Supporting Information

$K_2S_2O_8$-Prompted Rearrangement of Nitrones for the Synthesis of Benzo[d]oxazoles

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Contents

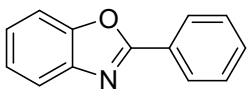
1. General information

^{1}H NMR and ^{13}C NMR spectra were recorded on 300MHz and 75MHz in $CDCl_3$ (^{1}H NMR and ^{13}C NMR spectra of 2bl and 2ak were recorded on 400MHz and 101MHz in $CDCl_3$). All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. Products were purified by flash chromatogrgraphy on 200-300 mesh silica gel. Unless otherwise noted, commercially reagents were used without further purification.

General procedure for the synthesis of 2 (2aa as an example)

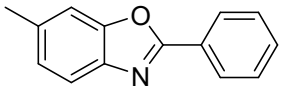
Synthesis of 2aa: A test tube was charged with nitrone (0.2 mmol), $K_2S_2O_8$ (0.6 mmol) in DCE (2 mL). The mixture was stirred at 120°C for 12 h. When the reaction was completed, the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 30:1) to yield the isolated product 2aa.

2. Characterization data for isolated compounds

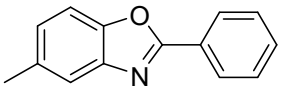


2-phenylbenzo[*d*]oxazole 2aa.[1,2] White solid (33.5 mg 86%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 – 8.23 (m, 2H), 7.83 – 7.76 (m, 1H), 7.64 – 7.57 (m, 1H), 7.57 – 7.51 (m, 3H), 7.41 – 7.33 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.00 (s), 150.72 (s), 142.06 (s), 131.48 (s),

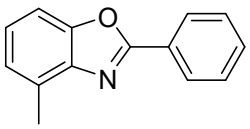
128.87 (s), 127.58 (s), 127.13 (s), 125.07 (s), 124.54 (s), 119.98 (s), 110.56 (s).



6-methyl-2-phenylbenzo[*d*]oxazole 2ab.[3] White solid (33.4 mg 80%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.16 – 8.08 (m, 2H), 7.53 (d, J = 8.1 Hz, 1H), 7.40 (dd, J = 6.6, 3.6 Hz, 3H), 7.25 (s, 1H), 7.05 (d, J = 8.1 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.48 (s), 150.98 (s), 139.86 (s), 135.47 (s), 131.18 (s), 128.78 (s), 127.38 (s), 125.73 (s), 119.27 (s), 110.68 (s), 77.42 (s), 77.00 (s), 76.58 (s), 21.73 (s).

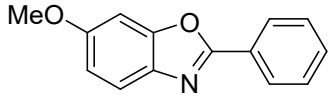


5-methyl-2-phenylbenzo[*d*]oxazole 2ac.[3] White solid (34.8 mg 83%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (dd, J = 6.8, 3.0 Hz, 2H), 7.55 (s, 1H), 7.53 – 7.48 (m, 3H), 7.45 (d, J = 8.3 Hz, 1H), 7.19 – 7.11 (m, 1H), 2.48 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.01 (s), 148.86 (s), 142.15 (s), 134.32 (s), 131.33 (s), 128.82 (s), 127.45 (s), 127.18 (s), 126.17 (s), 119.81 (s), 109.89 (s), 77.42 (s), 77.00 (s), 76.58 (s), 21.52 (s).

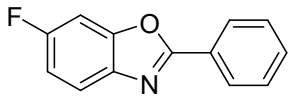


4-methyl-2-phenylbenzo[*d*]oxazole 2ad.[5] White solid (11.3 mg 27%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 – 8.23 (m, 2H), 7.54 – 7.47 (m, 3H), 7.39 (d, J = 8.0 Hz, 1H), 7.24 (t, J = 3.8 Hz, 1H), 7.14 (d, J = 7.4 Hz, 1H), 2.68 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.26 (s), 150.53 (s), 141.43 (s), 131.23 (s), 130.59 (s), 128.80 (s), 127.58 (s),

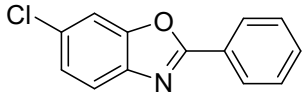
127.45 (s), 125.02 (s), 124.71 (s), 107.81 (s), 16.55 (s).



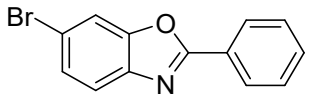
6-methoxy-2-phenylbenzo[*d*]oxazole 2ae.[6] White solid (26.7 mg 59%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.25 – 8.14 (m, 2H), 7.64 (d, J = 8.7 Hz, 1H), 7.56 – 7.45 (m, 3H), 7.11 (d, J = 2.3 Hz, 1H), 6.96 (dd, J = 8.7, 2.4 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.24 (s), 151.60 (s), 135.83 (s), 131.04 (s), 128.84 (s), 127.31 (s), 127.15 (s), 119.95 (s), 112.79 (s), 95.39 (s), 77.42 (s), 77.00 (s), 76.58 (s), 55.92 (s).



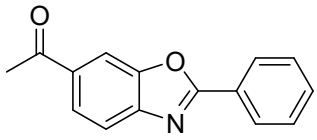
6-fluoro-2-phenylbenzo[*d*]oxazole 2af.[3] White solid (34.3 mg 82%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.15 – 8.09 (m, 2H), 7.60 (dd, J = 8.7, 4.9 Hz, 1H), 7.47 – 7.39 (m, 3H), 7.23 – 7.16 (m, 1H), 7.05 – 6.97 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.27 (s), 159.04 (s), 150.69 (d, J = 14.4 Hz), 138.42 (s), 131.56 (s), 128.92 (s), 127.46 (s), 126.88 (s), 120.22 (d, J = 10.1 Hz), 112.67 (s), 112.34 (s), 98.82 (s), 98.45 (s), 77.42 (s), 77.00 (s), 76.58 (s).



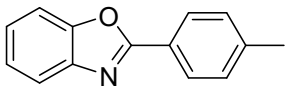
6-chloro-2-phenylbenzo[*d*]oxazole 2ag.[3] White solid (41.7 mg 91%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 – 8.14 (m, 2H), 7.65 (d, J = 8.5 Hz, 1H), 7.56 (d, J = 1.7 Hz, 1H), 7.54 – 7.44 (m, 3H), 7.35 – 7.27 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.64 (s), 150.87 (s), 140.85 (s), 131.74 (s), 130.63 (s), 128.91 (s), 127.61 (s), 126.66 (s), 125.23 (s), 120.42 (s), 111.18 (s).



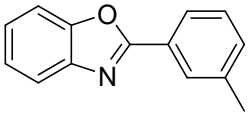
6-bromo-2-phenylbenzo[*d*]oxazole 2ah.[4] White solid (45.3 mg 83%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.23 (ddd, J = 5.5, 3.1, 1.5 Hz, 2H), 7.76 – 7.71 (m, 1H), 7.62 (d, J = 8.5 Hz, 1H), 7.57 – 7.49 (m, 3H), 7.49 – 7.44 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.49 (s), 151.17 (s), 141.29 (s), 131.79 (s), 128.93 (s), 127.98 (s), 127.65 (s), 126.62 (s), 120.90 (s), 117.92 (s), 114.07 (s), 77.42 (s), 77.00 (s), 76.58 (s).



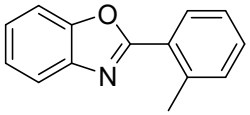
1-(2-phenylbenzo[d]oxazol-6-yl)ethan-1-one 2ak. White solid (22.3 mg 47%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 – 8.26 (m, 2H), 8.20 (d, J = 1.1 Hz, 1H), 8.03 – 7.99 (m, 1H), 7.84 – 7.78 (m, 1H), 2.69 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 196.94 (s), 165.88 (s), 150.77 (s), 146.14 (s), 134.38 (s), 132.31 (s), 129.08 (s), 128.02 (s), 126.56 (s), 125.52 (s), 119.69 (s), 110.81 (s), 26.91 (s).



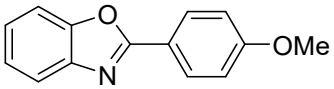
2-(p-tolyl)benzo[*d*]oxazole 2ba.[1] White solid (27.2 mg 65%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (d, J = 8.0 Hz, 2H), 7.78 – 7.71 (m, 1H), 7.59 – 7.53 (m, 1H), 7.32 (dd, J = 8.5, 3.8 Hz, 4H), 2.42 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.25 (s), 150.65 (s), 142.15 (s), 141.99 (s), 129.59 (s), 127.55 (s), 125.49 (s), 124.81 (s), 124.42 (s), 122.31 (s), 119.80 (s), 110.44 (s), 77.42 (s), 77.00 (s), 76.58 (s), 21.59 (s).



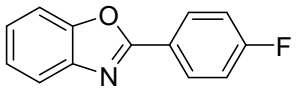
2-(m-tolyl)benzo[*d*]oxazole 2bb.[4] White solid (23.4 mg 56%); ^{1}H NMR (300 MHz, CDCl3) δ 8.05 (d, J = 7.6 Hz, 1H), 7.81 – 7.74 (m, 1H), 7.61 – 7.54 (m, 1H), 7.40 (d, J = 7.6 Hz, 1H), 7.35 (dd, J = 5.7, 3.5 Hz, 3H), 2.45 (s, 3H). 13C NMR (75 MHz, CDCl3) δ 150.59 (s), 141.94 (s), 138.67 (s), 132.32 (s), 128.76 (s), 128.09 (s), 126.84 (s), 124.98 (s), 124.64 (s), 124.48 (s), 119.85 (s), 110.51 (s), 77.42 (s), 77.00 (s), 76.58 (s), 21.32 (s).



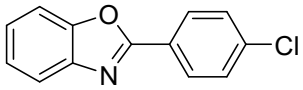
2-(o-tolyl)benzo[*d*]oxazole 2bc.[1] White solid (10.1 mg 56%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 (dd, J = 6.5, 3.0 Hz, 1H), 7.86 – 7.79 (m, 1H), 7.64 – 7.57 (m, 1H), 7.46 – 7.32 (m, 5H), 2.84 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.38 (s), 150.28 (s), 142.10 (s), 138.82 (s), 131.75 (s), 130.86 (s), 129.92 (s), 126.22 (s), 126.02 (s), 124.97 (s), 124.33 (s), 120.11 (s), 110.45 (s), 77.42 (s), 77.00 (s), 76.58 (s), 22.17 (s).



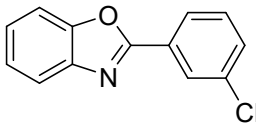
2-(4-methoxyphenyl)benzo[*d*]oxazole 2bd.[3] White solid (21.5 mg 51%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 (dd, J = 9.0, 2.1 Hz, 2H), 7.78 – 7.69 (m, 1H), 7.60 – 7.51 (m, 1H), 7.38 – 7.27 (m, 2H), 7.03 (dd, J = 8.9, 2.0 Hz, 2H), 3.89 (d, J = 2.0 Hz, 3H). ^{13}C NMR (75 MHz, CDCl) δ 163.08 (s), 162.20 (s), 150.50 (s), 142.04 (s), 129.30 (s), 124.55 (s), 124.37 (s), 119.49 (s), 114.25 (s), 110.32 (s), 77.42 (s), 77.00 (s), 76.58 (s), 55.37 (s).



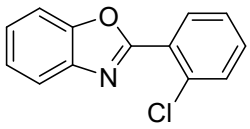
2-(4-fluorophenyl)benzo[*d*]oxazole 2be.[2] White solid (36.6 mg 88%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.29 – 8.20 (m, 2H), 7.80 – 7.71 (m, 1H), 7.59 – 7.52 (m, 1H), 7.38 – 7.30 (m, 2H), 7.24 – 7.15 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.44 (s), 163.09 (s), 162.11 (s), 150.73 (s), 142.03 (s), 129.79 (d, J = 8.9 Hz), 125.09 (s), 124.62 (s), 123.45 (s), 119.95 (s), 116.28 (s), 115.99 (s), 110.52 (s), 77.42 (s), 77.00 (s), 76.58 (s).



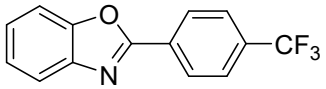
2-(4-chlorophenyl)benzo[*d*]oxazole 2bf.[1] White solid (43.5 mg 95%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 – 8.11 (m, 2H), 7.79 – 7.71 (m, 1H), 7.59 – 7.51 (m, 1H), 7.50 – 7.43 (m, 2H), 7.34 (dd, J = 6.0, 3.2 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.98 (s), 150.70 (s), 141.97 (s), 137.69 (s), 129.19 (s), 128.78 (s), 125.61 (s), 125.28 (s), 124.67 (s), 120.04 (s), 110.56 (s).



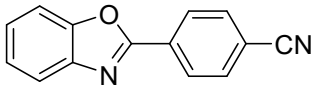
2-(3-chlorophenyl)benzo[*d*]oxazole 2bg.[8] White solid (39.4 mg 86%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.25 (t, J = 1.6 Hz, 1H), 8.13 (d, J = 7.3 Hz, 1H), 7.82 – 7.75 (m, 1H), 7.60 – 7.56 (m, 1H), 7.50 – 7.44 (m, 2H), 7.39 – 7.35 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.49 (s), 150.66 (s), 134.96 (s), 131.35 (s), 130.11 (s), 128.74 (s), 127.49 (s), 125.52 (s), 125.43 (s), 124.71 (s), 120.13 (s), 110.60 (s).



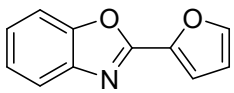
2-(2-chlorophenyl)benzo[*d*]oxazole 2bh.[8] White solid (16.5 mg 36%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.20 – 8.13 (m, 1H), 7.91 – 7.82 (m, 1H), 7.67 – 7.54 (m, 2H), 7.50 – 7.36 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.55 (s), 141.66 (s), 133.46 (s), 131.87 (s), 131.79 (s), 131.35 (s), 126.89 (s), 126.24 (s), 125.54 (s), 124.62 (s), 120.48 (s), 110.71 (s).



2-(4-(trifluoromethyl)phenyl)benzo[*d*]oxazole 2bi.[3] White solid (43.7 mg 83%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 – 8.33 (m, 2H), 7.83 – 7.75 (m, 3H), 7.64 – 7.57 (m, 1H), 7.43 – 7.36 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.44 (s), 150.85 (s), 141.90 (s), 133.18 (s), 132.74 (s), 130.43 (s), 127.82 (s), 125.87 (dd, J = 8.6, 4.8 Hz), 124.91 (s), 120.39 (s), 110.76 (s).

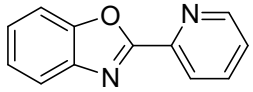


4-(benzo[*d*]oxazol-2-yl)benzonitrile 2bj.[2] White solid (39.2 mg 89%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.33 (dd, J = 8.2, 0.6 Hz, 2H), 7.83 – 7.75 (m, 3H), 7.60 (ddd, J = 4.6, 2.3, 0.7 Hz, 1H), 7.45 – 7.36 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.82 (s), 150.81 (s), 141.79 (s), 132.59 (s), 131.02 (s), 127.87 (s), 126.10 (s), 125.06 (s), 120.50 (s), 118.08 (s), 114.66 (s), 110.80 (s).



2-(furan-2-yl)benzo[*d*]oxazole 2bk.[7] White solid (10.1 mg 27%); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 – 7.72 (m, 1H), 7.70 – 7.65

(m, 1H), 7.60 – 7.52 (m, 1H), 7.40 – 7.31 (m, 2H), 7.28 (dd, J = 3.5, 0.6 Hz, 1H), 6.62 (dd, J = 3.5, 1.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.09 (s), 145.68 (s), 142.57 (s), 141.59 (s), 125.23 (s), 124.80 (s), 120.09 (s), 114.22 (s), 112.21 (s), 110.51 (s).



2bl

2-(pyridin-2-yl)benzo[d]oxazole 2bl.[9] White solid (14.9 mg 38%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, J = 4.4 Hz, 1H), 8.37 (d, J = 7.9 Hz, 1H), 7.93 – 7.80 (m, 2H), 7.72 – 7.64 (m, 1H), 7.49 – 7.36 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.43 (s), 151.03 (s), 150.28 (s), 146.04 (s), 141.74 (s), 137.09 (s), 126.03 (s), 125.57 (s), 124.92 (s), 123.43 (s), 120.62 (s), 111.22 (s).

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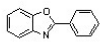
9. F. Zhu, J. L. Tao and Z. X. Wang, *Org Lett*, **2015**, *17*, 4926.

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



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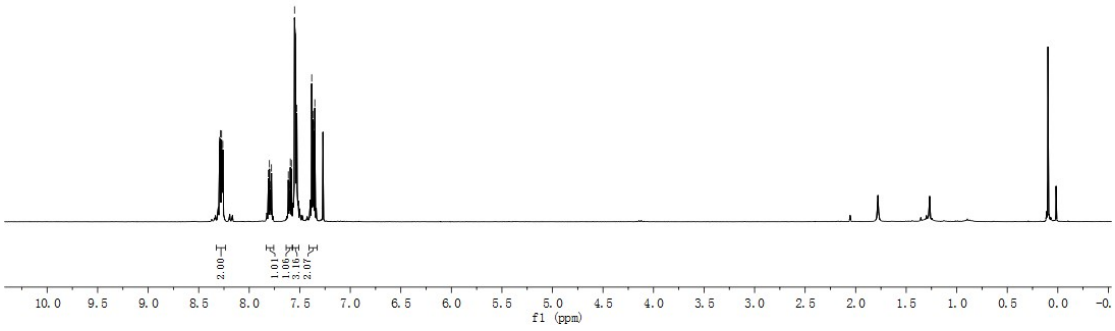

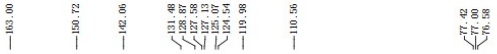

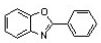

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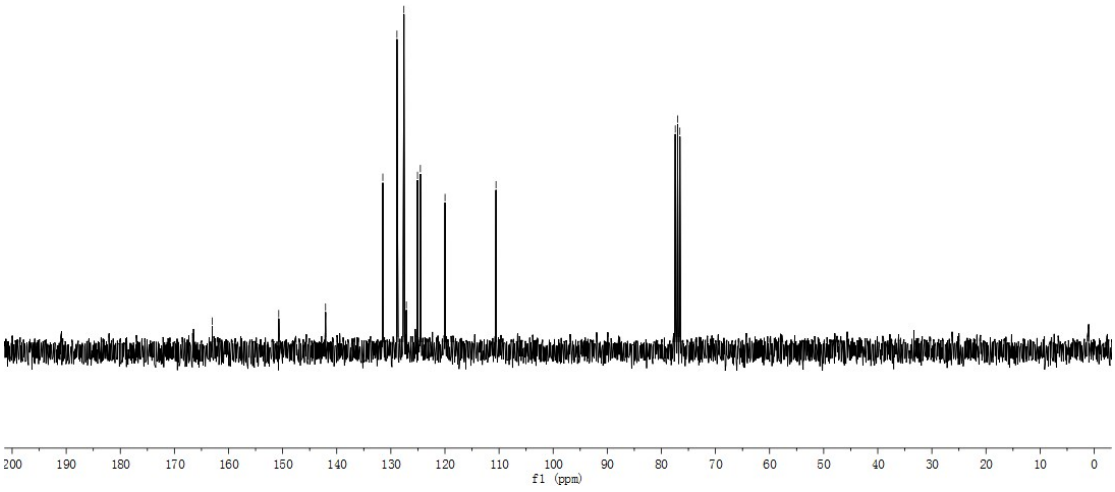

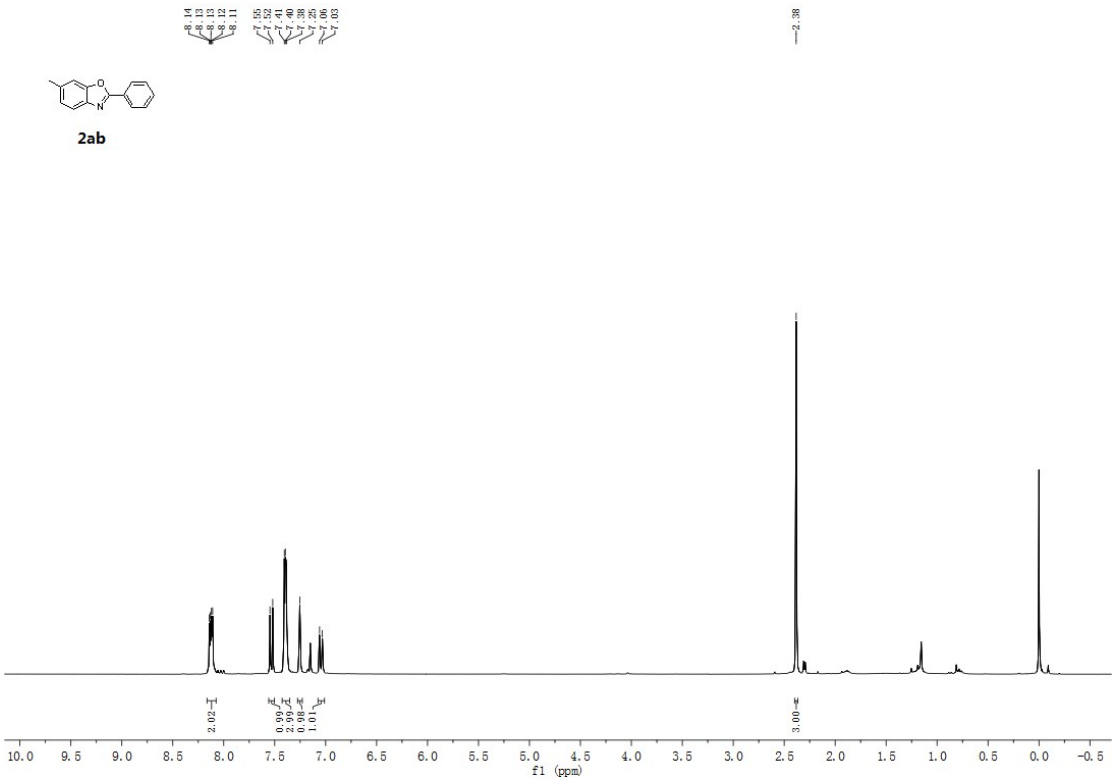
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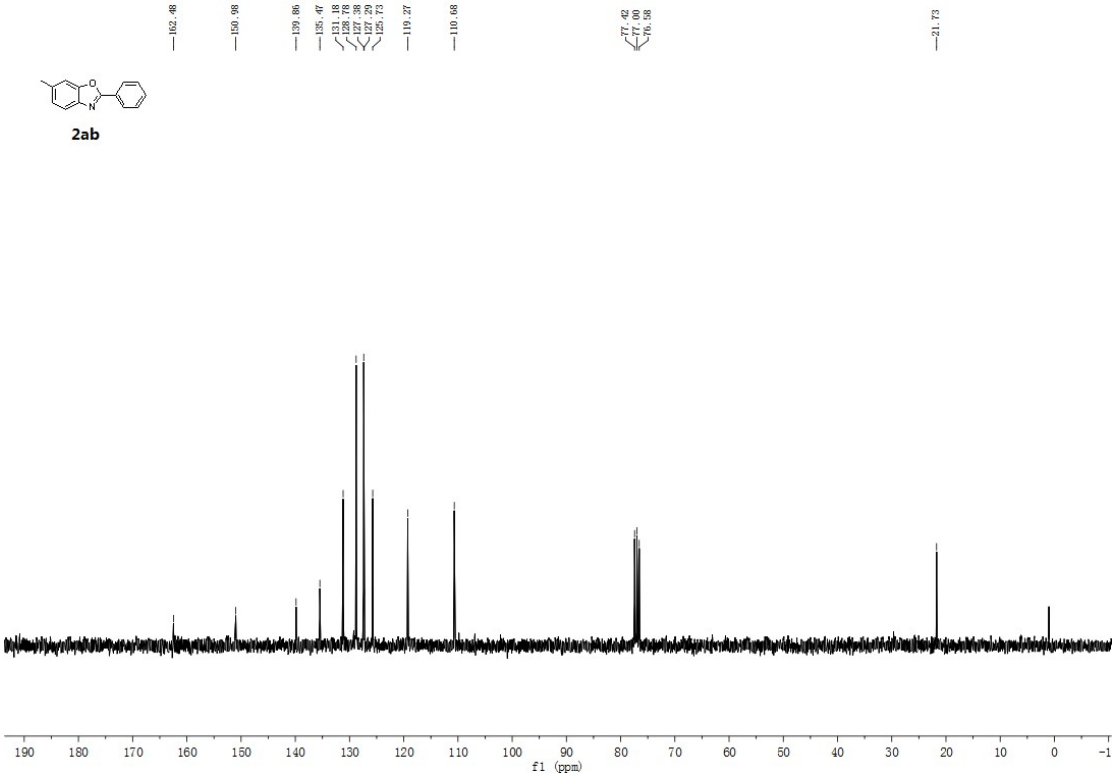
7.03
2.38
2.02
0.99
2.99
0.98
1.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

2ab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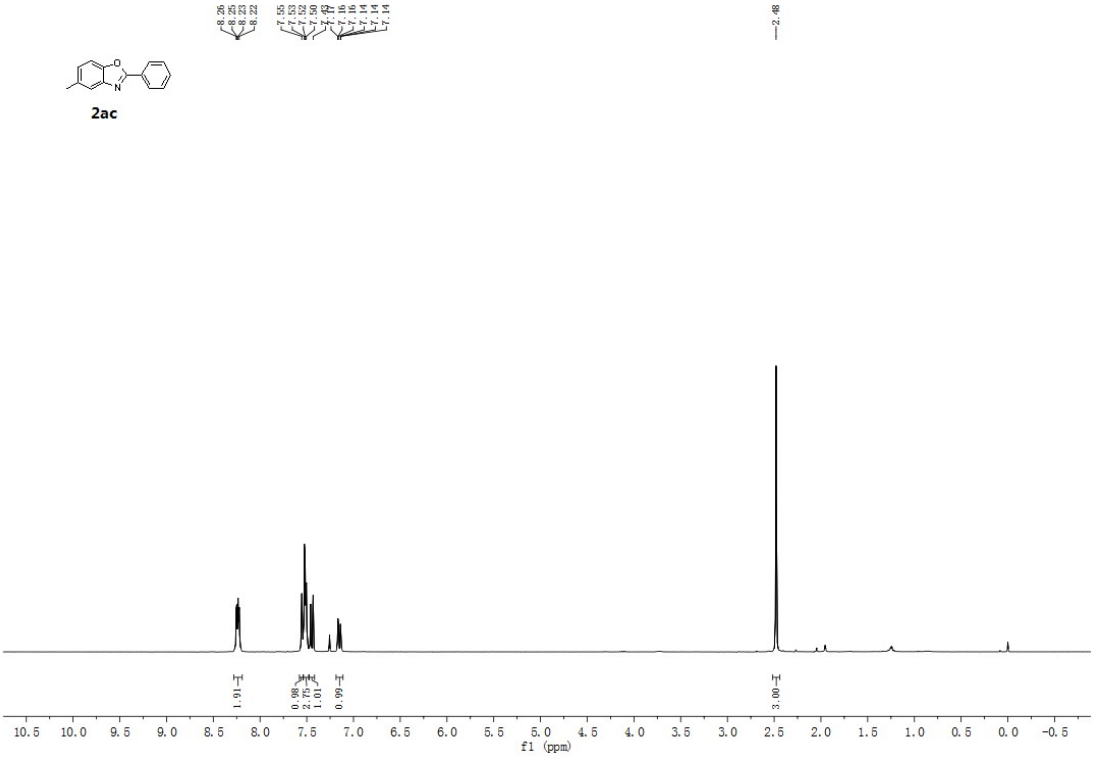
f1 (ppm)

2ab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7.14
2.48
1.91
0.98
2.75
1.01
0.99
3.00
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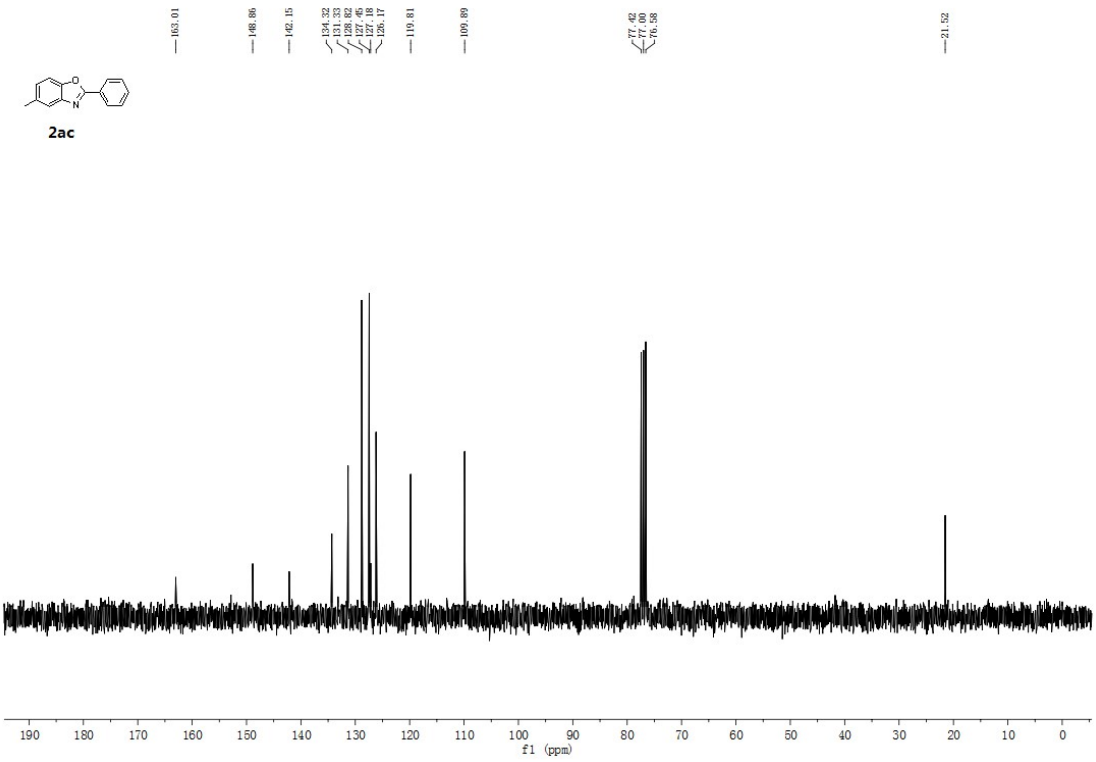
f1 (ppm)

2ac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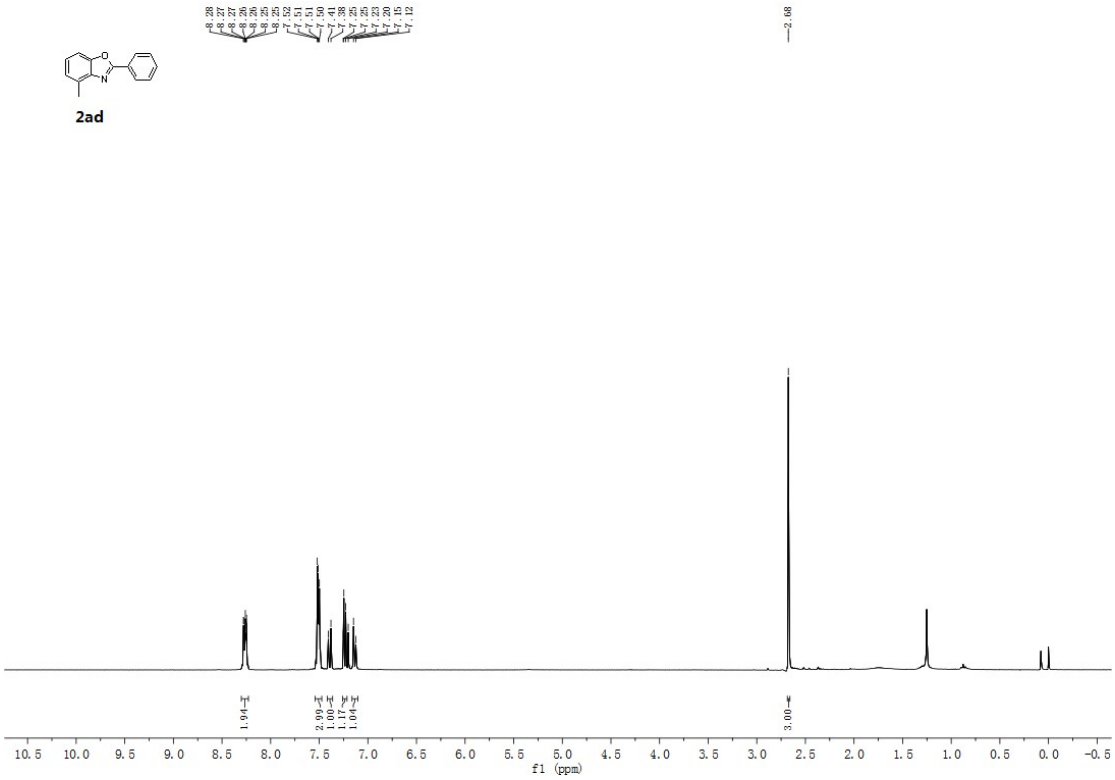
f1 (ppm)

2ac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7.25
7.23
7.20
7.15
7.12
2.68
1.94
2.99
1.00
1.17
1.04
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

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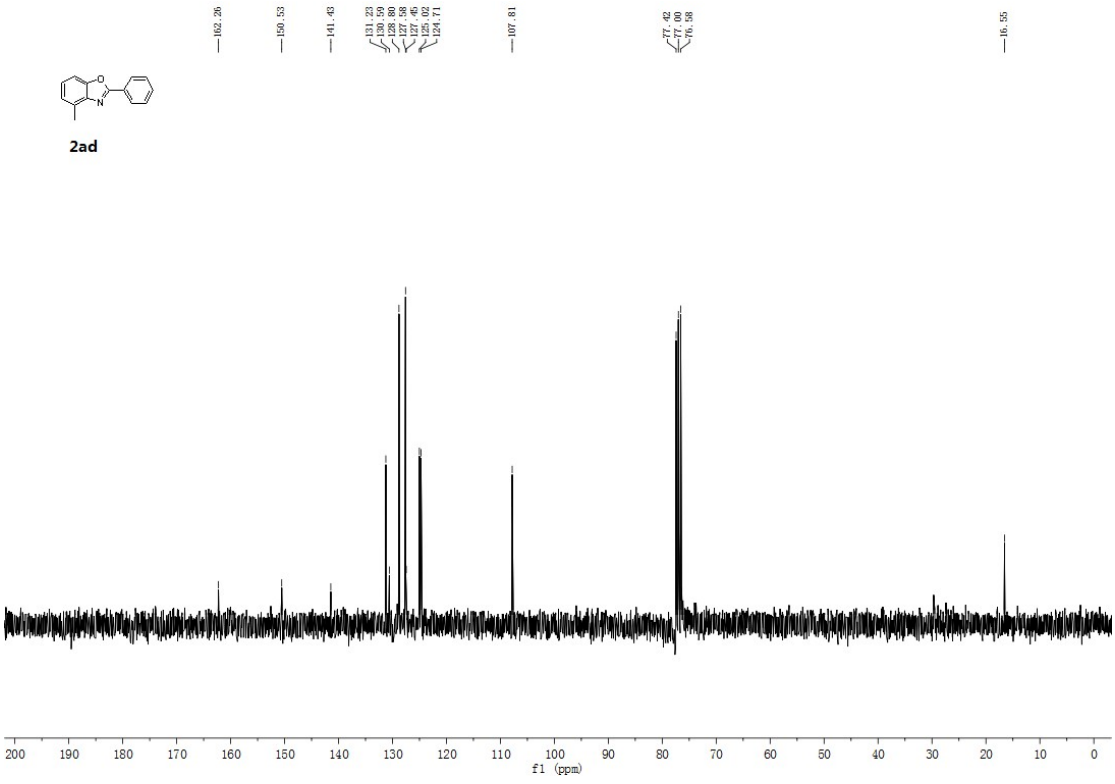
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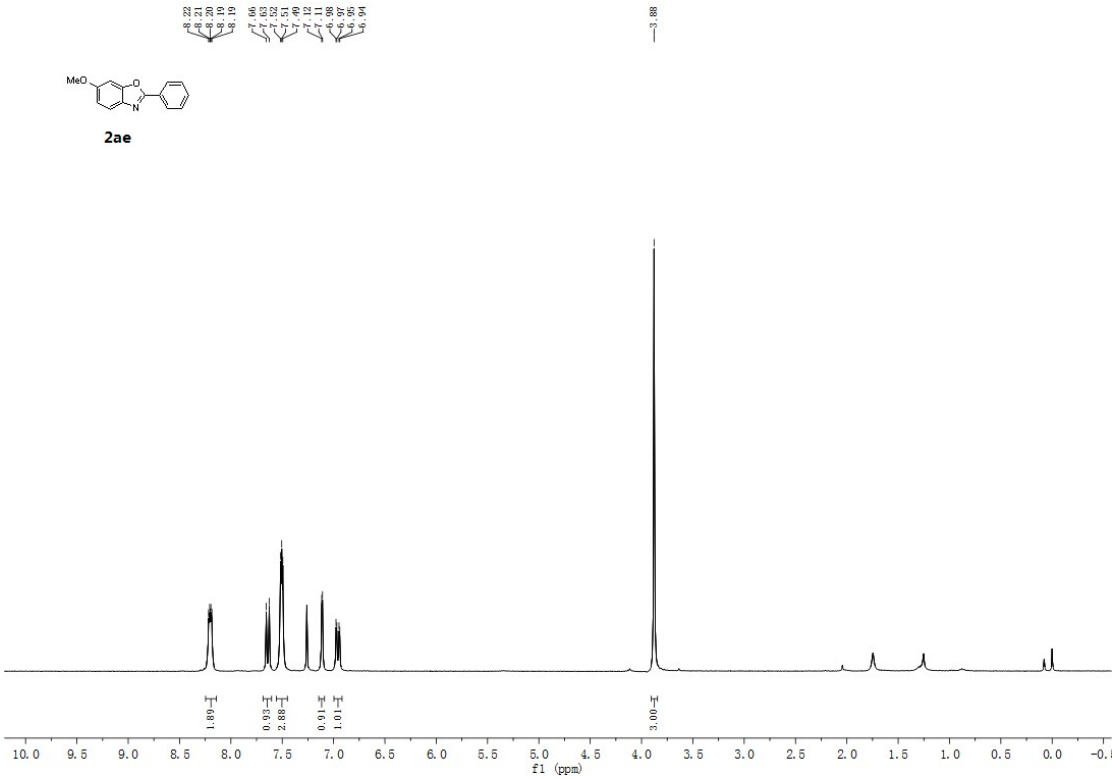
f1 (ppm)

2ad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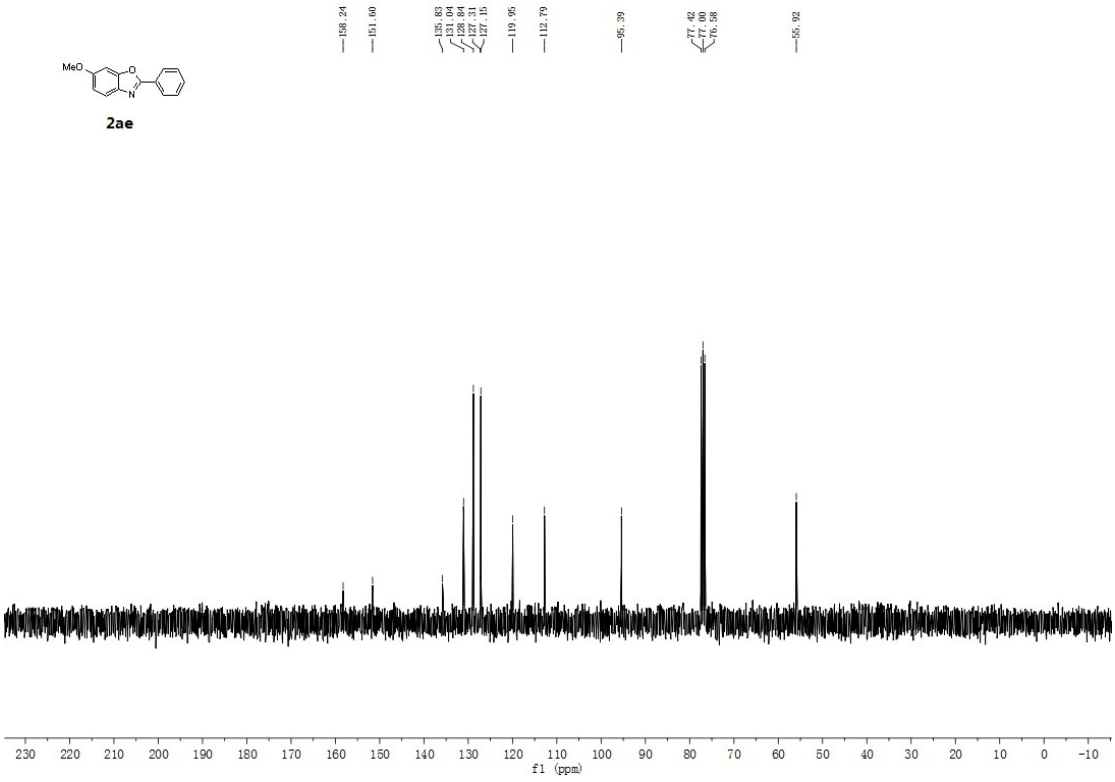
6.98
6.97
6.95
6.94
3.88
MeO
2ae
1.89
0.93
2.88
0.91
1.01
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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MeO
2ae
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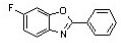
f1 (ppm)



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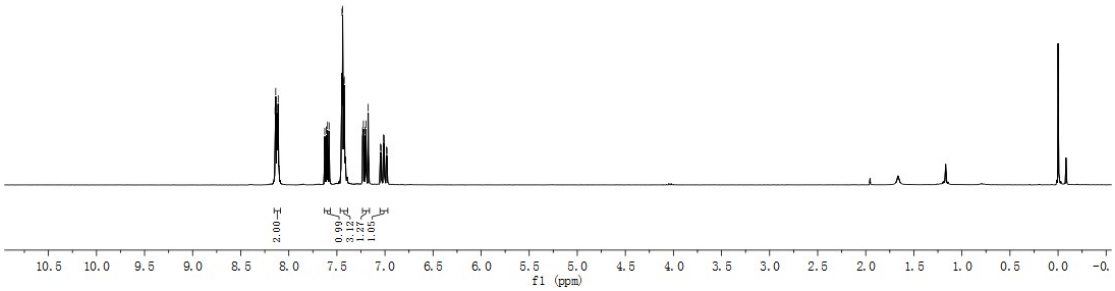

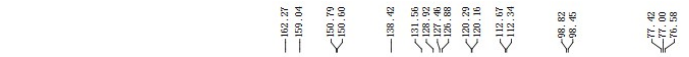

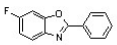

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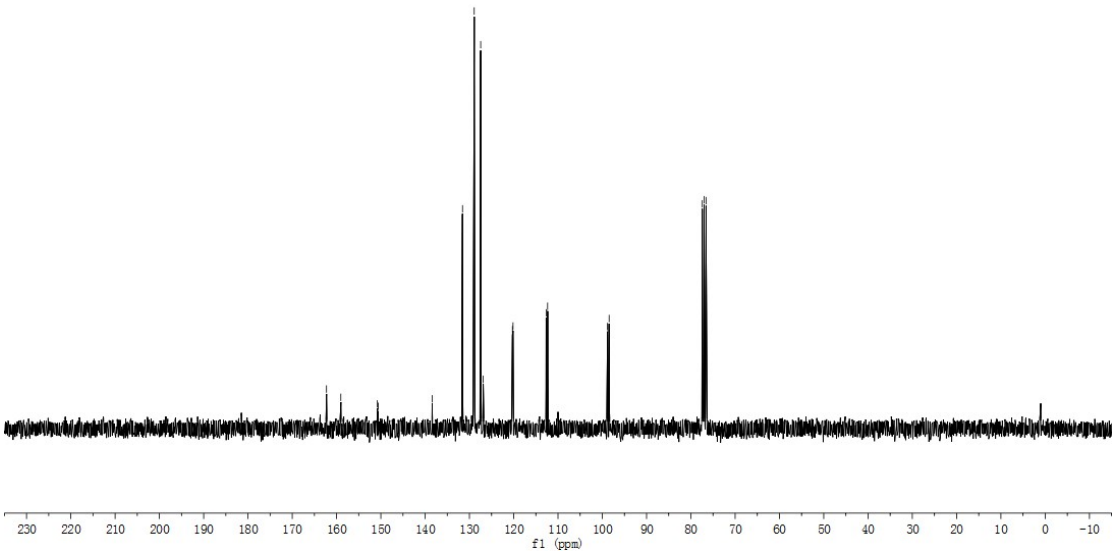

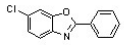

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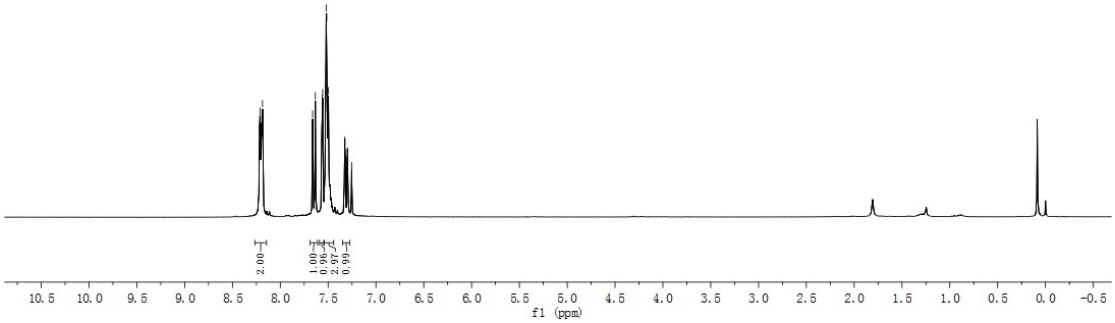
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0.99
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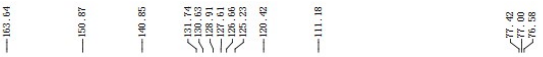
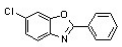
f1 (ppm)





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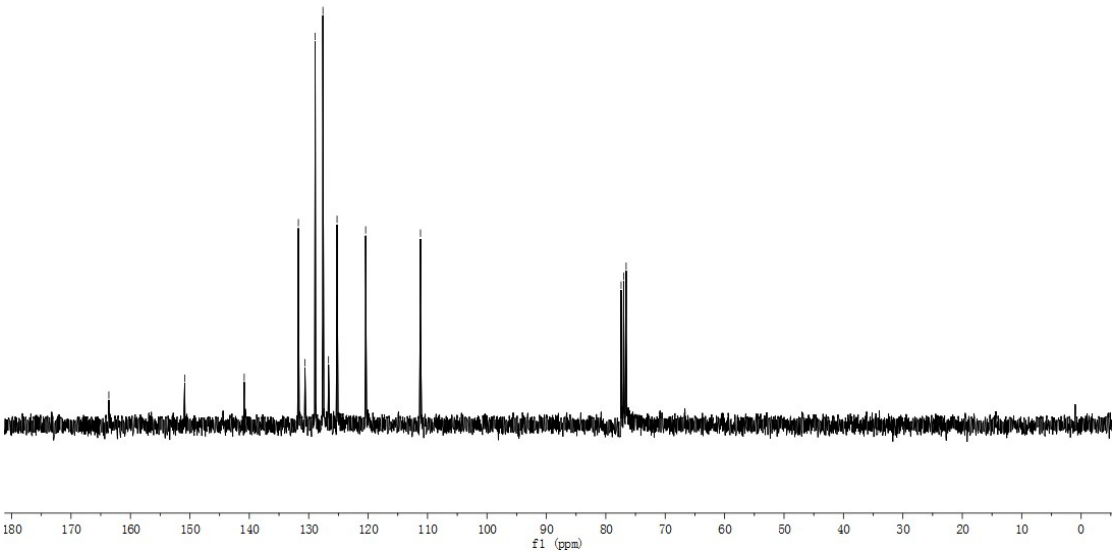
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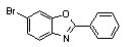
f1 (ppm)



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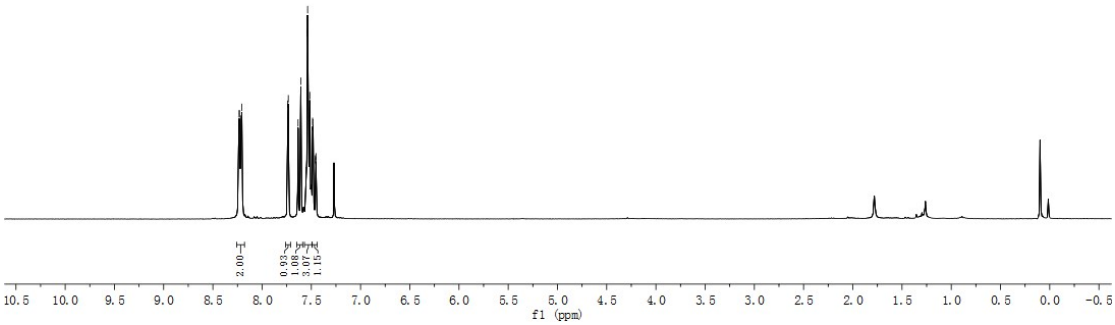

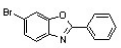

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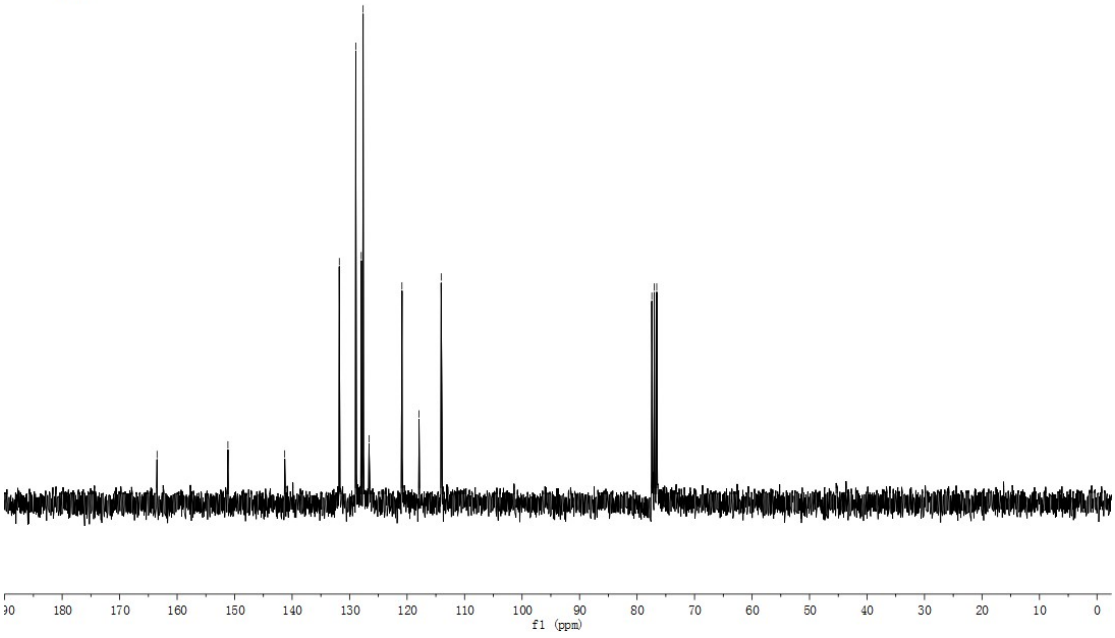

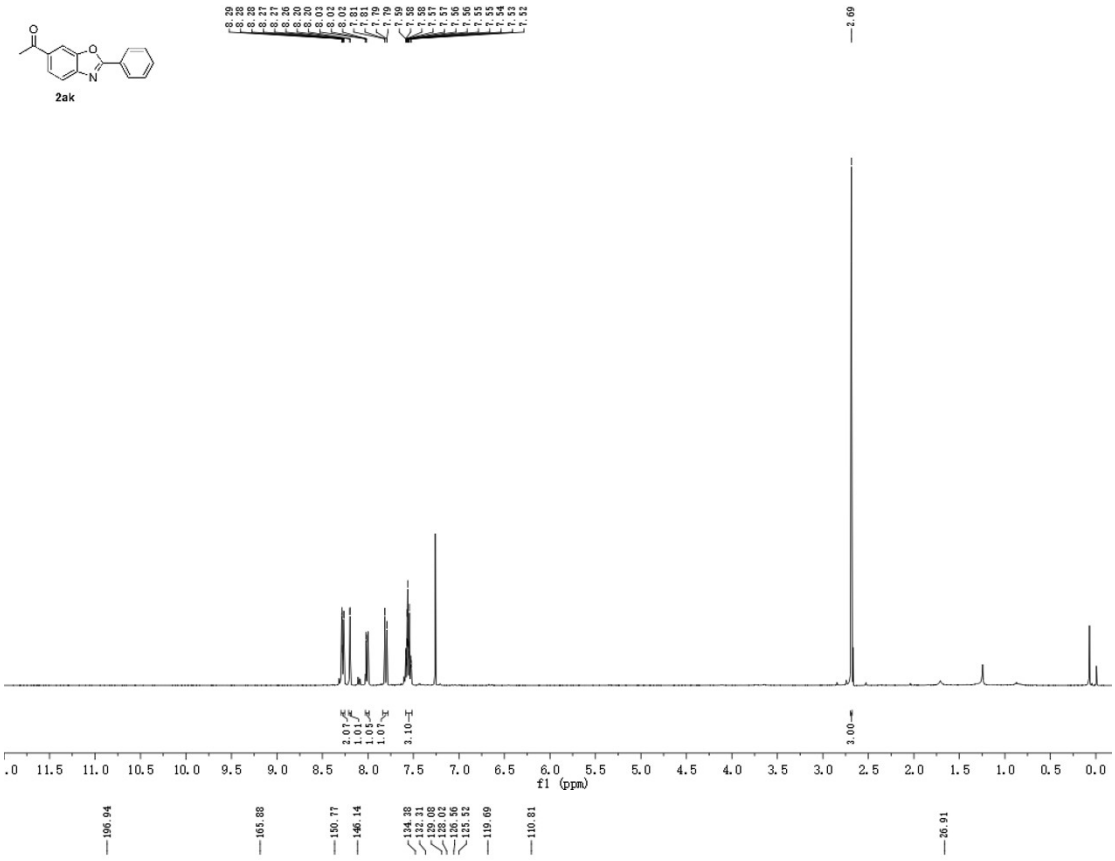
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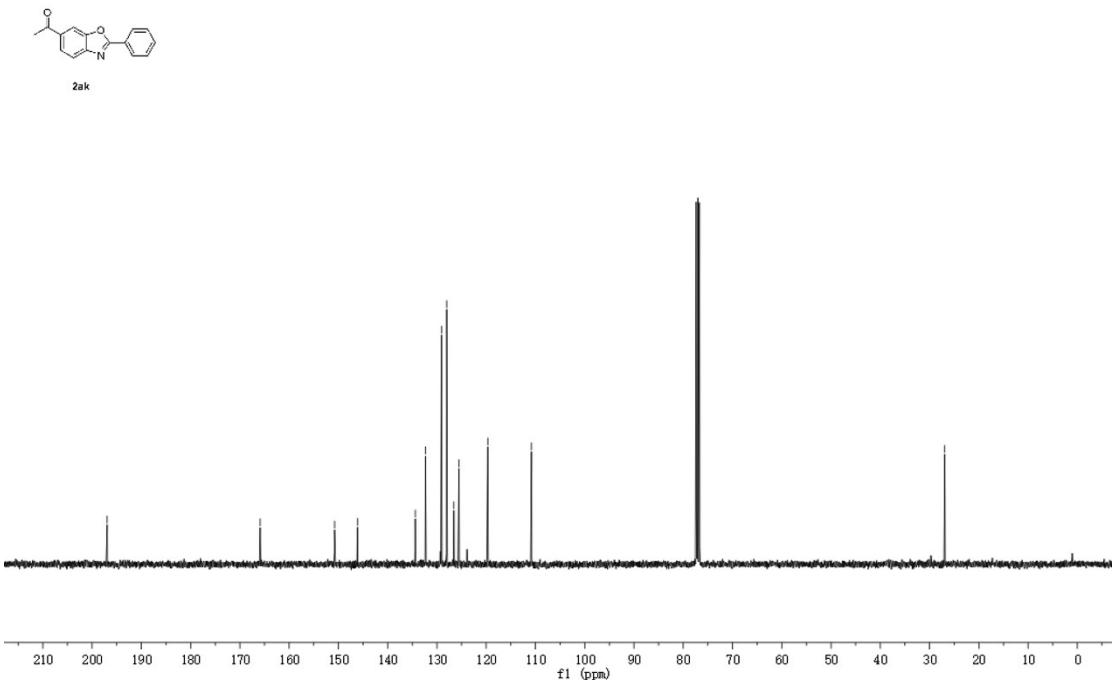
f1 (ppm)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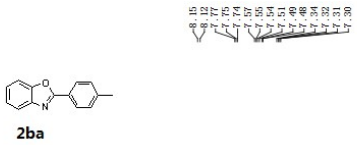

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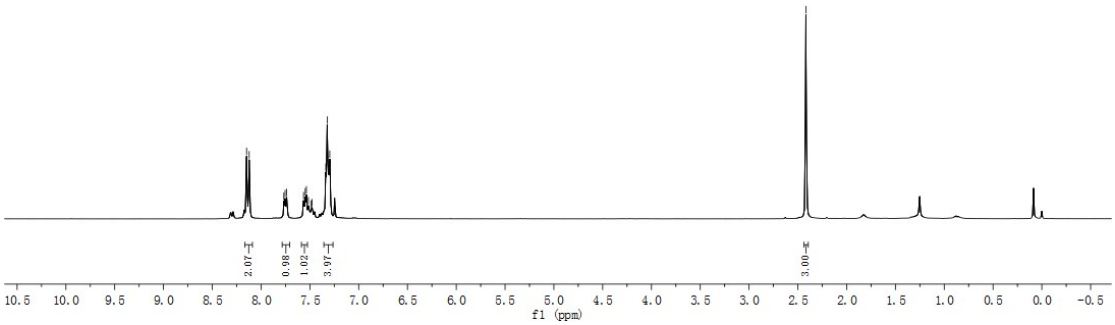

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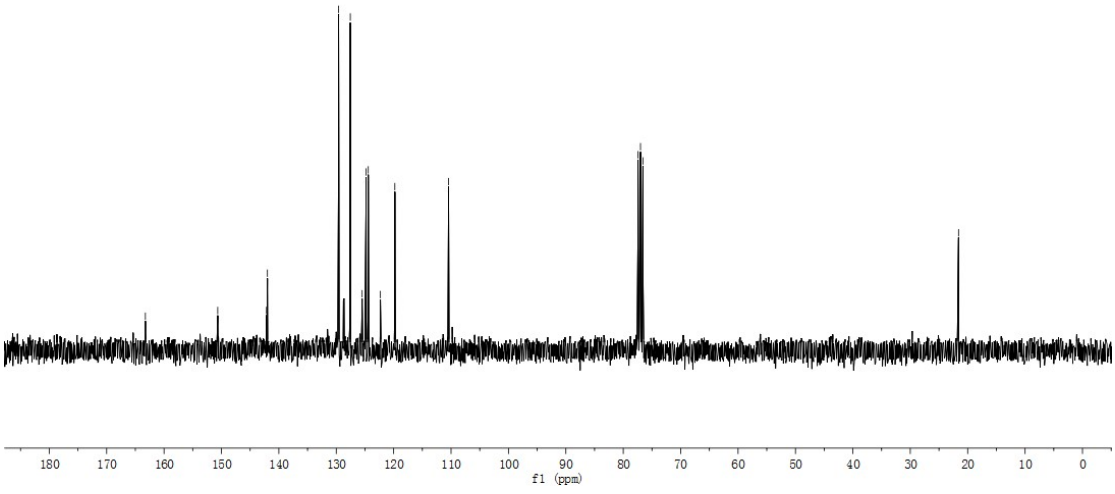

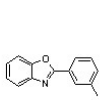

2bb

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7.39
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7.34
7.33
2.45
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1.00
1.02
1.14
2.94
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


150.59
141.94
138.67
132.32
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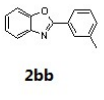

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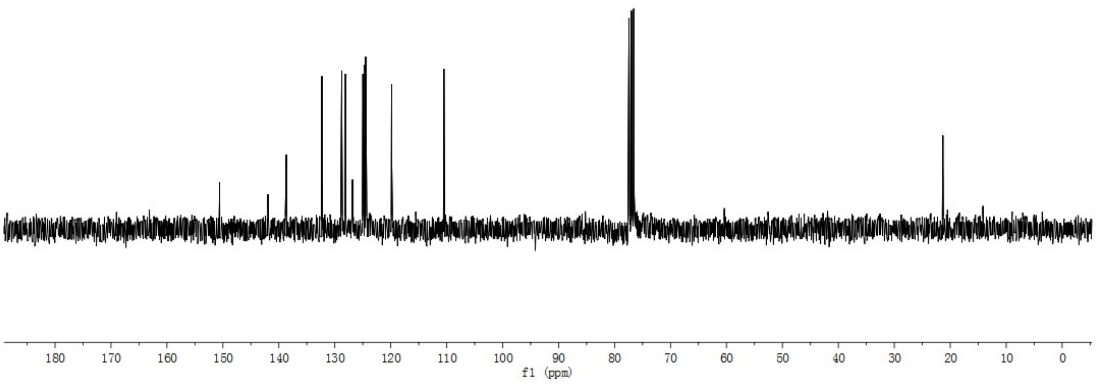
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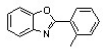

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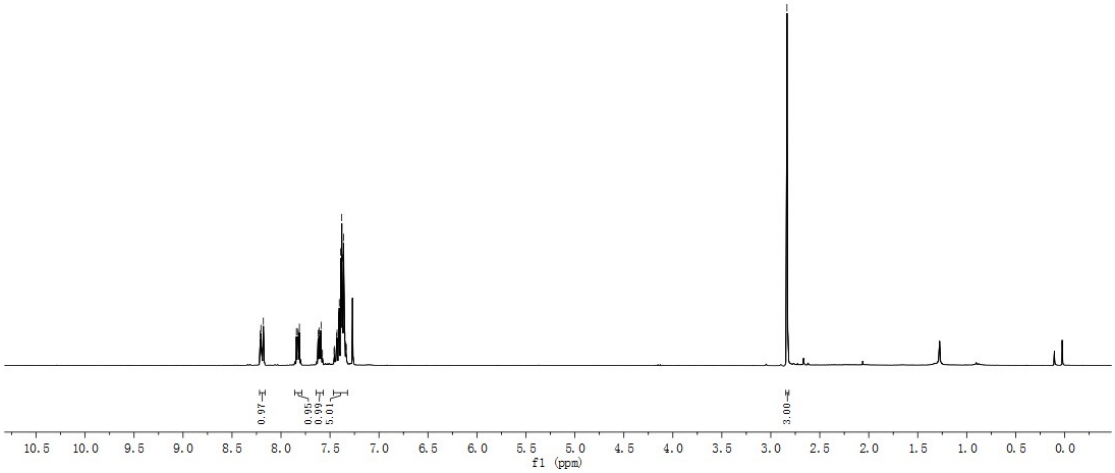
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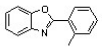

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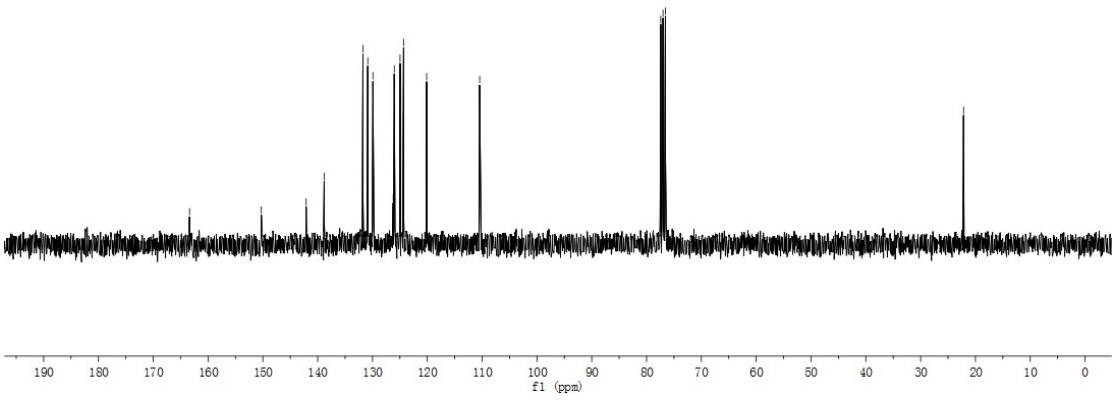
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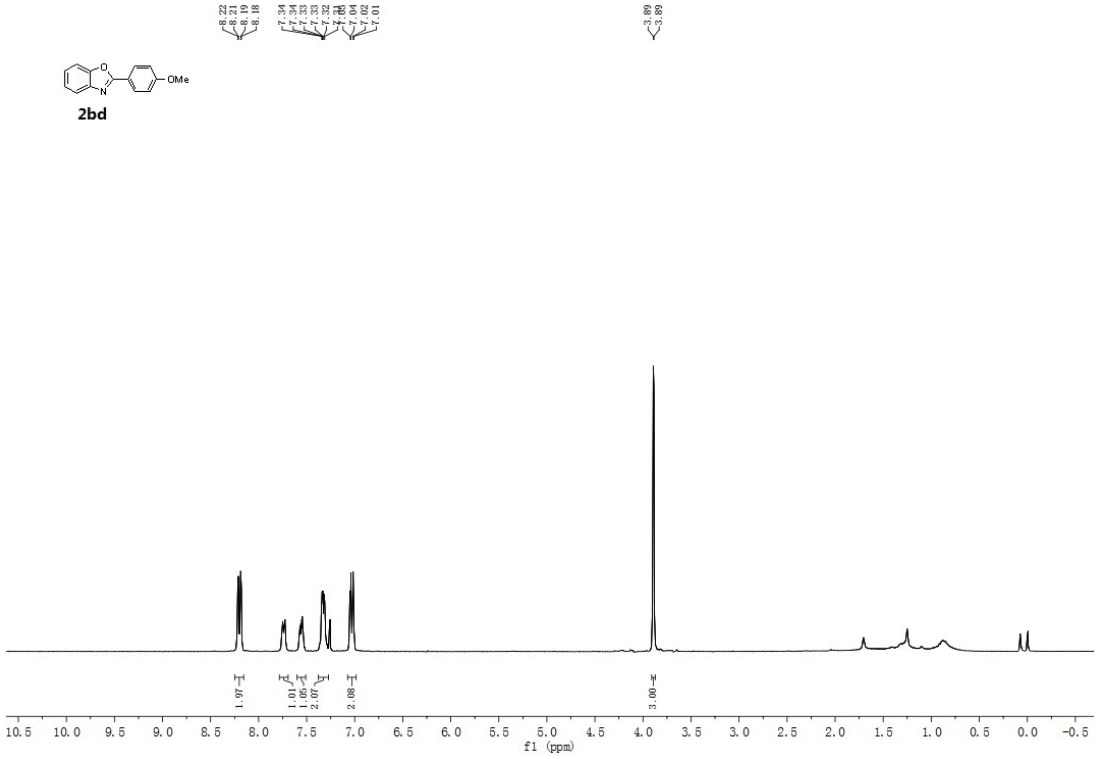
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OMe
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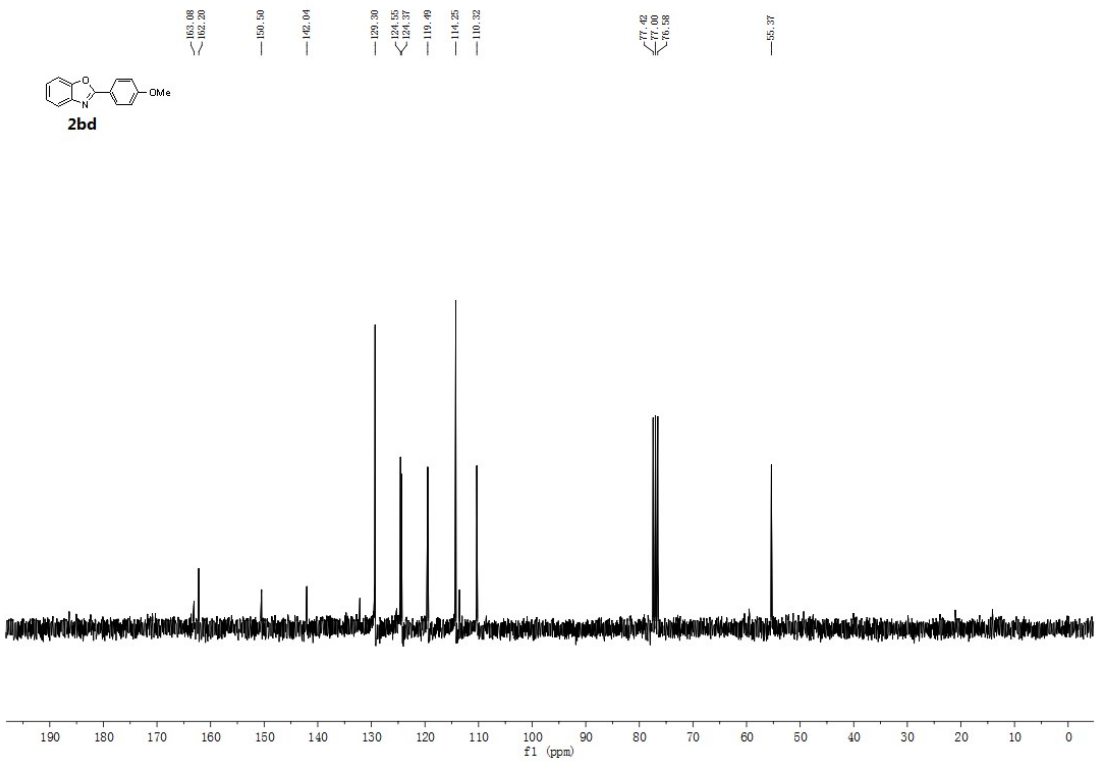
f1 (ppm)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55.37
OMe
2bd
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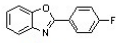
f1 (ppm)



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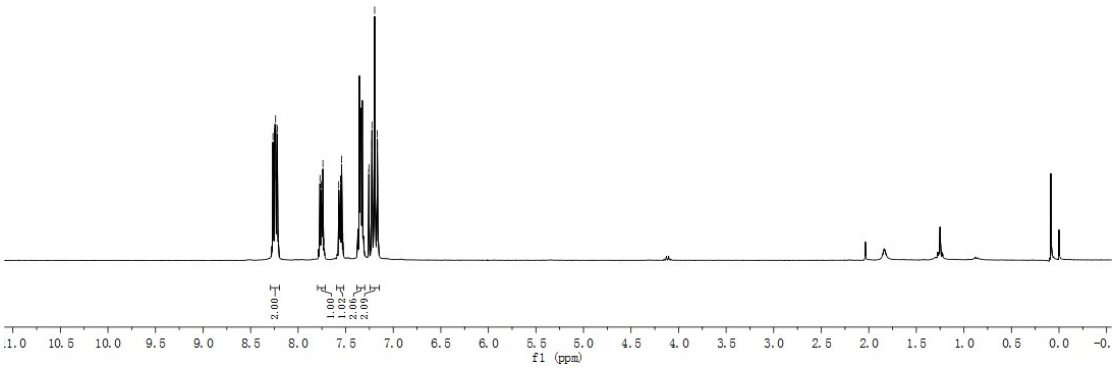

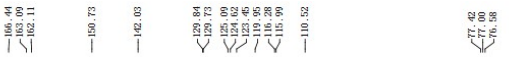

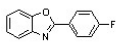

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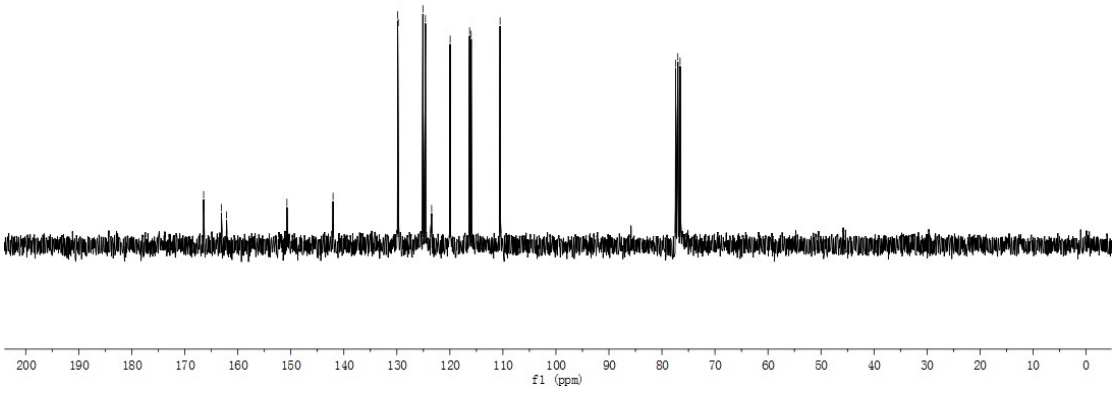

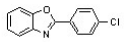

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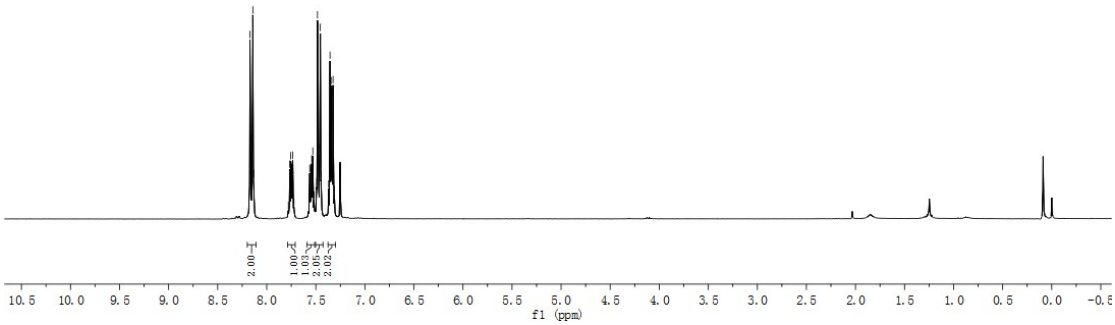
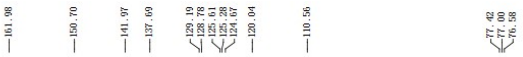
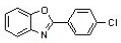

2.00
1.00
1.03
2.05
2.02
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)





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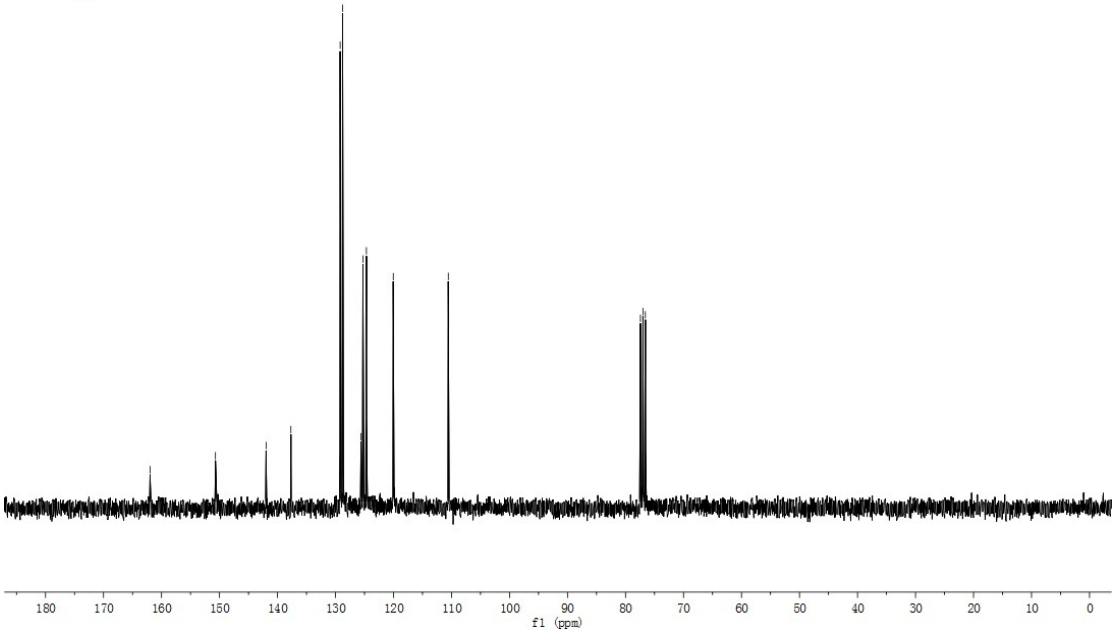
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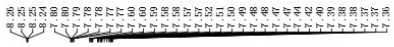

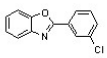

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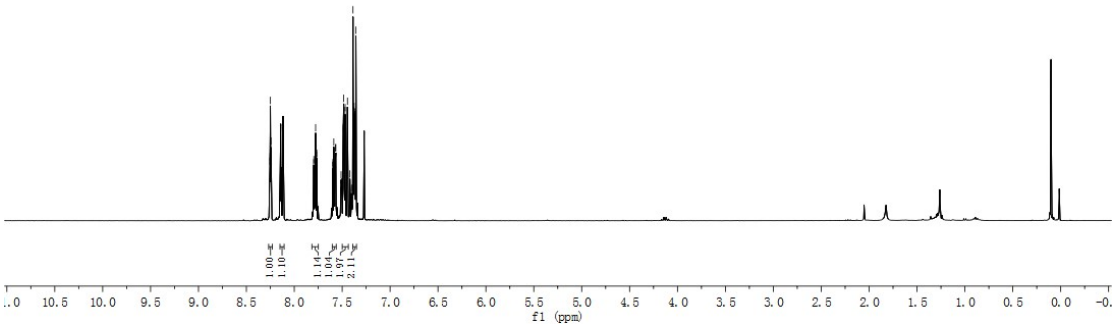

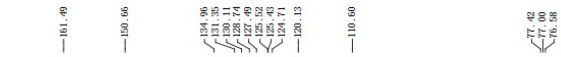

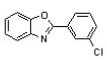

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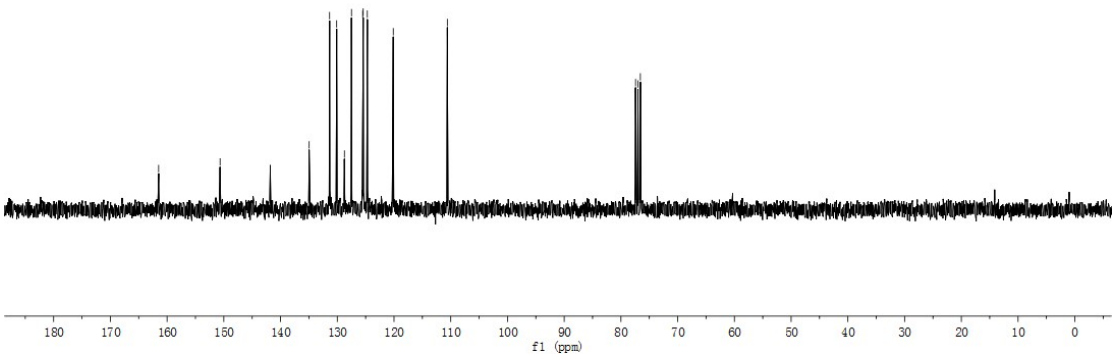

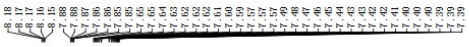

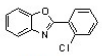

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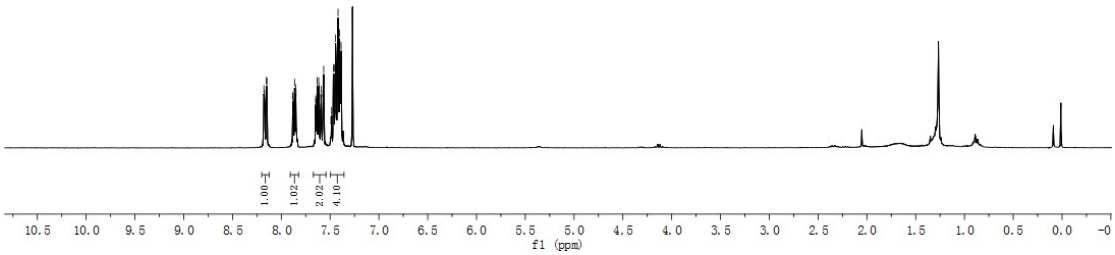

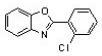

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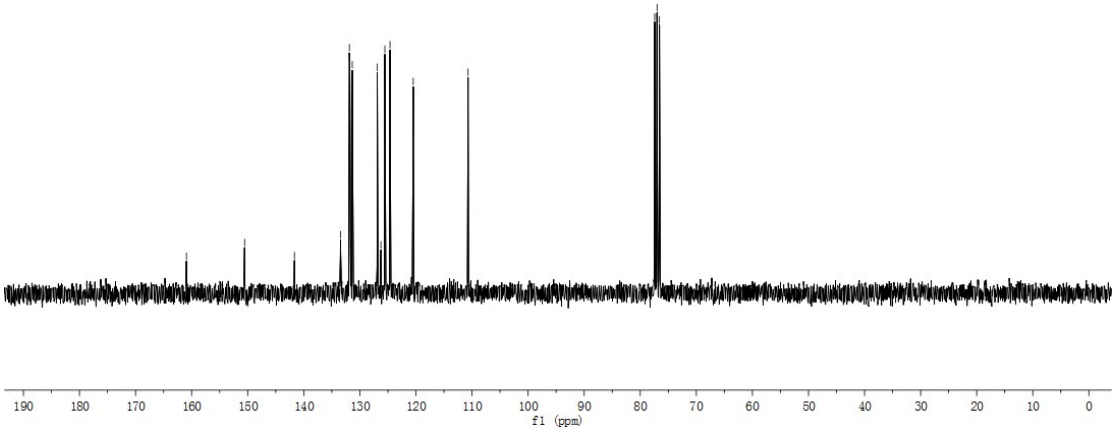

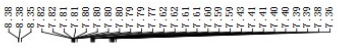

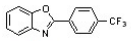

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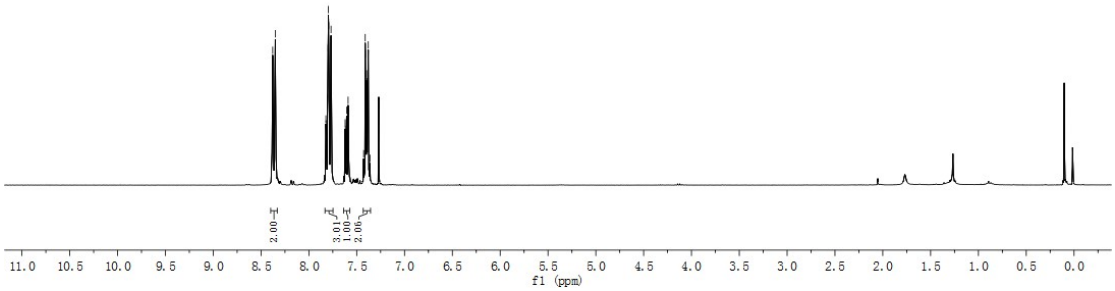

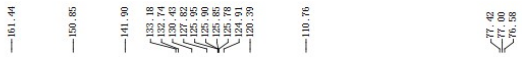

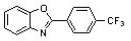

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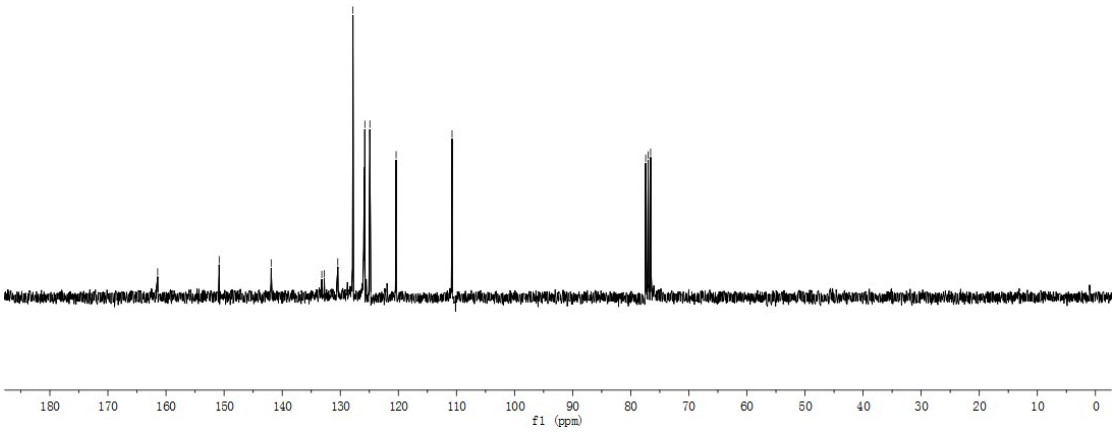

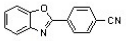

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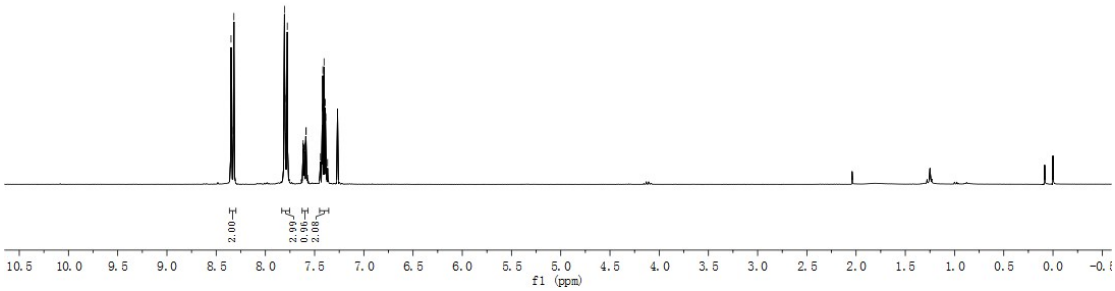

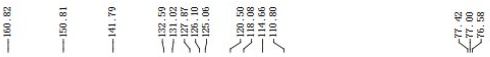

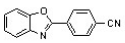

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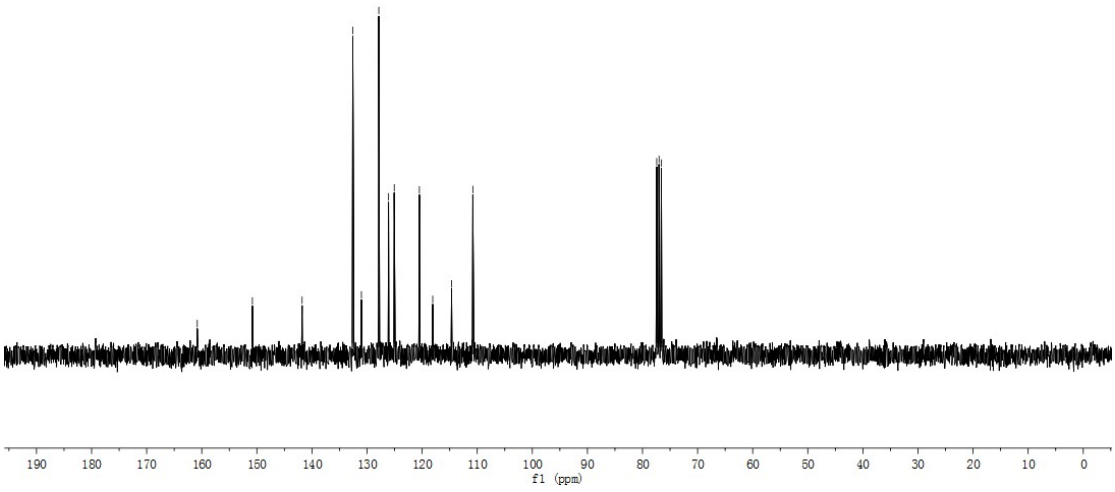

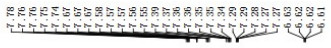

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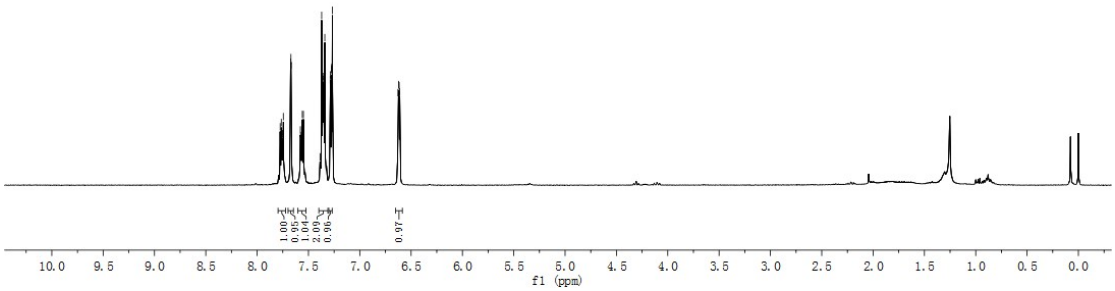

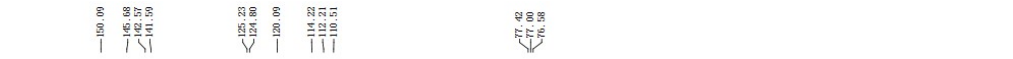

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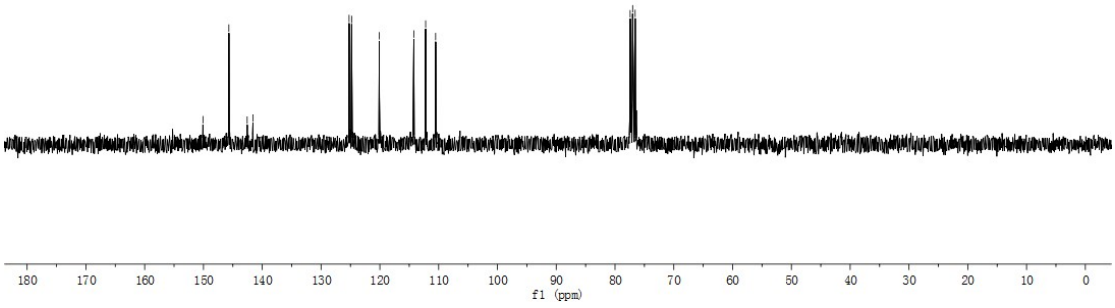

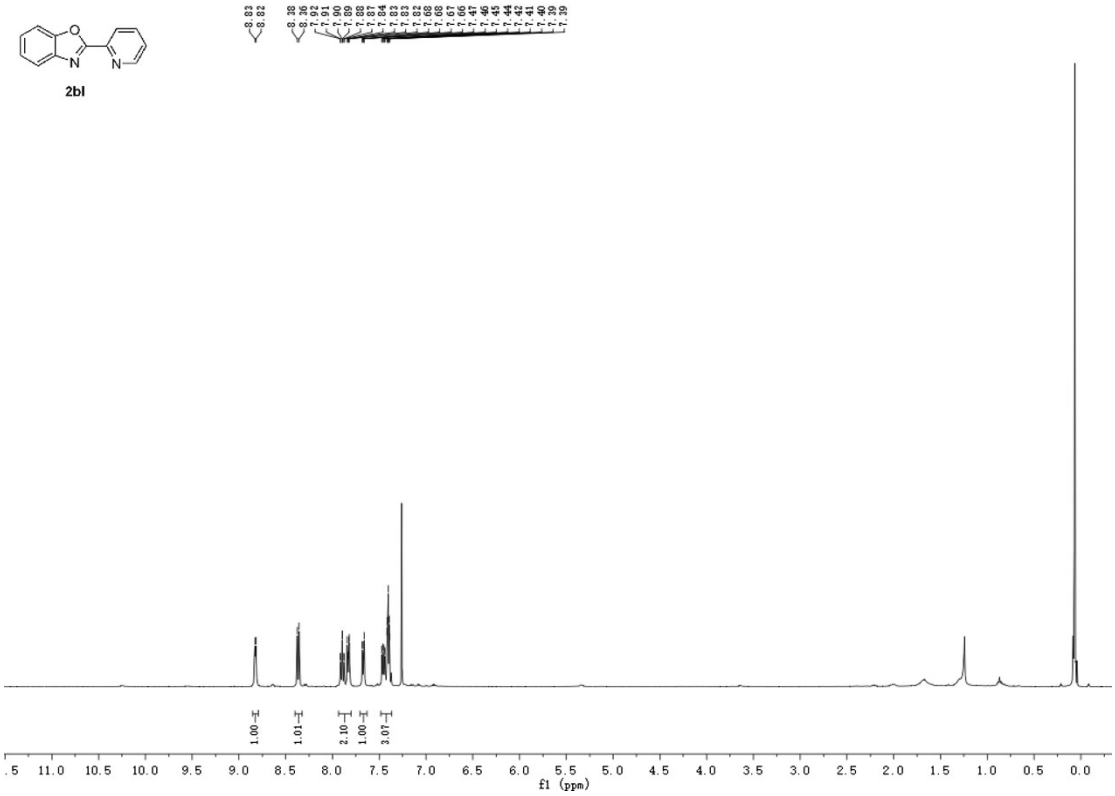
2bl
8.83
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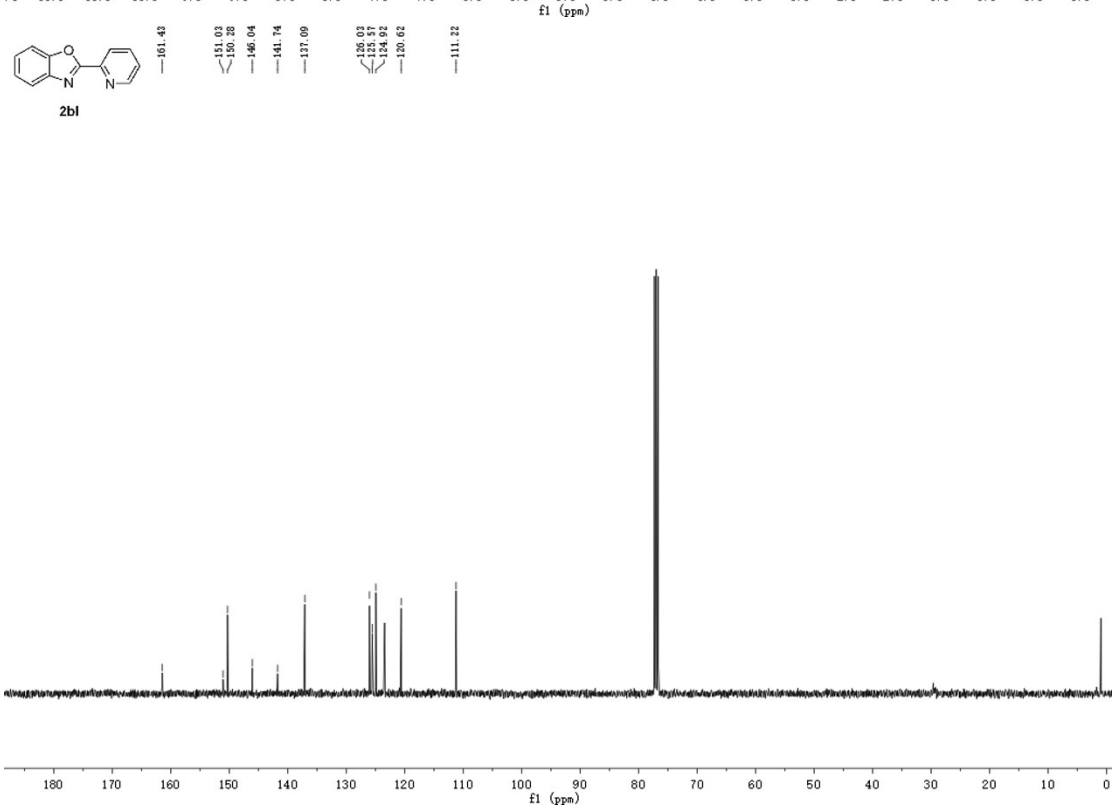
8.38
8.36
7.92
7.91
7.90
7.89
7.88
7.87
7.84
7.83
7.82
7.68
7.67
7.66
7.47
7.46
7.45
7.44
7.43
7.42
7.41
7.40
7.39
7.39
1.00
1.01
2.10
1.00
3.07
f1 (ppm)


2bl
161.43
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150.28
146.04
141.74
137.09
126.03
125.57
124.92
120.62
111.22
f1 (ppm)