Supporting Information

CuCl-Catalyzed Direct C-H Alkenylation of Benzoxazoles with Allyl Halides

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1. General information

All commercially available reagents were used directly without purification unless otherwise stated. All solvents were purified following standard procedures. For chromatography, 200-300 mesh silica gel (Qingdao, China) was employed. $^1$H and $^{13}$C NMR spectra were recorded at 500 and 125 MHz, respectively. Chemical shifts are reported in ppm using tetramethylsilane as internal standard when CDCl$_3$ was used as solvent. IR spectra were recorded on a FT-IR instrument. The HRMS analysis was obtained on a QTOF mass spectrometer. Melting points were determined with melting points apparatus and are uncorrected.

2. General procedure for the CuCl-catalyzed alkenylation of benzoxazoles with allyl halides

To a solution of benzoxazole (1.0 mmol), allyl halide (1.5 mmol) and tBuOLi (3.0 mmol) in toluene (3.0 mL) was added CuCl (0.1 mmol) under a N$_2$ atmosphere. The resulting mixture was heated at 110 °C for the indicated time. After completion of the reaction, the mixture was cooled to room temperature. The solvent was removed in a vacuum, and the resulting residue was purified on a silica gel column (Petroleum ether/EtOAc = 50:1) to provide the desired products 3.

3. Spectral data of C2-alkenyldbenzoxazole products 3

(E)-2-(Prop-1-en-1-yl)benzo[d]oxazole (3a) (E). Pale yellow oil; 111 mg, 70% yield; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3738, 3673, 2929, 2855, 2372, 1512, 1015, 821 cm$^{-1}$; $^1$H NMR (500 MHz, CDCl$_3$) $\delta$ 1.98 (dd, $J_1 = 1.5$ Hz, $J_2 = 7.0$ Hz, 3H), 6.44 (dd, $J_1 = 1.5$ Hz, $J_2 = 15.5$ Hz, 1H), 6.97-7.04 (m, 1H), 7.26-7.29 (m, 2H), 7.44-7.45 (m, 1H), 7.65-7.67 (m, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$) $\delta$ 18.7, 110.2, 118.2, 119.8, 124.3, 124.8, 139.0, 141.9, 150.3, 162.4; HRMS (ESI) calcd for C$_{10}$H$_{10}$NO [M+H]$^+$ 160.0757, found 160.0762.
(Z)-2-(Prop-1-en-1-yl)benzo[d]oxazole (3a) (Z). Pale yellow oil; 31 mg, 20% yield; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3740, 3663, 2926, 2852, 2367, 1512, 1265, 1021, 809, 695 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 2.34 (dd, J₁ = 1.5 Hz, J₂ = 7.0 Hz, 3H), 6.34-6.39 (m, 1H), 6.43 (dd, J₁ = 1.0 Hz, J₂ = 11.5 Hz, 1H), 7.31-7.33 (m, 2H), 7.50-7.52 (m, 1H), 7.72-7.73 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 16.1, 110.4, 116.2, 119.9, 124.4, 125.0, 139.6, 141.7, 149.9, 162.6.

2-(2-Methylprop-1-en-1-yl)benzo[d]oxazole (3b). White solid; 156 mg, 90% yield; m.p: 42-45 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3440, 3055, 2923, 1639, 1536, 1454, 1242, 1006, 968, 924, 850, 744, 615 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 1.98 (s, 3H), 2.33 (s, 3H), 6.22 (s, 1H), 7.26-7.29 (m, 2H), 7.46-7.47 (m, 1H), 7.68-7.70 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 21.0, 27.6, 110.1, 111.9, 119.6, 124.1, 124.4, 142.0, 149.7, 150.5, 162.8.

5-Methyl-2-(2-methylprop-1-en-1-yl)benzo[d]oxazole (3c). Pale yellow solid; 159 mg, 84% yield; m.p: 50-53 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3438, 2920, 1648, 1533, 1451, 1348, 1242, 1006, 965, 850, 741 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 1.99 (s, 3H), 2.32 (s, 3H), 2.42 (s, 3H), 6.21 (s, 1H), 7.05 (d, J = 8.5 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 7.46 (s, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 21.0, 27.6, 110.1, 111.6, 119.9, 124.1, 124.4, 142.0, 149.7, 150.5, 162.8; HRMS (ESI) calcd for C₁₂H₁₄NO [M+H]⁺ 188.1070, found 188.1067. Anal. Calcd for C₁₂H₁₃NO: C, 76.98; H, 7.00; N, 7.48. Found: C, 76.77; H, 7.13; N, 7.30.
6-Methyl-2-(2-methylprop-1-en-1-yl)benzo[d]oxazole (3d).
Pale yellow solid; 167 mg, 89% yield; m.p: 54-56 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3435, 3055, 2931, 1645, 1536, 1454, 1345, 1242, 1006, 965, 853, 744 cm\(^{-1}\); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 2.00 (s, 3H), 2.33 (s, 3H), 2.44 (s, 3H), 6.22 (s, 1H), 7.08 (d, \(J = 8.5\) Hz, 1H), 7.25 (s, 1H), 7.54 (d, \(J = 8.0\) Hz, 1H); \(^13\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 20.9, 21.7, 27.6, 110.38, 112.0, 118.9, 125.3, 134.8, 139.8, 149.8, 150.0, 162.4; HRMS (ESI) calcd for C\(_{12}\)H\(_{14}\)NO \([\text{M+H}]^+\) 188.1070, found 188.1065. Anal. Calcd for C\(_{12}\)H\(_{13}\)NO: C, 76.98; H, 7.00; N, 7.48. Found: C, 76.77; H, 7.27; N, 7.35.

5-Chloro-2-(2-methylprop-1-en-1-yl)benzo[d]oxazole (3e).
Pale yellow solid; 162 mg, 78% yield; m.p: 59-63 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3432, 3055, 2914, 1645, 1536, 1451, 1345, 1242, 1000, 965, 856, 747, 624 cm\(^{-1}\); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 2.01 (s, 3H), 2.32 (s, 3H), 6.19 (s, 1H), 7.20 (dd, \(J_1 = 2.0\) Hz, \(J_2 = 8.5\) Hz, 1H), 7.33 (d, \(J = 8.5\) Hz, 1H), 7.62 (d, \(J = 2.0\) Hz, 1H); \(^13\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 21.0, 27.7, 110.8, 111.5, 119.4, 124.6, 129.5, 143.1, 148.2, 151.9, 164.0; HRMS (ESI) calcd for C\(_{11}\)H\(_{11}\)ClNO \([\text{M+H}]^+\) 208.0524, found 208.0526. Anal. Calcd for C\(_{11}\)H\(_{10}\)ClNO: C, 63.62; H, 4.85; N, 6.75. Found: C, 63.66; H, 5.09; N, 6.41.

5-Bromo-2-(2-methylprop-1-en-1-yl)benzo[d]oxazole (3f).
Pale yellow solid; 201 mg, 80% yield; m.p: 62-65 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3090, 1804, 1657, 1539, 1452, 1249, 1141, 1045, 953 cm\(^{-1}\); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 2.04 (d, \(J = 1.0\) Hz, 3H), 2.34 (s, 1H), 6.21 (t, \(J = 1.0\) Hz, 1H), 7.32 (d, \(J = 8.5\) Hz, 1H), 7.37 (dd, \(J_1 = 2.0\) Hz, \(J_2 = 8.5\) Hz, 1H), 7.80 (d, \(J = 2.0\) Hz, 1H); \(^13\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 21.1,
27.8, 111.4, 111.5, 116.8, 122.5, 127.4, 143.6, 148.7, 152.1, 163.9; HRMS (ESI) calcd for C_{11}H_{10}BrNONa [M+Na]^+ 273.9837, found 273.9828.

6-Bromo-2-(2-methylprop-1-en-1-yl)benzo[d]oxazole (3g). Pale yellow solid; 218 mg, 87% yield; m.p: 77-79 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3099, 2979, 2911, 1884, 1654, 1539, 1427, 1257, 1133, 1045, 945, 906, 839, 806, 676, 588, 424 cm\(^{-1}\); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 2.02 (s, 3H), 2.32 (s, 3H), 6.19 (s, 1H), 7.39 (dd, \(J_1 = 1.5\) Hz, \(J_2 = 8.5\) Hz, 1H), 7.51 (d, \(J = 8.5\) Hz, 1H), 7.60 (d, \(J = 1.5\) Hz, 1H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 21.1, 27.7, 111.5, 113.7, 117.2, 120.5, 127.5, 141.2, 150.2, 151.8, 163.2; HRMS (ESI) calcd for C_{11}H_{11}BrNO [M+H]^+ 252.0019, found 252.0016.

7-Bromo-2-(2-methylprop-1-en-1-yl)benzo[d]oxazole (3h). Pale yellow solid; 193 mg, 77% yield; m.p: 57-59 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3079, 2917, 1919, 1654, 1548, 1421, 1348, 1262, 1215, 1127, 1068, 959, 836, 786, 736, 624 cm\(^{-1}\); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 2.04 (s, 3H), 2.36 (s, 3H), 6.27 (s, 1H), 7.15 (t, \(J = 8.0\) Hz, 1H), 7.39 (d, \(J = 8.0\) Hz, 1H), 7.59 (d, \(J = 8.0\) Hz, 1H); \(^{13}\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 21.1, 27.8, 102.1, 111.4, 118.6, 125.3, 127.5, 142.7, 147.9, 152.3, 162.9; HRMS (ESI) calcd for C_{11}H_{11}BrNO [M+H]^+ 252.0019, found 252.0024. Anal. Calcd for C_{11}H_{10}BrNO: C, 52.41; H, 4.00; N, 5.56. Found: C, 52.56; H, 4.18; N, 5.40.

2-(2-Methylprop-1-en-1-yl)-5-(trifluoromethyl)benzo[d]oxazole (3i). Pale yellow solid; 176 mg, 73% yield; m.p: 56-58 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3058, 2920, 1657, 1524, 1442, 1321, 1168, 1124, 1045, 933, 812, 656 cm\(^{-1}\);
$^1$H NMR (500 MHz, CDCl$_3$) δ 2.05 (d, $J$ = 1.0 Hz, 3H), 2.36 (d, $J$ = 0.5 Hz, 3H), 6.24-6.25 (m, 1H), 7.53 (t, $J$ = 0.8 Hz, 2H), 7.95 (s, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 21.1, 27.7, 110.5, 111.3, 117.1, 117.1, 121.6, 121.6, 142.2, 151.4, 152.9, 164.4; HRMS (ESI) calcd for C$_{12}$H$_{11}$F$_3$NO [M+H]$^+$ 242.0787, found 242.0785.

2-(Cyclohex-1-en-1-yl)benzo[d]oxazole (3k). Pale yellow solid; 159 mg, 80% yield; m.p: 29-31 ℃; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3432, 3055, 2923, 1639, 1533, 1454, 1242, 1006, 955, 847, 747, 623 cm$^{-1}$; $^1$H NMR (500 MHz, CDCl$_3$) δ 1.67-1.70 (m, 2H), 1.77-1.80 (m, 2H), 2.28 (dd, $J_1$ = 2.5Hz, $J_2$ = 6.5 Hz, 2H), 2.59 (t, $J$ = 3.0 Hz, 2H), 7.05-7.06 (m, 1H), 7.26-7.28 (m, 2H), 7.44-7.46 (m, 1H), 7.68-7.70 (m, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 21.7, 22.1, 24.7, 25.8, 110.1, 120.0, 124.0, 124.1, 124.7, 135.4, 142.0, 150.3, 164.1; HRMS (ESI) calcd for C$_{13}$H$_{14}$NO [M+H]$^+$ 200.1069, found 200.1076.

2-(Cyclohex-1-en-1-yl)-5-methylbenzo[d]oxazole (3l).

White solid; 149 mg, 70% yield; m.p: 50-53 ℃; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3426, 2923, 1651, 1542, 1460, 1345, 1236, 1101, 1003, 968, 850, 739 cm$^{-1}$; $^1$H NMR (500 MHz, CDCl$_3$) δ 1.67-1.71 (m, 2H), 1.76-1.80 (m, 2H), 2.28-2.30 (m, 2H), 2.43 (s, 3H), 2.59 (dd, $J_1$ = 5.5 Hz, $J_2$ = 7.5 Hz, 2H), 7.02-7.07 (m, 2H), 7.31 (d, $J$ = 8.5 Hz, 1H), 7.46 (s, 1H); $^{13}$C NMR (125 MHz, CDCl$_3$) δ 21.5, 21.9, 22.1, 24.7, 25.8, 109.5, 119.7, 125.7, 126.4, 133.8, 135.0, 142.1, 148.5, 164.3; HRMS (ESI) calcd for C$_{14}$H$_{16}$NO [M+H]$^+$ 214.1226, found 214.1231.

5-Chloro-2-(cyclohex-1-en-1-yl)benzo[d]oxazole (3m).

White solid; 175 mg, 75% yield; m.p: 60-62 ℃;
(recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3435, 3061, 2923, 1539, 1448, 1236, 1003, 968, 855, 736, 618 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 1.67-1.70 (m, 2H), 1.77-1.80 (m, 2H), 2.28 (dd, J₁ = 2.5 Hz, J₂ = 6.5 Hz, 2H), 2.59 (t, J = 3.0 Hz, 2H), 7.05-7.06 (t, J = 1.8 Hz, 1H), 7.25-7.28 (m, 1H), 7.44-7.46 (m, 1H), 7.68-7.70 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 21.8, 22.0, 24.6, 25.9, 110.9, 119.7, 124.9, 126.1, 129.5, 136.5, 143.1, 148.9, 165.4; HRMS (ESI) calcd for C₁₃H₁₂NOCl [M+H]⁺ 234.0680, found 234.0678.

4. General procedure for the synthesis of 1,3-diene containing benzoxazoles

To a solution of benzoxazole (1.5 mmol), 1,4-dibromobut-2-ene (1.0 mmol) and tBuOLi (3.0 mmol) in toluene (3.0 mL) was added CuCl (0.1 mmol) under a N₂ atmosphere. The resulting mixture was heated at 50 °C for the indicated time. After completion of the reaction, the mixture was cooled to room temperature. The solvent was removed in a vacuum, and the resulting residue was purified on a silica gel column (Petroleum ether/EtOAc = 50:1) to provide the desired products 6.

5. Spectral data of 1,3-diene containing benzoxazoles 6

(E)-2-(Buta-1,3-dien-1-yl)benzo[d]oxazole (6a). White solid; 128 mg, 75% yield; m.p: 32-34 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature) IR (KBr) 2926, 1527, 1451, 1242, 1000, 912, 850, 739 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 5.45 (d, J = 10.0 Hz, 1H), 5.60 (d, J = 16.5 Hz, 1H), 6.52-6.60 (m, 2H), 7.29-7.31 (m, 2H), 7.39 (dd, J₁ = 11.0 Hz, J₂ = 15.5 Hz, 1H), 7.46-7.50 (m, 1H), 7.68-7.70 (m, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 110.3, 117.9, 120.0, 123.8, 124.5, 125.2, 135.5, 140.0, 142.2, 150.4, 162.5; HRMS (ESI) calcd for C₁₁H₁₀NO [M+H]⁺ 172.0757, found 172.0752.

(E)-2-(buta-1,3-dien-1-yl)-5-methylbenzo[d]oxazole (6b).
White solid; 139 mg, 75% yield; m.p: 60-62 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3014, 1845, 1595, 1519, 1257, 1186, 1003, 924, 856, 800 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 2.46 (s, 3H), 5.46 (d, J = 10.0 Hz, 1H), 5.61 (d, J = 17.0 Hz, 1H), 6.51-6.61 (m, 2H), 7.12 (dd, J₁ = 1.0 Hz, J₂ = 8.5 Hz, 1H), 7.35-7.40 (m, 2H), 7.47 (s, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 21.5, 109.7, 118.0, 119.8, 123.6, 126.4, 134.3, 135.6, 139.6, 142.3, 148.6, 162.6; HRMS (ESI) calcd for C₁₂H₁₂NO [M+H]⁺ 186.0913, found 186.0912.

(E)-2-(Buta-1,3-dien-1-yl)-6-methylbenzo[d]oxazole (6c). White solid; 135 mg, 73% yield; m.p: 59-62 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3431, 2917, 1610, 1486, 1239, 1112, 965, 812, 594 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 2.48 (s, 3H), 5.45 (d, J = 10.0 Hz, 1H), 5.60 (d, J = 17.0 Hz, 1H), 6.51-6.61 (m, 2H), 7.13 (d, J = 8.5 Hz, 1H), 7.29 (s, 1H), 7.36 (dd, J₁ = 11.0 Hz, J₂ = 16.0 Hz, 1H), 7.55 (d, J = 8.5 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) 21.8, 110.5, 118.0, 119.2, 123.4, 125.7, 135.6, 135.8, 139.4, 140.0, 150.7, 164.9; HRMS (ESI) calcd for C₁₂H₁₂NO [M+H]⁺ 186.0913, found 186.0900.

(E)-2-(Buta-1,3-dien-1-yl)-5-chlorobenzo[d]oxazole (6d). White solid; 164 mg, 80% yield; m.p: 58-60 °C; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3014, 1586, 1524, 1445, 1257, 1012, 915, 906, 853, 792, 697, 591 cm⁻¹; ¹H NMR (500 MHz, CDCl₃) δ 5.49 (d, J = 10.0 Hz, 1H), 5.62 (d, J = 17.0 Hz, 1H), 6.47-6.60 (m, 2H), 7.25-7.28 (m, 1H), 7.35-7.40 (m, 2H), 7.64 (d, J = 2.0 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 111.0, 117.4, 119.8, 124.4, 125.4, 129.9, 135.4, 140.7, 143.3, 148.9, 163.7; HRMS (ESI) calcd for C₁₁H₉ClNO [M+H]⁺ 206.0211, found 206.0216.
(E)-2-(Buta-1, 3-dien-2-yl)-5-bromobenzo[d]oxazole (6e).  
White solid; 174 mg, 70% yield; m.p: 71-73 °C;  
(recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3087, 1845, 1583, 1519, 1445, 1251, 1165, 1000, 927, 862, 797, 680, 583 cm$^{-1}$;  
$^1$H NMR (500 MHz, CDCl$_3$) δ 5.49 (d, $J = 10.0$ Hz, 1H), 5.62 (d, $J = 17.0$ Hz, 1H), 6.48-6.60 (m, 2H), 7.32-7.41 (m, 3H), 7.79 (d, $J = 2.0$ Hz, 1H);  
$^{13}$C NMR (125 MHz, CDCl$_3$) δ 111.5, 117.2, 117.3, 122.8, 124.5, 128.1, 135.4, 140.8, 143.7, 149.4, 163.5; HRMS (ESI) calcd for C$_{11}$H$_9$NOBr [M+H]$^+$ 249.9862, found 249.9867.

(E)-6-Bromo-2-(buta-1,3-dien-1-yl)benzo[d]oxazole (6f).  
Pale yellow solid; 189mg, 76% yield; m.p: 70-72 °C;  
(recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 3017, 1604, 1457, 1262, 1000, 918, 800, 580 cm$^{-1}$;  
$^1$H NMR (500 MHz, CDCl$_3$) δ 5.51 (d, $J = 10.0$ Hz, 1H), 5.64 (d, $J = 17.0$ Hz, 1H), 6.52 (d, $J = 15.5$ Hz, 1H), 6.55-6.62 (m, 1H), 7.39 (t, $J = 8.0$ Hz, 1H), 7.44 (dd, $J_1 = 1.5$ Hz, $J_2 = 8.5$ Hz, 1H), 7.55 (d, $J = 8.5$ Hz, 1H), 7.66 (d, $J = 2.0$ Hz, 1H);  
$^{13}$C NMR (125 MHz, CDCl$_3$) δ 113.9, 117.4, 118.1, 120.8, 124.4, 128.0, 135.4, 140.6, 141.4, 151.0, 163.0; HRMS (ESI) calcd for C$_{11}$H$_9$BrNO [M+H]$^+$ 249.9862, found 249.9869.

(E)-7-Bromo-2-(buta-1,3-dien-1-yl)benzo[d]oxazole (6g).  
Pale yellow oil; 199 mg, 80% yield; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 2923, 1607, 1524, 1474, 1416, 1265, 1218, 1071, 1006, 909, 776, 733, 730, 621, 456 cm$^{-1}$;  
$^1$H NMR (500 MHz, CDCl$_3$) δ 5.52 (d, $J = 10.0$ Hz, 1H), 5.68 (d, $J = 16.5$ Hz, 1H), 6.54-6.63 (m, 2H), 7.21 (t, $J = 7.75$ Hz, 1H), 7.46-7.51 (m, 2H), 7.62 (dd, $J_1 = 0.5$ Hz, $J_2 = 8.0$ Hz, 1H);  
$^{13}$C NMR (125 MHz, CDCl$_3$) δ 102.3, 117.2, 118.9, 124.6, 125.7, 128.3, 135.4,
141.1, 142.9, 148.6, 162.6; HRMS (ESI) calcd for C_{11}H_{8}BrNONa [M+Na]^+ 271.9681, found 271.9705.

(E)-2-(Buta-1,3-dien-1-yl)-5-(trifluoromethyl)benzo[d]oxazole (6h). Colorless oil; 96 mg, 40% yield; (recrystallized from petroleum ether and ethyl acetate at room temperature); IR (KBr) 2958, 2926, 2855, 1725, 1460, 1380, 1324, 1257, 1124, 800 cm\(^{-1}\); \(^1\)H NMR (500 MHz, CDCl\(_3\)) \(\delta\) 5.52-5.54 (d, \(J = 10.0\) Hz, 1H), 5.65-5.68 (d, \(J = 17.0\) Hz, 1H), 6.54-6.64 (m, 2H), 7.42-7.48 (dd, \(J_1 = 11.0\) Hz, \(J_2 = 15.5\) Hz, 1H), 7.57-7.61 (m, 2H), 7.96 (s, 1H); \(^13\)C NMR (125 MHz, CDCl\(_3\)) \(\delta\) 110.7, 117.2, 117.5, 117.6, 122.4 (q, \(J_{C-F} = 265\) Hz), 124.8, 127.8, 135.3, 141.3, 142.3, 152.1, 164.1; HRMS (ESI) calcd for C\(_{12}\)H\(_9\)F\(_3\)NO [M+H]^+ 240.0631, found 240.0636.

6. Reference

(1) Xie, W.; Chang, S. Angew. Chem., Int. Ed. 2016, 55, 1876.
7. $^1$H and $^{13}$C NMR spectra

![NMR spectra of 3a (Z)](image-url)