Supporting Information

Visible light-mediated synthesis of quinazolinones from benzyl bromides and 2-aminobenzamides without using any photocatalyst or additive

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1. Experimental section

1.1 Instruments and reagents
All major chemicals and solvents were obtained from commercial sources and used without further purification. ^1^H NMR, ^13^C NMR and ^19^F spectra were recorded on a Bruker Avance III-500 spectrometer (Bruker, Switzerland).

1.2 General Methods for the Synthesis of quinazolinone derivatives
A mixture of benzyl bromide (0.1 mmol), 2-aminobenzamide (0.2 mmol) and methanol (2 mL) as added to the test tube. The reaction mixture was irradiated with a Blue LED (18 W) for 28 h under air atmosphere and stirred at 300–400 rpm. The reaction was monitored using TLC (PE: EtOAc = 6:1, v/v). The organic phase was concentrated under reduced pressure to give the crude product, which was purified by column chromatography to obtain the pure product.

1.3 Cyclic Voltammetry Experiment
Cyclic voltammetry (CV) was taken using a CHI6043E potentiostation. CV measurement of A was carried out in 0.1 M of nBu_4NBF_4/MeOH at a scan rate of 100 mV/s with the protection of N_2. The working electrode is a glassy carbon, the counter electrode is a Pt wire, and the reference electrode is saturated calomel electrode (SCE).

![Figure S1. Cyclic voltammograms of A](image)
1.4 UV-Visible Spectroscopy

Figure S2. UV-Visible absorption spectra

1.5 Determination of electron spin resonance (EPR)

Figure S3. EPR spectra

(a) A and hydrobromic acid in MeOH, under blue LED irritation 10 min;
(b) A and hydrobromic acid in MeOH, dark.

1.6 Confirmation of Formation of H$_2$O$_2$

We conducted the step of template reaction. After 28 hours of reaction, EtOAc (20 mL) was added in the reaction mixture. The organic phase was extracted with H$_2$O (3x10 mL). To this aqueous
layer, HCl and a solution of KI in H₂O were added successively and stirred well. Subsequently, a starch solution was added under vigorous stirring. Finally, the blue color appeared in several minutes. This experimental result indicated that the H₂O₂ was formed in the reaction could oxidize the iodide ions in acidic media to produce I₂, and then I₂ was trapped by the starch to form this deep blue complex (Figure S1).

\[
\begin{align*}
H_2O_2 & \quad + \quad I^- & \overset{H^+}{\longrightarrow} & \quad H_2O & \quad + \quad I_2 \\
I_2 & \quad + \quad \text{starch} & \longrightarrow & \quad I_2-\text{starch} \quad \text{(blue)}
\end{align*}
\]

Figure S4. Confirmation of Formation of H₂O₂
2. Characterization Data of Products

(3a) 2-phenylquinazolin-4(3H)-one \[^{[1]}\]

White solid, m.p. 235.2-236.4 °C. \(^1\)H NMR (500 MHz, DMSO-\(d_6\)) \(\delta\) 12.59 (s, 1H), 8.24 – 8.15 (m, 3H), 7.85 (td, \(J = 7.8, 7.2, 1.4\) Hz, 1H), 7.76 (d, \(J = 8.0\) Hz, 1H), 7.64 – 7.50 (m, 4H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 162.74, 152.78, 149.19, 135.08, 133.18, 131.87, 129.08, 128.24, 127.98, 127.06, 126.33, 121.44.

(3b) 2-(p-tolyl)quinazolin-4(3H)-one \[^{[1]}\]

White solid, m.p. 240.3-242.4 °C. \(^1\)H NMR (500 MHz, DMSO-\(d_6\)) \(\delta\) 12.51 (s, 1H), 8.14 (dd, \(J = 24.1, 7.7\) Hz, 3H), 7.88 – 7.81 (m, 1H), 7.74 (d, \(J = 8.1\) Hz, 1H), 7.52 (t, \(J = 7.4\) Hz, 1H), 7.36 (d, \(J = 8.1\) Hz, 2H), 2.40 (s, 3H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 162.73, 152.65, 149.28, 141.89, 135.01, 130.33, 129.64, 128.13, 127.87, 126.83, 126.30, 121.35, 21.45.

(3c) 2-(m-tolyl)quinazolin-4(3H)-one \[^{[2]}\]

White solid, m.p. 237.3-239.5 °C. \(^1\)H NMR (500 MHz, DMSO-\(d_6\)) \(\delta\) 12.51 (s, 1H), 8.16 (d, \(J = 7.7\) Hz, 1H), 8.04 (s, 1H), 7.98 (d, \(J = 7.4\) Hz, 1H), 7.85 (t, \(J = 7.5\) Hz, 1H), 7.75 (d, \(J = 8.1\) Hz, 1H), 7.53 (t, \(J = 7.4\) Hz, 1H), 7.47 – 7.34 (m, 2H), 2.42 (s, 3H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 162.74, 152.88, 149.16, 138.37, 135.04, 133.10, 132.46, 128.96, 128.75, 126.98, 126.31, 125.34, 121.42, 21.45.

(3d) 2-(o-tolyl)quinazolin-4(3H)-one \[^{[2]}\]

White solid, m.p. 212.5-213.8 °C. \(^1\)H NMR (500 MHz, DMSO-\(d_6\)) \(\delta\) 12.48 (s, 1H), 8.18 (d, \(J = 7.8\) Hz, 1H), 7.89 – 7.80 (m, 1H), 7.70 (d, \(J = 8.1\) Hz, 1H), 7.60 – 7.48 (m, 2H), 7.44 (t, \(J = 7.2\) Hz, 1H), 7.39 –
7.31 (m, 2H), 2.39 (s, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.24, 154.83, 149.19, 136.57, 134.93, 134.68, 130.99, 130.36, 129.60, 127.83, 127.10, 126.25, 126.16, 121.44, 20.04.

(3e) 2-(4-Fluorophenyl)quinazolin-4(3H)-one [3]

White solid, m.p. 283.1-284.9 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.61 (s, 1H), 8.26 (dd, $J = 8.6$, 5.5 Hz, 2H), 8.16 (d, $J = 7.7$ Hz, 1H), 7.85 (t, $J = 7.5$ Hz, 1H), 7.75 (d, $J = 8.1$ Hz, 1H), 7.53 (t, $J = 7.4$ Hz, 1H), 7.41 (t, $J = 8.8$ Hz, 2H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 165.49, 163.50, 162.71, 151.84, 149.08, 135.10, 130.87, 130.80, 129.67, 127.89, 127.07, 126.32, 121.32, 116.19, 116.01. $^{19}$F NMR (471 MHz, DMSO-$d_6$) $\delta$ -109.05.

(3f) 2-(4-Chlorophenyl)quinazolin-4(3H)-one [3]

White solid, m.p. 297.8-299.6 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.64 (s, 1H), 8.19 (dd, $J = 24.0$, 8.1 Hz, 3H), 7.85 (t, $J = 7.1$ Hz, 1H), 7.75 (d, $J = 8.1$ Hz, 1H), 7.64 (d, $J = 8.5$ Hz, 2H), 7.54 (t, $J = 7.4$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.64, 151.79, 149.02, 136.75, 135.13, 131.99, 130.08, 129.15, 127.98, 127.24, 126.34, 121.44.

(3g) 2-(4-Bromophenyl)quinazolin-4(3H)-one [3]

White solid, m.p. 293.1-295.2 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.64 (s, 1H), 8.22 – 8.06 (m, 3H), 7.89 – 7.82 (m, 1H), 7.76 (t, $J = 9.0$ Hz, 3H), 7.55 (t, $J = 7.4$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.62, 151.90, 149.02, 135.15, 132.35, 132.08, 130.26, 127.99, 127.26, 126.34, 125.71, 121.47.

(3h) 2-(2-Fluorophenyl)quinazolin-4(3H)-one [1]
White solid, m.p. 240.5-242.6 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.61 (s, 1H), 8.19 (d, $J = 7.8$ Hz, 1H), 7.87 (t, $J = 7.6$ Hz, 1H), 7.80 (t, $J = 7.0$ Hz, 1H), 7.75 (d, $J = 8.1$ Hz, 1H), 7.64 (q, $J = 6.3$ Hz, 1H), 7.58 (t, $J = 7.5$ Hz, 1H), 7.45 – 7.35 (m, 2H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 161.96, 161.02, 159.03, 150.41, 149.13, 135.07, 133.35, 133.28, 131.52, 131.51, 127.96, 127.50, 126.32, 125.09, 125.06, 122.79, 122.68, 121.56, 116.73, 116.56. $^{19}$F NMR (471 MHz, DMSO-$d_6$) $\delta$ -114.68.

(3i) 2-(4-(trifluoromethyl)phenyl)quinazolin-4(3$H$)-one $^{[3]}$

White solid, m.p. 283.8-295.7 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.78 (s, 1H), 8.38 (d, $J = 7.2$ Hz, 2H), 8.19 (d, $J = 7.2$ Hz, 1H), 8.02 – 7.70 (m, 4H), 7.57 (t, $J = 6.6$ Hz, 1H).$^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 151.60, 148.89, 137.04, 135.18, 131.68, 131.42, 129.17, 128.14, 127.56, 126.35, 125.96, 125.93, 125.49, 123.33, 121.65. $^{19}$F NMR (471 MHz, DMSO-$d_6$) $\delta$ -61.35.

(3j) 2-((1,1'-biphenyl)-4-yl)quinazolin-4(3$H$)-one $^{[4]}$

White solid, m.p. 288.1-290.5 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.63 (s, 1H), 8.32 (d, $J = 8.4$ Hz, 2H), 8.18 (d, $J = 7.8$ Hz, 1H), 7.86 (dd, $J = 10.5$, 7.9 Hz, 3H), 7.78 (t, $J = 7.2$ Hz, 3H), 7.53 (q, $J = 8.0$ Hz, 3H), 7.44 (t, $J = 7.3$ Hz, 1H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.72, 152.37, 149.24, 143.29, 139.41, 135.10, 132.00, 129.54, 128.84, 128.65, 127.99, 127.32, 127.22, 127.06, 126.34, 121.47.

(3k) 2-(naphthalen-1-yl)quinazolin-4(3$H$)-one $^{[3]}$

White solid, m.p. 289.8-291.9 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.71 (s, 1H), 8.24 (d, $J = 7.6$ Hz, 1H), 8.19 (d, $J = 7.6$ Hz, 1H), 8.13 (d, $J = 8.2$ Hz, 1H), 8.09 – 8.04 (m, 1H), 7.88 (t, $J = 7.5$ Hz, 1H), 7.81 (d, $J = 6.9$ Hz, 1H), 7.75 (d, $J = 8.0$ Hz, 1H), 7.69 – 7.56 (m, 4H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$
162.37, 154.13, 149.19, 135.01, 133.58, 132.18, 130.85, 130.71, 128.81, 128.16, 127.94, 127.55, 127.27, 126.84, 126.32, 125.69, 125.55, 121.70.

(3l) 3-methyl-2-phenylquinazolin-4(3H)-one [1]

White solid, m.p. 127.9-129.8 °C. \(^1^H\) NMR (500 MHz, DMSO-\(d_6\)) \(\delta\) 8.19 (d, \(J = 7.9\) Hz, 1H), 7.84 (t, \(J = 7.5\) Hz, 1H), 7.74 – 7.65 (m, 3H), 7.56 (s, 4H), 3.37 (s, 3H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 162.11, 156.60, 147.52, 135.86, 134.81, 130.26, 128.87, 128.73, 127.64, 127.34, 126.55, 120.61, 34.36.

(3m) 3-butyl-2-phenylquinazolin-4(3H)-one [5]

White solid, m.p. 112.4-114.1 °C. \(^1^H\) NMR (500 MHz, DMSO-\(d_6\)) \(\delta\) 8.20 (d, \(J = 7.9\) Hz, 1H), 7.85 (t, \(J = 7.5\) Hz, 1H), 7.71 – 7.61 (m, 3H), 7.56 (d, \(J = 6.0\) Hz, 4H), 3.97 – 3.81 (m, 2H), 1.48 (p, \(J = 7.4\) Hz, 2H), 1.07 (h, \(J = 7.3\) Hz, 2H), 0.66 (t, \(J = 7.3\) Hz, 3H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 161.59, 156.51, 147.34, 135.87, 134.91, 130.04, 128.83, 128.44, 127.63, 127.43, 126.64, 120.89, 45.28, 30.31, 19.76, 13.64.

(3n) 3-benzyl-2-phenylquinazolin-4(3H)-one [1]

White solid, m.p. 138.4-140.6 °C. \(^1^H\) NMR (500 MHz, DMSO-\(d_6\)) \(\delta\) 8.25 – 8.19 (m, 1H), 7.93 – 7.86 (m, 1H), 7.72 (d, \(J = 8.1\) Hz, 1H), 7.61 (t, \(J = 7.4\) Hz, 1H), 7.54 – 7.40 (m, 5H), 7.21 (t, \(J = 7.7\) Hz, 3H), 6.92 (d, \(J = 6.6\) Hz, 2H), 5.19 (s, 2H). \(^{13}\)C NMR (126 MHz, DMSO-\(d_6\)) \(\delta\) 161.85, 156.61, 147.42, 137.18, 135.59, 135.22, 130.17, 128.88, 128.69, 128.44, 127.82, 127.70, 127.55, 126.88, 126.72, 120.84, 48.68.

(3o) 6-methoxy-2-phenylquinazolin-4(3H)-one [1]
White solid, m.p. >300°C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.53 (s, 1H), 8.17 (d, $J$ = 7.0 Hz, 2H), 7.71 (d, $J$ = 8.8 Hz, 1H), 7.55 (d, $J$ = 7.4 Hz, 4H), 7.49 – 7.40 (m, 1H), 3.90 (s, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.49, 158.20, 150.54, 143.67, 133.25, 129.69, 129.04, 127.95, 124.58, 122.25, 56.11.

(3p) 6-fluoro-2-phenylquinazolin-4($3H$)-one $^{[4]}$

White solid; m.p: 274.2-276.6 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.70 (s, 1H), 8.18 (d, $J$ = 7.2 Hz, 2H), 7.84 (dd, $J$ = 8.6, 3.2 Hz, 2H), 7.74 (td, $J$ = 8.7, 2.9 Hz, 1H), 7.58 (dt, $J$ = 14.5, 7.0 Hz, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 162.16, 161.41, 159.46, 152.31, 146.08, 131.89, 130.81, 130.75, 129.08, 128.21, 123.63, 123.43, 122.67, 111.07, 110.89. $^{19}$F NMR (471 MHz, DMSO-$d_6$) $\delta$ -113.50.

(3q) 6-chloro-2-phenylquinazolin-4($3H$)-one $^{[1]}$

White solid, m.p. 276.9-279.0 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.74 (s, 1H), 8.18 (d, $J$ = 7.4 Hz, 2H), 8.08 (d, $J$ = 2.2 Hz, 1H), 7.86 (dd, $J$ = 8.7, 2.3 Hz, 1H), 7.76 (d, $J$ = 8.7 Hz, 1H), 7.59 (dt, $J$ = 25.5, 7.1 Hz, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 161.76, 153.25, 147.93, 135.15, 132.89, 132.06, 131.21, 130.20, 129.10, 128.30, 125.33.

(3r) 6-bromo-2-phenylquinazolin-4($3H$)-one $^{[1]}$

White solid; m.p. 283.8-286.3 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) $\delta$ 12.74 (s, 1H), 8.31 – 8.11 (m, 3H), 7.98 (d, $J$ = 7.8 Hz, 1H), 7.70 (d, $J$ = 8.4 Hz, 1H), 7.66 – 7.50 (m, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) $\delta$ 161.62, 153.36, 148.18, 137.86, 132.90, 132.08, 130.34, 129.10, 128.45, 128.31, 123.05, 119.39.

(3s) 7-chloro-2-phenylquinazolin-4($3H$)-one $^{[3]}$
White solid; m.p: 284.1-286.3 °C. $^1$H NMR (500 MHz, DMSO-$d_6$) δ 12.74 (s, 1H), 8.20 (dd, $J$ = 24.5, 4.4 Hz, 3H), 8.03 – 7.93 (m, 1H), 7.69 (d, $J$ = 8.7 Hz, 1H), 7.59 (dt, $J$ = 26.2, 7.1 Hz, 3H). $^{13}$C NMR (126 MHz, DMSO-$d_6$) δ 161.67, 153.40, 148.17, 137.87, 132.91, 132.08, 130.31, 129.10, 128.45, 128.31, 123.05, 119.39.

3. $^1$H-NMR, $^{13}$C-NMR and $^{19}$F-NMR spectra of products

$^1$H NMR spectra of compound 3a
$^{13}$C NMR spectra of compound 3a

$^1$H NMR spectra of compound 3b
$^{13}$C NMR spectra of compound 3b
$^1$H NMR spectra of compound 3c

$^{13}$C NMR spectra of compound 3c
$^1$H NMR spectra of compound 3d

$^{13}$C NMR spectra of compound 3d
$^1$H NMR spectra of compound 3e

$^{13}$C NMR spectra of compound 3e
$^{19}$F NMR spectra of compound 3e

$^1$H NMR spectra of compound 3f
$^{13}$C NMR spectra of compound 3f

$^1$H NMR spectra of compound 3g
$^{13}$C NMR spectra of compound 3g

$^1$H NMR spectra of compound 3h
$^{13}$C NMR spectra of compound 3h

$^{19}$F NMR spectra of compound 3h
$^1$H NMR spectra of compound 3i

$^{13}$C NMR spectra of compound 3i
$^{19}$F NMR spectra of compound 3i

$^1$H NMR spectra of compound 3j
$^{13}$C NMR spectra of compound 3j

$^1$H NMR spectra of compound 3k
$^{13}$C NMR spectra of compound 3k

$^1$H NMR spectra of compound 3l
$^{13}$C NMR spectra of compound 3l

![13C NMR spectra of compound 3l](image)

$^1$H NMR spectra of compound 3m

![$^1$H NMR spectra of compound 3m](image)
$^{13}$C NMR spectra of compound 3m

$^1$H NMR spectra of compound 3n
$^{13}$C NMR spectra of compound 3n

$^1$H NMR spectra of compound 3o
$^{13}$C NMR spectra of compound 3o

$^1$H NMR spectra of compound 3p
$^{13}$C NMR spectra of compound 3p

$^{19}$F NMR spectra of compound 3p
$^1$H NMR spectra of compound 3q

$^{13}$C NMR spectra of compound 3q
$^1$H NMR spectra of compound 3r

$^{13}$C NMR spectra of compound 3r
$^1$H NMR spectra of compound 3s

$^{13}$C NMR spectra of compound 3s
\textsuperscript{1}H NMR spectra of compound A

GC-MS of compound A
4. Reference