Electronic Supporting Information

A metal catalyst-free and one-pot synthesis of (3,4-dihydro-2H-benzo[b][1,4]oxazin-2-yl)methanol derivatives in water

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General methods: Unless stated otherwise, solvents and chemicals were obtained from commercial sources and used without further purification. Reactions were monitored by thin layer chromatography (TLC) on silica gel plates (60 F254) using EtOAc-Hexane as eluent and visualizing with ultraviolet light or iodine spray. Flash chromatography was performed on silica gel (230-400 mesh) using hexane and ethyl acetate. $^1$H and $^{13}$C NMR spectra were recorded in DMSO-$d_6$ solution by using a 400 MHz spectrometer. Proton chemical shifts (δ) are relative to tetramethylsilane (TMS, δ = 0.00) as internal standard and expressed in ppm. Spin multiplicities are given as s (singlet), d (doublet), t (triplet) and m (multiplet) as well as b (broad). Coupling constants (J) are given in hertz. Infrared spectra were recorded on a FT-IR spectrometer. Melting points were determined using melting point B-540 apparatus and are uncorrected. HRMS was determined using waters LCT premier XETOF ARE-047 apparatus.

General method for the preparation of (3,4-dihydro-2$H$-benzo[b][1,4]oxazin-2-yl)methanol derivatives (3)

To a stirred solution of sodium hydroxide (1.4 mmol) in water (5.0 mL) was added 2-aminophenol 1 (1.0 mmol) and stirring continued at room temperature for 10 min. To this was added (±)-epichlorohydrin 2 (1.2 mmol) and the mixture was stirred at room temperature for 20-70 minutes (See Table S-1). After completion of reaction (indicated by TLC), the mixture was treated with dil HCl (5%) until pH reach to 7 and then extracted with EtOAc (3 x 10 mL). The combined organic layer was collected, washed with cold water (2 x 10 mL), dried over anhydrous Na$_2$SO$_4$, filtered and concentrated under low vacuum. The crude product obtained was purified by column chromatography over silica gel using 10-30% EtOAc-Hexane.

*The work-up procedure can be avoided for compounds 3f-3n as these products were separated as oil in the reaction mixture. The oil separated can be collected and purified directly by using column chromatography.
Table S-1. Synthesis of (3,4-dihydro-2H-benzo[b][1,4]oxazin-2-yl)methanol derivatives (3)

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<th>Entry</th>
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<th>Time (min)</th>
<th>Yieldb (%)</th>
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</table>
Spectral data of synthesized compounds

(3,4-Dihydro-2H-benzo[b][1,4]oxazin-2-yl)methanol (3a)

Brown gum; Yield: 70%; \(^1H\) NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 6.65-6.62 (m, 2H), 6.56–6.54 (m, 1H), 6.47-6.43 (m, 1H), 5.67 (s, 1H), 4.91 (t, \(J = 6.0\) Hz, 1H), 3.96 - 3.94 (m, 1H), 3.60 - 3.56 (m, 1H), 3.51-3.48 (m, 1H), 3.35 – 3.34 (m, 1H), 3.04 - 3.01 (m, 1H). \(^{13}C\) NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 142.8, 134.4, 120.7, 116.7, 115.8, 114.5, 74.2, 61.5, 41.6. IR (CHCl\(_3\)): 3419, 3019, 2928, 2400, 1609, 1502, 1215, 928 cm\(^{-1}\); Mass: m/z (ES): 166.08 (M+H, 100%); HRMS: m/z (M+H) calcd for C\(_9\)H\(_{12}\)NO\(_2\): 166.0868; found: 166.0866.

\(^1H\) NMR (400 MHz, CDCl\(_3\)): \(\delta\) 6.79 (d, \(J = 8.1\) Hz, 1H), 6.75 (t, \(J = 8.1\) Hz, 1H), 6.66 (t, \(J = 8.1\) Hz, 1H), 6.58 (d, \(J = 8.1\) Hz, 1H), 4.17-4.25 (m, 1H), 3.83 (dd, \(J = 11.8, 4.4\) Hz, 1H), 3.77 (dd, \(J = 11.8, 5.9\) Hz, 1H), 3.35 (dd, \(J = 11.8, 2.9\) Hz, 1H), 3.28 (dd, \(J = 11.8, 7.3\) Hz, 1H).

(7-Nitro-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-yl)methanol (3b)

Orange solid; Yield: 65%, mp: 127 °C ; \(^1H\) NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 7.69 (d, \(J = 8.8\) Hz 1H), 7.51-7.47 (m, 2H), 6.64 (d, \(J=8.8,1H\)), 5.03 (t, \(J=6.0\)Hz,1H), 4.00-3.98 (m, 1H), 3.63-3.45 (m, 3H), 3.23-3.18 (m, 1H). \(^{13}C\) NMR (400 MHz, DMSO-\(d_6\)): \(\delta\) 142.1, 140.6, 135.5, 119.2, 111.8,
111.3, 73.5, 61.0, 40.8; IR (CHCl$_3$): 3419, 3020, 2400, 1600, 1516, 1215, 928 cm$^{-1}$; Mass: m/z (ES): 211.07 (M+H, 100%); HRMS: m/z (M+H) calcd for C$_9$H$_{11}$N$_2$O$_4$: 211.0719; found: 211.0722

(6-Chloro-3,4-dihydro-2$H$-benzo[b][1,4]oxazin-2-yl)methanol (3c)

Brown liquid; Yield: 70%; $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 6.64 (d, $J$= 8.8 Hz, 1H), 6.59 (s, 1H), 6.45-6.42 (m,1H), 6.05 (s, 1H), 4.93 (t, $J$=5.6 Hz,1H), 3.96-3.92 (m, 1H), 3.61-3.49 (m, 2H), 3.35-3.31 (m,1H), 3.06-3.01 (m, 1H); $^{13}$C NMR (400 MHz, DMSO-$d_6$): $\delta$ 141.5, 135.9, 124.3, 117.0, 115.6, 113.2, 74.2, 61.3, 41.0; IR (CHCl$_3$): 3427, 3019, 2400, 1609, 1498, 1215, 928 cm$^{-1}$; Mass: m/z (ES): 200.04 (M+H, 100%); HRMS: m/z (M+H) calcd for C$_9$H$_{11}$NO$_2$ Cl: 200.0478; found: 200.0492

(6-Bromo-3,4-dihydro-2$H$-benzo[b][1,4]oxazin-2-yl)methanol (3d)

Orange gum; Yield: 68%; $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 6.70 (d, $J$= 2Hz, 1H), 6.57 - 6.54 (m,2H), 6.04 (sb, 1H),4.93 (t, $J$ = 5.6 Hz,1H), 3.97- 3.95 (m, 1H), 3.60-3.47 (m,2H), 3.32 - 3.31 (m,1H), 3.05-3.03 (m, 1H).$^{13}$C NMR (400 MHz, DMSO-$d_6$): $\delta$ 141.9, 136.3, 118.4, 117.5, 116.0, 112.1, 74.1, 61.3, 41.0; IR (CHCl$_3$): 3412, 3019, 2400, 1601, 1497, 1215, 928 cm$^{-1}$; Mass: m/z (ES): 243.99(M+H, 40%), 245.99 (M+2, 60%); HRMS: m/z (M+H) calcd for C$_9$H$_{11}$NO$_2$ Br: 243.9973; found: 243.9978.

(7-Methyl-3,4-dihydro-2$H$-benzo[b][1,4]oxazin-2-yl)methanol (3e)
Light blue liquid; Yield: 68%; $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 6.56 - 6.54 (m, 2H), 6.31 (d, $J = 7.6$ Hz, 1H), 5.36 (d, $J = 5.6$, 1H), 4.92 (t, $J = 5.6$ Hz, 1H), 3.97 - 3.91 (m, 1H), 3.66 - 3.57 (m, 2H), 3.32 - 3.31 (m, 1H), 3.21 - 3.14 (m, 1H), 2.16 (s, 3H). $^{13}$C NMR (400 MHz, DMSO-$d_6$): $\delta$ 141.1, 134.5, 129.7, 117.1, 115.4, 112.2, 73.6, 61.5, 48.1, 20.8; IR (CHCl$_3$): 3419, 3019, 2400, 1609, 1502, 1215, 928 cm$^{-1}$; Mass: m/z (ES): 180.1 (M+H, 100%); HRMS: m/z (M+H) calcd for C$_{10}$H$_{14}$NO$_2$: 180.1025; found: 180.1022.

(4-Benzyl-3,4-dihydro-2$H$-benzo[b][1,4]oxazin-2-yl)methanol (3f)

Light green liquid; Yield: 78%; $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 7.35 - 7.22 (m, 5H), 6.72 - 6.65 (m, 3H), 6.54 - 6.50 (m, 1H), 4.95 (t, $J = 5.6$ Hz, 1H), 4.52 - 4.40 (m, 2H), 4.12 - 4.09 (m, 1H), 3.65 - 3.60 (m, 1H), 3.56 - 3.50 (m, 1H), 3.40 - 3.38 (m, 1H), 3.20 - 3.15 (m, 1H); $^{13}$C NMR (400 MHz, DMSO-$d_6$): $\delta$ 143.7, 138.8, 135.4, 128.9 (2C), 127.6 (2C), 127.3, 121.5, 117.5, 116.2, 112.7, 74.3, 61.9, 54.3, 49.21; IR (CHCl$_3$): 3683, 3409, 3019, 2400, 1606, 1504, 1215, 928 cm$^{-1}$; Mass: m/z (ES): 256.13(M+H, 100%); HRMS: m/z (M+H) calcd for C$_{16}$H$_{18}$NO$_2$: 256.1338; found: 256.1340.

(4-(4-Chlorobenzyl)-3,4-dihydro-2$H$-benzo[b][1,4]oxazin-2-yl)methanol (3g)
Orange solid; Yield: 76%, mp: 72°C; \( ^1\)H NMR (400 MHz, DMSO-\(d_6\)): \( \delta \) 7.39 (d, \( J = 8.8 \) Hz, 2H), 7.31 (d, \( J = 8.4 \) Hz, 2H), 6.72 - 6.68 (m, 2H), 6.67 - 6.64 (m, 1H), 6.55 - 6.51 (m, 1H), 4.97 - 4.94 (t, \( J = 5.6 \) Hz, 1H), 4.51 - 4.39 (m, 2H), 4.12 - 4.09 (m, 1H), 3.65 - 3.60 (m, 1H), 3.56 - 3.50 (m, 1H), 3.40 - 3.37 (m, 1H), 3.20 - 3.15 (m, 1H); \( ^{13}\)C NMR (400 MHz, DMSO-\(d_6\)): \( \delta \) 143.3, 137.4, 134.7, 131.3, 129.0 (2C), 128.4 (2C), 121.0, 117.2, 115.8, 112.2, 73.8, 61.4, 53.2, 48.7; IR (CHCl\(_3\)): 3684, 3410, 3019, 2400, 1606, 1504, 1215, 929 cm\(^{-1}\); Mass: m/z (ES): 290.09(M+H, 100%); HRMS: m/z (M+H) calcd for C\(_{16}\)H\(_{17}\)NO\(_2\)Cl: 290.0948; found: 290.0953.

(4-(2-Chlorobenzyl)-3,4-dihydro-2\(H\)-benzo[\(b\)][1,4]oxazin-2-yl)methanol (3h)

Light green gum; Yield: 78%; \( ^1\)H NMR (400 MHz, DMSO-\(d_6\)): \( \delta \) 7.51 - 7.47 (m, 1H), 7.32 - 7.26 (m, 3H), 6.75 - 6.73 (m, 1H), 6.72 - 6.68 (m, 1H), 6.66 - 6.52 (m, 1H), 6.48 - 6.44 (m, 1H), 4.98 (t, \( J = 5.8 \) Hz, 1H), 4.51 (s, 2H), 4.19 - 4.13 (m, 1H), 3.67 - 3.62 (m, 1H), 3.58 - 3.52 (m, 1H), 3.44 - 3.40 (m, 1H), 3.29 - 3.24 (m, 1H); \( ^{13}\)C NMR (400 MHz, DMSO-\(d_6\)): \( \delta \) 143.2, 135.1, 134.6, 132.1, 129.5, 128.6, 128.4, 127.3, 121.2, 117.3, 115.8, 111.8, 73.9, 61.4, 52.1, 48.8; IR (CHCl\(_3\)): 3683, 3411, 2924, 1606, 1505, 1220, 928 cm\(^{-1}\); Mass: m/z (ES): 290.09(M+H, 100%); HRMS: m/z (M+H) calcd for C\(_{16}\)H\(_{17}\)NO\(_2\)Cl: 290.0948; found: 290.0956.

(4-(3,4-Dimethoxybenzyl)-3,4-dihydro-2\(H\)-benzo[\(b\)][1,4]oxazin-2-yl)methanol (3i)
**Off white solid; Yield: 75%, mp: 64°C;**  $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 6.95-6.90 (m, 2H), 6.82 - 6.78 (m, 2H), 6.78 - 6.73 (m, 2H), 6.54 - 6.50 (m, 1H), 4.95 (t, $J$ = 5.2 Hz, 1H), 4.36 (s, 2H), 4.10 - 4.09 (m, 1H), 3.78 (s, 6H), 3.69 - 3.61 (m, 1H), 3.59 - 3.51 (m, 1H), 3.35 - 3.33 (m, 1H), 3.15 - 3.10 (m, 1H); $^{13}$C NMR (400 MHz, DMSO-$d_6$): $\delta$ 148.8, 147.7, 143.3, 135.1, 130.5, 121.0, 119.3, 117.1, 115.8, 112.5, 111.7, 111.1, 73.9, 61.5, 55.4, 53.6, 48.4; IR (CHCl$_3$): 3419, 3019, 2400, 1606, 1515, 928 cm$^{-1}$; Mass: m/z (ES): 316.15(M+H, 100%); HRMS: m/z (M+H) calcd for C$_{18}$H$_{22}$NO$_4$: 316.1549; found: 316.1536.

(4-Benzyl-6-chloro-3,4-dihydro-2$H$-benzo[b][1,4]oxazin-2-yl)methanol (3j)

**Brown liquid; Yield: 78%;**  $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 7.37 - 7.33 (m, 2H), 7.28 - 7.24 (m, 3H), 6.70 (d, $J$ = 8.8 Hz, 1H), 6.65 (s, 1H), 6.52 - 6.50 (m, 1H), 4.98 (t, $J$ = 5.2 Hz, 1H), 4.56 - 4.44 (m, 2H), 4.11 - 4.09 (m, 1H), 3.63 - 3.60 (m, 1H), 3.59 - 3.52 (m, 1H), 3.43 - 3.40 (m, 1H), 3.32 - 3.20 (m, 1H); $^{13}$C NMR (400 MHz, DMSO-$d_6$): $\delta$ 141.9, 137.7, 136.1, 128.5 (2C), 126.9 (3C), 124.9, 116.8, 115.9, 111.1, 73.8, 61.3, 53.5, 48.3; IR (CHCl$_3$): 3683, 3428, 3019, 2400, 1603, 1505, 1215, 928 cm$^{-1}$; Mass: m/z (ES): 290.09 (M+H, 100%); HRMS: m/z (M+H) calcd for C$_{16}$H$_{17}$NO$_2$Cl: 290.0948; found: 290.0961.

(4-(4-Chlorobenzyl)-7-methyl-3,4-dihydro-2$H$-benzo[b][1,4]oxazin-2-yl)methanol (3k)
Off white gum; Yield: 75%; $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 7.39 (d, $J=8.0$ Hz, 2H), 7.31 (d, $J=8.4$ Hz, 2H), 6.58 (d, $J=7.6$ Hz, 1H), 6.49 (s, 1H), 6.33 (d, $J=7.8$ Hz, 1H), 4.91 (t, $J=5.6$ Hz, 1H), 4.50 - 4.43 (m, 2H), 4.05 - 4.04 (m, 1H), 3.63 - 3.58 (m, 1H), 3.53 - 3.47 (m, 1H), 3.35 - 3.31 (m, 1H), 3.15 - 3.12 (m, 1H), 2.09 (s, 3H); $^{13}$C NMR (400 MHz, DMSO-$d_6$): $\delta$ 141.1, 137.5, 134.4, 131.3, 129.7 (2C), 129.0 (2C), 128.4, 117.6, 115.6, 112.7, 73.7, 61.4, 53.0, 48.6, 20.7; IR (CHCl$_3$): 3683, 3419, 3019, 2400, 1605, 1506, 1215, 928 cm$^{-1}$; Mass: m/z (ES): 304.11 (M+H, 100%); HRMS: m/z (M+H) calcd for C$_{17}$H$_{19}$ClNO$_2$: 304.1104; found: 304.1110.

(4-Benzyl-7-methyl-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-yl)methanol (3l)

Brown liquid; Yield: 77%; $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 7.35 - 7.23 (m, 5H), 6.58 (d, $J=8.0$ Hz, 1H), 6.53 (s, 1H), 6.32 (d, $J=8.0$ Hz, 1H), 4.94 (t, $J=6.0$ Hz, 1H), 4.51 - 4.44 (m, 2H), 4.06 - 4.05 (m, 1H), 3.63 - 3.57 (m, 1H), 3.53 - 3.47 (m, 1H), 3.35 - 3.34 (m, 1H), 3.15 - 3.11 (m, 1H), 2.09 (s, 3H); $^{13}$C NMR (400 MHz, DMSO-$d_6$): $\delta$ 141.1, 138.3, 134.6, 129.6 (2C), 128.4 (2C), 127.1, 126.8, 117.4, 115.5, 112.7, 73.7, 61.5, 53.7, 48.6, 20.7; IR (CHCl$_3$): 3683, 3420, 3019, 2400, 1605, 1505, 1215, 928 cm$^{-1}$; Mass: m/z (ES): 270.15 (M+H, 100%); HRMS: m/z (M+H) calcd for C$_{17}$H$_{20}$NO$_2$: 270.1494; found: 270.1500.

(4-(2-Fluorobenzyl)-3,4-dihydro-2H-benzo[b][1,4]oxazin-2-yl)methanol (3m)
Light blue liquid; Yield: 78%;\textsuperscript{1}H NMR (400 MHz, DMSO-\textit{d}_6): \delta 7.33 -7.29 (m, 2H), 7.22-7.13 (m, 2H), 6.71-6.67 (m, 3H), 6.57 -6.50 (m, 1H), 4.93 (t, \textit{J} = 6.0 Hz, 1H), 4.54 -4.45 (m, 2H), 4.09 -4.07 (m, 1H), 3.64 -3.59 (m, 1H), 3.55 -3.49 (m,1H), 3.41-3.37 (m,1H), 3.21 -3.16 (m, 1H); \textsuperscript{13}C NMR (400 MHz, DMSO-\textit{d}_6): 161.6 - 159.1 (C-F coupling \textit{J}=242.9), 143.3,134.6, 129.3, 129.3,124.8, 124.3, 121.1, 117.2, 115.8,115.4,112.0, 73.8, 61.4, 48.6, 47.8; IR (CHCl\textsubscript{3}): 3597, 3447, 3018, 2400, 1607, 1505, 1216, 929 cm\textsuperscript{-1}; Mass: m/z (ES): (M+H, 100%); HRMS: m/z (M+H) calcd for C\textsubscript{16}H\textsubscript{17}NO\textsubscript{2}F:274.1243; found: 274.1243

\textbf{(4-(4-Methoxybenzyl)-3,4-dihydro-2H-benzo[\textit{b}][1,4]oxazin-2-yl)methanol (3n)}

Yellow liquid; Yield: 75%;\textsuperscript{1}H NMR (400 MHz, DMSO-\textit{d}_6): \delta 7.22 (d, \textit{J} = 8.8 Hz, 2 H), 6.89 (d, \textit{J}= 8.8 Hz, 2H), 6.74 -6.68 (m, 3H), 6.53-6.49 (m,1H), 4.93 (t, \textit{J} = 6.0 Hz,1H), 4.43-4.33 (m, 2H), 4.19 -4.09 (m, 1H), 3.72 (s, 3H), 3.64 -3.58 (m, 1H), 3.54 -3.48 (m,1H), 3.36 -3.33 (m,1H), 3.14-3.10 (m, 1H); \textsuperscript{13}C NMR (400 MHz, DMSO-\textit{d}_6): 158.2, 143.3, 134.9, 129.9,128.5 (2C), 121.0, 117.0, 115.7, 113.8 (2C), 112.3, 73.8, 61.3, 54.9, 53.2, 48.4; IR (CHCl\textsubscript{3}): 3463, 3018, 2400, 1607, 1511, 1216, 927 cm\textsuperscript{-1}; Mass: m/z (ES): (M+H, 100%); HRMS: m/z (M+H) calcd for C\textsubscript{17}H\textsubscript{20}NO\textsubscript{3}:286.1443; found: 286.1456.