# Supporting Information

## Metal-Free TBHP-Mediated Oxidative Ring Openings of 2-Arylimidazopyridines Via Regioselective Cleavage of C−C and C−N Bonds

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## Table of contents

**General Information:**

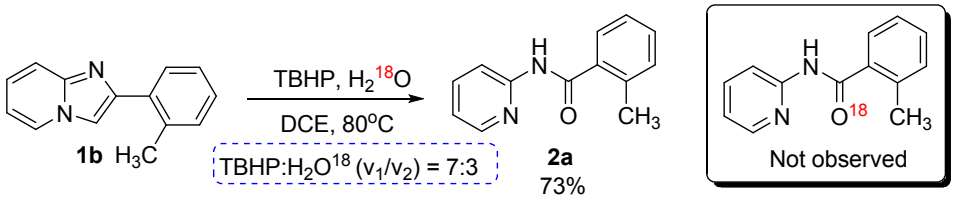
All commercially available reagent and chemicals were purchased from chemical suppliers and used as received without further purification. Column chromatography was performed on silica gel (200-300 mesh). Mass analyses and HRMS were obtained on a TOF mass spectrometer. $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded in $CDCl_3$ with TMS as internal standard (400 MHz $^{1}H$, 100 MHz $^{13}C$) at room temperature.

## Experiments of investigations on the mechanism

### (1) General procedure for $H_2{}^{18}O$ labeling experiment

A 25 mL Schlenk tube equipped with a magnetic stirring bar was charged with substituted 2-phenylimidazo[1,2-*a*]pyridines (**1b**) (0.4 mmol), TBHP (1.6 mmol, *tert*-butyl hydroperoxide 70 wt % in $H_2{}^{18}O$), and DCE (2.0 ml). The tube was sealed and then the mixture was allowed to stir under under air atmosphere at 80 $^{o}C$ for 18 h. After the reaction, the resulting mixture was concentrated under vacuum and the residue was purified by flash column chromatography using a mixture of petroleum ether and ethyl acetate (4:1) as an eluent. The products were measured by HRMS.

The HRMS spectra of products was listed as bellow (Figure 1).



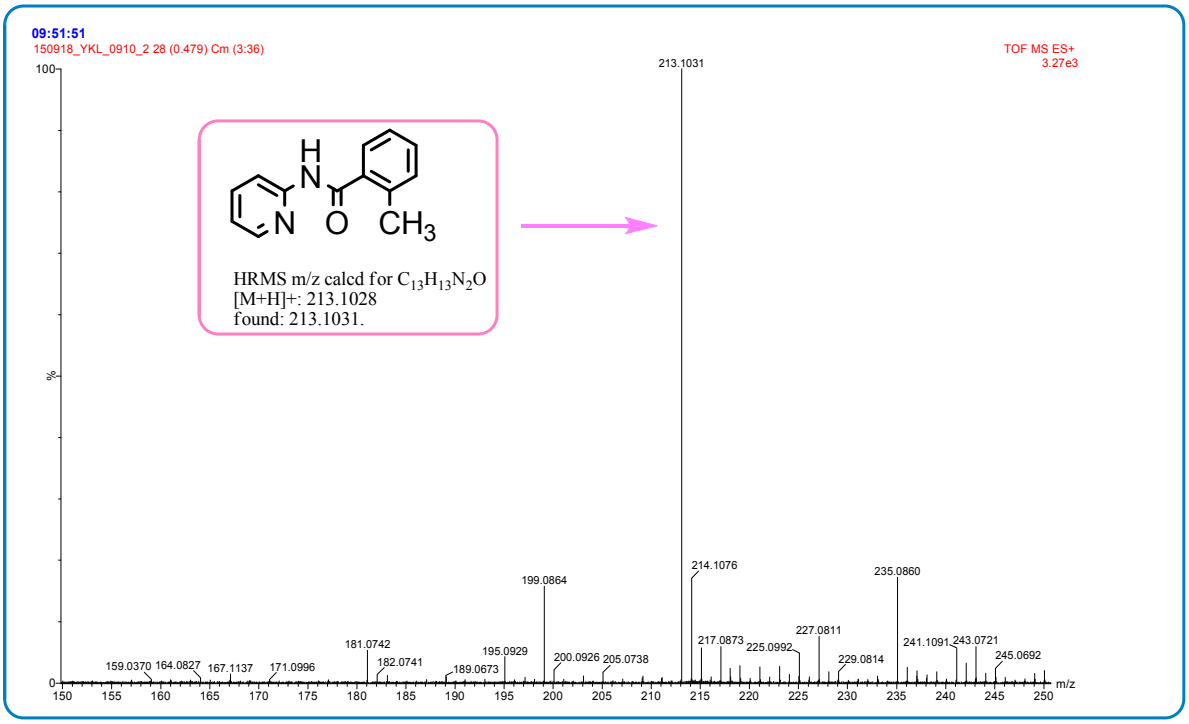
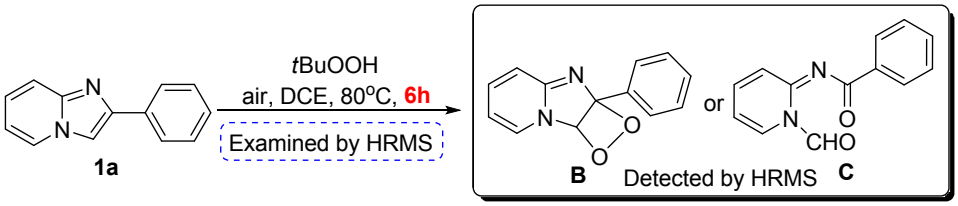



**Figure 1**. The HRMS spectral of $^{18}O$ labelled proudcts

**(2) Experiment procedure for the reaction of 1a with TBHP for a time.**

A 25 mL Schlenk tube equipped with a magnetic stirring bar was charged with substituted 2-phenylimidazo[1,2-*a*]pyridines (**1a**) (0.4 mmol), TBHP (4 equiv, *tert*-butyl hydroperoxide 70 wt % in water), and DCE (2.0 ml). The tube was sealed and then the mixture was allowed to stir under under air atmosphere at 80 $^{o}$C for about 6 h. Afterwards, 30 uL of the mixture was quickly taken out into a small tube and analyzed by HRMS. The HRMS spectra of products was listed as bellow (Figure 2).



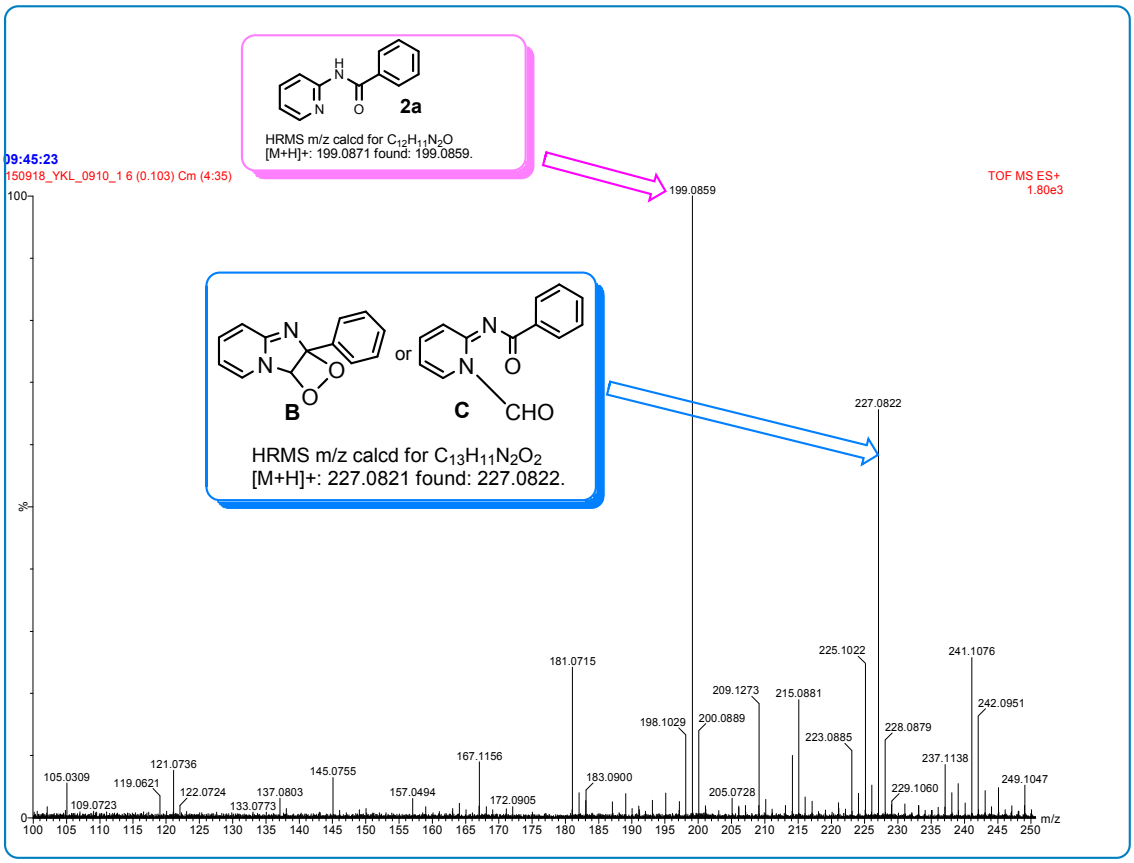
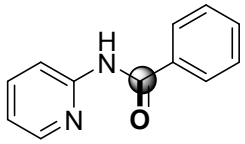



**Figure 2**. HRMS spectrum of the reaction mixture after reaction of **1a** with TBHP for 6h

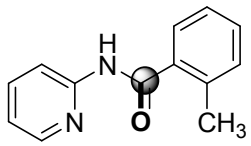
**General experimental procedures for synthesis of *N*-(pyridin-2-yl)benzamides:**

A 25 mL Schlenk tube equipped with a magnetic stirring bar was charged with substituted 2-phenylimidazo[1,2-*a*]pyridines (**1**) (0.4 mmol), TBHP (4 equiv, *tert*-butyl hydroperoxide 70 wt % in water), and DCE (2.0 ml). The tube was sealed and then the mixture was allowed to stir under under air atmosphere at 80 °C for 18 h. After completion of the reaction, the resulting solution was cooled down to room temperature, and the solvent was removed with the aid of a rotary evaporator. The residue was purified by column chromatography on silica gel using petroleum ether/ethyl acetate as eluent to provide the desired product (**2**).



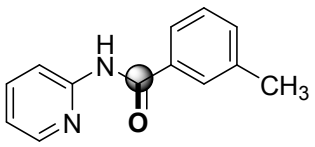
**2a**

***N*-(Pyridin-2-yl)benzamide (2a):**[1] Eluent petroleum ether/ethyl acetate (10:1). white solid, 58 mg, 73% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.4). $^{1}$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.38 (br, 1H), 8.43 (d, 1H, $J$ = 8.0 Hz), 8.14 (d, 1H, $J$ = 4.0 Hz), 7.95 (d, 2H, $J$ = 8.0 Hz), 7.75 (t, 1H, $J$ = 8.0 Hz), 7.55 (d, 1H, $J$ = 8.0 Hz), 7.47 (t, 2H, $J$ = 8.0 Hz), 7.03 (t, 1H, $J$ = 8.0 Hz), 3.80 (s, 3H), 3.75 (s, br, 2H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 166.1, 151.8, 147.6, 138.6, 134.4, 132.2, 128.7, 127.4, 119.8, 114.5. HRMS m/z calcd for $C_{12}H_{11}N_2O$ $[M+H]^+$: 199.0871 found: 199.0859.



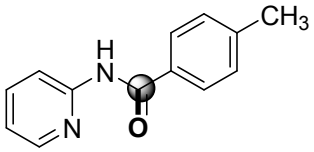
**2b**

**2-Methyl-*N*-(pyridin-2-yl)benzamide (2b):**[2] Eluent petroleum ether/ethyl acetate (10:1). white solid, 56 mg, 66% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^{1}$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.46 (br, 1H), 8.41 (d, 1H, $J$ = 8.0 Hz), 7.76-7.71 (m, 2H), 7.53 (d, 1H, $J$ = 8.0 Hz), 7.39 (t, 1H, $J$ = 8.0 Hz), 7.25 (t, 1H, $J$ = 8.0 Hz), 6.94 (t, 1H, $J$ = 8.0 Hz), 2.53 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 168.7, 151.8, 147.6, 138.5, 136.4, 136.2, 131.2, 130.5, 127.0, 125.9, 119.7, 114.3, 19.8. HRMS m/z calcd for $C_{13}H_{13}N_2O$ $[M+H]^+$: 213.1028 found: 213.1034.



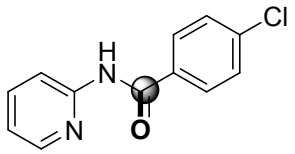
**2c**

**3-Methyl-*N*-(pyridin-2-yl)benzamide (2c):**[3] Eluent petroleum ether/ethyl acetate (10:1). white solid, 58 mg, 68% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.4). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 8.88 (br, 1H), 8.42 (d, 1H, $J$ = 8.0 Hz), 8.24 (d, 1H, $J$ = 4.0 Hz), 7.85 (d, 2H, $J$ = 8.0 Hz), 7.75 (t, 1H, $J$ = 8.0 Hz), 7.30 (d, 2H, $J$ = 8.0 Hz), 7.06 (t, 1H, $J$ = 8.0 Hz), 2.44 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.8, 151.8, 147.8, 142.8, 138.4, 131.5, 129.5, 127.3, 119.8, 114.2, 21.5. HRMS m/z calcd for $C_{13}H_{13}N_2O$ $[M+H]^+$: 213.1028 found: 213.1034.




**2d**

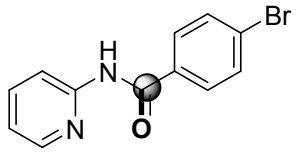
**4-Methyl-*N*-(pyridin-2-yl)benzamide (2d):**[4] Eluent petroleum ether/ethyl acetate (10:1). white solid, 55 mg, 65% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.6). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.15 (br, 1H), 8.42 (d, 1H, $J$ = 8.0 Hz), 8.16 (d, 1H, $J$ = 4.0 Hz), 7.84 (d, 2H, $J$ = 8.0 Hz), 7.75 (t, 1H, $J$ = 8.0 Hz), 7.27 (d, 2H, $J$ = 8.0 Hz), 7.02 (t, 1H, $J$ = 8.0 Hz), 2.42 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.9, 151.9, 147.8, 142.7, 138.4, 131.5, 129.4, 127.4, 119.7, 114.3, 21.5. HRMS m/z calcd for $C_{13}H_{13}N_2O$ $[M+H]^+$: 213.1028 found: 213.1034.




**2e**

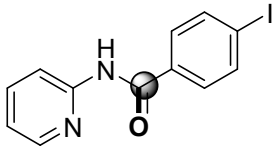
**4-Chloro-*N*-(pyridin-2-yl)benzamide (2e):**[5] Eluent petroleum ether/ethyl acetate (10:1). white solid, 54 mg, 58% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.3). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.17 (br, 1H), 8.39 (d, 1H, $J$ = 8.0 Hz), 7.89 (d,

2H, $J$ = 8.0 Hz), 7.77 (t, 1H, $J$ = 8.0 Hz), 7.46 (d, 2H, $J$ = 8.0 Hz), 7.06 (t, 1H, $J$ = 8.0 Hz). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 164.9, 151.6, 147.8, 138.6, 138.5, 132.8, 129.1, 128.8, 120.1, 114.4. HRMS m/z calcd for $C_{12}H_{10}ClN_2O$ $[M+H]^+$: 233.0482 found: 233.0481.



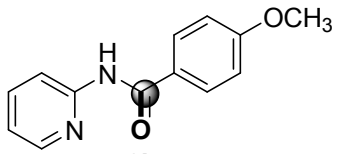

**2f**

**4-Bromo-*N*-(pyridin-2-yl)benzamide (2f):**[5] Eluent petroleum ether/ethyl acetate (10:1). white solid, 74 mg, 67% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.29 (br, 1H), 8.38 (d, 1H, $J$ = 8.0 Hz), 8.15 (d, 1H, $J$ = 4.0 Hz), 7.81 (d, 2H, $J$ = 8.0 Hz), 7.76 (t, 1H, $J$ = 8.0 Hz), 7.60 (d, 2H, $J$ = 8.0 Hz), 7.05 (t, 1H, $J$ = 8.0 Hz). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.0, 151.6, 147.8, 138.6, 133.2, 132.0, 129.0, 127.0, 120.1, 114.5. HRMS m/z calcd for $C_{12}H_{10}BrN_2O$ $[M+H]^+$: 276.9977, 278.9956 found: 276.9981, 278.9959.



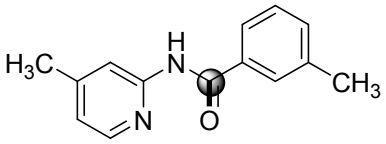

**2g**

**4-Iodo-*N*-(pyridin-2-yl)benzamide (2g):**[5] Eluent petroleum ether/ethyl acetate (10:1). white solid, 86 mg, 66% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.6). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.58 (br, 1H), 8.43 (d, 1H, $J$ = 8.0 Hz), 7.88-7.53 (m, 3H), 7.23 (d, 2H, $J$ = 8.0 Hz), 7.09 (dd, 1H, $J$ = 8.0 Hz). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.4, 151.6, 147.3, 138.9, 137.9, 133.7, 129.1, 120.0, 114.8, 99.5. HRMS m/z calcd for $C_{12}H_{10}IN_2O$ $[M+H]^+$: 324.9838 found: 324.9832.



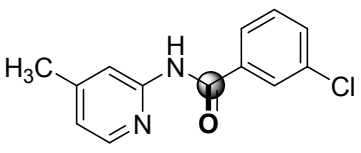
**2h**

**4-methoxy-*N*-(pyridin-2-yl)benzamide (2h):**[5] Eluent petroleum ether/ethyl acetate (10:1). white solid, 57 mg, 63% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.4). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 8.98 (br, 1H), 8.40 (d, 1H, $J$ = 8.0 Hz), 8.21 (d, 1H, $J$ = 8.0 Hz), 7.92 (d, 2H, $J$ = 8.0 Hz), 7.74 (t, 1H, $J$ = 8.0 Hz), 7.03 (t, 1H, $J$ = 8.0 Hz), 6.97 (d, 2H, $J$ = 8.0 Hz). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.4, 162.8, 151.9, 147.8, 138.4, 129.3, 126.5, 119.6, 114.3, 114.0, 55.5. HRMS m/z calcd for $C_{13}H_{13}N_2O_2$ $[M+H]^+$: 229.0977 found: 229.0973.



**2i**

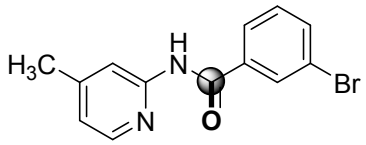
**3-Methyl-*N*-(4-methylpyridin-2-yl)benzamide (2i):** Eluent petroleum ether/ethyl acetate (10:1). white solid, 68 mg, 75% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.4). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.01 (br, 1H), 8.28 (s, 1H), 8.05 (d, 1H, $J$ = 4.0 Hz), 7.75-7.72 (m, 2H), 7.38 (d, 1H, $J$ = 4.0 Hz), 6.88 (d, 1H, $J$ = 4.0 Hz), 2.42 (d, 6H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 166.1, 151.8, 150.0, 147.4, 138.6, 134.4, 132.9, 128.7, 127.9, 124.4, 121.0, 114.8, 21.4, 21.3. HRMS m/z calcd for $C_{14}H_{15}N_2O$ $[M+H]^+$: 227.1184 found: 227.1187.



**2j**

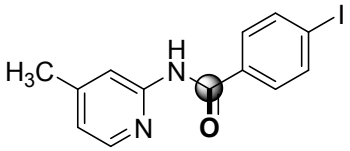
**3-Chloro-*N*-(4-methylpyridin-2-yl)benzamide (2j):** Eluent petroleum ether/ethyl

acetate (10:1). white solid, 58 mg, 59% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.44 (br, 1H), 8.23 (s, 1H), 7.96 (d, 1H, $J$ = 8.0 Hz), 7.92 (s, 1H), 7.51 (d, 1H, $J$ = 8.0 Hz), 7.39 (t, 1H, $J$ = 8.0 Hz), 6.86 (d, 1H, $J$ = 4.0 Hz), 2.40 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 164.8, 151.6, 150.2, 147.3, 136.3, 135.0, 132.1, 130.0, 127.8, 125.4, 121.3, 115.1, 21.4. HRMS m/z calcd for $C_{13}H_{12}ClN_2O$ $[M+H]^+$: 247.0638 found: 247.0634.




**2k**

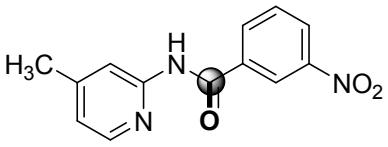
**3-Bromo-*N*-(4-methylpyridin-2-yl)benzamide (2k):** Eluent petroleum ether/ethyl acetate (10:1). white solid, 88 mg, 76% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.43 (br, 1H), 8.24 (s, 1H), 8.07 (s, 1H), 7.98 (s, 1H), 7.84 (d, 1H, $J$ = 8.0 Hz), 7.67 (d, 1H, $J$ = 8.0 Hz), 7.33 (t, 1H, $J$ = 8.0 Hz), 6.88 (d, 1H, $J$ = 4.0 Hz), 2.40 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 164.6, 151.6, 150.2, 147.3, 136.5, 135.0, 130.7, 130.2, 126.0, 122.9, 121.4, 115.1, 21.5. HRMS m/z calcd for $C_{13}H_{12}BrN_2O$ $[M+H]^+$: 291.0133, 293.0113 found: 291.0135, 293.0117.




**2l**

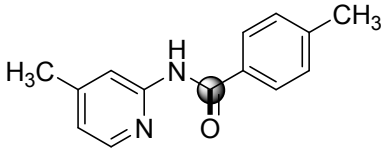
**4-Iodo-*N*-(4-methylpyridin-2-yl)benzamide (2l):** Eluent petroleum ether/ethyl acetate (10:1). white solid, 97 mg, 72% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.03 (br, 1H), 8.25-8.09 (m, 2H), 7.85 (d,

2H, $J$ = 8.0 Hz), 7.67 (d, 2H, $J$ = 8.0 Hz), 6.91 (s, 1H), 2.42 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.1, 151.4, 150.3, 147.2, 138.0, 133.8, 128.8, 121.3, 115.0, 99.4, 21.5. HRMS m/z calcd for $C_{13}H_{12}IN_2O$ $[M+H]^+$: 338.9994 found: 338.9992.



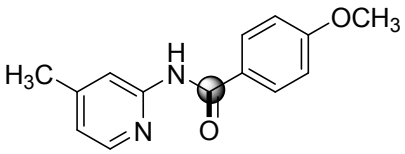

**2m**

***N*-(4-methylpyridin-2-yl)-3-nitrobenzamide (2m):** Eluent petroleum ether/ethyl acetate (10:1). white solid, 69 mg, 67% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.80 (br, 1H), 8.77 (s, 1H), 8.38 (d, 1H, $J$ = 8.0 Hz), 8.28 (d, 1H, $J$ = 8.0 Hz), 8.21 (s, 1H), 7.95 (s, 1H, $J$ = 4.0 Hz), 7.66 (t, 1H, $J$ = 8.0 Hz), 6.88 (d, 1H, $J$ = 4.0 Hz), 2.40 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 163.8, 151.4, 150.4, 148.3, 147.2, 136.2, 133.3, 129.9, 126.5, 122.6, 121.6, 115.4, 21.4. HRMS m/z calcd for $C_{13}H_{12}N_3O$ $[M+H]^+$: 258.0879 found: 258.0876.



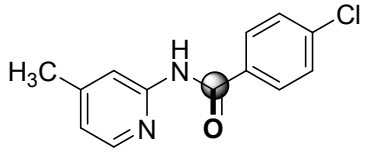

**2n**

**4-Methyl-*N*-(4-methylpyridin-2-yl)benzamide (2n):** Eluent petroleum ether/ethyl acetate (10:1). white solid, 68 mg, 75% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.6). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.08 (br, 1H), 8.28 (s, 1H), 8.08 (d, 1H, $J$ = 4.0 Hz), 7.86 (d, 2H, $J$ = 8.0 Hz), 7.30 (d, 2H, $J$ = 8.0 Hz), 6.89 (d, 1H, $J$ = 4.0 Hz), 2.44 (s, 3H), 2.41 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.8, 151.8, 150.1, 147.2, 142.7, 131.5, 129.4, 127.4, 120.9, 114.9, 21.5, 21.4. HRMS m/z calcd for $C_{14}H_{15}N_2O$ $[M+H]^+$: 227.1184 found: 227.1187.



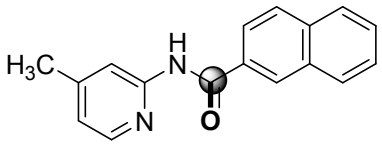
**2o**

**4-Methoxy-*N*-(4-methylpyridin-2-yl)benzamide (2o):**[6] Eluent petroleum ether/ethyl acetate (10:1). white solid, 69 mg, 71% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.4). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.01 (br, 1H), 8.25 (s, 1H), 8.05 (d, 1H, $J$ = 8.0 Hz), 7.91 (d, 2H, $J$ = 8.0 Hz), 6.96 (d, 2H, $J$ = 8.0 Hz), 6.86 (d, 1H, $J$ = 8.0 Hz), 3.87 (s, 3H), 2.39 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.4, 162.8, 151.9, 149.9, 147.3, 129.2, 126.6, 120.9, 114.8, 114.0, 55.4, 21.4. HRMS m/z calcd for $C_{14}H_{15}N_2O_2$ $[M+H]^+$: 243.1134 found: 243.1131.



**2p**

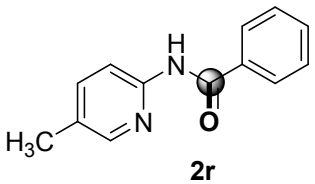
**4-Methoxy-*N*-(4-methylpyridin-2-yl)benzamide (2p):** Eluent petroleum ether/ethyl acetate (10:1). white solid, 60 mg, 61% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.22 (br, 1H), 8.24 (s, 1H), 8.02 (d, 1H, $J$ = 8.0 Hz), 7.89 (d, 2H, $J$ = 8.0 Hz), 7.46 (d, 2H, $J$ = 8.0 Hz), 6.89 (d, 2H, $J$ = 4.0 Hz), 2.42 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 164.9, 151.6, 150.2, 147.3, 138.5, 132.8, 129.0, 128.8, 121.3, 115.0, 21.5. HRMS m/z calcd for $C_{13}H_{12}ClN_2O$ $[M+H]^+$: 247.0638 found: 247.0634.



**2q**

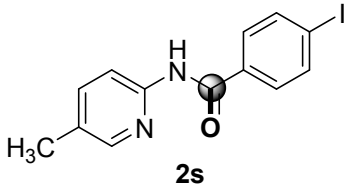
***N*-(4-Methylpyridin-2-yl)-2-naphthamide (2q):** Eluent petroleum ether/ethyl acetate

(10:1). white solid, 75 mg, 72% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.4). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.39 (br, 1H), 8.45 (s, 1H), 8.33 (s, 1H), 8.04-8.00 (m, 2H), 7.94-7.88 (m, 3H), 7.56 (dt, 2H, $J$ = 8.0 Hz), 6.84 (d, 1H, $J$ = 4.0 Hz), 2.41 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 166.0, 151.9, 150.1, 147.4, 135.0, 132.6, 131.7, 129.1, 128.7, 128.0, 127.8, 126.9, 123.7, 121.1, 114.9, 21.4. HRMS m/z calcd for $C_{17}H_{15}N_2O$ $[M+H]^+$: 263.1184 found: 263.1190.




**2r**

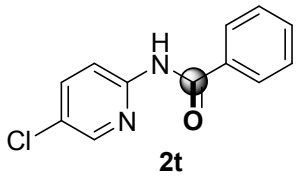
***N*-(5-Methylpyridin-2-yl)benzamide (2r):**[6] Eluent petroleum ether/ethyl acetate (10:1). white solid, 58 mg, 68% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.03 (br, 1H), 8.35 (d, 1H, $J$ = 8.0 Hz), 8.13 (d, 1H, $J$ = 8.0 Hz), 7.98 (d, 2H, $J$ = 8.0 Hz), 7.63-7.57 (m, 2H), 7.54-7.49 (m, 2H), 2.35 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.7, 149.5, 147.3, 139.3, 134.4, 132.1, 129.9, 128.8, 128.3, 127.3, 114.0, 17.8. HRMS m/z calcd for $C_{13}H_{13}N_2O$ $[M+H]^+$: 213.1028 found: 213.1034.




**2s**

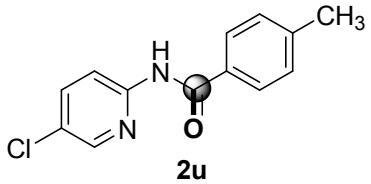
**4-Iodo-*N*-(5-methylpyridin-2-yl)benzamide (2s):** Eluent petroleum ether/ethyl acetate (10:1). white solid, 91 mg, 67% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 8.90 (br, 1H), 8.28 (d, 1H, $J$ = 8.0 Hz), 8.04 (s, 1H), 7.85 (d, 2H, $J$ = 8.0 Hz), 7.65 (d, 2H, $J$ = 8.0 Hz), 7.59 (d, 1H, $J$ = 8.0

Hz), 2.32 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.0, 149.3, 147.7, 139.1, 138.0, 133.9, 129.5, 128.8, 113.9, 99.2, 17.8. HRMS m/z calcd for $C_{13}H_{12}IN_2O$ $[M+H]^+$: 338.9994 found: 338.9992.



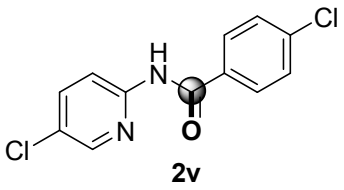

**2t**

***N*-(5-Chloropyridin-2-yl)benzamide (2t):**[7] Eluent petroleum ether/ethyl acetate (10:1). white solid, 54 mg, 58% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 8.80 (br, 1H), 8.41 (d, 1H, $J$ = 8.0 Hz), 8.21 (s, 1H), 7.93 (d, 2H, $J$ = 8.0 Hz), 7.74 (d, 1H, $J$ = 8.0 Hz), 7.60 (t, 1H, $J$ = 8.0 Hz), 7.52 (t, 2H, $J$ = 8.0 Hz), 2.35 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.7, 149.9, 146.5, 138.1, 134.0, 132.4, 128.9, 128.6, 127.5, 127.2, 114.9. HRMS m/z calcd for $C_{12}H_{10}ClN_2O$ $[M+H]^+$: 233.0482 found: 233.0481.



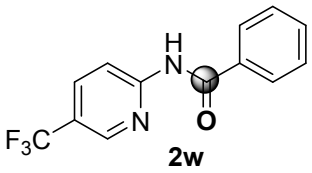

**2u**

***N*-(5-Chloropyridin-2-yl)-4-methylbenzamide (2u):**[8] Eluent petroleum ether/ethyl acetate (10:1). white solid, 61 mg, 62% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.6). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 8.80 (br, 1H), 8.41 (d, 1H, $J$ = 8.0 Hz), 8.18 (s, 1H), 7.82 (d, 2H, $J$ = 8.0 Hz), 7.72 (d, 1H, $J$ = 8.0 Hz), 7.30 (d, 2H, $J$ = 8.0 Hz), 2.41 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 165.6, 150.1, 146.5, 143.1, 138.0, 131.1, 129.5, 127.4, 127.3, 114.9, 21.5. HRMS m/z calcd for $C_{13}H_{12}ClN_2O$ $[M+H]^+$: 247.0638 found: 247.0634.



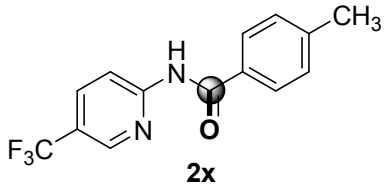

**2v**

**4-Chloro-*N*-(5-chloropyridin-2-yl)benzamide (2v):**[8] Eluent petroleum ether/ethyl acetate (10:1). white solid, 61 mg, 57% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.4). $^{1}$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 8.72 (br, 1H), 8.37 (d, 1H, $J$ = 8.0 Hz), 8.22 (s, 1H), 7.87 (d, 2H, $J$ = 8.0 Hz), 7.74 (d, 1H, $J$ = 8.0 Hz), 7.49 (d, 2H, $J$ = 8.0 Hz), 2.41 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 164.5, 149.7, 146.6, 138.9, 138.2, 132.3, 129.2, 128.8, 128.7, 114.9. HRMS m/z calcd for $C_{12}H_9Cl_2N_2O$ $[M+H]^+$: 267.0092 found: 267.0094.




**2w**

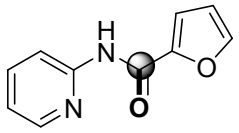
***N*-(5-(Trifluoromethyl)pyridin-2-yl)benzamide (2w):** Eluent petroleum ether/ethyl acetate (10:1). white solid, 67 mg, 63% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^{1}$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.18 (br, 1H), 8.56 (d, 1H, $J$ = 8.0 Hz), 8.41 (s, 1H), 7.99-7.93 (m, 3H), 7.62 (t, 1H, $J$ = 8.0 Hz), 7.52 (t, 2H, $J$ = 8.0 Hz), 2.41 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 166.1, 154.3, 145.3 (q, $J$ = 0.4), 135.8 (q, $J$ = 0.3), 133.8, 132.7, 128.9, 127.4, 123.5 (q, $J$ = 270), 122.6 (q, $J$ = 24.8), 113.6. HRMS m/z calcd for $C_{13}H_{10}F_3N_2O$ $[M+H]^+$: 267.0745 found: 267.0748.




**2x**

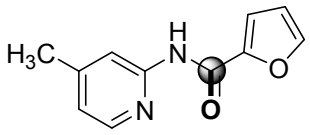
**4-Methyl-*N*-(5-(trifluoromethyl)pyridin-2-yl)benzamide (2x):** Eluent petroleum

ether/ethyl acetate (10:1). white solid, 74 mg, 66% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.4). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 9.18 (br, 1H), 8.55 (d, 1H, $J$ = 8.0 Hz), 8.37 (s, 1H), 7.96 (d, 1H, $J$ = 8.0 Hz), 7.83 (d, 2H, $J$ = 8.0 Hz), 7.31 (d, 2H, $J$ = 8.0 Hz), 2.45 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 166.1, 154.4, 145.3 (q, $J$ = 0.4), 143.5, 135.7 (q, $J$ = 0.3), 131.0, 129.6, 127.4, 123.2 (q, $J$ = 250.1), 122.4 (q, $J$ = 33.0), 113.5, 21.5. HRMS m/z calcd for $C_{14}H_{12}F_3N_2O$ $[M+H]^+$: 281.0902 found: 281.0905.




**2y**

***N*-(Pyridin-2-yl)furan-2-carboxamide (2y):**[6] Eluent petroleum ether/ethyl acetate (10:1). white solid, 39 mg, 52% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 8.81 (br, 1H), 8.33-8.35 (m, 2H), 7.76 (t, 1H, $J$ = 8.0 Hz), 7.55 (s, 1H), 7.29 (d, 1H, $J$ = 4.0 Hz), 7.09 (t, 1H, $J$ = 8.0 Hz), 6.59 (dd, 1H, $J$ = 4.0 Hz). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 156.2, 151.0, 148.0, 147.4, 144.7, 138.4, 119.9, 115.9, 114.1, 112.7. HRMS m/z calcd for $C_{10}H_9N_2O_2$ $[M+H]^+$: 189.0664 found: 189.0667.




**2z**

***N*-(4-Methylpyridin-2-yl)furan-2-carboxamide (2z):**[9] Eluent petroleum ether/ethyl acetate (10:1). white solid, 44 mg, 54% yield. (petroleum ether/ethyl acetate = 3:1, Rf = 0.5). $^1$H NMR ($CDCl_3$, 400 MHz, ppm) $\delta$ 8.77 (br, 1H), 8.19 (s, 1H), 8.18 (s, 1H), 7.54 (s, 1H), 7.28 (d, 1H, $J$ = 4.0 Hz), 6.90 (d, 1H, $J$ = 4.0 Hz), 6.92 (d, 1H, $J$ = 4.0 Hz), 6.58 (d, 1H, $J$ = 8.0 Hz), 2.41 (s, 3H). $^{13}$C NMR ($CDCl_3$, 100 MHz, ppm) $\delta$ 156.1,

151.0, 149.9, 147.6, 147.5, 144.7, 121.2, 115.8, 114.7, 112.6, 21.4. HRMS m/z calcd for $C_{11}H_{11}N_2O_2$ $[M+H]^+$: 203.0824 found: 203.0827.

**References**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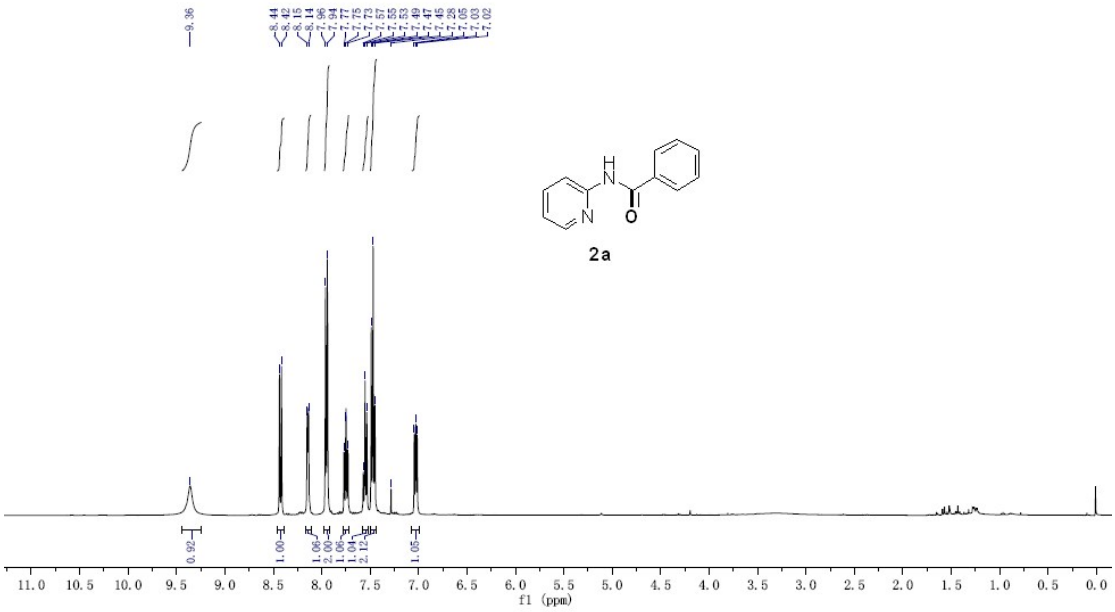
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8.14
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7.73
7.57
7.55
7.53
7.49
7.47
7.45
7.28
7.05
7.03
7.02
2a
0.92
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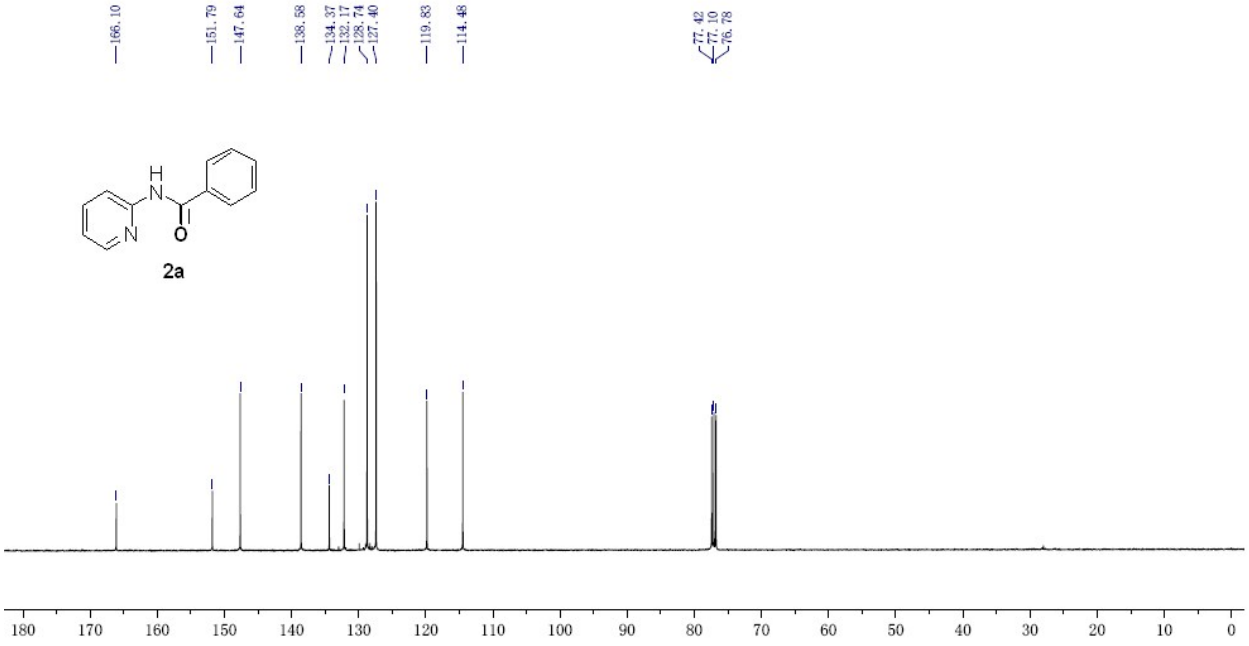
1.06
2.00
1.06
1.04
2.12
1.05
f1 (ppm)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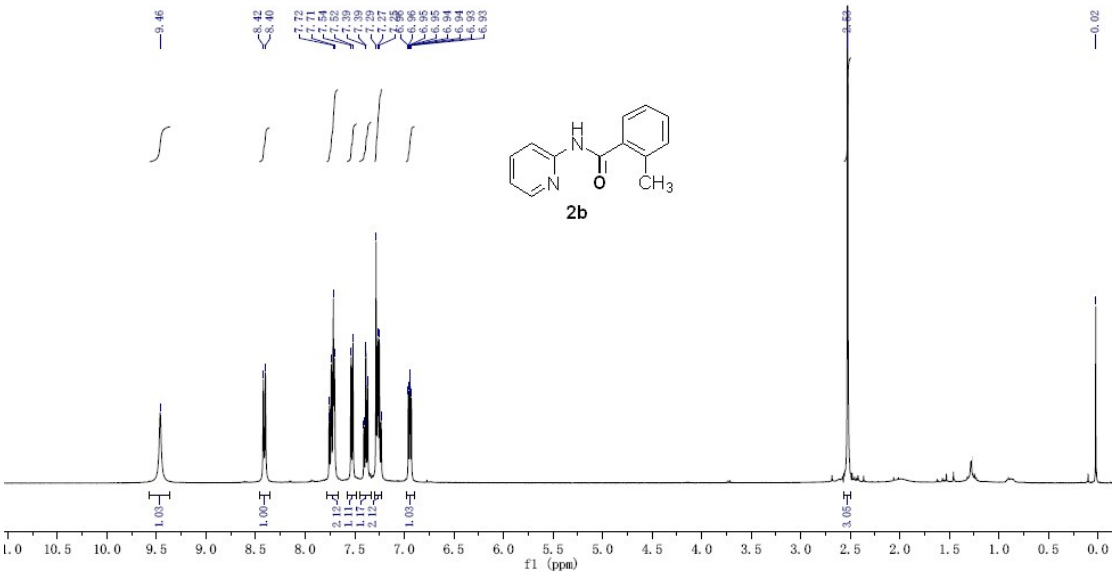
76.78
2a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6.95
6.94
6.93
6.93
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2.12
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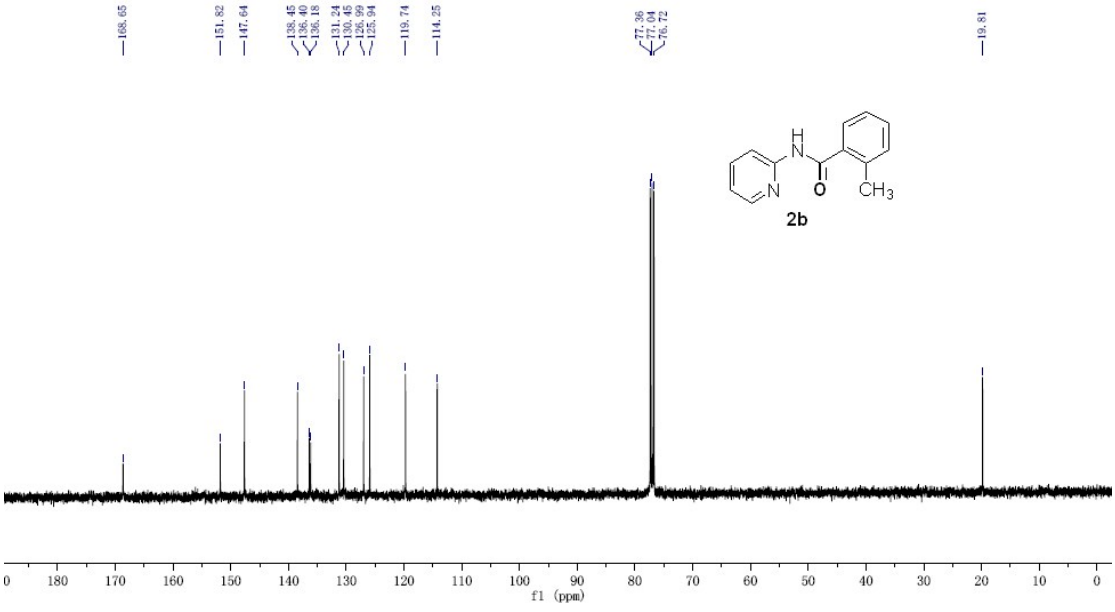
3.05
2b
f1 (ppm)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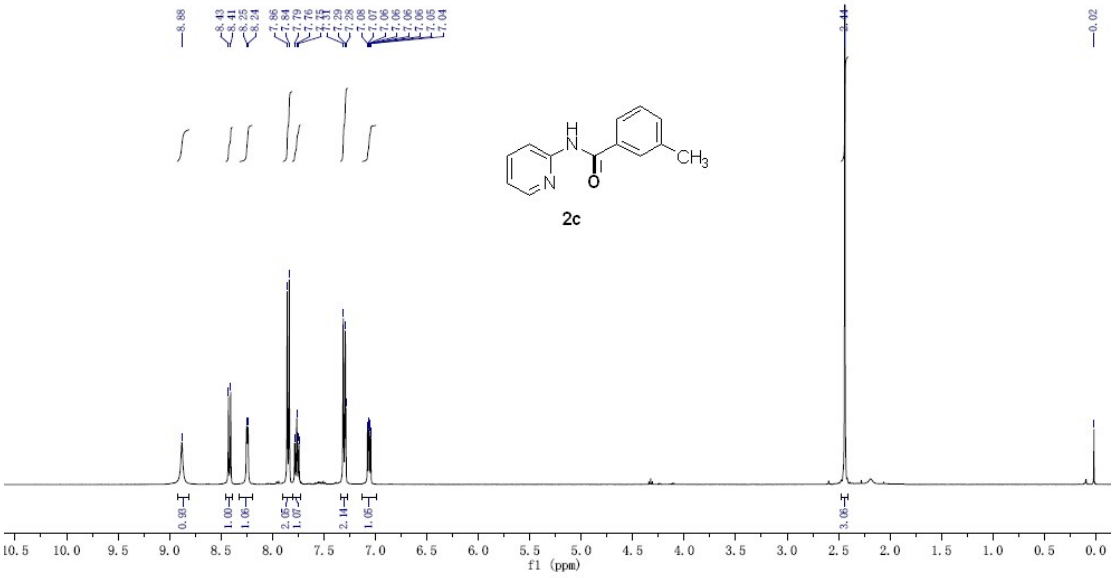
2b
f1 (ppm)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7.79
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7.07
7.06
7.06
7.05
7.05
7.04
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1.06
2.05
1.07
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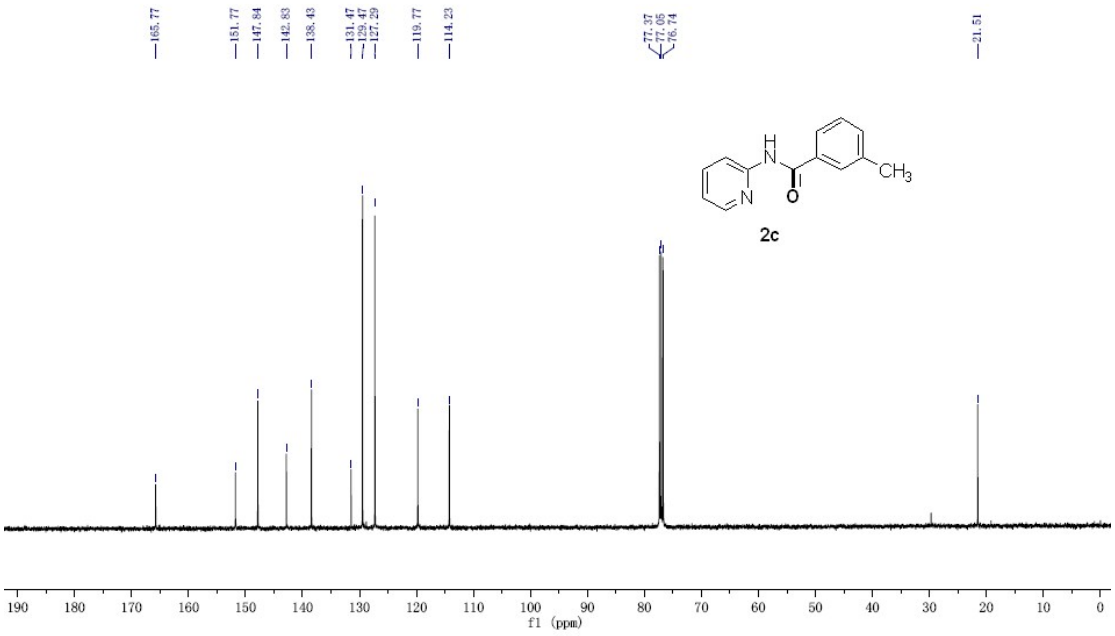
3.06
H
N
O
CH3
2c
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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O
CH3
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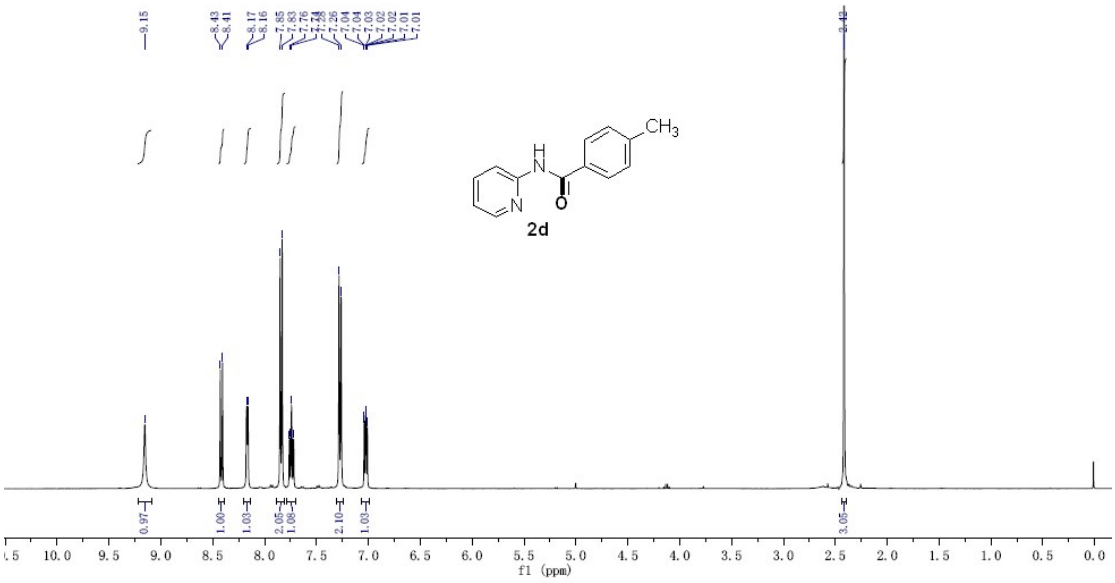
f1 (ppm)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7.01
2.43
0.97
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2.05
1.08
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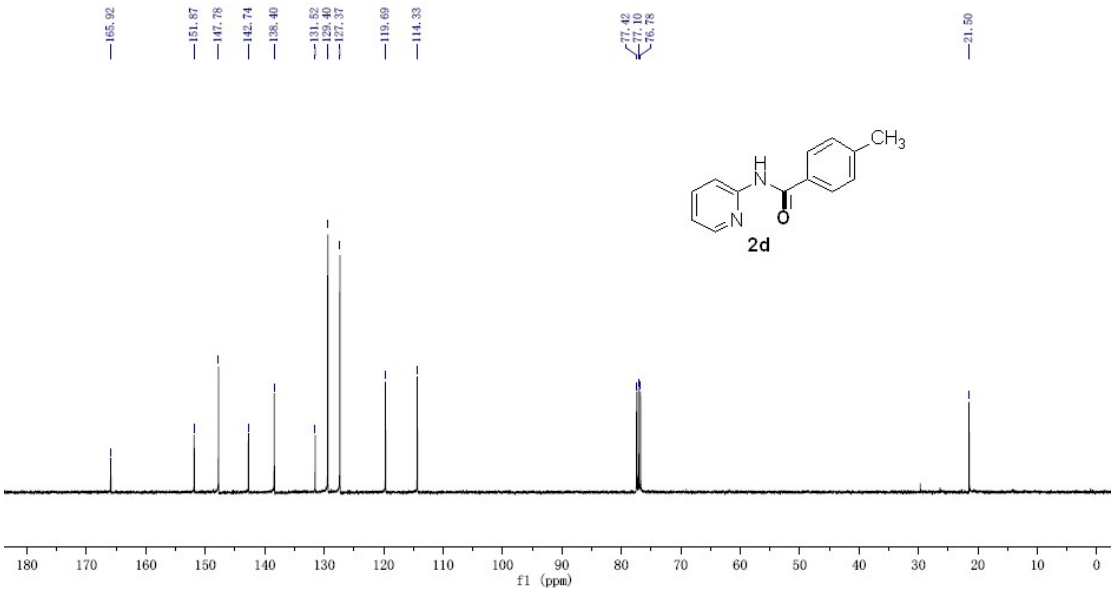
1.03
3.05
f1 (ppm)
CH3
N
H
O
2d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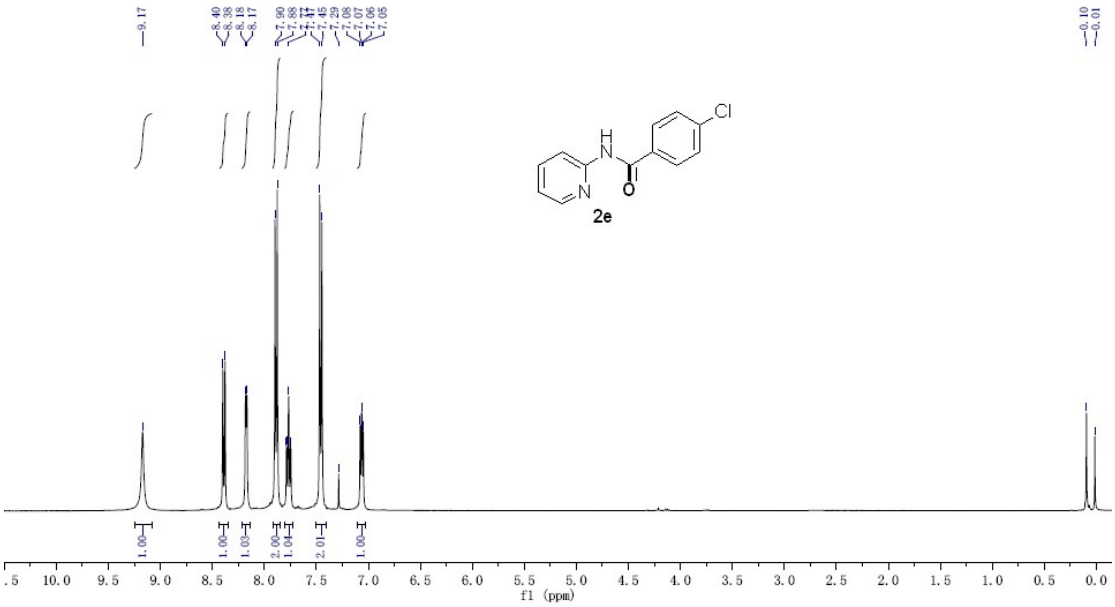
N
H
O
2d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0.01
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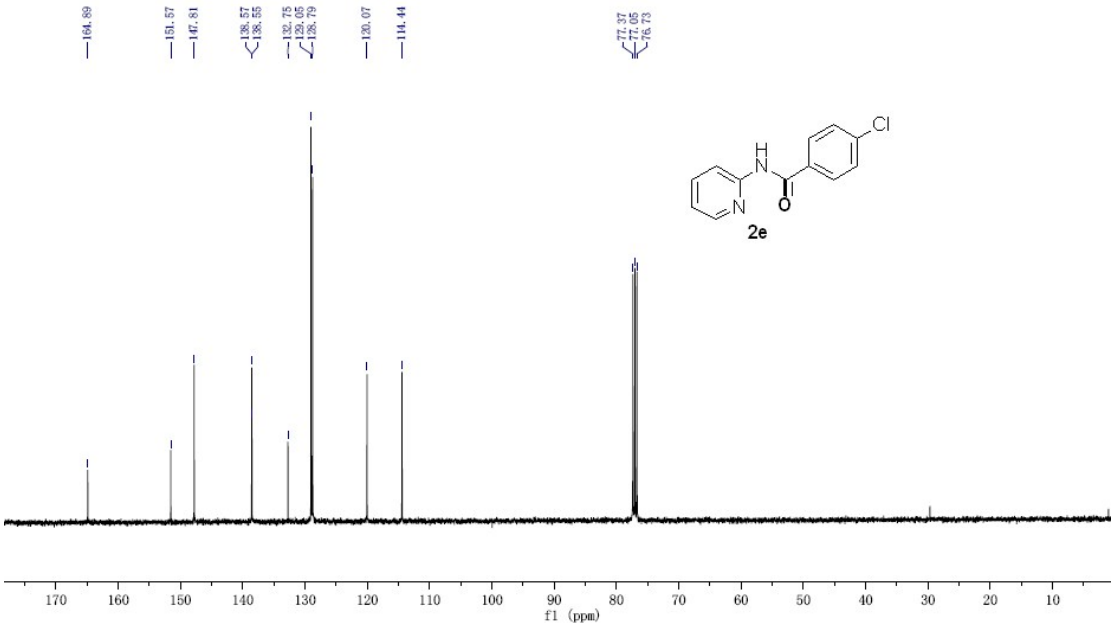
1.04
2.01
1.00
Cl
H
N
O
N
2e
f1 (ppm)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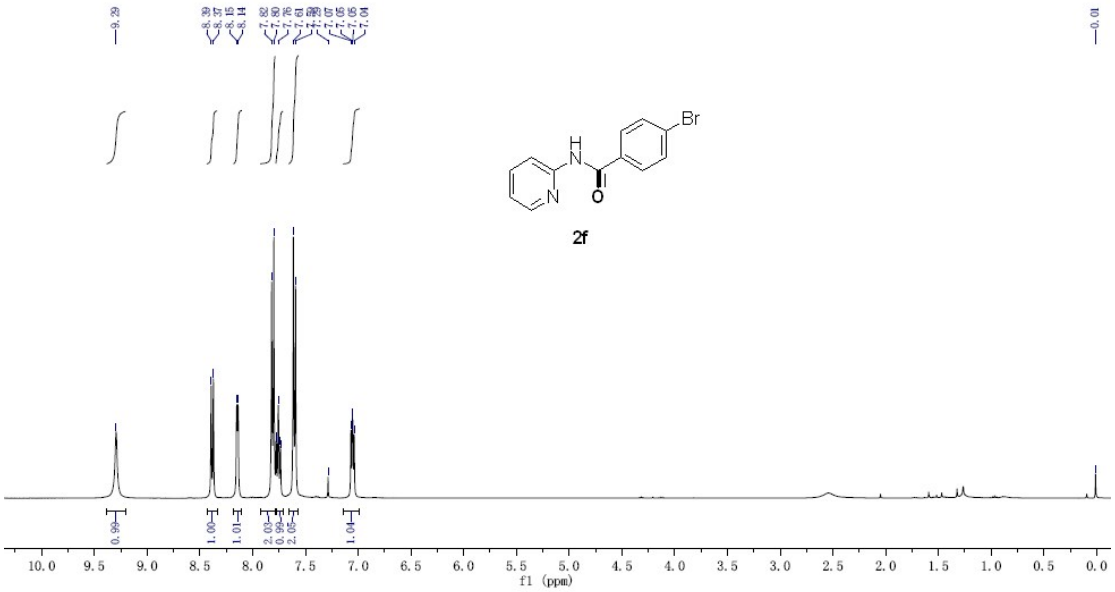
f1 (ppm)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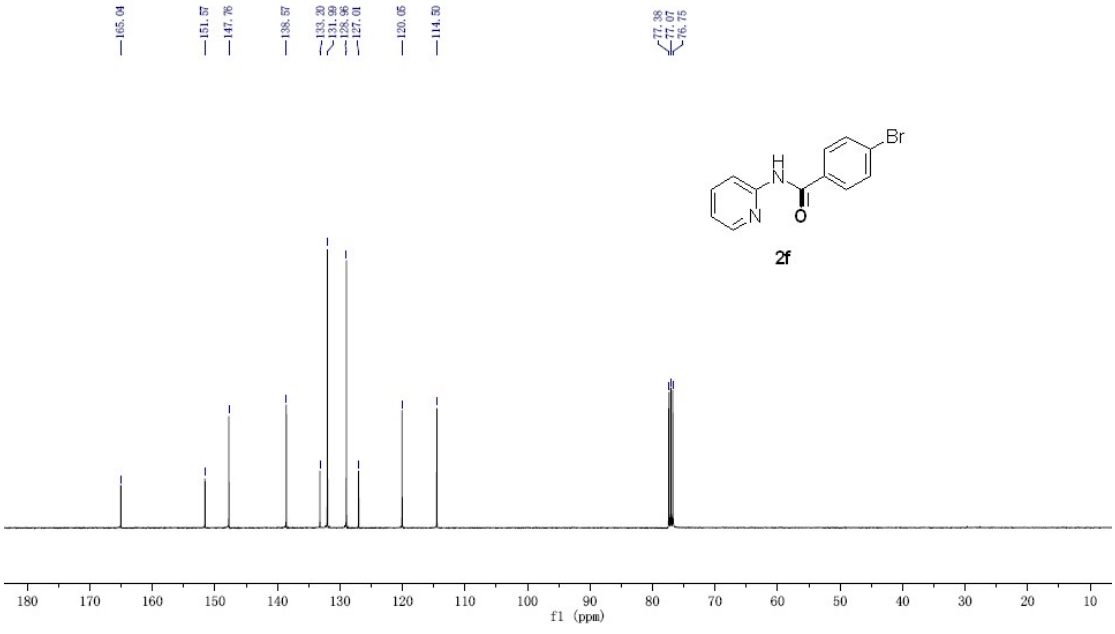
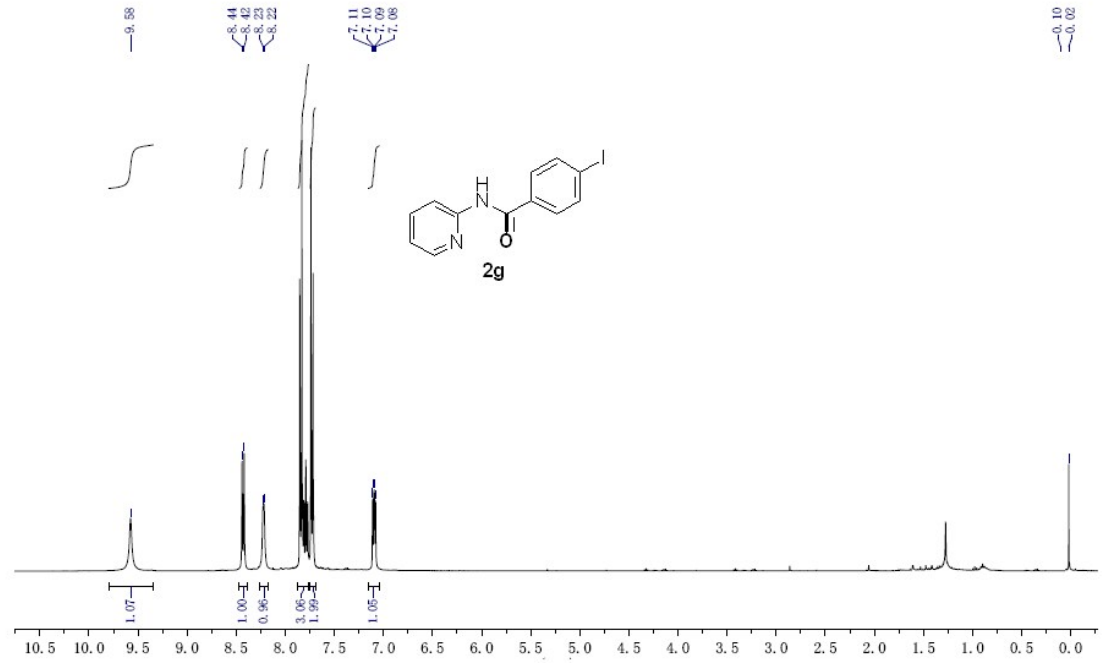
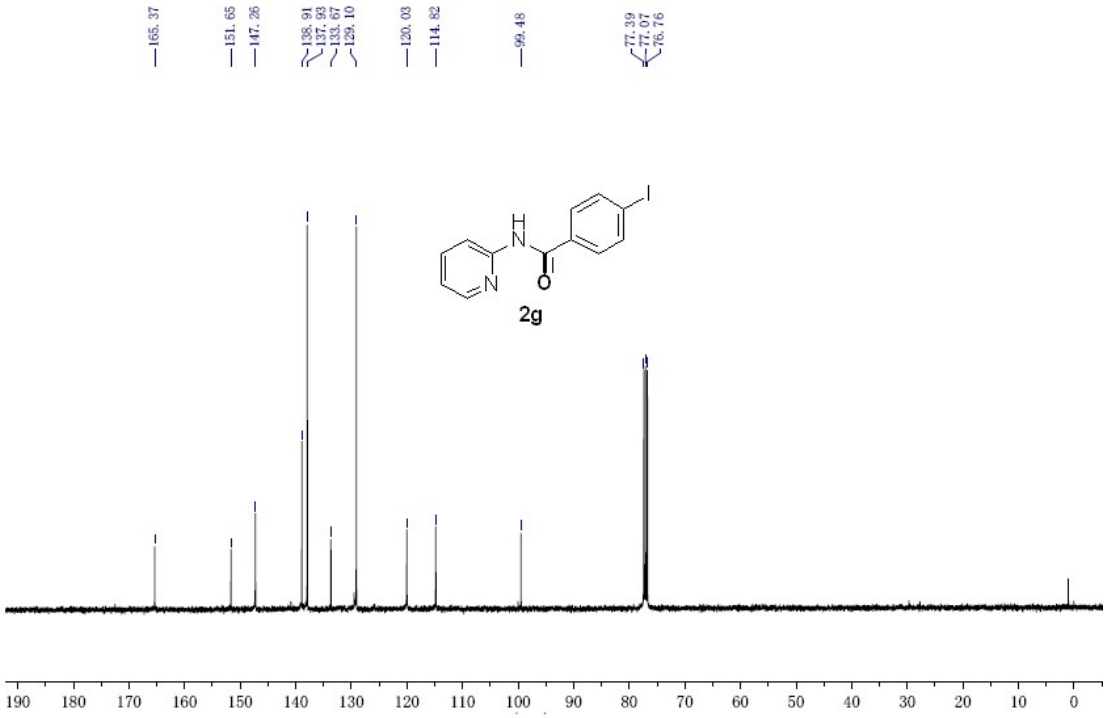
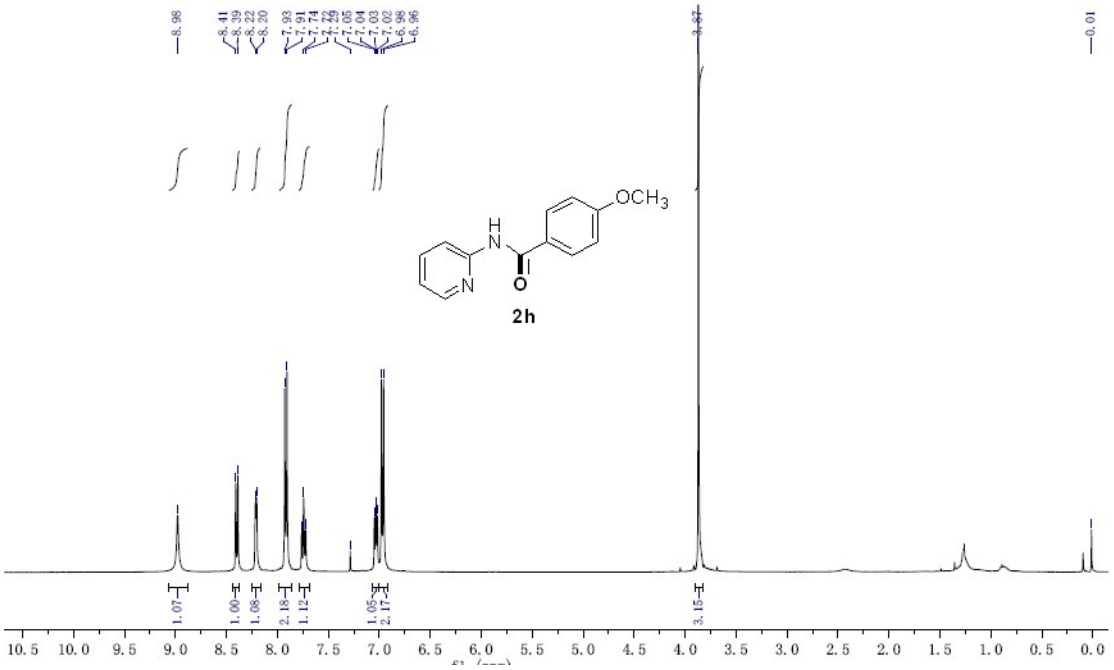
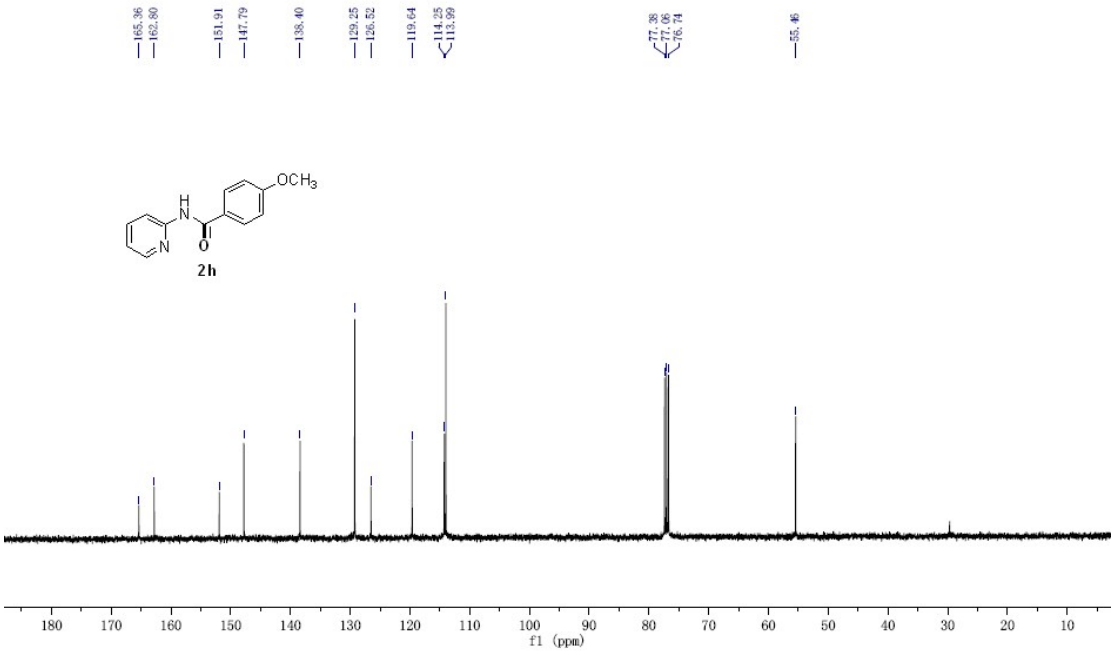
0.01
Br
H
N
O
2f
0.99
1.00
1.01
2.03
0.99
2.05
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

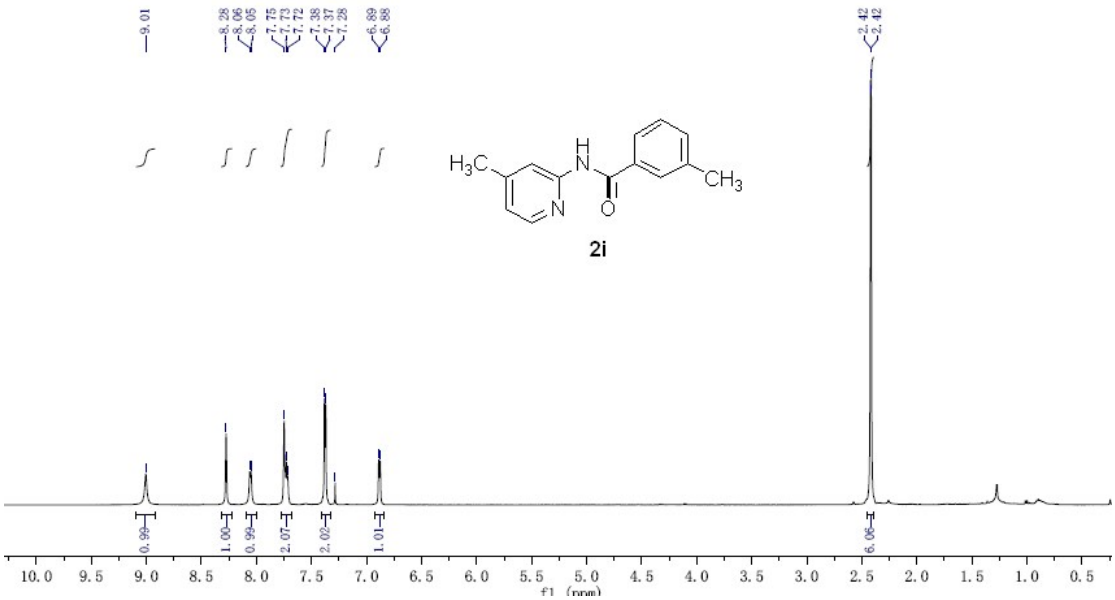

165.04
151.57
147.76
138.57
133.20
131.99
128.96
127.01
120.05
114.50
77.38
77.07
76.75
Br
H
N
O
2f
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

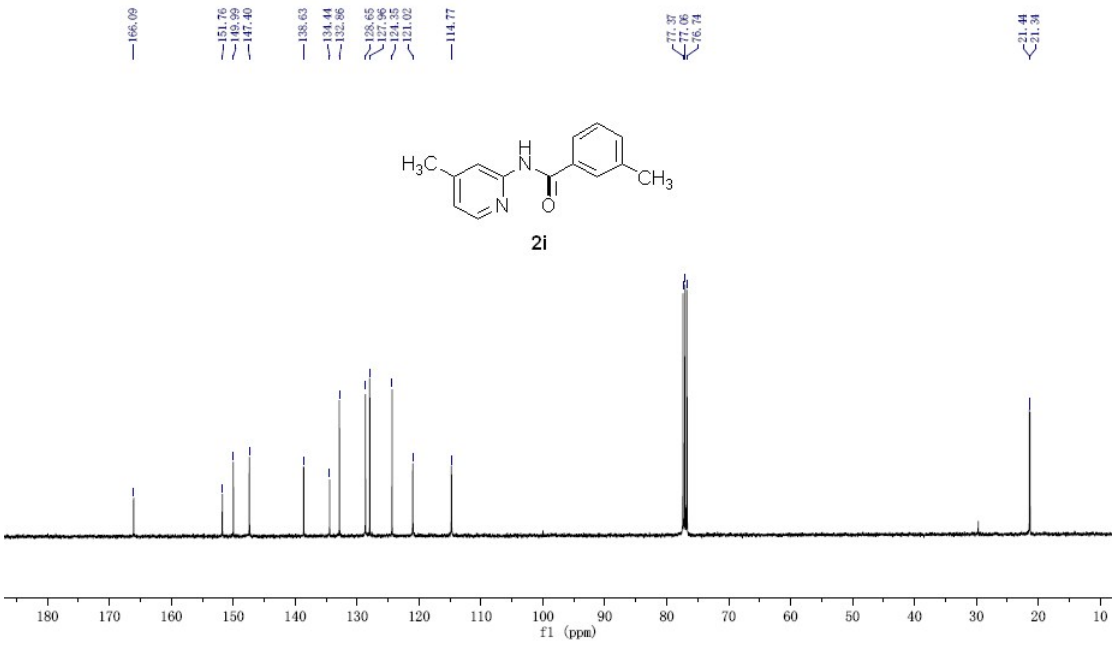

9.58
8.44
8.42
8.23
8.22
7.11
7.10
7.09
7.08
0.10
0.02
2g
1.07
1.00
0.96
3.06
1.99
1.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

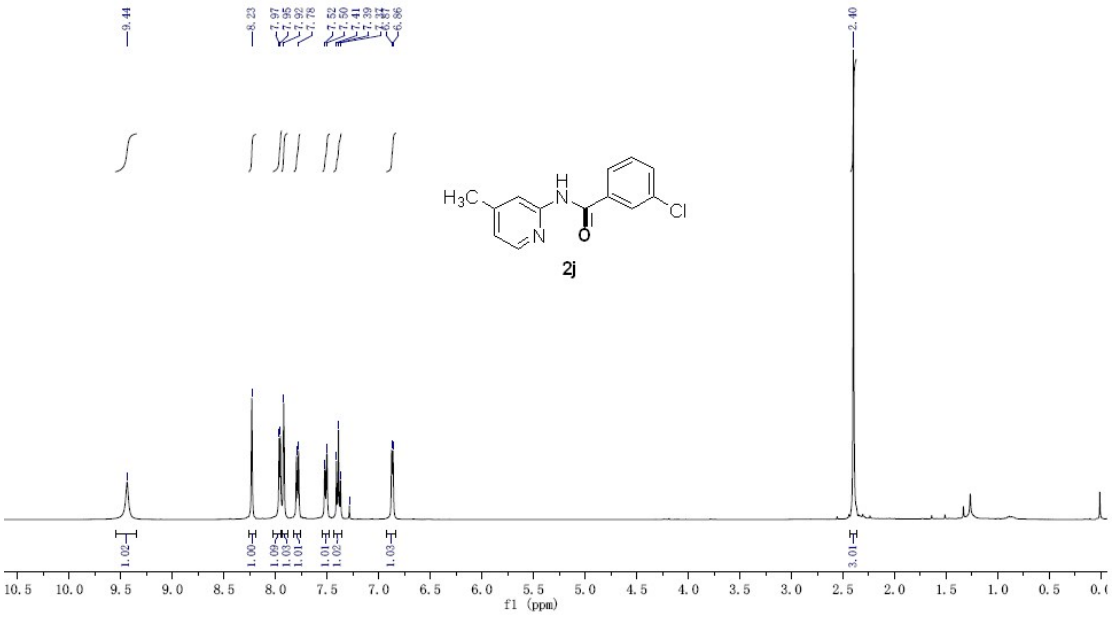

165.37
151.65
147.26
138.91
137.93
133.67
129.10
120.03
114.82
99.48
77.39
77.07
76.76
2g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

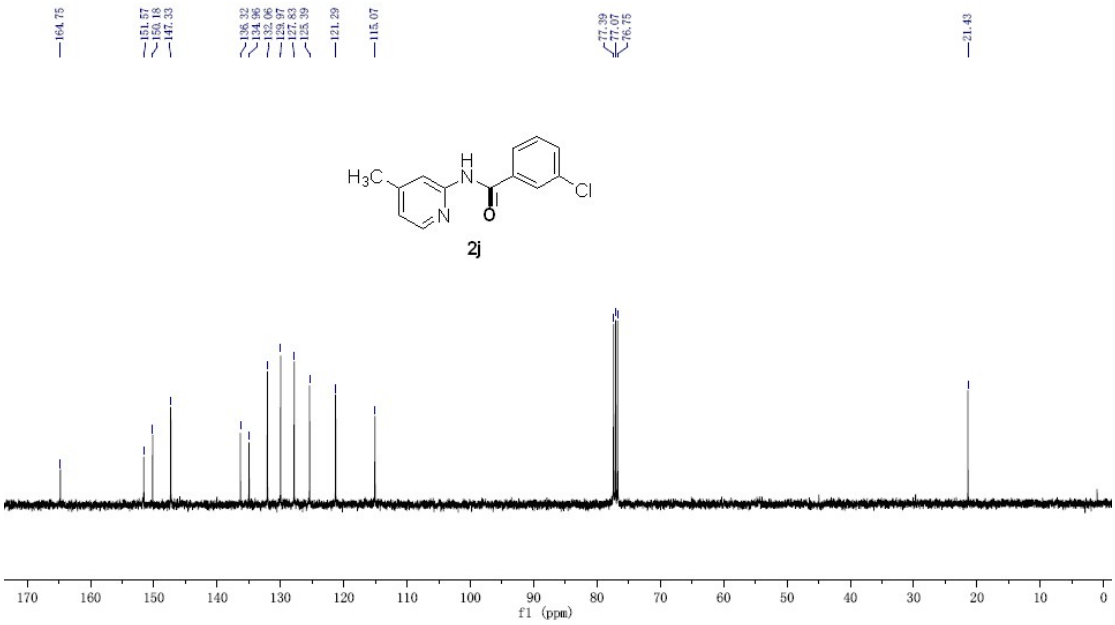

8.98
8.41
8.39
8.22
8.20
7.93
7.91
7.74
7.29
7.05
7.04
7.03
7.02
6.98
6.96
3.87
0.01
OCH3
H
N
O
N
2h
1.07
1.00
1.08
2.18
1.12
1.05
2.17
3.15
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

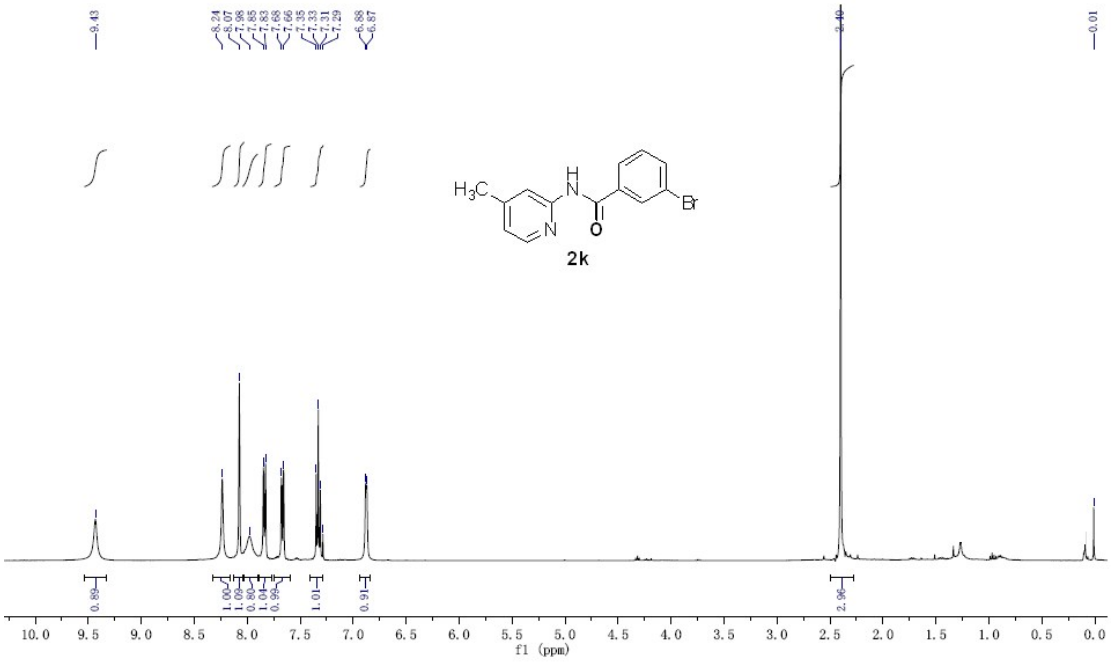

165.36
162.80
151.91
147.79
138.40
129.25
126.52
119.64
114.25
113.99
77.38
77.06
76.74
55.46
OCH3
H
N
O
N
2h
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

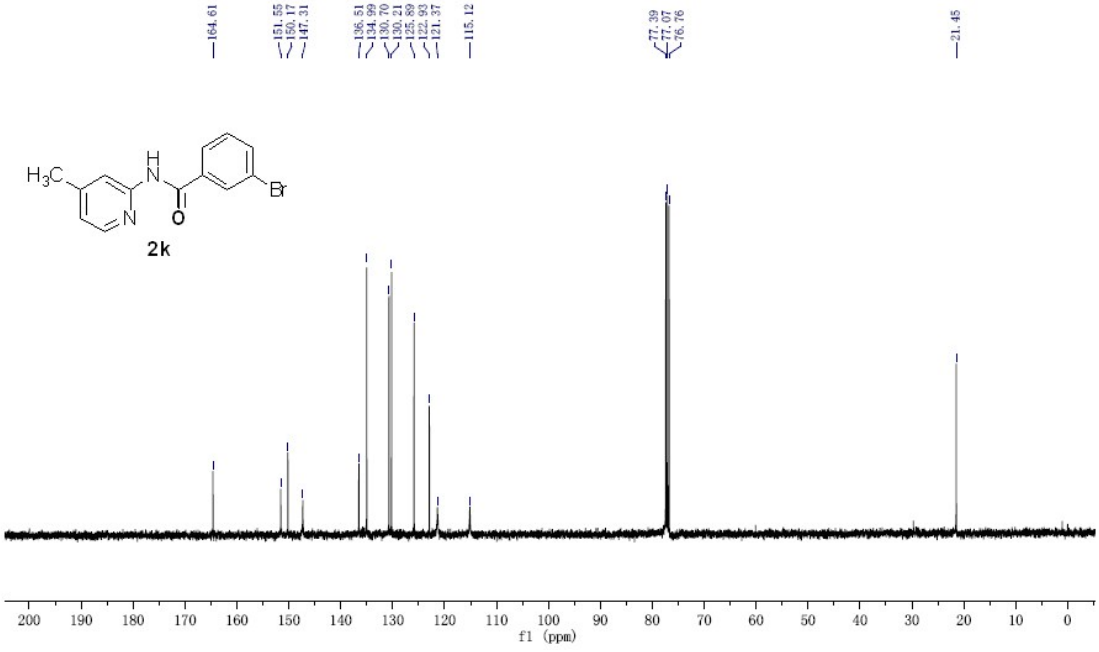

9.01
8.28
8.06
8.05
7.75
7.73
7.72
7.38
7.37
7.28
6.89
6.88
2.42
2.42
0.99
1.00
0.99
2.07
2.02
1.01
6.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

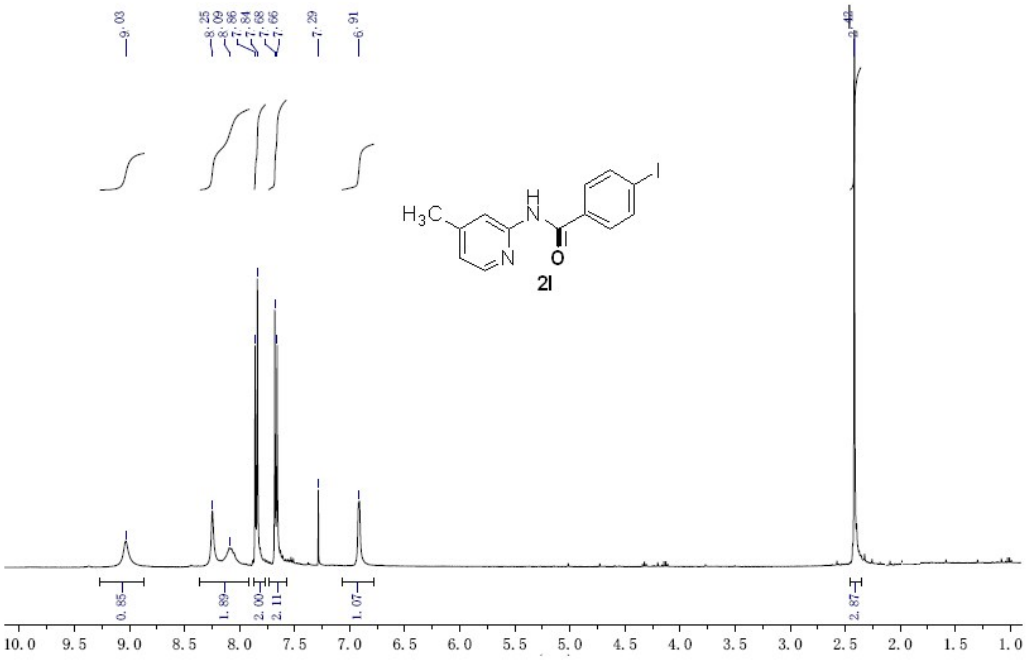

166.09
151.76
149.99
147.40
138.63
134.44
132.86
128.65
127.96
124.35
121.02
114.77
77.37
77.06
76.74
21.44
21.34
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

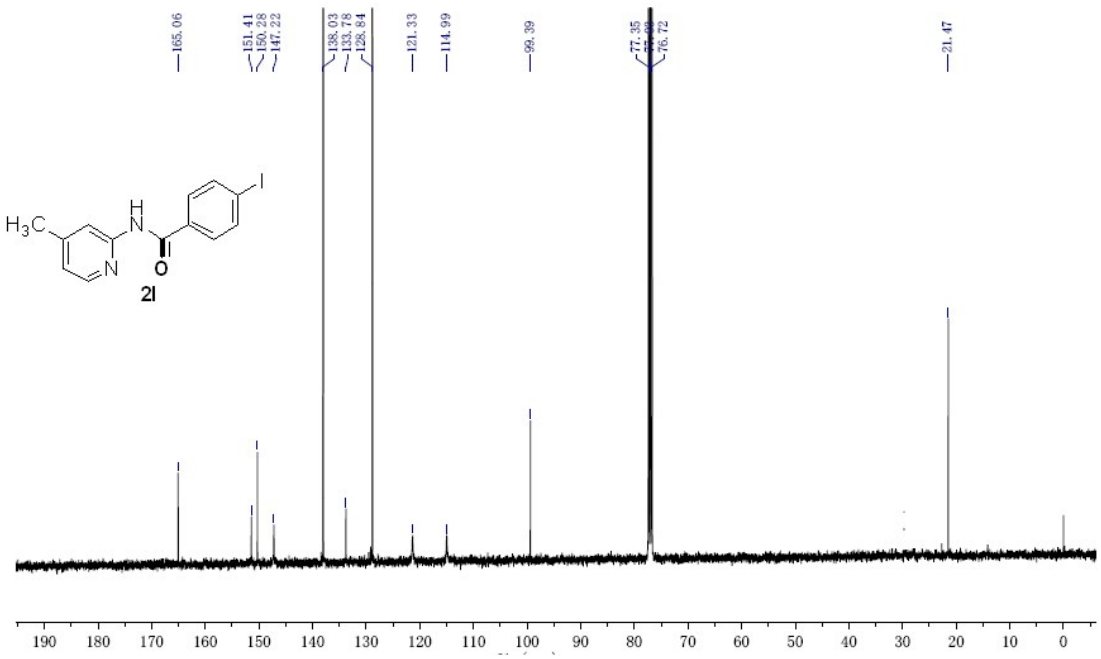

9.44
8.23
7.97
7.95
7.92
7.78
7.52
7.50
7.41
7.39
7.37
6.87
6.86
2.40
H3C
N
H
O
Cl
2j
1.02
1.00
1.09
1.03
1.01
1.01
1.02
1.03
3.01
f1 (ppm)

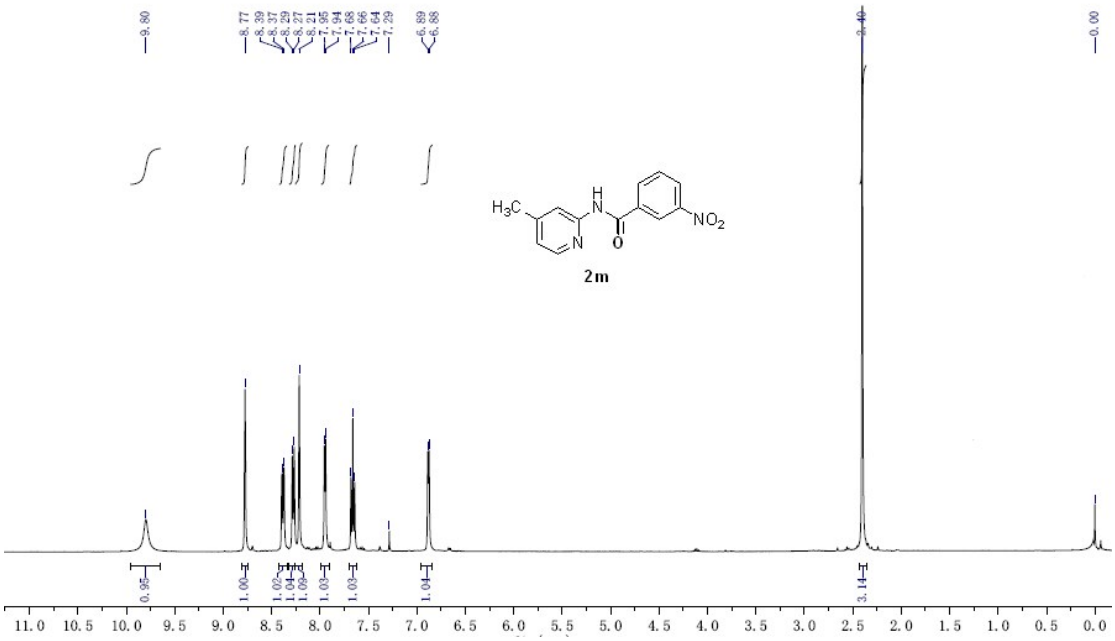

164.75
151.57
150.18
147.33
136.32
134.96
132.06
129.97
127.83
125.39
121.29
115.07
77.39
77.07
76.75
21.43
H3C
N
H
O
Cl
2j
f1 (ppm)


9.43
8.24
8.07
7.86
7.85
7.83
7.68
7.66
7.35
7.33
7.31
7.29
6.88
6.87
2.49
0.01
0.89
1.00
1.00
0.80
1.04
0.98
1.01
0.91
2.96
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)
H3C
N
H
N
O
Br
2k


164.61
151.55
150.17
147.31
136.51
134.99
130.70
130.21
125.89
122.93
121.37
115.12
77.39
77.07
76.76
21.45
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
H3C
N
H
N
O
Br
2k


9.03
8.25
8.09
7.86
7.84
7.68
7.66
7.29
6.91
2.47
H3C
N
H
N
O
I
2l
0.85
1.89
2.00
2.11
1.07
2.87
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


165.06
151.41
150.28
147.22
138.03
133.78
128.84
121.33
114.99
99.39
77.35
77.00
76.72
21.47
H3C
N
H
N
O
I
2l
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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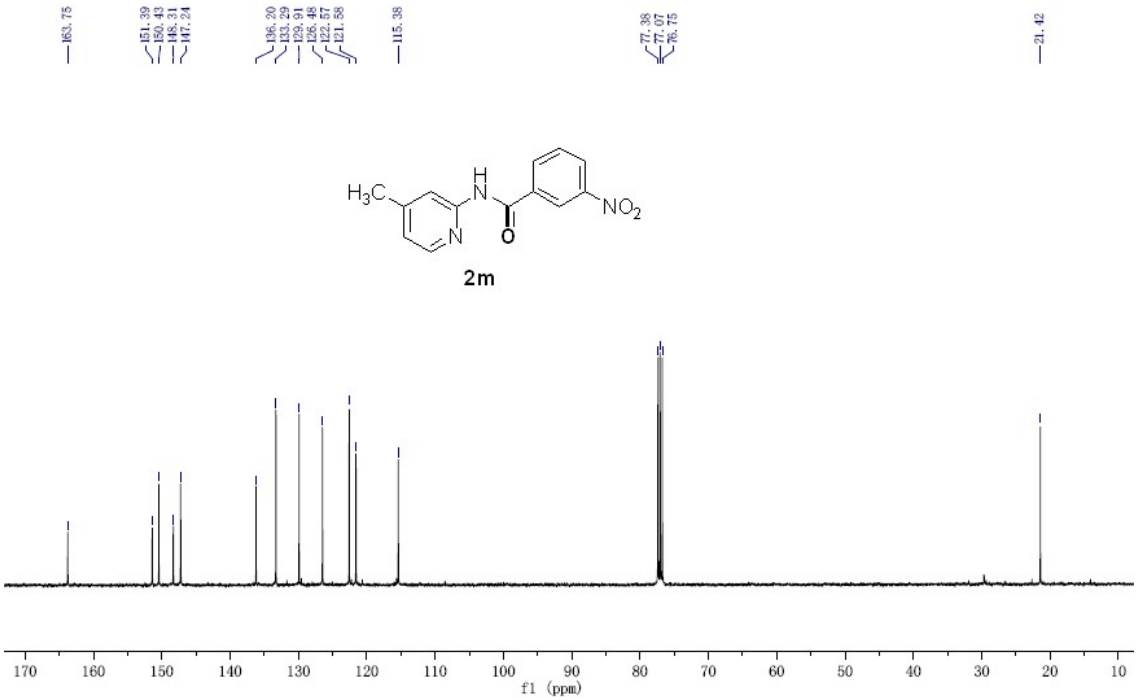
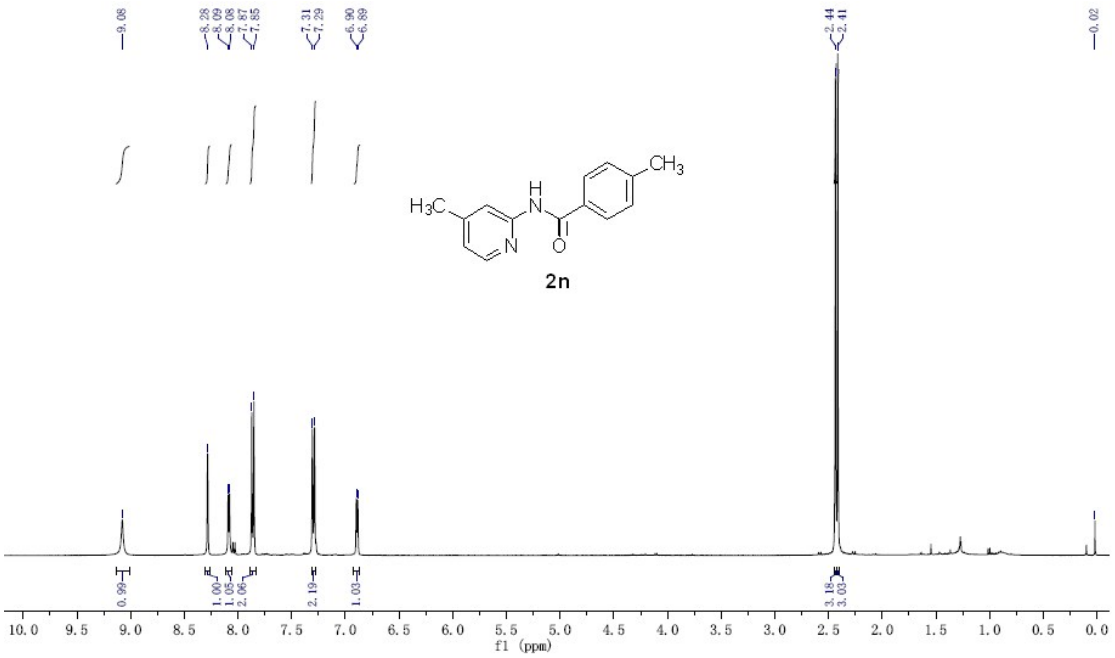
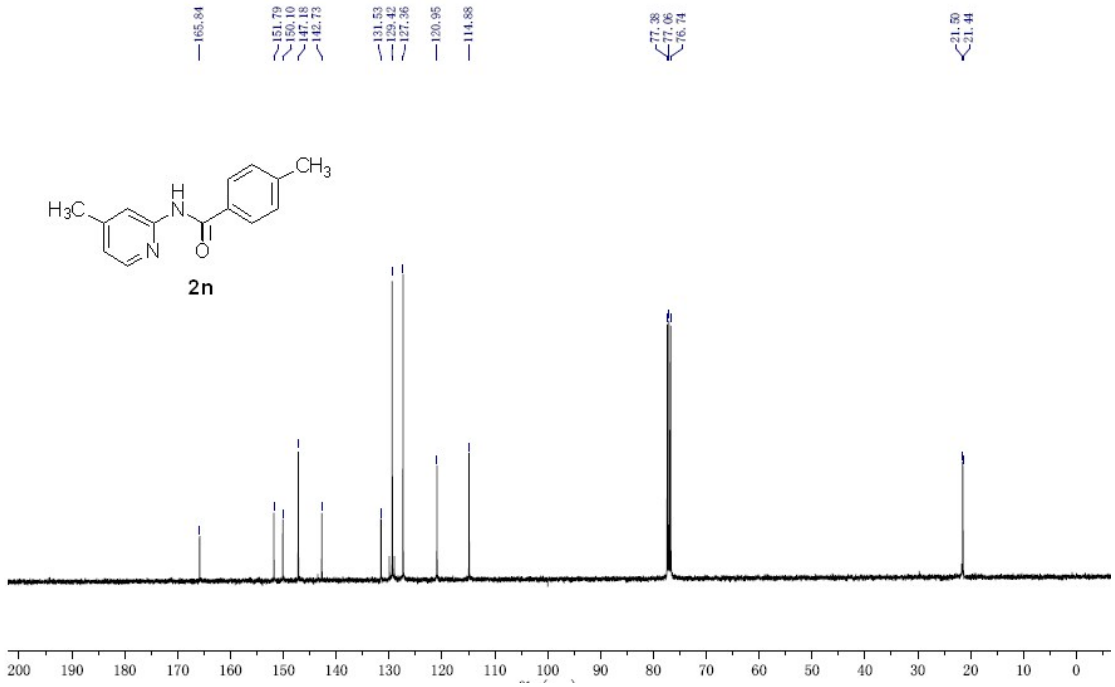
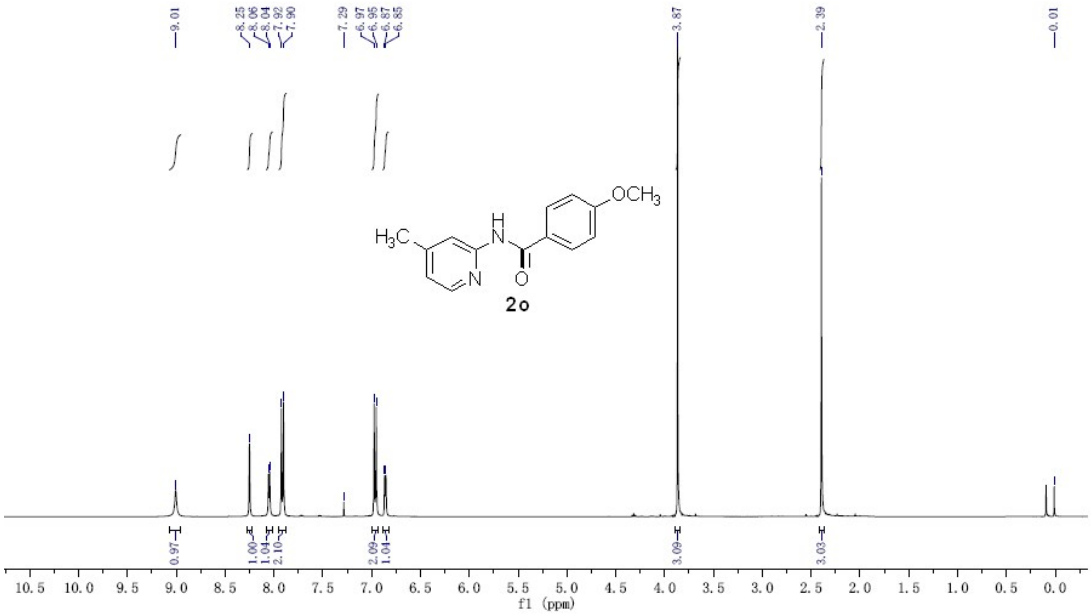
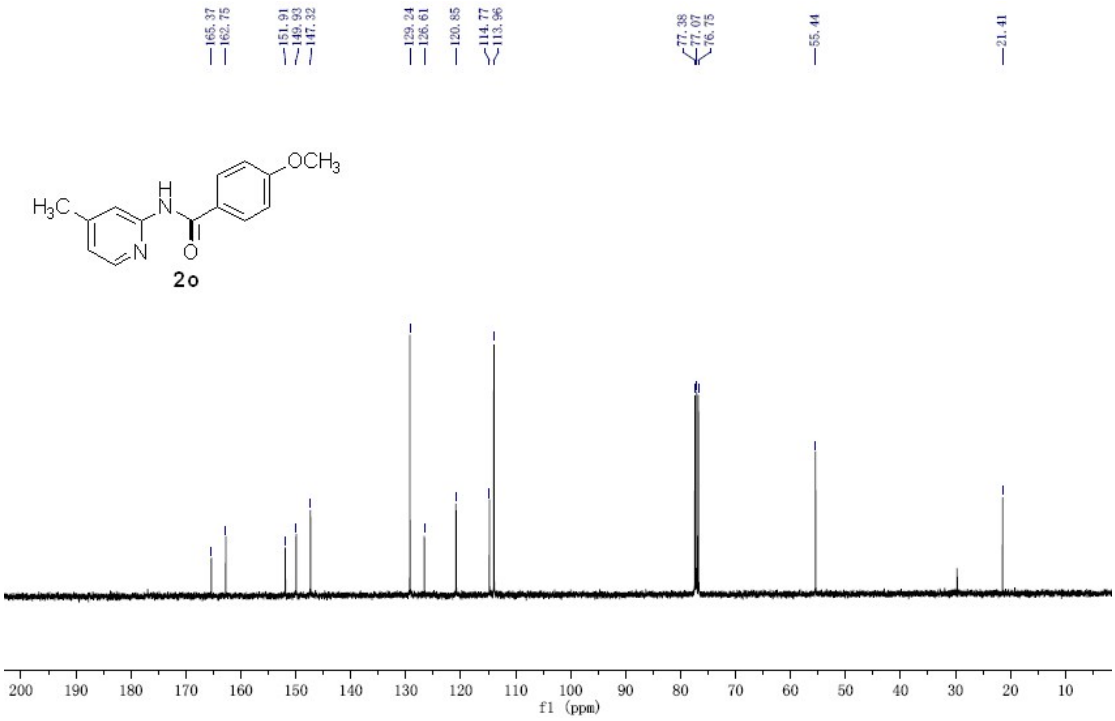
8.77
8.39
8.37
8.29
8.27
8.21
7.95
7.94
7.68
7.66
7.64
7.29
6.89
6.88
3.40
0.00
0.95
1.00
1.02
1.04
1.09
1.03
1.03
1.04
3.14
H3C
N
H
O
NO2
2m
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

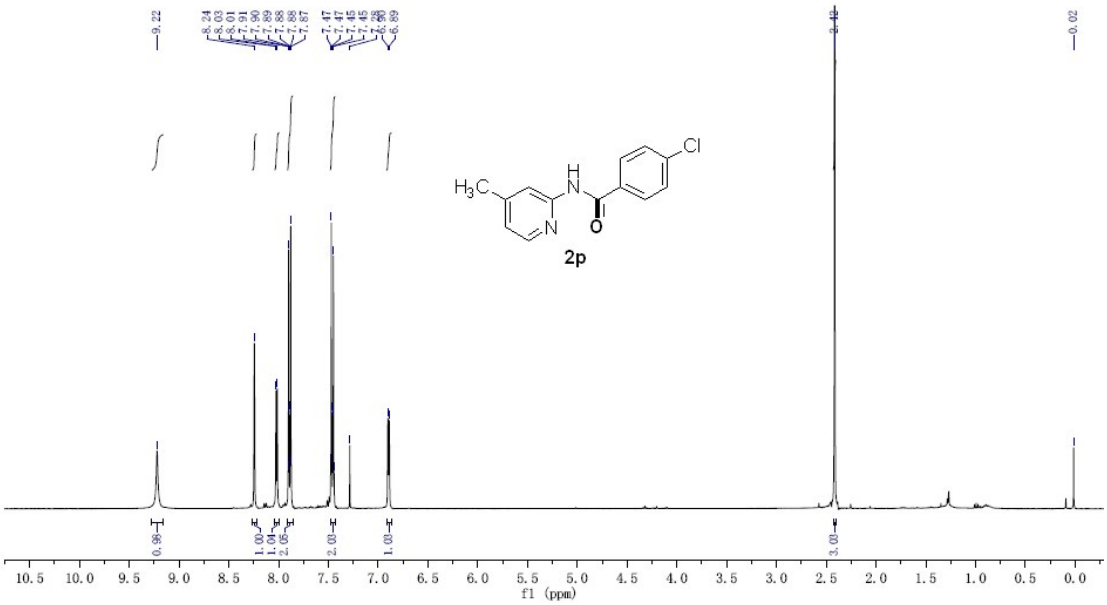

163.75
151.39
150.43
148.31
147.24
136.20
133.29
129.91
126.46
122.57
121.58
115.38
77.38
77.07
76.75
21.42
H3C
N
H
O
NO2
2m
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


9.08
8.28
8.09
8.08
7.87
7.85
7.31
7.29
6.90
6.89
2.44
2.41
0.02
0.99
1.00
1.08
2.06
2.19
1.03
3.18
3.03
H3C
CH3
H
N
O
N
2n
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)


165.84
151.79
150.10
147.18
142.73
131.53
129.42
127.36
120.95
114.88
77.38
77.06
76.74
21.50
21.44
H3C
CH3
H
N
O
N
2n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


9.01
8.05
8.03
8.04
7.92
7.90
7.29
6.97
6.95
6.87
6.85
3.87
2.39
0.01
OCH3
H3C
H
N
O
N
2o
0.97
1.00
1.04
2.10
2.09
1.04
3.09
3.03
f1 (ppm)


165.37
162.75
151.91
149.93
147.32
129.24
126.61
120.85
114.77
113.96
77.38
77.07
76.75
55.44
21.41
OCH3
H3C
H
N
O
N
2o
f1 (ppm)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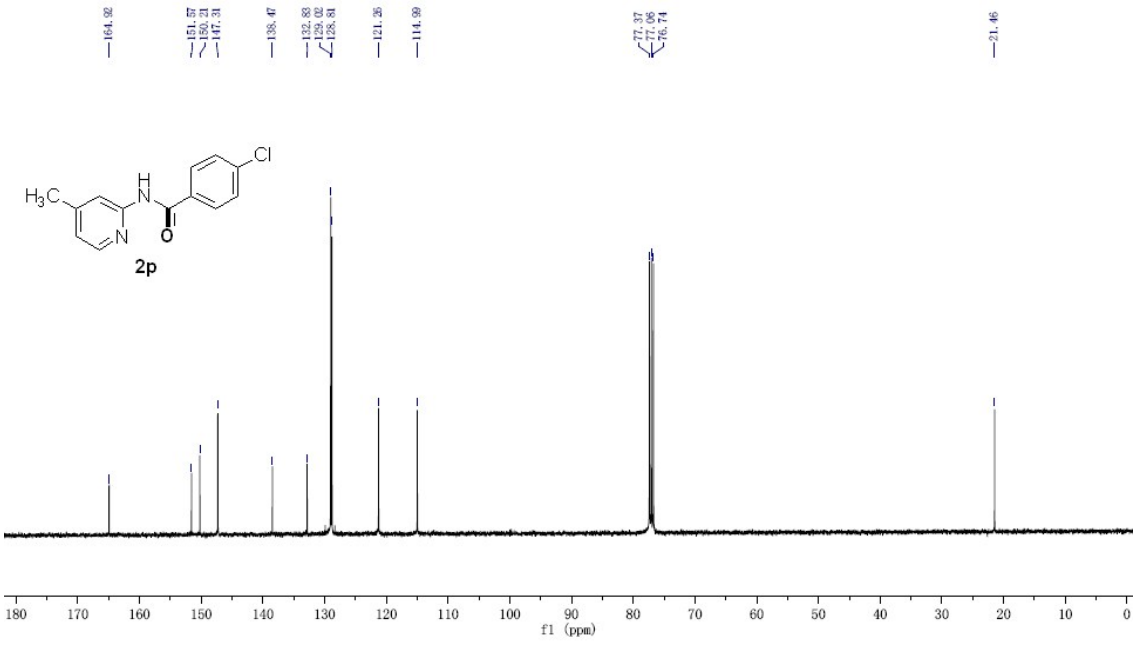
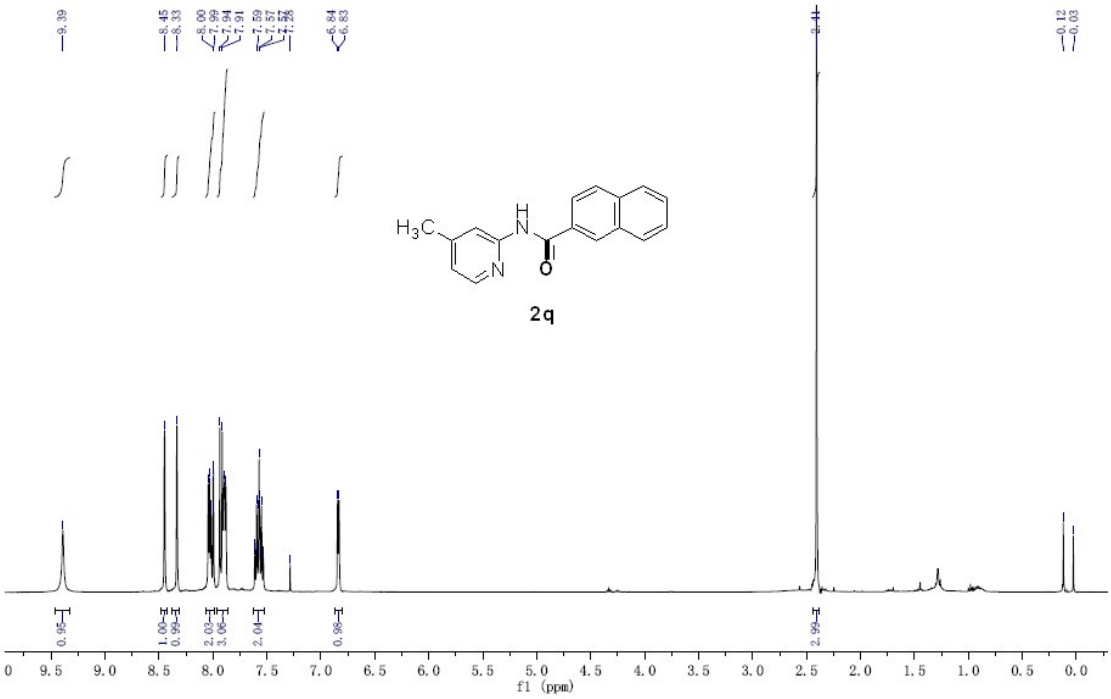
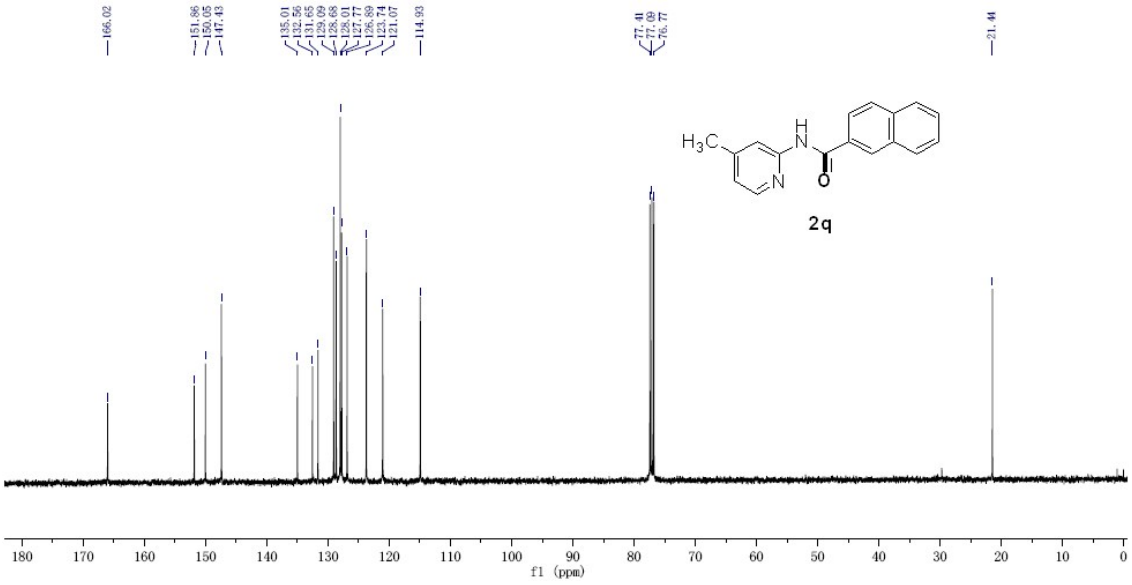
8.24
8.03
8.01
7.91
7.90
7.89
7.88
7.88
7.87
7.47
7.47
7.45
7.45
6.89
2.42
0.02
Cl
H
N
H3C
N
O
2p
0.99
1.00
1.04
2.05
2.03
1.03
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


164.92
151.57
150.21
147.31
138.47
132.83
129.02
128.81
121.26
114.99
77.37
77.06
76.74
21.46
Cl
H
N
H3C
N
O
2p
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.39
8.45
8.33
8.00
7.99
7.94
7.91
7.59
7.57
6.84
6.83
2.41
0.12
0.03
0.95
1.00
0.99
2.03
3.06
2.04
0.98
2.99
f1 (ppm)


H3C
N
H
O

2q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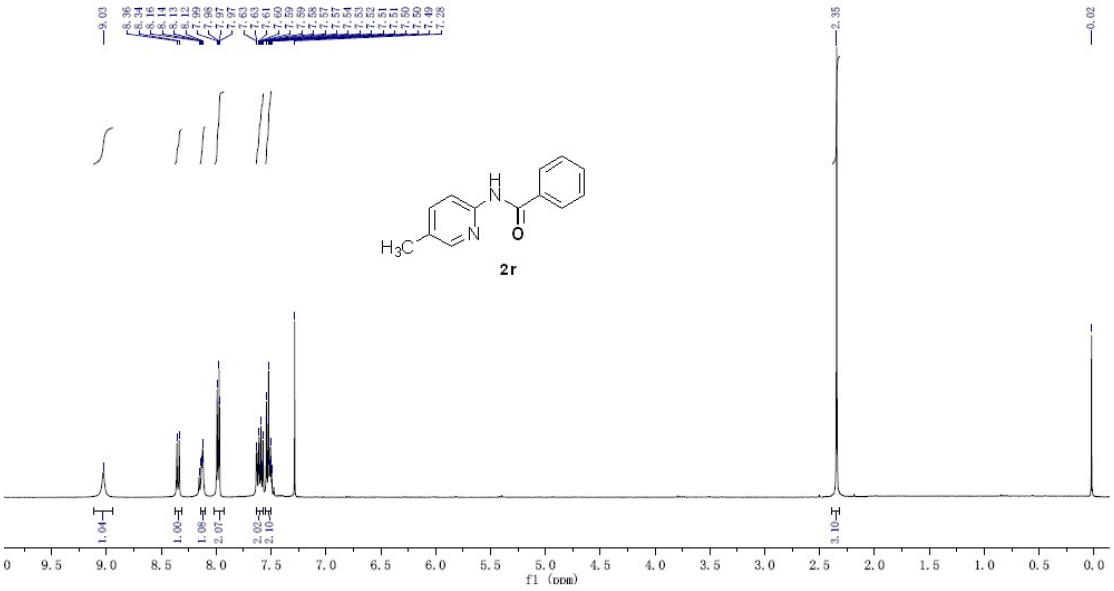
150.05
147.43
135.01
132.56
131.65
129.89
128.68
128.01
127.77
126.89
123.74
121.07
114.93
77.41
77.09
76.77
21.44
f1 (ppm)


H3C
N
H
O

2q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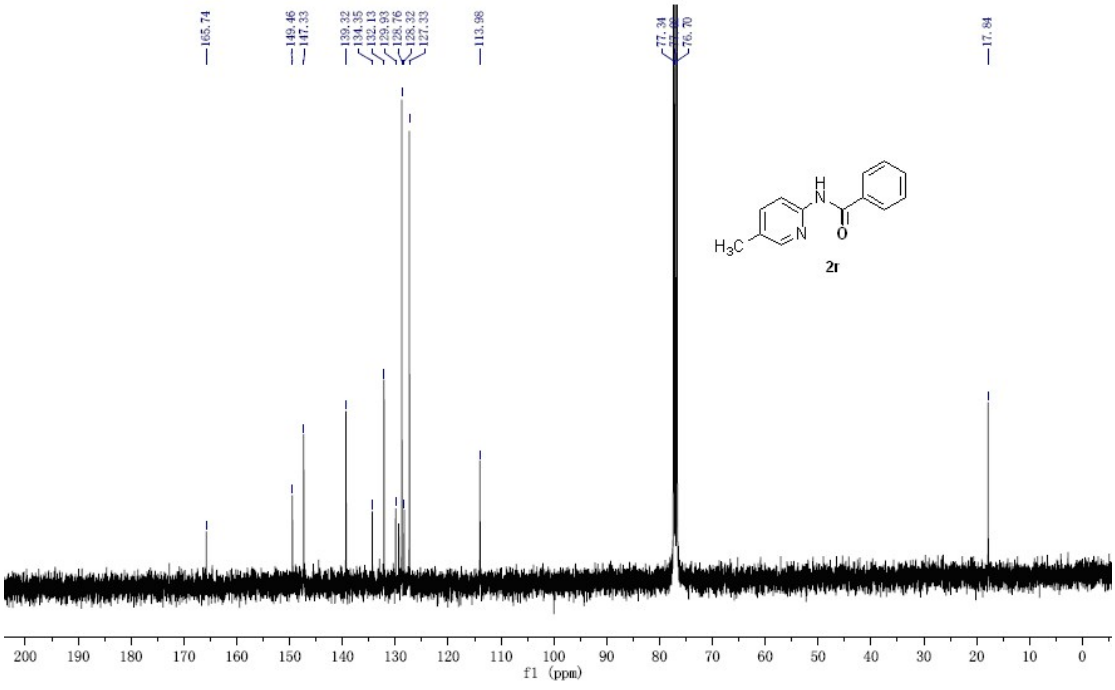
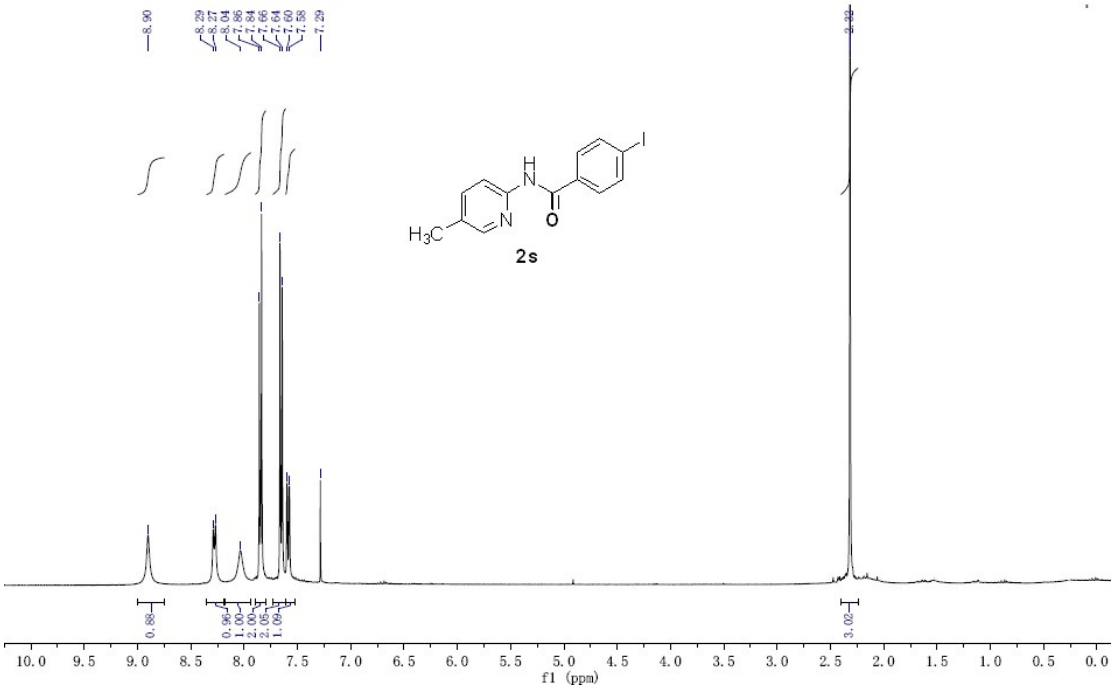
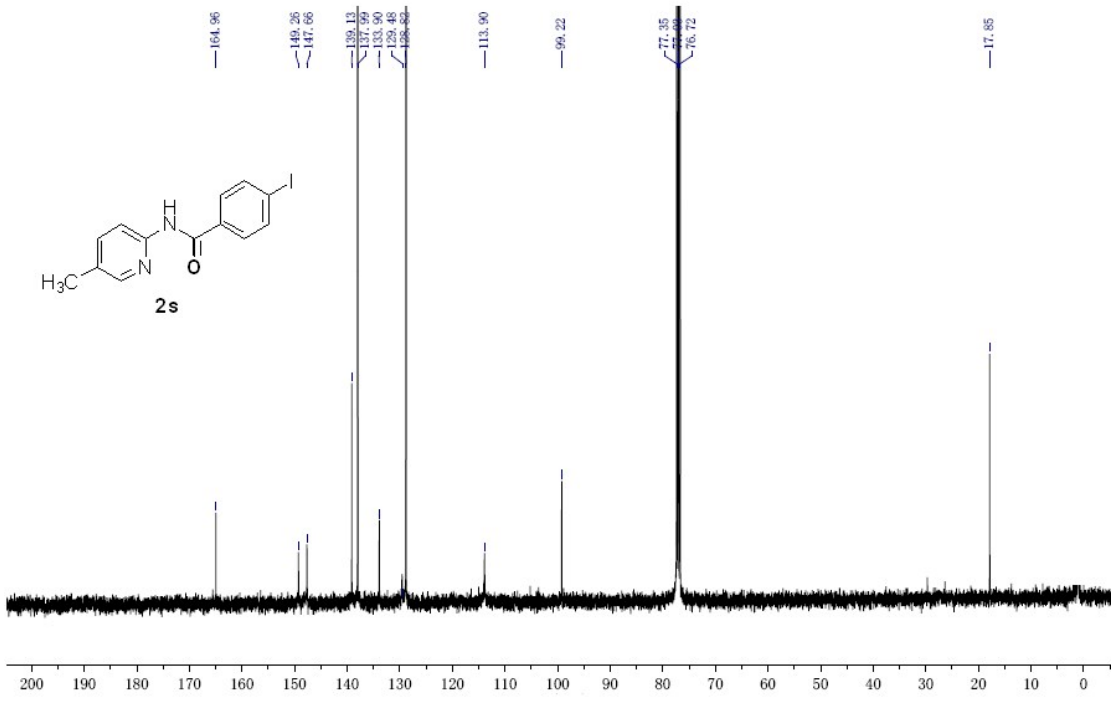
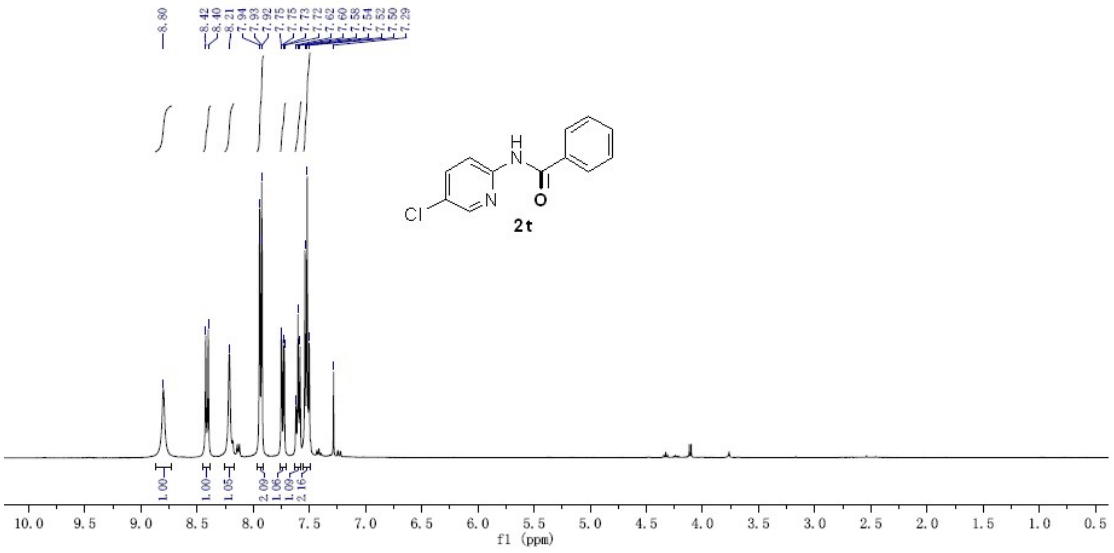
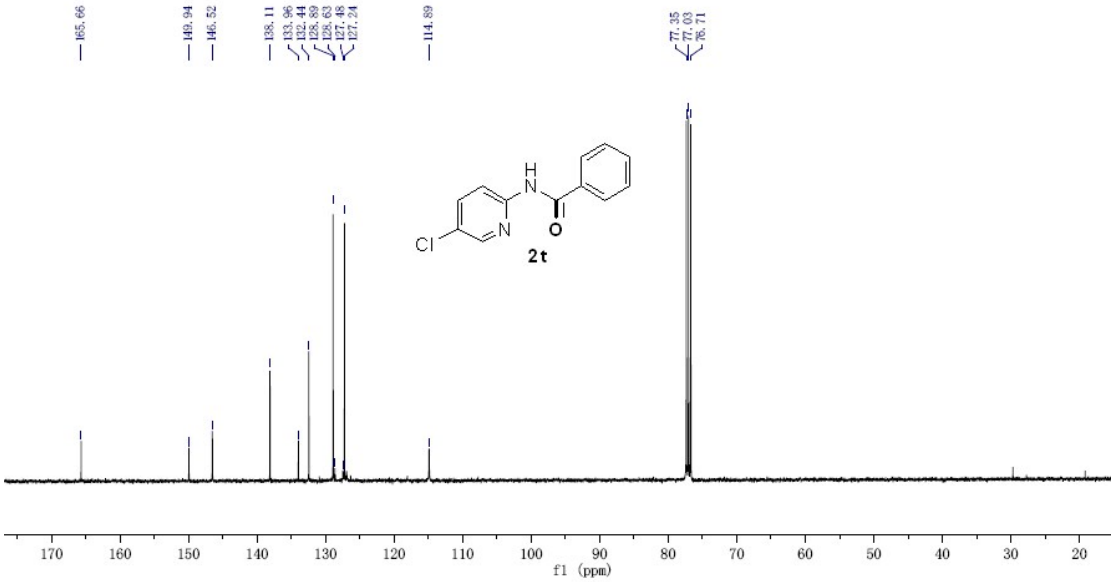
8.36
8.34
8.16
8.14
8.13
8.12
7.99
7.98
7.97
7.97
7.63
7.61
7.60
7.59
7.59
7.58
7.57
7.57
7.54
7.53
7.52
7.51
7.51
7.50
7.50
7.49
7.28
2.35
0.02
1.04
1.00
1.08
2.07
2.02
2.10
3.10
H
N
O
H3C
2r
f1 (ppm)

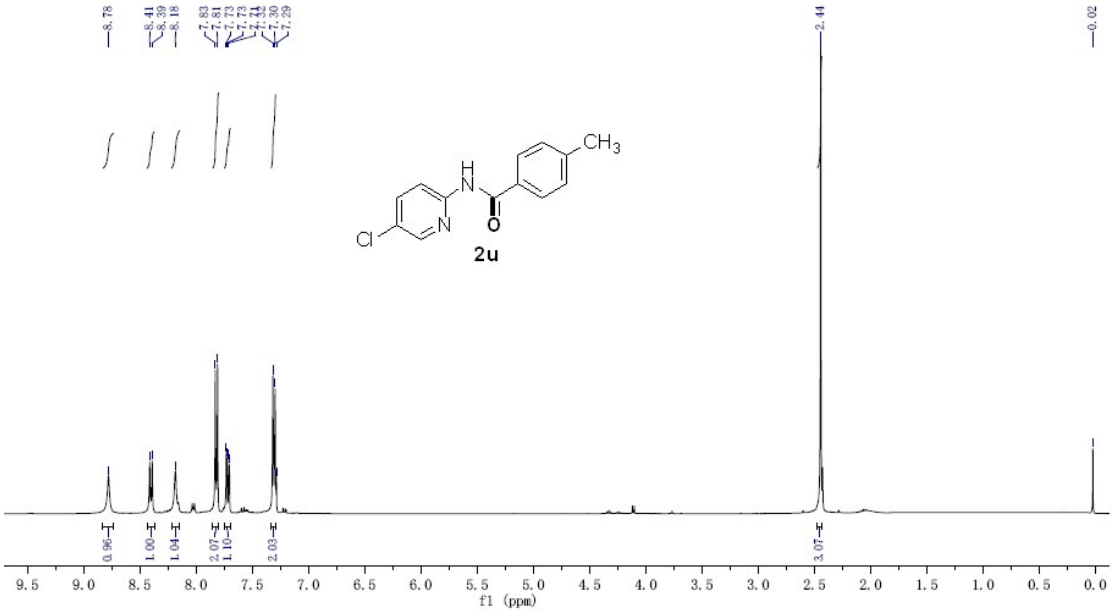

165.74
149.46
147.33
139.32
134.35
132.13
129.93
128.76
128.32
127.33
113.98
77.34
77.02
76.70
17.84
H
N
O
H3C
2r
f1 (ppm)

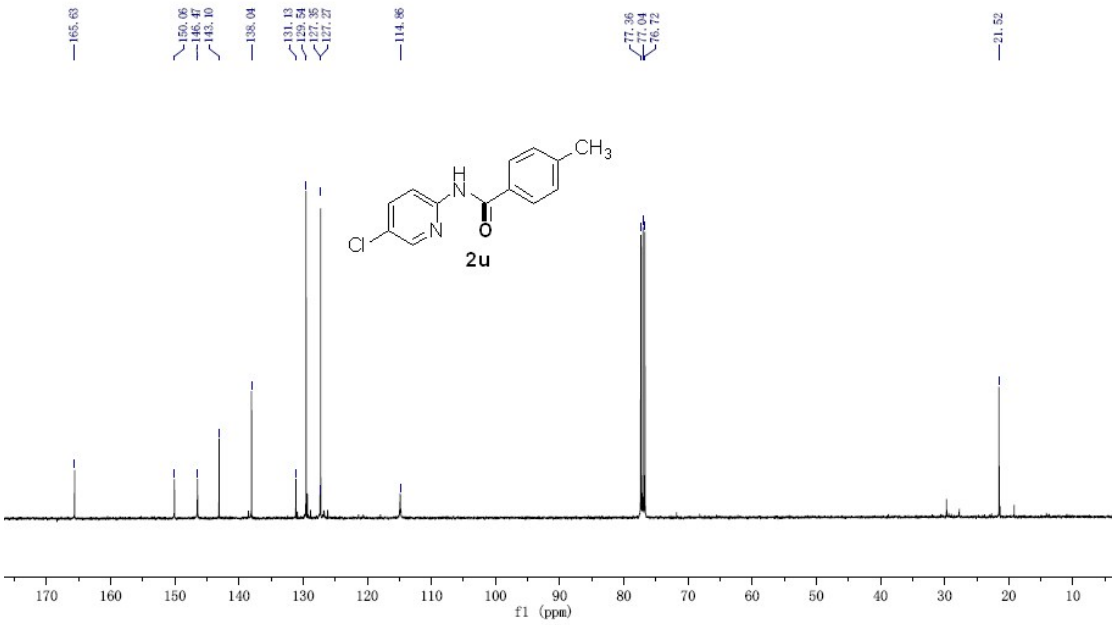

8.90
8.29
8.27
8.04
7.86
7.84
7.66
7.64
7.60
7.58
7.29
2.32
I
H
N
O
H3C
2s
0.88
0.96
1.00
2.05
1.09
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

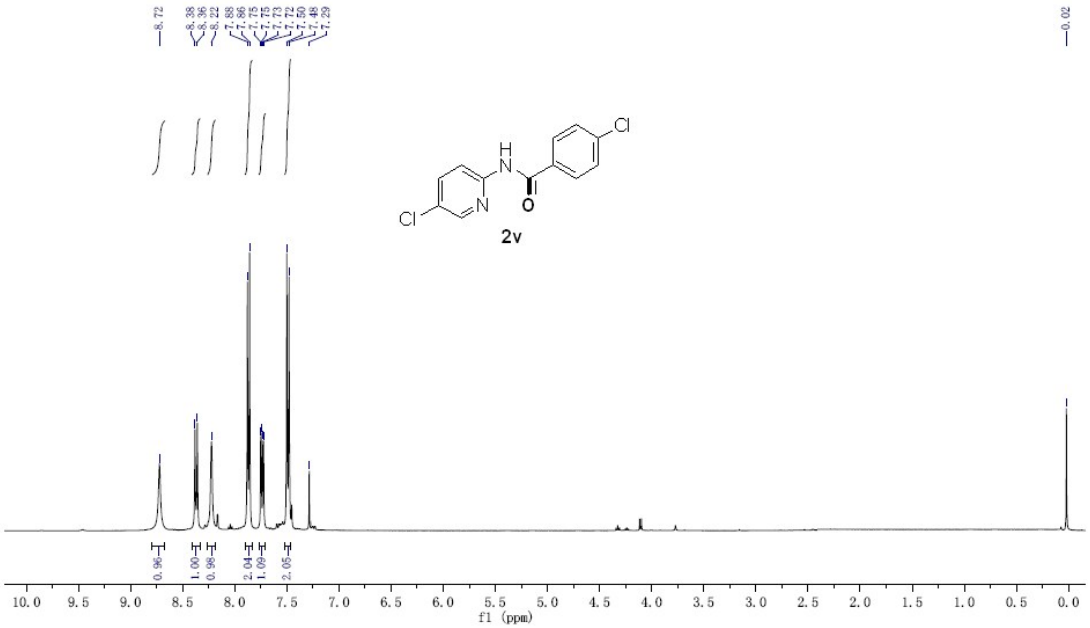

164.96
149.26
147.66
139.13
137.99
133.90
129.48
128.82
113.90
99.22
77.35
77.00
76.72
17.85
I
H
N
O
H3C
2s
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

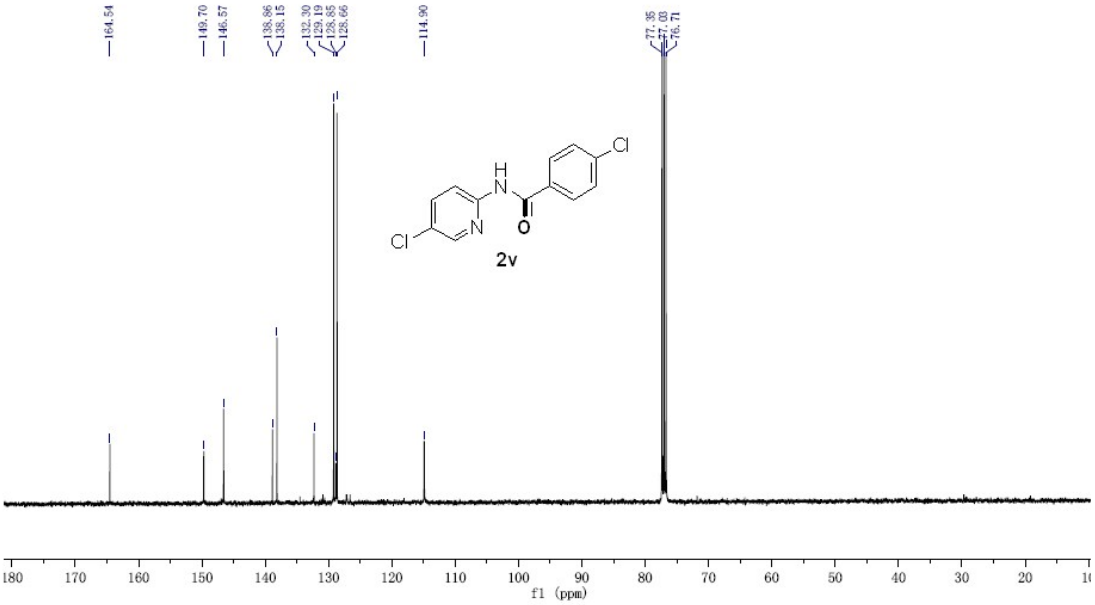

8.80
8.42
8.40
8.21
7.94
7.93
7.92
7.75
7.75
7.73
7.72
7.62
7.60
7.58
7.54
7.52
7.50
7.29
1.00
1.00
1.05
2.09
1.06
1.09
2.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)
H
N
O
N
Cl
2t

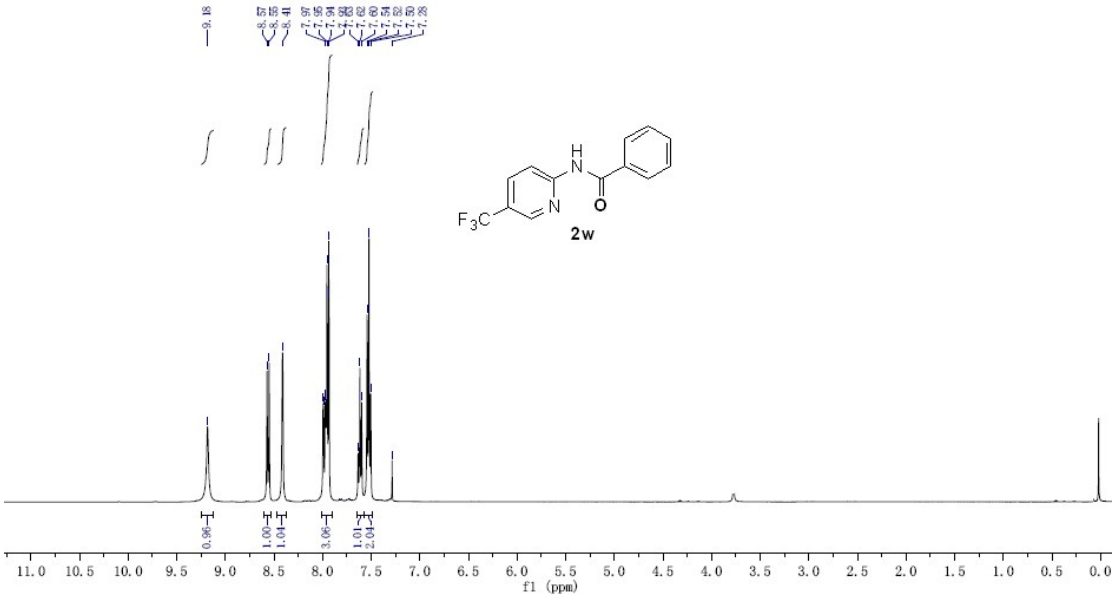

165.66
149.94
146.52
138.11
133.96
132.44
128.89
128.63
127.45
127.24
114.89
77.35
77.03
76.71
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)
H
N
O
N
Cl
2t

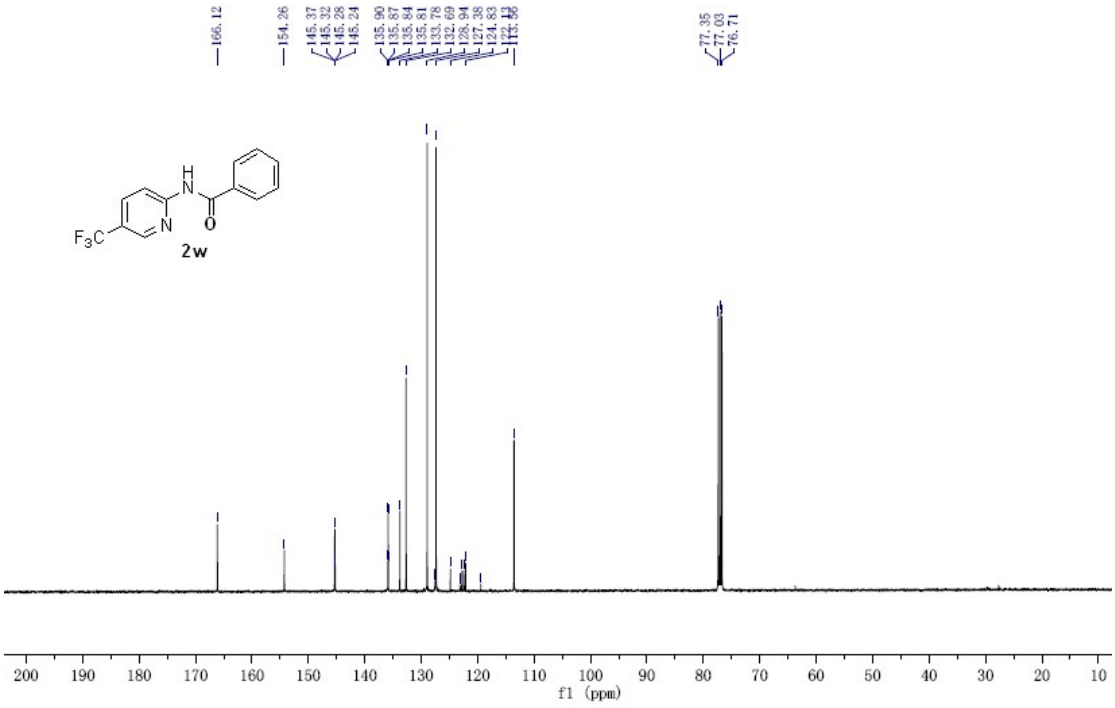

8.78
8.41
8.39
8.18
7.83
7.81
7.73
7.73
7.31
7.30
7.29
2.44
0.02
CH3
H
N
N
O
Cl
2u
0.96
1.00
1.04
2.07
1.10
2.03
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

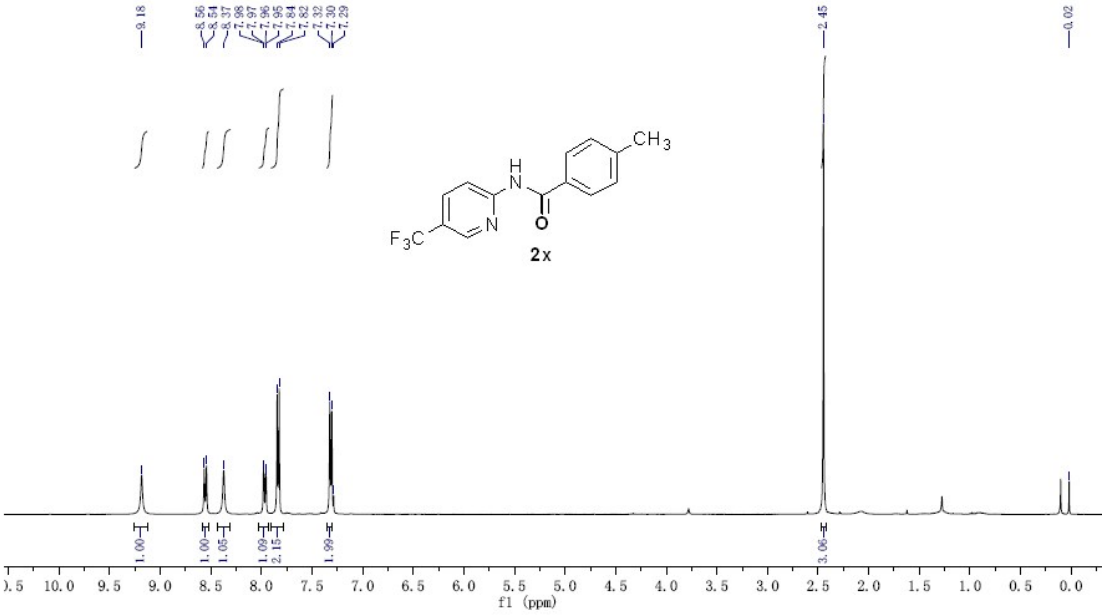

165.63
150.06
146.47
143.10
138.04
131.13
129.54
127.35
127.27
114.96
77.36
77.04
76.72
21.52
CH3
H
N
N
O
Cl
2u
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

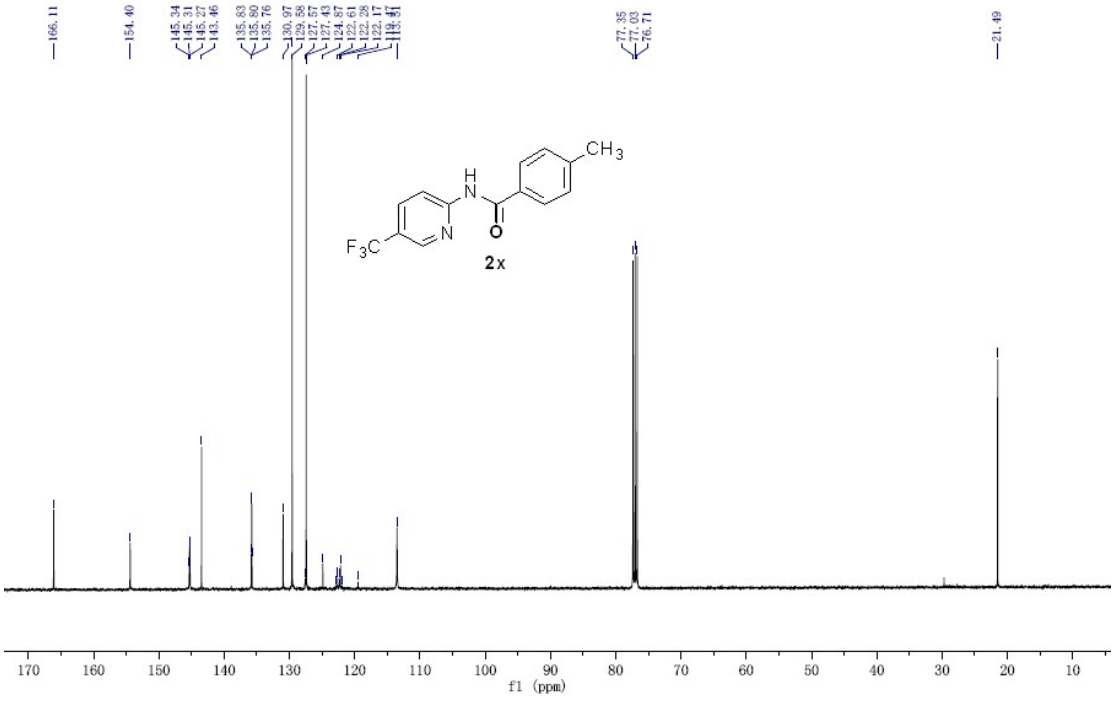

8.72
8.38
8.35
8.22
7.88
7.86
7.75
7.75
7.73
7.72
7.69
7.48
7.29
0.02
0.96
1.00
0.98
2.04
1.09
2.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
Cl
H
N
O
Cl
2v

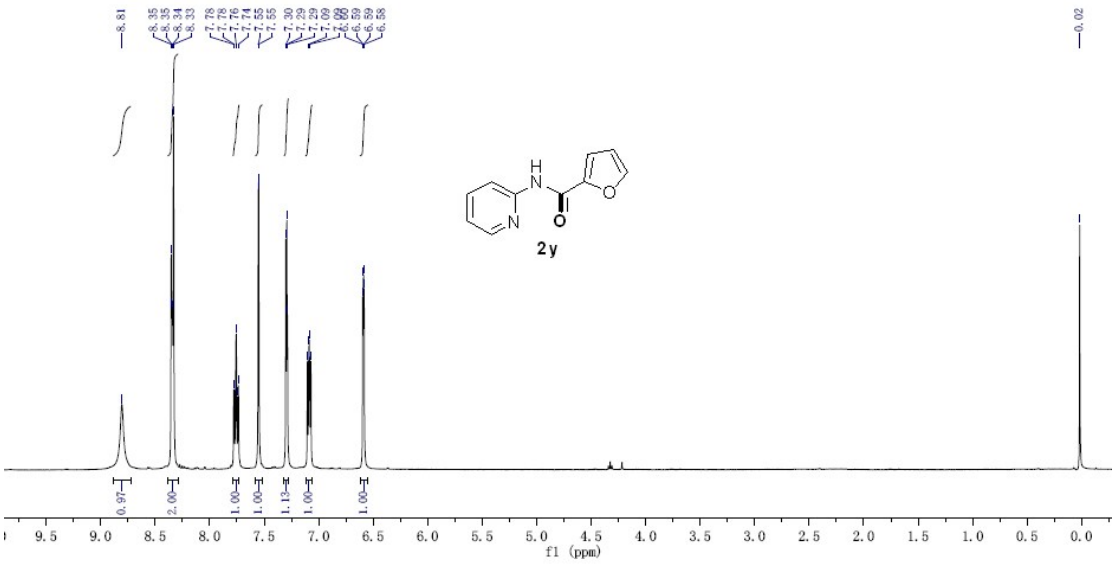

164.54
149.70
146.57
138.86
138.15
132.30
129.19
128.85
128.66
114.90
77.35
77.03
76.71
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)
Cl
H
N
O
Cl
2v

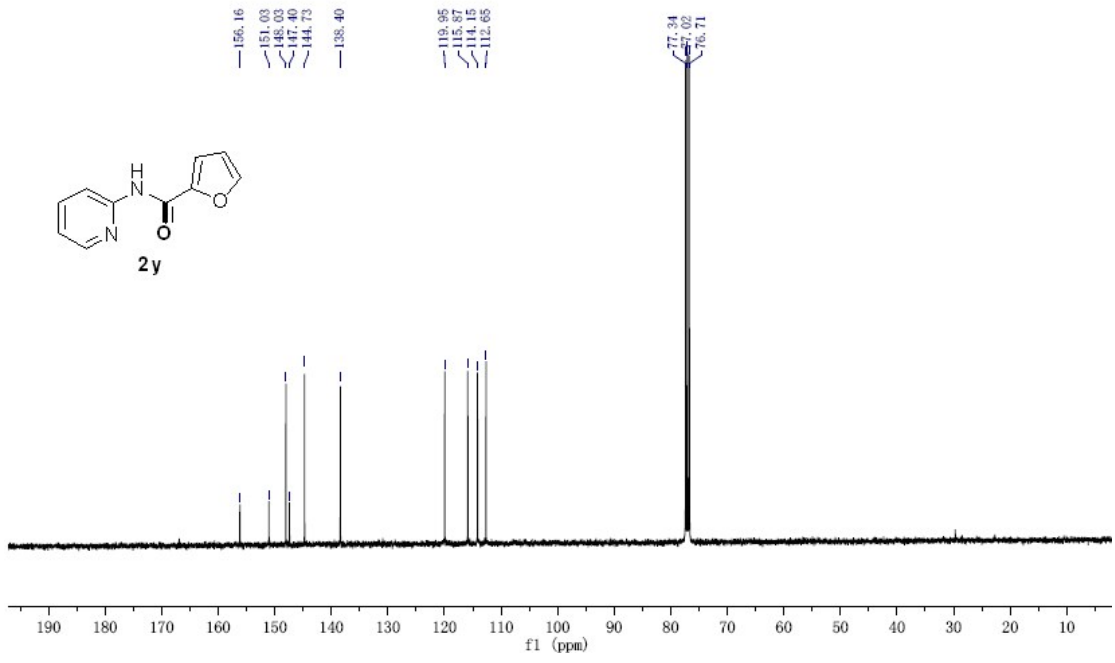

9.18
8.57
8.55
8.41
7.97
7.95
7.94
7.62
7.60
7.54
7.52
7.50
7.26
H
N
O
F3C
2w
0.96
1.00
1.04
3.06
1.01
2.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

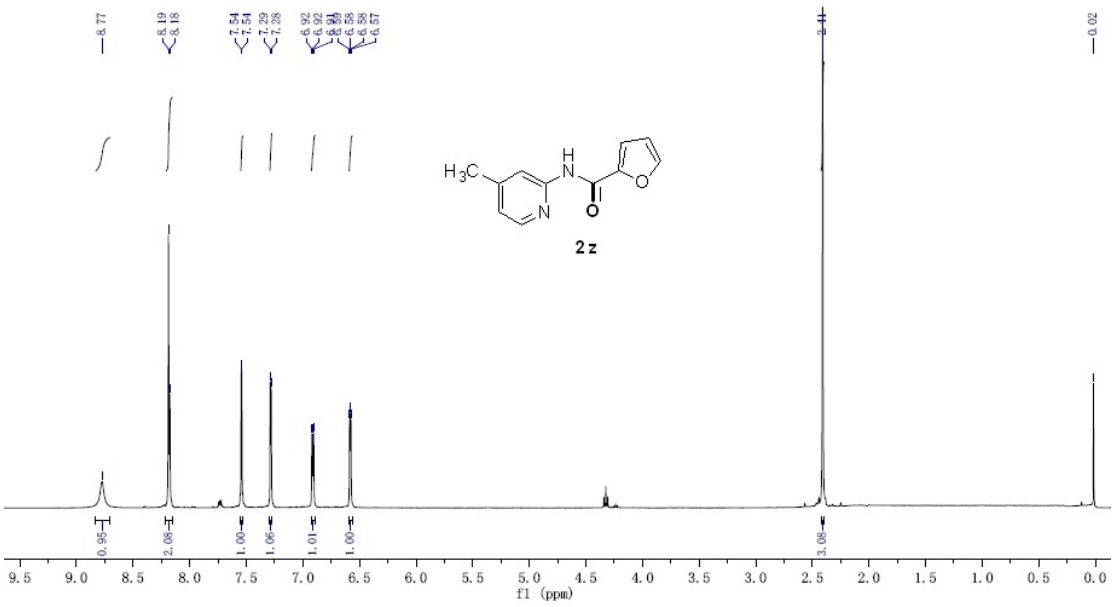

166.12
154.26
145.37
145.32
145.28
145.24
135.90
135.87
135.84
135.81
133.78
132.69
128.94
127.38
124.83
77.35
77.03
76.71
H
N
O
F3C
2w
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

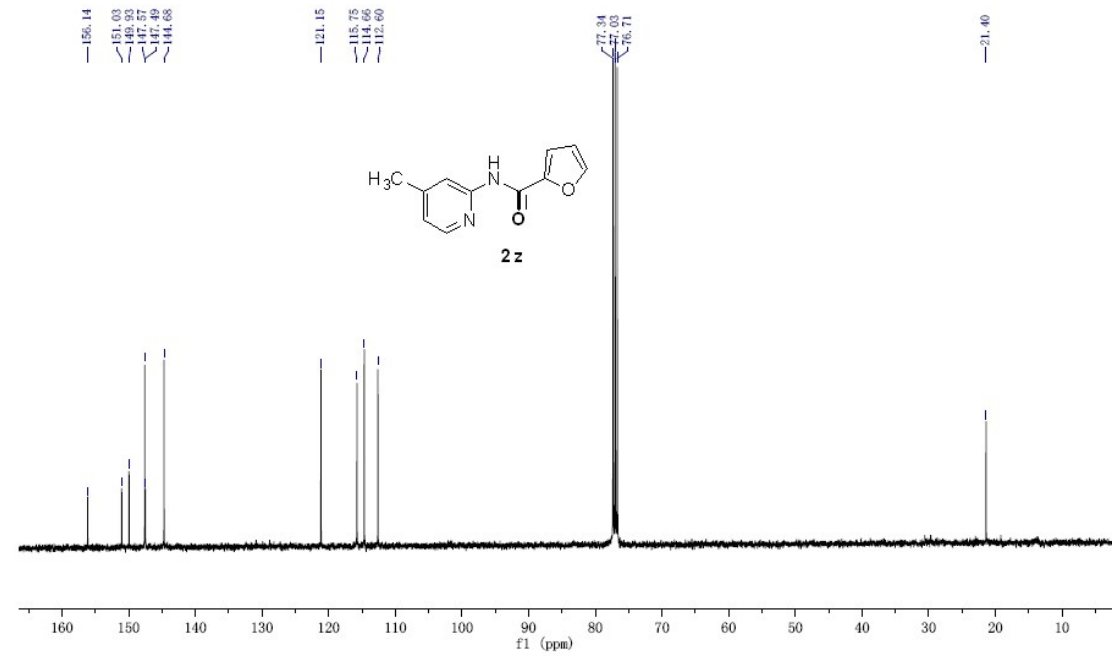

9.18
8.56
8.54
8.37
7.98
7.97
7.96
7.95
7.84
7.82
7.32
7.30
7.29
2.45
0.02
CH3
H
N
N
O
F3C
2x
1.00
1.00
1.05
1.09
2.15
1.99
3.06
f1 (ppm)


166.11
154.40
145.34
145.31
145.27
143.46
135.83
135.60
135.76
130.97
129.58
127.57
127.43
124.67
122.61
122.28
122.17
119.47
119.41
77.35
77.03
76.71
21.49
CH3
H
N
N
O
F3C
2x
f1 (ppm)


8.81
8.35
8.35
8.34
8.33
7.78
7.78
7.76
7.74
7.55
7.55
7.30
7.29
7.29
7.09
6.89
6.89
6.88
0.02
0.97
2.00
1.00
1.00
1.13
1.00
1.00
2y
f1 (ppm)


156.16
151.03
148.03
147.40
144.73
138.40
119.95
115.87
114.15
112.65
77.34
77.02
76.71
2y
f1 (ppm)


8.77
8.19
8.18
7.54
7.54
7.29
7.28
6.92
6.92
6.58
6.58
6.58
6.57
2.41
0.02
0.95
2.08
1.00
1.06
1.01
1.00
3.08
H3C
H
N
O
N
O
2z
f1 (ppm)


156.14
151.03
149.93
147.57
147.49
144.68
121.15
115.75
114.66
112.60
77.34
77.03
76.71
21.40
H3C
H
N
O
N
O
2z
f1 (ppm)