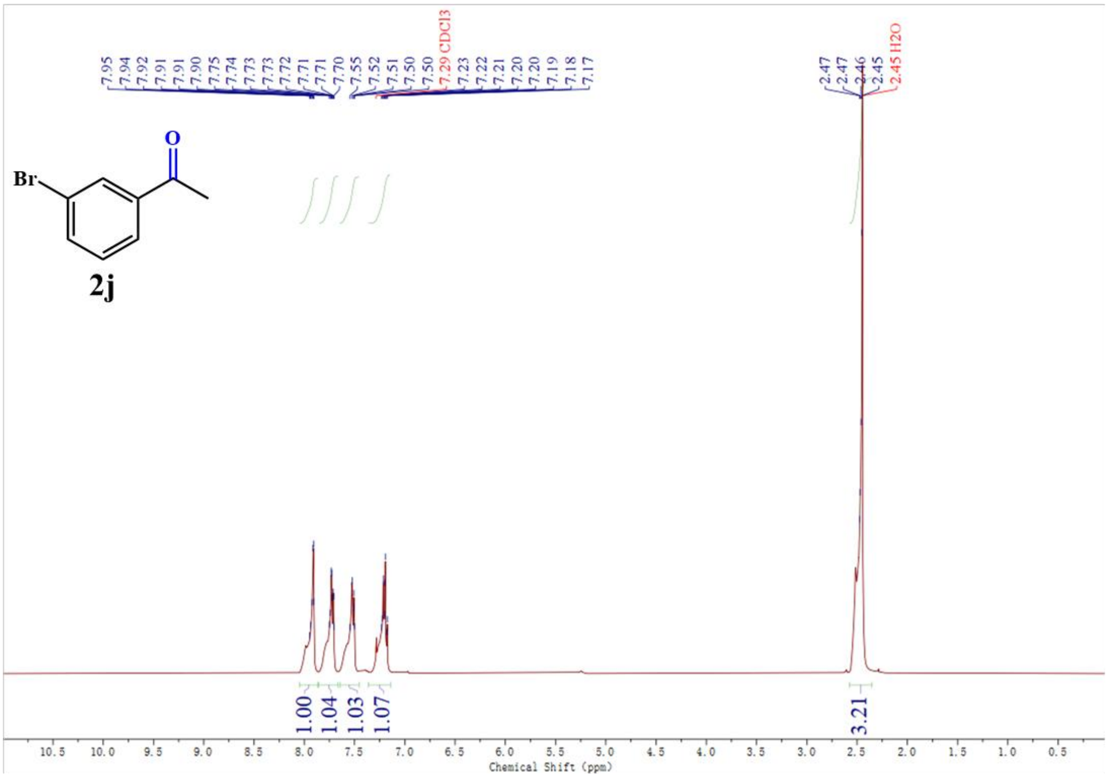


^{13}C NMR of **2i** in $CDCl_3$



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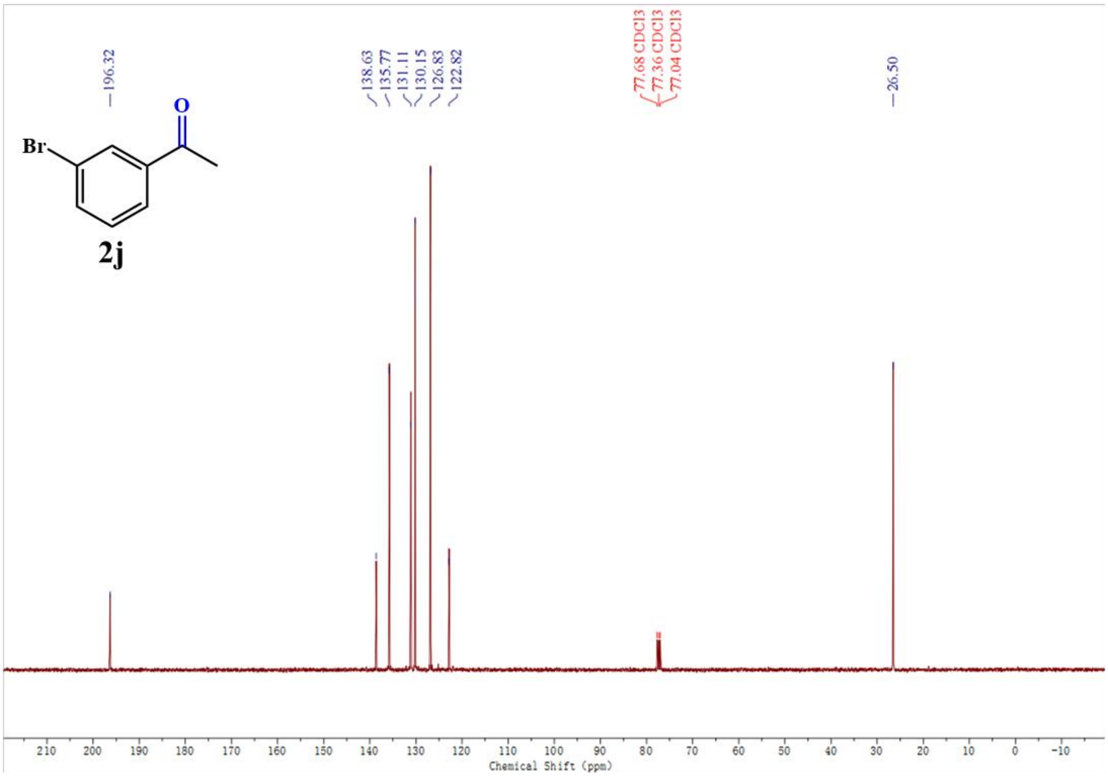

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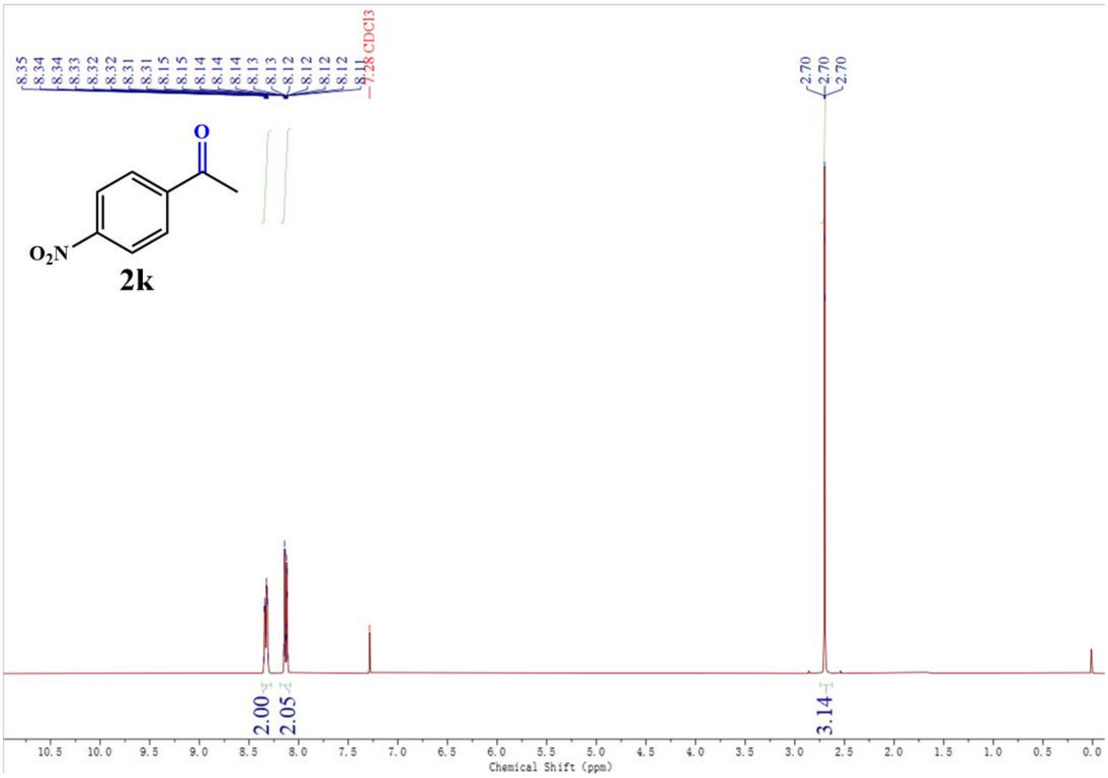

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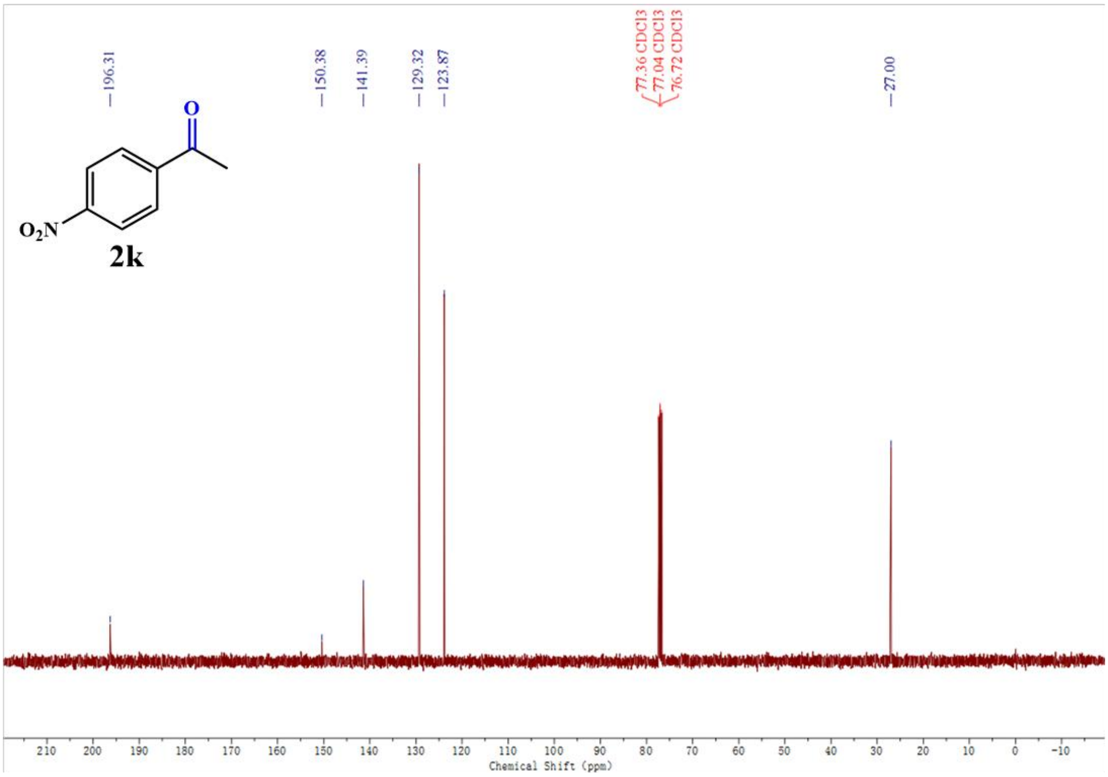

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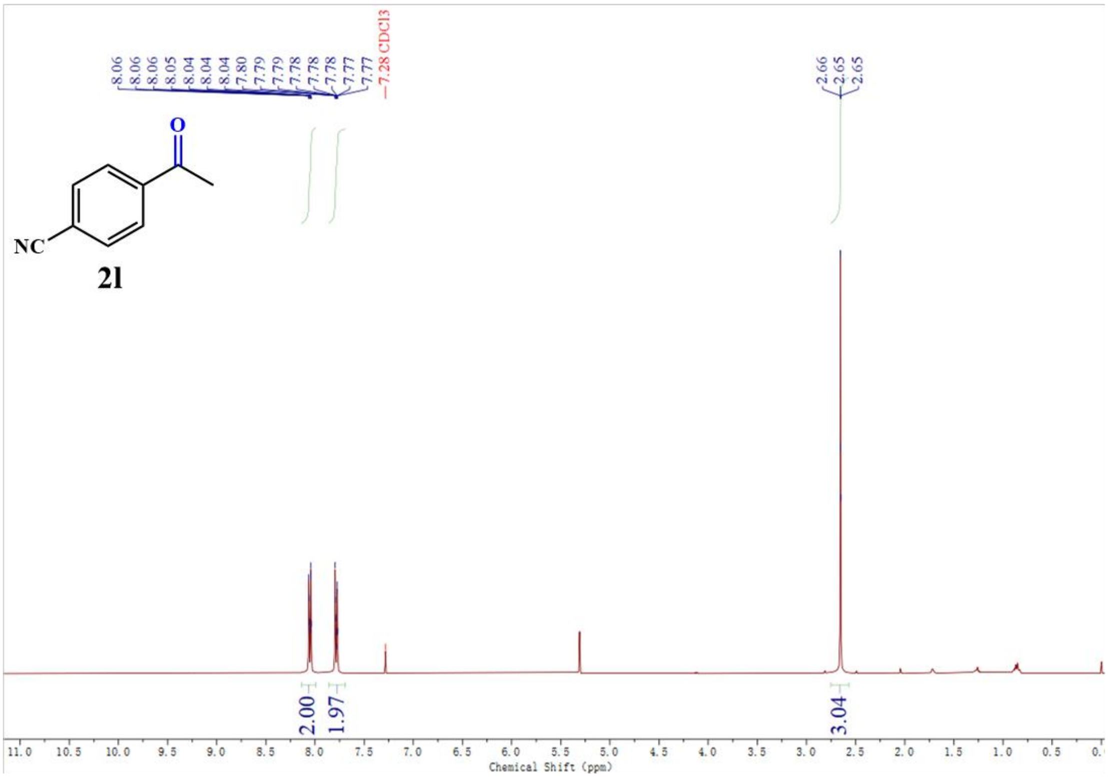

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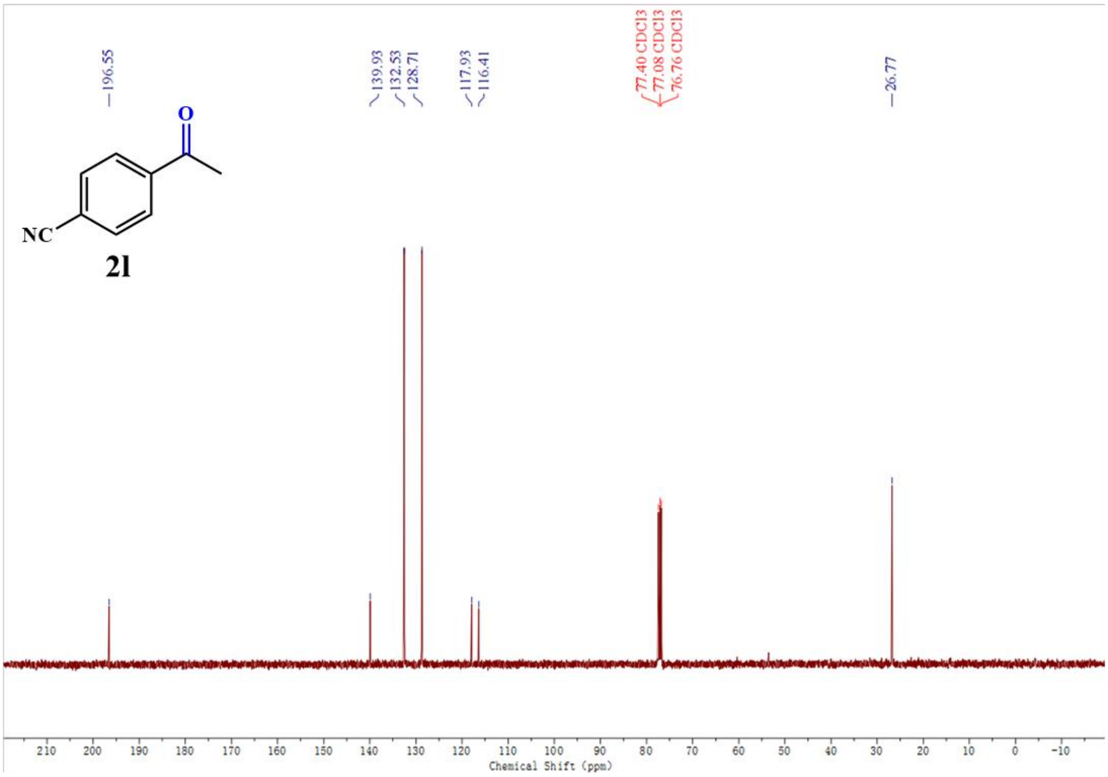

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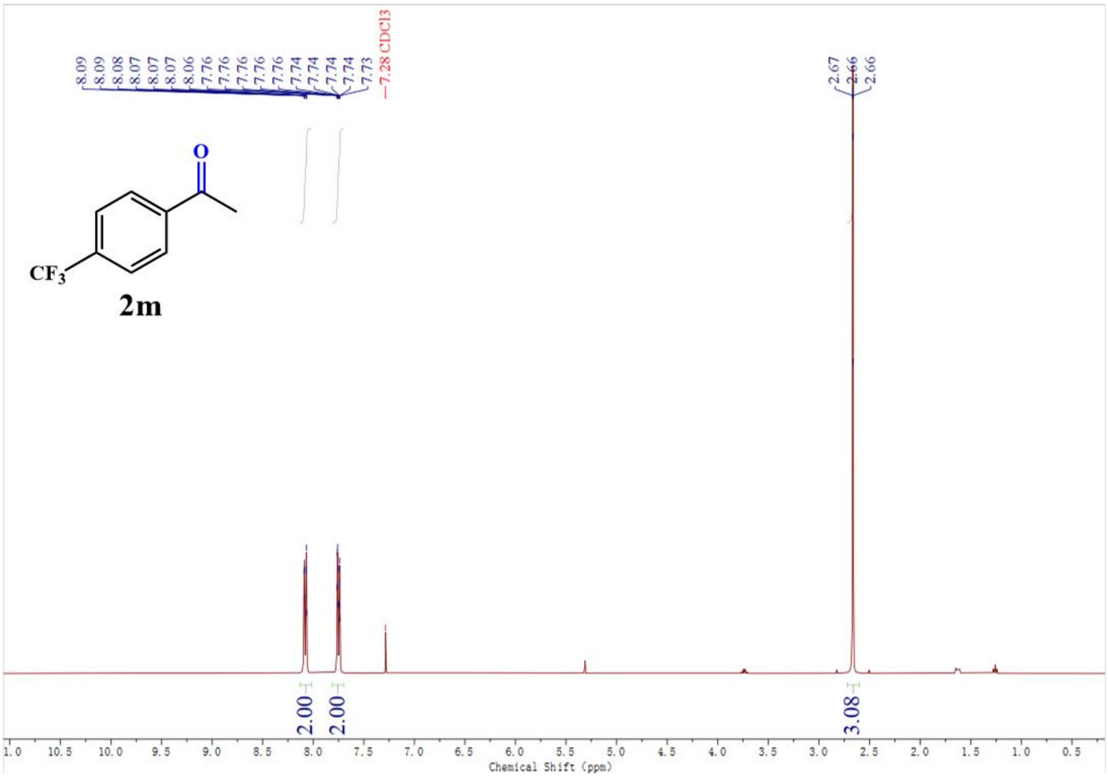

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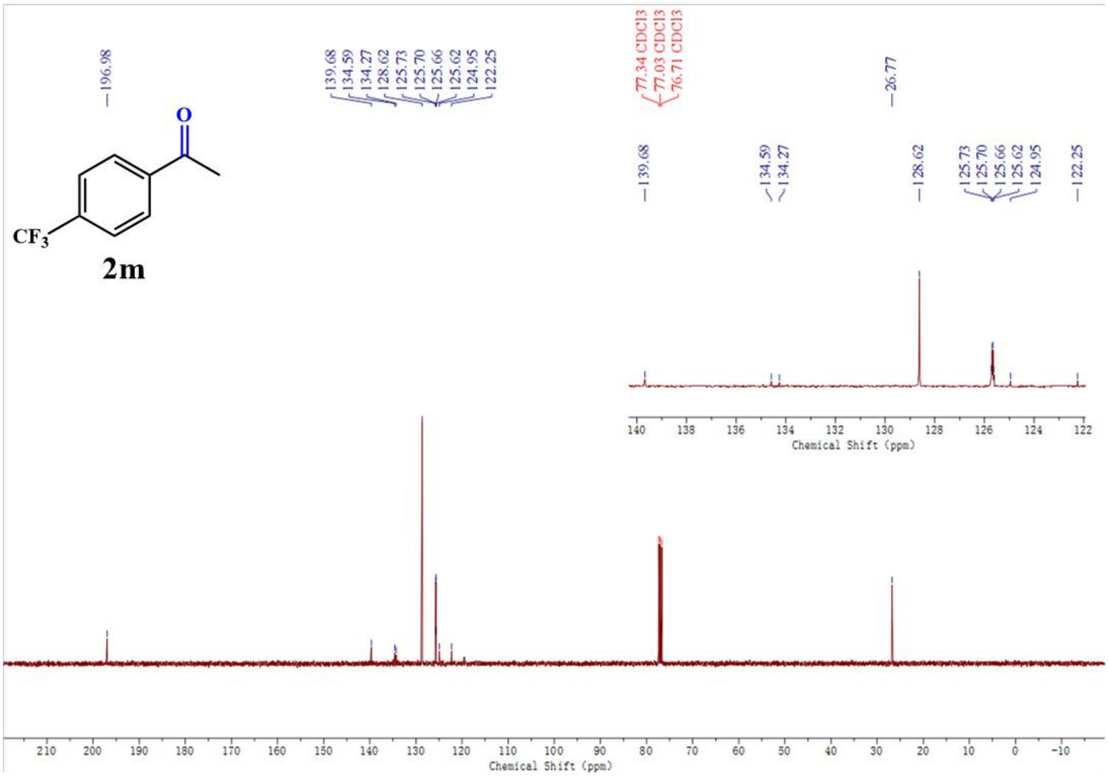

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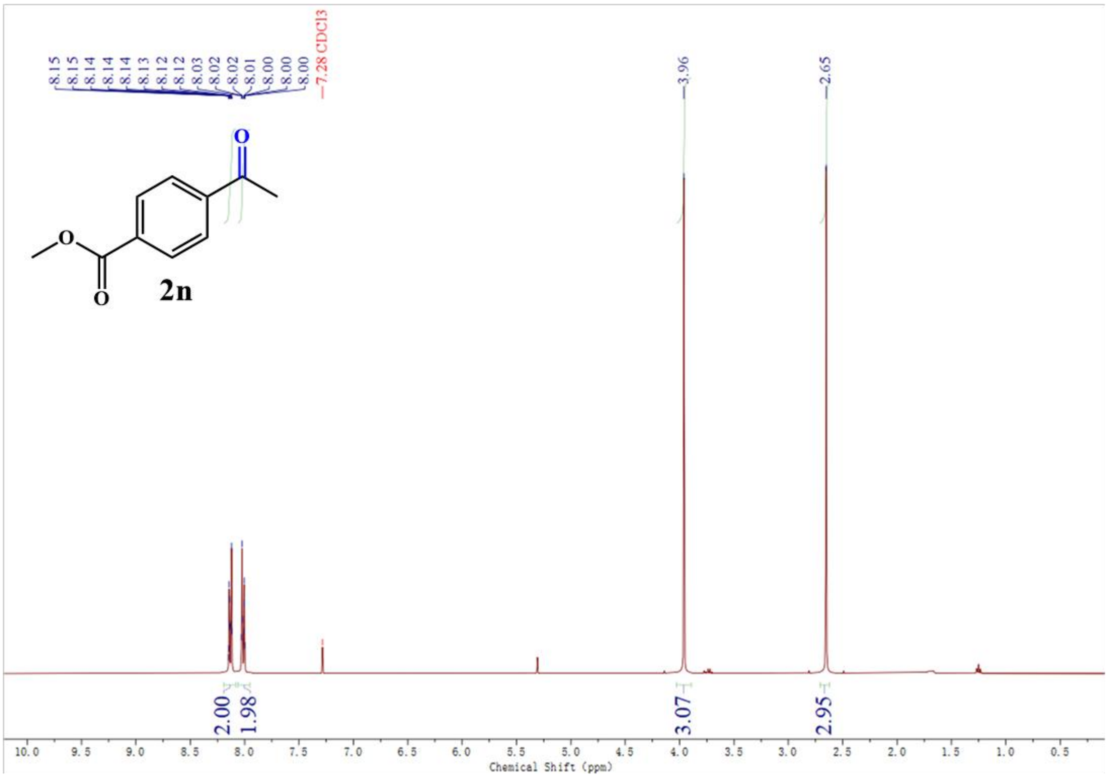

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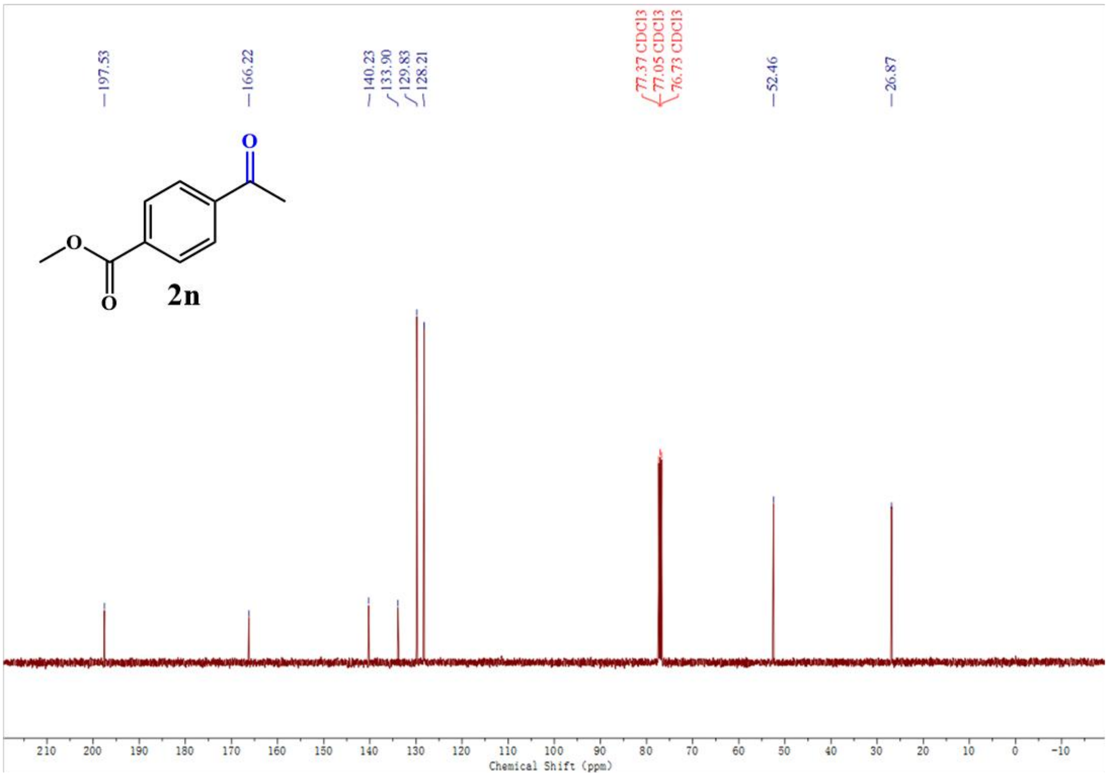

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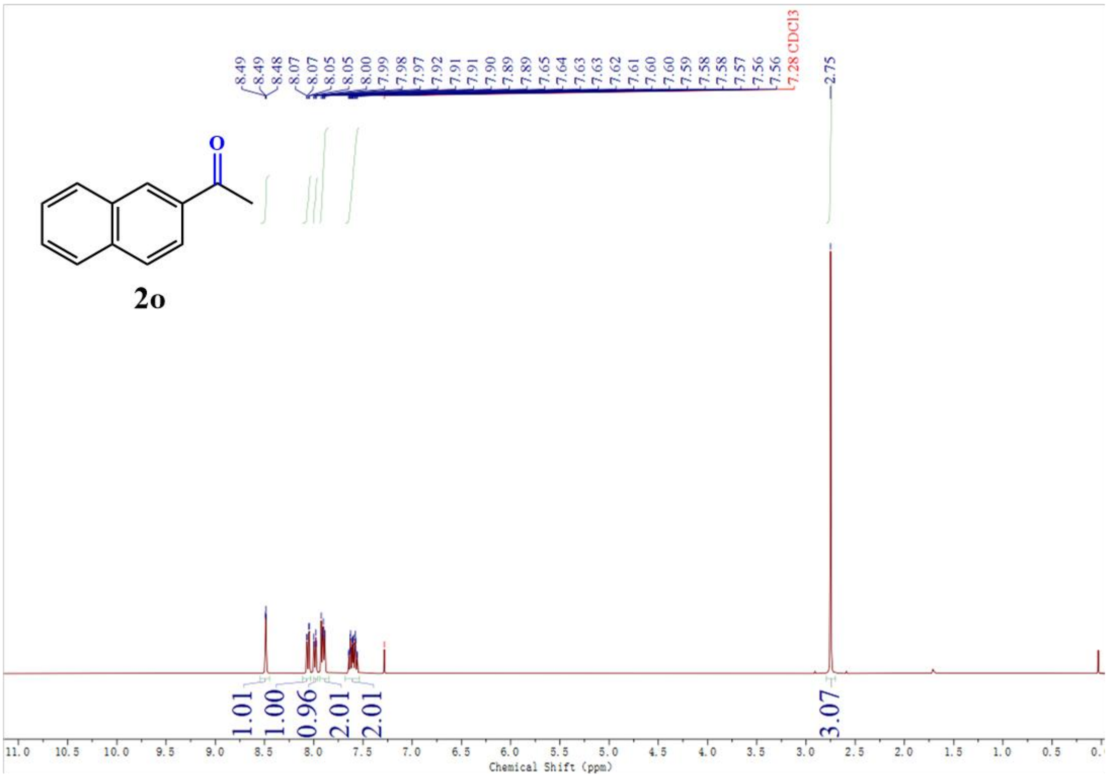

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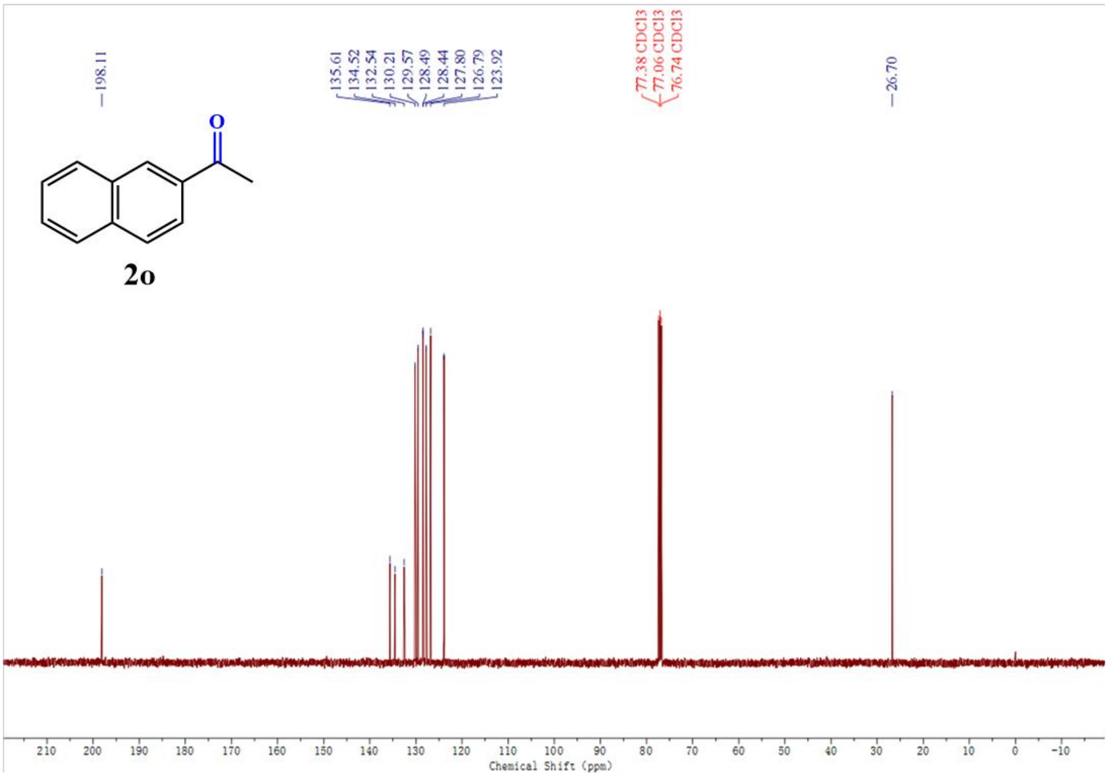

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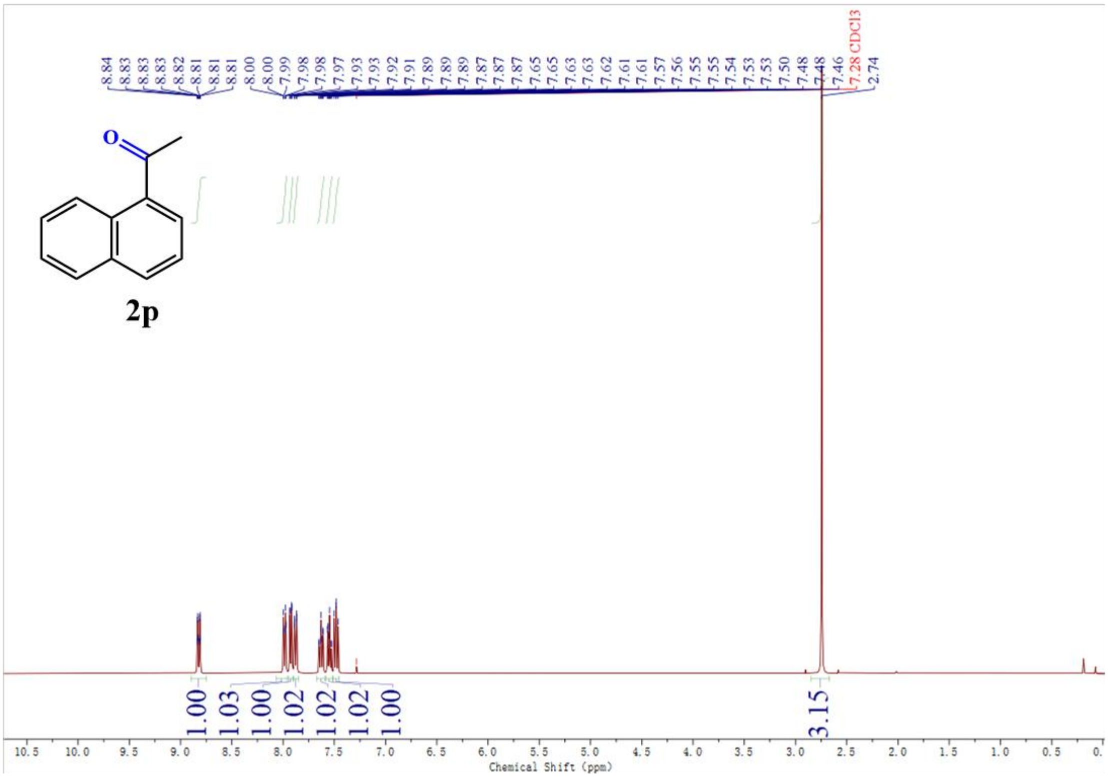

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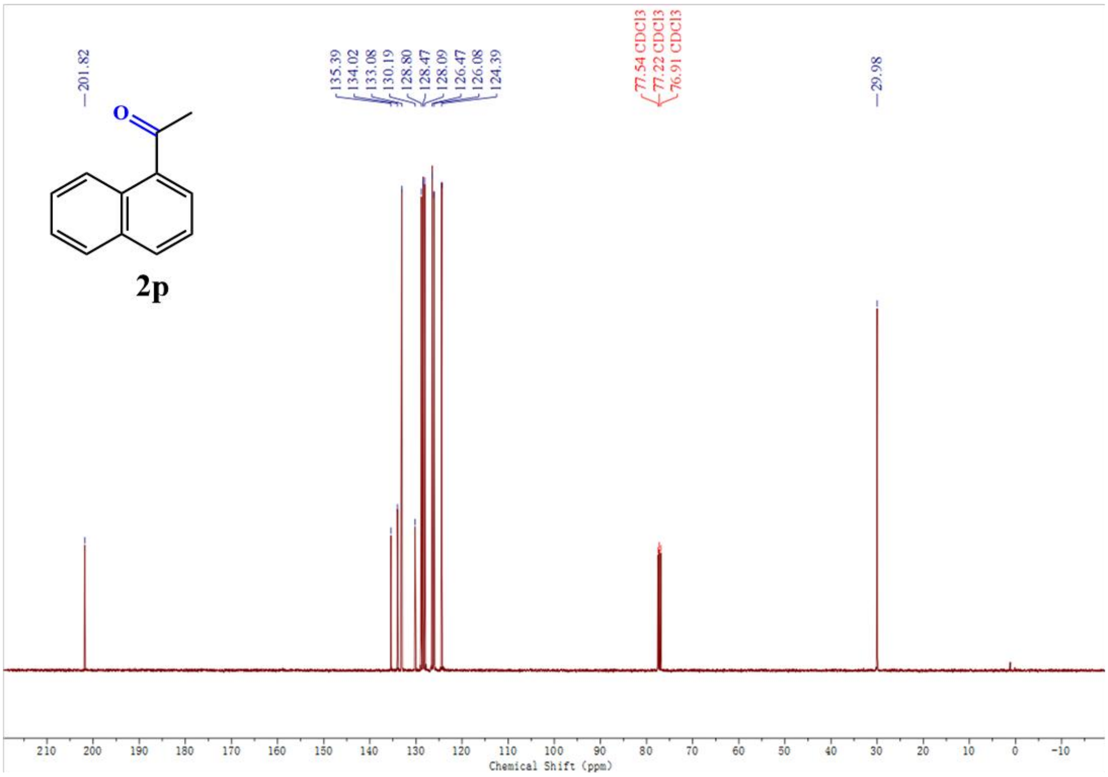

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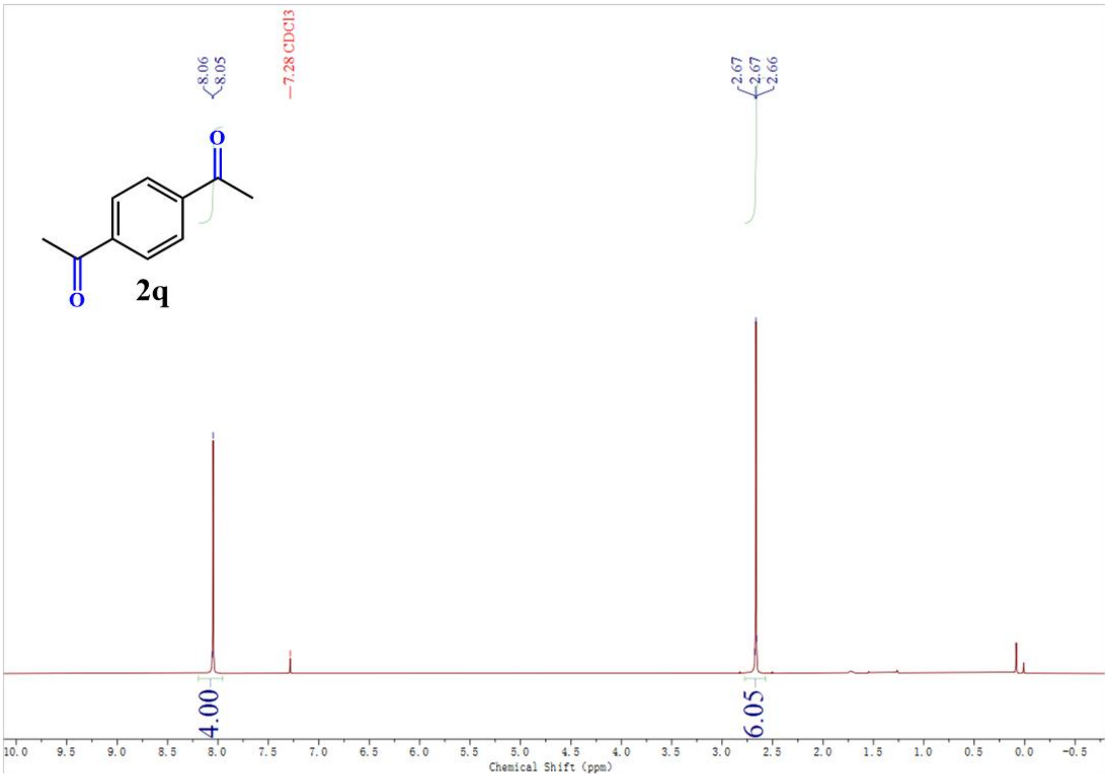

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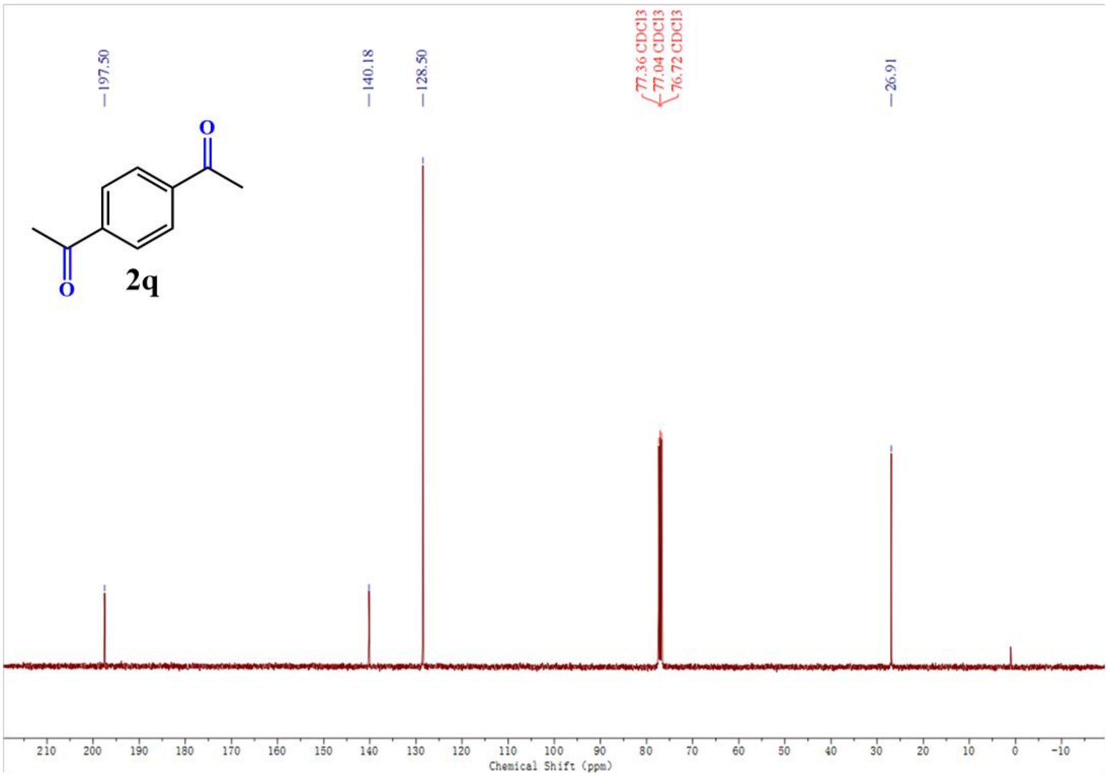

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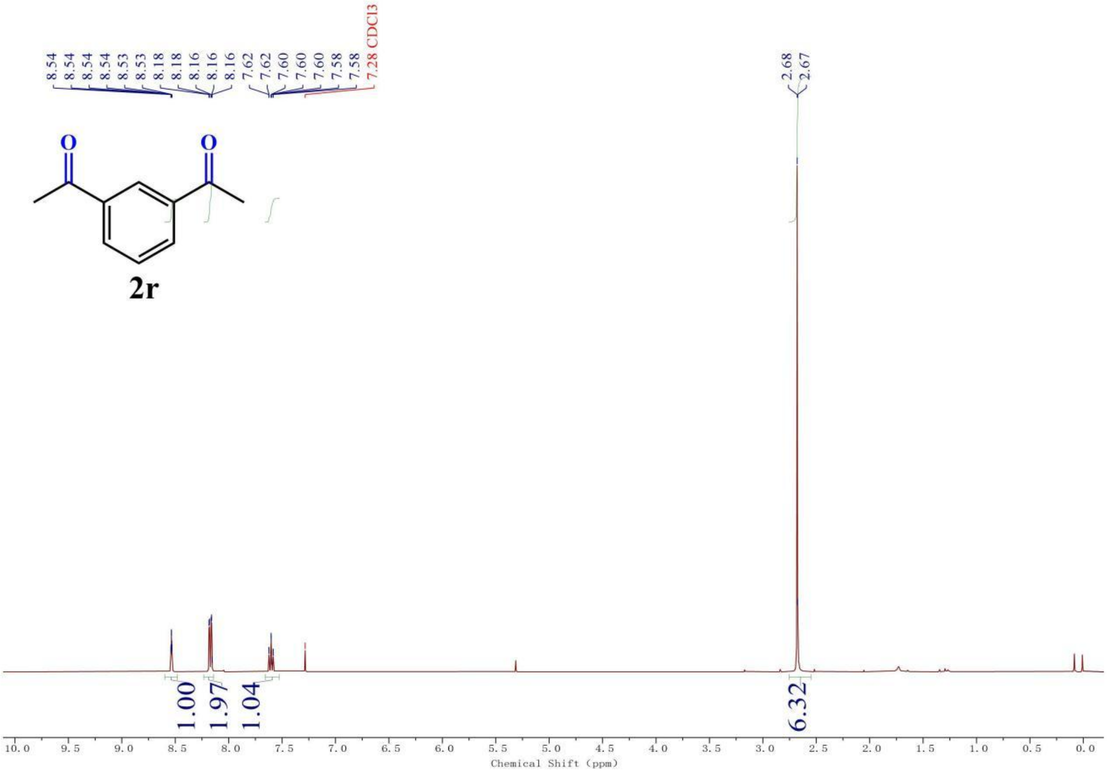
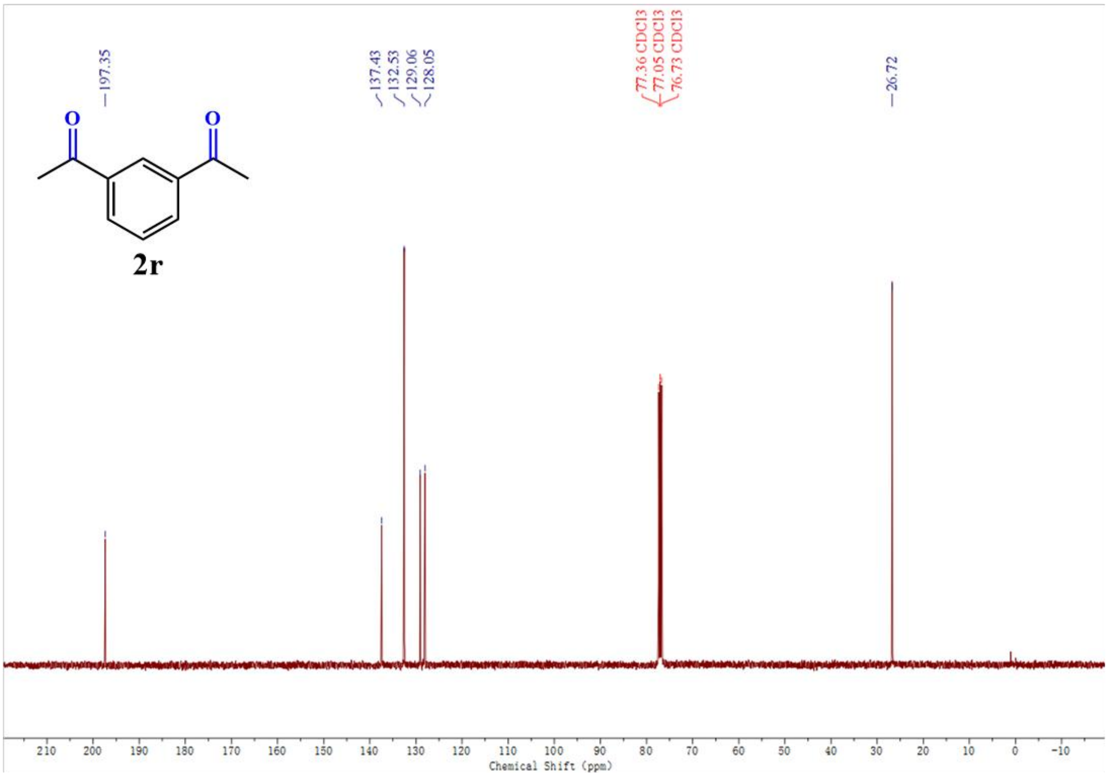
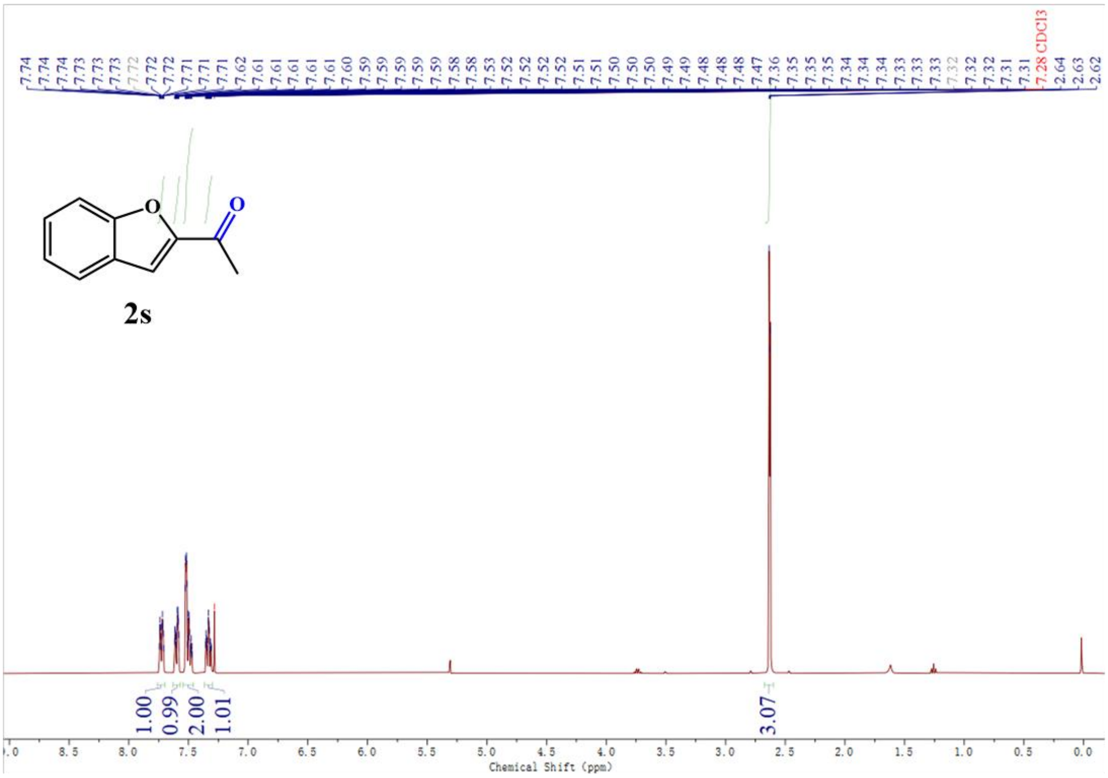


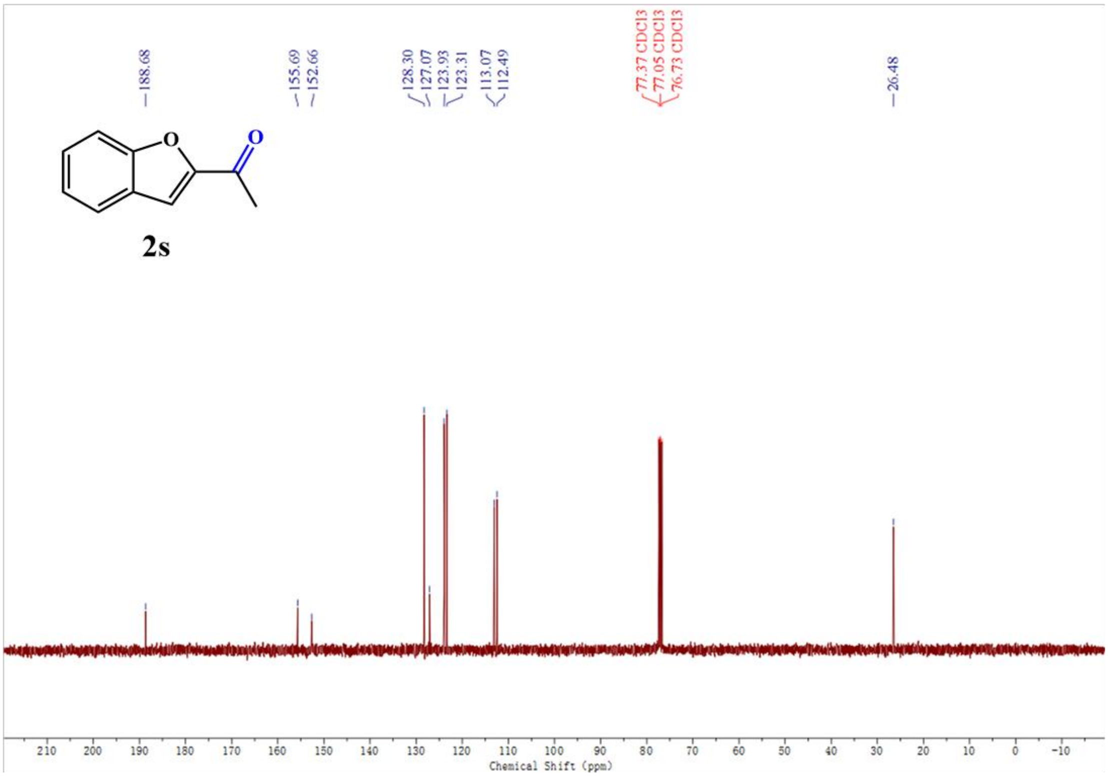
^{1}H NMR of **2r** in $CDCl_3$



^{13}C NMR of **2r** in $CDCl_3$



^{1}H NMR of **2s** in $CDCl_3$



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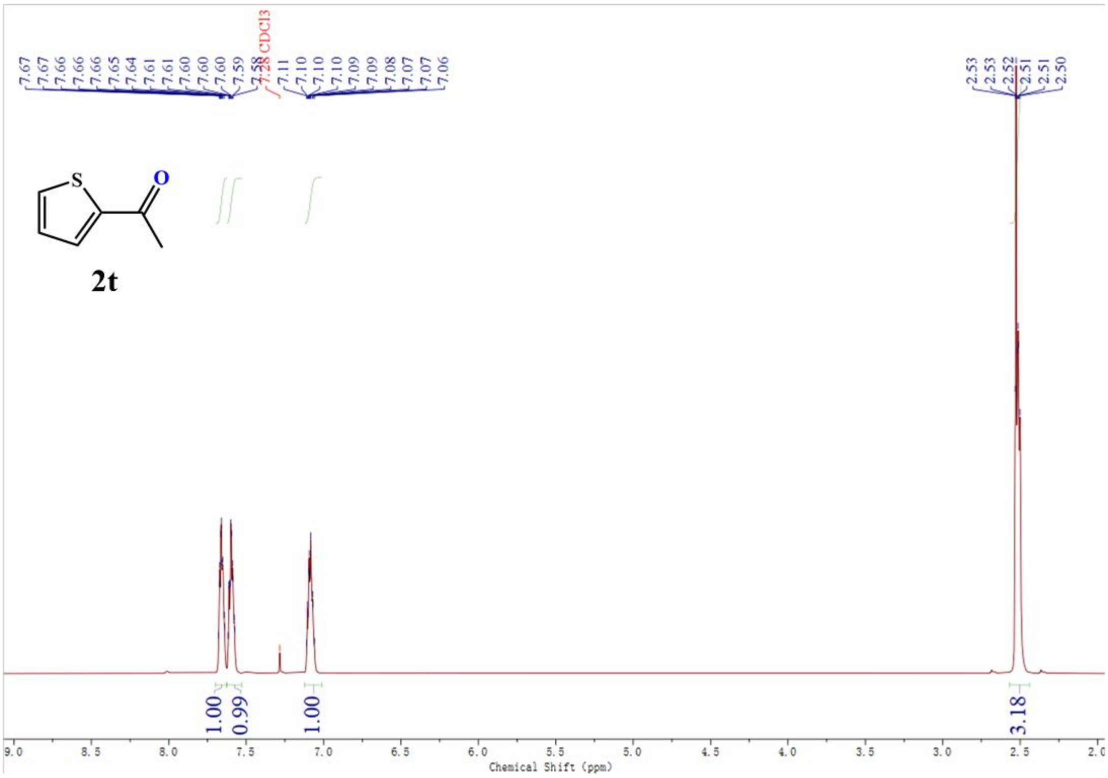
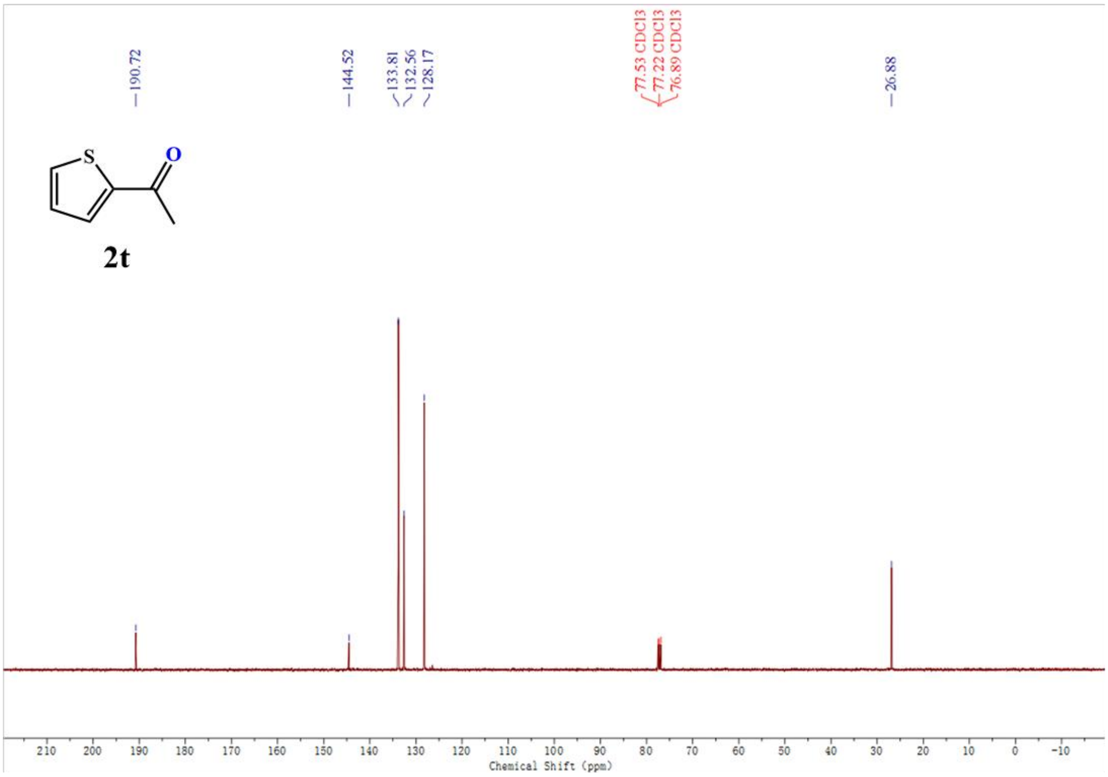
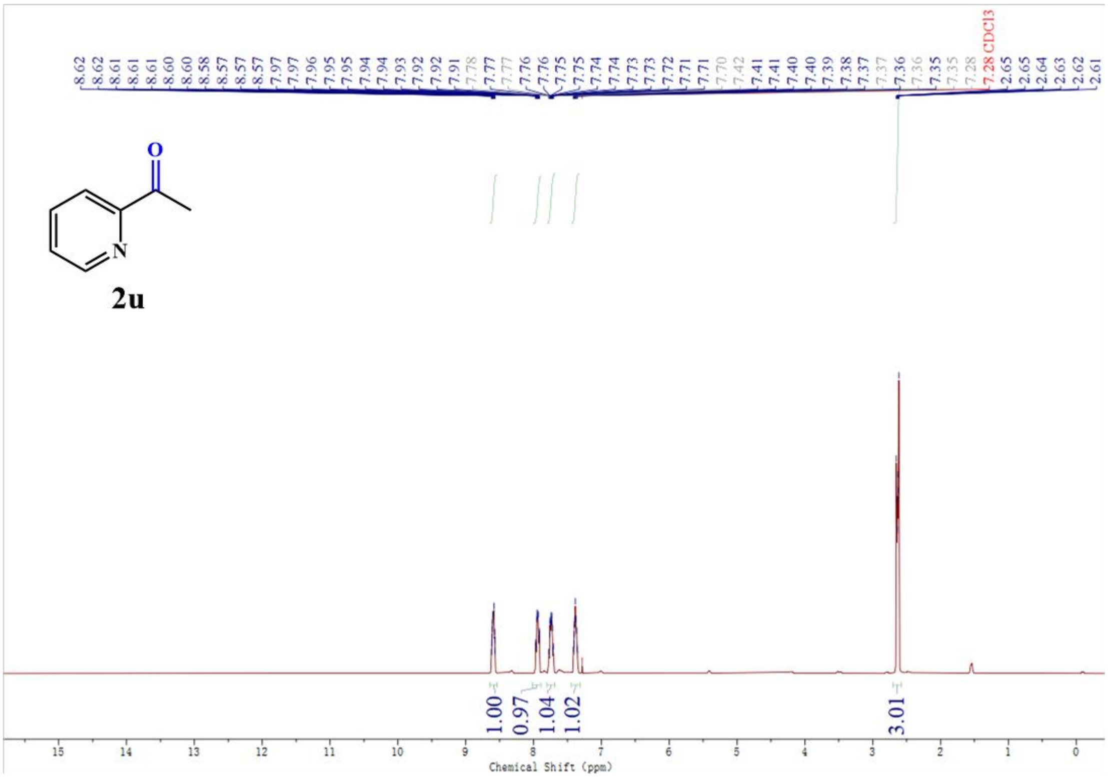


^{1}H NMR of **2t** in CDCl$_3$



^{13}C NMR of **2t** in CDCl$_3$



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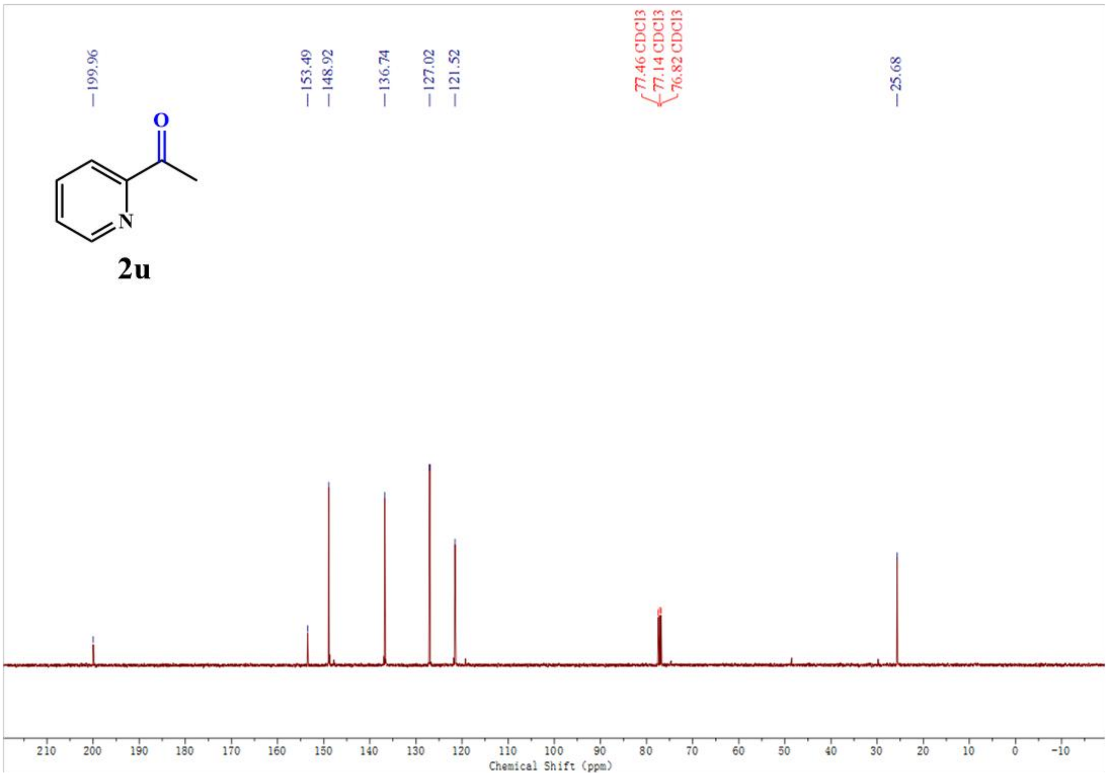

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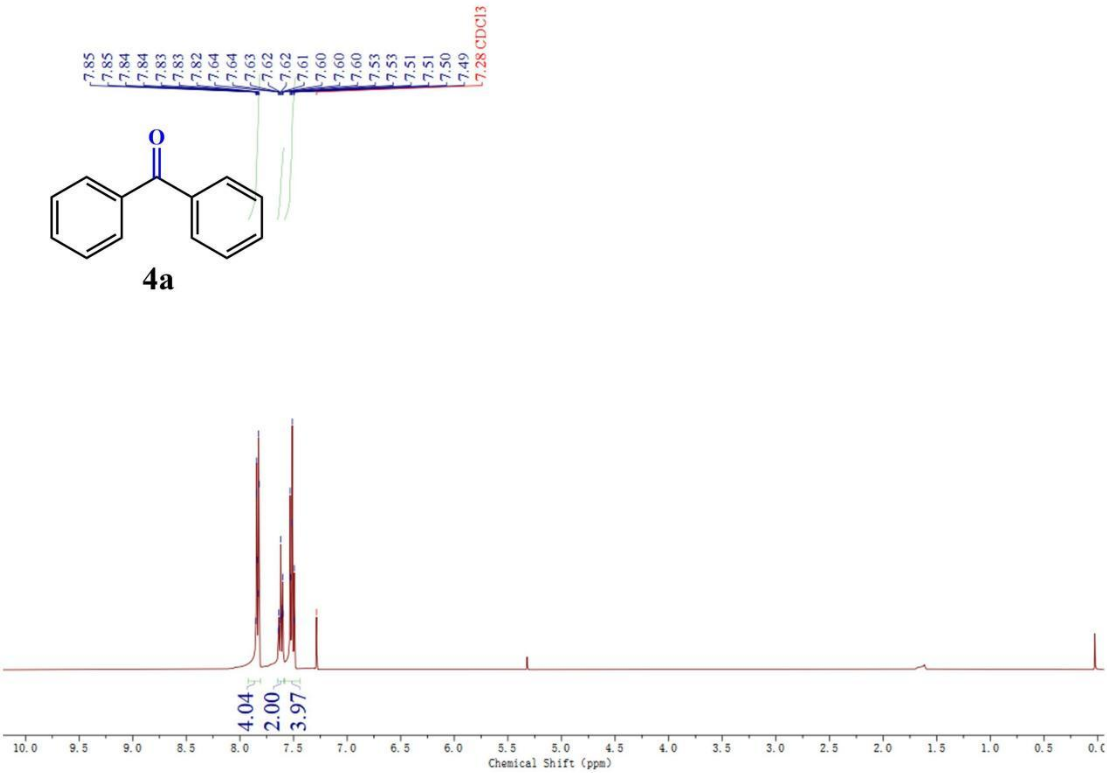
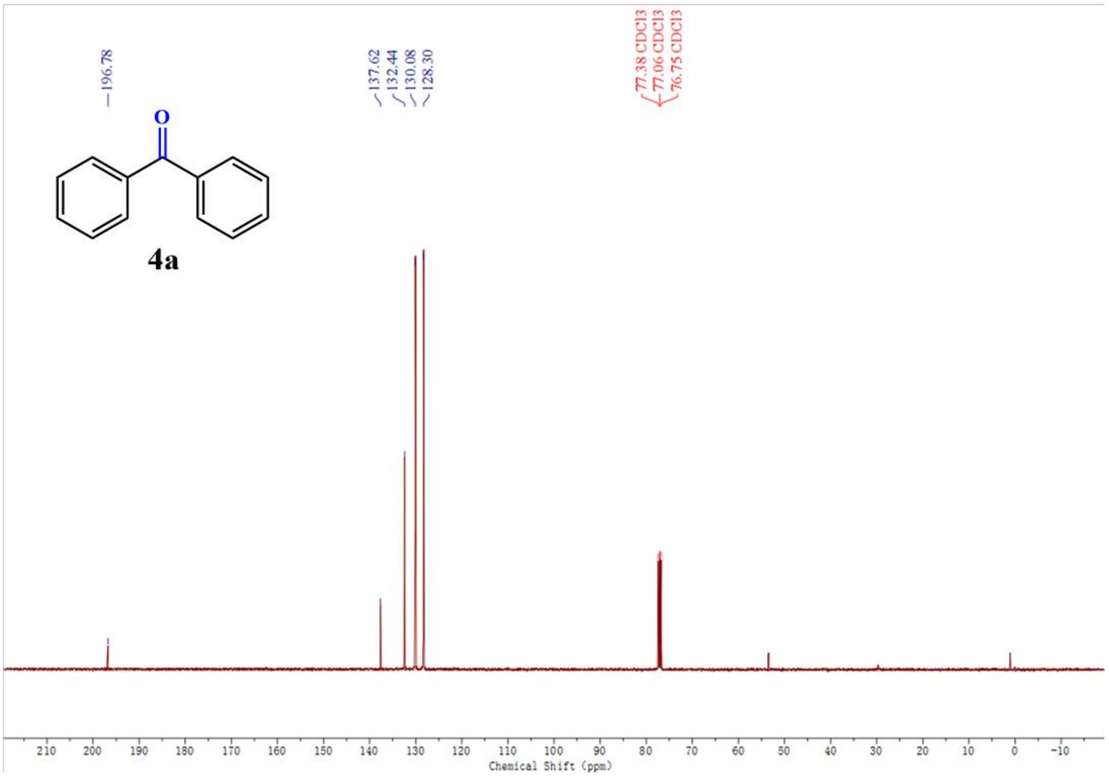
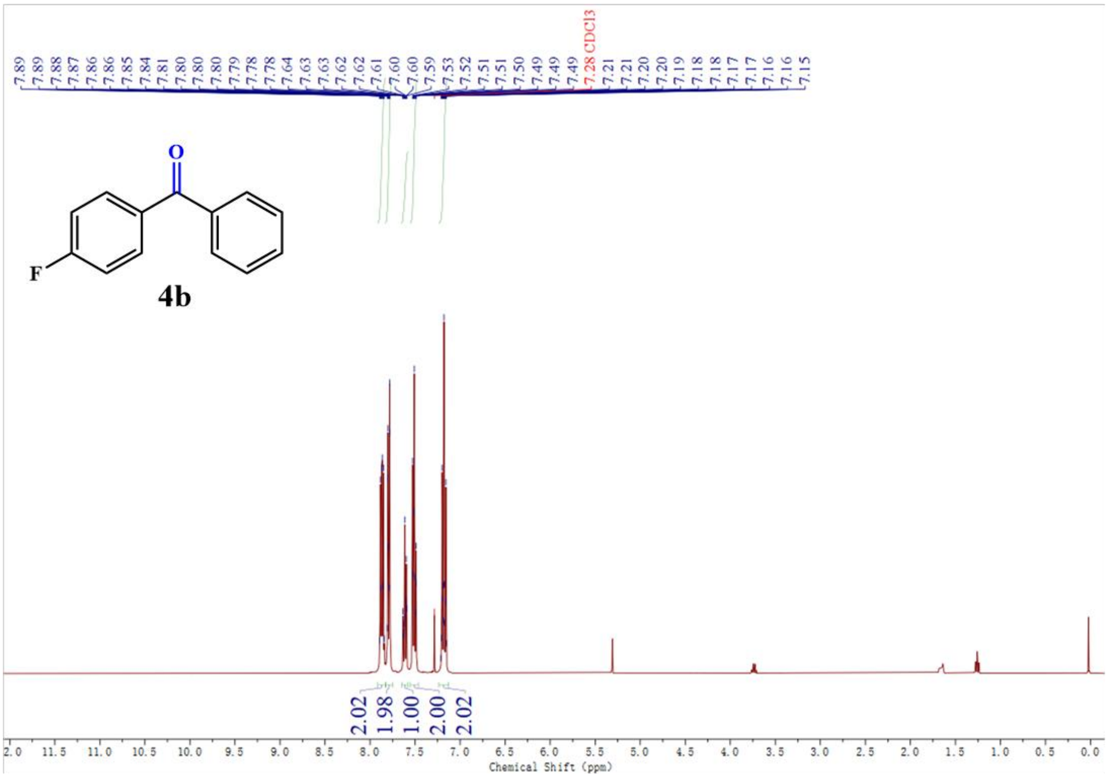


^{1}H NMR of **4a** in $CDCl_3$



^{13}C NMR of **4a** in $CDCl_3$



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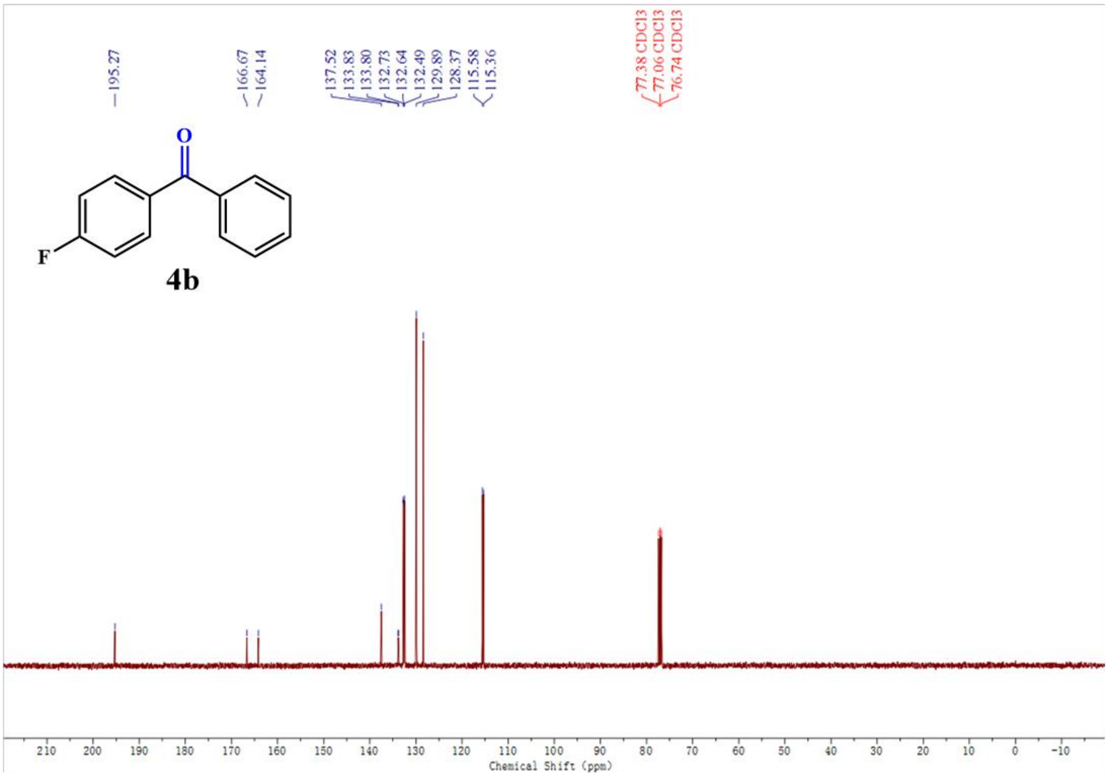

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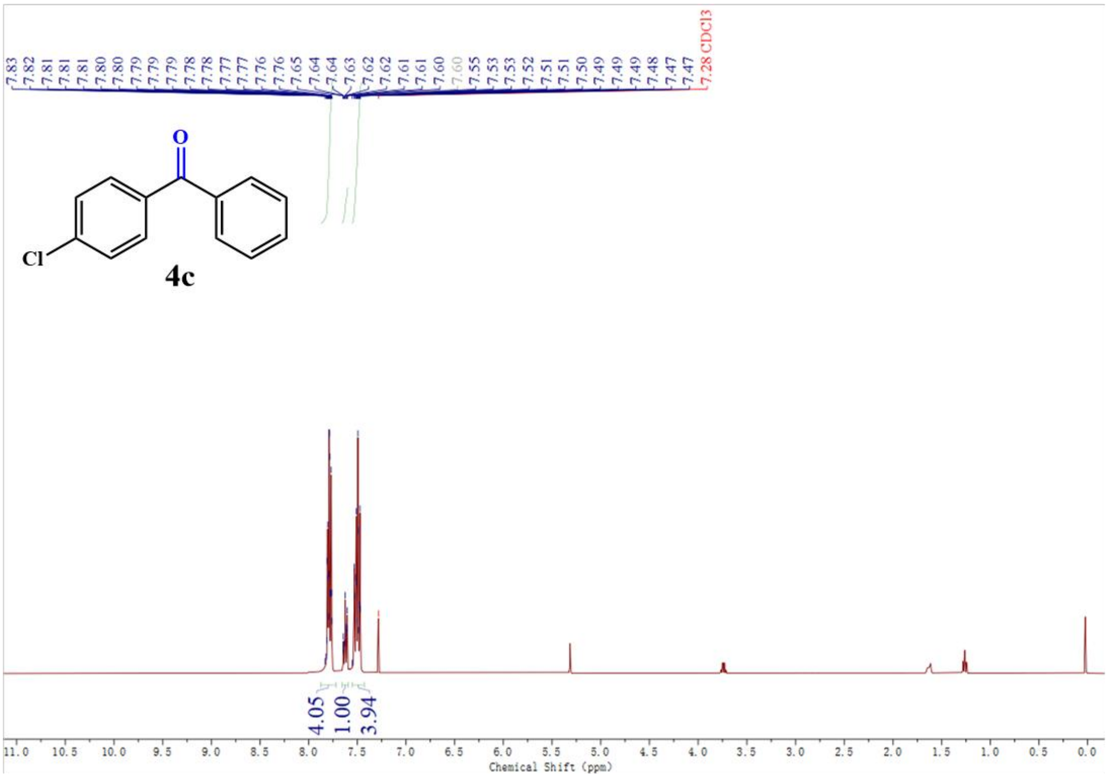
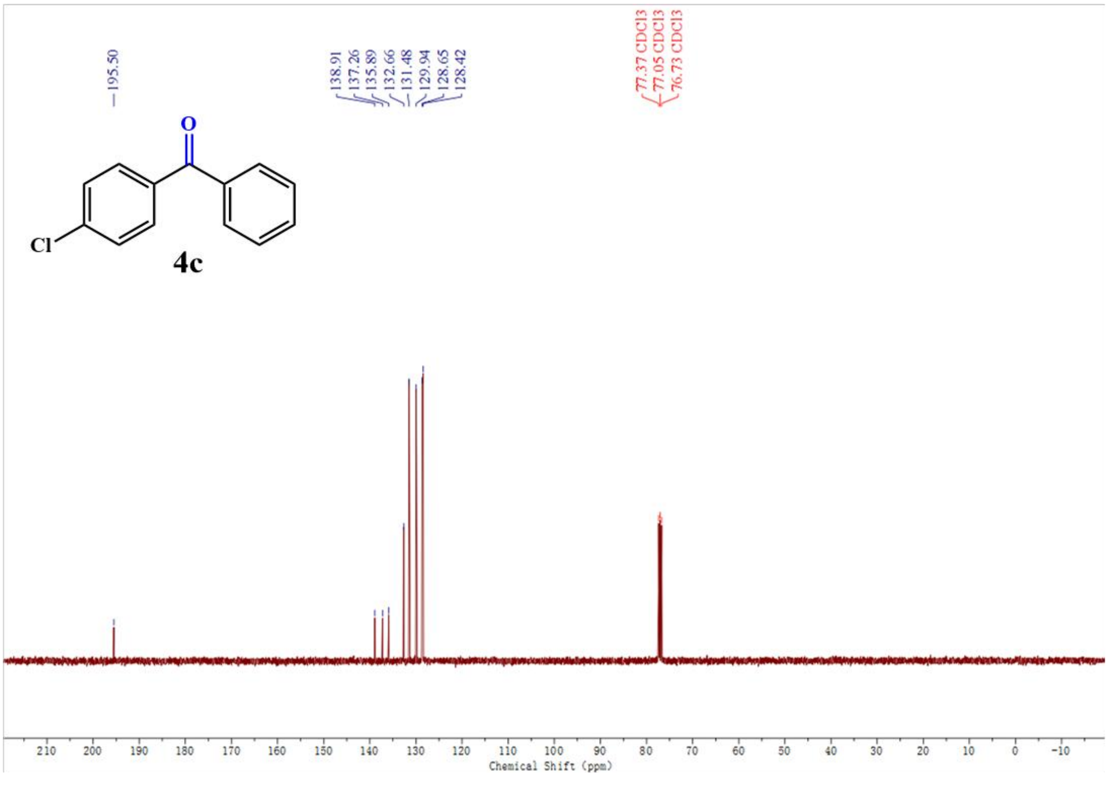
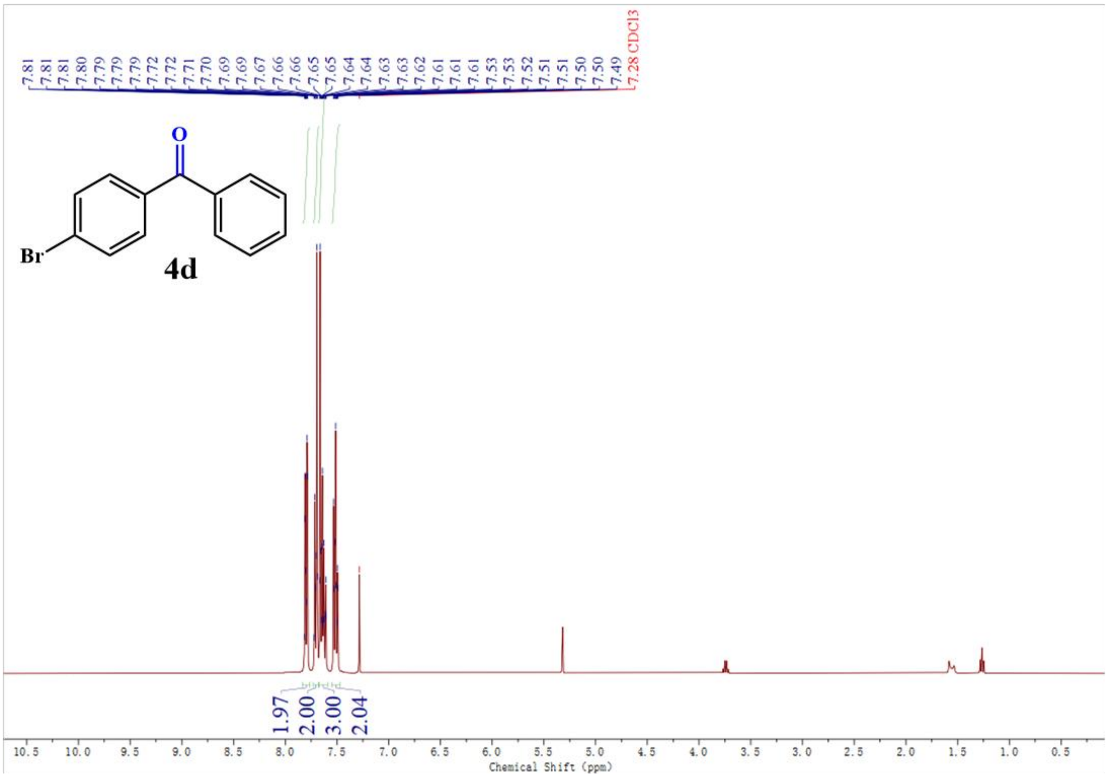


^{1}H NMR of **4c** in $CDCl_3$



^{13}C NMR of **4c** in $CDCl_3$



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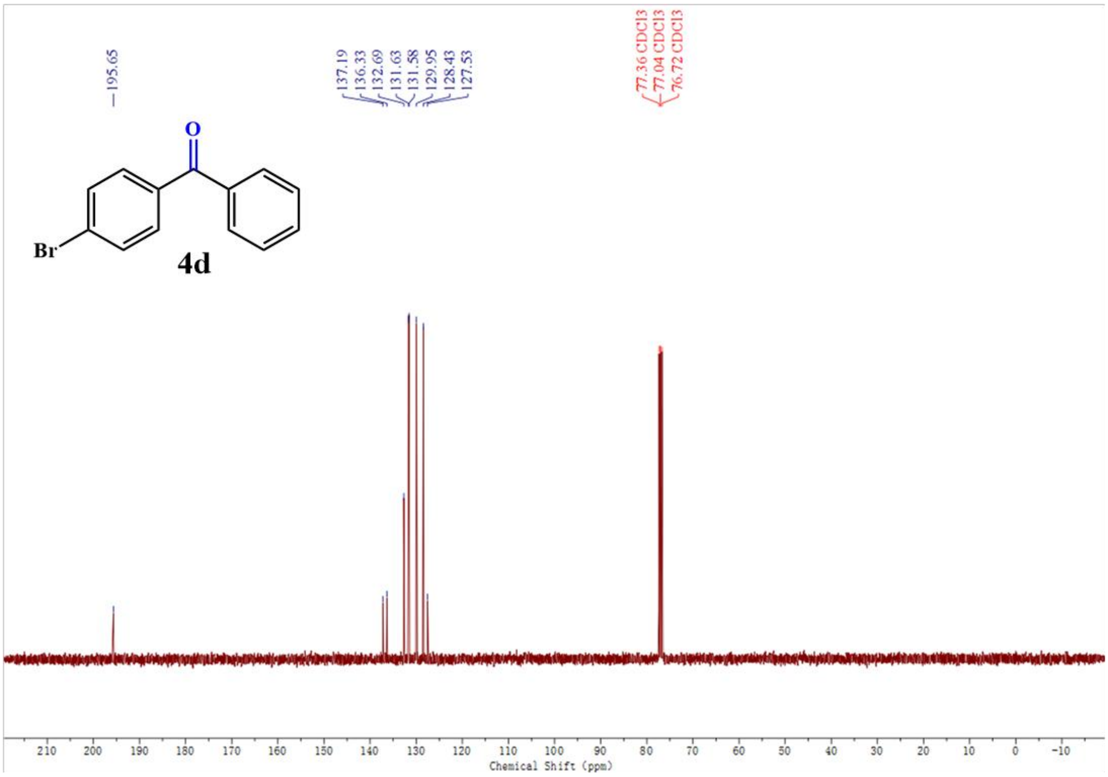

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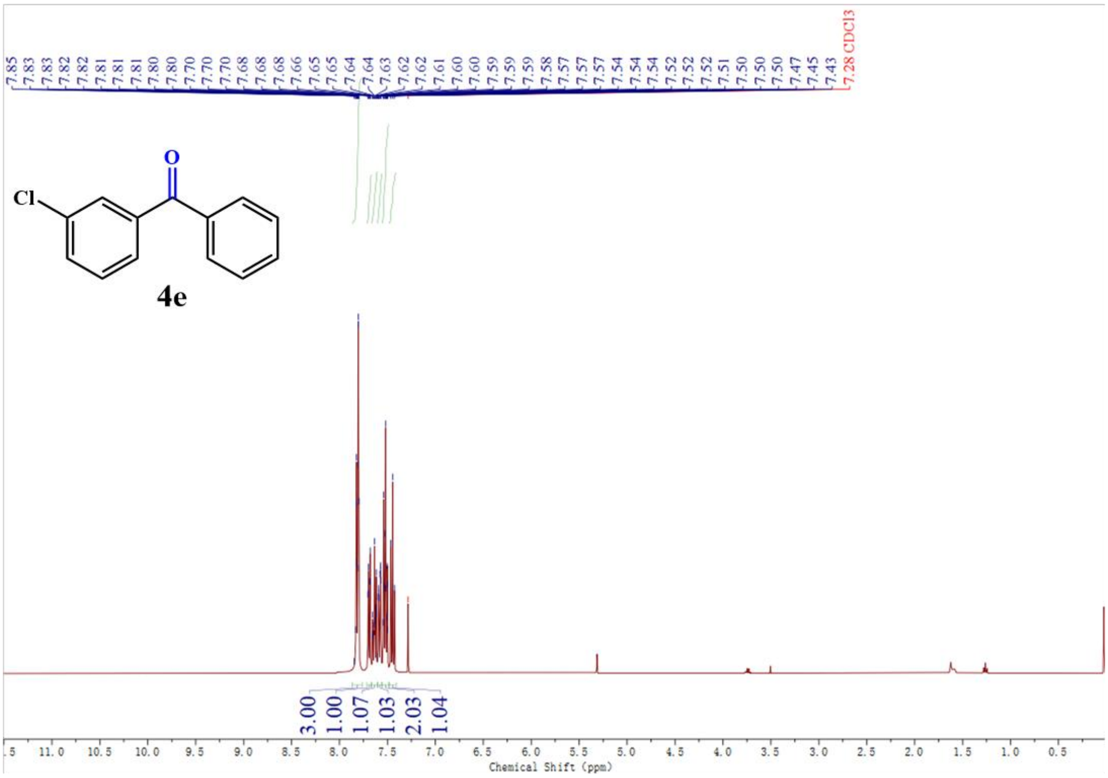

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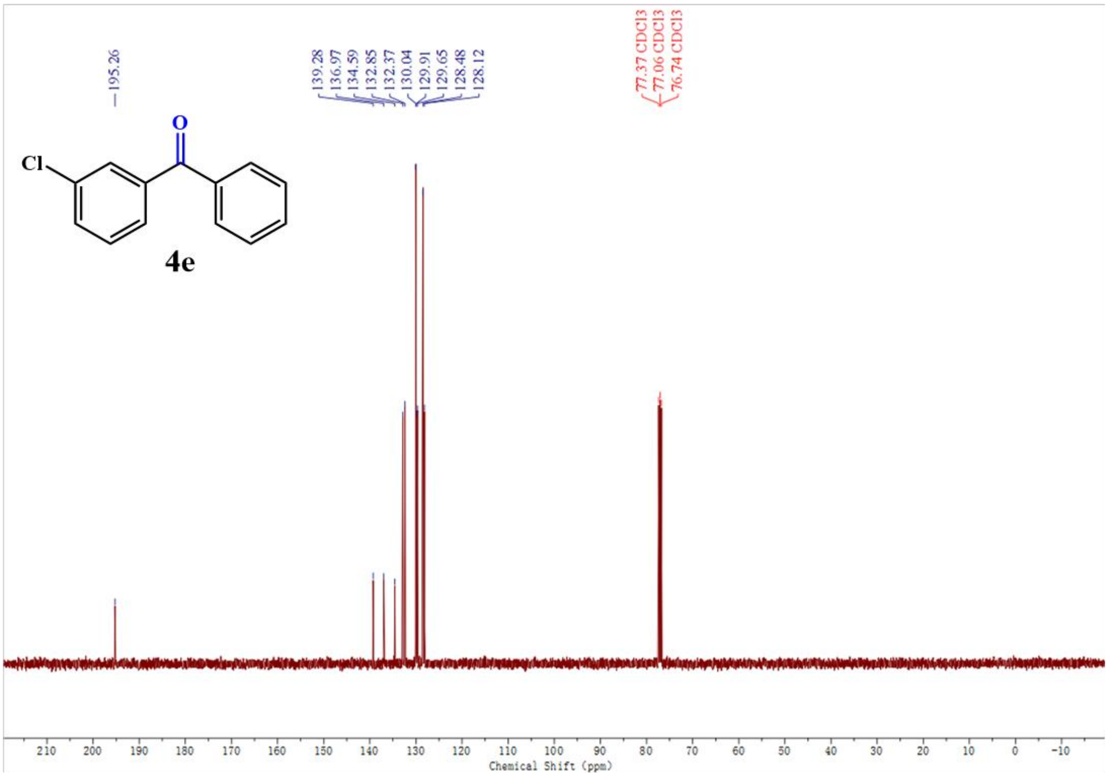

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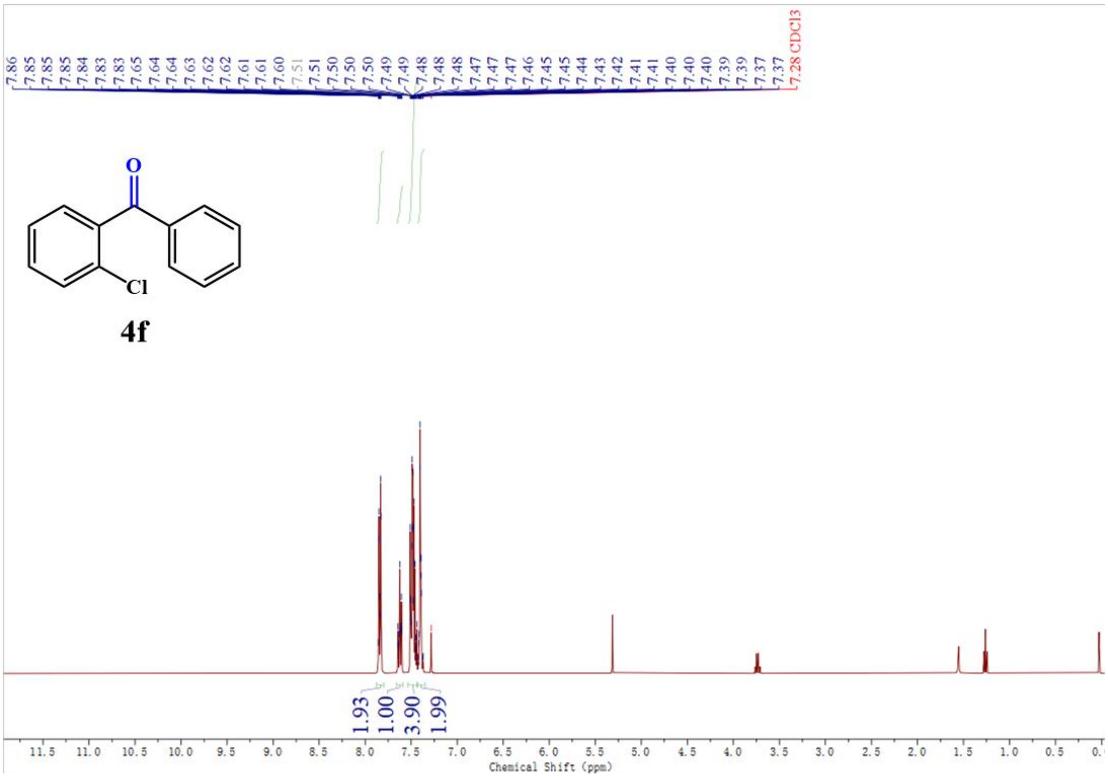

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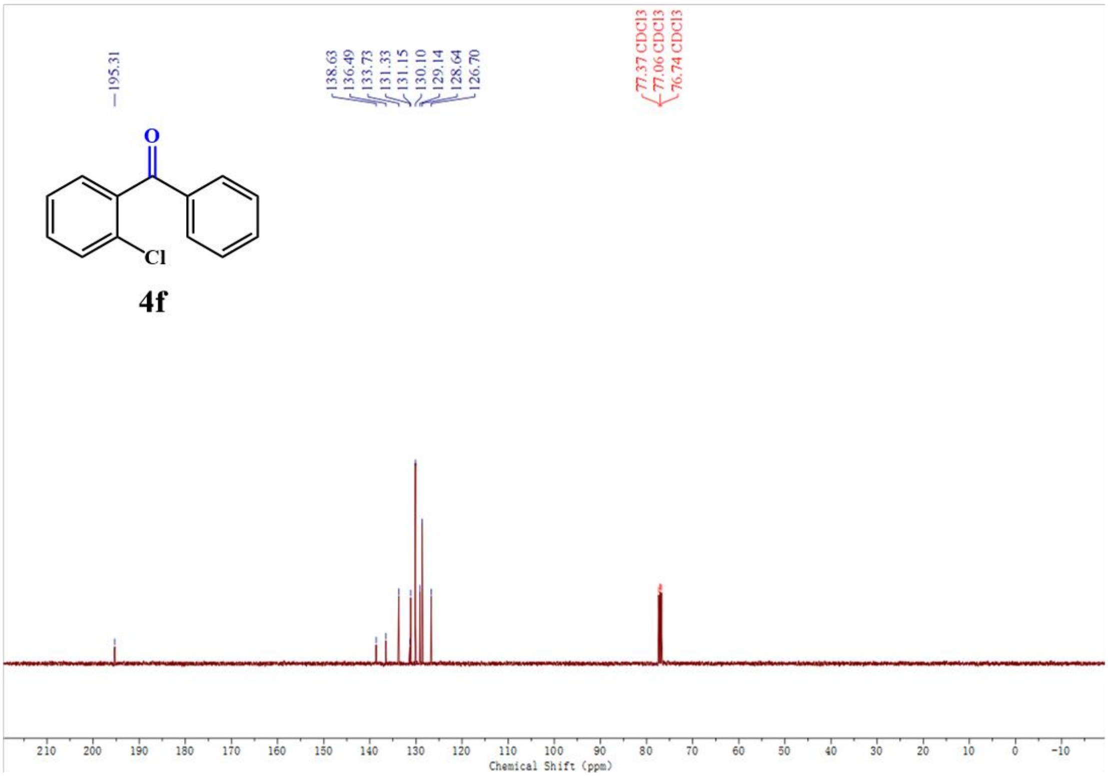

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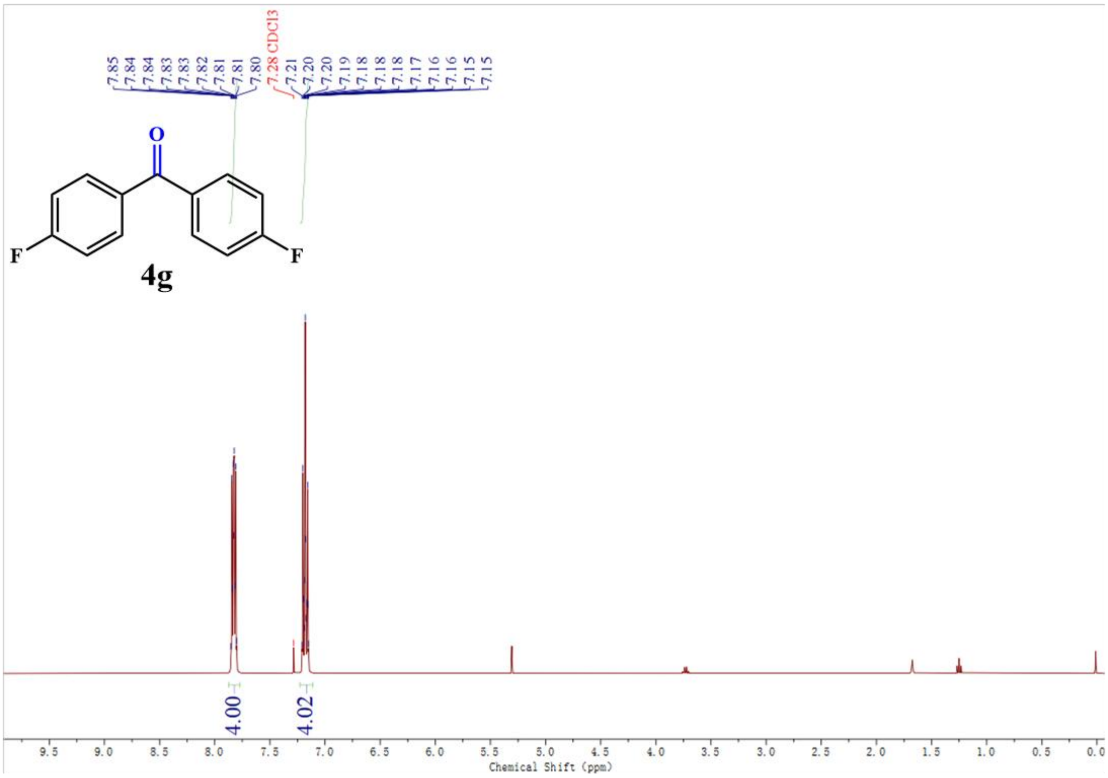

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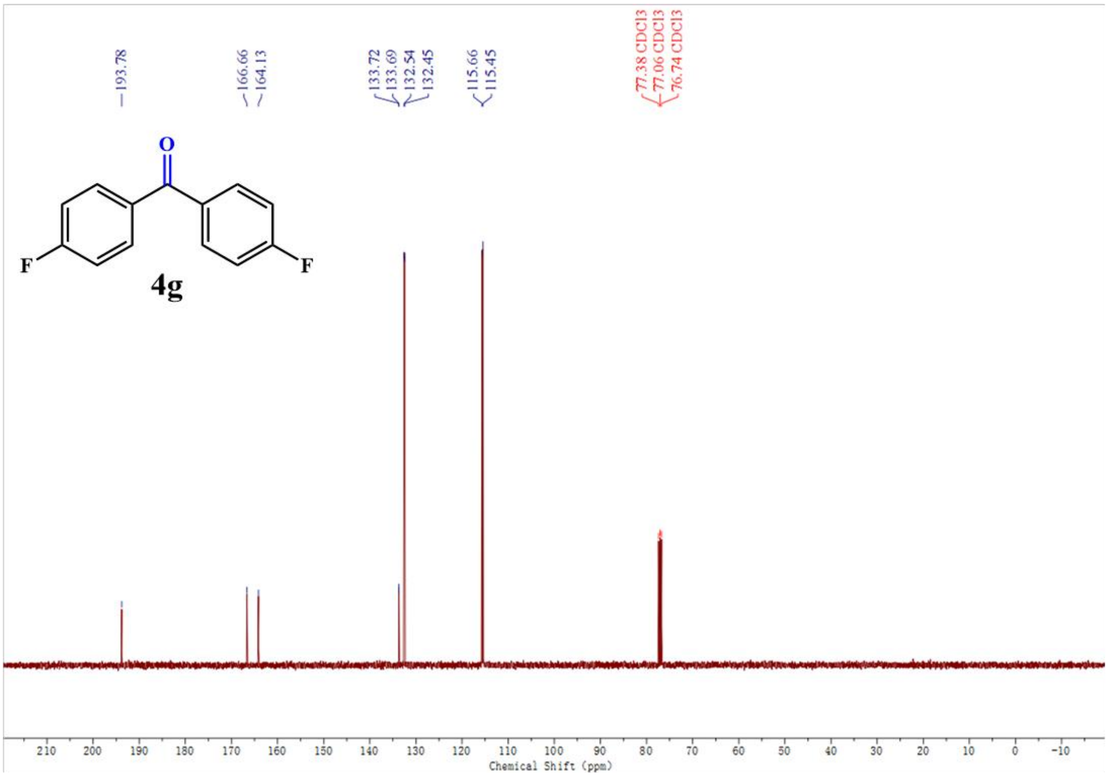

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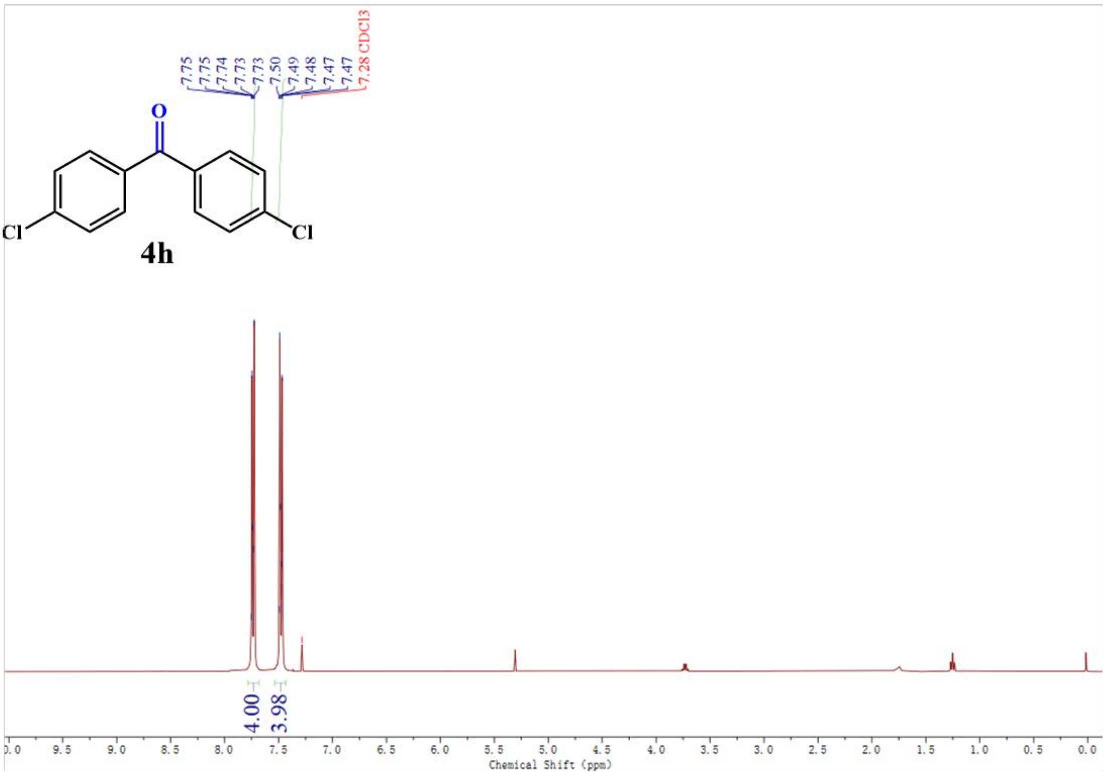

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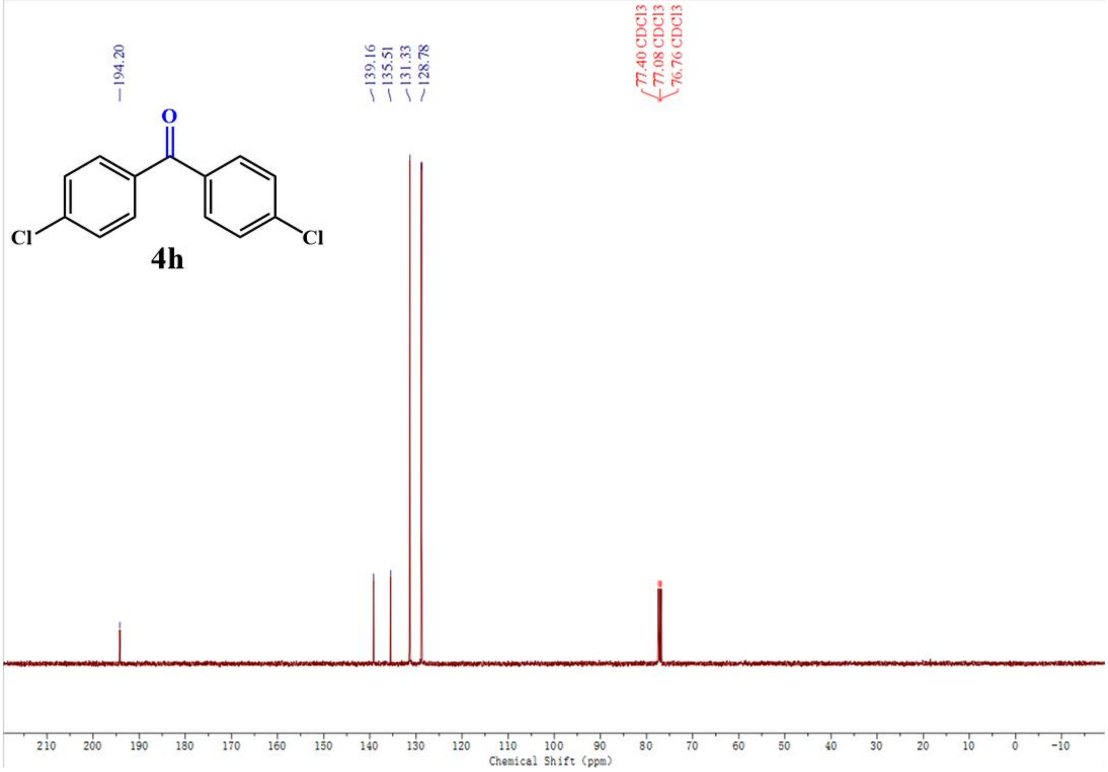

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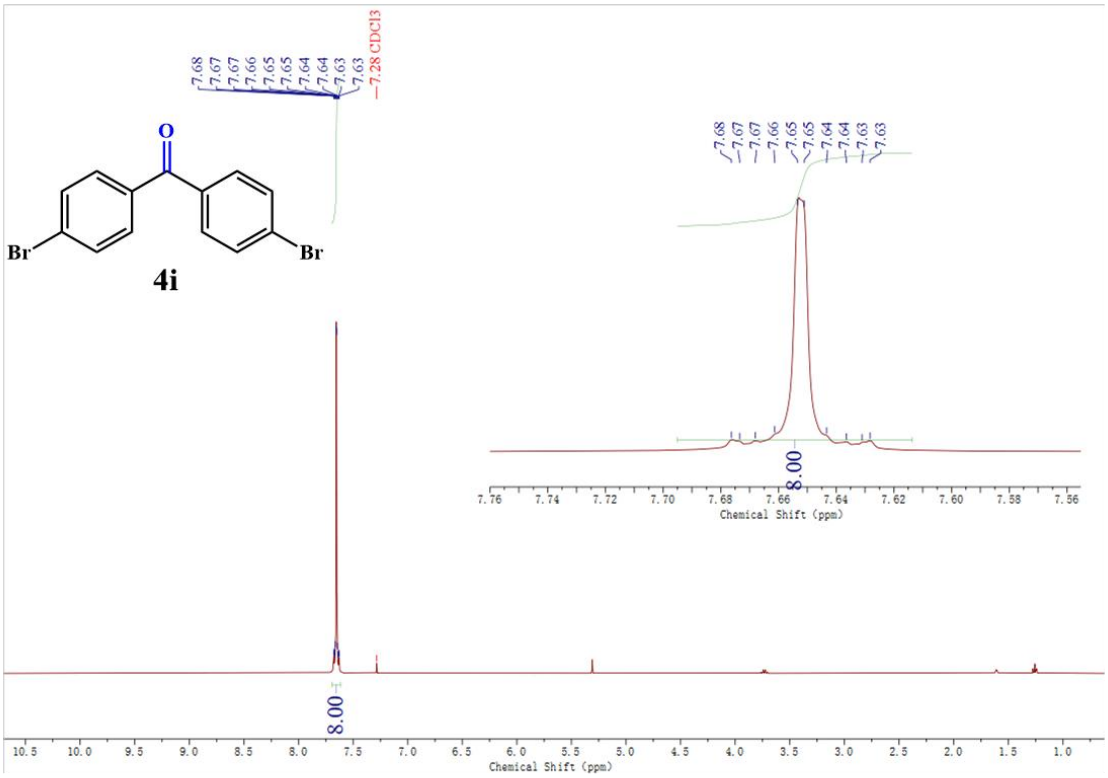

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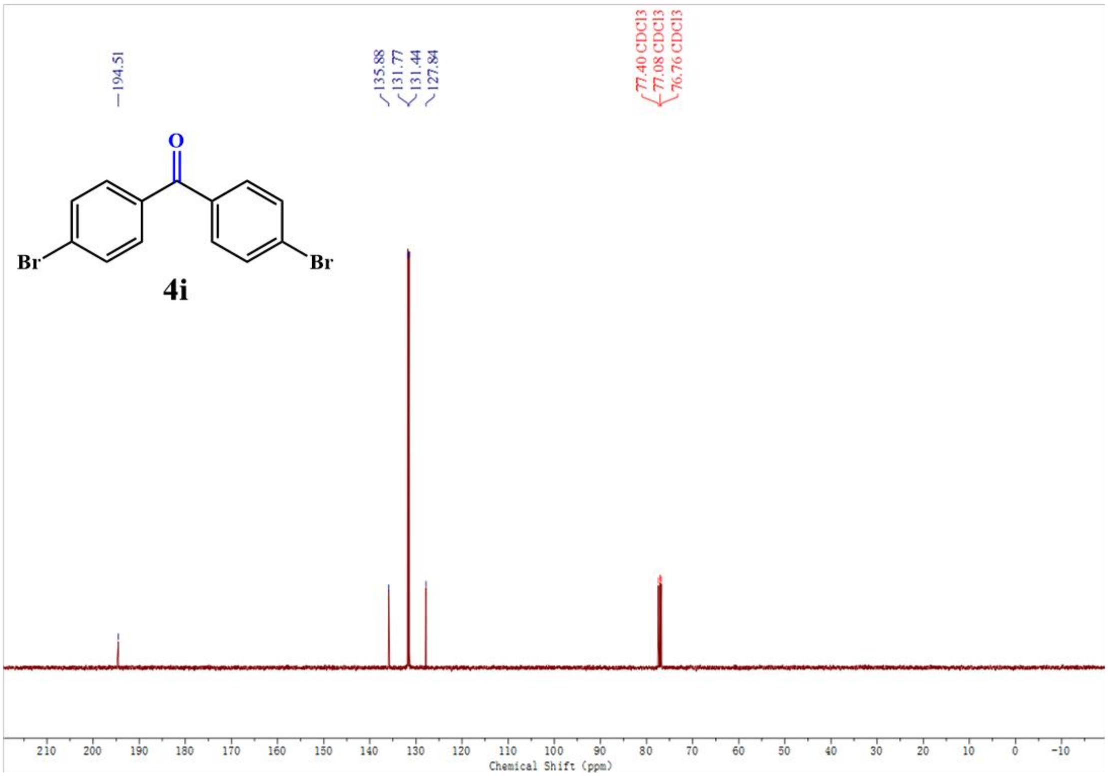

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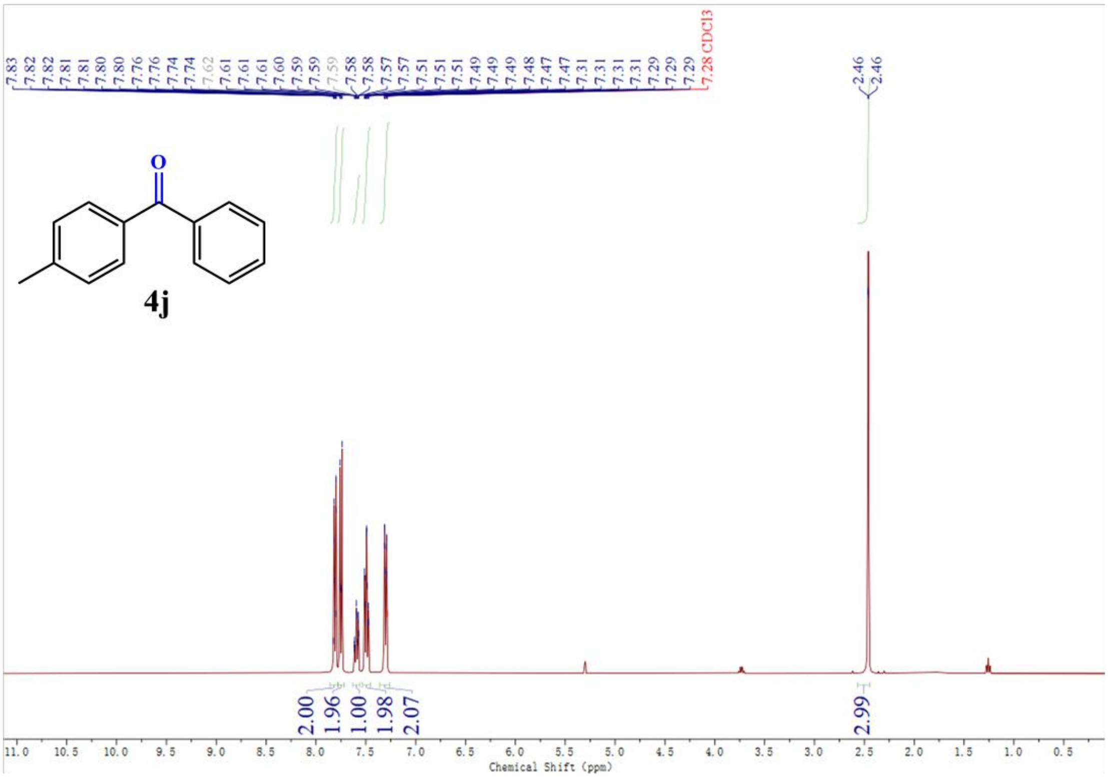

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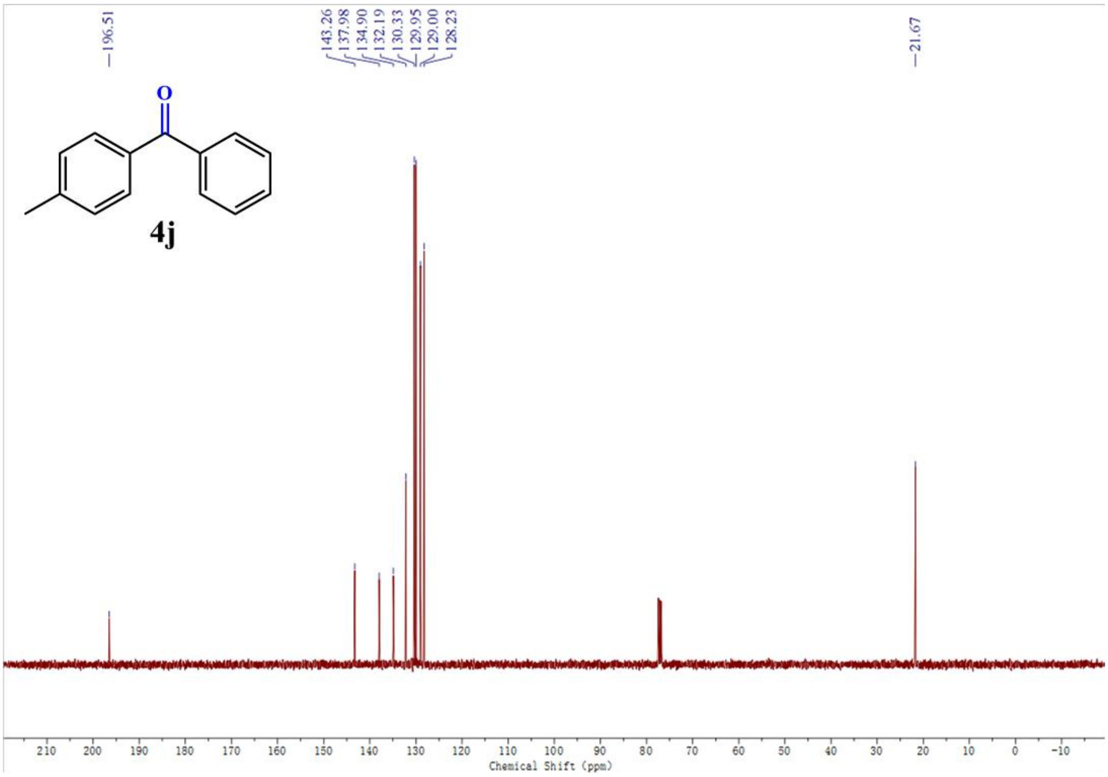

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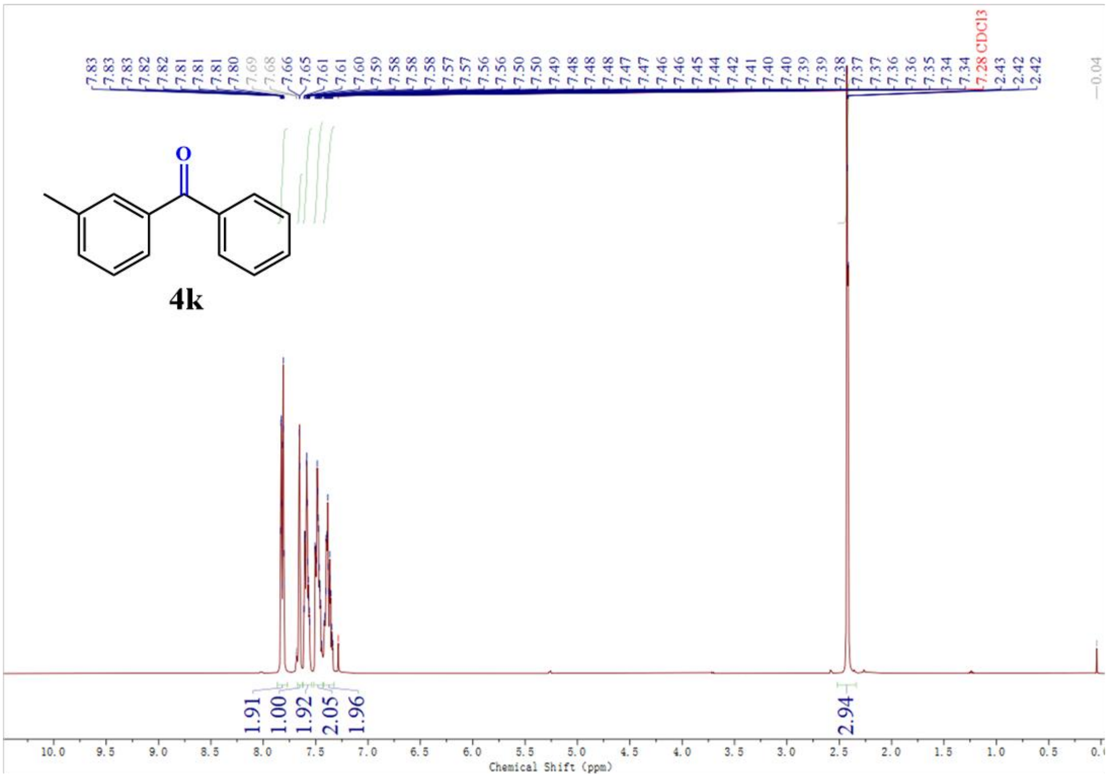

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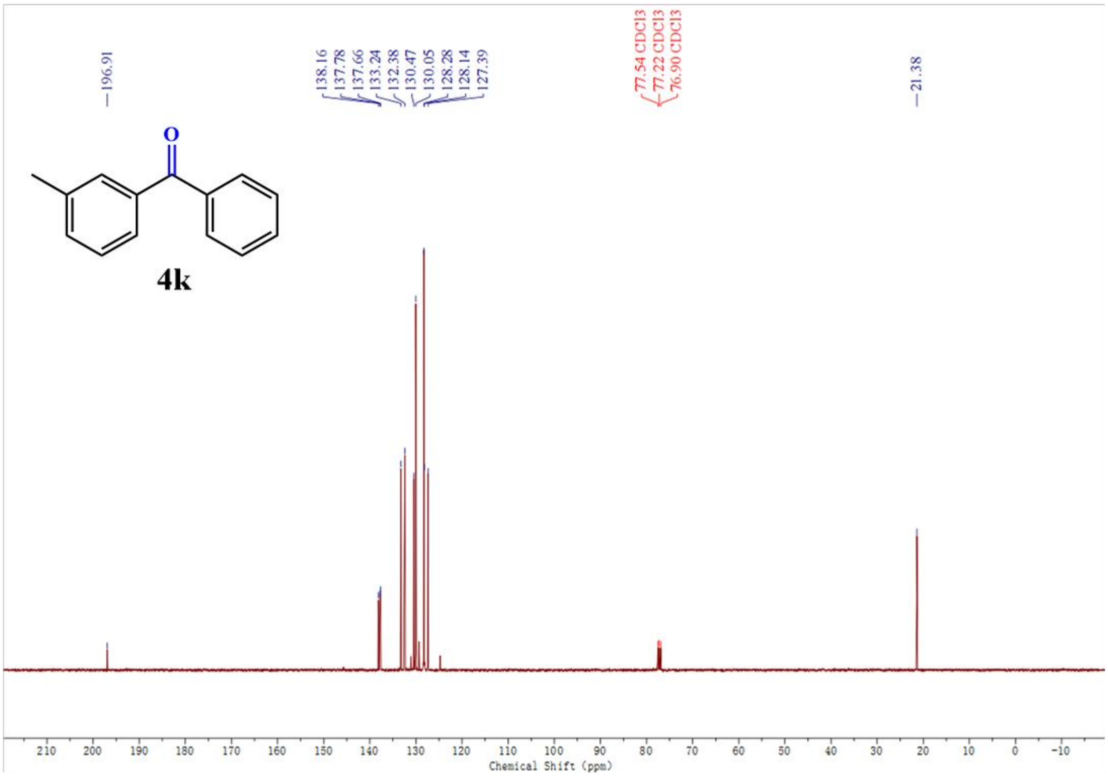

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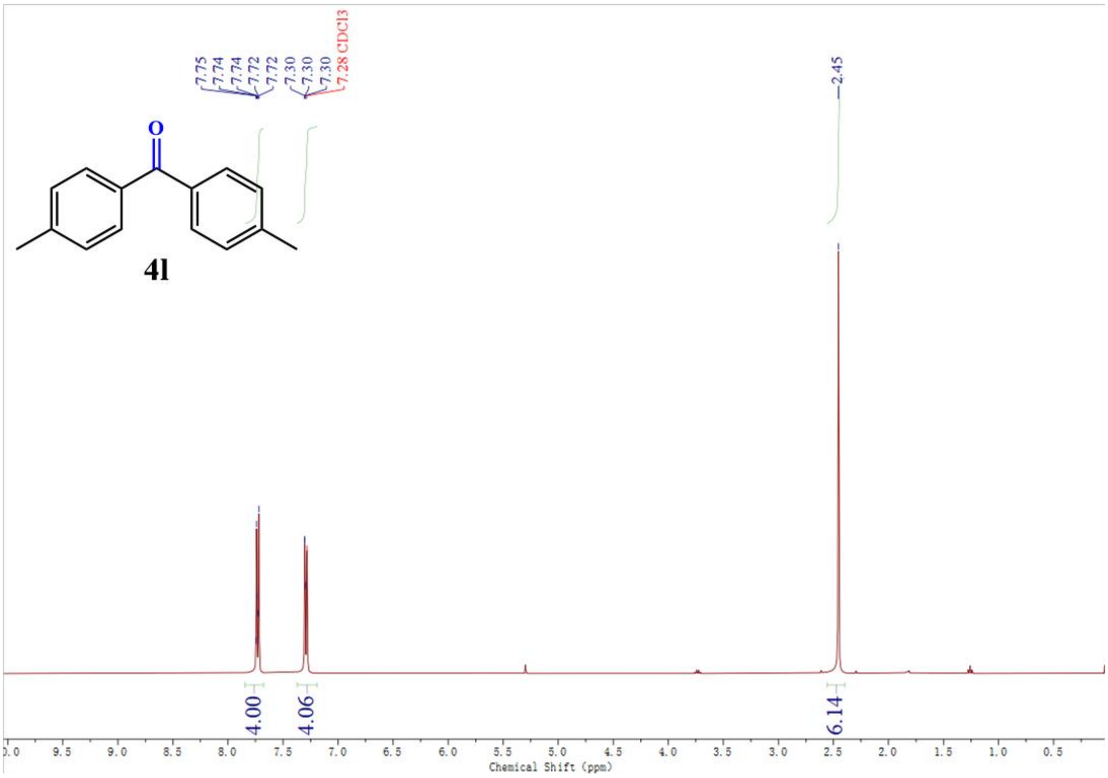

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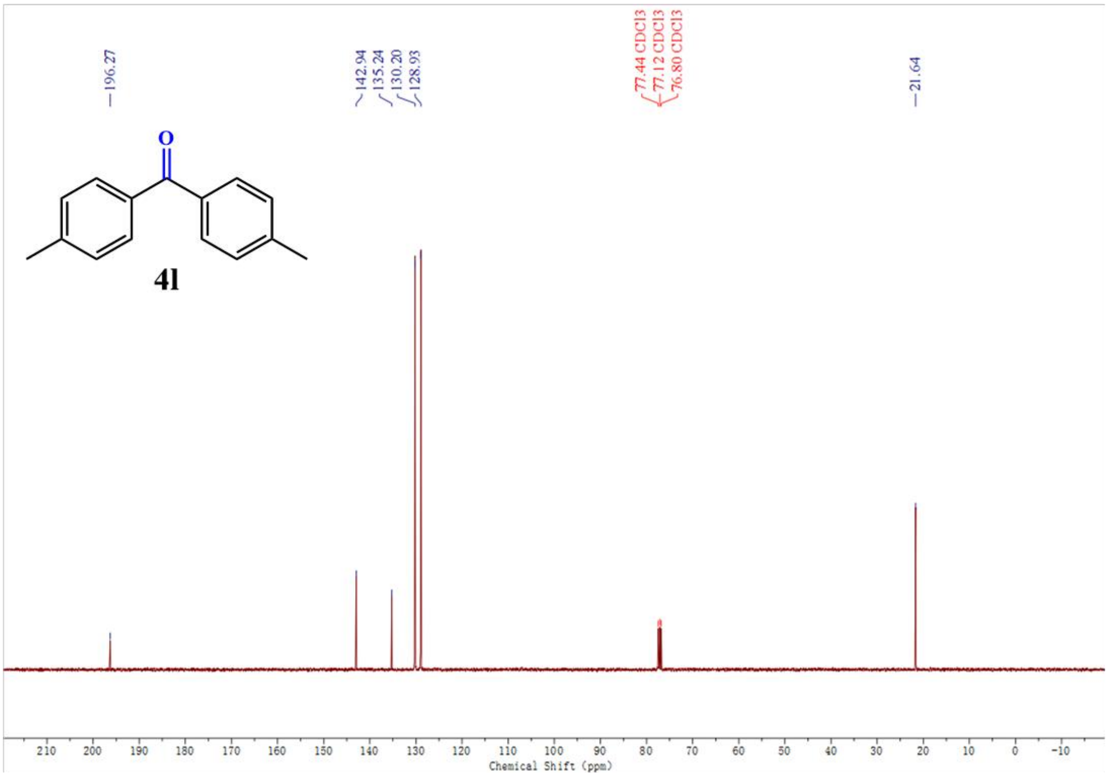

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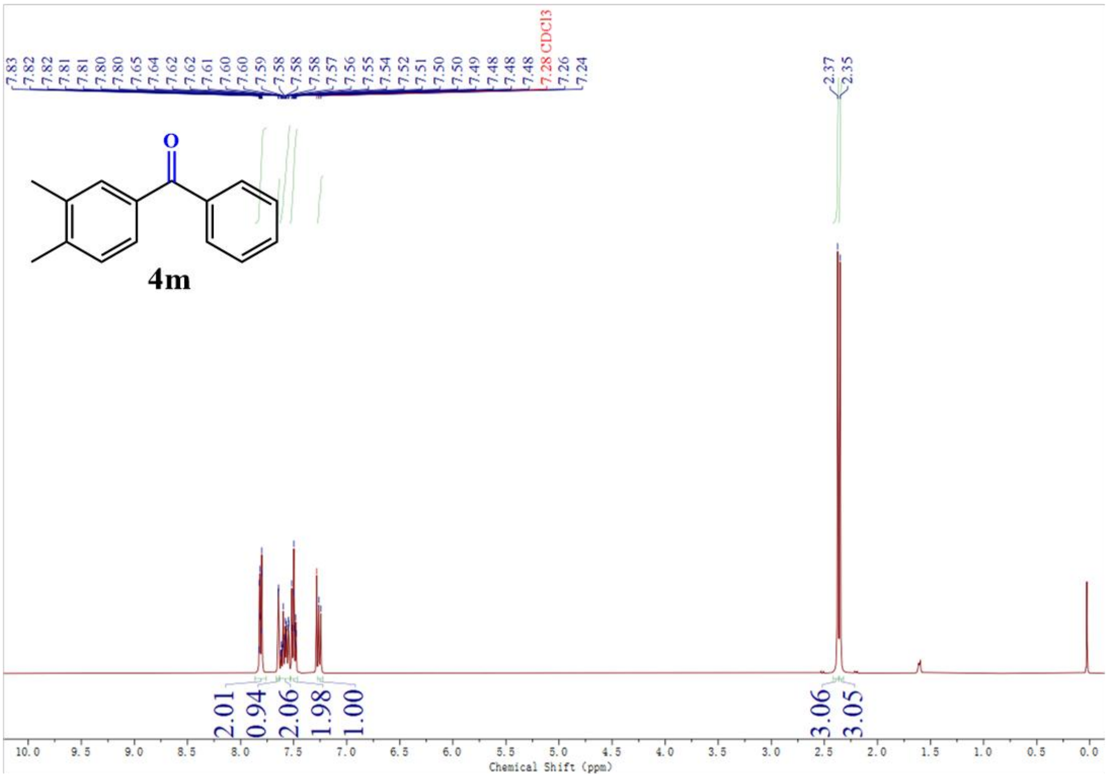

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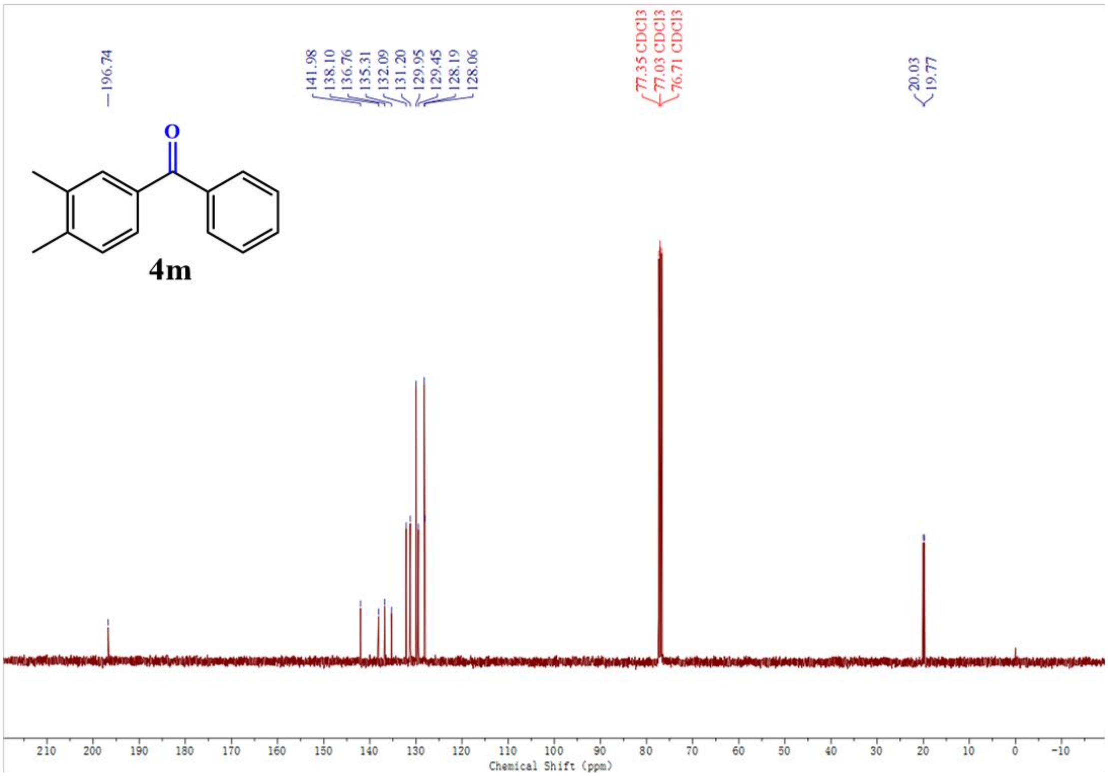

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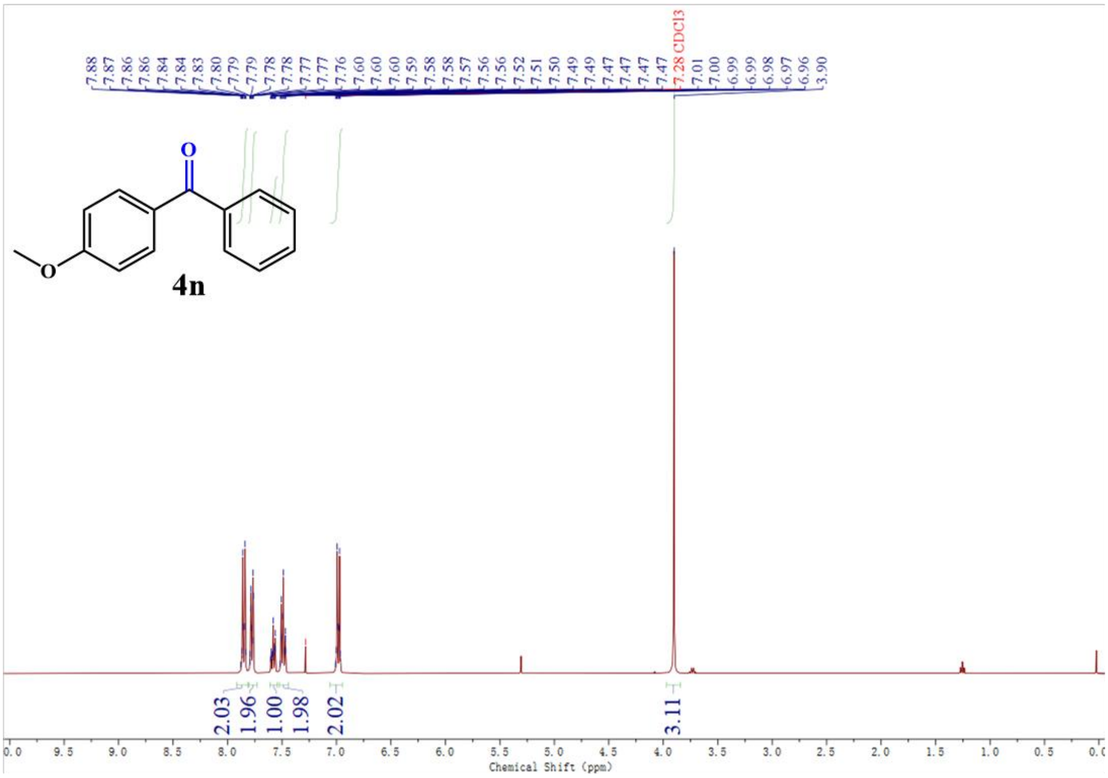

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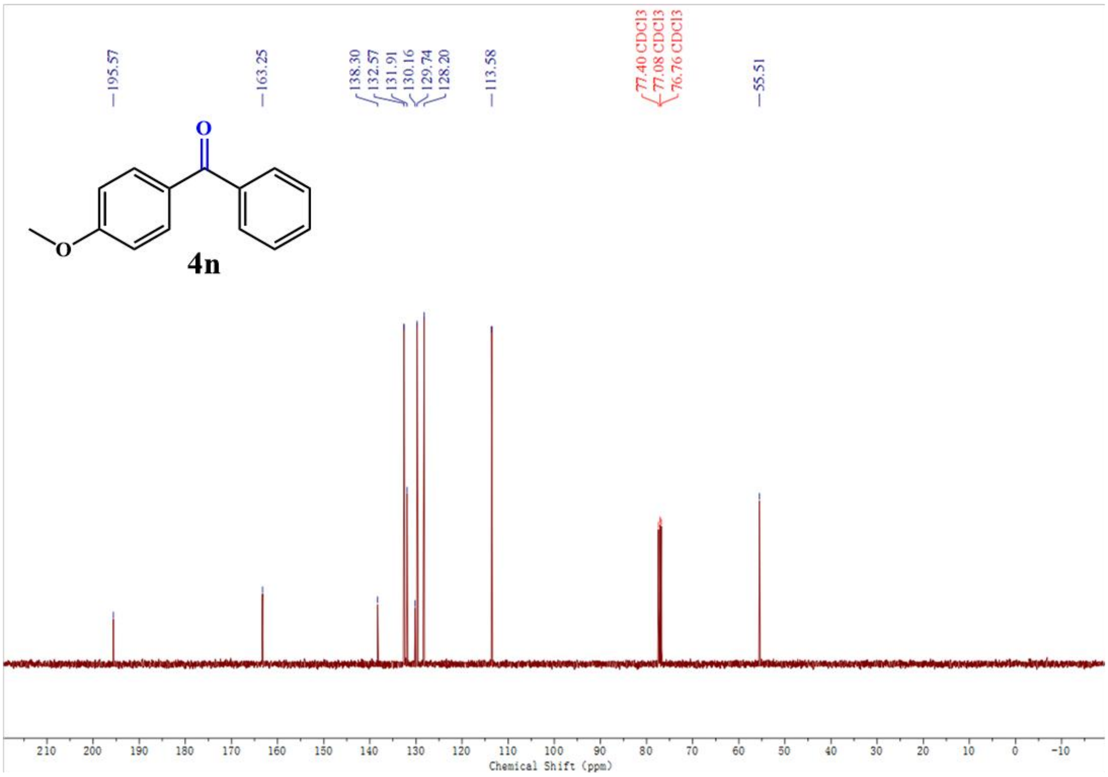

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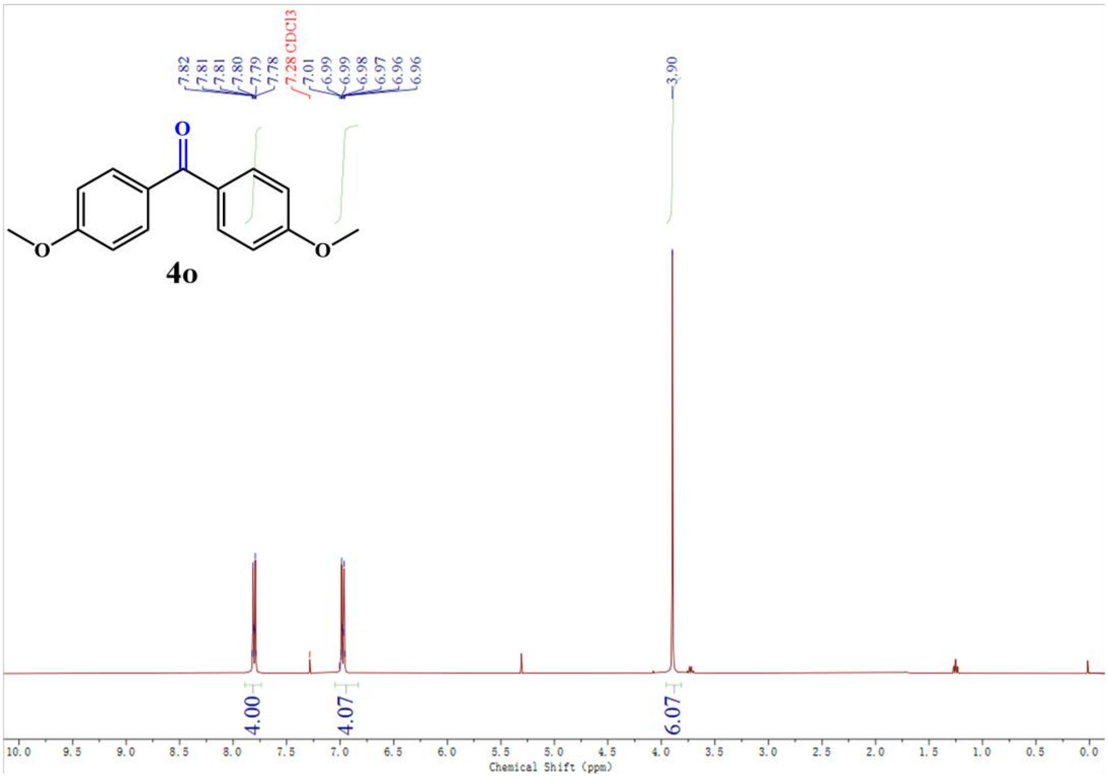

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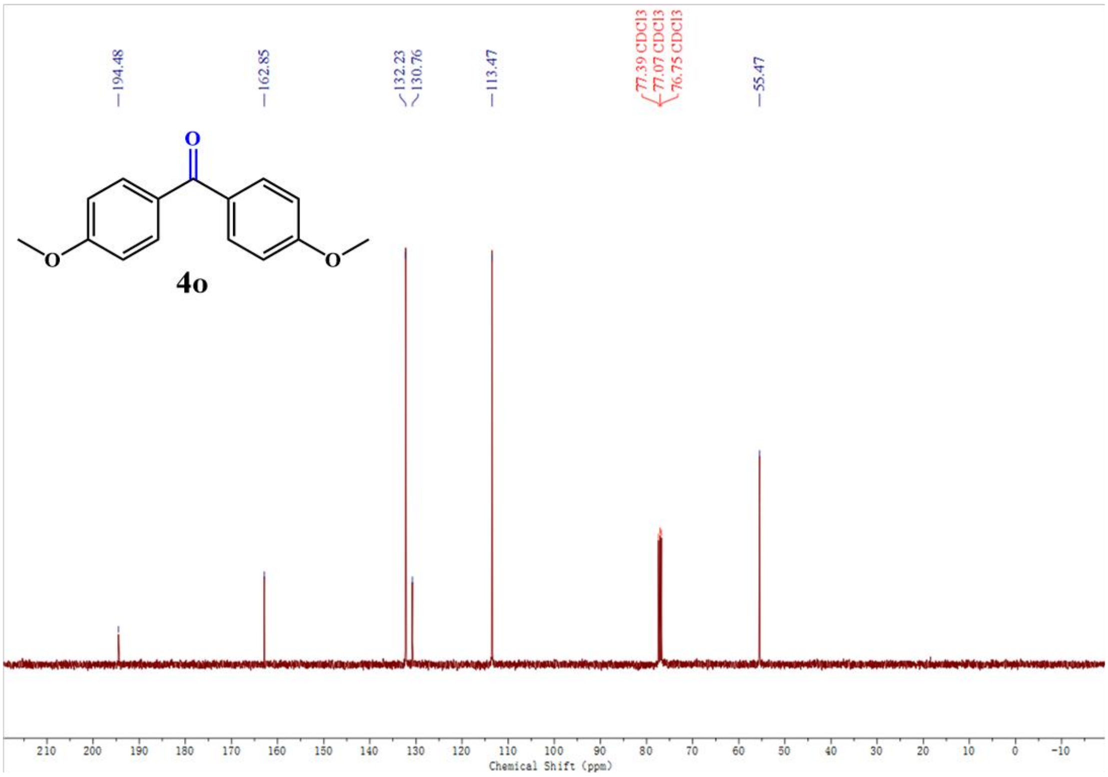

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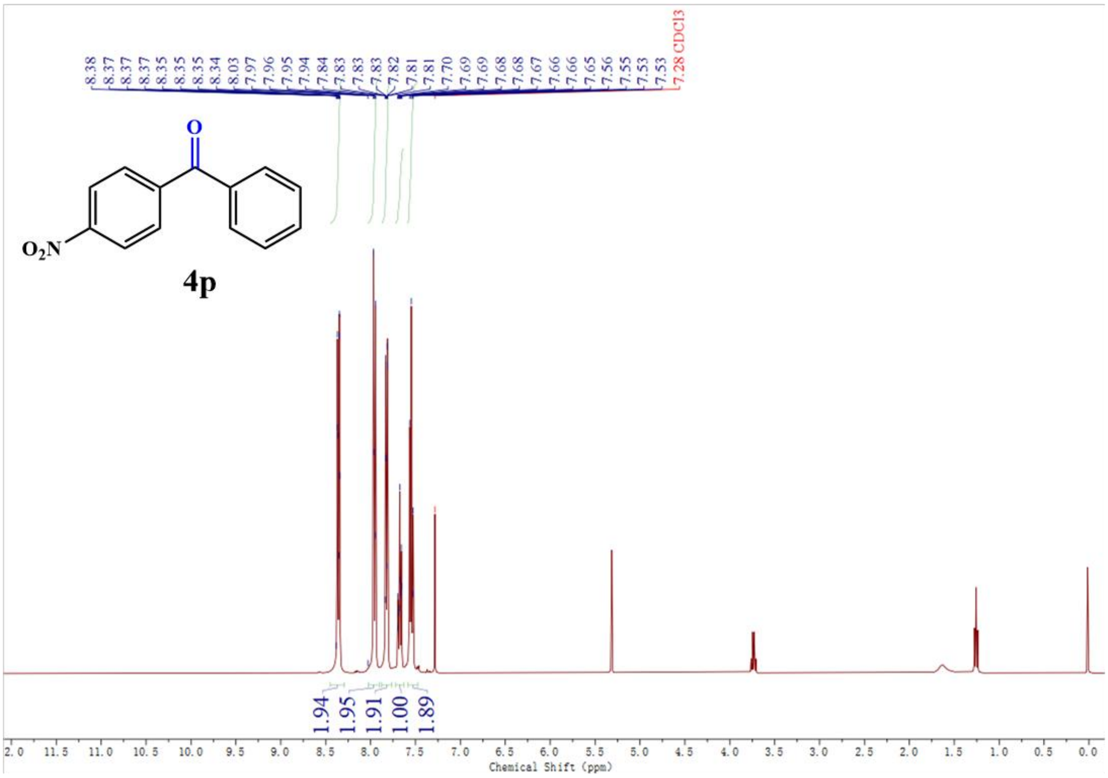

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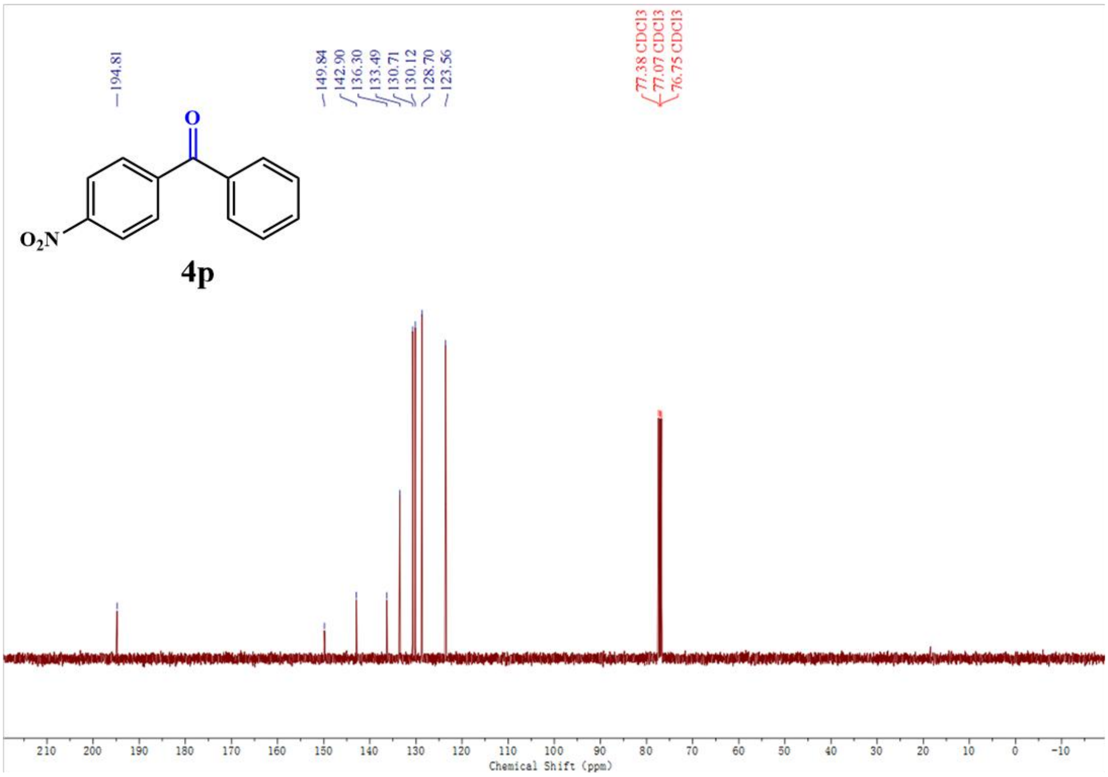

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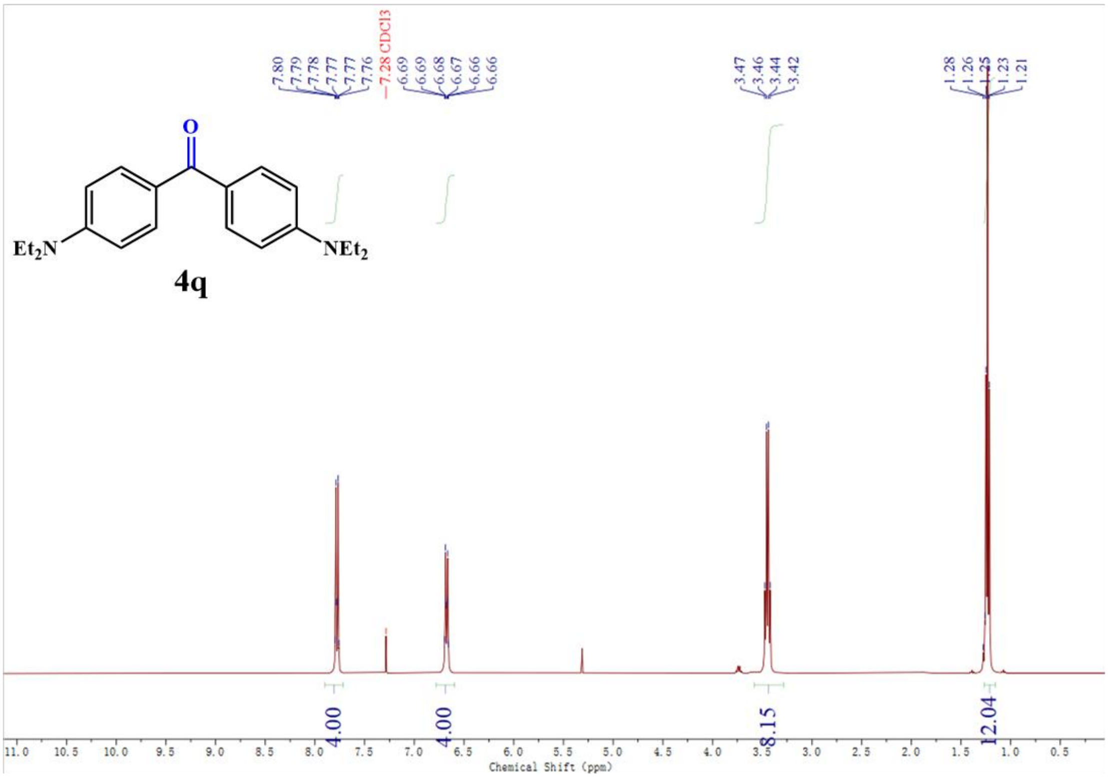

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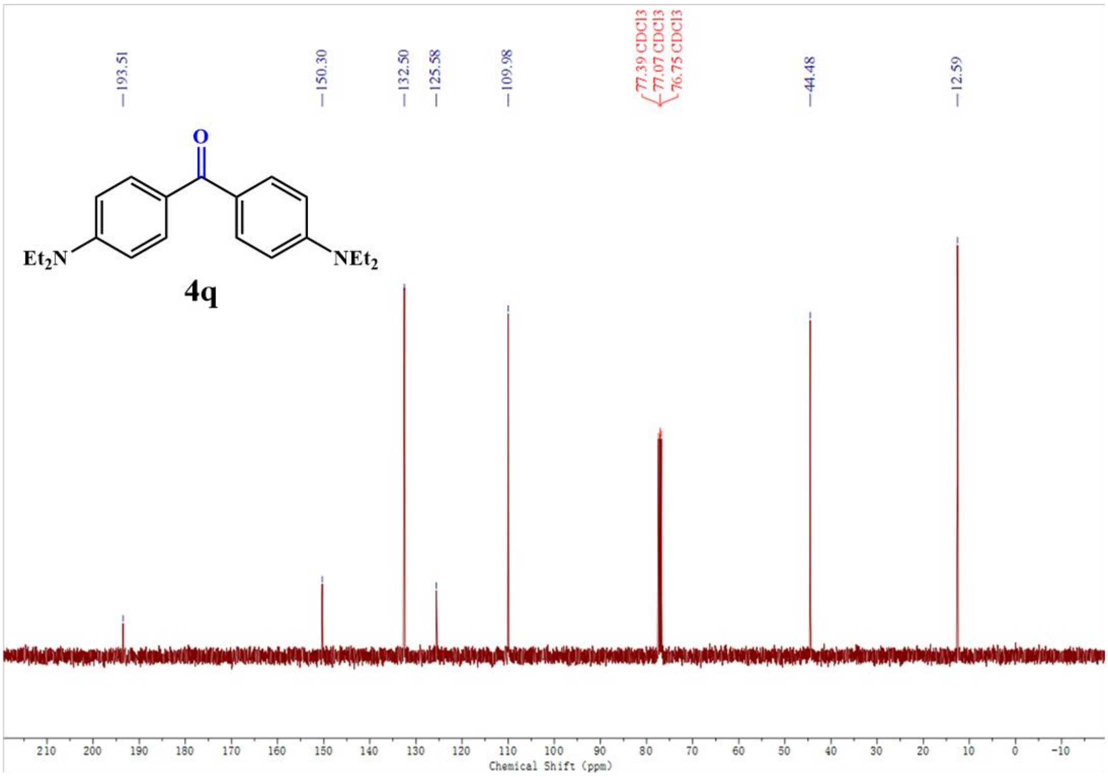

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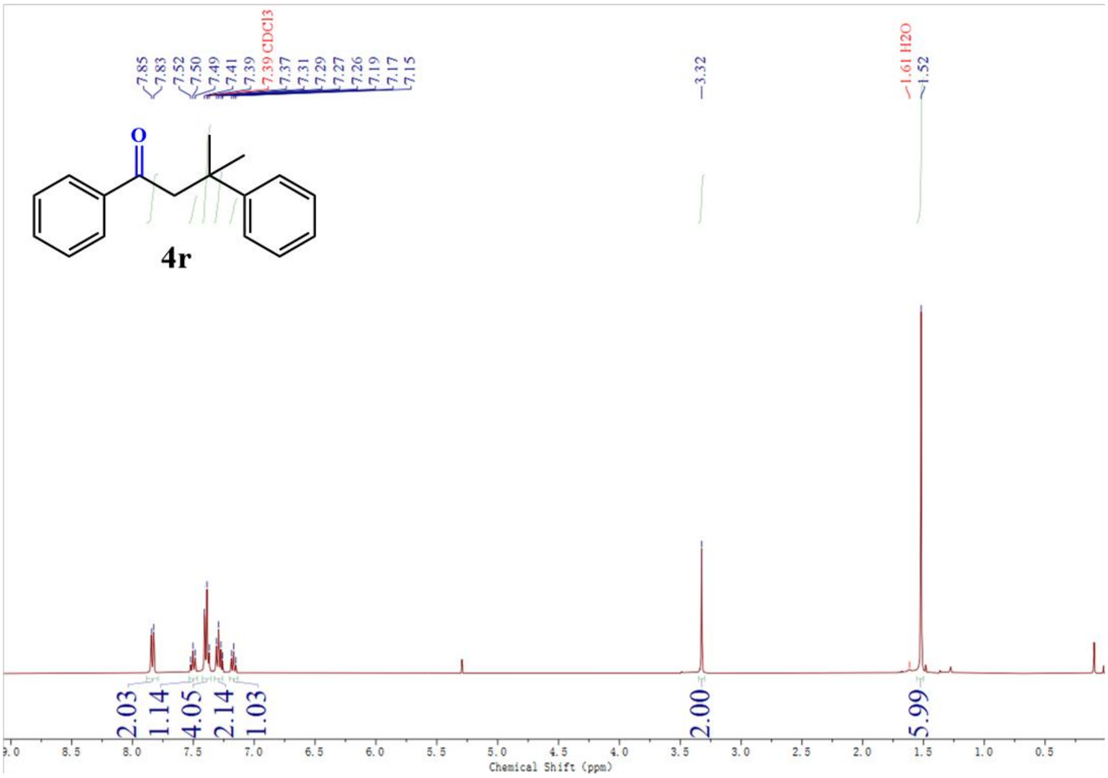

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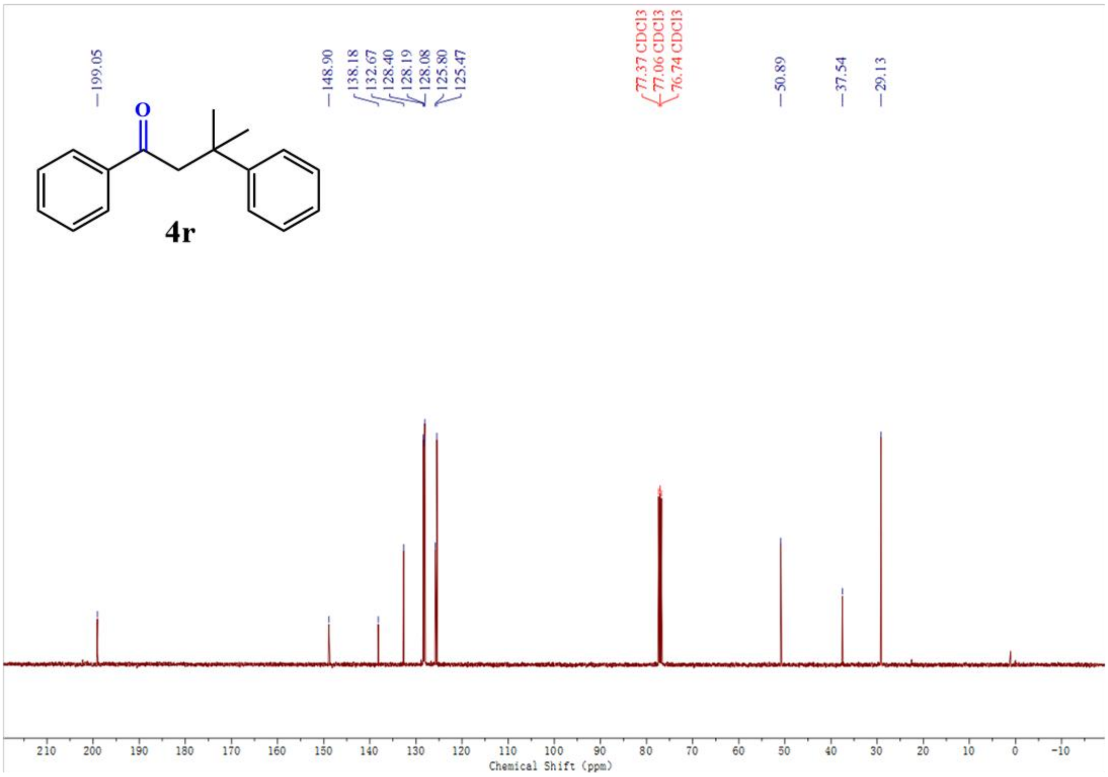

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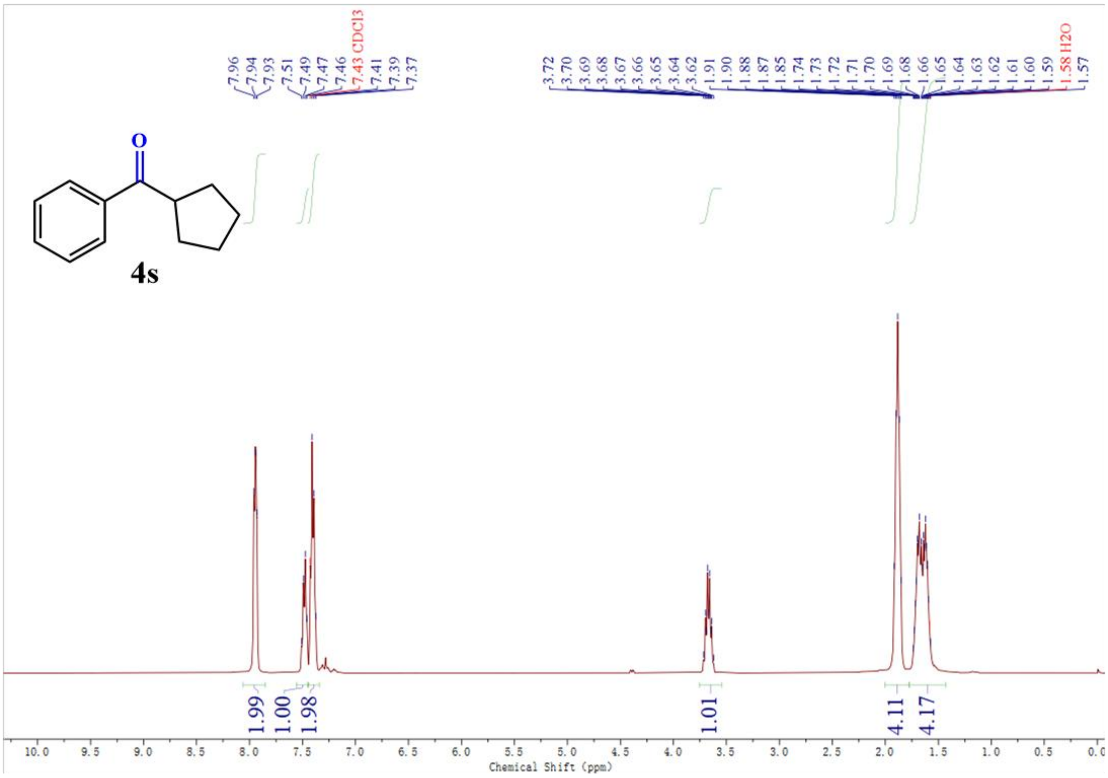

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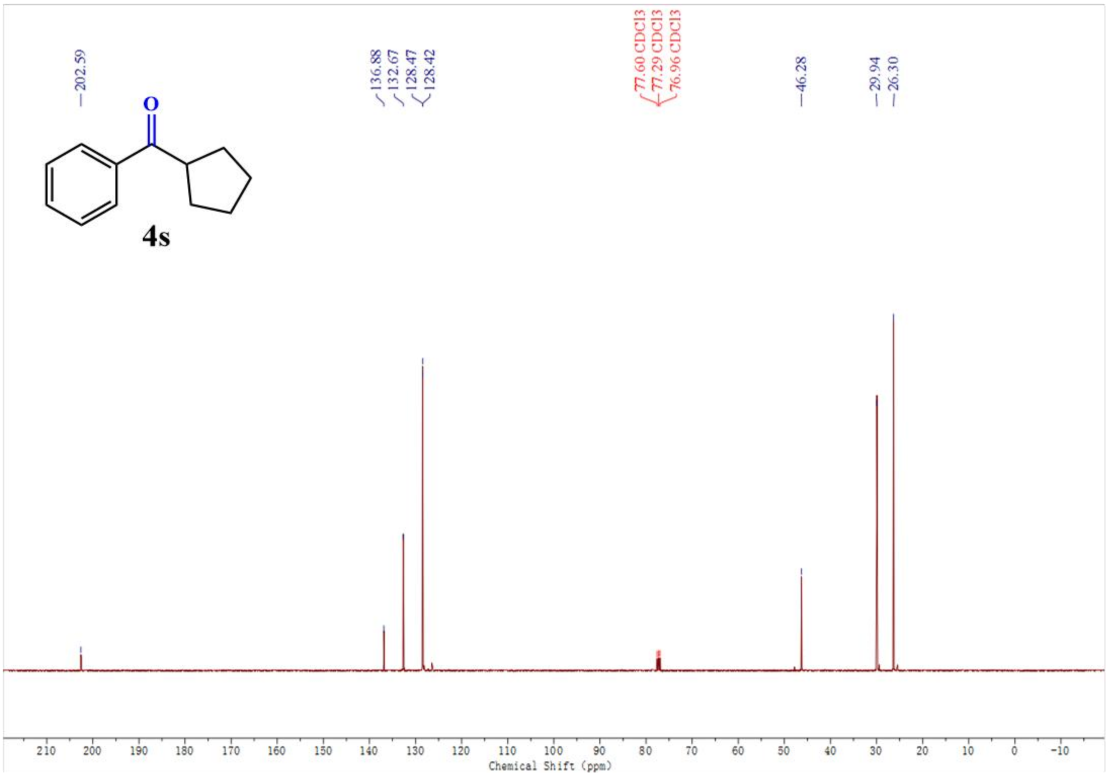

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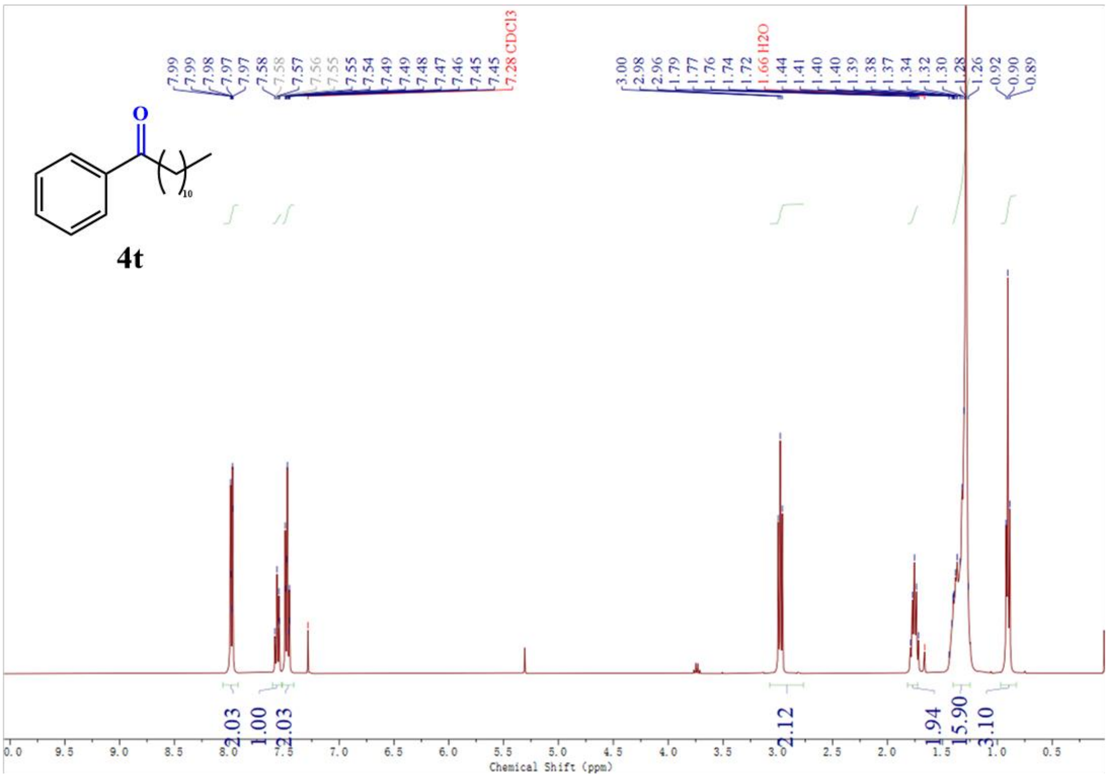

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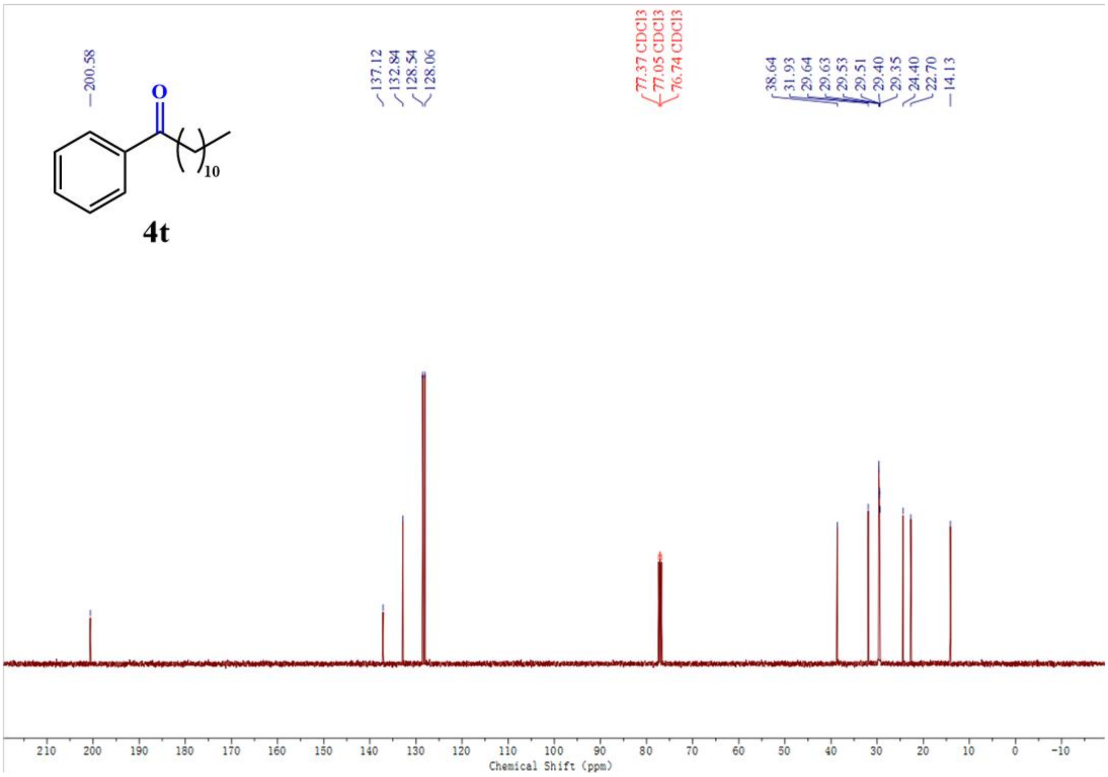
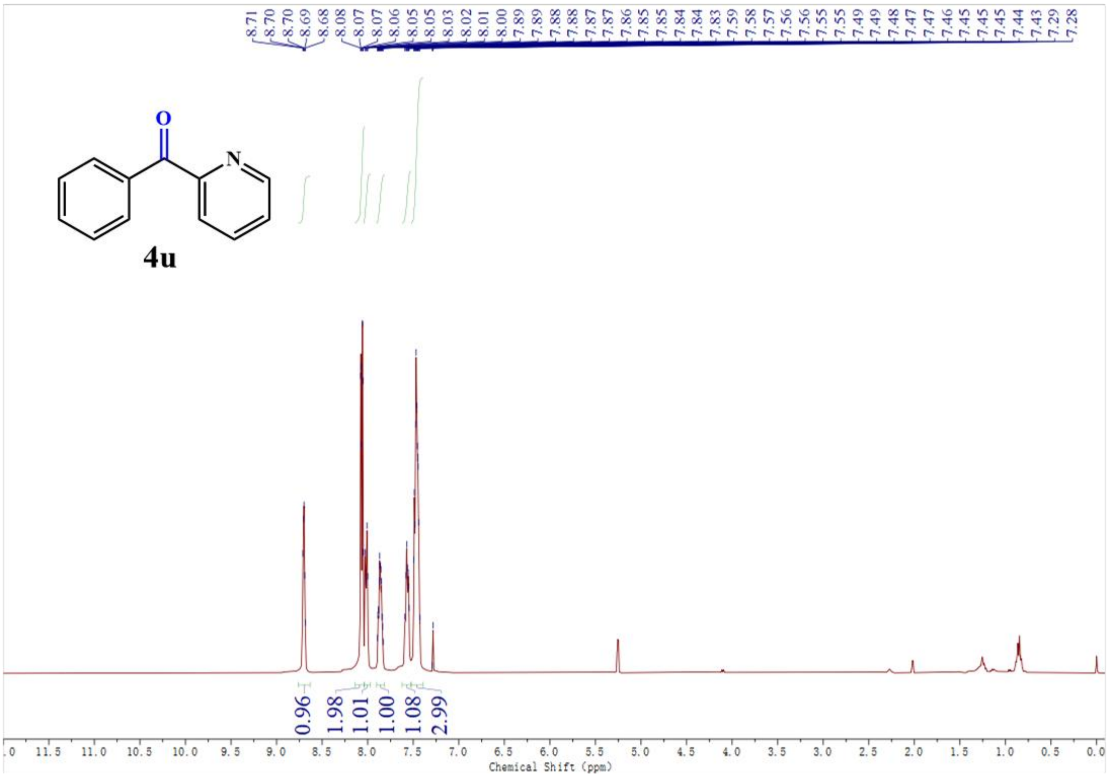
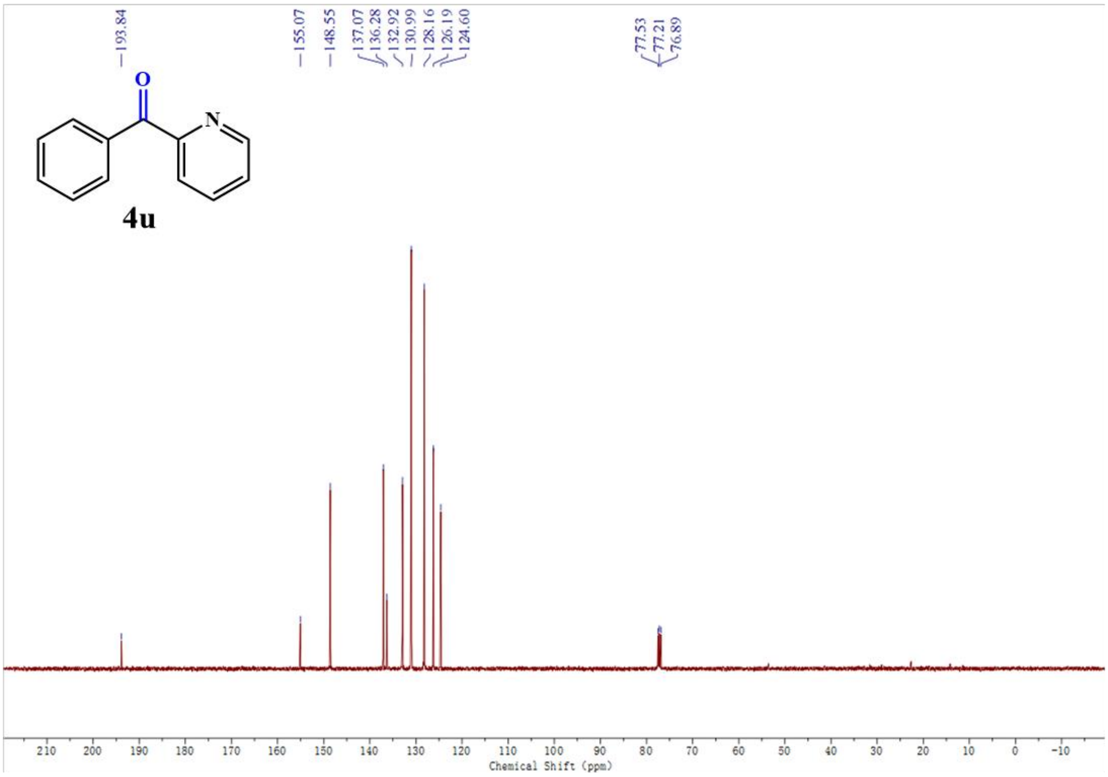


^{13}C NMR of **4t** in CDCl$_3$



^{1}H NMR of **4u** in $CDCl_3$



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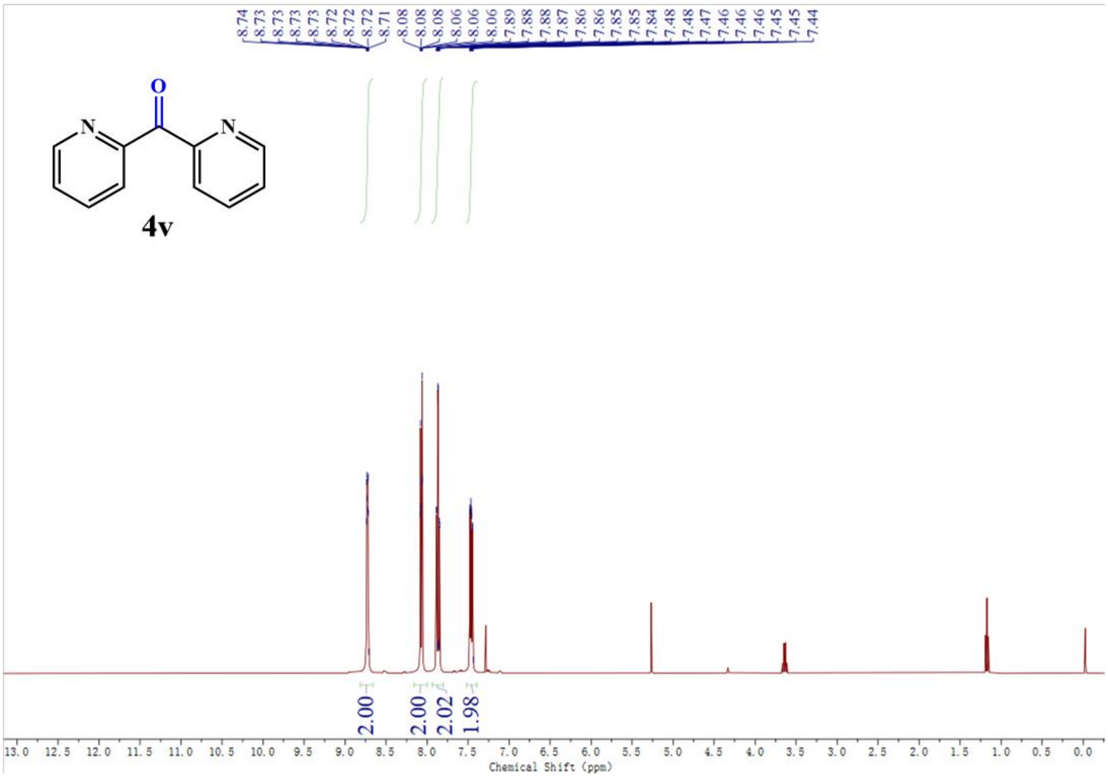

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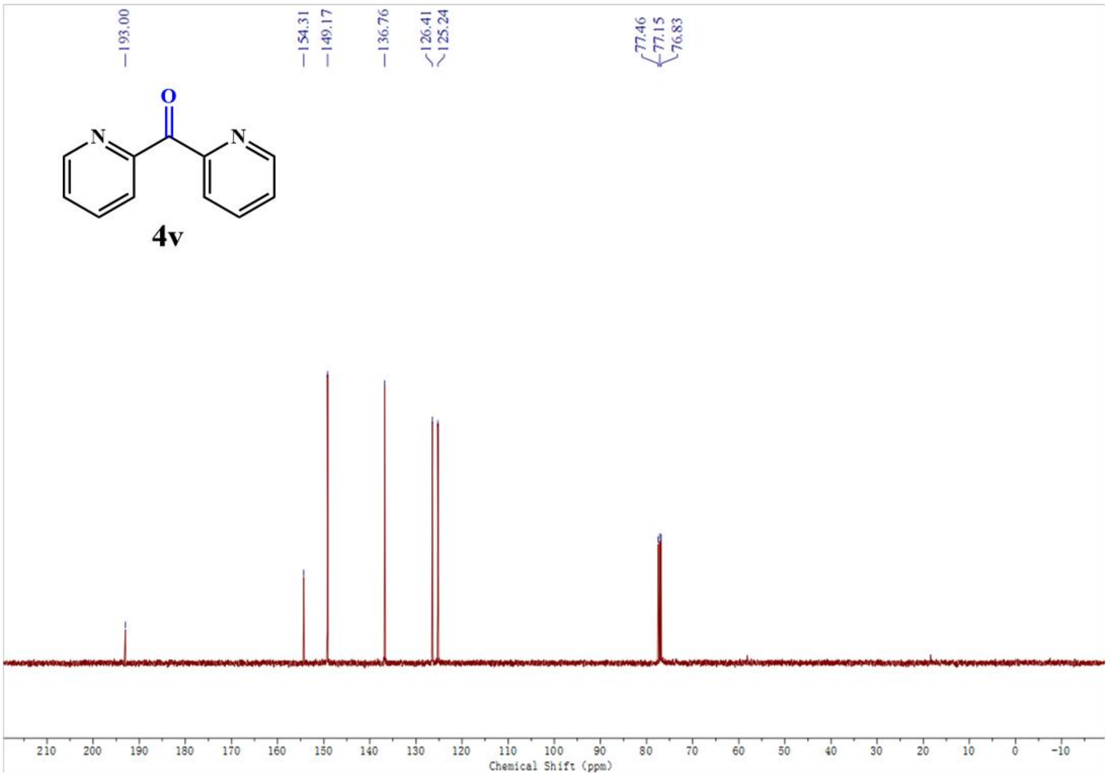

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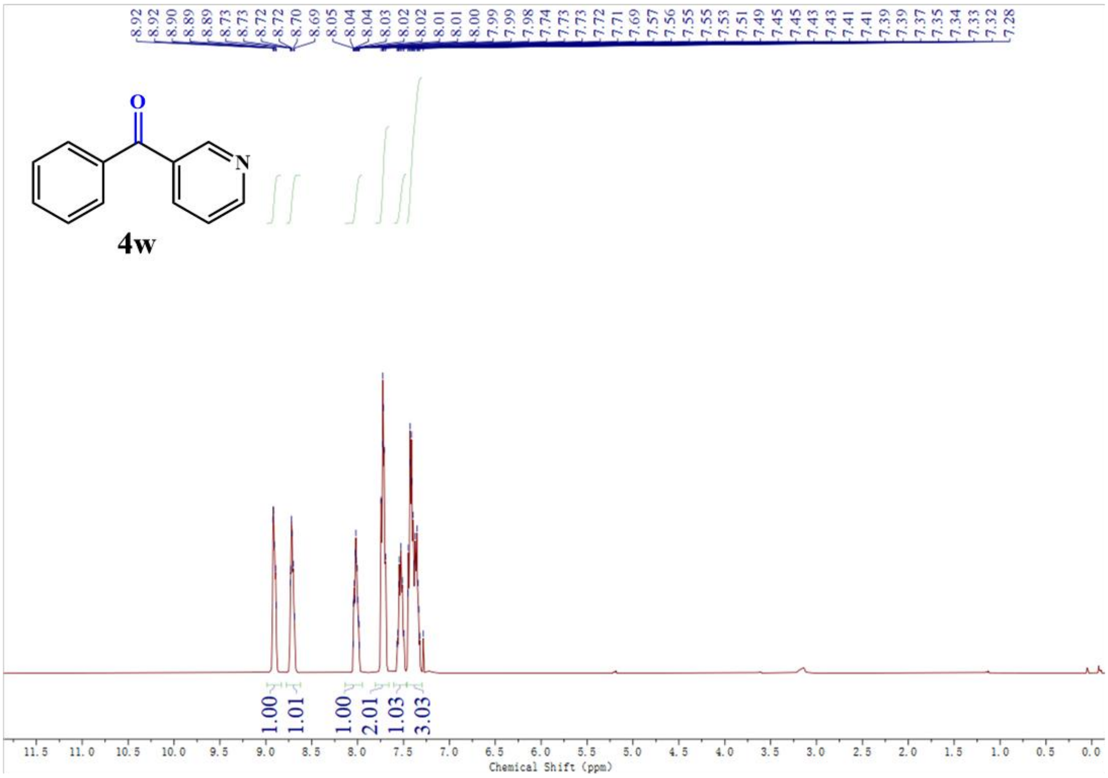
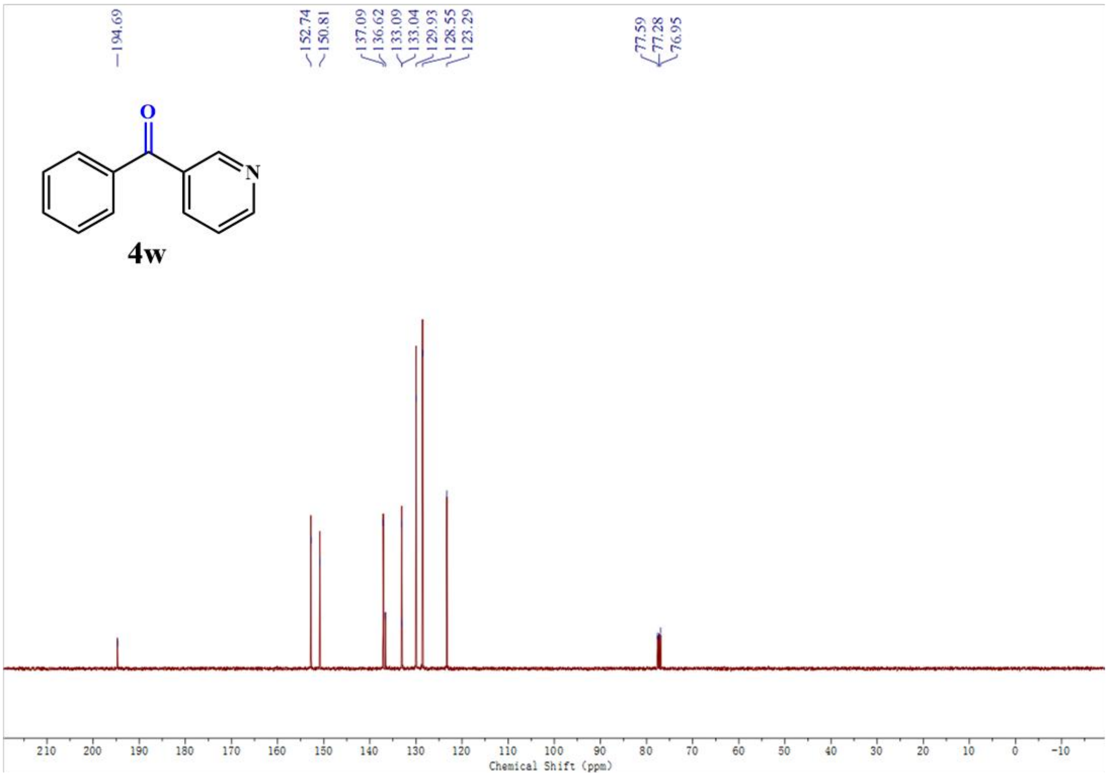
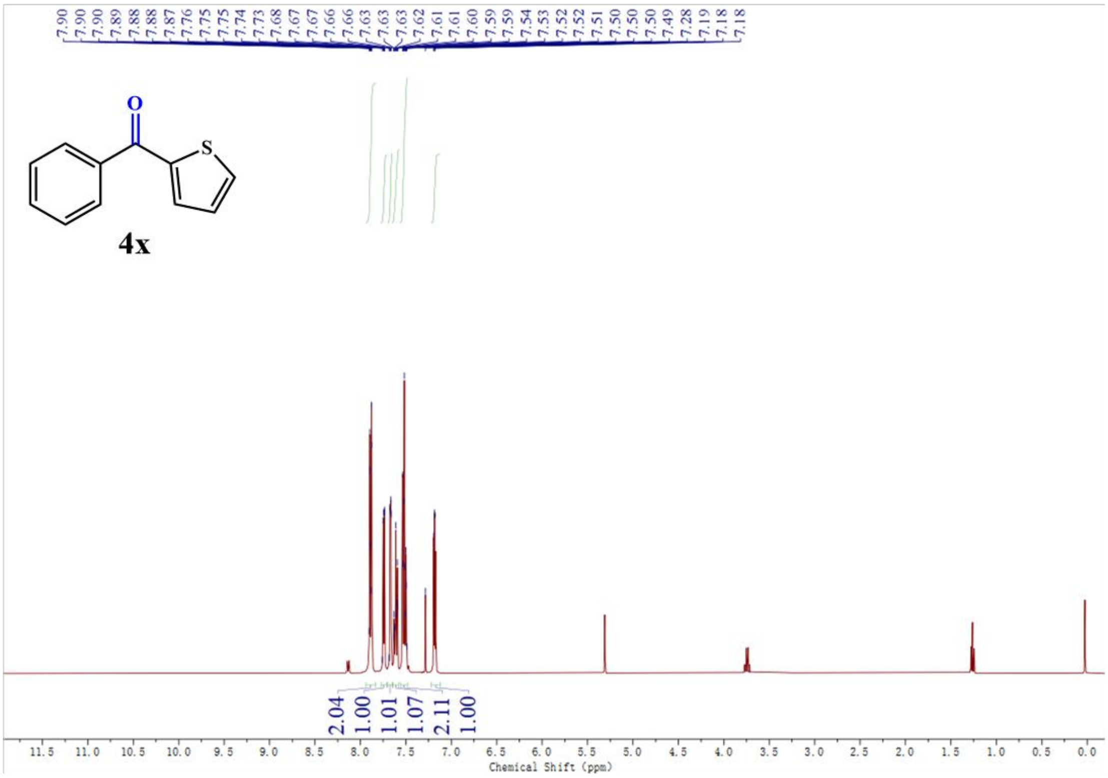


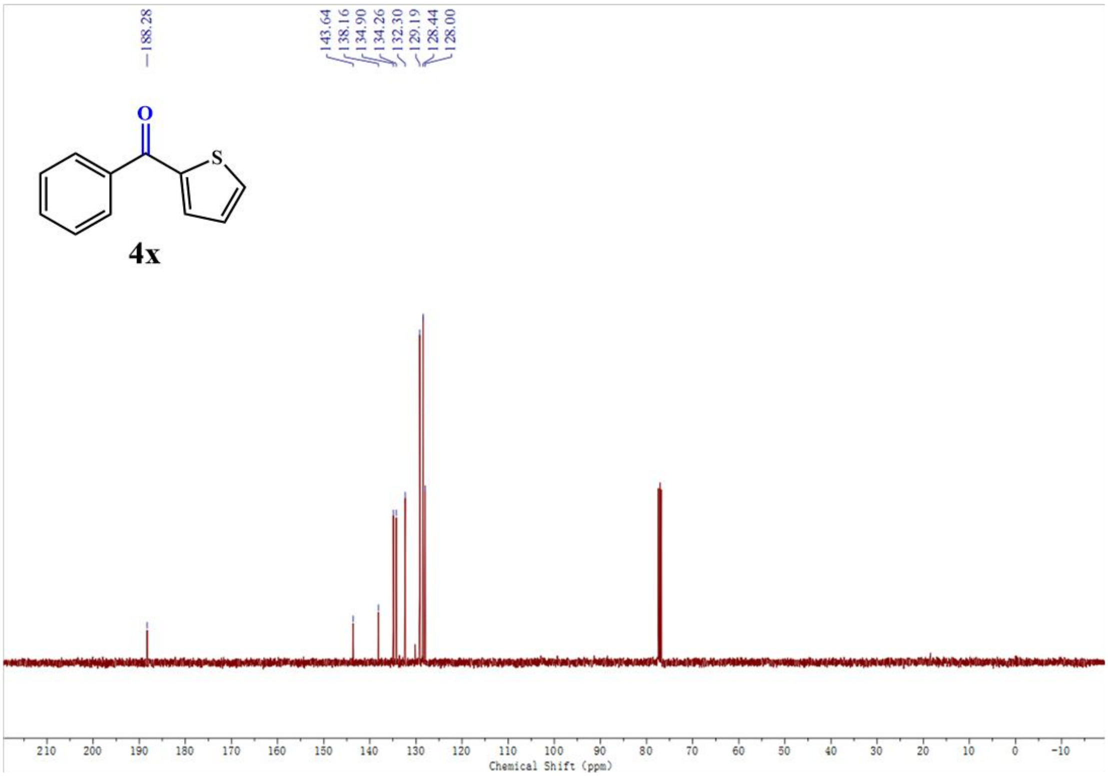
^{1}H NMR of **4w** in CDCl$_3$



^{13}C NMR of **4w** in CDCl$_3$



^{1}H NMR of **4x** in $CDCl_3$



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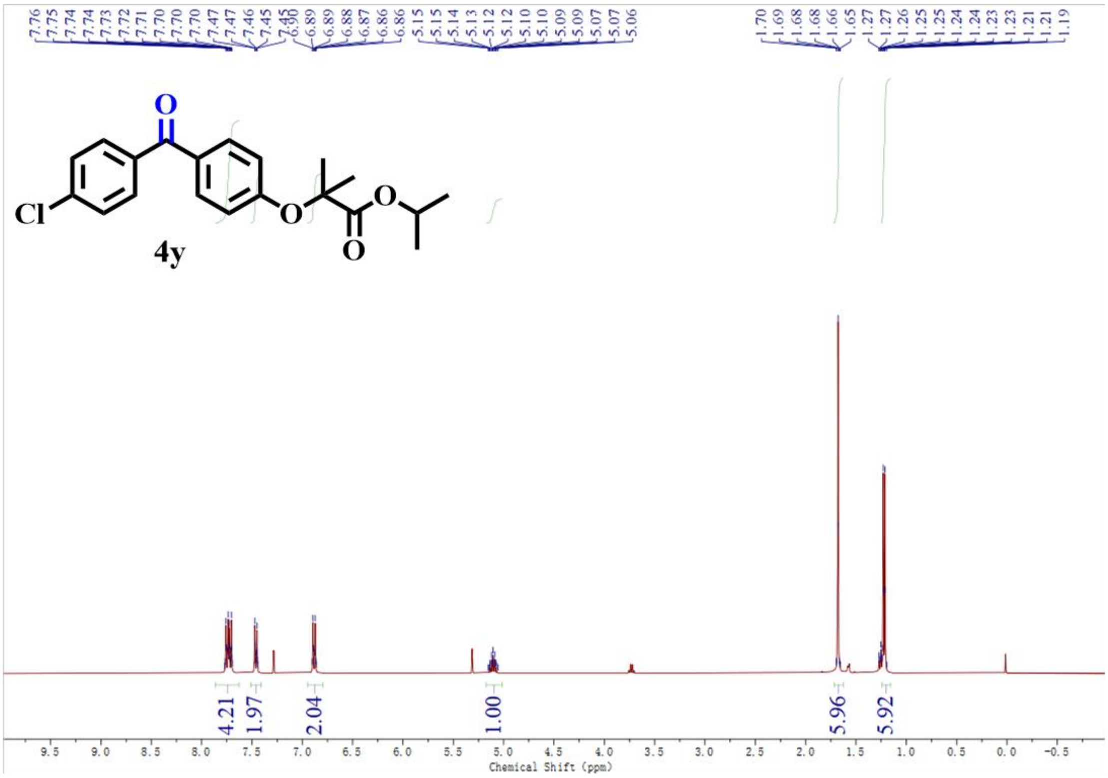

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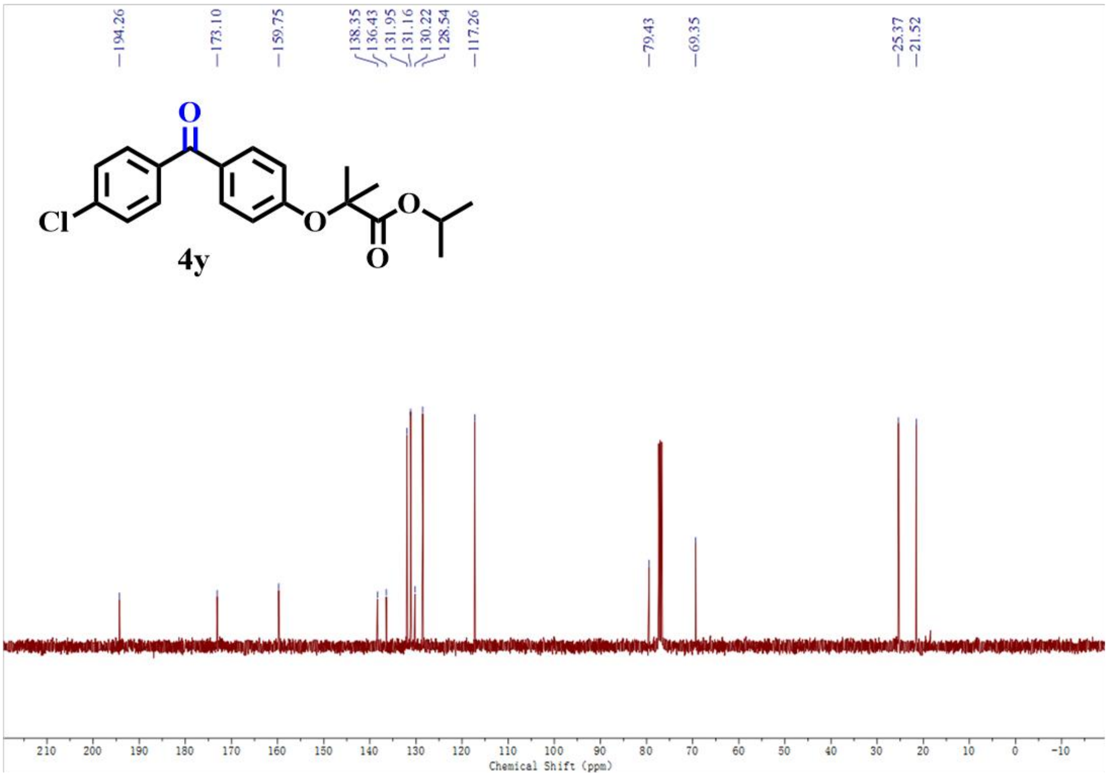

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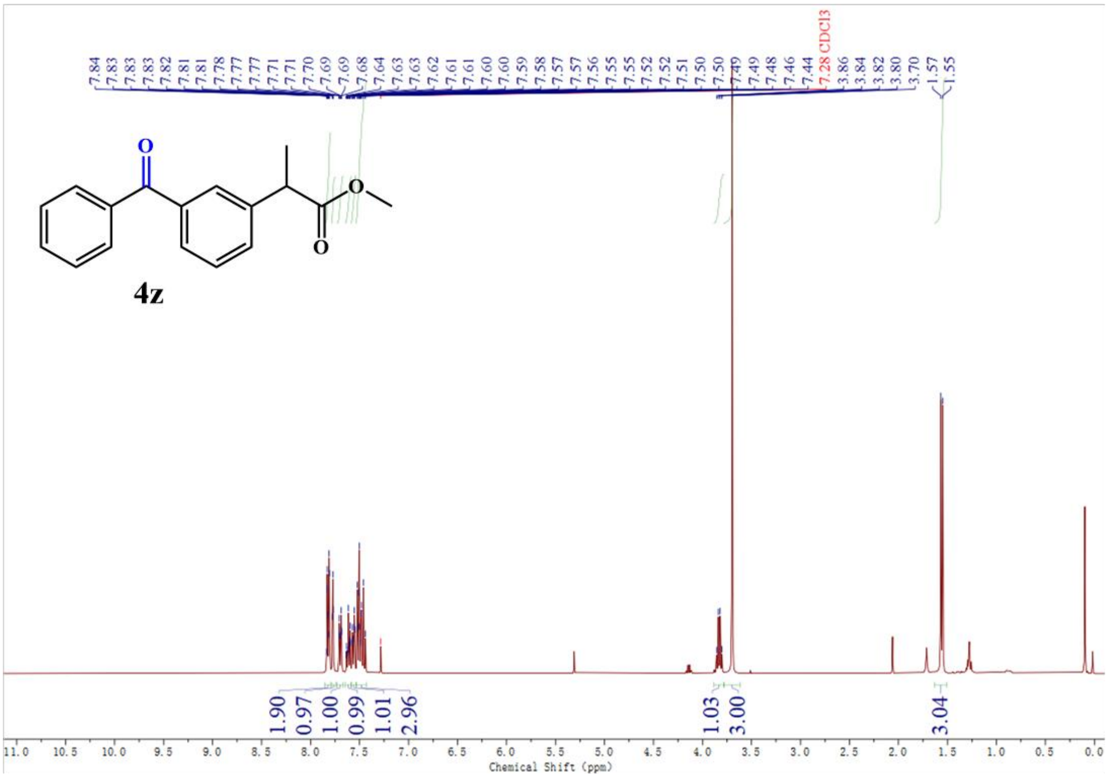

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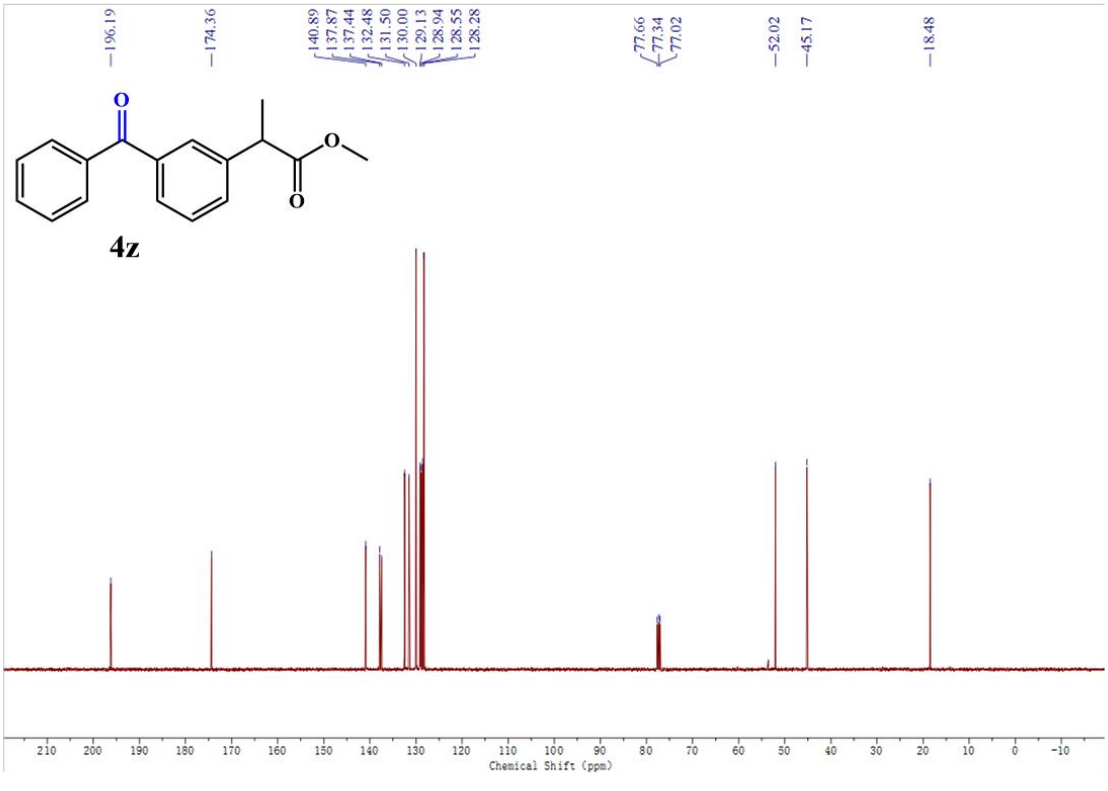

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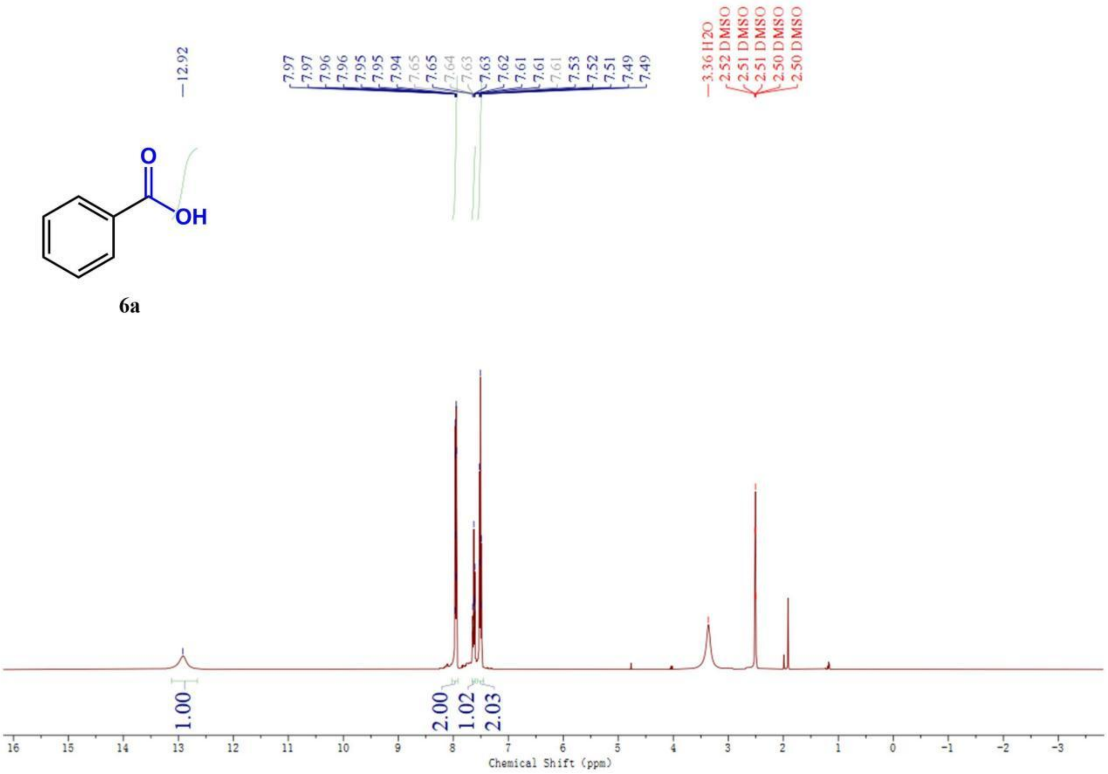
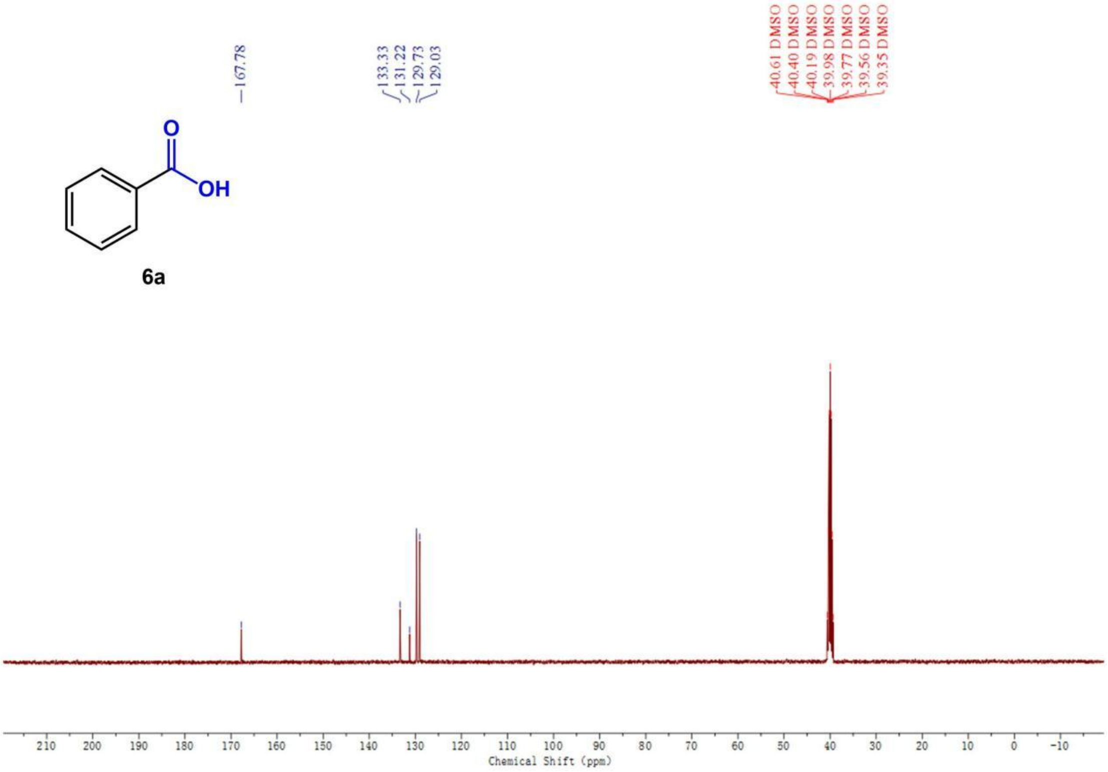


^{1}H NMR of **6a** in DMSO-d_6



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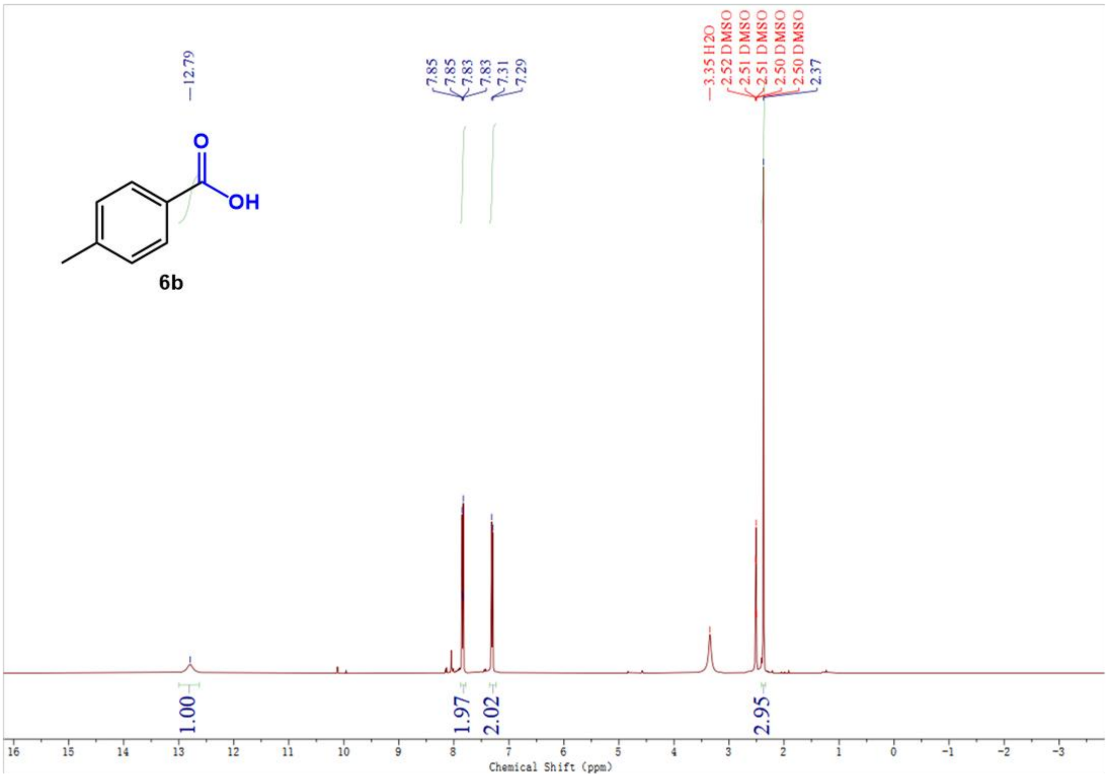
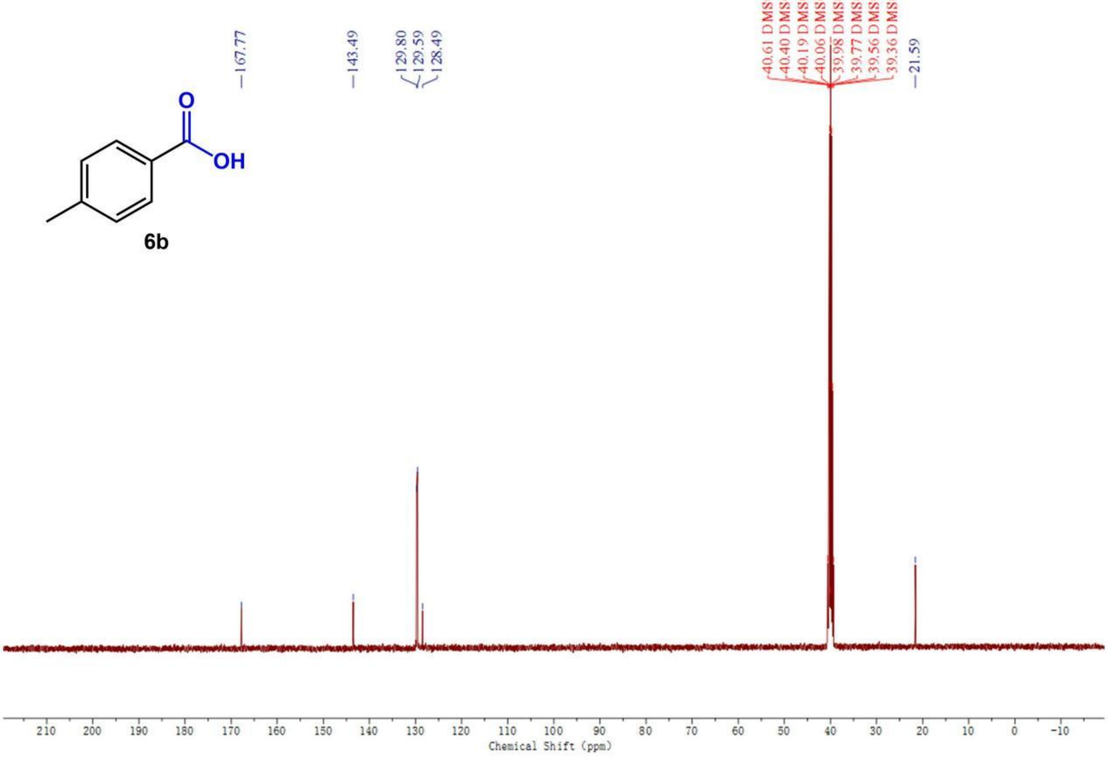


^{1}H NMR of **6b** in DMSO-d_6



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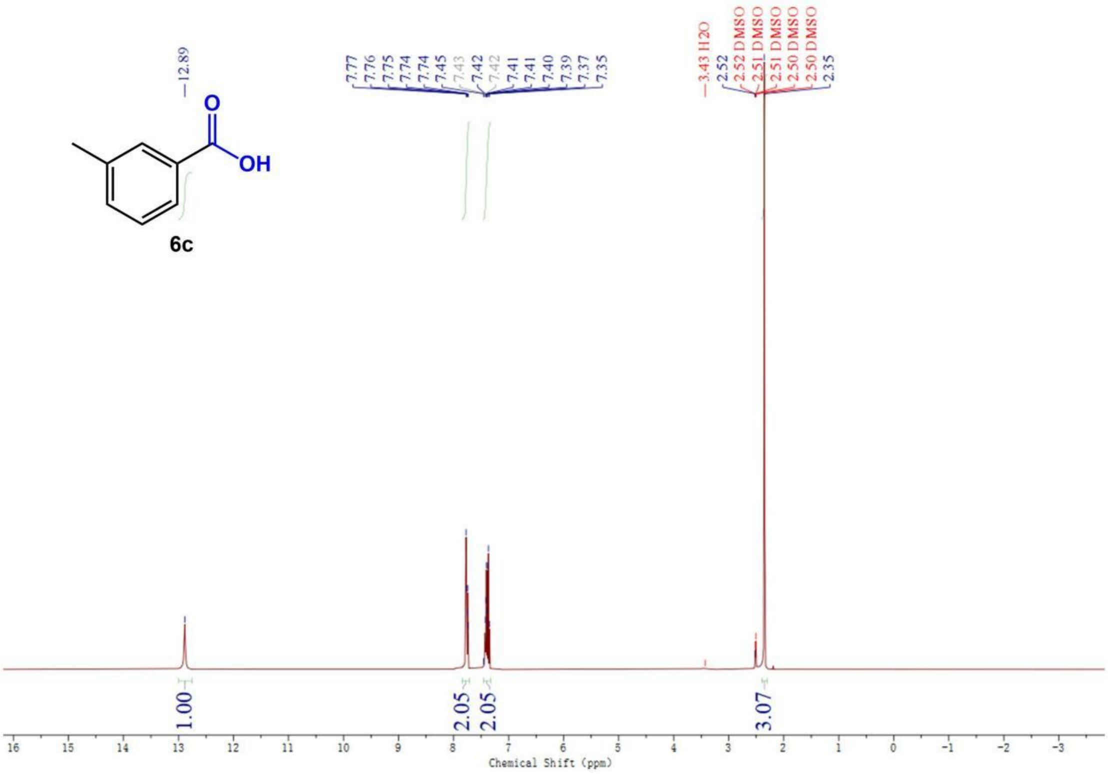
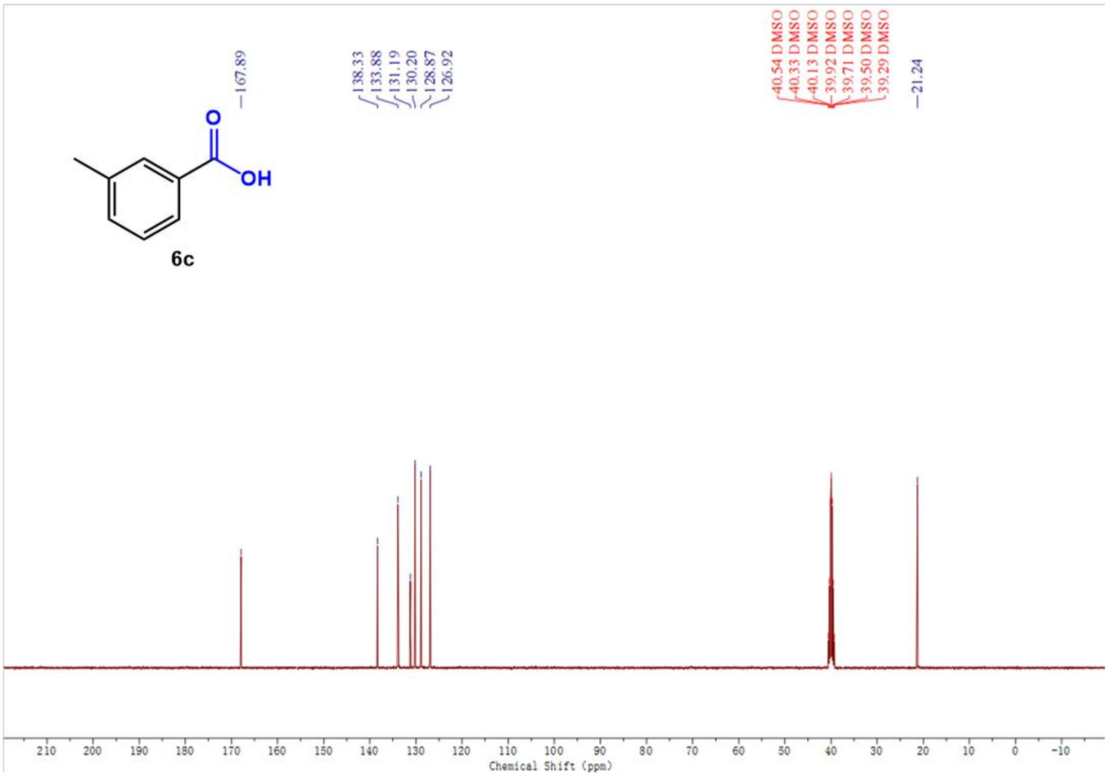


^{1}H NMR of **6c** in DMSO-d_6



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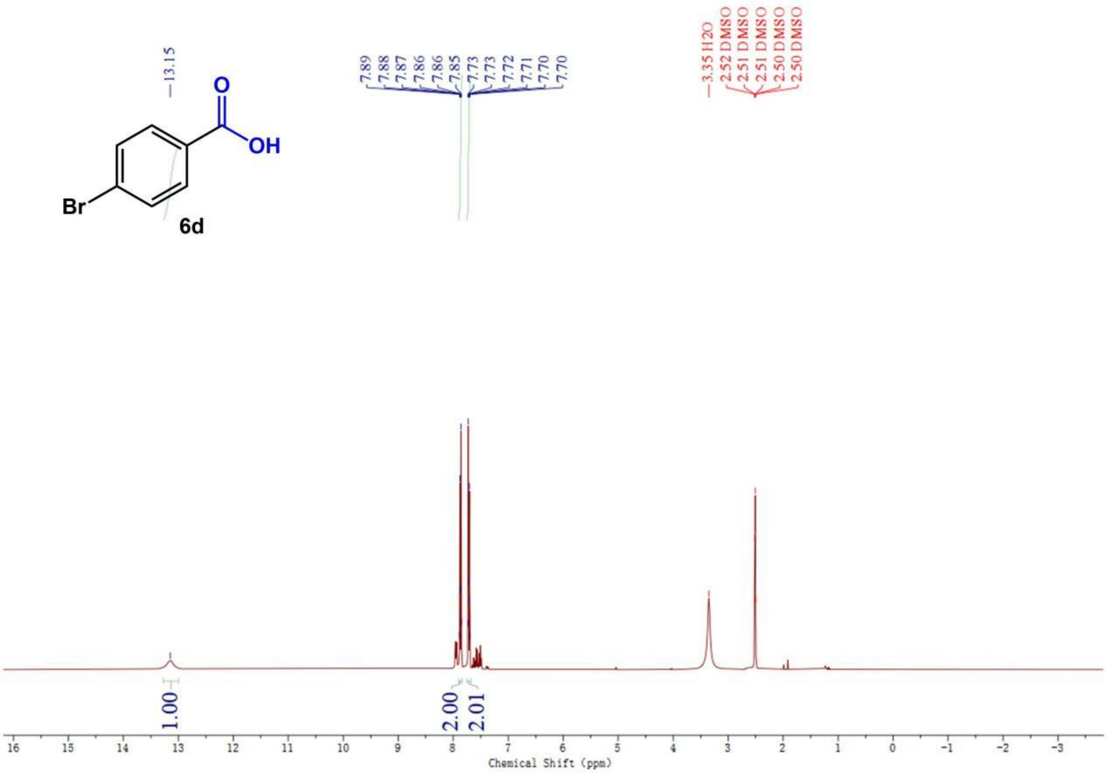
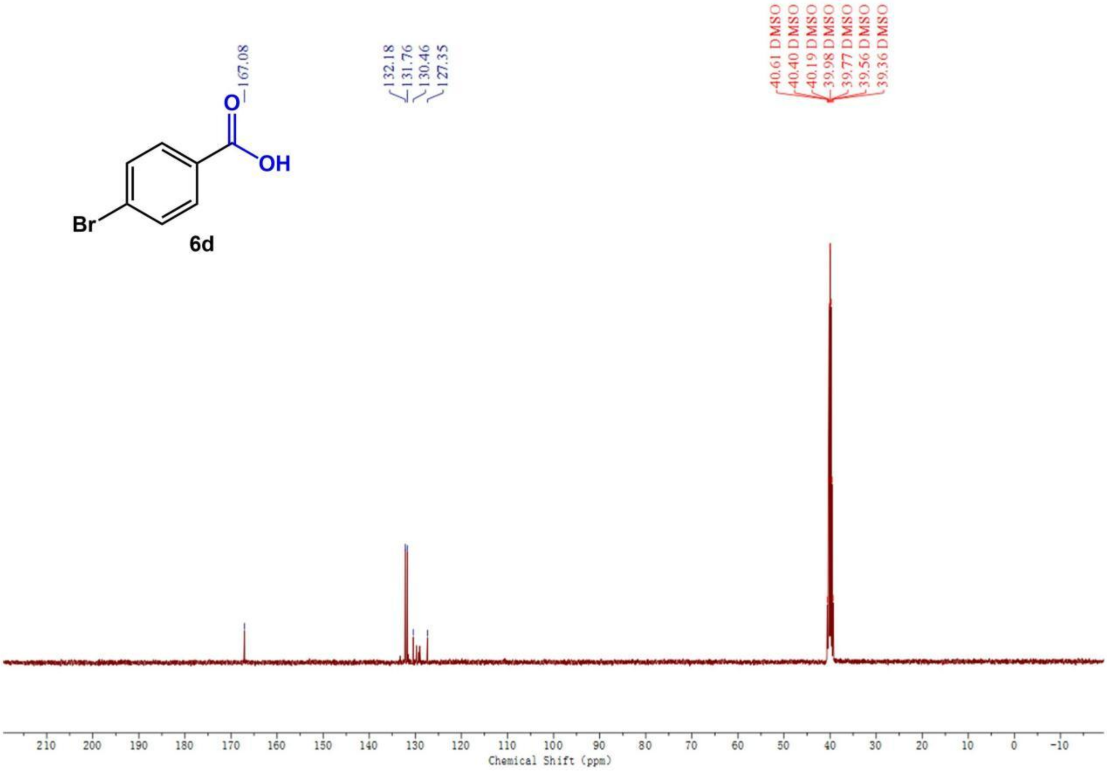


^{1}H NMR of **6d** in DMSO-d_6



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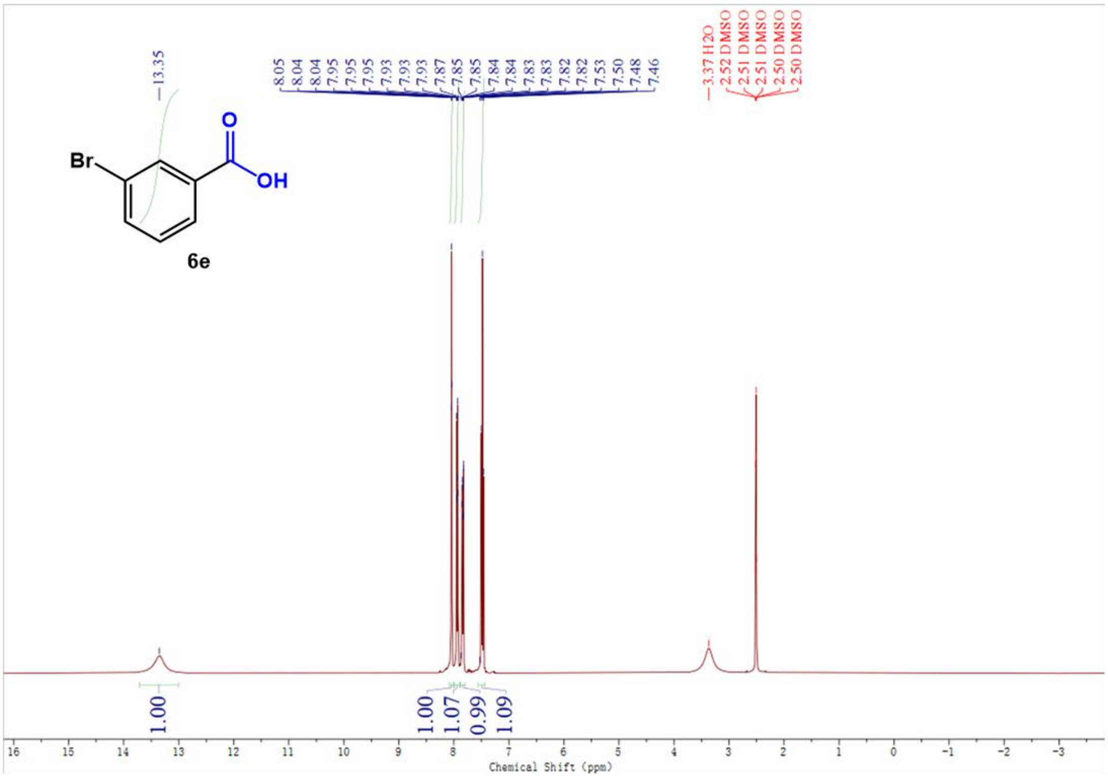
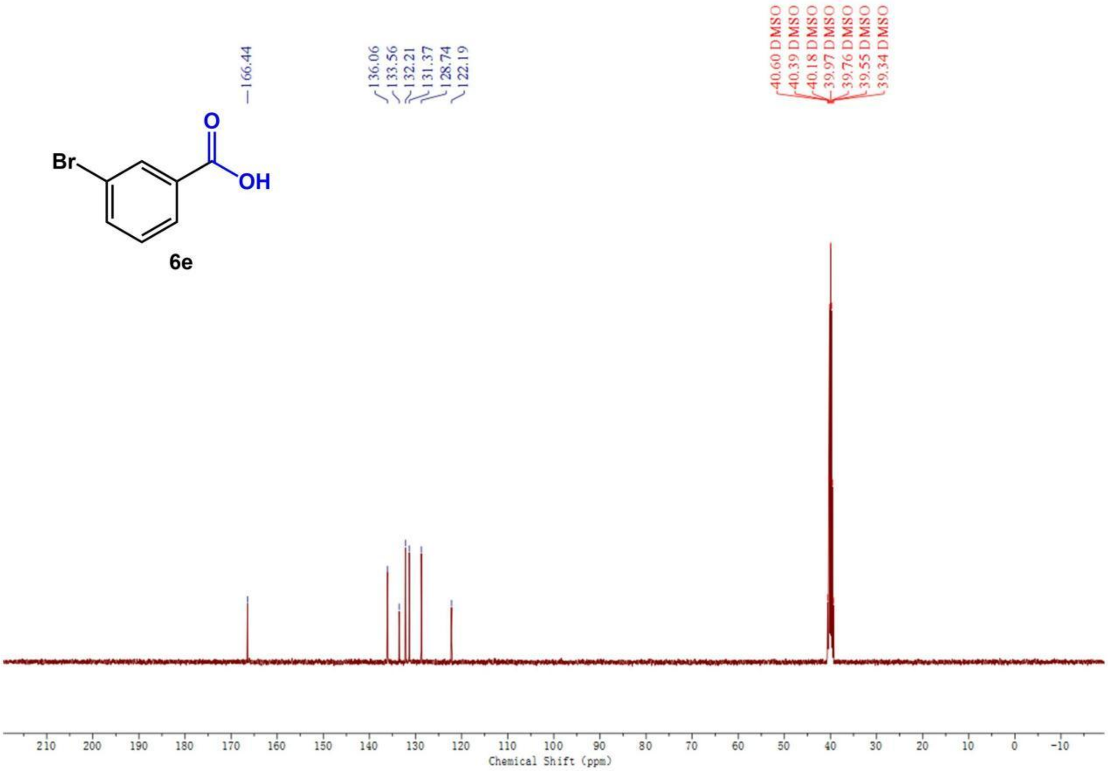


^{1}H NMR of **6e** in DMSO-d_6



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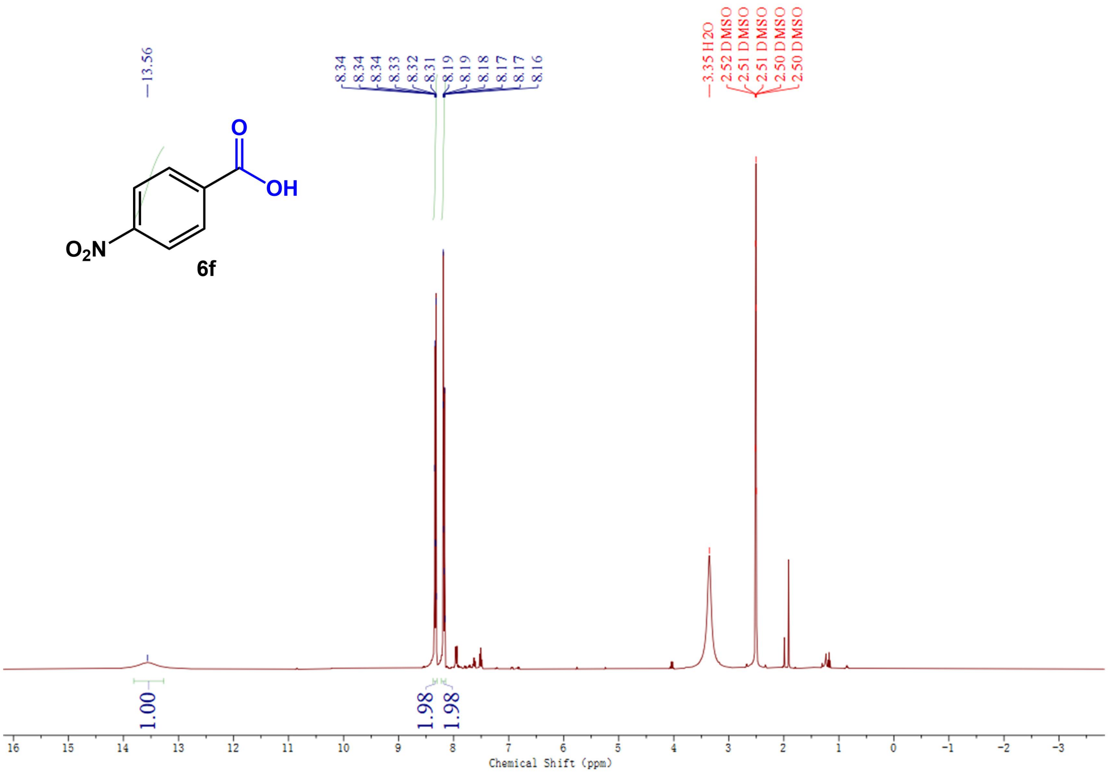
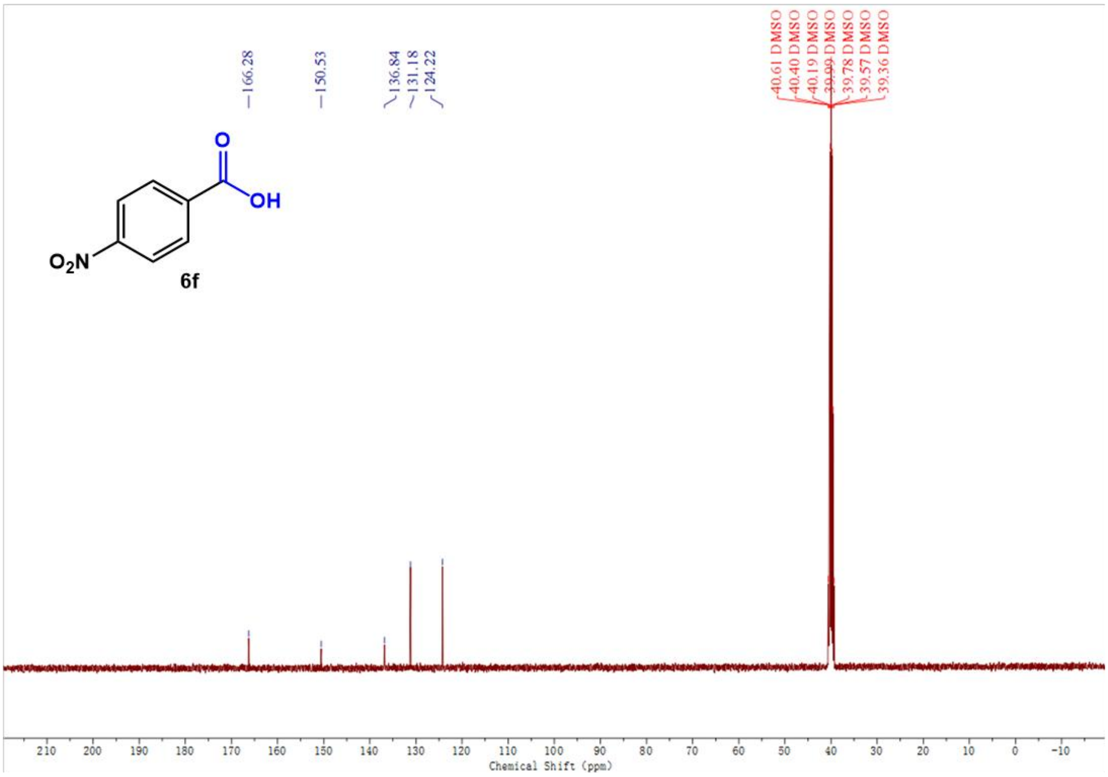


^{1}H NMR of **6f** in DMSO-d_6



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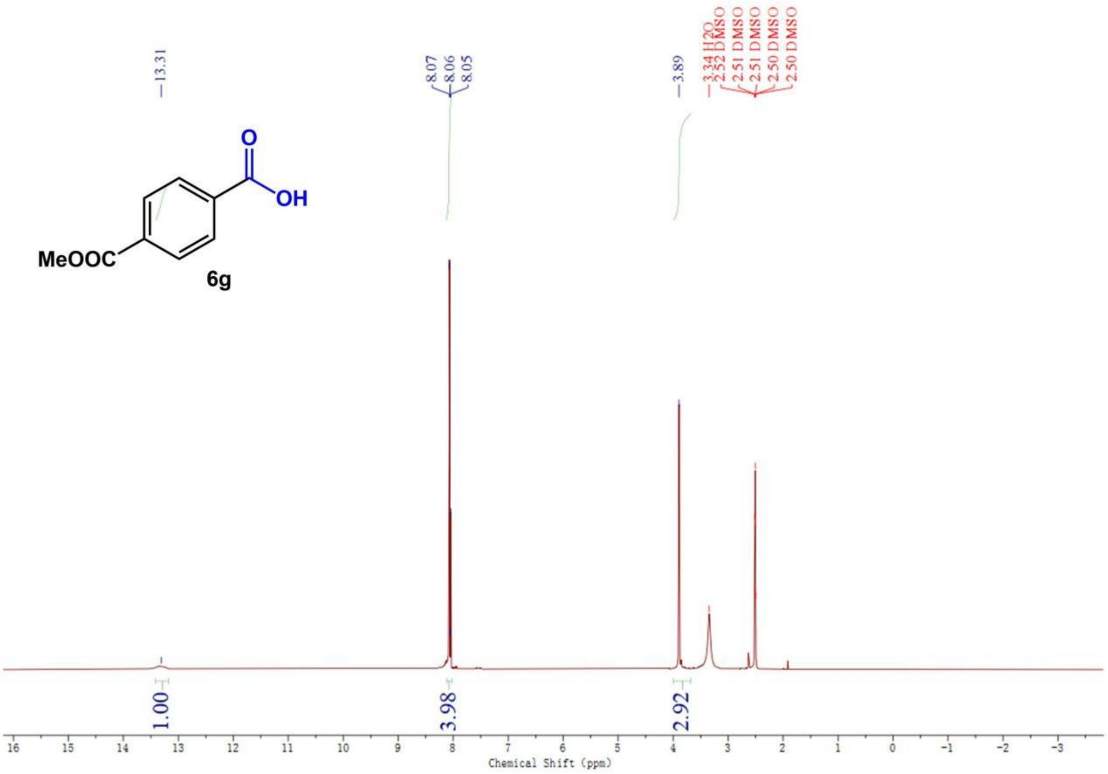
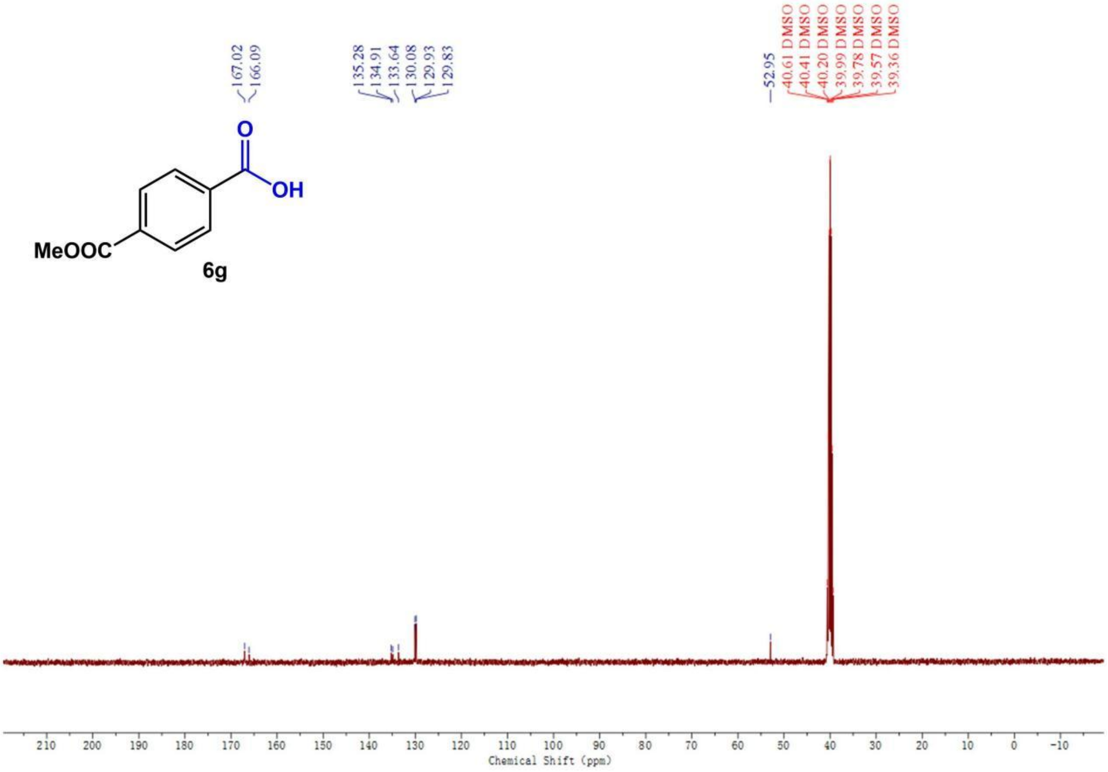


^{1}H NMR of **6g** in DMSO-*d*$_6$



^{13}C NMR of **6g** in DMSO-*d*$_6$

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