Supporting Information

Copper Supported on H^+-Modified Manganese Oxide Octahedral Molecular Sieves (Cu/H-OMS-2) as a Heterogeneous Biomimetic Catalyst for the Synthesis of 3-Aroylimidazopyridines and 3-Aroylimidazopyrimidines

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CONTENTS

1. General information

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without further purification. Metal salts were commercially available and were used directly. All experiments were carried out under air. Flash chromatography was carried out with Merck silica gel 60 (200-300 mesh). Analytical TLC was performed with Merck silica gel 60 F254 plates, and the products were visualized by UV detection. ^{1}H NMR and ^{13}C NMR (400 and 100 MHz respectively) spectra were recorded in $CDCl_3$. Chemical shifts (δ) are reported in ppm using TMS as internal standard, and spin-spin coupling constants (J) are given in Hz.

All supported catalysts are synthesized by wet impregnation in deionized water and $Cu(OH)_x$/OMS-2 is made by deposition-precipitation in water. The crystal phase and composition were determined by power X-ray diffraction using a X-Pert PRO X-ray diffractometer with Cu Ka radiation in the 2θ range of 10–90^{o}.

Infrared spectra of the materials were recorded on calcined powders dispersed in KBr (2 mg sample in 300 mg KBr) using a Perkin-Elmer One FTIR spectrometer with a resolution of 4 cm^{-1} operating in the range 500-2000 cm^{-1} with 4 scans per spectrum.

The morphologies of the samples were characterized by a TF20 transmission electron microscope and SM-5600LV scanning electron

microscope. Nitrogen adsorption-desorption measurements were performed at 76 K using an ASAP 2020M analyzer utilizing the BET model for the calculation of specific surface areas.

The reducibility of the catalysts was measured by the hydrogen temperature-programmed reduction (H_2-TPR) technique. A 50 mg of OMS-2, H-OMS-2 or Cu/H-OMS-2 was placed in a quartz reactor that was connected to a TPR apparatus and the reactor was heated from r.t. to 550 ^oC with a heating rate of 10 ^oC/min. The reducing atmosphere was the mixture of H_2 and N_2 with a total flow rate of 30 mL/min and the amount of H_2 uptake during the reduction was measured by a thermal conductivity detector (TCD).

The oxygen species of the catalysts was investigated by the oxygen temperature-programmed desorption (O_2-TPD) technique. A 50 mg of H-OMS-2 or Cu/H-OMS-2 was place in a quartz reactor that was connected to a TPD apparatus and the reactor was purged with He at room temperature for 1 h followed by heating to 950 ^oC at 10 ^oC/min in the same atmosphere.

The X-ray photoelectron spectroscopy (XPS) measurements were performed on a Kratos AXIS Ultra DLD high performance electron spectrometer using nonmonochromatized Al Kα excitation source ($h\nu$ = 1486.6 eV). Binding energies were calibrated by using the contaminant carbon (C 1s = 284.6 eV).

2. Experimental procedure

2.1 Preparation of H-OMS-2[1]

H-OMS-2 was synthesized by ion-exchange with homemade OMS-2. The concentrated HNO_3 (50 mL) was added to OMS-2 (2 g) and the slurry was stirred vigorously at 80 ^oC for 6 h. The product was filtered and washed by deionized water for many times. Then, the product was dried at 120 ^oC for 12 h in an oven and calcined at 280 ^oC for 6 h.

2.2 Preparation of Cu/H-OMS-2

Support H-OMS-2 (2 g) was added to a 50 mL round-bottom flask. A solution of $Cu(NO_3)_2 \cdot 3H_2O$ (0.15 g) in deionized water (10 mL) was added to H-OMS-2, and additional deionized water (10 mL) was added to wash down the sides of the flask. Then the flask was submerged into an ultrasound bath for 3 h at room temperature and stirred for further 20 h at room temperature. After that, the water was distilled under reduced pressure on a rotary evaporator at 80 ^oC for more than 2 h. Finally, the black powder was dried into an oven at 110 ^oC for 4 h followed by calcination at 350 ^oC under air for 2 h.

2.3 General procedure for Cu/H-OMS-2-catalyzed 3-aroylimidazo[1,2-*a*]pyridines synthesis

Cu/H-OMS-2 (12 mg, 0.7 mol%), 2-aminopyridine (0.6 mmol), chalcones (0.4 mmol) and $Cl_2CHCHCl_2$ (1.2 mL)/HOAc (0.1 mL)

were added to a flask with a bar. The flask was stirred at 100 °C for 20 h under air. After cooling to room temperature, the mixture was diluted with ethyl acetate and filtered. The filtrate was removed under reduced pressure to get the crude product, which was further purified by silica gel chromatography (petroleum/ethyl acetate = 4/1 as eluent) to yield corresponding product.

2.4 General procedure for Cu/H-OMS-2-catalyzed 3-aroylimidazo[1,2-*a*]pyrimidines synthesis

Cu/H-OMS-2 (12 mg, 0.7 mol%), 2-aminopyrimidine (0.6 mmol), chalcones (0.4 mmol) and $Cl_2CHCHCl_2$ (1.2 mL)/HOAc (0.1 mL) were added to a flask with a bar. The flask was stirred at 100 °C for 20 h under air. After cooling to room temperature, the mixture was diluted with ethyl acetate and filtered. The filtrate was removed under reduced pressure to get the crude product, which was further purified by silica gel chromatography (petroleum/ethyl acetate = 4/1 as eluent) to yield corresponding product.

2.5 General procedure for Cu/H-OMS-2-catalyzed one-pot reactions for the synthesis of 3-aroylimidazo[1,2-*a*]pyridines

Cu/H-OMS-2 (12 mg, 0.7 mol%), acetophenone (0.4 mmol), benzaldehyde (0.6 mmol), 2-aminopyridine (0.6 mmol) and Cl2CHCHCl2 (1.2 mL) were added to a flask with a bar. The mixture was stirred for 2 h at 100 °C, then, HOAc (0.1 mL) was

added to the mixture. The flask was stirred at 100 ^{o}C for another 20 h under air. After cooling to room temperature, the mixture was diluted with ethyl acetate and filtered. The filtrate was removed under reduced pressure to get the crude product, which was further purified by silica gel chromatography (petroleum/ethyl acetate = 4/1 as eluent) to yield corresponding product.

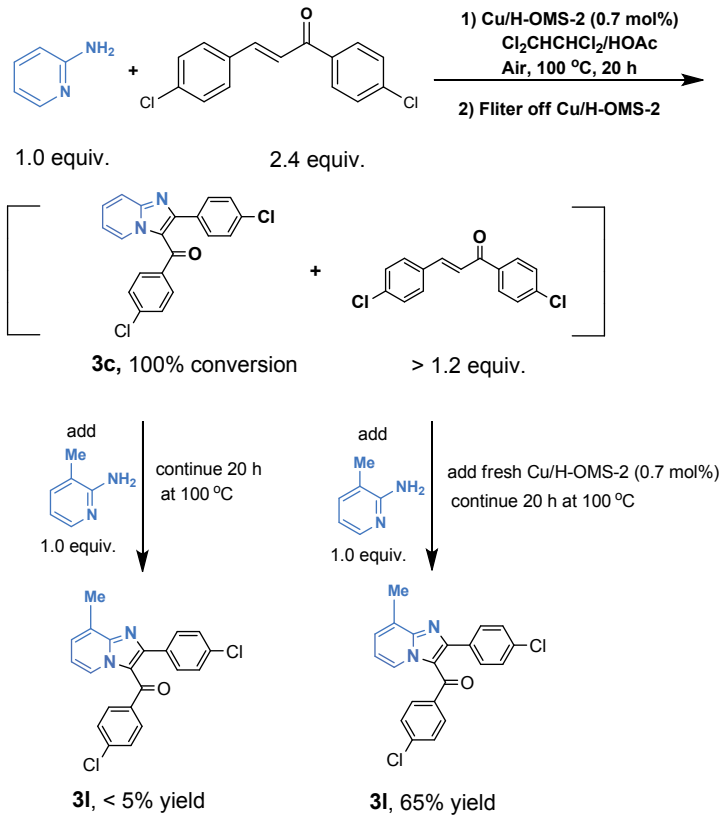
2.6 General procedure for catalyst recovery

Once the reaction was finished, the mixture was diluted with10 mL of EtOH. This mixture was centrifuged (2000 rpm, 20 min) and the solvent was subtracted using a syringe with a syringe filter (4 mm PTFE syringe filter, 0.2 um). The washing/centrifugation sequence was repeated many times. The residual solvent was completely removed under reduced pressure and the recovered Cu/H-OMS-2 was dried at 110 ^{o}C for 4 h. Then, the dried Cu/H-OMS-2 was put into the same tube with fresh reagents for the next run. This procedure was repeated for every cycle and the yield of the reaction was determined by ^{1}H NMR using Br_2CH_2 as internal standard.

3. Hot filtration experiment

Cu/H-OMS-2 (12 mg, 0.7 mol%), 2-aminopyridine (0.4 mmol, 1.0 equiv.), 4,4`-dichlorochalcones (0.96 mmol, 2.4 equiv.) and $Cl_2CHCHCl_2$ (1.2 mL)/HOAc (0.1 mL) were added to a flask with a

bar. The flask was stirred at 100 °C for about 20 h under air. Then, the catalyst was removed after filtering a totally converted reaction mixture. Next, another aminopyridine (1.0 equiv., 2-amino-3-methyl-pyridine) were added into the filtrate together, and then the filtrate was treated with the rest of 4,4'-dichlorochalcones (>1.2 equiv.) under the standard conditions. Consequently, **3l** was hardly isolated, while 65% yield of **3l** was obtained if fresh Cu/H-OMS-2 was put into the filtrate (Scheme S1). Inductively coupled plasma-atomic emission spectroscopy (ICP-AES) was used to analyze the reaction solution after filtration of the catalyst, which showed 0.5 ppm of copper leached from Cu/H-OMS-2.



Scheme S1. The hot filtration experiment.

4. The SEM image of Cu/H-OMS-2

As shown in Fig. S1, Cu/H-OMS-2 have a typical nano-rod morphology.

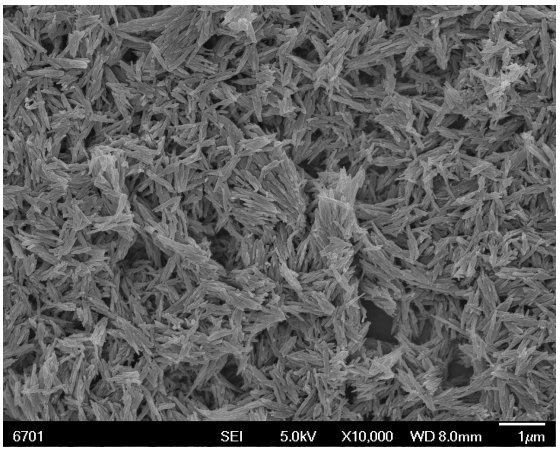


Figure S1. SEM image of Cu/H-OMS-2.

5. XPS analysis of the catalysts

Fig. S2 shows the Mn 2p XPS of H-OMS-2 and Cu/H-OMS-2. It was found that the support and the catalyst all contain Mn^{3+} and Mn^{4+}.[2] For Cu/H-OMS-2, we can see that the binding energies of Mn $2p_{3/2}$ and Mn $2p_{1/2}$ are essentially identical to those of support H-OMS-2. Importantly, compared to those of H-OMS-2, the binding energy of Mn 2p of Cu/H-OMS-2 are slightly higher. This observation indicates that there is an electronic interaction between the catalytic metal Cu and ETM OMS-2.

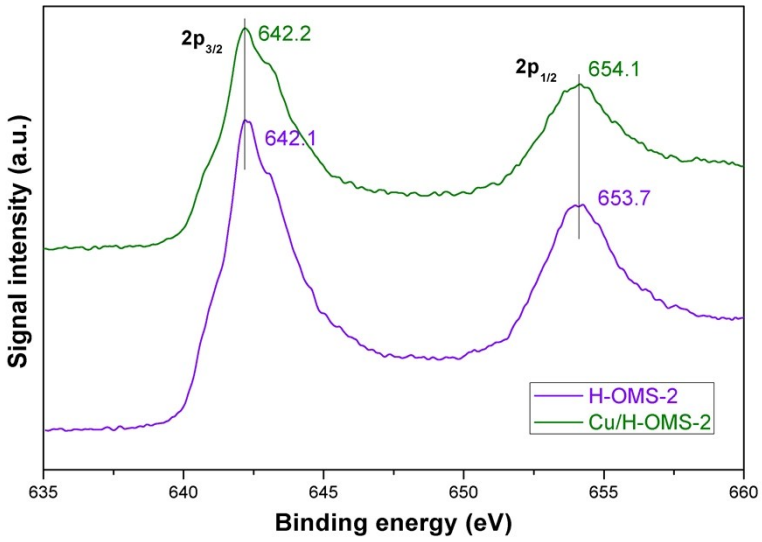


Figure S2. XPS profile of Mn 2p.

6. O_2-TPD of the catalysts

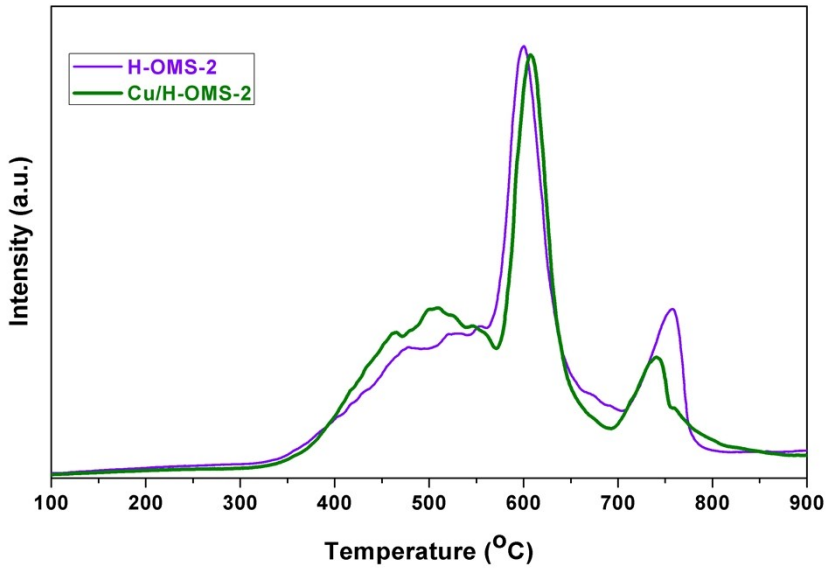


Figure S3. O_2-TPD of H-OMS-2 and Cu/H-OMS-2.

7. The morphology of used Cu/H-OMS-2

TEM was employed to observe the morphology of retrieved Cu/H-OMS-2 after the first run. Fig. S4 showed that the used catalyst remains the nano-rod morphology.

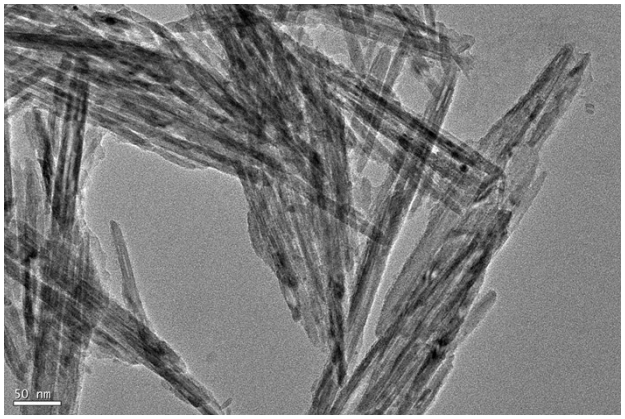
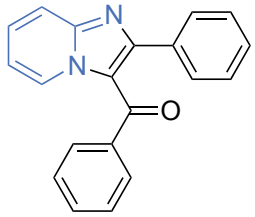


Fig S4. TEM image of used Cu/OMS-2.

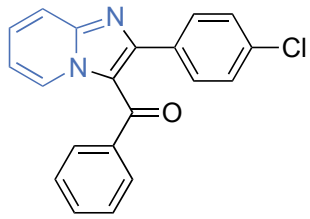
8. Characterization of products

phenyl(2-phenylimidazo[1,2-*a*]pyridin-3-yl)methanone (**3a**)[3]



White solid, isolated yield 89%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.55 (d, 1H, J = 7.2 Hz), 7.81 (d, 1H, J = 9.2 Hz), 7.54-7.50 (m, 3H), 7.33-7.24 (m, 3H), 7.11-7.08 (m, 6H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.3, 155.0, 147.4, 138.6, 133.9, 131.8, 130.2, 129.5, 129.2, 128.2, 127.7, 120.0, 117.5, 114.6.

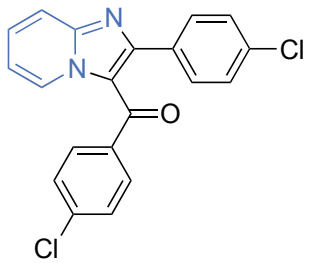
(2-(4-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (**3b**)[3]



White solid, isolated yield 76%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.53 (d, 1H, J = 7.2 Hz), 7.83 (d, 1H, J = 9.2 Hz), 7.57-7.54 (m, 1H), 7.53-7.44

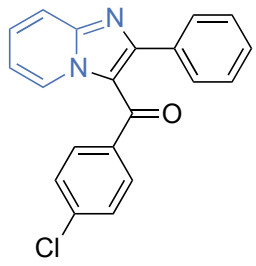
(m, 2H), 7.43-7.42 (m, 2H), 7.31-7.29 (m, 1H), 7.14-7.11 (m, 3H), 7.07-7.05 (m, 2H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.8, 155.1, 147.5, 137.9, 137.0, 133.7, 130.9, 130.2, 129.4, 128.5, 128.2, 127.9, 127.8, 119.8, 117.5, 114.8.

(4-chlorophenyl)(2-(4-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)methanone (**3c**)[4]



White solid, isolated yield 82%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.50 (d, 1H, J = 6.8 Hz), 7.81 (d, 1H, J = 8.8 Hz), 7.58-7.54 (m, 1H), 7.45 (d, 2H, J = 8.4 Hz), 7.27 (d, 2H, J = 8.0 Hz), 7.14-7.12 (m, 5H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.6, 153.5, 147.5, 138.4, 136.9, 134.9, 132.3, 131.4, 130.9, 129.6, 128.2, 128.1, 119.8, 117.5, 114.9, 113.9.

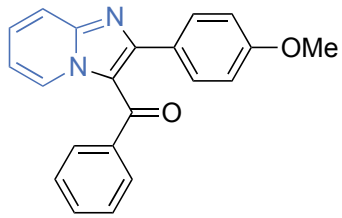
(4-chlorophenyl)(2-phenylimidazo[1,2-*a*]pyridin-3-yl)methanone (**3d**)[3]



White solid, isolated yield 88%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.54 (d, 1H, J = 7.2 Hz), 7.81 (d, 1H, J = 8.8 Hz), 7.58-7.50 (m, 3H), 7.36-7.34 (m, 1H), 7.26 (d, 2H, J = 8.0 Hz), 7.17-7.06 (m, 5H); ^{13}C NMR (100MHz,

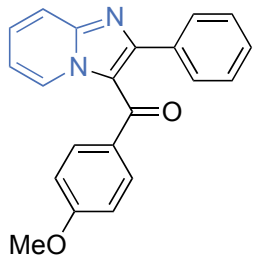
$CDCl_3$): δ = 187.2, 153.5, 147.4, 138.5, 134.4, 132.5, 131.9, 131.3, 129.5, 129.4, 128.3, 127.9, 120.0, 117.5, 114.8.

(2-(4-methoxyphenyl)imidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (**3f**)[4]



White solid, isolated yield 79%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.53 (d, 1H, *J* = 7.2 Hz), 7.78 (d, 1H, *J* = 8.8 Hz), 7.54-7.51 (m, 3H), 7.28-7.26 (m, 3H), 7.18-7.08 (m, 3H), 7.61 (d, 2H, *J* = 8.8 Hz), 3.72 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.4, 159.7, 154.8, 147.4, 138.7, 138.6, 131.7, 131.5, 129.6, 129.1, 128.2, 127.8, 119.6, 117.2, 114.4, 114.0, 113.3, 55.2.

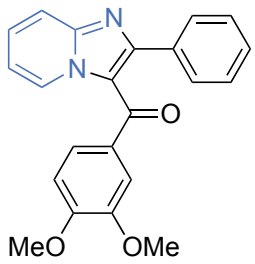
(4-methoxyphenyl)(2-phenylimidazo[1,2-*a*]pyridin-3-yl)methanone (**3g**)[4]



White solid, isolated yield 65%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.32 (d, 1H, *J* = 7.2 Hz), 7.78 (d, 1H, *J* = 8.8 Hz), 7.49-7.47 (m, 2H), 7.31-7.29 (m, 2H), 7.09-7.06 (m, 2H), 6.99-6.95 (m, 3H), 6.52 (d, 2H, *J* = 8.8 Hz), 3.66 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 186.1, 162.7, 153.7, 151.5, 147.6, 147.2, 138.4, 131.9, 130.2, 128.7, 128.2, 127.8, 119.7, 117.4,

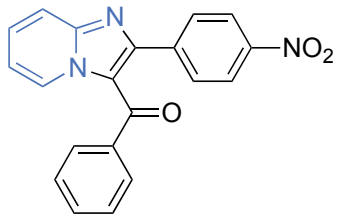
114.1, 113.1, 55.3.

(3,4-dimethoxyphenyl)(2-phenylimidazo[1,2-*a*]pyridin-3-yl)methanone (**3h**)[4]



White solid, isolated yield 45%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.53 (d, 1H, J = 7.2 Hz), 7.79 (d, 1H, J = 8.8 Hz), 7.58-7.50 (m, 3H), 7.32-7.26 (m, 1H), 7.16-7.10 (m, 3H), 7.07 (d, 1H, J = 6.4 Hz), 7.00 (d, 1H, J = 7.2 Hz), 6.72 (d, 1H, J = 8.4 Hz), 3.81 (s, 3H), 3.66 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.2, 154.6, 149.3, 148.2, 147.4, 138.8, 131.9, 129.6, 129.2, 128.2, 127.9, 126.6, 123.3, 119.7, 117.3, 114.4, 113.3, 110.6, 55.9, 55.7.

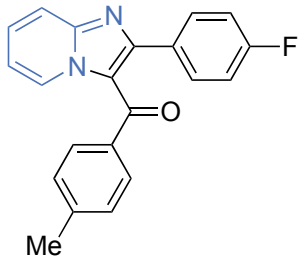
(2-(4-nitrophenyl)imidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (**3i**)[3]



Pale yellow solid, isolated yield 84%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.45 (d, 1H, J = 7.2 Hz), 7.87 (d, 2H, J = 8.8 Hz), 7.76 (d, 1H, J = 9.2 Hz), 7.53-7.49 (m, 1H), 7.44-7.41 (m, 4H), 7.26-7.22 (m, 1H), 7.09-7.05 (m, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 186.8, 151.8, 147.7, 140.6, 138.4, 132.4, 130.9, 129.7, 129.5, 128.2, 128.1, 122.8, 119.7, 117.7,

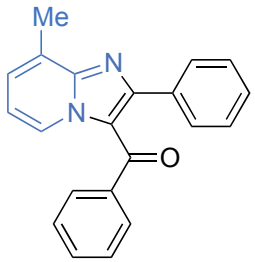
115.2, 113.9.

(2-(4-fluorophenyl)imidazo[1,2-*a*]pyridin-3-yl)(*p*-tolyl)methanone (**3j**)



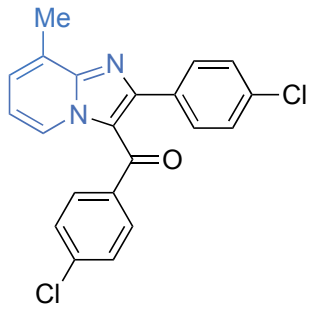
White solid, isolated yield 60%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.46 (d, 1H, J = 7.2 Hz), 7.84 (d, 1H, J = 8.8 Hz), 7.55-7.51 (m, 1H), 7.42 (d, 2H, J = 8.0 Hz), 7.34-7.31 (m, 2H), 7.11-7.07 (m, 1H), 6.93 (d, 2H, J = 8.0 Hz), 6.83-6.78 (m, 2H), 2.28 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.0, 161.5, 152.9, 142.9, 131.9, 131.8, 130.1, 129.7, 129.2, 129.1, 128.6, 128.1, 117.3, 114.9, 114.7, 114.6, 21.5. HRMS (ESI) m/z: Found: 331.3433. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 331.3549.

(8-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (**3k**)[4]



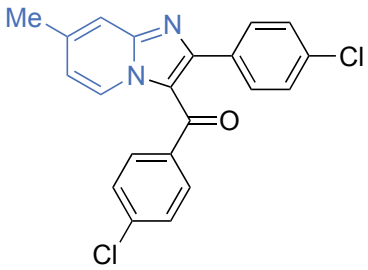
White solid, isolated yield 72%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.41 (d, 1H, J = 7.2 Hz), 7.50-7.48 (m, 2H), 7.34-7.31 (m, 3H), 7.26-7.22 (m, 2H), 7.11-6.99 (m, 6H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.5, 154.6, 138.8, 134.2, 131.6, 130.3, 129.5, 128.4, 128.1, 127.7, 127.6, 127.5, 125.9, 114.6, 17.1.

(4-chlorophenyl)(2-(4-chlorophenyl)-8-methylimidazo[1,2-*a*]pyridin-3-yl)methanone (**3l**)[4]



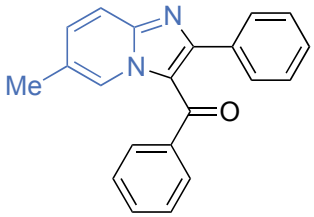
White solid, isolated yield 71%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.35 (d, 1H, J = 7.2 Hz), 7.42 (d, 2H, J = 8.4 Hz), 7.35 (d, 1H, J = 6.8 Hz), 7.28-7.26 (m, 2H), 7.12-7.10 (m, 4H), 7.04-7.01 (m, 1H), 2,73 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.7, 153.1, 147.7, 138.3, 137.0, 134.7, 132.6, 131.5, 130.8, 128.5, 128.2, 128.1, 127.6, 125.9, 120.3, 114.9, 17.0.

(4-chlorophenyl)(2-(4-chlorophenyl)-7-methylimidazo[1,2-*a*]pyridin-3-yl)methanone (**3n**)



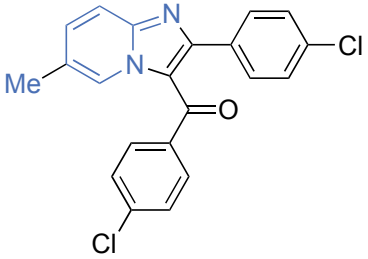
White solid, isolated yield 70%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.40 (d, 1H, J = 7.2 Hz), 7.56 (s, 1H), 7.44-7.42 (m, 2H), 7.27-7.23 (m, 2H), 7.13-7.11 (m, 4H), 6.98-6.95 (m, 1H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.4, 153.9, 147.9, 141.8, 138.2, 137.1, 134.8, 132.5, 131.3, 130.8, 128.1, 128.0, 127.4, 119.6, 117.5, 116.1, 21.6. HRMS (ESI) m/z: Found: 382.2583. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 382.2549.

(6-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)(phenyl)methanone (**3o**)[5]



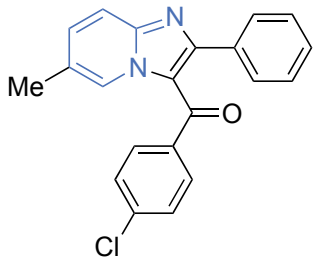
White solid, isolated yield 66%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.37 (s, 1H), 7.71 (d, 1H, J = 7.2 Hz), 7.51-7.49 (m, 2H), 7.39-7.37 (m, 1H), 7.31-7.23 (m, 3H), 7.10-7.07 (m, 5H), 2.45 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.3, 154.9, 146.4, 138.8, 134.1, 132.1, 131.7, 130.2, 129.6, 128.1, 127.7, 126.2, 124.6, 119.9, 116.7, 18.5.

(4-chlorophenyl)(2-(4-chlorophenyl)-6-methylimidazo[1,2-*a*]pyridin-3-yl)methanone (**3p**)[5]



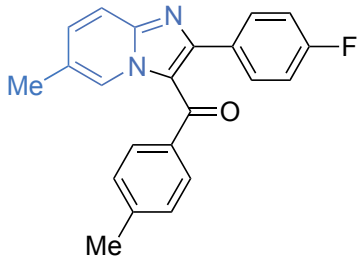
White solid, isolated yield 64%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.31 (s, 1H), 7.71 (d, 1H, J = 7.2 Hz), 7.44-7.42 (m, 3H), 7.26-7.23 (m, 2H), 7.12-7.10 (m, 4H), 2.45 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.5, 153.3, 146.5, 138.3, 136.9, 134.7, 132.5, 131.3, 130.9, 128.2, 128.1, 126.1, 125.9, 119.8, 116.7, 18.5.

(4-chlorophenyl)(6-methyl-2-phenylimidazo[1,2-*a*]pyridin-3-yl)methanone (**3q**)[4]



White solid, isolated yield 69%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.36 (s, 1H), 7.13 (d, 1H, J = 7.2 Hz), 7.43-7.41 (m, 2H), 7.30-7.26 (m, 2H), 7.19-7.17 (m, 1H), 7.13-7.09 (m, 2H), 7.05-7.03 (m, 2H), 2.45 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.8, 154.9, 146.5, 137.8, 137.2, 133.9, 132.4, 130.9, 130.2, 128.4, 127.9, 127.8, 126.2, 124.8, 119.7, 116.8, 18.5.

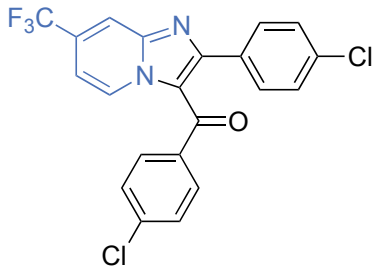
(2-(4-fluorophenyl)-6-methylimidazo[1,2-*a*]pyridin-3-yl)(*p*-tolyl)methanone (**3r**)



White solid, isolated yield 53%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.21 (s, 1H), 7.61 (d, 1H, J = 7.2 Hz), 7.34-7.19 (m, 4H), 7.85 (d, 2H, J = 8.0 Hz), 7.73-7.69 (m, 2H), 2.36 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.0, 163.9, 161.5, 153.1, 146.2, 142.7, 135.9, 132.0, 131.9, 131.8, 130.5, 129.7, 128.5, 126.0, 124.5, 119.9, 116.6, 114.9, 114.6, 21.5, 18.5. HRMS (ESI) m/z: Found: 345.3833. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 345.3824.

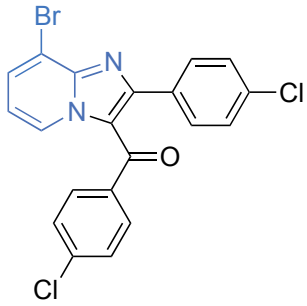
(4-chlorophenyl)(2-(4-chlorophenyl)-7-

(trifluoromethyl)imidazo[1,2-*a*]pyridin-3-yl)methanone (**3s**)[5]



White solid, isolated yield 39%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.82 (s, 1H), 7.92 (d, 1H, J = 7.2 Hz), 7.70-7.68 (m, 1H), 7.48-7.46 (m, 2H), 7.30-7.27 (m, 2H), 7.17-7.15 (m, 4H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.8, 154.3, 150.7, 147.2, 140.9, 139.2, 136.1, 135.5, 131.4, 130.9, 128.9, 128.5, 128.4, 125.4, 120.6, 118.2, 113.8, 111.9.

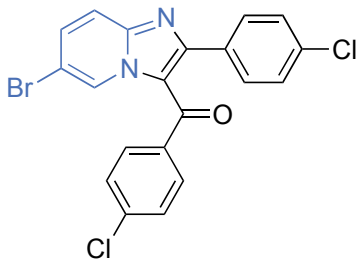
(8-bromo-2-(4-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)(4-chlorophenyl)methanone (**3t**)



White solid, isolated yield 45%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.42 (d, 1H, J = 7.2 Hz), 7.97 (d, 1H, J = 7.2 Hz), 7.83-7.78 (m, 1H), 7.48-7.43 (m, 2H), 7.32-7.27 (m, 2H), 7.17-7.08 (m, 4H), 6.98 (t, 1H, J = 6.8 Hz); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.9, 153.4, 145.4, 143.8, 131.8, 131.6, 130.9, 129.3, 128.3, 128.2, 127.3, 121.8, 121.1, 114.9, 111.7. HRMS (ESI) m/z: Found: 447.1266. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 447.1236.

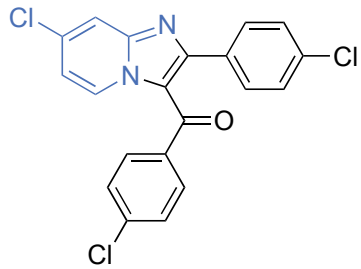
(6-bromo-2-(4-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)(4-

chlorophenyl)methanone (**3u**)



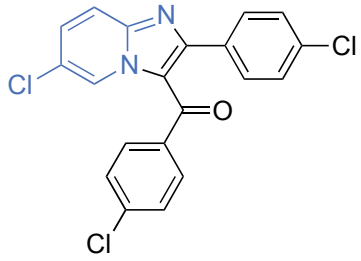
White solid, isolated yield 42%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.64 (s, 1H), 7.72 (d, 1H, J = 7.2 Hz), 7.45-7.43 (m, 3H), 7.25 (d, 2H, J = 6.0 Hz), 7.15-7.13 (m, 4H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.6, 153.4, 145.9, 138.8, 136.4, 135.2, 133.0, 131.8, 131.4, 130.9, 128.8, 128.3, 128.2, 118.0, 109.8. HRMS (ESI) m/z: Found: 447.1247. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 447.1236.

(7-chloro-2-(4-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)(4-chlorophenyl)methanone (**3v**)



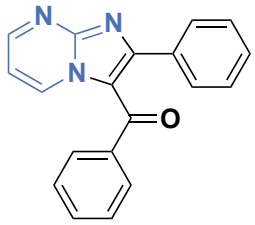
White solid, isolated yield 55%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.41 (d, 1H, J = 7.2 Hz), 7.77 (s, 1H), 7.44-7.42 (m, 2H), 7.26-7.23 (m, 3H), 7.14-7.12 (m, 4H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.6, 147.5, 138.7, 136.5, 136.2, 135.2, 131.9, 131.4, 130.9, 129.3, 128.6, 128.5, 128.3, 128.2, 116.5, 116.3. HRMS (ESI) m/z: Found: 402.6766. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 402.6744.

(6-chloro-2-(4-chlorophenyl)imidazo[1,2-*a*]pyridin-3-yl)(4-chlorophenyl)methanone (**3w**)



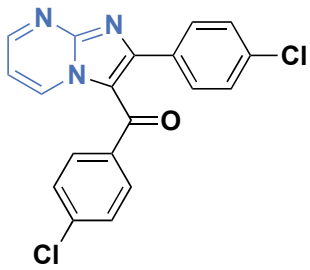
White solid, isolated yield 52%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.55 (s, 1H), 7.77 (d, 1H, J = 7.2 Hz), 7.54-7.51 (m, 1H), 7.45-7.43 (m, 2H), 7.26-7.24 (m, 2H), 7.14-7.12 (m, 4H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.6, 153.4, 145.7, 138.8, 136.3, 135.2, 131.7, 131.2, 130.9, 128.7, 128.3, 128.2, 126.2, 123.3, 119.9, 117.7. HRMS (ESI) m/z: Found: 402.6769. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 402.6744.

phenyl(2-phenylimidazo[1,2-*a*]pyrimidin-3-yl)methanone (**4a**)[6]



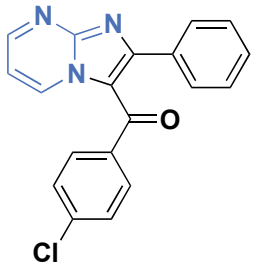
White solid, isolated yield 76%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.76 (d, 1H, J = 7.2 Hz), 8.80 (d, 1H, J = 7.2 Hz), 7.52-7.50 (m, 2H), 7.40-7.38 (m, 2H), 7.31-7.28 (m, 1H), 7.17-7.09 (m, 6H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.5, 155.9, 153.5, 149.9, 137.9, 135.9, 133.1, 132.2, 130.4, 129.5, 128.8, 127.9, 127.8, 118.1, 110.7.

(4-chlorophenyl)(2-(4-chlorophenyl)imidazo[1,2-*a*]pyrimidin-3-yl)methanone (**4b**)[6]



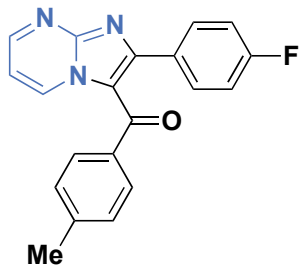
White solid, isolated yield 82%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.68 (d, 1H, J = 7.2 Hz), 8.81 (d, 1H, J = 7.2 Hz), 7.45 (d, 2H, J = 8.4 Hz), 7.32 (d, 2H, J = 8.4 Hz), 7.15-7.12 (m, 5H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.7, 154.4, 153.8, 149.9, 138.9, 136.1, 135.9, 135.4, 131.5, 131.4, 130.8, 128.3, 128.2, 117.9, 110.9.

(4-chlorophenyl)(2-phenylimidazo[1,2-*a*]pyrimidin-3-yl)methanone (**4c**)[6]



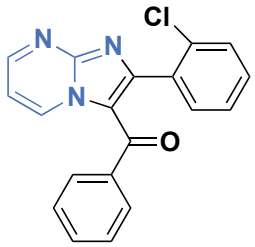
White solid, isolated yield 81%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.73 (d, 1H, J = 7.2 Hz), 8.80 (d, 1H, J = 7.2 Hz), 7.73 (d, 2H, J = 8.4 Hz), 7.36 (d, 2H, J = 8.4 Hz), 7.22-7.20 (m, 1H), 7.18-7.06 (m, 5H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 185.9, 156.2, 153.7, 150.1, 138.5, 136.2, 135.9, 132.8, 130.8, 130.4, 129.1, 128.2, 127.9, 117.9, 110.9.

(2-(4-fluorophenyl)imidazo[1,2-*a*]pyrimidin-3-yl)(*p*-tolyl)methanone (**4d**)



Pale yellow solid, isolated yield 46%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.68 (d, 1H, J = 7.2 Hz), 8.80 (d, 1H, J = 7.2 Hz), 7.44-7.40 (m, 3H), 7.16-7.13 (m, 2H), 6.97 (d, 2H, J = 8.0 Hz), 7.85-7.80 (t, 2H, J = 8.4 Hz), 2.30 (s, 3H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.1, 154.1, 153.3, 149.8, 143.5, 135.9, 135.1, 132.3, 132.2, 129.7, 129.3, 128.7, 127.4, 115.1, 114.8, 110.7, 21.6. HRMS (ESI) m/z: Found: 332.3466. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 332.3414.

(2-(2-chlorophenyl)imidazo[1,2-*a*]pyrimidin-3-yl)(phenyl)methanone (**4e**)



Yellow solid, isolated yield 25%. ^{1}H NMR (400MHz, $CDCl_3$): δ = 9.76 (d, 1H, J = 7.2 Hz), 8.77 (d, 1H, J = 7.2 Hz), 7.43-7.41 (m, 3H), 7.33-7.32 (m, 1H), 7.19-7.13 (m, 1H), 7.03-6.99 (m, 5H); ^{13}C NMR (100MHz, $CDCl_3$): δ = 187.3, 153.6, 152.8, 149.9, 137.8, 136.2, 133.4, 133.2, 131.9, 130.1, 129.3, 129.2, 128.6, 127.4, 126.4, 111.7. HRMS (ESI) m/z: Found: 334.7767. Calcd for $C_{14}H_{11}IN_2O$: $(M+H)^+$ 334.7715.

Reference:

[1] R. Kumar, S. Sithambaram, S. L. Suib, *J. Catal*., **2009**, *262*, 304-313.

[2] X. Liu, Z. Jin, J. Lu, X. Wang, M. Luo, *Chem. Eng. J*., **2010**, *162*, 151-157.

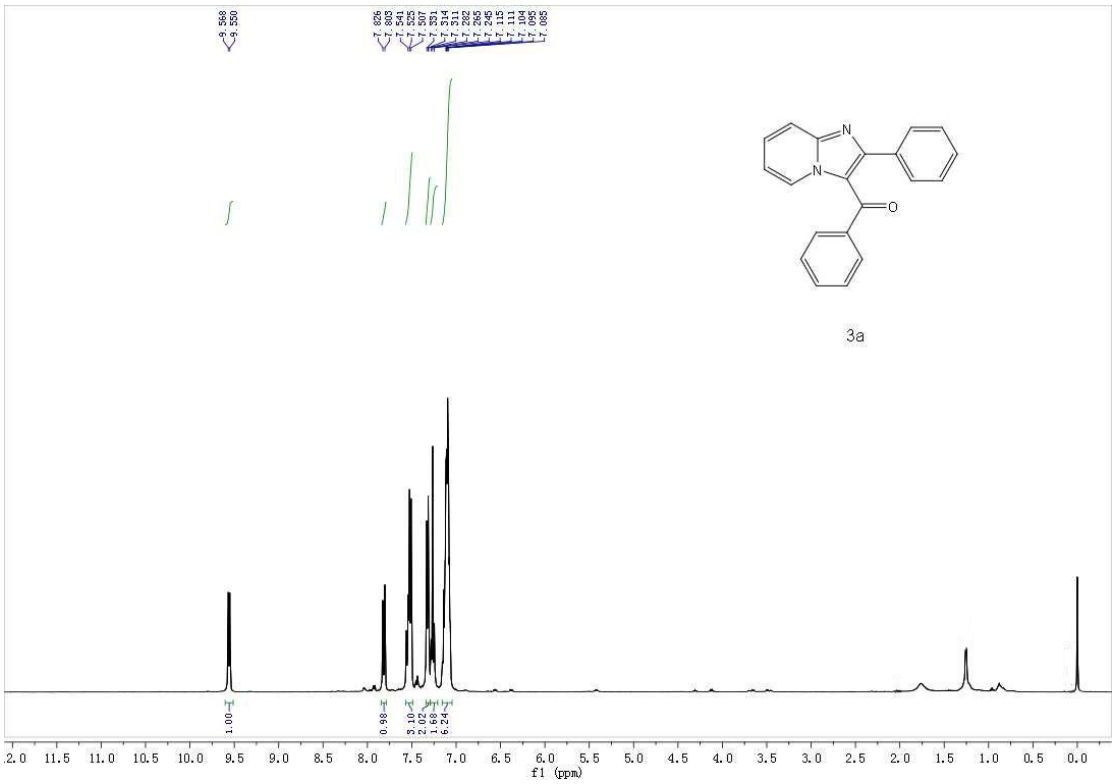
[3] K. Monir, A. K. Bagdi, S. Mishra, A. Majee, A. Hajra, *Adv. Synth. Catal*., **2014**, *356*, 1105 – 1112.

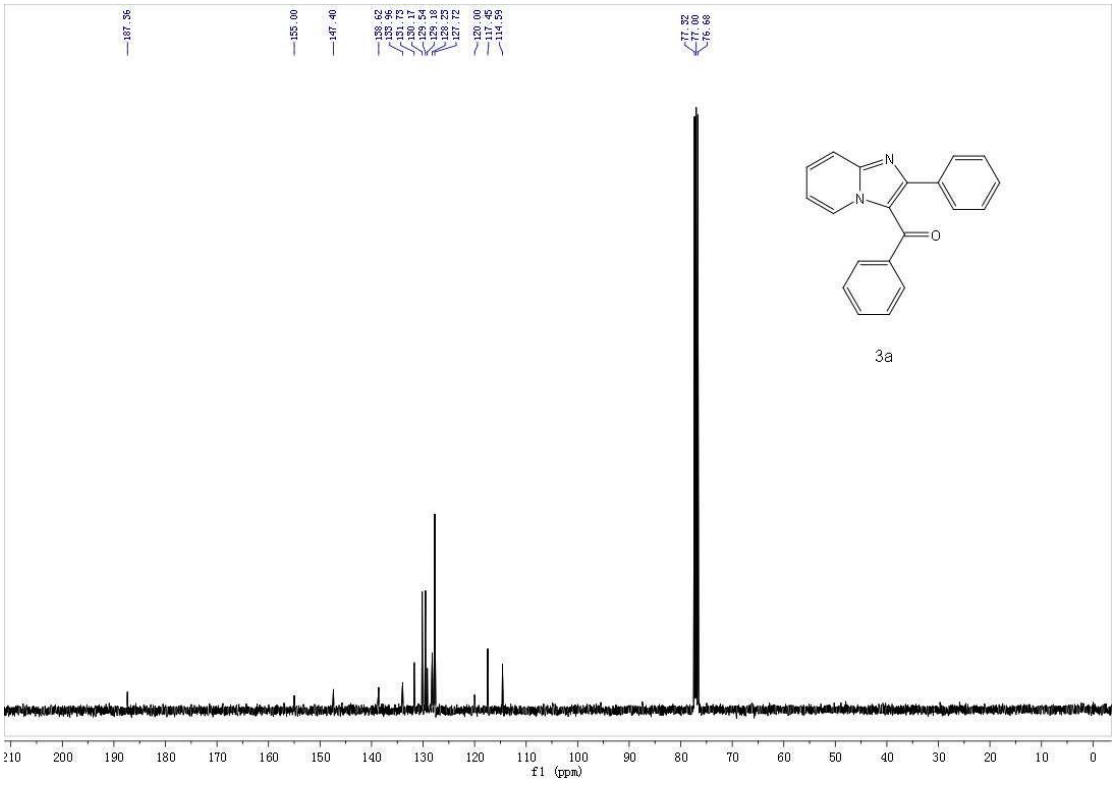
[4] P. Kaswan, K. Pericherla, H. K. Saini, A. Kumar, *RSC Adv*., **2015**, *5*, 3670–3677.

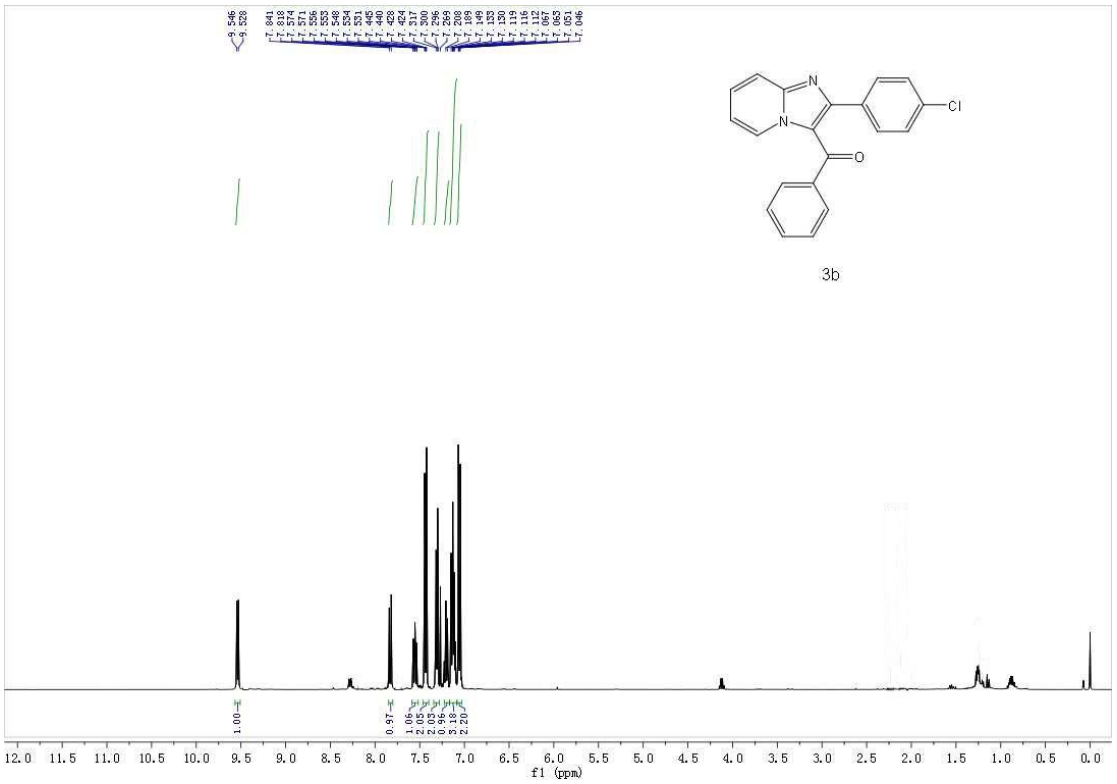
[5] P. Kaswan, K. Pericherla, Rajnikant, A. Kumar, *Tetrahedron*, **2014**, *70*, 8539-8544.

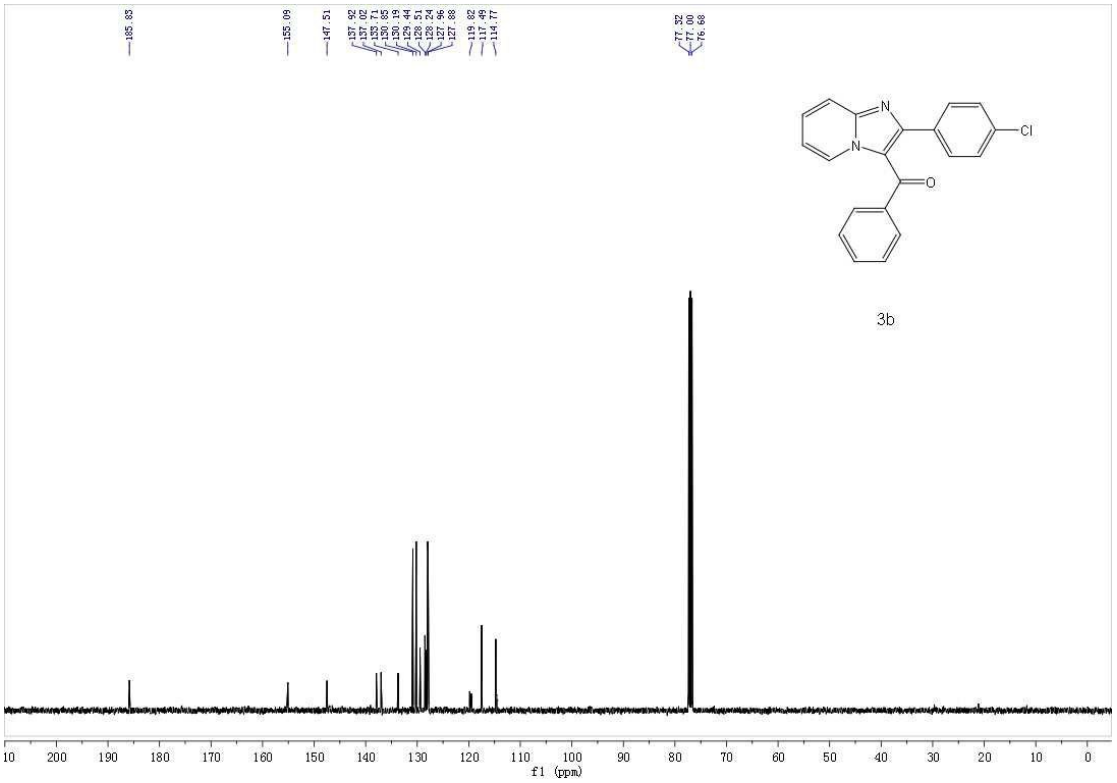
[6] K. R. Reddy, A. S. Reddy, R. Shankar, R. Kant, P. Das, *Asian J. Org. Chem.,* **2015**, *4*, 537-583.

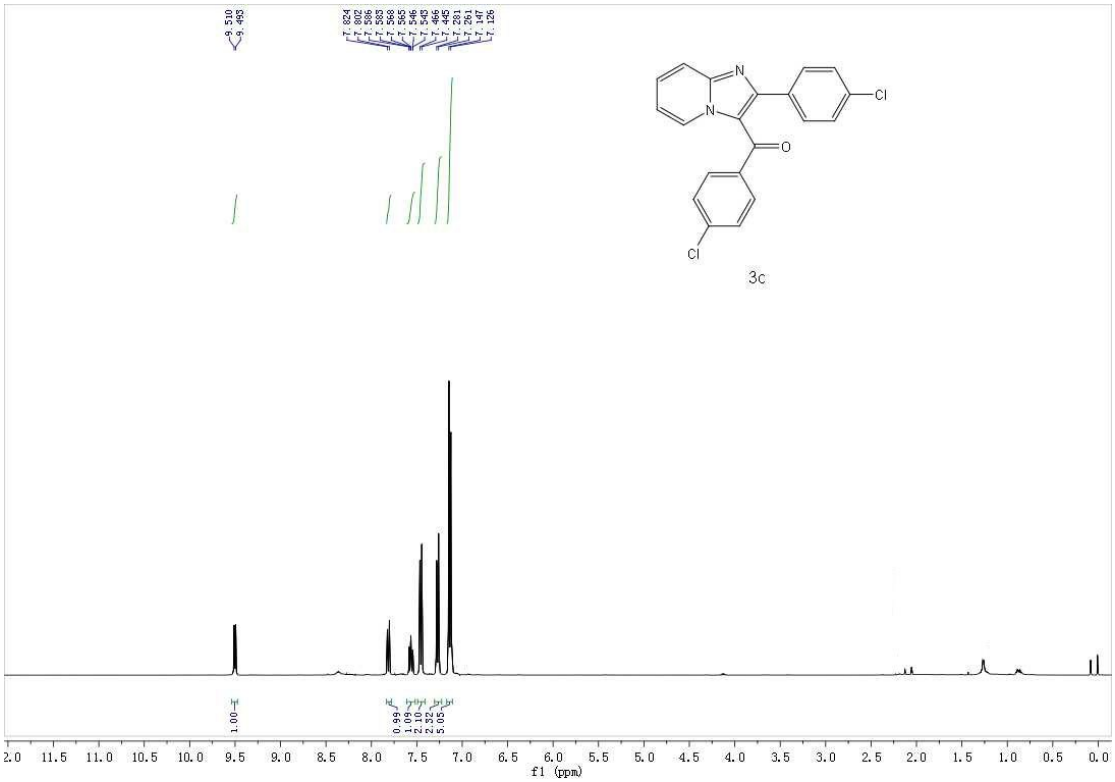
9. Copies of ^{1}H and ^{13}C spectra

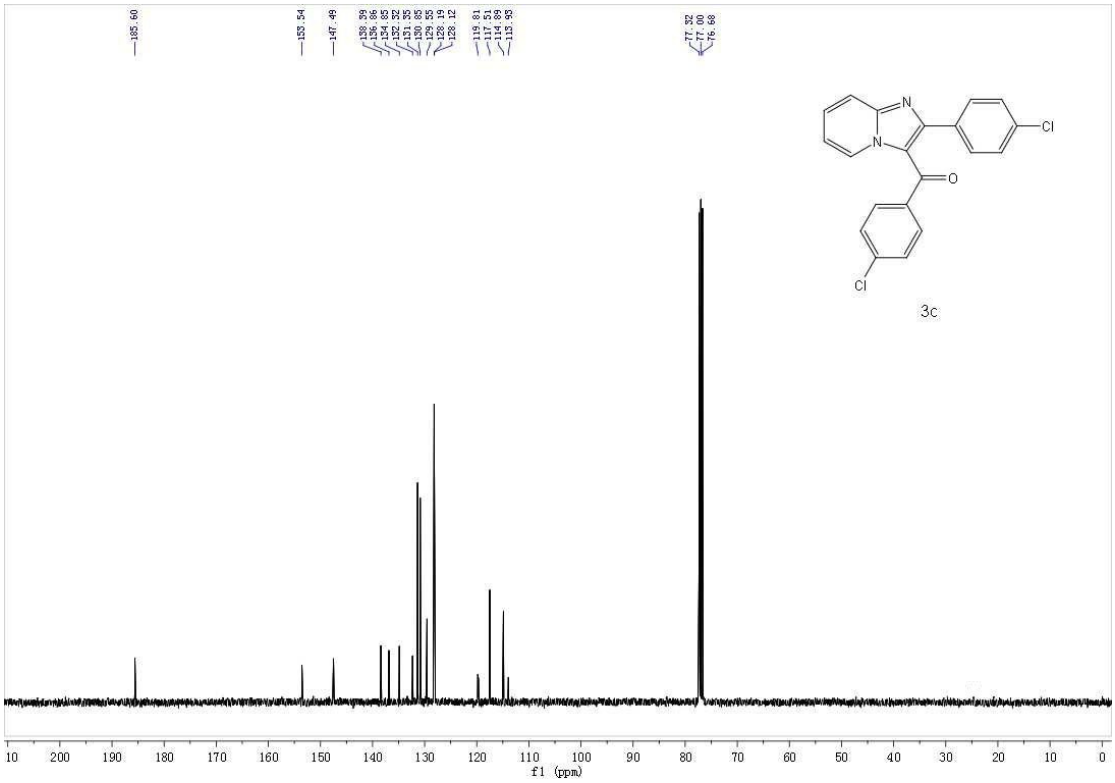


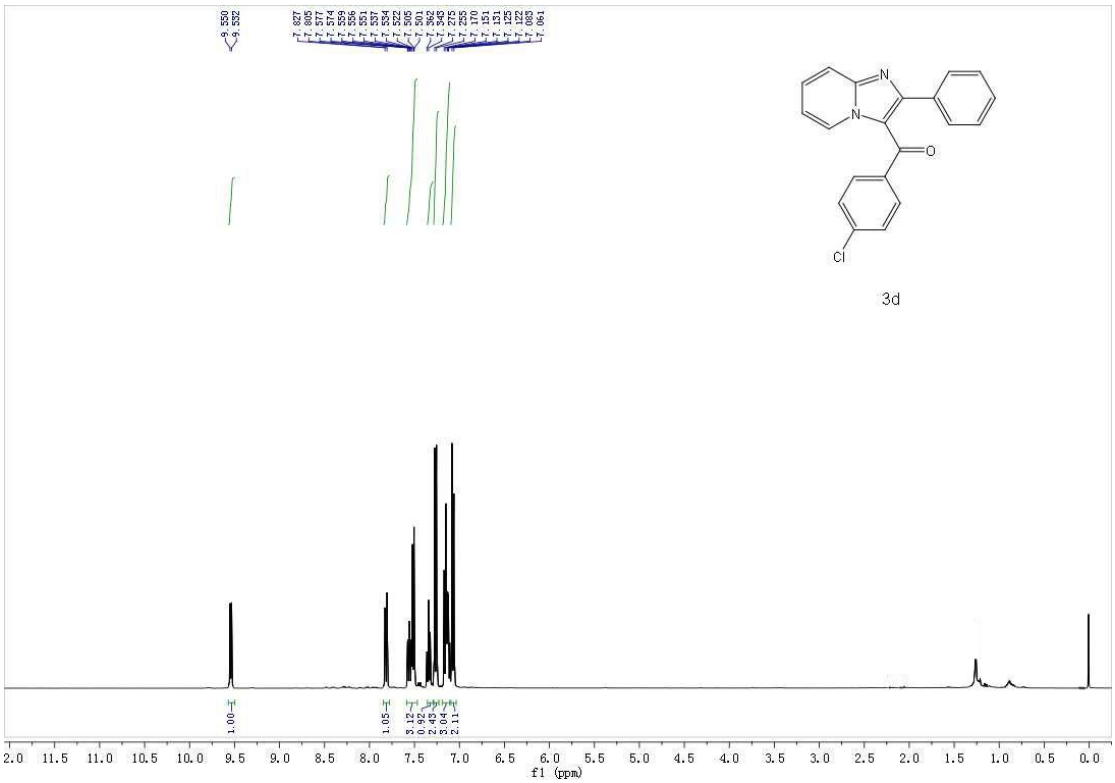



9.546
9.528
7.841
7.818
7.814
7.571
7.571
7.556
7.553
7.548
7.534
7.531
7.445
7.440
7.428
7.427
7.317
7.300
7.296
7.269
7.208
7.189
7.149
7.133
7.130
7.119
7.116
7.112
7.067
7.065
7.051
7.046
N
N
Cl
O
3b
1.00
0.97
1.06
2.05
2.05
3.18
2.20
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


185.83
155.09
147.51
137.92
137.02
135.71
130.05
130.19
129.44
128.51
128.24
127.96
127.88
119.82
117.49
114.77
77.32
77.00
76.68
N
N
Cl
O
3b
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.510
9.493
7.924
7.602
7.596
7.583
7.568
7.555
7.546
7.543
7.466
7.445
7.261
7.147
7.126
N
N
Cl
O
Cl
3c
1.00
0.99
1.09
2.10
2.25
5.05
f1 (ppm)


185.60
153.54
147.49
138.39
135.86
134.85
132.32
131.35
130.85
130.55
128.19
128.12
119.81
117.91
114.88
113.93
77.32
77.00
76.68
N
N
Cl
O
Cl
3c
f1 (ppm)


9.550
9.532
7.827
7.805
7.577
7.574
7.559
7.556
7.551
7.537
7.534
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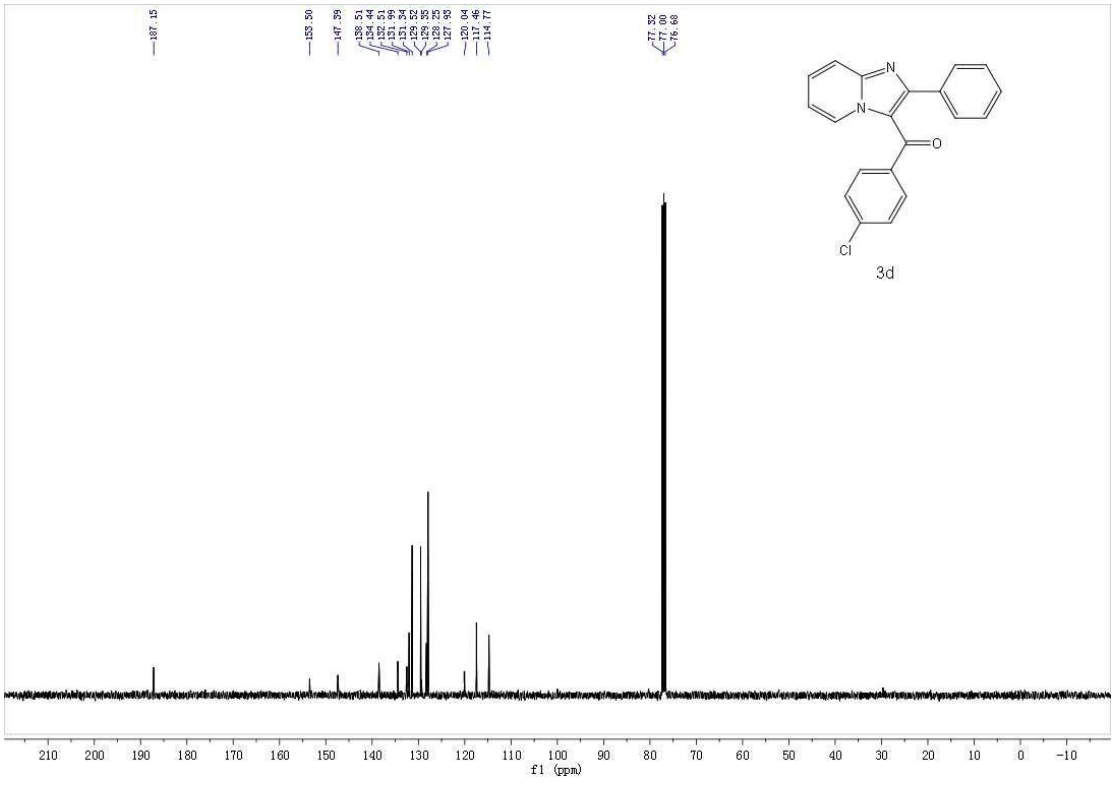
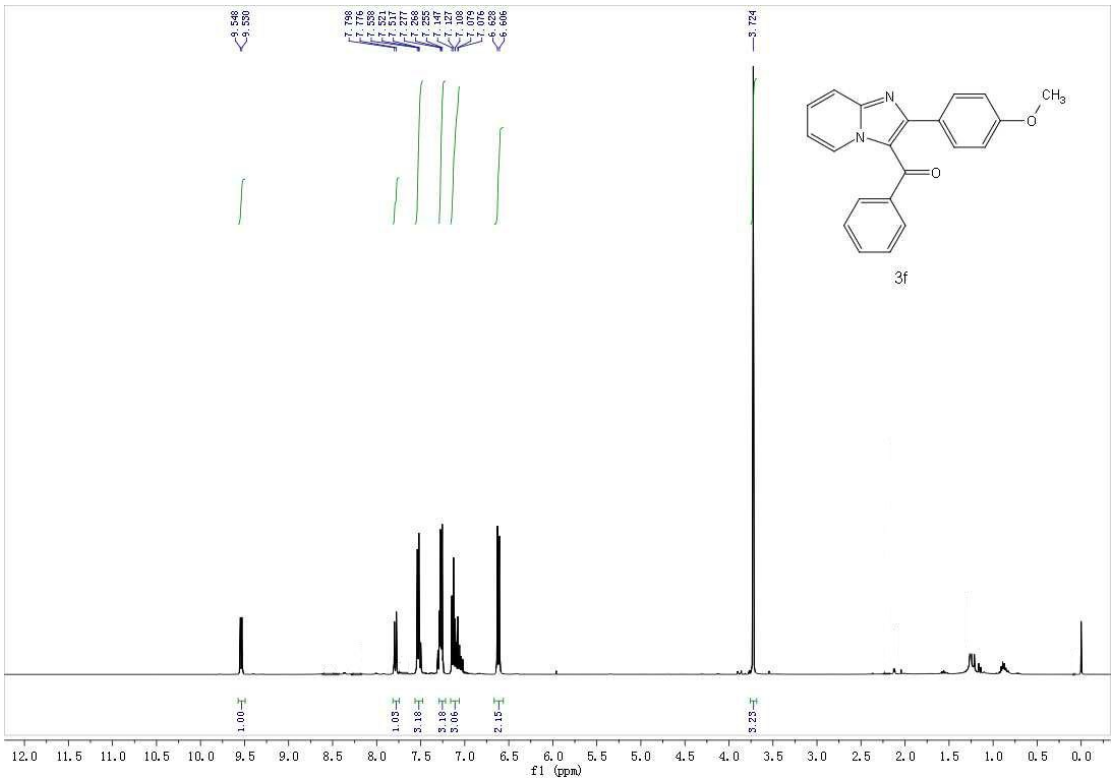
7.505
7.501
7.352
7.348
7.275
7.255
7.170
7.151
7.131
7.125
7.122
7.065
7.061
N
N
O
Cl
3d
1.00
1.05
3.12
0.92
2.03
3.04
2.11
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


187.15
153.50
147.39
138.51
134.44
132.51
131.99
131.54
129.52
129.35
128.25
127.93
120.04
117.46
114.77
77.32
77.00
76.68
N
N
O
Cl
3d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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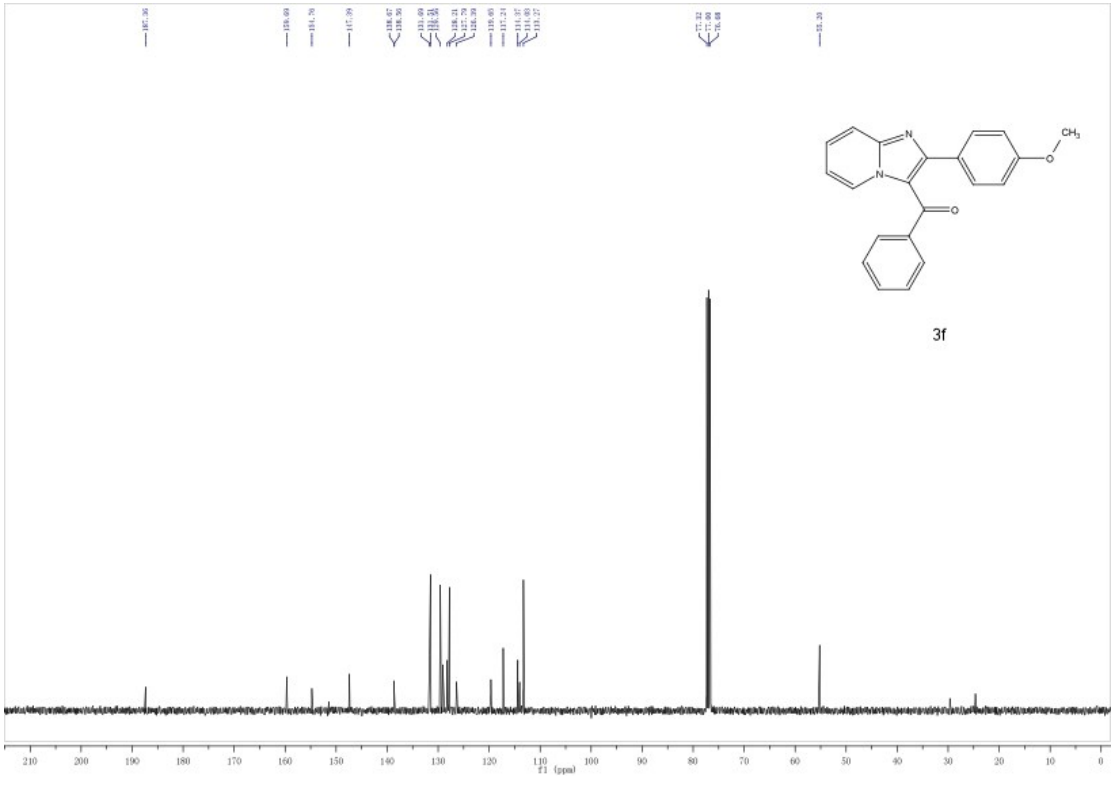
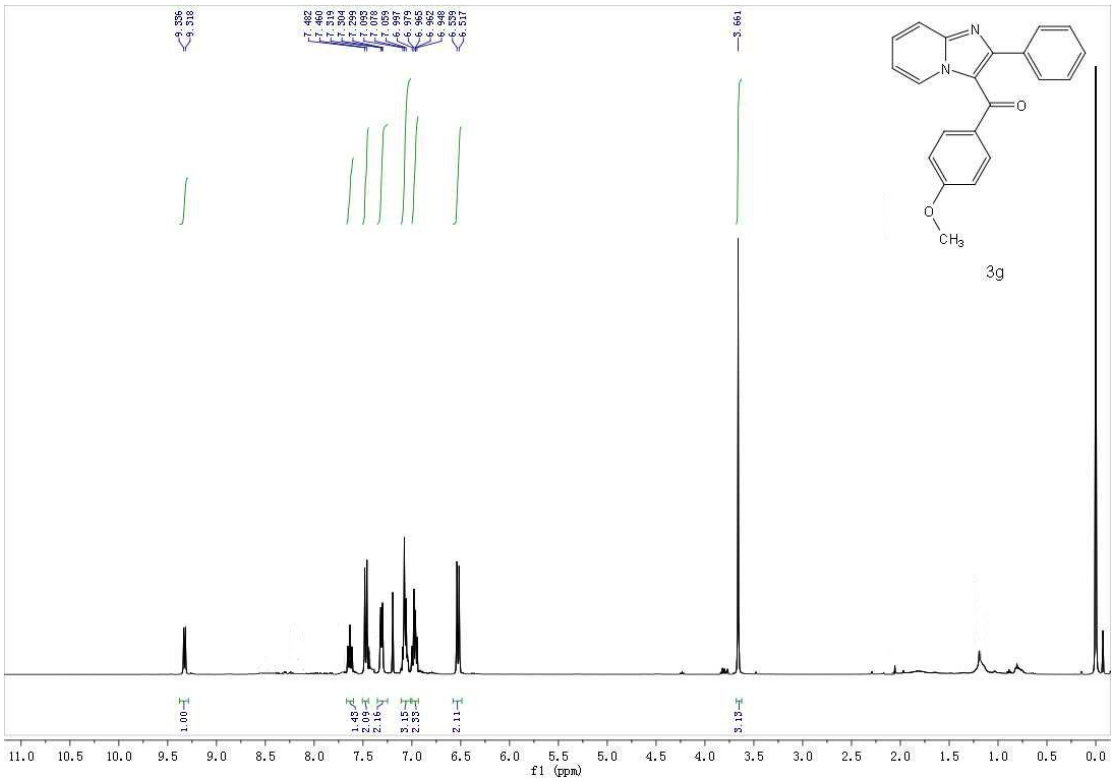
9.530
7.798
7.776
7.538
7.521
7.517
7.277
7.268
7.255
7.147
7.127
7.108
7.079
7.076
6.628
6.606
3.724
1.00
1.03
3.18
3.18
3.06
2.15
3.23
f1 (ppm)
3f


f1 (ppm)
3f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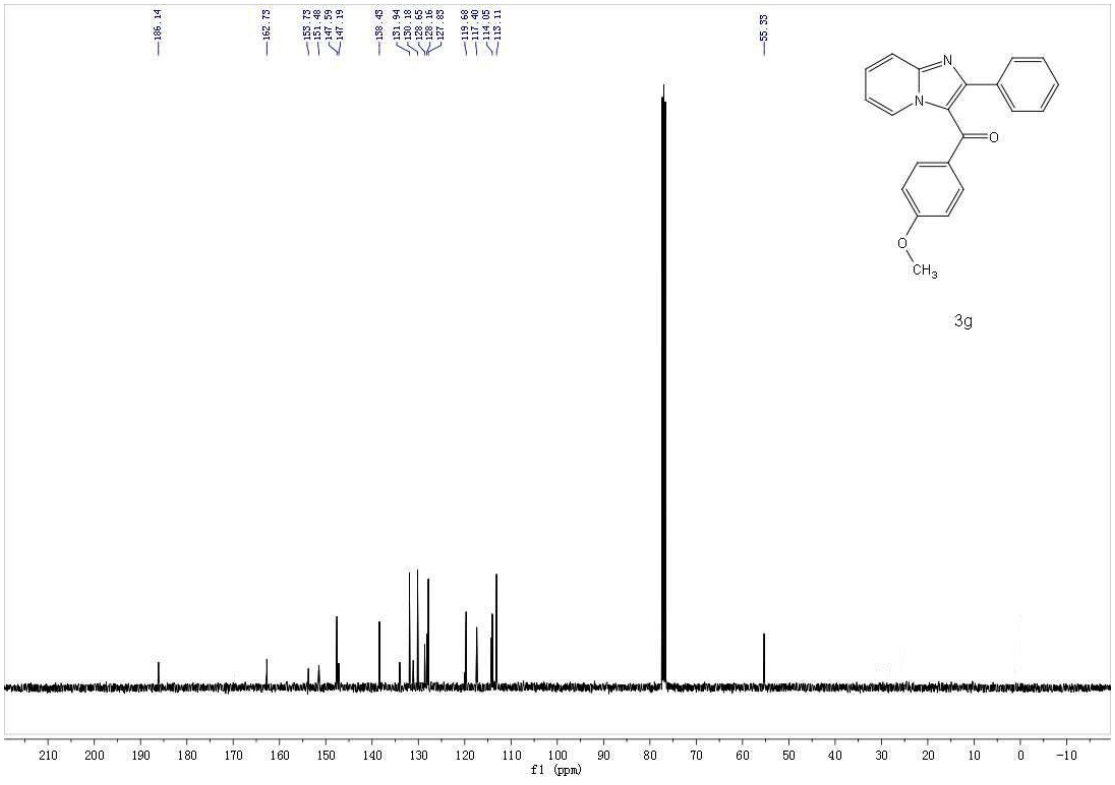
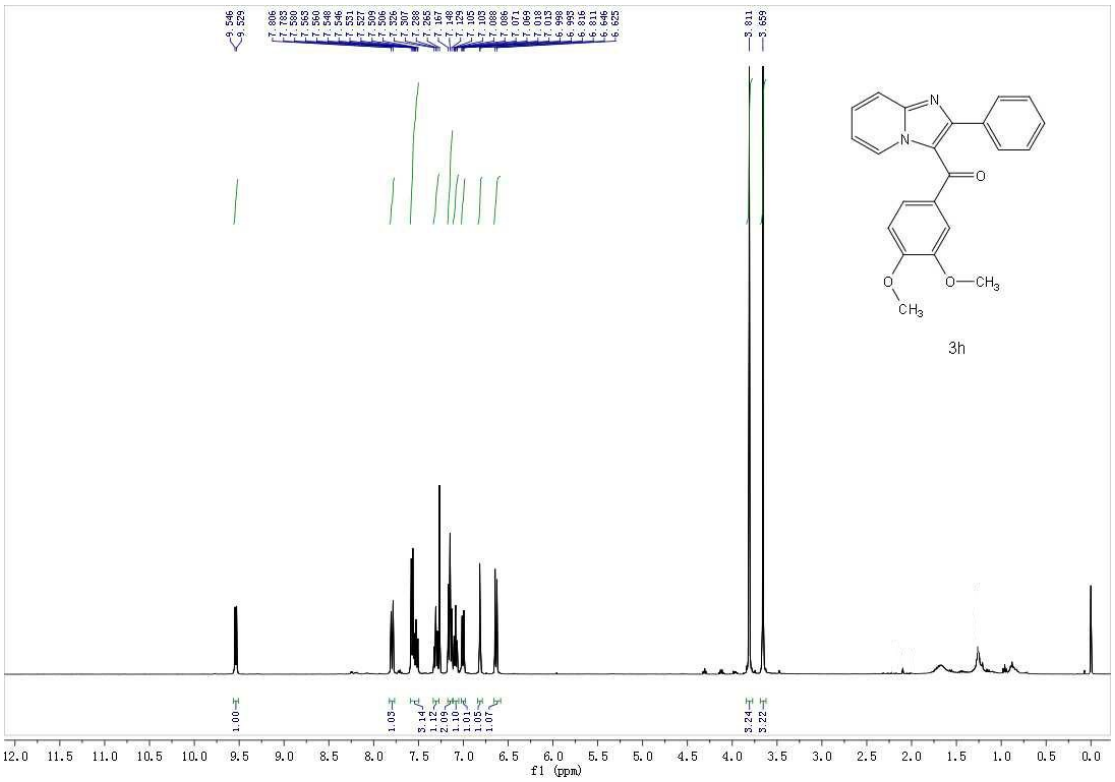
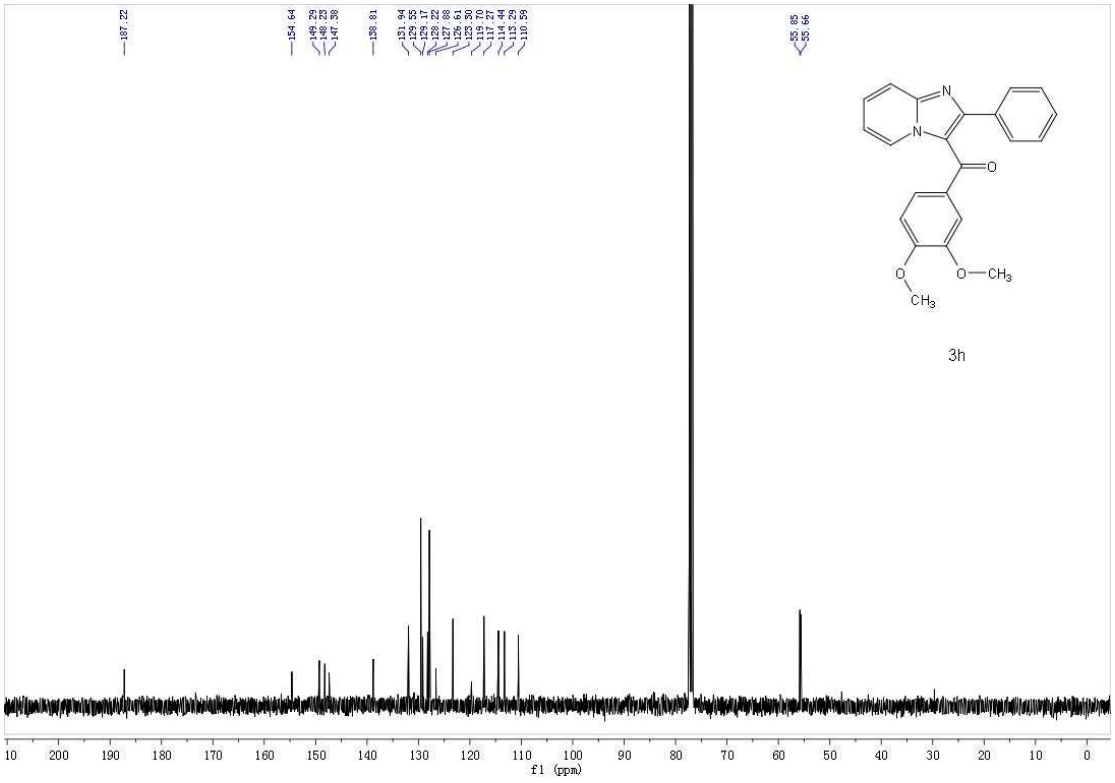
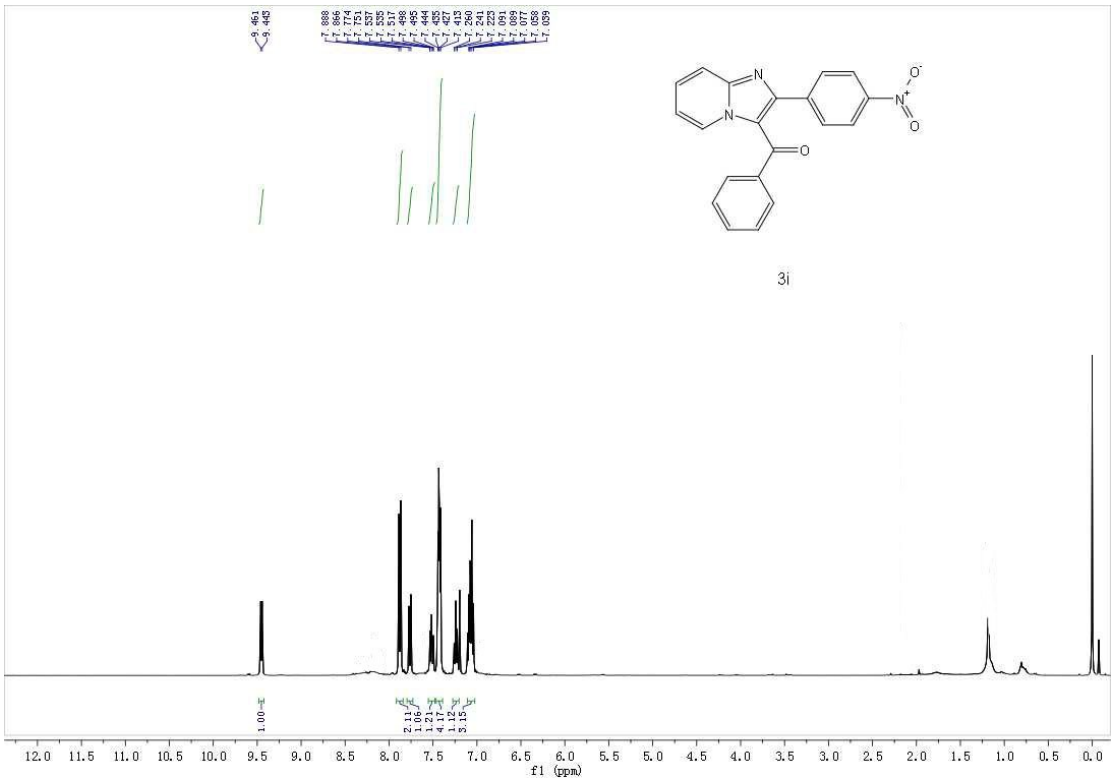
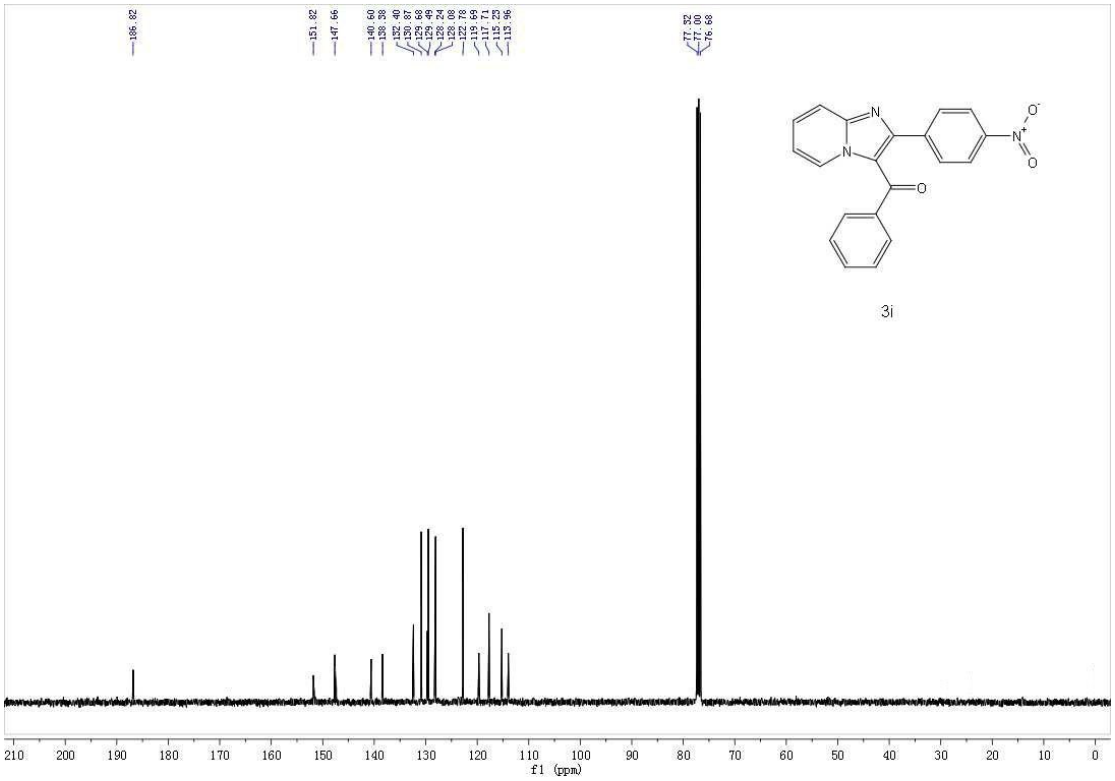
9.318
7.482
7.460
7.315
7.304
7.299
7.093
7.078
7.059
6.997
6.979
6.965
6.957
6.948
6.539
6.517
3.661
1.00
1.43
2.09
2.16
5.15
2.33
2.11
3.13
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
N
N
O
O
CH3
3g

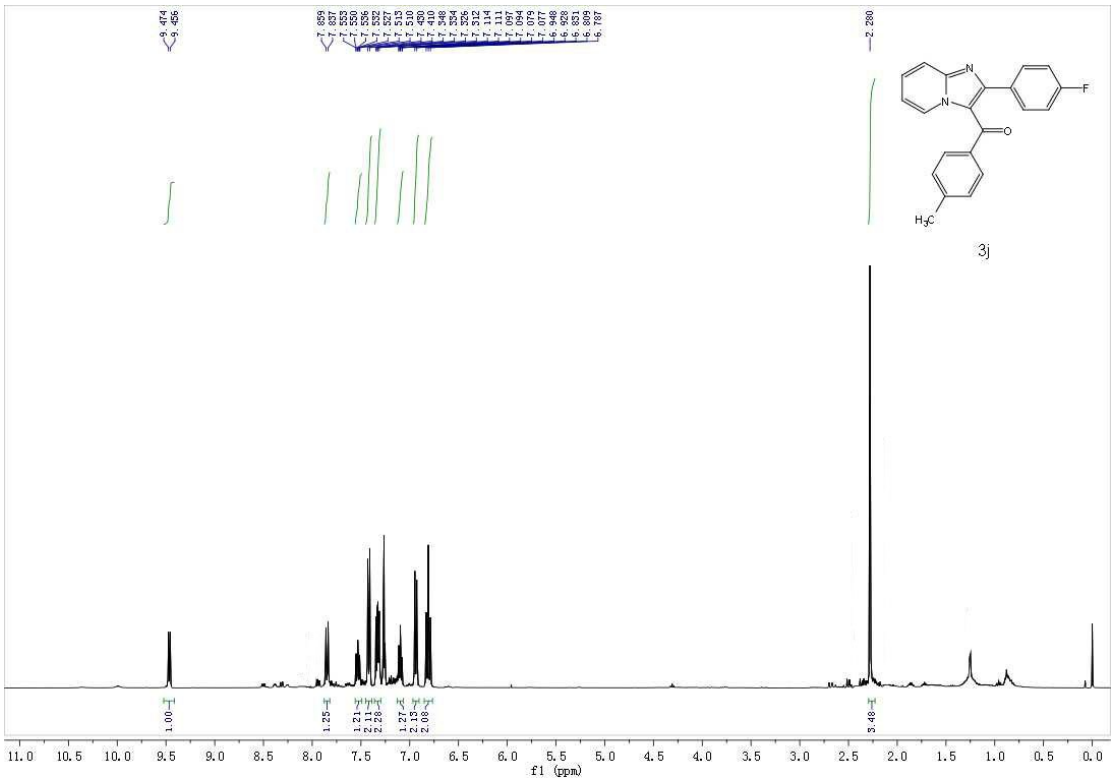

186.14
162.73
155.73
153.46
147.59
147.19
138.45
131.94
130.18
128.65
128.15
127.83
119.68
117.40
114.85
113.11
55.53
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
N
N
O
O
CH3
3g


9.546
9.529
7.806
7.783
7.580
7.563
7.560
7.548
7.546
7.531
7.527
7.507
7.506
7.326
7.307
7.298
7.265
7.167
7.148
7.129
7.105
7.103
7.088
7.086
7.071
7.064
7.018
7.013
6.998
6.995
6.816
6.811
6.646
6.625
3.811
3.659
1.00
1.03
3.14
1.12
2.10
1.01
1.05
1.07
3.24
3.22
f1 (ppm)
3h


187.22
154.64
149.29
148.23
147.38
138.81
131.94
129.55
129.17
128.22
127.88
126.51
125.30
119.70
117.27
114.44
113.29
110.59
55.85
55.66
f1 (ppm)
3h


9.461
9.445
7.888
7.866
7.774
7.751
7.537
7.535
7.517
7.498
7.495
7.444
7.435
7.427
7.415
7.260
7.241
7.223
7.091
7.089
7.077
7.058
7.039
O
N
O
O
3i
1.00
2.11
1.05
2.21
4.17
1.12
5.15
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


186.82
151.82
147.66
140.60
138.38
132.40
130.87
129.68
129.46
128.24
128.08
122.78
119.69
117.71
115.23
113.96
77.32
77.00
76.68
O
N
O
O
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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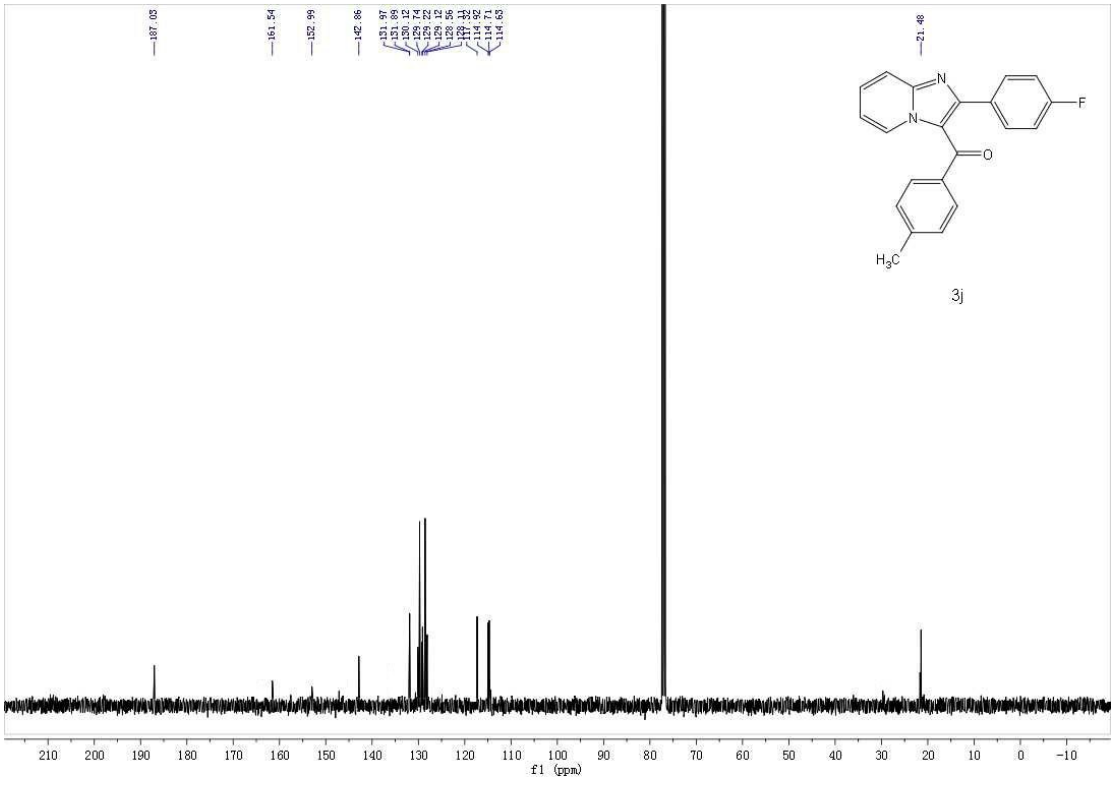
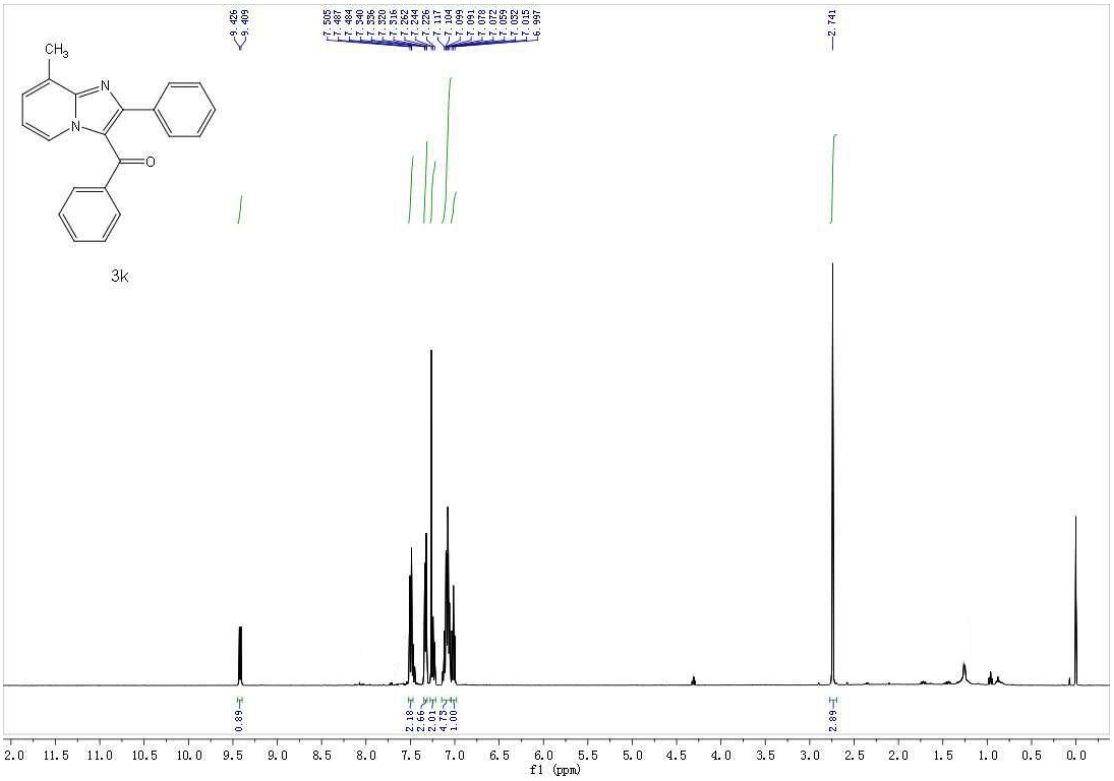
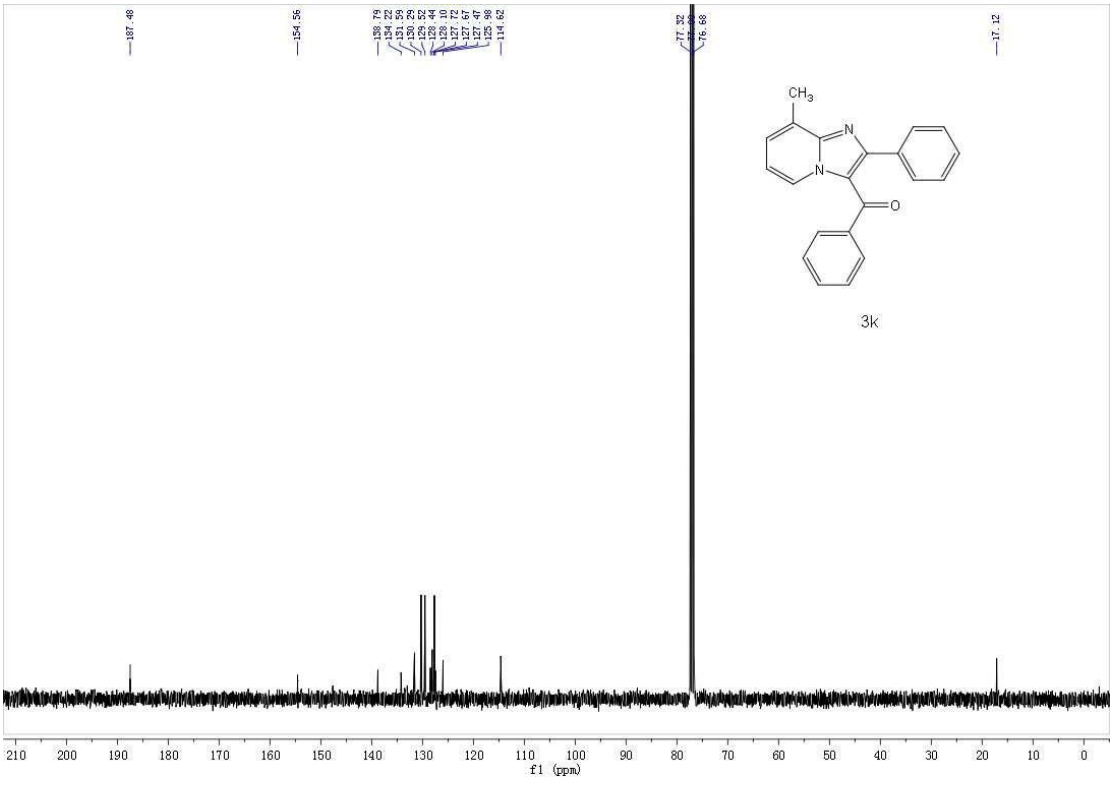
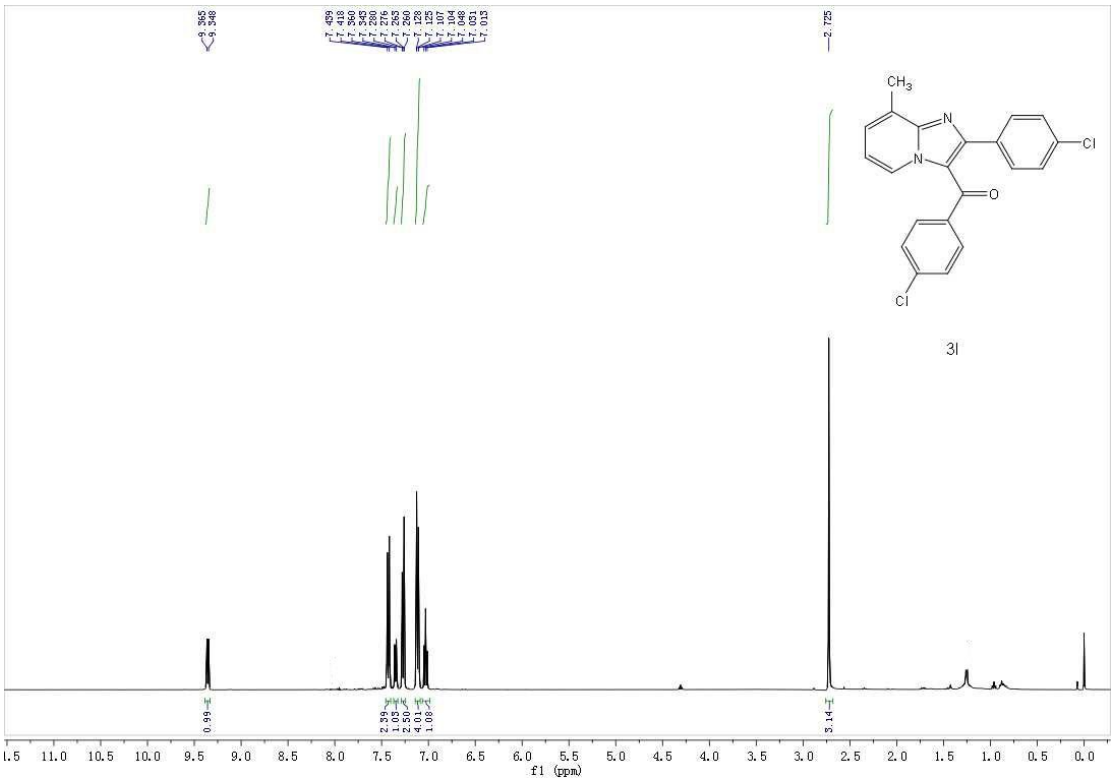
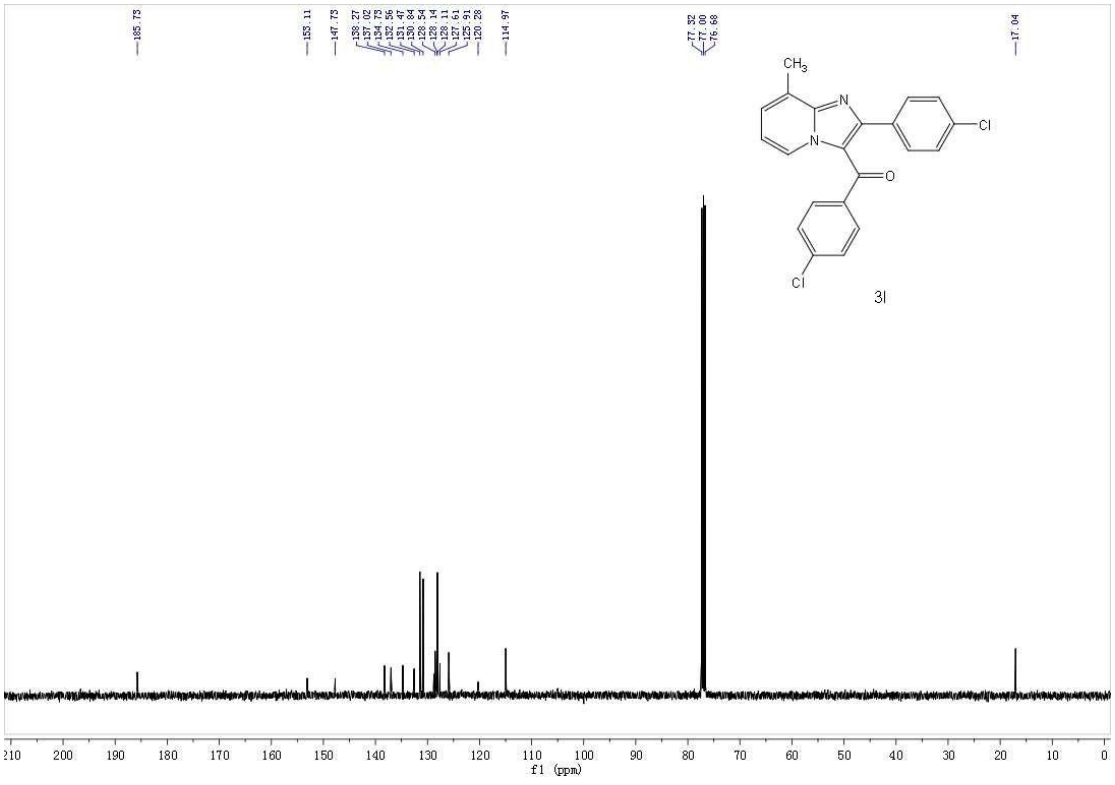
9.456
7.659
7.657
7.553
7.550
7.536
7.532
7.527
7.513
7.510
7.480
7.440
7.436
7.394
7.326
7.312
7.114
7.111
7.097
7.094
7.079
7.077
6.948
6.928
6.831
6.809
6.787
2.280
F
O
H3C
3j
1.00
1.25
1.21
2.11
2.28
1.27
2.13
2.08
3.48
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

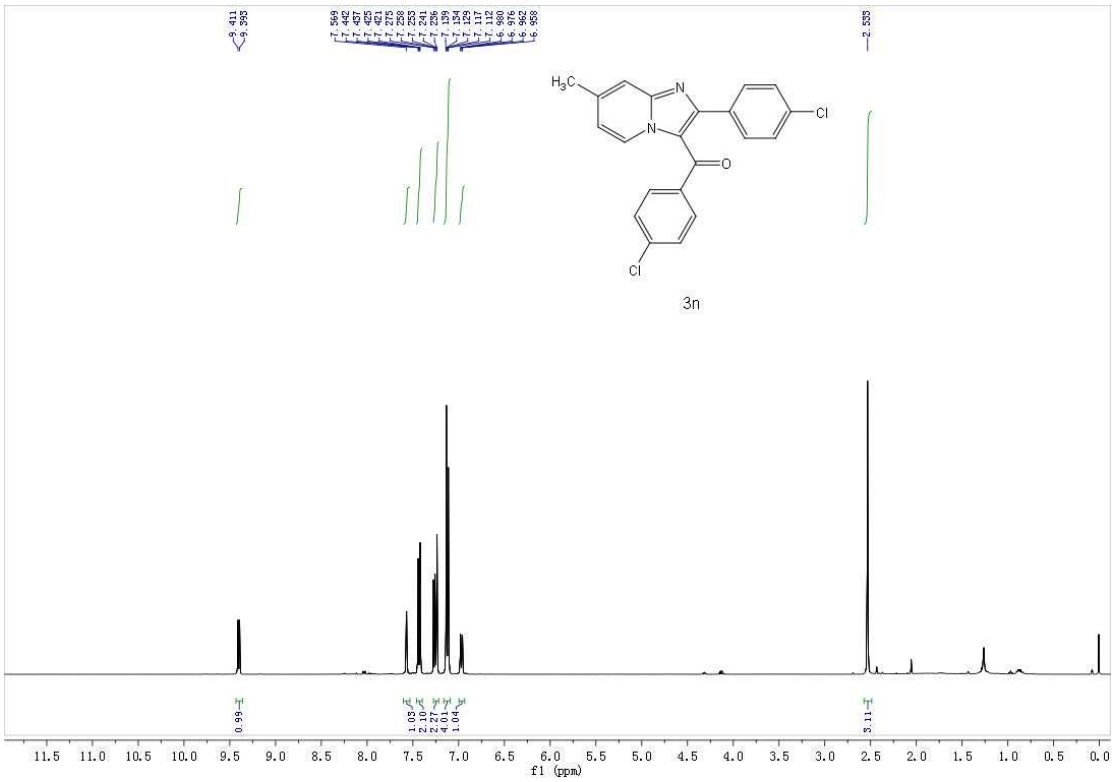

187.03
161.54
152.99
142.86
131.97
131.89
130.12
129.74
129.72
129.12
128.56
117.32
117.11
114.92
114.71
114.63
21.48
F
O
H3C
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


CH3
N
N
O
3k
9.426
9.409
7.505
7.487
7.484
7.360
7.356
7.320
7.316
7.262
7.244
7.226
7.117
7.104
7.099
7.081
7.078
7.072
7.059
7.052
7.035
6.997
2.741
0.89
2.18
2.66
2.01
4.13
1.00
2.89
f1 (ppm)


187.48
154.56
138.79
134.22
131.58
130.29
129.52
128.44
128.10
127.72
127.67
127.47
125.98
114.62
77.32
76.68
17.12
CH3
N
N
O
3k
f1 (ppm)


9.365
9.348
7.459
7.418
7.360
7.345
7.280
7.276
7.263
7.260
7.128
7.125
7.107
7.104
7.048
7.031
7.015
2.725
CH3
N
N
Cl
O
Cl
3l
0.99
2.39
1.03
2.50
4.01
1.08
3.14
f1 (ppm)


185.73
153.11
147.73
138.27
137.02
134.73
132.96
131.47
130.84
128.54
128.14
128.11
127.61
125.91
120.28
114.97
77.32
77.00
76.68
17.04
CH3
N
N
Cl
O
Cl
3l
f1 (ppm)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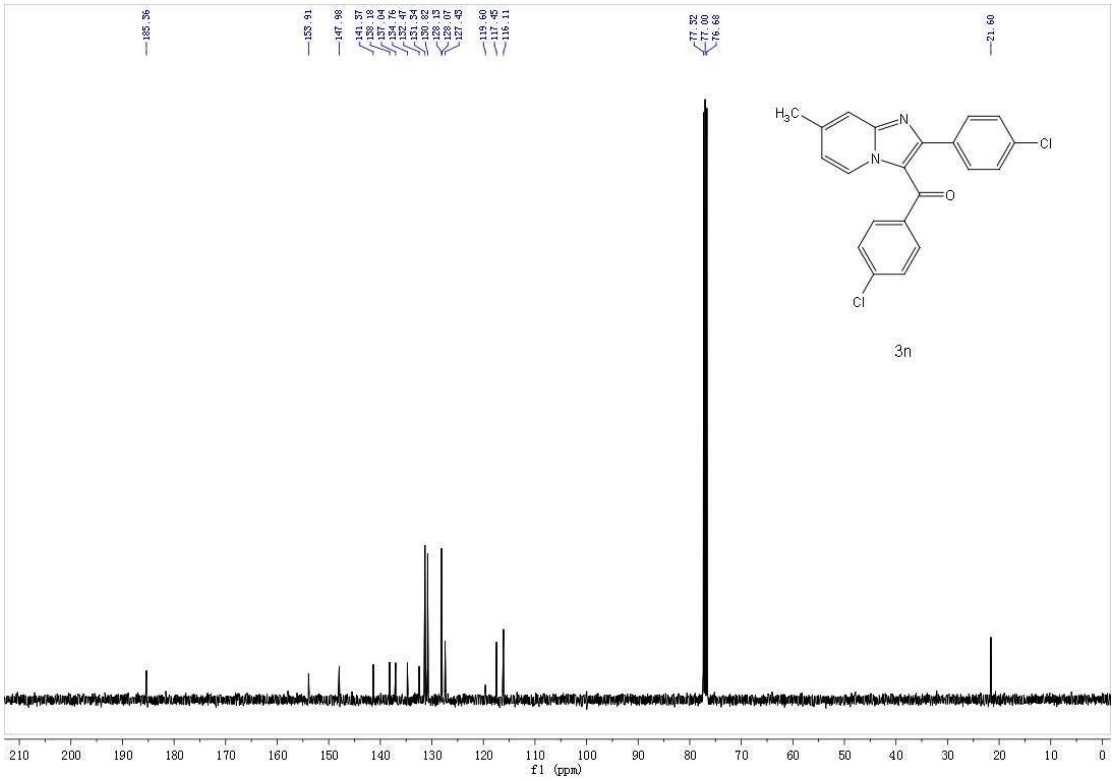
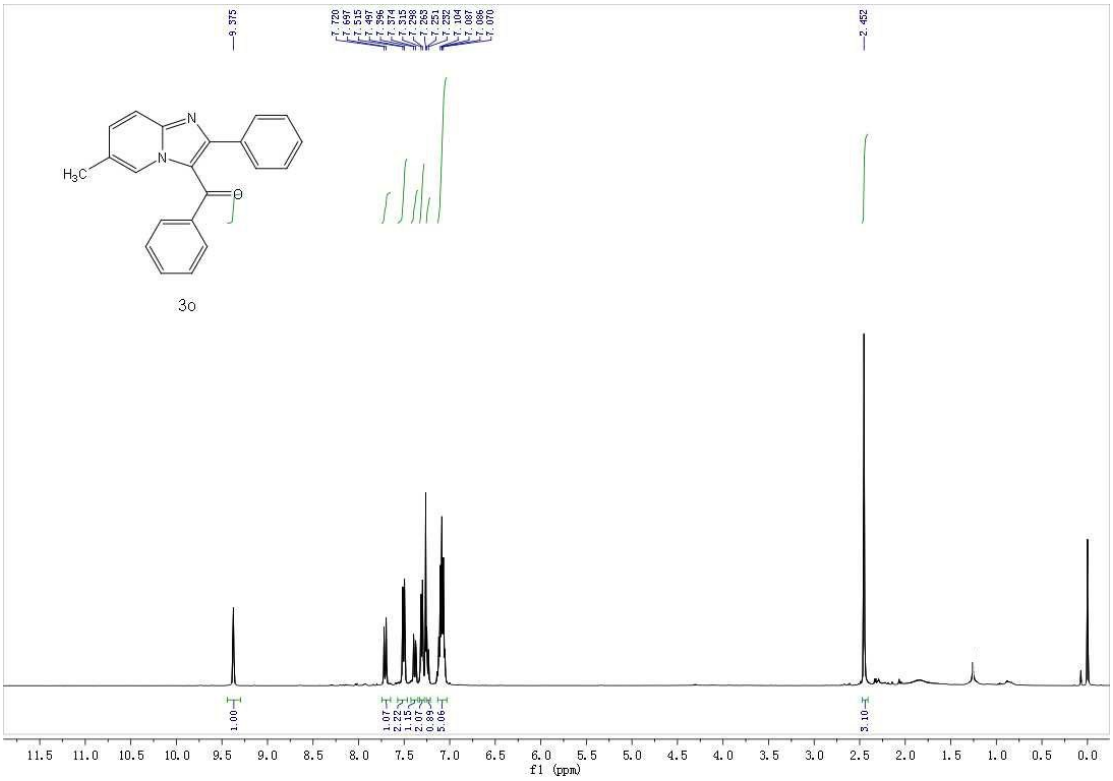
7.569
7.447
7.437
7.425
7.421
7.275
7.258
7.253
7.241
7.236
7.159
7.154
7.129
7.117
7.112
6.990
6.976
6.962
6.958
2.535
H3C
N
N
O
Cl
Cl
3n
0.99
1.03
2.10
2.27
4.01
1.04
3.11
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


185.36
153.91
147.98
141.57
138.18
137.04
134.76
132.47
131.34
130.82
128.13
128.07
127.45
119.60
117.45
116.11
77.32
77.00
76.68
21.60
H3C
N
N
O
Cl
Cl
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.497
7.396
7.374
7.315
7.286
7.263
7.251
7.232
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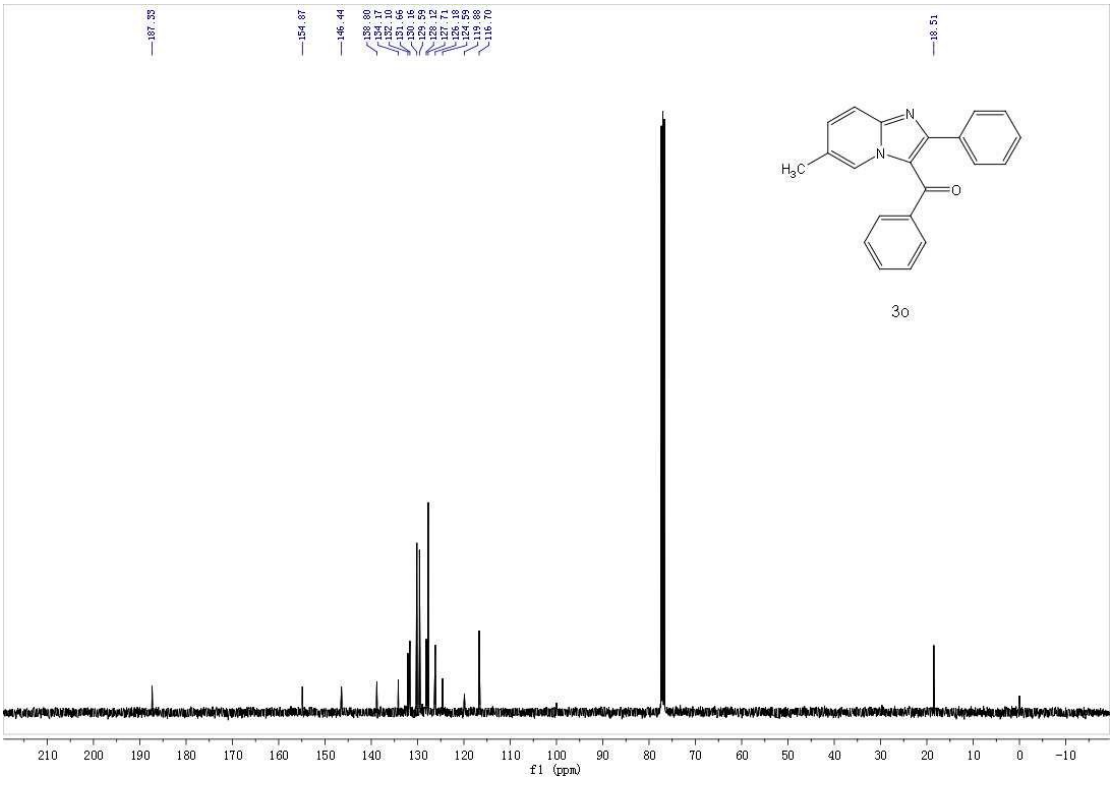
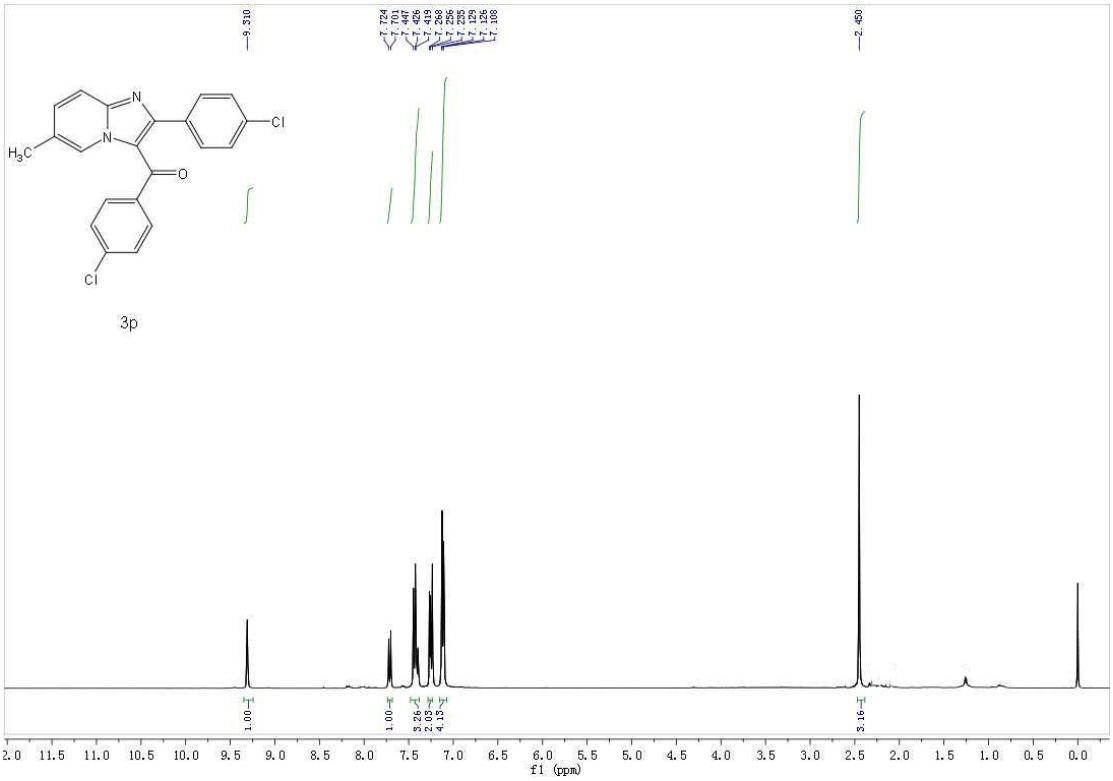
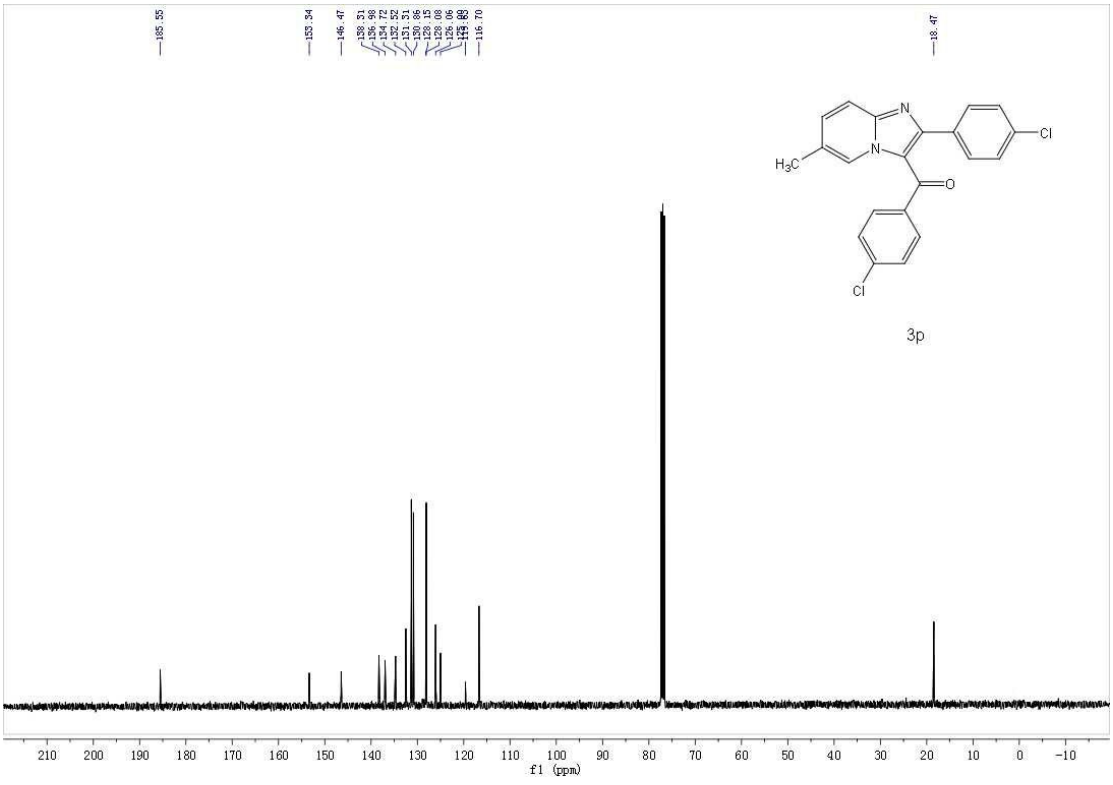
7.087
7.086
7.070
2.452
N
N
H3C
O
3o
1.00
1.07
2.22
1.15
2.07
0.89
1.00
3.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

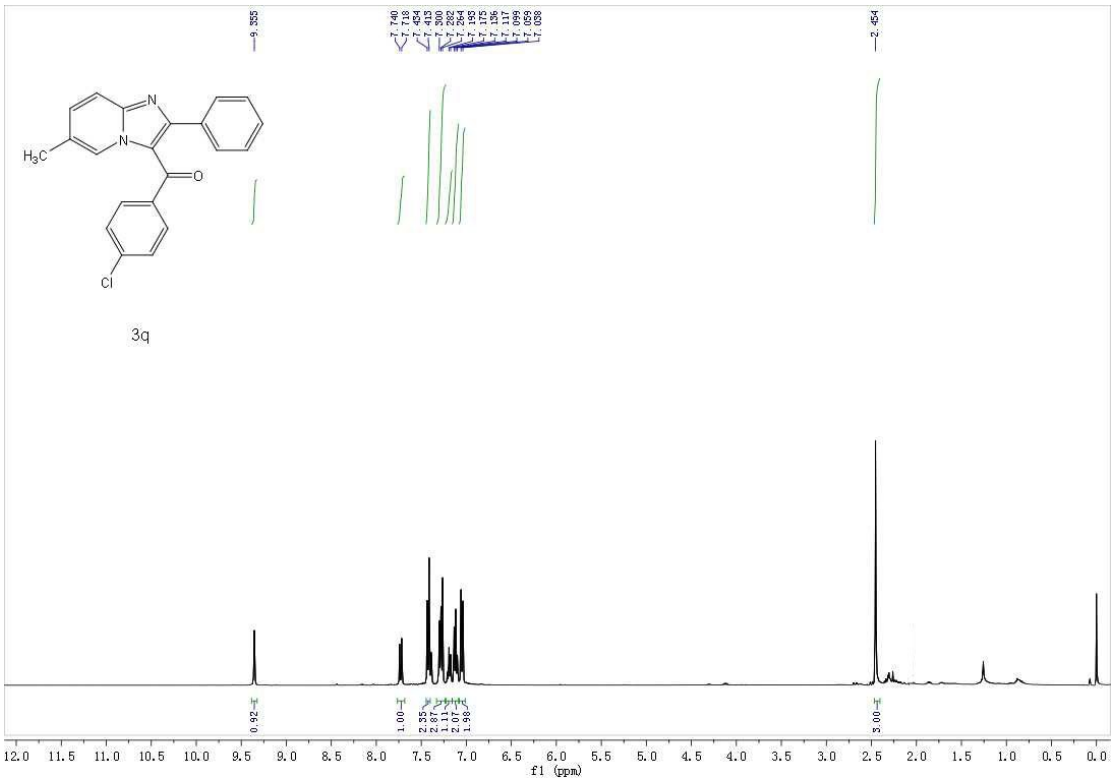

187.33
154.87
146.44
138.80
134.17
132.10
131.66
130.16
129.59
128.12
127.71
126.18
124.59
119.88
116.70
18.51
N
N
H3C
O
3o
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


9.510
7.724
7.701
7.447
7.426
7.419
7.268
7.256
7.235
7.129
7.125
7.108
2.450
N
N
O
Cl
Cl
H3C
1.00
1.00
5.26
2.13
4.13
3.16
f1 (ppm)

3p


185.55
153.34
146.47
138.51
135.69
134.72
132.52
131.51
130.86
130.15
128.08
126.06
116.70
18.47
N
N
O
Cl
Cl
H3C
f1 (ppm)

3p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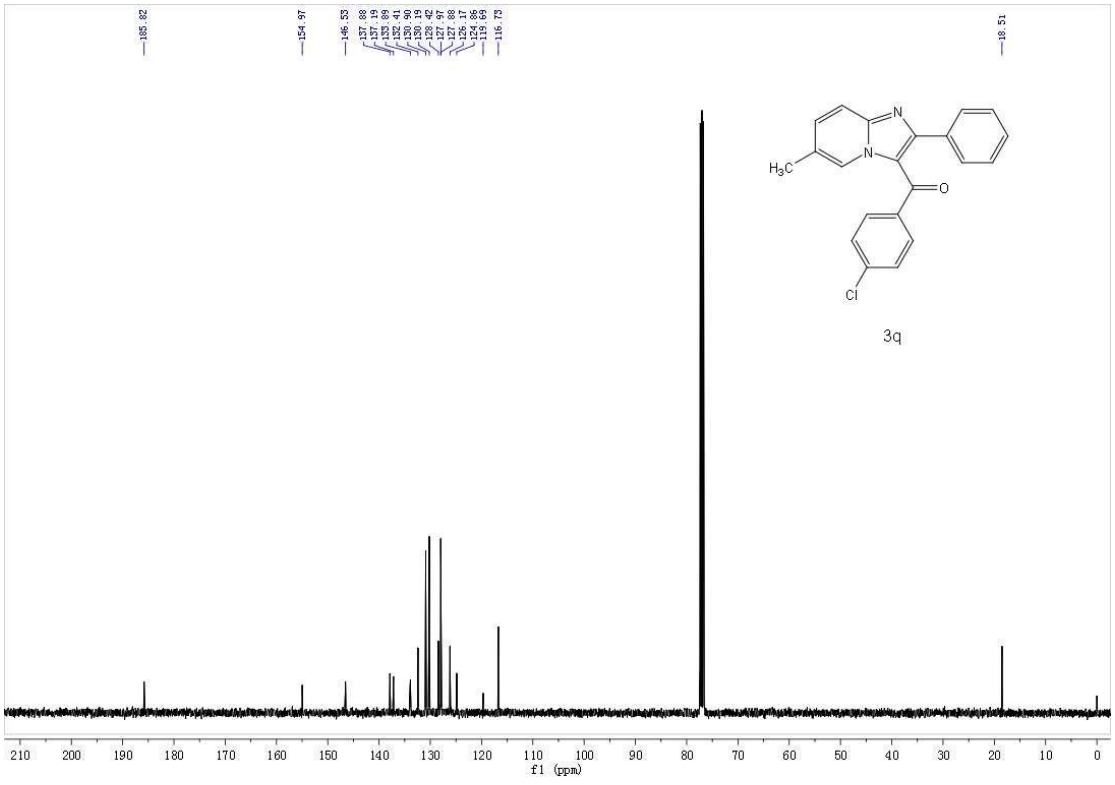
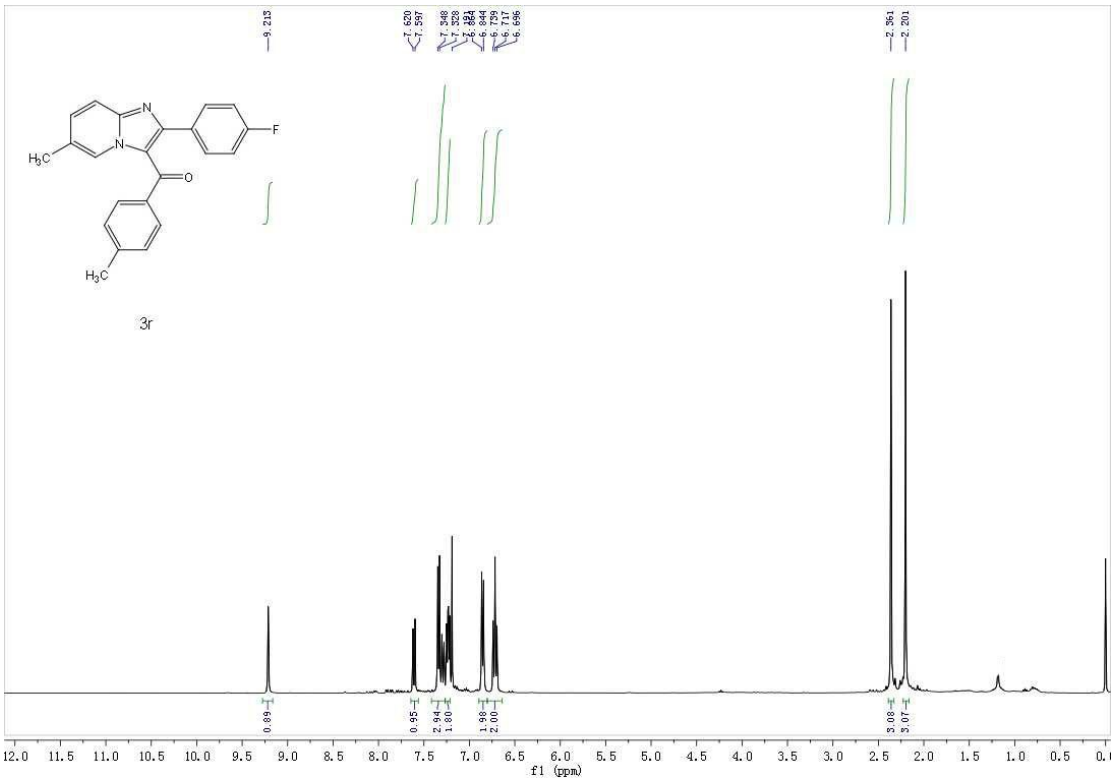
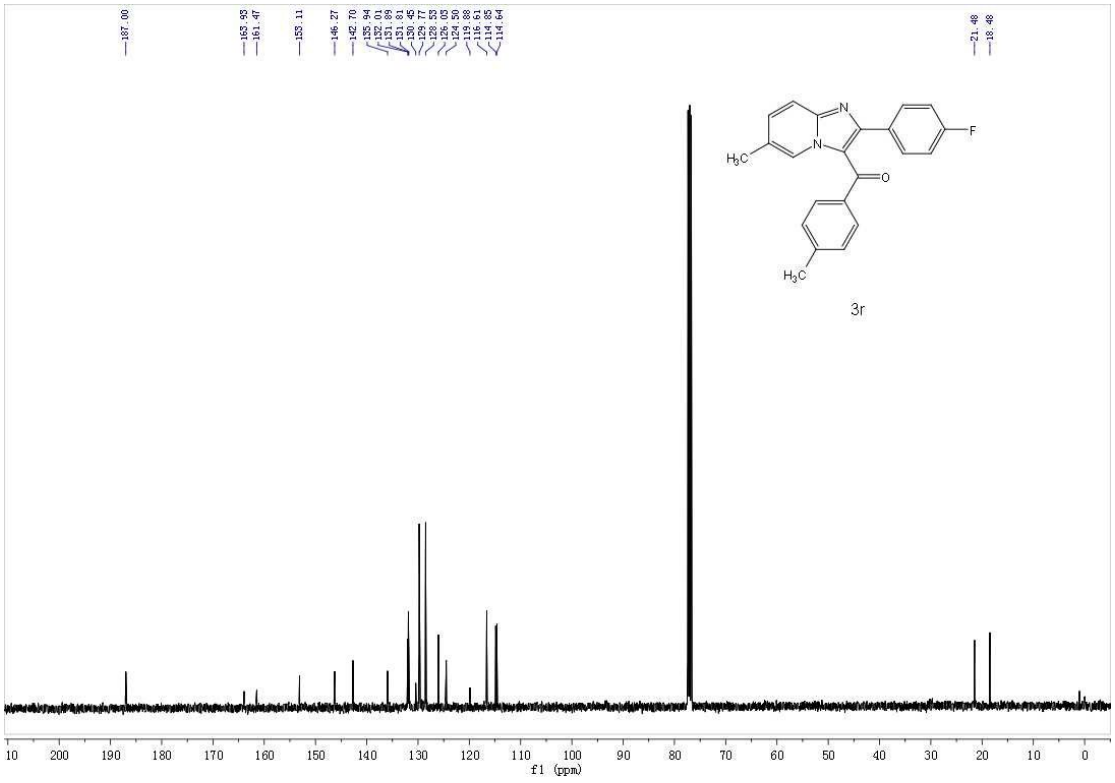
7.718
7.454
7.433
7.300
7.282
7.264
7.195
7.175
7.136
7.117
7.099
7.059
7.038
2.454
N
N
H3C
O
Cl
3q
0.92
1.00
2.35
2.87
2.17
2.01
1.98
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

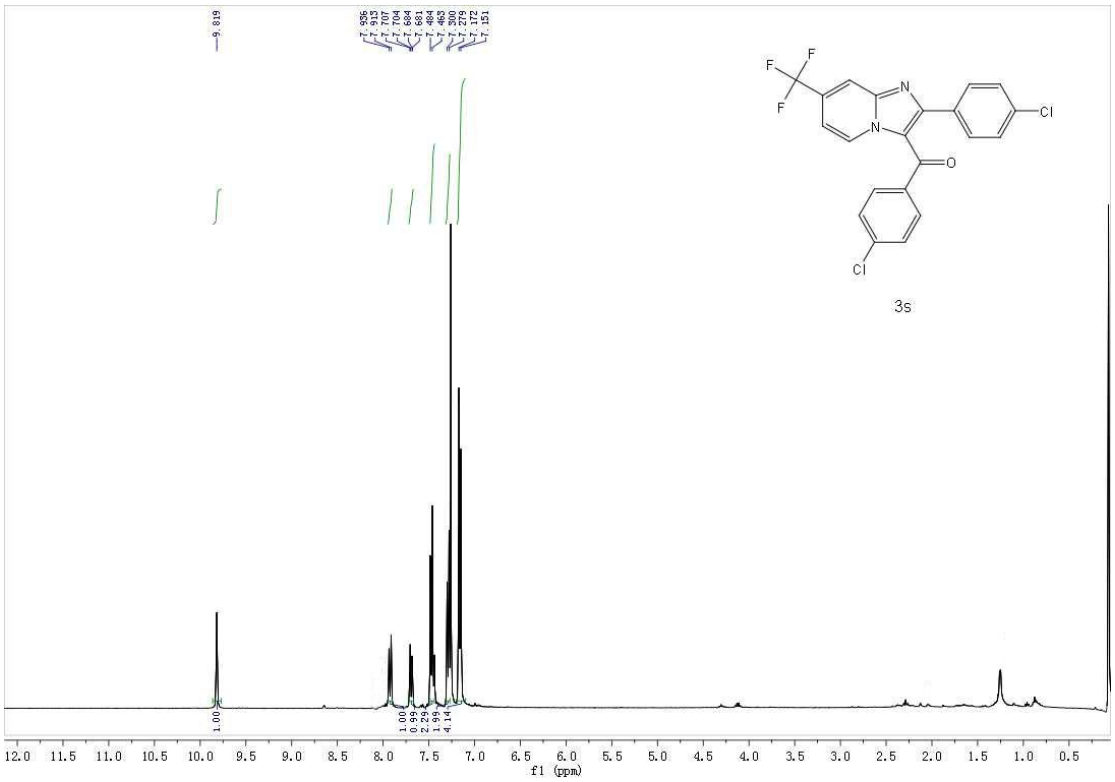

185.82
154.97
146.53
137.88
137.19
133.89
132.41
130.90
130.19
128.47
127.97
127.88
126.17
124.66
119.95
116.73
18.51
N
N
H3C
O
Cl
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

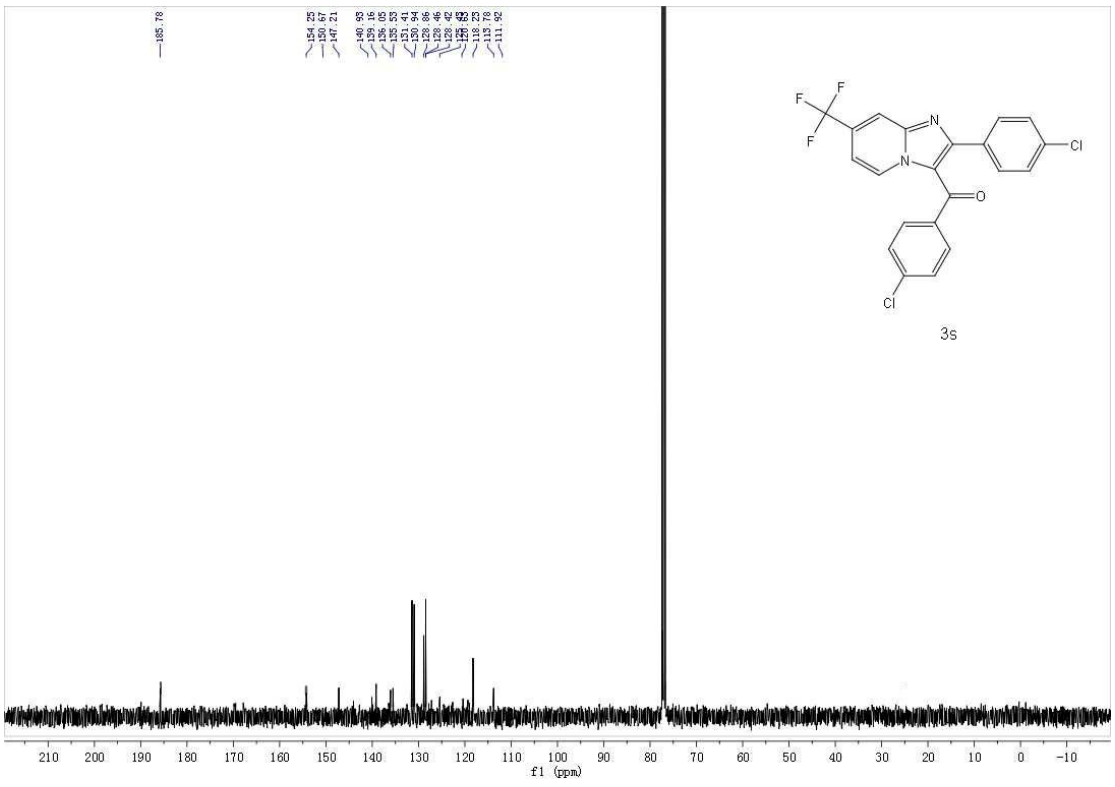

9.213
7.620
7.597
7.348
7.328
6.844
6.739
6.717
6.696
2.361
2.201
0.89
0.95
2.94
1.80
1.98
2.00
3.08
3.07
f1 (ppm)

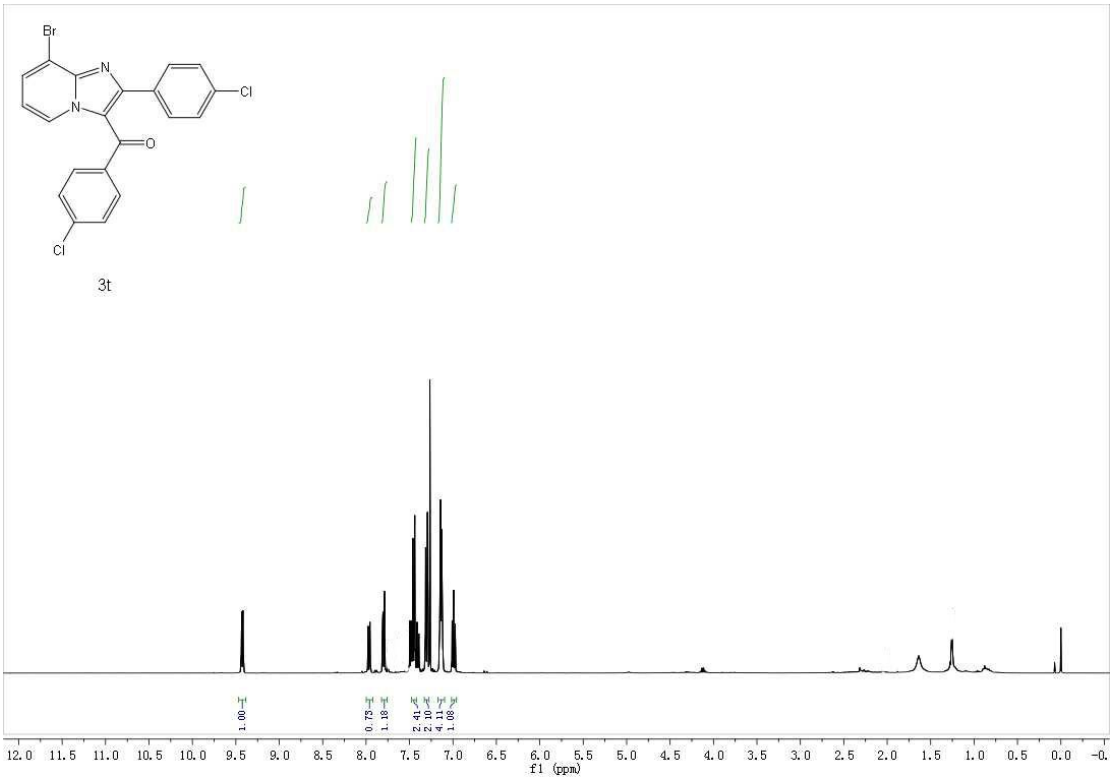
3r

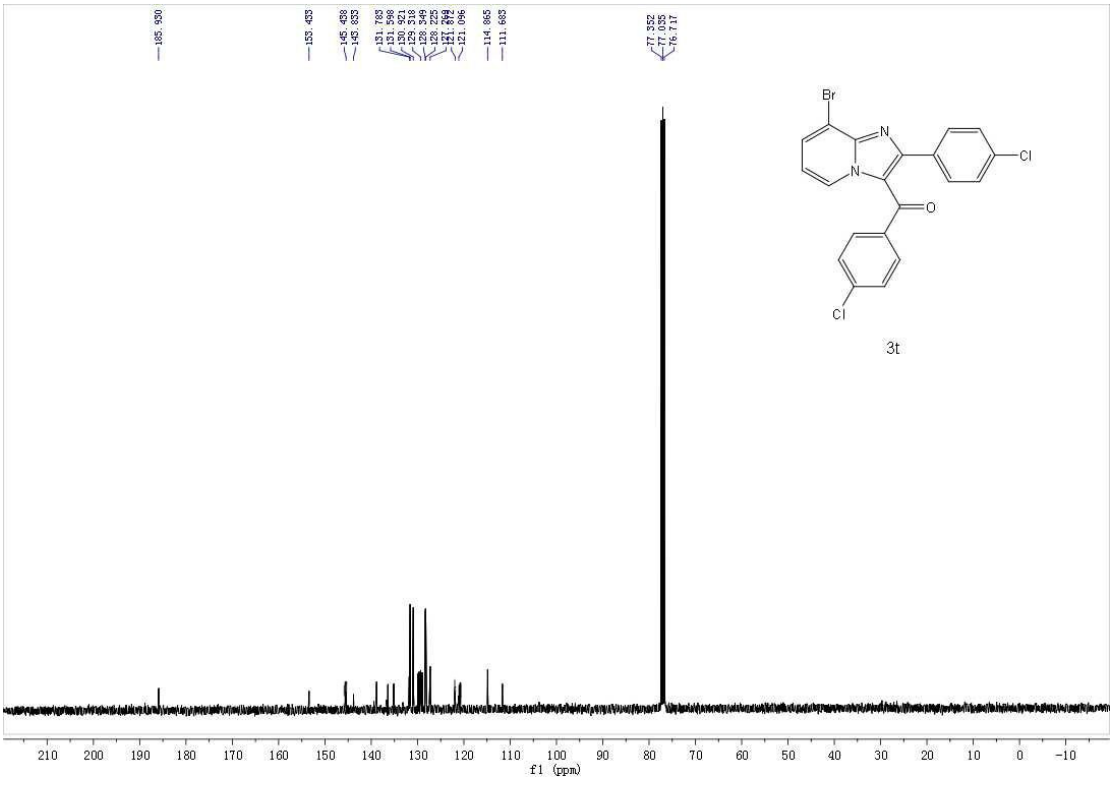

187.00
163.93
161.47
153.11
146.27
142.70
135.94
132.01
131.88
131.81
130.45
129.77
128.53
126.85
124.90
119.88
116.61
114.85
114.64
21.48
18.48
f1 (ppm)

3r


9.819
7.936
7.917
7.707
7.704
7.684
7.681
7.664
7.463
7.300
7.279
7.172
7.151
1.00
1.03
0.99
2.29
1.98
4.14
F
F
F
N
N
Cl
O
Cl
3s
f1 (ppm)


185.78
154.25
150.67
147.21
140.93
139.16
136.05
135.53
131.41
130.94
128.86
128.46
128.42
118.23
115.76
111.92
F
F
F
N
N
Cl
O
Cl
3s
f1 (ppm)


Br
N
N
Cl
O
Cl
3t
1.00
0.73
1.18
2.41
2.10
4.11
1.08
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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153.433
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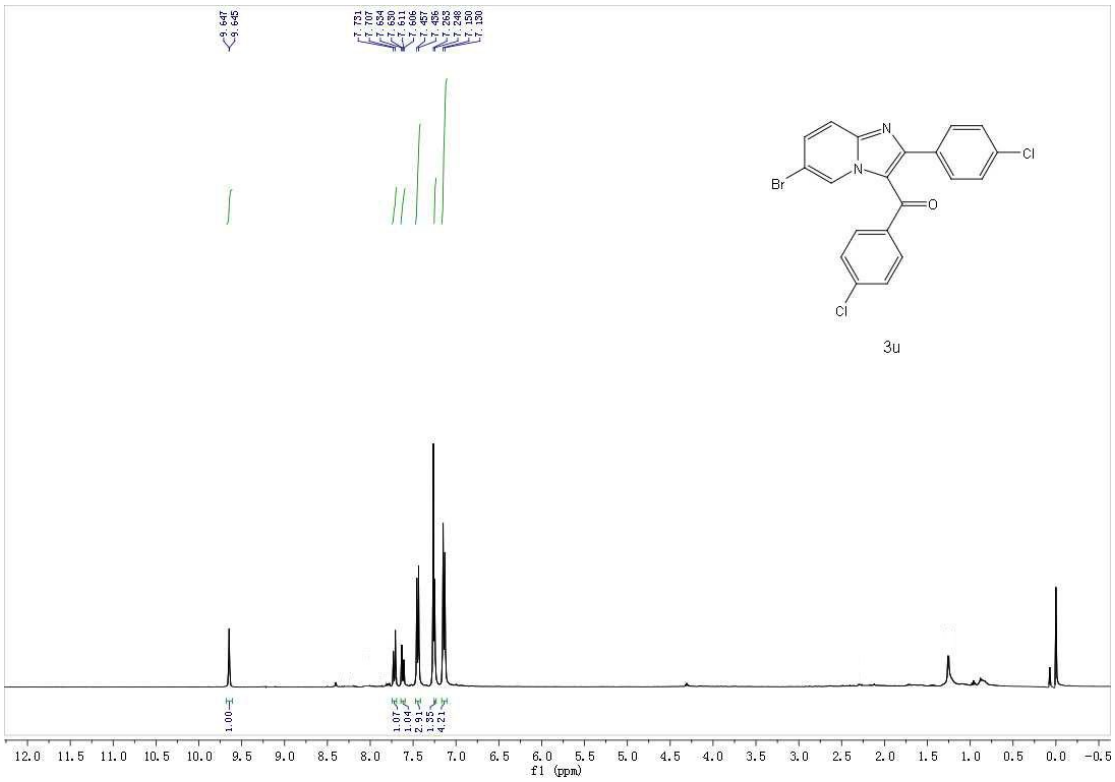
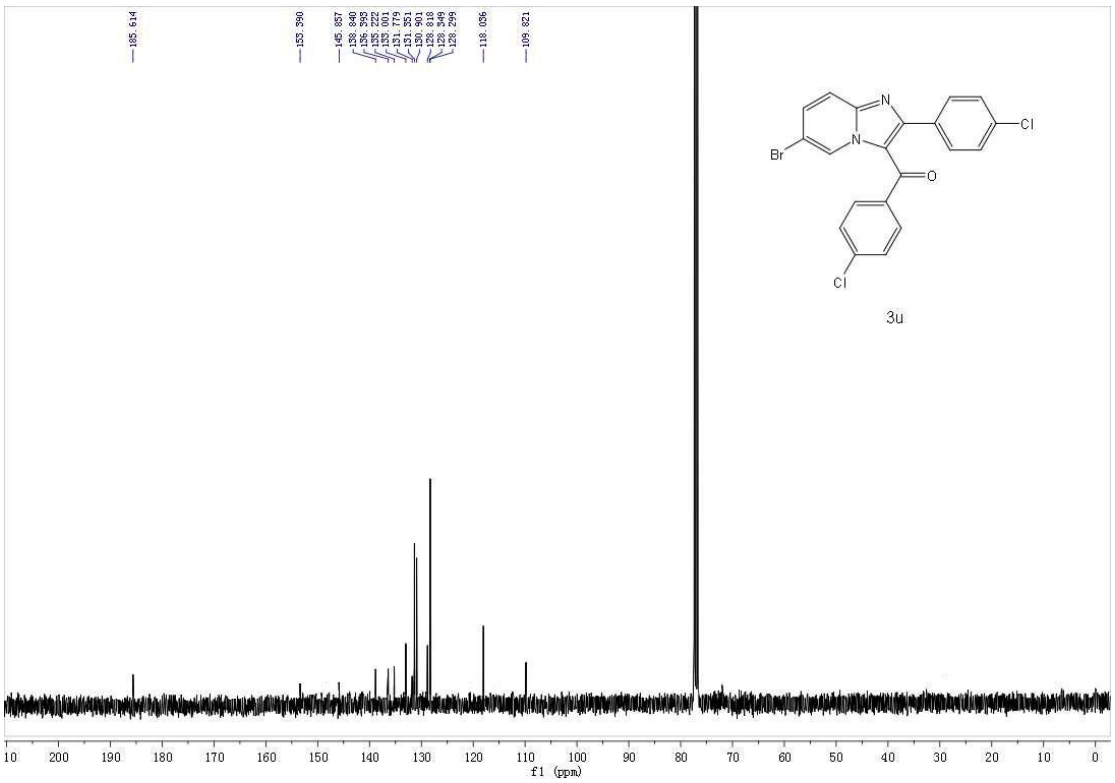
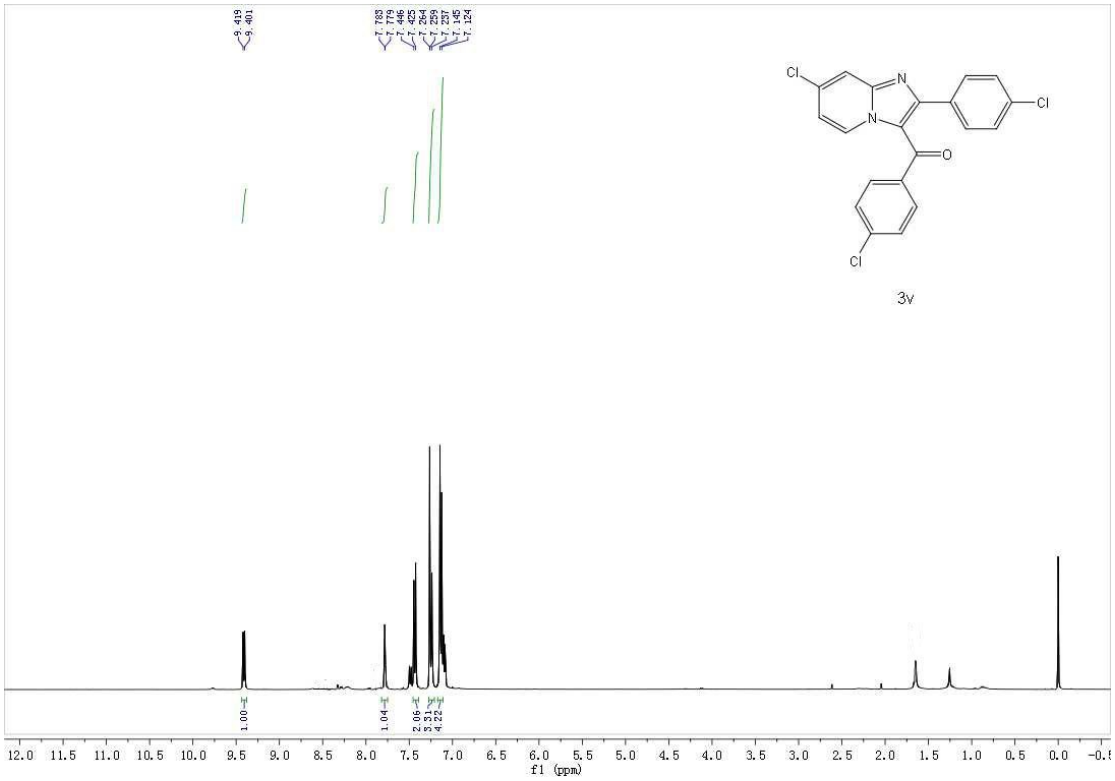
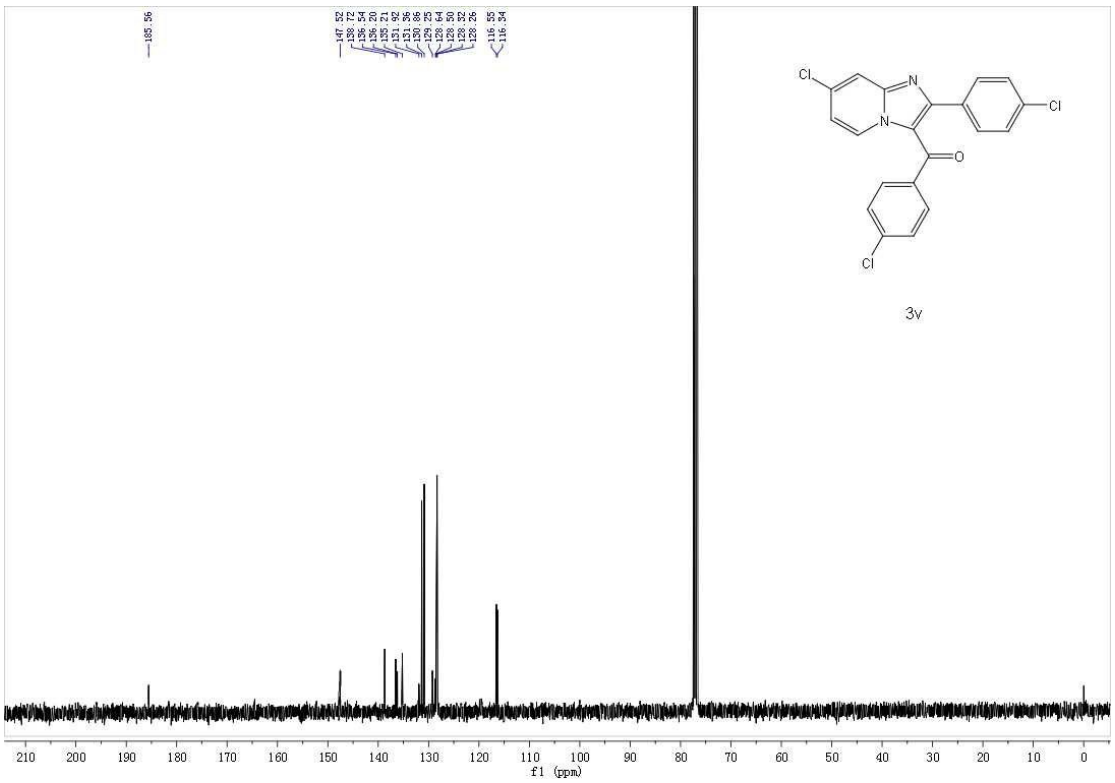
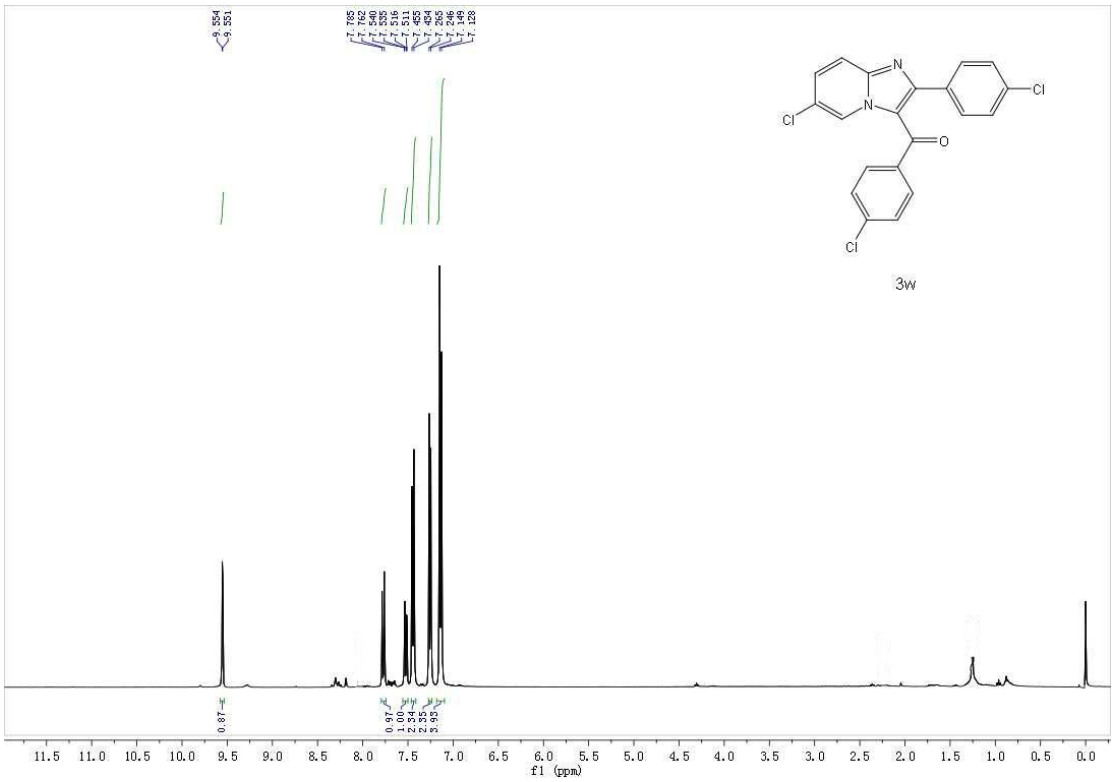
145.833
131.783
131.598
131.531
129.313
128.349
128.225
121.844
121.096
114.865
111.683
77.352
77.055
76.717
Br
N
N
Cl
O
Cl
3t
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

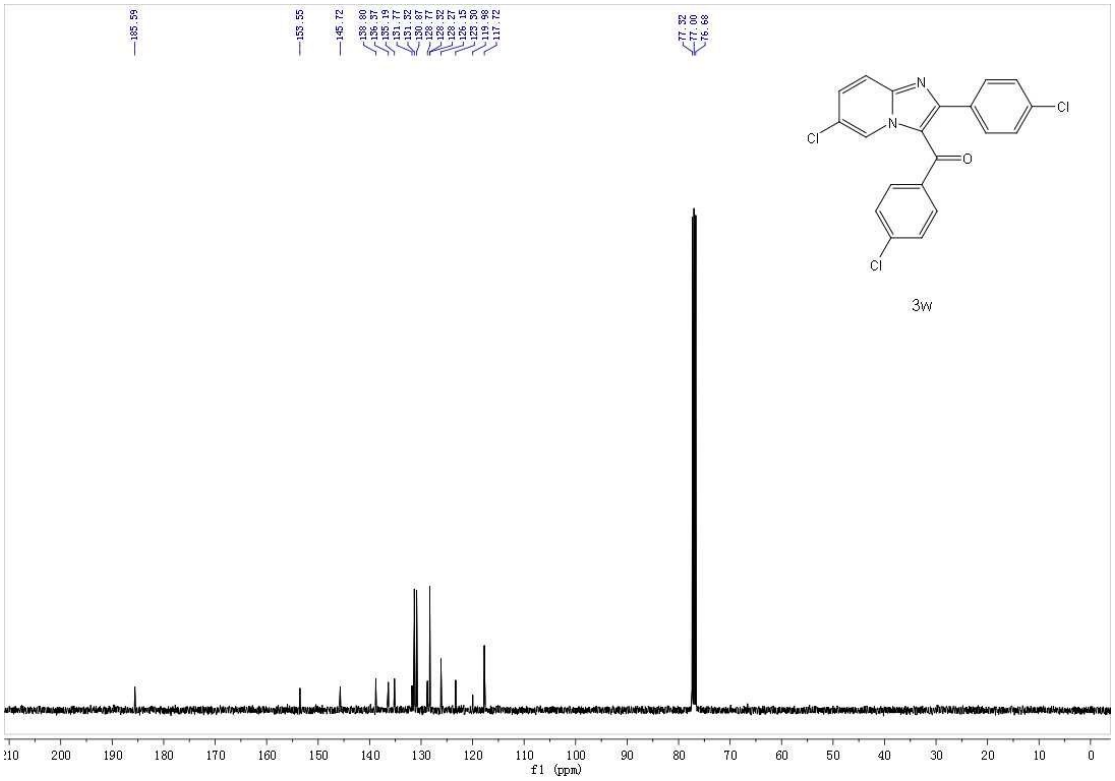

9.647
9.645
7.731
7.707
7.634
7.630
7.611
7.606
7.457
7.456
7.263
7.260
7.150
7.130
Br
N
N
O
Cl
Cl
3u
1.00
1.07
1.04
2.91
1.97
4.21
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

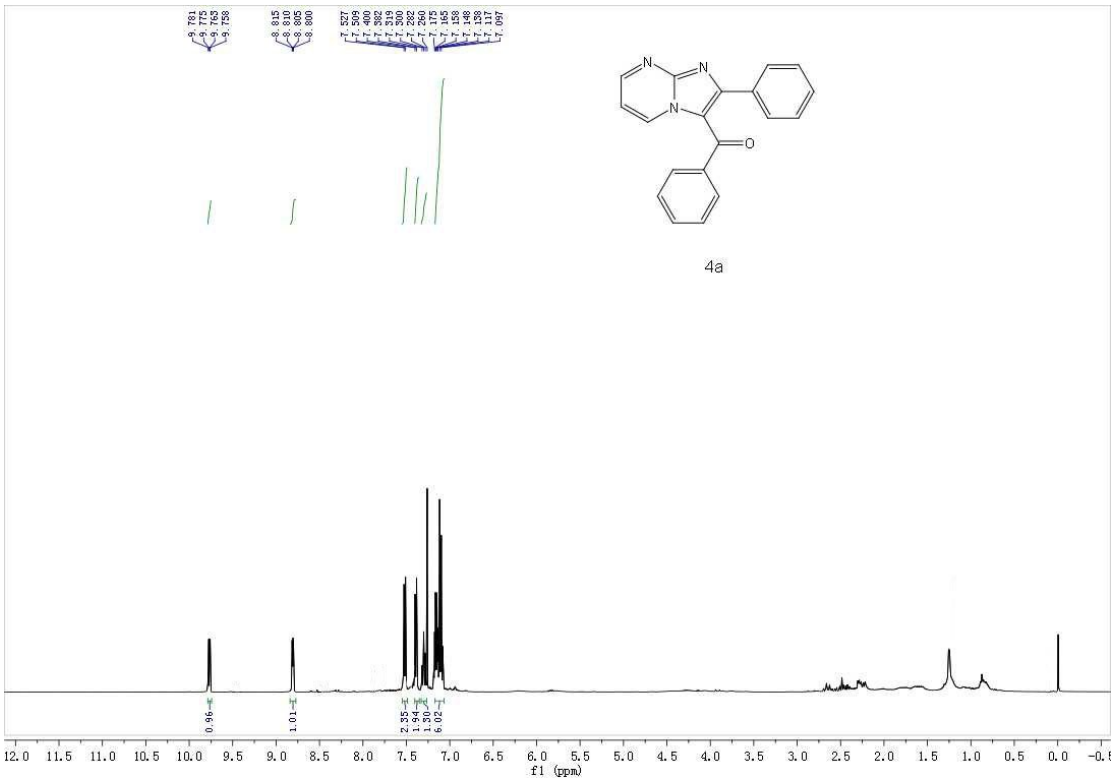

185.614
153.390
145.857
138.840
136.598
135.072
133.070
131.779
131.351
130.901
130.818
128.349
128.299
118.036
109.821
Br
N
N
O
Cl
Cl
3u
10 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

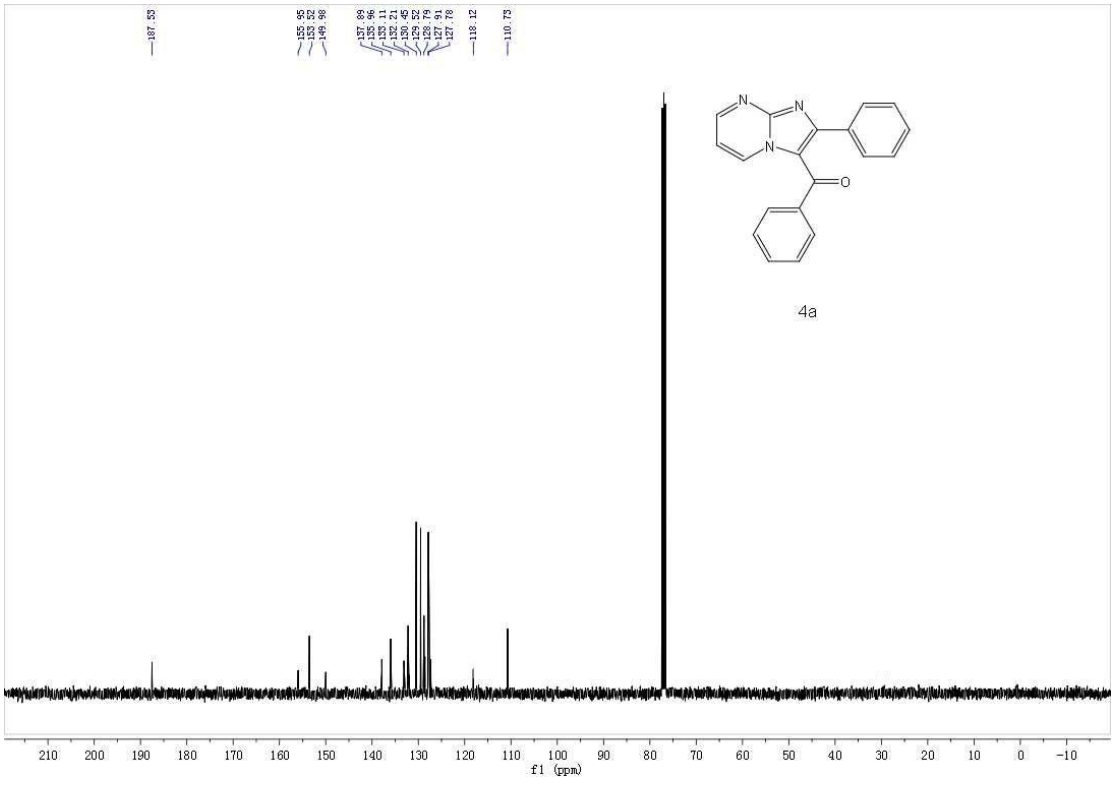

9.419
9.401
7.788
7.779
7.446
7.425
7.264
7.259
7.237
7.145
7.124
Cl
N
N
O
Cl
Cl
3v
1.00
1.04
2.05
3.91
4.22
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

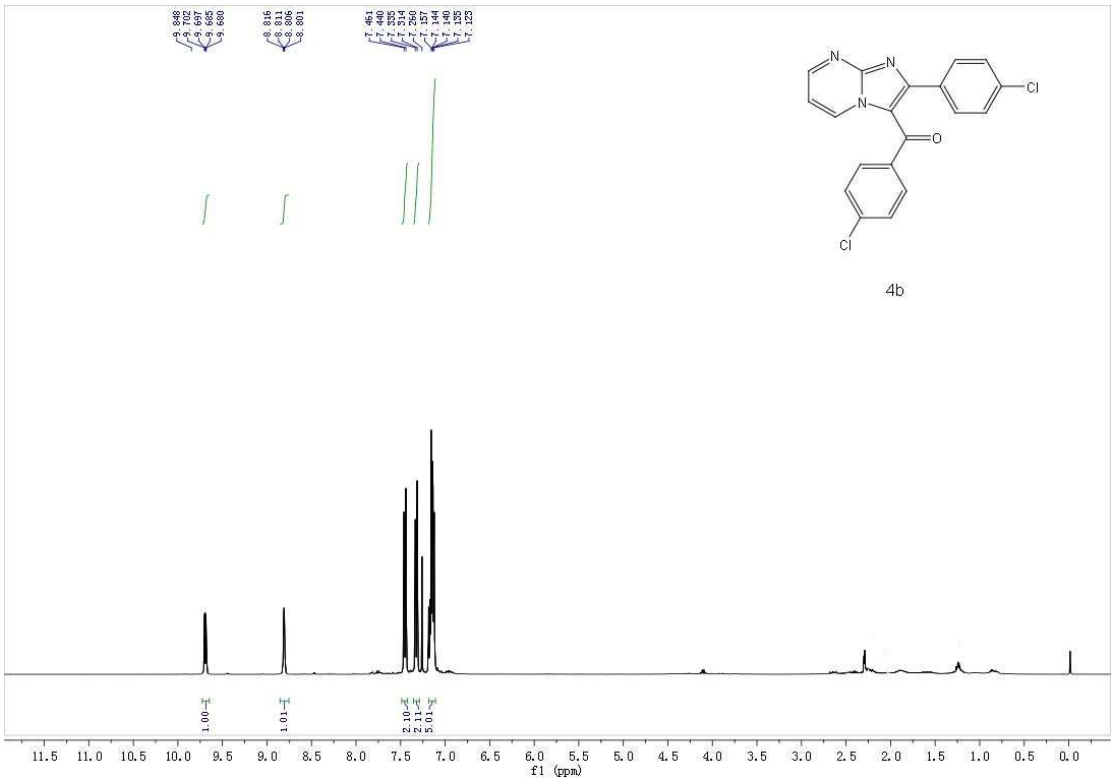

185.56
147.52
138.72
135.54
135.20
131.92
131.36
129.86
129.35
128.64
128.50
128.32
128.26
116.55
116.34
Cl
N
N
O
Cl
Cl
3v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

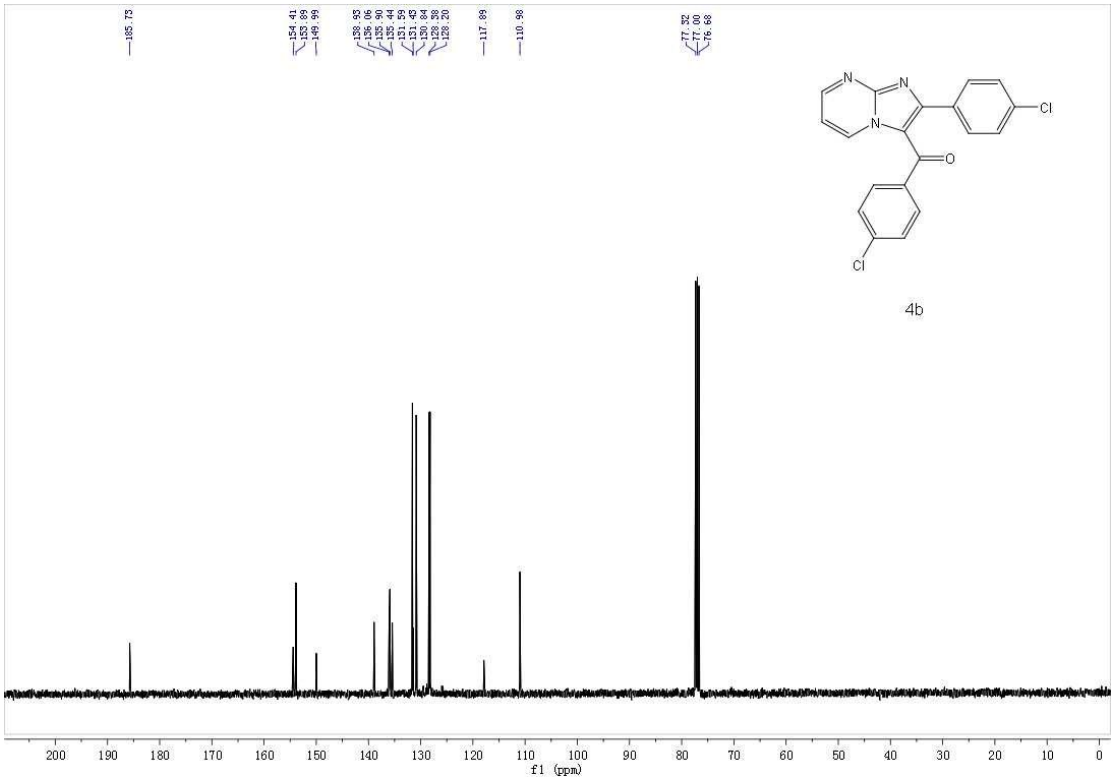

9.554
9.551
7.785
7.762
7.540
7.535
7.516
7.511
7.455
7.454
7.265
7.246
7.149
7.128
Cl
N
N
Cl
O
Cl
3w
0.87
0.97
1.04
2.34
2.35
5.95
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

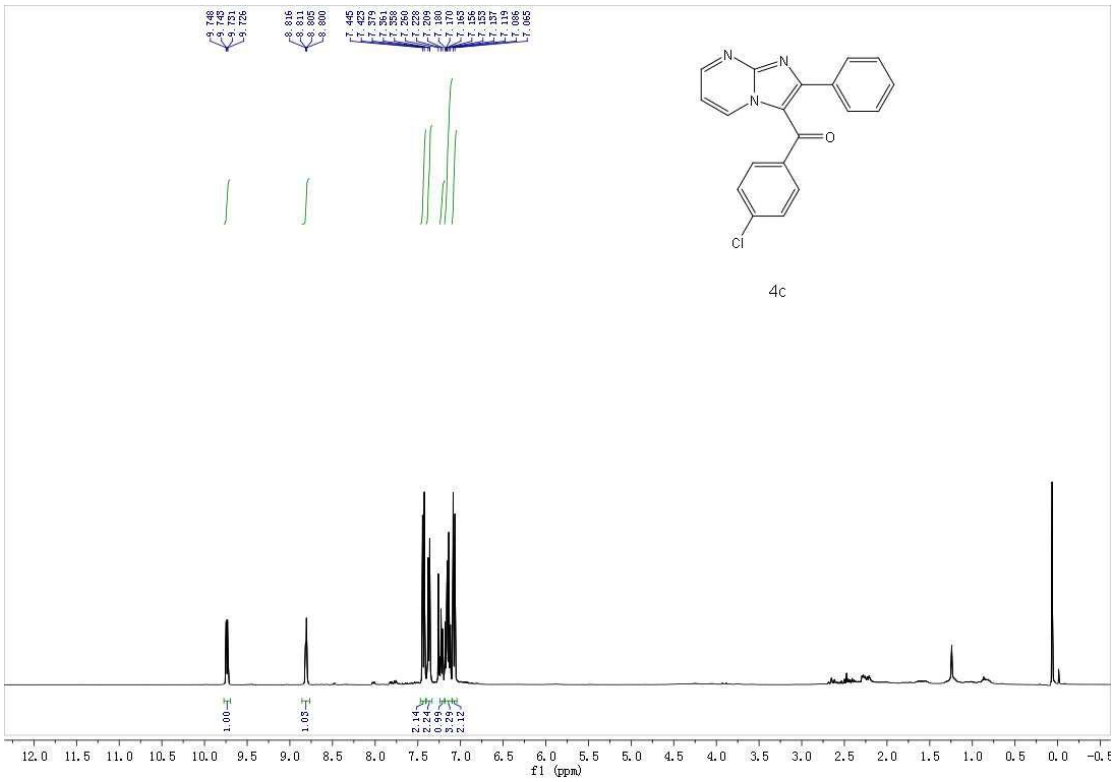

185.59
153.55
145.72
138.80
135.37
135.19
131.77
131.32
130.97
130.77
128.52
128.27
126.15
123.30
119.99
117.72
77.32
77.00
76.68
Cl
N
N
Cl
O
Cl
3w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

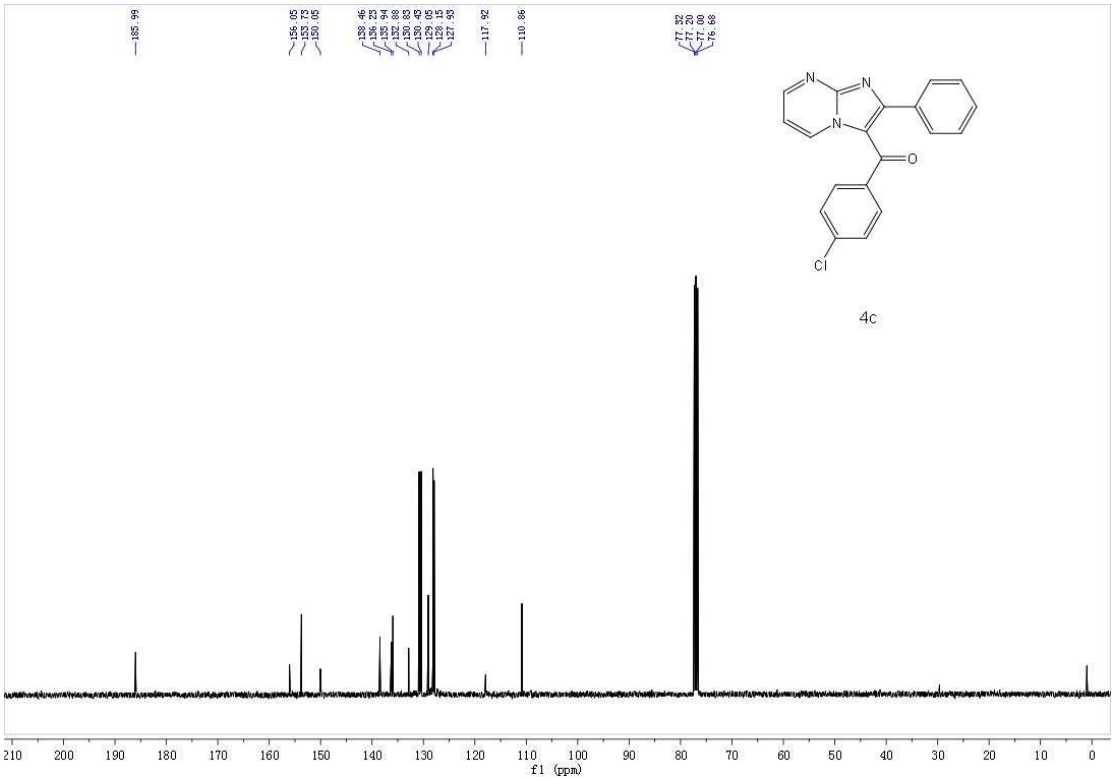

9.781
9.775
9.763
9.758
8.815
8.810
8.805
8.800
7.527
7.509
7.400
7.382
7.319
7.300
7.282
7.260
7.175
7.165
7.158
7.148
7.138
7.117
7.097
4a
0.96
1.01
2.35
1.93
1.30
6.02
f1 (ppm)

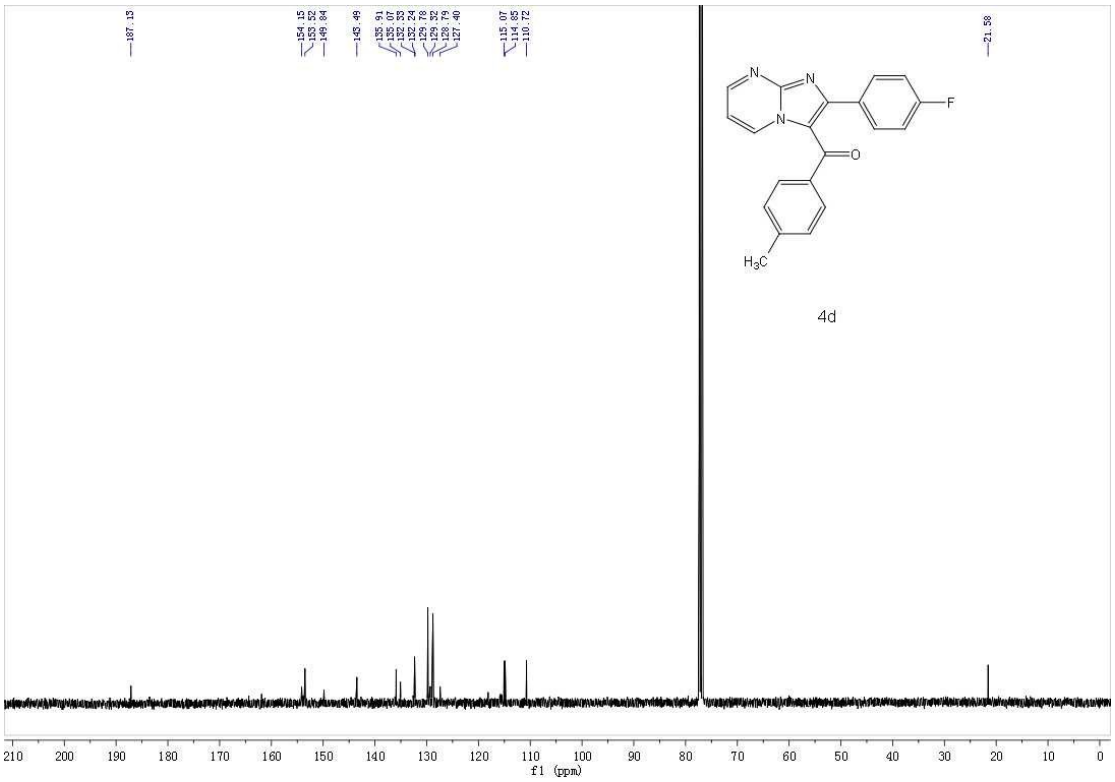

187.53
155.95
153.52
149.98
137.69
135.96
133.11
132.21
130.45
129.32
128.79
127.91
127.78
118.12
110.73
4a
f1 (ppm)

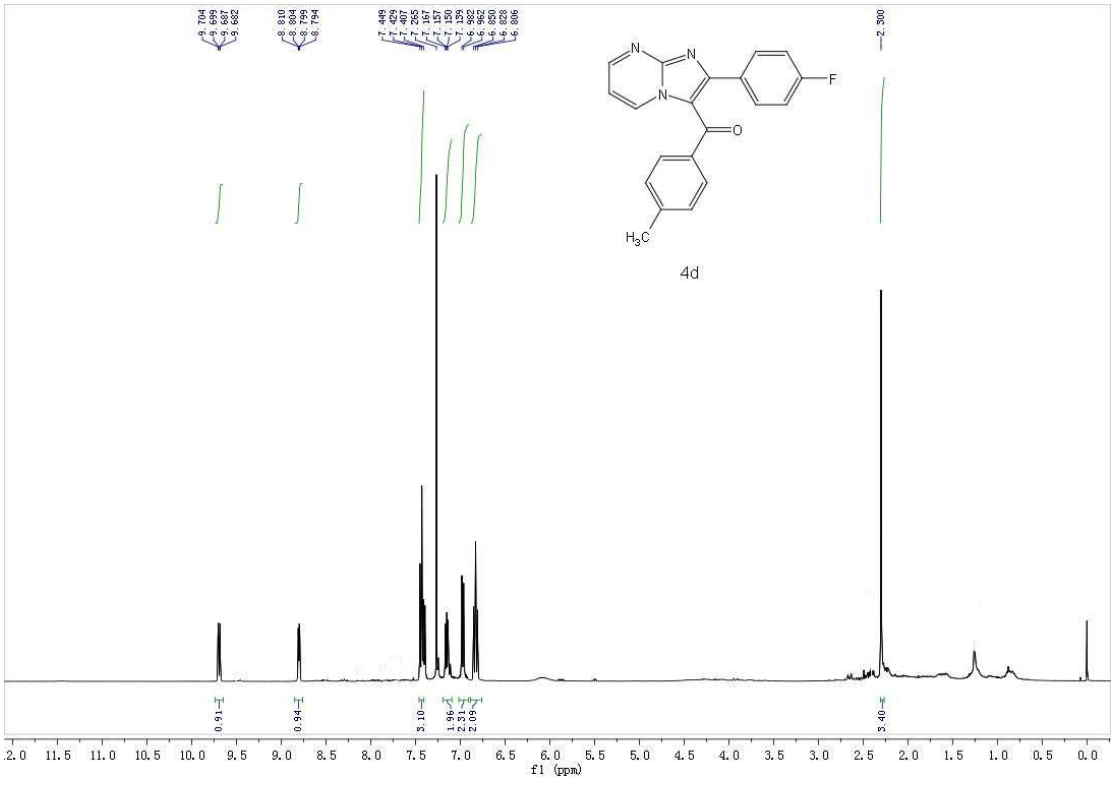

9.848
9.702
9.697
9.685
9.680
8.816
8.811
8.806
8.801
7.461
7.440
7.335
7.314
7.260
7.157
7.144
7.140
7.135
7.123
N
N
N
Cl
O
Cl
4b
1.00
1.01
2.10
2.11
5.01
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

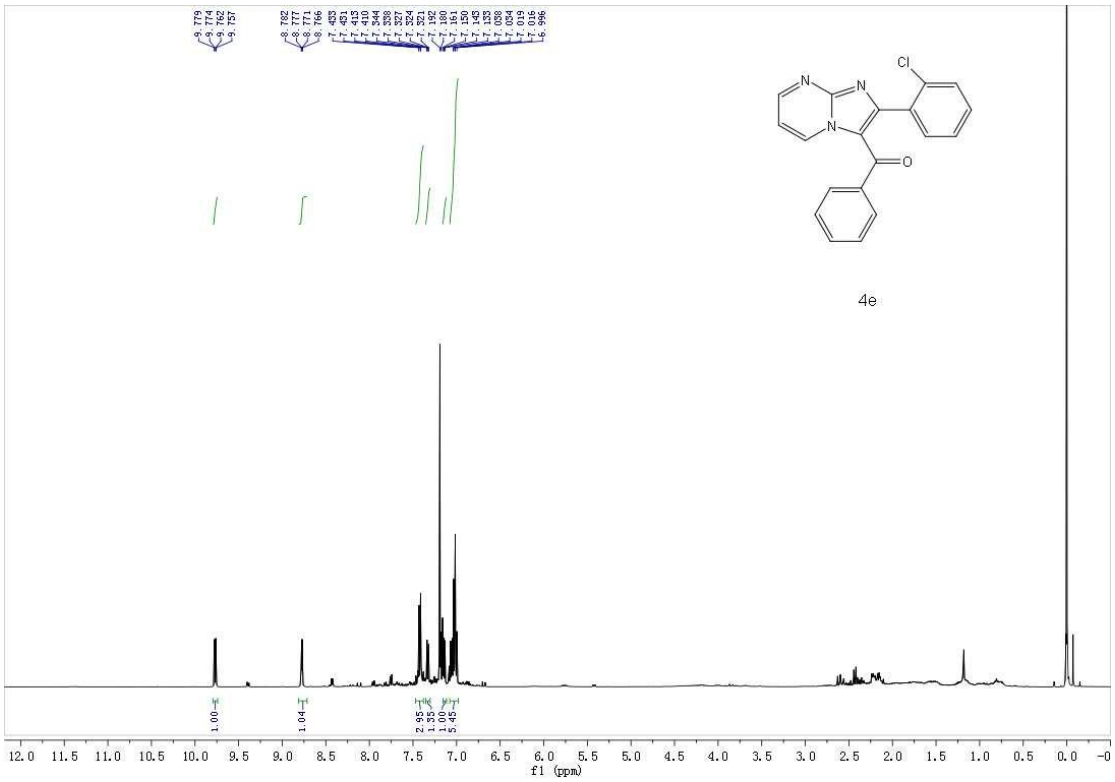

185.73
154.41
153.88
149.99
138.93
136.06
135.90
135.44
131.88
131.45
130.84
129.38
128.20
117.89
110.98
77.32
77.00
76.68
N
N
N
Cl
O
Cl
4b
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

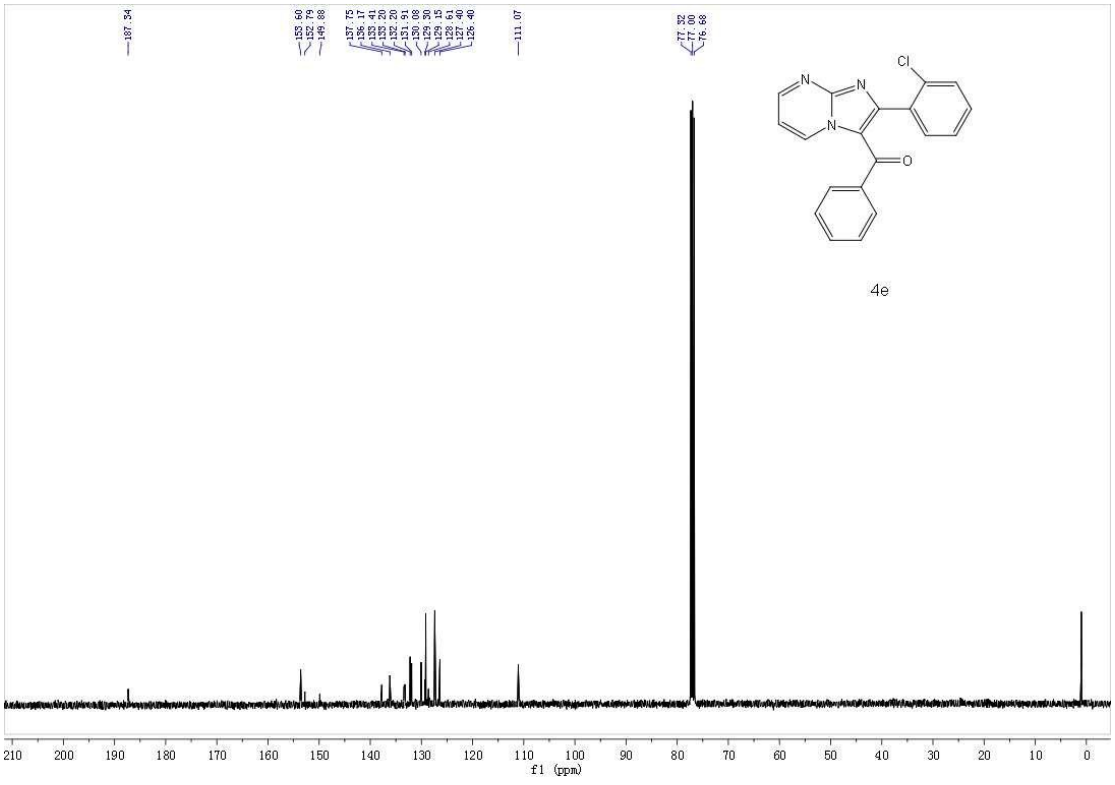

9.748
9.745
9.731
9.726
8.816
8.811
8.805
8.800
7.445
7.423
7.375
7.361
7.358
7.260
7.223
7.209
7.180
7.170
7.163
7.155
7.153
7.137
7.119
7.086
7.065
N
N
N
O
Cl
4c
1.00
1.03
2.14
2.24
0.99
3.29
2.12
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

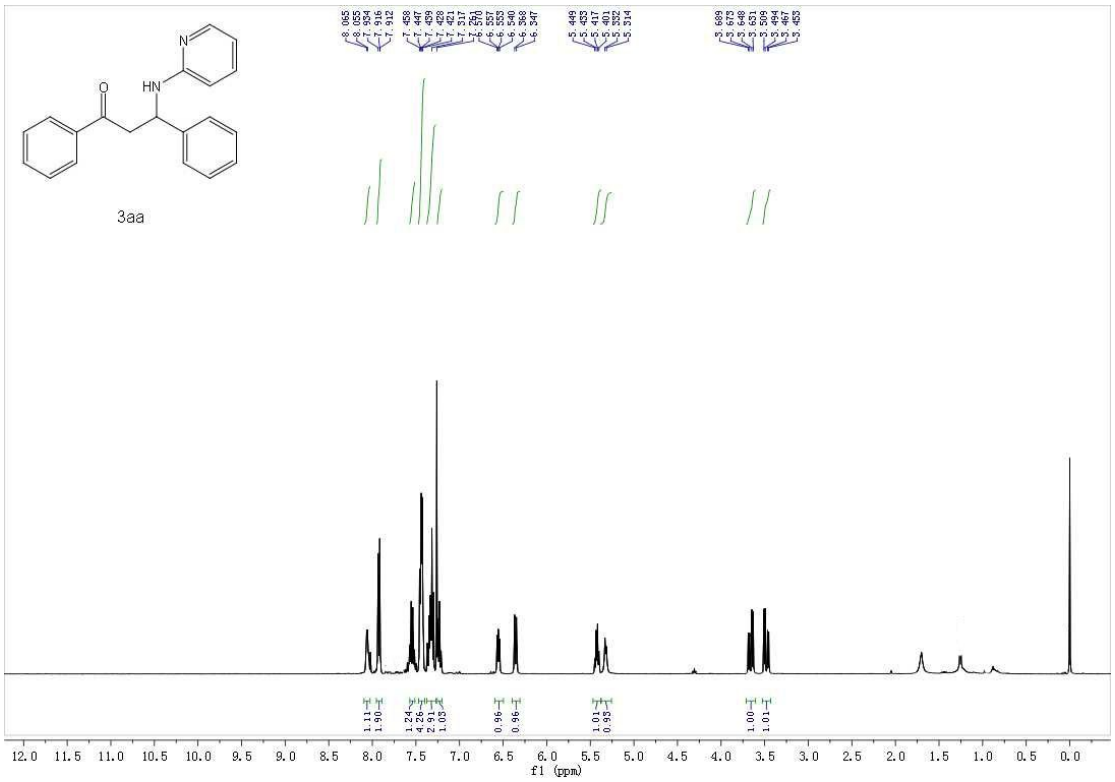

185.99
156.05
153.73
150.06
138.46
136.23
135.94
132.88
130.83
130.45
129.65
128.15
127.93
117.92
110.86
77.32
77.20
77.00
76.68
N
N
N
O
Cl
4c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


187.13
154.15
153.52
149.84
145.49
135.91
135.07
133.93
132.24
129.78
129.32
125.79
127.40
115.07
114.85
110.72
21.58
N
N
N
F
O
H3C
4d
f1 (ppm)


9.704
9.699
9.687
9.682
8.810
8.804
8.799
8.794
7.449
7.429
7.407
7.255
7.167
7.157
7.150
7.139
6.962
6.850
6.828
6.806
2.500
N
N
N
F
O
H3C
4d
0.91
0.94
3.10
1.96
2.91
2.09
3.40
f1 (ppm)


9.779
9.774
9.762
9.757
8.782
8.777
8.771
8.766
7.493
7.491
7.453
7.451
7.413
7.410
7.344
7.339
7.327
7.324
7.321
7.192
7.180
7.161
7.150
7.145
7.133
7.059
7.054
7.019
7.016
6.996
1.00
1.04
2.95
1.33
1.00
5.45
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)
Cl
N
N
N
O
4e


187.34
153.60
152.79
149.88
137.75
136.17
135.44
133.20
132.20
131.91
131.88
129.30
129.15
128.61
127.40
126.40
111.07
77.32
77.00
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Cl
N
N
N
O
4e


3aa
f1 (ppm)