Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Palladium/Copper-Catalyzed Decarbonylative Heteroarylation of Amides via C-N Bond Activation

Ping-Xin Zhou,*[a] Shuai Shi,[b] Jia Wang,[a] Yalei Zhang,[a] Changzheng Li*[a] and Chunpo Ge*[a]

[a] *School of Basic Medical Sciences, Xinxiang Medical University, Xinxiang, 453003, China*

[b] *School of Foreign Language, Xinxiang Medical University, Xinxiang, 453003, China*

E-mail: zhoupingxin518@yahoo.com, changzhengli@xxmu.edu.cn and gecp1987@ xxmu.edu.cn

Table of Contents

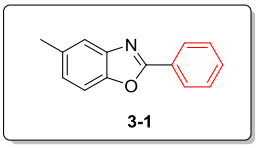
1. General remarks

The desired product was purified by flash column chromatography, silica gel (200~300 mesh). ^{1}H NMR spectra and ^{13}C NMR spectra were recorded on 400 MHz in CDCl3 and TMS as internal standard. All products were further characterized by HRMS (high resolution mass spectra). Copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. 1,4-dioxane were dried over sodium with benzophenone-ketyl intermediate as indicator. Commercially available reagents and solvents were used without further purification. *N*-glutarimide amide **1**[1] and heteroarenes **2**[2] were synthesized according to the literature procedure. For **3-3**, **3-5**, **3-8**, **3-9**, **3-10**, **3-11** and **3-30** are new compounds. For others **3** are known compounds.[3]

2. General procedure for the preparation of the products 3

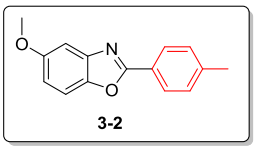
An oven-dried Schlenk tube under a nitrogen atmosphere was charged with **1** (0.4 mmol, 2.0 equiv), **2** (0.2 mmol, 1.0 equiv), $Pd(PPh_3)_2Cl_2$ (10 mol %), dppe (20 mol %), CuBr (20 mol %), Na_2CO_3 (0.26 mmol, 1.3 equiv), 1,4-dioxane (0.5 mL). The mixture was stirred at room temperature for 20 minutes and then stirred at 160 ℃ for 24 h. The resulting mixture was cooled to room temperature and filtered through Celite eluting with EtOAc. The volatiles were evaporated under reduced pressure and the residue was purified by silica gel flash chromatography to afford the desired products **3**.

3. Spectral data of compound 3



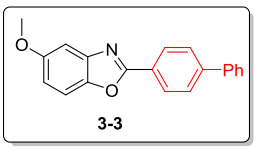
3-1

5-methyl-2-phenylbenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.28-8.26 (m, 2H), 7.59 (s, 1H), 7.59-7.54 (m, 3H), 7.47 (d, *J* = 8.5 Hz, 1H), 7.19-7.17 (m, 1H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.09, 148.96, 142.23, 134.39, 131.38, 128.86, 127.53, 127.27, 126.22, 119.88, 109.93, 21.53; HRMS (ESI) m/z: calcd for $C_{14}H_{12}NO$, $[M+H]^+$: 210.0841; Found: 210.0914.



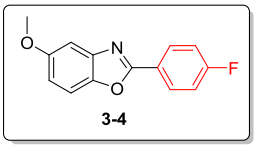
3-2

5-methoxy-2-(p-tolyl)benzo[d]oxazole: white solid; NMR yield; HRMS (ESI) m/z: calcd for $C_{15}H_{14}NO_2$, $[M+H]^+$: 240.0946; Found: 240.1021.



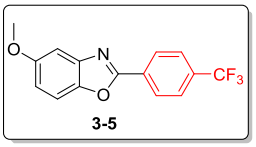
3-3

2-([1,1'-biphenyl]-4-yl)-5-methoxybenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.33-8.31 (m, 2H), 7.79-7.77 (m, 2H), 7.70-7.68 (m, 2H), 7.53-7.49 (m, 3H), 7.46-7.43 (m, 1H), 7.30 (d, *J* = 2.5 Hz, 1H), 7.00-6.98 (m, 1H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.65, 157.39, 145.44, 144.06, 143.01, 139.98, 128.93, 128.03, 127.92, 127.52, 127.14, 126.03, 113.68, 110.70, 102.82, 55.93; HRMS (ESI) m/z: calcd for $C_{20}H_{16}NO_2$, $[M+H]^+$: 302.1103; Found: 302.1176.



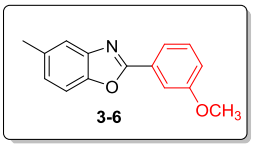
3-4

2-(4-fluorophenyl)-5-methoxybenzo[d]oxazole: yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.25-8.22 (m, 2H), 7.54 (d, *J* = 2.0 Hz, 1H), 7.47-7.45 (m, 1H), 7.26-7.20 (m, 2H), 6.98-6.96 (m, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 165.95, 163.43, 162.86, 157.40, 145.37, 142.84, 131.38, 129.68, 129.60, 128.87, 127.45, 123.54, 116.24, 116.02, 113.68, 110.67, 102.81, 55.90; HRMS (ESI) m/z: calcd for $C_{14}H_{11}FNO_2$, $[M+H]^+$: 244.0696; Found: 244.0770.



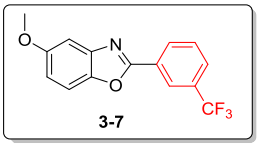
3-5

5-methoxy-2-(4-(trifluoromethyl)phenyl)benzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.35 (d, *J* = 8.0 Hz, 2H), 7.80 (d, *J* = 3.0 Hz, 2H), 7.50 (d, *J* = 9.0 Hz, 1H), 7.29-7.28 (m, 1H), 7.02 (dd, *J* = 9.0, 2.0 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.14, 157.59, 145.49, 142.71, 132.96, 130.48, 127.66, 125.93, 125.90, 125.86, 125.82, 122.38, 114.63, 110.94, 102.90, 55.91; HRMS (ESI) m/z: calcd for $C_{15}H_{11}F_3NO_2$, $[M+H]^+$: 294.0664; Found: 294.0734.



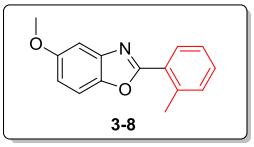
3-6

2-(3-methoxyphenyl)-5-methylbenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.86 (d, *J* = 7.5 Hz, 1H), 7.80-7.79 (m, 1H), 7.59 (s, 1H), 7.49-7.43 (m, 2H), 7.20-7.18 (m, 1H), 7.11-7.09 (m, 1H), 3.94 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.00, 159.88, 148.95, 142.21, 134.40, 129.95, 128.46, 126.28, 120.02, 119.88, 118.20, 111.75, 109.93, 55.50, 21.54; HRMS (ESI) m/z: calcd for $C_{15}H_{14}NO_2$, $[M+H]^+$: 240.0946; Found: 240.1020.

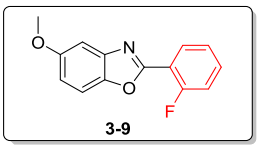


3-7

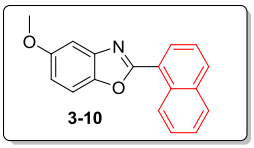
5-methoxy-2-(3-(trifluoromethyl)phenyl)benzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.52 (d, *J* = 2.5 Hz, 1H), 8.43-8.41 (m, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.69-7.67 (m, 1H), 7.52-7.50 (m, 1H), 7.29 (t, *J* = 2.5 Hz, 1H), 7.03-7.00 (m, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.18, 157.59, 145.43, 142.67, 131.38, 130.42, 129.50, 128.87, 128.09, 127.82, 127.78, 127.74, 127.71, 127.45, 124.34, 114.46, 110.91, 102.89, 55.91; HRMS (ESI) m/z: calcd for $C_{15}H_{11}F_3NO_2$, $[M+H]^+$: 294.0664; Found: 294.0733.



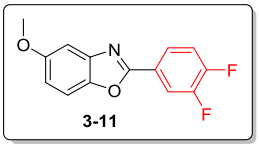
5-methoxy-2-(o-tolyl)benzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.20-8.18 (m, 1H), 7.49 (d, *J* = 9.0 Hz, 1H), 7.46-7.41 (m, 1H), 7.37 (d, *J* = 7.0 Hz, 2H), 7.33 (d, *J* = 3.0 Hz, 1H), 7.00-6.98 (m, 1H), 3.91 (s, 3H), 2.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.18, 157.23, 144.91, 142.89, 138.68, 131.77, 130.80, 129.79, 126.28, 126.04, 113.73, 110.61, 102.85, 55.94, 22.26; HRMS (ESI) m/z: calcd for $C_{15}H_{14}NO_2$, $[M+H]^+$: 240.0946; Found: 240.1019.



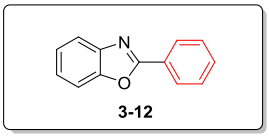
2-(2-fluorophenyl)-5-methoxybenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.25-8.22 (m, 1H), 7.55-7.51 (m, 2H), 7.34-7.27 (m, 3H), 7.02-6.99 (m, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.98, 160.14, 160.08, 159.40, 157.42, 145.11, 145.09, 142.58, 133.00, 132.91, 130.36, 130.35, 124.44, 116.95, 114.30, 110.83, 102.93, 55.90; HRMS (ESI) m/z: calcd for $C_{14}H_{11}FNO_2$, $[M+H]^+$: 244.0696; Found: 244.0764.



5-methoxy-2-(naphthalen-1-yl)benzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 9.50 (d, *J* = 8.5 Hz, 1H), 8.43 (d, *J* = 7.5 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.64 (t, *J* = 3.0 Hz, 1H), 7.61 (d, *J* = 5.0 Hz, 2H), 7.55 (d, *J* = 8.5 Hz, 1H), 7.41-7.40 (m, 1H), 7.04-7.02 (m, 1H), 3.94 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ: 163.59, 157.33, 144.82, 143.11, 133.95, 132.19, 130.61, 129.16, 128.66, 127.85, 126.41, 126.29, 124.94, 123.69, 113.98, 110.64, 103.00, 55.97; HRMS (ESI) m/z: calcd for $C_{18}H_{14}NO_2$, $[M+H]^+$: 276.0946; Found: 276.1017.

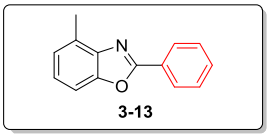


2-(3,4-difluorophenyl)-5-methoxybenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.07-8.03 (m, 1H), 8.01-7.98 (m, 1H), 7.47 (d, *J* = 9.0 Hz, 1H), 7.35-7.25 (m, 2H), 7.00-6.98 (m, 1H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.69, 157.53, 153.63, 151.73, 151.22, 149.24, 145.43, 142.71, 131.38, 128.87, 127.44, 124.07, 117.95, 116.58, 114.18, 110.80, 102.84, 55.91; HRMS (ESI) m/z: calcd for $C_{14}H_{10}F_2NO_2$, $[M+H]^+$: 262.0601; Found:262.0675.



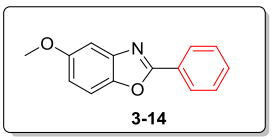
3-12

2-phenylbenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.31-8.29 (m, 2H), 7.83-7.81 (m, 1H), 7.63-7.61 (m, 1H), 7.58-7.56 (m, 3H), 7.40-7.38 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.03, 150.73, 142.06, 131.53, 128.91, 127.61, 127.13, 125.11, 124.58, 120.00, 110.59; HRMS (ESI) m/z: calcd for $C_{13}H_{10}NO$, $[M+H]^+$: 196.0684; Found: 196.0754.



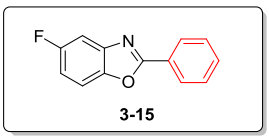
3-13

4-methyl-2-phenylbenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.32-8.30 (m, 2H), 7.56-7.55 (m, 3H), 7.45-7.43 (m, 1H), 7.29-7.26 (m, 1H), 7.19-7.17 (m, 1H), 2.72 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 162.28, 150.55, 141.45, 131.28, 130.61, 128.84, 127.61, 127.45, 125.05, 124.75, 107.85, 16.61; HRMS (ESI) m/z: calcd for $C_{14}H_{12}NO$, $[M+H]^+$: 210.0841; Found: 210.0917.



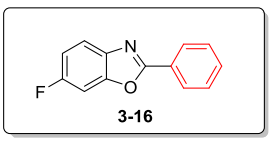
3-14

5-methoxy-2-phenylbenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.26-8.25 (m, 2H), 7.55-7.54 (m, 3H), 7.48 (d, *J* = 8.5 Hz, 1H), 7.29 (d, *J* = 3.0 Hz, 1H), 6.97 (dd, *J* = 9.0, 2.0 Hz, 1H), 3.90 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 163.79, 157.40, 145.42, 142.93, 131.41, 128.89, 127.49, 127.27, 113.72, 110.72, 102.88, 55.94; HRMS (ESI) m/z: calcd for $C_{14}H_{12}NO_2$, $[M+H]^+$: 226.0790; Found: 226.0865.



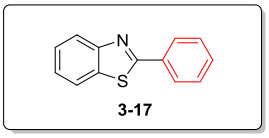
3-15

5-fluoro-2-phenylbenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.27-8.26 (m, 2H), 7.59-7.53 (m, 4H), 7.49-7.47 (m, 1H), 7.13-7.09 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.75, 161.32, 158.93, 147.07, 142.96, 131.82, 128.96, 127.66, 126.82, 112.83, 112.57, 110.88, 110.78, 106.52, 106.27; HRMS (ESI) m/z: calcd for $C_{13}H_9FNO$, $[M+H]^+$: 214.0590; Found: 214.0662.



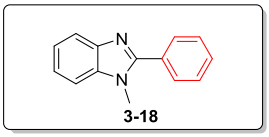
3-16

6-fluoro-2-phenylbenzo[d]oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.25-8.23 (m, 2H), 7.72 (dd, *J* = 8.5, 5.0 Hz, 1H), 7.57-7.55 (m, 3H), 7.33 (dd, *J* = 8.0, 2.5 Hz, 1H), 7.15-7.11 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.67, 161.86, 159.43, 150.75, 138.37, 131.60, 128.95, 127.46, 126.84, 120.28, 120.18, 112.66, 112.42, 98.81, 98.53; HRMS (ESI) m/z: calcd for $C_{13}H_9FNO$, $[M+H]^+$: 214.0590; Found: 214.0664.



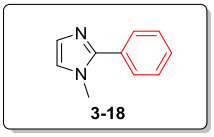
3-17

2-phenylbenzo[d]thiazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.14-8.11 (m, 3H), 7.95-7.93 (m, 1H), 7.55-7.52 (m, 4H), 7.44-7.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.07, 154.11, 135.04, 133.59, 130.97, 129.02, 127.55, 126.32, 125.19, 123.22, 121.62; HRMS (ESI) m/z: calcd for $C_{13}H_{10}NS$, $[M+H]^+$: 212.0456; Found: 212.0529.



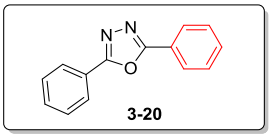
3-18

1-methyl-2-phenyl-1H-benzo[d]imidazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.88-7.86 (m, 1H), 7.79 (dd, *J* = 7.5, 2.0 Hz, 2H), 7.57-7.53 (m, 3H), 7.42-7.40 (m, 1H), 7.36-7.34 (m, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.75, 142.91, 136.55, 130.18, 129.72, 129.43, 128.67, 122.76, 122.43, 119.81, 109.63, 31.68; HRMS (ESI) m/z: calcd for $C_{14}H_{13}N_2$, $[M+H]^+$: 209.1000; Found: 209.1070.



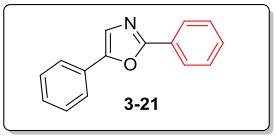
3-18

1-methyl-2-phenyl-1H-imidazole: white solid; NMR yield; HRMS (ESI) m/z: calcd for $C_{10}H_{11}N_2$, $[M+H]^+$: 159.0844; Found: 159.0917.



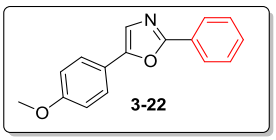
3-20

2,5-diphenyl-1,3,4-oxadiazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.19-8.17 (m, 4H), 7.59-7.57 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 164.58, 131.72, 129.07, 126.93, 123.91; HRMS (ESI) m/z: calcd for $C_{14}H_{10}N_2ONa$, $[M+Na]^+$: 245.0793; Found: 245.0688.



3-21

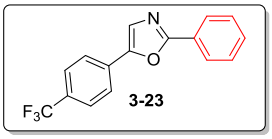
2,5-diphenyloxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.16-8.14 (m, 2H), 7.77-7.75 (m, 2H), 7.54-7.47 (m, 6H), 7.39-7.37 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.13, 151.24, 130.33, 128.93, 128.82, 128.44, 127.99, 127.42, 126.27, 124.18, 123.43; HRMS (ESI) m/z: calcd for $C_{15}H_{12}NO$, $[M+H]^+$: 222.0841; Found: 222.0913.



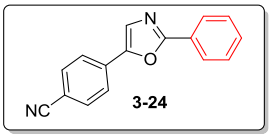
3-22

5-(4-methoxyphenyl)-2-phenyloxazole: yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.14-8.12 (m, 2H), 7.70-7.68 (m, 2H), 7.51-7.48 (m, 3H), 7.36 (s, 1H), 7.02-7.00 (m, 2H), 3.89 (s, 3H); ^{13}C

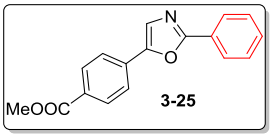
NMR (125 MHz, $CDCl_3$) δ: 160.56, 159.83, 151.33, 130.13, 128.80, 127.58, 126.15, 125.76, 121.95, 120.88, 114.42, 55.39; HRMS (ESI) m/z: calcd for $C_{16}H_{14}NO_2$, $[M+H]^+$: 252.0946; Found: 252.1017.



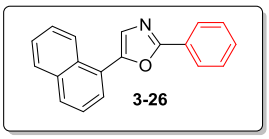
2-phenyl-5-(4-(trifluoromethyl)phenyl)oxazole: white solid; ^1H NMR (500 MHz, $CDCl_3$) δ: 8.15-8.13 (m, 2H), 7.84-7.82 (m, 2H), 7.72-7.71 (m, 2H), 7.57 (s, 1H), 7.53-7.52 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.98, 149.82, 131.20, 130.75, 130.18, 128.90, 127.07, 126.47, 126.03, 126.00, 125.97, 125.93, 125.23, 124.20; HRMS (ESI) m/z: calcd for $C_{16}H_{11}F_3NO$, $[M+H]^+$: 290.0714; Found: 290.0788.



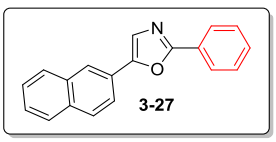
5-(4-isocyanophenyl)-2-phenyloxazole: white solid; ^1H NMR (500 MHz, $CDCl_3$) δ: 8.14-8.12 (m, 2H), 7.83-7.81 (m, 2H), 7.74 (d, *J* = 8.0 Hz, 2H), 7.61 (s, 1H), 7.53-7.52 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 162.38, 149.32, 132.80, 131.88, 130.97, 128.94, 126.81, 126.52, 126.24, 124.32, 118.57, 111.46; HRMS (ESI) m/z: calcd for $C_{16}H_{11}N_2O$, $[M+H]^+$: 247.0793; Found: 247.0867.



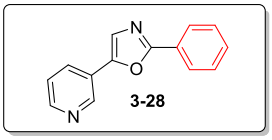
methyl 4-(2-phenyloxazol-5-yl)benzoate: white solid; ^1H NMR (500 MHz, $CDCl_3$) δ: 8.16-8.12 (m, 4H), 7.81-7.79 (m, 2H), 7.58 (d, *J* = 1.5 Hz, 1H), 7.54-7.51 (m, 3H), 3.97 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 166.50, 161.96, 150.24, 131.95, 130.70, 130.30, 129.61, 128.89, 127.11, 126.47, 125.43, 123.82, 52.24; HRMS (ESI) m/z: calcd for $C_{17}H_{14}NO_3$, $[M+H]^+$: 280.0875; Found: 280.0970



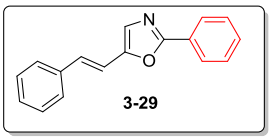
5-(naphthalen-1-yl)-2-phenyloxazole: white solid; ^1H NMR (500 MHz, $CDCl_3$) δ: 8.42-8.40 (m, 1H), 8.22-8.20 (m, 2H), 7.97-7.93 (m, 2H), 7.88-7.86 (m, 1H), 7.64-7.53 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 161.53, 150.52, 133.90, 130.42, 130.10, 129.58, 128.89, 128.77, 127.49, 127.12, 126.81, 126.42, 126.36, 126.27, 125.37, 125.33, 124.91; HRMS (ESI) m/z: calcd for $C_{19}H_{14}NO$, $[M+H]^+$: 272.0997; Found: 272.1072.



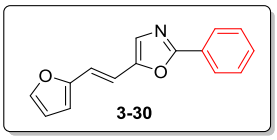
5-(naphthalen-2-yl)-2-phenyloxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.23-8.20 (m, 3H), 7.95-7.92 (m, 2H), 7.89-7.87 (m, 1H), 7.81 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.59-7.52 (m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.32, 151.36, 133.38, 133.09, 130.42, 128.85, 128.76, 128.21, 127.86, 127.38, 126.82, 126.52, 126.36, 125.25, 123.93, 122.92, 122.06; HRMS (ESI) m/z: calcd for $C_{19}H_{14}NO$, $[M+H]^+$: 272.0997; Found: 272.1072



2-phenyl-5-(pyridin-3-yl)oxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.68-8.66 (m, 1H), 8.18-8.16 (m, 2H), 7.84-7.77 (m, 3H), 7.52-7.50 (m, 3H), 7.26-7.24 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.97, 150.77, 149.96, 147.37, 136.89, 130.68, 128.85, 127.19, 126.96, 126.56, 122.83, 119.19; HRMS (ESI) m/z: calcd for $C_{14}H_{11}N_2O$, $[M+H]^+$: 223.0793; Found: 223.0867.



(E)-2-phenyl-5-styryloxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.15-8.13 (m, 2H), 7.55-7.50 (m, 5H), 7.43-7.40 (m, 2H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.22-7.19 (m, 2H), 6.97 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 161.10, 150.36, 136.41, 130.42, 129.47, 128.83, 128.25, 127.37, 126.58, 126.51, 126.41, 113.10; HRMS (ESI) m/z: calcd for $C_{17}H_{14}NO$, $[M+H]^+$: 248.0997; Found:248.1073.



(E)-5-(2-(furan-2-yl)vinyl)-2-phenyloxazole: white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ: 8.12-8.10 (m, 2H), 7.50-7.45 (m, 4H), 7.16 (s, 1H), 6.97 (d, *J* = 16.0 Hz, 1H), 6.87 (d, *J* = 16.0 Hz, 1H), 6.47-6.44 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ: 160.99, 152.41, 150.13, 142.79, 130.40, 128.81, 127.32, 126.60, 126.37, 116.98, 111.95, 111.31, 110.05; HRMS (ESI) m/z: calcd for $C_{15}H_{12}NO_2$, $[M+H]^+$: 238.0790; Found: 238.0862.

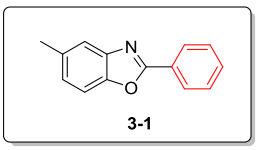
4. References

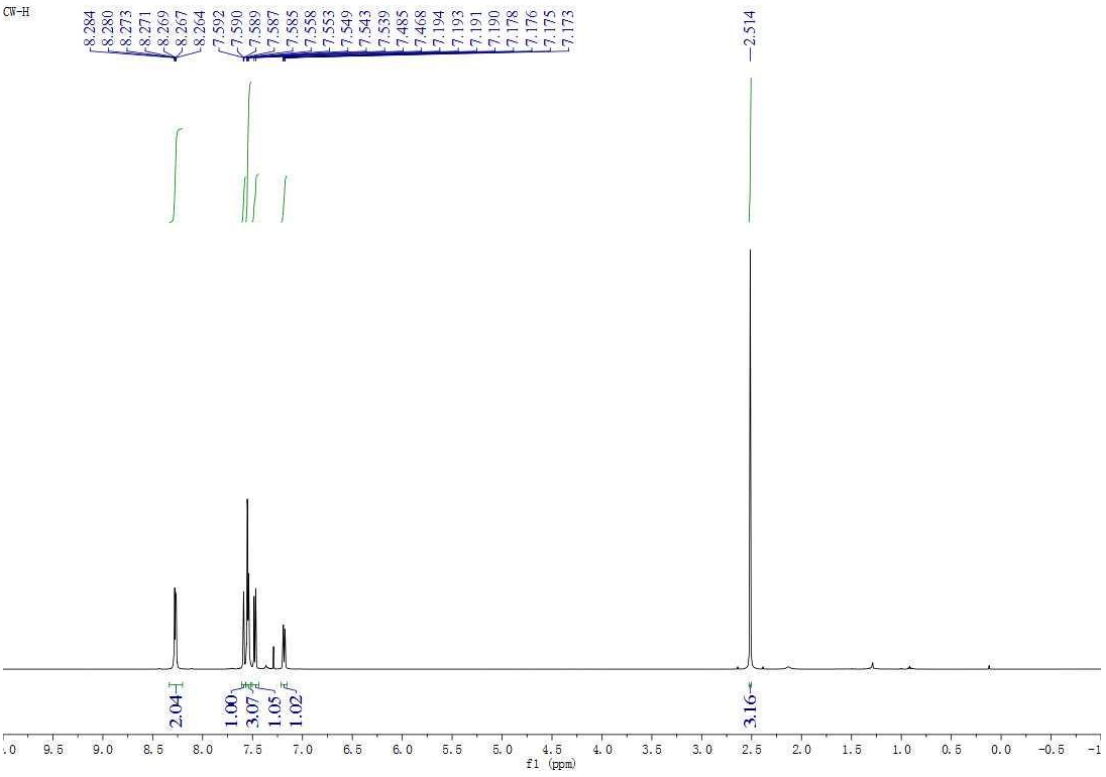
1. Meng, G.; Szostak, M. *Org. Lett.*, **2016**, *18*, 796.

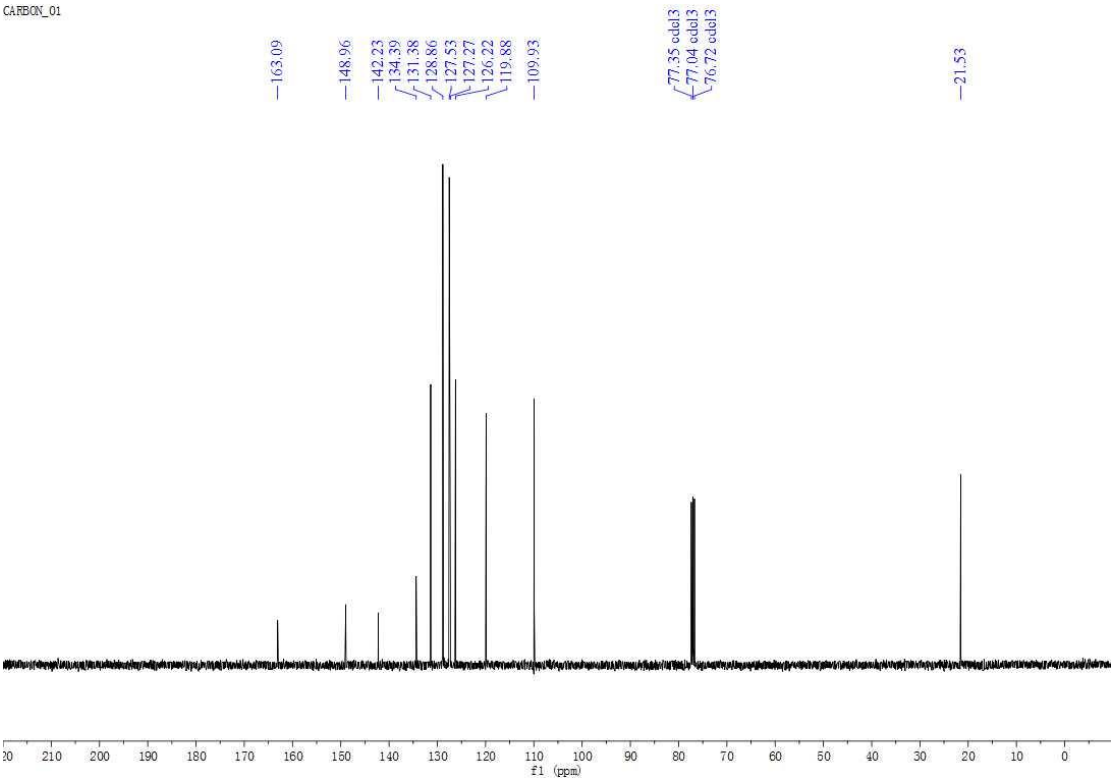
2 (a) Besselièvre, F.; Mahuteau-Betzer, F.; Grierson, D. S.; Piguel, S. *J. Org. Chem*. **2008**, *73*, 3278. (b) Li, Y.; Liu, J.; Xie, Y.; Zhang, R.; Jin, K.; Wang, X.; Duan. C. *Org. Biomol. Chem*. **2012**, *10*, 3715.

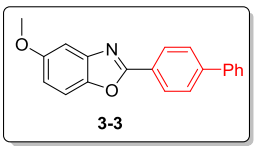
3. (a) Ohnmacht, S. A.; Mamone, P.; Culshaw, A. J.; Greaney, M. F. *Chem. Commun*. **2008**, 1241. (b) Jiang, H.; Huang, H.; Cao, H.; Qi, C. *Org. Lett*. **2010**, *12*, 5561. (c) Cheung, **C. W.**; Buchwald, S. L. *J. Org. Chem*. **2012**, *77*, 7526. (d) Tang, L.; Guo, X.; Yang, Y.; Zha, Z.; Wang, Z. *Chem. Commun*. **2014**, *50*, 6145. (e) Chatterjee, T.; Cho, J. Y.; Cho, E. J. *J. Org. Chem*. **2016**, *81*, 6995. (f) Meng, X.; Wang, Y.; Wang, Y.; Chen, B.; Jing, Z.; Chen, G.; Zhao, P. *J. Org. Chem*. **2017**, *82*, 6922. (g) Hanson, M. G.; Olson, N. M.; Yi, Z.; Wilson, G.; Kalyani. D. *Org. Lett.* **2017**, *19*, 4271.

5. 1H and 13C NMR spectra for compound 3

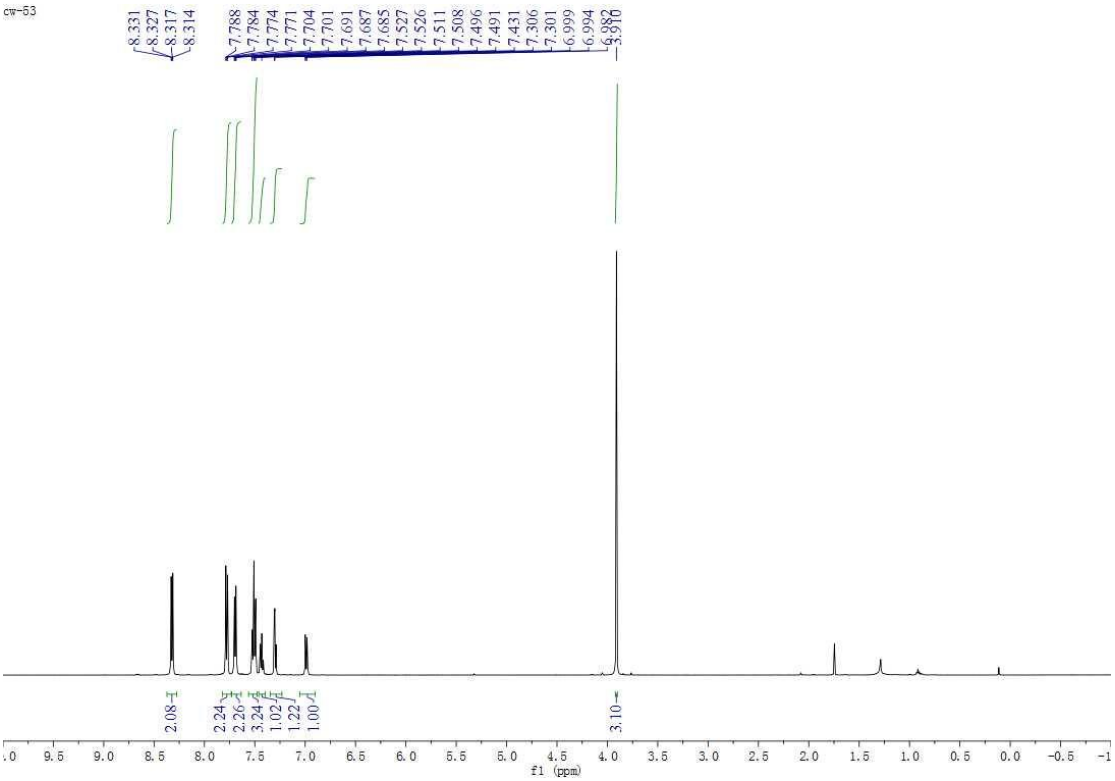


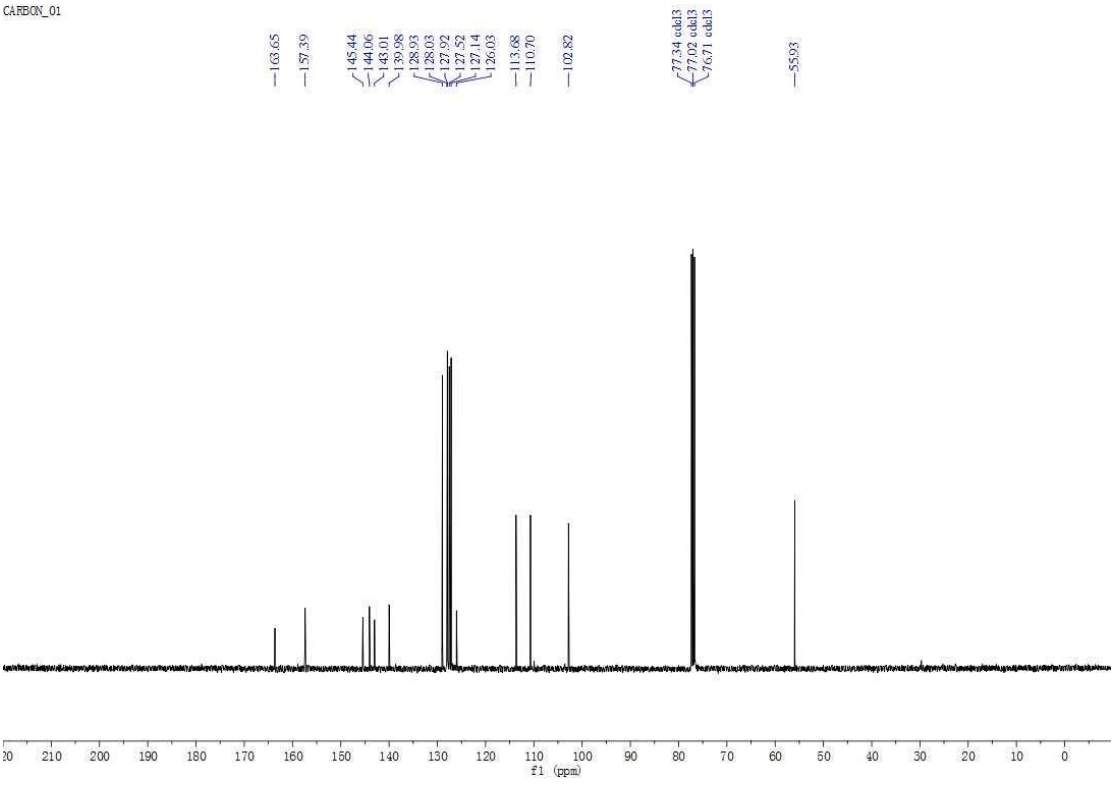


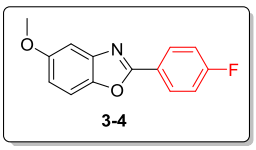



O
N
O
Ph

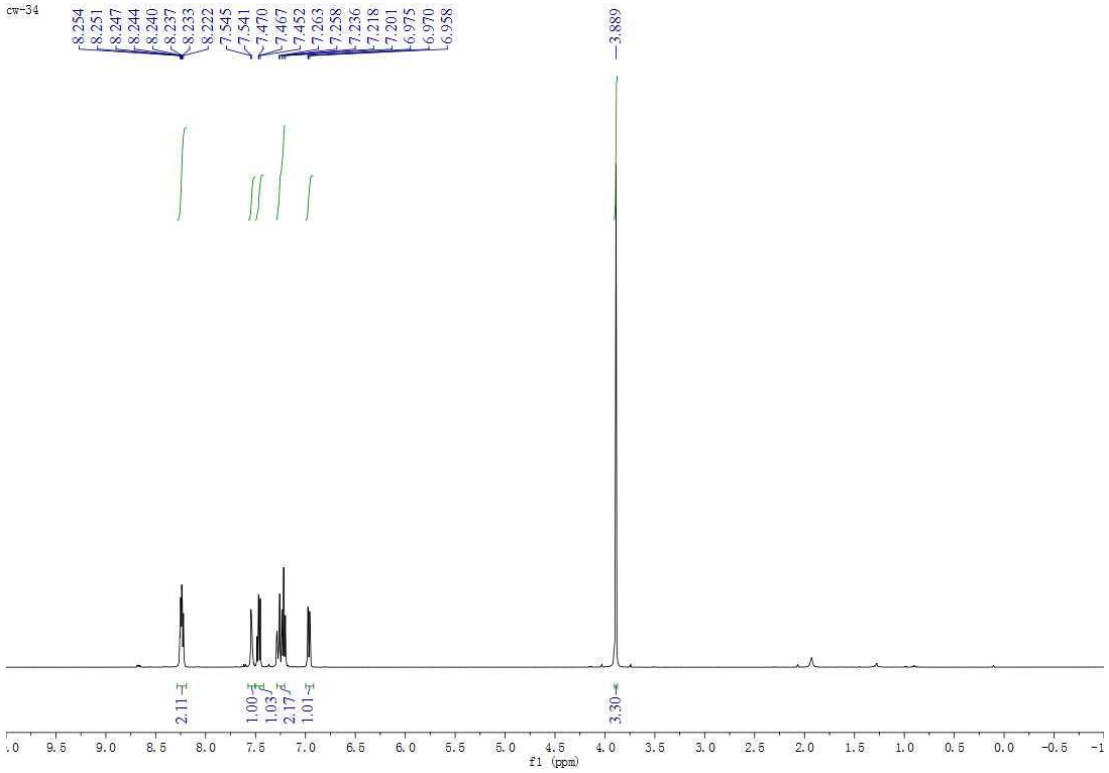
3-3


cw-53
8.331
8.327
8.317
8.314
7.788
7.784
7.774
7.771
7.704
7.701
7.691
7.687
7.685
7.527
7.526
7.511
7.508
7.496
7.491
7.431
7.306
7.301
6.999
6.994
6.982
3.910
2.08
2.24
2.26
3.24
1.02
1.22
1.00
3.10
f1 (ppm)


CARBON_01
163.65
157.39
145.44
144.06
143.01
139.98
128.93
128.03
127.92
127.52
127.14
126.03
113.68
110.70
102.82
77.34 cdcl3
77.02 cdcl3
76.71 cdcl3
55.93
f1 (ppm)


O
N
O
F

3-4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8.251
8.247
8.244
8.240
8.237
8.233
8.222
7.545
7.541
7.470
7.467
7.452
7.263
7.258
7.236
7.218
7.201
6.975
6.970
6.958
3.889
2.11
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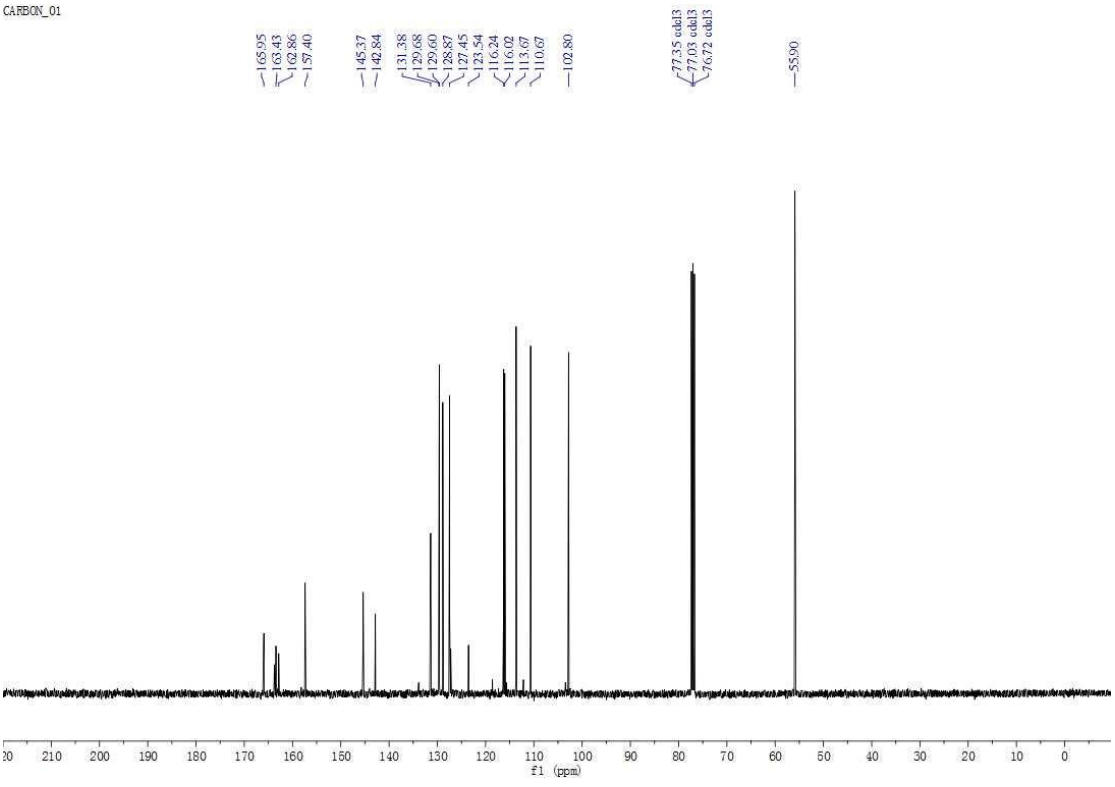
1.03
2.17
1.01
3.30
f1 (ppm)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163.43
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157.40
145.37
142.84
131.38
129.68
129.60
128.87
127.45
123.54
116.24
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113.67
110.67
102.80
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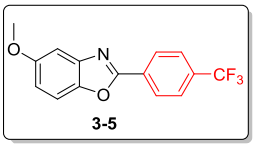
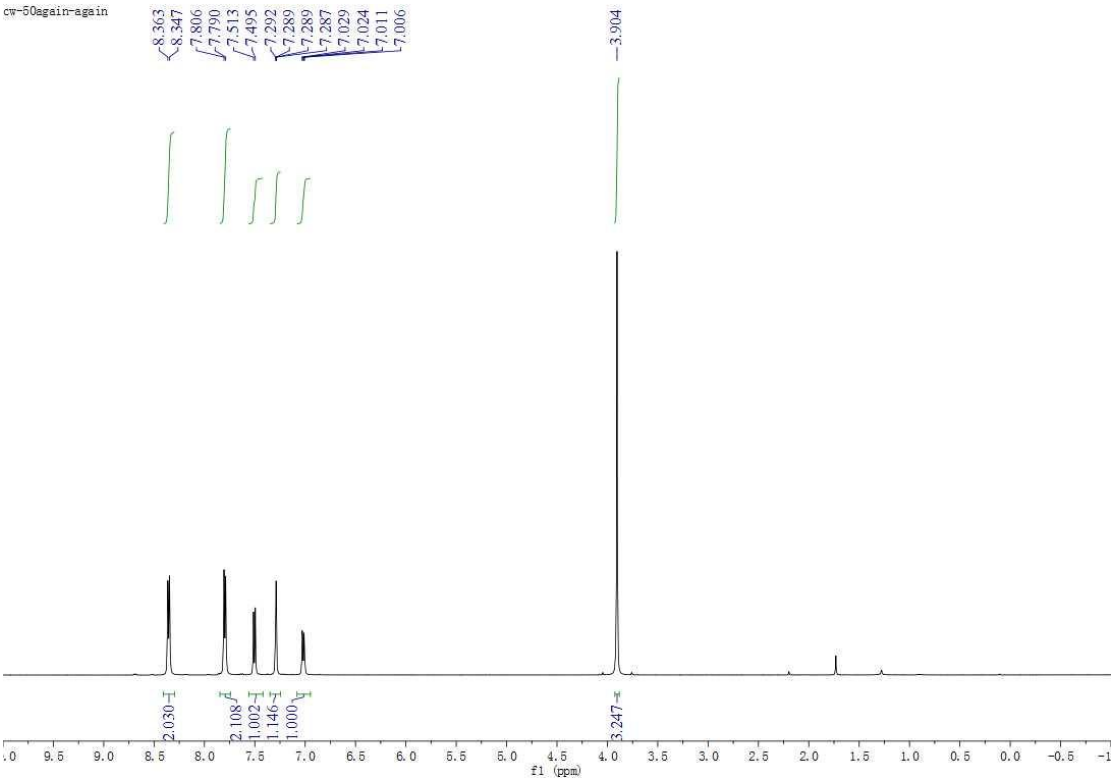
77.03 cdcl3
76.72 cdcl3
55.90
f1 (ppm)


O
N
O
CF3

3-5


cw-50again-again
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7.790
7.513
7.495
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7.289
7.289
7.287
7.029
7.024
7.011
7.006
3.904
2.030
2.108
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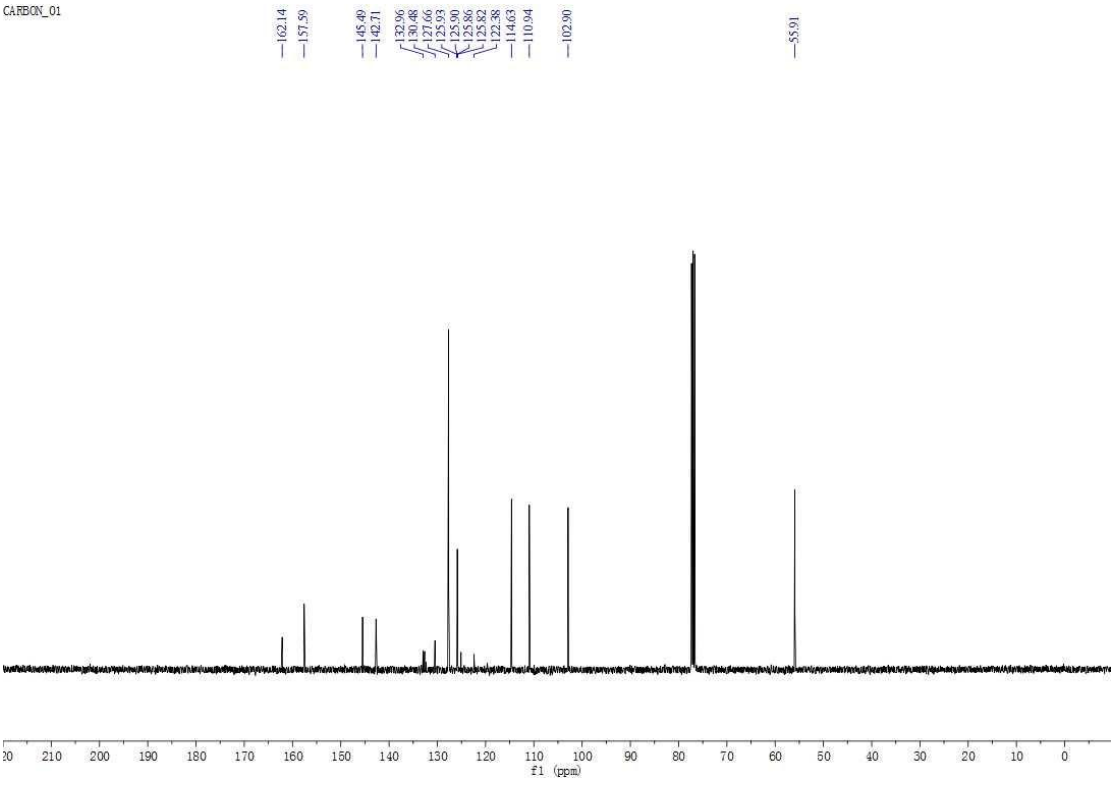
1.146
1.000
3.247
f1 (ppm)


CARBON_01
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127.66
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125.86
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110.94
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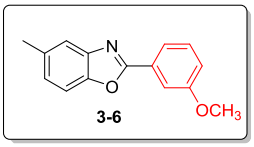
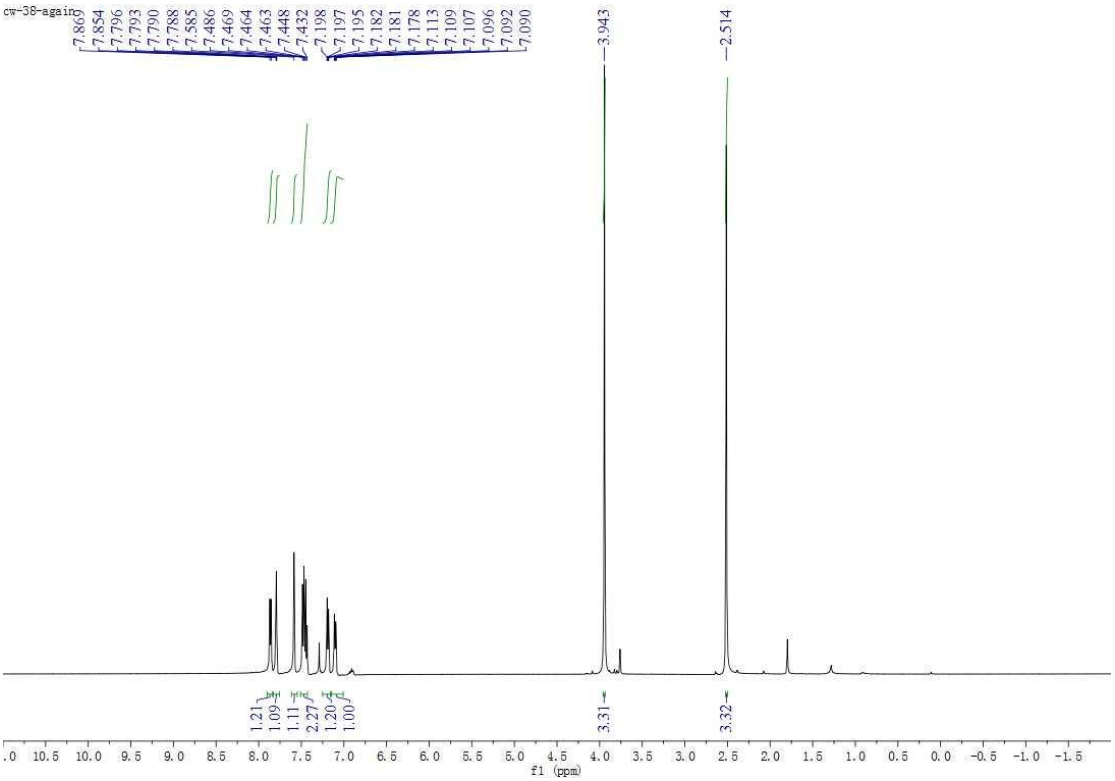
55.91
f1 (ppm)


N
O
OCH3

3-6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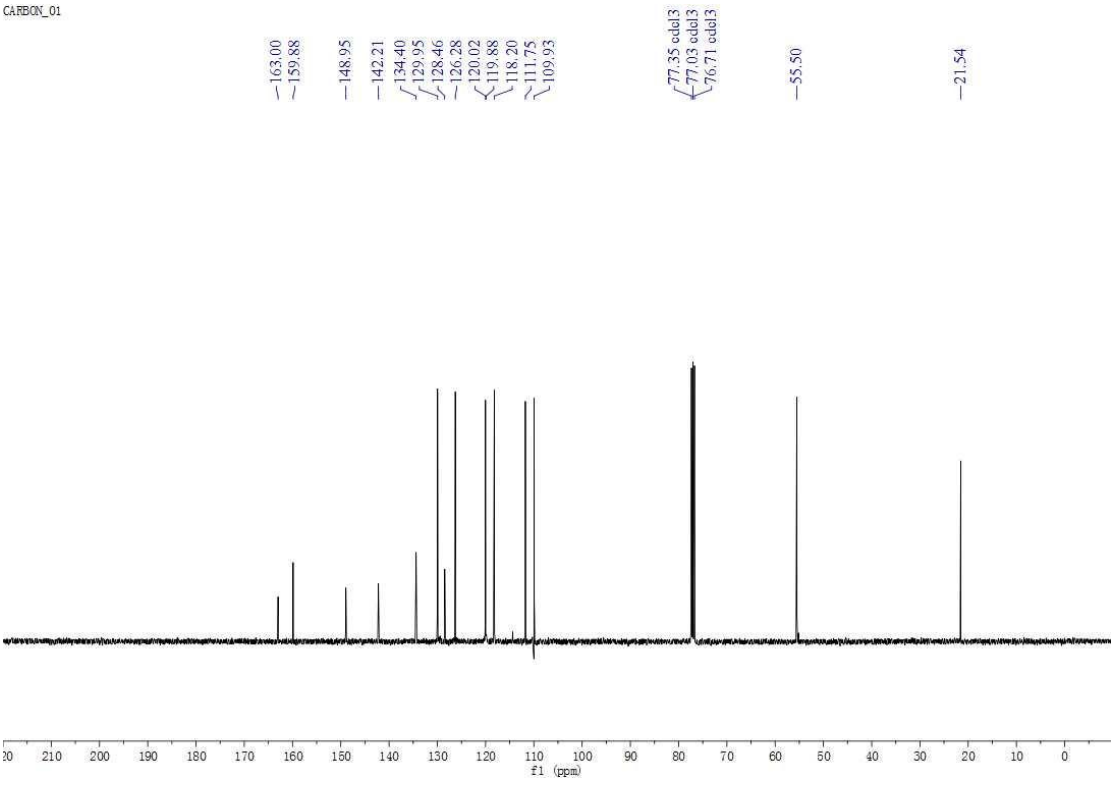
7.869
7.854
7.796
7.793
7.790
7.788
7.585
7.486
7.469
7.464
7.463
7.448
7.432
7.198
7.197
7.195
7.182
7.181
7.178
7.113
7.109
7.107
7.096
7.092
7.090
3.943
2.514
1.21
1.09
1.11
2.27
1.20
1.00
3.31
3.32
f1 (ppm)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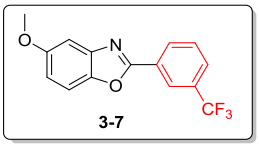
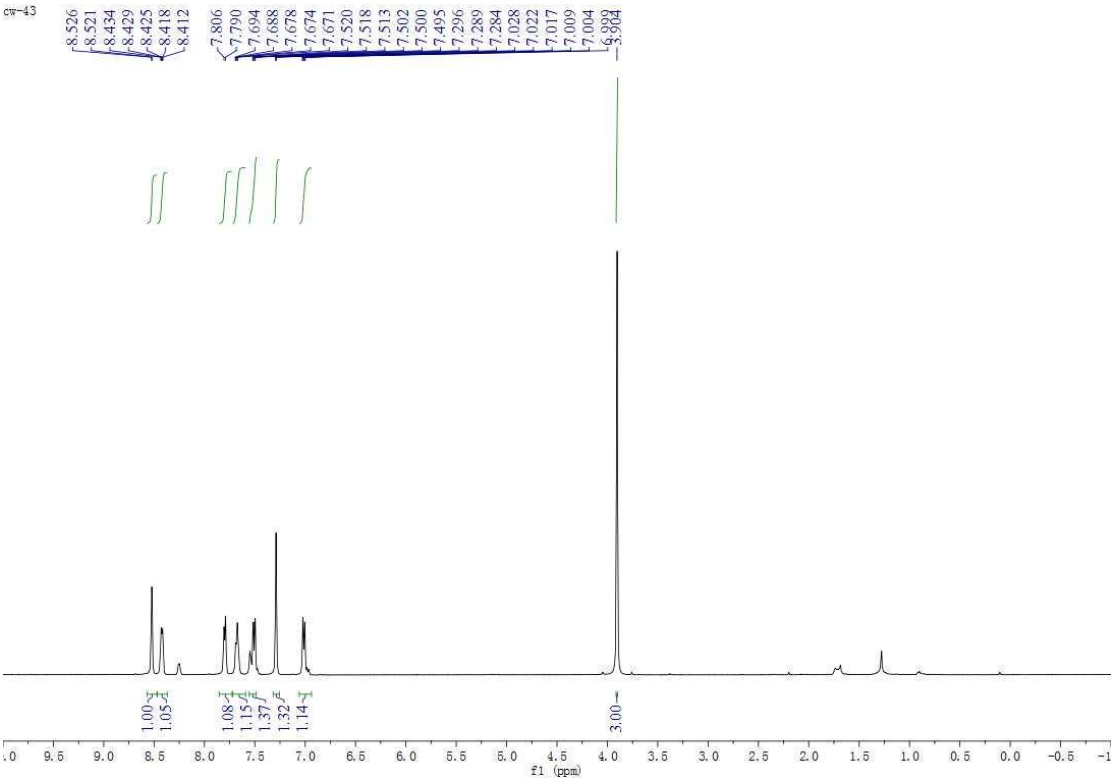
21.54
f1 (ppm)


O
N
O
CF3

3-7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8.425
8.418
8.412
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7.790
7.694
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7.674
7.671
7.520
7.518
7.513
7.502
7.500
7.495
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7.289
7.284
7.028
7.022
7.017
7.009
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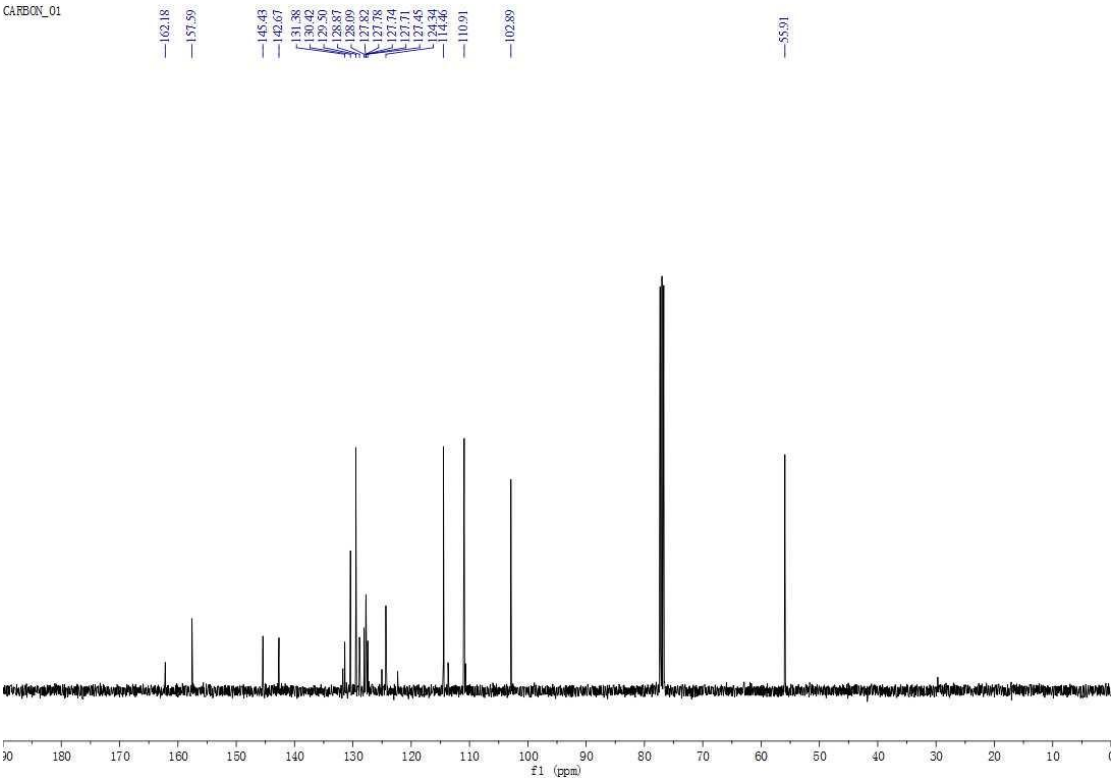
1.32
1.14
3.00
f1 (ppm)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110.91
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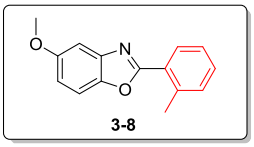
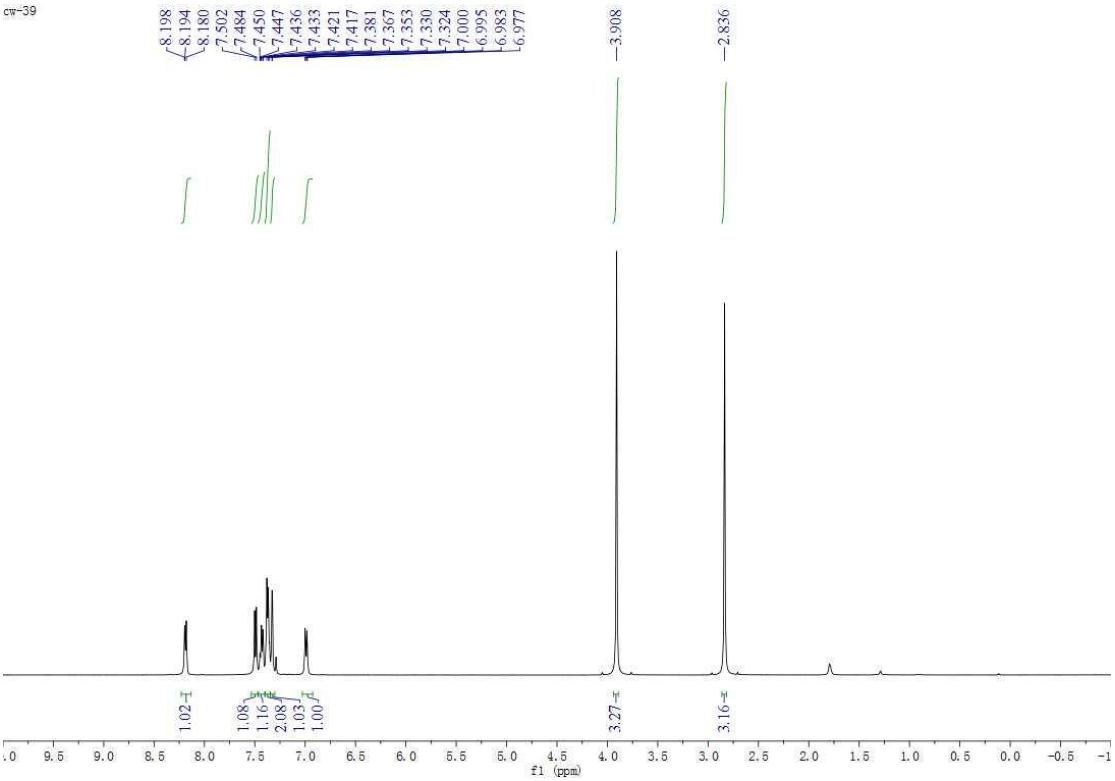
55.91
f1 (ppm)


O
N
O

3-8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7.367
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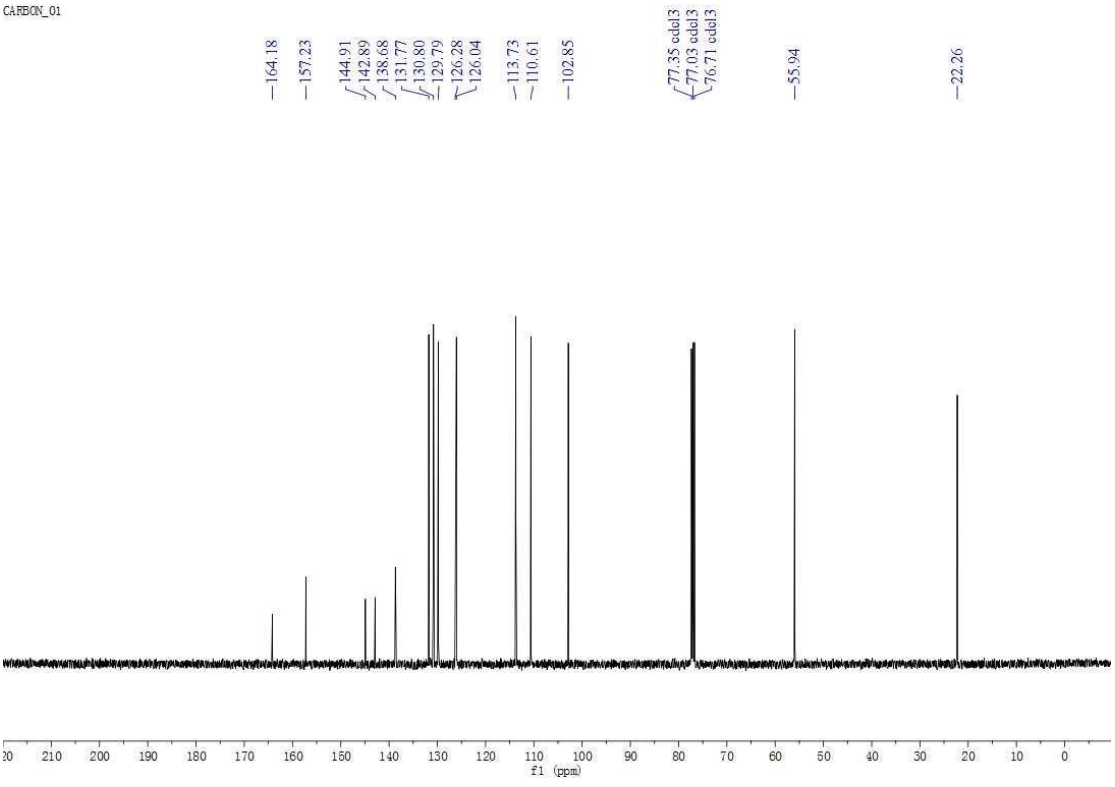
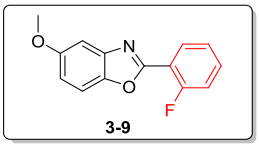
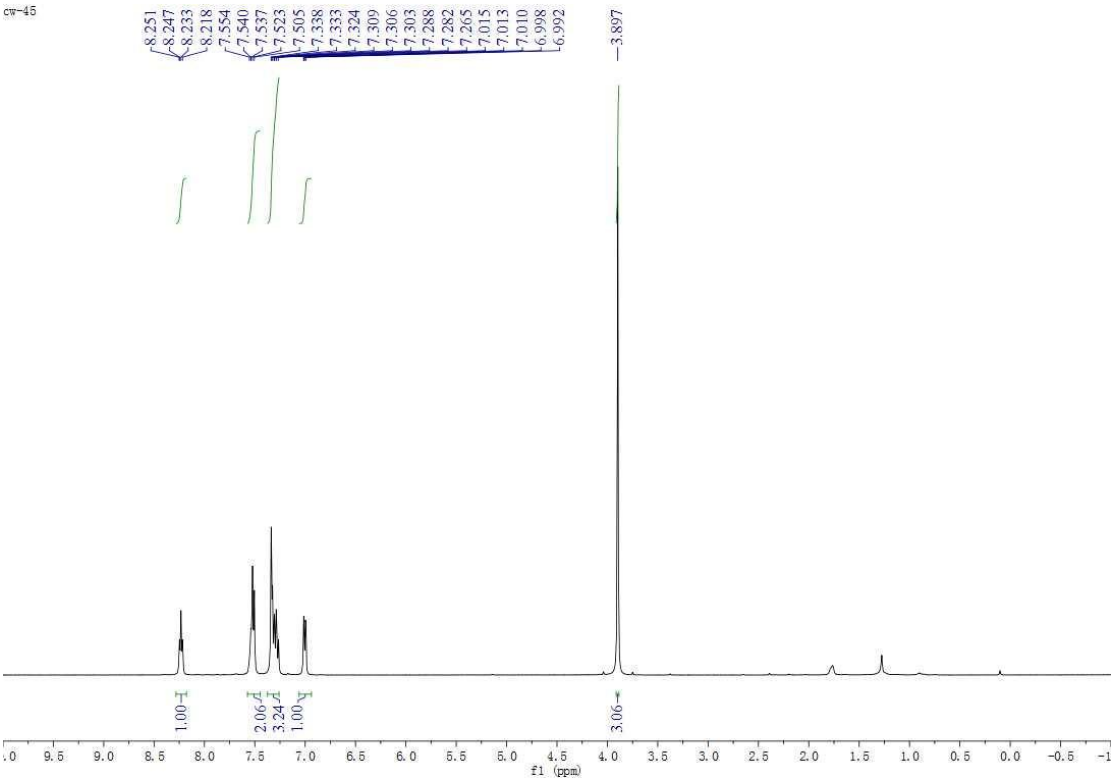
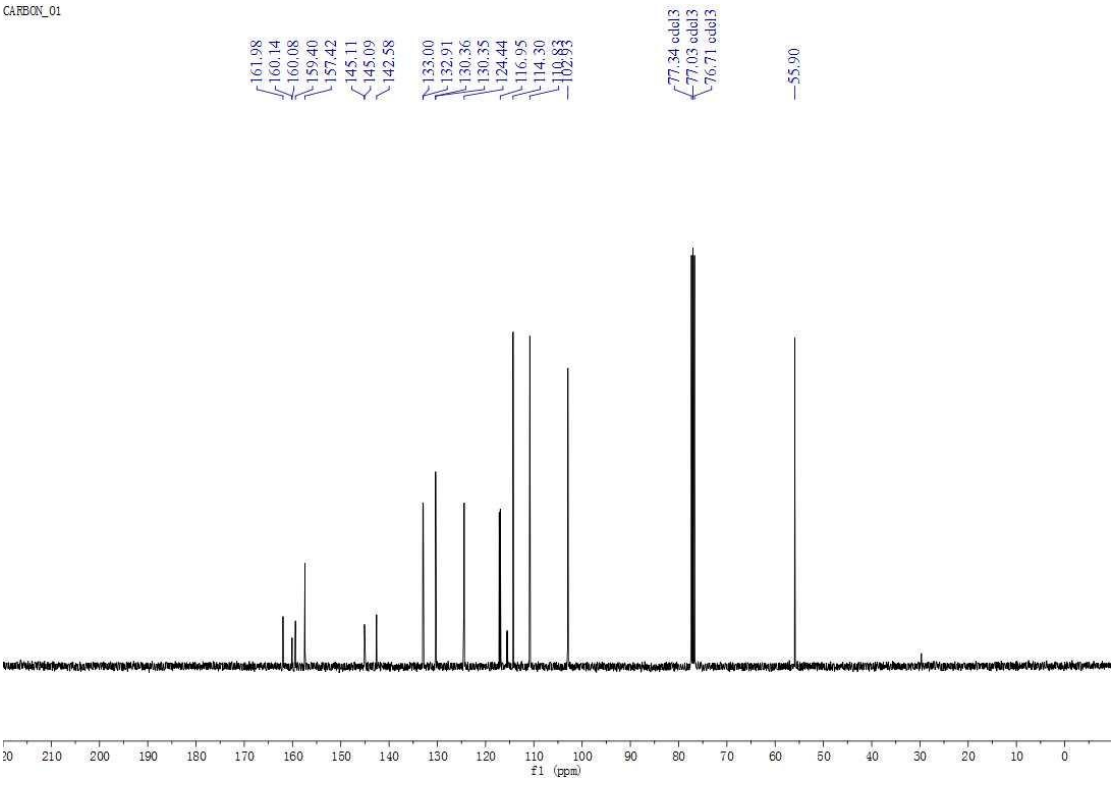
7.330
7.324
7.000
6.995
6.983
6.977
3.908
2.836
1.02
1.08
1.16
2.08
1.03
1.00
3.27
3.16
f1 (ppm)

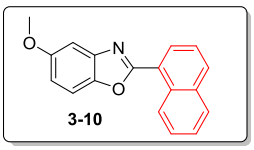

CARBON_01
164.18
157.23
144.91
142.89
138.68
131.77
130.80
129.79
126.28
126.04
113.73
110.61
102.85
77.35 cdcl3
77.03 cdcl3
76.71 cdcl3
55.94
22.26
f1 (ppm)


O
N
O
F

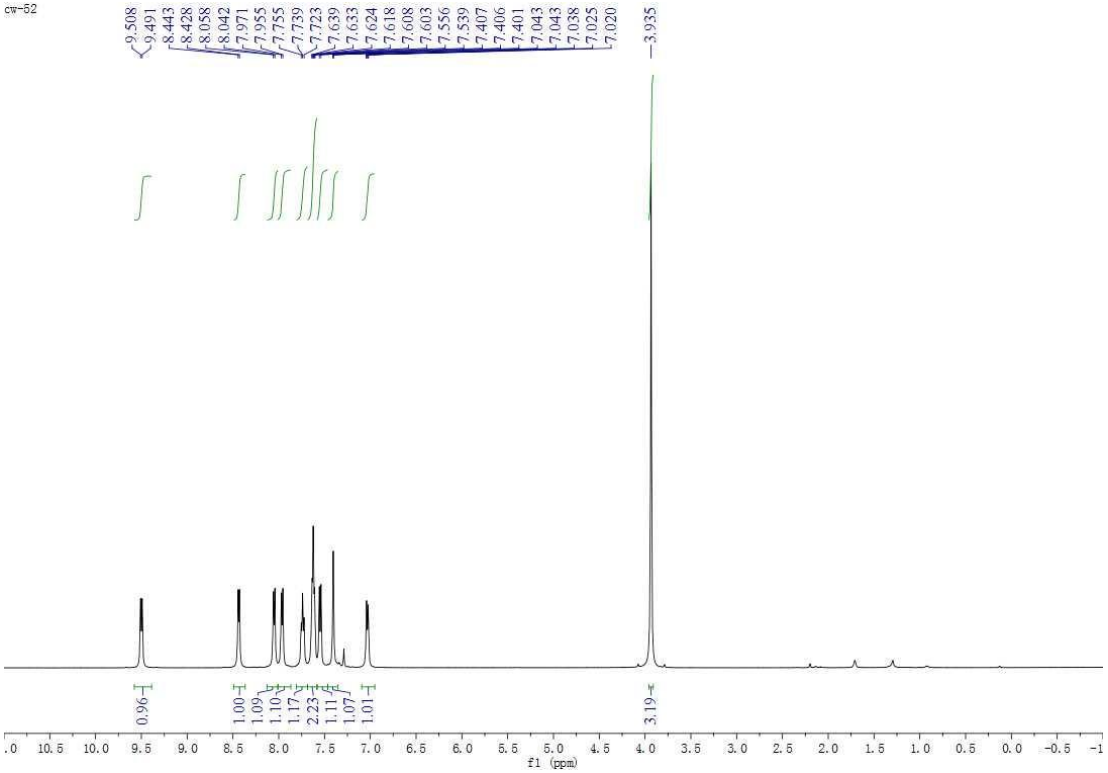
3-9

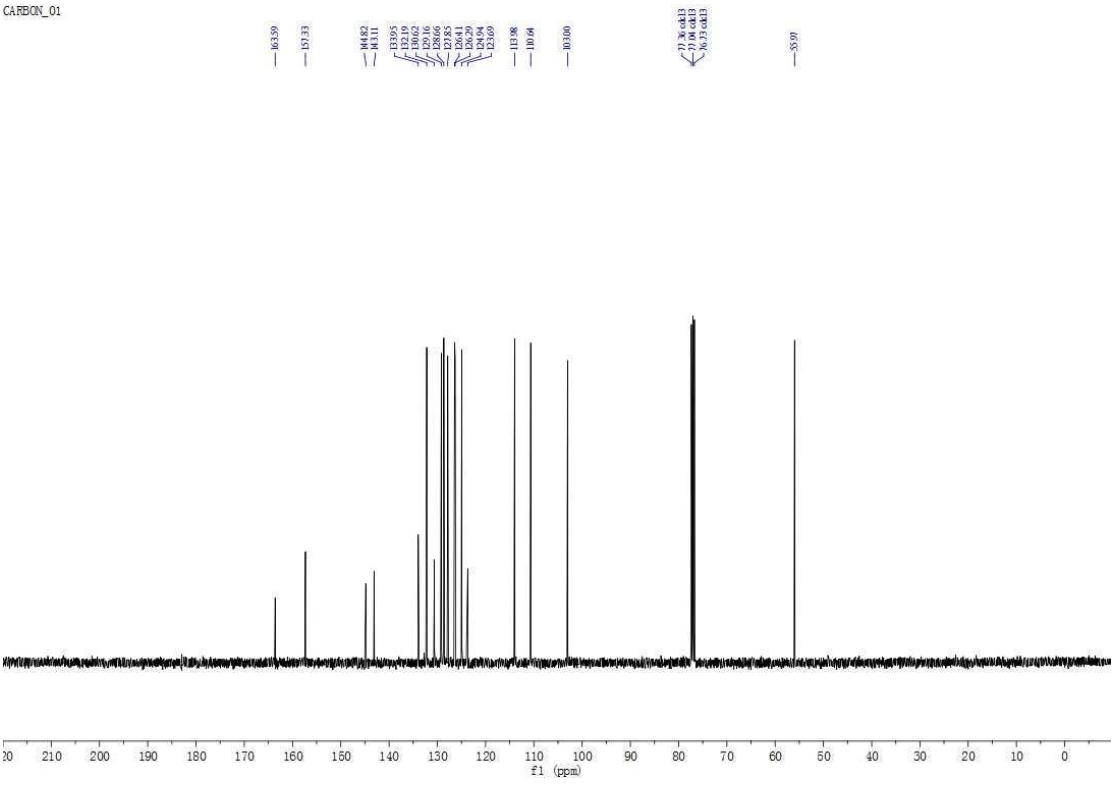

cw-45
8.251
8.247
8.233
8.218
7.554
7.540
7.537
7.523
7.505
7.338
7.333
7.324
7.309
7.306
7.303
7.288
7.282
7.265
7.015
7.013
7.010
6.998
6.992
3.897
1.00
2.06
3.24
1.00
3.06
f1 (ppm)

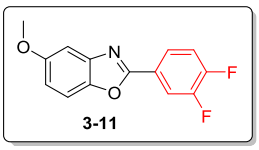

CARBON_01
161.98
160.14
160.08
159.40
157.42
145.11
145.09
142.58
133.00
132.91
130.36
130.35
124.44
116.95
114.30
77.34 cdcl3
77.03 cdcl3
76.71 cdcl3
55.90
f1 (ppm)


O
N
O

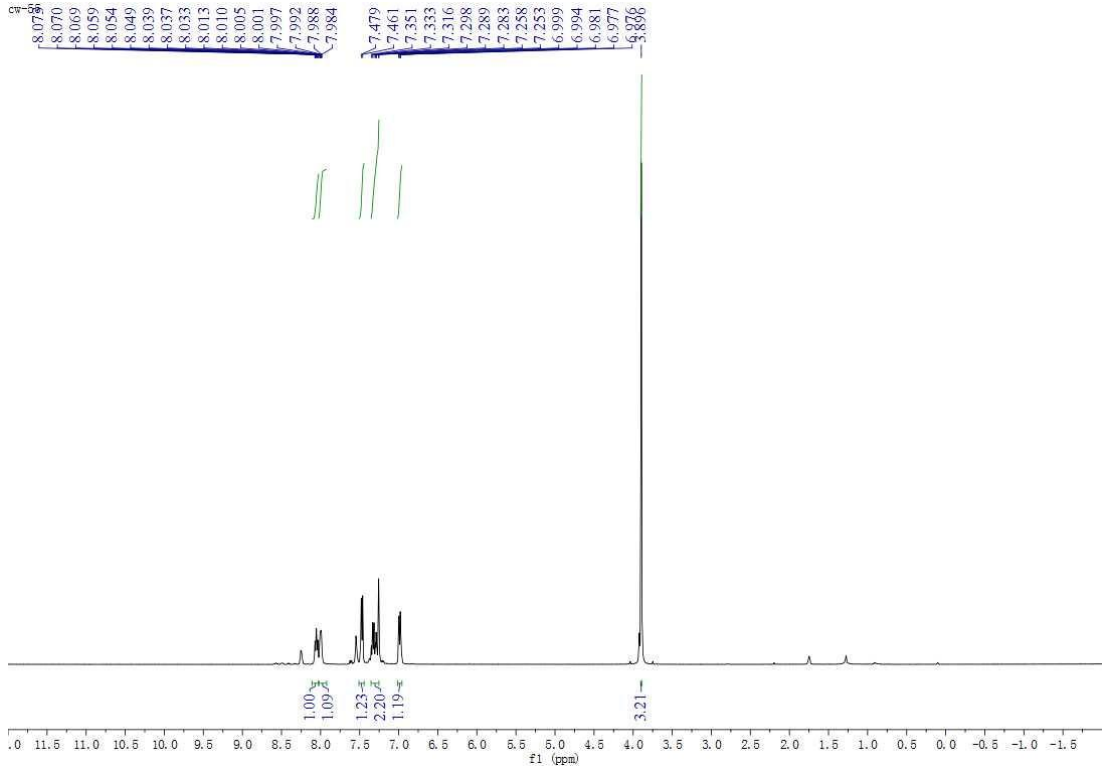
3-10

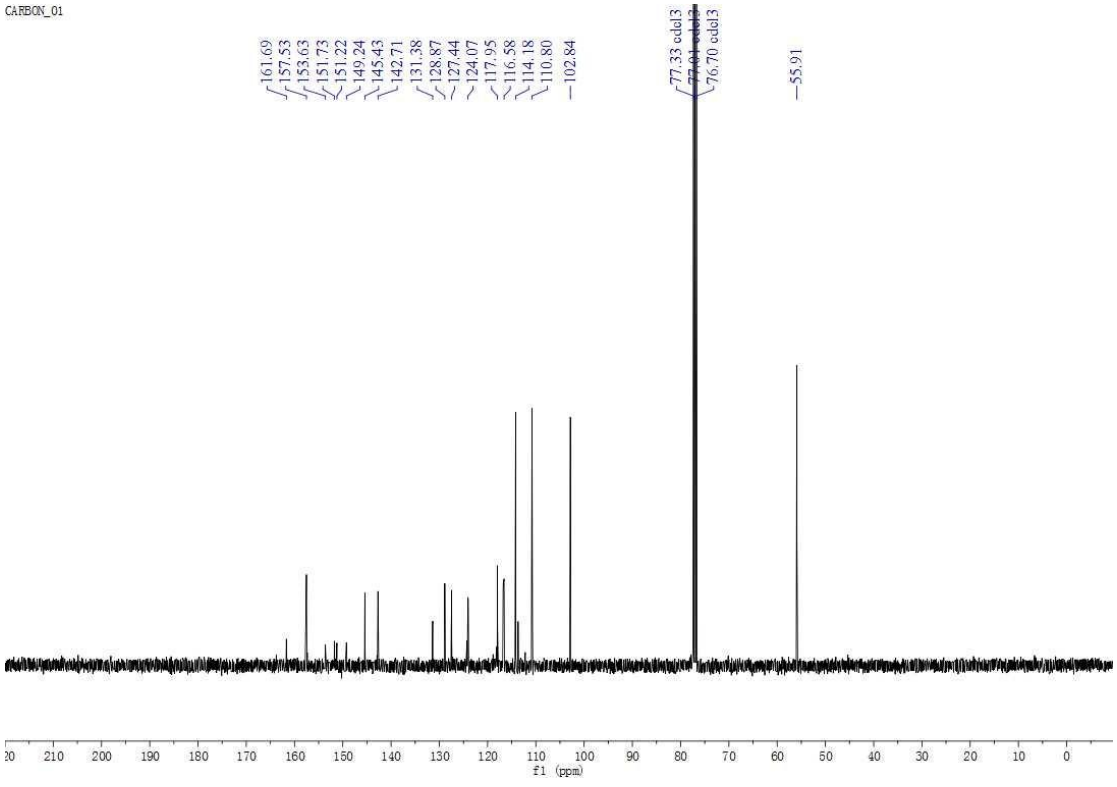

cw-52
9.508
9.491
8.443
8.428
8.058
8.042
7.971
7.955
7.755
7.739
7.723
7.639
7.633
7.624
7.618
7.608
7.603
7.556
7.539
7.407
7.406
7.401
7.043
7.043
7.038
7.025
7.020
3.935
0.96
1.00
1.09
1.10
1.17
2.23
1.11
1.07
1.01
3.19
f1 (ppm)

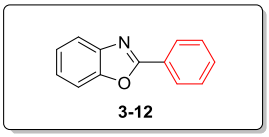

CARBON_01
163.59
157.33
144.82
143.11
133.95
132.19
130.62
129.16
128.66
127.85
126.41
126.29
124.94
123.69
113.98
110.64
103.00
77.36 cdcl3
77.04 cdcl3
76.73 cdcl3
55.91
f1 (ppm)


O
N
O
F
F

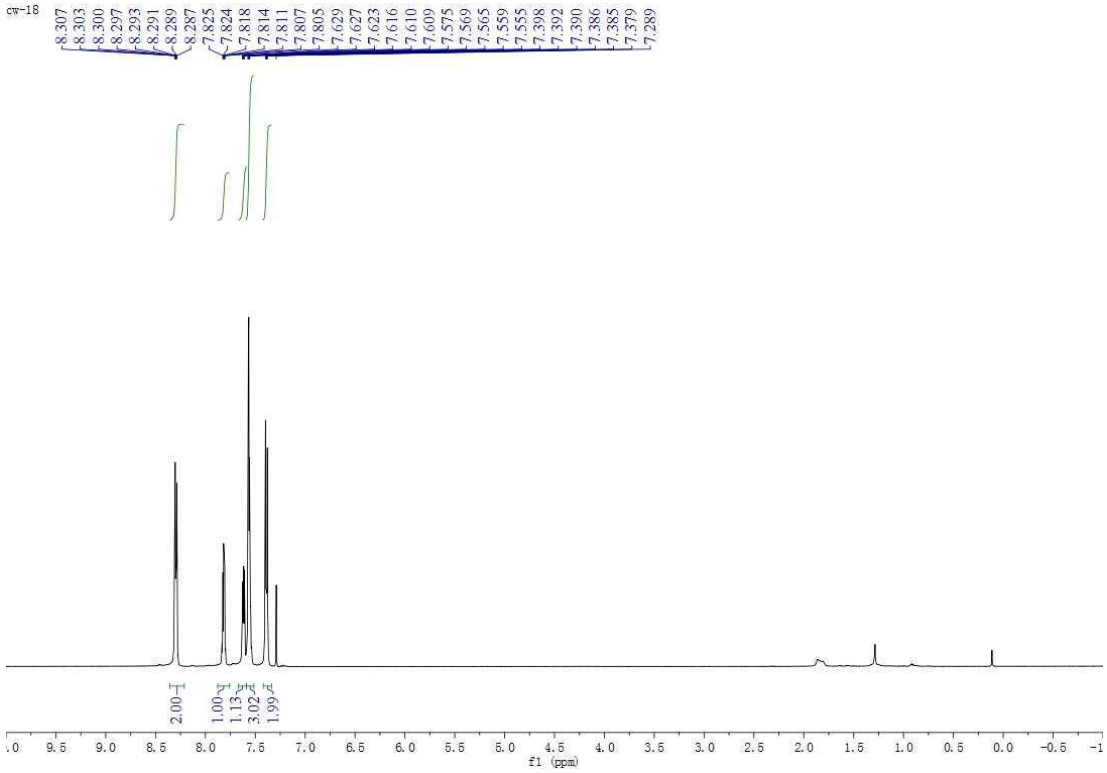
3-11

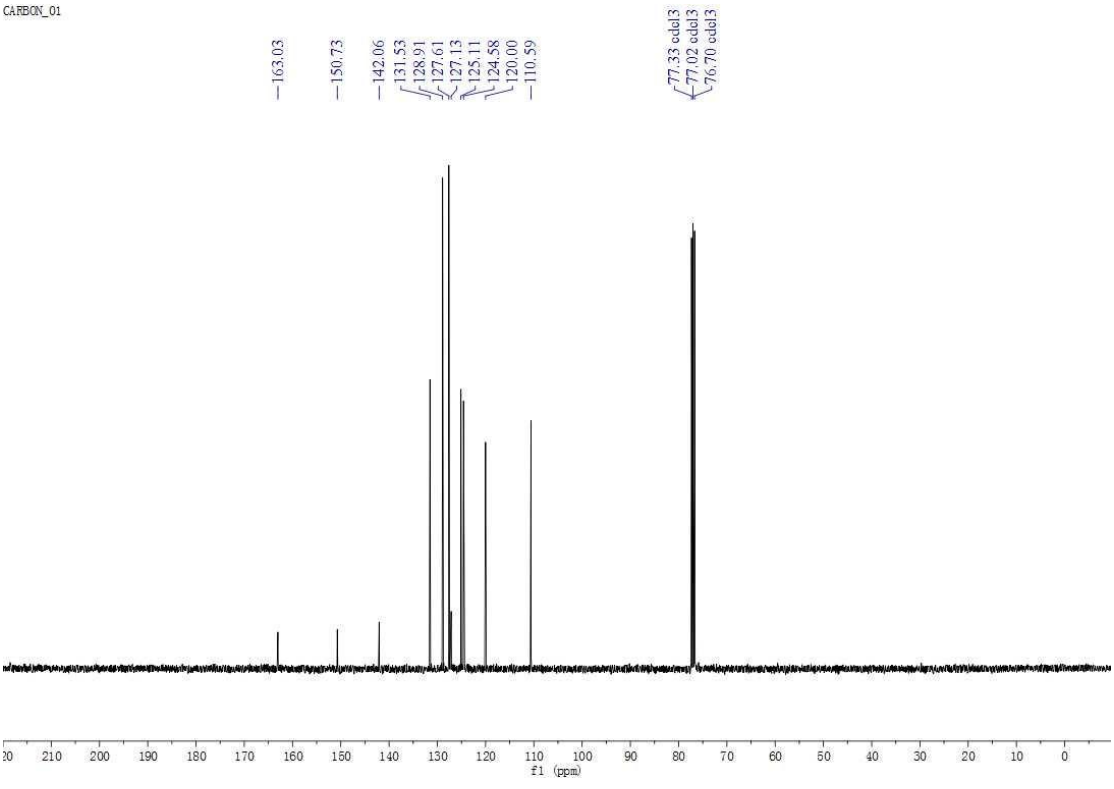

8.079
8.070
8.069
8.059
8.054
8.049
8.039
8.037
8.033
8.013
8.010
8.005
8.001
7.997
7.992
7.988
7.984
7.479
7.461
7.351
7.333
7.316
7.298
7.289
7.283
7.258
7.253
6.999
6.994
6.981
6.977
3.896
1.00
1.09
1.23
2.20
1.19
3.21
f1 (ppm)

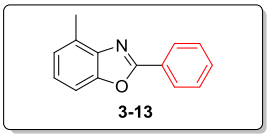

CARBON_01
161.69
157.53
153.63
151.73
151.22
149.24
145.43
142.71
131.38
128.87
127.44
124.07
117.95
116.58
114.18
110.80
102.84
77.33 cdcl3
77.01 cdcl3
76.70 cdcl3
55.91
f1 (ppm)



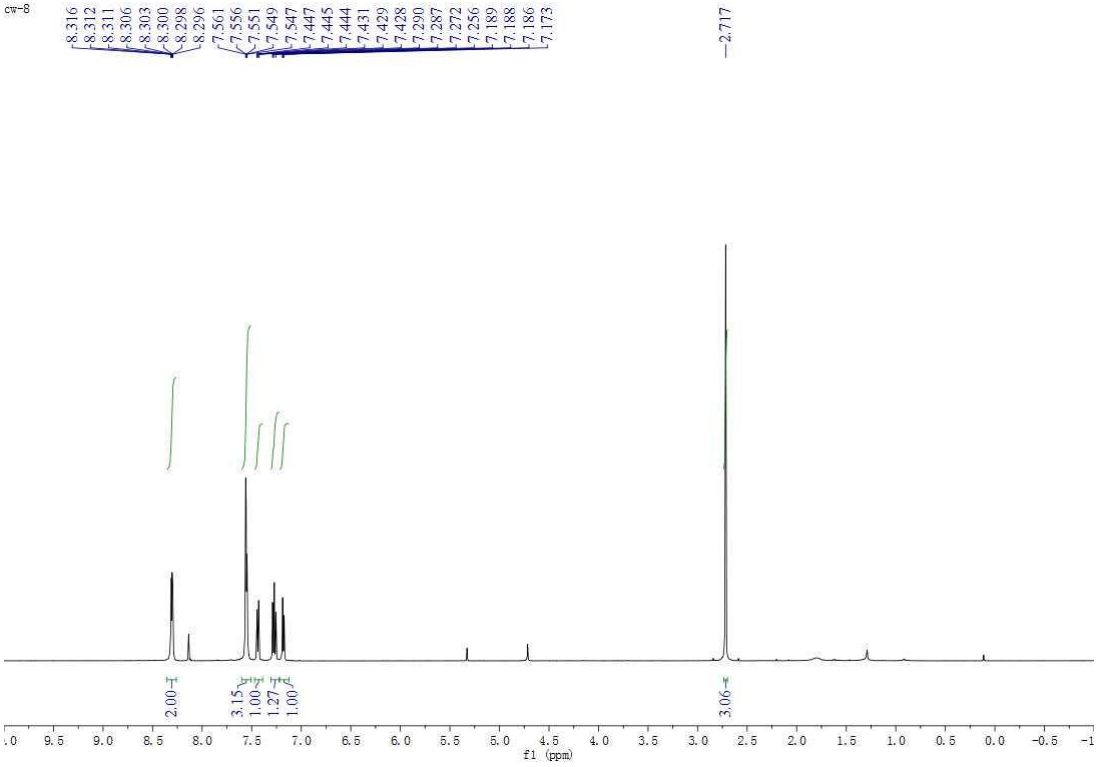
3-12

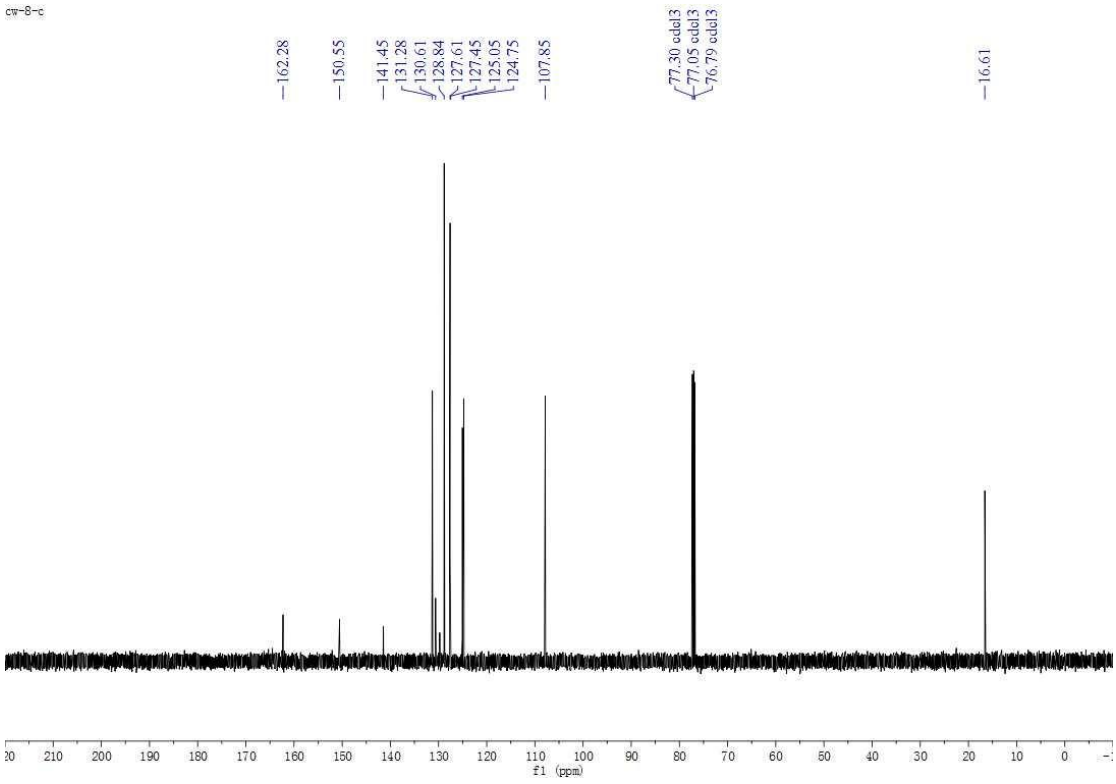

cw-18
8.307
8.303
8.300
8.297
8.293
8.291
8.289
8.287
7.825
7.824
7.818
7.814
7.811
7.807
7.805
7.629
7.627
7.623
7.616
7.610
7.609
7.575
7.569
7.565
7.559
7.555
7.398
7.392
7.390
7.386
7.385
7.379
7.289
2.00
1.00
1.13
3.02
1.99
f1 (ppm)

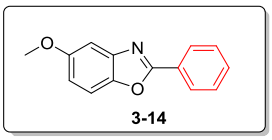

CARBON_01
163.03
150.73
142.06
131.53
128.91
127.61
127.13
125.11
124.58
120.00
110.59
77.33 cdcl3
77.02 cdcl3
76.70 cdcl3
f1 (ppm)


N
O

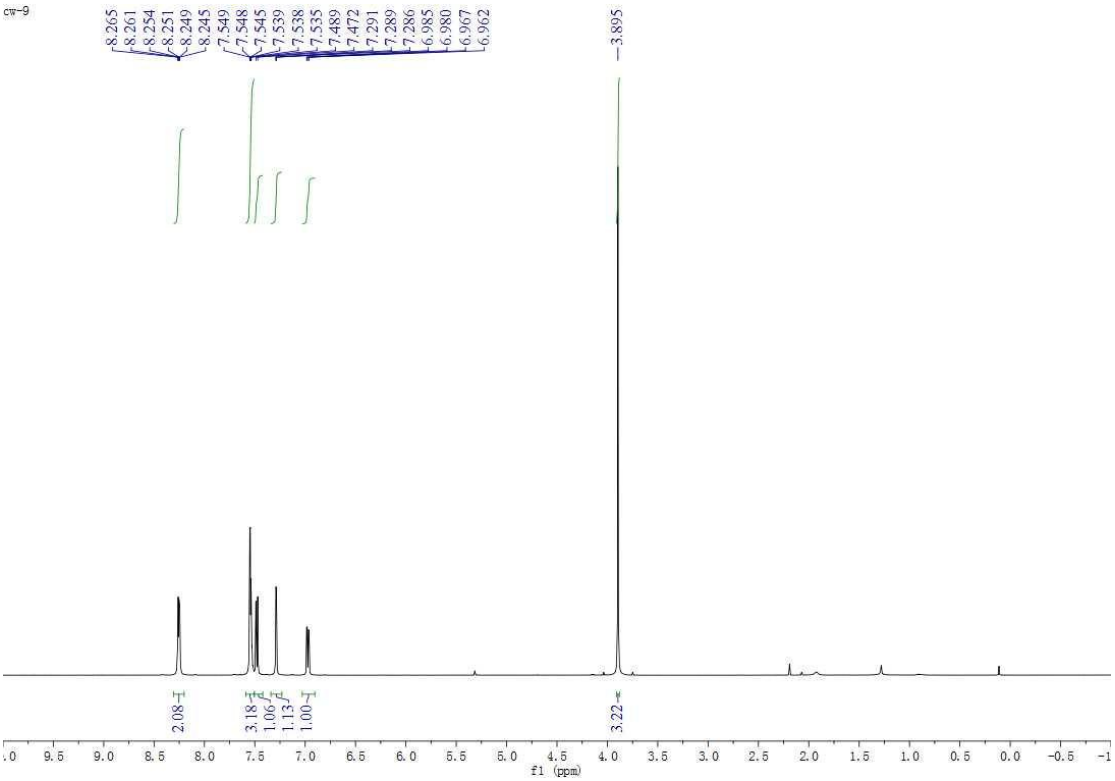
3-13

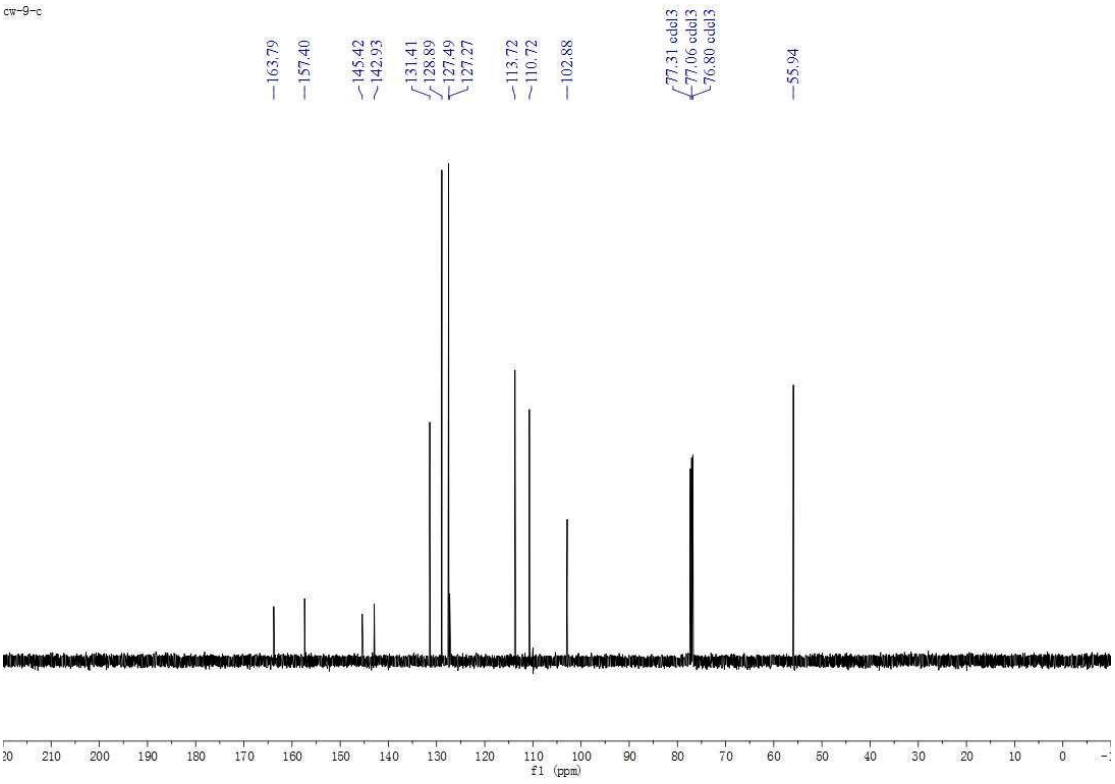

cw-8
8.316
8.312
8.311
8.306
8.303
8.300
8.298
8.296
7.561
7.556
7.551
7.549
7.547
7.447
7.445
7.444
7.431
7.429
7.428
7.290
7.287
7.272
7.256
7.189
7.188
7.186
7.173
2.717
2.00
3.15
1.00
1.27
1.00
3.06
f1 (ppm)

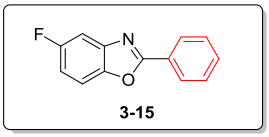

cw-8-c
162.28
150.55
141.45
131.28
130.61
128.84
127.61
127.45
125.05
124.75
107.85
77.30 cdcl3
77.05 cdcl3
76.79 cdcl3
16.61
f1 (ppm)



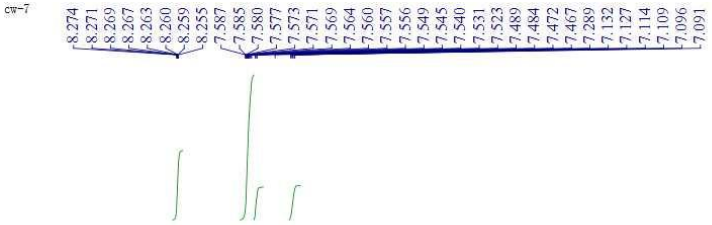
3-14

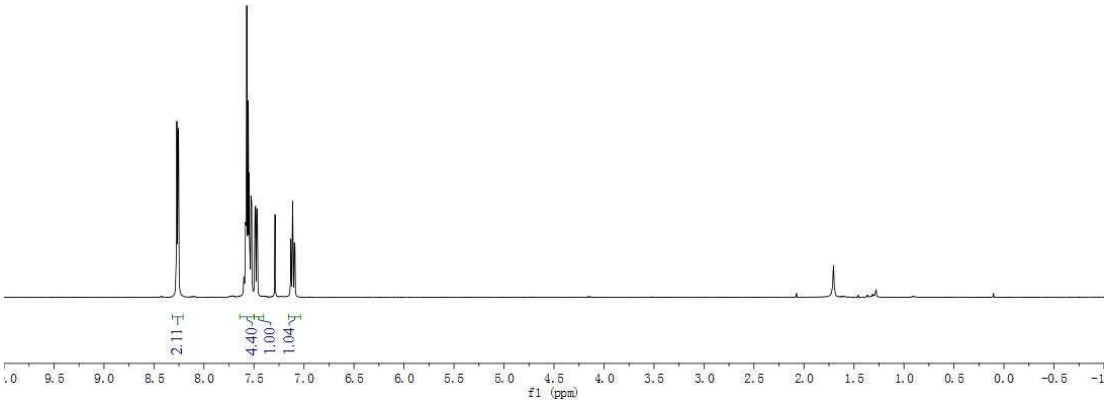

cw-9
8.265
8.261
8.254
8.251
8.249
8.245
7.549
7.548
7.545
7.539
7.538
7.535
7.489
7.472
7.291
7.289
7.286
6.985
6.980
6.967
6.962
3.895
2.08
3.18
1.06
1.13
1.00
3.22
f1 (ppm)

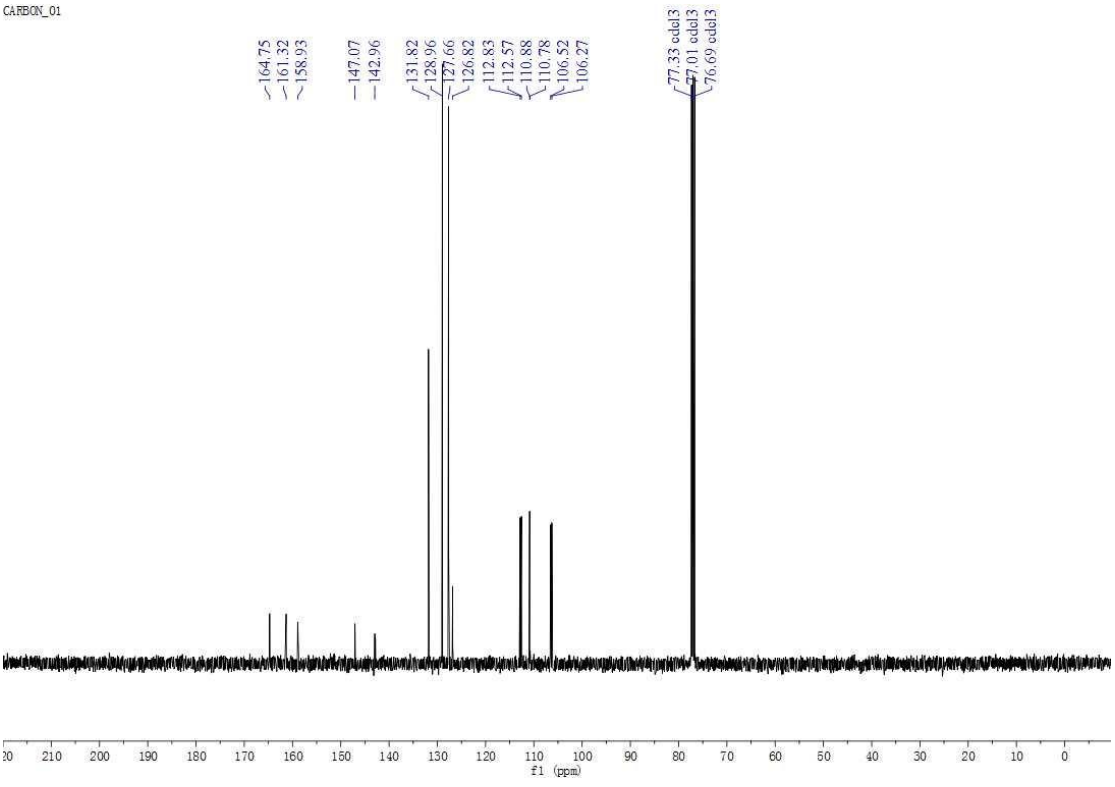

cw-9-c
163.79
157.40
145.42
142.93
131.41
128.89
127.49
127.27
113.72
110.72
102.88
77.31 cdcl3
77.06 cdcl3
76.80 cdcl3
55.94
f1 (ppm)

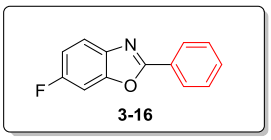

F
N
O

3-15

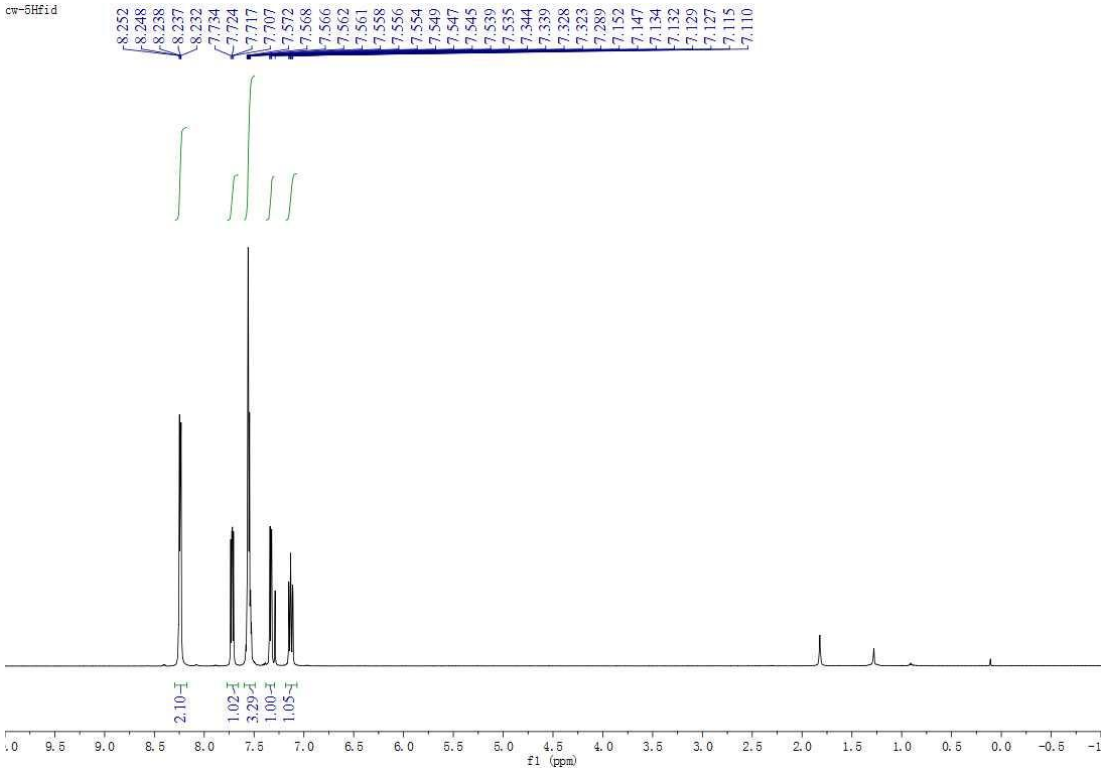

cw-7
8.274
8.271
8.269
8.267
8.263
8.260
8.259
8.255
7.587
7.585
7.580
7.577
7.573
7.571
7.569
7.564
7.560
7.557
7.556
7.549
7.545
7.540
7.531
7.523
7.489
7.484
7.472
7.467
7.289
7.132
7.127
7.114
7.109
7.096
7.091

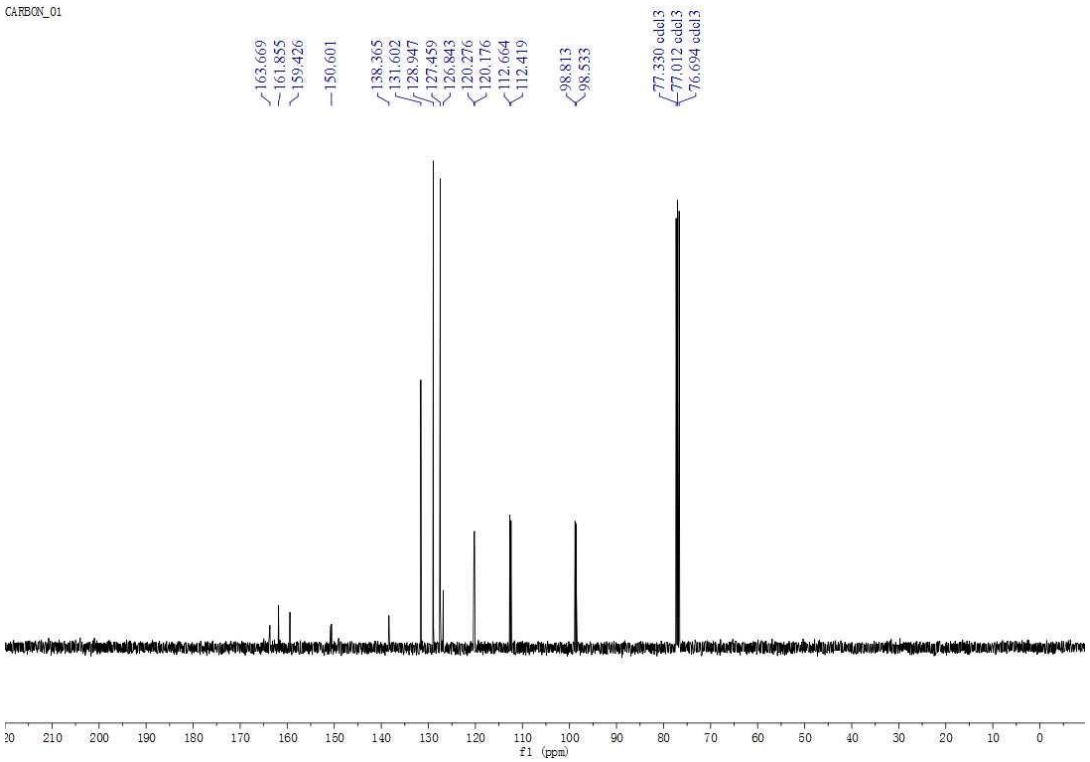

2.11
4.40
1.00
1.04
f1 (ppm)

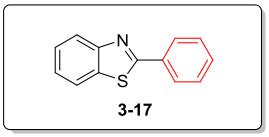

CARBON_01
164.75
161.32
158.93
147.07
142.96
131.82
128.96
127.66
126.82
112.83
112.57
110.88
110.78
106.52
106.27
77.33 cdcl3
77.01 cdcl3
76.69 cdcl3
f1 (ppm)


N
O
F

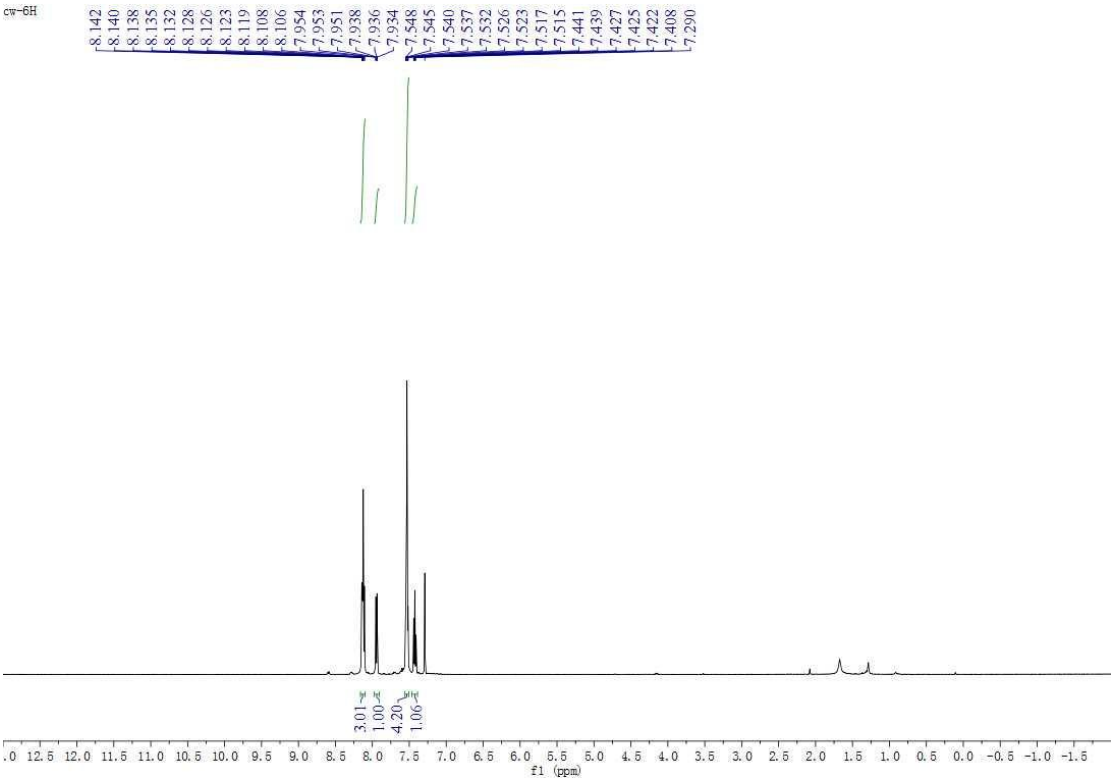
3-16

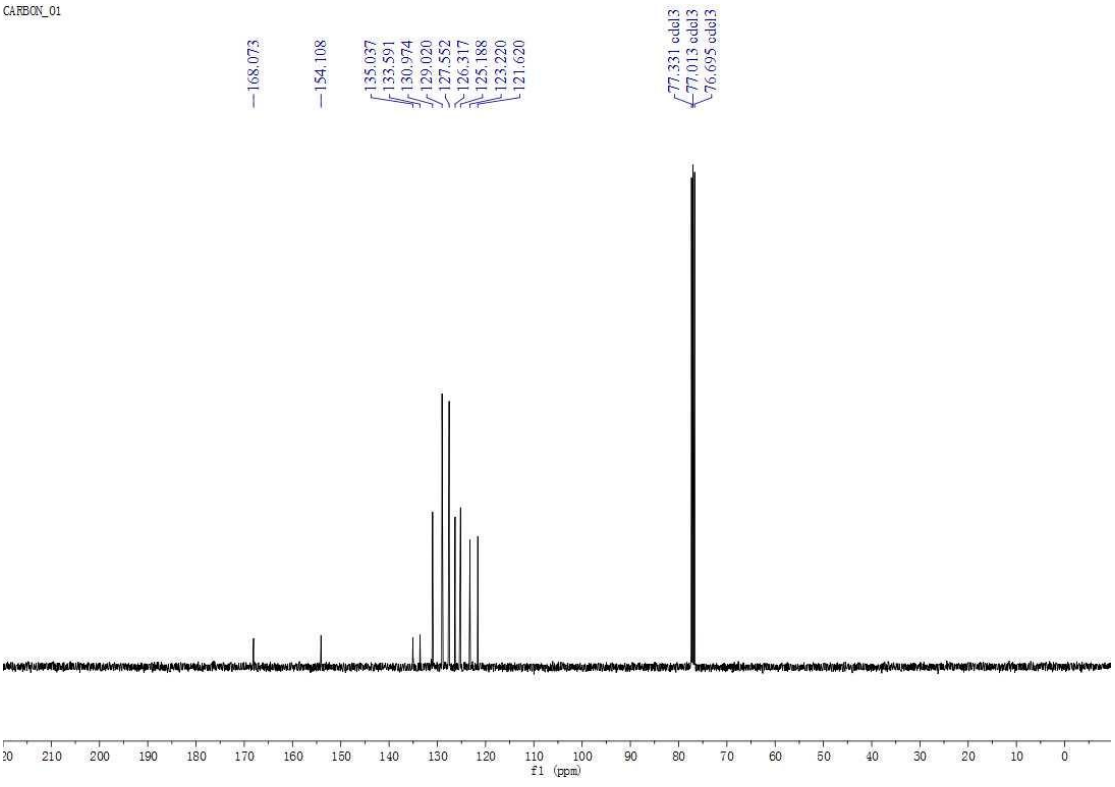

cw-5Hfid
8.252
8.248
8.238
8.237
8.232
7.734
7.724
7.717
7.707
7.572
7.568
7.566
7.562
7.561
7.558
7.556
7.554
7.549
7.547
7.545
7.539
7.535
7.344
7.339
7.328
7.323
7.289
7.152
7.147
7.134
7.132
7.129
7.127
7.115
7.110
2.10
1.02
3.29
1.00
1.05
f1 (ppm)

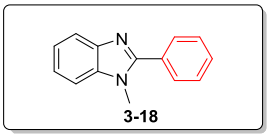

CARBON_01
163.669
161.855
159.426
150.601
138.365
131.602
128.947
127.459
126.843
120.276
120.176
112.664
112.419
98.813
98.533
77.330 cdcl3
77.012 cdcl3
76.694 cdcl3
f1 (ppm)


N
S

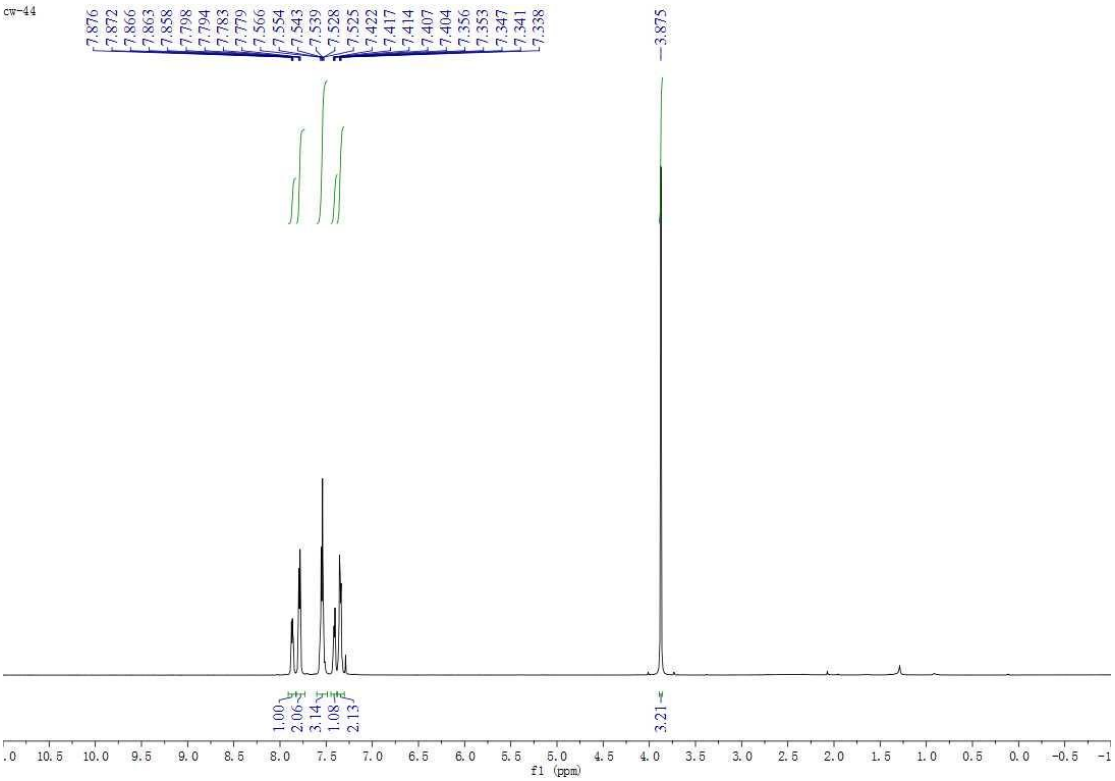
3-17

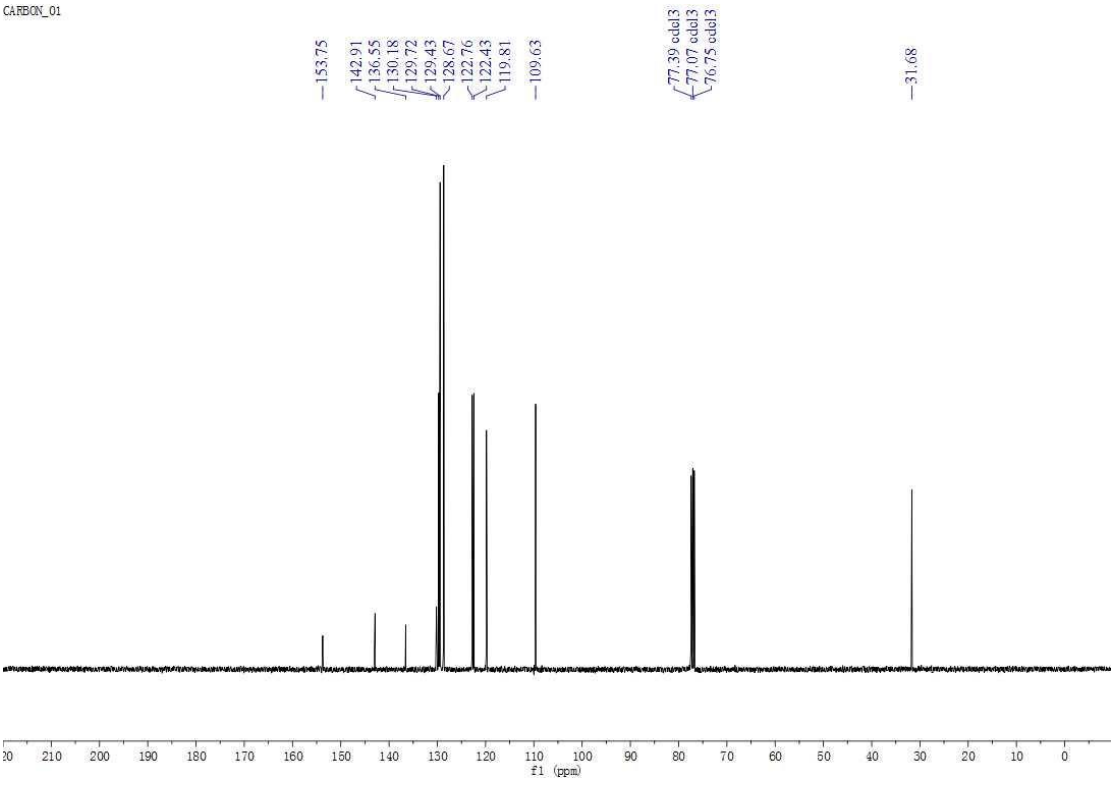

cw-6H
8.142
8.140
8.138
8.135
8.132
8.128
8.126
8.123
8.119
8.108
8.106
7.954
7.953
7.951
7.938
7.936
7.934
7.548
7.545
7.540
7.537
7.532
7.526
7.523
7.517
7.515
7.441
7.439
7.427
7.425
7.422
7.408
7.290
3.01
1.00
4.20
1.06
f1 (ppm)

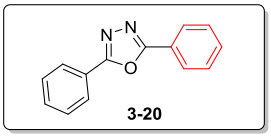

CARBON_01
168.073
154.108
135.037
133.591
130.974
129.020
127.552
126.317
125.188
123.220
121.620
77.331 cdcl3
77.013 cdcl3
76.695 cdcl3
f1 (ppm)

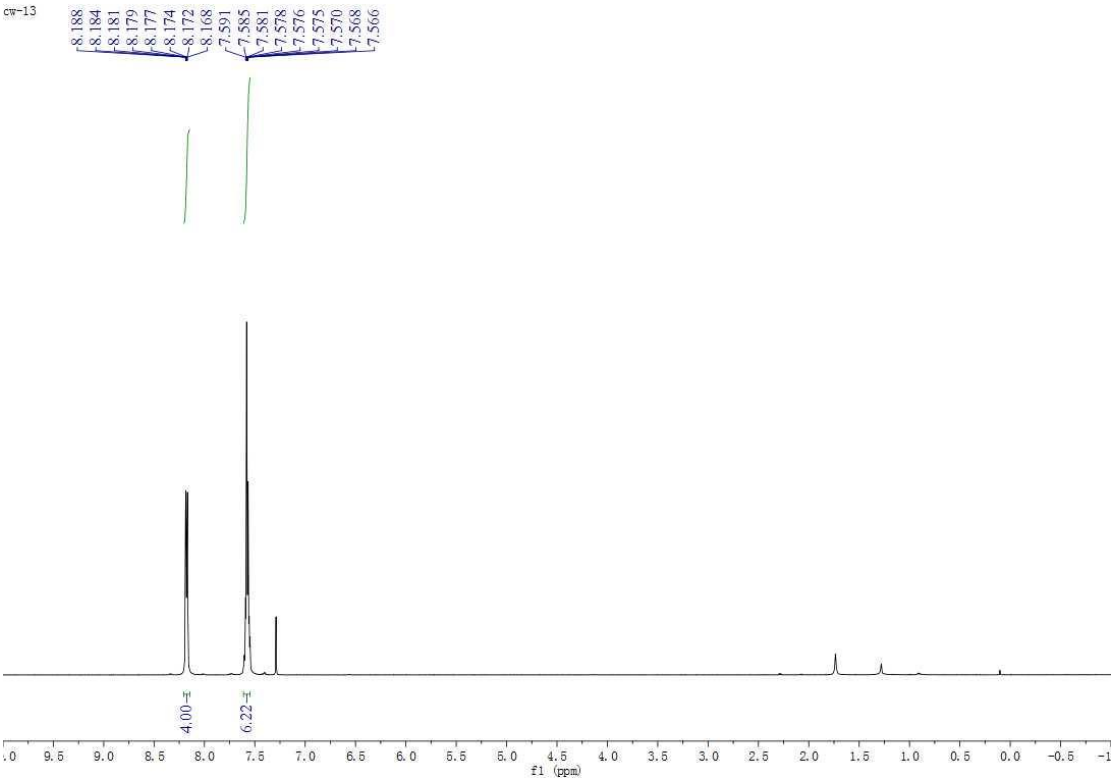


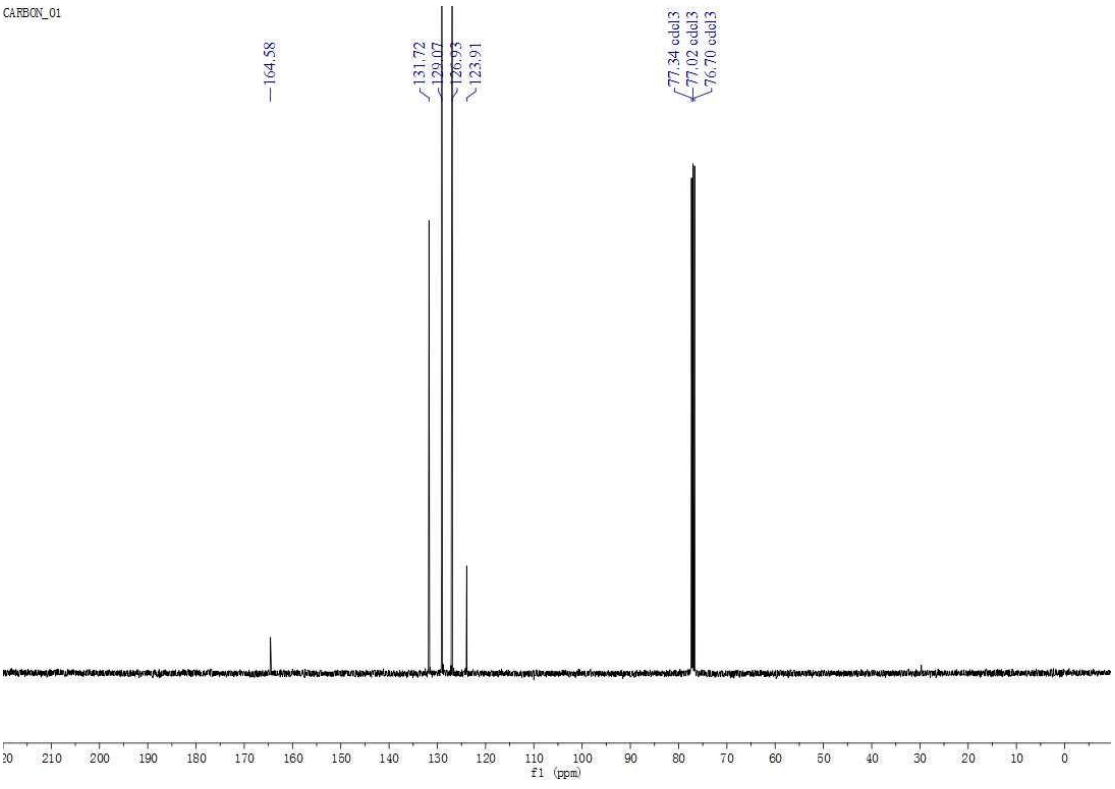
3-18

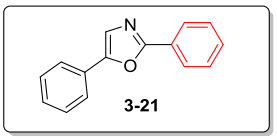

cw-44
7.876
7.872
7.866
7.863
7.858
7.798
7.794
7.783
7.779
7.566
7.554
7.543
7.539
7.528
7.525
7.422
7.417
7.414
7.407
7.404
7.356
7.353
7.347
7.341
7.338
3.875
1.00
2.06
3.14
1.08
2.13
3.21
f1 (ppm)

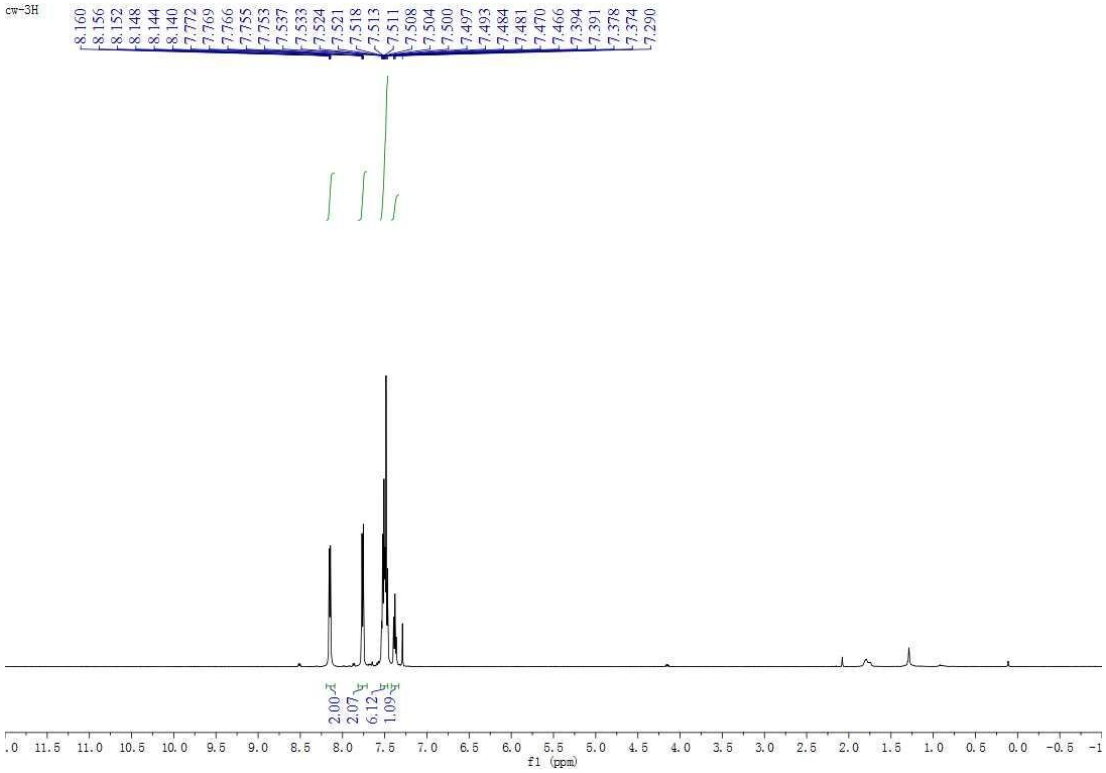

CARBON_01
153.75
142.91
136.55
130.18
129.72
129.43
128.67
122.76
122.43
119.81
109.63
77.39 cdcl3
77.07 cdcl3
76.75 cdcl3
31.68
f1 (ppm)

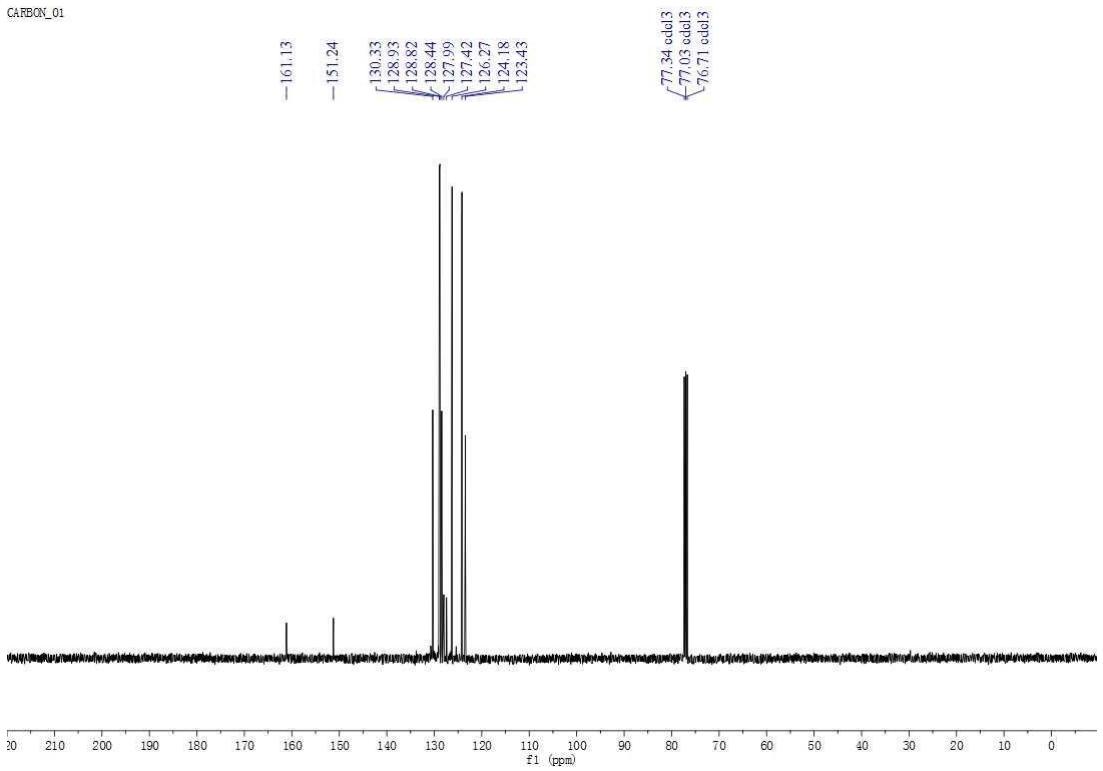

3-20

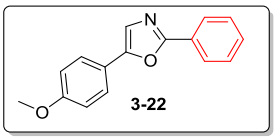

cw-13
8.188
8.184
8.181
8.179
8.177
8.174
8.172
8.168
7.591
7.585
7.581
7.578
7.576
7.575
7.570
7.568
7.566
4.00
6.22
f1 (ppm)


CARBON_01
164.58
131.72
129.07
126.93
123.91
77.34 cdcl3
77.02 cdcl3
76.70 cdcl3
f1 (ppm)

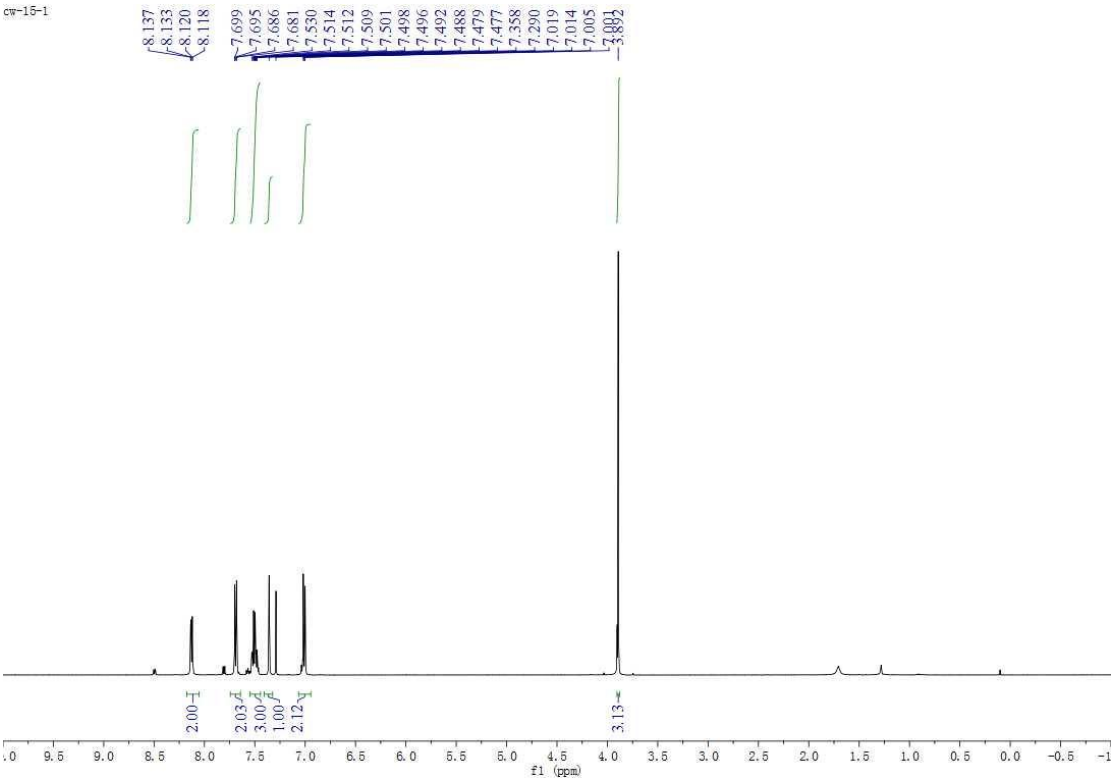

3-21

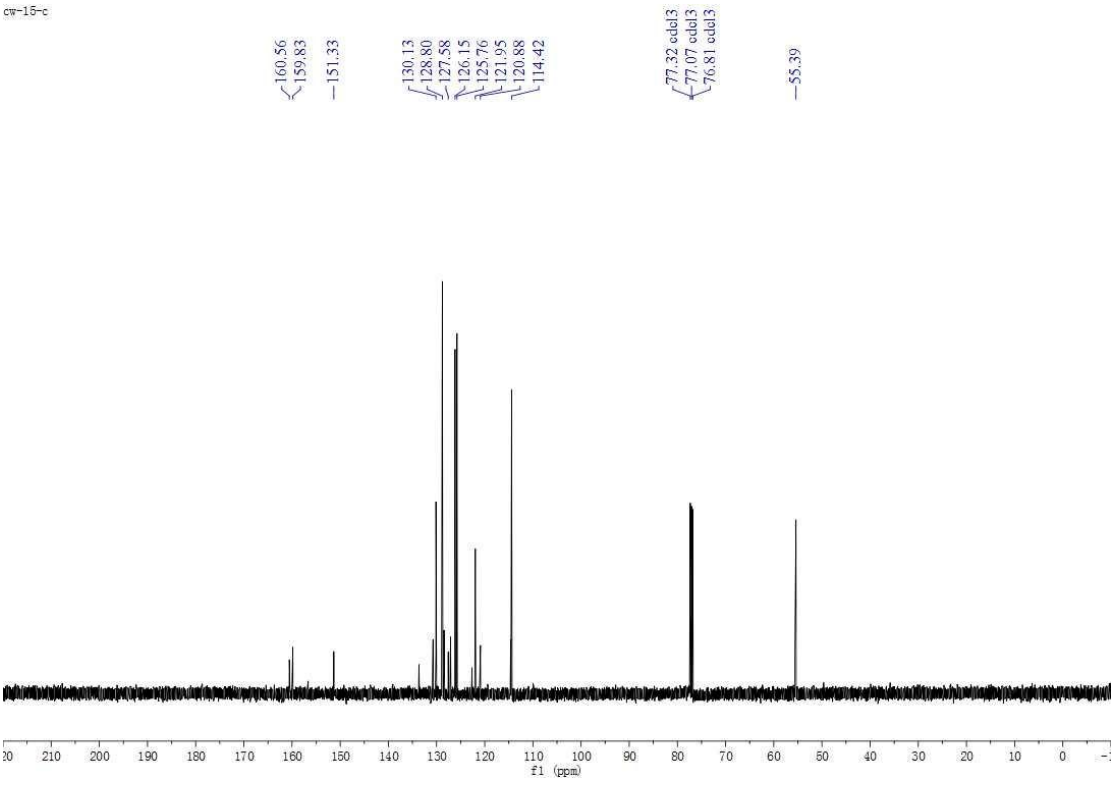

cw-3H
8.160
8.156
8.152
8.148
8.144
8.140
7.772
7.769
7.766
7.755
7.753
7.537
7.533
7.524
7.521
7.518
7.513
7.511
7.508
7.504
7.500
7.497
7.493
7.484
7.481
7.470
7.466
7.394
7.391
7.378
7.374
7.290
2.00
2.07
6.12
1.09
f1 (ppm)

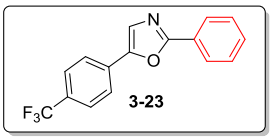

CARBON_01
161.13
151.24
130.33
128.93
128.82
128.44
127.99
127.42
126.27
124.18
123.43
77.34 cdcl3
77.03 cdcl3
76.71 cdcl3
f1 (ppm)

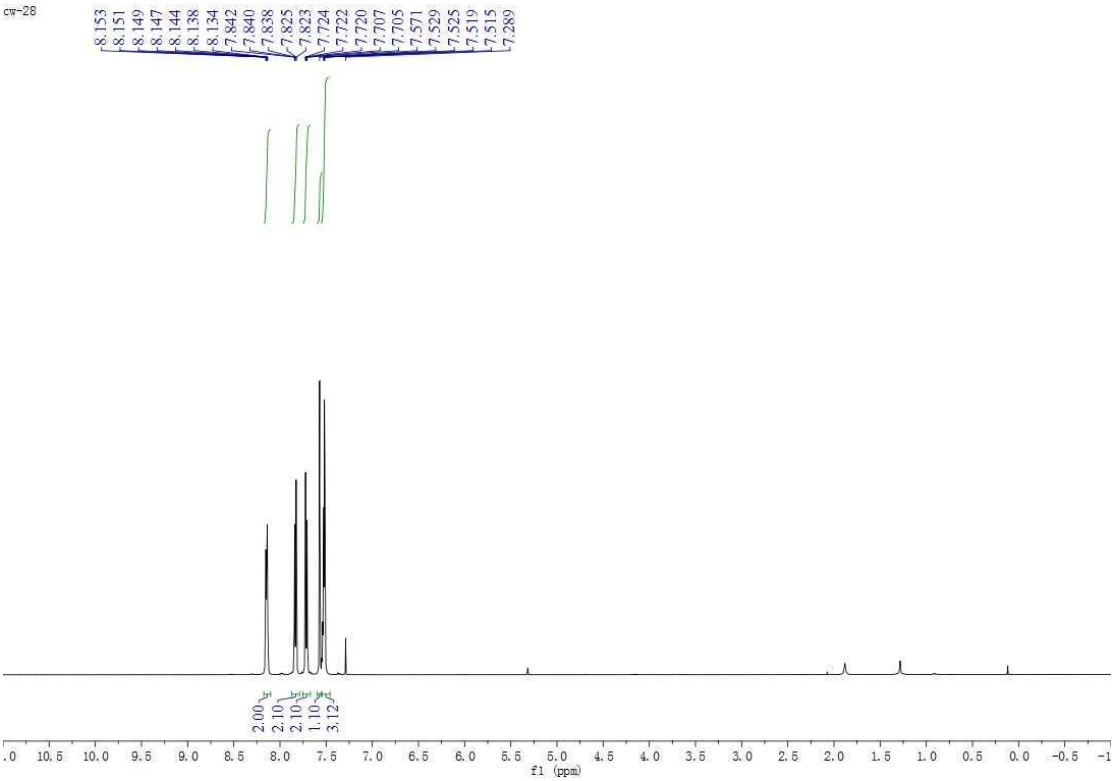

N
O
O

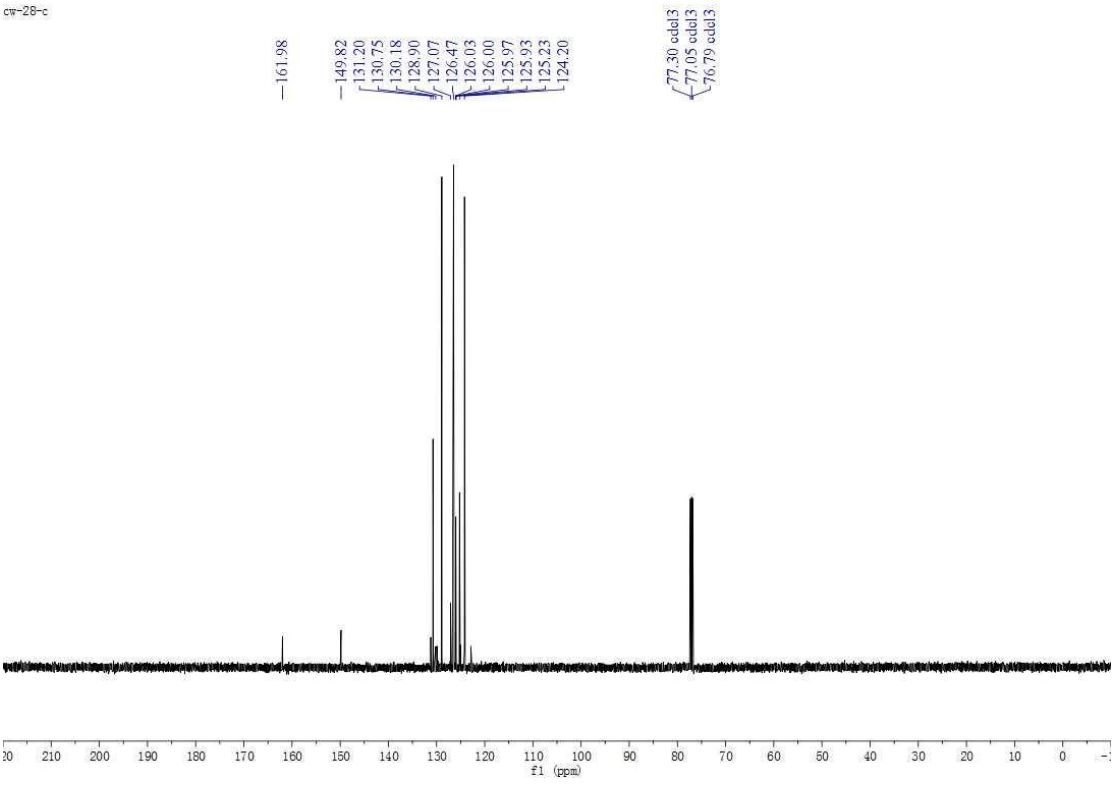
3-22

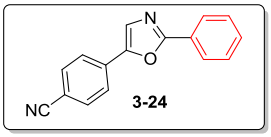

cw-15-1
8.137
8.133
8.120
8.118
7.699
7.695
7.686
7.681
7.530
7.514
7.512
7.509
7.501
7.498
7.496
7.492
7.488
7.479
7.477
7.358
7.290
7.019
7.014
7.005
3.892
2.00
2.03
3.00
1.00
2.12
3.13
f1 (ppm)

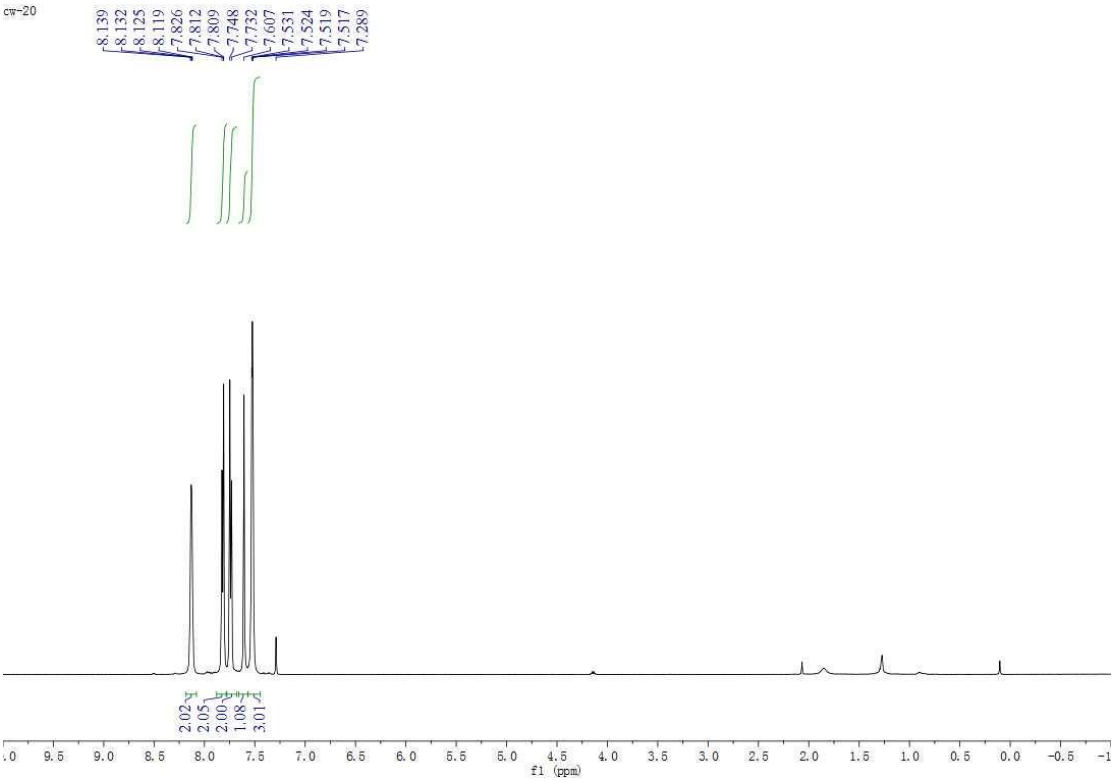

cw-15-c
160.56
159.83
151.33
130.13
128.80
127.58
126.15
125.76
121.95
120.88
114.42
77.32 cdcl3
77.07 cdcl3
76.81 cdcl3
55.39
f1 (ppm)

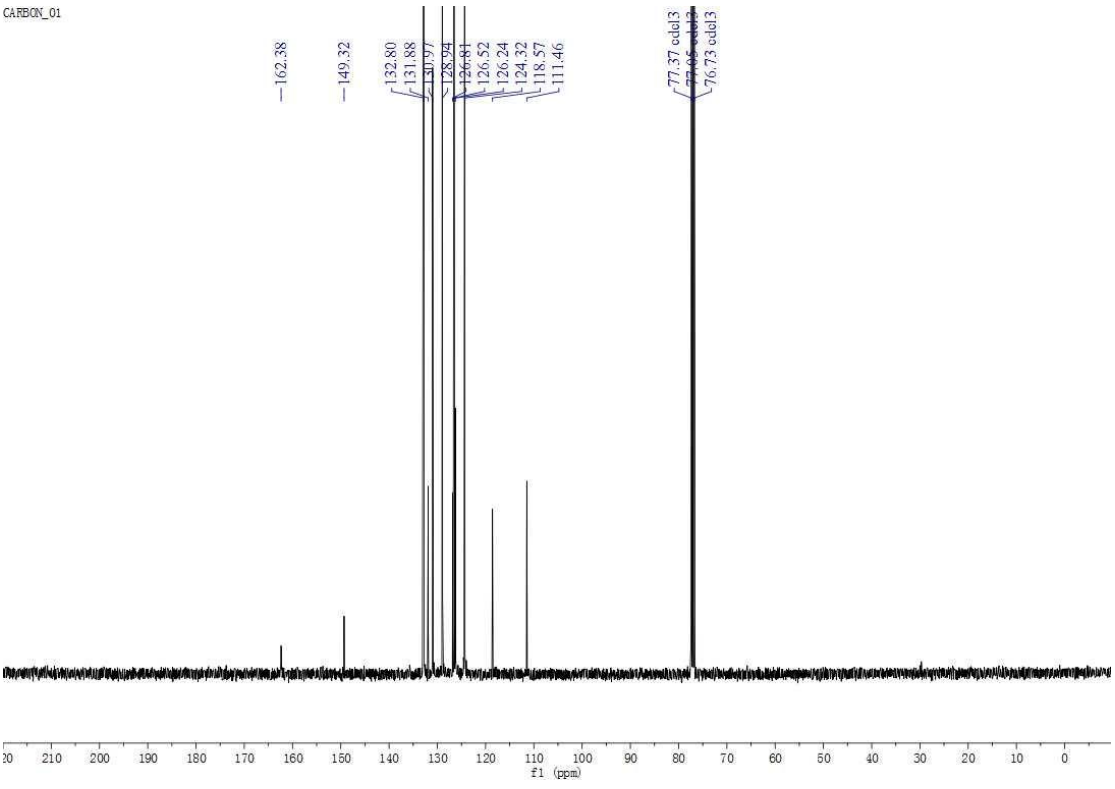

N
O
F3C
3-23

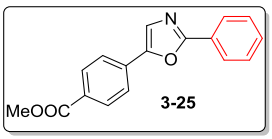

cw-28
8.153
8.151
8.149
8.147
8.144
8.138
8.134
7.842
7.840
7.838
7.825
7.823
7.724
7.722
7.720
7.707
7.705
7.571
7.529
7.525
7.519
7.515
7.289
2.00
2.10
2.10
1.10
3.12
f1 (ppm)

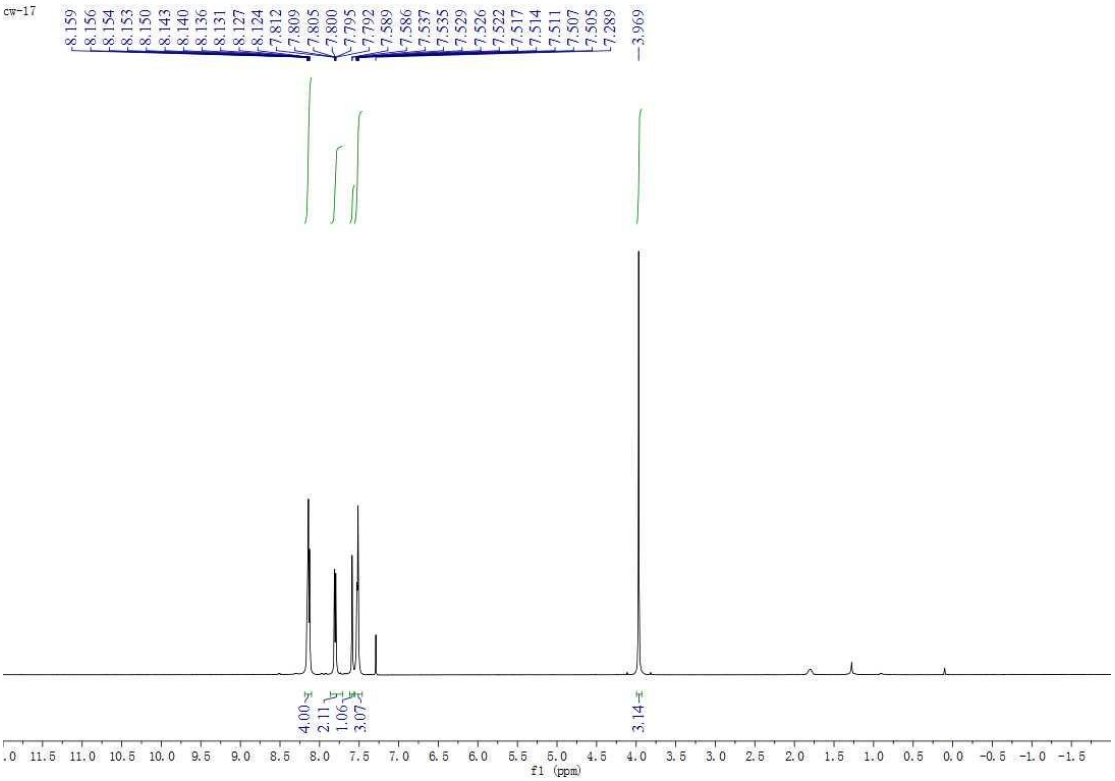

cw-28-c
161.98
149.82
131.20
130.75
130.18
128.90
127.07
126.47
126.03
126.00
125.97
125.93
125.23
124.20
77.30 cdcl3
77.05 cdcl3
76.79 cdcl3
f1 (ppm)

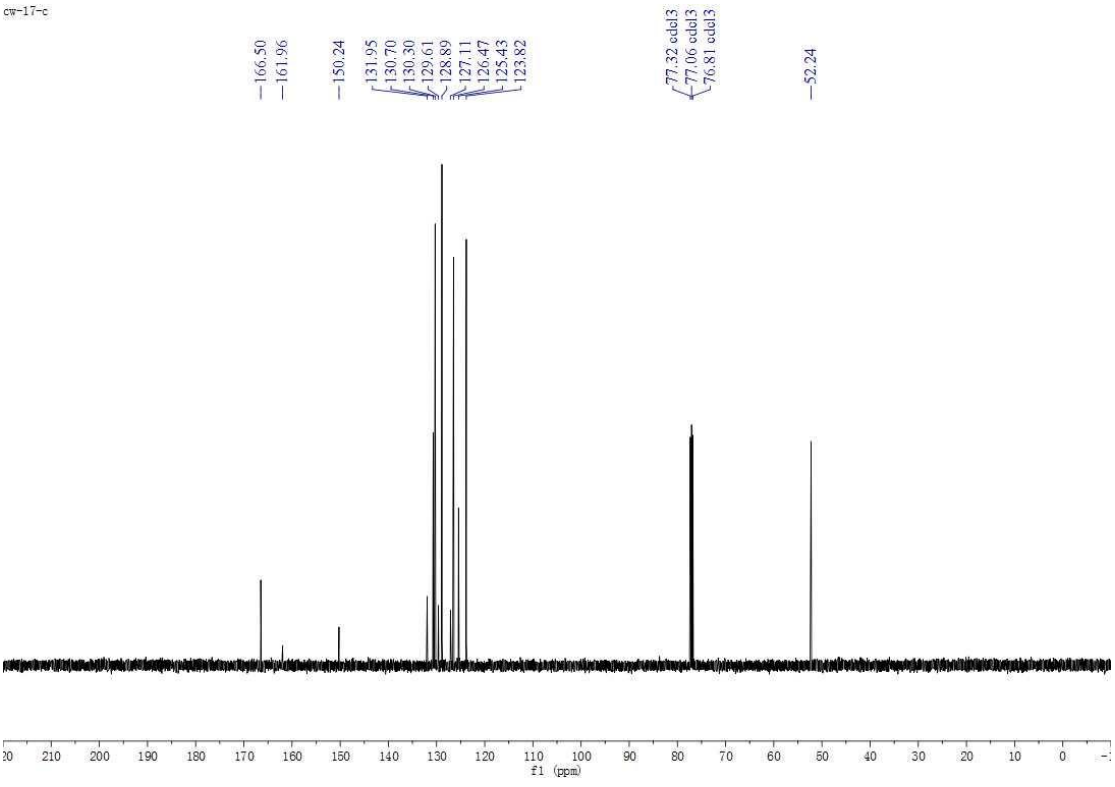

N
O
NC
3-24

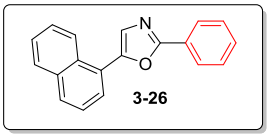

cw-20
8.139
8.132
8.125
8.119
7.826
7.812
7.809
7.748
7.732
7.607
7.531
7.524
7.519
7.517
7.289
2.02
2.05
2.00
1.08
3.01
f1 (ppm)

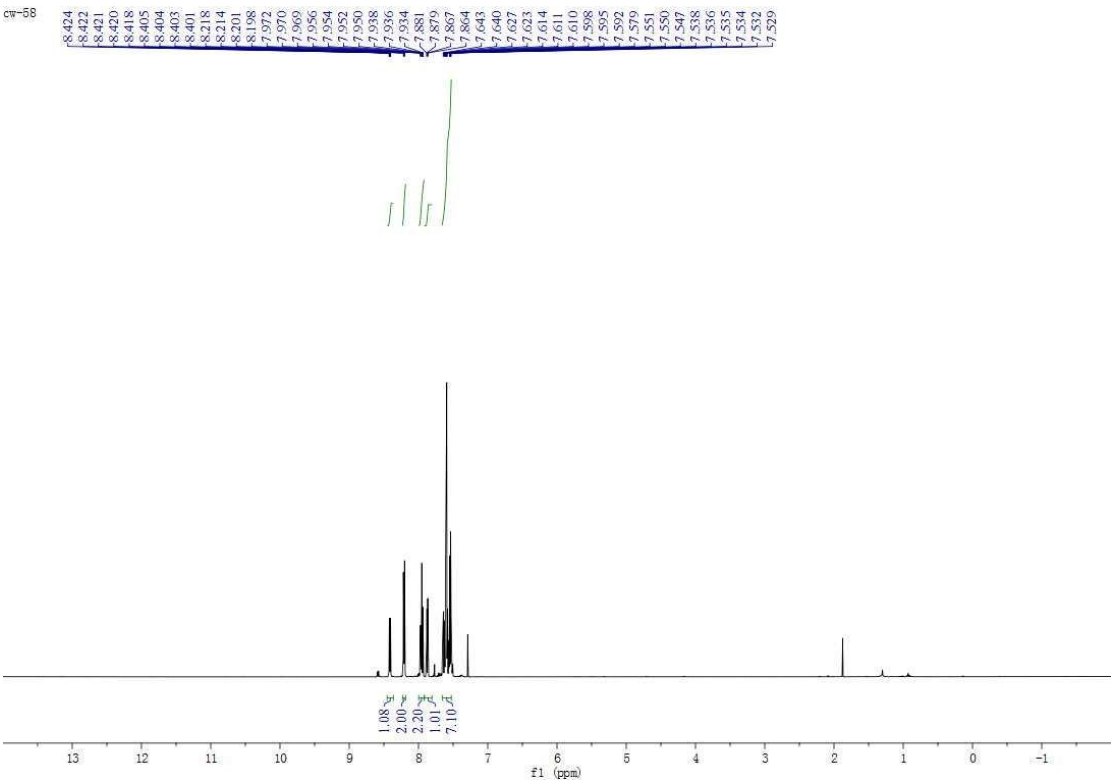

CARBON_01
162.38
149.32
132.80
131.88
130.97
128.94
126.81
126.52
126.24
124.32
118.57
111.46
77.37 cdcl3
76.73 cdcl3
f1 (ppm)

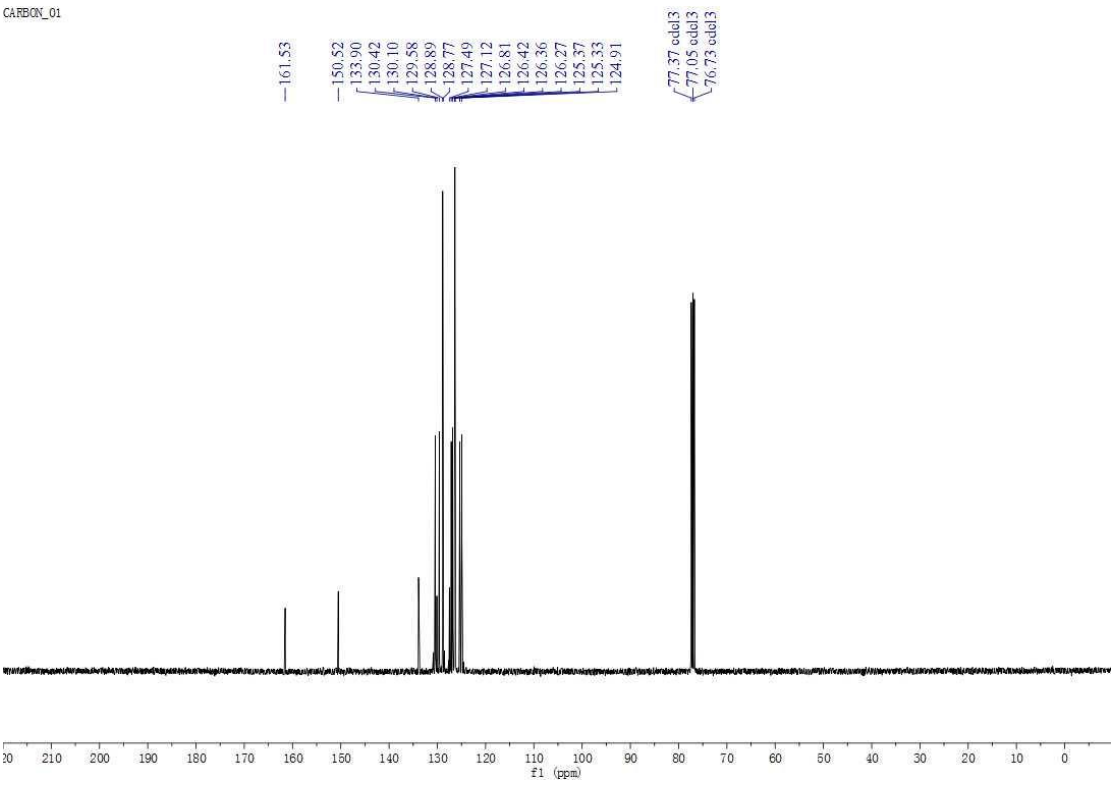

N
O
MeOOC
3-25

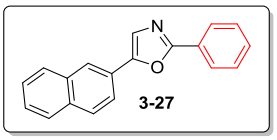

cw-17
8.159
8.156
8.154
8.153
8.150
8.143
8.140
8.136
8.131
8.127
8.124
7.812
7.809
7.805
7.800
7.795
7.792
7.589
7.586
7.537
7.535
7.529
7.526
7.522
7.517
7.514
7.511
7.507
7.505
7.289
3.969
4.00
2.11
1.06
3.07
3.14
f1 (ppm)

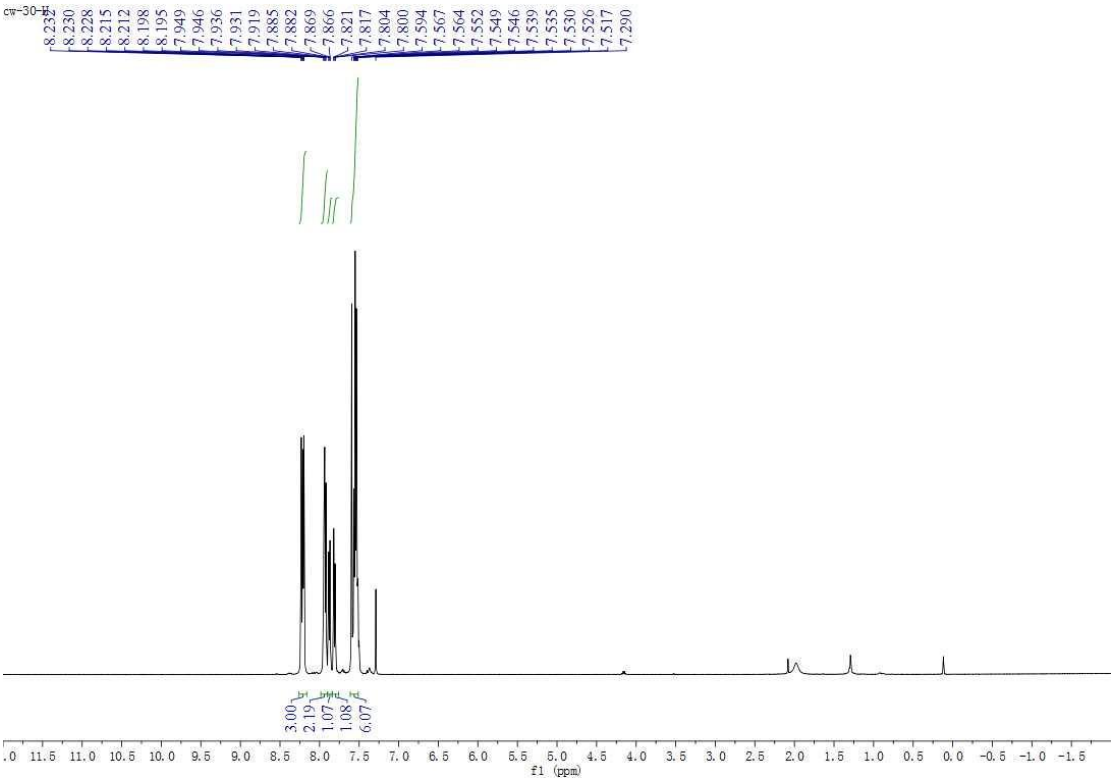

cw-17-c
166.50
161.96
150.24
131.95
130.70
130.30
129.61
128.89
127.11
126.47
125.43
123.82
77.32 cdcl3
77.06 cdcl3
76.81 cdcl3
52.24
f1 (ppm)

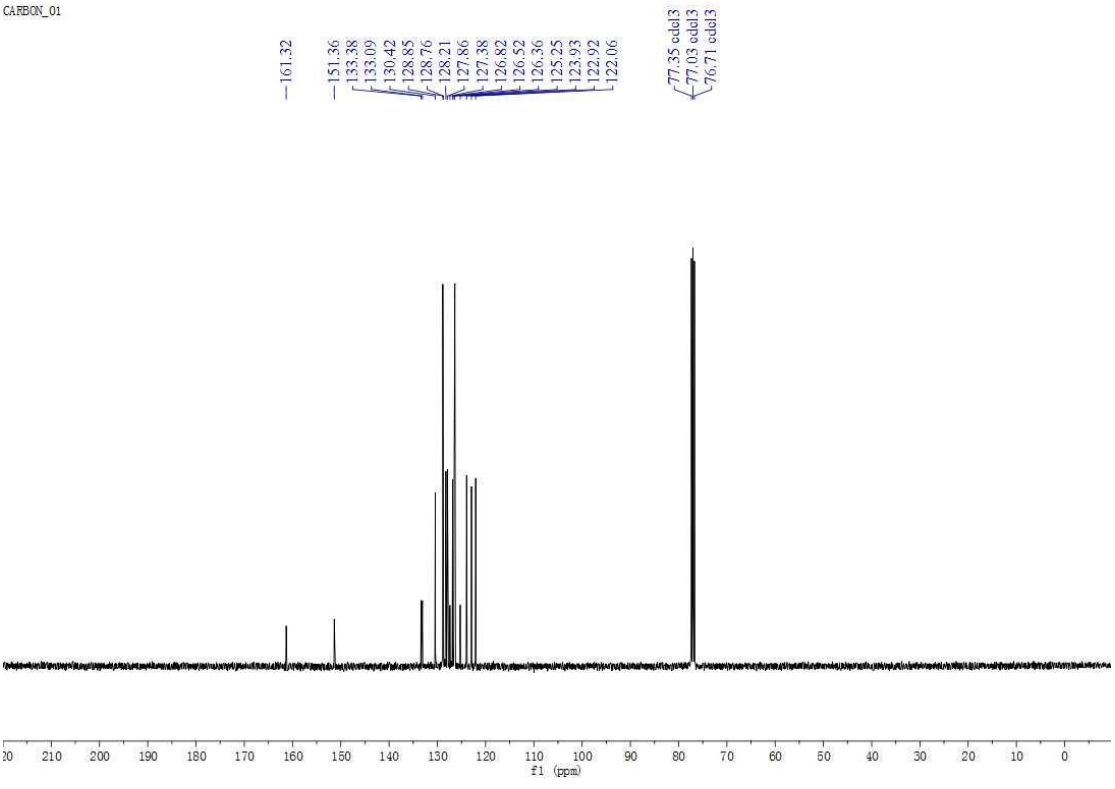

3-26

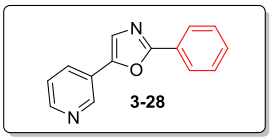

cw-68
8.424
8.422
8.421
8.420
8.418
8.405
8.404
8.403
8.401
8.218
8.214
8.201
8.198
7.972
7.970
7.969
7.956
7.954
7.952
7.950
7.938
7.936
7.934
7.881
7.879
7.867
7.864
7.643
7.640
7.627
7.623
7.614
7.611
7.610
7.598
7.595
7.592
7.579
7.551
7.550
7.547
7.538
7.536
7.535
7.534
7.532
7.529
1.08
2.00
2.20
1.01
7.10
f1 (ppm)


CARBON_01
161.53
150.52
133.90
130.42
130.10
129.58
128.89
128.77
127.49
127.12
126.81
126.42
126.36
126.27
125.37
125.33
124.91
77.37 cdcl3
77.05 cdcl3
76.73 cdcl3
f1 (ppm)

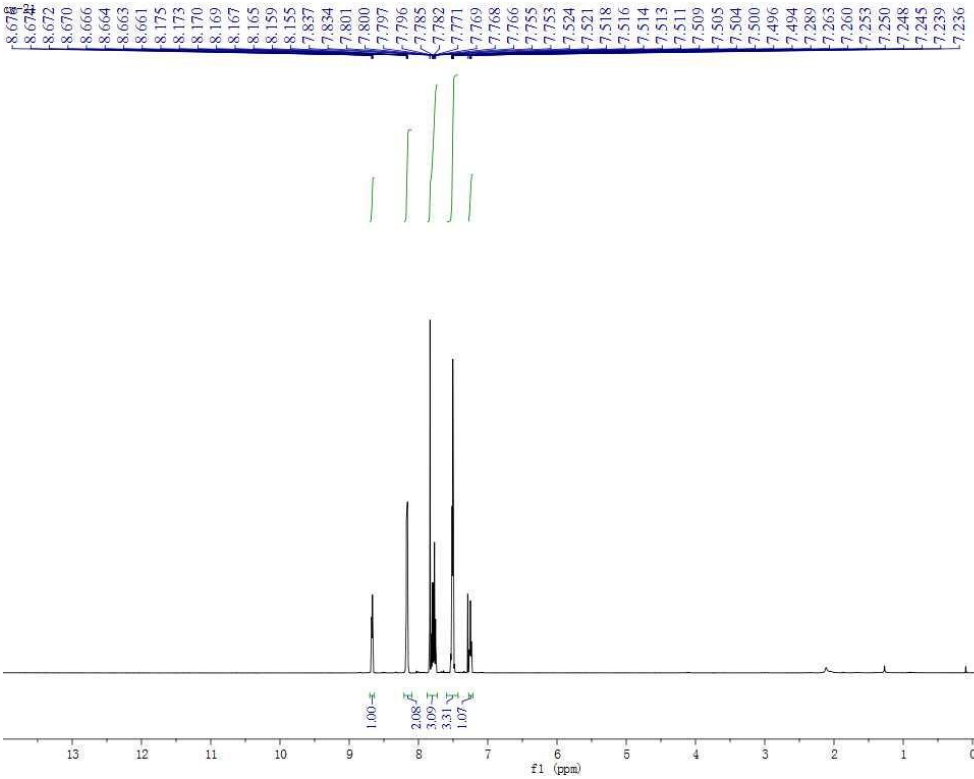

N
O
3-27


cw-30-H
8.232
8.230
8.228
8.215
8.212
8.198
8.195
7.949
7.946
7.936
7.931
7.919
7.885
7.882
7.869
7.866
7.821
7.817
7.804
7.800
7.594
7.567
7.564
7.552
7.549
7.546
7.539
7.535
7.530
7.526
7.517
7.290
3.00
2.19
1.07
1.08
6.07
f1 (ppm)

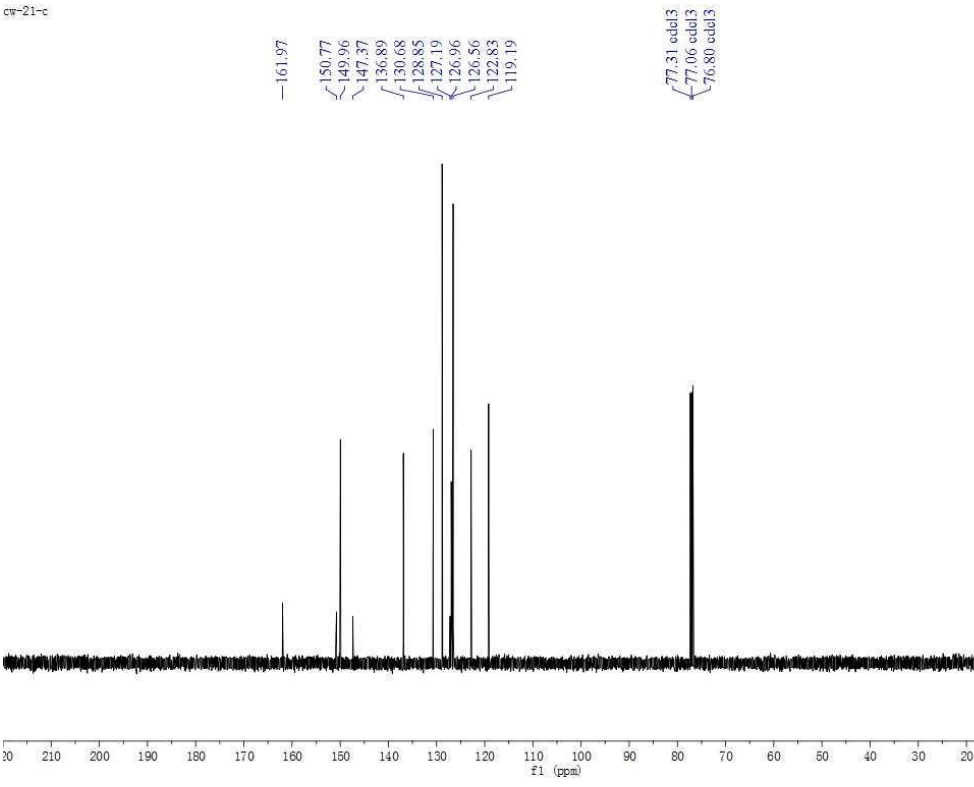

CARBON_01
161.32
151.36
133.38
133.09
130.42
128.85
128.76
128.21
127.86
127.38
126.82
126.52
126.36
125.25
123.93
122.92
122.06
77.35 cdcl3
77.03 cdcl3
76.71 cdcl3
f1 (ppm)

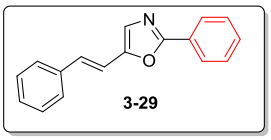

N
O
N

3-28


8.678
8.674
8.672
8.670
8.666
8.664
8.663
8.661
8.175
8.173
8.170
8.169
8.167
8.165
8.159
8.155
7.837
7.834
7.801
7.800
7.797
7.796
7.785
7.782
7.771
7.769
7.768
7.766
7.755
7.753
7.524
7.521
7.518
7.516
7.514
7.513
7.511
7.509
7.505
7.504
7.500
7.496
7.494
7.289
7.263
7.260
7.253
7.250
7.248
7.245
7.239
7.236
1.00
2.08
3.09
3.31
1.07
f1 (ppm)

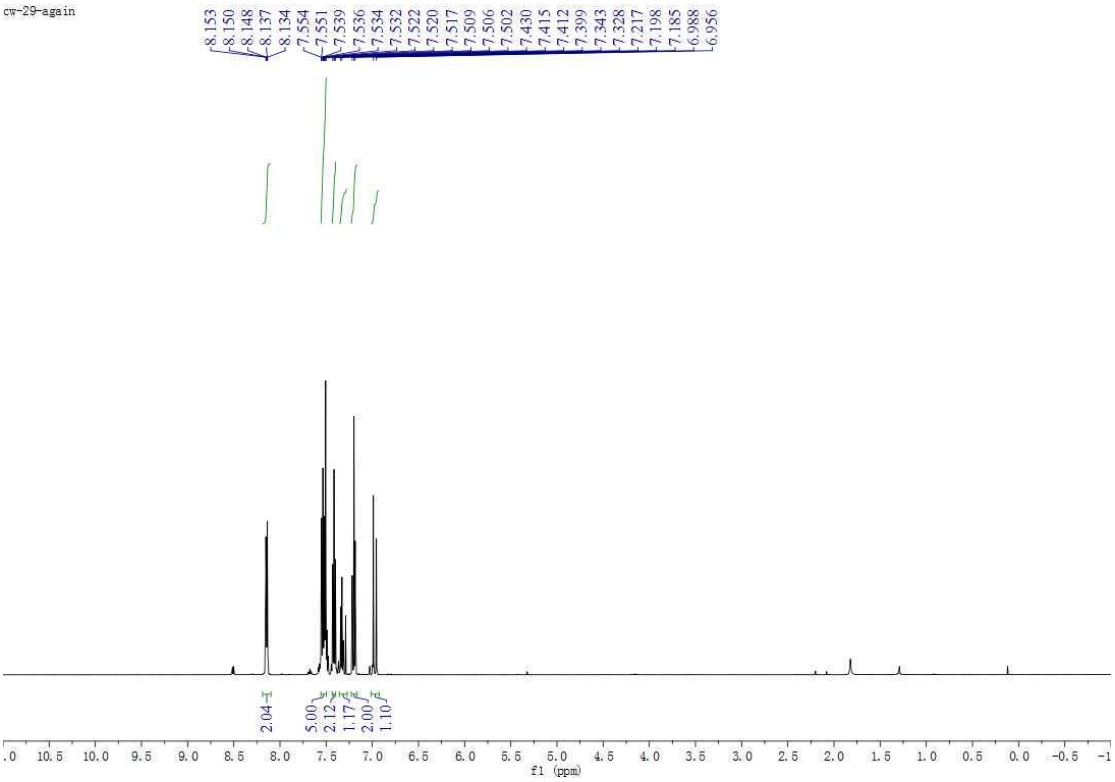
cw-21-c


161.97
150.77
149.96
147.37
136.89
130.68
128.85
127.19
126.96
126.56
122.83
119.19
77.31 cdcl3
77.06 cdcl3
76.80 cdcl3
f1 (ppm)

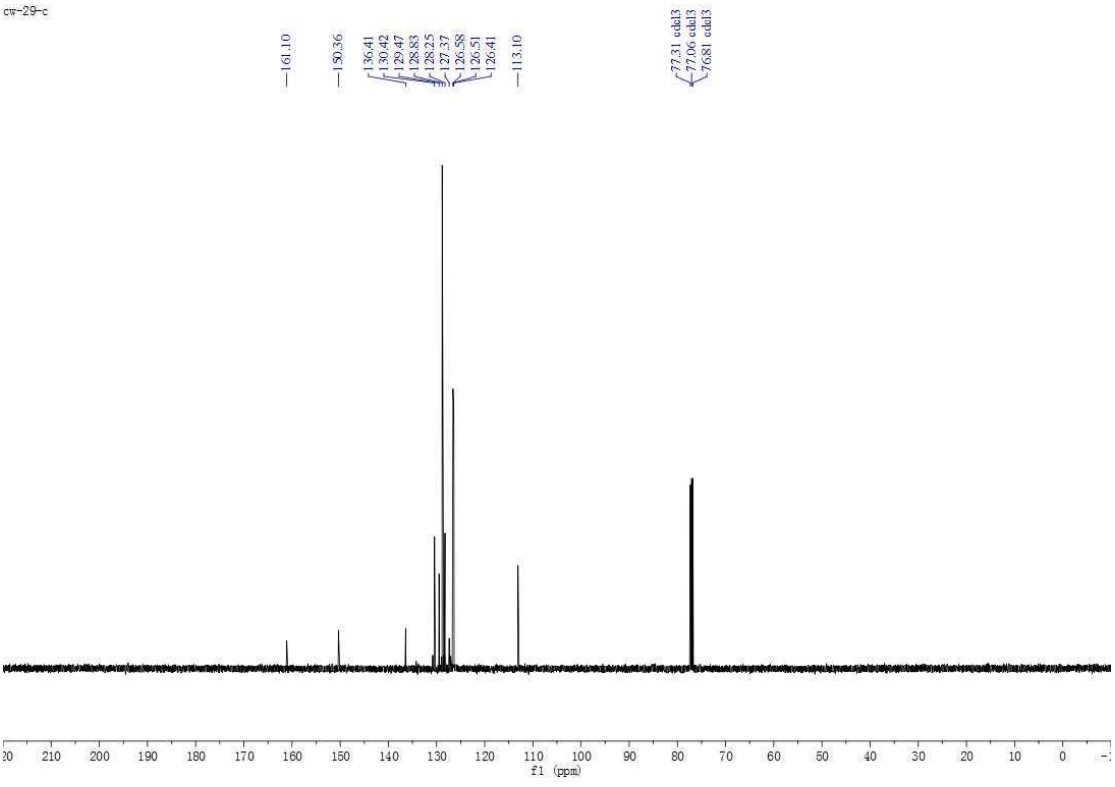


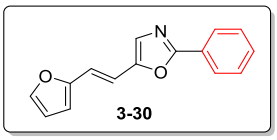
3-29

cw-29-again



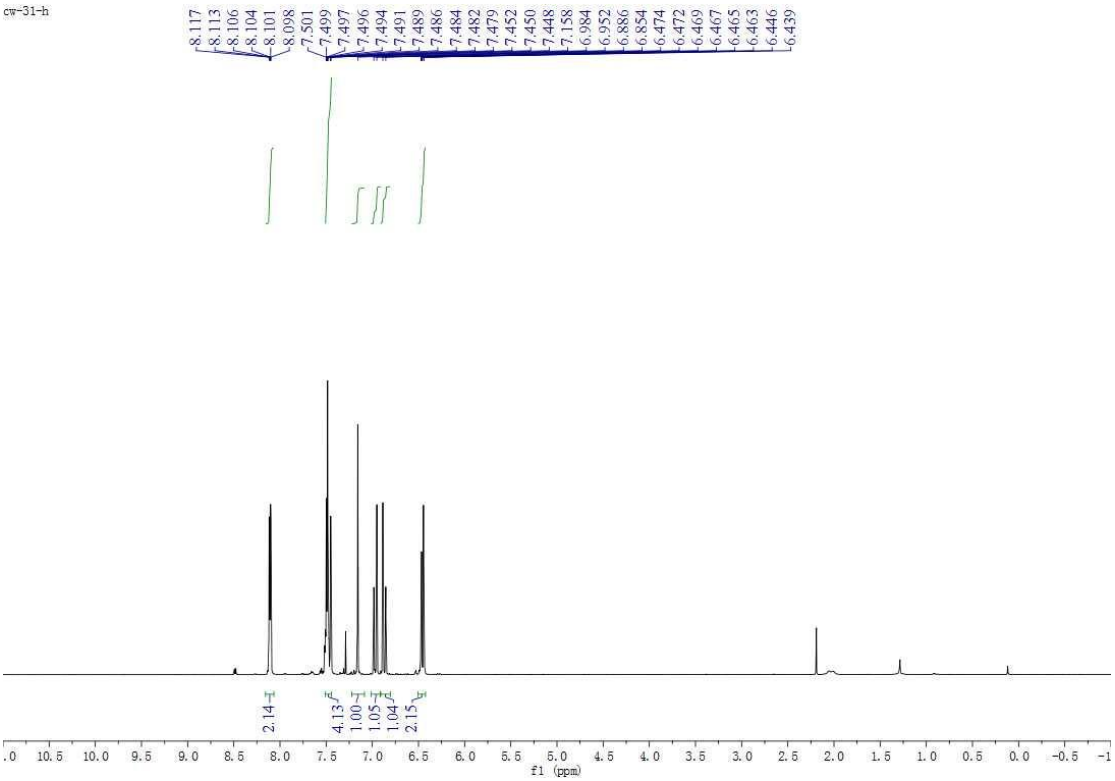
cw-29-c





3-30

cw-31-h



CW-31-C