Supporting Information

Copper-Catalyzed Oxidative Functionalization of Benzylic
C–H Bonds with Quinazoline 3-Oxides

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1. General considerations

All reactions were carried out in oven-dried glassware. All methylarenes were obtained from commercial sources and used as received. All the reactions were monitored by thin-layer chromatography (TLC). Products purification was done using silica gel column chromatography. $^1$H/$^13$C NMR spectra were recorded on Bruker avance 400 MHz and Bruker AMX 400 MHz spectrometer at 400/100 MHz, respectively, in CDCl$_3$ unless otherwise stated, using either TMS or the undeuterated solvent residual signal as the reference. Chemical shifts are given in ppm and are measured relative to CDCl$_3$ or DMSO-d$_6$ as an internal standard. Mass spectra were obtained by the electrospray ionization time-of-flight (ESI-TOF) mass spectrometry. GC yields were obtained using biphenyl as an internal standard. Flash column chromatography purification of compounds was carried out by gradient elution using ethyl acetate (EA) in light petroleum ether (PE).

2. General experimental procedure for the synthesis of quinazolin-4-ones

A mixture of Quinazoline 3-oxides (0.2 mmol), alkyl arenes (4 mmol), CuSO$_4$ (0.006 mmol), TBAI (0.04 mmol), NaI (0.1 mmol) and TBHP (5.5 M in decane) (0.4 mmol) in DCM (2 mL) was stirred at 70 °C for 12 h. After the reaction was completion (monitored by TLC), the contents were cooled to room temperature and then extracted with ethyl acetate (3 x 10 mL). The combined organic phase was evaporated under reduced pressure to afford the crude product which was further purified by flash chromatography on silica gel gradient with elution of ethyl acetate in petroleum ether to obtain the quinazolin-4-ones.
3. Characterization of products

3-(Benzyloxy)quinazolin-4(3H)-one (3a)

White solid (40.8 mg, 81 %); ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, 1H), 7.82–7.73 (m, 2H), 7.68 (d, J = 8.1 Hz, 1H), 7.56–7.50 (m, 1H), 7.45–7.34 (m, 5H), 5.32 (s, 2H); ¹³C NMR (101 MHz, CDCl₃) δ 157.4, 146.9, 144.7, 134.3, 133.2, 130.0, 129.7, 128.9, 127.8, 127.3, 126.7, 123.5, 79.3; HRMS (ESI) calcd for C₁₅H₁₂N₂O₂ [M + Na⁺]: 275.0796, found: 275.0795.

3-(2-Chlorobenzyloxy)quinazolin-4(3H)-one (3b)

White solid (50.9 mg, 89%); ¹H NMR (400 MHz, CDCl₃) δ 8.37 (d, J = 8.0 Hz, 1H), 7.93 (s, 1H), 7.78 (t, J = 8.0 Hz, 1H), 7.71 (d, J = 8.0 Hz, 1H), 7.55 (t, J = 8.0 Hz, 1H), 7.46 (d, J = 7.9 Hz, 2H), 7.36 (t, J = 8.0 Hz, 1H), 7.32–7.23 (m, 1H), 5.49 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 157.5, 147.0, 144.5, 135.3, 134.4, 132.6, 131.3, 131.1, 130.0, 127.9, 127.4 (2C), 126.7, 123.5, 76.3; HRMS (ESI) calcd for C₁₅H₁₁ClN₂O₂ [M + Na⁺]: 309.0407, found: 309.0403.

3-((4-Bromobenzyl)oxy)quinazolin-4(3H)-one (3c)

White solid (46.7 mg, 71 %); ¹H NMR (400 MHz, CDCl₃) δ 8.37–8.33 (m, 1H), 7.87 (s, 1H), 7.82–7.74 (m, 1H), 7.70 (d, J = 8.2 Hz, 1H), 7.57–7.49 (m, 3H), 7.33 (d, J = 8.3 Hz, 2H), 5.28 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 157.4, 147.0, 144.4, 134.4, 132.3, 132.2, 131.6, 128.0, 127.5, 126.7, 124.1, 123.5, 78.5; HRMS (ESI) calcd for C₁₅H₁₁BrN₂O₂ [M + Na⁺]: 331.0082, found: 331.0086.

3-((4-Iodobenzyl)oxy)quinazolin-4(3H)-one (3d)

White solid (67.3 mg, 89 %); ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, J = 7.9 Hz, 1H), 7.87 (s, 1H), 7.82–7.76 (m, 1H), 7.76–7.69 (m, 3H), 7.58–7.52 (m, 1H), 7.19 (d, J = 7.9 Hz, 2H), 5.27 (s, 2H); ¹³C
NMR (100 MHz, CDCl$_3$) $\delta$ 157.4, 146.9, 144.4, 138.2, 134.5, 132.9, 131.7, 127.9, 127.5, 126.7, 123.5, 96.0, 78.7; HRMS (ESI) calcd for C$_{15}$H$_{11}$IN$_2$O$_2$ [M + H]$^+$: 378.9943, found: 378.9938.

3-((2-Methylbenzyl)oxy)quinazolin-4(3H)-one (3e)

White solid (47.9 mg, 90 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.28–8.24 (m, 1H), 7.69 (s, 1H), 7.68–7.62 (m, 1H), 7.59 (d, $J$ = 7.9 Hz, 1H), 7.45–7.39 (m, 1H), 7.23–7.12 (m, 3H), 7.08–7.02 (m, 1H), 5.28 (s, 2H), 2.43 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.5, 147.0, 144.6, 138.5, 134.3, 131.5, 131.4, 130.9, 130.1, 127.9, 127.3, 126.7, 126.3, 123.5, 77.6, 19.0; HRMS (ESI) calcd for C$_{16}$H$_{14}$N$_2$O$_2$ [M + Na]$^+$: 289.0953, found: 289.0952.

3-((3-Methylbenzyl)oxy)quinazolin-4(3H)-one (3f)

White solid (44.7 mg, 84 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.39–8.34 (m, 1H), 7.85–7.82 (m, 1H), 7.79–7.72 (m, 1H), 7.68 (d, $J$ = 8.1 Hz, 1H), 7.57–7.49 (m, 1H), 7.29–7.17 (m, 4H), 5.28 (s, 2H), 2.34 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.5, 147.0, 144.8, 138.8, 134.3, 133.2, 130.7, 130.5, 128.8, 127.8, 127.3, 127.1, 126.7, 123.6, 79.5, 21.3; HRMS (ESI) calcd for C$_{16}$H$_{14}$N$_2$O$_2$ [M + Na]$^+$: 289.0953, found: 289.0952.

3-((4-Methylbenzyl)oxy)quinazolin-4(3H)-one (3g)

White solid (45.8 mg, 86 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.36 (d, $J$ = 8.0 Hz, 1H), 7.80–7.72 (m, 2H), 7.68 (d, $J$ = 8.0 Hz, 1H), 7.56–7.49 (m, 1H), 7.32–7.25 (m, 2H), 7.18 (d, $J$ = 7.7 Hz, 2H), 5.29 (s, 2H), 2.35 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.5, 147.0, 144.9, 139.8, 134.3, 130.3, 130.2, 129.7, 127.8, 127.3, 126.7, 123.6, 79.2, 21.3; HRMS (ESI) calcd for C$_{16}$H$_{14}$N$_2$O$_2$ [M + Na]$^+$: 289.0953, found: 289.0950.

3-((4-Methoxybenzyl)oxy)quinazolin-4(3H)-one (3h)
White solid (50.8 mg, 90 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.38–8.32 (m, 1H), 7.78–7.71 (m, 2H), 7.67 (d, $J = 7.4$ Hz, 1H), 7.55–7.47 (m, 1H), 7.36–7.30 (m, 2H), 6.90–6.85 (m, 2H), 5.25 (s, 2H), 3.79 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 160.7, 157.5, 147.0, 144.9, 134.2, 131.7, 127.8, 127.2, 126.7, 125.4, 123.5, 114.3, 78.9, 55.3; HRMS (ESI) calcd for C$_{16}$H$_{14}$N$_2$O$_3$ [M + Na]$^+$: 305.0902, found: 305.0901.

3-(((4-(tert-Butyl)benzyl)oxy)quinazolin-4(3H)-one (3i)

White solid (52.4 mg, 85 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.37 (d, $J = 8.0$ Hz, 1H), 7.85 (s, 1H), 7.79–7.73 (m, 1H), 7.69 (d, $J = 8.2$ Hz, 1H), 7.56–7.50 (m, 1H), 7.44–7.34 (m, 4H), 5.30 (s, 2H), 1.31 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.5, 152.9, 147.0, 144.9, 134.3, 130.3, 129.9, 127.8, 127.3, 126.7, 125.9, 123.6, 79.3, 34.8, 31.3; HRMS (ESI) calcd for C$_{19}$H$_{20}$N$_2$O$_2$ [M + Na]$^+$: 331.1422, found: 331.1418.

3-(((3,5-Dimethylbenzyl)oxy)quinazolin-4(3H)-one (3j)

White solid (49.3 mg, 88 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.36 (d, $J = 7.9$ Hz, 1H), 7.86 (s, 1H), 7.80–7.71 (m, 1H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.56–7.46 (m, 1H), 7.03 (d, $J = 10.6$ Hz, 3H), 5.24 (s, 2H), 2.29 (s, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.5, 147.0, 144.9, 138.6, 134.3, 133.1, 131.3, 127.8, 127.3, 126.7, 123.6, 79.6, 21.2; HRMS (ESI) calcd for C$_{17}$H$_{16}$N$_2$O$_2$ [M + Na]$^+$: 303.1109, found: 303.1110.

3-((3,4,5-Trimethoxybenzyl)oxy)quinazolin-4(3H)-one (3k)

White solid (56.1 mg, 82%); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.37 (d, $J = 8.0$ Hz, 1H), 7.93 (s, 1H), 7.82–7.75 (m, 1H), 7.71 (d, $J = 8.1$ Hz, 1H), 7.58–7.51 (m, 1H), 6.66 (s, 2H), 5.26 (s, 2H), 3.85 (s, 3H), 3.82 (s, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.5, 153.6, 146.9, 144.6, 139.2, 134.4, 128.6, 127.9, 127.4, 126.6, 123.5, 107.1, 79.7, 60.9, 56.2; HRMS (ESI) calcd for C$_{18}$H$_{18}$N$_2$O$_5$ [M + Na]$^+$: 365.1113, found: 365.1118.
4-(((4-Oxoquinazolin-3(4H)-yl)oxy)methyl)benzonitrile (3l)

White solid (39.3 mg, 71 %); ^1H NMR (400 MHz, CDCl$_3$) $\delta$ 8.35 (d, $J$ = 7.8 Hz, 1H), 8.00 (s, 1H), 7.84–7.77 (m, 1H), 7.76–7.69 (m, 3H), 7.63 (d, $J$ = 7.7 Hz, 2H), 7.60–7.52 (m, 1H), 5.39 (s, 2H); ^13C NMR (100 MHz, CDCl$_3$) $\delta$ 157.3, 146.9, 144.0, 138.3, 134.6, 132.7, 130.1, 128.0, 127.7, 126.7, 123.5, 118.2, 113.5, 78.3; HRMS (ESI) calcd for C$_{16}$H$_{11}$N$_3$O$_2$ [M + H]$^+$: 278.0930, found: 278.0926.

3-((4-Propionylbenzyl)oxy)quinazolin-4(3H)-one (3m)

White solid (40.8 mg, 65 %); ^1H NMR (400 MHz, CDCl$_3$) $\delta$ 8.36 (d, $J$ = 8.0 Hz, 1H), 7.99 (d, $J$ = 8.0 Hz, 2H), 7.91 (s, 1H), 7.81–7.75 (m, 1H), 7.70 (d, $J$ = 8.1 Hz, 1H), 7.59–7.52 (m, 3H), 5.38 (s, 2H), 3.03 (q, $J$ = 7.2 Hz, 2H), 1.23 (t, $J$ = 7.2 Hz, 3H); ^13C NMR (100 MHz, CDCl$_3$) $\delta$ 200.1, 157.4, 146.9, 144.4, 137.9, 137.8, 134.5, 130.0, 128.6, 127.9, 127.5, 126.7, 123.5, 78.6, 32.0, 8.1; HRMS (ESI) calcd for C$_{18}$H$_{16}$N$_2$O$_3$ [M + Na]$^+$: 331.1059, found: 331.1062.

Methyl 4-(((4-oxoquinazolin-3(4H)-yl)oxy)methyl)benzoate (3n)

White solid (32.9 mg, 53 %); ^1H NMR (400 MHz, CDCl$_3$) $\delta$ 8.36 (d, $J$ = 8.0 Hz, 1H), 8.07 (d, $J$ = 7.9 Hz, 2H), 7.90 (s, 1H), 7.81–7.75 (m, 1H), 7.70 (d, $J$ = 8.1 Hz, 1H), 7.57–7.50 (m, 3H), 5.38 (s, 2H), 3.93 (s, 3H); ^13C NMR (100 MHz, CDCl$_3$) $\delta$ 166.4, 157.4, 146.9, 144.3, 138.0, 134.4, 131.3, 130.2, 129.7, 127.9, 127.5, 126.7, 123.5, 78.6, 52.3; HRMS (ESI) calcd for C$_{17}$H$_{14}$N$_2$O$_4$ [M + Na]$^+$: 333.0851, found: 333.0850.

3-((3-Nitrobenzyl)oxy)quinazolin-4(3H)-one (3o)
White solid (29.1 mg, 49 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.41–8.35 (m, 2H), 8.32–8.27 (m, 1H), 8.05 (s, 1H), 7.89 (d, $J$ = 7.6 Hz, 1H), 7.84–7.78 (m, 1H), 7.74 (d, $J$ = 8.1 Hz, 1H), 7.66–7.61 (m, 1H), 7.60–7.55 (m, 1H), 5.44 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.3, 148.5, 146.9, 143.9, 135.6, 135.3, 134.6, 130.1, 128.0, 127.7, 126.8, 124.5, 124.4, 123.5, 78.0; HRMS (ESI) calcd for C$_{15}$H$_{13}$N$_3$O$_4$ [M + H]$^+$: 298.0828, found: 298.0823.

3-((4-(Pyridin-2-yl)benzyl)oxy)quinazolin-4(3$H$)-one (3p)

White solid (52.6 mg, 80 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.70 (d, $J$ = 4.7 Hz, 1H), 8.37 (d, $J$ = 8.0 Hz, 1H), 8.03 (d, $J$ = 8.2 Hz, 2H), 7.86 (s, 1H), 7.79–7.71 (m, 3H), 7.68 (d, $J$ = 8.0 Hz, 1H), 7.57–7.51 (m, 3H), 7.29–7.22 (m, 1H), 5.39 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.5, 156.4, 149.8, 147.0, 144.7, 140.7, 136.9, 134.4, 133.9, 130.5, 127.9, 127.5, 127.4, 126.7, 123.5, 122.6, 120.7, 79.0; HRMS (ESI) calcd for C$_{20}$H$_{15}$N$_3$O$_2$ [M + Na]$^+$: 352.1062, found: 352.1060.

3-((4'-Methyl-[1,1'-biphenyl]-4-yl)methoxy)quinazolin-4(3$H$)-one (3q)

White solid (56.8 mg, 83 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.40–8.36 (m, 1H), 7.87 (s, 1H), 7.80–7.74 (m, 1H), 7.69 (d, $J$ = 7.8 Hz, 1H), 7.60 (d, $J$ = 8.2 Hz, 2H), 7.57–7.51 (m, 1H), 7.48 (d, $J$ = 8.2 Hz, 4H), 7.28–7.23 (m, 2H), 5.36 (s, 2H), 2.39 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.6, 147.0, 144.8, 142.6, 137.6, 137.3, 134.4, 131.8, 130.6, 129.6, 127.9, 127.5, 127.4, 126.8, 123.6, 79.2, 21.2; HRMS (ESI) calcd for C$_{22}$H$_{18}$N$_2$O$_2$ [M + Na]$^+$: 365.1266, found: 365.1268.

3-(Naphthalen-2-ylmethoxy)quinazolin-4(3$H$)-one (3r)

Yellow solid (48.3 mg, 80 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.38 (d, $J$ = 7.8 Hz, 1H), 7.91–7.81 (m, 4H), 7.81–7.70 (m, 2H), 7.67–7.57 (m, 2H), 7.55–7.44 (m, 3H), 5.48 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.5, 147.0, 144.7, 134.3, 133.7, 133.1, 130.7, 129.8, 129.0, 128.2, 127.9, 127.8, 127.3, 127.0, 126.7, 126.6, 123.6, 79.6; HRMS (ESI) calcd for C$_{19}$H$_{14}$N$_2$O$_2$ [M + Na]$^+$: 325.0953, found: 325.0949.
3-(Naphthalen-1-ylmethoxy)quinazolin-4(3H)-one (3s)

Yellow solid (52.5 mg, 87 %); \(^1\)H NMR (400 MHz, CDCl\(_3\) \(\delta\) 8.47 (d, \(J = 8.4\) Hz, 1H), 8.38 (d, \(J = 8.0\) Hz, 1H), 7.92–7.85 (m, 2H), 7.76–7.49 (m, 6H), 7.41–7.31 (m, 2H), 5.79 (s, 2H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\) \(\delta\) 157.6, 146.9, 144.6, 134.3, 133.9, 132.1, 130.9, 130.0, 129.9, 127.9, 127.4, 127.3, 126.7, 126.5, 125.2, 124.0, 123.5, 77.5; HRMS (ESI) calcd for C\(_{19}\)H\(_{14}\)N\(_2\)O\(_2\) [M + Na]\(^+\): 325.0953, found: 325.0954.

3-(Quinolin-8-ylmethoxy)quinazolin-4(3H)-one (3t)

White solid (51.5 mg, 85 %); \(^1\)H NMR (400 MHz, CDCl\(_3\) \(\delta\) 8.91–8.82 (m, 1H), 8.40 (d, \(J = 7.6\) Hz, 1H), 8.18 (d, \(J = 7.7\) Hz, 1H), 7.91–7.80 (m, 2H), 7.78–7.70 (m, 1H), 7.66 (d, \(J = 7.7\) Hz, 1H), 7.57–7.47 (m, 2H), 7.46–7.38 (m, 1H), 6.03 (s, 2H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\) \(\delta\) 157.6, 150.4, 146.9, 146.6, 145.1, 145.0, 130.0, 128.3, 127.6, 127.0, 126.6, 126.1, 123.6, 121.5, 75.8; HRMS (ESI) calcd for C\(_{18}\)H\(_{13}\)N\(_3\)O\(_2\) [M + Na]\(^+\): 326.0905, found: 326.0900.

3-(Thiophen-2-ylmethoxy)quinazolin-4(3H)-one (3u)

White solid (45.9 mg, 89 %); \(^1\)H NMR (400 MHz, CDCl\(_3\) \(\delta\) 8.36 (d, \(J = 8.0\) Hz, 1H), 7.80–7.73 (m, 2H), 7.69 (d, \(J = 8.1\) Hz, 1H), 7.57–7.50 (m, 1H), 7.42 (d, \(J = 4.7\) Hz, 1H), 7.06–7.03 (m, 1H), 7.01–6.95 (m, 1H), 5.52 (s, 2H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\) \(\delta\) 157.5, 147.0, 144.7, 134.9, 134.4, 130.0, 129.1, 127.9, 127.6, 127.3, 126.7, 123.5, 72.2; HRMS (ESI) calcd for C\(_{13}\)H\(_{10}\)N\(_2\)O\(_2\)S [M + H]\(^+\): 281.0361, found: 281.0365.

3-(Thiophen-3-ylmethoxy)quinazolin-4(3H)-one (3v)

White solid (36.1 mg, 70 %); \(^1\)H NMR (400 MHz, CDCl\(_3\) \(\delta\) 8.36 (d, \(J = 8.0\) Hz, 1H), 7.80–7.73 (m, 2H), 7.69 (d, \(J = 8.1\) Hz, 1H), 7.56–7.50 (m, 1H), 7.41–7.36 (m, 1H), 7.33 (s, 1H), 7.20 (d, \(J = 4.9\) Hz, 1H), 5.35 (s, 2H); \(^1^3\)C NMR (100 MHz, CDCl\(_3\) \(\delta\) 157.5, 147.0, 144.7, 134.4, 134.3, 128.1, 127.9, 127.7,
127.4, 127.3, 126.7, 123.5, 73.2; HRMS (ESI) calcd for C$_{13}$H$_{10}$N$_2$O$_2$S [M + Na]$^+$: 281.0361, found: 281.0363.

3-(Benz[b]thiophen-3-ylmethoxy)quinazolin-4(3H)-one (3w)

White solid (46.8 mg, 76 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.38 (d, $J = 7.9$ Hz, 1H), 8.15 (d, $J = 8.0$ Hz, 1H), 7.89 (d, $J = 8.0$ Hz, 1H), 7.79–7.72 (m, 1H), 7.68–7.63 (m, $J = 8.2$ Hz, 2H), 7.56–7.46 (m, 3H), 7.45–7.40 (m, 1H), 5.61 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.6, 147.0, 144.5, 140.6, 137.7, 134.4, 130.1, 128.7, 127.9, 127.4, 126.7, 125.0, 123.5, 123.1, 122.1, 72.2; HRMS (ESI) calcd for C$_{17}$H$_{12}$N$_2$O$_2$S [M + Na]$^+$: 331.0517, found: 331.0514.

3-(1-Phenylethoxy)quinazolin-4(3H)-one (3x)

Colorless liquid (38.3 mg, 72 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.34 (d, $J = 8.0$ Hz, 1H), 7.75–7.68 (m, 1H), 7.64–7.59 (m, 2H), 7.53–7.46 (m, 1H), 7.40–7.30 (m, 5H), 5.59 (q, $J = 6.5$ Hz, 1H), 1.81–1.76 (m, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.7, 146.8, 145.0, 138.3, 134.2, 129.6, 129.0, 127.7, 127.2, 126.7, 123.4, 84.7, 19.8; HRMS (ESI) calcd for C$_{16}$H$_{14}$N$_2$O$_2$ [M + Na]$^+$: 289.0953, found: 289.0950.

3-(1-Phenylpropoxy)quinazolin-4(3H)-one (3y)

Colorless liquid (32.5 mg, 58%); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.25 (d, $J = 7.8$ Hz, 1H), 7.67–7.61 (m, 1H), 7.55–7.48 (m, 2H), 7.45–7.39 (m, 1H), 7.29–7.20 (m, 5H), 5.23 (t, $J = 7.2$ Hz, 1H), 2.31–2.19 (m, 1H), 1.97–1.86 (m, 1H), 0.97 (t, $J = 7.4$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.7, 146.8, 145.1, 137.3, 134.2, 129.5, 129.0, 128.2, 127.7, 127.2, 126.6, 123.5, 90.3, 27.3, 10.1; HRMS (ESI) calcd for C$_{17}$H$_{16}$N$_2$O$_2$ [M + Na]$^+$: 303.1109, found: 303.1107.

3-((1,2,3,4-Tetrahydronaphthalen-1-yl)oxy)quinazolin-4(3H)-one (3z)

Colorless liquid (42.0 mg, 72 %); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.40–8.36 (m, 1H), 7.81–7.70 (m, 3H), 7.58–7.51 (m, 1H), 7.42 (d, $J = 7.5$ Hz, 1H), 7.32–7.25 (m, 1H), 7.21–7.11 (m, 2H), 5.58 (t, $J = 3.3$ Hz, 1H), 3.00–2.92 (m, 1H), 2.86–2.75 (m, 1H), 2.42–2.34 (m, 1H), 2.25–2.10 (m, 1H), 1.98–1.84 (m, 2H);
C NMR (100 MHz, CDCl$_3$) δ 158.0, 147.0, 145.5, 138.4, 134.3, 131.5, 131.2, 129.5, 129.3, 127.9, 127.3, 126.7, 126.1, 123.6, 81.6, 28.9, 26.7, 17.7; HRMS (ESI) calcd for C$_{18}$H$_{16}$N$_2$O$_2$ [M + Na]$^+$: 315.1109, found: 315.1108.

2-Methyl-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4a)

White solid (30 mg, 83%); $^1$H NMR (400 MHz, CDCl$_3$) δ 8.22 (d, $J = 7.6$ Hz, 1H), 7.68–7.62 (m, 1H), 7.55 (d, $J = 8.1$ Hz, 1H), 7.42–7.35 (m, 1H), 7.31–7.09 (m, 4H), 5.24 (s, 2H), 2.50 (s, 3H), 2.41 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 158.2, 153.9, 146.5, 138.6, 134.3, 131.8, 131.2, 130.8, 129.8, 127.1, 126.6, 126.5, 126.3, 122.6, 76.3, 20.3, 19.1; HRMS (ESI) calcd for C$_{17}$H$_{16}$N$_2$O$_2$ [M + Na]$^+$: 303.1109, found: 303.1107.

2-Ethyl-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4b)

White solid (52.9 mg, 90%); $^1$H NMR (400 MHz, CDCl$_3$) δ 8.30 (d, $J = 7.6$ Hz, 1H), 7.77–7.70 (m, 1H), 7.68 (d, $J = 8.3$ Hz, 1H), 7.49–7.43 (m, 1H), 7.40 (d, $J = 7.4$ Hz, 1H), 7.34–7.28 (m, 1H), 7.28–7.18 (m, 3H), 5.32 (s, 1H), 2.83 (q, $J = 7.4$ Hz, 2H), 2.59 (s, 3H), 1.33 (t, $J = 7.4$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 157.9, 156.9, 146.1, 138.0, 133.7, 131.4, 130.5, 130.2, 129.2, 126.8, 126.1, 125.9, 125.8, 122.0, 75.9, 25.6, 18.6, 10.3; HRMS (ESI) calcd for C$_{18}$H$_{18}$N$_2$O$_2$ [M + Na]$^+$: 317.1266, found: 317.1270.

3-((2-Methylbenzyl)oxy)-2-propylquinazolin-4(3H)-one (4c)

White solid (46.8 mg, 76%); $^1$H NMR (400 MHz, CDCl$_3$) δ 8.32–8.29 (m, 1H), 7.76–7.71 (m, 1H), 7.67 (d, $J = 7.6$ Hz, 1H), 7.49–7.43 (m, 1H), 7.40 (d, $J = 7.5$ Hz, 1H), 7.35–7.30 (m, 1H), 7.29–7.20 (m, 2H), 5.32 (s, 2H), 2.76 (t, $J = 7.6$ Hz, 2H), 2.59 (s, 3H), 1.87–1.76 (m, 2H), 0.99 (t, $J = 7.4$ Hz, 3H); $^{13}$C NMR (101 MHz, CDCl$_3$) δ 158.4, 156.6, 146.6, 138.7, 134.2, 131.9, 131.0, 130.7, 129.7, 127.3, 126.6, 126.4, 126.3, 122.5, 76.4, 34.8, 20.1, 19.1, 13.9; HRMS (ESI) calcd for C$_{19}$H$_{20}$N$_2$O$_2$ [M + Na]$^+$: 331.1422, found: 331.1423.
3-(((2-Methylbenzyl)oxy)-2-phenylquinazolin-4(3H)-one (4d)

White solid (61.6 mg, 90 %); \( ^1H \) NMR (400 MHz, CDCl\(_3\) \( \delta \) 8.40 (d, \( J = 8.0 \) Hz, 1H), 7.79 (d, \( J = 4.0 \) Hz, 2H), 7.71 (d, \( J = 8.0 \) Hz, 2H), 7.59–7.47 (m, 2H), 7.42 (t, \( J = 7.4 \) Hz, 2H), 7.24–7.15 (m, 1H), 7.09–6.97 (m, 1H), 6.79 (d, \( J = 7.2 \) Hz, 1H), 4.98 (s, 2H), 2.13 (s, 3H); \( ^{13}C \) NMR (100 MHz, CDCl\(_3\) \( \delta \) 158.3, 154.0, 146.6, 138.9, 134.5, 132.4, 131.5, 131.0, 130.5, 130.4, 129.6, 129.6, 128.2, 128.0, 127.0, 126.8, 125.9, 122.7, 76.0, 18.4; HRMS (ESI) calcd for C\(_{22}\)H\(_{18}\)N\(_2\)O\(_2\) [M + Na\(^+\)]: 365.1266, found: 365.1262.

6-Fluoro-3-(((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4e)

White solid (49.4 mg, 87 %); \( ^1H \) NMR (400 MHz, CDCl\(_3\) \( \delta \) 8.40–8.32 (m, 1H), 7.76 (s, 1H), 7.36–7.29 (m, 2H), 7.29–7.19 (m, 3H), 7.19–7.13 (m, 1H), 5.37 (s, 2H), 2.52 (s, 3H); \( ^{13}C \) NMR (10 MHz, CDCl\(_3\) \( \delta \) 156.4, 145.3, 138.0, 131.0, 130.7, 130.5, 129.7, 129.0, 125.9, 119.7, 115.8, 112.9, 99.5, 77.2, 18.5; HRMS (ESI) calcd for C\(_{16}\)H\(_{13}\)FN\(_2\)O\(_2\) [M + Na\(^+\)]: 307.0859, found: 307.0850.

6-Chloro-3-(((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4f)

White solid (42.0 mg, 70 %); \( ^1H \) NMR (400 MHz, CDCl\(_3\) \( \delta \) 8.32 (s, 1H), 7.76–7.65 (m, 2H), 7.62 (d, \( J = 8.6 \) Hz, 1H), 7.34–7.19 (m, 3H), 7.19–7.11 (m, 1H), 5.37 (s, 2H), 2.52 (s, 3H); \( ^{13}C \) NMR (100 MHz, CDCl\(_3\) \( \delta \) 156.5, 145.5, 144.8, 138.5, 134.8, 133.4, 131.5, 131.2, 131.0, 130.2, 129.5, 126.4, 126.1, 124.6, 77.6, 19.0; HRMS (ESI) calcd for C\(_{16}\)H\(_{13}\)ClN\(_2\)O\(_2\) [M + Na\(^+\)]: 323.0563, found: 323.0559.

7-Methoxy-3-(((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4g)

White solid (42.6 mg, 72 %); \( ^1H \) NMR (400 MHz, CDCl\(_3\) \( \delta \) 8.24 (d, \( J = 8.9 \) Hz, 1H), 7.73 (s, 1H), 7.33–7.21 (m, 3H), 7.18–7.12 (m, 1H), 7.11–7.03 (m, 2H), 5.36 (s, 2H), 3.90 (s, 3H), 2.52 (s, 3H); \( ^{13}C \) NMR (100 MHz, CDCl\(_3\) \( \delta \) 164.5, 157.2, 149.2, 145.2, 138.5, 131.5 (2C), 130.9, 130.0, 128.2, 126.3, 117.3, 116.8, 108.6, 77.6, 55.7, 19.0; HRMS (ESI) calcd for C\(_{17}\)H\(_{16}\)N\(_2\)O\(_3\) [M + Na\(^+\)]: 319.1059, found: 319.1055.
6,7-Dimethoxy-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4h)

![Chemical structure]

White solid (43.7 mg, 67%); ^1H NMR (400 MHz, CDCl$_3$) $\delta$ 7.70 (s, 1H), 7.66 (s, 1H), 7.33–7.23 (m, 3H), 7.19–7.14 (m, 1H), 7.07 (s, 1H), 5.38 (s, 2H), 4.02 (s, 3H), 3.98 (s, 3H), 2.54 (s, 3H); ^13C NMR (100 MHz, CDCl$_3$) $\delta$ 157.0, 154.9, 149.4, 143.3, 143.2, 138.5, 131.5 (2C), 130.9, 130.0, 126.3, 116.9, 108.2, 105.5, 77.6, 56.4, 56.3, 19.0; HRMS (ESI) calcld for C$_{18}$H$_{18}$N$_2$O$_4$ [M + Na]$^+$: 349.1164, found: 349.1166.

6,7-Dimethoxy-2-methyl-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4i)

![Chemical structure]

White solid (29.9 mg, 56%); ^1H NMR (400 MHz, CDCl$_3$) $\delta$ 7.60 (s, 1H), 7.37 (d, $J = 7.4$ Hz, 1H), 7.35–7.29 (m, 1H), 7.27 (d, $J = 8.2$ Hz, 1H), 7.24–7.19 (m, 1H), 7.04 (s, 1H), 5.33 (s, 2H), 4.04–3.93 (m, 6H), 2.60 (s, 3H), 2.47 (s, 3H); ^13C NMR (100 MHz, CDCl$_3$) $\delta$ 157.7, 155.0, 152.4, 148.8, 142.8, 138.6, 131.9, 131.2, 130.7, 129.8, 126.3, 115.7, 107.5, 105.3, 76.3, 56.3 (2C), 20.1, 19.1; HRMS (ESI) calcld for C$_{19}$H$_{20}$N$_2$O$_4$ [M + H]$^+$: 363.1321, found: 363.1325.

2-Ethyl-6,7-dimethoxy-3-((2-methylbenzyl)oxy)quinazolin-4(3H)-one (4j)

![Chemical structure]

White solid (41.8 mg, 62%); ^1H NMR (400 MHz, CDCl$_3$) $\delta$ 7.62 (s, 1H), 7.41 (d, $J = 7.4$ Hz, 1H), 7.36–7.31 (m, 1H), 7.30–7.21 (m, 2H), 7.09 (s, 1H), 5.33 (s, 2H), 4.01 (s, 6H), 2.82 (q, $J = 7.6$ Hz, 2H), 2.61 (s, 3H), 1.33 (t, $J = 7.4$ Hz, 3H); ^13C NMR (100 MHz, CDCl$_3$) $\delta$ 157.9, 156.0, 154.9, 154.9, 148.8, 142.9, 138.6, 131.9, 131.0, 130.7, 129.7, 126.2, 115.7, 107.5, 105.3, 76.4, 56.3 (2C), 26.0, 19.1, 10.9; HRMS (ESI) calcld for C$_{20}$H$_{22}$N$_2$O$_4$ [M + Na]$^+$: 377.1477, found: 377.1478.

7-((2-Methylbenzyl)oxy)-1,3]dioxolo[4,5-g]quinazolin-8(7H)-one (4k)

![Chemical structure]

White solid (33.5, 54%); ^1H NMR (400 MHz, CDCl$_3$) $\delta$ 7.65 (d, $J = 11.9$ Hz, 2H), 7.35–7.19 (m, 3H), 7.20–7.11 (m, 1H), 7.02 (s, 1H), 6.13 (s, 2H), 5.36 (s, 2H), 2.52 (s, 3H); ^13C NMR (100 MHz, CDCl$_3$) $\delta$ 156.9, 153.5, 147.9, 144.9, 143.2, 138.5, 131.5, 131.4, 130.9, 130.1, 126.3, 118.6, 106.2, 103.4, 102.5, 77.5, 19.0; HRMS (ESI) calcld for C$_{17}$H$_{14}$N$_2$O$_4$ [M + Na]$^+$: 333.0851, found: 333.0847.
4. Copies of $^1$H NMR & $^{13}$C NMR Spectra

$^1$H NMR and $^{13}$C NMR for compound 3a
$^1$H NMR and $^{13}$C NMR for compound 3b
$^1$H NMR and $^{13}$C NMR for compound 3e
$^1$H NMR and $^{13}$C NMR for compound 3d
\(^1\text{H NMR and }^{13}\text{C NMR for compound 3e}\)
$^1$H NMR and $^{13}$C NMR for compound 3f
$^1$H NMR and $^{13}$C NMR for compound 3g
$^1$H NMR and $^{13}$C NMR for compound 3h
$^1$H NMR and $^{13}$C NMR for compound 3i
$^1$H NMR and $^{13}$C NMR for compound 3j
$^{1}H$ NMR and $^{13}C$ NMR for compound 3k
\(^1\text{H NMR and }^{13}\text{C NMR for compound } 31\)
$^1$H NMR and $^{13}$C NMR for compound 3m
$^1$H NMR and $^{13}$C NMR for compound 3n
$^1$H NMR and $^{13}$C NMR for compound 3o
$^1$H NMR and $^{13}$C NMR for compound 3p
$^1$H NMR and $^{13}$C NMR for compound 3q
$^1$H NMR and $^{13}$C NMR for compound 3r
$^1$H NMR and $^{13}$C NMR for compound 3s
$^1$H NMR and $^{13}$C NMR for compound 3t
$^1$H NMR and $^{13}$C NMR for compound 3u
$^1$H NMR and $^{13}$C NMR for compound 3v
$^1\text{H NMR and } ^{13}\text{C NMR for compound 3w}$
$^1$H NMR and $^{13}$C NMR for compound 3x
$^1$H NMR and $^{13}$C NMR for compound 3y
$^1$H NMR and $^{13}$C NMR for compound 3z
\(^1\)H NMR and \(^{13}\)C NMR for compound 4a
$^1\text{H} \text{NMR and } ^{13}\text{C} \text{ NMR for compound 4b}$
$^1$H NMR and $^{13}$C NMR for compound 4c
\(^1\)H NMR and \(^13\)C NMR for compound 4d
$^1$H NMR and $^{13}$C NMR for compound 4e
$^1$H NMR and $^{13}$C NMR for compound 4f
$^1$H NMR and $^{13}$C NMR for compound 4g
$^1$H NMR and $^{13}$C NMR for compound 4h
$^1$H NMR and $^{13}$C NMR for compound 4i
$^1$H NMR and $^{13}$C NMR for compound 4j
$^1$H NMR and $^{13}$C NMR for compound 4k