Supporting Information

Metal free C−O bond cleavage: a new strategy for the synthesis of substituted oxazoles

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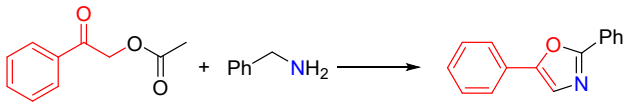
1. General remarks

All non-aqueous reactions and manipulations were performed in air atmosphere. All solvents were purchased from Energy Chemical, Aladdin and used without further treatment. The reactions were monitored by GC (7820A, Hubei University of Science and Technology) and GC-MS (QP2010, Hunan University). The electron ionization (EI) method was used as the ionization method for the HRMS measurement, and the mass analyzer type is TOF for EI. The ^{1}H NMR and ^{13}C NMR spectra were recorded on a Brucker ADVANCE III spectrometer at 400 MHz and 100 MHz, respectively (Hubei University of Science and Technology). Flash column chromatography was performed using silica gel 40-70 μm (200-300 mu). Amines and azide compounds were purchased from Energy Chemical and used without further treatment.

2. General procedure

A 10-mL Schlenk-type tube equipped with a magnetic stir bar was charged with substituted 2-oxo-2-phenylethyl acetate **1a-1l** (0.2 mmol), primary amine **2a-2m** (0.24 mmol), K_2CO_3 (0.4 mmol), I_2 (0.4 mmol), under N_2 atmospheres, ethyl acetate (2 mL) was added at room temperature, and then the reaction mixture was stirred at 80 °C for 8 h, the reaction was monitored by GC or GC-MS. After completion of the reaction, the resulting solution was cooled to room temperature, and neutralized with saturated NaCl solution. The product was extracted with ethyl acetate, dried over anhydrous Mg_2SO_4 and concentrated in vacuum. The crude product was purified by flash column chromatography on silica gel and eluted with ethyl acetate/Petroleum ether (1/5-1/10) give analytically pure product.

Table S1 Optimization of the model reaction condition of bases[a]



1a **2a** **3a**

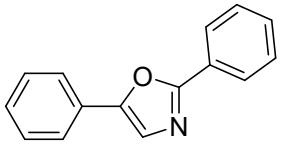
Entry	Additive	Solvent	**3a**%[b]
1	$NaOH/I_2$	ethyl acetate	35%
2	KOH/I_2	ethyl acetate	47%
3	NEt_3/I_2	ethyl acetate	trace

4	Na_2CO_3/I_2	ethyl acetate	63%
5	Cs_2CO_3/I_2	ethyl acetate	52%
6	C_4H_9OK /I_2	ethyl acetate	81%
7	K_2CO_3/I_2	ethyl acetate	90%

[a]Reaction conditions: 2-oxo-2-phenylethyl acetate **1a** (0.2 mmol), benzylamine **2a** (0.24 mmol), I_2 (0.4 mmol), base (0.4 mmol), ethyl acetate (2 mL), N_2 in 25 mL schlenk tube, 80 °C, 8 h. [b]Isolated yield.

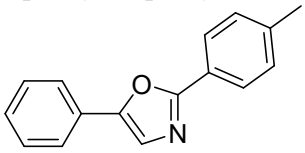
3. ^{1}H NMR and ^{13}C NMR data of products

2,5-diphenyloxazole (3a)[1]



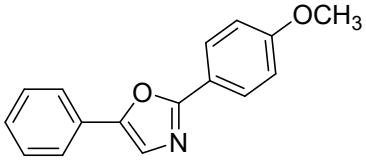
Following the general procedure (EtOAc/Petroleum ether 1:20), **3a** was obtained as a colorless solid, isolated yield: 88%, m.p. 66-68 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (q, 2H, *J* = 4.0 Hz), 7.71 (d, 2H, *J* = 7.6 Hz), 7.42-7.50 (m, 6H), 7.34 (t, 1H, *J* = 7.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.2, 151.3, 130.4, 128.9, 128.8, 128.5, 128.1, 127.5, 126.3, 124.2, 123.5; GC-MS: m/z = 221.25.

5-phenyl-2-(p-tolyl)oxazole (3b)[2]



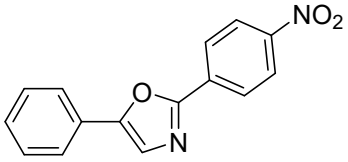
Following the general procedure (EtOAc/Petroleum ether 1:5), **3b** was obtained as a colorless solid, isolated yield: 85%, m.p. 71-73 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.00 (d, 2H, *J* = 8.0 Hz), 7.71 (d, 2H, *J* = 7.6 Hz), 7.44 (t, 3H, *J* = 7.0 Hz), 7.33 (d, 1H, *J* = 7.6 Hz), 7.28 (d, 2H, *J* = 8.0 Hz), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.1, 151.0, 140.7, 129.6, 128.9, 128.3, 128.2, 126.3, 124.8, 124.2, 123.4, 21.6; GC-MS: m/z = 235.09.

2-(4-methoxyphenyl)-5-phenyloxazole (3c)[1]



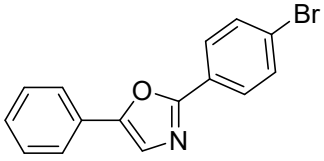
Following the general procedure (EtOAc/Petroleum ether 1:5), **3c** was obtained as a colorless solid, isolated yield: 84%, m.p. 78-79 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.71 (t, 3H, *J* = 6.6 Hz), 7.64 (s, 1H), 7.34-7.46 (m, 5H), 7.00 (q, 1H, *J* = 4.2 Hz), 3.89 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.1, 159.9, 151.3, 129.9, 128.9, 128.7, 128.5, 128.0, 124.2, 123.4, 118.8, 116.9, 111.0, 55.5; GC-MS: m/z = 251.09.

2-(4-nitrophenyl)-5-phenyloxazole (3d)[3]



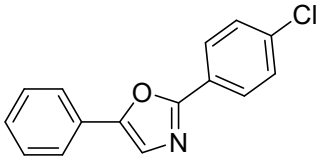
Following the general procedure (EtOAc/Petroleum ether 1:5), **3d** was obtained as a colorless solid, isolated yield: 81%, m.p. 209-213 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.34 (d, 2H, *J* = 9.2 Hz), 8.13-8.15 (m, 2H), 7.86 (d, 2H, *J* = 8.8 Hz), 7.66 (s, 1H), 7.52 (t, 3H, *J* = 3.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.8, 149.1, 147.2, 133.8, 131.1, 129.0, 126.9, 126.8, 126.7, 124.6, 124.5; GC-MS: m/z = 266.25.

2-(4-bromophenyl)-5-phenyloxazole (3e)[4]



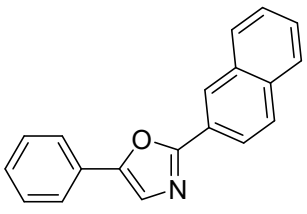
Following the general procedure (EtOAc/Petroleum ether 1:5), **3e** was obtained as a colorless solid, isolated yield: 79%, m.p. 100-102 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94 (d, 2H, *J* = 8.8 Hz), 7.69 (d, 2H, *J* = 7.6 Hz), 7.69 (d, 2H, *J* = 8.8 Hz), 7.41-7.45 (m, 3H), 7,34 (t, 1H, *J* = 7.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 171.1, 160.3, 151.6, 132.1, 128.9, 128.6, 127.8, 127.7, 126.4, 124.8, 124.2, 123.6; GC-MS: m/z = 298.99.

2-(4-chlorophenyl)-5-phenyloxazole (3f)[5]



Following the general procedure (EtOAc/Petroleum ether 1:5), **3f** was obtained as a colorless solid, isolated yield: 80%, m.p. 103-105 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.04 (d, 2H, *J* = 8.8 Hz), 7.71 (d, 2H, *J* = 7.6 Hz), 7.42-7.56 (m, 5H), 7.34 (t, 1H, *J* = 7.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.2, 151.6, 136.4, 129.1, 128.9, 128.6, 127.9, 127.5, 125.9, 124.3, 123.6; GC-MS: m/z = 255.04.

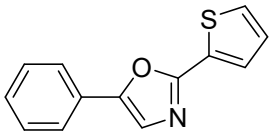
2-(naphthalen-2-yl)-5-phenyloxazole (3g)[2]



Following the general procedure (EtOAc/Petroleum ether 1:5), **3i** was obtained as a colorless solid, isolated yield: 85%, m.p. 99-102 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.60 (s, 1H),8.19 (d, 1H, *J* = 8.4 Hz), 7.77-7.93 (m, 5H), 7.47-7.56 (m, 5H), 7.38 (t, 1H, *J* = 7.2

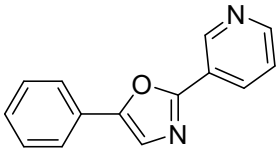
Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.4, 151.5, 134.2, 133.1, 128.9, 128.73, 128.71, 128.5, 128.1, 127.9, 127.3, 126.8, 126.2, 124.8, 124.3, 123.6, 123.2; GC-MS: m/z = 271.09.

5-phenyl-2-(thiophen-2-yl)oxazole (3h)[5]



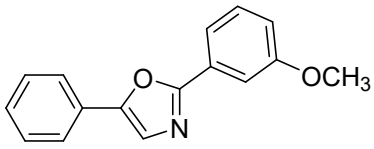
Following the general procedure (EtOAc/Petroleum ether 1:5), **3g** was obtained as a colorless solid, isolated yield: 78%, m.p. 72-74 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.74 (d, 1H, *J* = 3.6 Hz), 7.71 (d, 2H, *J* = 7.6 Hz), 7.42-7.46 (m, 3H), 7.36 (s, 1H), 7.34 (t, 1H, *J* = 7.4 Hz), 7.14 (q, 1H, *J* = 4.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 157.4, 150.9, 130.1, 128.9, 128.5, 128.3, 127.9, 127.8, 127.6, 124.2, 123.3; GC-MS: m/z = 227.04.

5-phenyl-2-(pyridin-3-yl)oxazole (3i)[1]



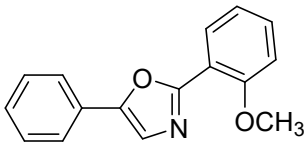
Following the general procedure (EtOAc/Petroleum ether 1:5), **3h** was obtained as a colorless solid, isolated yield: 81%, m.p. 77-79 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.35 (d, 1H, *J* = 1.2 Hz), 8.69 (d, 1H, *J* = 3.2 Hz), 8.36 (d, 1H, *J* = 8.0 Hz), 7.73 (d, 2H, *J* = 7.6 Hz), 7.36-7.49 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.7, 152.1, 150.9, 147.5, 133.5, 129.0, 128.9, 127.6, 124.4, 123.8, 123.7; GC-MS: m/z = 238.11.

2-(3-methoxyphenyl)-5-phenyloxazole (3j)[6]



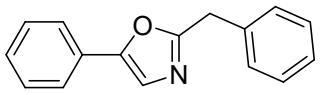
Following the general procedure (EtOAc/Petroleum ether 1:5), **3j** was obtained as a colorless solid, isolated yield: 80%, m.p. 81-84 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.71 (t, 2H, *J* = 6.6 Hz), 7.64 (s, 1H), 7.34-7.46 (m, 5H), 7.00 (q, 1H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.1, 159.9, 151.3, 129.9, 128.9, 128.7, 128.5, 128.0, 124.2, 123.4, 118.8, 116.9, 111.0, 55.5; GC-MS: m/z = 251.09.

diphenyl benzylphosphoramidate (3k)[3]



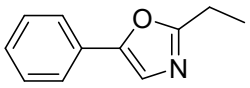
Following the general procedure (EtOAc/Petroleum ether 1:5), **3j** was obtained as a colorless solid, isolated yield: 74%, m.p. 77-79 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.74 (t, 2H, *J* = 6.6 Hz), 7.65 (s, 1H), 7.33-7.47 (m, 5H), 7.01 (q, 1H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.1, 159.9, 151.4, 130.0, 129.0, 128.7, 128.5, 128.0, 124.3, 123.5, 118.8, 116.9, 111.0, 55.5; GC-MS: m/z = 251.09.

2-benzyl-5-phenyloxazole (3l)[2]



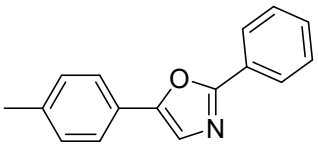
Following the general procedure (EtOAc/Petroleum ether 1:10), **3l** was obtained as a colorless solid, isolated yield: 70%, m.p. 71-72C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.31 (d, 2H, *J* = 7.2 Hz), 7.47 (t, 2H, *J* = 7.6 Hz), 7.24-7.49 (m, 7H), 4.18 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.7, 138.3, 125.5, 134.4, 131.2, 128.83, 128.75, 127.1, 126.8, 124.1, 122.0, 40.6; GC-MS: m/z = 235.09.

2-ethyl-5-phenyloxazole (3m)[1]



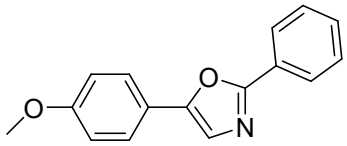
Following the general procedure (EtOAc/Petroleum ether 1:10), **3m** was obtained as a colorless liquid, isolated yield: 71%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.75 (d, 2H, *J* = 7.2 Hz), 7.34 (t, 2H, *J* = 7.6 Hz), 7.19 (t, 1H, *J* = 7.4 Hz), 7.09 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 149.7, 139.9, 134.5, 128.5, 126.3, 124.7, 114.7, 20.3, 11.2; GC-MS: m/z = 173.08.

2-phenyl-5-(p-tolyl)oxazole (3n)[1]



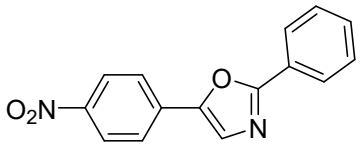
Following the general procedure (EtOAc/Petroleum ether 1:10), **3n** was obtained as a colorless solid, isolated yield: 85%, m.p. 69-71 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (d, 2H, *J* = 8.0 Hz), 7.60 (d, 2H, *J* = 8.0 Hz), 7.45-7.50 (m, 3H), 7.39 (s, 1H), 7.24 (d, 2H, *J* = 7.6 Hz), 2,39 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.9, 151.5, 138.5, 130.2, 129.6, 128.8, 127.6, 126.2, 125.3, 124.2, 122.8, 21.4; GC-MS: m/z = 235.09.

5-(4-methoxyphenyl)-2-phenyloxazole (3o)[1]



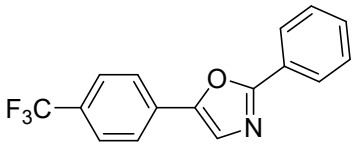
Following the general procedure (EtOAc/Petroleum ether 1:10), **3o** was obtained as a colorless solid, isolated yield: 84%, m.p. 88-89 °C. ^{1}H ($CDCl_3$, 400 MHz): δ 8.10 (d, 2H, *J* = 6.4 Hz), 7.64 (d, 2H, *J* = 8.8 Hz), 7.42-7.49 (m, 3H), 7.32 (s, 1H), 6.97 (d, 2H, *J* = 8.8 Hz), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 160.6, 159.9, 151.4, 130.1, 128.8, 127.7, 126.2, 125.8, 122.0, 121.0, 114.5, 55.4; GC-MS: m/z = 251.09.

5-(4-nitrophenyl)-2-phenyloxazole (3p)[7]



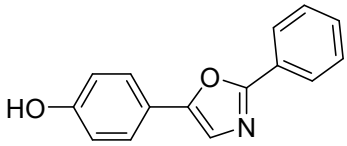
Following the general procedure (EtOAc/Petroleum ether 1:10), **3p** was obtained as a colorless solid, isolated yield: 89%, m.p. 112-115 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.31 (d, 2H, *J* = 9.2 Hz), 8.13-8.15 (m, 2H), 7.86 (d, 2H, *J* = 8.8 Hz), 7.66 (s, 1H), 7.52 (d, 3H, *J* = 3.2 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.8, 149.1, 147.2, 133.8, 131.1, 129.0, 126.9, 126.8, 126.7, 124.6, 124.5; GC-MS: m/z = 266.06.

2-phenyl-5-(4-(trifluoromethyl)phenyl)oxazole (3q)[1]



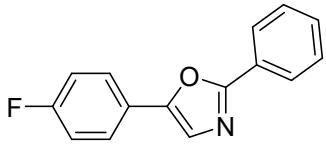
Following the general procedure (EtOAc/Petroleum ether 1:10), **3q** was obtained as a colorless solid, isolated yield: 74%, m.p. 203-205 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (q, 2H, *J* = 3.8 Hz), 7.81 (d, 2H, *J* = 8.0 Hz), 7.69 (d, 2H, *J* = 8.0 Hz), 7.56 (s, 1H), 7.49 (q, 3H, *J* = 2.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.0, 149.9, 131.6, 131.2 (d, $J_{c\text{-}f}$ = 94 Hz), 130.8, 129.9 128.9, 127.1, 126.5, 126.0 (d, $J_{c\text{-}f}$ = 4.0 Hz), 125.2, 124.2; GC-MS: m/z = 289.07.

4-(2-phenyloxazol-5-yl)phenol (3r)[6]



Following the general procedure (EtOAc/Petroleum ether 1:10), **3r** was obtained as a colorless solid, isolated yield: 81%, m.p. > 250 °C. ^{1}H NMR (DMSO-*d*, 400 MHz): δ 9.89 (s, 1H), 8.06 (t, 2H, *J* = 6.4 Hz), 7.65 (d, 2H, *J* = 8.8 Hz), 7.59 (s, 1H), 7.49-7.57 (m, 3H), 6.87 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR (DMSO-*d*, 100 MHz): δ 159.7, 158.5, 151.8, 130.8, 129.6, 127.5, 126.3, 126.2, 122.3, 119.0, 116.4; GC-MS: m/z = 237.07.

5-(4-fluorophenyl)-2-phenyloxazole (3s)[1]



Following the general procedure (EtOAc/Petroleum ether 1:10), **3s** was obtained as a colorless solid, isolated yield: 79%, m.p. 72-74 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.09 (q, 2H, *J* = 7.2 Hz), 7.69-7.72 (m, 2H), 7.47-7.49 (m, 3H), 7.38 (s, 1H), 7.15 (d, 2H, *J* = 8.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.2 (d, $J_{c\text{-}f}$ = 30 Hz), 150.5, 130.4, 129.1, 128.9, 129.9, 127.2, 126.3, 126.1 (d, $J_{c\text{-}f}$ = 8.0 Hz), 123.1, 116.0 (d, $J_{c\text{-}f}$ = 22 Hz); GC-MS: m/z = 239.07.

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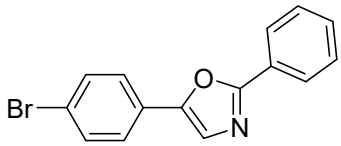
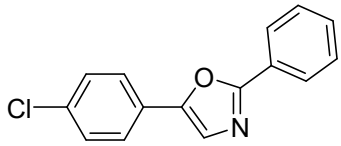
5-(4-bromophenyl)-2-phenyloxazole (3t)[6]



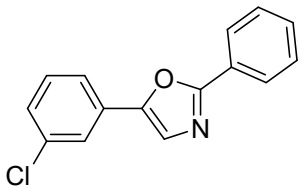
Following the general procedure (EtOAc/Petroleum ether 1:10), **3t** was obtained as a colorless solid, isolated yield: 81%, m.p. 101-103 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.09 (q, 2H, *J* = 4.0 Hz), 7.58 (s, 4H), 7.45-7.49 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.5, 150.3, 132.2, 130.5, 128.9, 127.3, 127.0, 126.4, 125.7, 124.0, 123.3; GC-MS: m/z = 298.99.

5-(4-chlorophenyl)-2-phenyloxazole (3u)[1]



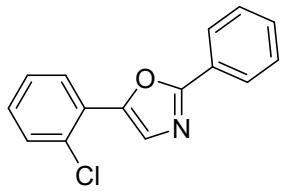
Following the general procedure (EtOAc/Petroleum ether 1:10), **3u** was obtained as a colorless solid, isolated yield: 80%, m.p. 110-112 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.09 (q, 2H, *J* = 3.8 Hz), 7.62 (d, 2H, *J* = 8.4 Hz), 7.46-7.50 (m, 3H), 7.41 (d, 2H, *J* = 3.6 Hz), 7.39 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.4, 150.3, 134.2, 130.5, 129.2, 128.9, 127.3, 126.5, 126.4, 125.4, 123.9; GC-MS: m/z = 255.04.

5-(3-chlorophenyl)-2-phenyloxazole (3v)[4]



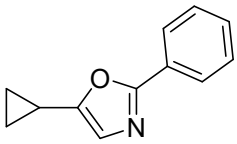
Following the general procedure (EtOAc/Petroleum ether 1:10), **3v** was obtained as a colorless solid, isolated yield: 81%, 102-104 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.11 (m, 2H), 7.69 (s, 1H), 7.57 (d, 1H, *J* = 8.0 Hz), 7.46-7.49 (m, 4H), 7.36 (t, 1H, *J* = 8.0 Hz), 7.28 (d, 1H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.6, 149.9, 135.1, 130.6, 130.2, 129.7, 128.9, 128.4, 127.2, 126.4, 124.4, 124.2, 122.2; GC-MS: m/z = 255.04

5-(2-chlorophenyl)-2-phenyloxazole (3w)[7]



Following the general procedure (EtOAc/Petroleum ether 1:10), **3w** was obtained as a colorless solid, isolated yield: 74%, 101-102 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (q, 2H, *J* = 3.8 Hz), 7.72 (s, 1H), 7.59 (d, 1H, *J* = 8.0 Hz), 7.48-7.51 (m, 4H), 7.36 (t, 1H, *J* = 8.0 Hz), 7.31 (d, 1H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.6, 149.9, 135.1, 130.6, 130.3, 129.7, 128.9, 128.4, 127.3, 126.4, 124.5, 124.2, 122.3; GC-MS: m/z = 255.04.

5-cyclopropyl-2-phenyloxazole (3x)[4]



Following the general procedure (EtOAc/Petroleum ether 1:10), **3x** was obtained as a colorless solid, isolated yield: 69%, 70-72 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.99 (q, 2H, *J* = 3.8 Hz), 7.40-7.45 (m, 3H), 6.81 (s, 1H), 1.92-1.99 (m, 1H), 0.97-1.00 (m, 2H), 0.85-0.88 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.1, 154.6, 129.9, 128.7, 127.8, 126.0, 122.6, 6.7, 6.5; GC-MS: m/z = 185.08.

4. References

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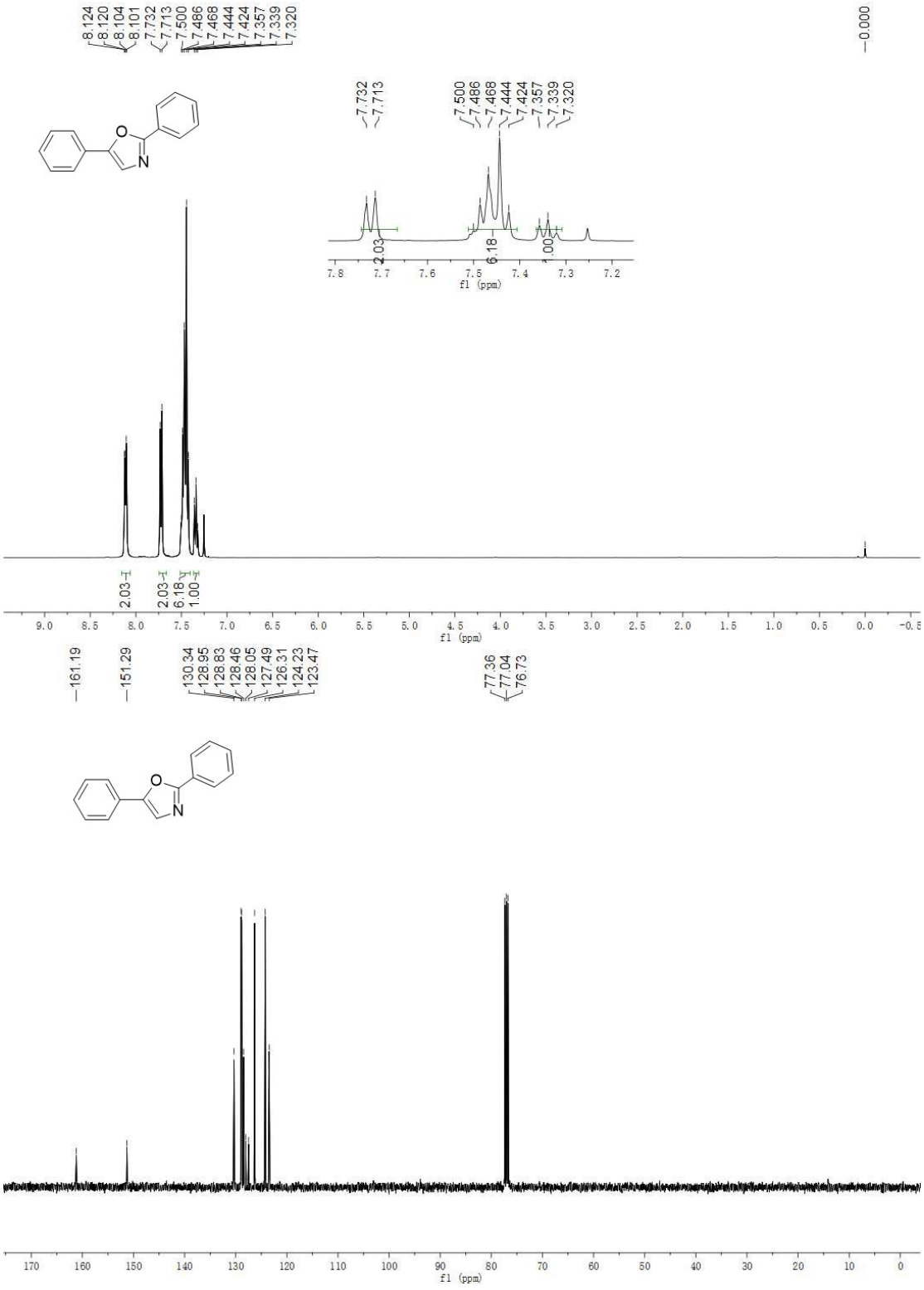
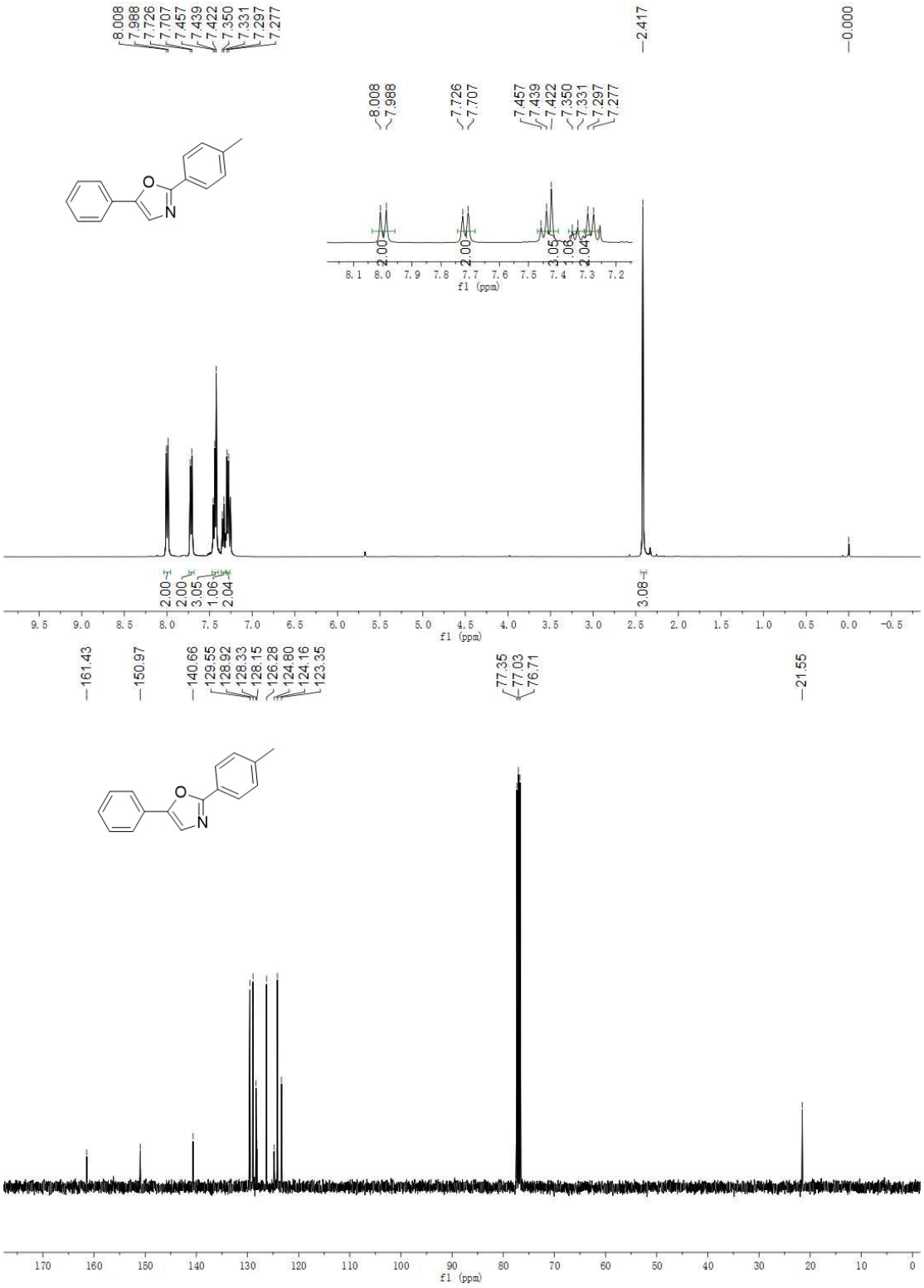
Copies of ^{1}H NMR and ^{13}C NMR spectra

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7.350
7.331
7.297
7.277
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0.000
f1 (ppm)
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150.97
140.66
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128.15
126.28
124.80
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123.35
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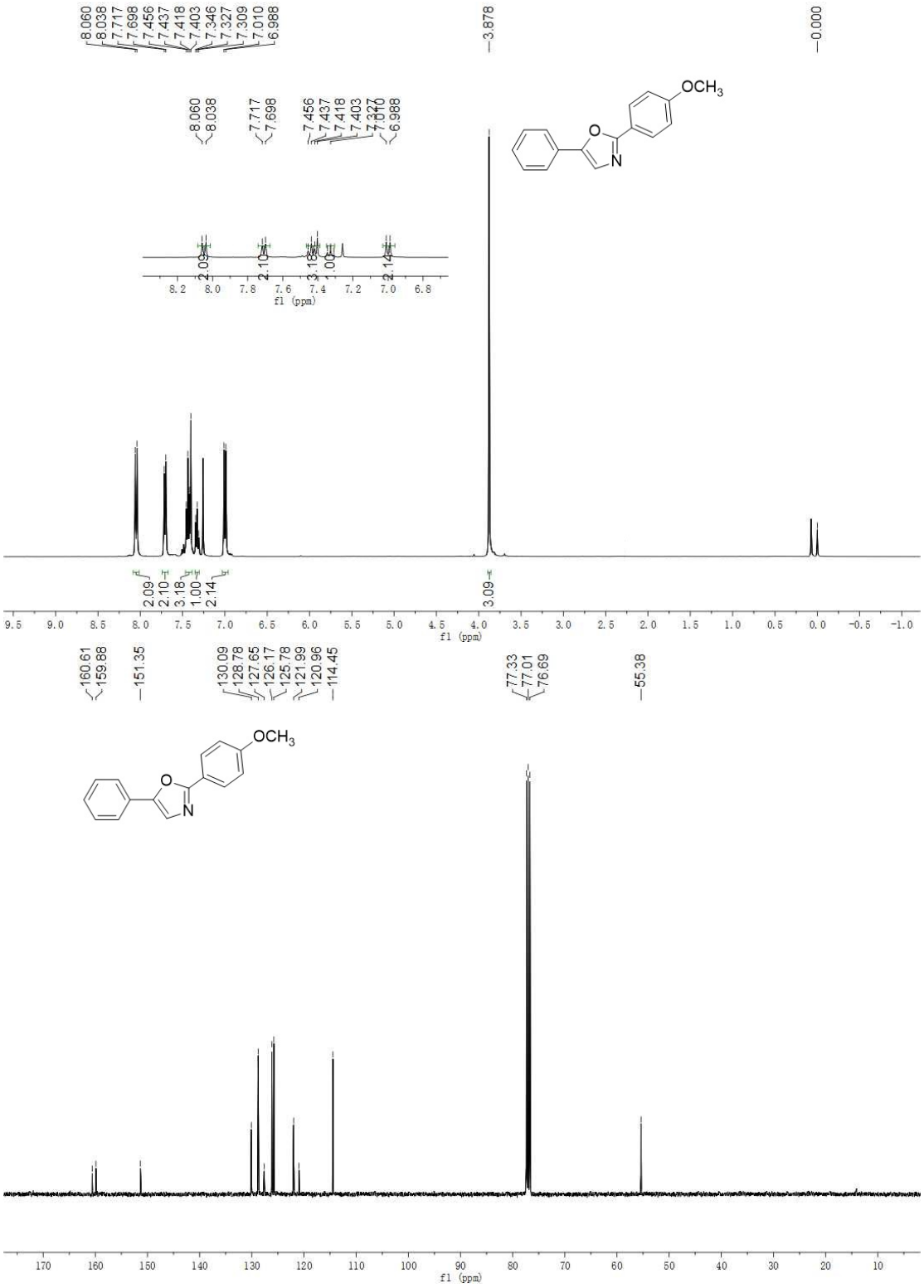
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7.403
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7.327
7.309
7.010
6.988
3.878
0.000
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O
N
2.09
2.10
3.18
1.00
2.14
3.09
f1 (ppm)
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159.88
151.35
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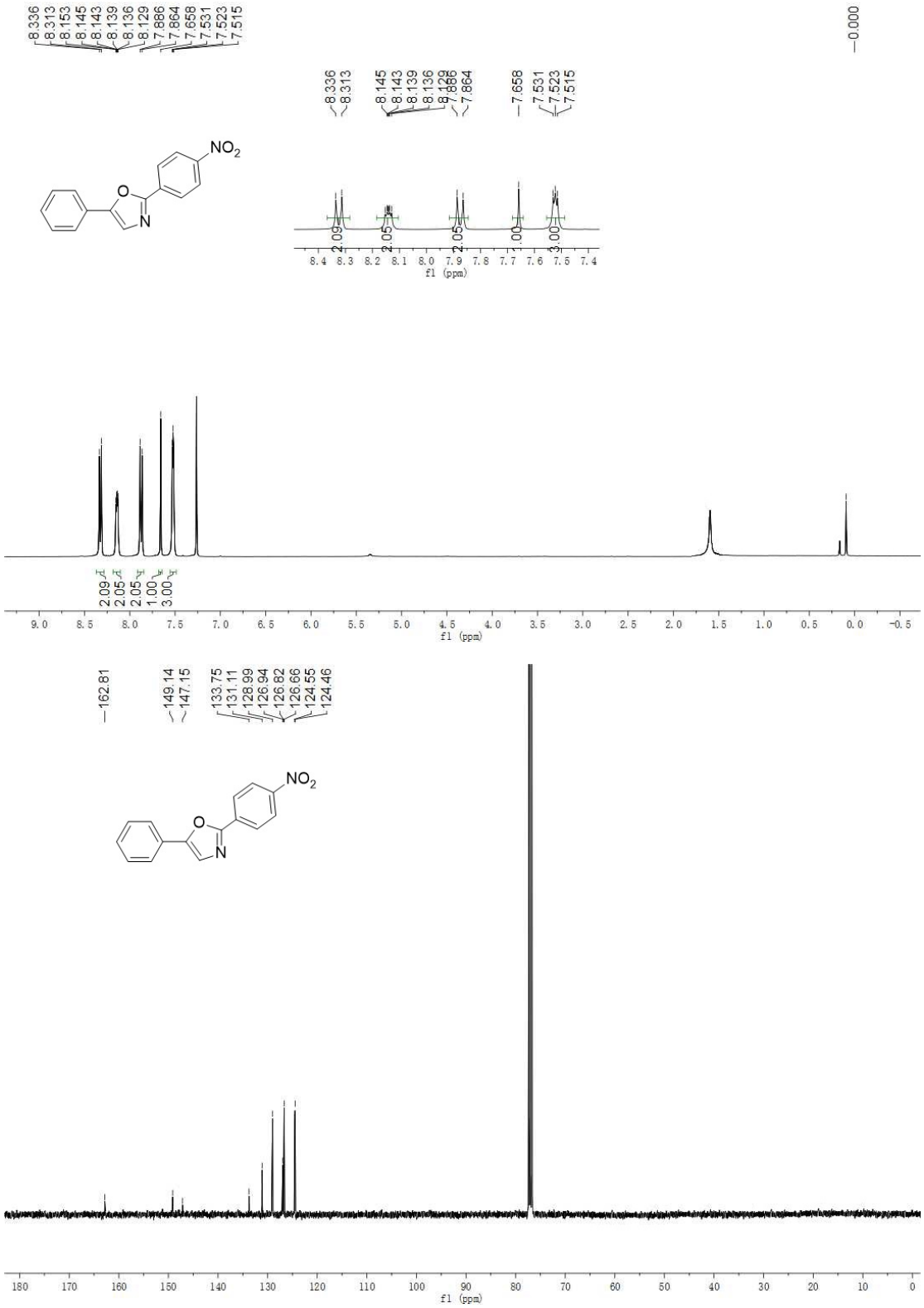
77.01
76.69
55.38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7.523
7.515
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O
N
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2.05
2.05
1.00
3.00
f1 (ppm)
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126.94
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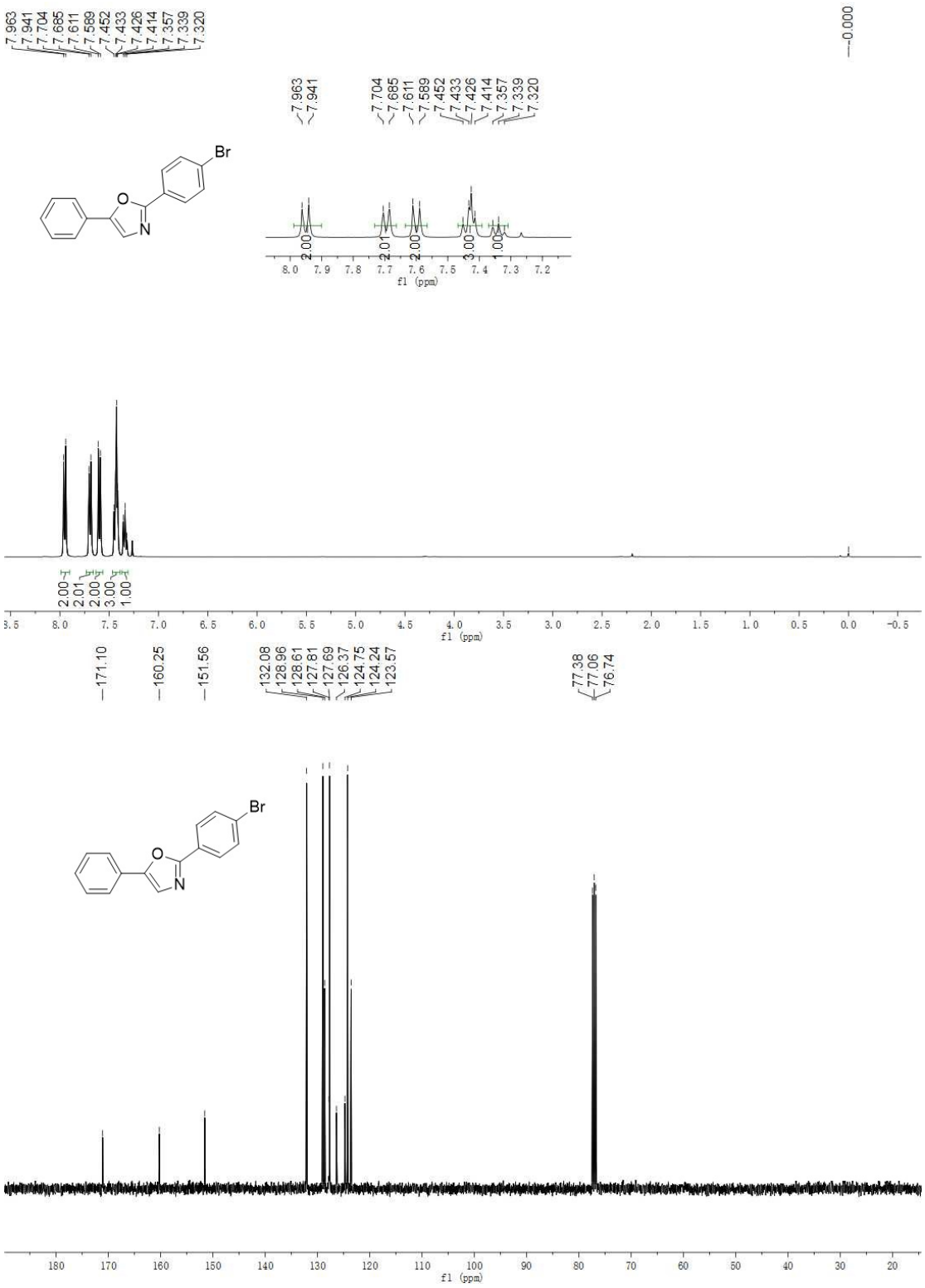
124.55
124.46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7.320
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Br
O
N
2.00
2.01
2.00
3.00
1.00
f1 (ppm)
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124.24
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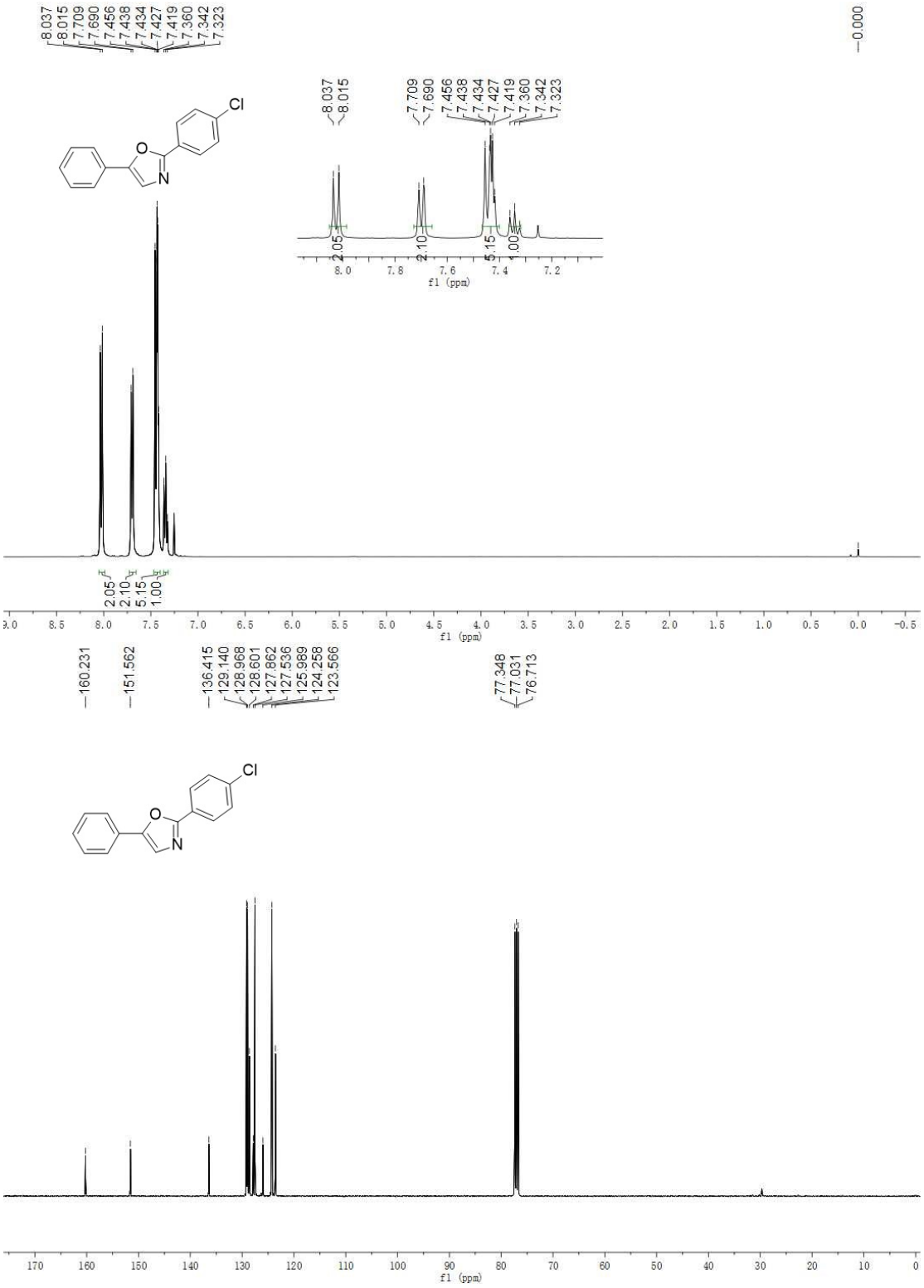
77.38
77.06
76.74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Cl
O
N
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2.10
5.15
1.00
f1 (ppm)
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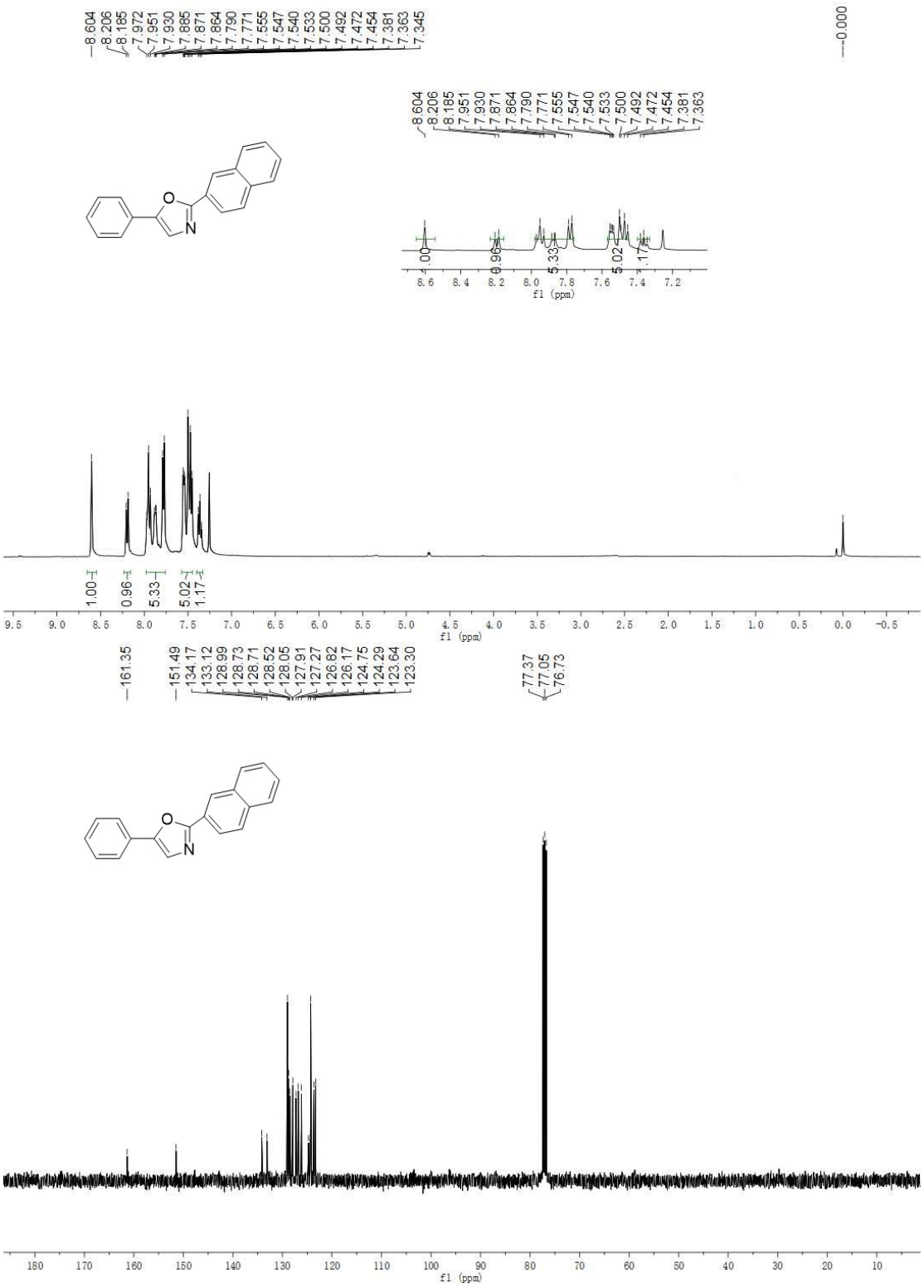
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7.547
7.540
7.533
7.500
7.492
7.472
7.454
7.381
7.363
7.345
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1.00
0.96
5.33
5.02
1.17
f1 (ppm)
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134.17
133.12
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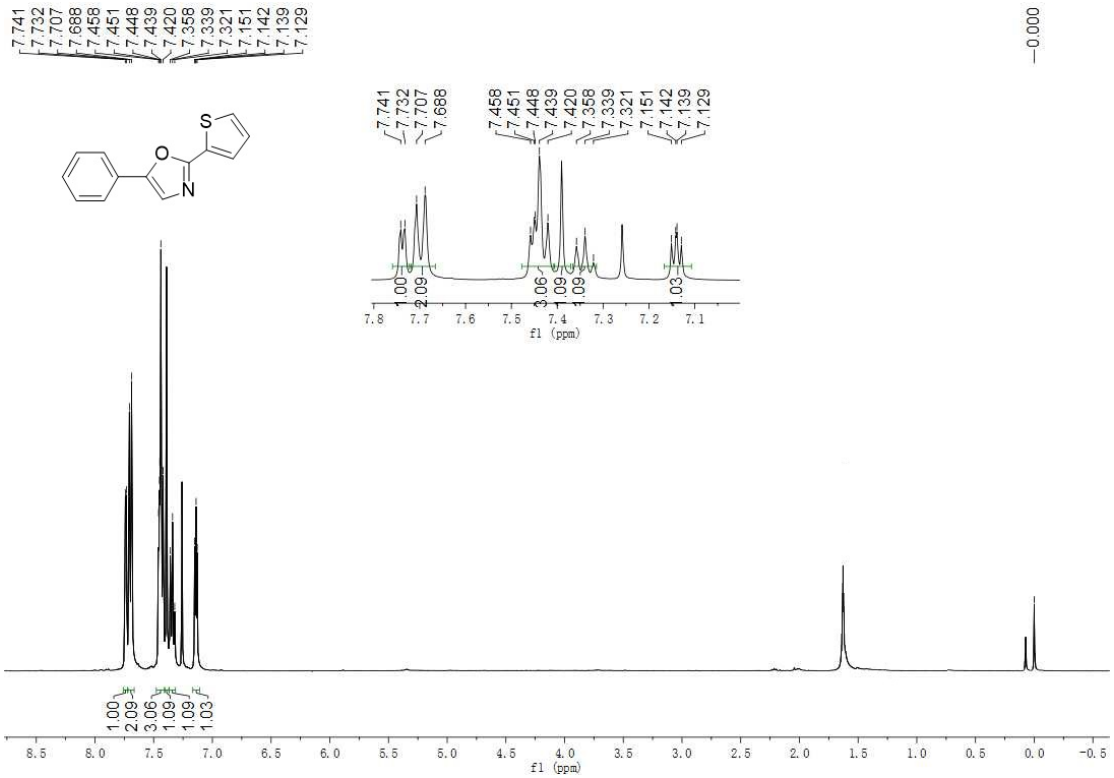
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7.151
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S
O
N
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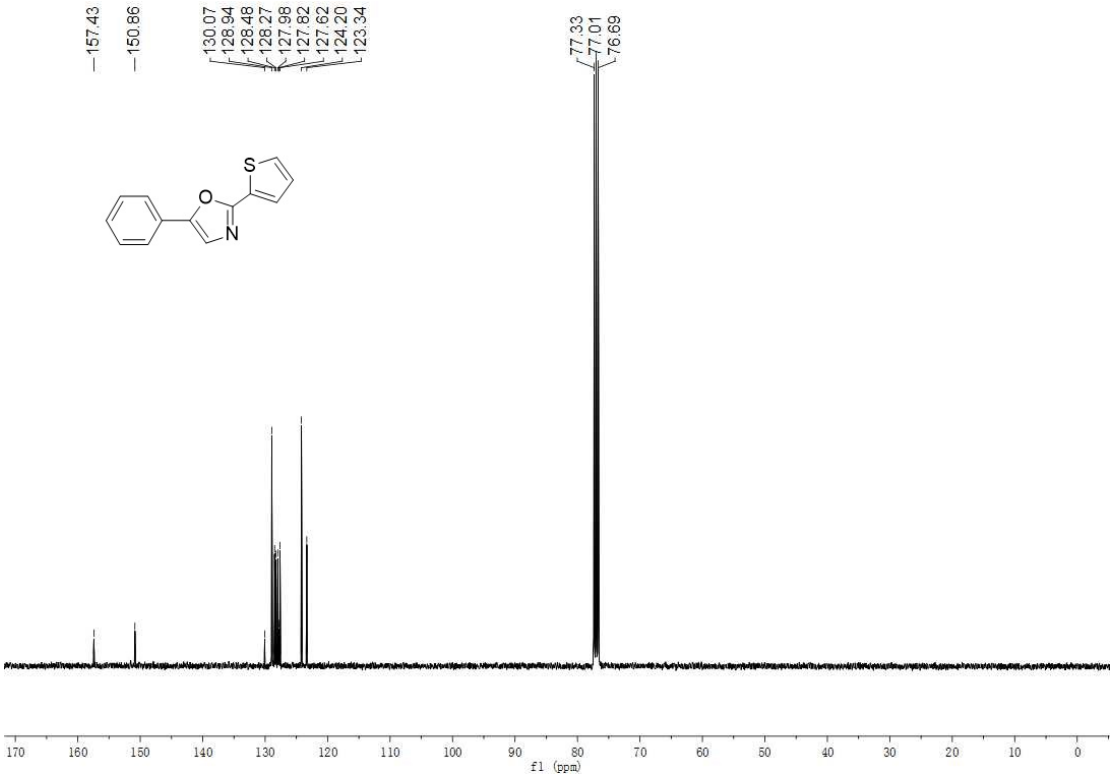
1.09
1.09
1.03
f1 (ppm)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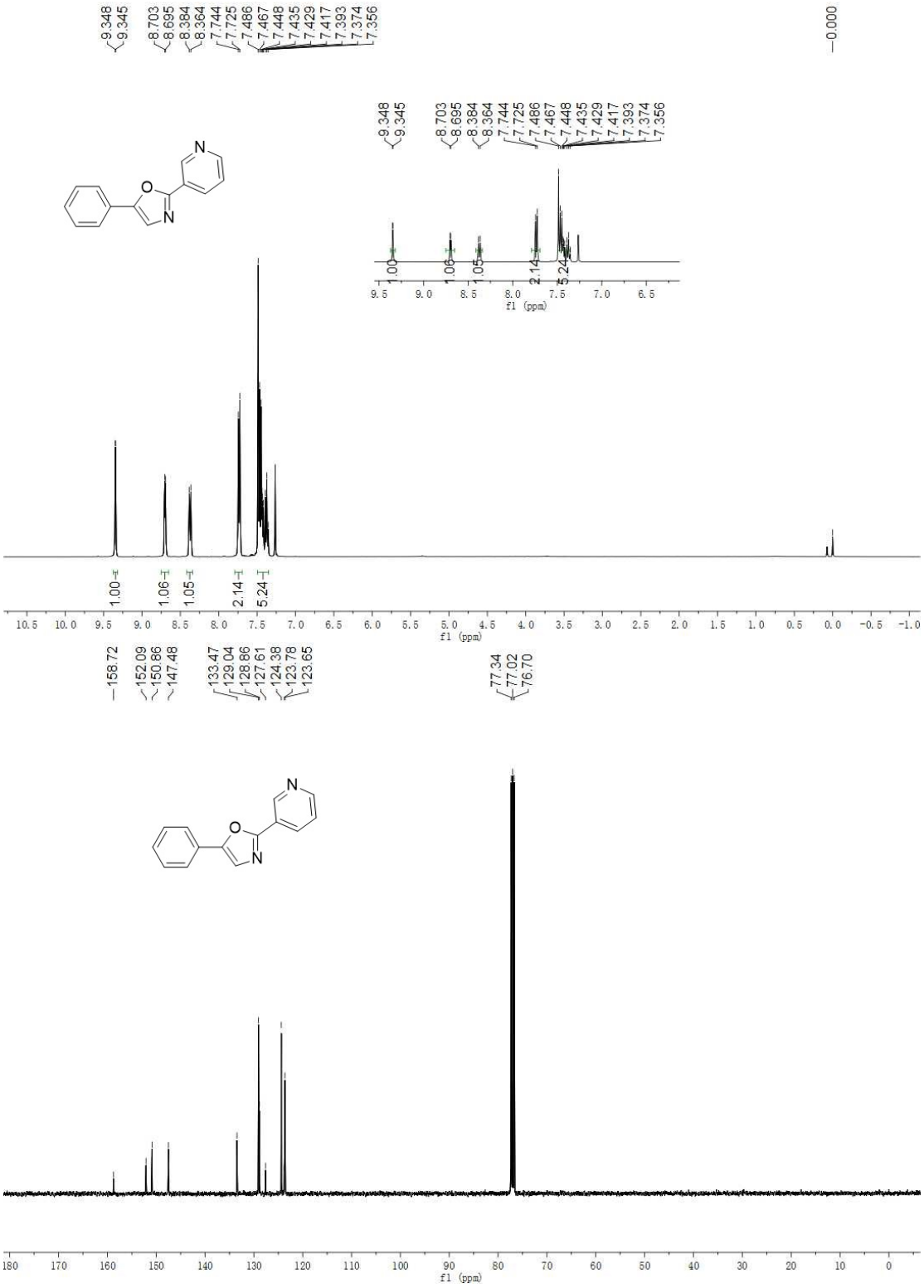
O
N
f1 (ppm)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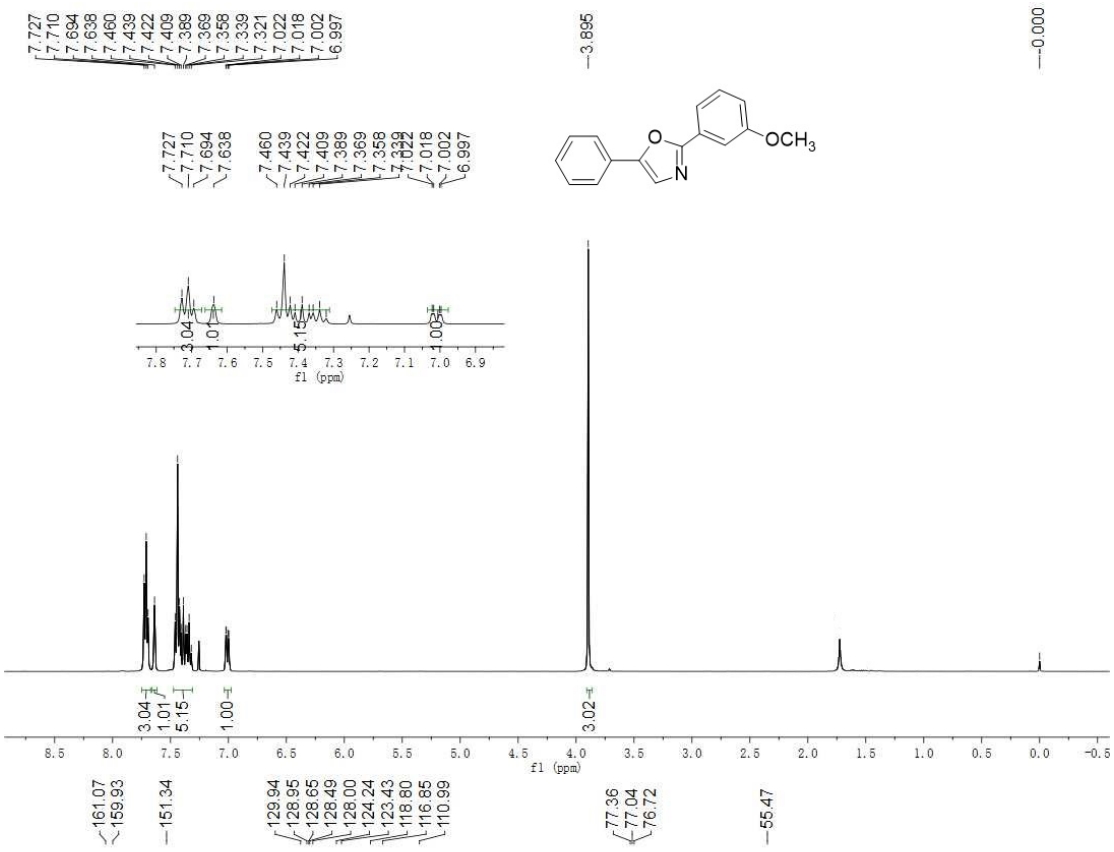
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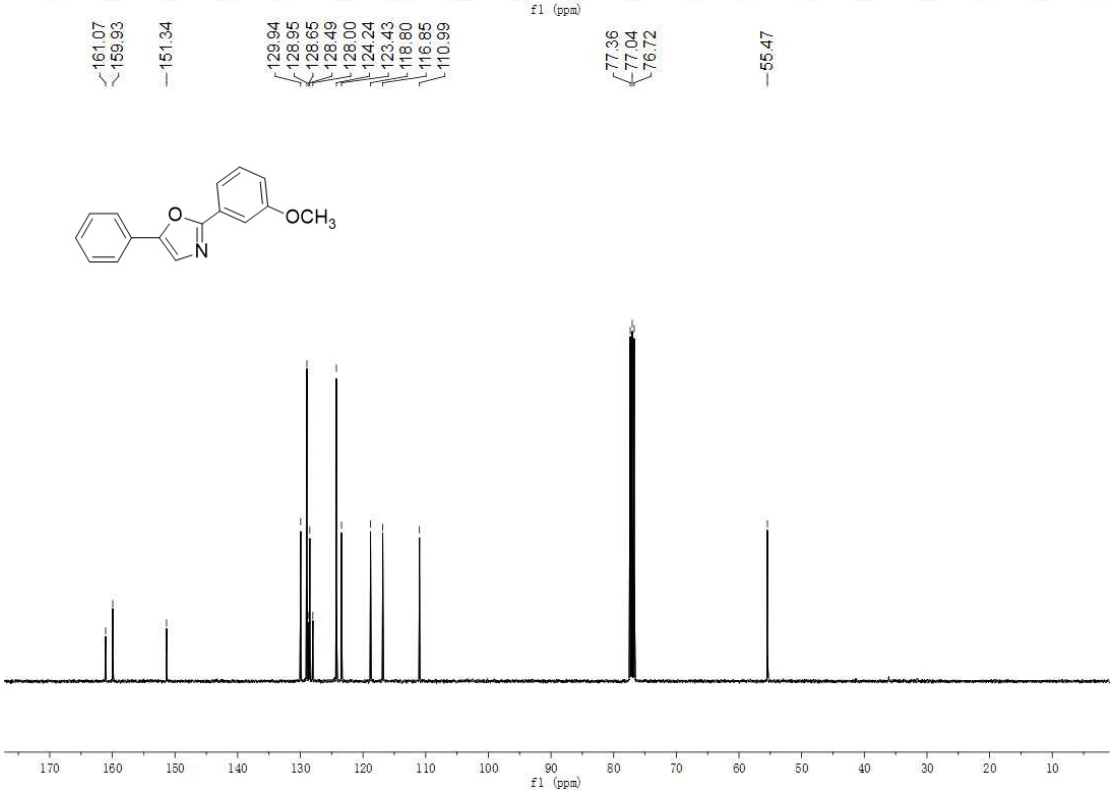
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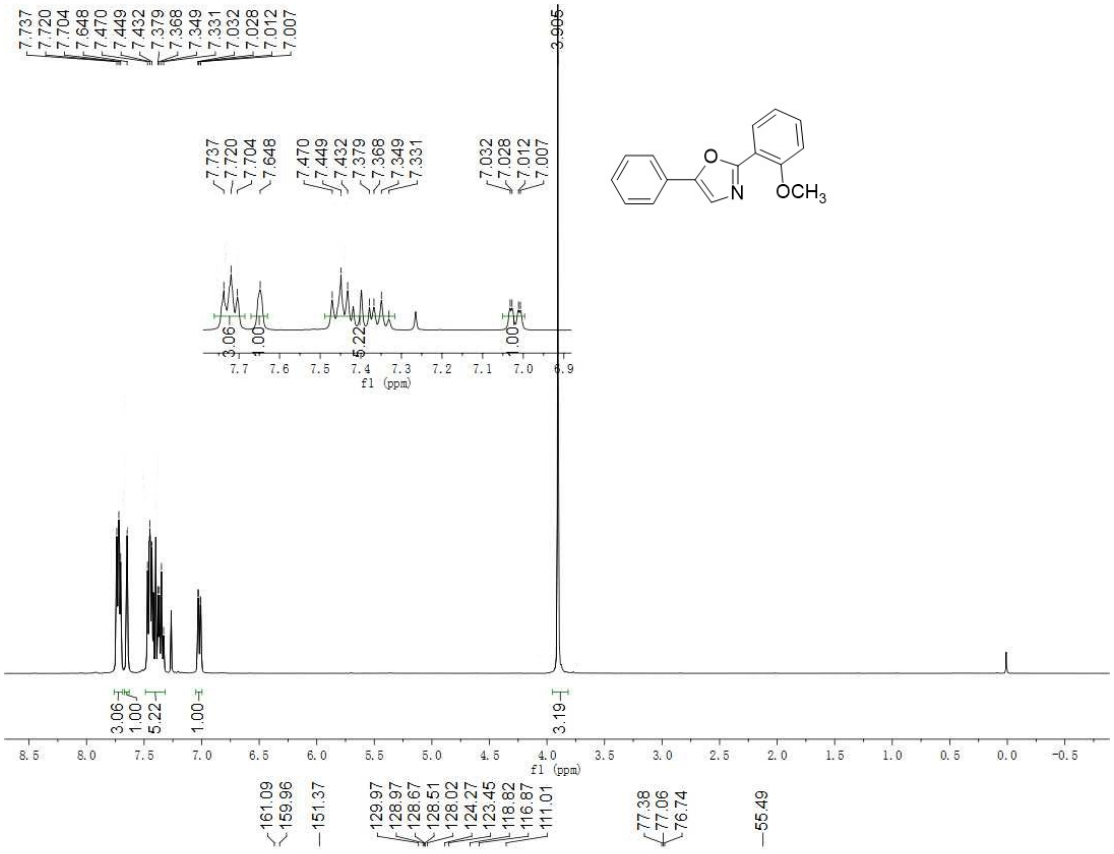
N
f1 (ppm)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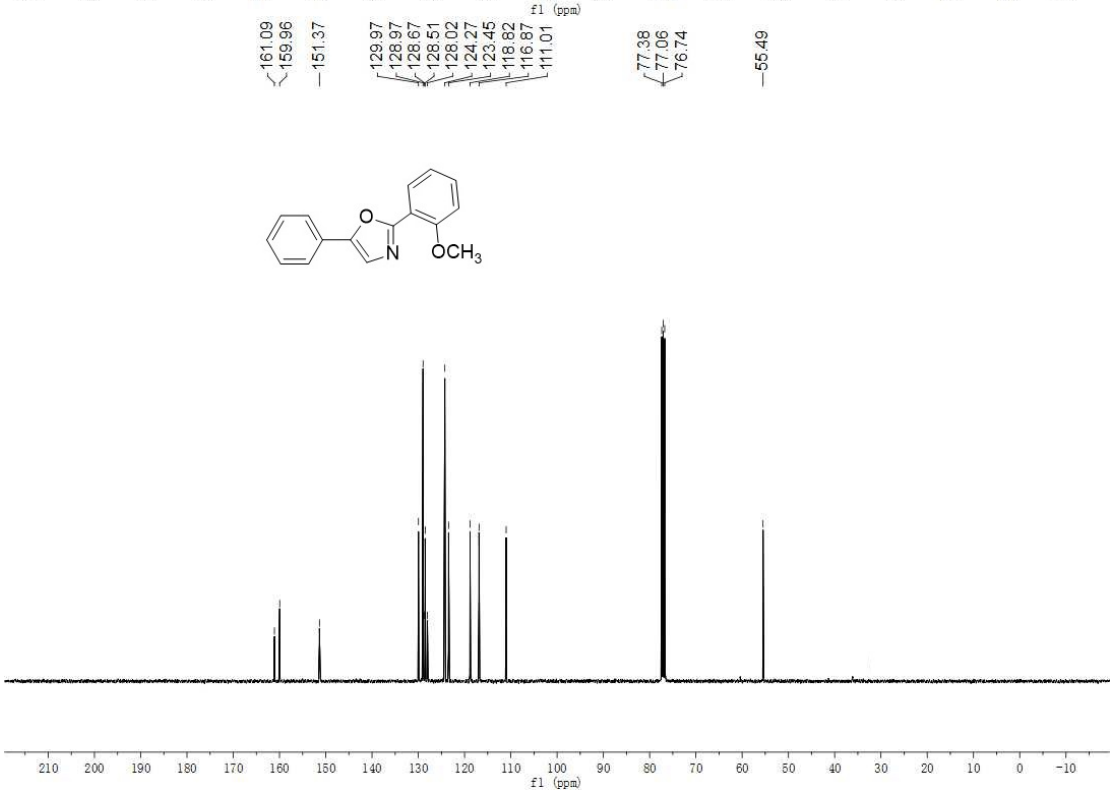
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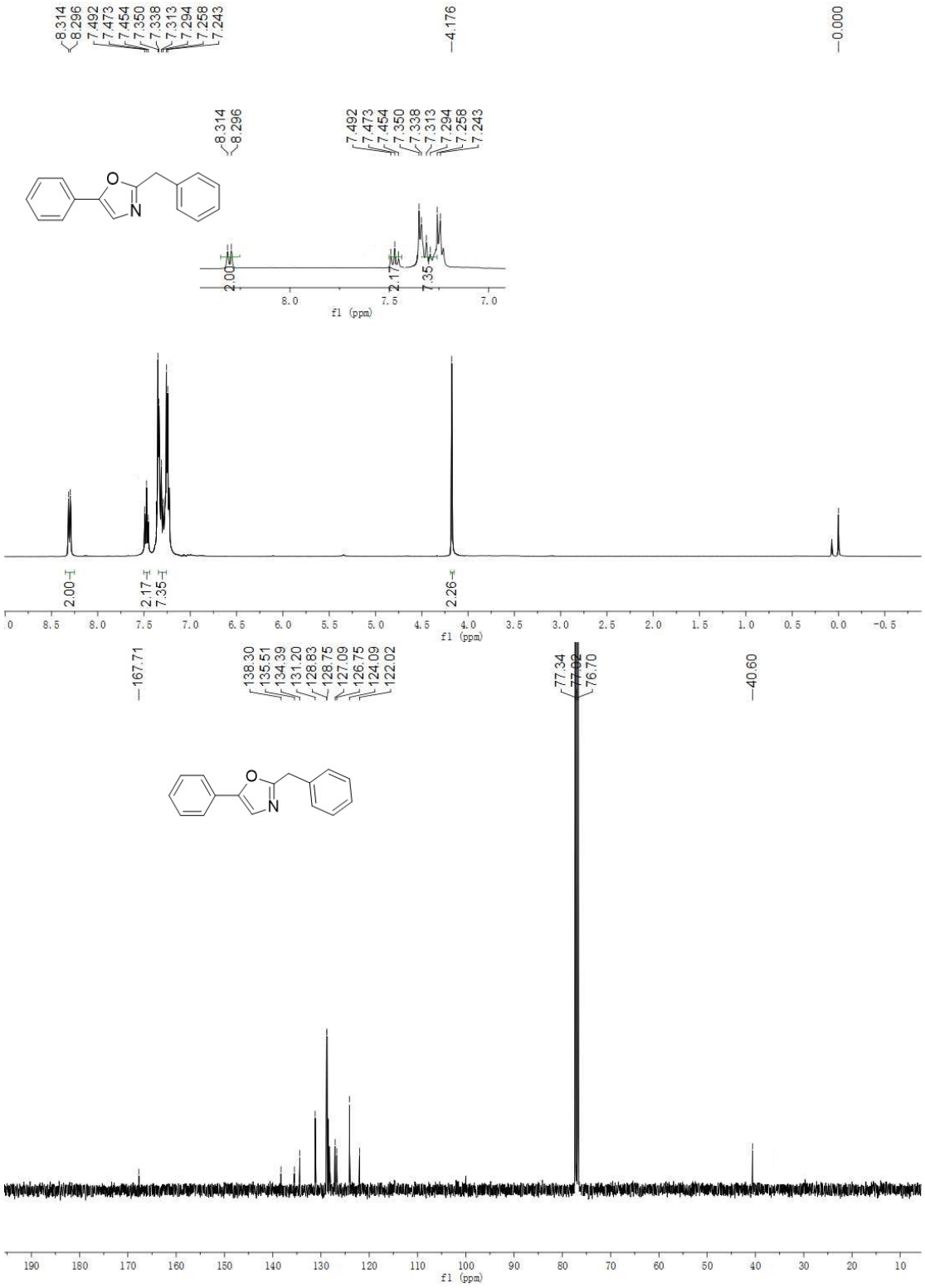
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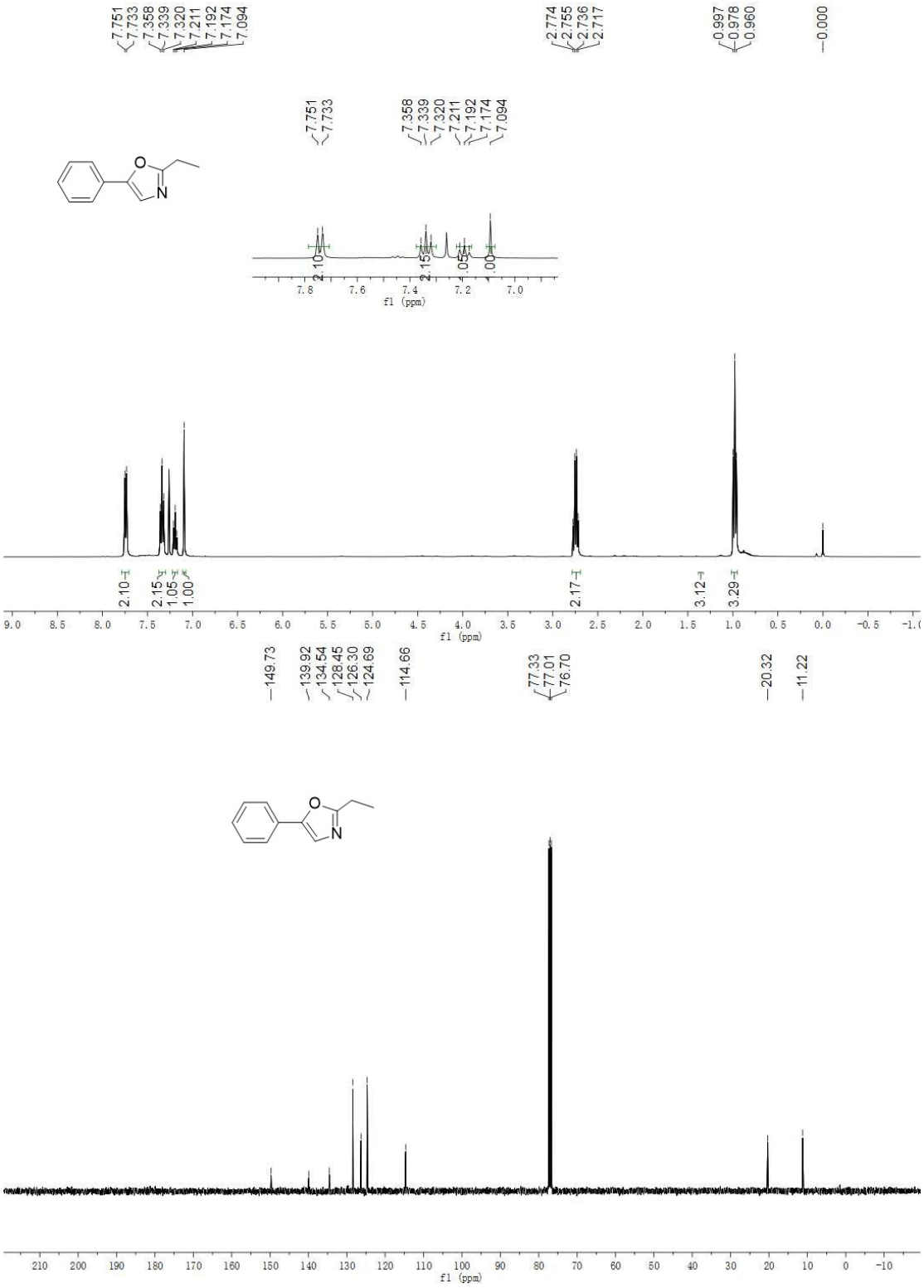
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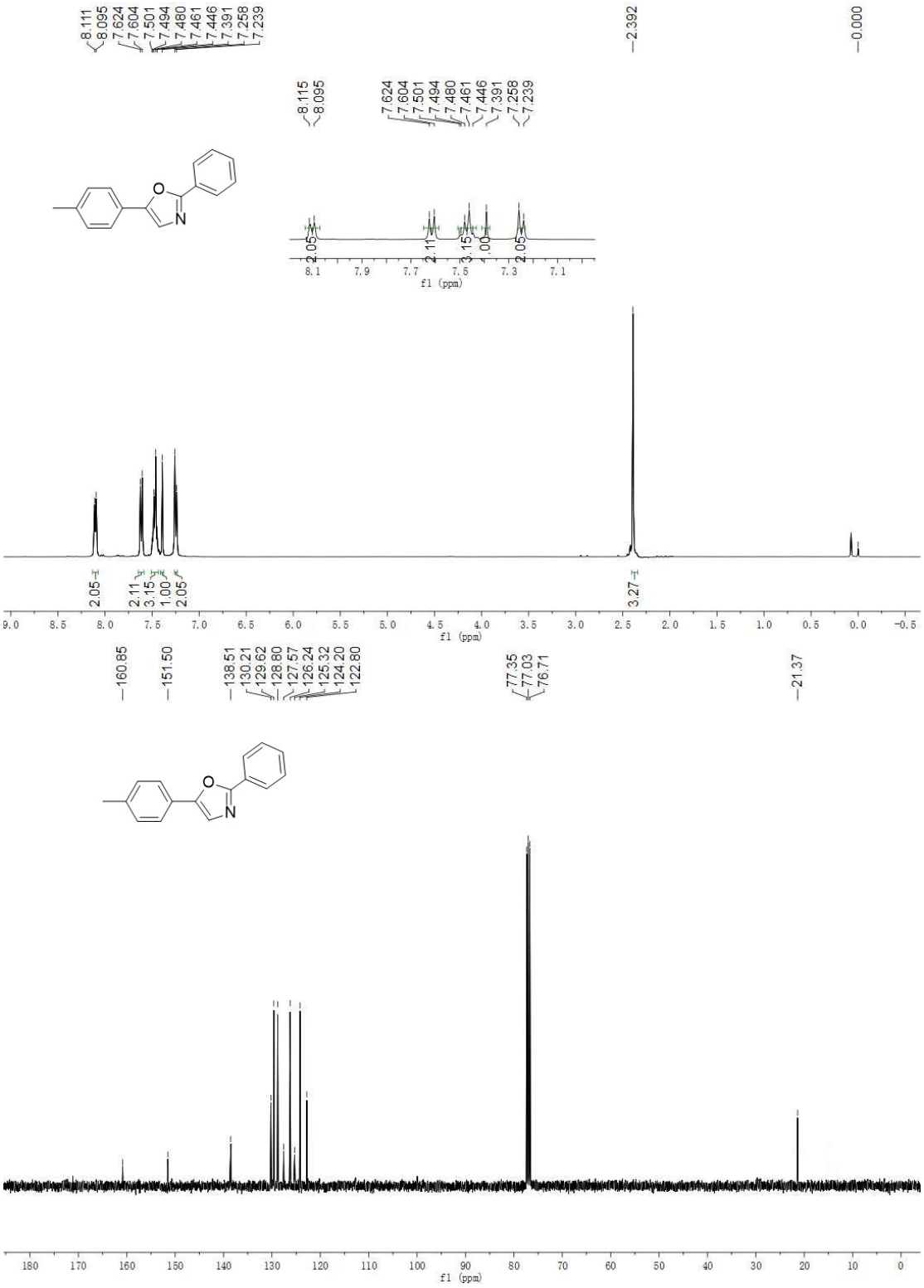
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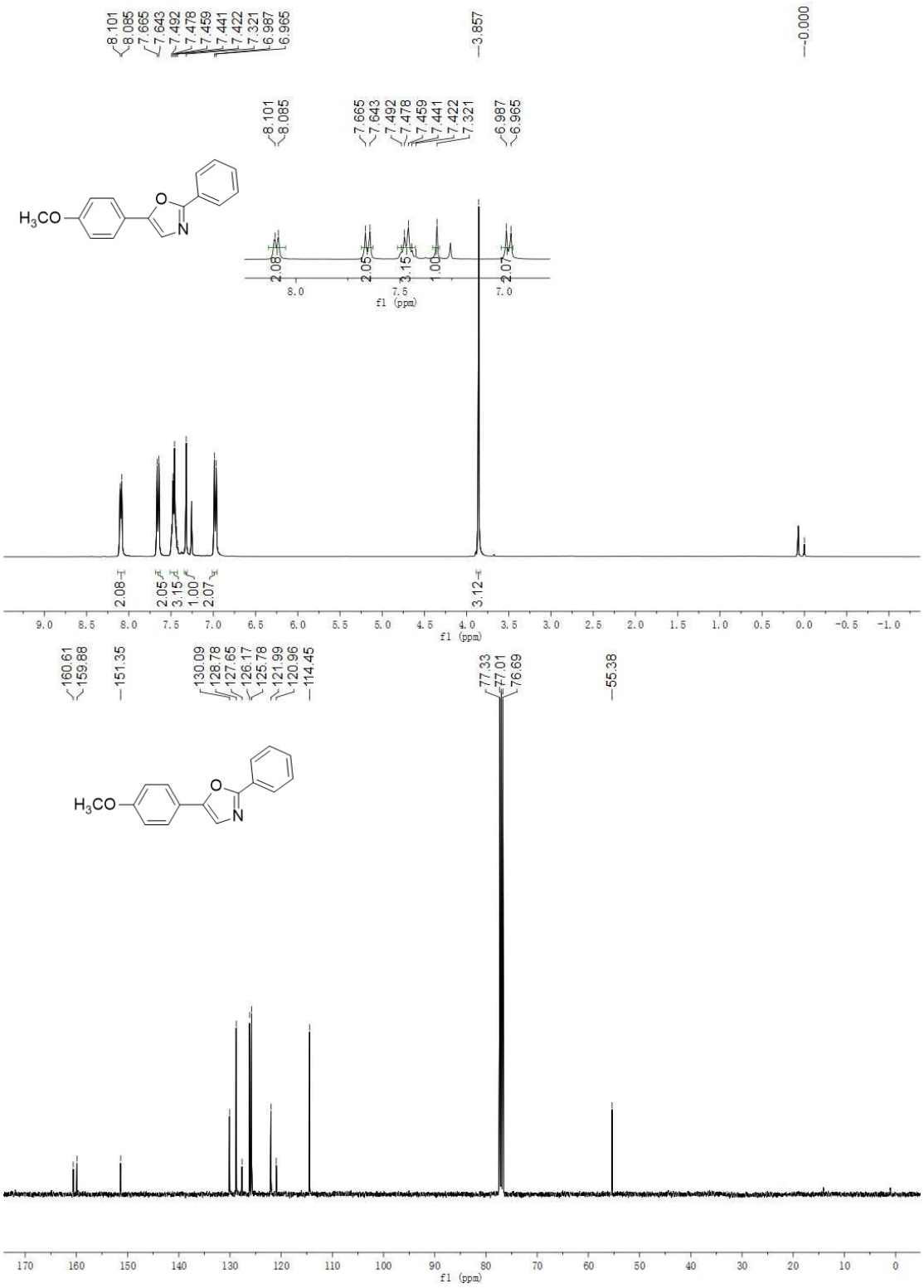
N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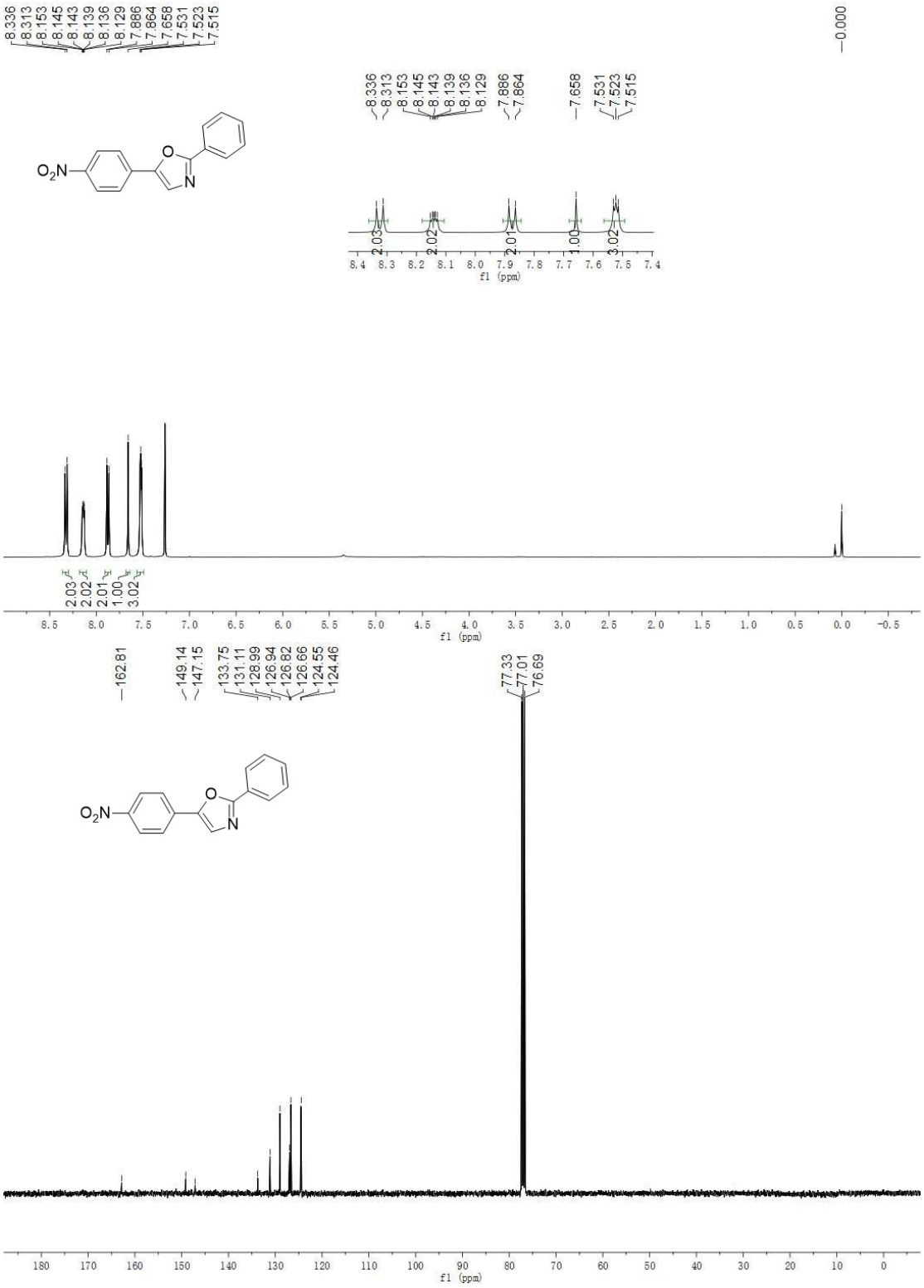
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2.02
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1.00
3.02
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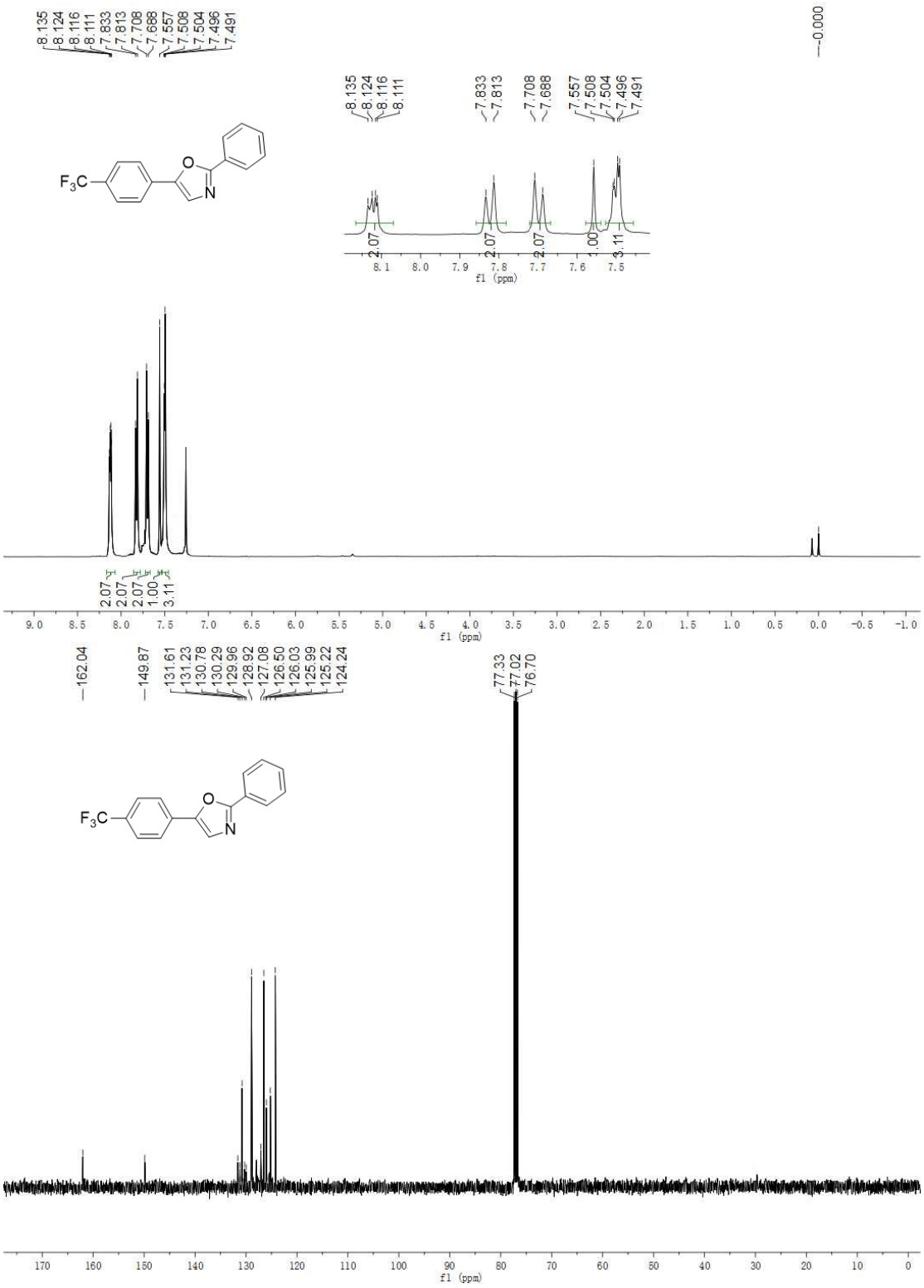
77.01
76.69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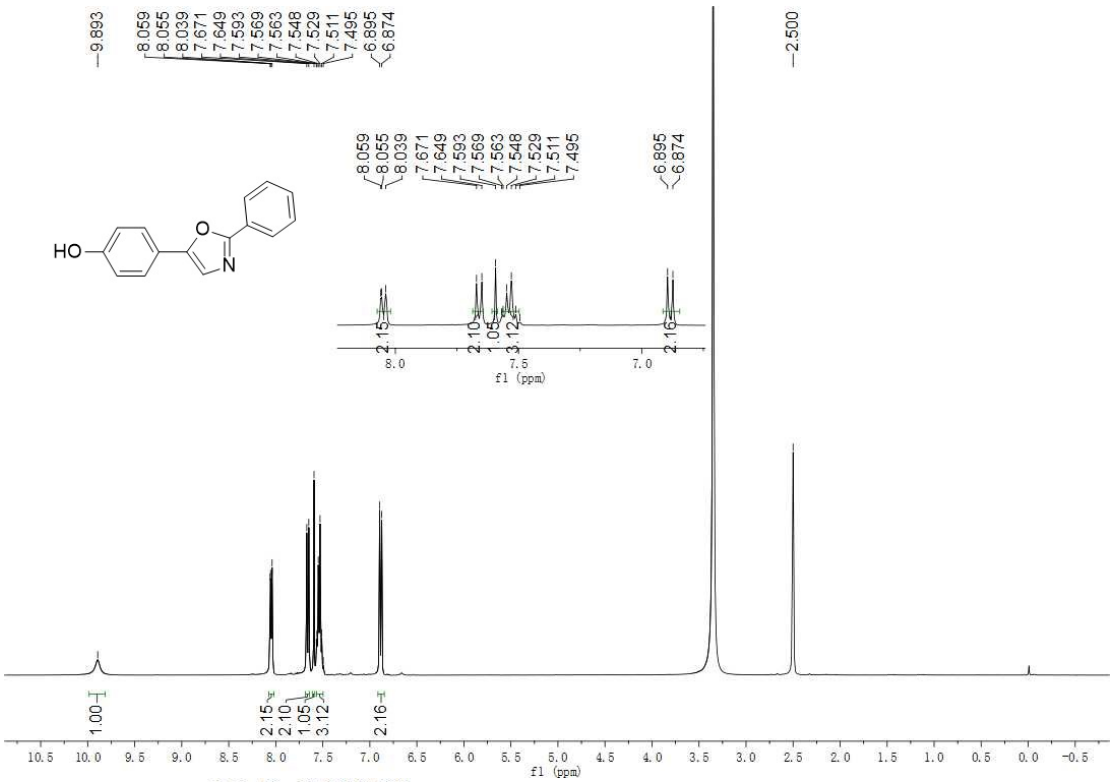
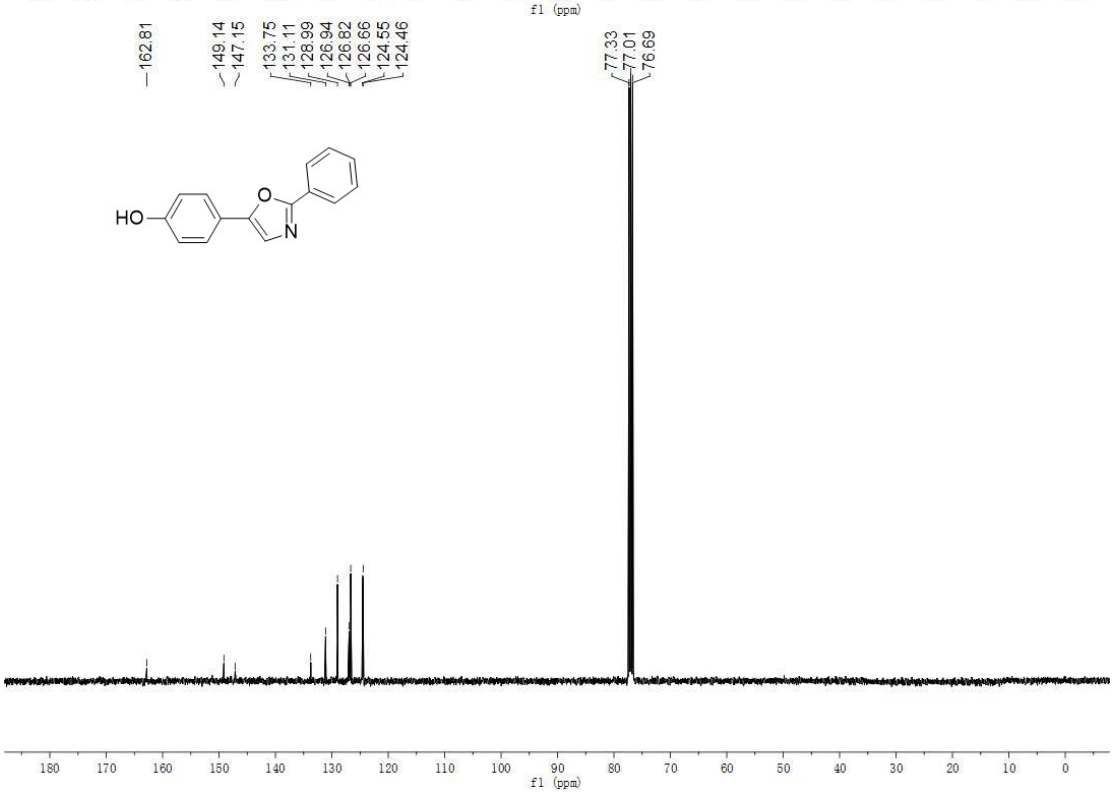
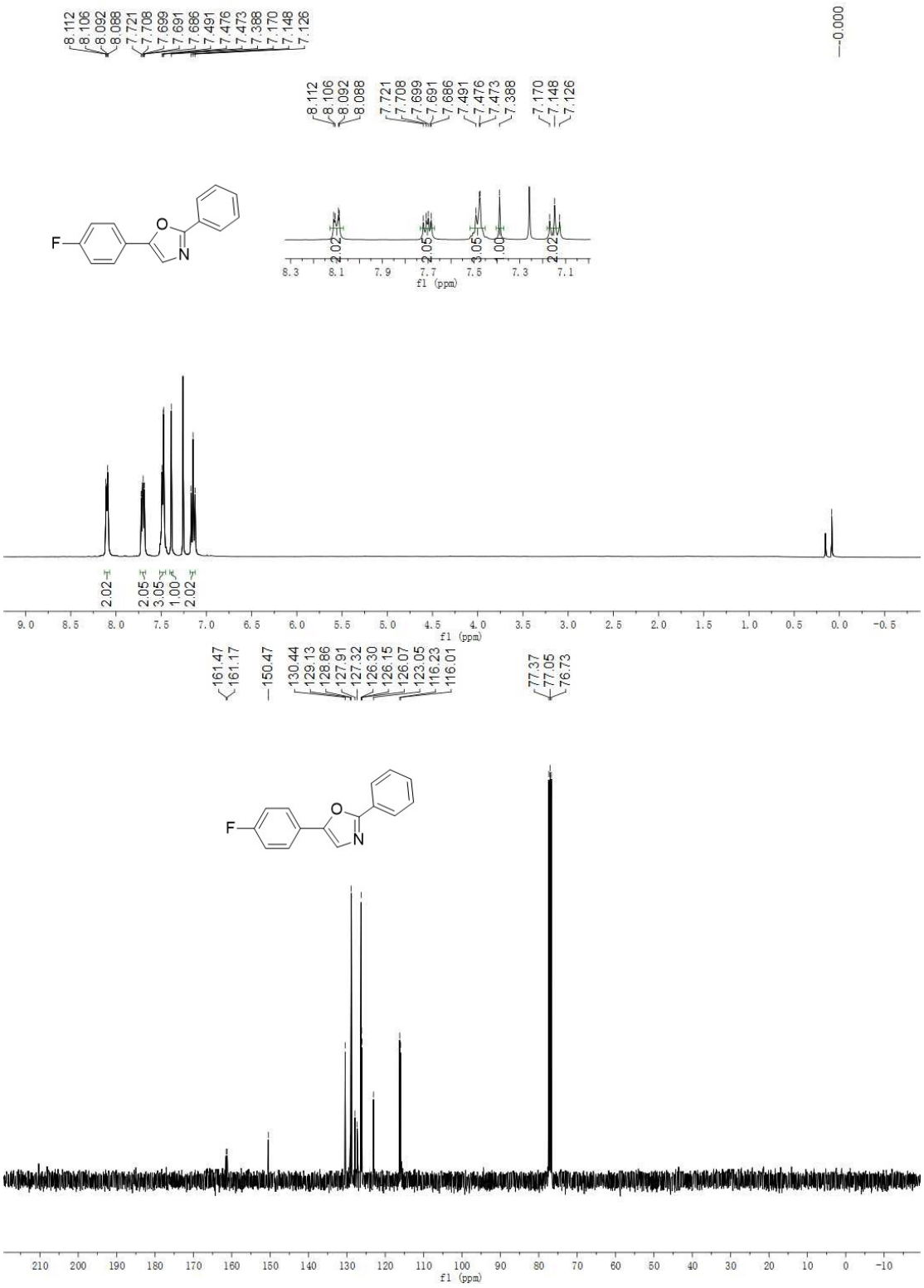
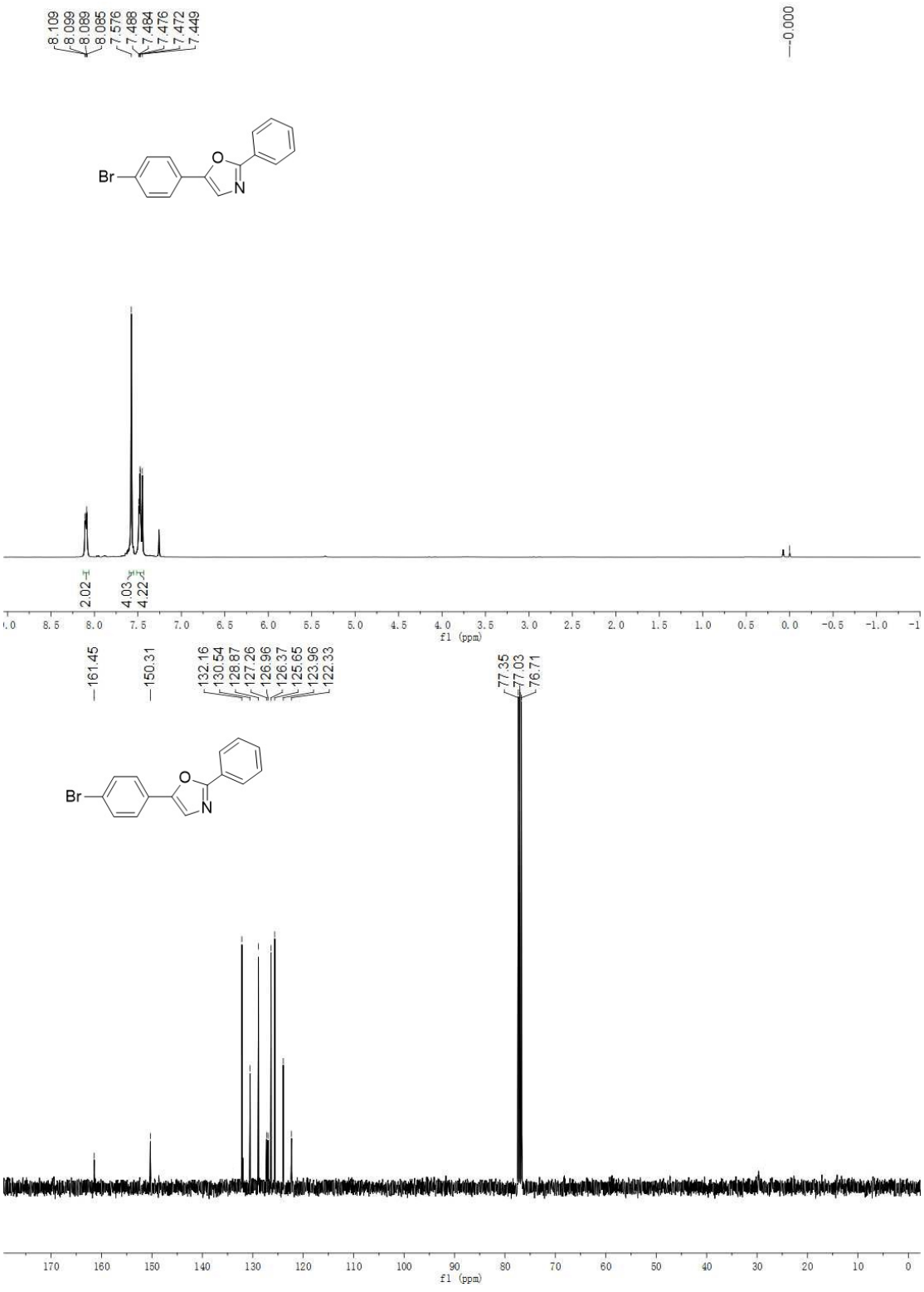
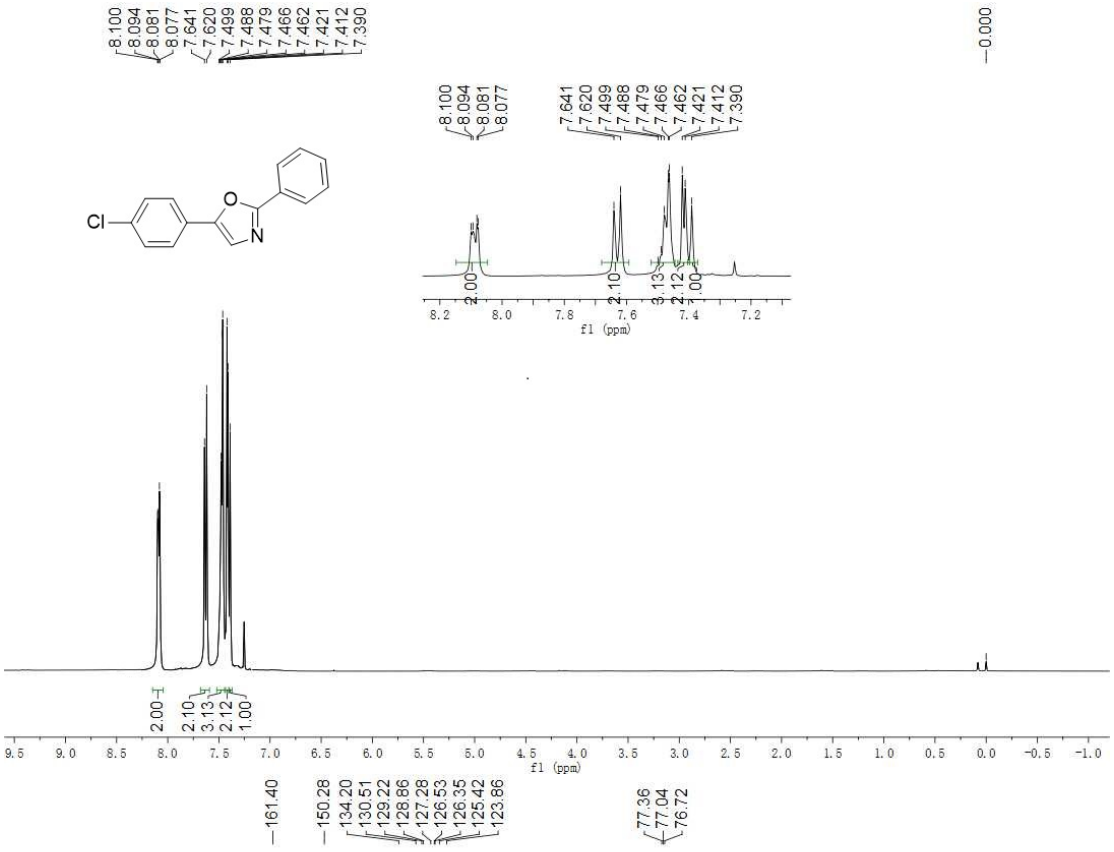
O
N
2.07
2.07
2.07
1.00
3.11
f1 (ppm)
162.04
149.87
131.61
131.23
130.78
130.29
129.96
128.92
127.08
126.50
126.03
125.99
125.22
124.24
77.33
77.02
76.70

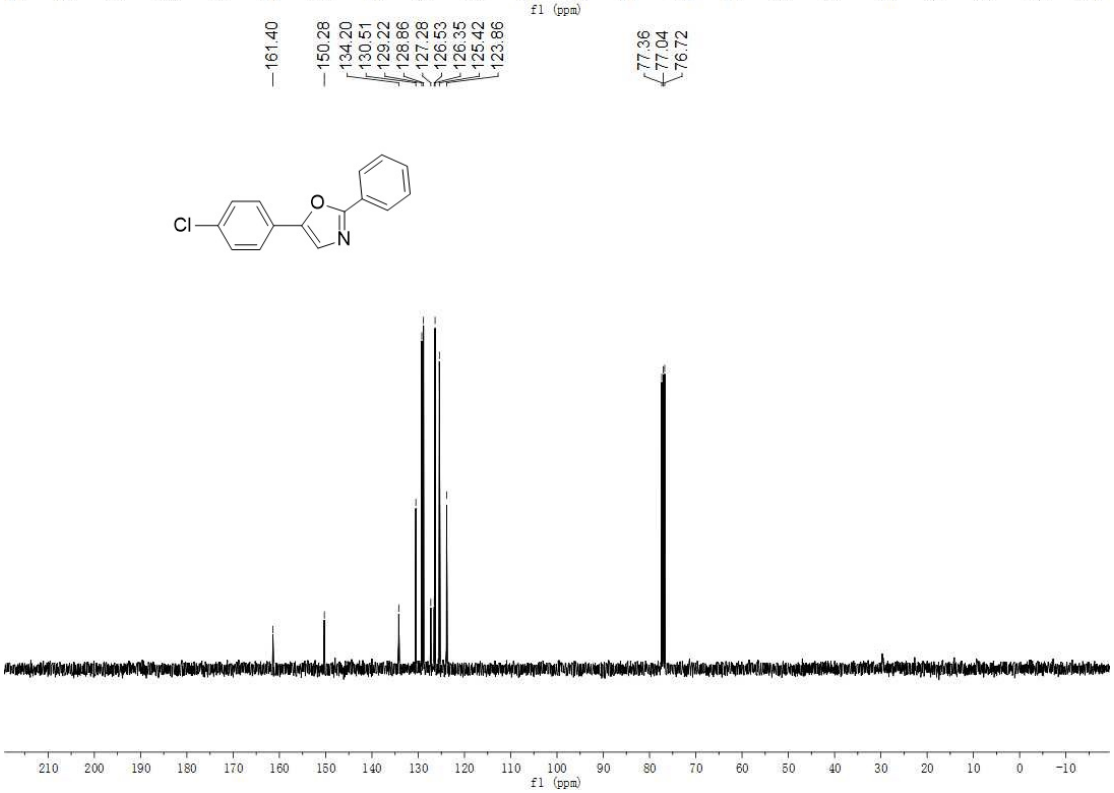

9.893
8.059
8.055
8.039
7.671
7.649
7.593
7.569
7.563
7.548
7.529
7.511
7.495
6.895
6.874
2.500
HO
O
N
1.00
2.15
2.10
1.05
3.12
2.16
f1 (ppm)

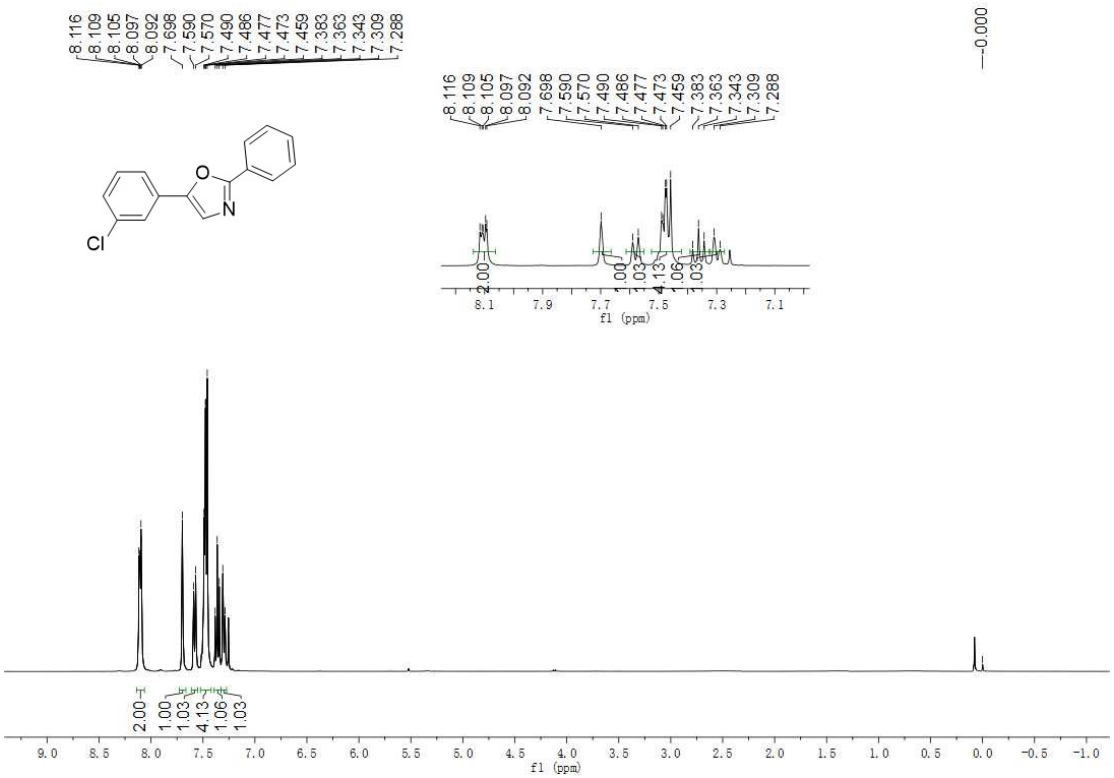

162.81
149.14
147.15
133.75
131.11
128.99
126.94
126.82
126.66
124.55
124.46
77.33
77.01
76.69
HO
O
N
f1 (ppm)

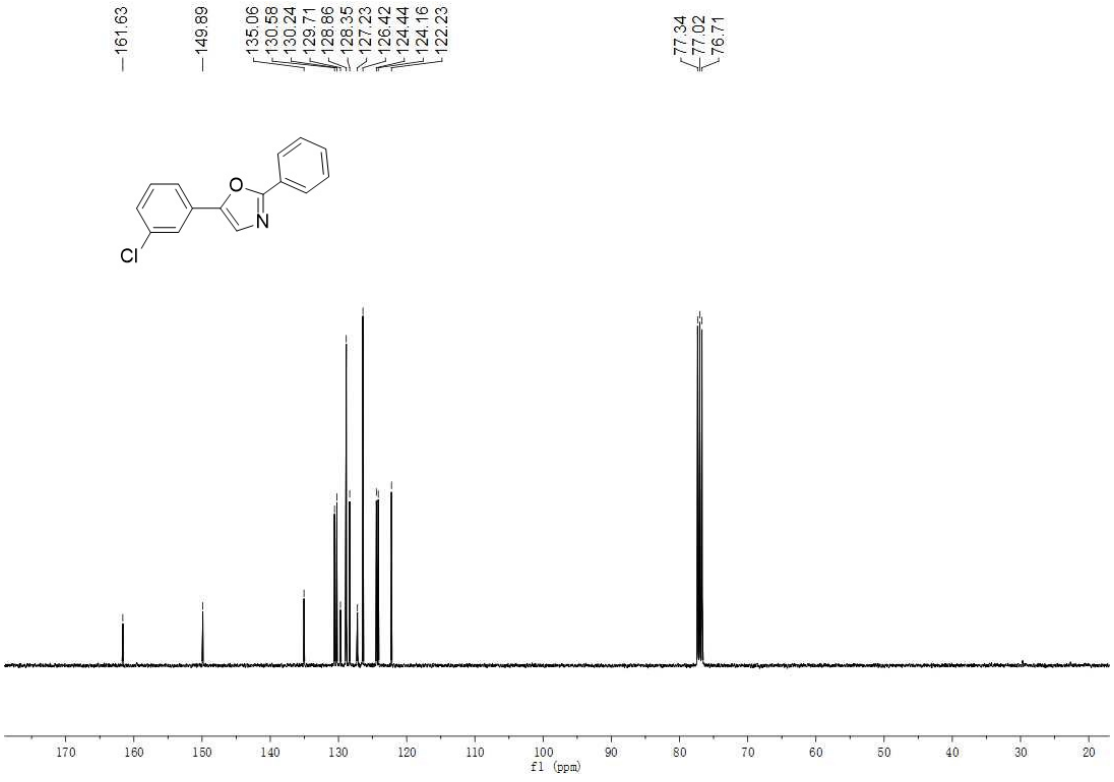

8.112
8.106
8.092
8.088
7.721
7.708
7.699
7.691
7.686
7.491
7.476
7.473
7.388
7.170
7.148
7.126
0.000
F
O
N
2.02
2.05
3.05
1.00
2.02
f1 (ppm)
161.47
161.17
150.47
130.44
129.13
128.86
127.91
127.32
126.30
126.15
126.07
123.05
116.23
116.01
77.37
77.05
76.73

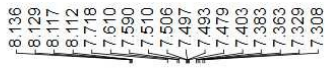

8.109
8.099
8.089
8.085
7.576
7.488
7.484
7.476
7.472
7.449
0.000
Br
O
N
2.02
4.03
4.22
f1 (ppm)
161.45
150.31
132.16
130.54
128.87
127.26
126.96
126.37
125.65
123.96
122.33
77.35
77.03
76.71
Br
O
N
f1 (ppm)

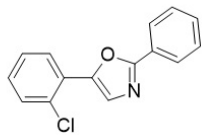

8.100
8.094
8.081
8.077
7.641
7.620
7.499
7.488
7.479
7.466
7.462
7.421
7.412
7.390
0.000
Cl
O
N
2.00
2.10
3.13
2.12
1.00
f1 (ppm)

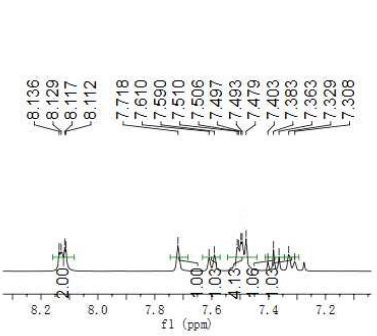

161.40
150.28
134.20
130.51
129.22
128.86
127.28
126.53
126.35
125.42
123.86
77.36
77.04
76.72
Cl
O
N
f1 (ppm)


8.116
8.109
8.105
8.097
8.092
7.698
7.590
7.570
7.490
7.486
7.477
7.473
7.459
7.383
7.363
7.343
7.309
7.288
-0.000
O
N
Cl
2.00
1.00
1.03
4.13
1.06
1.03
f1 (ppm)

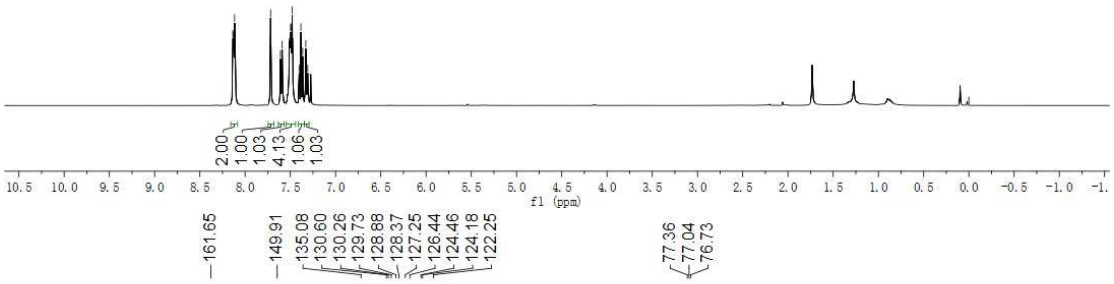

161.63
149.89
135.06
130.58
130.24
129.71
128.86
128.35
127.23
126.42
124.44
124.16
122.23
77.34
77.02
76.71
O
N
Cl
f1 (ppm)


8.136
8.129
8.117
8.112
7.718
7.610
7.590
7.510
7.506
7.497
7.493
7.479
7.403
7.383
7.363
7.329
7.308

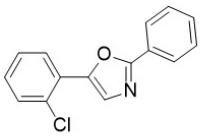

O
N
Cl

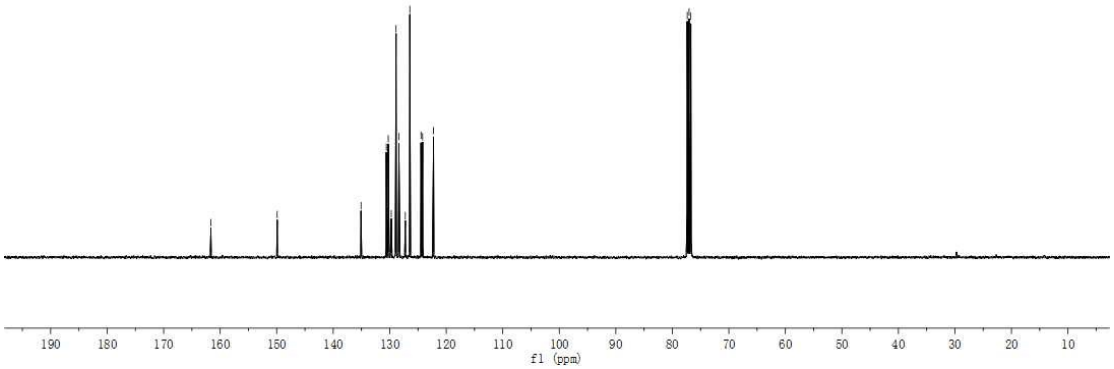

8.136
8.129
8.117
8.112
7.718
7.610
7.590
7.510
7.506
7.497
7.493
7.479
7.403
7.383
7.363
7.329
7.308
2.00
1.00
1.03
4.13
1.06
1.03
8.2
8.0
7.8
7.6
7.4
7.2
f1 (ppm)

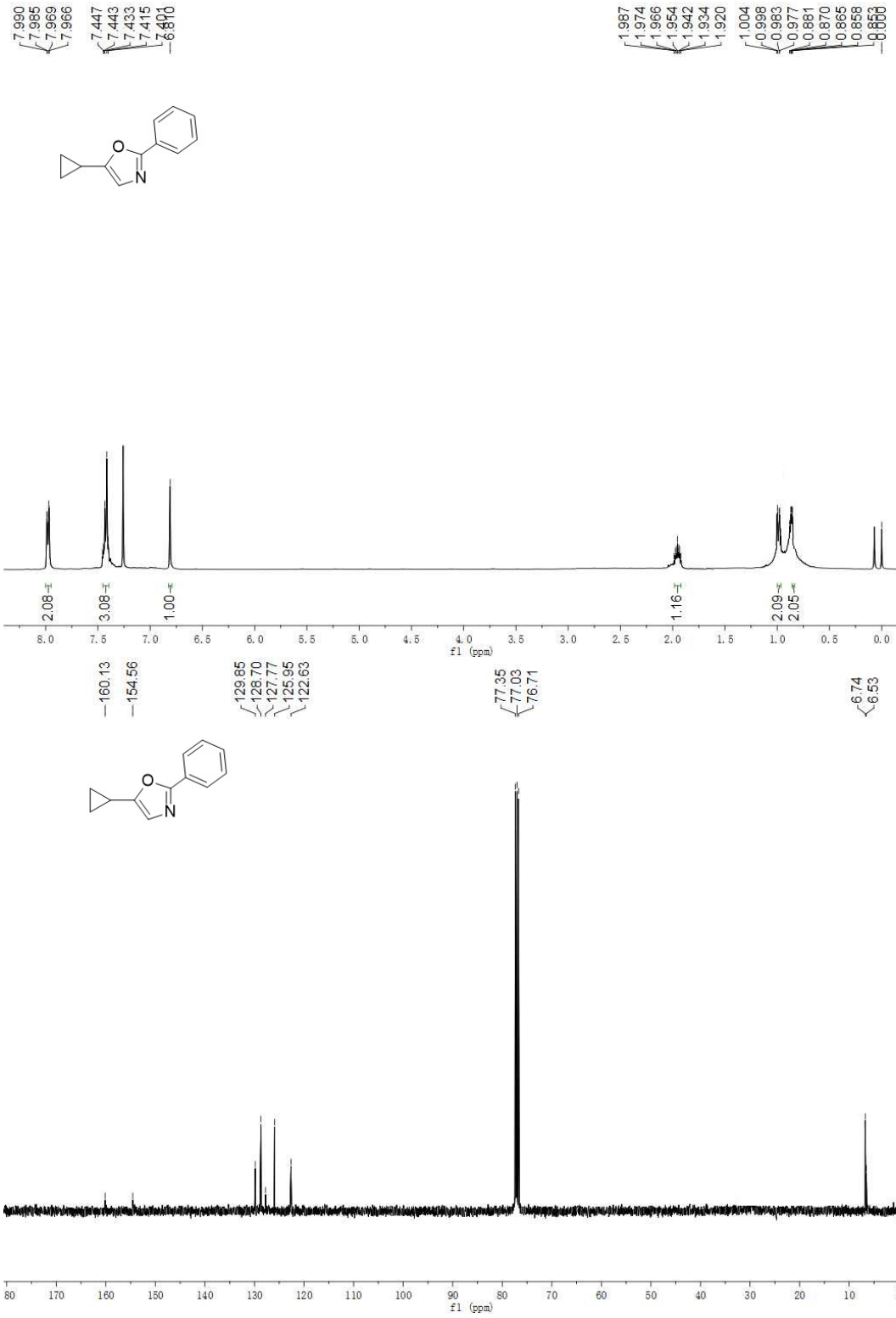

0.000


2.00
1.00
1.03
4.13
1.06
1.03
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
f1 (ppm)

161.65
149.91
135.08
130.60
130.26
129.73
128.88
128.37
127.25
126.44
124.46
124.18
122.25
77.36
77.04
76.73


O
N
Cl


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.990
7.985
7.969
7.966
7.447
7.443
7.433
7.415
7.401
6.810
1.987
1.974
1.966
1.954
1.942
1.934
1.920
1.004
0.998
0.983
0.977
0.881
0.870
0.865
0.658
2.08
3.08
1.00
1.16
2.09
2.05
f1 (ppm)
160.13
154.56
129.85
128.70
127.77
125.95
122.63
77.35
77.03
76.71
6.74
6.53
f1 (ppm)