Supporting Information

Transition-Metal-Free β-C-H Bond Carbonylation of Enamides or Amides with a Trifluoromethyl Group as CO Surrogate for the Synthesis of 1,3-Oxazin-6-ones

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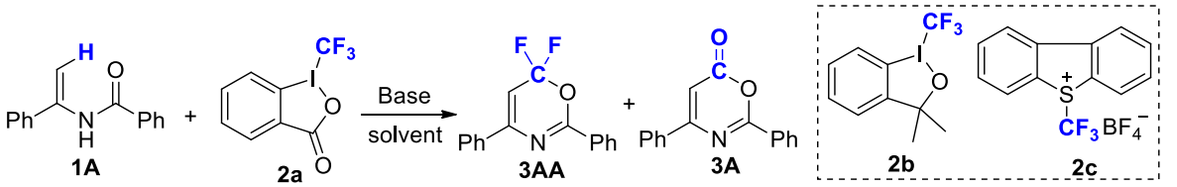
General information

All reactions were carried out under argon (Ar) atmosphere using Schlenk techniques with magnetic stirring. Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. Ethyl acetate (EA) was purchased anhydrous from commercial sources and transferred under an argon atmosphere. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F254 plates. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040-0.063 mm). Visualization on TLC was achieved by use of UV light (254 nm) or iodine.^{1}H,^{13}C and ^{19}F NMR spectra were recorded on Bruker DPX spectrometers (400 MHz or 500 MHz), (100 MHz or 125MHz) and (376 MHz) in $CDCl_3$ with tetramethylsilane (TMS) as internal standard. Chemical shifts are reported in ppm and coupling constants are given in Hz. Data for ^{1}H NMR are recorded as follows: chemical shift (ppm), multiplicity(s, singlet; d, doublet; t, triplet; q, quarter; m, multiplet), coupling constant (Hz), integration. Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm). ^{19}F NMR spectra were recorded on a Bruker DPX 400 MHz spectrometer [$CFCl_3$ as an external reference (0 ppm)]. HMRS were obtained on a Bruker Apex IV RTMS.

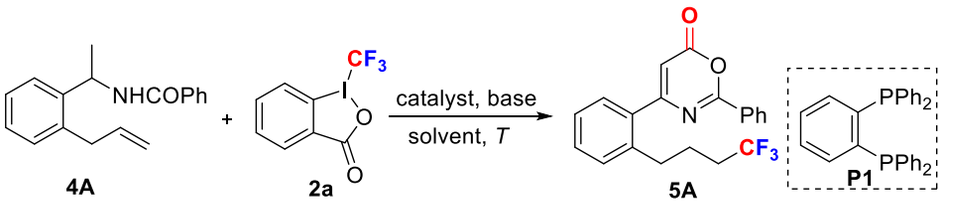
Table S1. Screening reaction conditions for the substrate 1A.[a]



entry	Base (x equiv.)	Solvent	*T* (°C)	*t* (h)	Yield(%) **3AA**[b]	**3A**[c]
1	K_3PO_4 (2)	DCM	80	12	29	--[f]
2	Cs_2CO_3 (3)	DCM	45	8	38	--[f]
3	DABCO (3)	DCM	45	8	3	--[f]
4	NaOAc (3)	DCM	45	8	--[f]	--[f]
5	K_3PO_4 (3)	CH_3Cl	45	12	52	--[f]
6	K_3PO_4 (3)	DMSO	45	12	55	--[f]
8	K_3PO_4 (3)	DMF	45	12	62	--[f]
9	K_3PO_4(3)	CH_3CN	45	12	93	--[f]
10[d]	K_3PO_4 (3)	CH_3CN	45	12	--[f]	--[f]
11[e]	K_3PO_4 (3)	CH_3CN	45	12	--[f]	--[f]
12	K_3PO_4(3)/H_2O(5)	CH_3CN	45	6	36	32
13	K_3PO_4(3)	CH_3CN/H_2O (2:1)	45	6	--[f]	79
14	K_3PO_4(5)	CH_3CN/H_2O (2:1)	45	6	--[f]	85
15	K_3PO_4(3)	CH_3CN/H_2O (2:0.8)	45	6	--[f]	83
16	K_3PO_4(3)	CH_3CN/H_2O (2:0.2)	45	6	--[f]	84
17	--	CH_3CN/H_2O (2:1)	45	6	--[f]	--[f]

[a] Conditions: **1A** (0.1 mmol), **2a** (0.12 mmol). [b] Determined by ^{1}HNMR spectroscopy using CH_2Br_2 as internal standard. [c] Determined by ^{19}F NMR spectroscopy with $PhCF_3$ as internal standard. [d] **2a** was replaced with **2b**. [e] **2a** was replaced with **2c**. [f] Product was not detected.

Table S2. Screening reaction conditions for the substrate 4A.[a]



entry	catalyst	base	solvent	*T* (°C)	*t* (h)	Yield (%)
1	--	K_3PO_4	CH_3CN/H_2O(2:1)	80	16	trace
2	P1	--	EA	80	16	20
3	P1	Cs_2CO_3	EA	80	16	51
4	P1	K_2CO_3	EA	80	16	42
5	P1	K_2PO_4	EA	80	16	40
6	Et_4NI	Cs_2CO_3	EA	80	36	45
7	TBAI	Cs_2CO_3	EA	80	36	50
8	TBAI	K_2CO_3	EA	80	16	53
9	TBAI	K_3PO_4	EA	80	16	55
10	TBAI	$NaHCO_3$	EA	80	16	6
11	TBAI	Na_2CO_3	EA	80	16	5
12	TBAI	K_3PO_4	NMP	80	16	trace
13	TBAI	K_3PO_4	DMF	80	16	5
14	TBAI	K_3PO_4	CH_3CN	80	16	54
15	TBAI	K_3PO_4	CH_3CN/H_2O (5.0 equiv.)	80	16	50

Conditions: **4A** (0.1 mmol), **2a** (0.22 mmol), catalyst (20 mol %), base (4.0 equiv.) under Ar.
[b] Yield of **5** was determined by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard.

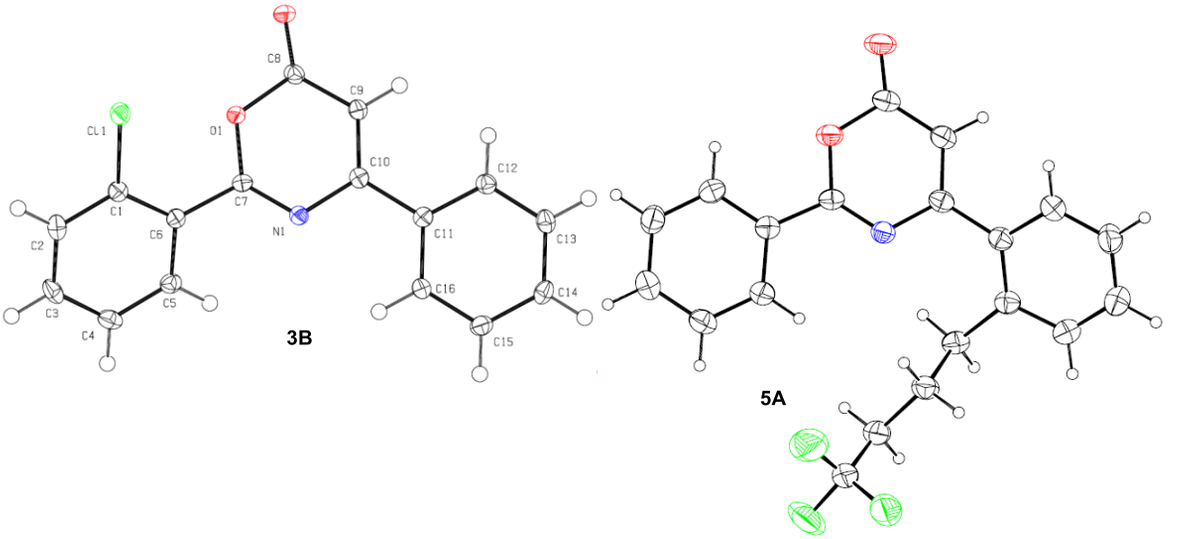
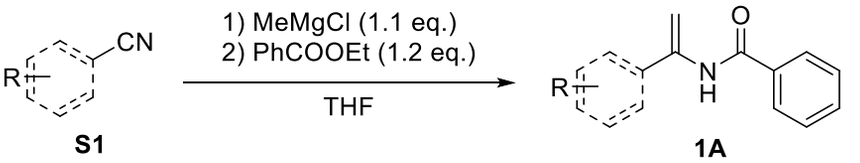


Figure S1. X-ray structures of **3B** and **5A**.

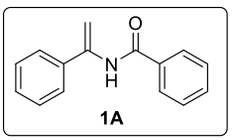
General procedure for the preparation of substrates

1) Representative procedure for the synthesis of 1[1]

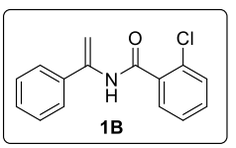


S1 1A

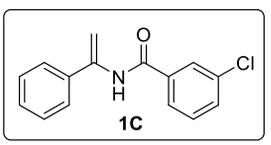
***N*-(1-Phenylvinyl)benzamide (1A)** Benzonitrile **S1** (15 mmol) and methyl magnesium chloride in THF (3.0 M, 5.5 mL, 16.5 mmol, Aldrich) were mixed under argon atmosphere, followed by heating to reflux for 30 min. After cooling to room temperature, the solution thus obtained was added to a solution of ethyl benzoate (2.70 g, 18 mmol) in THF (5.0 mL) at 0 ℃. After 4 h, ether (20 mL) and water (10 ml) were added. After vigorous stirring for 5 min, the mixture was filtered through Celite pad. The solution were extracted with EtOAc (3×30 mL), washed with brine, dried with anhydrous Na_2SO_4, filtered, and concentrated *in vacuo*. The residue was purified by flash column chromatography on silica gel (ethyl acetate/petroleum ether = 1/15-1/5) to give *N*-(1-Phenylvinyl)benzamide **1A** (837 mg, 25%) as a white solid.



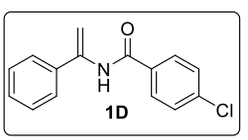
***N*-(1-Phenylvinyl)benzamide (1A)**
White solid (836.6 mg, 25% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.82 (m, 2H), 7.56-7.45 (m, 6H), 7.43-7.35 (m, 3H), 6.05 (s, 1H), 5.21 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.22, 140.55, 138.48, 134.77, 131.82, 128.79, 128.74, 128.65, 126.90, 126.00, 103.00.
HRMS (ESI) calcd. for $C_{15}H_{14}ON$ $[M+H]^+$ 224.1070, found 224.1065.



2-Chloro-*N*-(1-phenylvinyl)benzamide (1B)
White solid (694.2 mg, 18% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (m, 1H), 7.58 (s, 1H), 7.52-7.50 (m, 2H), 7.44-7.34 (m, 6H), 6.11 (s, 1H), 5.23 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.07, 140.39, 138.13, 135.13, 131.65, 130.44, 130.31, 128.78, 128.75, 127.28, 126.051, 103.29.
HRMS (ESI) calcd. for $C_{15}H_{13}ONCl$ $[M+H]^+$ 258.0680, found 258.0676.

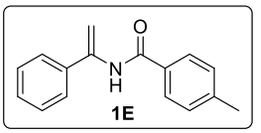


3-Chloro-*N*-(1-phenylvinyl)benzamide (1C)
White solid (771.3 mg, 20% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.81 (m, 1H), 7.70-7.68 (m, 1H), 7.53-7.38 (m, 8H), 6.02 (s, 1H), 5.24 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 164.84, 140.39, 138.24, 136.58, 135.00, 131.88, 130.08, 128.90, 128.87, 127.33, 126.03, 124.95, 103.53.
HRMS (ESI) calcd. for $C_{15}H_{13}ONCl$ $[M+H]^+$ 258.0680, found 258.0678.

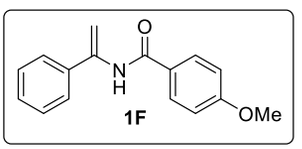


4-Chloro-*N*-(1-phenylvinyl)benzamide (1D)
White solid (1157.0 mg, 30% yield).

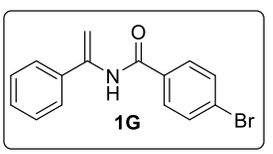
^{1}HNMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.5 Hz, 2H), 7.53 (s, 1H), 7.47 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.43-7.35 (m, 5H), 5.98 (s, 1H), 5.22 (s, 1H).
^{13}CNMR (125 MHz, $CDCl_3$) δ 165.19, 140.45, 138.24, 138.10, 133.07, 128.98, 128.84, 128.81, 128.38, 125.99, 103.47.
HRMS (ESI) calcd. for $C_{15}H_{13}ONCl$ $[M+H]^+$ 258.0680, found 258.0679.



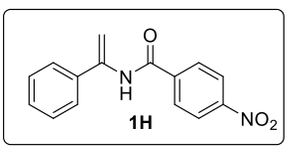
4-Methyl-*N*-(1-phenylvinyl)benzamide (1E)
White solid (711.9 mg, 20% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.0Hz, 2H), 7.54-7.47 (m, 3H), 7.45-7.35 (m, 3H), 7.31-7.28 (m, 2H), 6.04 (s, 1H), 5.19 (s, 1H), 2.41 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.14, 142.39, 140.59, 138.66, 131.96, 129.43, 128.81, 128.75, 126.91, 126.04, 102.66, 21.47.
HRMS (ESI) calcd. for $C_{16}H_{16}ON$ $[M+H]^+$ 238.1226, found 238.1222.



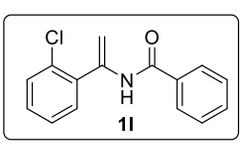
4-Methoxy-*N*-(1-phenylvinyl)benzamide (1F)
White solid (1215.8 mg, 32% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.78 (m, 2H), 7.51-7.48 (m, 2H), 7.43-7.35 (m, 4H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.01 (s, 1H), 5.18 (s, 1H), 3.86 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.70, 162.48, 140.69, 138.76, 128.81, 128.79, 128.72, 127.05, 126.06, 113.97, 102.54, 55.45.
HRMS (ESI) calcd. for $C_{16}H_{16}O_2$ N $[M+H]^+$ 254.1176, found 254.1171.



4-Bromo-*N*-(1-phenylvinyl)benzamide (1G)
White solid (1360.0 mg, 35% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dt, *J* = 8.8, 2.4 Hz, 2H), 7.61 (dt, *J* = 8.4, 2.4 Hz, 2H), 7.51-7.35 (m, 6H), 6.02 (s, 1H), 5.23 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.24, 140.42, 138.33, 133.61, 132.03, 128.89, 128.8, 128.52, 126.61, 126.02, 103.34.
HRMS (ESI) calcd. for $C_{15}H_{13}ONBr$ $[M+H]^+$ 302.0175, found 302.0169.

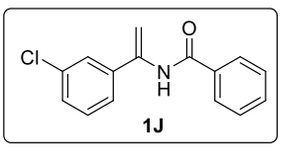


4-Nitro-*N*-(1-phenylvinyl)benzamide (1H)
Yellow solid (684.2 mg, 17% yield).
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.5 Hz, 2H), 7.99 (d, *J* = 9.0 Hz, 2H), 7.55-7.47 (m, 3H), 7.44-7.40 (m, 3H), 6.06 (s, 1H), 5.29 (s, 1H).
^{13}CNMR (125 MHz, $CDCl_3$) δ 164.17, 149.73, 140.27, 137.93, 129.1, 129.10, 128.97, 128.17, 126.01, 124.04, 104.16.
HRMS (ESI) calcd. for $C_{15}H_{13}O_3N_2$ $[M+H]^+$ 269.0921, found 269.0918.



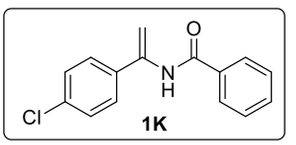
***N*-(1-(2-Chlorophenyl)vinyl)benzamide (1I)**
White solid (579.8 mg, 15% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.78 (m, 2H), 7.58 (s, 1H),

7.52-7.48 (m, 1H), 7.47-7.37 (m, 4H), 7.33-7.26 (m, 2H), 6.18 (s, 1H), 4.95 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.74, 139.29, 137.33, 134.63, 132.00, 131.71, 131.32, 129.87, 128.62, 127.11, 126.90, 105.07.
HRMS (ESI) calcd. for $C_{15}H_{13}ONCl$ $[M+H]^+$ 258.0680, 258.0678.



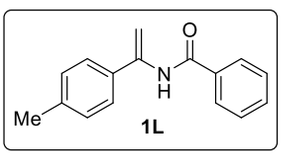
1J

***N*-(1-(3-Chlorophenyl)vinyl)benzamide (1J)**
White solid (541.2 mg, 14% yield)**.**
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.81 (m, 2H), 7.62-7.44 (m, 5H), 7.38-7.28 (m, 3H), 5.98-5.93 (m, 1H), 5.23-5.22 (m, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.21, 140.18, 139.53, 134.74, 134.48, 132.01, 130.04, 128.82, 127.01, 126.96, 126.27, 124.21, 104.49.
HRMS (ESI) calcd. for $C_{15}H_{13}ONCl$ $[M+H]^+$ 258.0680, found 258.0676.



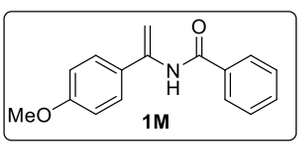
1K

***N*-(1-(4-Chlorophenyl)vinyl)benzamide (1K)**
White solid (734.4 mg, 19% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.80 (m, 2H), 7.67 (s, 1H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 2H), 7.40-7.38 (m, 2H), 7.33-7.31 (m, 2H), 5.86 (s, 1H), 5.19 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.25, 139.75, 136.62, 134.46, 134.34, 131.90, 128.80, 128.68, 127.29, 126.96, 104.28.
HRMS (ESI) calcd. for $C_{15}H_{13}ONCl$ $[M+H]^+$ 258.0680, found 258.0677.



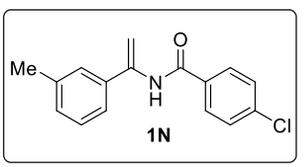
1L

***N*-(1-(p-tolyl)vinyl)benzamide (1L)**
White solid (676.3 mg, 19% yield)**.**
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.6 Hz, 2H), 7.56-7.38 (m, 6H), 7.26-7.20 (m, 2H), 6.01 (s, 1H), 5.18 (s, 1H), 2.38 (s, 3H).
^{13}CNMR (100 MHz, $CDCl_3$) δ 166.18, 140.46, 138.78, 135.71, 134.89, 131.81, 129.48, 128.77, 126.89, 125.90, 102.18, 21.18.
HRMS (ESI) calcd. for $C_{16}H_{16}ON$ $[M+H]^+$ 238.1226, found 238.1222.



1M

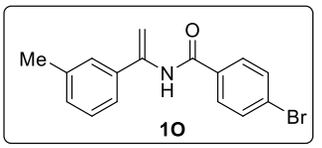
***N*-(1-(4-Methoxyphenyl)vinyl)benzamide (1M)**
White solid (1140.0 mg, 30% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84-7.82 (m, 2H), 7.54 (tt, *J* = 7.6, 2.4 Hz, 1H), 7.49-7.40 (m, 5H), 6.93-6.90 (m, 2H), 5.93 (s, 1H), 5.14 (s, 1H), 3.83 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.19, 160.00, 140.14, 134.86, 131.80, 130.98, 128.75, 127.29, 126.90, 114.11, 101.83, 55.34.
HRMS (ESI) calcd. for $C_{16}H_{16}O_2N$ $[M+H]^+$ 254.1176, found 254.1172.



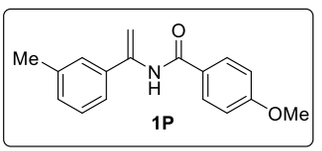
1N

4-Chloro-*N*-(1-(m-tolyl)vinyl)benzamide (1N)
White solid (1222.7 mg, 30% yield).
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.70 (dt, *J* = 8.4, 2.4 Hz, 2H), 7.35 (dt, *J* = 8.4, 2.4 Hz, 2H), 7.23-7.21 (m, 3H), 7.14-7.12 (m, 1H), 5.85 (s, 1H), 5.16 (s, 1H), 2.33 (s, 3H).

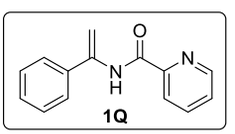
^{13}CNMR (100 MHz, $CDCl_3$) δ 165.20, 140.60, 138.30, 138.00, 137.83, 132.91, 129.41, 128.72, 128.49, 128.40, 126.58, 122.95, 103.57, 21.33.
HRMS (ESI) calcd. for $C_{16}H_{15}ONCl$ $[M+H]^+$ 272.0837, found 272.0833.



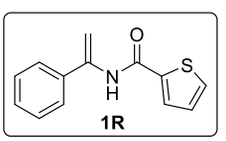
4-Bromo-*N*-(1-(m-tolyl)vinyl)benzamide (1O)
White solid (1944.6 mg, 41% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.22-7.14 (m, 4H), 5.85 (s, 1H), 5.17 (s, 1H), 2.34 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.29, 140.57, 138.30, 137.97, 133.37, 131.70, 129.42, 128.56, 128.49, 126.58, 126.32, 122.95, 103.57, 21.35.
HRMS (ESI) calcd. for $C_{16}H_{15}ONBr[M+H]^+$ 316.0332, found 316.0329.



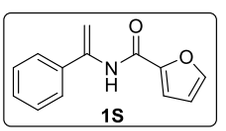
4-Methoxy-*N*-(1-(m-tolyl)vinyl)benzamide (1P)
White solid (1122.7 mg, 28% yield).
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.80 (dt, *J* = 8.8, 2.8 Hz, 2H), 7.44 (s, 1H), 7.29-7.28 (m, 3H), 7.20-7.18 (m, 1H), 6.97-6.94 (m, 2H), 6.00 (s, 1H), 5.16 (s, 1H), 3.86 (s, 3H), 2.39 (s, 3H).
^{13}CNMR (100 MHz, $CDCl_3$) δ 165.72, 162.45, 140.81, 138.77, 138.55, 129.50, 128.81, 128.71, 127.10, 126.79, 123.14, 113.96, 102.29, 55.45, 21.48.
HRMS (ESI) calcd. for $C_{17}H_{18}O_2N$ $[M+H]^+$ 268.1332, found 268.1327.



***N*-(1-Phenylvinyl)picolinamide (1Q)**
White solid (538.3 mg, 16% yield).
^{1}HNMR (400 MHz, $CDCl_3$) δ 8.74-8.71 (m, 2H), 7.72-7.64 (m, 3H), 7.47-7.34 (m, 5H), 6.02 (s, 1H), 5.27 (s, 1H).
^{13}CNMR (100 MHz, $CDCl_3$) δ 164.25, 150.75, 150.69, 141.76, 140.18, 137.89, 129.00, 128.92, 128.89, 126.00, 120.75, 104.26.
HRMS (ESI) calcd. for $C_{14}H_{13}ON_2$ $[M+H]^+$ 225.1022, found 225.1018.

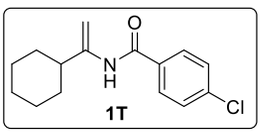


***N*-(1-Phenylvinyl)thiophene-2-carboxamide (1R)**
yellow solid (928.7 mg, 27% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (s, 1H), 7.58 (dd, *J* = 4.0, 1.2 Hz, 1H), 7.50 (dd, *J* = 5.2, 1.2 Hz, 1H), 7.47-7.44 (m, 2H), 7.39-7.34 (m, 3H), 7.07 (dd, *J* = 4.8, 3.6 Hz, 1H), 5.89 (s, 1H), 5.19 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 160.54, 140.22, 139.07, 138.03, 130.71, 128.61, 128.59, 128.24, 127.68, 125.87, 103.53.
HRMS (ESI) calcd. for $C_{13}H_{12}ONS$ $[M+H]^+$ 230.0634, found 230.0632.



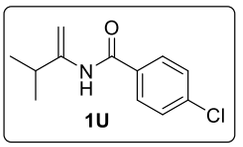
***N*-(1-Phenylvinyl)furan-2-carboxamide (1S)**
Yellow sticky liquid(511.7 mg, 16% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.41-7.38 (m, 3H), 7.31-7.26 (m, 3H), 7.11 (dd, *J* = 3.6, 0.8 Hz, 1H), 6.42 (dd, *J* = 3.6, 2.0 Hz, 1H), 5.96 (s, 1H), 5.13 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 156.37, 147.20, 143.89, 139.52, 137.58, 128.23, 128.21, 125.38, 114.59, 111.98, 102.51.
HRMS (ESI) calcd. for $C_{13}H_{12}O_2N$ $[M+H]^+$ 214.0863, found 214.0859.



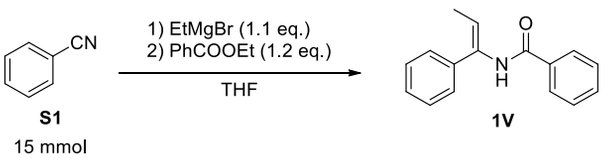
1T

4-Chloro-*N*-(1-cyclohexylvinyl)benzamide (1T)
White solid (554.0 mg, 14% yield)**.**
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.36 (d, *J* = 7.2 Hz, 2H), 7.21 (s, 1H), 5.71 (s, 1H), 4.66 (s, 1H), 2.09-2.03 (m, 1H), 1.91-1.68 (m, 5H), 1.34-1.15 (m, 5H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.13, 145.87, 137.64, 133.64, 128.78, 128.20, 98.15, 43.69, 31.71, 26.64, 25.96.
HRMS (ESI) calcd. for $C_{15}H_{19}ONCl$ $[M+H]^+$ 264.1150, found 264.1146.

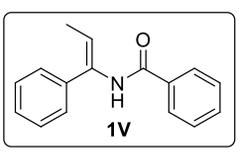


1U

4-Chloro-*N*-(3-methylbut-1-en-2-yl)benzamide (1U)
White solid (335.6 mg, 10% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.44-7.41 (m, 2H), 7.01 (s, 1H), 5.75 (s, 1H), 4.72 (s, 1H), 2.50-2.40 (m, 1H), 1.17 (d, *J* = 6.8 Hz, 6H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.03, 146.23, 137.86, 133.71, 128.99, 128.18, 97.81, 33.91, 21.13.
HRMS (ESI) calcd. for $C_{12}H_{15}ONCl$ $[M+H]^+$ 224.0837, found 224.0833.



S1
15 mmol
1V

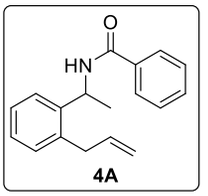


1V

(*E*)-*N*-(1-Phenylprop-1-en-1-yl)benzamide (1V)
White solid (747.5 mg, 21% yield).
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (d, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.43 (d, *J* = 7.5 Hz, 2H), 7.33-7.25 (m, 4H), 6.03 (q, *J* = 7.0 Hz, 1H), 1.84 (d, *J* = 7.0 Hz, 3H).
^{13}CNMR (125 MHz, $CDCl_3$) δ 165.43, 138.05, 134.22, 134.03, 131.86, 128.73, 128.45, 127.82, 127.27, 125.54, 121.10, 14.19.
HRMS (ESI) calcd. for $C_{16}H_{16}ON^+[M+H]^+$ 238.1226, found 238.1223.

2) Procedure for the synthesis of 4

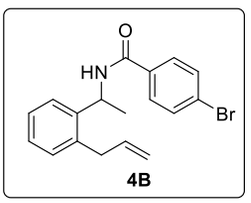
Syntheis of **4A-4E** has already been reported in our previous work. [2]



***N*-(1-(2-Allylphenyl)ethyl)benzamide (4A)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.2 Hz, 2H), 7.51-7.39 (m, 4H), 7.30-7.23 (m, 3H), 6.50 (d, *J* = 6.8 Hz, 1H), 6.09-5.99 (m, 1H), 5.57 (dq, *J* = 7.2, 6.8 Hz, 1H) 5.10-5.02 (m, 2H), 3.68 (dd, *J* = 16.0, 6.8 Hz, 1H), 3.49 (dd, *J* = 16.0, 5.6 Hz, 1H), 1.61 (d, *J* = 6.8 Hz, 3H).

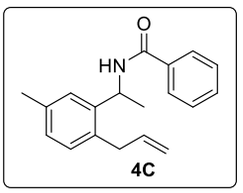
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.30, 141.08, 137.66, 137.13, 134.44, 131.32, 130.25, 128.42, 127.54, 126.87, 126.81, 125.23, 115.92, 45.39, 36.75, 21.48.



***N*-(1-(2-Allylphenyl)ethyl)-4-bromobenzamide (4B)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.41-7.37 (m, 1H), 7.26-7.18 (m, 3H), 6.55 (d, *J* = 7.2 Hz, 1H), 6.03-5.93 (m, 1H), 5.49 (dq, *J* = 7.2, 6.8 Hz, 1H), 5.04 (dq, *J* = 10.0, 1.6 Hz, 1H), 4.98 (dq, *J* = 17.2, 2.0 Hz, 1H), 3.62 (dd, *J* = 16.0, 6.4 Hz, 1H), 3.55 (ddt, *J* = 16.0, 6.0, 1.6 Hz, 1H), 1.55 (d, *J* = 6.8 Hz, 3H).

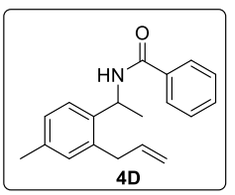
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.40, 140.88, 138.00, 137.09, 133.24, 131.59, 130.31, 128.53, 127.62, 126.84, 125.96, 125.24, 115.95, 45.55, 36.74, 21.43.



***N*-(1-(2-Allyl-5-methylphenyl)ethyl)benzamide (4C)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.71 (m, 2H), 7.44 (tt, *J* = 7.6, 2.0 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 8.0 Hz, 1H), 7.02 (s, 1H), 6.43 (d, *J* = 7.2 Hz, 1H), 6.04-5.94 (m, 1H), 5.49 (dq, *J* = 7.2, 6.8 Hz, 1H), 5.05-4.98 (m, 2H), 3.63 (dd, *J* = 16.0, 6.8 Hz, 1H), 3.45 (dd, *J* = 16.0, 6.0 Hz, 1H), 2.31 (s, 3H), 1.55 (d, *J* = 6.8 Hz, 3H).

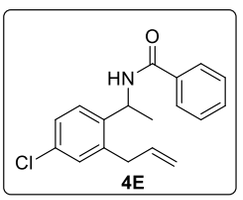
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.23, 138.07, 137.53, 137.22, 137.14, 134.49, 131.25, 130.92, 128.37, 127.47, 126.85, 125.22, 115.81, 45.17, 36.74, 21.45, 20.93.



***N*-(1-(2-Allyl-4-methylphenyl)ethyl)benzamide (4D)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.23 (m, 2H), 7.48 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.42-7.39 (m, 2H), 7.20 (s, 1H), 7.10 (d, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.27 (d, *J* = 6.8 Hz, 1H), 6.04-5.94 (m, 1H), 5.50 (dq, *J* = 7.2, 6.8 Hz, 1H), 5.04-4.97 (m, 2H), 3.59 (dd, *J* = 16.0, 6.4 Hz, 1H), 3.43 (dd, *J* = 16.0, 5.6 Hz, 1H), 2.35 (s, 3H), 1.57 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.25, 140.80, 137.40, 136.30, 134.63, 134.52, 131.32, 130.27, 128.44, 128.34, 126.88, 125.96, 115.72, 45.43, 36.42, 21.50, 21.17.



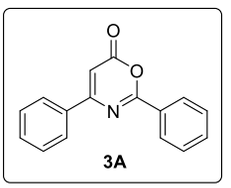
***N*-(1-(2-Allyl-4-chlorophenyl)ethyl)benzamide (4E)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.72 (m, 2H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 2H), 7.32-7.30 (m, 1H), 7.18-7.16 (m, 2H), 6.62 (d, *J* = 6.8 Hz, 1H), 6.01-5.91 (m, 1H), 5.44 (dq, *J* = 7.2, 6.8 Hz,

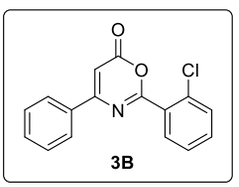
1H), 5.08 (dd, *J* = 10.0, 1.2 Hz, 1H), 5.01 (dd, *J* = 17.2, 5.6 Hz, 1H), 3.61 (dd, *J* = 16.0, 6.8 Hz, 1H), 3.42 (dd, *J* = 16.0, 5.6 Hz, 1H), 1.52 (d, *J* = 6.8 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.40, 139.87, 139.55, 136.20, 134.16, 132.97, 131.44, 129.91, 128.43, 126.88, 126.78, 126.69, 116.64, 45.02, 36.43, 21.48.

General procedure for the synthesis of products 3

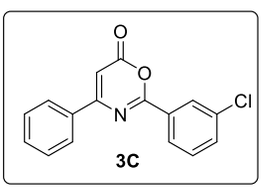
To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **1** (0.2 mmol), Togni's reagent **2a** (75 mg, 0.24 mmol) and potassium phosphate (212 mg, 1.0 mmol). The tube was evacuated and backfilled with Argon for three times and CH_3CN/H_2O (2.0 mL/1.0 mL) was added *via* syringe, then the tube was stirred at 45 ℃. After reaction completed (monitored by TLC), the reaction solution was concentrated *in vacuo* and the crude residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 4/1-20/1) to give the corresponding products **3**.



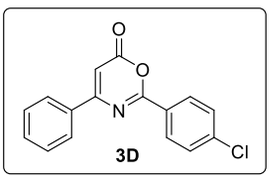
2,4-Diphenyl-6H-1,3-oxazin-6-one (3A)
White solid (39.9 mg, 80% yield).
^{1}HNMR (400 MHz, $CDCl_3$) δ 8.38-8.35 (m, 2H), 8.13-8.10 (m, 2H), 7.65-7.60 (m, 1H), 7.58-7.50 (m, 5H), 6.61 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 163.09, 161.78, 159.86, 134.36, 133.34, 131.89, 129.94, 128.90, 128.77, 128.68, 127.31, 101.65.
HRMS (ESI) calcd. for $C_{16}H_{12}O_2N$ $[M+H]^+$ 250.0863, found 250.0860



2-(2-Chlorophenyl)-4-phenyl-6H-1,3-oxazin-6-one (3B)
White solid (46.0 mg, 81% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-8.08 (m, 2H), 8.04 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.58-7.47 (m, 5H), 7.42 (td, *J* = 8.0, 1.6 Hz, 1H), 6.65 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 161.87, 161.51, 159.58, 134.07, 133.97, 132.90, 132.04, 131.79, 131.57, 129.35, 128.99, 127.48, 126.90, 102.11.
HRMS (ESI) calcd. for $C_{16}H_{11}O_2NCl$ $[M+H]^+$ 284.0473, found 284.0470.

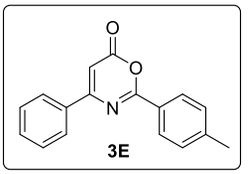


2-(3-Chlorophenyl)-4-phenyl-6H-1,3-oxazin-6-one (3C)
White solid (39.7 mg, 70% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35-8.33 (m, 1H), 8.24-8.22 (m, 1H), 8.10-8.08 (m, 2H), 7.60-7.46 (m, 5H), 6.62 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 161.84, 161.70, 159.38, 135.08, 134.12, 133.32, 132.09, 131.74, 130.12, 129.01, 128.66, 127.37, 126.74, 102.12.
HRMS (ESI) calcd. for $C_{16}H_{11}O_2NCl$ $[M+H]^+$ 284.0473, found 284.0470.

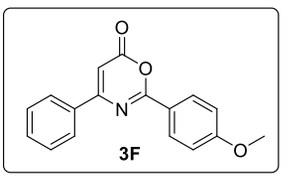


2-(4-Chlorophenyl)-4-phenyl-6H-1,3-oxazin-6-one (3D)
White solid (40.3 mg, 71% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30-8.27 (m, 2H), 8.09-8.07 (m, 2H), 7.58-7.49 (m, 5H), 6.60 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 162.26, 161.77, 159.52, 139.90,

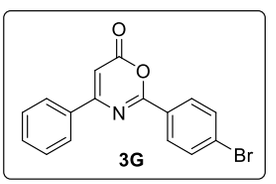
134.23, 132.02, 129.99, 129.21, 128.97, 128.45, 127.33, 101.80.
HRMS (ESI) calcd. for $C_{16}H_{11}O_2NCl$ $[M+H]^+$ 284.0473, found 284.0471.



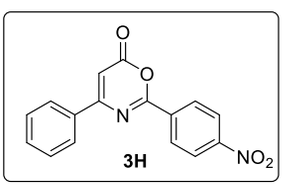
4-Phenyl-2-(p-tolyl)-6H-1,3-oxazin-6-one (3E)
White solid (44.8 mg, 85% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.4 Hz, 2H), 8.11-8.09 (m, 2H), 7.56-7.50 (m, 3H), 7.33 (d, *J* = 8.0 Hz, 2H), 6.58 (s, 1H), 2.46 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 163.39, 162.03, 160.11, 144.36, 134.58, 131.84, 129.59, 128.91, 128.77, 127.36, 127.28, 101.36, 21.79.
HRMS (ESI) calcd. for $C_{17}H_{14}O_2N$ $[M+H]^+$ 264.1019, found 264.1016.



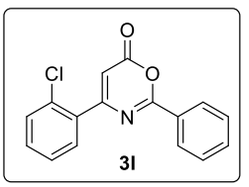
2-(4-Methoxyphenyl)-4-phenyl-6H-1,3-oxazin-6-one (3F)
White solid (45.2 mg, 81% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33-8.30 (m, 2H), 8.10-8.07 (m, 2H), 7.54-7.50 (m, 3H), 7.03-6.99 (m, 2H), 6.54 (s, 1H), 3.91 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 163.91, 163.20, 162.17, 160.22, 134.70, 131.76, 130.85, 128.87, 127.32, 122.37, 114.22, 100.71, 55.55.
HRMS (ESI) calcd. for $C_{17}H_{14}O_3N$ $[M+H]^+$ 280.0968, found 280.0964.



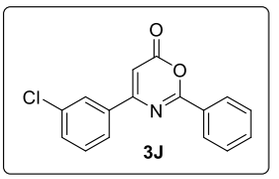
2-(4-Bromophenyl)-4-phenyl-6H-1,3-oxazin-6-one (3G)
White solid (53.2 mg, 81% yield).
^{1}HNMR (400 MHz, $CDCl_3$) δ 8.23-8.20 (m, 2H), 8.10-8.07 (m, 2H), 7.69-7.66 (m, 2H), 7.57-7.50 (m, 3H), 6.61 (s, 1H).
^{13}CNMR (100 MHz, $CDCl_3$) δ 162.40, 161.78, 159.52, 134.21, 132.20, 132.04, 130.09, 128.98, 128.91, 128.61, 127.34, 101.88.
HRMS (ESI) calcd. for $C_{16}H_{11}O_2NBr$ $[M+H]^+$ 327.9968, found 327.9963.



2-(4-Nitrophenyl)-4-phenyl-6H-1,3-oxazin-6-one (3H)
White solid (26.5 mg, 45% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56-8.52 (m, 2H), 8.40-8.37 (m, 2H), 8.12-8.09 (m, 2H), 7.62-7.53 (m, 3H), 6.69 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 161.51, 160.97, 158.81, 150.58, 135.47, 133.83, 132.33, 129.70, 129.12, 127.38, 124.96, 102.78.
HRMS (ESI) calcd. for $C_{16}H_{11}O_4N_2$ $[M+H]^+$ 295.0713, found 295.0711.



4-(2-Chlorophenyl)-2-phenyl-6H-1,3-oxazin-6-one (3I)
White solid (45.4 mg, 80% yield).
^{1}HNMR (400 MHz, $CDCl_3$) δ 8.30-8.27 (m, 2H), 7.80-7.75 (m, 1H), 7.62-7.57 (m, 1H), 7.52-7.48 (m, 3H), 7.43-7.38 (m, 2H), 6.64 (s, 1H).
^{13}CNMR (100 MHz, $CDCl_3$) δ 163.12, 161.24, 159.05, 134.49, 133.38, 132.52, 131.37, 130.85, 130.81, 129.71, 128.75, 128.63, 127.01, 108.14.
HRMS (ESI) calcd. for $C_{16}H_{11}O_2NCl$ $[M+H]^+$ 284.0473, found 284.0469.



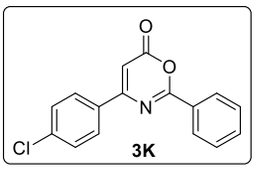
4-(3-Chlorophenyl)-2-phenyl-6H-1,3-oxazin-6-one (3J)

White solid (34.0 mg, 60% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35-8.31 (m, 2H), 8.09-8.08 (m, 1H), 7.93-7.90 (m, 1H), 7.65-7.61 (m, 1H), 7.56-7.49 (m, 3H), 7.47-7.42 (m, 1H), 6.56 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.40, 160.31, 159.37, 136.19, 135.13, 133.54, 131.72, 130.13, 129.68, 128.82, 128.73, 127.47, 125.23, 102.37.

HRMS (ESI) calcd. for $C_{16}H_{11}O_2NCl$ $[M+H]^+$ 284.0473, found 284.0469.



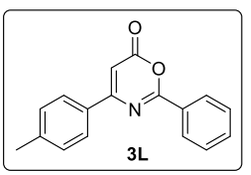
4-(4-Chlorophenyl)-2-phenyl-6H-1,3-oxazin-6-one (3K)

White solid (47.7 mg, 84% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36-8.33 (m, 2H), 8.04 (d, *J* = 8.8 Hz, 2H), 7.65-7.61 (m, 1H), 7.56-7.48 (m, 4H), 6.57 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.39, 160.67, 159.60, 138.23, 133.53, 132.88, 129.83, 129.24, 128.85, 128.75, 128.64, 101.72.

HRMS (ESI) calcd. for $C_{16}H_{11}O_2NCl$ $[M+H]^+$ 284.0473, found 284.0470.



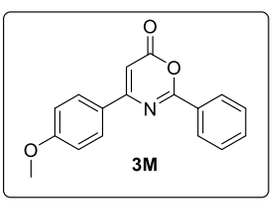
2-Phenyl-4-(p-tolyl)-6H-1,3-oxazin-6-one (3L)

White solid (38.4 mg, 73% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36-8.34 (m, 2H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.63-7.59 (m, 1H), 7.55-7.50 (m, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 6.55 (s, 1H), 2.44 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.96, 161.79, 160.03, 142.62, 133.26, 131.61, 130.06, 129.66, 128.76, 128.68, 127.32, 100.78, 21.56.

HRMS (ESI) calcd. for $C_{17}H_{14}O_2N$ $[M+H]^+$ 264.1019, found 264.1016.



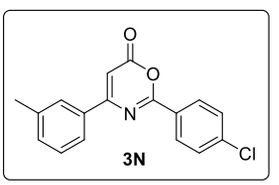
4-(4-Methoxyphenyl)-2-phenyl-6H-1,3-oxazin-6-one (3M)

White solid (44.7 mg, 80% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35-8.32 (m, 2H), 8.06 (dt, *J* = 9.2, 2.8 Hz, 2H), 7.60 (tt, *J* = 7.6, 1.6 Hz, 1H), 7.53-7.49 (m, 2H), 7.00 (dt, *J* = 10.0, 3.2 Hz, 2H), 6.47 (s, 1H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.81, 162.76, 161.33, 160.09, 133.20, 130.09, 129.18, 128.73, 128.63, 126.72, 114.28, 99.48, 55.45.

HRMS (ESI) calcd. for $C_{17}H_{14}O_3N$ $[M+H]^+$ 280.0968, found 280.0965.



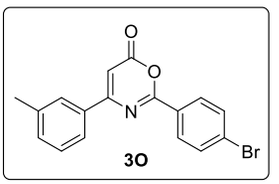
2-(4-Chlorophenyl)-4-(m-tolyl)-6H-1,3-oxazin-6-one (3N)

White solid (51.8 mg, 87% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.8 Hz, 2H), 7.85-7.83 (m, 2H), 7.48 (d, *J* = 8.8 Hz, 2H), 7.41-7.33 (m, 2H), 6.54 (s, 1H), 2.45 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.03, 161.77, 159.44, 139.76, 138.66, 134.09, 132.78, 129.90, 129.10, 128.80, 128.42, 127.78, 124.46, 101.62, 21.46.

HRMS (ESI) calcd. for $C_{17}H_{13}O_2NCl$ $[M+H]^+$ 298.0629, found 298.0626.



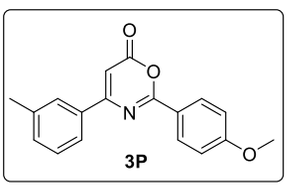
2-(4-Bromophenyl)-4-(m-tolyl)-6H-1,3-oxazin-6-one (3O)

White solid (58.9 mg, 86% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dt, *J* = 9.2, 2.4 Hz, 2H), 7.86-7.84 (m, 2H), 7.65 (dt, *J* = 8.8, 2.4 Hz, 2H), 7.41-7.34 (m, 2H), 6.56 (s, 1H), 2.45 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 162.19, 161.81, 159.46, 138.69, 134.10, 132.81, 132.11, 130.02, 128.88, 128.82, 128.49, 127.80, 124.49, 101.72, 21.5.

HRMS (ESI) calcd. for $C_{17}H_{13}O_2NBr$ $[M+H]^+$ 342.0124, found 342.0120.



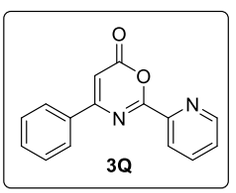
2-(4-Methoxyphenyl)-4-(m-tolyl)-6H-1,3-oxazin-6-oneone (3P)

White solid (46.9 mg, 80% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (dt, *J* = 8.8, 3.2 Hz, 2H), 7.85-7.83 (m, 2H), 7.39-7.31 (m, 2H), 6.98 (dt, *J* = 8.8, 3.2 Hz, 2H), 6.47 (s, 1H), 3.88 (s, 3H), 2.44 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.75, 162.93, 162.12, 160.13, 138.50, 134.51, 132.50, 130.71, 128.67, 127.77, 124.41, 122.28, 114.09, 100.50, 55.45, 21.43.

HRMS (ESI) calcd. for $C_{18}H_{16}O_3N$ $[M+H]^+$ 294.1125, found 294.1119.



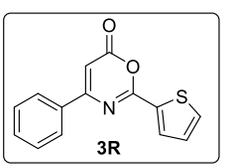
4-Phenyl-2-(pyridin-2-yl)-6H-1,3-oxazin-6-one (3Q)

White solid (21.0 mg, 42% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, *J* = 4.8 Hz, 2H), 8.15 (dd, *J* = 4.4, 2.0 Hz, 2H), 8.10-8.07 (m, 2H), 7.60-7.51 (m, 3H), 6.68 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 161.32, 161.16, 158.78, 150.76, 137.32, 133.74, 132.27, 129.06, 127.33, 121.63, 103.15.C。

HRMS (ESI) calcd. for $C_{15}H_{11}O_2N_2$ $[M+H]^+$ 251.0815, found 251.0811.



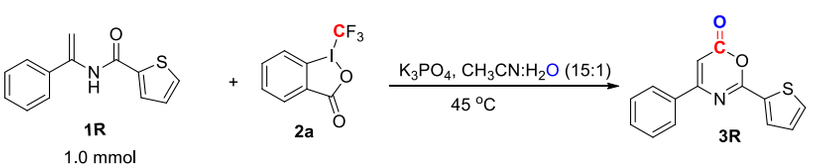
4-Phenyl-2-(thiophen-2-yl)-6H-1,3-oxazin-6-one (3R)

White solid (28.6 mg, 56% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05-8.00 (m, 3H), 7.66 (dt, *J* = 4.8, 1.6 Hz, 1H), 7.56-7.46 (m, 3H), 7.20-7.17 (m, 1H), 6.51 (s, 1H).

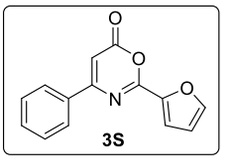
^{13}C NMR (100 MHz, $CDCl_3$) δ 162.07, 159.60, 159.31, 134.14, 134.09, 133.60, 132.75, 131.90, 128.86, 128.54, 127.26, 100.71.

HRMS (ESI) calcd. for $C_{14}H_{10}O_2NS$ $[M+H]^+$ 256.0427, found 256.0423.

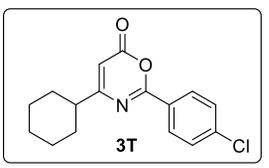


To a flame-dried Schlenk tube (100 ml) equipped with a magnetic stir bar were added **1R** (1.0 mmol), Togni's reagent **2a** (375 mg, 1.2 mmol) and potassium phosphate (1.06 g, 5.0 mmol). The tube was evacuated and backfilled with Argon for three times and CH_3CN/H_2O (15.0 mL/1.0 mL) was added *via* syringe, then the tube was stirred at 45 ℃ for 7 h. After reaction completed (monitored by TLC), the reaction solution was concentrated *in vacuo* and the crude residue was purified by silica gel column chromatography (petroleum

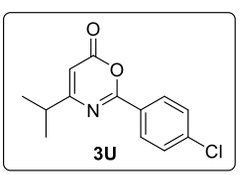
ether/EtOAc = 10/1) to give the corresponding product **3R** (153.0 mg, 60%).



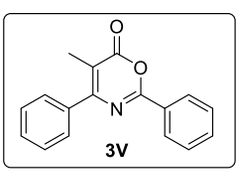
2-(Furan-2-yl)-4-phenyl-6H-1,3-oxazin-6-one (3S)
White solid (34.0 mg, 71% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-8.04 (m, 2H), 7.73-7.72 (m, 1H), 7.56-7.48 (m, 3H), 7.46 (dd, *J* = 3.6, 0.8 Hz, 1H), 6.64 (dd, *J* = 3.6, 1.6 Hz, 1H), 6.53 (s, 1H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 162.22, 158.85, 155.42, 147.56, 144.65, 134.24, 131.94, 128.94, 127.33, 118.56, 112.82, 101.33.
HRMS (ESI) calcd. for $C_{14}H_{10}O_3N$ $[M+H]^+$ 240.0655, found 240.0652.



2-(4-Chlorophenyl)-4-cyclohexyl-6H-1,3-oxazin-6-one (3T)
White solid (41.7 mg, 72% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 8.8 Hz, 2H), 5.96 (s, 1H), 2.43-2.36 (m, 1H), 1.97-1.71 (m, 5H), 1.46-1.19 (m, 5H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 173.34, 161.91, 159.39, 139.44, 129.74, 128.98, 128.38, 103.46, 44.85, 30.46, 25.82, 25.72.
HRMS (ESI) calcd. for $C_{16}H_{17}O_2NCl$ $[M+H]^+$ 290.0942, found 290.0940.



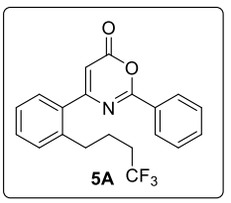
2-(4-Chlorophenyl)-4-isopropyl-6H-1,3-oxazin-6-one (3U)
White solid (35.0 mg, 70% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.4 Hz, 2H), 7.48 (d, *J* = 8.8 Hz, 2H), 6.04 (s, 1H), 2.81-2.75 (m, 1H), 1.29 (d, *J* = 6.8 Hz, 6H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 174.40, 162.12, 159.45, 139.58, 129.84, 129.09, 128.42, 103.31, 35.25, 20.27.
HRMS (ESI) calcd. for $C_{13}H_{13}O_2NCl$ $[M+H]^+$ 250.0629, found 250.0627.



5-Methyl-2,4-diphenyl-6H-1,3-oxazin-6-one (3V)
White solid (35.8 mg, 68% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 6.8 Hz, 2H), 7.71-7.68 (m, 2H), 7.59-7.55 (m, 1H), 7.53-7.47 (m, 5H), 2.25 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 161.79, 159.65, 158.69, 136.55, 132.81, 130.01, 129.90, 129.16, 128.71, 128.27, 128.24, 114.65, 13.39.
HRMS (ESI) calcd. for $C_{17}H_{14}O_2N$ $[M+H]^+$ 264.1019, found 264.1013.

General procedure for the synthesis of products 5

To a flame-dried Schlenk tube equipped with a magnetic stir bar were added **4** (0.2 mmol), Togni's reagent **2a** (139 mg, 0.44 mmol), potassium phosphate (170 mg, 0.8 mmol) and Bu_4NI (20 mol %, 14.8 mg). The tube was evacuated and backfilled with argon for three times, and wet EtOAc (3.0 mL) was added *via* syringe. Then the tube was stirred at 80 ℃. After reaction completed (monitored by TLC), the reaction solution was concentrated *in vacuo* and the crude residue was purified by silica gel column chromatography (petroleum ether/EtOAc = 10/1-20/1) to give the corresponding products **5**.



2-Phenyl-4-(2-(4,4,4-trifluorobutyl)phenyl)-6H-1,3-oxazin-6-one (5A)

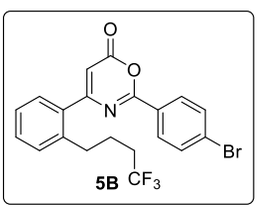
White solid (36.6 mg, 51% yield).

^{1}HNMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.4 Hz, 2H), 7.63-7.59 (m, 1H), 7.53-7.43 (m, 4H), 7.36-7.32 (m, 2H), 6.30 (s, 1H), 2.90 (t, *J* = 8.0 Hz, 2H), 2.11-2.00 (m, 4H).

^{13}CNMR (100 MHz, $CDCl_3$) δ 166.22, 162.89, 159.08, 139.58, 135.84, 133.52, 130.56, 130.30, 129.73, 129.48, 128.89, 128.63, 126.98 (q, J_{CF} =274.6 H_Z), 126.73, 107.05, 33.49 (q, J_{CF} =28.3 H_Z), 32.28, 23.87 (q, J_{CF} =2.5 H_Z).

^{19}FNMR (376 MHz, $CDCl_3$) δ -66.20.

HRMS (ESI) calcd. for $C_{20}H_{17}O_2NF_3^+[M+H]^+$ 360.1206, found 360.1198.



2-(4-Bromophenyl)-4-(2-(4,4,4-trifluorobutyl)phenyl)-6H-1,3-oxazin-6-one (5B)

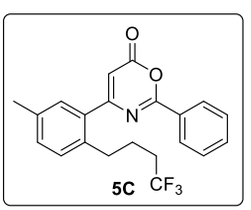
White solid (50.8 mg, 58% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.8 Hz, 2H), 7.65 (d, *J* = 8.8 Hz, 2H), 7.48-7.41 (m, 2H), 7.36-7.32 (m, 2H), 6.31 (s, 1H), 2.88 (t, *J* = 8.0 Hz, 2H), 2.14-2.04 (m, 2H), 2.03-1.93 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.14, 162.16, 158.77, 139.50, 135.66, 132.31, 130.69, 130.33, 130.00, 129.50, 128.86, 128.63, 126.95 (q, J_{CF} = 274.8.0), 126.81, 107.29, 33.49 (q, J_{CF} = 28.5), 32.28, 23.88 (q, J_{CF} = 3.1 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.14.

HRMS (ESI) calcd. for $C_{20}H_{16}O_2NBrF_3^+[M+H]^+$ 438.0311, found 438.0305.



4-(5-methyl-2-(4,4,4-trifluorobutyl)phenyl)-2-phenyl-6H-1,3-oxazin-6-one (5C)

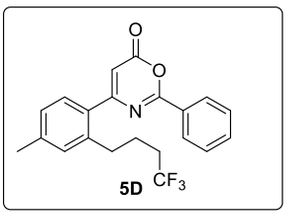
White solid (44.8 mg, 60% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27-8.25 (m, 2H), 7.63-7.59 (m, 1H), 7.53-7.49 (m, 2H), 7.36-7.34 (m, 1H), 7.16-7.14 (m, 2H), 6.28 (s, 1H), 2.88 (t, *J* = 7.6 Hz, 2H), 2.41 (s, 3H), 2.15-1.94 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.30, 162.75, 159.29, 140.95, 139.63, 133.48, 132.99, 131.17, 129.84, 129.62, 128.90, 128.64, 127.51, 127.01 (q, J_{CF} = 274.8 Hz), 106.61, 33.59 (q, J_{CF} = 28.4 Hz), 32.36, 23.99 (q, J_{CF} = 3.0 Hz), 21.32.

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.19.

HRMS (ESI) calcd. for $C_{21}H_{19}O_2NF_3^+[M+H]^+$ 374.1362, found 374.1357.



4-(4-Methyl-2-(4,4,4-trifluorobutyl)phenyl)-2-phenyl-6H-1,3-oxazin-6-one (5D)

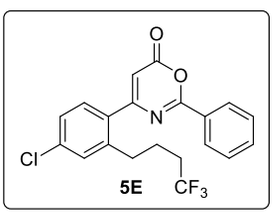
White solid (42.6 mg, 57% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 7.6 Hz, 2H), 7.63-7.59 (m, 1H), 7.56-7.49 (m, 2H), 7.28-7.21 (m, 3H), 6.28 (s, 1H), 2.86 (t, *J* = 8.0 Hz, 2H), 2.39 (s, 3H), 2.13-1.92 (m, 4H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.44, 162.85, 159.22, 136.49, 136.45, 135.68, 133.53, 131.32, 130.29, 130.04, 129.75, 128.90, 128.65, 127.01 (q, J_{CF} = 274.8 Hz), 106.92, 33.48 (q, J_{CF} = 28.4 Hz), 31.87, 23.94 (q, J_{CF} = 2.6 Hz), 20.88.

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.20.

HRMS (ESI) calcd. for $C_{21}H_{19}O_2NF_3^+[M+H]^+$ 374.1362, found 374.1354.



4-(4-Chloro-2-(4,4,4-trifluorobutyl)phenyl)-2-phenyl-6H-1,3-oxazin-6-one (5E)

White solid (38.6 mg, 49% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26-8.24 (m, 2H), 7.62 (tt, *J* = 7.6, 1.6 Hz, 1H), 7.53-7.49 (m, 2H), 7.40-7.31 (m, 3H), 6.27 (s, 1H), 2.88 (t, *J* = 8.0 Hz, 2H), 2.15-1.94 (m, 4H).

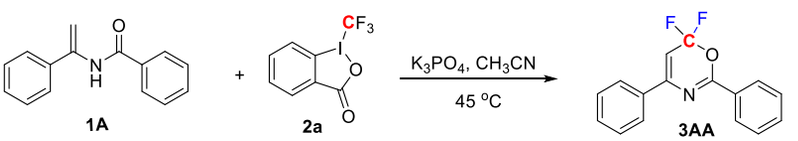
^{13}C NMR (100 MHz, $CDCl_3$) δ 165.11, 163.20, 158.86, 141.62, 136.63, 134.26, 133.72, 130.84, 130.33, 129.59, 128.97, 128.67, 127.00, 126.86 (q, J_{CF} = 274.7 Hz), 107.18, 33.49 (q, J_{CF} = 28.6 Hz), 32.22, 23.75 (q, J_{CF} = 2.9 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -66.16.

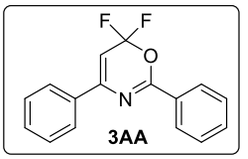
HRMS (ESI) calcd. for $C_{20}H_{16}O_2NClF_3^+[M+H]^+$ 394.0816, found 394.0812.

Experiment for mechanistic studies

1) Synthesis of intermediate of the reaction



To a flame-dried Schlenk tube equipped with a magnetic stir bar was added **1A** (44.7 mg, 0.2 mmol), Togni's reagent **2a** (75.8 mg, 0.24 mmol) and potassium phosphate (212.3 mg, 1.0 mmol). The tube was evacuated and backfilled with Argon for three times and dry CH_3CN (2.0 mL) was added *via* syringe. The tube was then stirred at 45 ℃. After reaction completed (monitored by TLC), the reaction solution was concentrated *in vacuo* and the crude residue was immediately purified by silica gel column chromatography (Hexane) after having deactivated silica gel with Et_3N. 6,6-Difluoro-2,4-diphenyl-6H-1,3-oxazine **3AA** could be obtained as a White solid.



3AA

6,6-Difluoro-2,4-diphenyl-6H-1,3-oxazine (3AA)

White solid (48.8 mg, 90% yield).

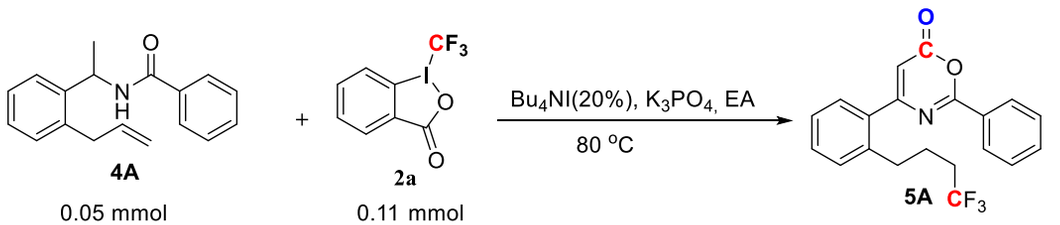
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29-8.26 (m, 2H), 8.00-7.98 (m, 2H), 7.61-7.57 (m, 1H), 7.53-7.47 (m, 5H), 6.16 (s, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 154.35, 147.67 (t, J_{CF} = 13.8 Hz), 134.73, 132.71, 130.31, 129.98, 128.70, 128.63, 128.39, 126.45, 121.50 (t, J_{CF} = 243.4 Hz), 97.71 (t, J_{CF} = 32.5 Hz).

^{19}F NMR (376 MHz, $CDCl_3$) δ -36.81.

HRMS (ESI) calcd. for $C_{16}H_{12}F_2NO^+[M+H]^+$ 272.0887, found 272.0882.

2) Control experiment in the presence of radical scavengers



trapping reagents	yield (^{19}FNMR %)
TEMPO (2.2 equiv)	trace
BHT (2.2 equiv)	6%
Benzoquinone (2.2 equiv)	7%

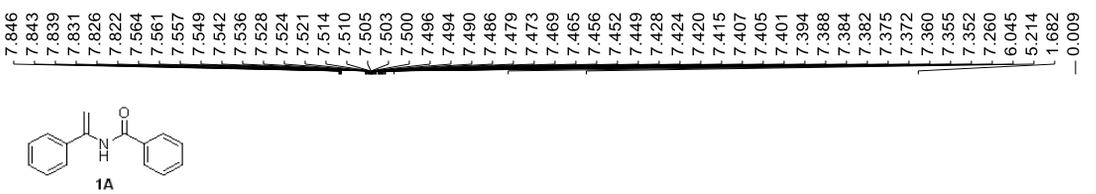
To a flame-dried Schlenk tube equipped with a magnetic stir bar was added **4A** (13 mg, 0.05 mmol), Togni's reagent **2a** (34 mg, 0.11 mmol), K_3PO_4 (42 mg, 0.2 mmol), TBAI (3.7 mg, 0.001 mmol) and radical scavenger (2.2 equiv.). The tube was evacuated and backfilled with Ar for three times, and then EtOAc (1.0 mL) were added *via* syringe. After stirring for 18 h at 80 ℃, the reaction mixture was cooled to room temperature. α,α,α-Trifluorotoluene (internal standard, 7.3 mg, 0.05 mmol) was added. ^{19}F NMR analysis of this reaction mixture showed that **5A** was formed in trace amount when TEMPO (17 mg, 0.11 mmol) was used as radical scavenger. By employing BHT (24 mg, 0.11 mmol) and BQ (12 mg, 0.11 mmol) as radical scanvengers, **5A** was formed in 6% yield and 7% yield respectively.

Reference

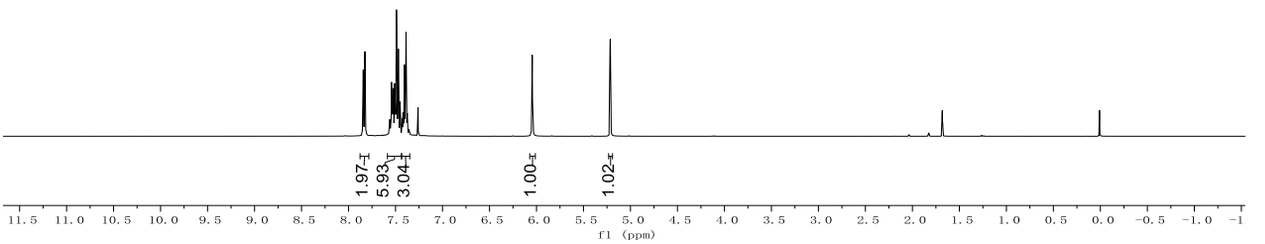
1 H. Kiyohara, R. Matsubara and S. Kobayashi, *Org. Lett.*, 2006, **8**, 5333.

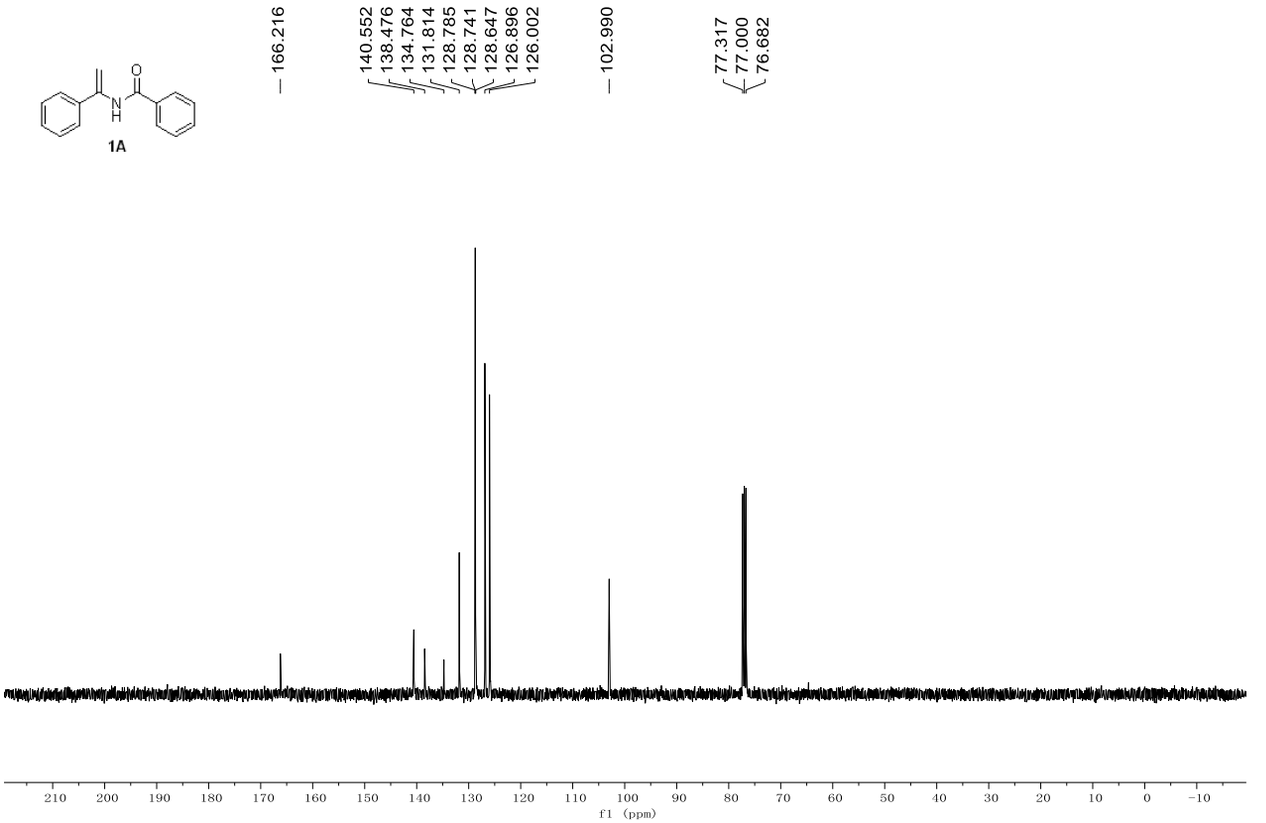
2 P. Yu, S.-C. Zheng, N.-Y. Yang, B. Tan and X.-Y. Liu, *Angew. Chem., Int. Ed.*, 2015, **127**, 4113.

NMR spectra



1A

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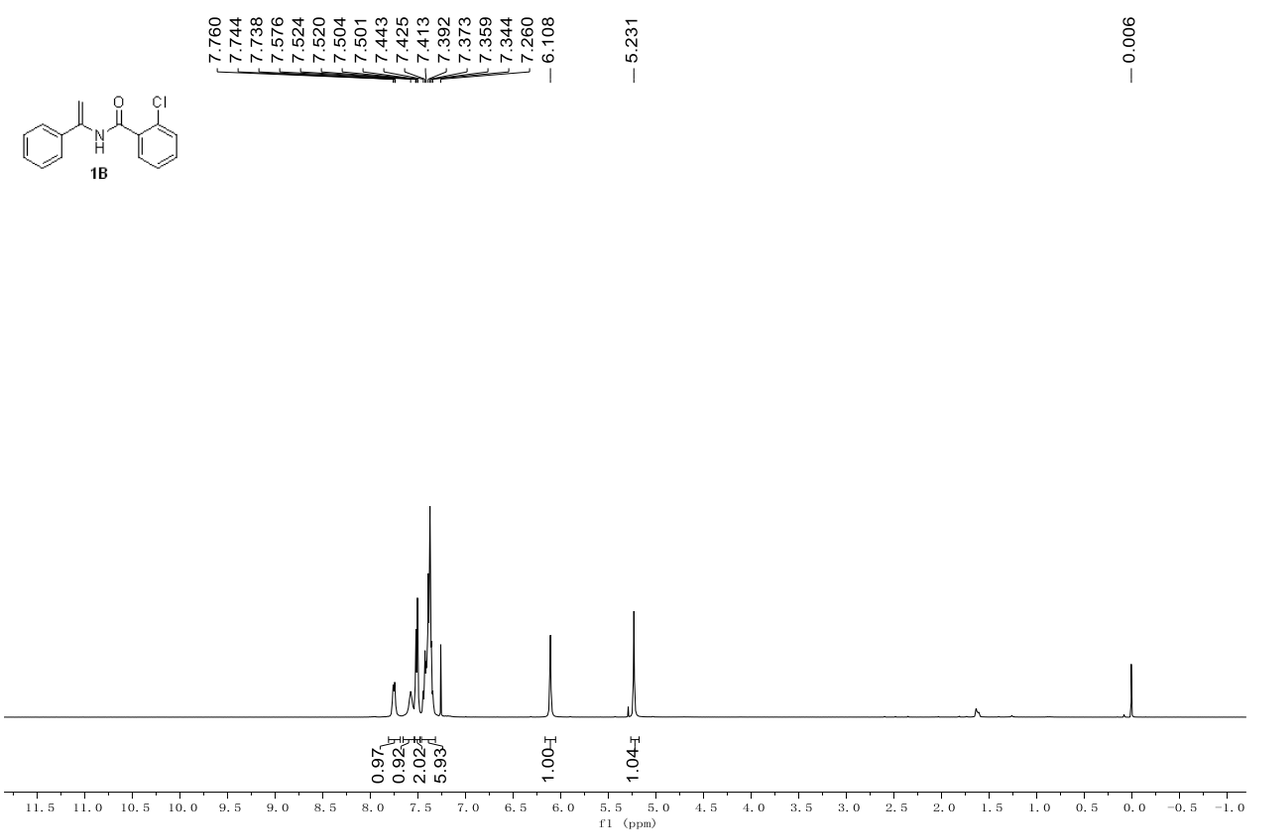
138.476
134.764
131.814
128.785
128.741
128.647
126.896
126.002
102.990
77.317
77.000
76.682
1A
f1 (ppm)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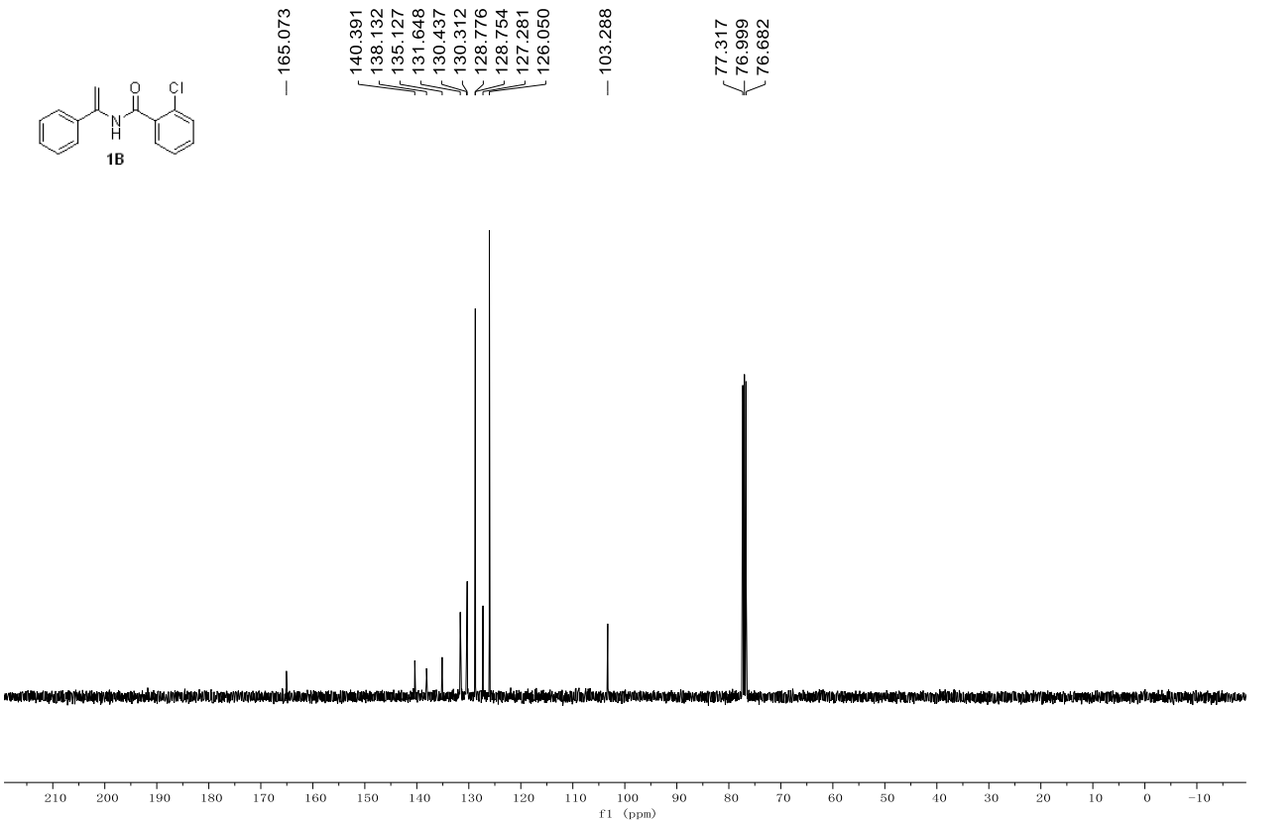
7.744
7.738
7.576
7.524
7.520
7.504
7.501
7.443
7.425
7.413
7.392
7.373
7.359
7.344
7.260
6.108
5.231
0.006
1B
0.97
0.92
2.02
5.93
1.00
1.04
f1 (ppm)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127.281
126.050
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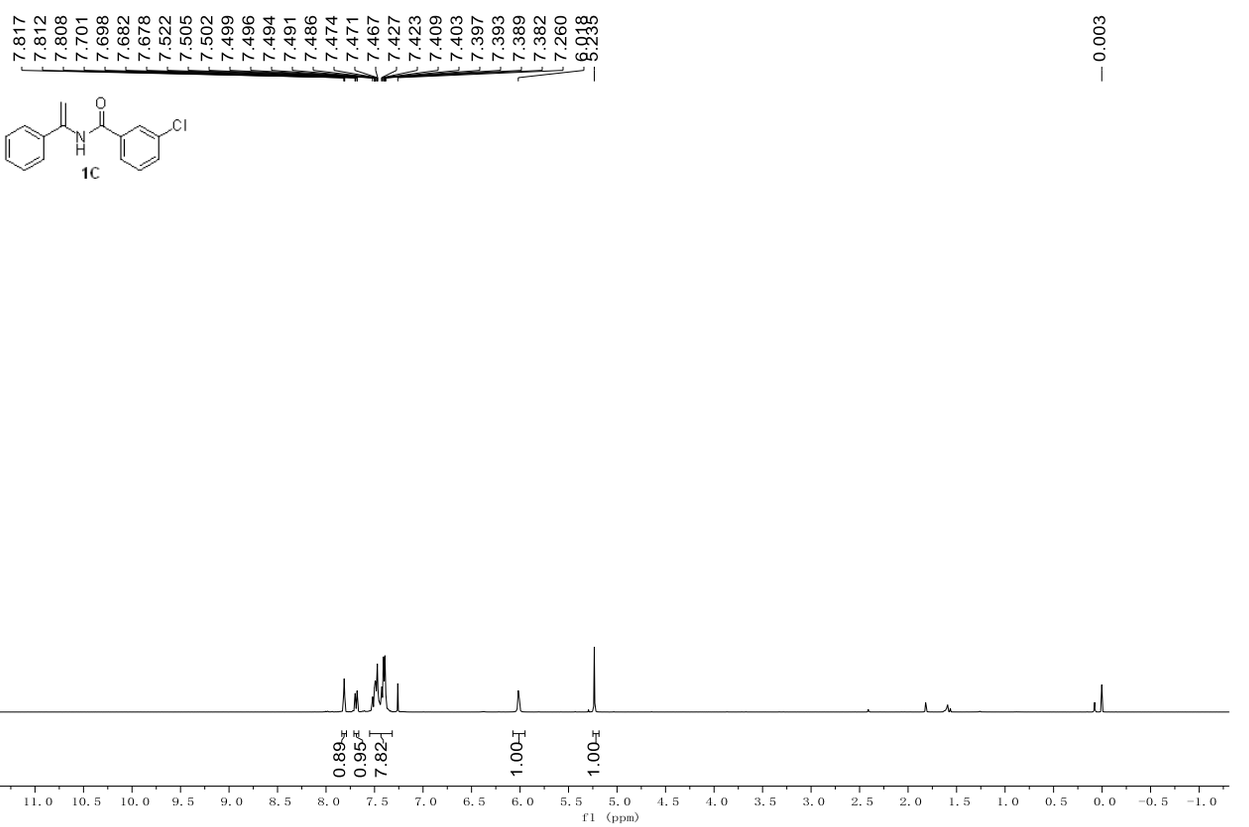
77.317
76.999
76.682
1B
f1 (ppm)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7.812
7.808
7.701
7.698
7.682
7.678
7.522
7.505
7.502
7.499
7.496
7.494
7.491
7.486
7.474
7.471
7.467
7.427
7.423
7.409
7.403
7.397
7.393
7.389
7.382
7.260
6.018
5.235
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1C
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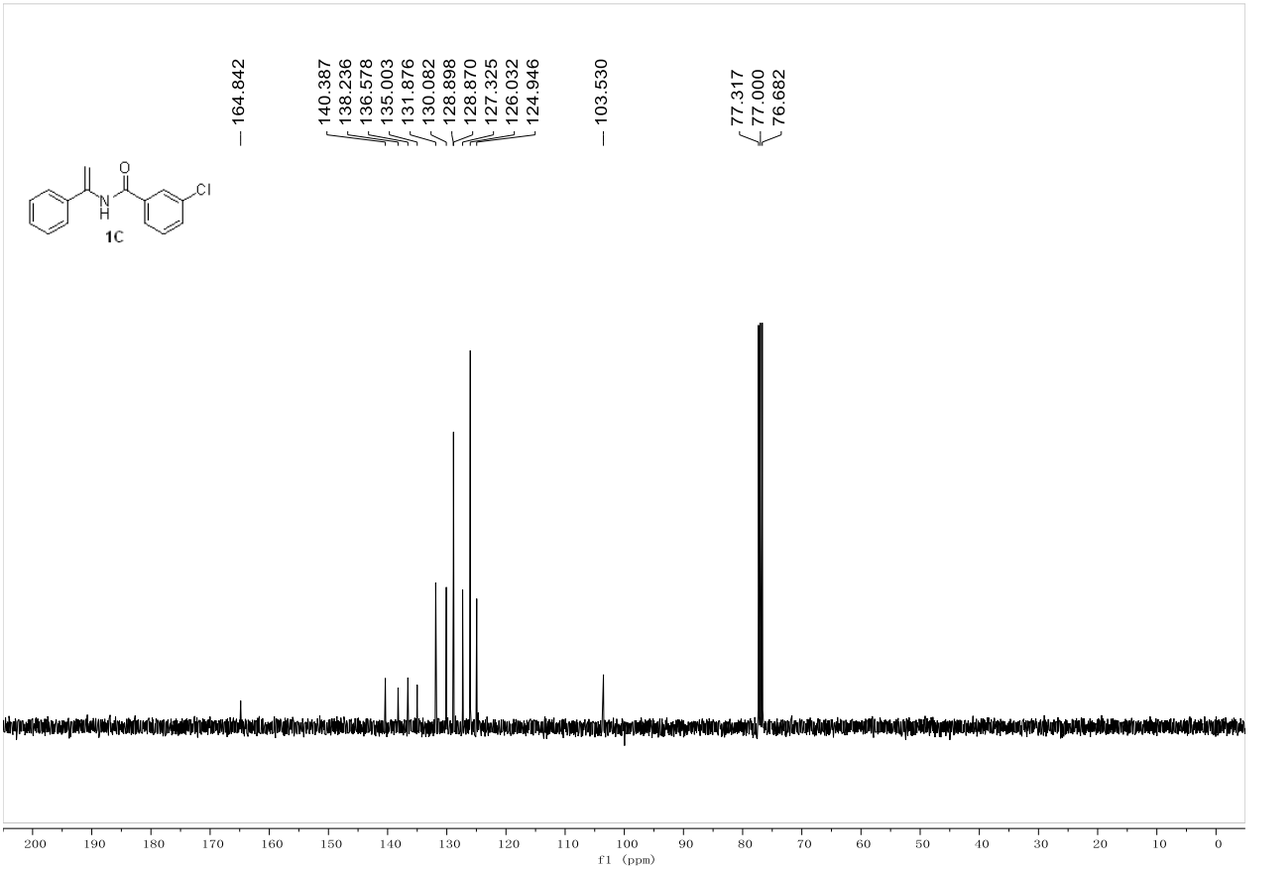
7.82
1.00
1.00
f1 (ppm)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124.946
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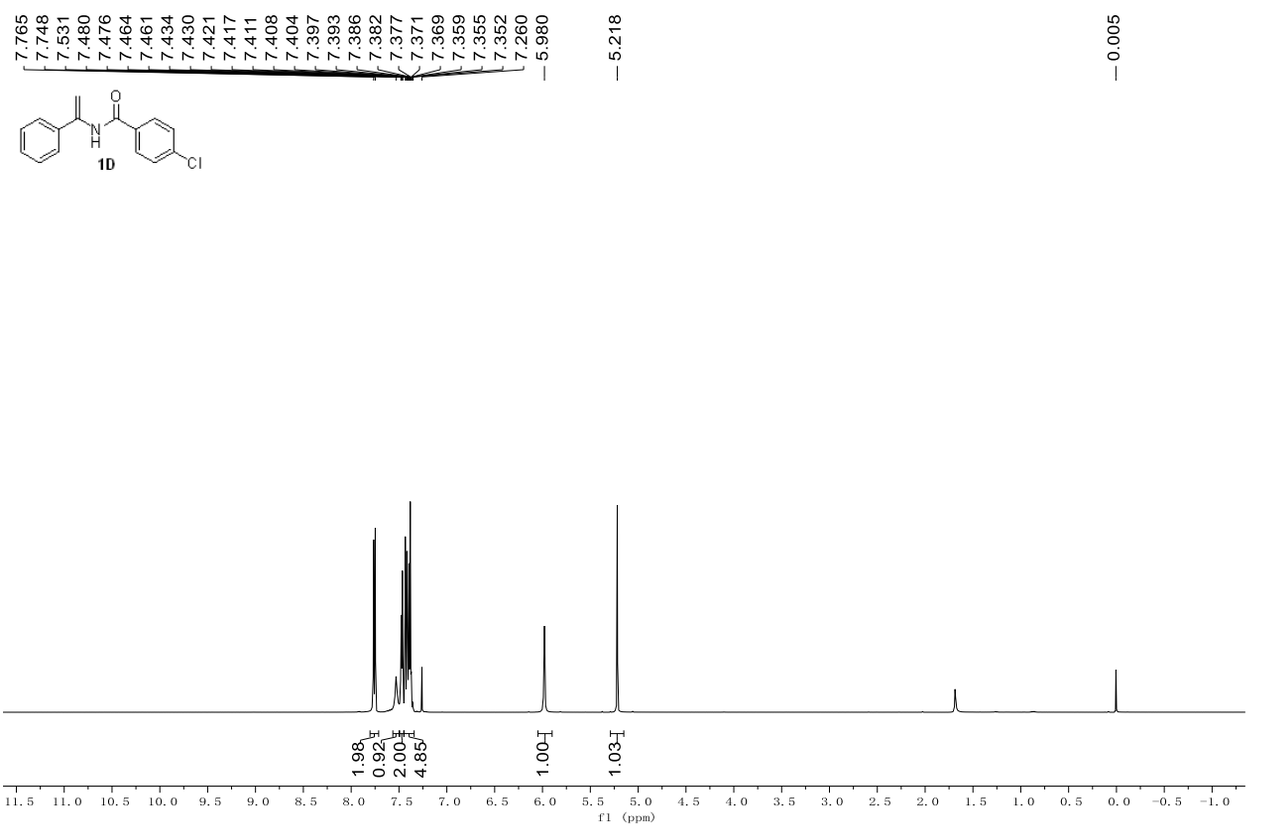
77.317
77.000
76.682
1C
f1 (ppm)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7.531
7.480
7.476
7.464
7.461
7.434
7.430
7.421
7.417
7.411
7.408
7.404
7.397
7.393
7.386
7.382
7.377
7.371
7.369
7.359
7.355
7.352
7.260
5.980
5.218
0.005
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1.98
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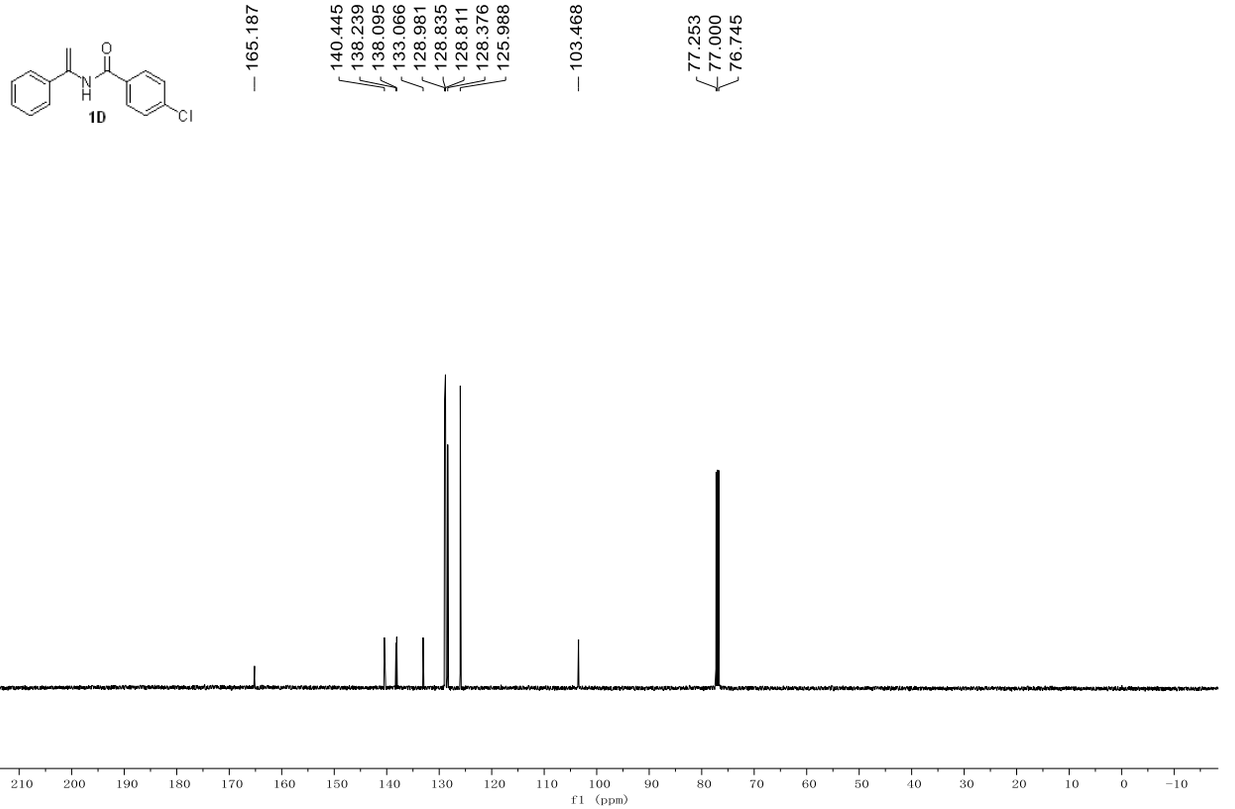
2.00
4.85
1.00
1.03
f1 (ppm)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133.066
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128.835
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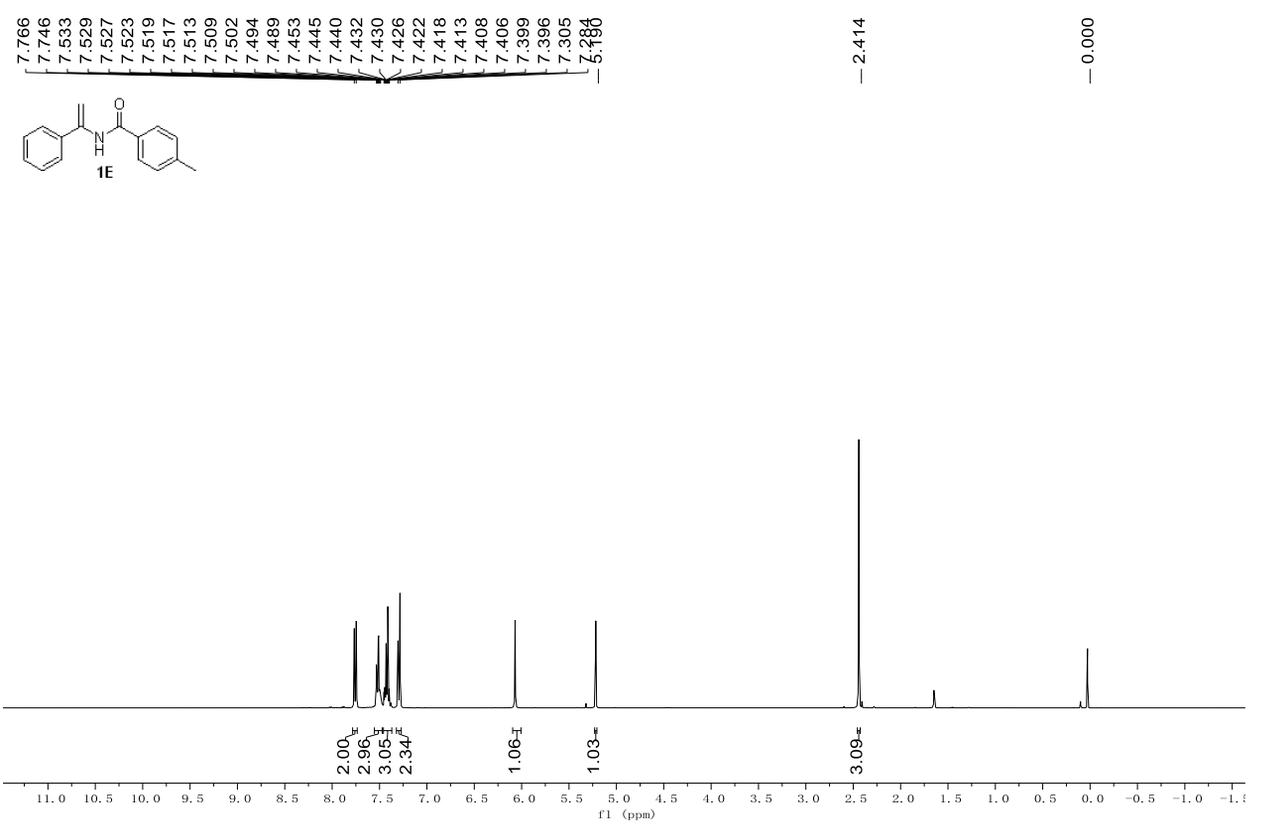
128.376
125.988
103.468
77.253
77.000
76.745
f1 (ppm)


1E
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7.746
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7.529
7.527
7.523
7.519
7.517
7.513
7.509
7.502
7.494
7.489
7.453
7.445
7.440
7.432
7.430
7.426
7.422
7.418
7.413
7.408
7.406
7.399
7.396
7.305
7.284
5.190
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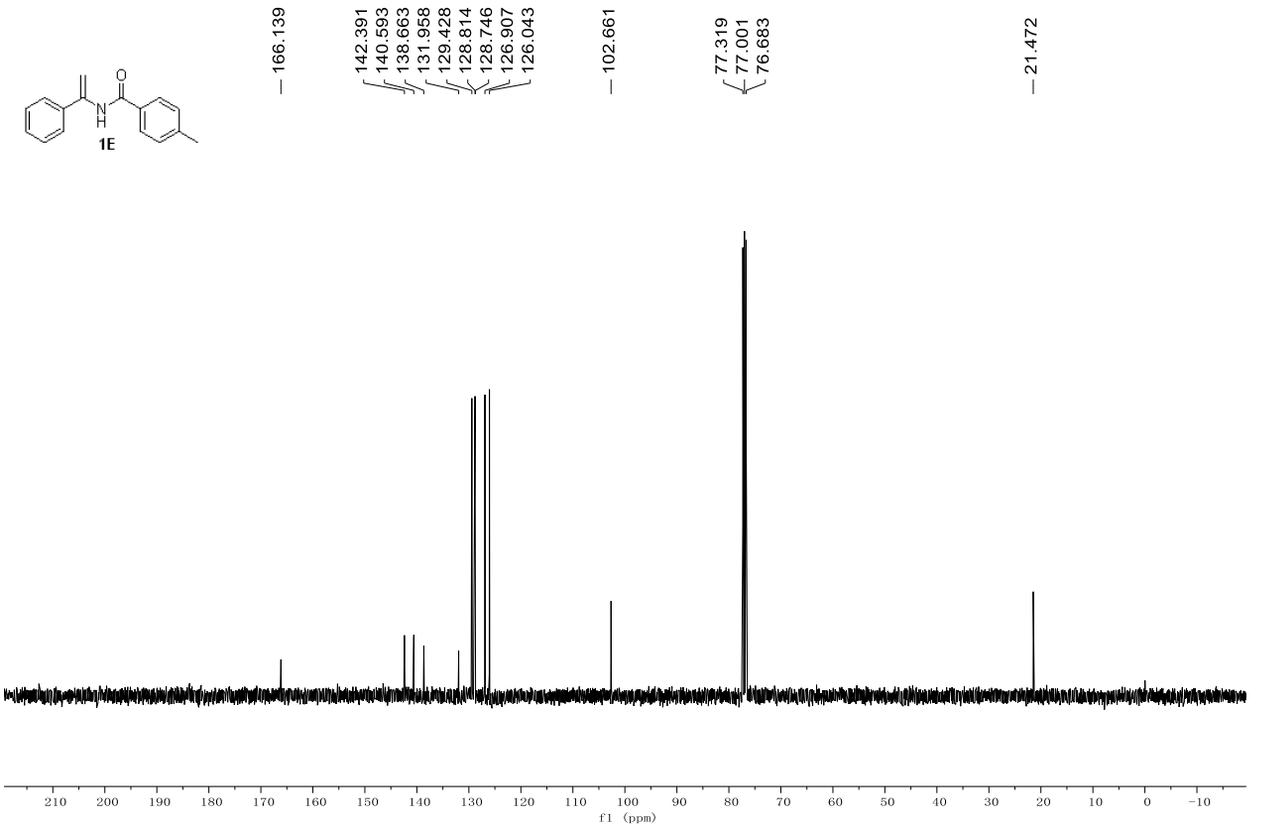
0.000
2.00
2.96
3.05
2.34
1.06
1.03
3.09
f1 (ppm)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102.661
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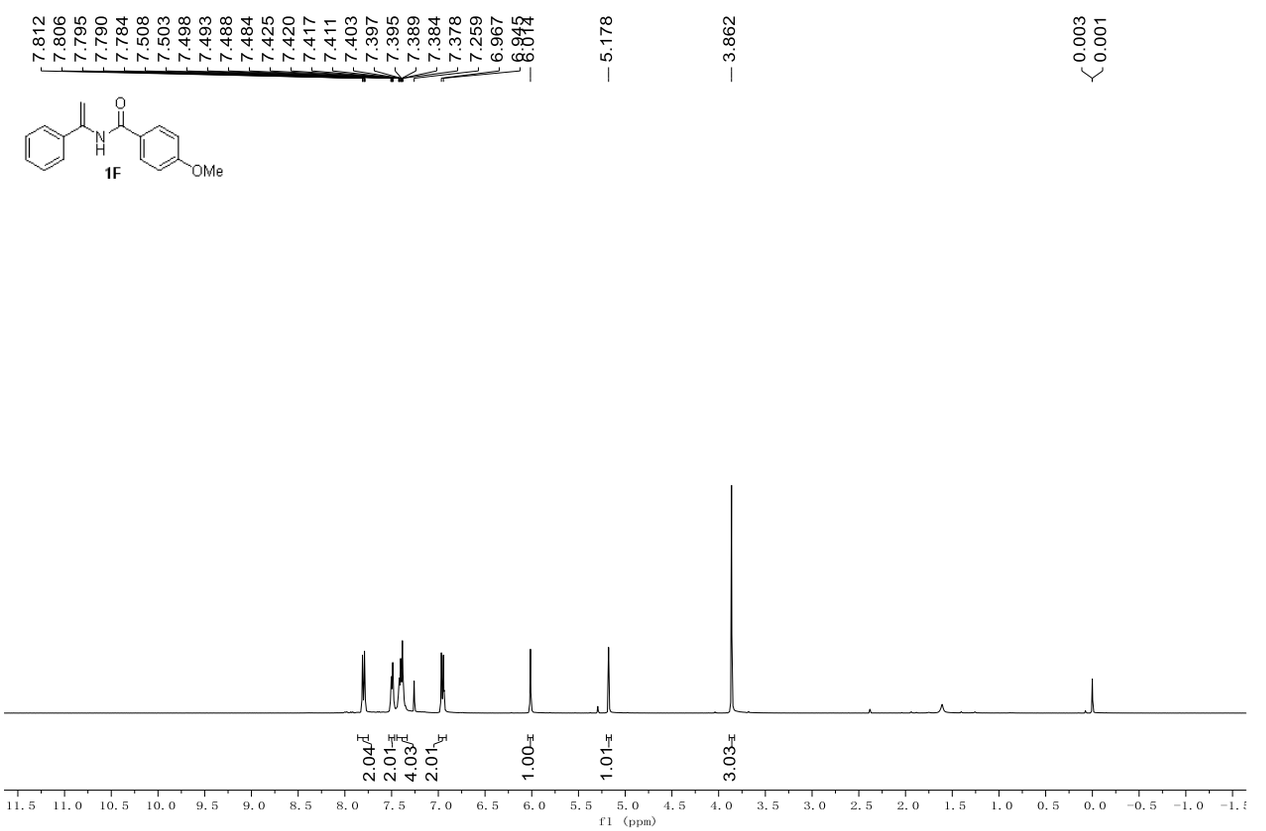
77.001
76.683
21.472
1E
f1 (ppm)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7.488
7.484
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7.420
7.417
7.411
7.403
7.397
7.395
7.389
7.384
7.378
7.259
6.967
6.945
6.914
5.178
3.862
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2.04
2.01
4.03
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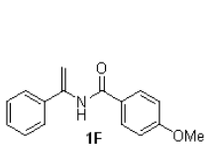
1.01
3.03
1F
OMe
f1 (ppm)



1F

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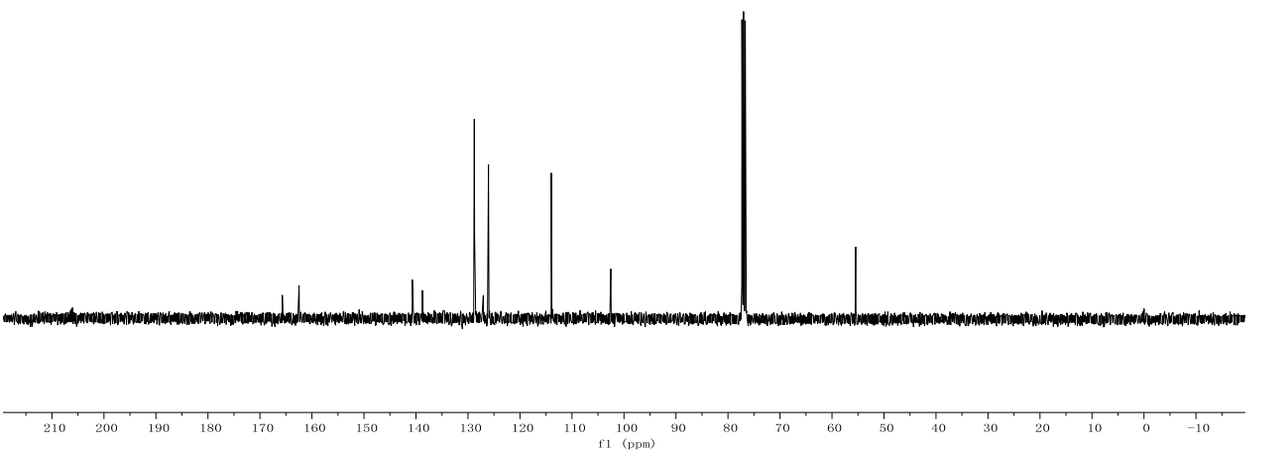
55.445



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7.507
7.502
7.500
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7.490
7.485
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7.423
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7.407
7.403
7.398
7.395
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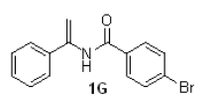
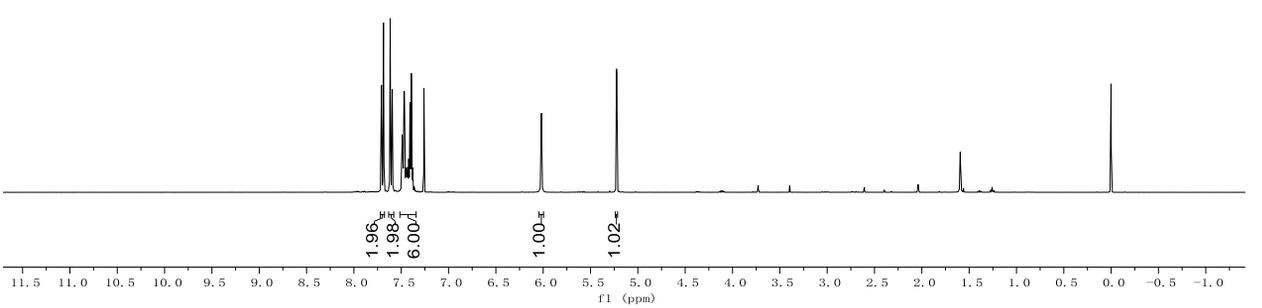
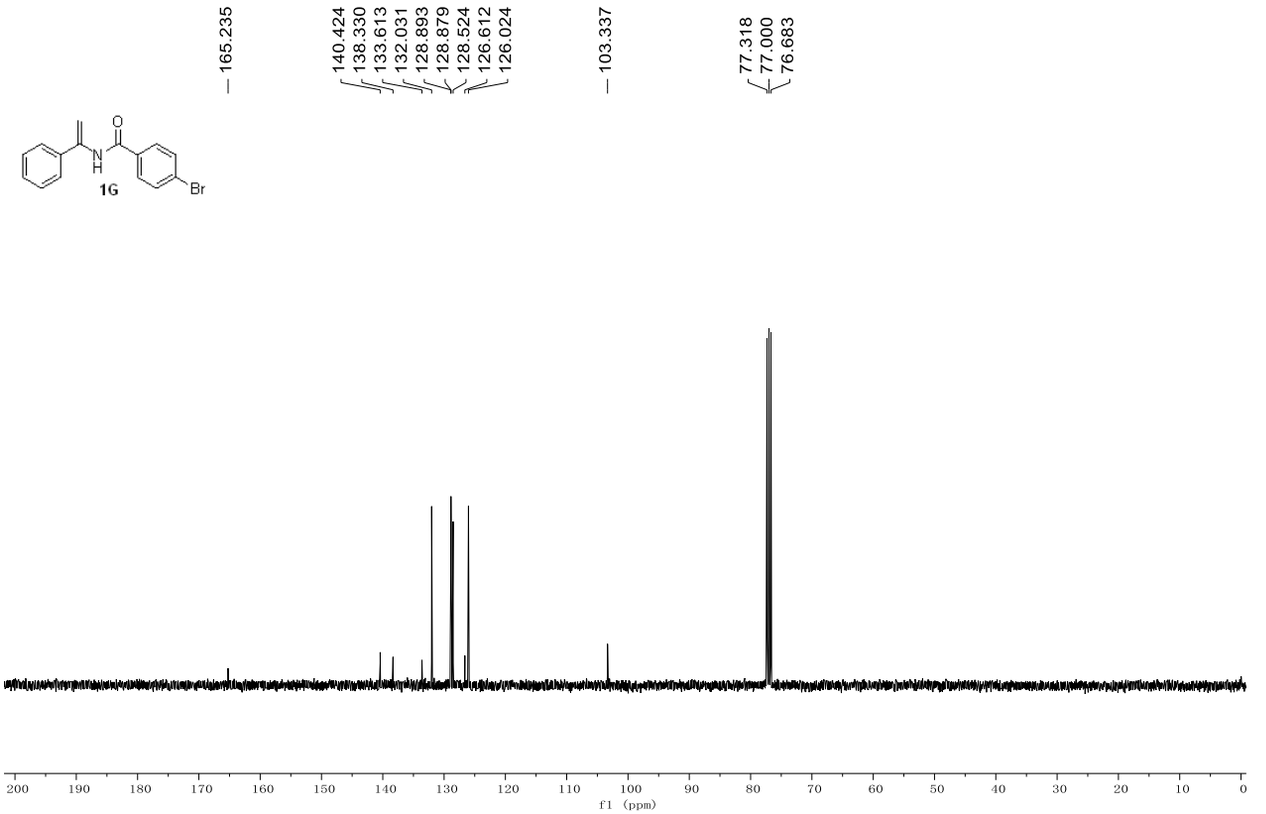


1G

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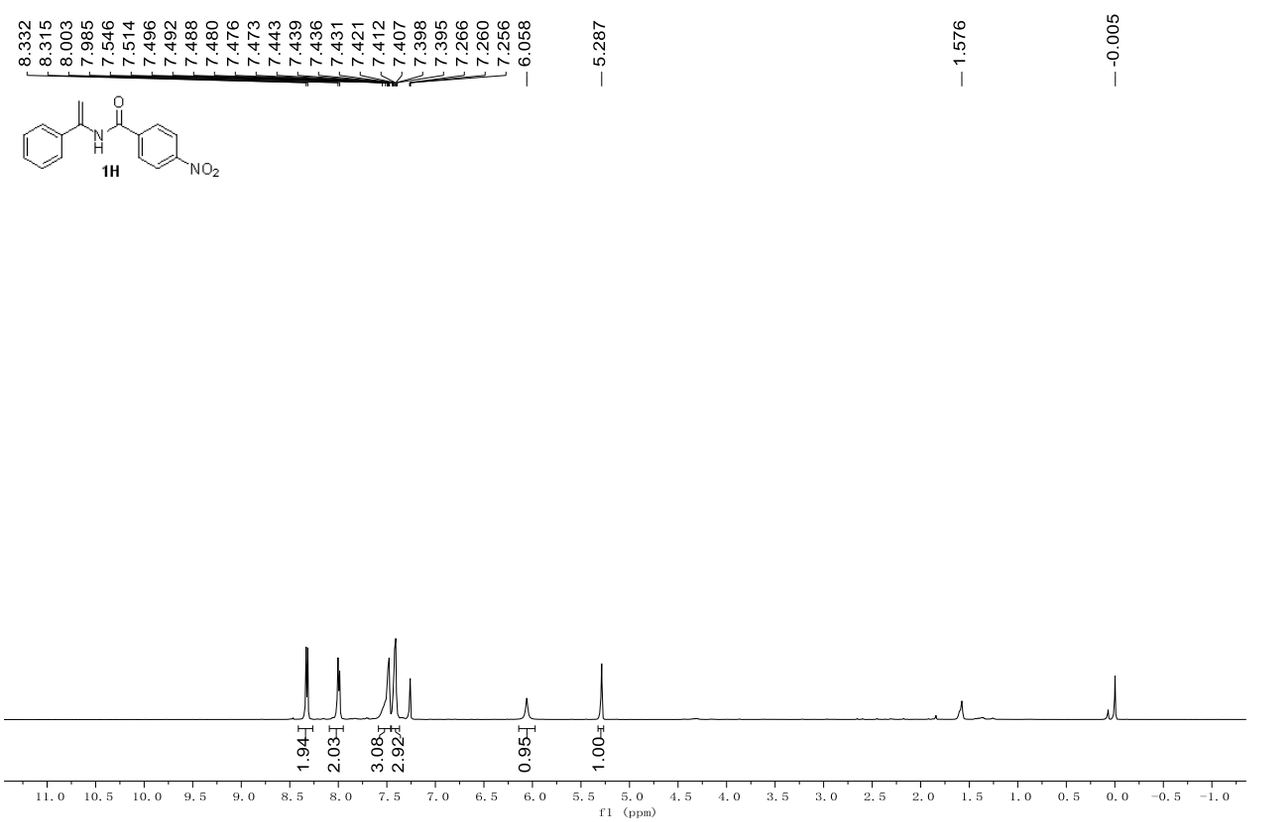
77.000
76.683
1G
Br
f1 (ppm)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7.443
7.439
7.436
7.431
7.421
7.412
7.407
7.398
7.395
7.266
7.260
7.256
6.058
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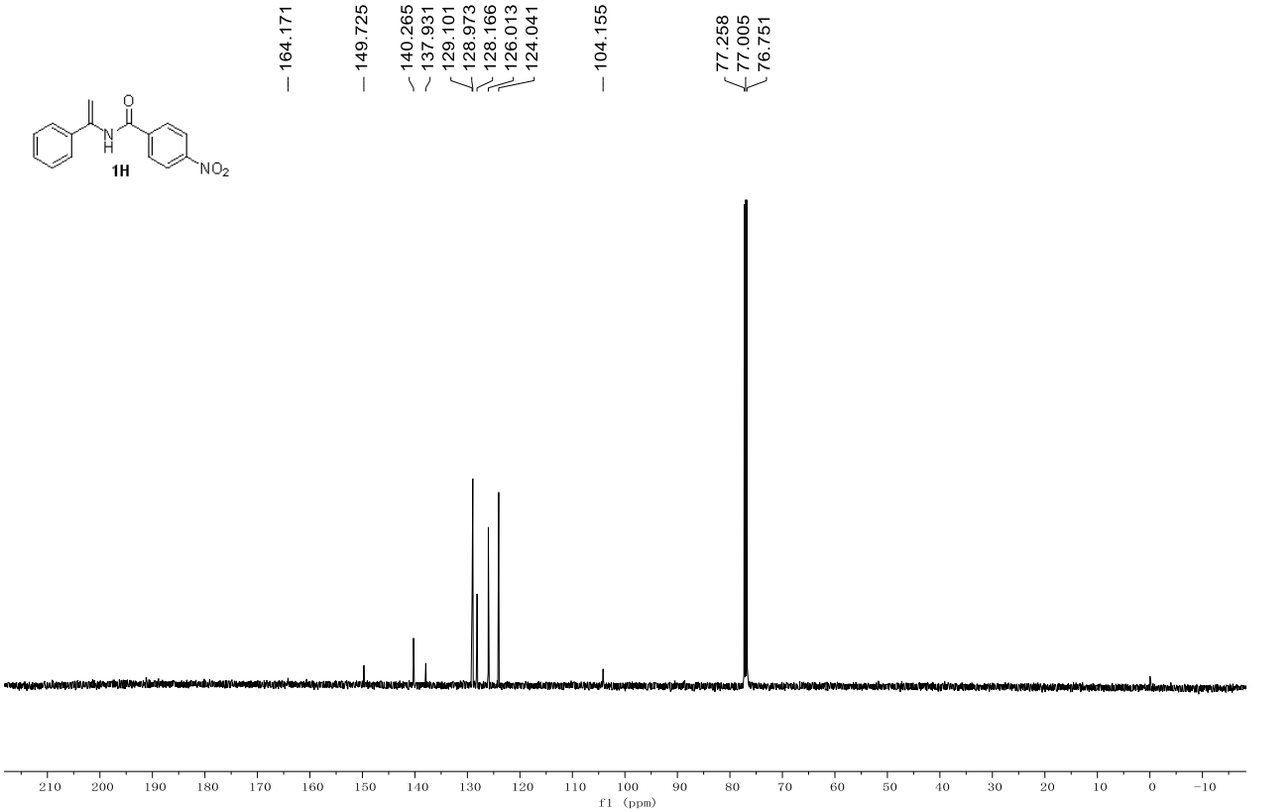
1.00
f1 (ppm)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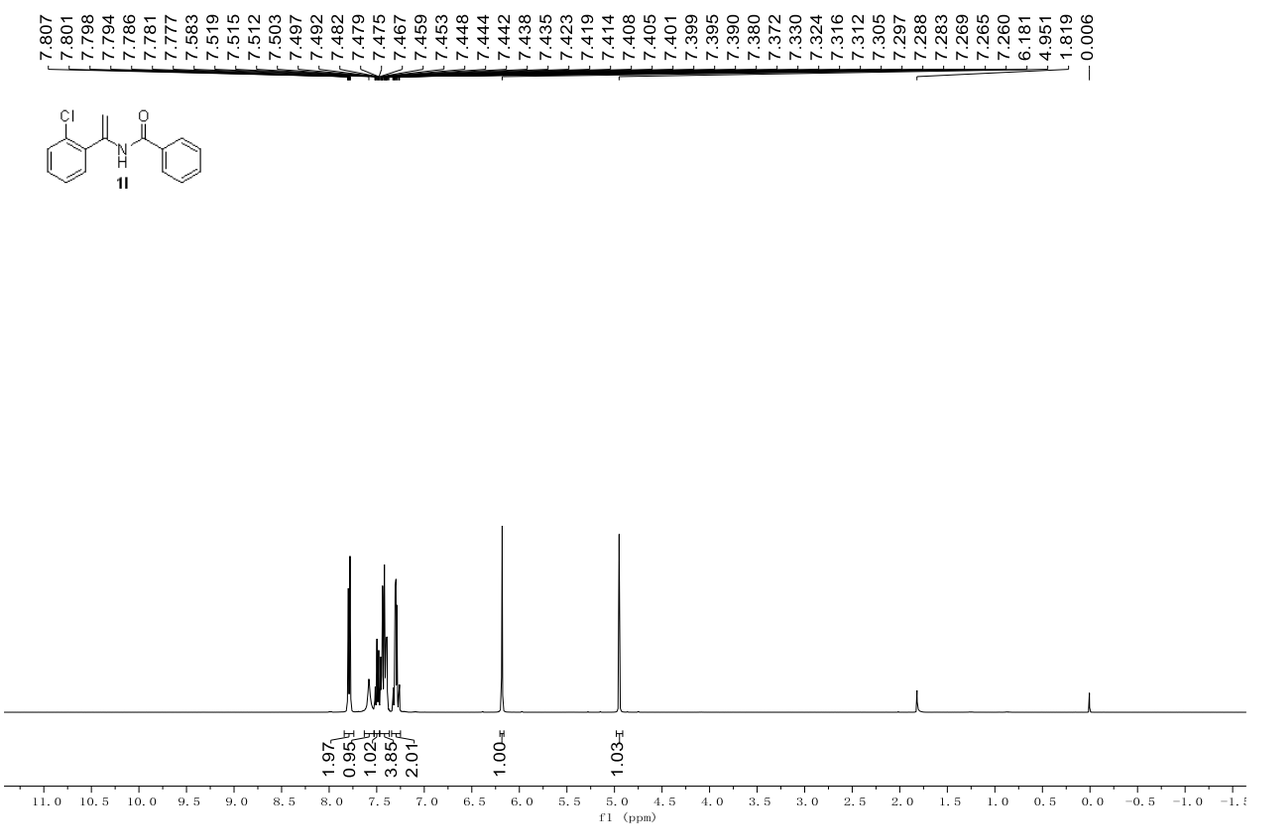
f1 (ppm)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7.288
7.283
7.269
7.265
7.260
6.181
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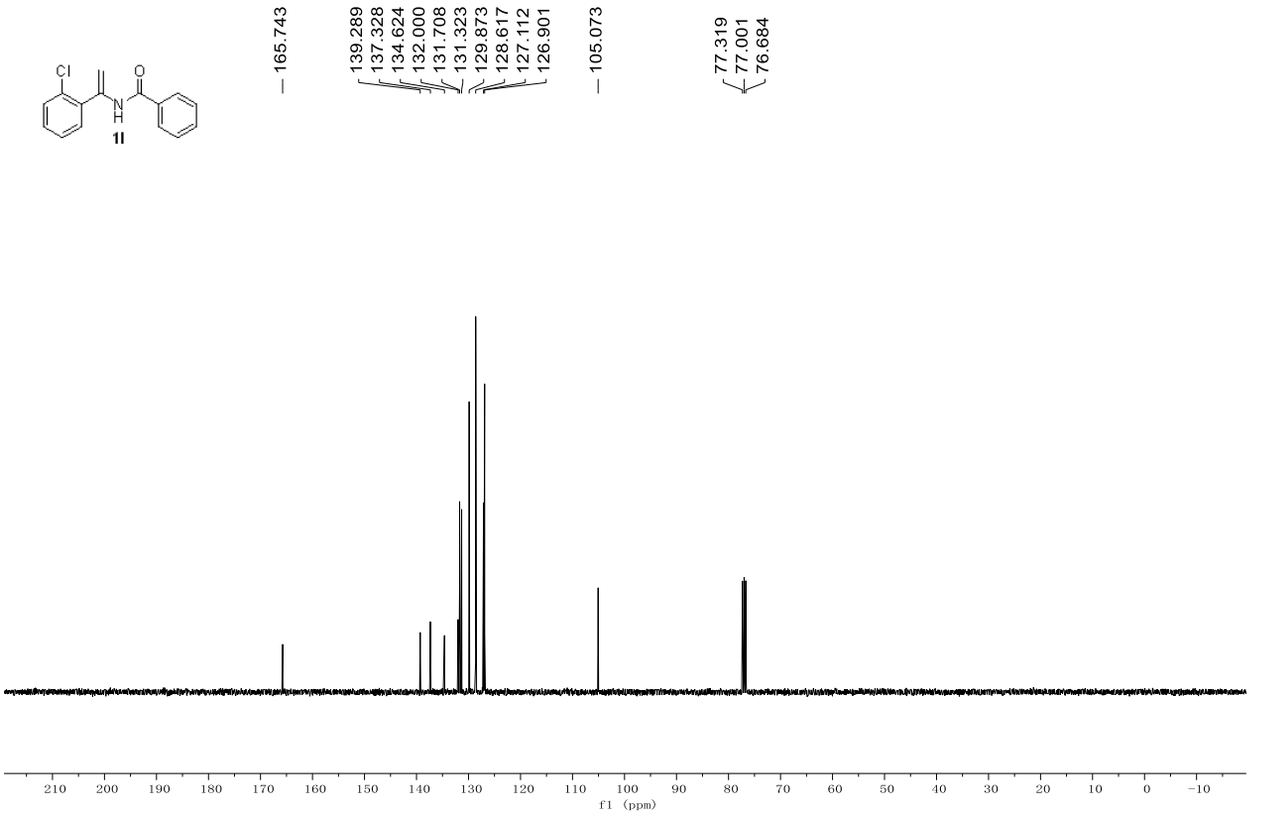
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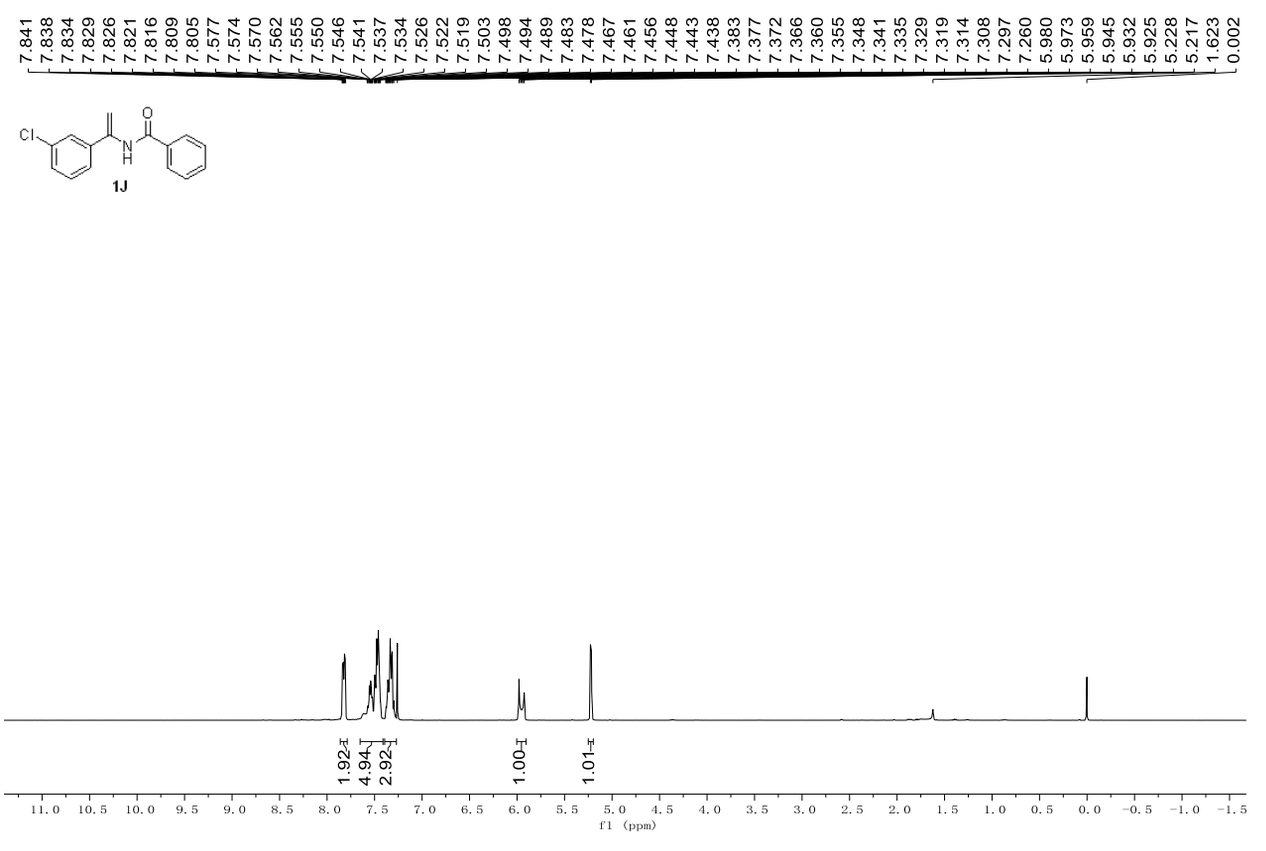
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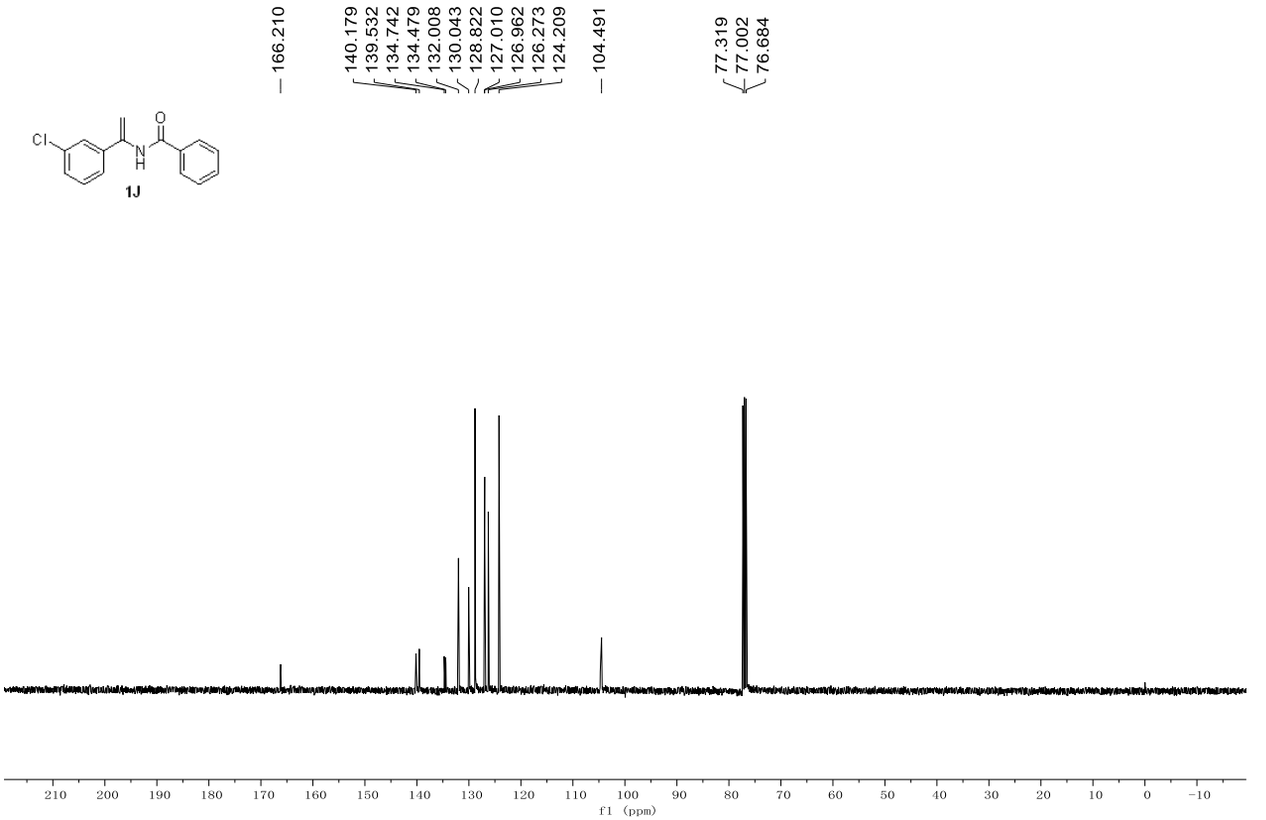
f1 (ppm)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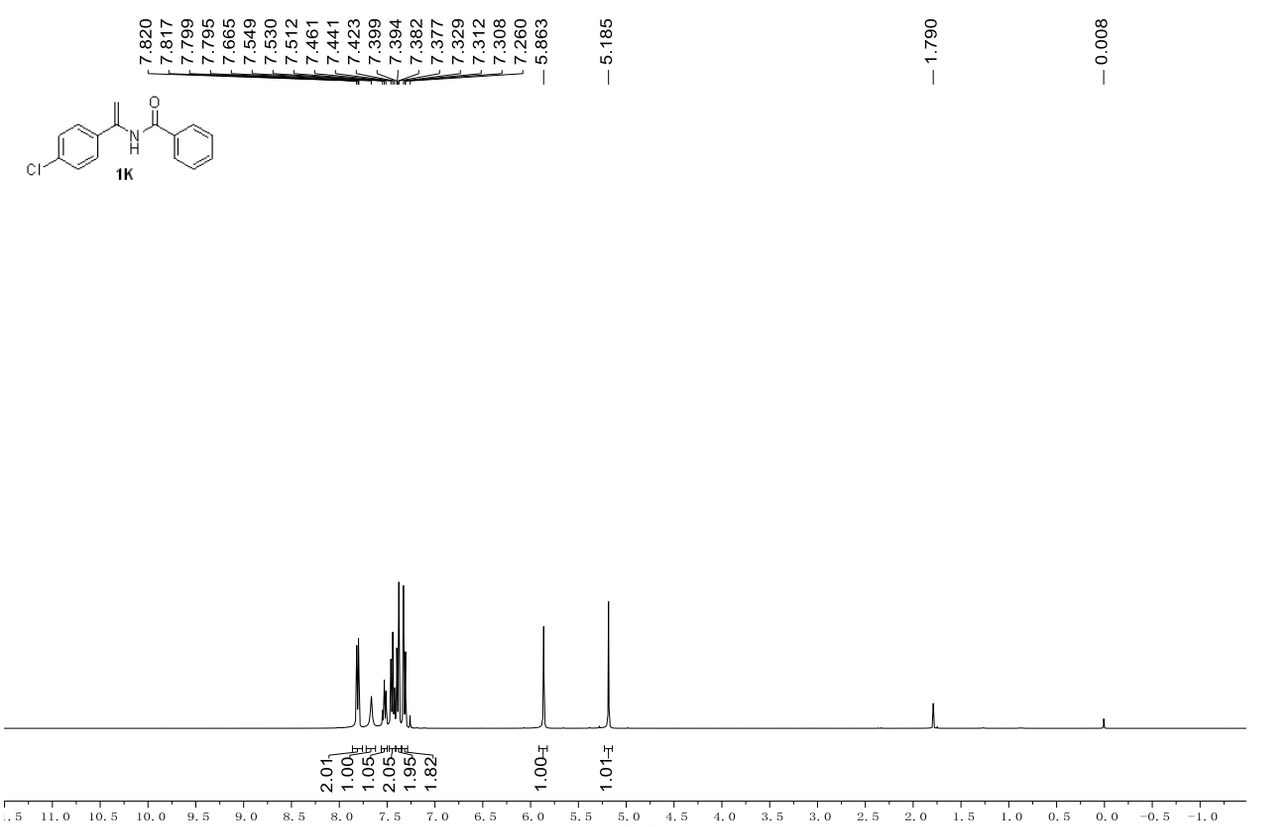
104.491
77.319
77.002
76.684
Cl
O
N
H
1J
f1 (ppm)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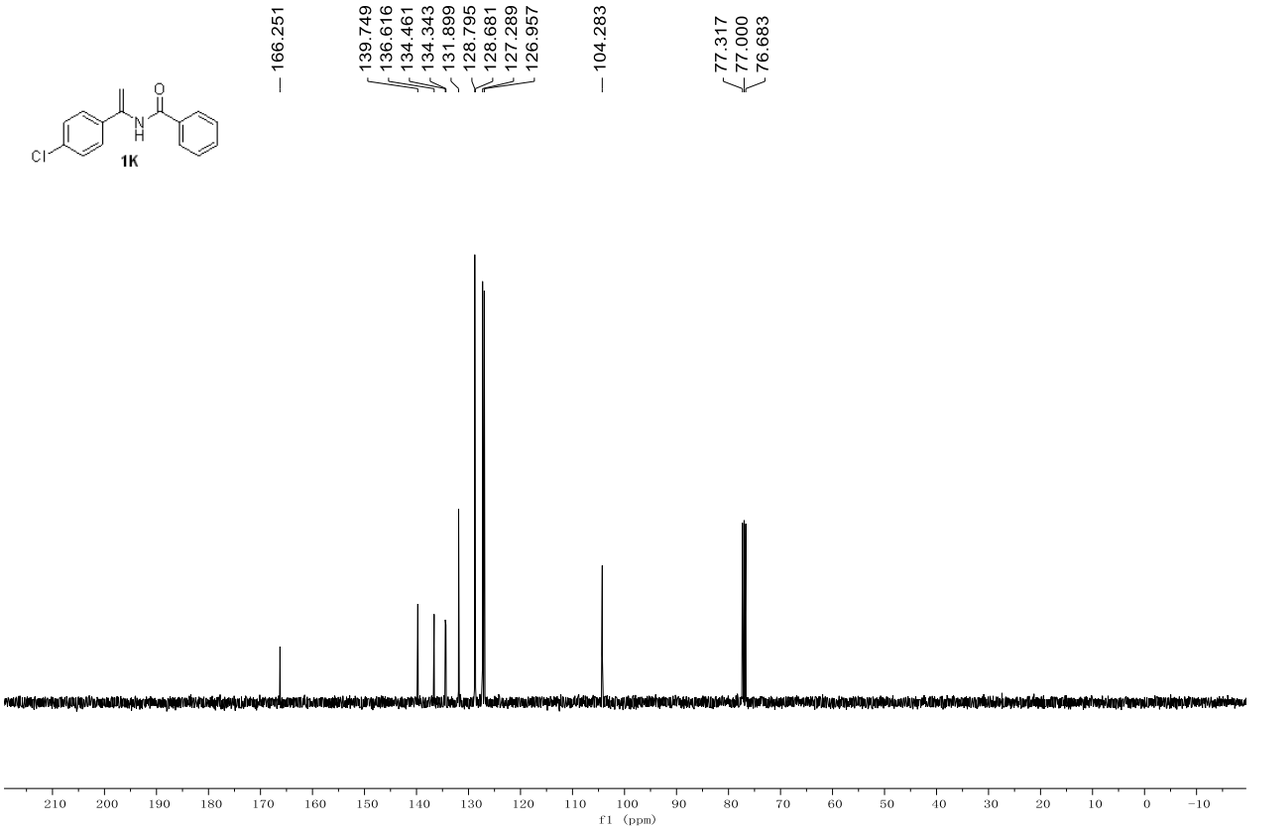
7.817
7.799
7.795
7.665
7.549
7.530
7.512
7.461
7.441
7.423
7.399
7.394
7.382
7.377
7.329
7.312
7.308
7.260
5.863
5.185
1.790
0.008
Cl
O
N
H
1K
2.01
1.00
1.05
2.05
1.95
1.82
1.00
1.01
f1 (ppm)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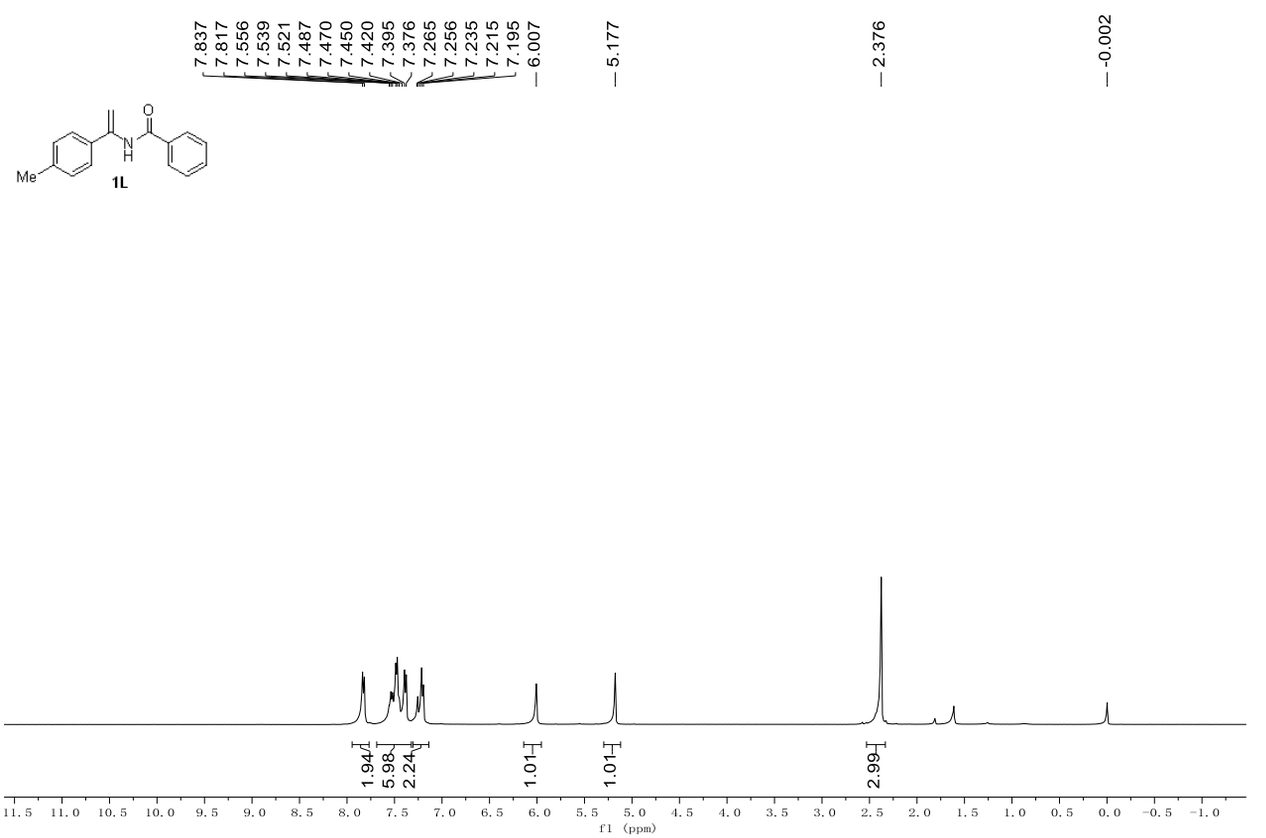
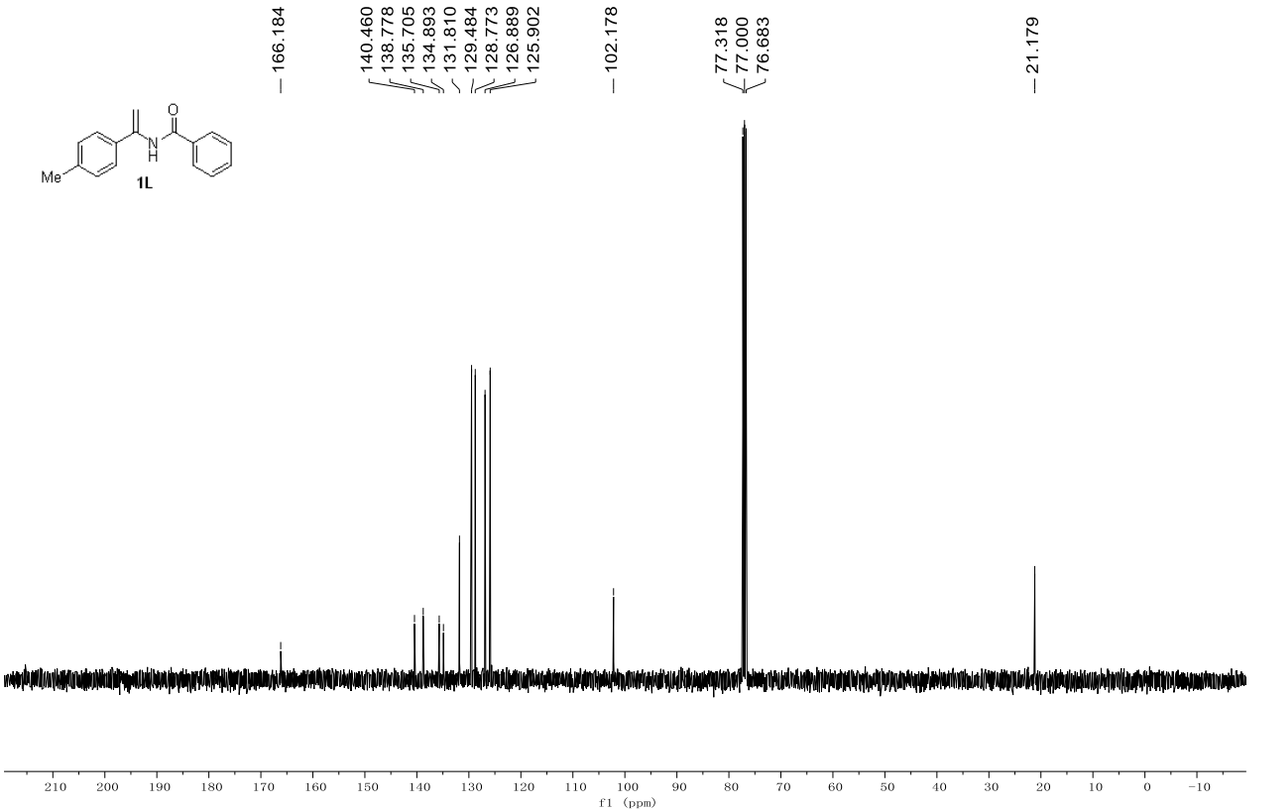
139.749
136.616
134.461
134.343
131.899
128.795
128.681
127.289
126.957
104.283
77.317
77.000
76.683
Cl
1K
f1 (ppm)


7.837
7.817
7.556
7.539
7.521
7.487
7.470
7.450
7.420
7.395
7.376
7.265
7.256
7.235
7.215
7.195
6.007
5.177
2.376
-0.002
Me
1L
1.94
5.98
2.24
1.01
1.01
2.99
f1 (ppm)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135.705
134.893
131.810
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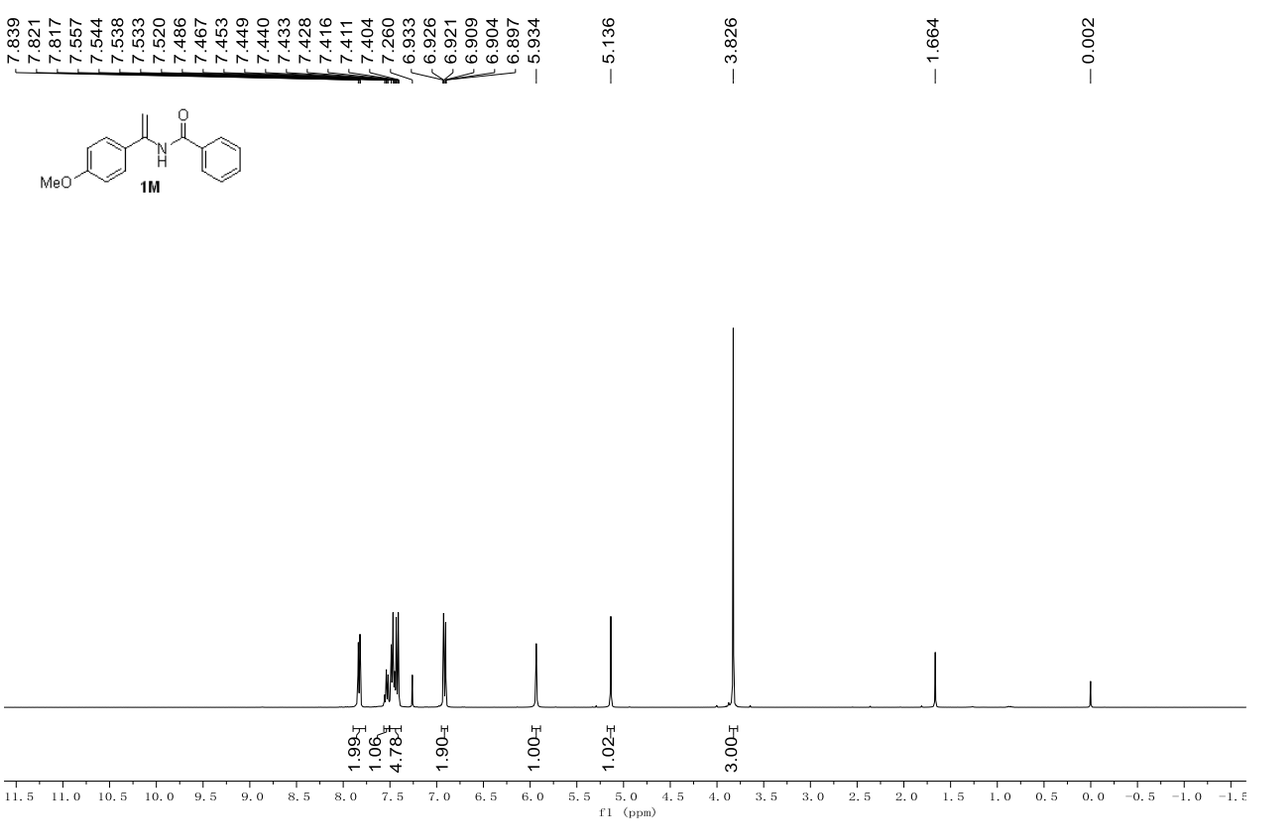
128.773
126.889
125.902
102.178
77.318
77.000
76.683
21.179
Me
1L
f1 (ppm)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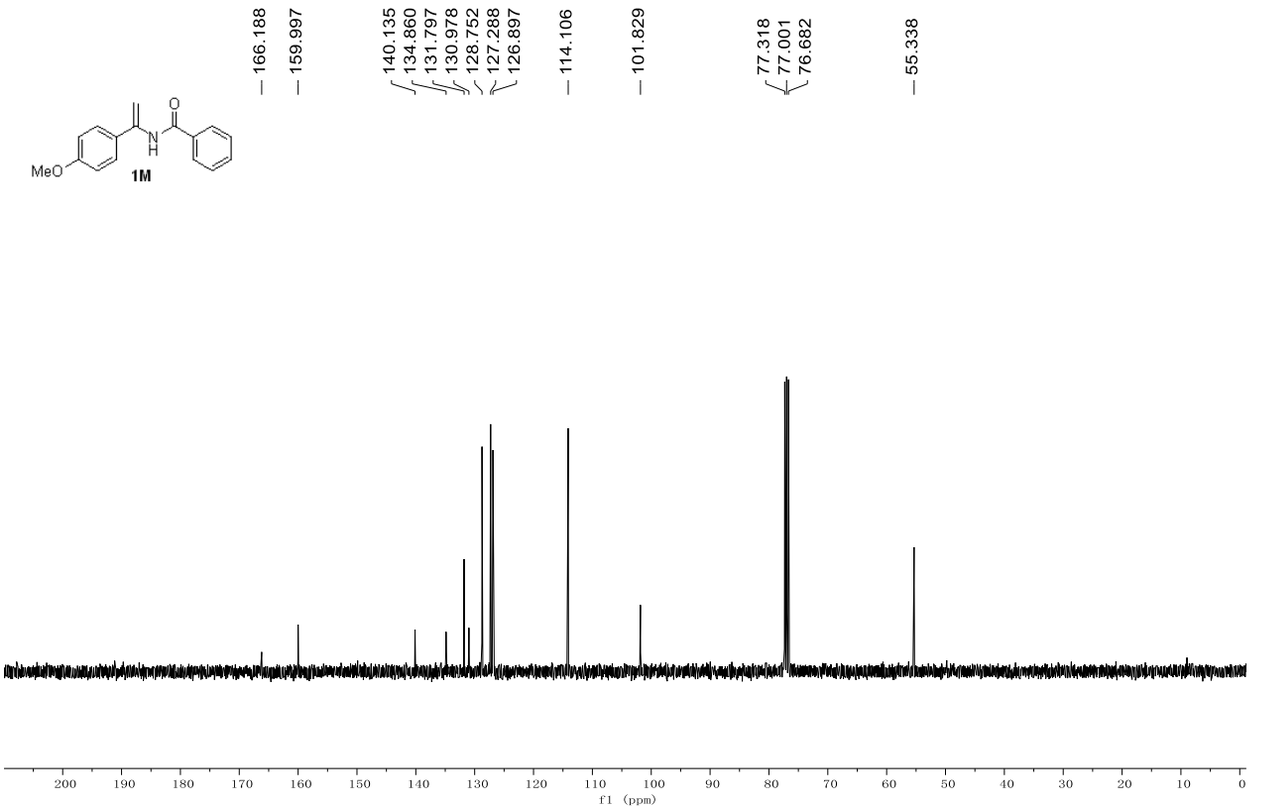
7.817
7.557
7.544
7.538
7.533
7.520
7.486
7.467
7.453
7.449
7.440
7.433
7.428
7.416
7.411
7.404
7.260
6.933
6.926
6.921
6.909
6.904
6.897
5.934
5.136
3.826
1.664
0.002
MeO
1M
1.99
1.06
4.78
1.90
1.00
1.02
3.00
f1 (ppm)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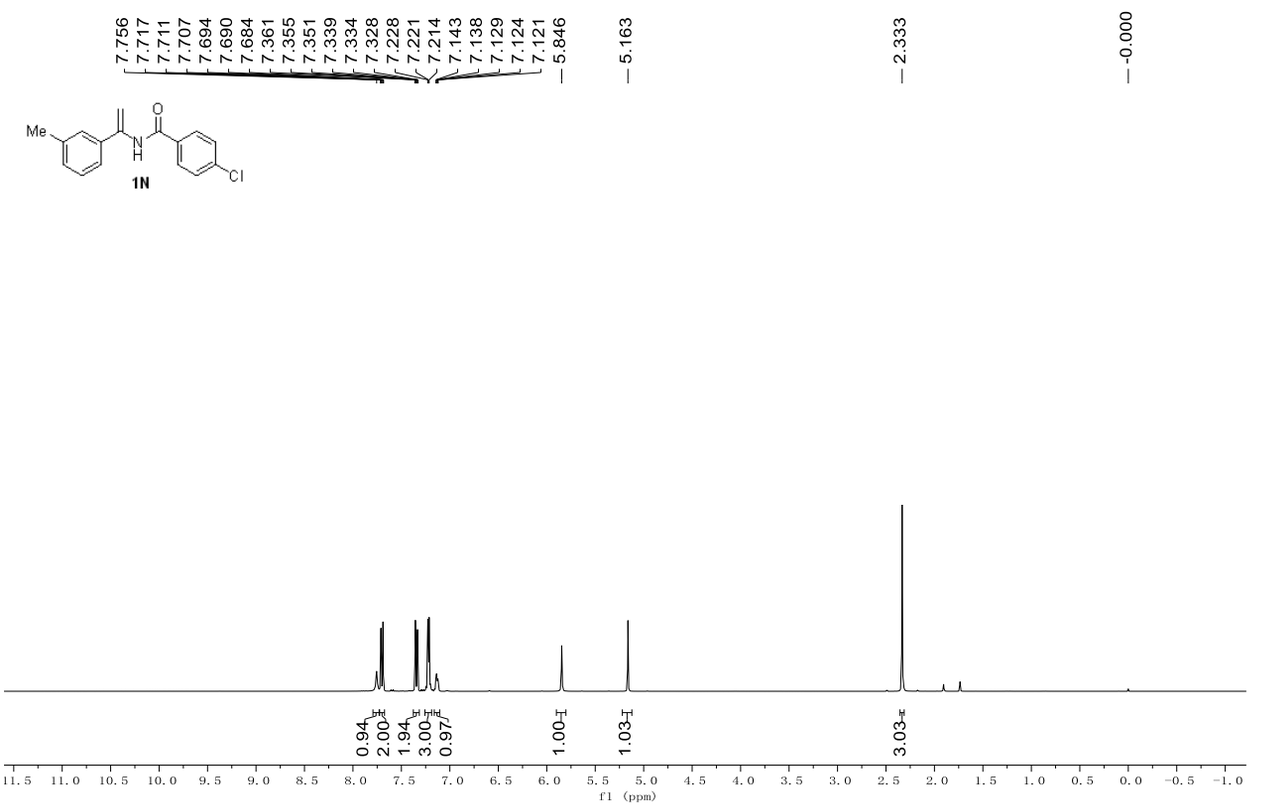
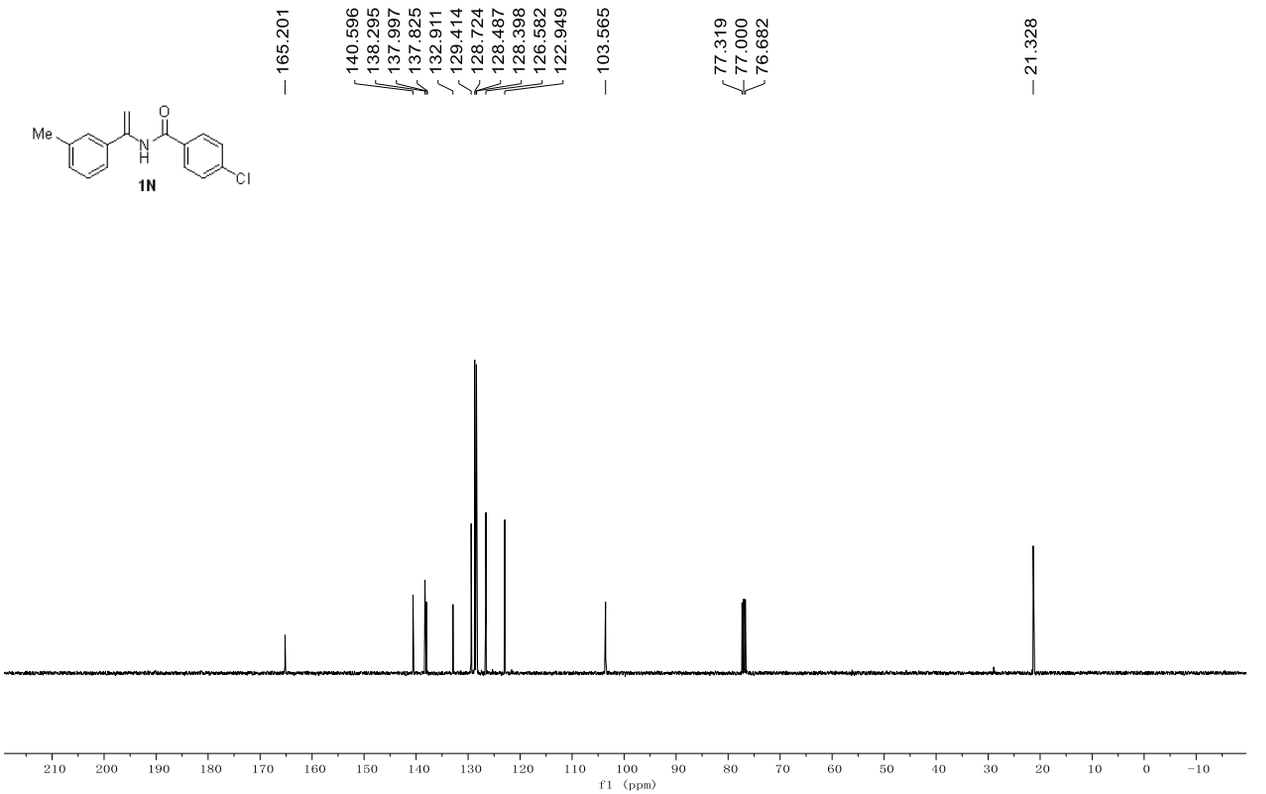
159.997
140.135
134.860
131.797
130.978
128.752
127.288
126.897
114.106
101.829
77.318
77.001
76.682
55.338
MeO
1M
f1 (ppm)


7.756
7.717
7.711
7.707
7.694
7.690
7.684
7.361
7.355
7.351
7.339
7.334
7.328
7.228
7.221
7.214
7.143
7.138
7.129
7.124
7.121
5.846
5.163
2.333
-0.000
Me
Cl
1N
0.94
2.00
1.94
3.00
0.97
1.00
1.03
3.03
f1 (ppm)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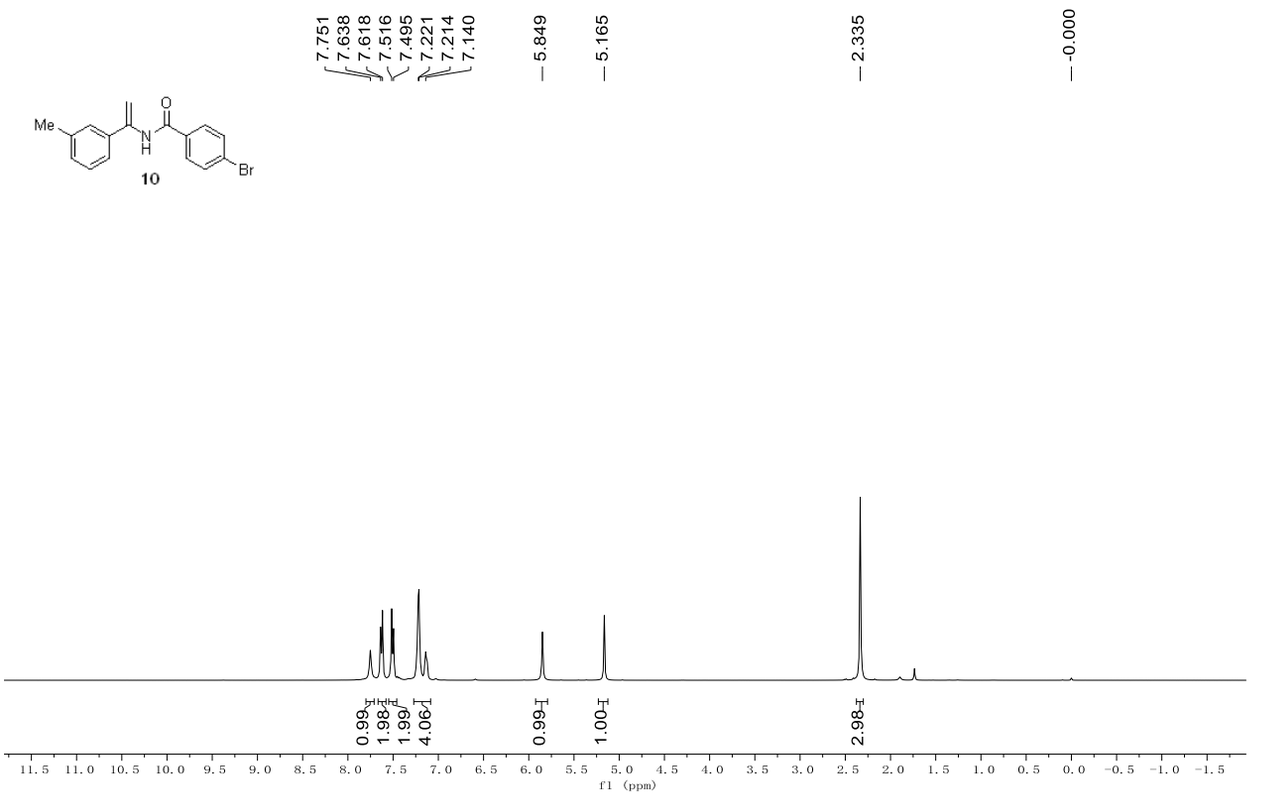
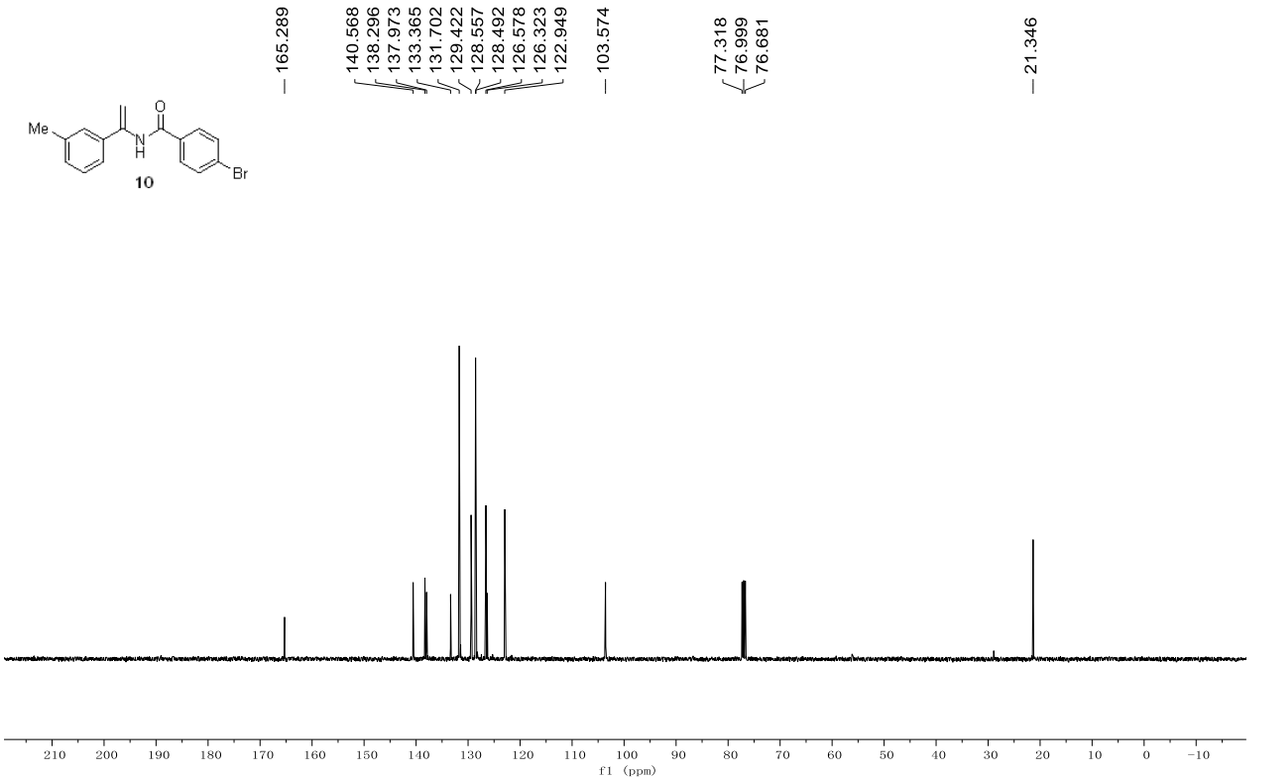
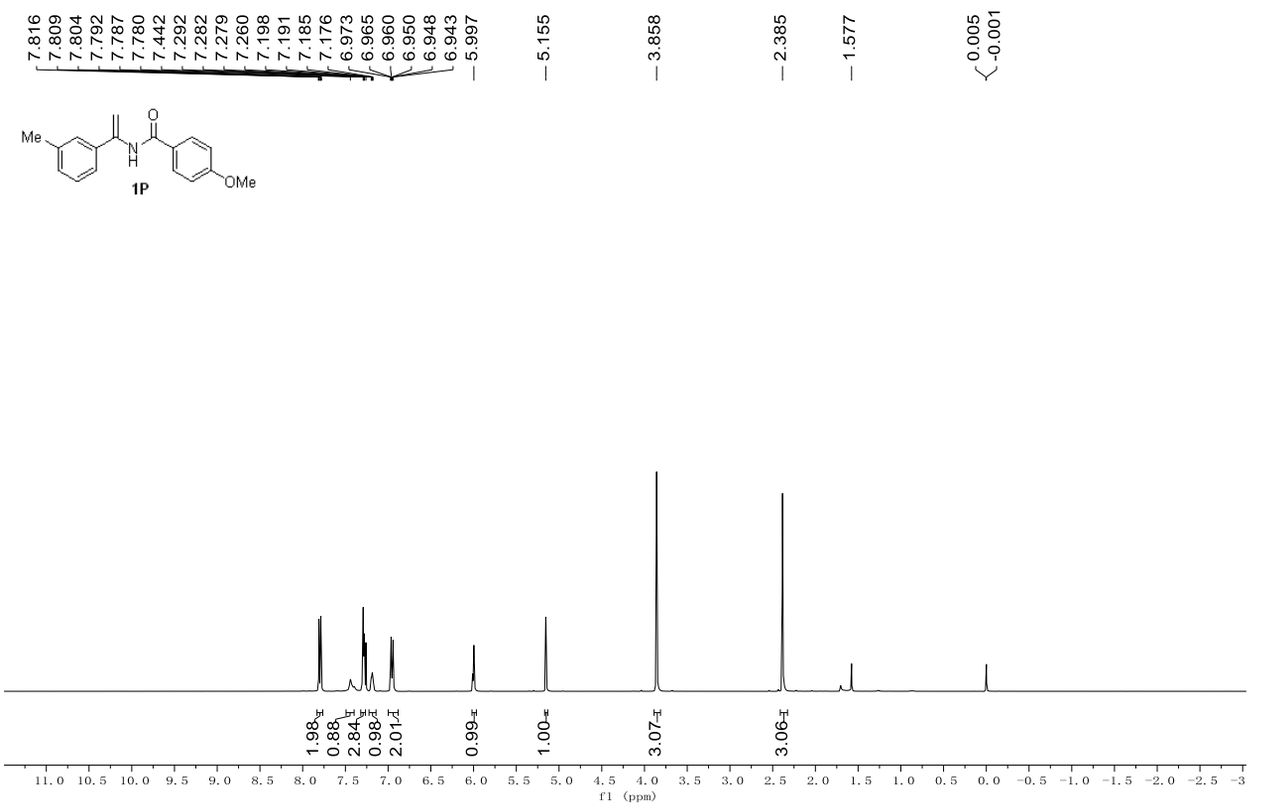
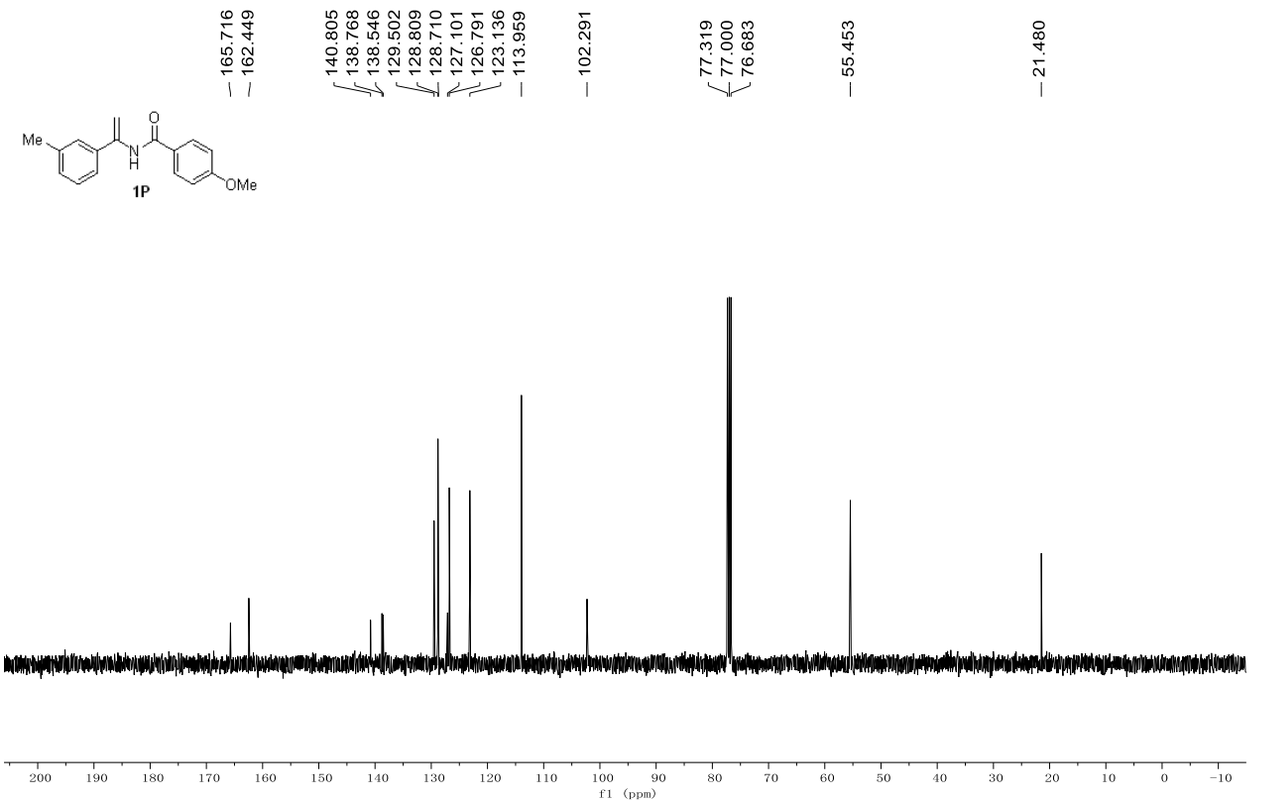
140.596
138.295
137.997
137.825
132.911
129.414
128.724
128.487
128.398
126.582
122.949
103.565
77.319
77.000
76.682
21.328
Me
O
N
H
Cl
1N
f1 (ppm)


7.751
7.638
7.618
7.516
7.495
7.221
7.214
7.140
5.849
5.165
2.335
-0.000
Me
O
N
H
Br
10
0.99
1.98
1.99
4.06
0.99
1.00
2.98
f1 (ppm)


165.289
140.568
138.296
137.973
133.365
131.702
129.422
128.557
128.492
126.578
126.323
122.949
103.574
77.318
76.999
76.681
21.346
Me
Br
10
f1 (ppm)


7.816
7.809
7.804
7.792
7.787
7.780
7.442
7.292
7.282
7.279
7.260
7.198
7.191
7.185
7.176
6.973
6.965
6.960
6.950
6.948
6.943
5.997
5.155
3.858
2.385
1.577
0.005
-0.001
Me
OMe
1P
1.98
0.88
2.84
0.98
2.01
0.99
1.00
3.07
3.06
f1 (ppm)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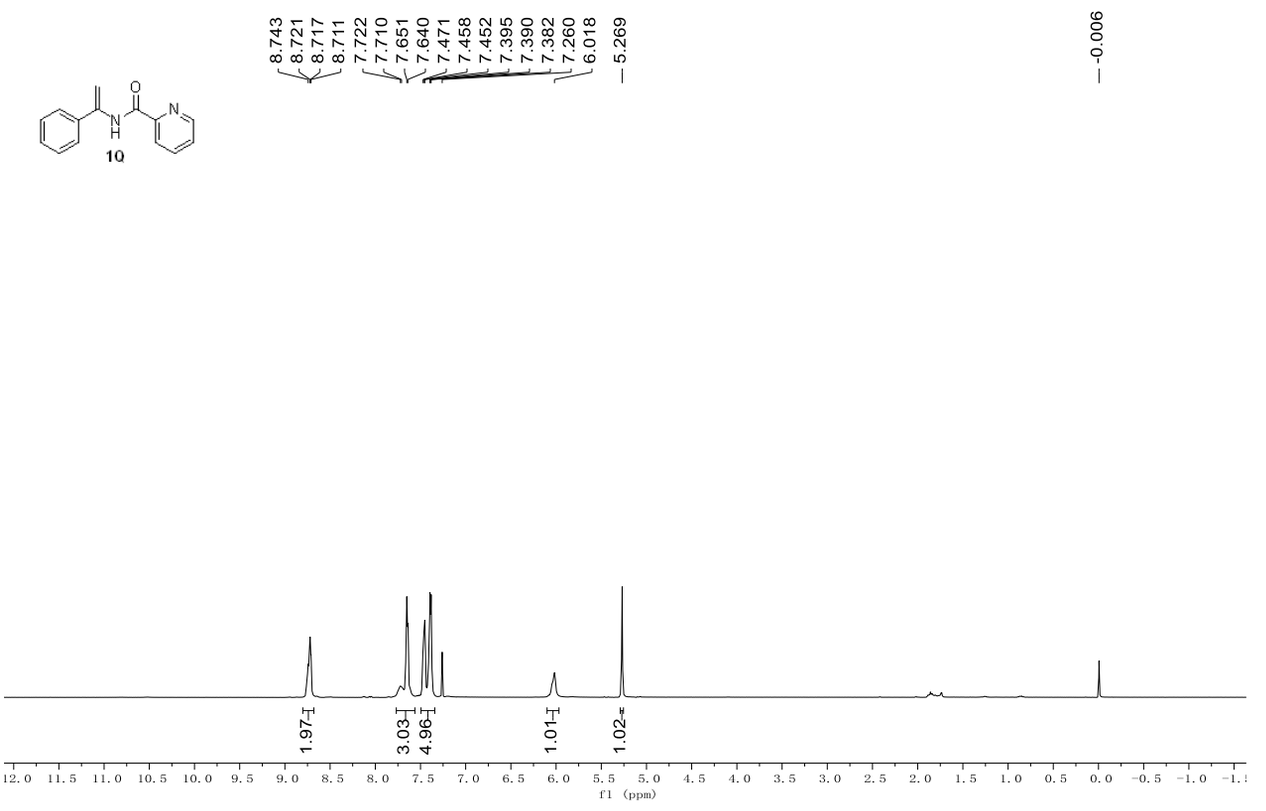
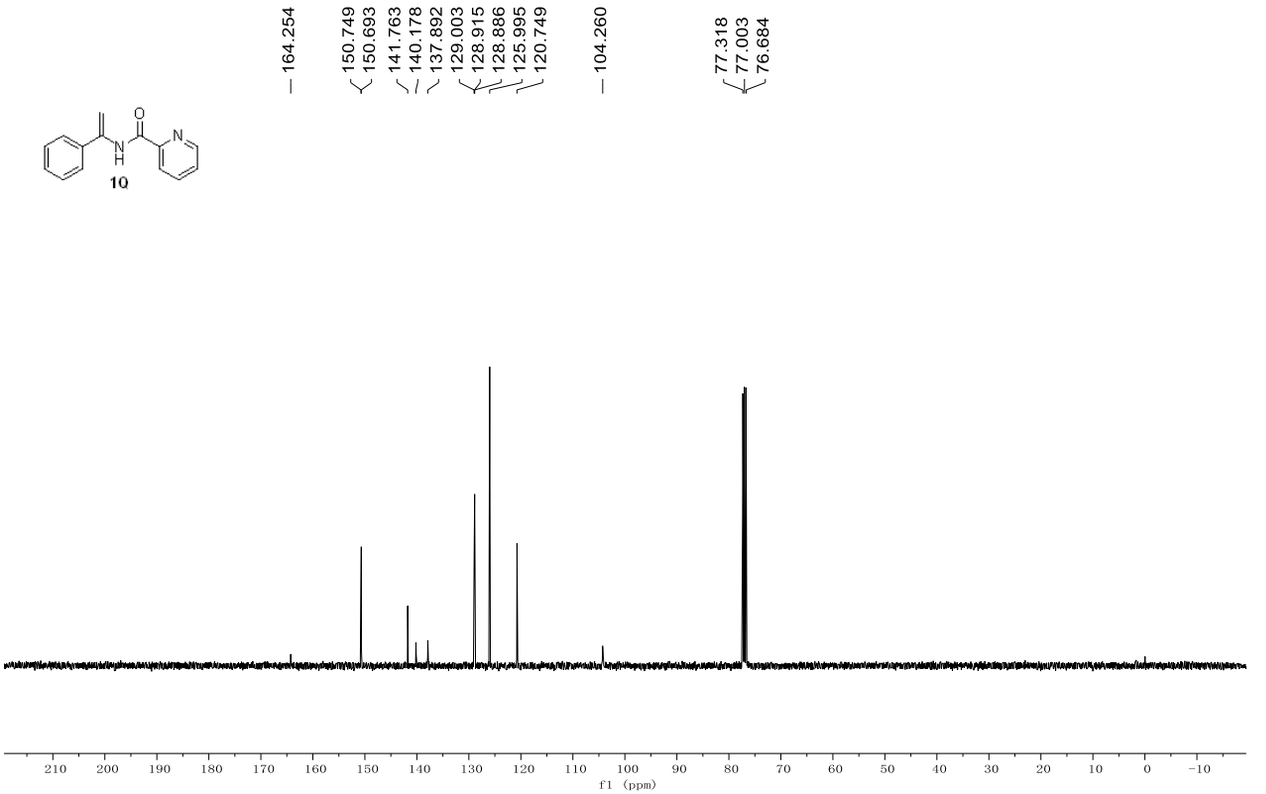
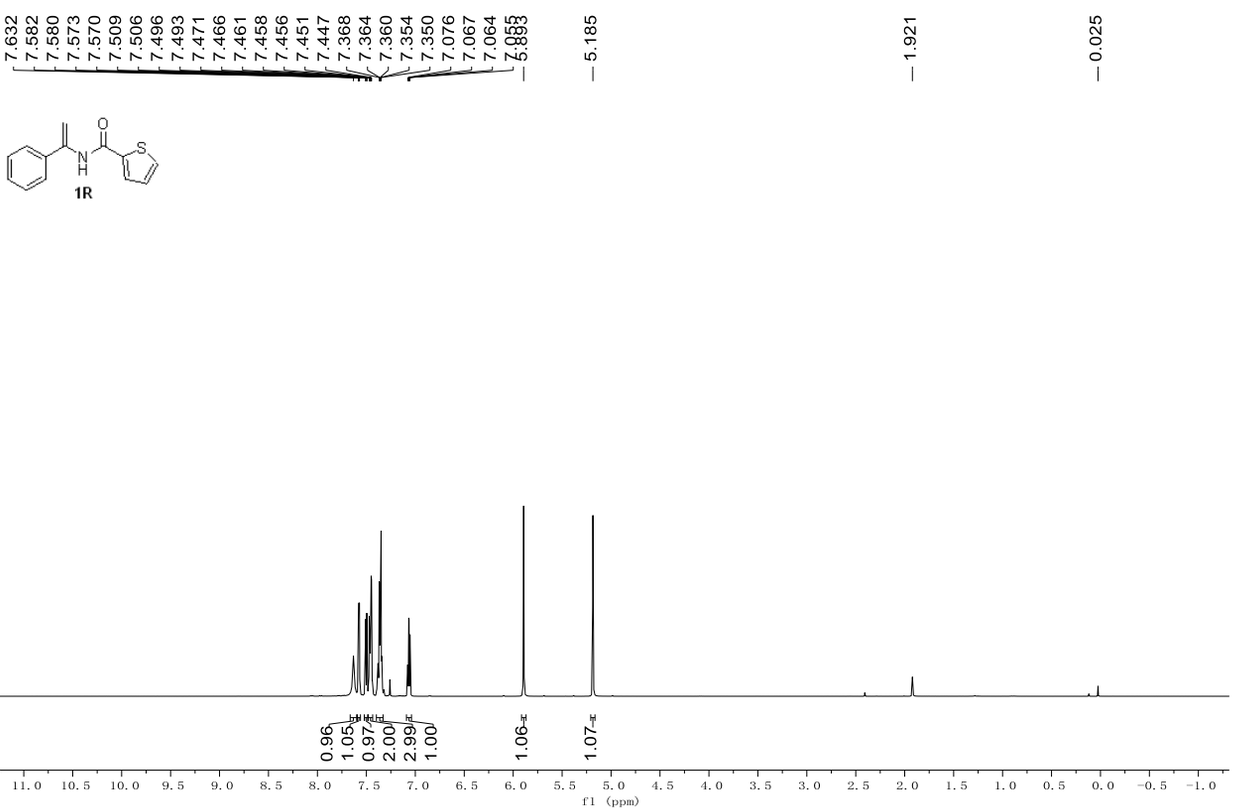
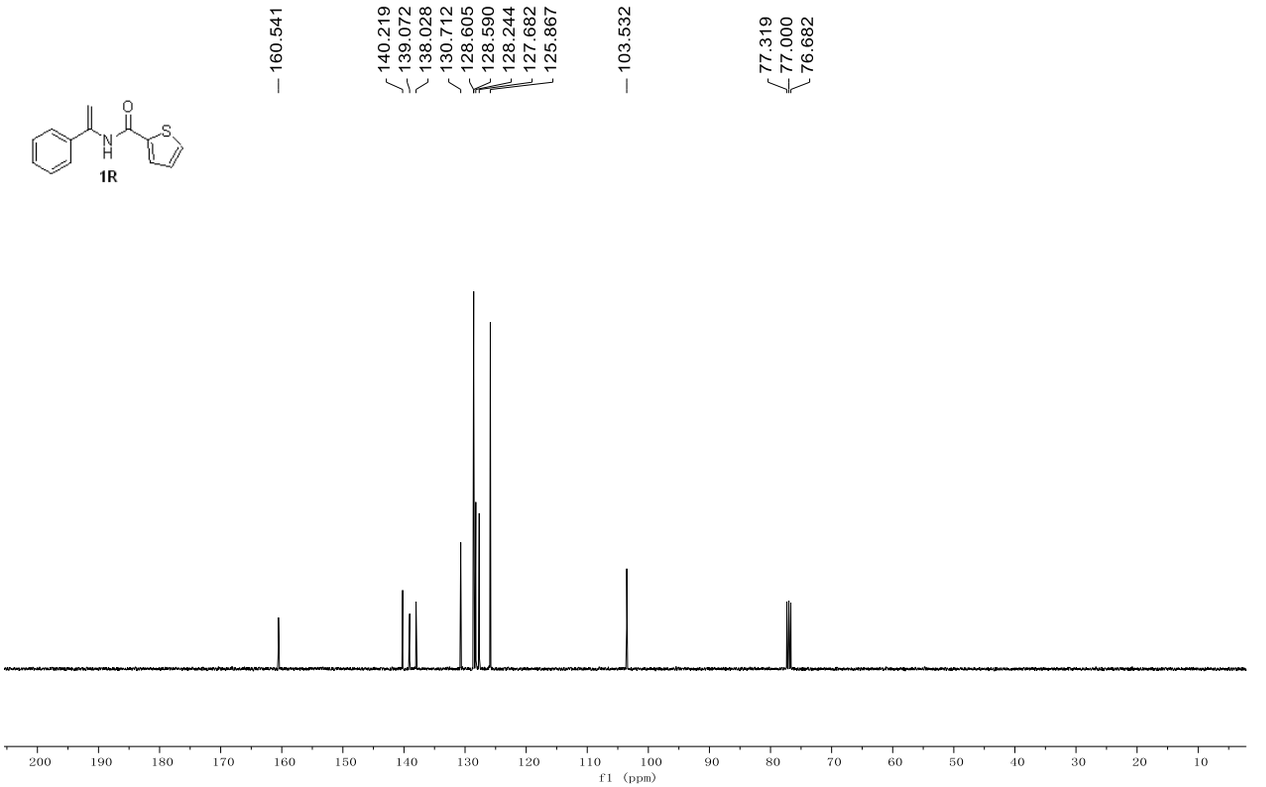
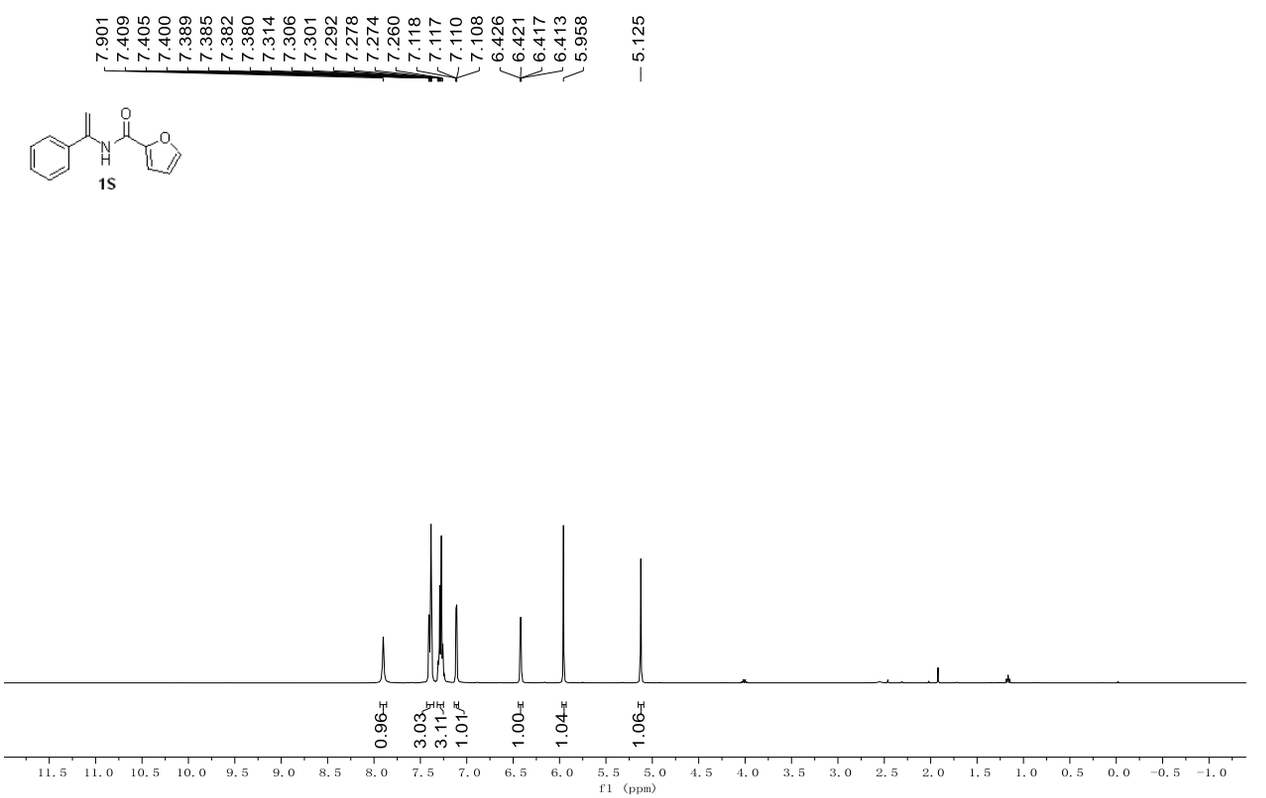
162.449
140.805
138.768
138.546
129.502
128.809
128.710
127.101
126.791
123.136
113.959
102.291
77.319
77.000
76.683
55.453
21.480
Me
OMe
1P
f1 (ppm)


8.743
8.721
8.717
8.711
7.722
7.710
7.651
7.640
7.471
7.458
7.452
7.395
7.390
7.382
7.260
6.018
5.269
-0.006
1.97
3.03
4.96
1.01
1.02
1Q
f1 (ppm)


164.254
150.749
150.693
141.763
140.178
137.892
129.003
128.915
128.886
125.995
120.749
104.260
77.318
77.003
76.684
1Q
f1 (ppm)


7.632
7.582
7.580
7.573
7.570
7.509
7.506
7.496
7.493
7.471
7.466
7.461
7.458
7.456
7.451
7.447
7.368
7.364
7.360
7.354
7.350
7.076
7.067
7.064
5.185
1.921
0.025
1R
0.96
1.05
0.97
2.00
2.99
1.00
1.06
1.07
f1 (ppm)


160.541
140.219
139.072
138.028
130.712
128.605
128.590
128.244
127.682
125.867
103.532
77.319
77.000
76.682
1R
f1 (ppm)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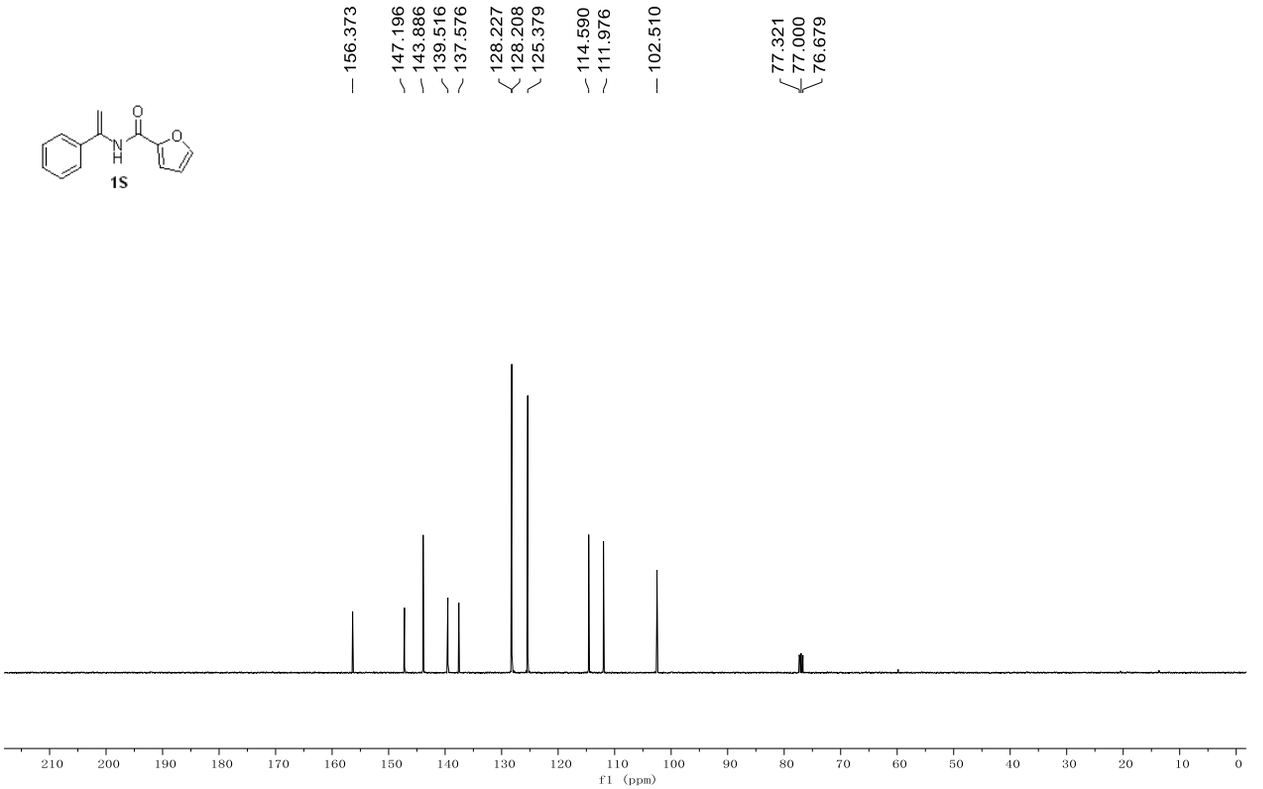
7.409
7.405
7.400
7.389
7.385
7.382
7.380
7.314
7.306
7.301
7.292
7.278
7.274
7.260
7.118
7.117
7.110
7.108
6.426
6.421
6.417
6.413
5.958
5.125
1S
0.96
3.03
3.11
1.01
1.00
1.04
1.06
f1 (ppm)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143.886
139.516
137.576
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125.379
114.590
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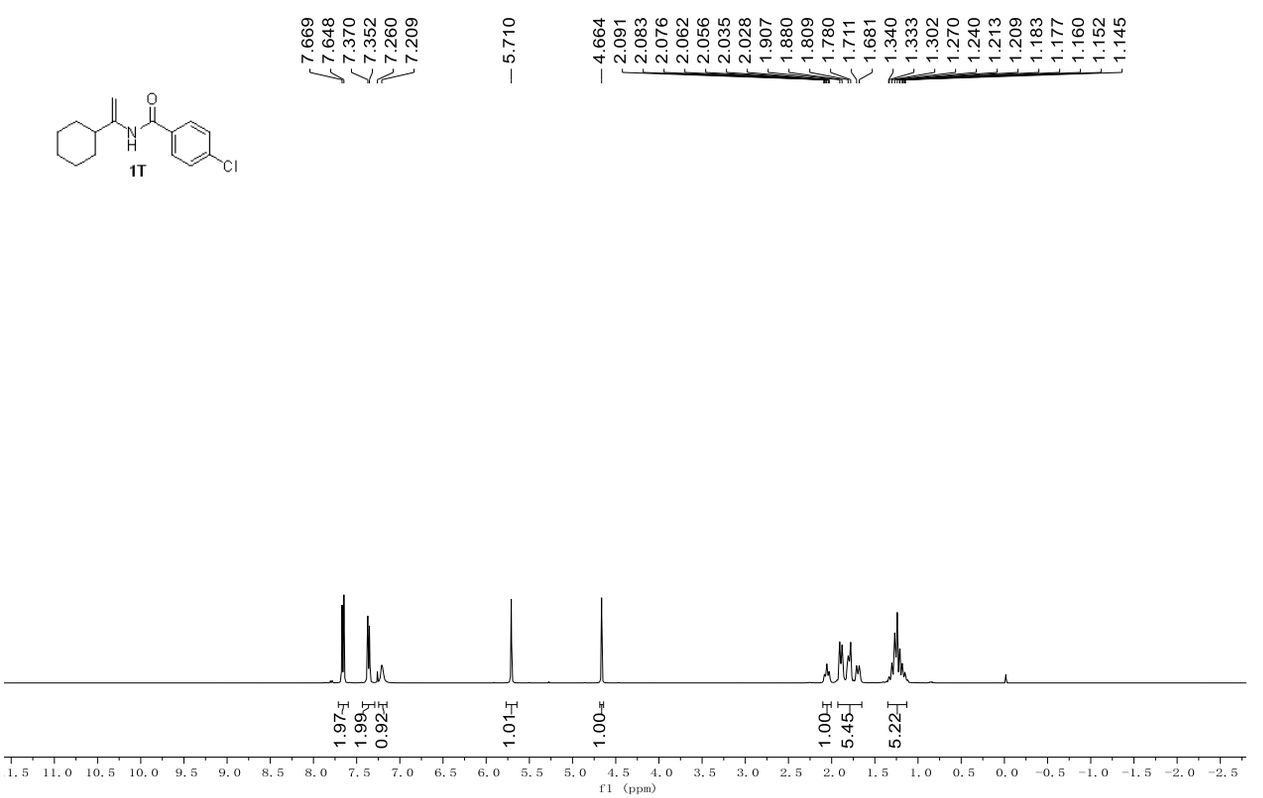
102.510
77.321
77.000
76.679
1S
f1 (ppm)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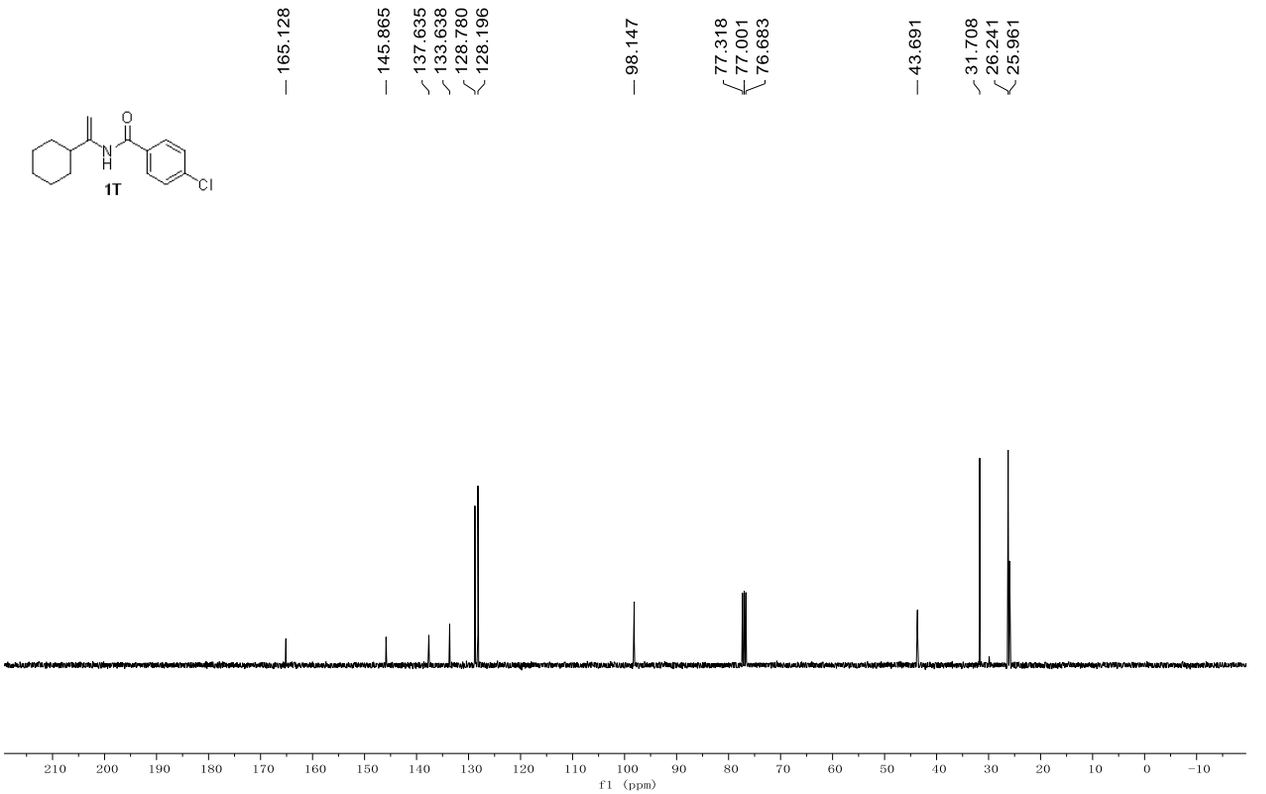
7.370
7.352
7.260
7.209
5.710
4.664
2.091
2.083
2.076
2.062
2.056
2.035
2.028
1.907
1.880
1.809
1.780
1.711
1.681
1.340
1.333
1.302
1.270
1.240
1.213
1.209
1.183
1.177
1.160
1.152
1.145
Cl
1T
1.97
1.99
0.92
1.01
1.00
1.00
5.45
5.22
f1 (ppm)


165.128
145.865
137.635
133.638
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128.196
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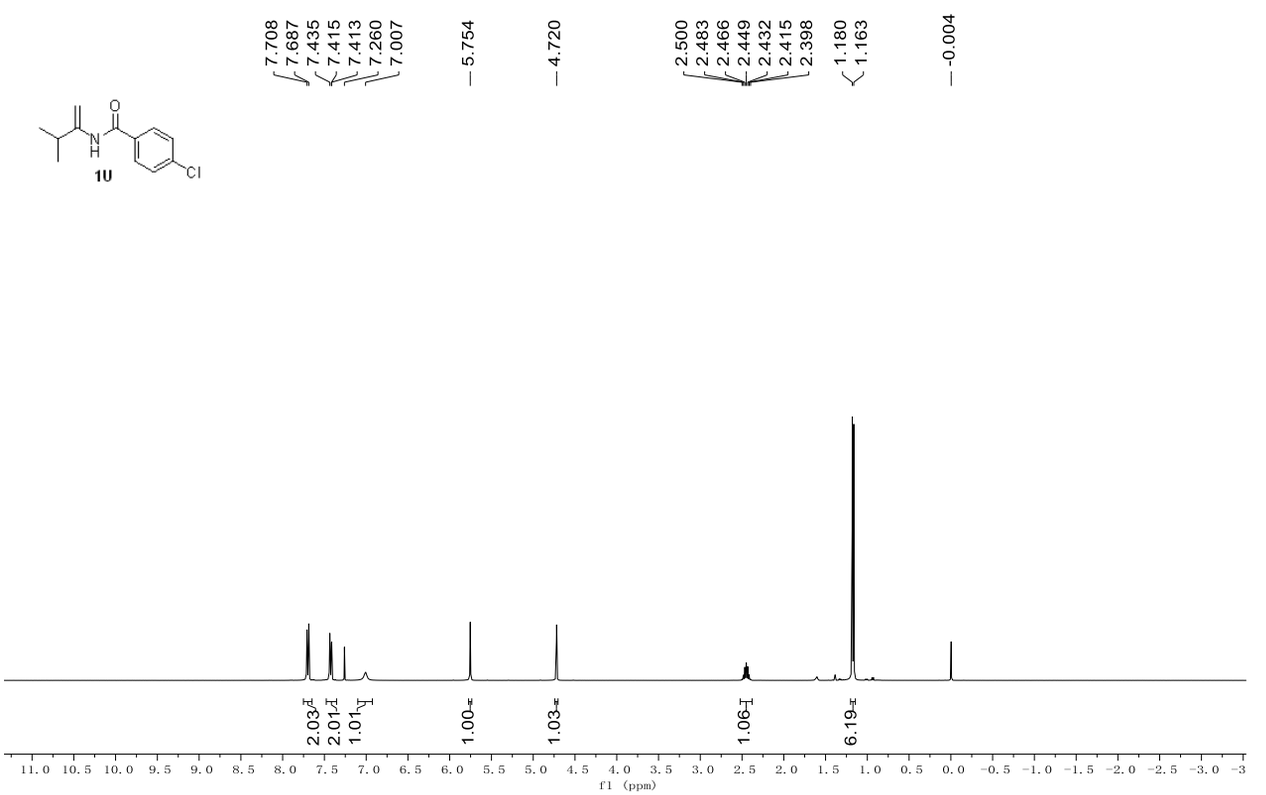
77.318
77.001
76.683
43.691
31.708
26.241
25.961
1T
f1 (ppm)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7.413
7.260
7.007
5.754
4.720
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2.483
2.466
2.449
2.432
2.415
2.398
1.180
1.163
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1U
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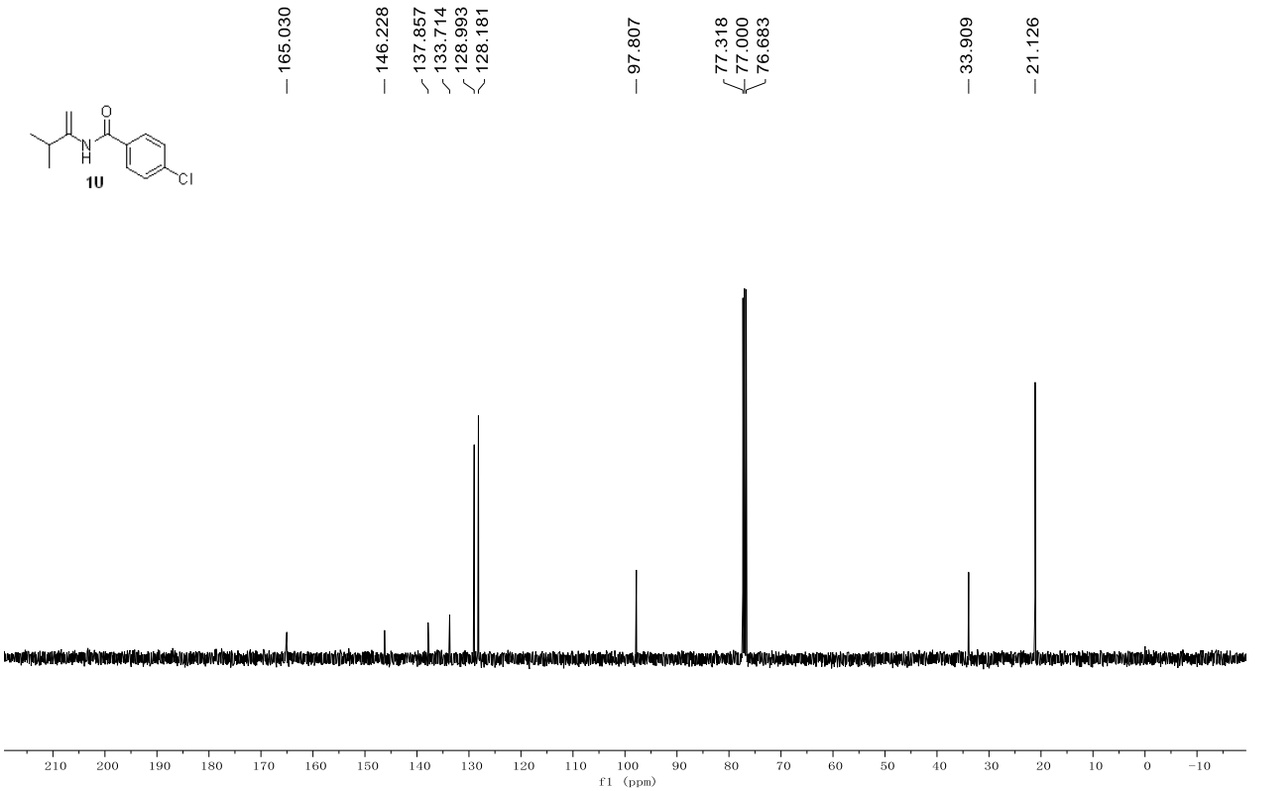
2.01
1.01
1.00
1.03
1.06
6.19
f1 (ppm)


165.030
146.228
137.857
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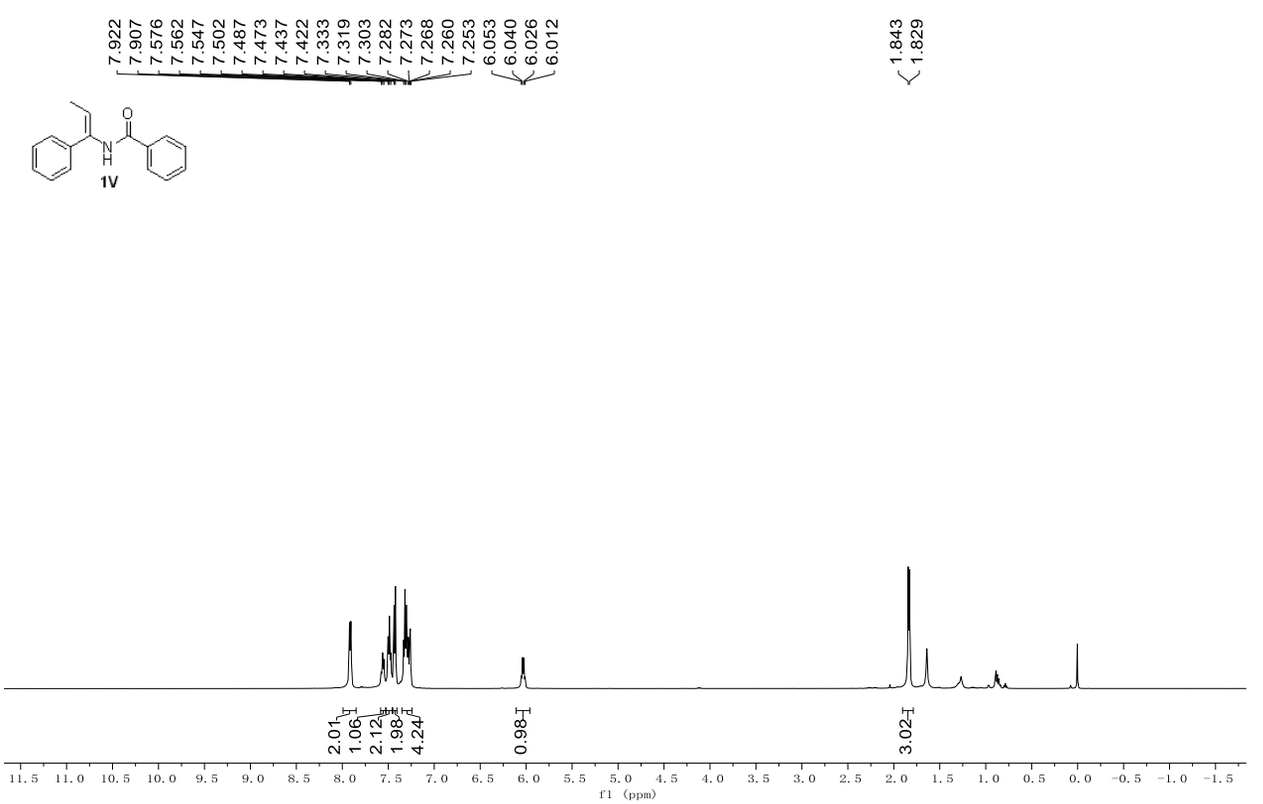
128.181
97.807
77.318
77.000
76.683
33.909
21.126
1U
Cl
f1 (ppm)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7.907
7.576
7.562
7.547
7.502
7.487
7.473
7.437
7.422
7.333
7.319
7.303
7.282
7.273
7.268
7.260
7.253
6.053
6.040
6.026
6.012
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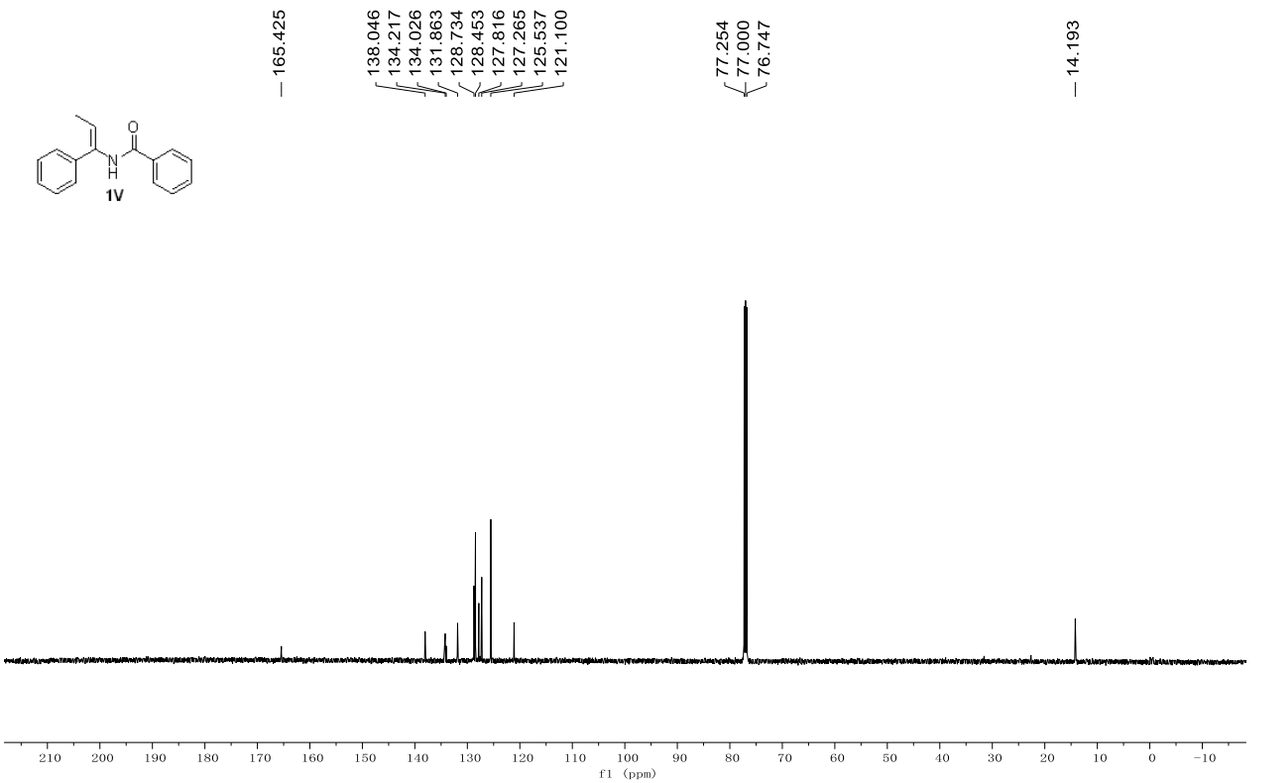
1.829
1V
2.01
1.06
2.12
1.98
4.24
0.98
3.02
f1 (ppm)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134.026
131.863
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127.816
127.265
125.537
121.100
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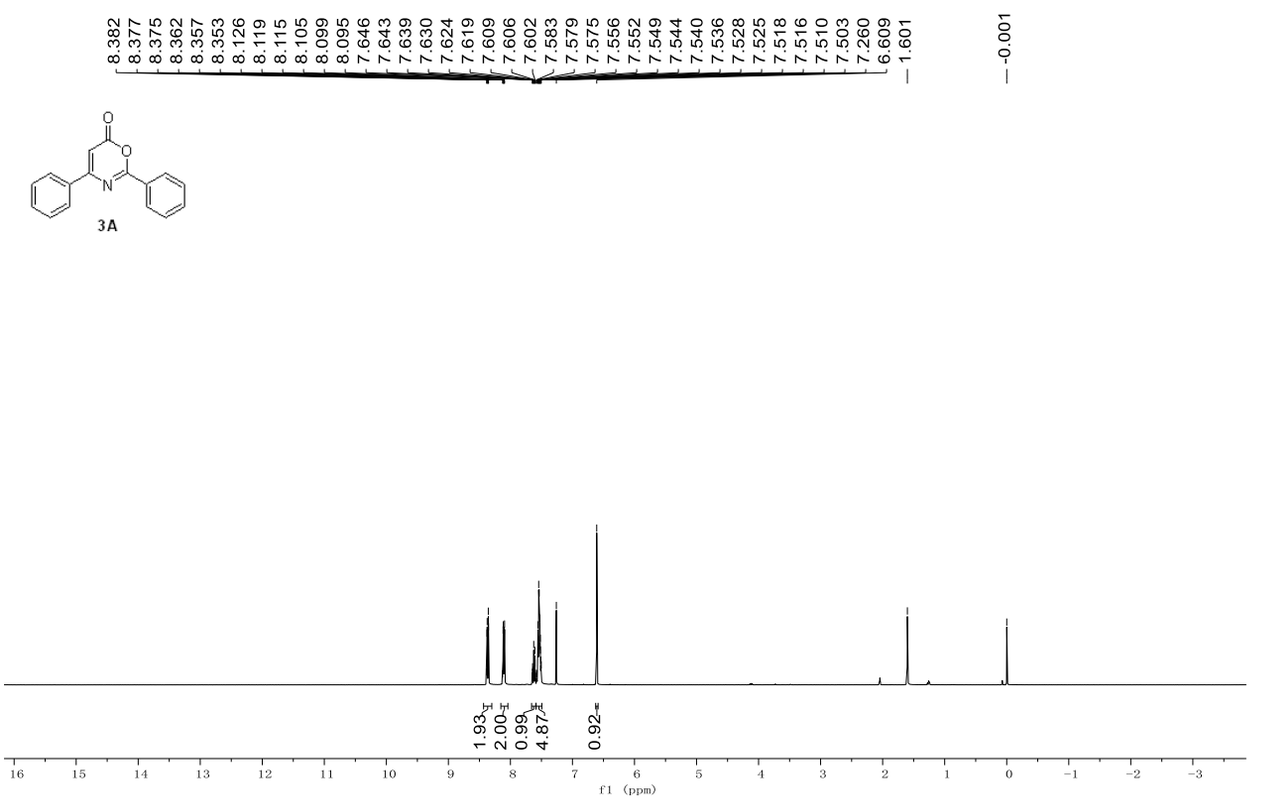
77.000
76.747
14.193
1V
f1 (ppm)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8.353
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8.119
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8.105
8.099
8.095
7.646
7.643
7.639
7.630
7.624
7.619
7.609
7.606
7.602
7.583
7.579
7.575
7.556
7.552
7.549
7.544
7.540
7.536
7.528
7.525
7.518
7.516
7.510
7.503
7.260
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2.00
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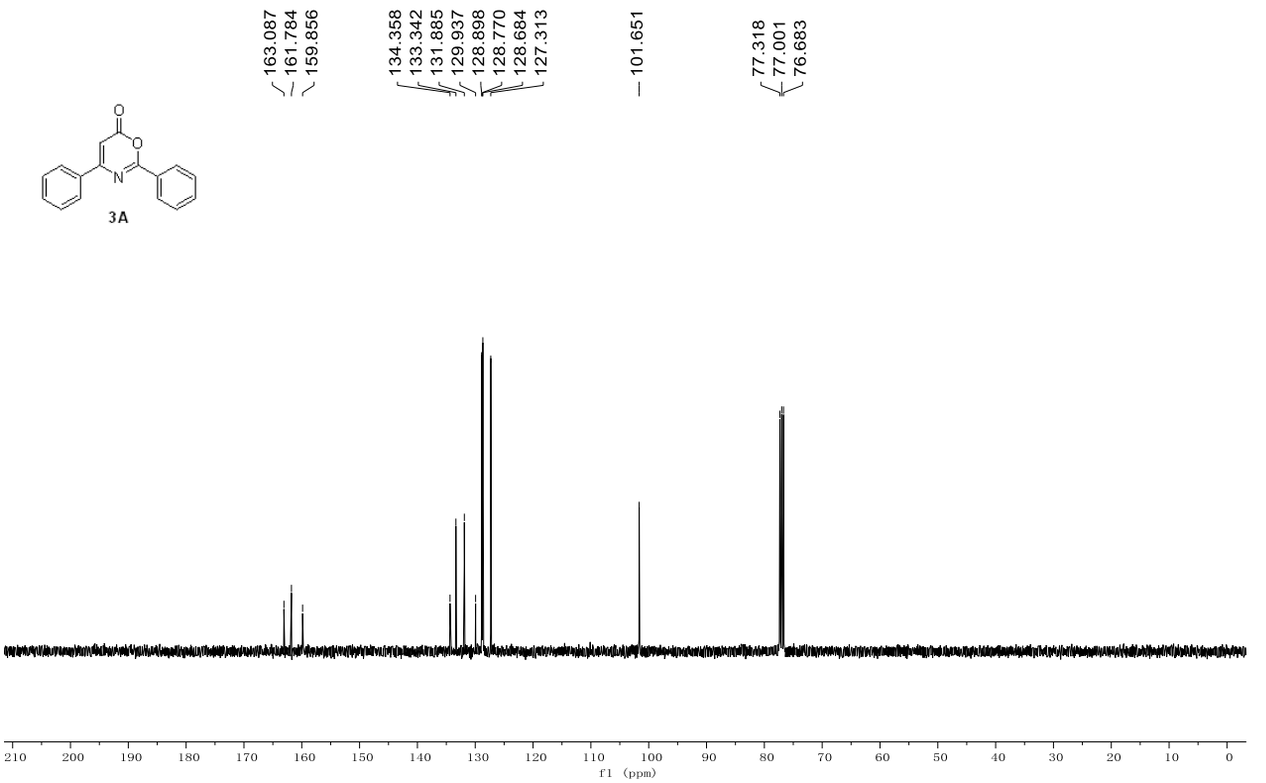
0.92
f1 (ppm)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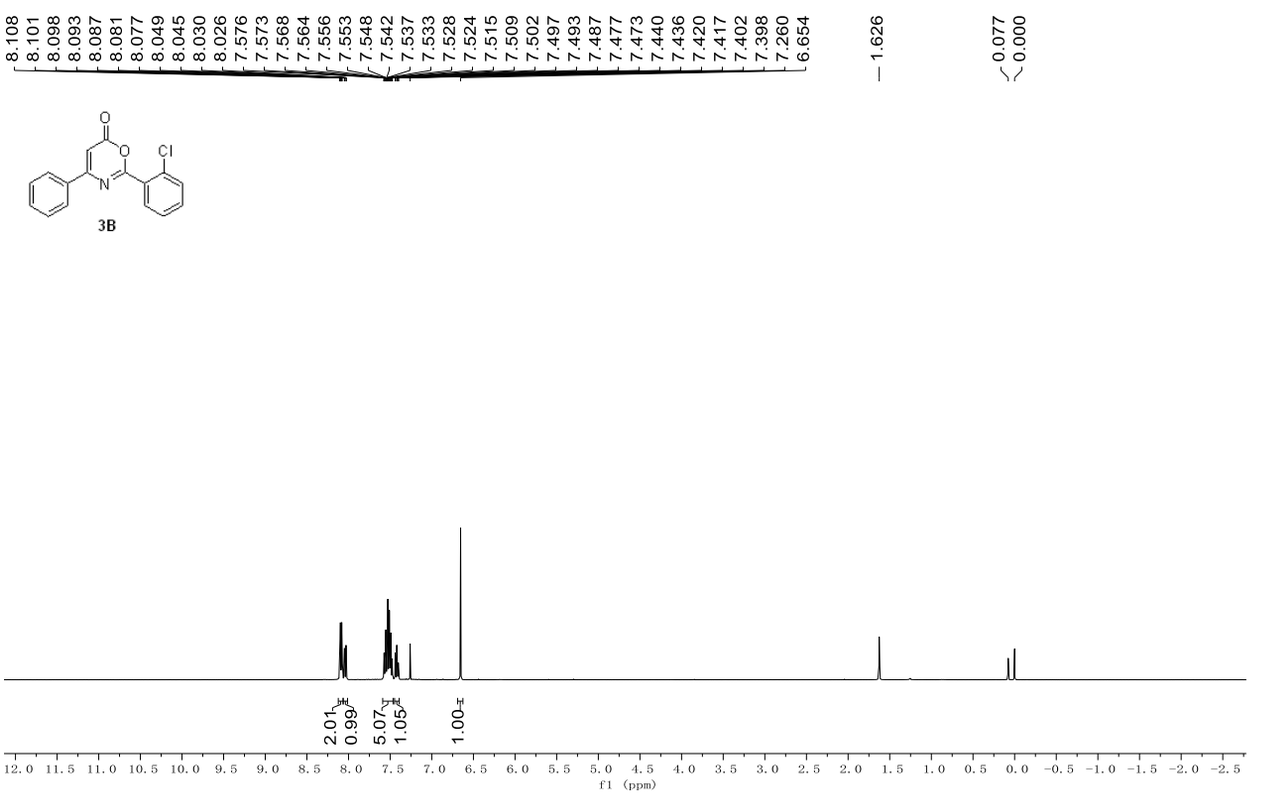
127.313
101.651
77.318
77.001
76.683
3A
f1 (ppm)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8.098
8.093
8.087
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8.077
8.049
8.045
8.030
8.026
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7.573
7.568
7.564
7.556
7.553
7.548
7.542
7.537
7.533
7.528
7.524
7.515
7.509
7.502
7.497
7.493
7.487
7.477
7.473
7.440
7.436
7.420
7.417
7.402
7.398
7.260
6.654
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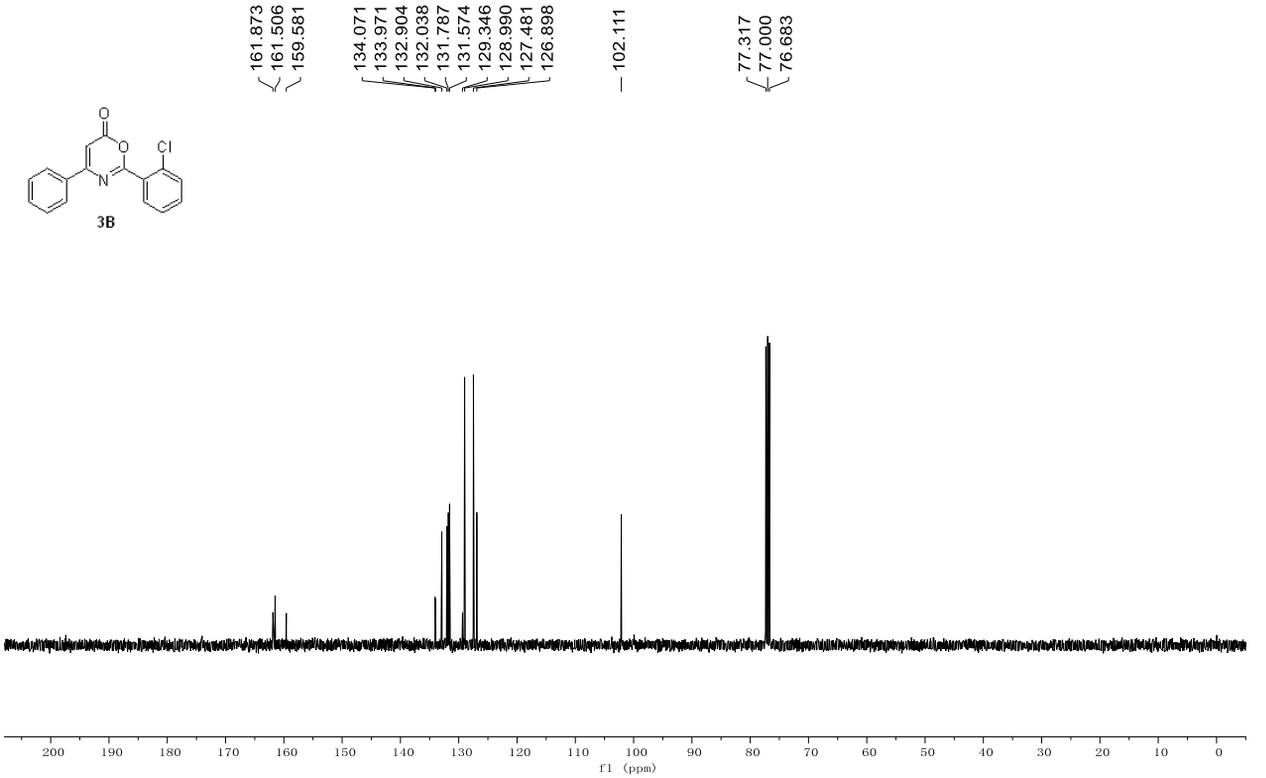
0.077
0.000
Cl
3B
2.01
0.99
5.07
1.05
1.00
f1 (ppm)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161.506
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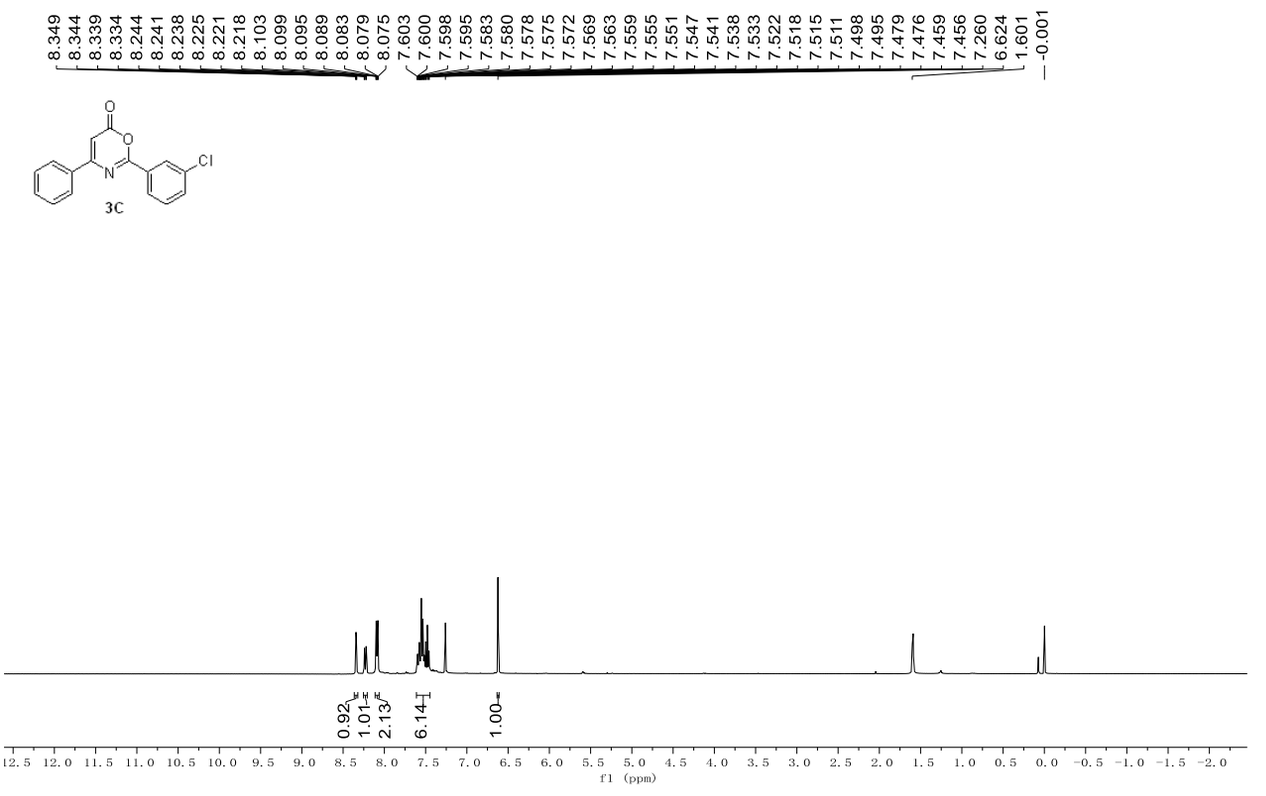
134.071
133.971
132.904
132.038
131.787
131.574
129.346
128.990
127.481
126.898
102.111
77.317
77.000
76.683
O
O
N
Cl
3B
f1 (ppm)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8.334
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8.238
8.225
8.221
8.218
8.103
8.099
8.095
8.089
8.083
8.079
8.075
7.603
7.600
7.598
7.595
7.583
7.580
7.578
7.575
7.572
7.569
7.563
7.559
7.555
7.551
7.547
7.541
7.538
7.533
7.522
7.518
7.515
7.511
7.498
7.495
7.479
7.476
7.459
7.456
7.260
6.624
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O
O
N
Cl
3C
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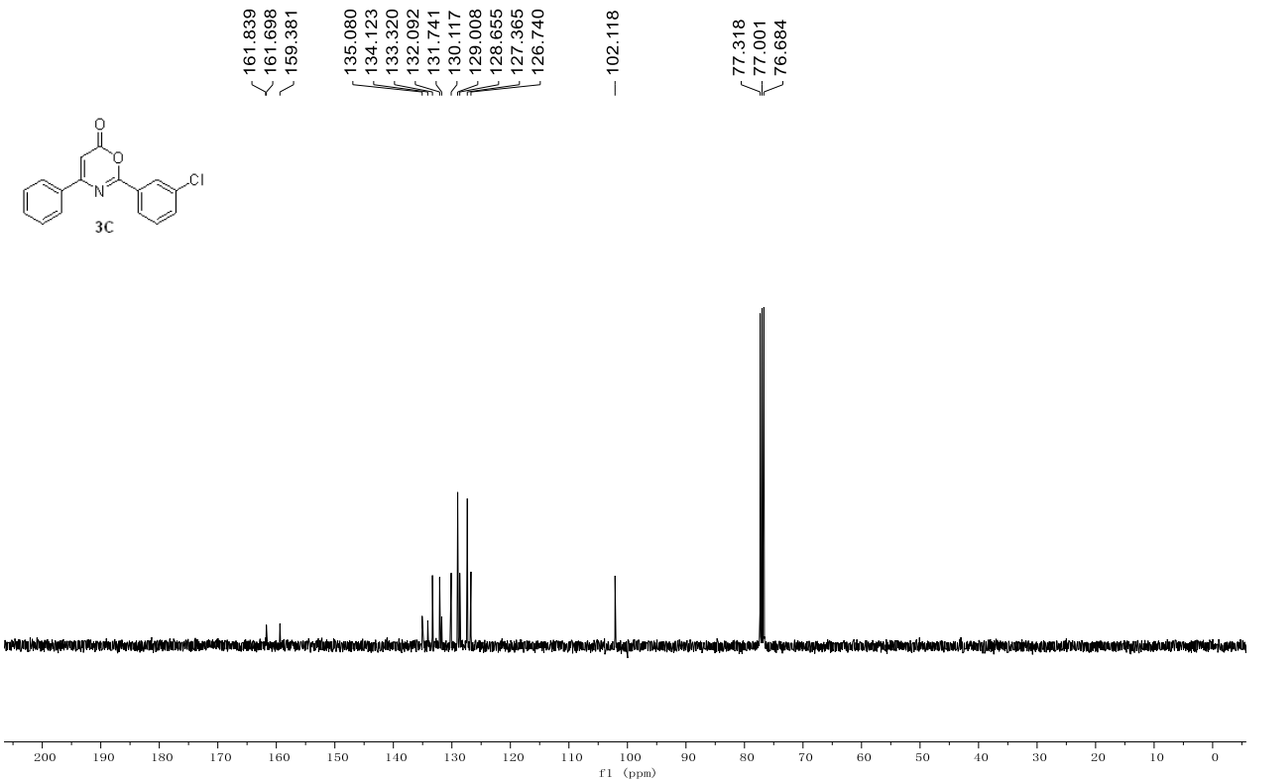
2.13
6.14
1.00
f1 (ppm)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133.320
132.092
131.741
130.117
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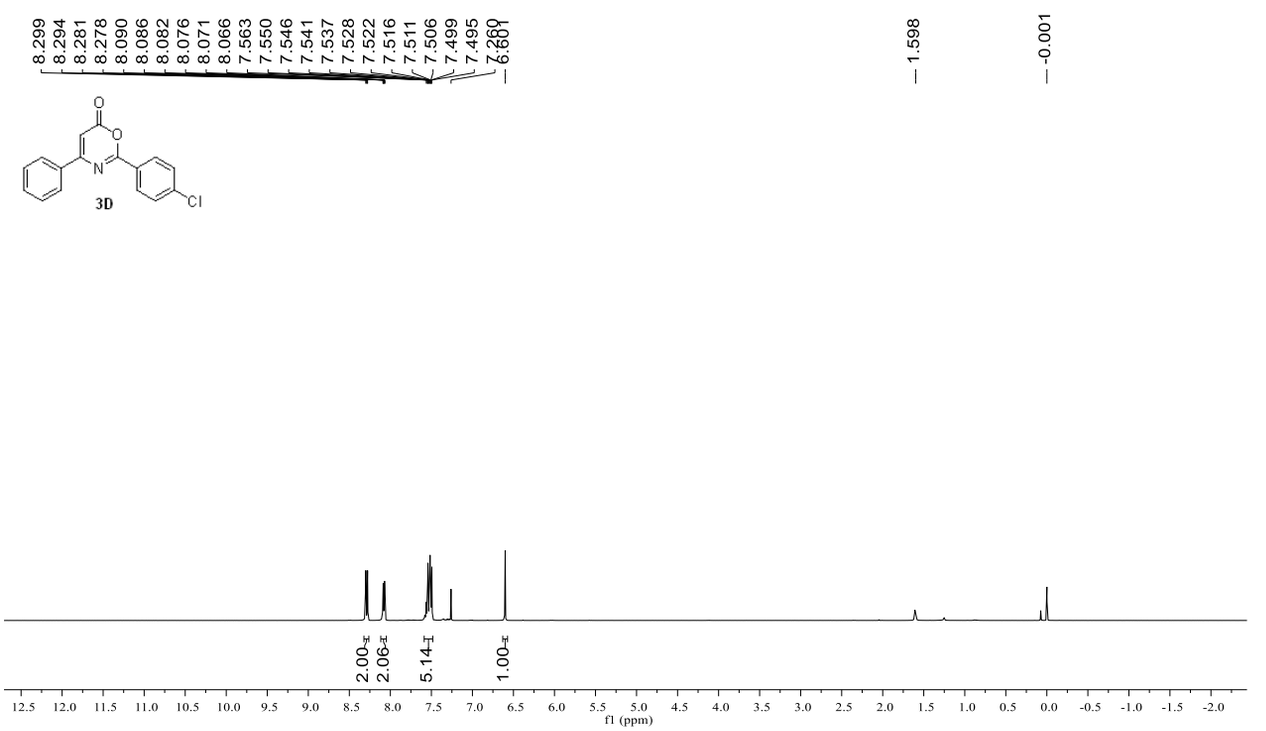
128.655
127.365
126.740
102.118
77.318
77.001
76.684
O
O
N
Cl
3C
f1 (ppm)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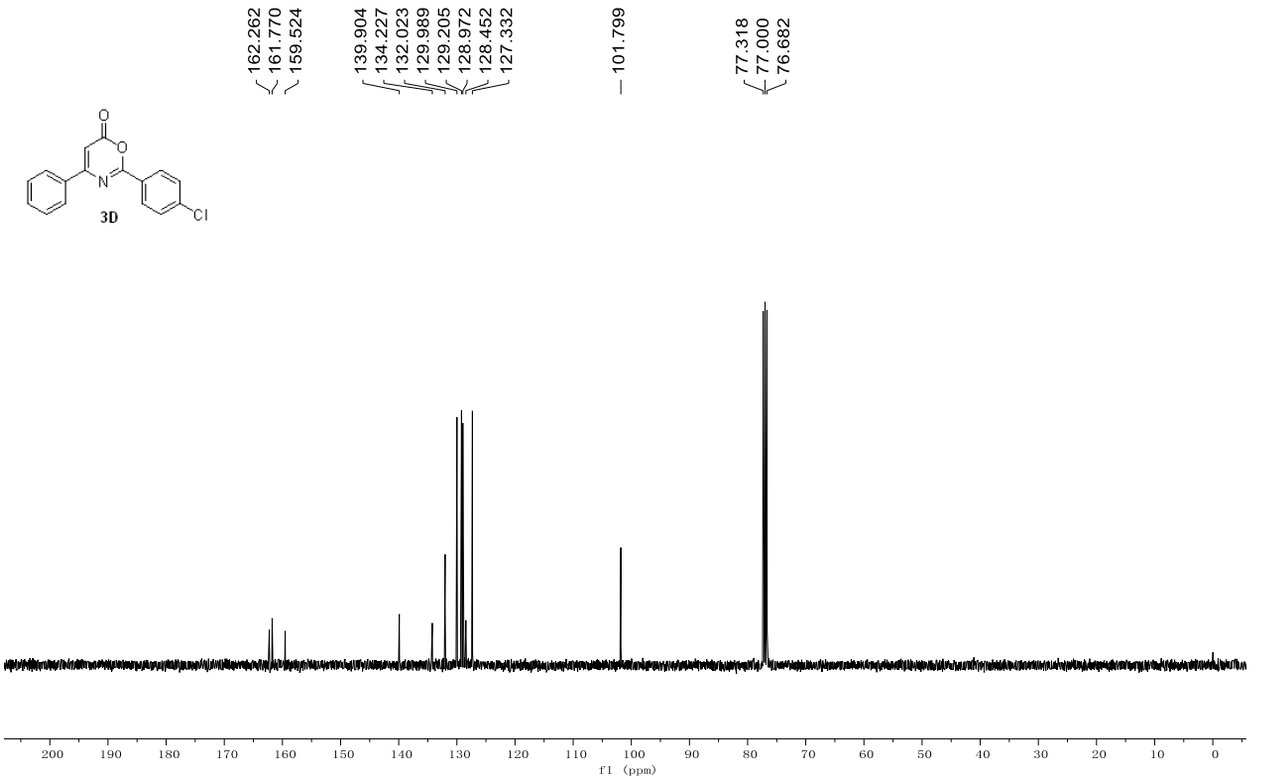
8.281
8.278
8.090
8.086
8.082
8.076
8.071
8.066
7.563
7.550
7.546
7.541
7.537
7.528
7.522
7.516
7.511
7.506
7.499
7.495
7.260
6.601
1.598
-0.001
O
O
N
Cl
3D
2.00
2.06
5.14
1.00
f1 (ppm)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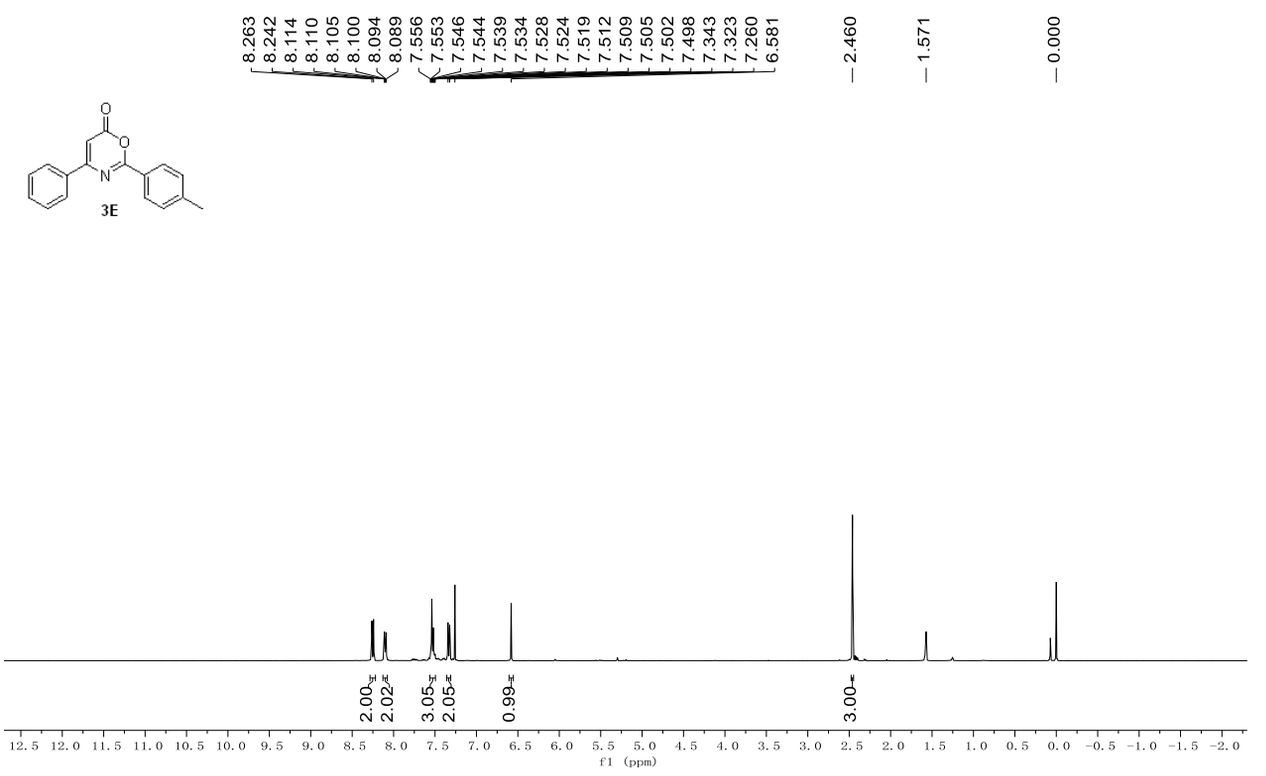
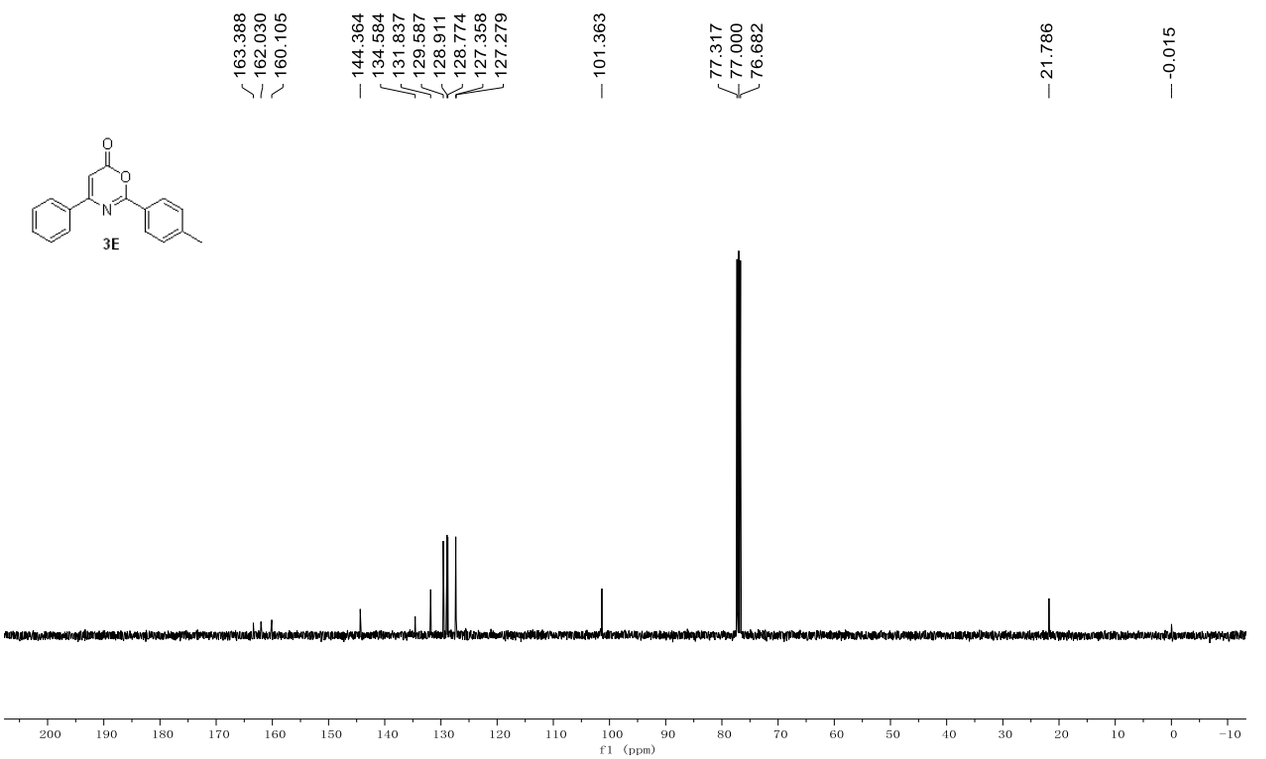
161.770
159.524
139.904
134.227
132.023
129.989
129.205
128.972
128.452
127.332
101.799
77.318
77.000
76.682
O
O
N
Cl
3D
f1 (ppm)


8.263
8.242
8.114
8.110
8.105
8.100
8.094
8.089
7.556
7.553
7.546
7.544
7.539
7.534
7.528
7.524
7.519
7.512
7.509
7.505
7.502
7.498
7.343
7.323
7.260
6.581
2.460
1.571
0.000
O
O
N
3E
2.00
2.02
3.05
2.05
0.99
3.00
f1 (ppm)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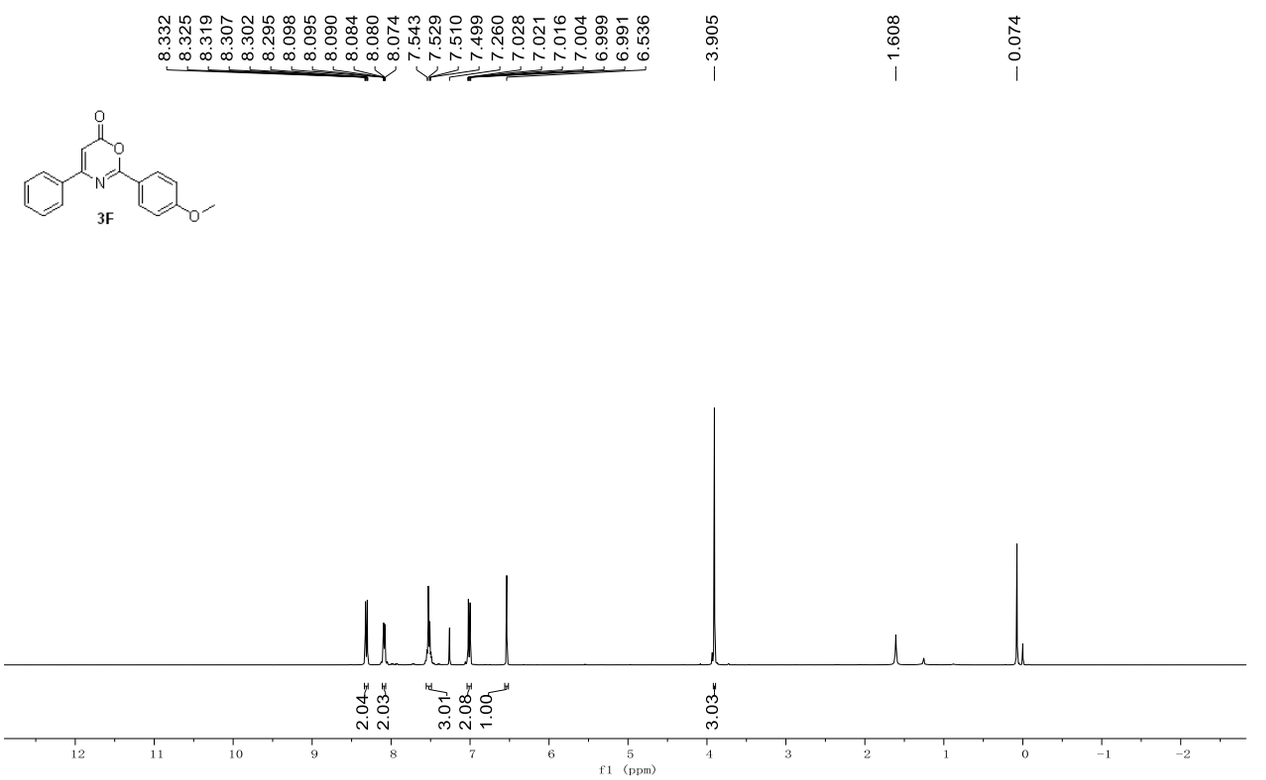
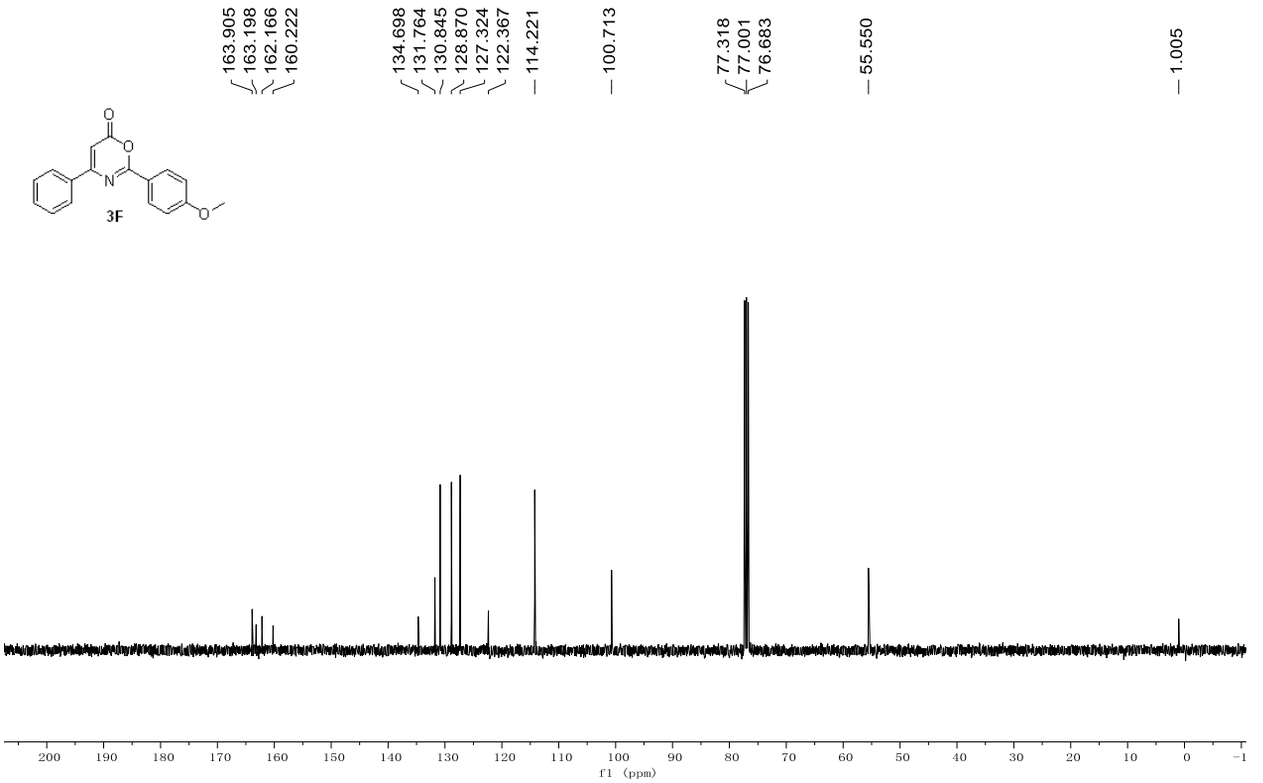
162.030
160.105
144.364
134.584
131.837
129.587
128.911
128.774
127.358
127.279
101.363
77.317
77.000
76.682
21.786
-0.015
3E
f1 (ppm)


8.332
8.325
8.319
8.307
8.302
8.295
8.098
8.095
8.090
8.084
8.080
8.074
7.543
7.529
7.510
7.499
7.260
7.028
7.021
7.016
7.004
6.999
6.991
6.536
3.905
1.608
0.074
3F
2.04
2.03
3.01
2.08
1.00
3.03
f1 (ppm)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163.198
162.166
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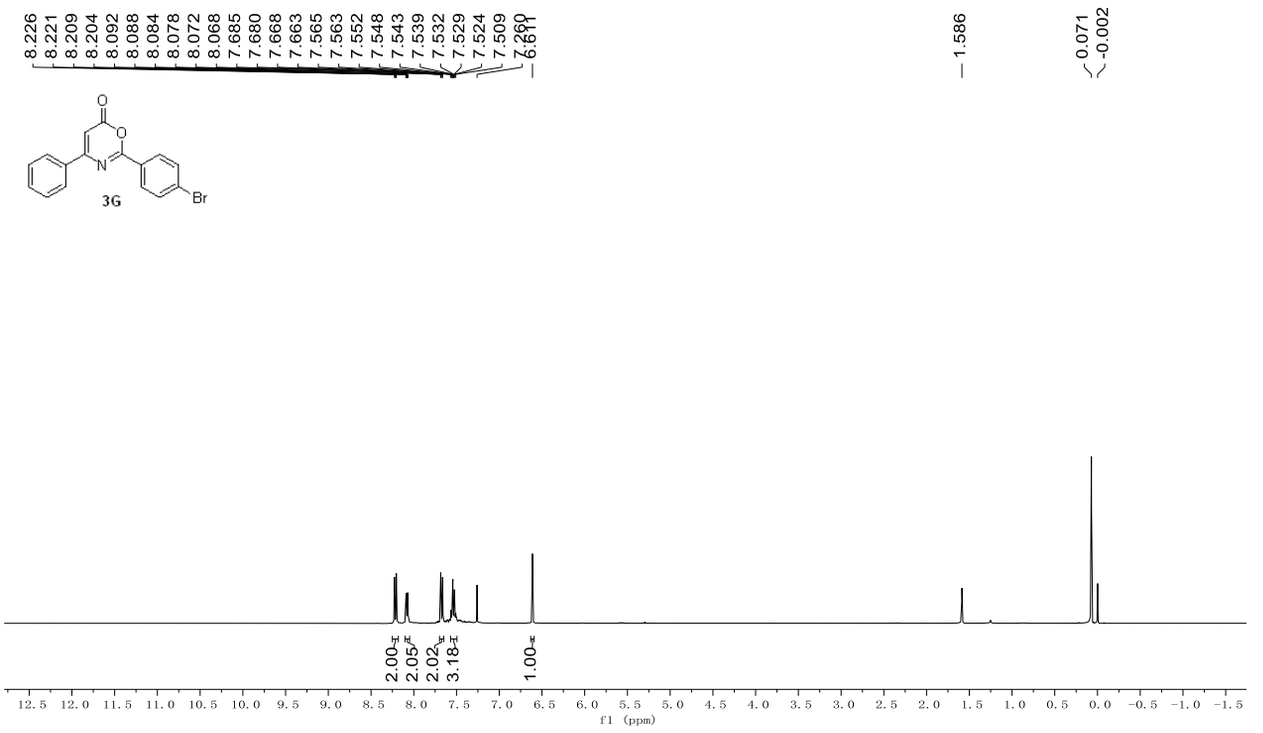
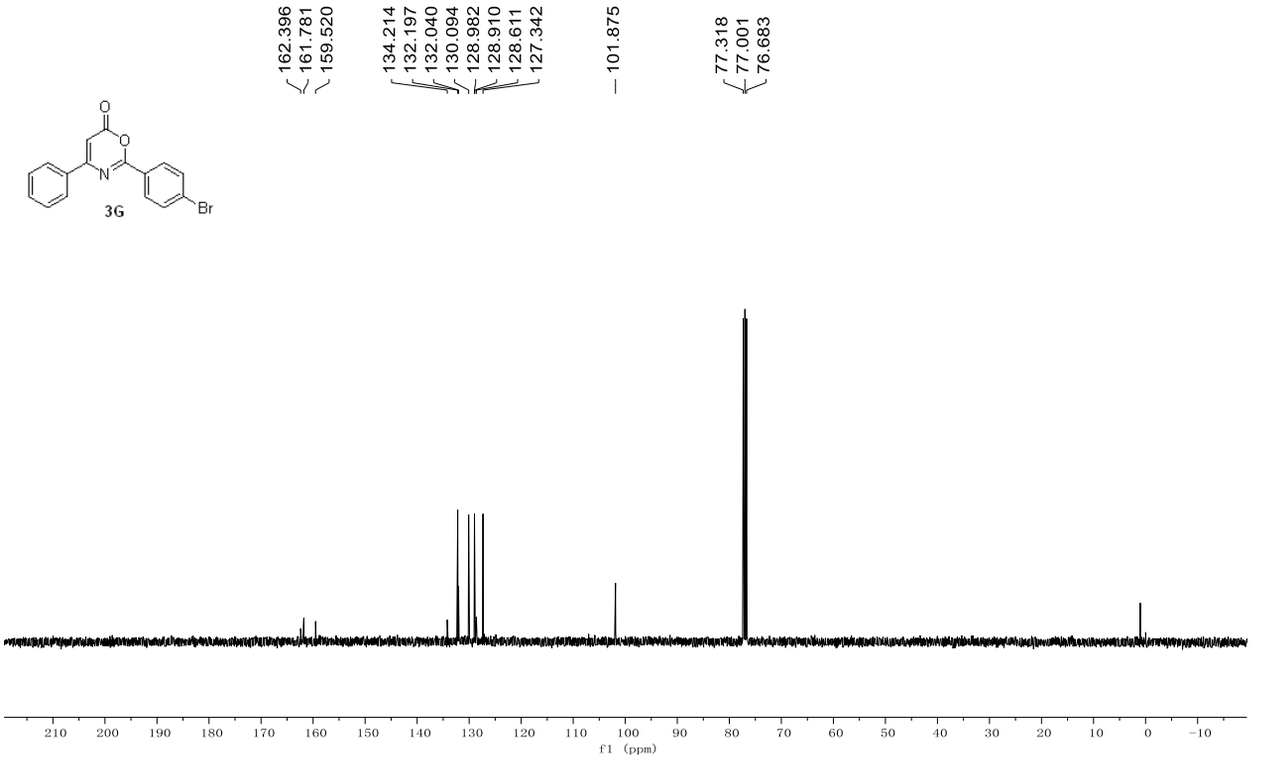
134.698
131.764
130.845
128.870
127.324
122.367
114.221
100.713
77.318
77.001
76.683
55.550
1.005
3F
f1 (ppm)


8.226
8.221
8.209
8.204
8.092
8.088
8.084
8.078
8.072
8.068
7.685
7.680
7.668
7.663
7.565
7.563
7.552
7.548
7.543
7.539
7.532
7.529
7.524
7.509
7.260
6.611
1.586
0.071
-0.002
3G
Br
2.00
2.05
2.02
3.18
1.00
f1 (ppm)


162.396
161.781
159.520
134.214
132.197
132.040
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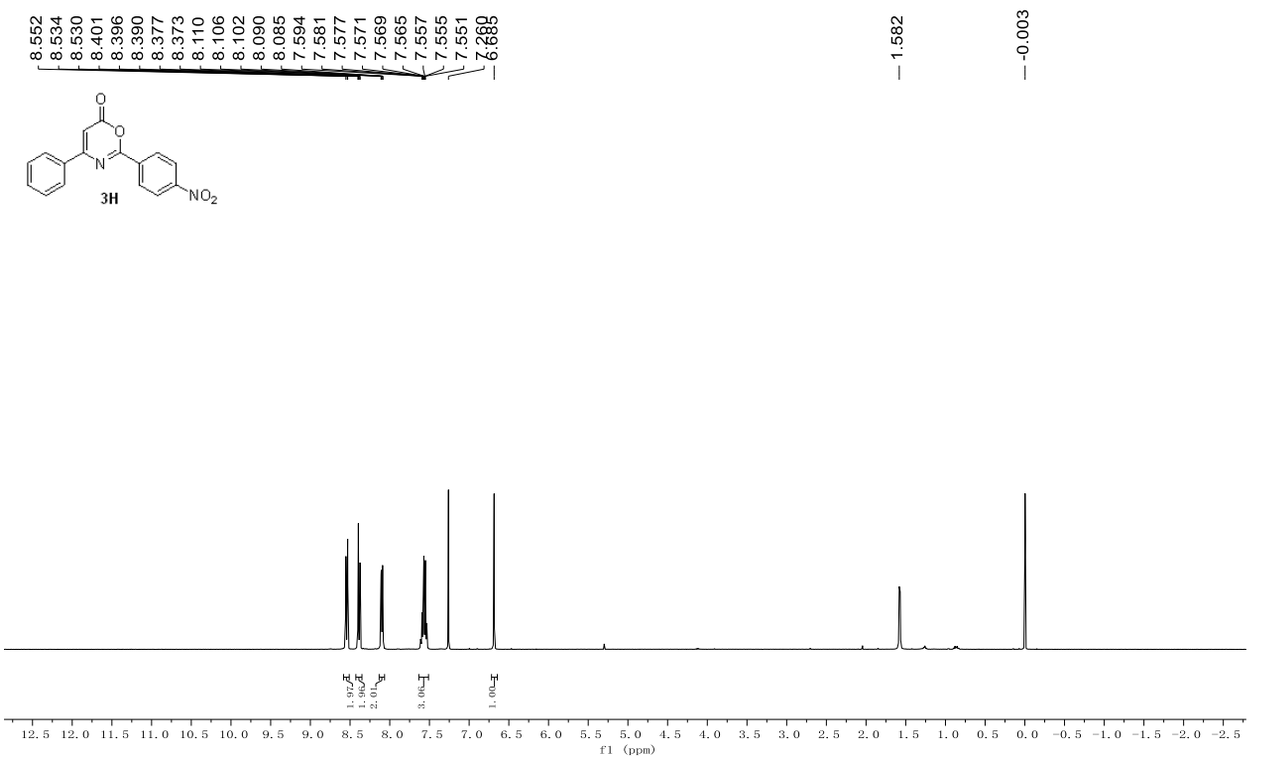
128.982
128.910
128.611
127.342
101.875
77.318
77.001
76.683
3G
Br
f1 (ppm)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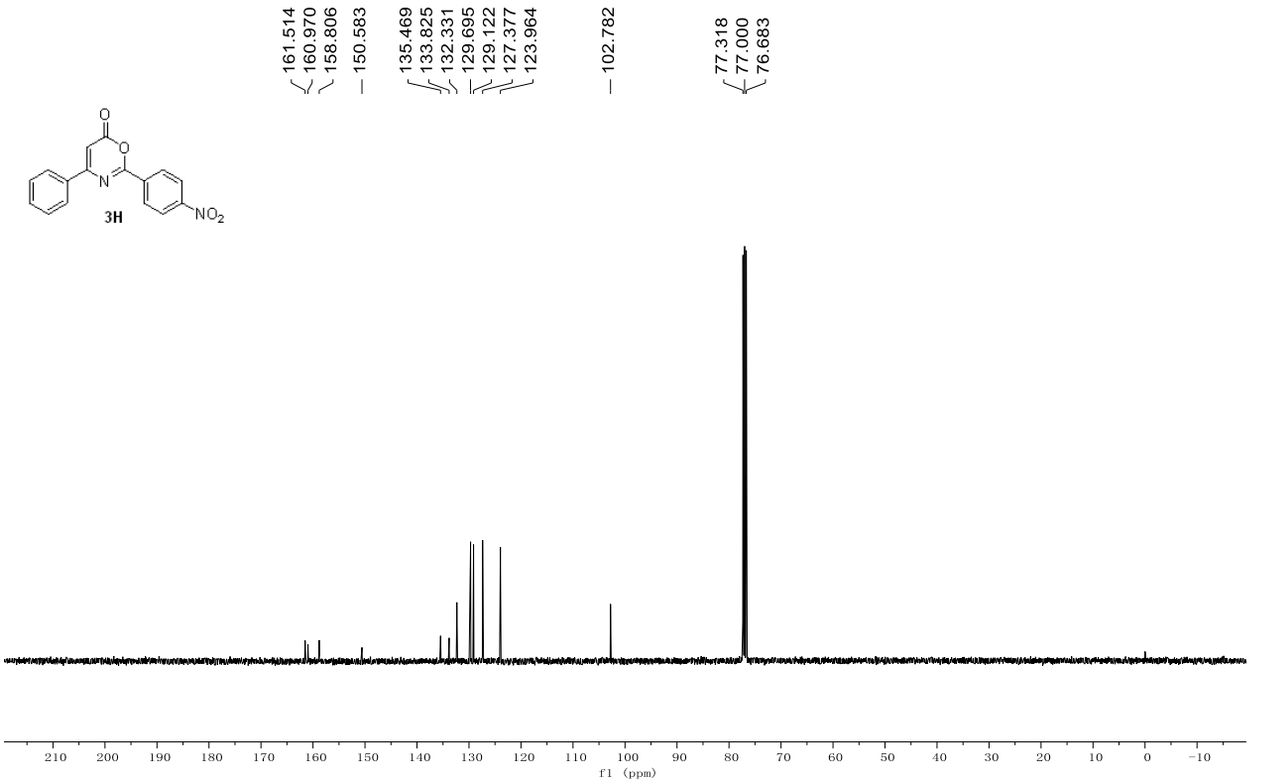
8.530
8.401
8.396
8.390
8.377
8.373
8.110
8.106
8.102
8.090
8.085
7.594
7.581
7.577
7.571
7.569
7.565
7.557
7.555
7.551
1.582
-0.003
3H
NO2
1.97
1.96
2.01
3.06
1.00
f1 (ppm)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160.970
158.806
150.583
135.469
133.825
132.331
129.695
129.122
127.377
123.964
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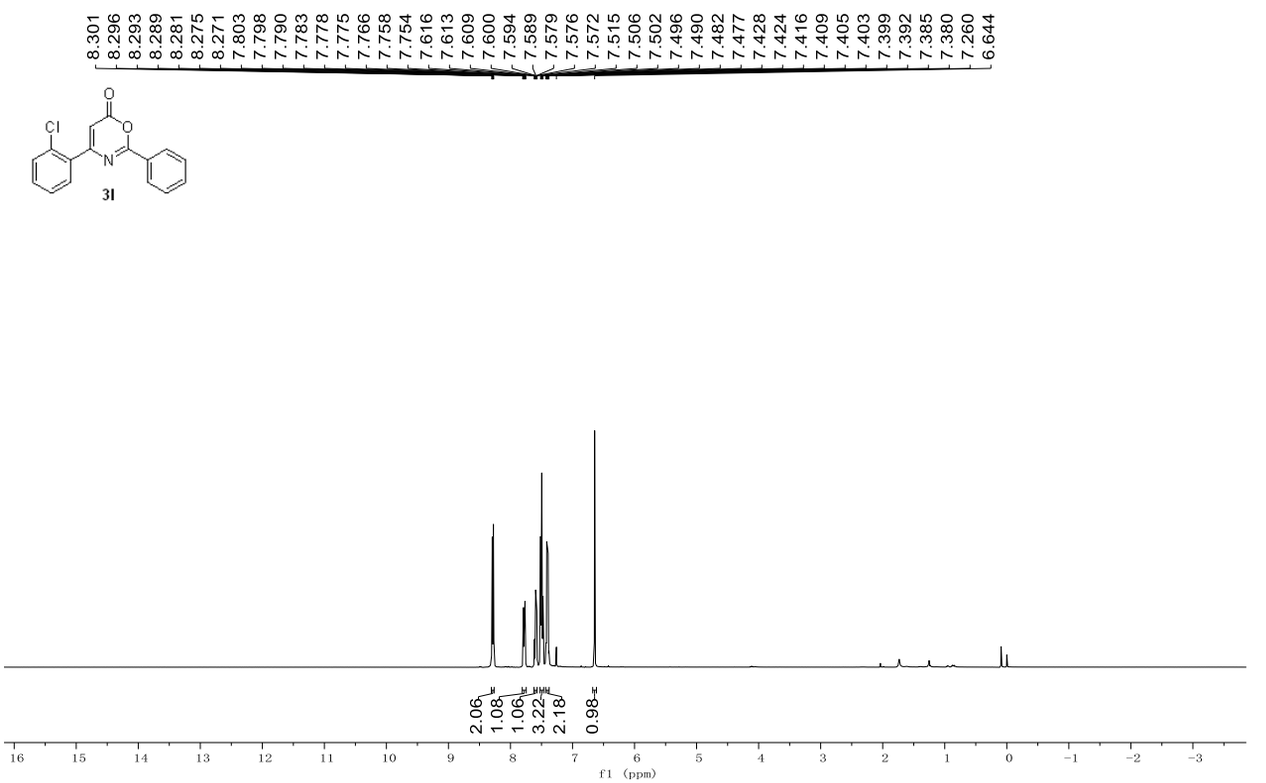
77.318
77.000
76.683
3H
f1 (ppm)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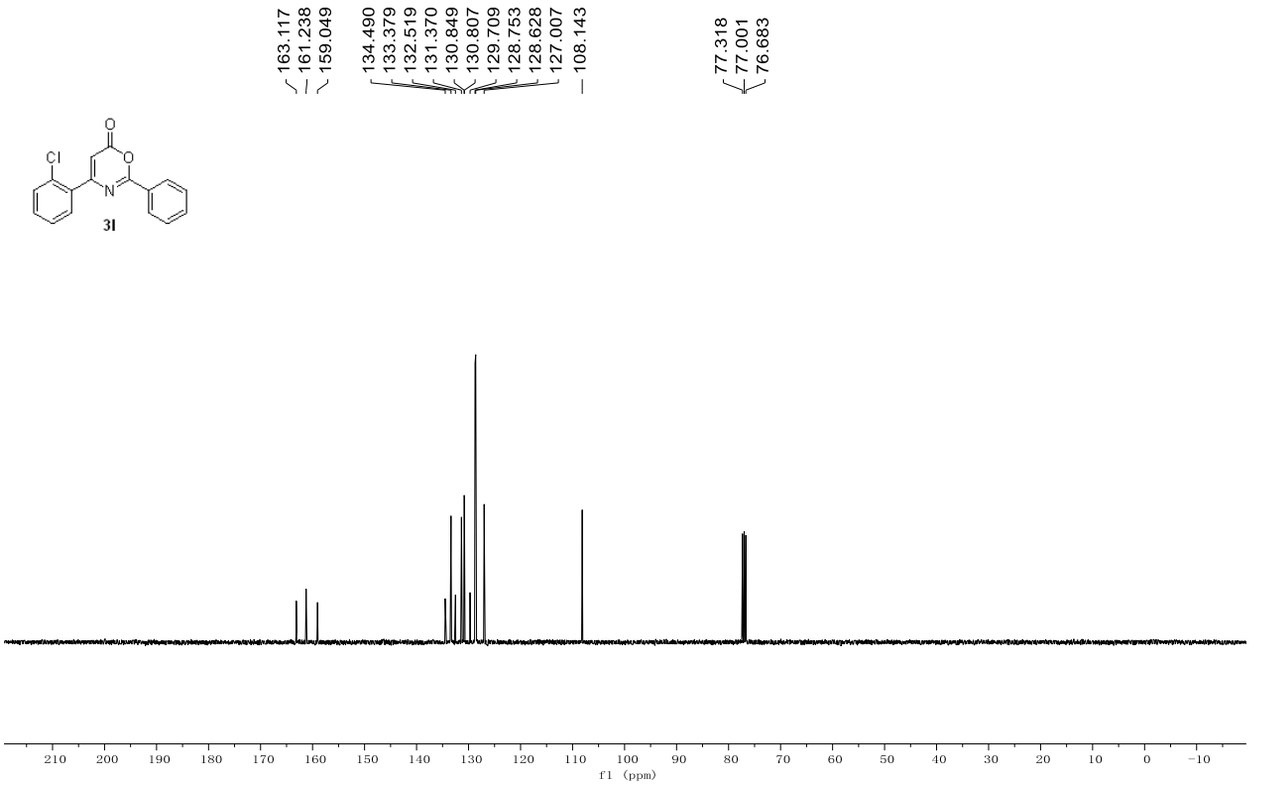
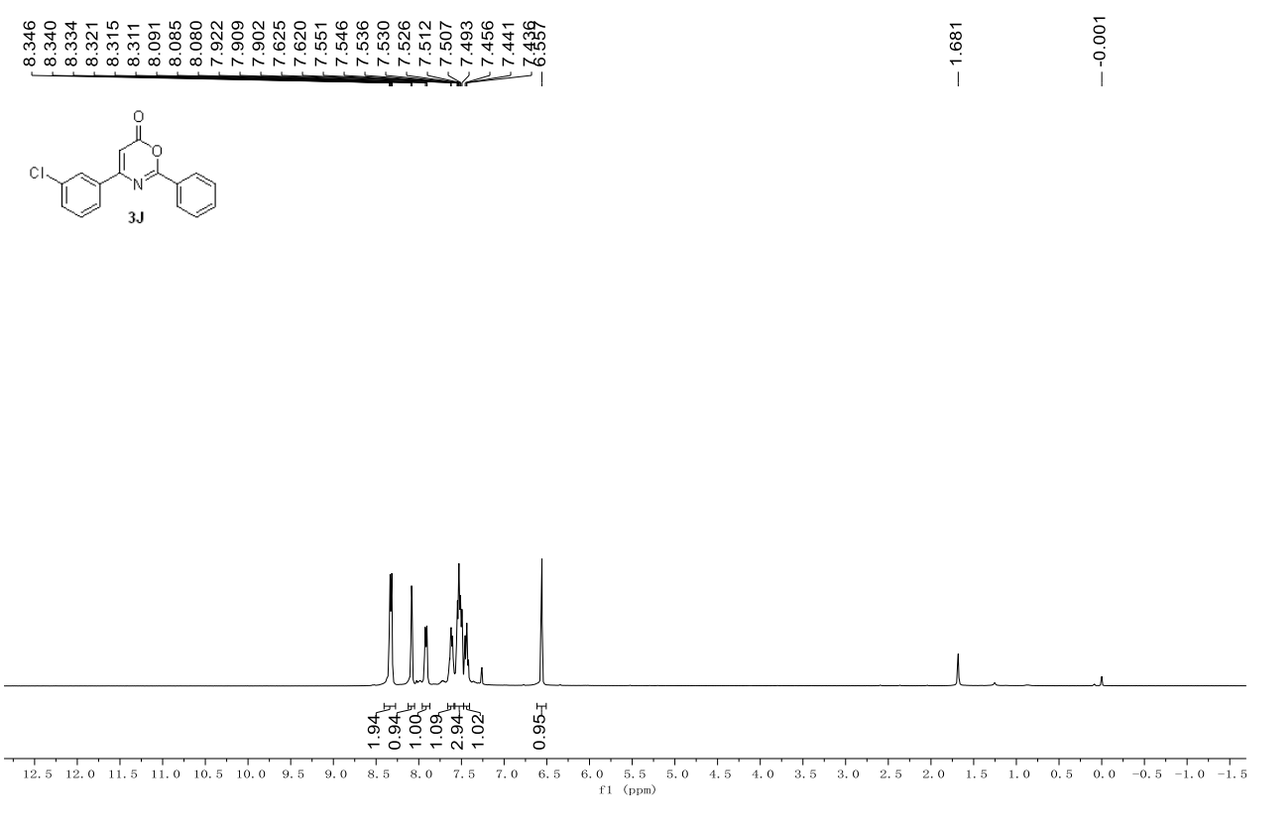
8.289
8.281
8.275
8.271
7.803
7.798
7.790
7.783
7.778
7.775
7.766
7.758
7.754
7.616
7.613
7.609
7.600
7.594
7.589
7.579
7.576
7.572
7.515
7.506
7.502
7.496
7.490
7.482
7.477
7.428
7.424
7.416
7.409
7.405
7.403
7.399
7.392
7.385
7.380
7.260
6.644
3I
2.06
1.08
1.06
3.22
2.18
0.98
f1 (ppm)


163.117
161.238
159.049
134.490
133.379
132.519
131.370
130.849
130.807
129.709
128.753
128.628
127.007
108.143
77.318
77.001
76.683
Cl
O
O
N
3I
f1 (ppm)


8.346
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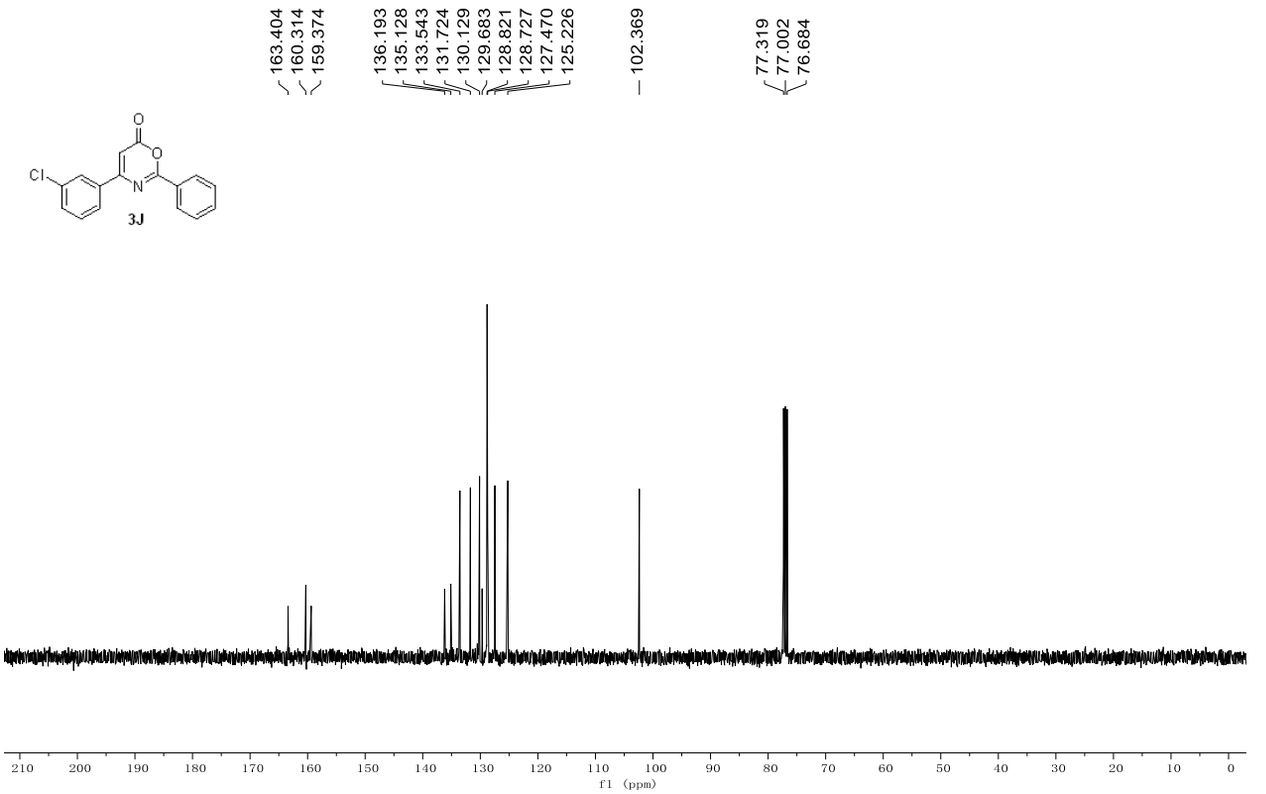
8.334
8.321
8.315
8.311
8.091
8.085
8.080
7.922
7.909
7.902
7.625
7.620
7.551
7.546
7.536
7.530
7.526
7.512
7.507
7.493
7.456
7.441
7.436
6.557
1.681
-0.001
Cl
O
O
N
3J
1.94
0.94
1.00
1.09
2.94
1.02
0.95
f1 (ppm)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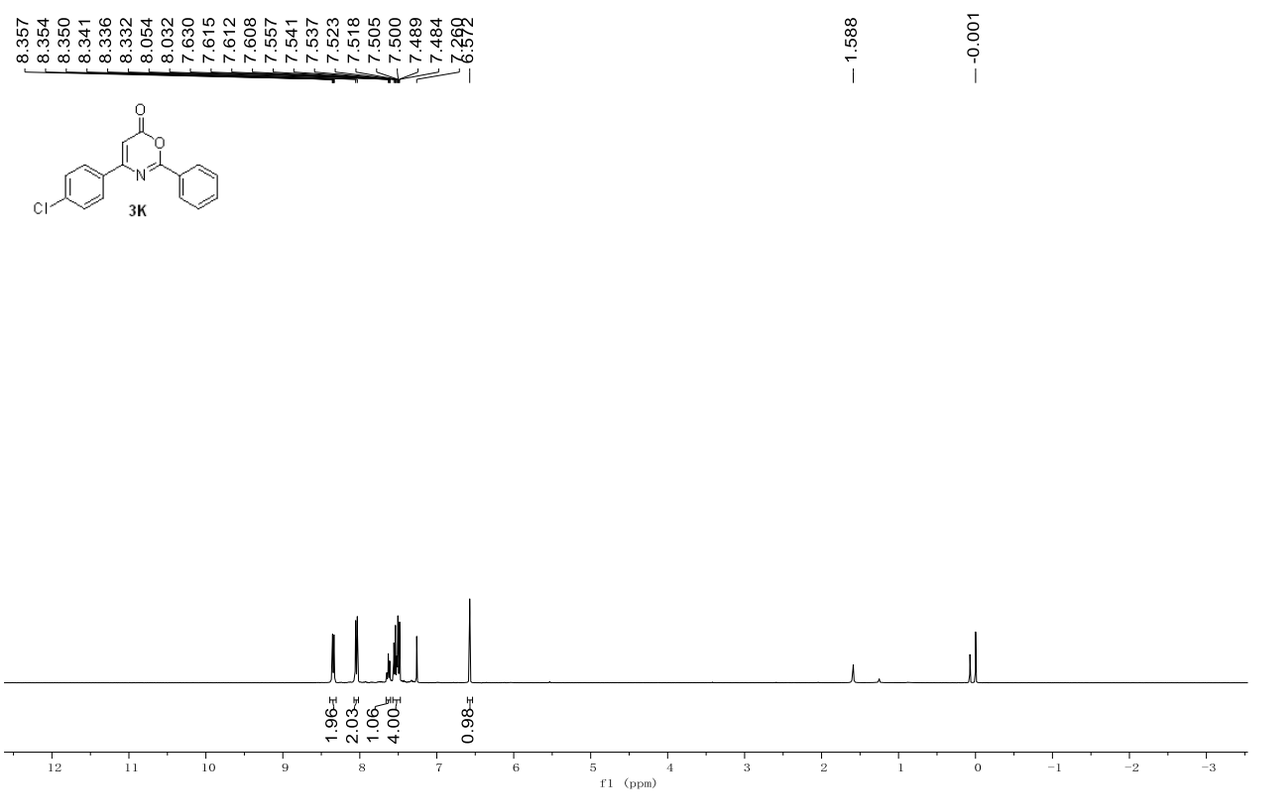
159.374
136.193
135.128
133.543
131.724
130.129
129.683
128.821
128.727
127.470
125.226
102.369
77.319
77.002
76.684
Cl
O
O
N
3J
f1 (ppm)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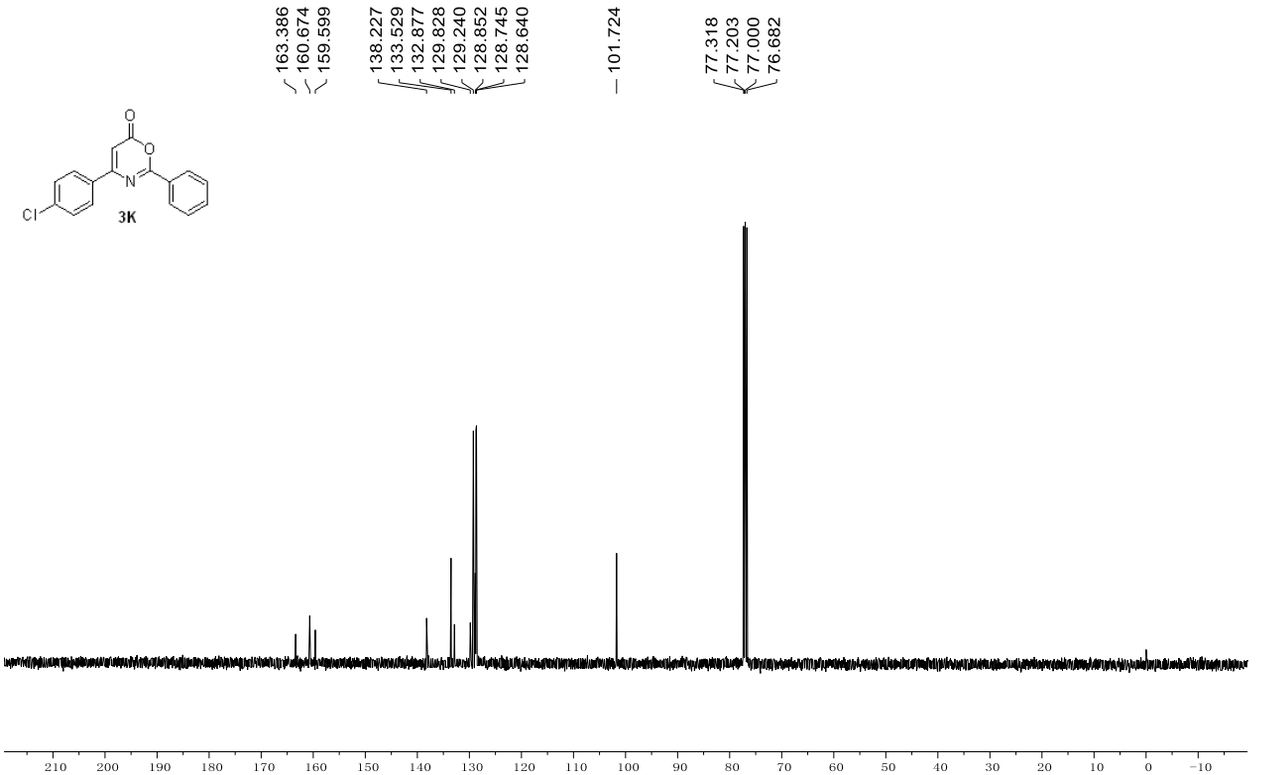
8.354
8.350
8.341
8.336
8.332
8.054
8.032
7.630
7.615
7.612
7.608
7.557
7.541
7.537
7.523
7.518
7.505
7.500
7.489
7.484
6.572
1.588
-0.001
Cl
O
O
N
3K
1.96
2.03
1.06
4.00
0.98
f1 (ppm)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159.599
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132.877
129.828
129.240
128.852
128.745
128.640
101.724
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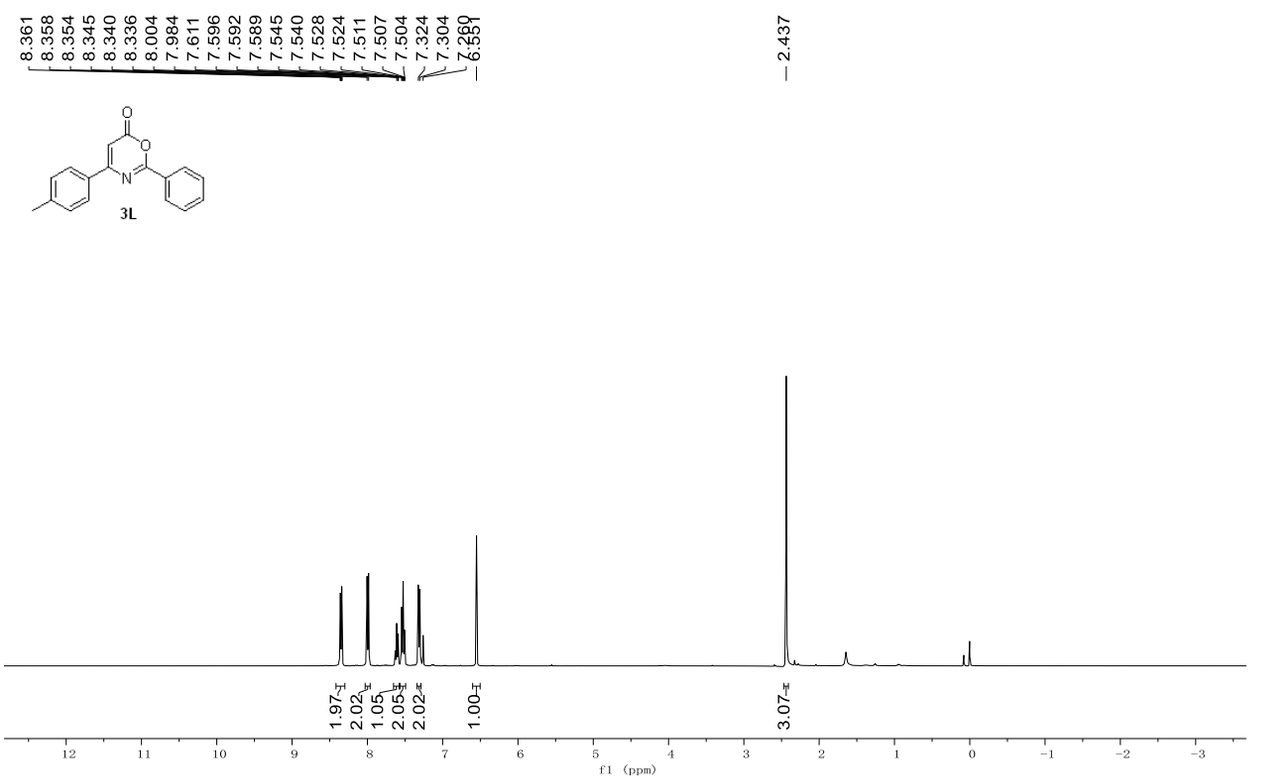
77.203
77.000
76.682
O
O
N
Cl
3K
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10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8.358
8.354
8.345
8.340
8.336
8.004
7.984
7.611
7.596
7.592
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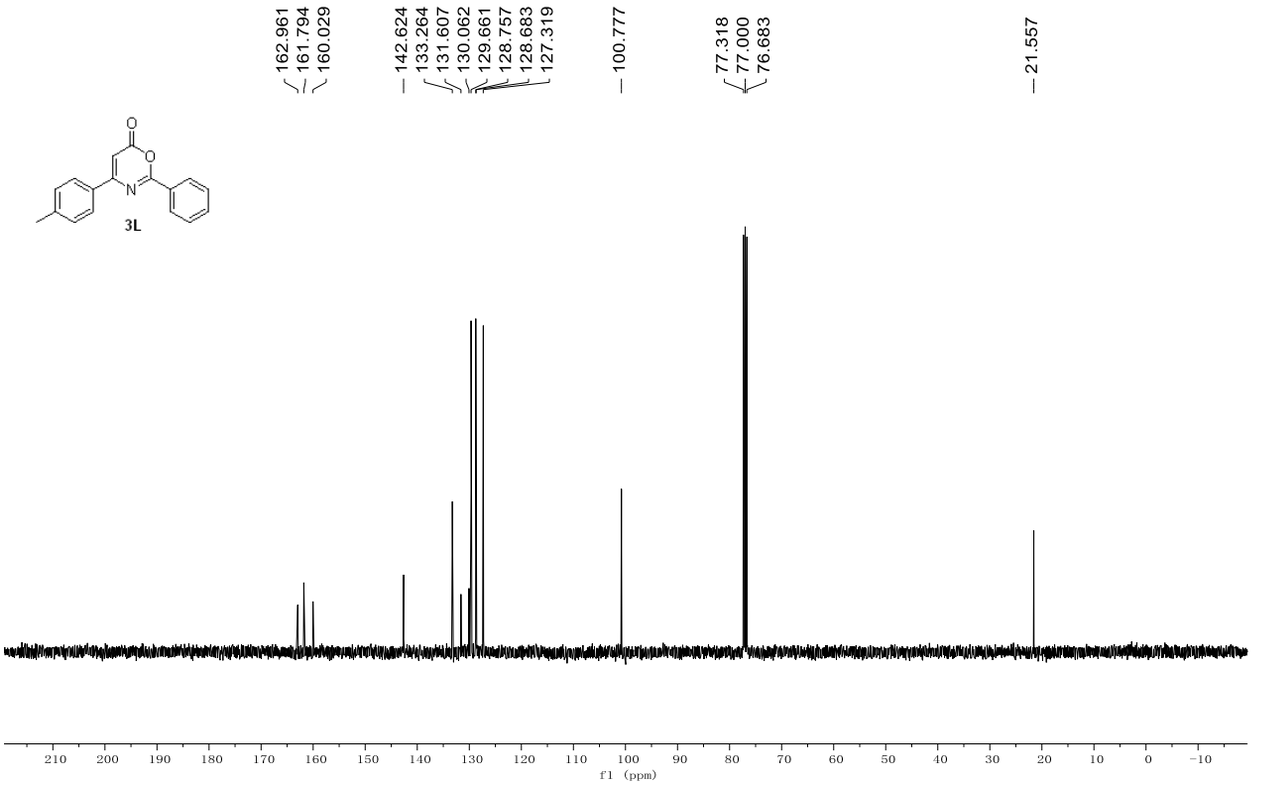
7.545
7.540
7.528
7.524
7.511
7.507
7.504
7.324
7.304
7.260
6.551
2.437
O
O
N
3L
1.97
2.02
1.05
2.05
2.02
1.00
3.07
12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 −3
f1 (ppm)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129.661
128.757
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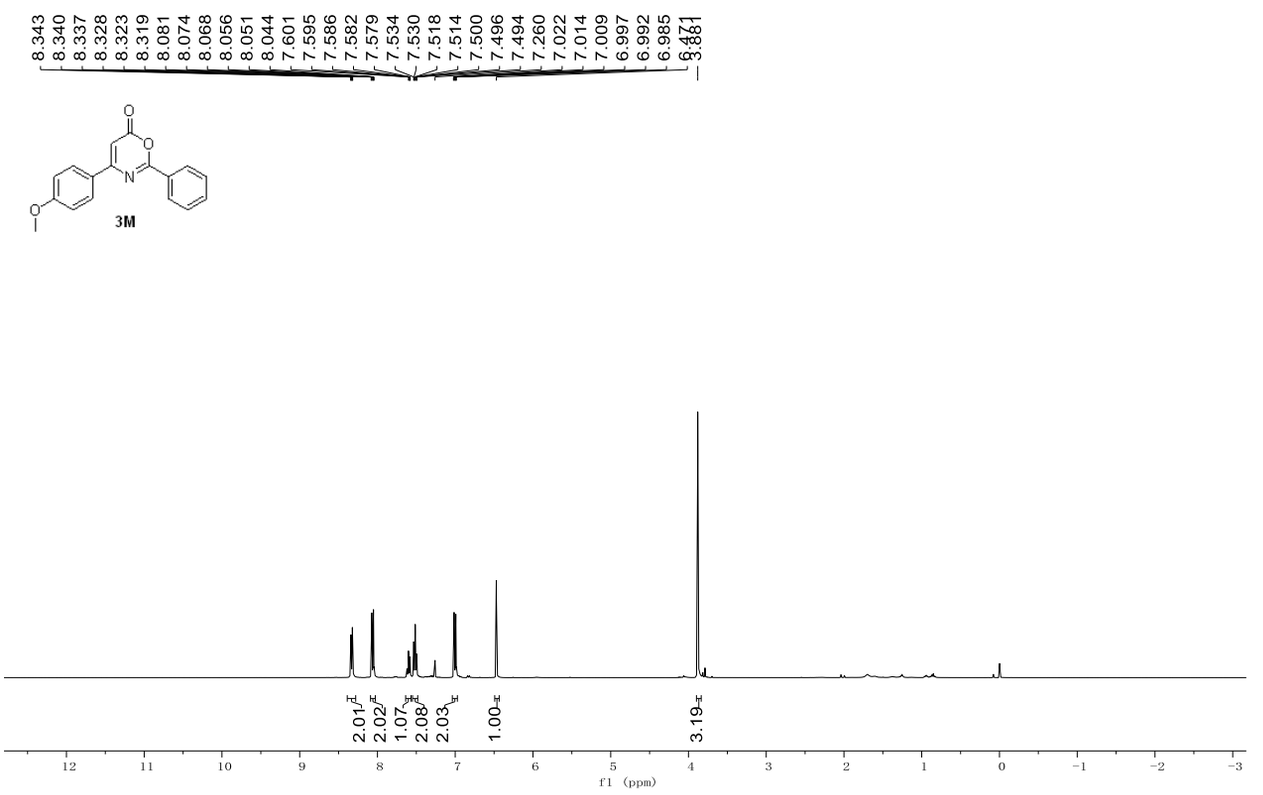
100.777
77.318
77.000
76.683
21.557
3L
f1 (ppm)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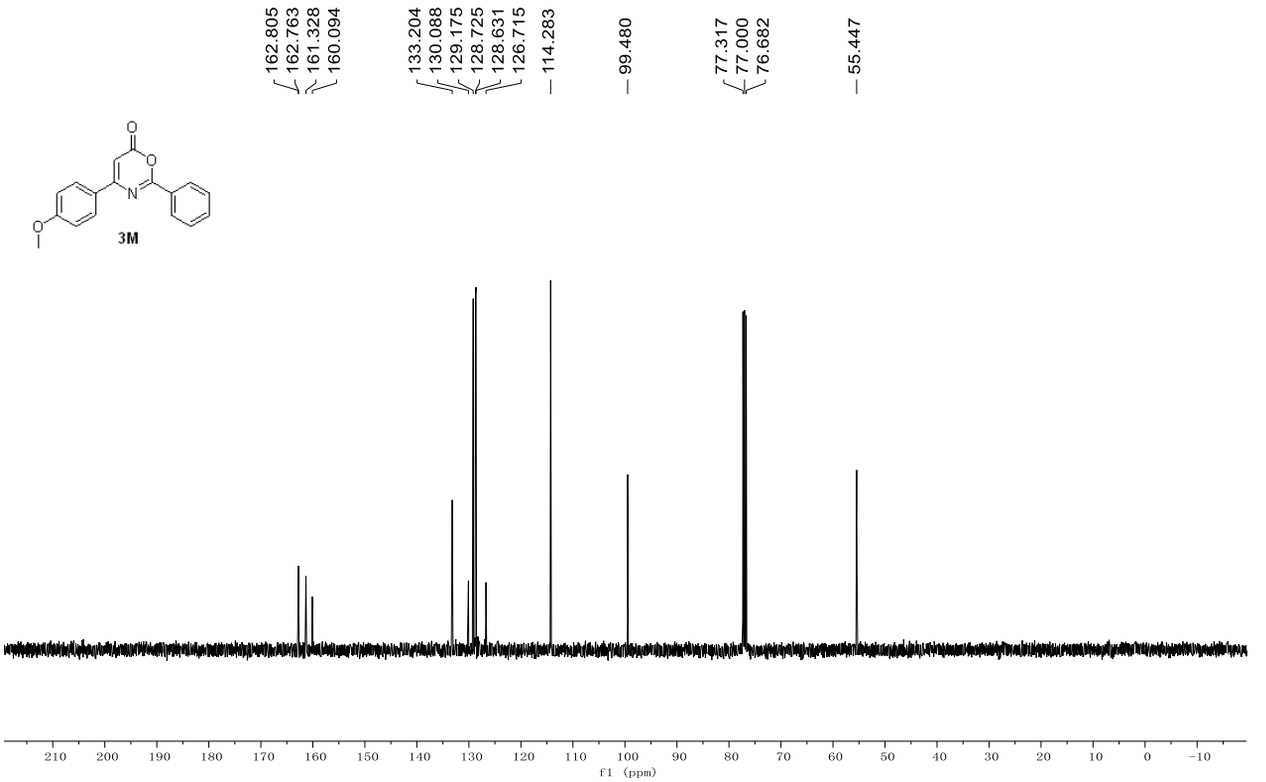
8.328
8.323
8.319
8.081
8.074
8.068
8.056
8.051
8.044
7.601
7.595
7.586
7.582
7.579
7.534
7.530
7.518
7.514
7.500
7.496
7.494
7.260
7.022
7.014
7.009
6.997
6.992
6.985
6.471
3.881
3M
2.01
2.02
1.07
2.08
2.03
1.00
3.19
f1 (ppm)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160.094
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130.088
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128.725
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114.283
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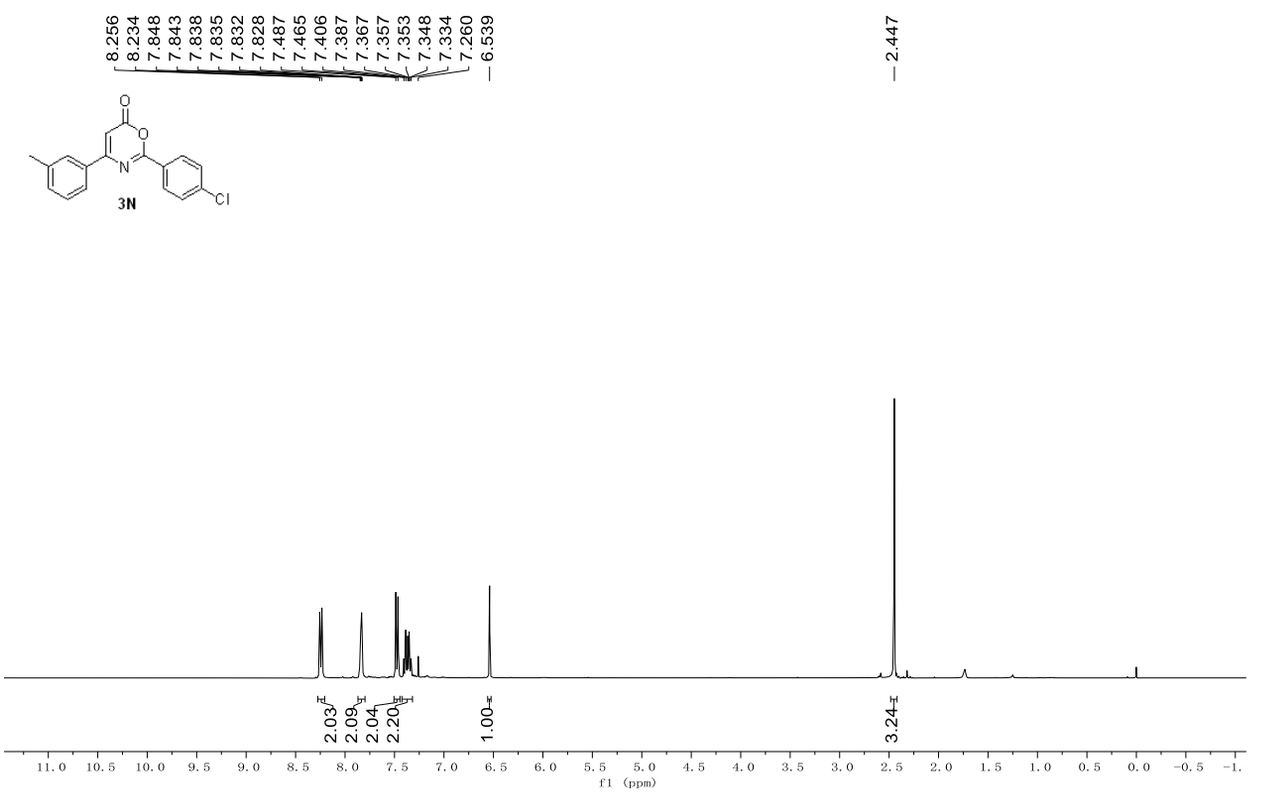
77.000
76.682
55.447
3M
f1 (ppm)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7.838
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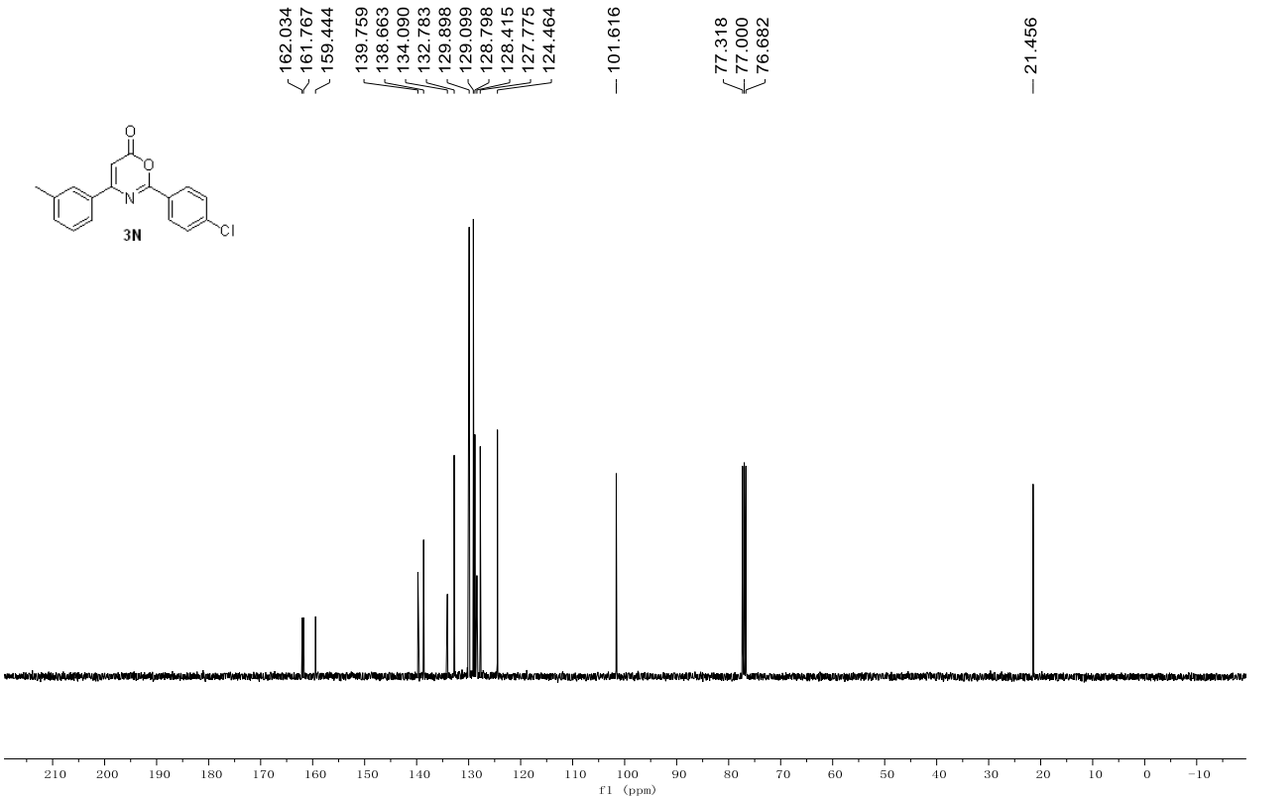
7.832
7.828
7.487
7.465
7.406
7.387
7.367
7.357
7.353
7.348
7.334
7.260
6.539
2.447
3N
2.03
2.09
2.04
2.20
1.00
3.24
f1 (ppm)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134.090
132.783
129.898
129.099
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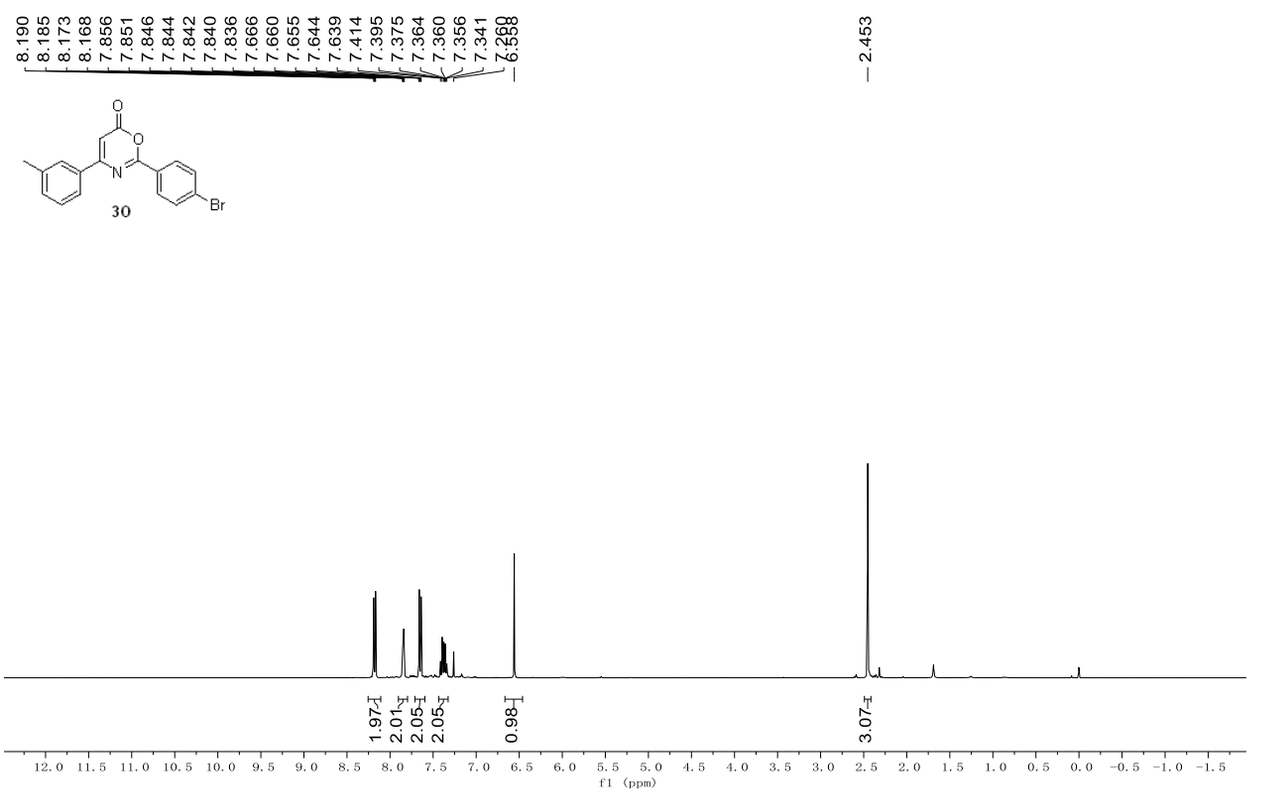
127.775
124.464
101.616
77.318
77.000
76.682
21.456
3N
Cl
f1 (ppm)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7.836
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7.655
7.644
7.639
7.414
7.395
7.375
7.364
7.360
7.356
7.341
7.260
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2.453
30
Br
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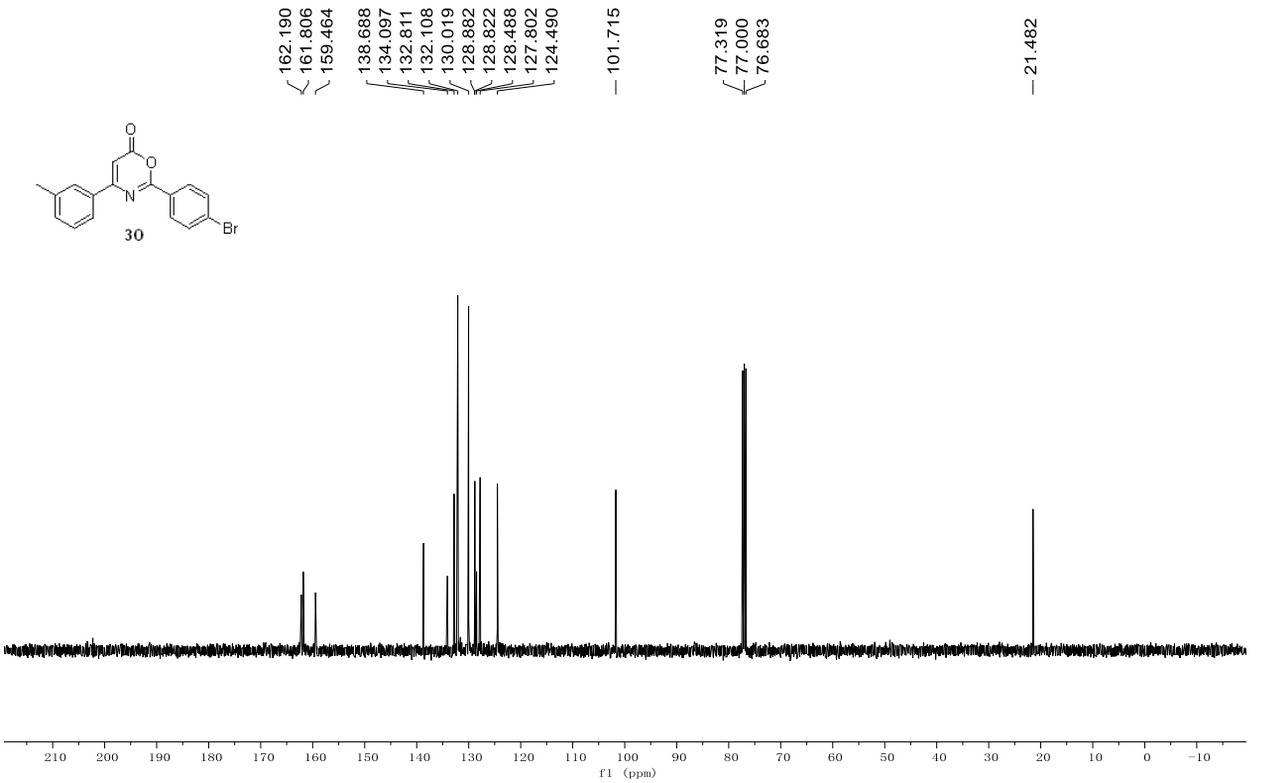
2.01
2.05
2.05
0.98
3.07
f1 (ppm)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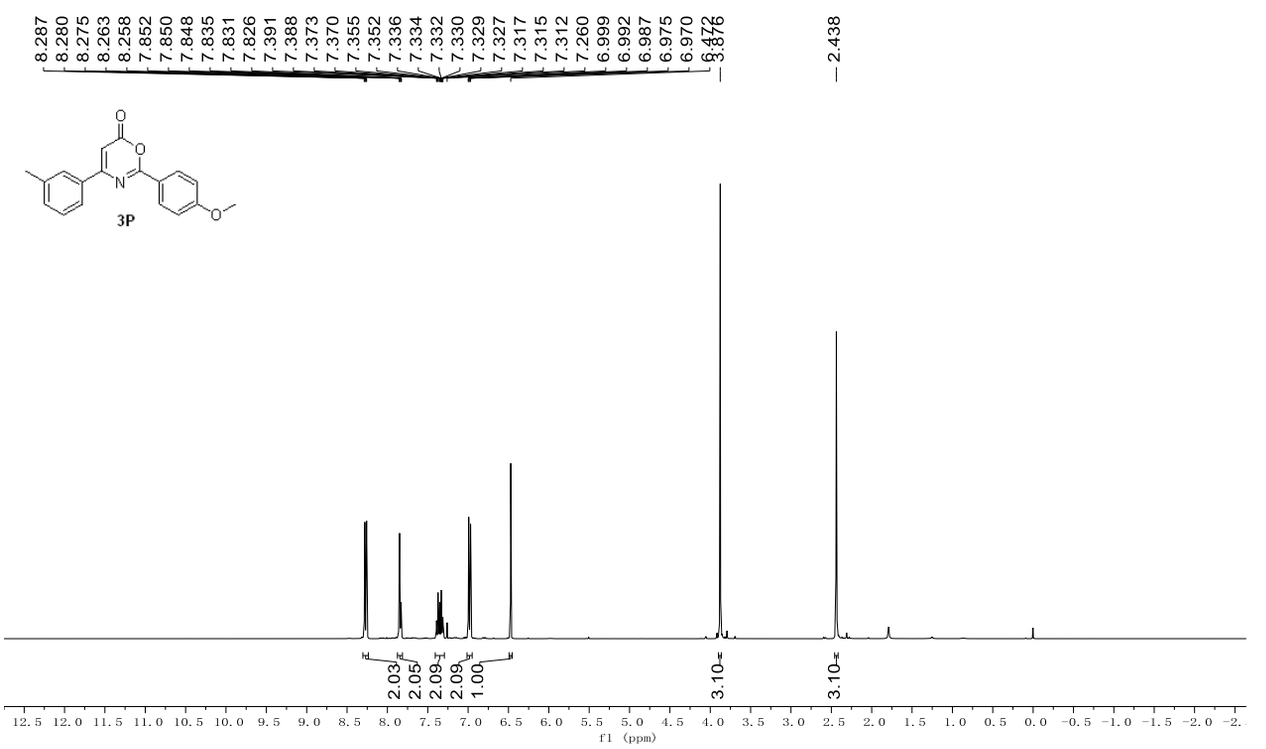
128.822
128.488
127.802
124.490
101.715
77.319
77.000
76.683
21.482
O
O
N
Br
3O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)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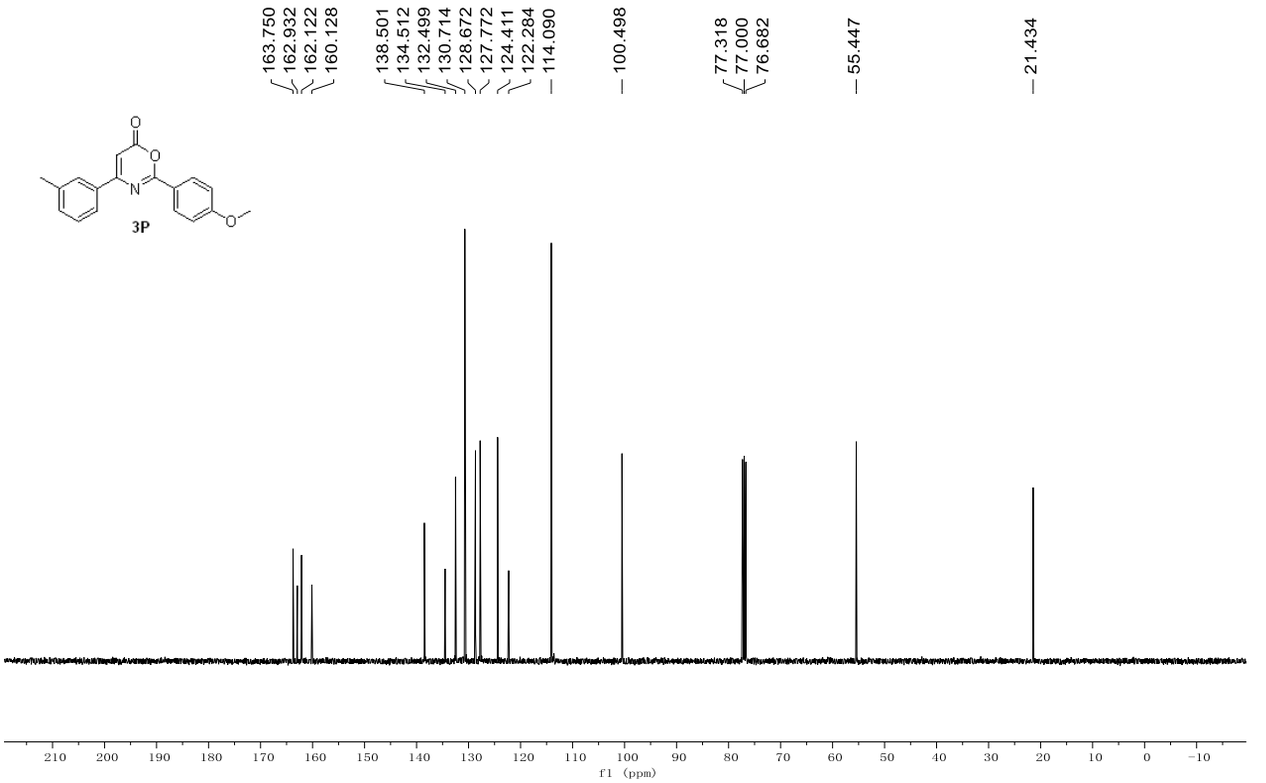
7.391
7.388
7.373
7.370
7.355
7.352
7.336
7.334
7.332
7.330
7.329
7.327
7.317
7.315
7.312
7.260
6.999
6.992
6.987
6.975
6.970
3.876
2.438
O
O
N
O
3P
2.03
2.05
2.09
2.09
1.00
3.10
3.10
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0 −2.
f1 (ppm)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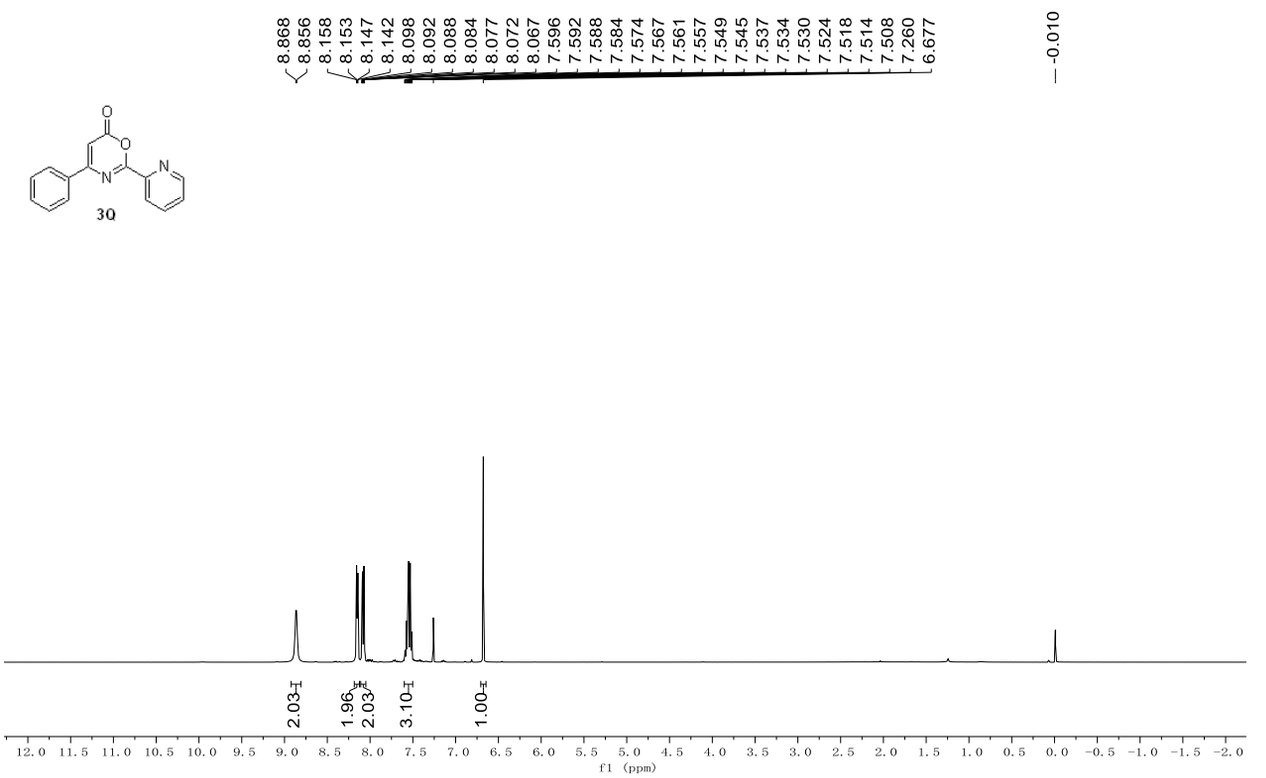
138.501
134.512
132.499
130.714
128.672
127.772
124.411
122.284
114.090
100.498
77.318
77.000
76.682
55.447
21.434
3P
f1 (ppm)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8.092
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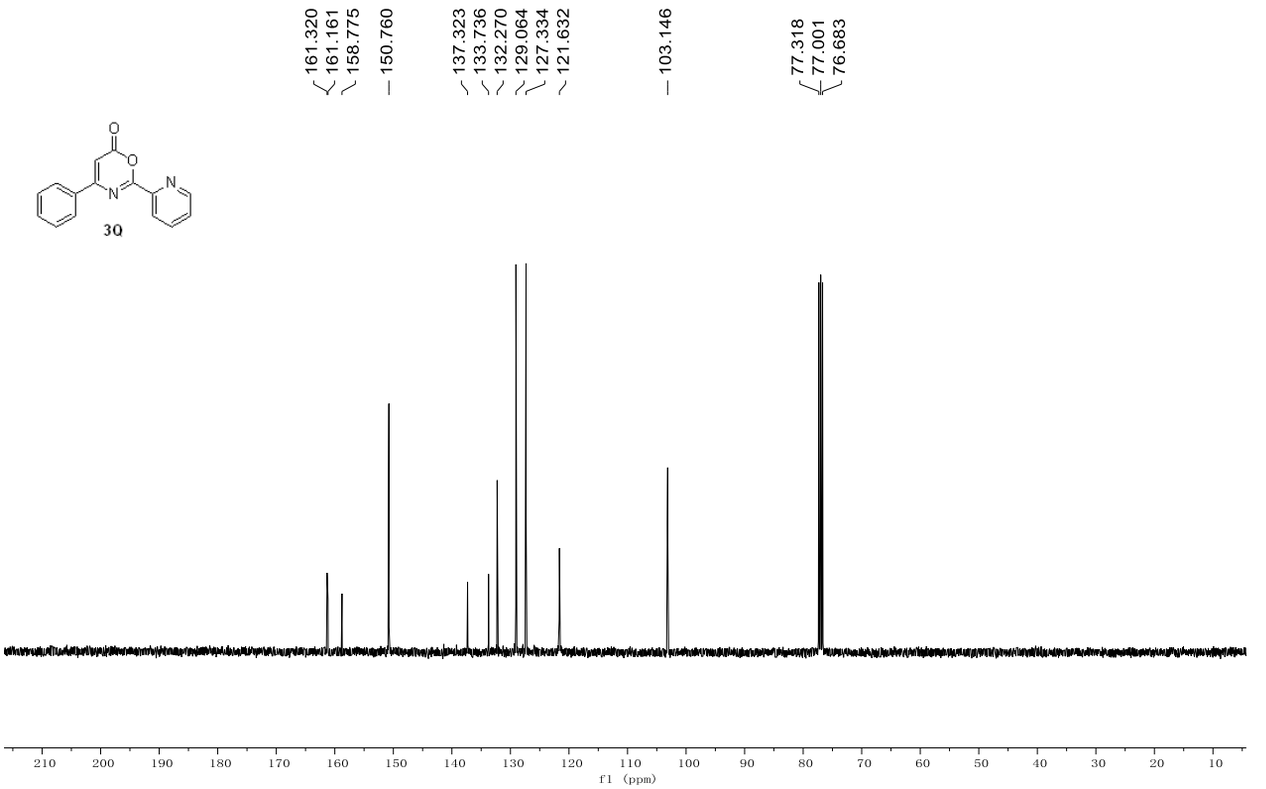
8.084
8.077
8.072
8.067
7.596
7.592
7.588
7.584
7.574
7.567
7.561
7.557
7.549
7.545
7.537
7.534
7.530
7.524
7.518
7.514
7.508
7.260
6.677
-0.010
3Q
2.03
1.96
2.03
3.10
1.00
f1 (ppm)


161.320
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150.760
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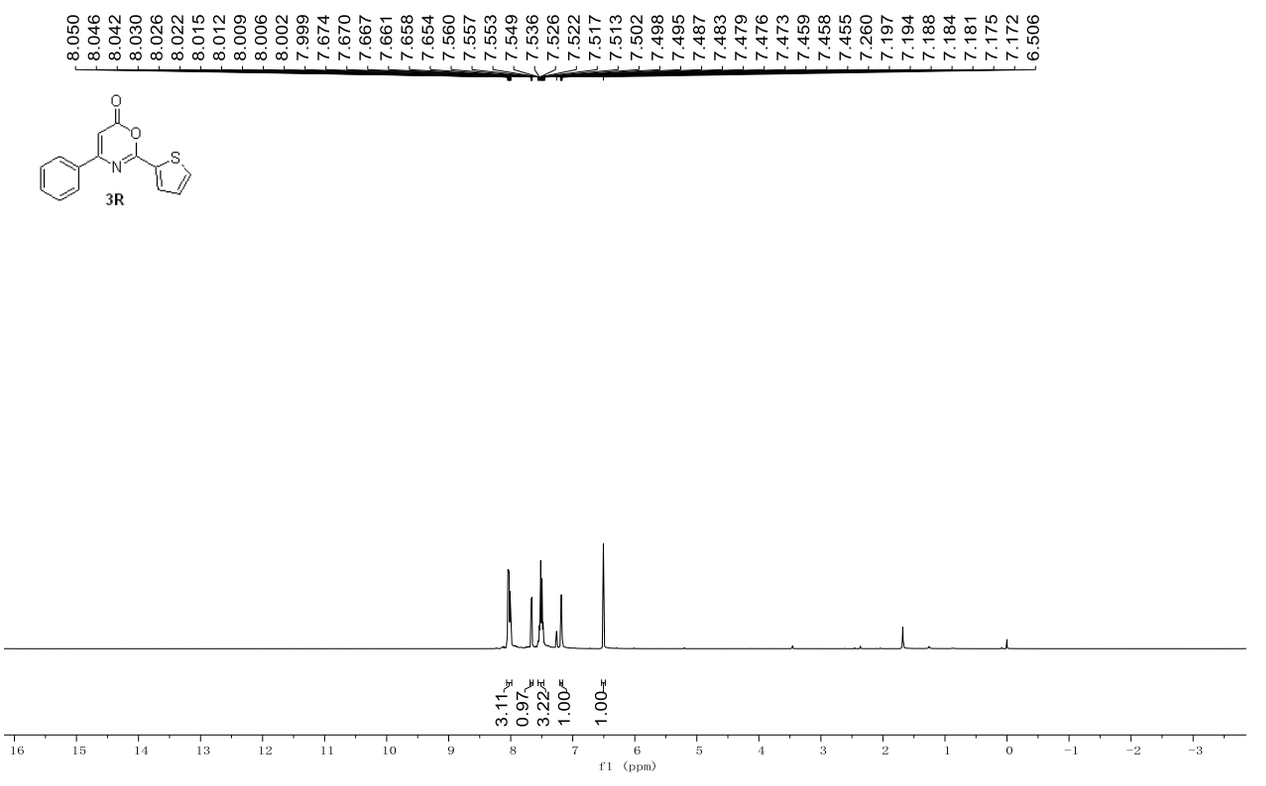
127.334
121.632
103.146
77.318
77.001
76.683
3Q
f1 (ppm)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8.026
8.022
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8.009
8.006
8.002
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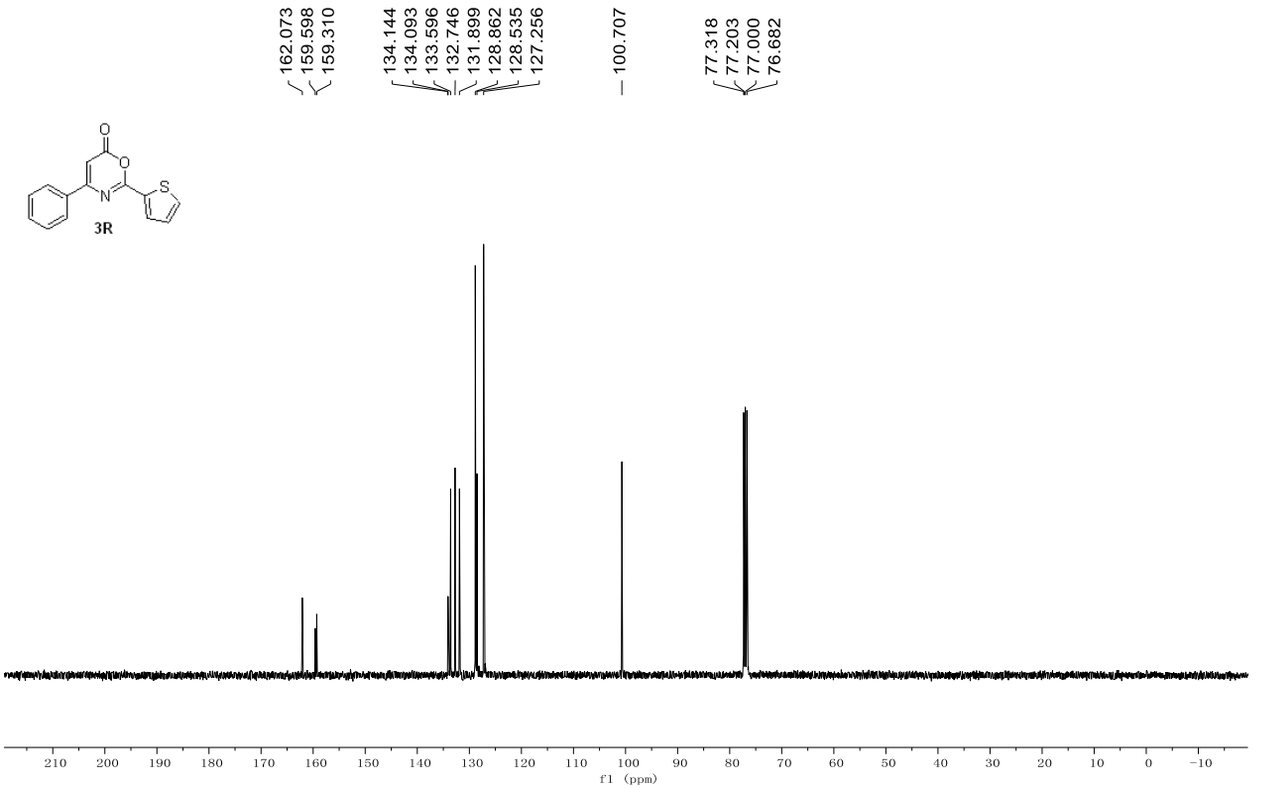
7.674
7.670
7.667
7.661
7.658
7.654
7.560
7.557
7.553
7.549
7.536
7.526
7.522
7.517
7.513
7.502
7.498
7.495
7.487
7.483
7.479
7.476
7.473
7.459
7.458
7.455
7.260
7.197
7.194
7.188
7.184
7.181
7.175
7.172
6.506
3R
3.11
0.97
3.22
1.00
1.00
f1 (ppm)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159.598
159.310
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134.093
133.596
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131.899
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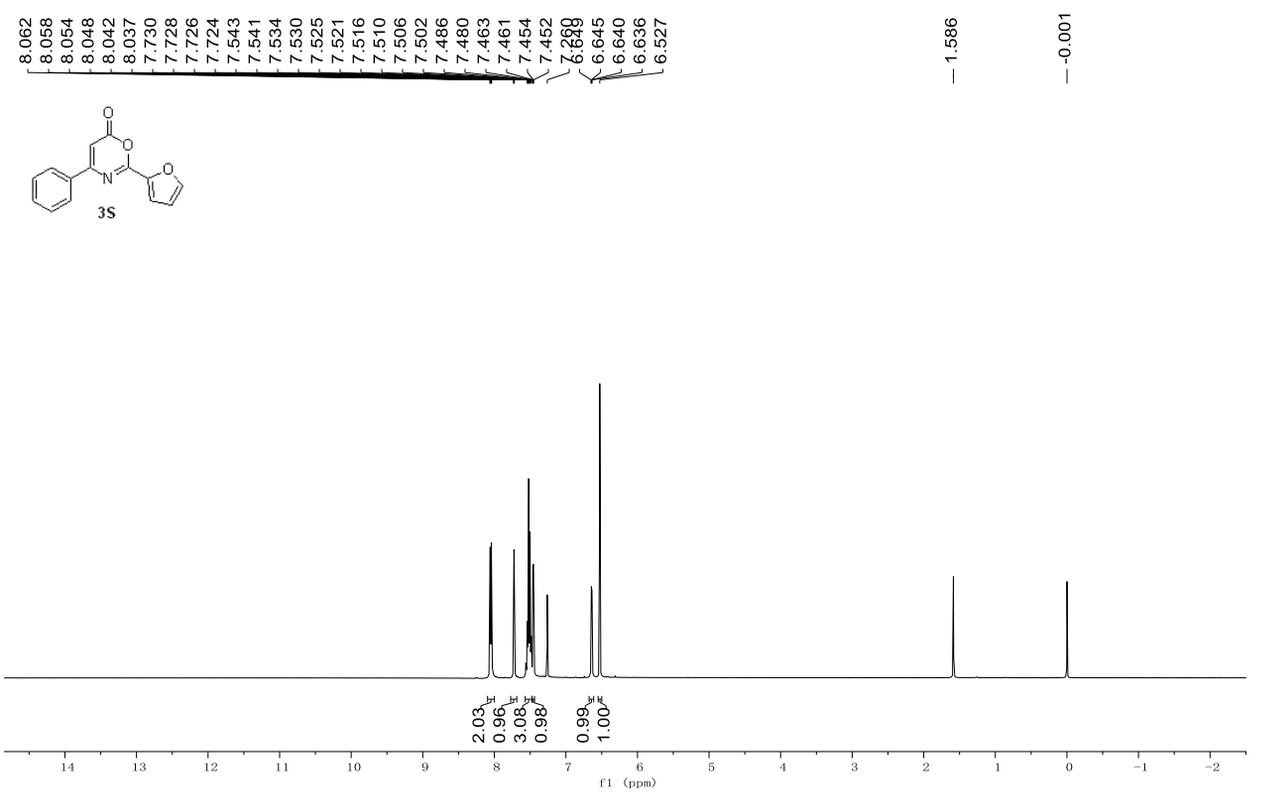
128.535
127.256
100.707
77.318
77.203
77.000
76.682
3R
f1 (ppm)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7.543
7.541
7.534
7.530
7.525
7.521
7.516
7.510
7.506
7.502
7.486
7.480
7.463
7.461
7.454
7.452
6.645
6.640
6.636
6.527
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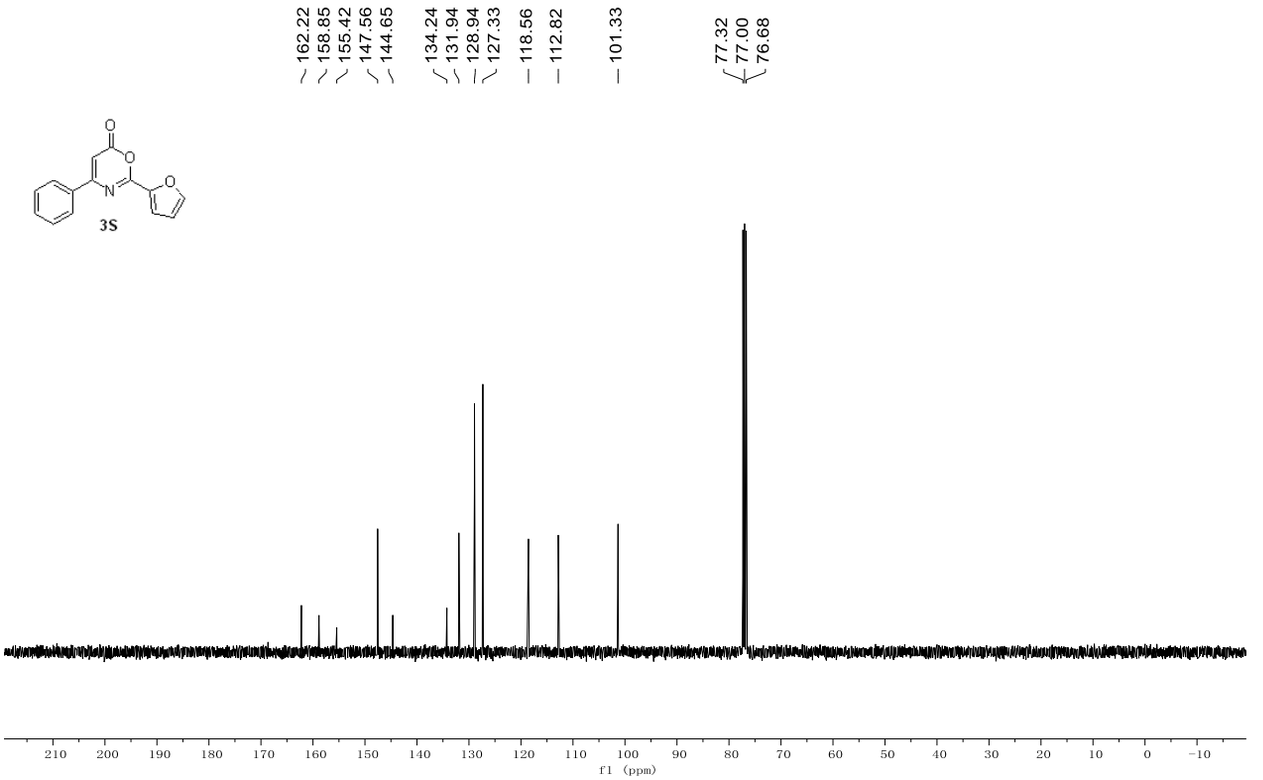
3S
2.03
0.96
3.08
0.98
0.99
1.00
f1 (ppm)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155.42
147.56
144.65
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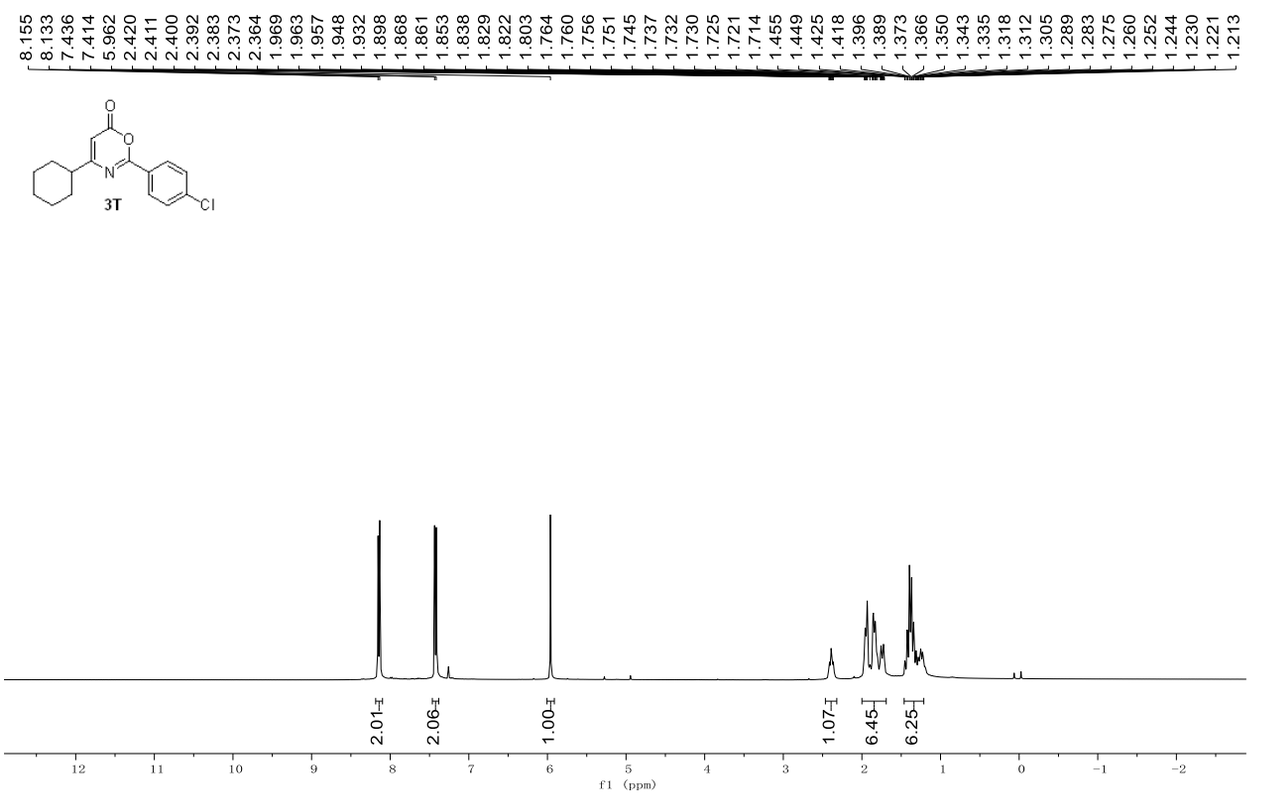
131.94
128.94
127.33
118.56
112.82
101.33
77.32
77.00
76.68
3S
f1 (ppm)


8.155
8.133
7.436
7.414
5.962
2.420
2.411
2.400
2.392
2.383
2.373
2.364
1.969
1.963
1.957
1.948
1.932
1.898
1.868
1.861
1.853
1.838
1.829
1.822
1.803
1.764
1.760
1.756
1.751
1.745
1.737
1.732
1.730
1.725
1.721
1.714
1.455
1.449
1.425
1.418
1.396
1.389
1.373
1.366
1.350
1.343
1.335
1.318
1.312
1.305
1.289
1.283
1.275
1.260
1.252
1.244
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3T
Cl
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1.00
1.07
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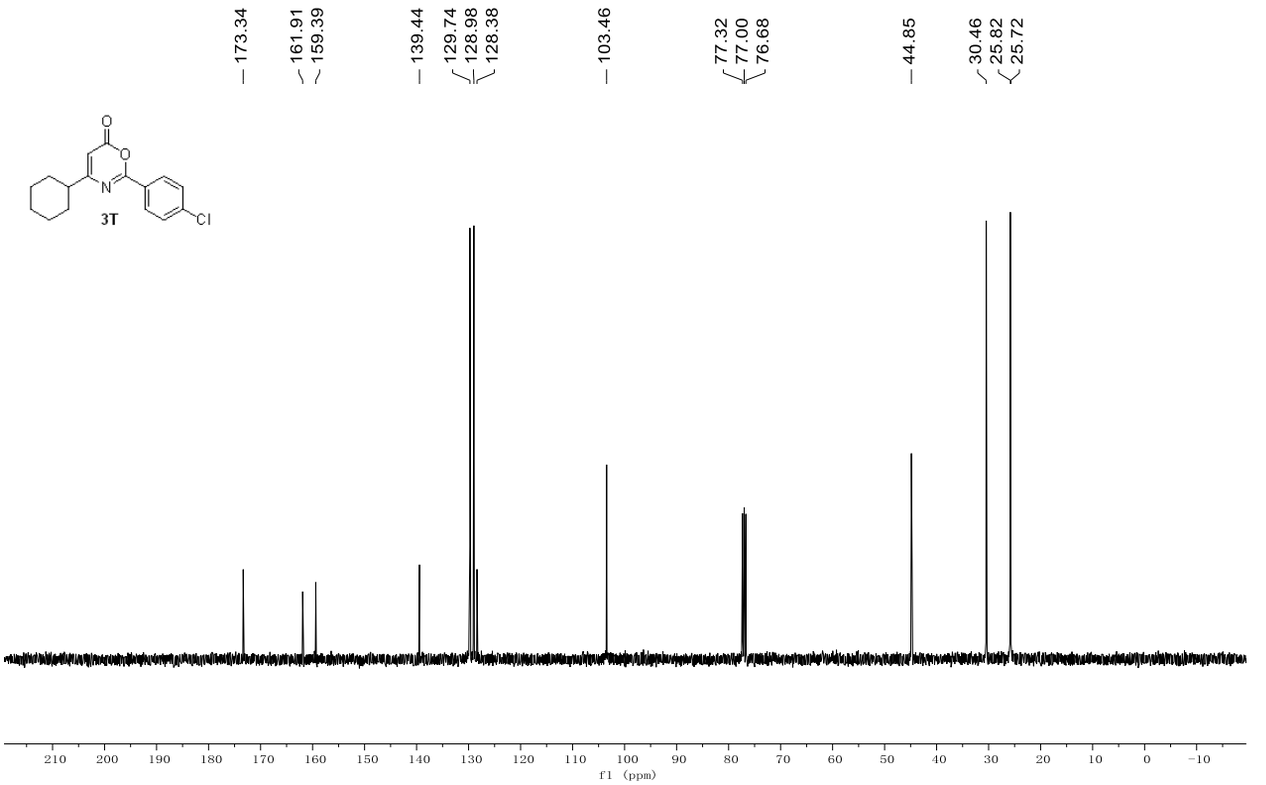
6.25
f1 (ppm)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128.98
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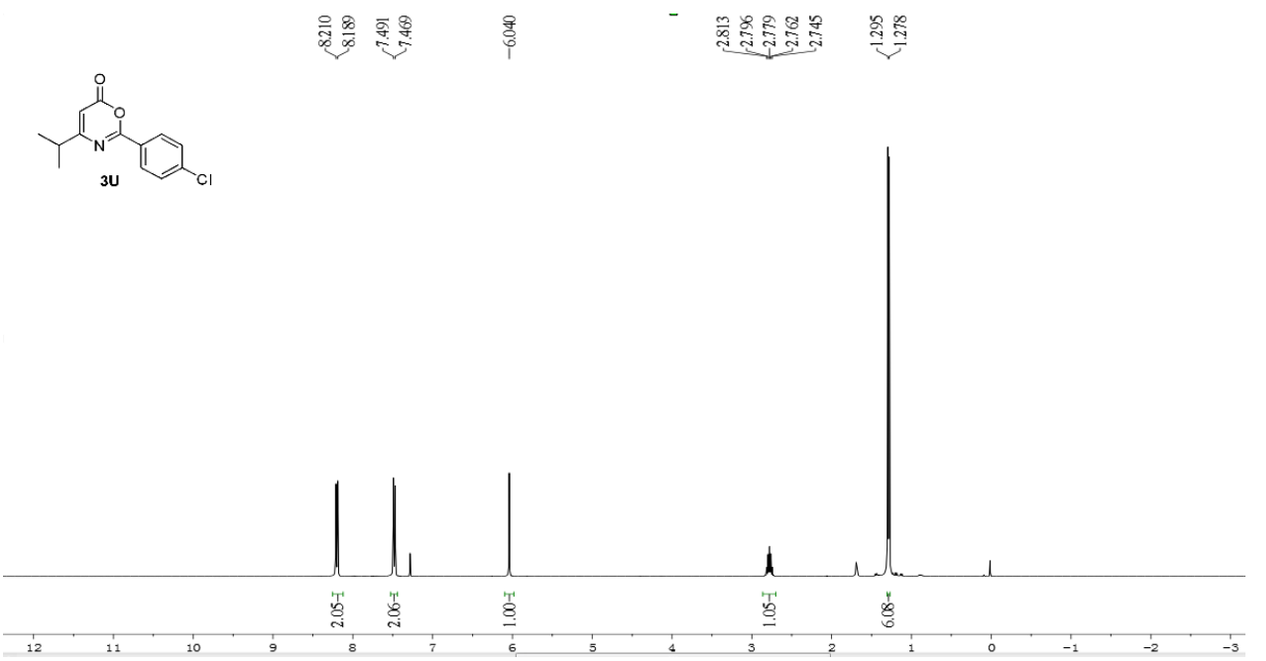
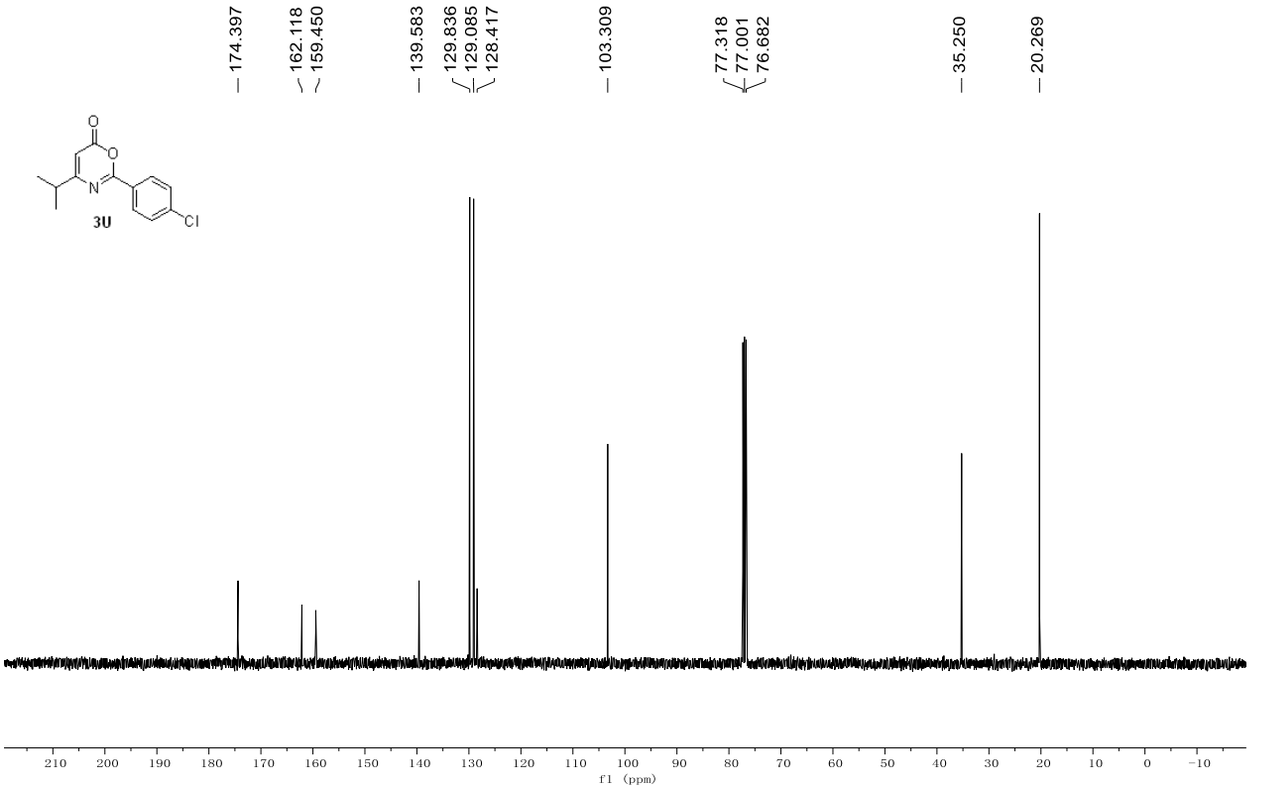
103.46
77.32
77.00
76.68
44.85
30.46
25.82
25.72
3T
Cl
f1 (ppm)


8.210
8.189
7.491
7.469
6.040
2.813
2.796
2.779
2.762
2.745
1.295
1.278
3U
Cl
2.05
2.06
1.00
1.05
6.08


174.397
162.118
159.450
139.583
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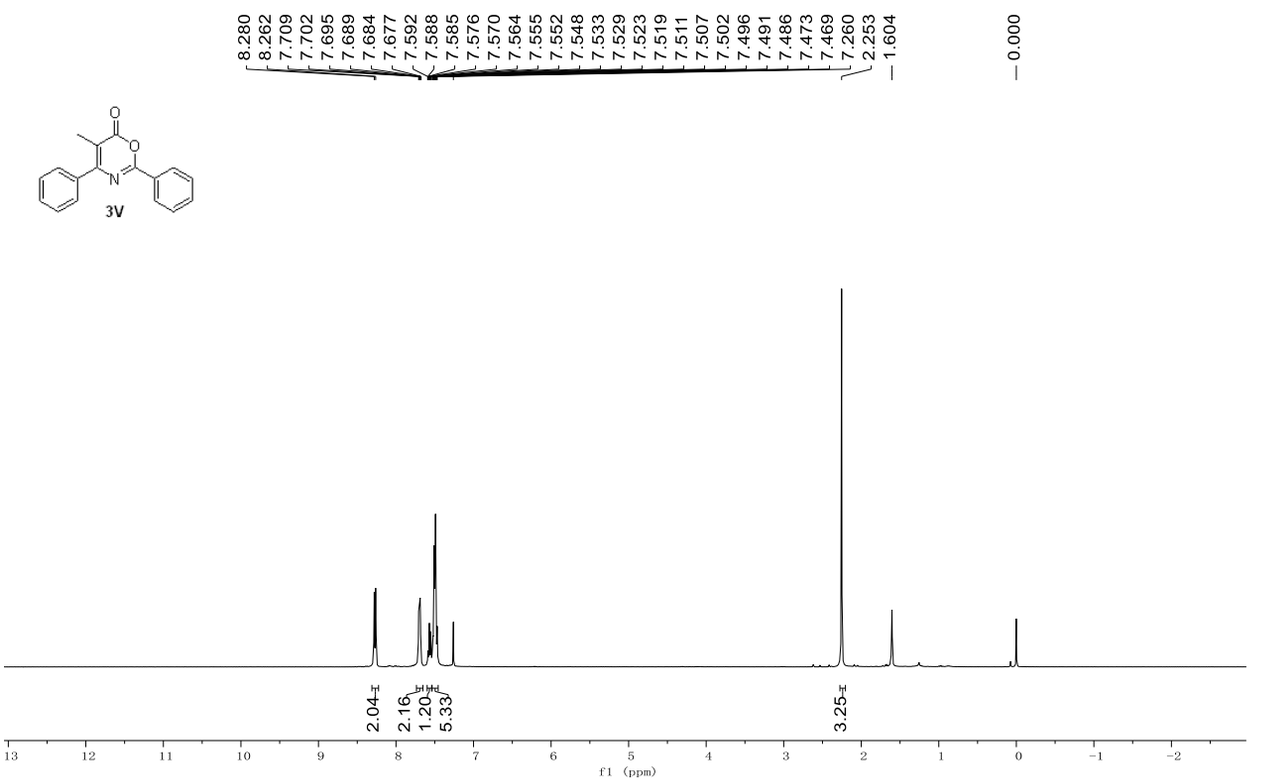
128.417
103.309
77.318
77.001
76.682
35.250
20.269
3U
Cl
f1 (ppm)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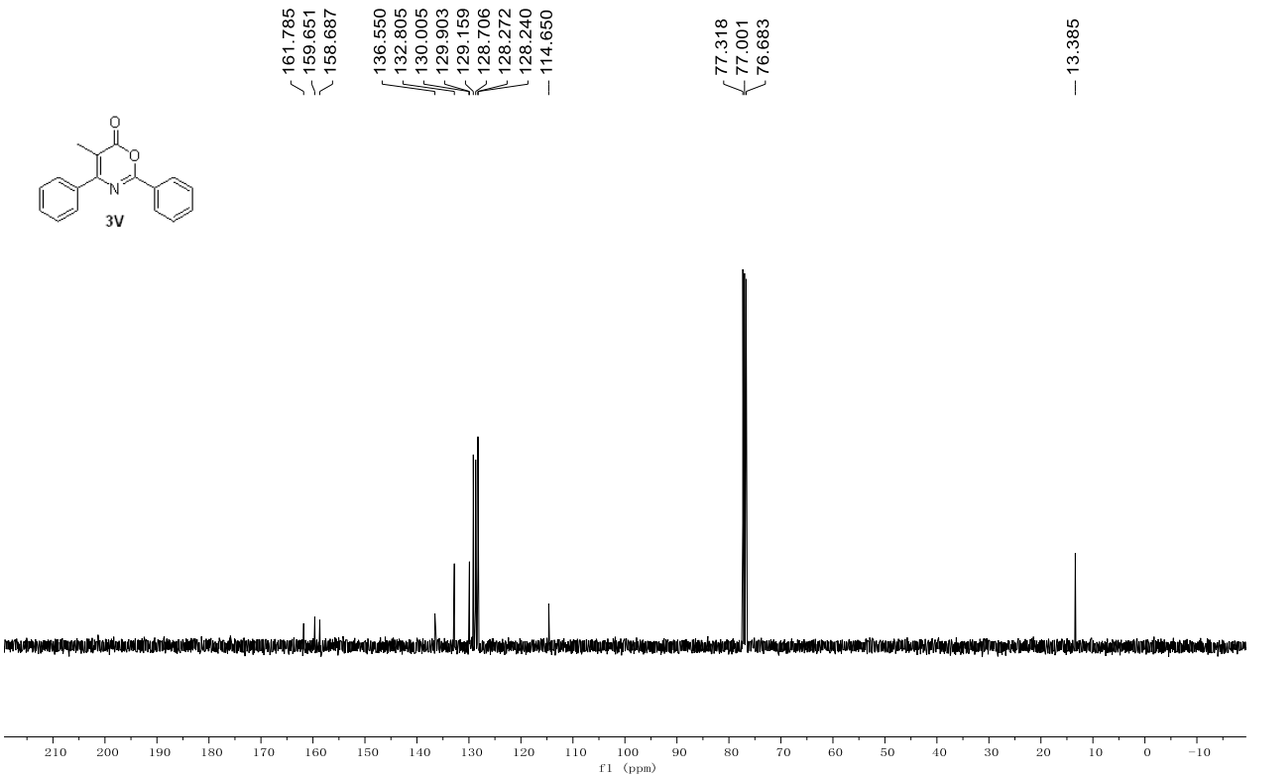
8.262
7.709
7.702
7.695
7.689
7.684
7.677
7.592
7.588
7.585
7.576
7.570
7.564
7.555
7.552
7.548
7.533
7.529
7.523
7.519
7.511
7.507
7.502
7.496
7.491
7.486
7.473
7.469
7.260
2.253
1.604
0.000
3V
2.04
2.16
1.20
5.33
3.25
f1 (ppm)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158.687
136.550
132.805
130.005
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129.159
128.706
128.272
128.240
114.650
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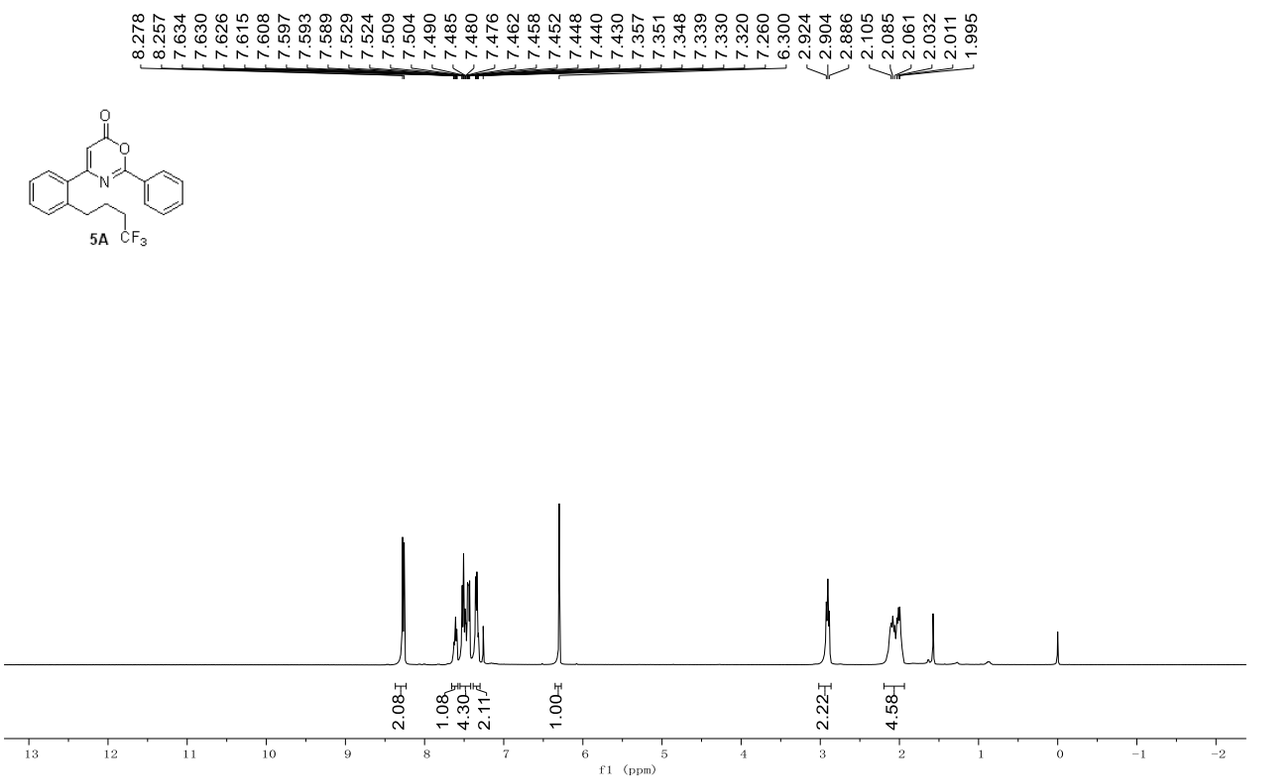
77.001
76.683
13.385
3V
f1 (ppm)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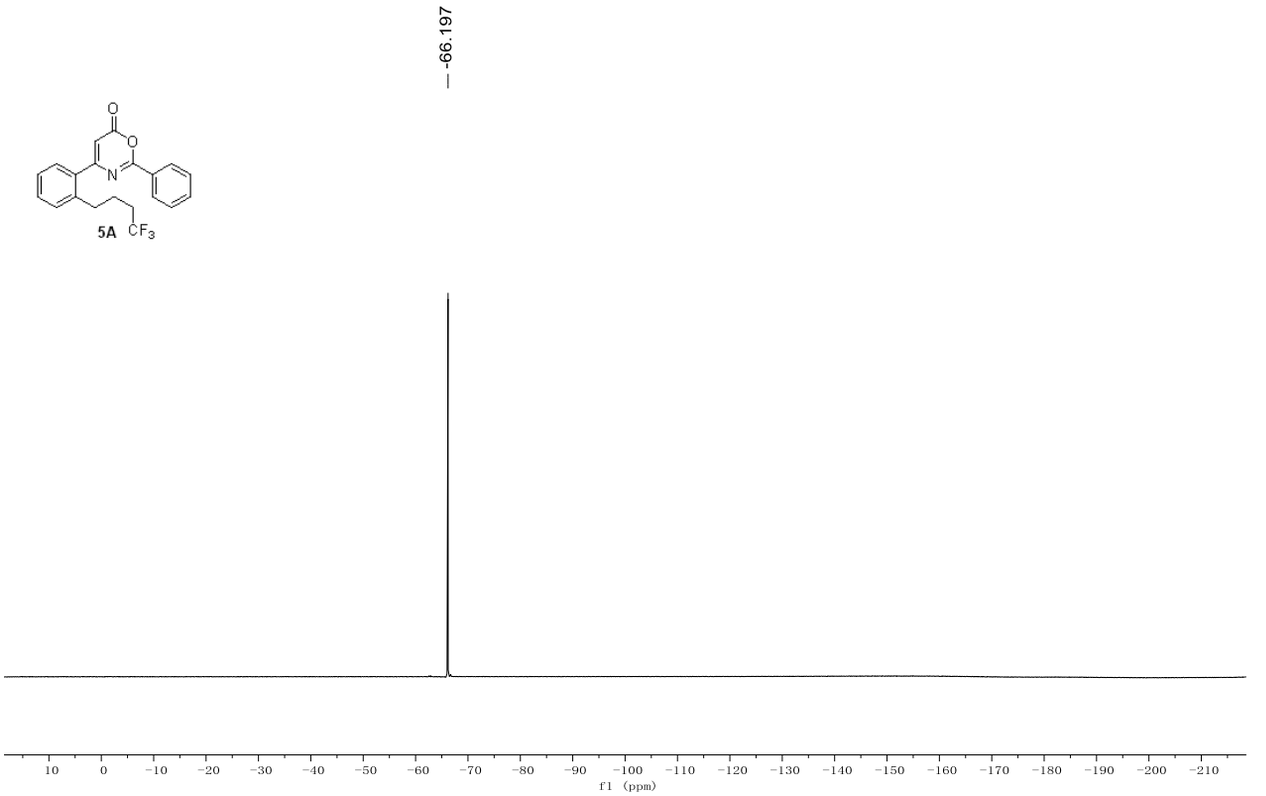
8.257
7.634
7.630
7.626
7.615
7.608
7.597
7.593
7.589
7.529
7.524
7.509
7.504
7.490
7.485
7.480
7.476
7.462
7.458
7.452
7.448
7.440
7.430
7.357
7.351
7.348
7.339
7.330
7.320
7.260
6.300
2.924
2.904
2.886
2.105
2.085
2.061
2.032
2.011
1.995
5A
CF3
2.08
1.08
4.30
2.11
1.00
2.22
4.58
f1 (ppm)


-66.197
5A
CF3
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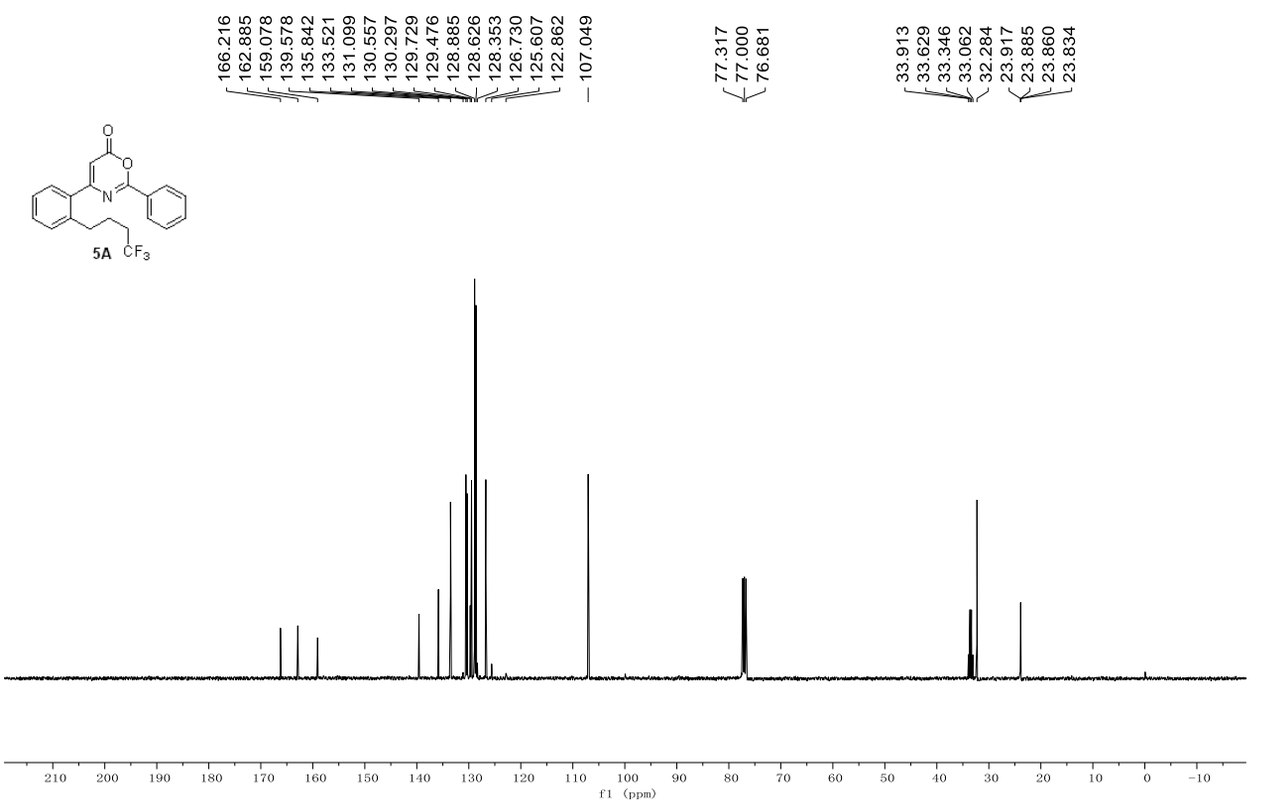
f1 (ppm)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135.842
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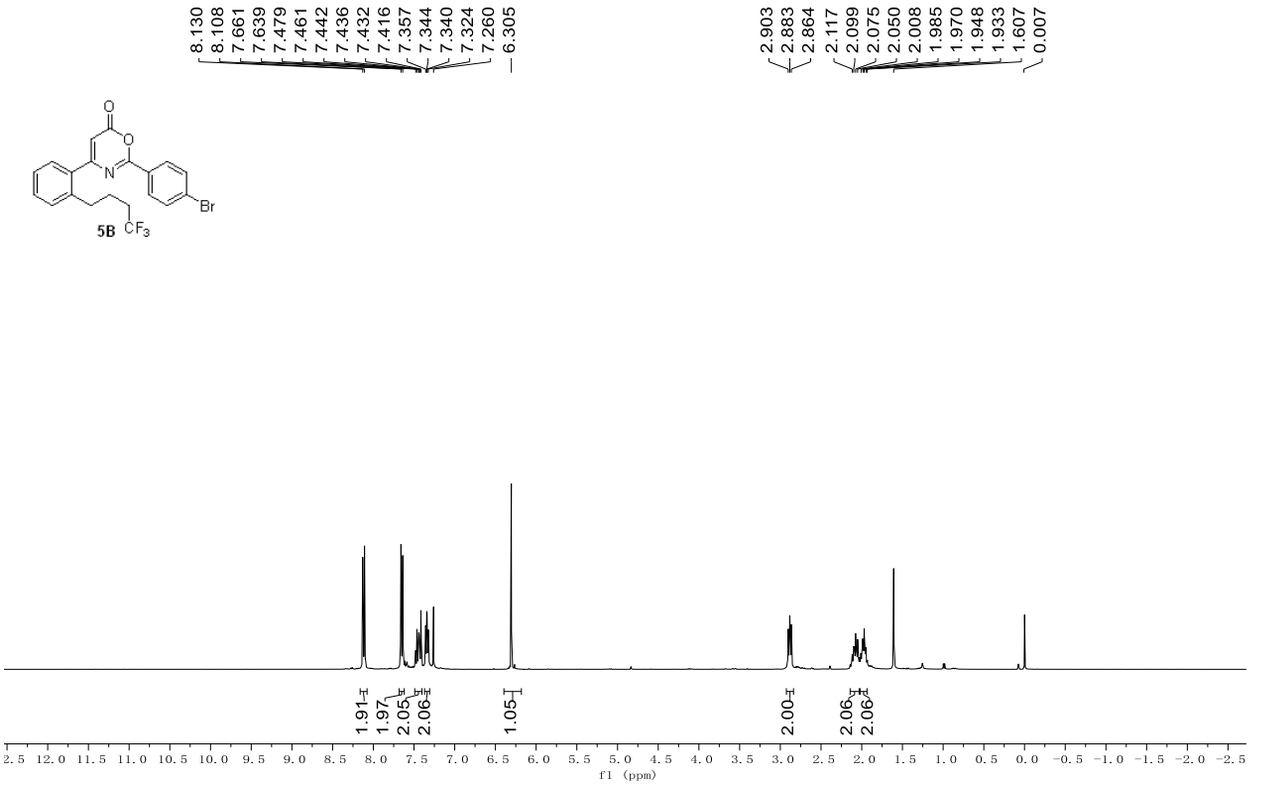
129.476
128.885
128.626
128.353
126.730
125.607
122.862
107.049
77.317
77.000
76.681
33.913
33.629
33.346
33.062
32.284
23.917
23.885
23.860
23.834
5A
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.639
7.479
7.461
7.442
7.436
7.432
7.416
7.357
7.344
7.340
7.324
7.260
6.305
2.903
2.883
2.864
2.117
2.099
2.075
2.050
2.008
1.985
1.970
1.948
1.933
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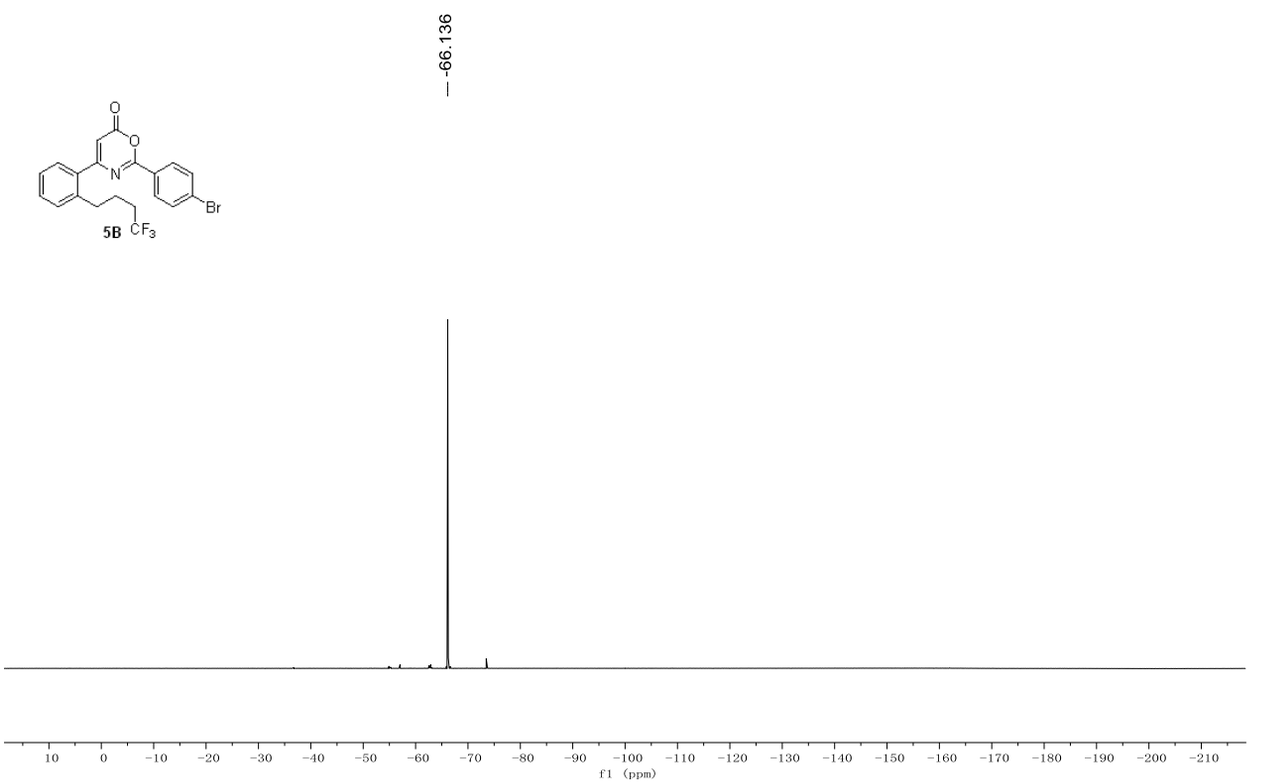
5B
1.91
1.97
2.05
2.06
1.05
2.00
2.06
2.06
f1 (ppm)


-66.136
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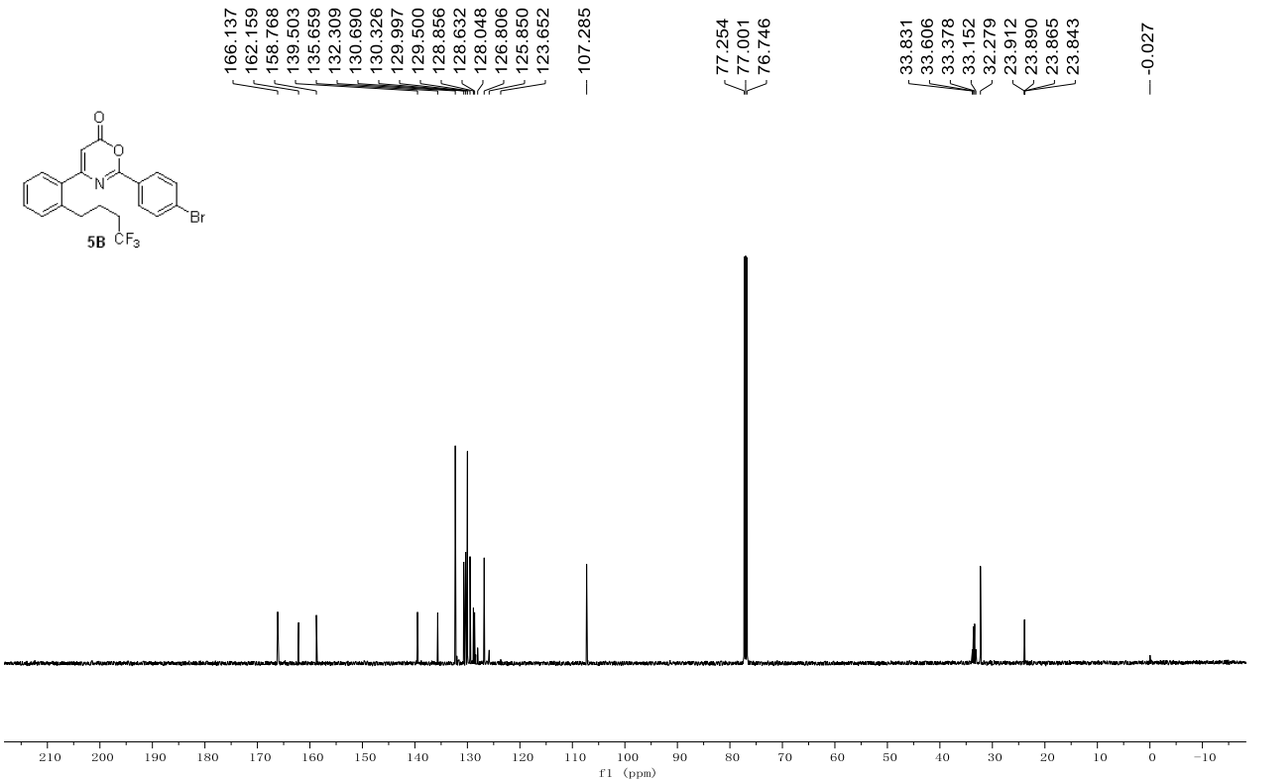
f1 (ppm)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132.309
130.690
130.326
129.997
129.500
128.856
128.632
128.048
126.806
125.850
123.652
107.285
77.254
77.001
76.746
33.831
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33.152
32.279
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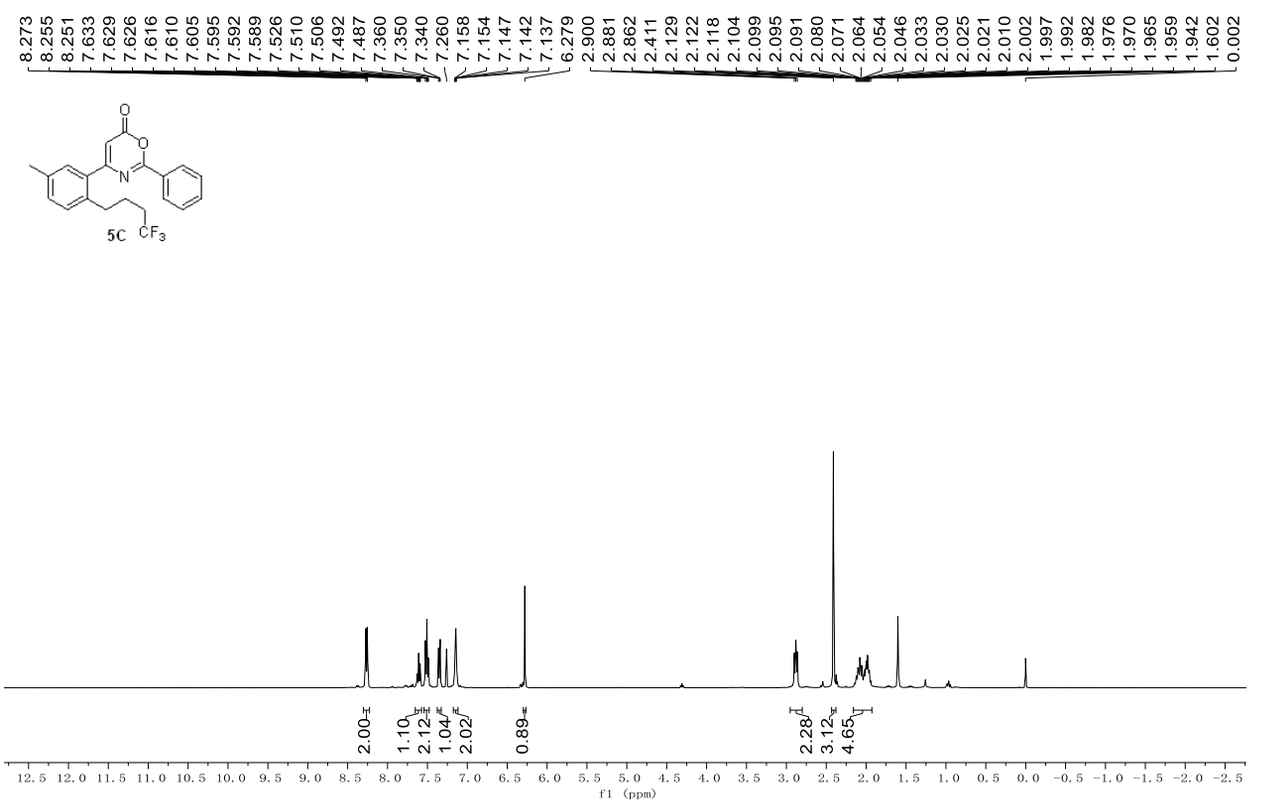
23.890
23.865
23.843
-0.027
5B
f1 (ppm)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8.255
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7.610
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7.595
7.592
7.589
7.526
7.510
7.506
7.492
7.487
7.360
7.350
7.340
7.260
7.158
7.154
7.147
7.142
7.137
6.279
2.900
2.881
2.862
2.411
2.129
2.122
2.118
2.104
2.099
2.095
2.091
2.080
2.071
2.064
2.054
2.046
2.033
2.030
2.025
2.021
2.010
2.002
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1.992
1.982
1.976
1.970
1.965
1.959
1.942
1.602
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1.04
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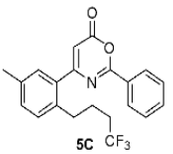
2.28
3.12
4.65
f1 (ppm)


5C
CF3

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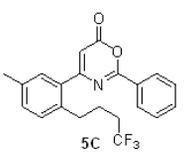
5C
CF3

166.300
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140.951
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131.173
129.837
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128.900
128.636
128.385
127.513
125.637
122.871
106.610
77.318
77.001
76.683
34.013
33.729
33.445
33.162
32.356
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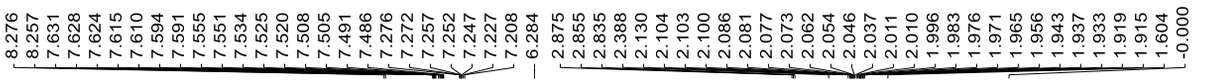
23.953
21.319
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.534
7.525
7.520
7.508
7.505
7.491
7.486
7.276
7.272
7.257
7.252
7.247
7.227
7.208
6.284
2.875
2.855
2.835
2.388
2.130
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2.103
2.100
2.086
2.081
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2.046
2.037
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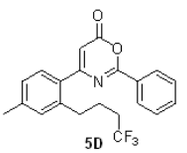
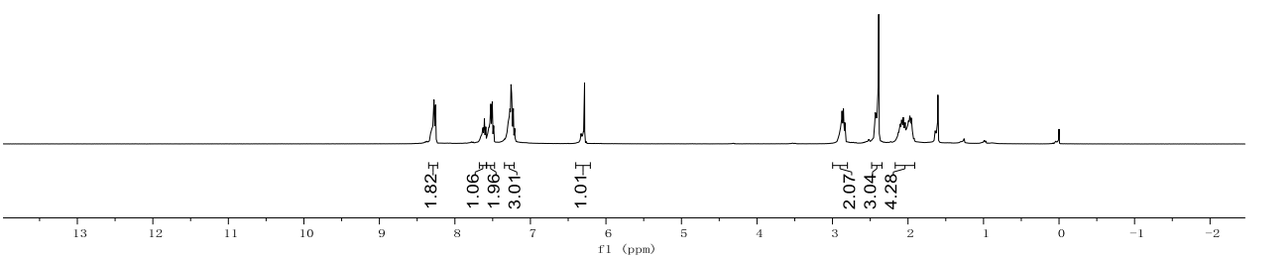
-0.000


O
O
N
CF3

5D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1.96
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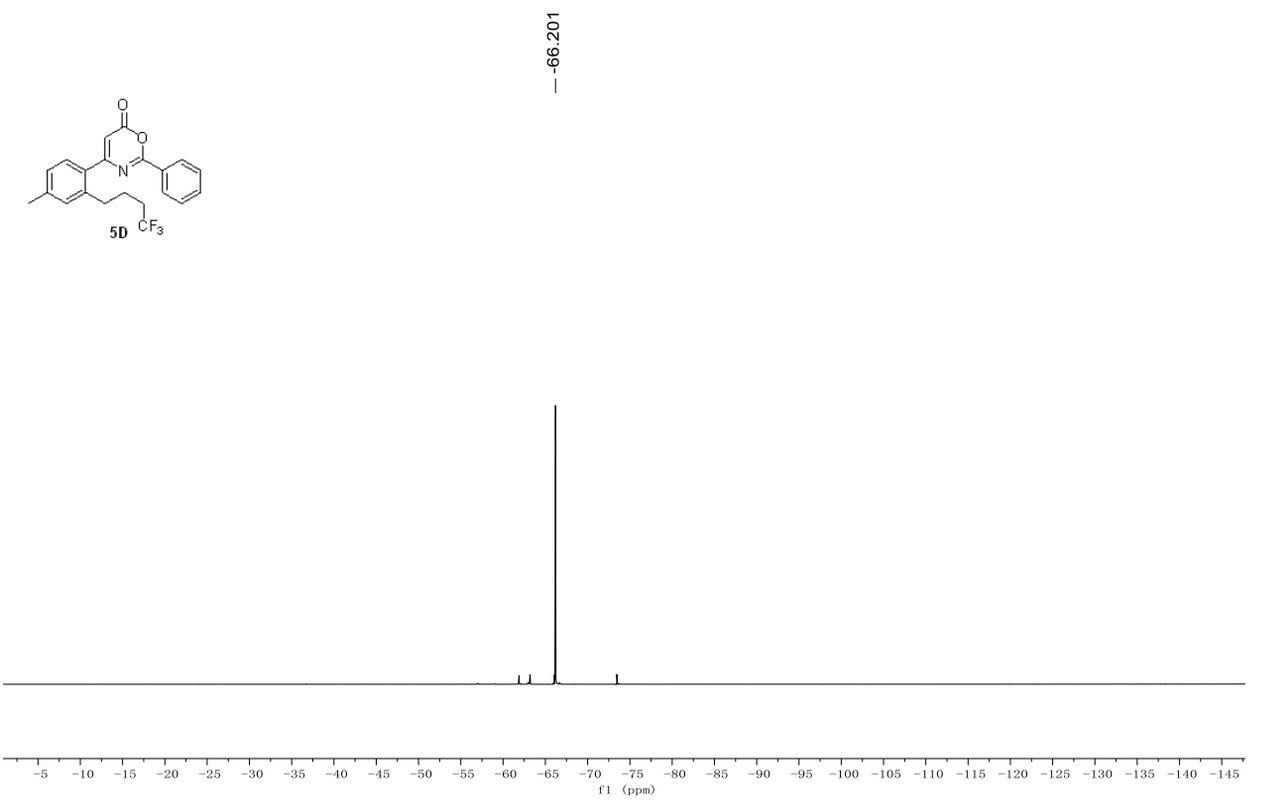
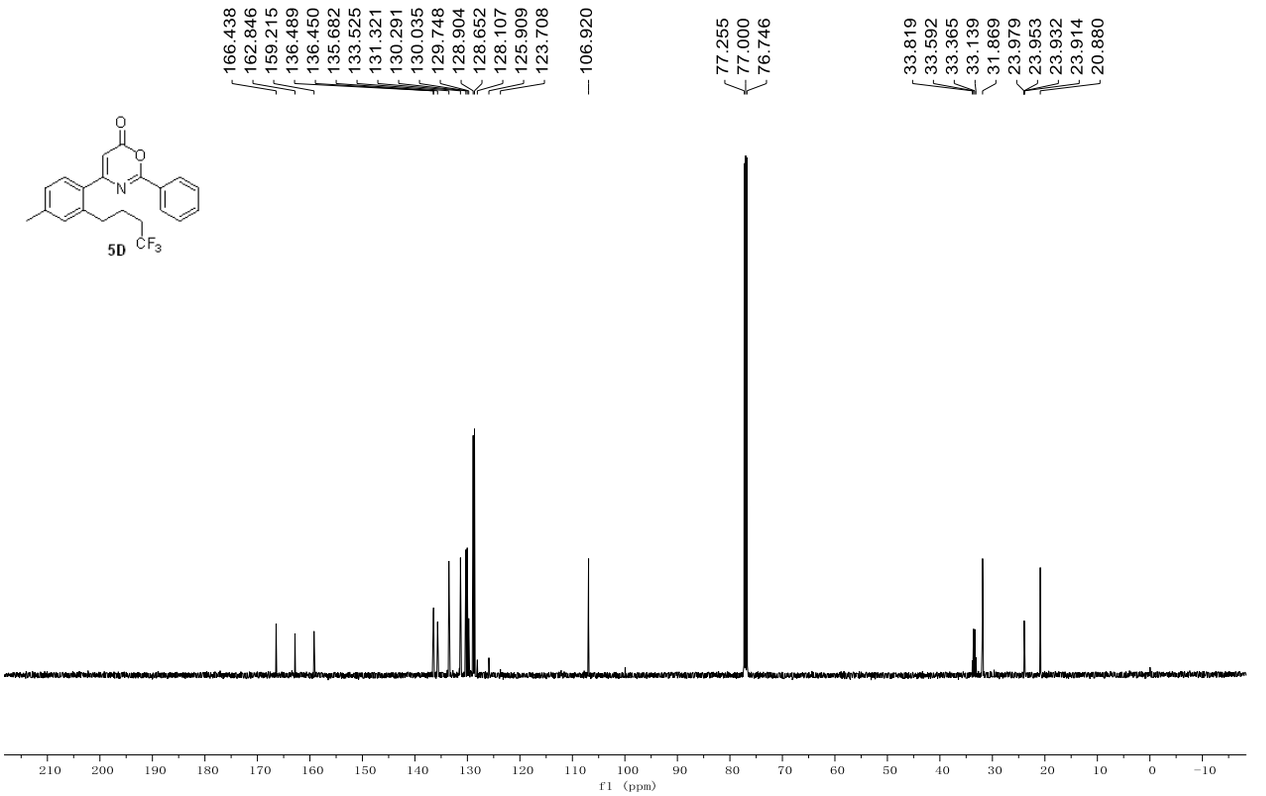
1.01
2.07
3.04
4.28
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
f1 (ppm)


-66.201
−5
−10
−15
−20
−25
−30
−35
−40
−45
−50
−55
−60
−65
−70
−75
−80
−85
−90
−95
−100
−105
−110
−115
−120
−125
−130
−135
−140
−145
f1 (ppm)

O
O
N
CF3

5D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130.035
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128.904
128.652
128.107
125.909
123.708
106.920
77.255
77.000
76.746
33.819
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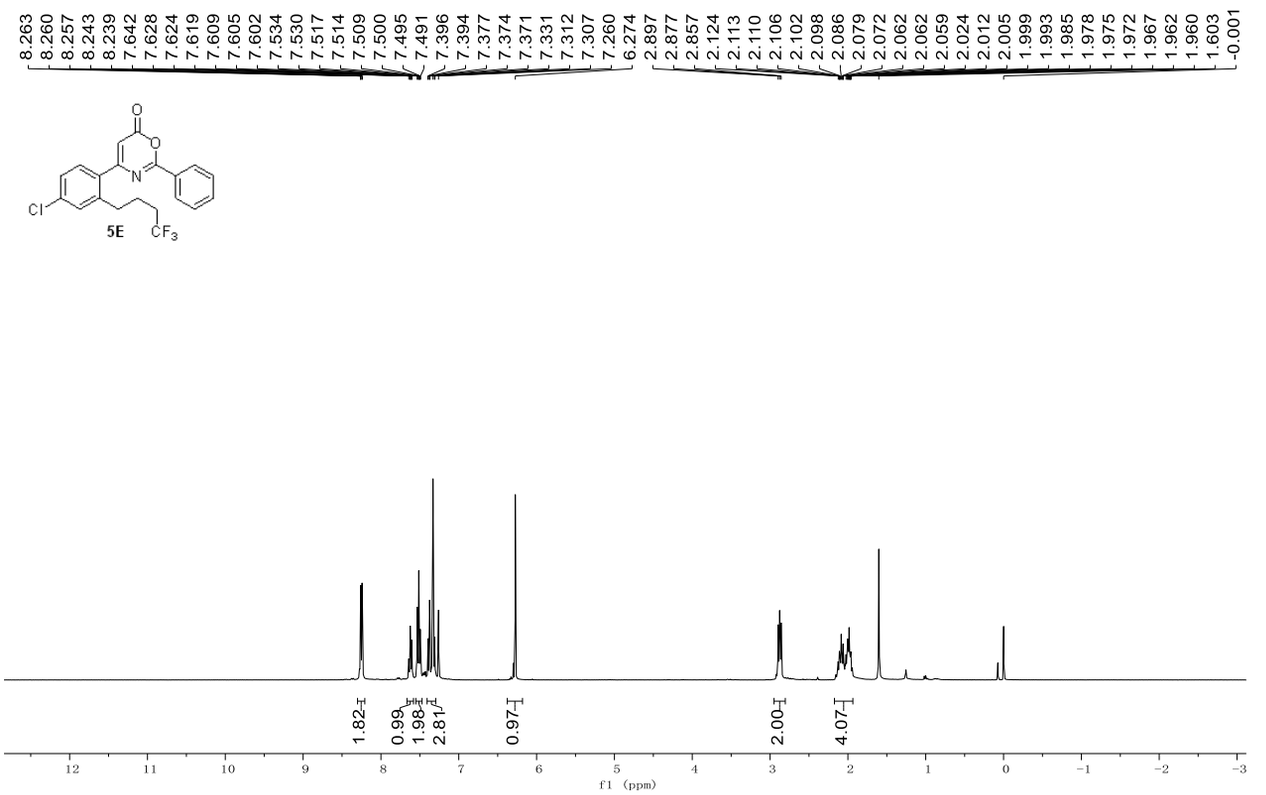
5D
f1 (ppm)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7.624
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7.609
7.605
7.602
7.534
7.530
7.517
7.514
7.509
7.500
7.495
7.491
7.396
7.394
7.377
7.374
7.371
7.331
7.312
7.307
7.260
6.274
2.897
2.877
2.857
2.124
2.113
2.110
2.106
2.102
2.098
2.086
2.079
2.072
2.062
2.062
2.059
2.024
2.012
2.005
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1.978
1.975
1.972
1.967
1.962
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5E
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0.99
1.98
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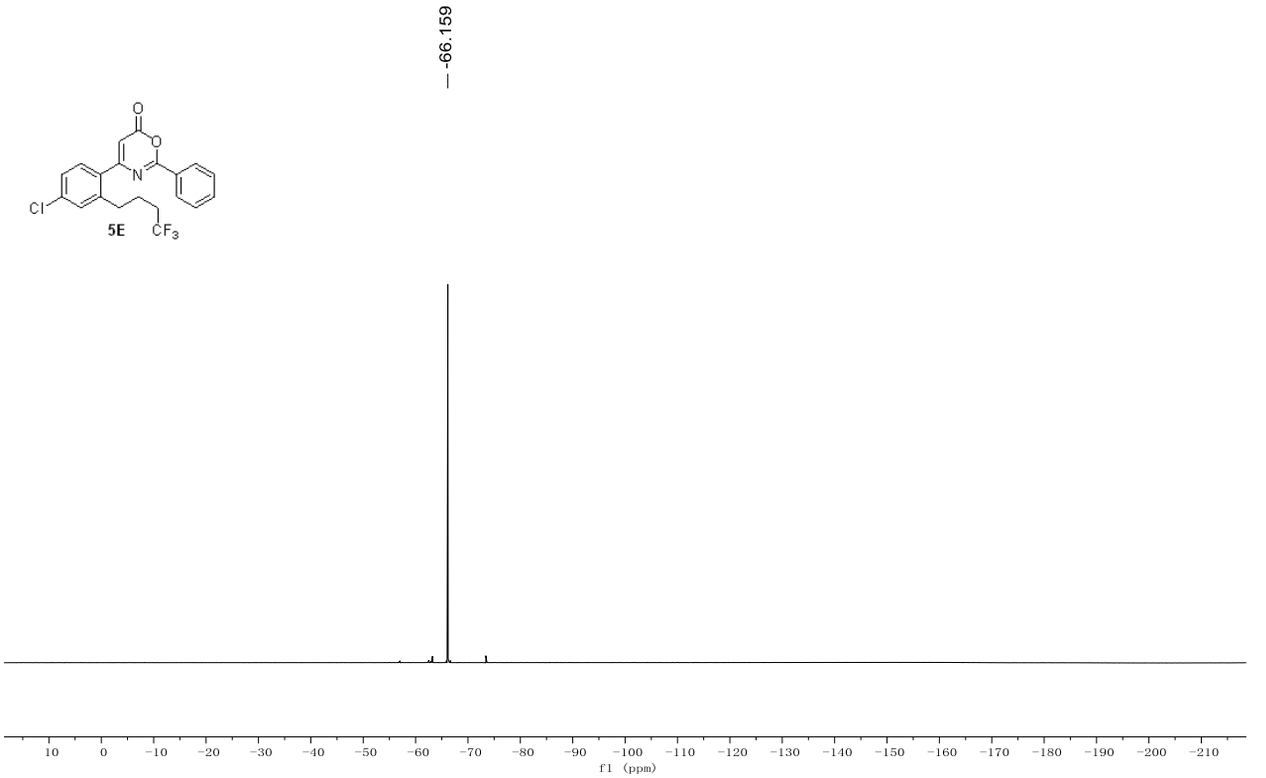
0.97
2.00
4.07
f1 (ppm)


-66.159
5E
CF3
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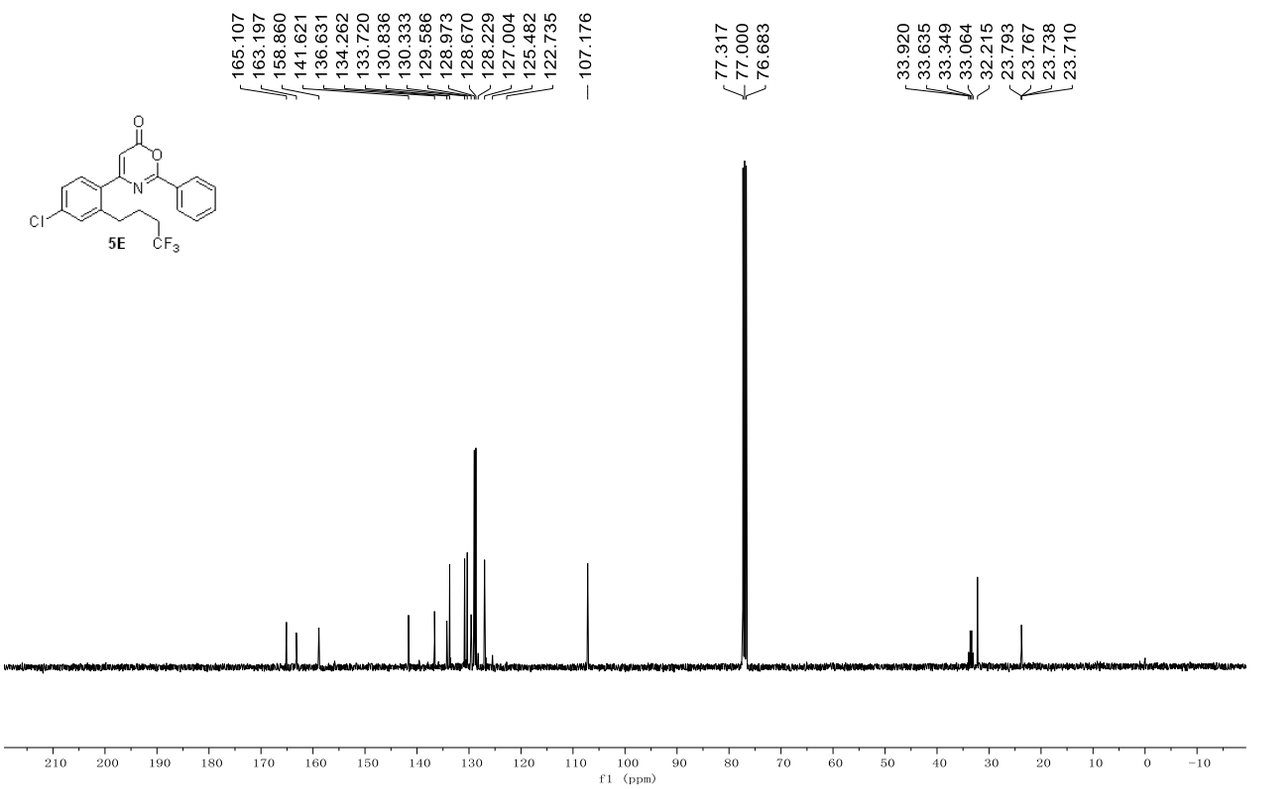
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130.333
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128.670
128.229
127.004
125.482
122.735
107.176
77.317
77.000
76.683
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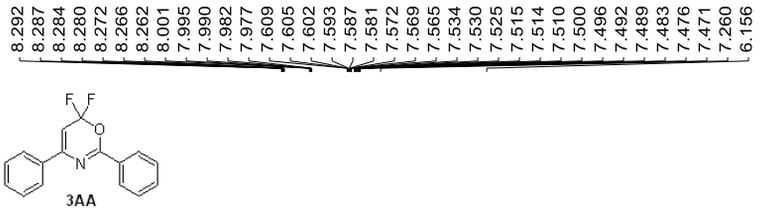
32.215
23.793
23.767
23.738
23.710
5E
CF3
f1 (ppm)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7.609
7.605
7.602
7.593
7.587
7.581
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7.530
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7.515
7.514
7.510
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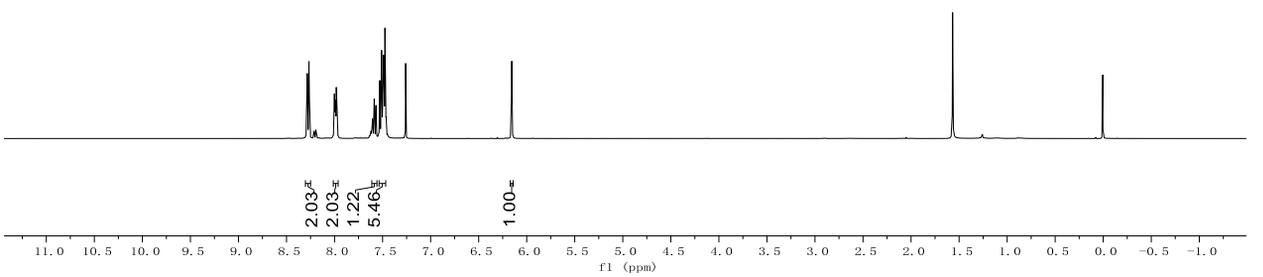
F
F
O
N

3AA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2.03
1.22
5.46
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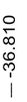
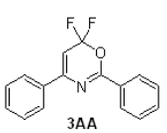
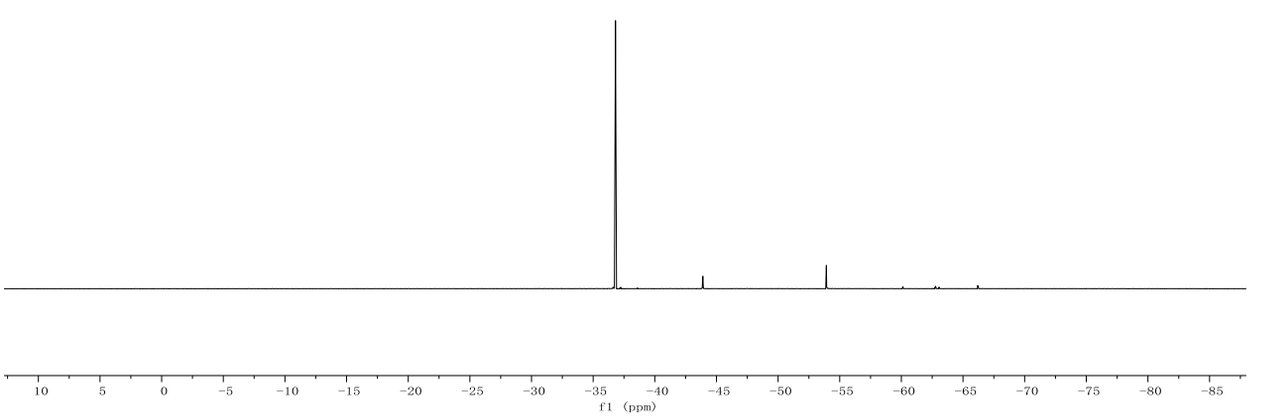
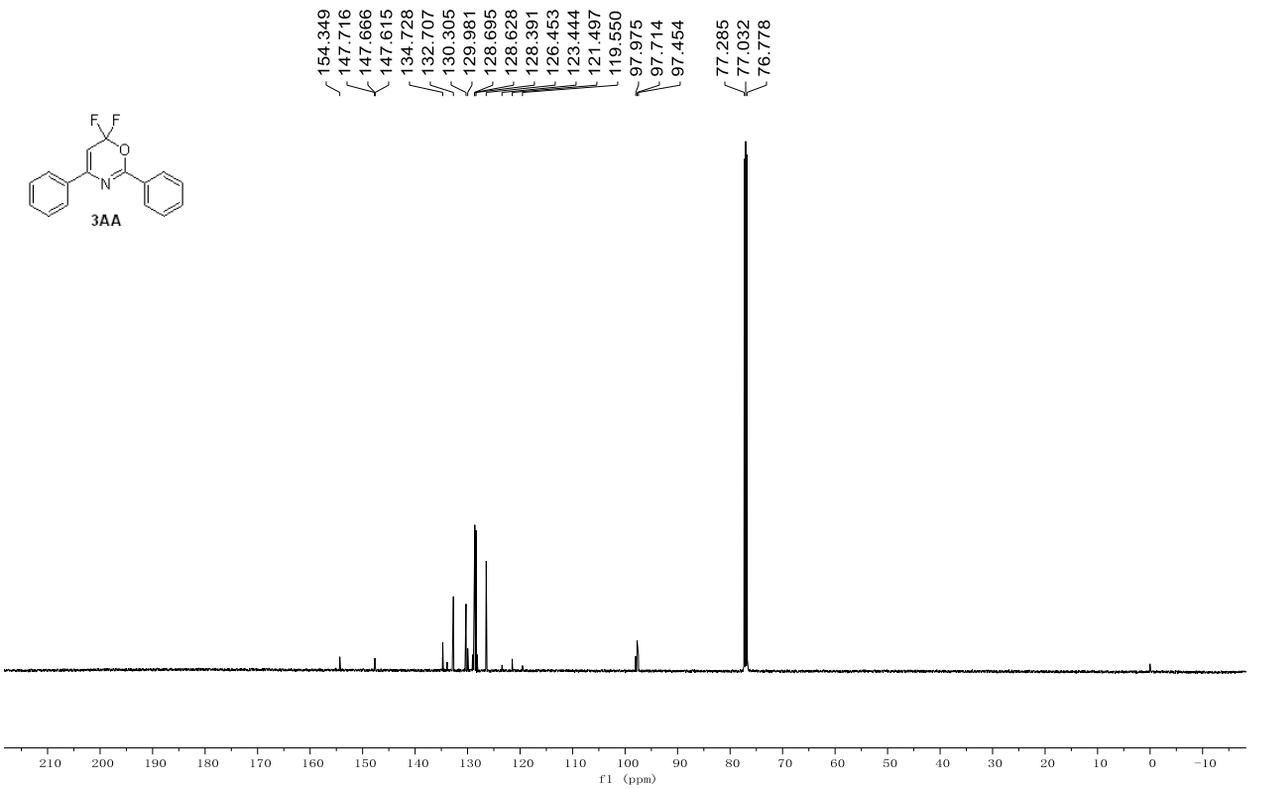
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0
f1 (ppm)


-36.810


F
F
O
N

3AA


10 5 0 −5 −10 −15 −20 −25 −30 −35 −40 −45 −50 −55 −60 −65 −70 −75 −80 −85
f1 (ppm)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147.716
147.666
147.615
134.728
132.707
130.305
129.981
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128.628
128.391
126.453
123.444
121.497
119.550
97.975
97.714
97.454
77.285
77.032
76.778
F
F
O
N
3AA
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)