Supporting Information for:

Visible light-driven oxidative coupling of dibenzylamine and substituted anilines with 2D WSe_2 nanomesh material

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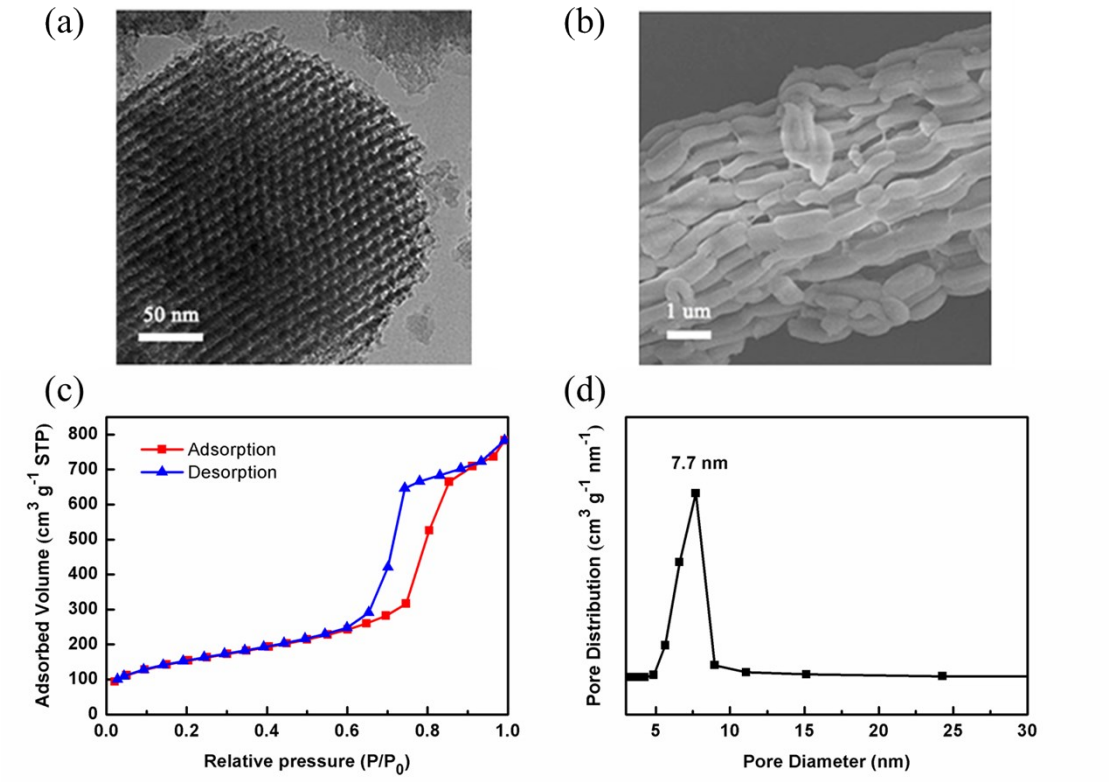


Figure S1. (a) TEM image of the SBA-15; (b) SEM image of the SBA-15; (c) N_2 adsorption-desorption isotherms for SBA-15; (d) Pore size distributions of the SBA-15.

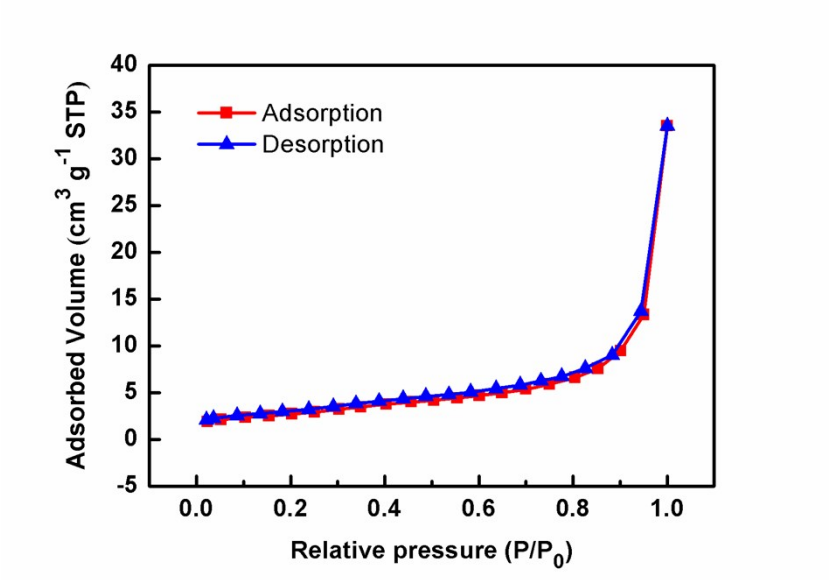
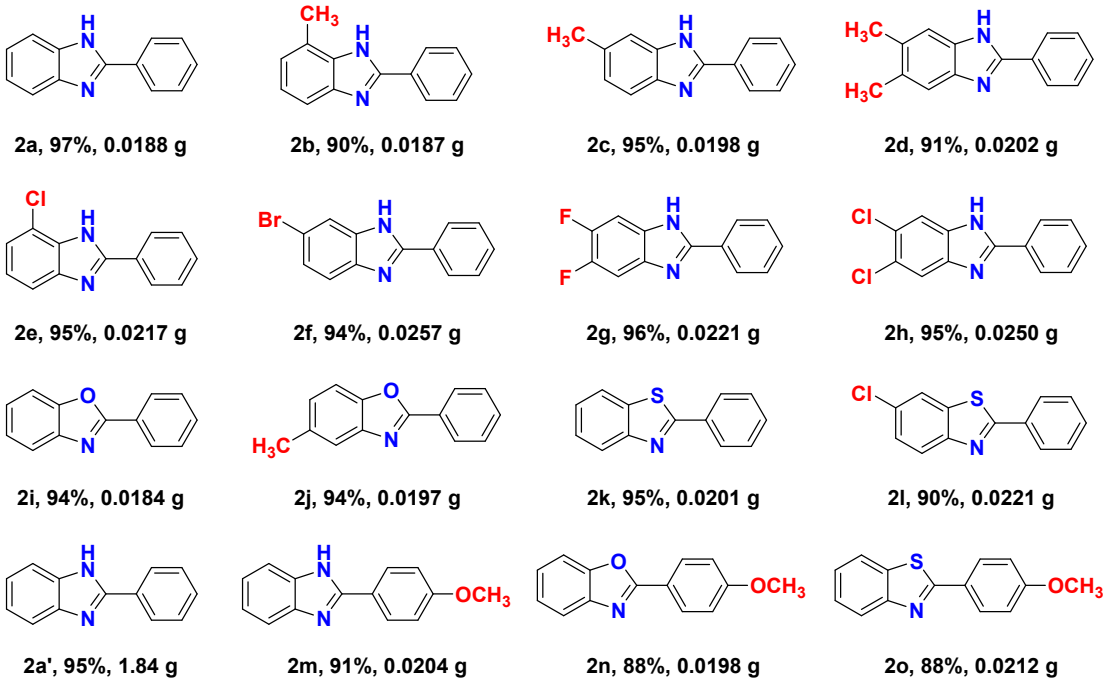


Figure S2. N_2 adsorption-desorption isotherms for the WSe_2 nanomesh.

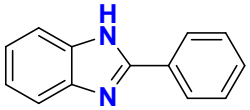


Scheme S1. Isolated yield and quantity of the synthesized compounds.

Results and Discussion

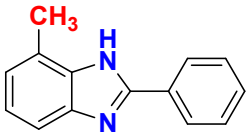
Characterization of the products

2-Phenyl-1*H*-benzo[*d*]imidazole (2a) [1]



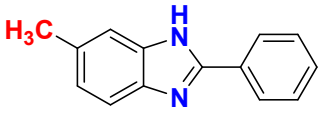
^{1}H NMR (500 MHz, DMSO) δ 12.97 (s, 1H), 8.24 (dd, J = 5.2, 3.3 Hz, 2H), 7.69 – 7.54 (m, 4H), 7.53 – 7.48 (m, 1H), 7.29 – 7.18 (m, 2H); ^{13}C NMR (126 MHz, DMSO) δ 151.73, 130.67, 130.30, 129.42, 126.93, 122.61; HRMS (ESI+): Calculated for $C_{13}H_{10}N_2H$: $[M+H]^+$ 195.0917, Found 195.0919.

7-Methyl-2-phenyl-1*H*-benzo[*d*]imidazole (2b) [2]



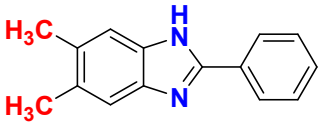
^{1}H NMR (500 MHz, DMSO) δ 12.71 (d, J = 130.5 Hz, 1H), 8.20 (s, 2H), 7.63 – 7.32 (m, 4H), 7.10 (t, J = 7.5 Hz, 1H), 7.00 (d, J = 7.2 Hz, 1H), 2.59 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 151.23, 130.81, 130.14, 129.32, 127.04, 122.62, 17.39; HRMS (ESI+): Calculated for $C_{14}H_{12}N_2H$: $[M+H]^+$ 209.1073, Found 209.1076.

6-Methyl-2-phenyl-1*H*-benzo[*d*]imidazole (2c) [1]



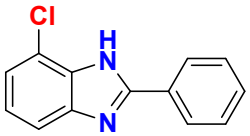
^{1}H NMR (500 MHz, DMSO) δ 12.77 (s, 1H), 8.20 – 8.11 (m, 2H), 7.50 (ddd, J = 11.1, 9.2, 4.2 Hz, 4H), 7.38 (s, 1H), 7.03 (dd, J = 8.1, 0.9 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 151.36, 130.77, 130.12, 129.37, 126.77, 124.04, 21.81; HRMS (ESI+): Calculated for $C_{14}H_{12}N_2H$: $[M+H]^+$ 209.1073, Found 209.1073.

5,6-Dimethyl-2-phenyl-1*H*-benzo[*d*]imidazole (2d) [3]



^{1}H NMR (500 MHz, DMSO) δ 12.65 (s, 1H), 8.21 – 8.10 (m, 2H), 7.53 (t, J = 7.5 Hz, 2H), 7.49 – 7.32 (m, 3H), 2.33 (s, 6H); ^{13}C NMR (126 MHz, DMSO) δ 150.81, 130.93, 129.91, 129.32, 126.68, 20.50; HRMS (ESI+): Calculated for $C_{15}H_{14}N_2H$: $[M+H]^+$ 223.1230, Found 223. 1234.

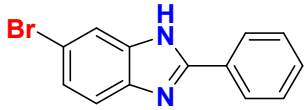
7-Chloro-2-phenyl-1*H*-benzo[*d*]imidazole (2e) [4]



^{1}H NMR (500 MHz, DMSO) δ 13.27 (s, 1H), 8.23 (d, J = 7.3 Hz, 2H), 7.63 – 7.50 (m, 4H),

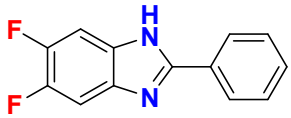
7.29 (d, J = 7.5 Hz, 1H), 7.23 (t, J = 7.8 Hz, 1H); ^{13}C NMR (126 MHz, DMSO) δ 152.51, 141.27, 136.68, 130.75, 130.05, 129.50, 127.16, 123.80, 123.19, 122.02, 111.01; HRMS (ESI+): Calculated for $C_{13}H_9ClN_2H$: $[M+H]^+$ 229.0527, Found 229.0530.

6-Bromo-2-phenyl-1*H*-benzo[*d*]imidazole (2f) [5]



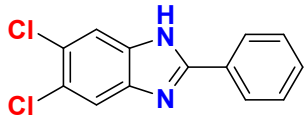
^{1}H NMR (500 MHz, DMSO) δ 13.12 (s, 1H), 8.25 – 8.12 (m, 2H), 7.80 (s, 1H), 7.64 – 7.46 (m, 4H), 7.35 (dd, J = 8.5, 1.7 Hz, 1H); ^{13}C NMR (126 MHz, DMSO) δ 152.94, 130.70, 130.12, 129.48, 127.08, 125.45, 114.75; HRMS (ESI+): Calculated for $C_{13}H_9BrN_2H$: $[M+H]^+$ 273.0022, Found 273.0023.

5,6-Difluoro-2-phenyl-1*H*-benzo[*d*]imidazole (2g) [6]



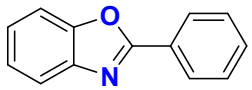
^{1}H NMR (500 MHz, DMSO) δ 13.20 (s, 1H), 8.19 – 8.14 (m, 2H), 7.71 (s, 1H), 7.61 – 7.49 (m, 4H); ^{13}C NMR (126 MHz, DMSO) δ 153.73, 130.59, 130.11, 129.47, 126.89; HRMS (ESI+): Calculated for $C_{13}H_8F_2N_2H$: $[M+H]^+$ 231.0729, Found 231.0738.

5,6-Dichloro-2-phenyl-1*H*-benzo[*d*]imidazole (2h) [7]



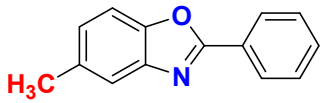
^{1}H NMR (500 MHz, DMSO) δ 13.25 (s, 1H), 8.17 (d, J = 7.0 Hz, 2H), 7.94 – 7.74 (m, 2H), 7.60 – 7.50 (m, 3H); ^{13}C NMR (126 MHz, DMSO) δ 154.29, 130.98, 129.76, 129.50, 127.20; HRMS (ESI+): Calculated for $C_{13}H_8Cl_2N_2H$: $[M+H]^+$ 263.0138, Found 263.0142.

2-Phenylbenzo[*d*]oxazole (2i) [8]



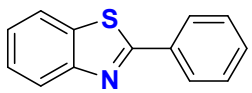
^{1}H NMR (500 MHz, DMSO) δ 8.24 (dt, J = 3.9, 2.3 Hz, 2H), 7.88 – 7.78 (m, 2H), 7.69 – 7.60 (m, 3H), 7.49 – 7.41 (m, 2H); ^{13}C NMR (126 MHz, DMSO) δ 162.70, 150.68, 141.97, 132.37, 129.74, 127.71, 126.89, 125.95, 125.31, 120.29, 111.37; HRMS (ESI+): Calculated for $C_{13}H_9NOH$: $[M+H]^+$ 196.0757, Found 196.0763.

5-Methyl-2-phenylbenzo[*d*]oxazole (2j) [8]



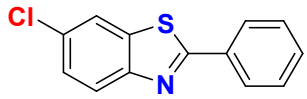
^{1}H NMR (500 MHz, DMSO) δ 8.20 (dd, J = 7.8, 1.7 Hz, 2H), 7.83 – 7.43 (m, 5H), 7.25 (dd, J = 8.3, 1.1 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 162.76, 148.92, 142.17, 134.71, 132.28, 129.74, 127.63, 127.01, 126.95, 120.08, 110.76, 21.46; HRMS (ESI+): Calculated for $C_{14}H_{11}NOH$: $[M+H]^+$ 210.0914, Found 210.0922.

2-Phenylbenzo[*d*]thiazole (2k) [9]



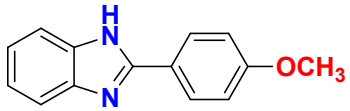
^{1}H NMR (500 MHz, DMSO) δ 8.22 – 8.05 (m, 4H), 7.63 – 7.55 (m, 4H), 7.49 (td, J = 7.8, 1.1 Hz, 1H); ^{13}C NMR (126 MHz, DMSO) δ 167.75, 154.06, 134.96, 133.35, 131.83, 129.82, 127.66, 127.10, 125.98, 123.37, 122.77; HRMS (ESI+): Calculated for $C_{13}H_9NSH$: $[M+H]^+$ 212.0529, Found 212.0526.

6-Chloro-2-phenylbenzo[*d*]thiazole (2l) [9]



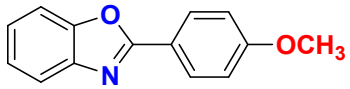
^{1}H NMR (500 MHz, DMSO) δ 8.20 (d, J = 8.6 Hz, 1H), 8.15 (d, J = 2.0 Hz, 1H), 8.12 – 8.09 (m, 2H), 7.64 – 7.57 (m, 3H), 7.53 (dd, J = 8.6, 2.1 Hz, 1H); ^{13}C NMR (126 MHz, DMSO) δ 170.15, 154.93, 133.73, 132.98, 132.29, 131.90, 129.96, 127.80, 126.12, 124.37, 122.76; HRMS (ESI+): Calculated for $C_{13}H_8ClNSH$: $[M+H]^+$ 246.0139, Found 246.0141.

2-(4-Methoxyphenyl)-1*H*-benzo[*d*]imidazole (2m) [1]



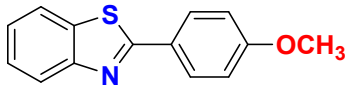
^{1}H NMR (500 MHz, DMSO) δ 12.92 (s, 1H), 7.78 (dd, *J* = 7.9, 1.0 Hz, 2H), 7.61 (s, 2H), 7.47 (t, *J* = 7.9 Hz, 1H), 7.25 – 7.19 (m, 2H), 7.09 – 7.04 (m, 1H), 3.88 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 160.11, 151.55, 131.93, 130.57, 122.68, 119.21, 116.34, 111.86, 55.76; HRMS (ESI+): Calculated for $C_{14}H_{12}N_2OH$: $[M+H]^+$ 225.1023, Found 225.1013.

2-(4-Methoxyphenyl)benzo[*d*]oxazole (2n) [8]



^{1}H NMR (500 MHz, DMSO) δ 8.16 – 8.09 (m, 2H), 7.79 – 7.68 (m, 2H), 7.41 – 7.34 (m, 2H), 7.16 – 7.09 (m, 2H), 3.85 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 162.84, 162.60, 150.58, 142.18, 129.56, 125.37, 125.10, 119.87, 119.24, 115.18, 111.11, 55.93; HRMS (ESI+): Calculated for $C_{14}H_{11}NO_2Na$: $[M+Na]^+$ 248.0682, Found 248.0681.

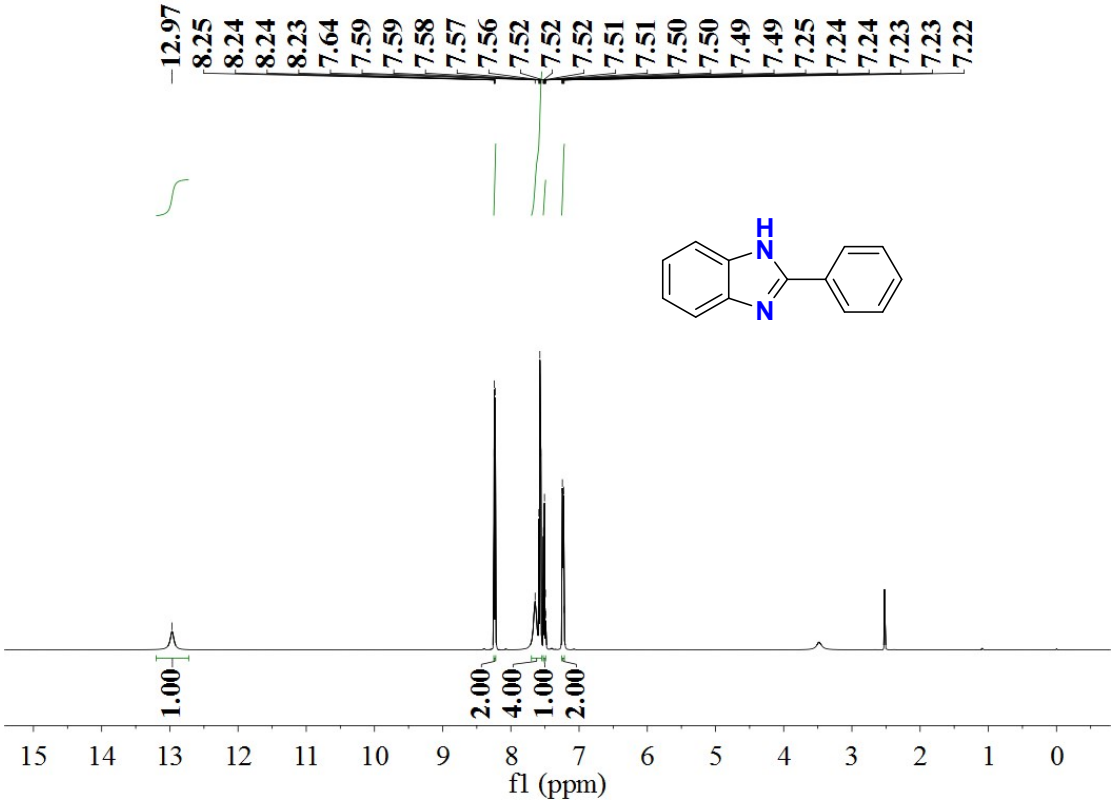
2-(4-Methoxyphenyl)benzo[*d*]thiazole (2o) [9]



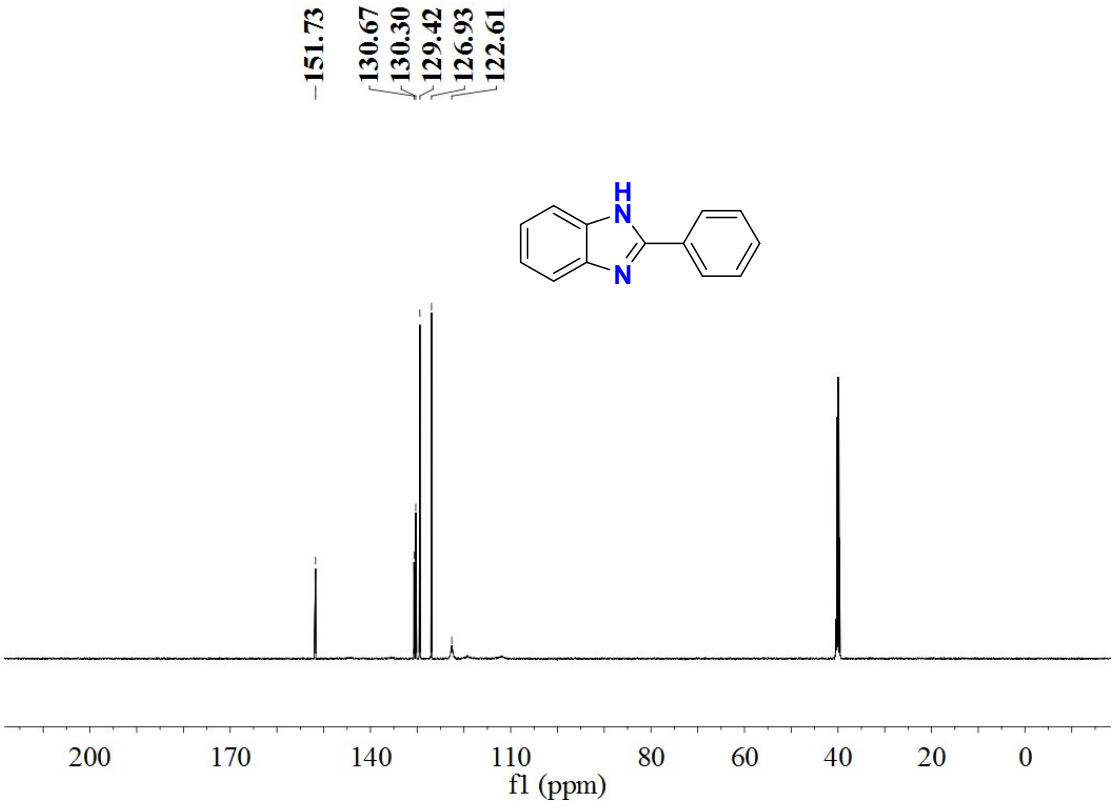
^{1}H NMR (500 MHz, DMSO) δ 8.10 (dd, *J* = 7.9, 0.5 Hz, 1H), 8.06 – 7.99 (m, 3H), 7.52 (ddd, *J* = 8.2, 7.3, 1.2 Hz, 1H), 7.46 – 7.39 (m, 1H), 7.14 – 7.09 (m, 2H), 3.85 (s, 3H); ^{13}C NMR (126 MHz, DMSO) δ 167.52, 162.26, 154.16, 134.72, 129.34, 126.97, 126.01, 125.56, 122.95, 122.64, 115.21, 55.95; HRMS (ESI+): Calculated for $C_{14}H_{11}NOSNa$: $[M+Na]^+$ 264.0453, Found 264.0449.

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

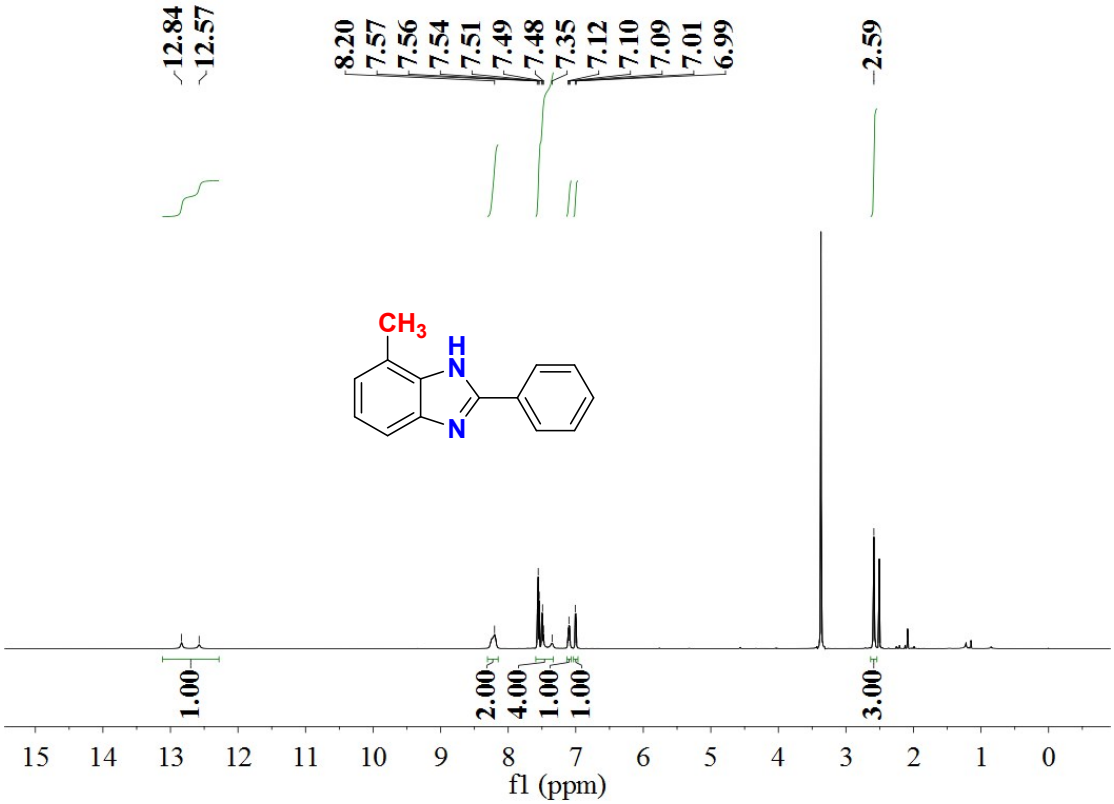
2a ^{1}H NMR



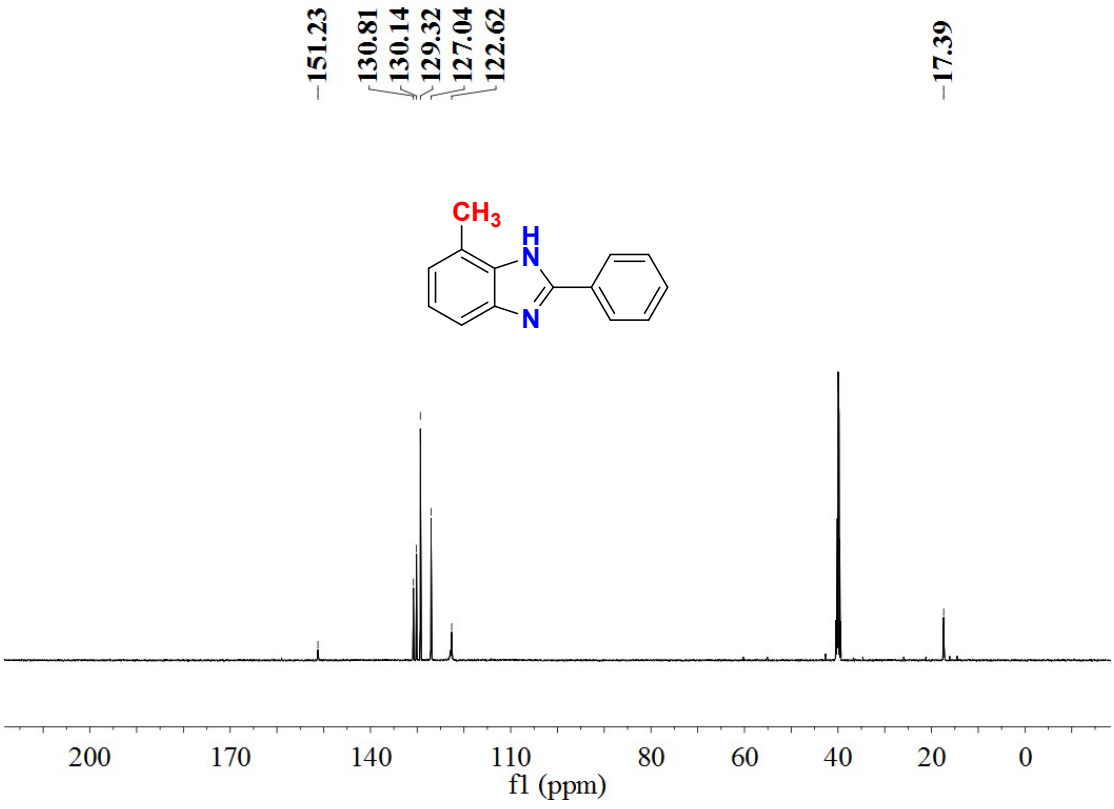
2a ^{13}C NMR



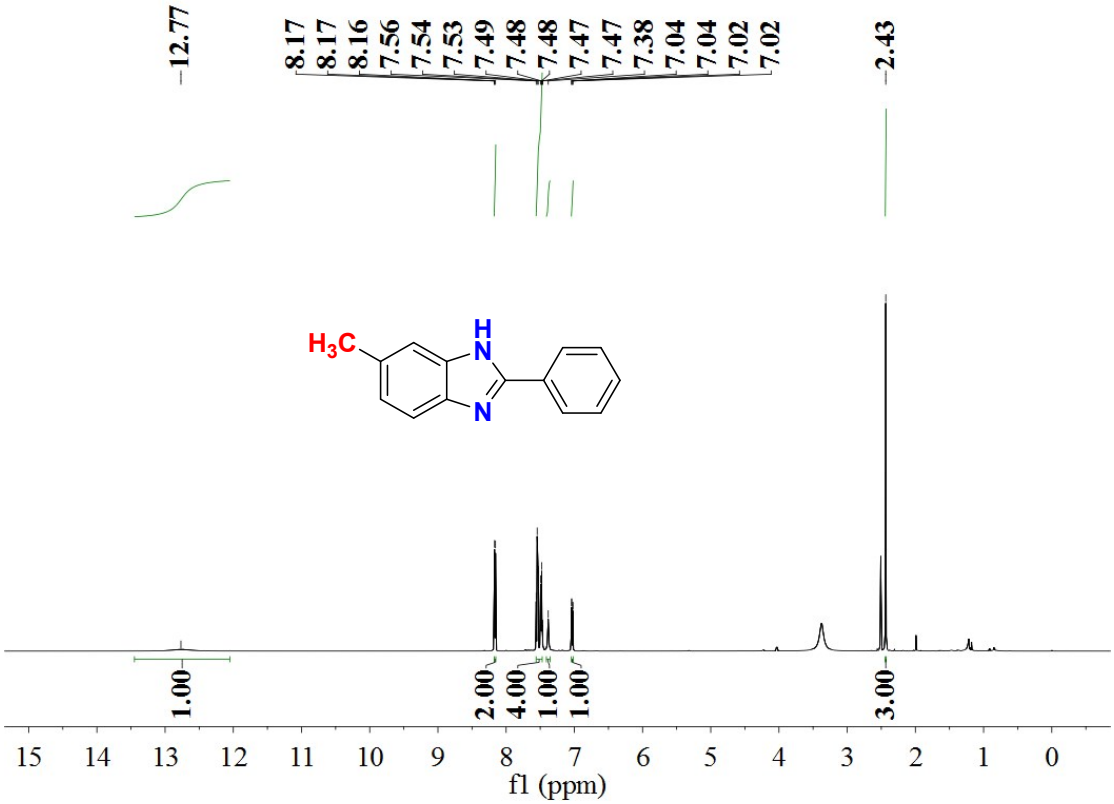
2b ^{1}H NMR



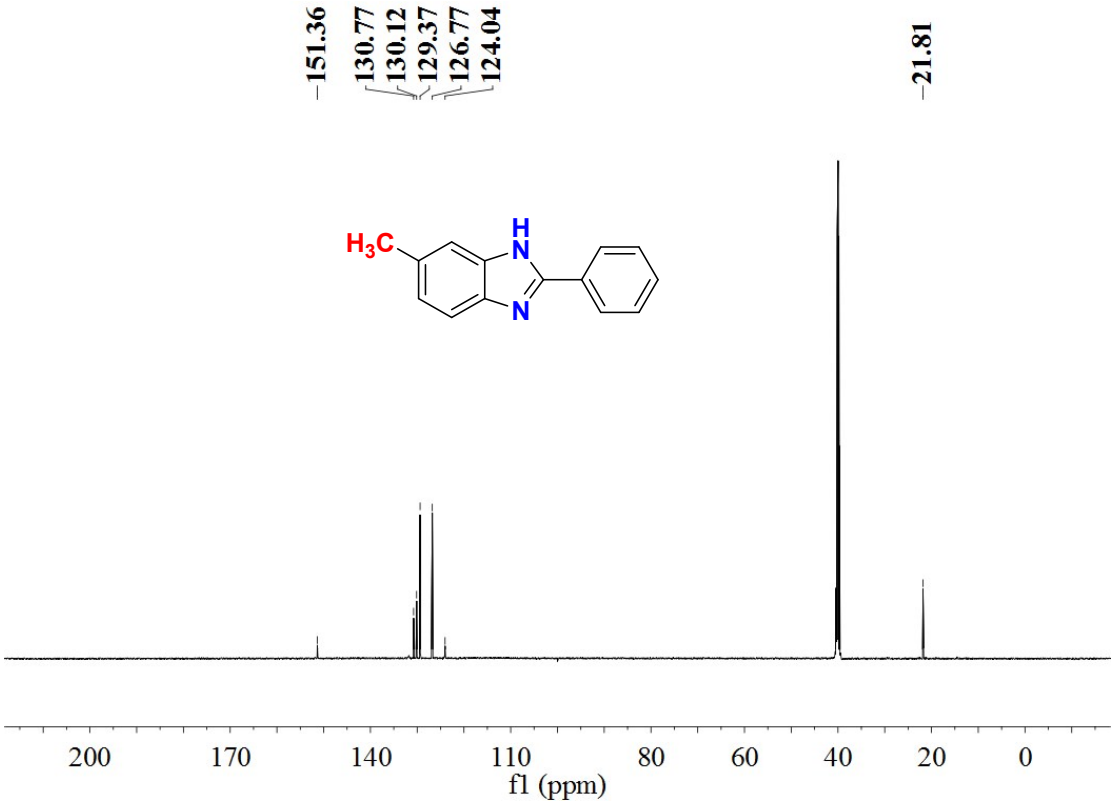
2b ^{13}C NMR



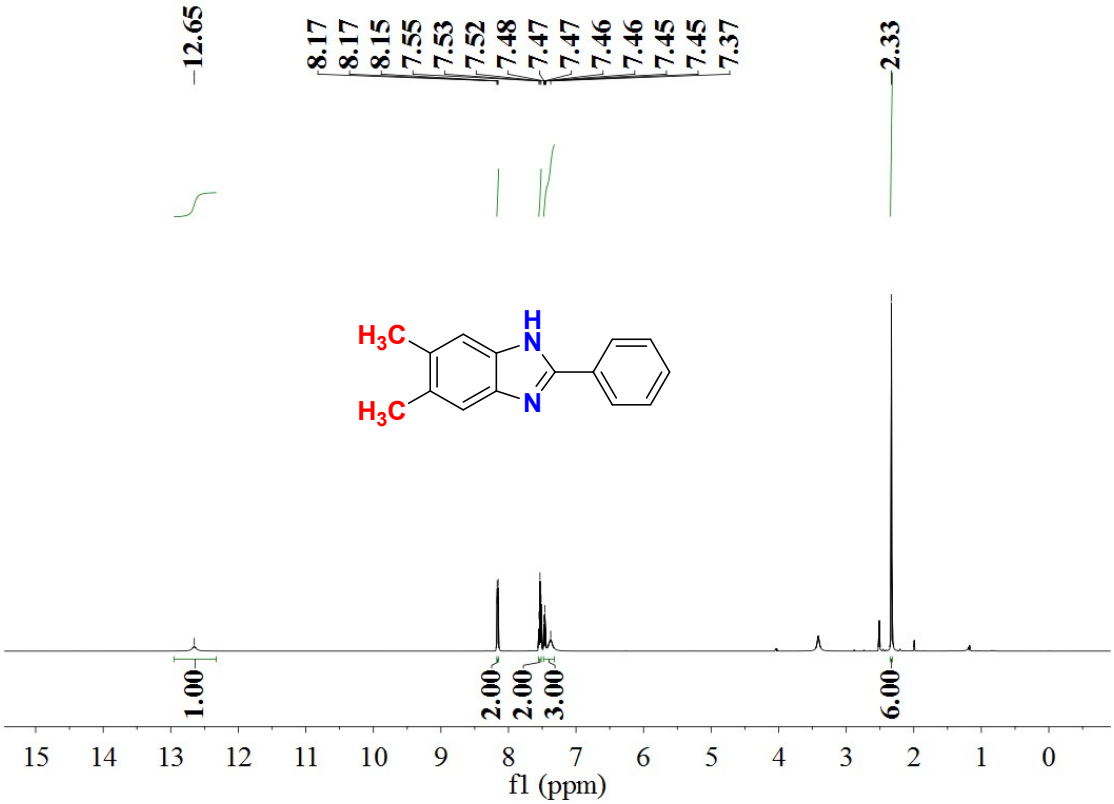
2c ^{1}H NMR



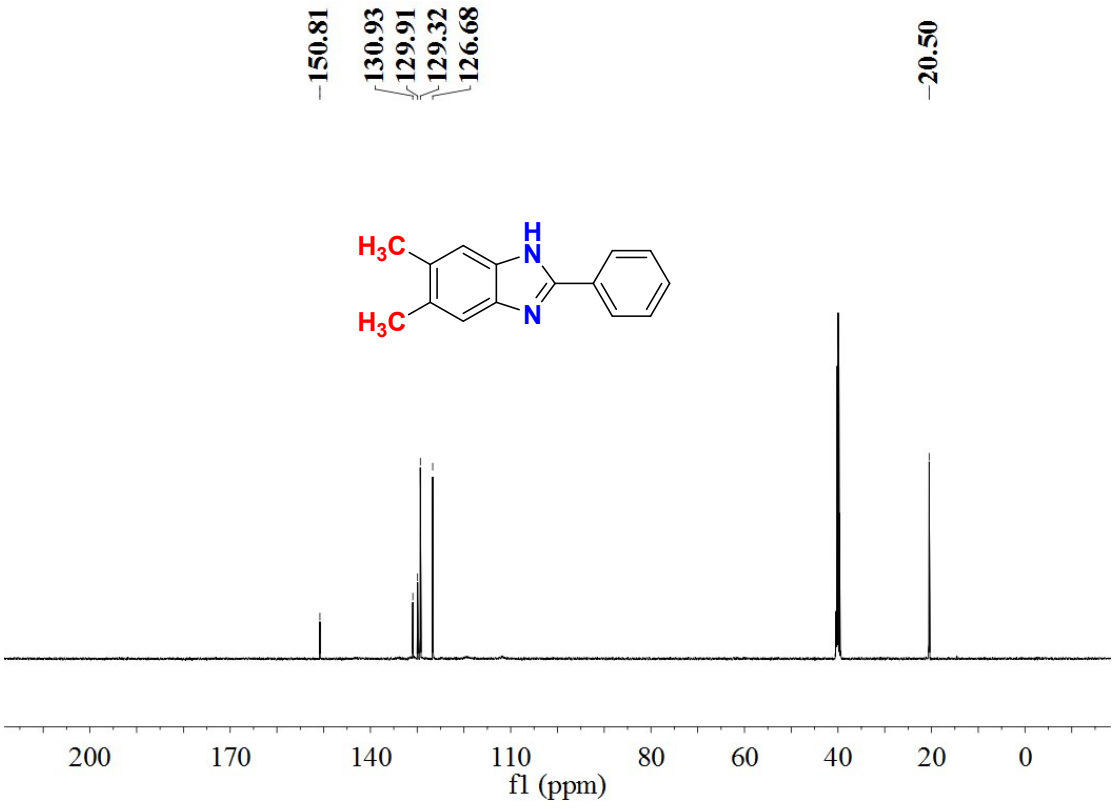
2c ^{13}C NMR



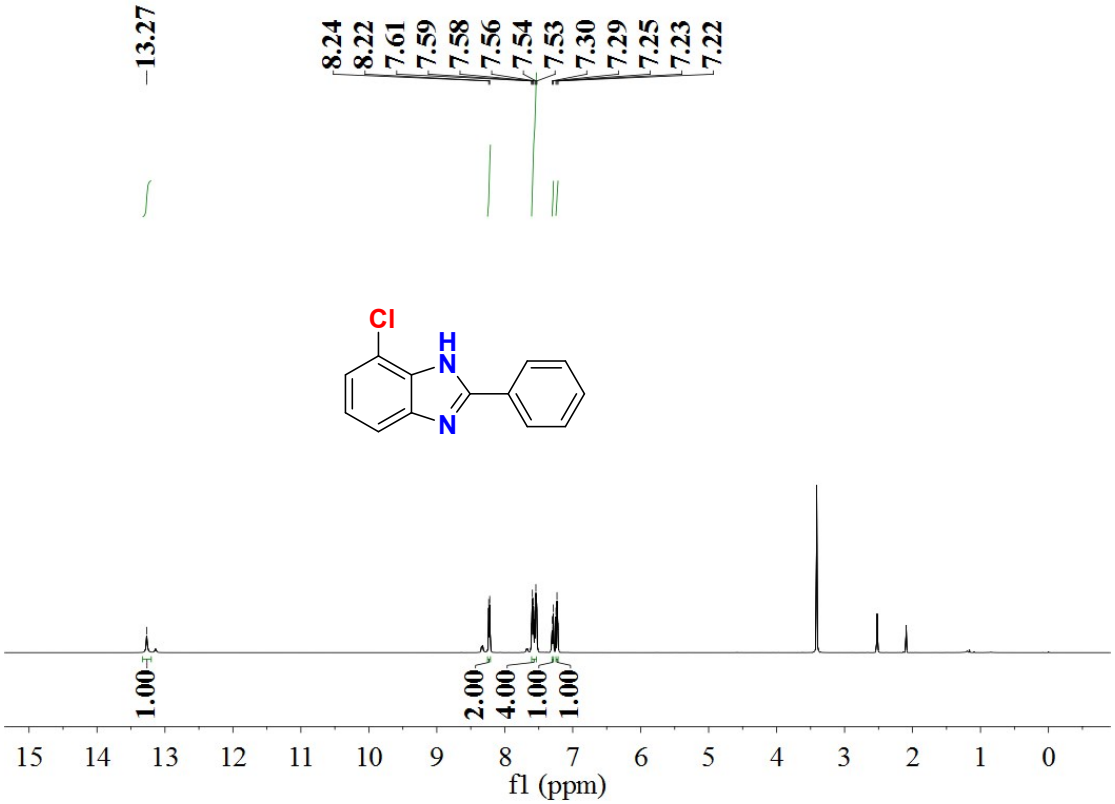
2d ^{1}H NMR



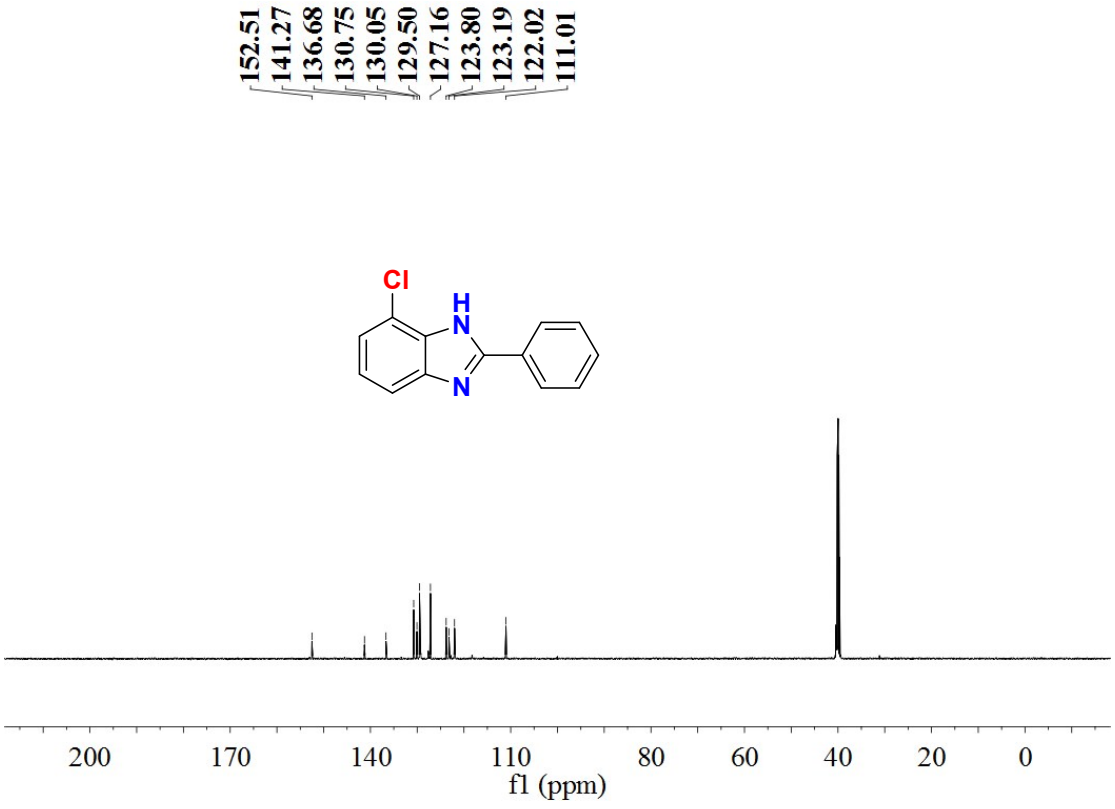
2d ^{13}C NMR



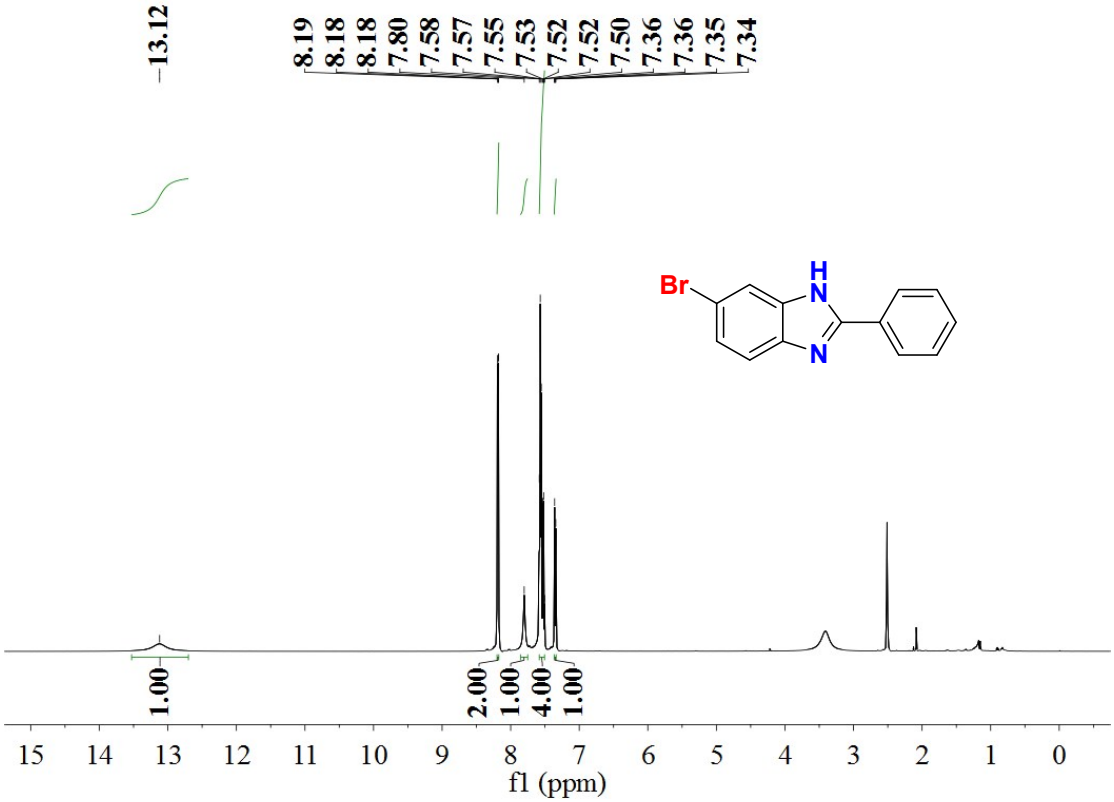
2e ^{1}H NMR



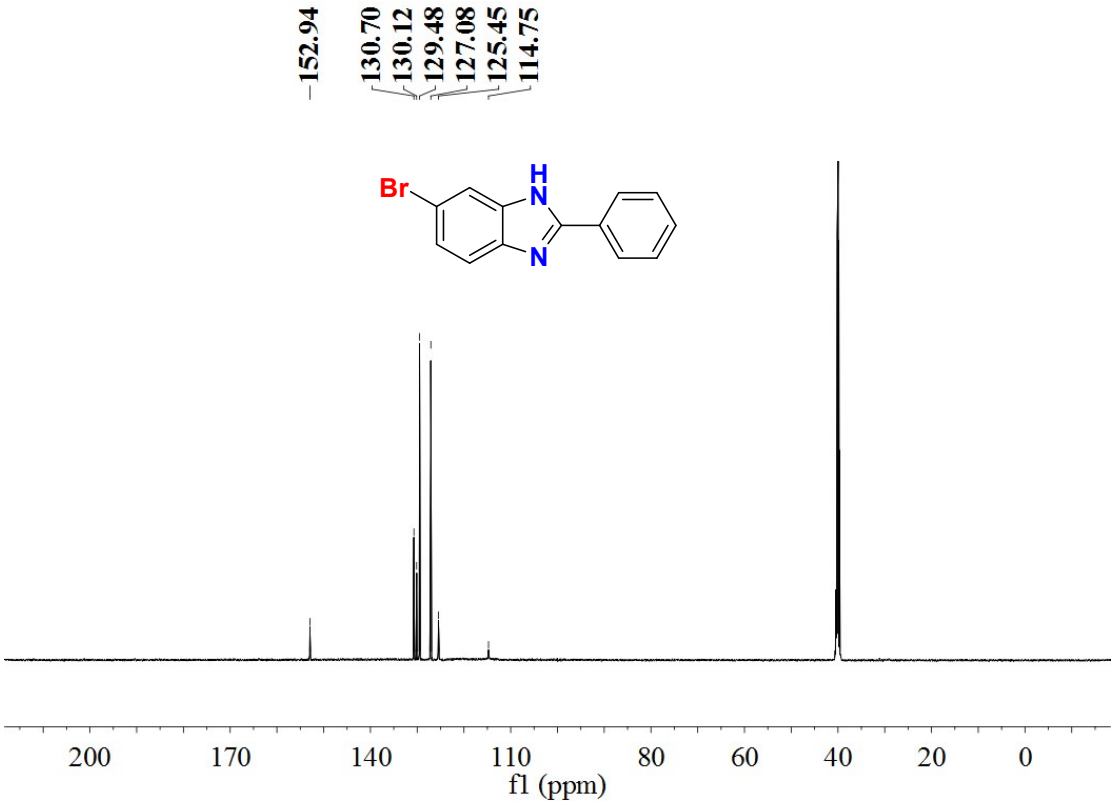
2e ^{13}C NMR



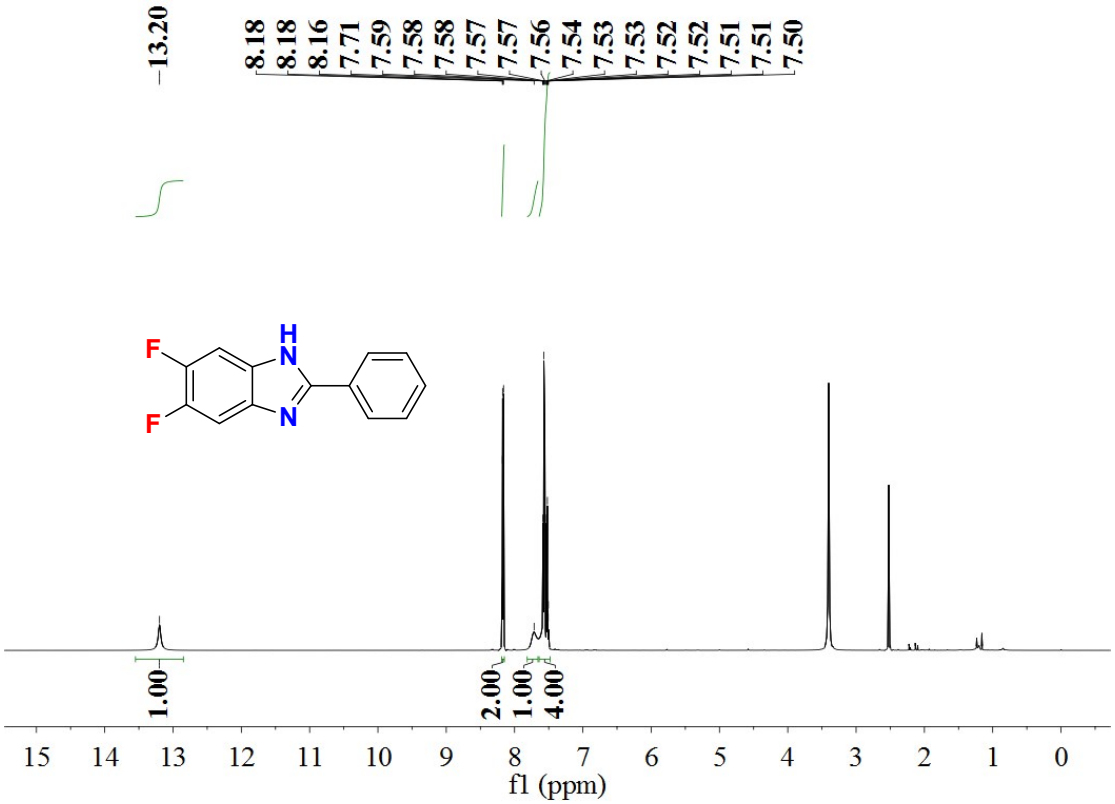
2f ^{1}H NMR



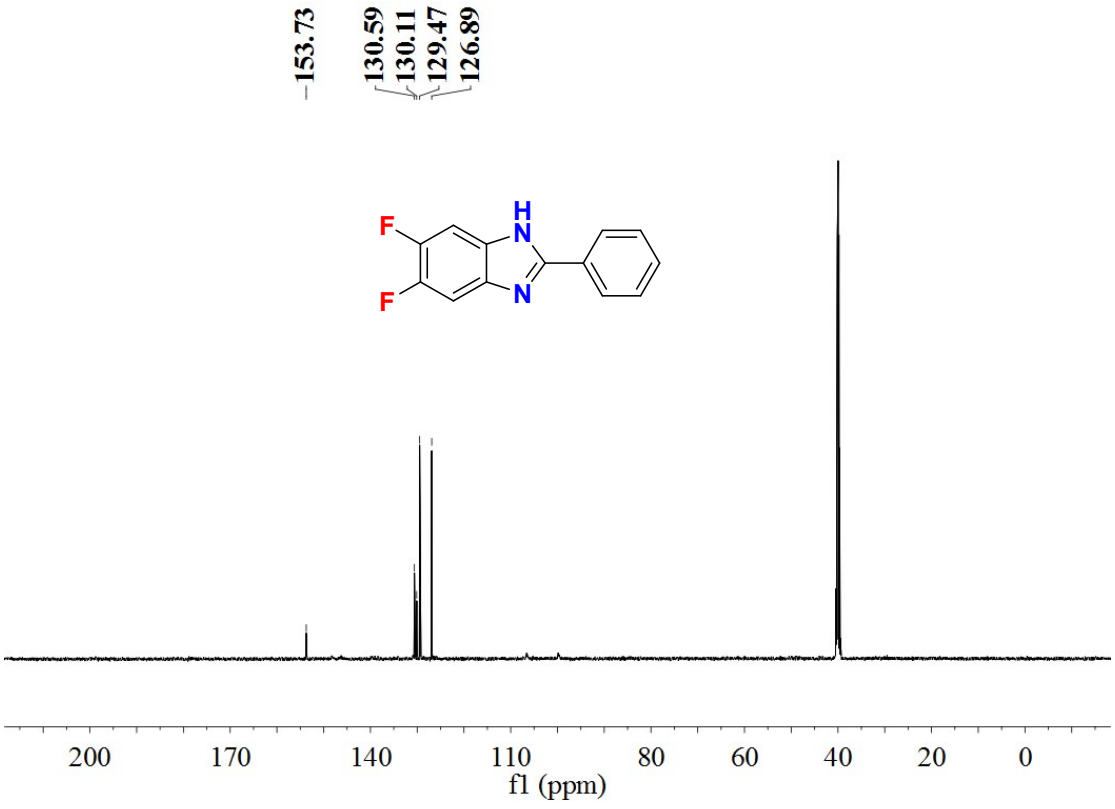
2f ^{13}C NMR



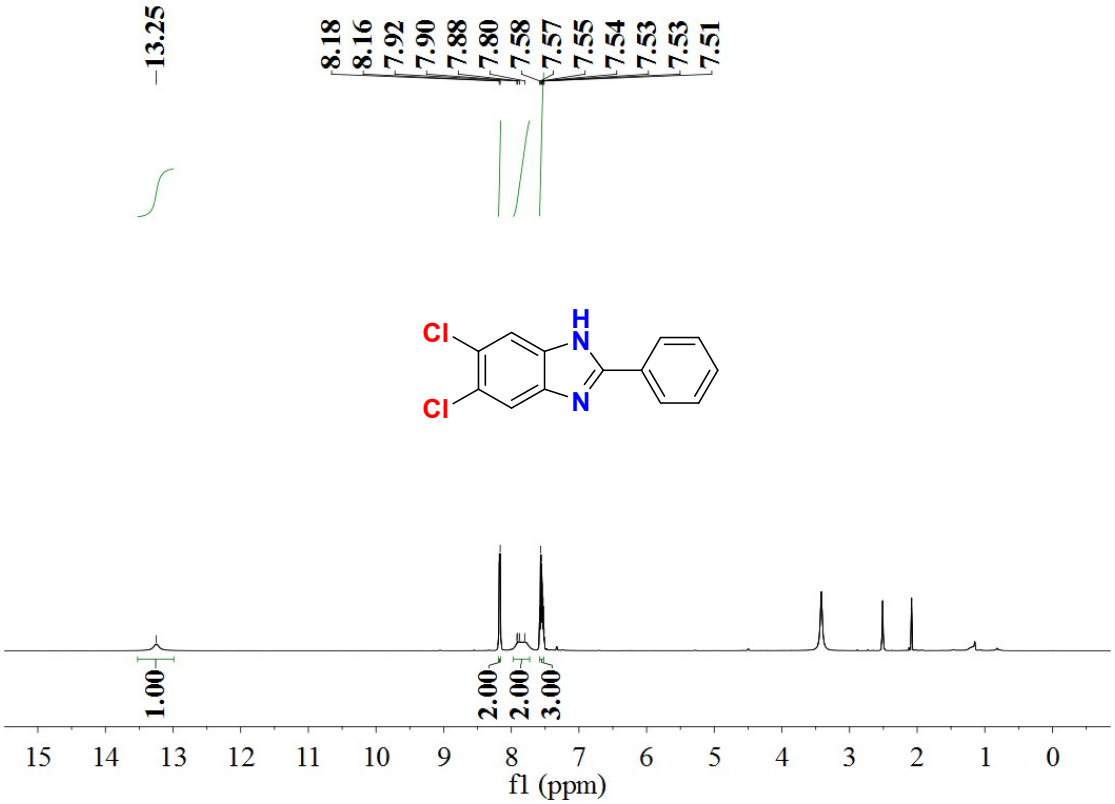
2g ^{1}H NMR



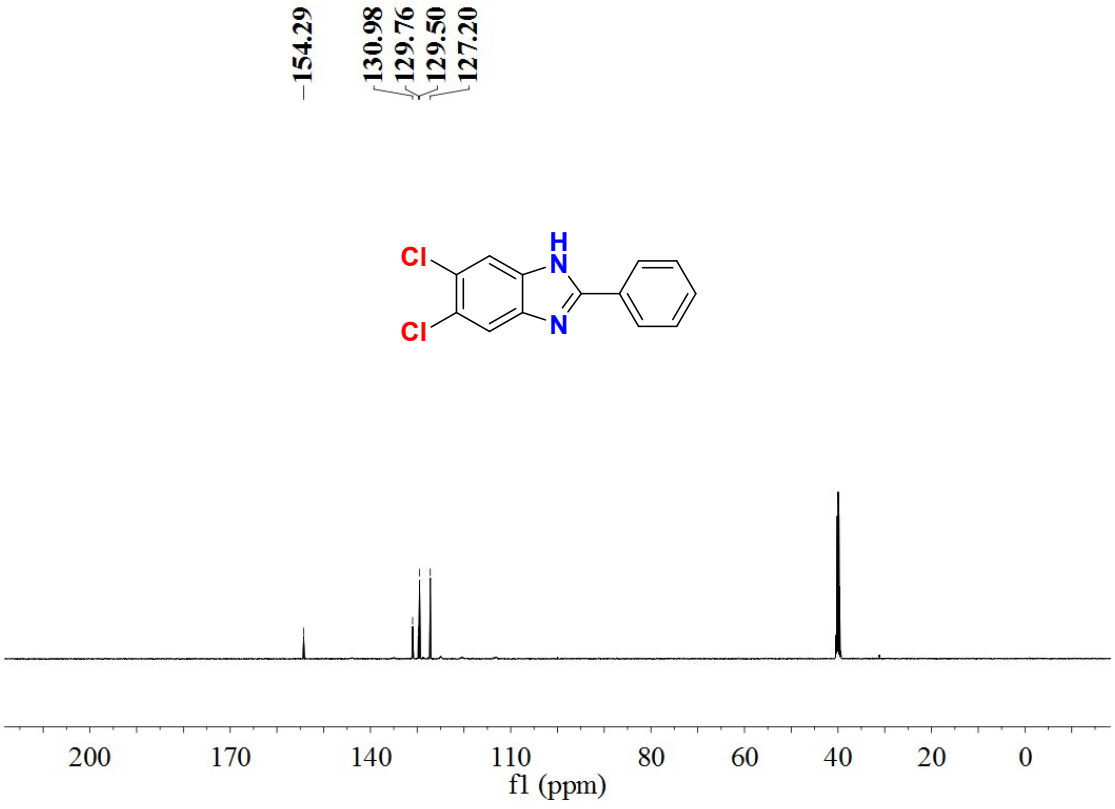
2g ^{13}C NMR



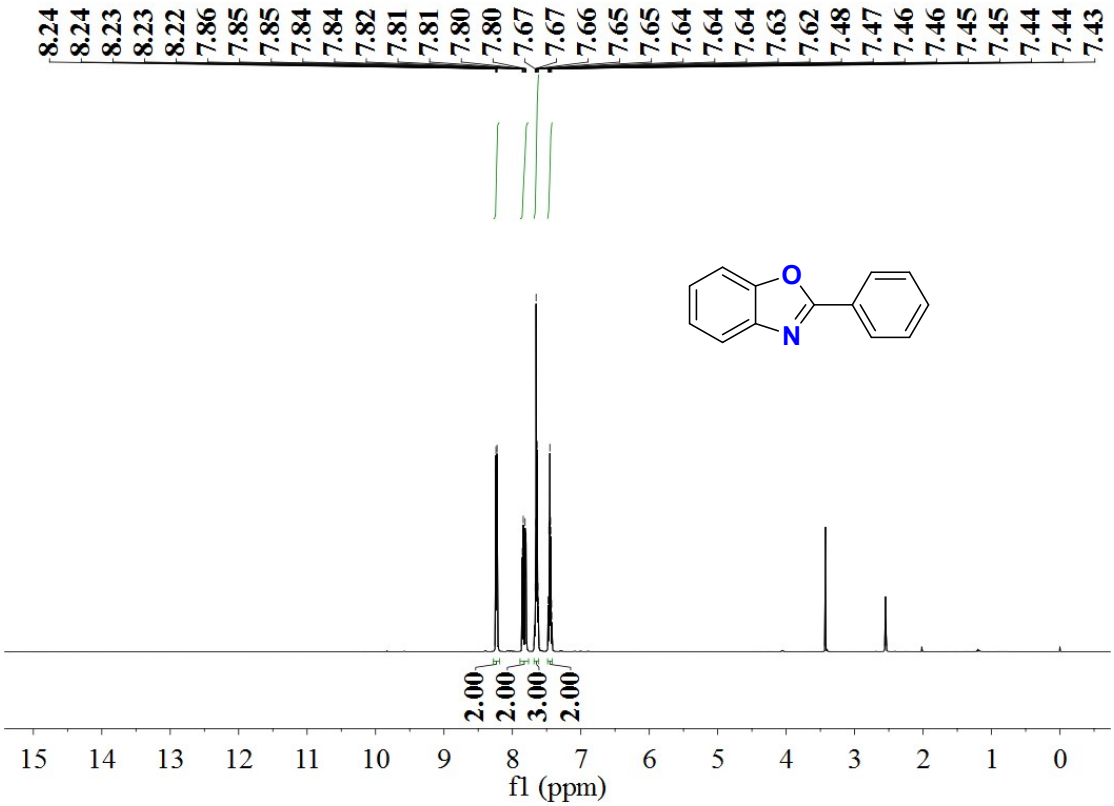
2h ^{1}H NMR



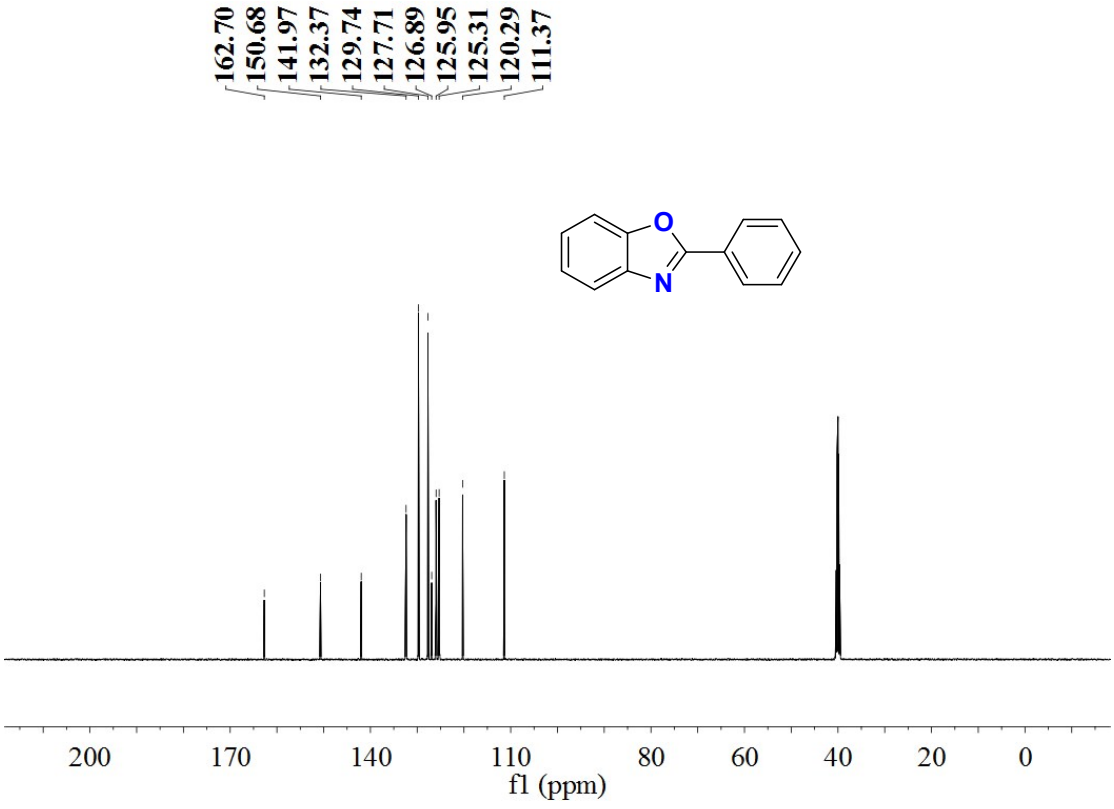
2h ^{13}C NMR



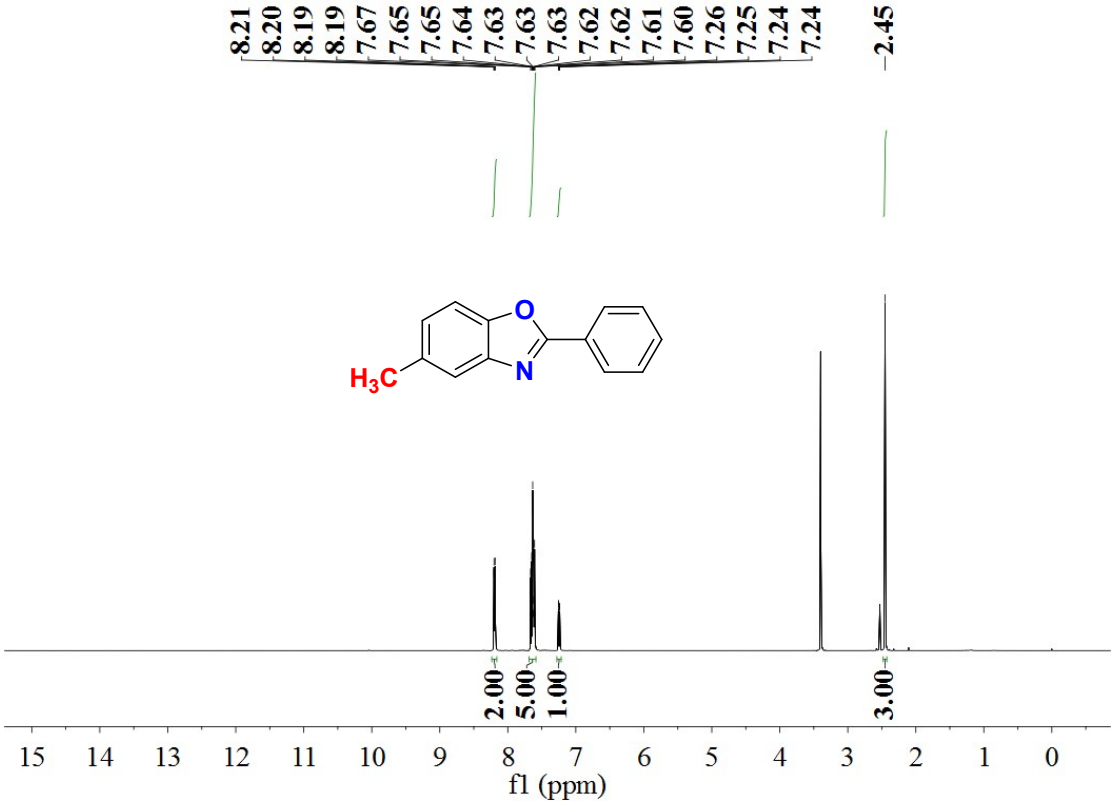
2i ^{1}H NMR



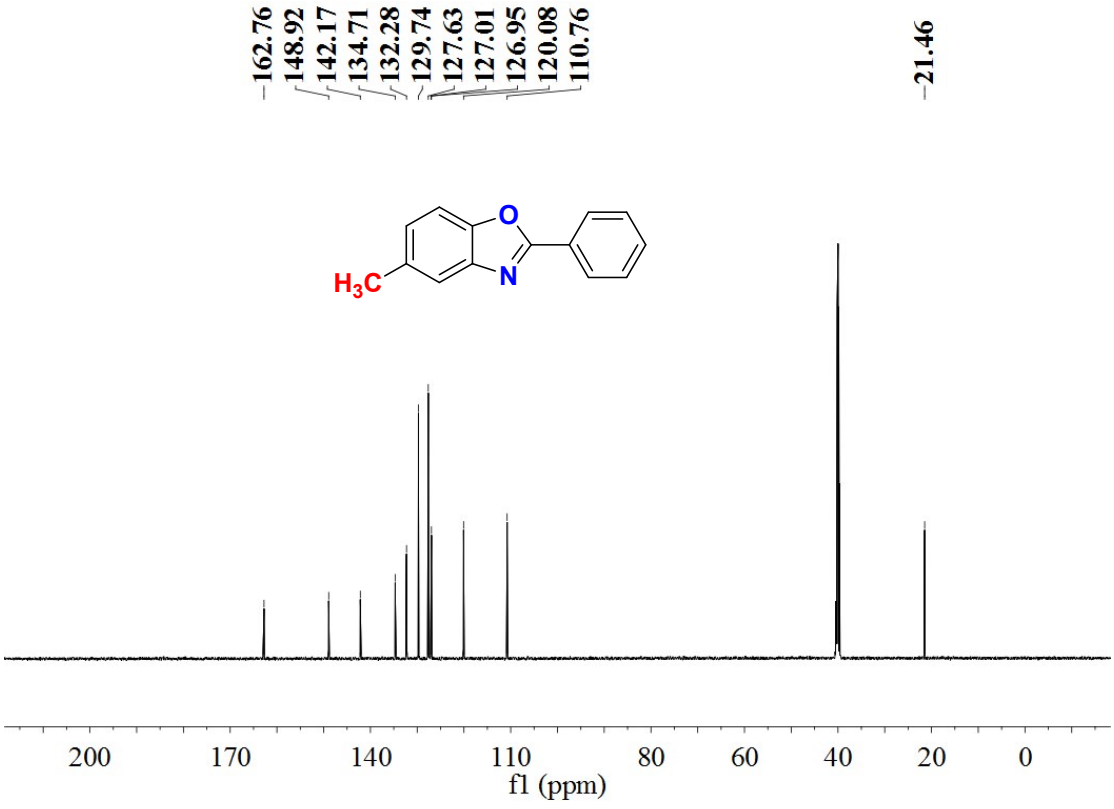
2i ^{13}C NMR



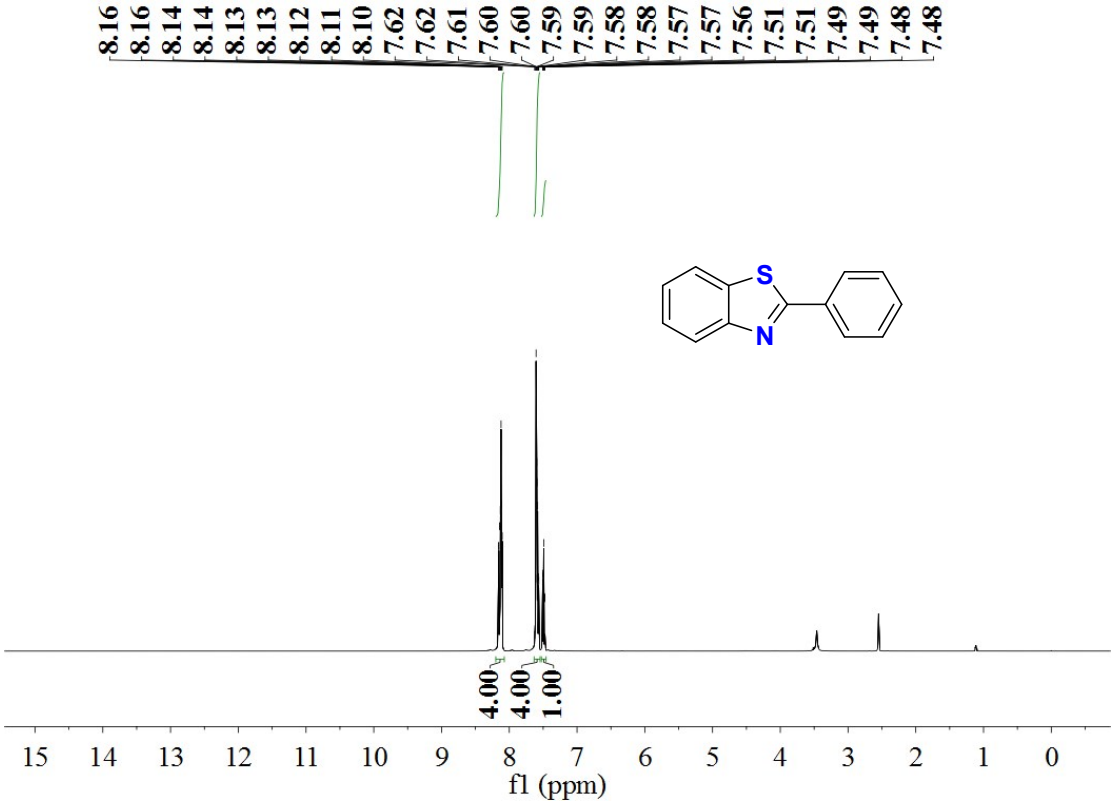
2j ^{1}H NMR



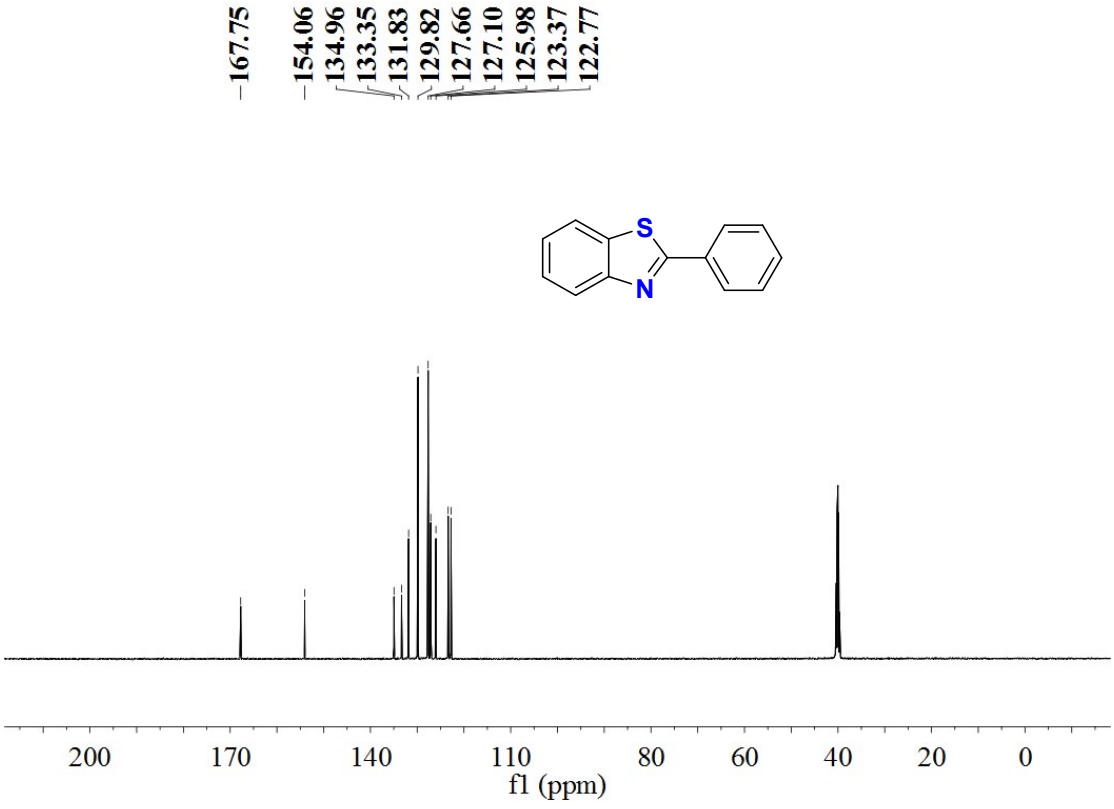
2j ^{13}C NMR



2k ^{1}H NMR



2k ^{13}C NMR



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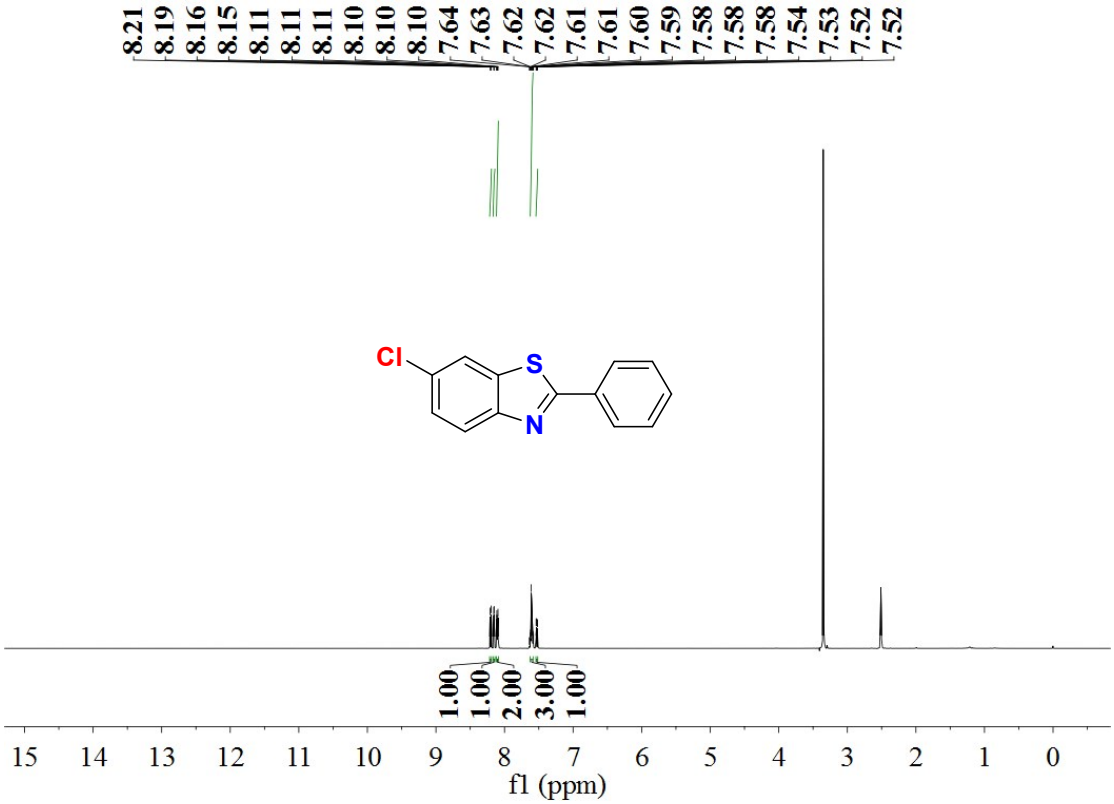

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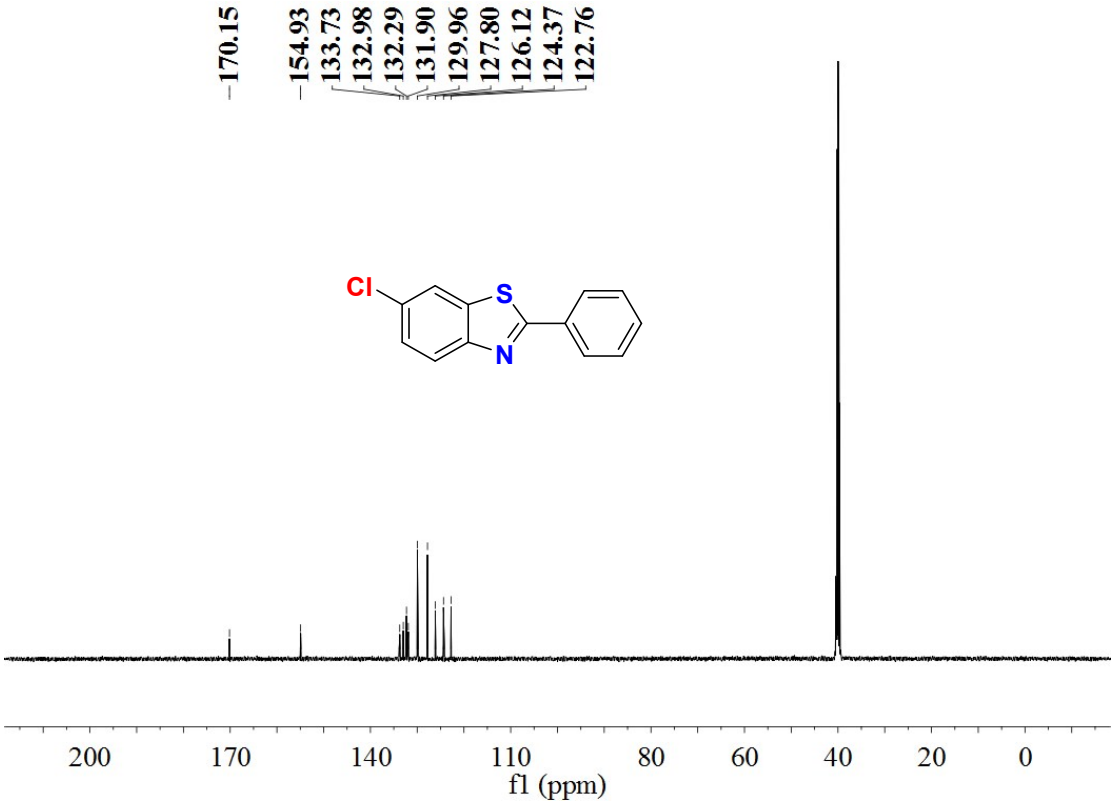
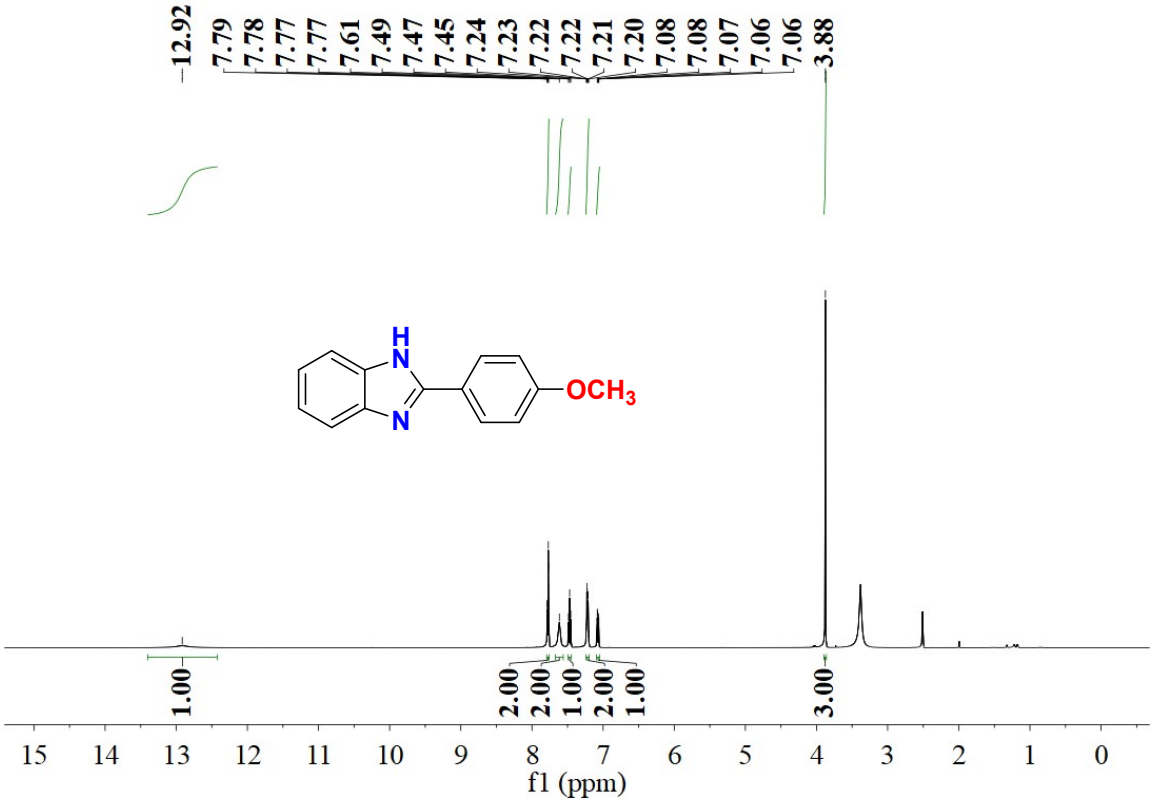


2m ^{1}H NMR



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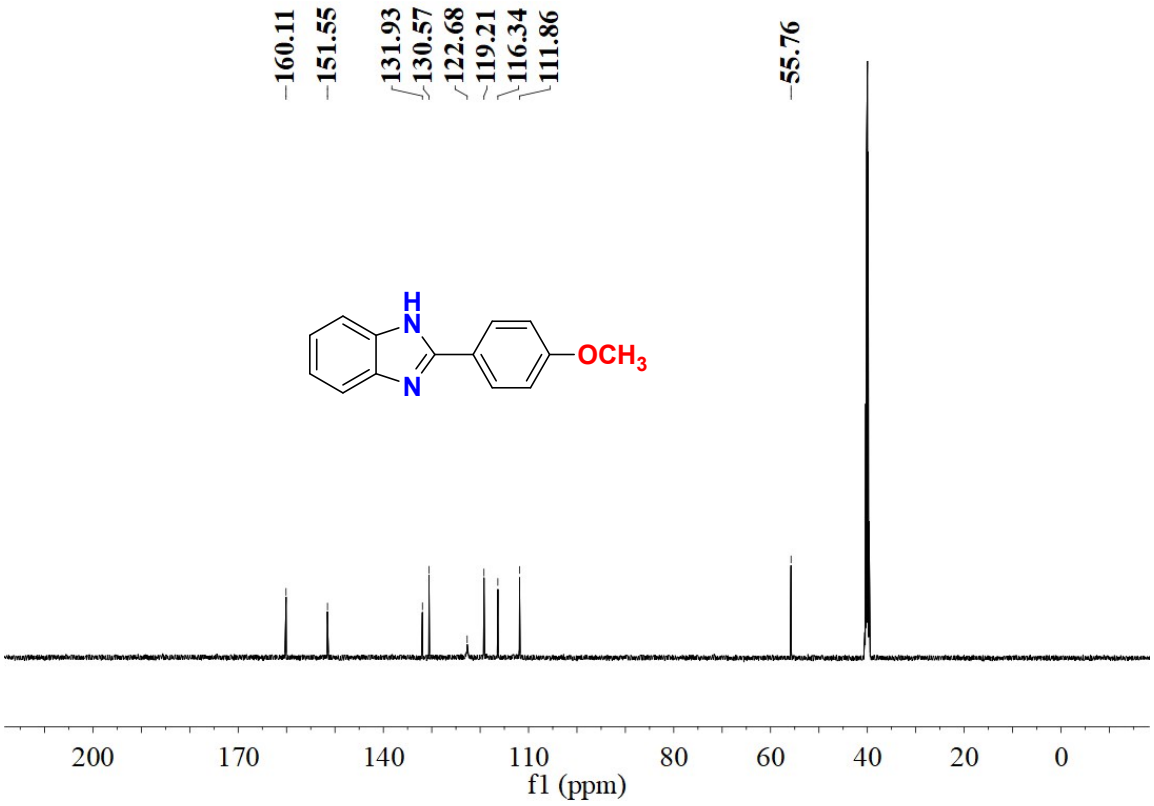
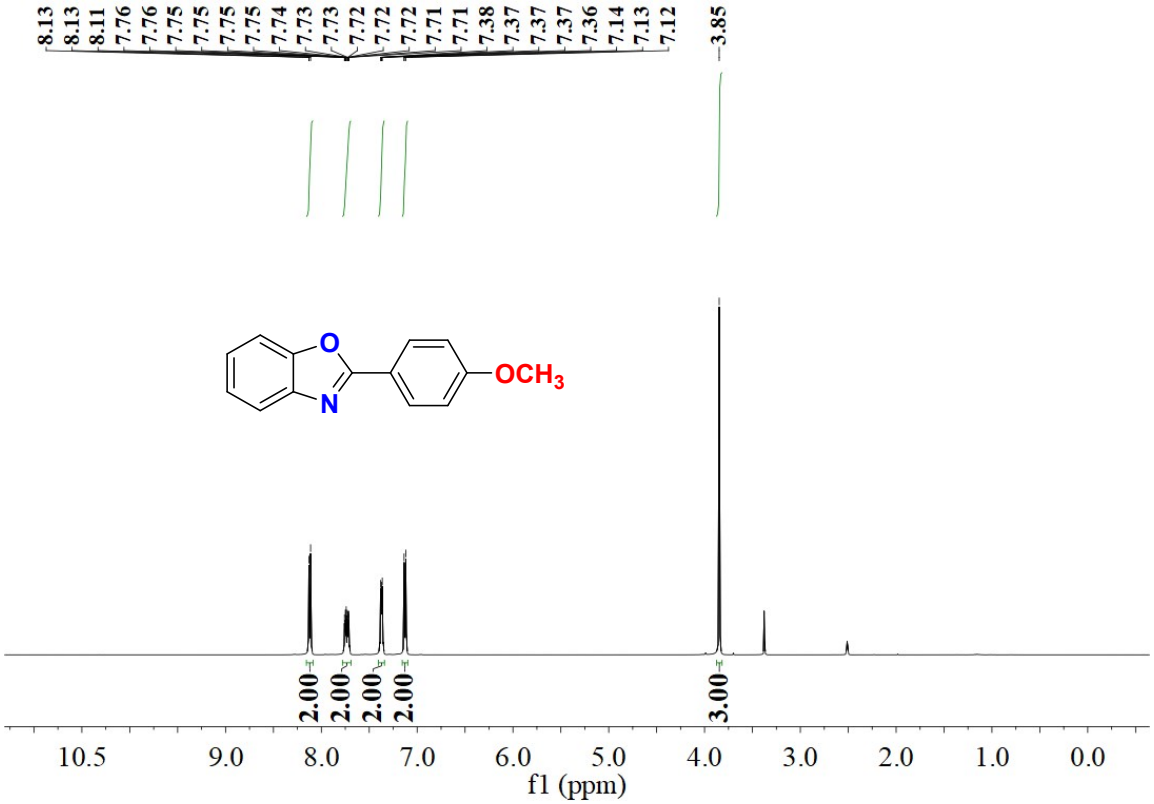
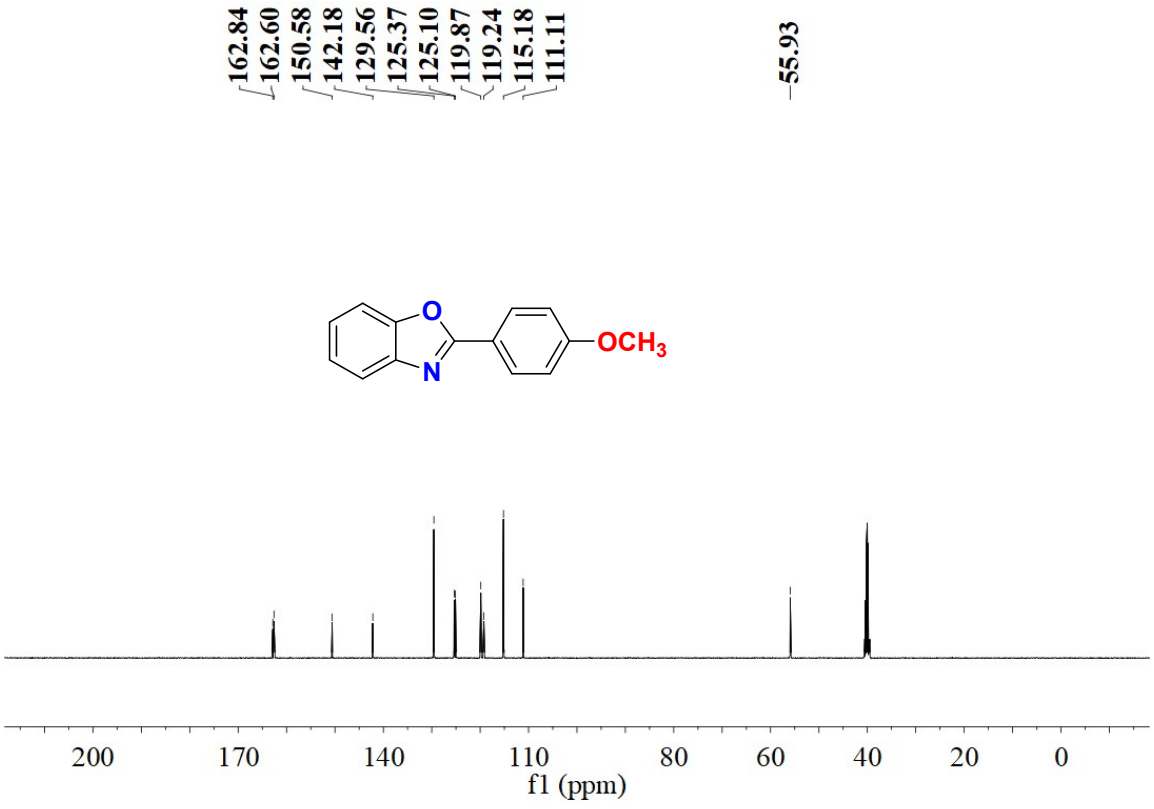


2n ^{1}H NMR



2n ^{13}C NMR



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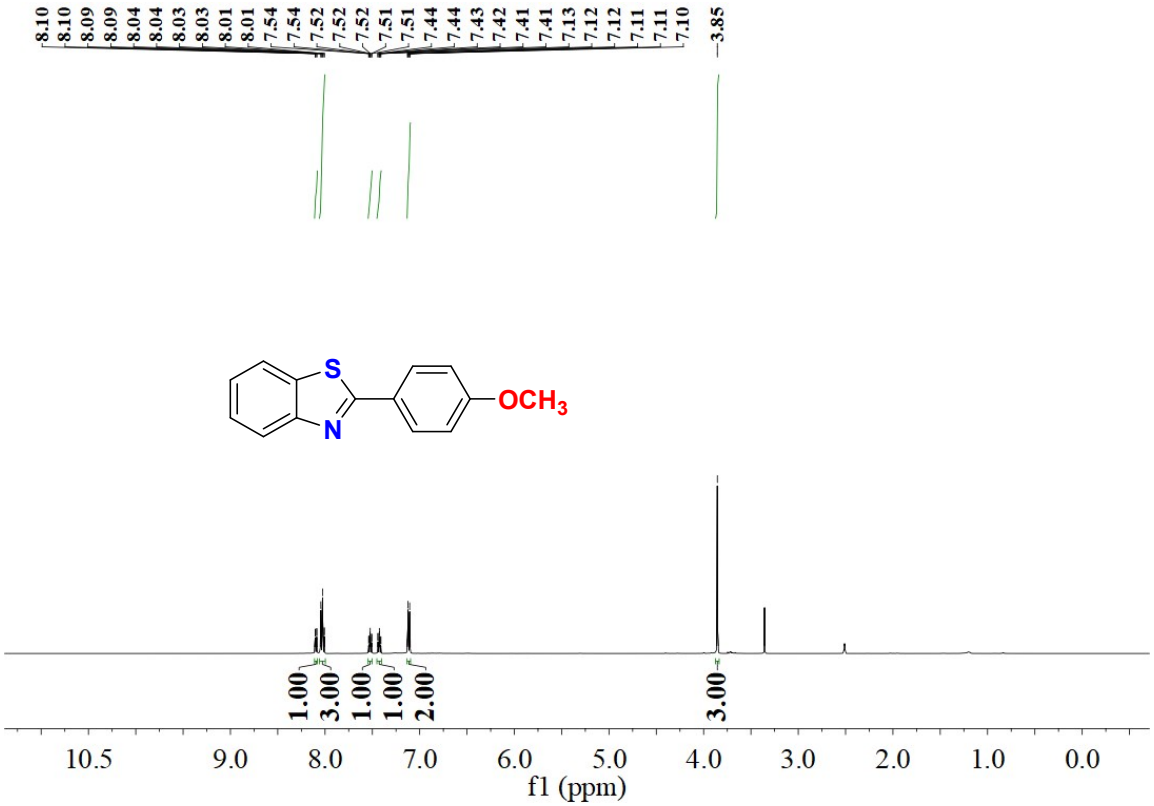
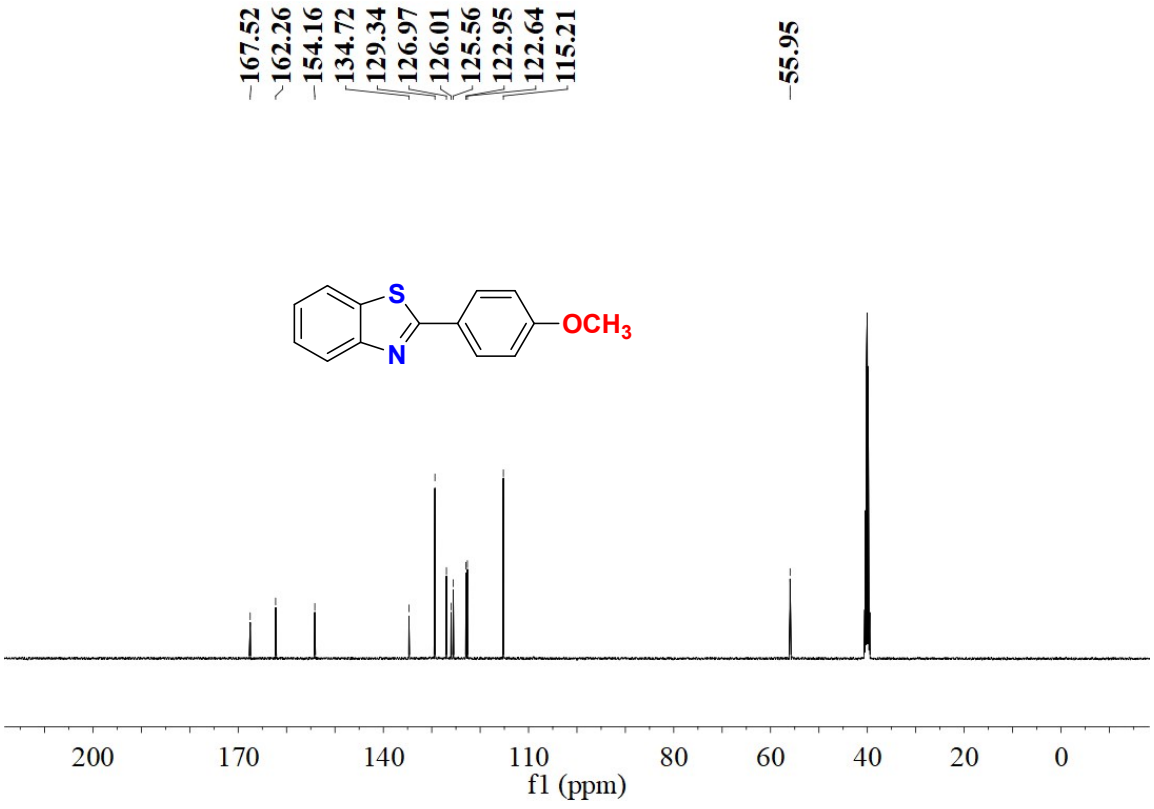


2o ^{13}C NMR



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