Supporting Information for

Electrochemical Oxidative Decarboxylative of α-Oxocarboxylic Acids

towards the Synthesis of Quinazolines and Quinazolinones

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General information

All glassware was oven dried at 110 °C for hours and cooled down under vacuum. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. The instrument for electrolysis is dual display potentiostat (DJS-292B) (made in China). The anodic electrode was graphite rod (ϕ 6 mm, hard) and cathodic electrode was nickel plate (1.5 cm × 1.5 cm × 0.1 cm). Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 °C). ¹H, ¹³C and ¹⁹F NMR data were recorded with Bruker Advance III (400 MHz) spectrometers with tetramethylsilane as an internal standard. All chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. All chemical shifts are reported relative to tetramethylsilane and *d*-solvent peaks, respectively.

General procedures

General procedure for the synthesis of 3-10:



In a 25 mL three-necked bottle equipped with a magnetic stir bar, C rod (ϕ 6 mm) was used as anode and Ni (1.5 cm × 1.5 cm × 0.1 cm) was used as cathode. (2aminophenyl)(phenyl)methanone (0.2 mmol), NH₄I (0.8 mmol, 116.0 mg) were added and charged with N₂ for three times. The glyoxylic acid **2** (0.4 mmol, 60 uL) and DMSO (10.0 mL) were added sequently to the bottle via syringes. The Electrolysis experiment was performed at 12 mA, 100 °C for 3 hours. When the reaction was finished, the reaction mixture was washed with water and extracted with ethyl acetate (10 mL x 3). The organic layers were combined, dried with Na₂SO₄, and concentrated. The pure product was obtained by flash column chromatography on silica gel.

General procedure for the synthesis of 11-22:



In a 25 mL three-necked bottle equipped with a magnetic stir bar, C rod (\$\$\op\$ 6 mm) was used as

anode and Ni (1.5 cm \times 1.5 cm \times 0.1 cm) was used as cathode. (2aminophenyl)(phenyl)methanone 1 (0.2 mmol, 39.4 mg), α -keto acids (0.4 mmol) NH₄I (0.8 mmol, 116.0 mg) were added and charged with N₂ for three times. The DMSO (10.0 mL) was added sequently to the bottle via syringes. The Electrolysis experiment was performed at 12 mA, 100 °C for 3 hours. When the reaction was finished, the reaction mixture was washed with water and extracted with ethyl acetate (10 mL x 3). The organic layers were combined, dried with Na₂SO₄, and concentrated. The pure product was obtained by flash column chromatography on silica gel. **General procedure for the synthesis of 23-38:**



In a 25 mL three-necked bottle equipped with a magnetic stir bar, C rod (ϕ 6 mm) was used as anode and Ni (1.5 cm × 1.5 cm × 0.1 cm) was used as cathode. 2-Amino-N-substitutedbenzamide (0.2 mmol), NH₄I (0.8 mmol, 116.0 mg) were added and charged with N₂ for three times. The glyoxylic acid **2** (0.4 mmol, 60 uL) and DMSO (10.0 mL) were added sequently to the bottle via syringes. The Electrolysis experiment was performed at 12 mA, 100 °C for 3 hours. When the reaction was finished, the reaction mixture was washed with water and extracted with ethyl acetate (10 mL x 3). The organic layers were combined, dried with Na₂SO₄, and concentrated. The pure product was obtained by flash column chromatography on silica gel.

General procedure for the synthesis of 39-46:



In a 25 mL three-necked bottle equipped with a magnetic stir bar, C rod (ϕ 6 mm) was used as anode and Ni (1.5 cm × 1.5 cm × 0.1 cm) was used as cathode. 2-Aminobenzamide (0.2 mmol, 27.2 mg), α -keto acids (0.4 mmol) NH₄I (0.8 mmol, 116.0 mg) were added and charged with N₂ for three times. The DMSO (10.0 mL) was added sequently to the bottle via syringes. The Electrolysis experiment was performed at 12 mA, 100 °C for 3 hours. When the reaction was finished, the reaction mixture was washed with water and extracted with ethyl acetate (10 mL x 3). The organic layers were combined, dried with Na₂SO₄, and concentrated. The pure product was obtained by flash column chromatography on silica gel.





In a 250 mL three-necked bottle equipped with a magnetic stir bar, C rod (ϕ 6 mm) was used as anode and Ni (1.5 1.5 cm × 0.1 cm) was used as cathode. cm Х (2-Aminophenyl)(phenyl)methanone 1 (10 mmo1, 1.97 g), NH₄I (40.0 mmol, 5.80 g) were added and charged with N₂ for three times. The glyoxylic acid 2 (20.0 mmol, 3.0 mL) and DMSO (100.0 mL) were added sequently to the bottle via syringes. The Electrolysis experiment was performed at 12 mA for 24 h. When the reaction was finished, the reaction mixture was washed with water and extracted with ethyl acetate (100 mL x 3). The organic layers were combined, dried with Na₂SO₄, and concentrated. The pure product was obtained by flash column chromatography on silica gel.



		C(+):Ni(-) I = 12 mA Electrolyte, DMSO	O NH
	NH ₂ O	12 mA, 3 h, 100 °C, N ₂ undivided cell	23
Entry	Electrolyte		Yield of 23 (%) ^b
1	NH ₄ I		74
2	KI		57
3	ⁿ Bu ₄ NBF ₄		39
4	ⁿ Bu ₄ NPF ₆		36
5			0

^{*a*}Reaction conditions: C anode, Ni cathode, constant current = 12 mA, **2-aminobenzamide** (0.2 mmol), **2-oxoacetic acid** (0.4 mmol), electrolyte (0.8 mmol), in 10.0 mL DMSO at 100 °C under N₂ for 3 h. ^{*b*}Yields shown are of isolated products.

GC-MS result for 49, 50, 51 and 52





Figure S1. GC-MS result for 49



Figure S2. GC-MS result for 50



Figure S3. GC-MS result for 51

Figure S4. GC-MS result for 52

Electrochemical procedures for cyclic voltammetry

Cyclic voltammetry was performed in a three-electrode cell connected to a schlenk line under nitrogen at 35 °C. The working electrode was a steady glassy carbon disk electrode, the counter electrode was a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. 10.0 mL of DMSO and 0.1 mmol of ⁿBu₄NBF₄ were added to the electrochemical cell in all experiments. The scan rate was 0.05 V/s, from 0 V to 2.5 V

Figure S5. A) Cyclic voltammetry of NH₄I (0.1 mmol) in DMSO (10 mL) with ⁿBu₄NBF₄ (0.1 mmol) under nitrogen at a scan rate of v = 0.05 V/s, from 0 V to 2.0 V. B) Cyclic voltammetry of I (0.1 mmol) in DMSO (10 mL) with ⁿBu₄NBF₄ (0.1 mmol) under nitrogen at a scan rate of v = 0.05 V/s, from 0 V to 2.5 V. C) Cyclic voltammetry of 47 (0.1 mmol) in DMSO (10 mL) with ⁿBu₄NBF₄ (0.1 mmol) under nitrogen at a scan rate of v =0.05 V/s, from 0 V to 2.5 V.

Detail descriptions for products

4-phenylquinazoline 3^[1]: 38.8 mg, 82% yield, a white solid, mp. 97 - 98 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.39 (s, 1H), 8.13 (t, *J* = 7.9 Hz, 2H), 7.92 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.82 – 7.74 (m, 2H), 7.65 – 7.54 (m, 4H). ¹³C NMR (101 MHz, CDCl₃) δ 168.43, 154.71, 151.13, 137.12, 133.73, 130.09, 129.97, 128.94, 128.67, 127.76, 127.13, 123.19.

4-(4-Fluorophenyl)quinazoline 4^[1]:35.9 mg, 80% yield, a light yellow solid, mp. 91 - 93 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.36 (s, 1H), 8.11 (t, J = 8.3 Hz, 2H), 7.93 (t, J = 8.0 Hz, 1H), 7.80 (dd, J = 8.6, 5.4 Hz, 2H), 7.63 (t, J = 7.7 Hz, 1H), 7.27 (t, J = 8.6 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 167.23, 165.24, 162.75, 154.60, 151.15, 133.82, 133.21 (d, $J_{C-F} = 3.3$ Hz), 132.03 (d, $J_{C-F} = 8.5$ Hz), 129.03, 127.92, 126.78, 123.04, 115.84 (d, $J_{C-F} = 21.8$ Hz). ¹⁹F NMR (377 MHz, CDCl₃) δ -110.29.

4-(4-Chlorophenyl)quinazoline 5^[1]:39.9 mg, 83% yield, a light yellow solid, mp. 116 - 118 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.38 (s, 1H), 8.11 (dd, *J* = 16.5, 8.4 Hz, 2H), 7.94 (t, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.64 (t, *J* = 8.3 Hz, 1H), 7.57 (d, *J* = 8.6 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 167.14, 154.65, 151.19, 136.49, 135.53, 133.90, 131.33, 129.10, 128.99, 128.00, 126.67, 122.99.

4-(4-Bromophenyl)quinazoline 6^[1]: 23.2 mg, 41% yield, a white solid, mp. 152 - 153 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.38 (s, 1H), 8.11 (dd, *J* = 18.4, 8.4 Hz, 2H), 7.94 (t, *J* = 8.3 Hz, 1H), 7.73 (d, *J* = 8.5 Hz, 2H), 7.70 - 7.59 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 167.15, 154.62, 151.14, 135.95, 133.88, 131.91, 131.52, 129.06, 127.98, 126.62, 124.81, 122.89.

4-Cyclohexylquinazoline 7^[1]: 26.7 mg, 63% yield, oily liquid. ¹H NMR (400 MHz, CDCl₃) δ 9.25 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.91 – 7.80 (m, 1H), 7.64 (t, *J* = 7.1 Hz, 1H), 3.56 (tt, *J* = 11.7, 3.2 Hz, 1H), 1.98 – 1.80 (m, 7H), 1.59 – 1.47 (m, 2H), 1.44 – 1.36 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 175.13, 154.76, 150.08, 133.33, 129.34, 127.37, 124.20, 123.27, 41.30, 32.05, 26.54, 26.03.

Quinazoline 8^[1]: 9.6 mg, 37% yield, a light yellow solid, mp. 47 - 49 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.41 (s, 1H), 9.35 (s, 1H)., 8.06 (d, J = 8.8 Hz, 1H), 7.93 (dd, J = 7.7, 6.4 Hz, 2H), 7.68 (t, J = 7.5 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 160.22, 155.24, 149.98, 134.17, 128.37, 127.93, 127.18, 125.06.

6-Chloro-4-phenylquinazoline 9^[1]: 34.1 mg, 71% yield, a light yellow solid, mp. 134 - 135 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.38 (s, 1H), 8.11 (d, *J* = 2.2 Hz, 1H), 8.07 (d, *J* = 9.0 Hz, 1H), 7.85 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.77 (dd, *J* = 6.7, 2.8 Hz, 2H), 7.63 – 7.58 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 167.67, 154.85, 149.63, 136.55, 134.73, 133.54, 130.71, 130.40, 129.86, 128.89, 125.84, 123.72.

6-Bromo-4-phenylquinazoline 10^[1]: 29.4 mg, 52% yield, a light yellow solid, mp. 145 - 147 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.39 (s, 1H), 8.27 (s, 1H), 8.03 – 7.94 (m, 2H), 7.77 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.65 – 7.57 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 167.48, 154.85, 149.76, 137.22, 136.47, 130.71, 130.38, 129.84, 129.12, 128.85, 124.11, 121.57.

2,4-Diphenylquinazoline 11^[2]: 47.4 mg, 84% yield, a light yellow solid, mp. 114 - 115 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.69 (d, *J* = 6.3 Hz, 2H), 8.15 (dd, *J* = 12.1, 8.5 Hz, 2H), 7.93 - 7.83 (m, 3H), 7.66 - 7.58 (m, 3H), 7.58 - 7.46 (m, 4H). ¹³C NMR (101 MHz, CDCl₃) δ 168.34, 160.26, 151.99, 138.20, 137.67, 133.56, 130.51, 130.19, 129.93, 129.16, 128.67, 128.54, 127.03, 121.70.

4-Phenyl-2-(p-tolyl)quinazoline 12^[2]: 42.1 mg, 71% yield, a white solid, mp. 162 - 163 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.59 (d, *J* = 8.2 Hz, 2H), 8.17 - 8.08 (m, 2H), 7.92 - 7.83 (m, 3H), 7.64 - 7.57 (m, 3H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.33 (d, J = 8.1 Hz, 2H), 2.45 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 168.28, 160.34, 151.99, 140.78, 137.75, 135.46, 133.53, 130.23, 129.92, 129.34, 129.07, 128.65, 128.56, 127.05, 126.82, 121.63, 21.59.

4-Phenyl-2-(*m*-tolyl)quinazoline 13^[2]: 53.3 mg, 90% yield, a yellow solid, mp. 89 – 91 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.49 (d, *J* = 8.1 Hz, 2H), 8.14 (dd, *J* = 13.5, 8.4 Hz, 2H), 7.96 – 7.84 (m, 3H), 7.65 – 7.58 (m, 3H), 7.55 (t, *J* = 7.1 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.32 (d, *J* = 7.7 Hz, 1H), 2.49 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 168.35, 160.45, 152.00, 138.20, 137.71, 133.58, 131.38, 130.24, 129.96, 129.18, 128.58, 128.51, 127.07, 126.99, 125.93, 121.71, 21.61.

4-Phenyl-2-(*o*-tolyl)quinazoline 14^[2]: 31.4 mg, 53% yield, a white solid, mp. 71 – 72 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.16 (d, *J* = 8.4 Hz, 2H), 8.01 – 7.95 (m, 1H), 7.92 – 7.79 (m, 3H), 7.65 – 7.50 (m, 4H), 7.38 – 7.28 (m, 3H), 2.67 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 168.08, 163.43, 151.70, 138.86, 137.51, 137.43, 133.67, 131.31, 130.77, 130.19, 129.97, 129.29, 129.14, 128.62, 127.36, 127.03, 126.04, 121.04, 21.34.

2-(4-(*tert***-Butyl)phenyl)-4-phenylquinazoline 15^[2]:** 42.0 mg, 62% yield, a yellow solid, mp. 103 - 105 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.60 (d, *J* = 8.5 Hz, 2H), 8.12 (dd, *J* = 14.5, 8.4 Hz, 2H), 7.89 – 7.84 (m, 3H), 7.63 – 7.49 (m, 6H), 1.38 (s, 9H). ¹³C NMR (101 MHz, CDCl₃) δ 168.23, 160.41, 153.82, 152.06, 137.79, 135.54, 133.49, 130.24, 129.90, 129.15, 128.55, 128.49, 127.04, 126.81, 125.56, 121.61, 34.90, 31.34.

2-(4-Methoxyphenyl)-4-phenylquinazoline 16^[2]: 28.7 mg, 46% yield, a white solid, mp. 159 -

160 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.66 (d, *J* = 8.9 Hz, 2H), 8.11 (t, *J* = 8.3 Hz, 2H), 7.88 (dd, *J* = 6.5, 3.2 Hz, 3H), 7.62 – 7.58 (m, 3H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 8.9 Hz, 2H), 3.90 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 168.25, 161.78, 160.05, 152.01, 137.77, 133.54, 130.87, 130.35, 130.20, 129.91, 128.91, 128.55, 127.06, 126.59, 121.42, 113.88, 55.42.

2-(4-Fluorophenyl)-4-phenylquinazoline 17^[2]: 43.8 mg, 73% yield, a light yellow solid, mp. 155 - 156 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.70 (dd, *J* = 8.8, 5.7 Hz, 2H), 8.13 (dd, *J* = 8.4, 4.0 Hz, 2H), 7.87 (dd, *J* = 6.4, 2.6 Hz, 3H), 7.63 – 7.58 (m, 3H), 7.55 (t, *J* = 7.7 Hz, 1H), 7.20 (t, *J* = 8.7 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 168.44, 165.91, 163.43, 159.32, 151.95, 137.59, 134.38 (d, *J*_{C-F} = 2.9 Hz), 133.71, 130.78 (d, *J*_{C-F} = 8.7 Hz), 130.19, 130.04, 129.07, 128.60, 127.09 (d, *J*_{C-F} = 1.0 Hz), 121.60, 115.48 (d, *J*_{C-F} = 21.6 Hz). ¹⁹F NMR (376 MHz, CDCl₃) δ -110.77.

2-(4-Chlorophenyl)-4-phenylquinazoline 18^[2]: 35.4 mg, 54% yield, a white solid, mp. 190 - 191 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.64 (d, *J* = 8.6 Hz, 2H), 8.12 (dd, *J* = 8.4, 3.6 Hz, 2H), 7.93 – 7.83 (m, 3H), 7.64 – 7.52 (m, 4H), 7.48 (d, *J* = 8.6 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 168.46, 159.22, 151.91, 137.53, 136.73, 133.75, 130.20, 130.07, 130.03, 129.13, 128.75, 128.62, 127.26, 127.10, 121.73.

2-(4-Bromophenyl)-4-phenylquinazoline 19^[2]: 54.7 mg, 76% yield, a white solid, mp. 140 - 142 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.58 (d, *J* = 8.5 Hz, 2H), 8.14 (dd, *J* = 8.4, 4.6 Hz, 2H), 7.94 – 7.84 (m, 3H), 7.66 – 7.55 (m, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 168.49, 159.30, 151.89, 137.51, 137.14, 133.78, 131.72, 130.29, 130.20, 130.09, 129.13, 128.62, 127.30, 127.12, 125.34, 121.77.

2-(3,5-Dimethylphenyl)-4-phenylquinazoline 20^[2]: 35.4 mg, 54% yield, a light yellow solid, mp. 160 - 161 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.30 (s, 2H), 8.13 (dd, *J* = 16.3, 8.3 Hz, 2H), 7.90 – 7.86 (m, 3H), 7.65 – 7.58 (m, 3H), 7.53 (t, *J* = 7.6 Hz, 1H), 7.14 (s, 1H), 2.44 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 168.34, 160.60, 151.97, 138.11, 137.72, 133.56, 132.38, 130.25, 129.95, 129.11, 128.59, 127.07, 126.93, 126.46, 121.74, 21.50.

2-(Naphthalen-1-yl)-4-phenylquinazoline 21^[3]: 48.5 mg, 73% yield, a yellow solid, mp. 172 - 173 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.79 (d, *J* = 8.3 Hz, 1H), 8.26 – 8.17 (m, 3H), 8.00 – 7.85 (m, 5H), 7.66 – 7.48 (m, 7H). ¹³C NMR (101 MHz, CDCl₃) δ 168.53, 162.82, 151.77, 137.48, 136.58, 134.26, 133.82, 131.40, 130.29, 130.20, 130.01, 129.73, 129.22, 128.66, 128.50, 127.53, 127.11, 126.78, 126.13, 125.85, 125.37, 121.32.

2-(Naphthalen-2-yl)-4-phenylquinazoline 22^[2]: 53.2 mg, 80% yield, a white solid, mp. 173 - 174 °C. ¹H NMR (400 MHz, CDCl₃) δ 9.24 (s, 1H), 8.81 (dd, *J* = 8.6, 1.6 Hz, 1H), 8.20 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 8.06 – 8.01 (m, 1H), 7.98 (d, J = 8.7 Hz, 1H), 7.95 – 7.86 (m, 4H), 7.67 – 7.59 (m, 3H), 7.58 – 7.49 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 168.43, 160.24, 152.07, 137.73, 135.61, 134.72, 133.64, 133.45, 130.26, 130.00, 129.32, 129.20, 129.02, 128.62, 128.18, 127.75, 127.11, 127.08, 127.00, 126.15, 125.62, 121.79.

Quinazolin-4(3*H***)-one 23**^[4]: 21.6 mg, 74% yield, a white solid, mp. 215 - 217 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.29 (s, 1H), 8.17 - 8.07 (m, 2H), 7.86 - 7.80 (m, 1H), 7.68 (d, J = 7.9 Hz, 1H), 7.56 - 7.51 (m, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 161.21, 149.21, 145.89, 134.81, 127.69, 127.23, 126.30, 123.06.

3-Methylquinazolin-4(3*H***)-one 24**^[4]: 30.7 mg, 96% yield, a white solid, mp. 104 - 105 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.29 (d, *J* = 8.0 Hz, 1H), 8.04 (s, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 3.58 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 161.59, 148.24, 146.80, 134.20, 127.45, 127.33, 126.53, 121.94, 34.14.

3-Butylquinazolin-4(3*H***)-one 25**^[4]: 36.4 mg, 90% yield, a white solid, mp. 61 - 62 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.31 (dd, *J* = 8.0, 1.3 Hz, 1H), 8.04 (s, 1H), 7.78 – 7.73 (m, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.53 – 7.48 (m, 1H), 4.04 – 3.97 (m, 2H), 1.82 – 1.72 (m, 2H), 1.41 (dq, *J* = 14.8, 7.4 Hz, 2H), 0.97 (t, J = 7.3 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 161.07, 148.02, 146.64, 134.19, 127.36, 127.28, 126.72, 122.17, 46.88, 31.44, 19.93, 13.70.

3-Allylquinazolin-4(3*H***)-one 26**^[4]: 25.6 mg, 76% yield, a white solid, mp. 56 - 58 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.31 (d, *J* = 8.0 Hz, 1H), 8.01 (s, 1H), 7.79 – 7.66 (m, 2H), 7.50 (t, *J* = 7.5 Hz, 1H), 6.03 – 5.94 (m, 1H), 5.28 (t, *J* = 14.9 Hz, 2H), 4.63 (d, *J* = 5.7 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 160.85, 148.07, 146.24, 134.33, 131.84, 127.50, 127.38, 126.81, 122.09, 118.90, 48.37.

3-Cyclopropylquinazolin-4(3H)-one 27^[5]: 30.2 mg, 81% yield, a white solid, mp. 95 - 97 °C. ¹H

NMR (400 MHz, CDCl₃) δ 8.29 (d, J = 8.0 Hz, 1H), 8.10 (s, 1H), 7.73 (t, J = 7.6 Hz, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.48 (t, J = 7.5 Hz, 1H), 3.27 – 3.20 (m, 1H), 1.20 (q, J = 6.8 Hz, 2H), 0.92 (dd, J = 6.1, 4.3 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 162.33, 147.54, 146.84, 134.28, 127.34, 126.59, 121.80, 29.35, 6.54.

3-Cyclohexylquinazolin-4(*3H*)-one 28^[4]: 37.9 mg, 83% yield, a white solid, mp. 118 - 119 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.30 (d, *J* = 8.7 Hz, 1H), 8.11 (s, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.68 (d, *J* = 7.5 Hz, 1H), 7.48 (t, *J* = 7.4 Hz, 1H), 4.84 – 4.77 (m, 1H), 2.0 – 1.91 (m, 4H), 1.77 (d, *J* = 13.2 Hz, 1H), 1.68 – 1.58 (m, 2H), 1.55 – 1.46 (m, 2H), 1.32 – 1.17 (m, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 160.71, 147.50, 143.93, 134.13, 127.25, 127.12, 126.97, 121.93, 53.34, 32.62, 25.91, 25.29.

3-Benzylquinazolin-4(3*H***)-one 29**^[4]: 29.3 mg, 62% yield, a white solid, mp. 115 - 117 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.32 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.11 (s, 1H), 7.78 – 7.72 (m, 1H), 7.70 (d, *J* = 7.3 Hz, 1H), 7.50 (t, *J* = 8.1 Hz, 1H), 7.35 – 7.30 (m, 5H), 5.19 (s, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 161.09, 148.02, 146.39, 135.72, 134.37, 129.06, 128.34, 128.02, 127.53, 127.43, 126.90, 122.20, 49.65.

3-(Furan-2-ylmethyl)quinazolin-4(3*H***)-one 30**^[4]: 43.4 mg, 96% yield, a white solid, mp. 117 - 119 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.29 (d, *J* = 8.0 Hz, 1H), 8.16 (s, 1H), 7.76 – 7.65 (m, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.36 (s, 1H), 6.45 (d, *J* = 3.0 Hz, 1H), 6.33 (s, 1H), 5.17 (s, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 160.61, 148.29, 147.85, 145.96, 143.10, 134.28, 127.42, 127.29, 126.71, 122.00, 110.71, 109.90, 42.03.

3-(Thiophen-2-ylmethyl)quinazolin-4(3*H***)-one 31**^[5]: 41.2 mg, 85% yield, a white solid, mp. 126 - 127 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.32 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.14 (s, 1H), 7.74 (t, *J* = 8.3 Hz, 1H), 7.68 (d, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 8.1 Hz, 1H), 7.26 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.14 (d, *J* = 3.1 Hz, 1H), 6.96 (dd, *J* = 5.1, 3.5 Hz, 1H), 5.33 (s, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 160.78, 147.98, 145.82, 137.50, 134.43, 127.87, 127.56, 127.48, 127.13, 126.86, 126.72, 122.08, 44.33.

3-(2-(1*H***-Indol-3-yl)ethyl)quinazolin-4(3***H***)-one 32**^[4]: 50.9 mg, 88% yield, a white solid, mp. 162 - 163 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.37 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.33 (s, 1H), 7.77 – 7.70 (m, 1H), 7.64 (dd, *J* = 8.0, 4.7 Hz, 2H), 7.54 – 7.48 (m, 2H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.20 (t, *J* = 7.0 Hz, 1H), 7.12 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 2.3 Hz, 1H), 4.29 (t, *J* = 6.8 Hz, 2H), 3.26 (t, *J* = 6.7 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 161.17, 148.16, 146.79, 136.50, 134.21, 127.37, 127.18, 126.85, 126.68, 122.86, 122.38, 122.13, 119.76, 118.40, 111.57, 111.25, 47.59, 24.97.

3-Phenylquinazolin-4(3*H***)-one 33**^[4]: 32.9 mg, 74% yield, a white solid, mp. 139 – 140 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.28 (d, *J* = 7.8 Hz, 1H), 8.07 (s, 1H), 7.71 (q, *J* = 8.0 Hz, 2H), 7.50 – 7.37 (m, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 160.39, 147.54, 145.83, 137.19, 134.26, 129.32, 128.77, 127.31, 127.26, 126.81, 126.73, 122.04.

3-(*p***-Tolyl)quinazolin-4(3***H***)-one 34^[4]: 44.5 mg, 94% yield, a white solid, mp. 148 - 149 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.37 (d,** *J* **= 7.9 Hz, 1H), 8.12 (s, 1H), 7.84 - 7.73 (m, 2H), 7.55 (t,** *J* **= 7.4 Hz, 1H), 7.36 - 7.29 (m, 4H), 2.44 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.94, 147.92,**

146.32, 139.29, 134.90, 134.57, 130.28, 127.62, 127.58, 127.21, 126.76, 21.26.

3-(4-Methoxyphenyl)quinazolin-4(3*H***)-one 35**^[4]: 38.8 mg, 77% yield, a white solid, mp. 210 - 211 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.34 (d, *J* = 7.9 Hz, 1H), 8.10 (s, 1H), 7.83 – 7.69 (m, 2H), 7.53 (t, *J* = 7.9 Hz, 1H), 7.32 (d, *J* = 8.6 Hz, 2H), 7.03 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.96, 159.80, 147.81, 146.36, 134.43, 130.06, 128.06, 127.49, 127.46, 127.06, 122.27, 114.73, 55.53.

3-(4-Chlorophenyl)quinazolin-4(3*H***)-one 36**^[6]: 42.0 mg, 82% yield, a white solid, mp. 191 - 192 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.35 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.08 (s, 1H), 7.83 – 7.75 (m, 2H), 7.54 (dd, *J* = 16.9, 8.4 Hz, 3H), 7.38 (d, *J* = 8.7 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 160.57, 147.71, 145.52, 135.81, 135.11, 134.73, 129.82, 128.29, 127.80, 127.62, 127.13, 122.15.

3-(4-Bromophenyl)quinazolin-4(3*H***)-one 37**^[4]: 33.6 mg, 56% yield, a white solid, mp. 213 - 214 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.35 (s, 1H), 8.21 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.90 (t, *J* = 8.4 Hz, 1H), 7.77 (t, *J* = 9.3 Hz, 3H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.54 (d, *J* = 8.6 Hz, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 160.37, 148.16, 147.34, 137.32, 135.25, 132.63, 130.25, 127.98, 127.82, 126.93, 122.39, 122.31.

3-(Naphthalen-1-yl)quinazolin-4(3*H***)-one 38**^[6]: 36.5 mg, 67% yield, a white solid, mp. 97 - 99 °C. ¹H NMR (400 MHz, CDCl₃) δ 8.42 (d, *J* = 8.0 Hz, 1H), 8.11 (s, 1H), 8.04 (d, *J* = 8.3 Hz, 1H), 7.98 (d, *J* = 7.9 Hz, 1H), 7.85 (s, 2H), 7.65 – 7.49 (m, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 161.04, 148.09, 146.81, 134.70, 134.32, 134.00, 130.25, 129.67, 128.58, 127.74, 127.70, 127.65, 127.25, 126.91, 125.92, 125.43, 122.32, 121.96.

2-Phenylquinazolin-4(3*H***)-one 39**^[6]: 43.1 mg, 97% yield, a white solid, mp. 238 - 240 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.55 (s, 1H), 8.20 – 8.15 (m, 3H), 7.88 – 7.81 (m, 1H), 7.75 (d, *J* = 7.6 Hz, 1H), 7.63 – 7.49 (m, 4H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 162.80, 152.86, 149.14, 135.08, 133.20, 131.87, 129.09, 128.24, 127.90, 127.07, 126.33, 121.42.

2-(*p***-Tolyl)quinazolin-4(3***H***)-one 40^[6]: 43.0 mg, 91% yield, a white solid, mp. 245 - 246 °C. ¹H NMR (400 MHz, DMSO-***d***₆) δ 12.47 (s, 1H), 8.15 (dd,** *J* **= 7.9, 1.2 Hz, 1H), 8.10 (d,** *J* **= 8.2 Hz, 2H), 7.83 (t,** *J* **= 6.9 Hz, 1H), 7.73 (d,** *J* **= 7.7 Hz, 1H), 7.51 (t,** *J* **= 6.9 Hz, 1H), 7.36 (d,** *J* **= 8.0 Hz, 2H), 2.39 (s, 3H). ¹³C NMR (101 MHz, DMSO-***d***₆) δ 162.79, 152.74, 149.24, 141.94, 135.06, 130.35, 129.67, 128.15, 127.84, 126.88, 126.32, 121.33, 21.46.**

2-(*m***-Tolyl)quinazolin-4(3***H***)-one 41^[6]: 29.8 mg, 63% yield, a white solid, mp. 221 - 223 °C. ¹H NMR (400 MHz, DMSO-***d***₆) δ 12.48 (s, 1H), 8.16 (d,** *J* **= 7.9 Hz, 1H), 8.03 (s, 1H), 7.97 (d,** *J* **= 7.2 Hz, 1H), 7.84 (t,** *J* **= 6.9 Hz, 1H), 7.75 (d,** *J* **= 7.9 Hz, 1H), 7.52 (t,** *J* **= 7.0 Hz, 1H), 7.48 – 7.37 (m, 2H), 2.41 (s, 3H). ¹³C NMR (101 MHz, DMSO-***d***₆) δ 162.74, 152.91, 149.20, 138.40, 135.08, 133.11, 132.49, 128.99, 128.75, 127.89, 127.02, 126.32, 125.36, 121.41, 21.44.**

2-(o-Tolyl)quinazolin-4(3H)-one 42^[6]: 35.9 mg, 76% yield, a white solid, mp. 215 - 217 °C. ¹H

NMR (400 MHz, DMSO- d_6) δ 12.45 (s, 1H), 8.17 (d, J = 8.6 Hz, 1H), 7.84 (t, J = 7.6 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.53 (dd, J = 16.0, 7.7 Hz, 2H), 7.44 (t, J = 7.4 Hz, 1H), 7.39 – 7.33 (m, 2H), 2.39 (s, 3H). ¹³C NMR (101 MHz, DMSO- d_6) δ 162.26, 154.85, 149.19, 136.57, 134.96, 134.69, 131.00, 130.37, 129.59, 127.83, 127.13, 126.25, 126.17, 121.43, 20.02.

2-(4-Methoxyphenyl)quinazolin-4(3*H***)-one 43**^[6]: 43.4 mg, 86% yield, a white solid, mp. 249 – 251 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.41 (s, 1H), 8.19 (d, *J* = 8.9 Hz, 2H), 8.14 (d, *J* = 7.9 Hz, 1H), 7.86 – 7.78 (m, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 162.79, 162.34, 152.35, 149.40, 135.06, 129.94, 127.76, 126.64, 126.30, 125.26, 121.13, 114.48, 55.94.

2-(4-Fluorophenyl)quinazolin-4(3*H***)-one 44**^[6]: 41.3 mg, 86% yield, a white solid, mp. 286 - 288 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.58 (s, 1H), 8.25 (dd, *J* = 8.7, 5.5 Hz, 2H), 8.16 (d, *J* = 7.6 Hz, 1H), 7.84 (t, *J* = 7.6 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.39 (t, *J* = 8.8 Hz, 2H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 165.75, 163.01 (d, *J*_{C-F} = 53.1 Hz), 151.90, 149.05, 135.11, 130.84 (d, *J*_{C-F} = 9.0 Hz), 129.70 (d, *J*_{C-F} = 2.9 Hz), 127.86, 127.09, 126.33, 121.32, 116.10 (d, *J*_{C-F} = 21.9 Hz).

2-(4-Chlorophenyl)quinazolin-4(3*H***)-one 45**^[6]: 31.3 mg, 61% yield, a white solid, mp. 295 – 296 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.61 (s, 1H), 8.23 – 8.13 (m, 3H), 7.89 – 7.82 (m, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 8.7 Hz, 2H), 7.58 – 7.51 (m, 1H). ¹³C NMR (101 MHz, DMSO-*d*₆) δ 162.05, 152.11, 148.39, 134.34, 132.45, 131.13, 128.34, 127.49, 127.15, 126.32, 125.58, 120.68.

2-(Naphthalen-2-yl)quinazolin-4(3H)-one 46^[6]: 34.3 mg, 63% yield, a light yellow solid, mp.
249 - 250 °C. ¹H NMR (400 MHz, DMSO-d₆) δ 12.74 (s, 1H), 8.88 (s, 1H), 8.37 (d, J = 9.4 Hz, 1H), 8.25 (d, J = 7.7 Hz, 1H), 8.18 - 8.04 (m, 3H), 7.93 (t, J = 7.2 Hz, 1H), 7.87 (d, J = 7.9 Hz, 1H), 7.76 - 7.66 (m, 2H), 7.61 (t, J = 7.3 Hz, 1H). ¹³C NMR (101 MHz, DMSO-d₆) δ 162.72, 152.72, 149.25, 135.17, 134.61, 132.75, 130.42, 129.44, 128.67, 128.58, 128.42, 128.14, 128.04, 127.41, 127.18, 126.38, 124.97, 121.51.

N-(2-Benzoylphenyl)benzamide 48^[2]: 3.0 mg, < 5% yield, a white solid, mp. 81 - 82 °C. ¹H NMR (400 MHz, CDCl₃) δ 12.01 (s, 1H), 8.94 (d, *J* = 8.1 Hz, 1H), 8.10 (dd, *J* = 8.1, 1.8 Hz, 2H), 7.74 (d, *J* = 6.8 Hz, 2H), 7.70 - 7.48 (m, 8H), 7.22 - 7.05 (t, *J* = 7.3 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 200.36, 165.86, 141.19, 138.81, 134.70, 134.61, 134.10, 132.46, 132.09, 129.86, 128.87, 128.38, 127.45, 123.13, 122.21, 121.46.

Copies of product NMR spectra

4-Phenylquinazoline (3)

4-(4-Fluorophenyl)quinazoline (4)

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm)

-	1	-	1			-	· · ·					1	1		· · ·	-	1 1	1	 1		22 - 3	-	1	-	1	-		-	-	-	-	_		1	-	т
	10		0	-1	0	-20	-30	-40)	-50	-60	-7	70	-80	-90	f1	-100 (ppm))	-12	20		-1	140	1			160	0		-18	30		-2	00		

4-(4-Chlorophenyl)quinazoline (5)

4-(4-Bromophenyl)quinazoline (6)

4-Cyclohexylquinazoline (7)

Quinazoline (8)

160.22 -155.24 149.98 134.17 128.37 127.93 127.18 125.06

6-Chloro-4-phenylquinazoline (9)

6-Bromo-4-phenylquinazoline (10)

9.38 8.14 8.12 8.12 8.12 8.12 7.72 7.729 7.729 7.729 7.729 7.728 7.728 7.728 7.728 7.728 7.728 7.728 7.728 7.728 7.768

4-Phenyl-2-(p-tolyl)quinazoline (12)

130 120 110 100 90 f1 (ppm)

4-Phenyl-2-(*m*-tolyl)quinazoline (13)

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 f1 (ppm)

4-Phenyl-2-(o-tolyl)quinazoline (14)

2-(4-Methoxyphenyl)-4-phenylquinazoline (16)

¹H NMR

2-(4-Fluorophenyl)-4-phenylquinazoline (17)

90	60	30	0	-20	-50	-80	-110	-150	-190	-230	-270	
1.1.1.1.1.1	1000	1.5		1.	1000	ft	(ppm)	1.5556.00		1000		

2-(4-Chlorophenyl)-4-phenylquinazoline (18)

46	8	2228233328
88	29	22228888888888
-	-	
1		

2-(4-Bromophenyl)-4-phenylquinazoline (19)

8.55 8.57 8.57 8.15 8.15 8.15 8.15 7.92 7.29 7.29 7.28 7.28 7.28 7.28 7.28 7.28 7.28 7.26 7.76 7.56 7.55 7.55

2-(3,5-Dimethylphenyl)-4-phenylquinazoline (20)

2-(Naphthalen-1-yl)-4-phenylquinazoline (21)

~8.80 ~8.80 ~8.80 ~8.80 ~8.20 ~8.78 ~8.20 ~8.78 ~8.20 ~8.22 ~8.22 ~8.22 ~8.22 ~8.22 ~8.22 ~1.72 ~9.62 ~1.72 ~9.62 ~1.72 ~9.62 ~1.72 ~9.72

2-(Naphthalen-2-yl)-4-phenylquinazoline (22)

Quinazolin-4(3H)-one (23)

¹³C NMR

3-Methylquinazolin-4(3*H*)-one (24)

3-Butylquinazolin-4(3*H*)-one (25)

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

3-Allylquinazolin-4(3*H*)-one (26)

3-Cyclopropylquinazolin-4(3H)-one (27)

1.44 1.17 1.17 1.17 1.17 1.17 1.17 1.17	3.2
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3-Cyclohexylquinazolin-4(3*H*)-one (28)

3-Benzylquinazolin-4(3*H*)-one (29)

3-(Furan-2-ylmethyl)quinazolin-4(3*H*)-one (30)

¹³C NMR

f1 (ppm)

3-(Thiophen-2-ylmethyl)quinazolin-4(3H)-one (31)

¹³C NMR

-44.33

3-(2-(1*H*-Indol-3-yl)ethyl)quinazolin-4(3*H*)-one (32)

3-Phenylquinazolin-4(3*H*)-one (33)

3-(*p*-Tolyl)quinazolin-4(3*H*)-one (34)

3-(4-Methoxyphenyl)quinazolin-4(3*H*)-one (35)

-55.53

3-(4-Chlorophenyl)quinazolin-4(3H)-one (36)

3-(4-Bromophenyl)quinazolin-4(3*H*)-one (37)

90 80 f1 (ppm)

3-(Naphthalen-1-yl)quinazolin-4(3H)-one (38)

¹³C NMR

2-Phenylquinazolin-4(3*H*)-one (39)

0 180 100 90 f1 (ppm) 130 120

2-(*p*-Tolyl)quinazolin-4(3*H*)-one (40)

2-(o-Tolyl)quinazolin-4(3H)-one (42)

1H NMR

2-(4-Methoxyphenyl)quinazolin-4(3*H*)-one (43)

2-(4-Fluorophenyl)quinazolin-4(3H)-one (44)

2-(4-Chlorophenyl)quinazolin-4(3*H*)-one (45)

2-(Naphthalen-2-yl)quinazolin-4(3H)-one (46)

100 90 f1 (ppm)

N-(2-Benzoylphenyl)benzamide (48)

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