Supporting Information Renewable Energy-Driven Synthesis of Bioactive Quinolinones through Photocatalytic and Electrochemical Activation

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A. Instrumentation and Chemicals

All purchased reagents and solvents were used without further purification unless otherwise noted. All the raw material, catalyzed and additives were purchased from WuXi AppTec. The chemical shifts are referenced to signals at 7.26 and 77.0 ppm, respectively. TLC was performed by using commercially prepared 100-400 mesh silica gel plates and visualization was effected at 254 nm. ¹H and ¹³C NMR spectras were recorded using a Bruker DRX-500 spectrometer using CDCl₃, DMSO- d_6 or CD₃OD as solvent. Chemical shifts of ¹H NMR were reported relative to CDCl₃ (δ 7.26), DMSO- d_6 (δ 2.50) or CD₃OD (δ 3.31). Chemical shifts of ¹³C NMR were reported relative to CDCl₃ (δ 77.0), DMSO- d_6 (δ 39.52) or CD₃OD (δ 49.0). The data of HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). Melting points were determined with a Büchi Melting Point B-545 instrument.

B. Preparation of substrates

1. Synthetic procedure for the preparation of 1b-1h, 1j-1o



A mixture of 2-bromoaniline (1 mmol) and phenylboric acid (1 mmol), Cs_2CO_3 (3 mmol), PdCl₂(dppf)·CH₂Cl₂ (9.0 mol%) were added to the solvent THF 10 mL and H₂O 1mL, stirring at 110 °C reflux for 16 hours, cooling to room temperature after reaction, dilution with H₂O (30 mL), extraction with EtOAc (50 mL × 3). The combined organic extract was washed with saturated NaHCO₃, dried over anhydrous Na₂SO₄ and evaporated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding starting materials **1b-1o**.

2. Synthetic procedure for the preparation of 1q-1r



A mixture of 2-bromoaniline (1 mmol) and 1-Cyclopentenylboronic acid (1 mmol), Cs_2CO_3 (3 mmol), $PdCl_2(dppf) \cdot CH_2Cl_2$ (9.0mol%) were added to the solvent THF 10 mL and H_2O 1 mL, stirring at 110 °C reflux for 16 hours, cooling to room temperature after reaction, dilution with H_2O (30 mL), extraction with EtOAc (50 mL × 3). The combined organic extract was washed with saturated NaHCO₃, dried over anhydrous Na₂SO₄ and evaporated in vacuo. The residue was purified by column chromatography on silica gel to afford the corresponding starting materials **1q-1r**.

3. Synthetic procedure for the preparation of 1s-1ab



A mixture of aniline (5.5 mmol), phenylacetylene (3.0 mmol) and Mg (NTf₂)₂ (5 mol%) was added to 6 mL HFIP and stirred in an oil bath at 70 °C for 24 hours. After the reaction, filtration, concentration under reduced pressure. The residue was purified by column chromatography on silica gel to afford the corresponding starting materials **1s-1ab**.

4. Synthetic procedure for the preparation of 1i,1p



Methyl triphenyl phosphorus bromide was added to THF at 0 °C, and then KO'Bu was slowly added, and the mixture turned yellow after addition. Heat the mixture to room temperature and stir for 1 h. The reaction was cooled to 0 °C, and 2-aminobenzophenone was added to the mixture, Heat to room temperature and continue the reaction for 4 h. After the reaction, filtration, concentration under reduced pressure. The residue was purified by column chromatography on silica gel to afford the corresponding starting materials **1i**, **1p**.

C. Optimization of Reaction Conditions

NH ₂	Sunlight, 4 h CO ballon, Solvent Pd(OAc) ₂ (5 mol%) TBAB (0.8 equiv.), HOAc (1.0 equiv.)	
Entry	Solvent	Yield (%)
1	THF	40
2	DCM	63
3	DMF	0
4	DMSO	trace
5	EtOH	0
6	CH ₃ CN	87

Table S1 Solvent screening

^{*a*}Reaction conditions: **1a** (0.2 mmol), Pd(OAc)₂ (5 mol%), TBAB (0.8 equiv), HOAc (1.0 equiv), CH₃CN (3 mL), CO balloon, sunlight irradiation for 4 h at room temperature. ^{*b*}Isolated yield.

Table S2 Catalysts screening

	Sunlight, 4 h CO ballon, CH ₃ CN ★ Catalysts (5 mol %) TBAB (0.8 equiv.), HOAc (1.0 equiv.)	
Entry	Catalysts	Yield (%)
1	$Pd(TFA)_2$	33
2	PdCl ₂	0
3	Pd(PPh ₃)Cl ₂	0
4	Pd(PPh) ₄	54
5	Pd(OAc) ₂	87
6	Cu(OAc) ₂	0
7	CuCl ₂	0
8	FeCl ₃	0
9	Fe(NO ₃) ₃	0
10	NiCl ₂	0
11	Ni(OAc) ₂	0

^{*a*}Reaction conditions: **1a** (0.2 mmol), Pd(OAc)₂ (5 mol%), TBAB (0.8 equiv), HOAc (1.0 equiv), CH₃CN (3 mL), CO balloon, sunlight irradiation for 4 h at room temperature. ^{*b*}Isolated yield.

Table S3 additive screening



2	KI	80
3	TEAB	85
4	TBAI	71
5	NaCl	32
6	ⁿ Bu ₄ NOAc	10
7	KF	22
8	0.2 TBAB	23
9	0.4TBAB	48
10	0.6TBAB	73
11	0.8TBAB	87
12	1.0TBAB	88

^{*a*}Reaction conditions: **1a** (0.2 mmol), Pd(OAc)₂ (5 mol%), TBAB (0.8 equiv), HOAc (1.0 equiv), CH₃CN (3 mL), CO balloon, sunlight irradiation for 4 h at room temperature. ^{*b*}Isolated yield.

Table S4 base/acid screening



^{*a*}Reaction conditions: **1a** (0.1 mmol), Pd(OAc)₂ (5 mol%), TBAB (0.8 equiv), HOAc (1.0 equiv), CH₃CN (3 mL), CO balloon, sunlight irradiation for 4 h at room temperature. ^{*b*}Isolated yield.

D. Analytical data for the compounds

4-methylquinolin-2(1*H*)-one (2a)



Yield 27.8 mg (87%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.61 (s, 1H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 7.8 Hz, 1H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.19 (t, *J* = 7.7 Hz, 1H), 6.40 (s, 1H), 2.42 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.1, 148.4, 139.1, 130.8, 125.2, 122.1, 121.3, 120.1, 115.9, 18.9. HRMS (ESI): m/z calculated for C₁₀H₉NO requires 160.0757 for [M+H]⁺, found 160.0756.

4,6-dimethylquinolin-2(1*H*)-one (2b)



Yield 27.7 mg (80%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.53 (s, 1H), 7.49 (s, 1H), 7.33-7.30 (m, 1H), 7.21 (d, *J* = 8.3 Hz, 1H), 6.36 (s, 1H), 2.40 (s, 3H), 2.36 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.0, 148.1, 137.1, 131.9, 131.0, 124.8, 121.3, 120.0, 115.8, 21.1, 19.0. HRMS (ESI): m/z calculated for C₁₁H₁₁NO requires 174.0913 for [M+H]⁺, found 174.0922.

4,7-dimethylquinolin-2(1*H*)-one (2c)



Yield 25.3 mg (73%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.52 (s, 1H), 7.58 (d, *J* = 8.2 Hz, 1H), 7.09 (s, 1H), 7.02 (d, *J* = 8.3 Hz, 1H), 6.31 (s, 1H), 2.37 (d, *J* = 10.7 Hz, 6H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.6, 148.9, 141.1, 139.0, 125.1, 123.9, 119.9, 118.1, 115.8, 21.6, 18.9. HRMS (ESI): m/z calculated for C₁₁H₁₁NO requires 174.0913 for [M+H]⁺, found 174.0921.

4,8-dimethylquinolin-2(1H)-one (2d)



Yield 23.2 mg (67%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 10.69 (s, 1H), 7.55 (d, *J* = 9.7 Hz, 1H), 7.34 (d, *J* = 9.6 Hz, 1H), 7.15-7.06 (m, 1H), 6.41 (d, *J* = 8.2 Hz, 1H), 2.42 (s, 6H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.4, 148.9, 137.5, 132.1, 124.0, 123.2, 121.9, 121.1, 120.1, 19.3, 17.9. HRMS (ESI): m/z calculated for C₁₁H₁₁NO requires 174.0913 for [M+H]⁺, found 174.0922.

6-methoxy-4-methylquinolin-2(1*H*)-one (2e)



Yield 25.7 mg (68%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.52-11.48 (m, 1H), 7.26-7.23 (m, 1H), 7.17 (dd, J = 5.9, 3.1 Hz, 1H), 7.14-7.12 (m, 1H), 6.39 (d, J = 6.2 Hz, 1H), 3.81 (d, J = 6.1 Hz, 3H), 2.41 (d, J = 6.2 Hz, 3H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 161.7, 154.6, 148.0, 133.5, 121.7, 120.7, 119.5, 117.1, 107.2, 55.9, 19.1. HRMS (ESI): m/z calculated for C₁₁H₁₁NO₂ requires 190.0863 for [M+H]⁺, found 190.0871.

6-(tert-butyl)-4-methylquinolin-2(1H)-one (2f)



Yield 37.8 mg (88%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.53 (s, 1H), 7.59-7.57 (m, 2H), 7.26 (d, *J* = 8.5 Hz, 1H), 6.37 (s, 1H), 2.43 (s, 3H), 1.31 (d, *J* = 3.2 Hz, 9H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.1, 148.5, 144.4, 137.0, 128.6, 121.2, 120.6, 119.5, 115.8, 34.7, 31.6, 19.0. HRMS (ESI): m/z calculated for C₁₄H₁₇NO requires 216.1383 for [M+H]⁺, found 216.1392.

6-fluoro-4-methylquinolin-2(1*H*)-one (2g)



Yield 20.2 mg (57%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.68 (s, 1H), 7.51 (dd, J = 9.9, 2.9 Hz, 1H), 7.40 (td, J = 8.7, 2.9 Hz, 1H), 7.32 (dd, J = 9.1, 5.1 Hz, 1H), 6.46 (s, 1H), 2.40 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 161.8, 157.5 (d, $J_{C-F} = 236.3$ Hz), 147.9, 135.8, 122.4, 120.9 (d, $J_{C-F} = 8.8$ Hz), 118.7 (d, $J_{C-F} = 23.8$ Hz), 117.6 (d, $J_{C-F} = 8.8$ Hz), 110.5 ($J_{C-F} = 22.5$ Hz), 18.9. ¹⁹F NMR (471 MHz, DMSO- d_6) δ -120.85. HRMS (ESI): m/z calculated for C₁₀H₈FNO requires 178.0663 for [M+H]⁺, found 178.0671.

6-chloro-4-methylquinolin-2(1H)-one (2h)



Yield 22.8 mg (59%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.74 (s, 1H), 7.75-7.71 (m, 1H), 7.55 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.31 (d, *J* = 8.7 Hz, 1H), 6.46 (s, 1H), 2.41 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.9, 147.7, 137.9, 130.7, 126.2, 124.6, 122.4, 121.4, 117.7, 18.9. HRMS (ESI): m/z calculated for C₁₀H₈ClNO requires 194.0367 for [M+H]⁺, found 194.0376.

6-bromo-4-methylquinolin-2(1H)-one (2i)



Yield 31.8 mg (67%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.74 (s, 1H), 7.86-7.83 (m, 1H), 7.68-7.63 (m, 1H), 7.25 (d, J = 8.6 Hz, 1H), 6.44 (s, 1H), 2.41 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 161.9, 147.6, 138.2, 133.4, 127.5, 122.4, 121.9, 118.0, 114.0, 18.9. HRMS (ESI): m/z calculated for C₁₀H₈BrNO requires 237.9862 for [M+H]⁺, found 237.9871.

4-methyl-6-nitroquinolin-2(1*H*)-one (2j)



Yield 22.8 mg (56%, yellow solid); ¹H NMR (500 MHz, DMSO- d_6) δ 12.19 (s, 1H), 8.52-8.50 (m, 1H), 8.35 (dd, J = 9.0, 2.6 Hz, 1H), 7.44 (d, J = 9.1 Hz, 1H), 6.58 (s, 1H), 2.51 (s, 3H). ¹³C{¹H} NMR (125)

MHz, DMSO- d_6) δ 162.3, 148.8, 143.6, 142.0, 125.6, 122.9, 121.6, 119.7, 116.9, 18.7. HRMS (ESI): m/z calculated for C₁₀H₈N₂O₃ requires 205.0608 for [M+H]⁺, found 205.0617.

6-acetyl-4-methylquinolin-2(1H)-one (2k)



Yield 27.4 mg (68%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.88 (s, 1H), 8.23 (d, J = 2.0 Hz, 1H), 8.04 (dd, J = 8.8, 2.0 Hz, 1H), 7.35 (dd, J = 8.5, 1.7 Hz, 1H), 6.46 (s, 1H), 2.61 (d, J = 1.9 Hz, 3H), 2.48 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 197.1, 162.2, 148.9, 142.4, 130.9, 130.2, 126.3, 122.0, 119.5, 116.1, 27.0, 18.8. HRMS (ESI): m/z calculated for C₁₂H₁₁NO₂ requires 202.0863 for [M+H]⁺, found 202.0871.

methyl 4-methyl-2-oxo-1,2-dihydroquinoline-6-carboxylate (2l)



Yield 28.6 mg (66%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.92 (s, 1H), 8.23 (d, *J* = 2.0 Hz, 1H), 8.04-8.00 (m, 1H), 7.36 (dd, *J* = 8.5, 2.1 Hz, 1H), 6.48 (s, 1H), 3.87 (d, *J* = 2.0 Hz, 3H), 2.46 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 166.3, 162.2, 148.5, 142.5, 131.1, 126.9, 123.2, 122.2, 119.6, 116.2, 52.6, 18.8. HRMS (ESI): m/z calculated for C₁₂H₁₁NO₃ requires 218.0812 for [M+H]⁺, found 218.0820.

4-methyl-6-(trifluoromethyl)quinolin-2(1*H*)-one (2m)



Yield 26.3 mg (58%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.96 (s, 1H), 7.98 (s, 1H), 7.84-7.80 (m, 1H), 7.46 (d, J = 8.7 Hz, 1H), 6.52 (s, 1H), 2.48 (s, 3H). ¹³C NMR (125 MHz, DMSO) δ 162.1, 148.4, 141.7, 127.1 (d, $J_{C-F} = 2.5$ Hz), 125.9, 123.8, 122.7 (q, $J_{C-F} = 5.4$ Hz), 122.4, 119.7, 116.9, 18.8. ¹⁹F NMR (471 MHz, DMSO- d_6) δ -59.90. HRMS (ESI): m/z calculated for C₁₁H₈F₃NO requires 228.0631 for [M+H]⁺, found 228.0639.

4,6,7-trimethylquinolin-2(1*H*)-one (2n)



Yield 29.9 mg (80%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.43 (d, *J* = 8.2 Hz, 1H), 7.43 (d, *J* = 8.6 Hz, 1H), 7.05 (d, *J* = 8.5 Hz, 1H), 6.28 (d, *J* = 8.6 Hz, 1H), 2.37 (d, *J* = 8.5 Hz, 3H), 2.26 (d, *J* = 8.6 Hz, 6H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.1, 148.1, 140.0, 137.5, 130.4, 125.2, 120.3, 118.2, 116.2, 20.3, 19.5, 18.9. HRMS (ESI): m/z calculated for C₁₂H₁₃NO requires 188.1070 for [M+H]⁺, found 188.1079.

4-methylbenzo[h]quinolin-2(1H)-one (2o)



Yield 34.7 mg (83%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.04-11.85 (m, 1H), 8.88 (d, *J* = 8.1 Hz, 1H), 8.00-7.96 (m, 1H), 7.77 (d, *J* = 8.8 Hz, 1H), 7.70 – 7.61 (m, 3H), 6.55 (s, 1H), 2.53 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.7, 149.5, 135.9, 134.1, 128.8, 128.3, 127.0, 122.9, 122.5, 122.4, 122.1, 121.0, 116.1, 19.7. HRMS (ESI): m/z calculated for C₁₄H₁₁NO requires 210.0913 for [M+H]⁺, found 210.0921.

3,4-dimethylquinolin-2(1*H*)-one (2p)



Yield 14.2 mg (41%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.63 (s, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.43 (s, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.18 (d, *J* = 7.9 Hz, 1H), 2.40 (s, 3H), 2.12 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.3, 142.5, 137.5, 129.5, 127.1, 124.8, 122.0, 120.4, 115.5, 15.4, 13.1. HRMS (ESI): m/z calculated for C₁₁H₁₁NO requires 174.0913 for [M+H]⁺, found 174.0921.

1,2,3,5-tetrahydro-4*H*-cyclopenta[c]quinolin-4-one (2q)



Yield 17.4 mg (47%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.60 (s, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.17 (t, *J* = 7.5 Hz, 1H), 3.08 (t, *J* = 7.8 Hz, 2H), 2.76 (t, *J* = 7.5 Hz, 2H), 2.09 (p, *J* = 7.6 Hz, 2H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.0, 151.6, 139.3, 133.3, 129.8, 125.2, 122.1, 118.4, 115.7, 32.0, 30.8, 22.7. HRMS (ESI): m/z calculated for C₁₂H₁₁NO requires 186.0913 for [M+H]⁺, found 186.0921.

7,8,9,10-tetrahydrophenanthridin-6(5H)-one (2r)



Yield 31.9 mg (80%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.61 (s, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.43 (t, J = 7.7 Hz, 1H), 7.28 (d, J = 8.2 Hz, 1H), 7.17 (t, J = 7.7 Hz, 1H), 2.81 (s, 2H), 2.46 (s, 2H), 1.81-1.76 (m, 2H), 1.74-1.69 (m, 2H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 162.1, 143.1, 137.3, 129.4, 128.5, 123.7, 122.0, 120.0, 115.6, 25.3, 24.1, 22.0, 21.9. HRMS (ESI): m/z calculated for C₁₃H₁₃NO requires 200.1070 for [M+H]⁺, found 200.1079.

4-phenylquinolin-2(1*H*)-one (2s)



Yield 36.3 mg (82%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.91 (s, 1H), 7.54-7.40 (m, 8H), 7.13 (d, *J* = 7.4 Hz, 1H), 6.48-6.31 (m, 1H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.8, 152.0, 139.8, 137.2, 131.1, 129.3, 129.2, 129.2, 126.6, 122.4, 121.7, 118.8, 116.3. HRMS (ESI): m/z calculated for C₁₅H₁₁NO requires 222.0913 for [M+H]⁺, found 222.0922.

4-(p-tolyl)quinolin-2(1*H*)-one (2t)



Yield 36.2 mg (77%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.87 (s, 1H), 7.52 (t, *J* = 7.7 Hz, 1H), 7.43-7.38 (m, 2H), 7.37-7.30 (m, 4H), 7.13 (t, *J* = 7.6 Hz, 1H), 6.36 (d, *J* = 3.4 Hz, 1H), 2.39 (d, *J* = 3.7 Hz, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.8, 152.0, 139.8, 138.8, 134.3, 131.0, 129.7, 129.1, 126.7, 122.3, 121.5, 118.9, 116.3, 21.3. HRMS (ESI): m/z calculated for C₁₆H₁₃NO requires 236.1070 for [M+H]⁺, found 236.1079.

4-(m-tolyl)quinolin-2(1*H*)-one (2u)



Yield 40.4 mg (86%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.90 (s, 1H), 7.51 (t, J = 7.8 Hz, 1H), 7.42-7.36 (m, 3H), 7.30 (d, J = 7.6 Hz, 1H), 7.27-7.21 (m, 2H), 7.12 (t, J = 7.7 Hz, 1H), 6.37 (s, 1H), 2.37 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 161.9, 152.1, 139.8, 138.5, 137.1, 131.0, 129.8, 129.6, 129.0, 126.7, 126.2, 122.3, 121.5, 118.9, 116.3, 21.4. HRMS (ESI): m/z calculated for C₁₆H₁₃NO requires 236.1070 for [M+H]⁺, found 236.1078.

4-(o-tolyl)quinolin-2(1*H*)-one (2v)



Yield 36.7 mg (78%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.91 (s, 1H), 7.50 (t, J = 7.7 Hz, 1H), 7.43-7.34 (m, 3H), 7.31 (t, J = 7.2 Hz, 1H), 7.19 (d, J = 7.4 Hz, 1H), 7.07 (t, J = 7.6 Hz, 1H), 6.92 (d, J = 8.0 Hz, 1H), 6.33 (s, 1H), 2.04 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 162.0, 152.0, 139.5, 136.9, 135.5, 131.0, 130.6, 129.2, 129.0, 126.5, 126.4, 122.4, 121.8, 119.3, 116.2, 19.8. HRMS (ESI): m/z calculated for C₁₆H₁₃NO requires 236.1070 for [M+H]⁺, found 236.1079.

4-(4-fluorophenyl)quinolin-2(1H)-one (2w)



Yield 35.4 mg (74%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.92 (s, 1H), 7.52 (d, *J* = 7.1 Hz, 3H), 7.42-7.33 (m, 4H), 7.14 (t, *J* = 7.7 Hz, 1H), 6.41 (s, 1H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.8 (d, *J*_{*C*-*F*} = 245 Hz), 161.7, 150.9, 139.8, 133.5 (d, *J*_{*C*-*F*} = 3.8 Hz), 131.4 (d, *J*_{*C*-*F*} = 8.8 Hz), 131.1, 126.5, 122.2 (d, *J*_{*C*-*F*} = 56.3 Hz), 118.8, 116.3, 116.2, 116.0. ¹⁹F NMR (471 MHz, DMSO-*d*₆) δ -113.01. HRMS (ESI): m/z calculated for C₁₅H₁₀FNO requires 240.0819 for [M+H]⁺, found 240.0828. **4-(4-chlorophenyl)quinolin-2(1***H***)-one (2x)**





Yield 39.8 mg (78%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 11.93 (s, 1H), 7.59 (d, J = 7.5 Hz, 2H), 7.55-7.47 (m, 3H), 7.40 (d, J = 8.1 Hz, 1H), 7.34 (d, J = 8.0 Hz, 1H), 7.14 (t, J = 7.6 Hz, 1H), 6.42 (s, 1H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 161.7, 150.7, 139.8, 136.0, 134.1, 131.2, 131.1, 129.2, 126.5, 122.5, 122.0, 118.6, 116.3. HRMS (ESI): m/z calculated for C₁₅H₁₀ClNO requires 256.0524 for [M+H]⁺, found 256.0528.

4-(4-bromophenyl)quinolin-2(1*H*)-one (2y)



Yield 41.3 mg (69%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.93 (s, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.54 (t, *J* = 7.8 Hz, 1H), 7.42 (dd, *J* = 16.1, 8.3 Hz, 3H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.42 (s, 1H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.7, 150.8, 139.8, 136.3, 132.1, 131.4,

131.2, 126.5, 122.8, 122.5, 121.9, 118.5, 116.3. HRMS (ESI): m/z calculated for $C_{15}H_{10}BrNO$ requires 300.0019 for [M+H]⁺, found 300.0029.

6-methyl-4-phenylquinolin-2(1*H*)-one (2z)



Yield 29.1 mg (62%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.83 (s, 1H), 7.54 (p, *J* = 6.1 Hz, 3H), 7.46 (d, *J* = 6.2 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.31 (d, *J* = 8.3 Hz, 1H), 7.15 (s, 1H), 6.35 (s, 1H), 2.25 (s, 3H). ¹³C {¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.7, 151.8, 137.8, 137.3, 132.3, 131.3, 129.2, 129.2, 129.1, 126.0, 121.7, 118.8, 116.2, 21.1. HRMS (ESI): m/z calculated for C₁₆H₁₃NO requires 236.1070 for [M+H]⁺, found 236.1080.

4-([1,1'-biphenyl]-4-yl)quinolin-2(1*H*)-one (2aa)



Yield 30.3 mg (51%, white solid); mp 245.2-249.7 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.90 (s, 1H), 7.84 (d, *J* = 7.8 Hz, 2H), 7.77 (d, *J* = 7.6 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 3H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.43 (d, *J* = 7.6 Hz, 2H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.46 (s, 1H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.8, 151.6, 141.0, 139.9, 139.8, 136.2, 131.1, 129.9, 129.6, 128.3, 127.5, 127.3, 126.7, 122.4, 121.7, 118.8, 116.3. HRMS (ESI): m/z calculated for C₂₁H₁₅NO requires 298.1226 for [M+H]⁺, found 298.1228.

4-(phenanthren-9-yl)quinolin-2(1*H*)-one (2ab)



Yield 53.3 mg (83%, white solid); mp 162.5-165.1 °C. ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.03 (s, 1H), 8.95 (dd, *J* = 17.5, 8.3 Hz, 2H), 8.06 (d, *J* = 7.8 Hz, 1H), 7.90 (s, 1H), 7.79 (t, *J* = 7.7 Hz, 1H), 7.72 (q, *J* = 7.7 Hz, 2H), 7.52 (dq, *J* = 13.7, 7.3, 6.4 Hz, 3H), 7.46 (d, *J* = 8.3 Hz, 1H), 6.96 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 8.0 Hz, 1H), 6.61 (s, 1H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.0, 151.0, 139.4, 133.6, 131.3, 131.1, 130.4, 130.3, 130.1, 129.4, 128.1, 127.8, 127.8, 127.7, 127.7, 127.0, 126.7, 123.9, 123.4, 123.1, 122.4, 120.0, 116.2. HRMS (ESI): m/z calculated for C₂₃H₁₅NO requires 322.1226 for [M+H]⁺, found 322.1227.

pyrrolo[1,2-a]quinoxalin-4(5H)-one (2ah)



Yield 22.1 mg (60%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 11.27 (s, 1H), 8.09 (d, *J* = 2.6 Hz, 1H), 7.95 (d, *J* = 8.1 Hz, 1H), 7.30-7.25 (m, 2H), 7.20 (d, *J* = 7.8 Hz, 1H), 7.06 (d, *J* = 3.8 Hz, 1H), 6.68 (d, *J* = 3.3 Hz, 1H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 155.9, 128.6, 126.2, 123.5, 123.3, 123.0, 118.5, 117.0, 115.3, 113.5, 112.2. HRMS (ESI): m/z calculated for C₁₁H₈N₂O requires 185.0709 for [M+H]⁺, found 185.0718.

pyrazolo[1,5-a]quinoxalin-4(5H)-one (2ai)



Yield 27.4 mg (74%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 9.25 (s, 1H), 8.15 (s, 1H), 7.93 (d, J = 8.2 Hz, 1H), 7.80 (s, 1H), 7.48 (d, J = 6.3 Hz, 1H), 7.25-7.17 (m, 1H), 6.56 (d, J = 2.0 Hz, 1H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 153.2, 141.2, 132.3, 131.6, 131.6, 128.2, 124.9, 124.8, 124.4, 107.6. HRMS (ESI): m/z calculated for C₁₀H₇N₃O requires 186.0662 for [M+H]⁺, found 186.0659.

furo[3,4-c]quinolin-4(5H)-one (2aj)



Yield 11.1 mg (30%, white solid); ¹H NMR (500 MHz, DMSO-d₆) δ 11.92 (s, 1H), 8.26 (s, 1H), 8.02 (d,

J = 7.9 Hz, 1H), 7.51-7.40 (m, 3H), 7.28 (t, J = 7.5 Hz, 1H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 153.5, 149.7, 142.5, 137.2, 131.0, 129.0, 124.6, 122.6, 116.5, 115.7, 107.2. HRMS (ESI): m/z calculated for C₁₁H₇NO₂ requires 186.0550 for [M+H]⁺, found 186.0558.

benzo[j]phenanthridin-6(5H)-one (2ak)



Yield 32.4 mg (66%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 8.01 (s, 1H), 7.92 (d, J = 4.2 Hz, 3H), 7.88 (s, 1H), 7.56-7.50 (m, 2H), 7.49 (d, J = 8.3 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 7.31 (d, J = 7.7 Hz, 1H), 7.17 (t, J = 7.5 Hz, 1H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 153.8, 136.7, 136.5, 133.7, 133.4, 132.6, 130.9, 128.6, 128.5, 128.3, 128.3, 127.9, 127.8, 126.7, 126.7, 124.1, 124.0. HRMS (ESI): m/z calculated for C₁₇H₁₁NO requires 246.0913 for [M+H]⁺, found 246.0919.

phenanthridin-6(5H)-one (2A)



Yield 26.2 mg (67%, white solid); ¹H NMR (500 MHz, DMSO- d_6) δ 7.99 (s, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 7.40 (s, 1H), 7.38 (s, 1H), 7.36-7.29 (m, 1H), 7.23 (d, J = 7.7 Hz, 1H), 7.15 (t, J = 7.3 Hz, 1H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 154.0, 139.2, 136.1, 133.9, 130.8, 129.7, 129.5, 129.2, 128.2, 127.8, 124.8, 124.3, 118.4. HRMS (ESI): m/z calculated for C₁₃H₉NO requires 196.0757 for [M+H]+, found 196.0762.

6-chloro-4-phenylquinolin-2(1H)-one (2B)

Yield 31.2 mg (61%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 12.06 (s, 1H), 7.59-7.55 (m, 2H), 7.53 (d, *J* = 6.9 Hz, 2H), 7.46 (dd, *J* = 7.5, 1.9 Hz, 2H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.26 (d, *J* = 2.4 Hz, 1H), 6.46 (s, 1H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.6, 150.9, 138.5, 136.5, 131.0, 129.5, 129.4, 129.1, 126.3, 125.4, 122.9, 120.1, 118.3. HRMS (ESI): m/z calculated for $C_{15}H_{10}CINO$ requires 256.0524 for $[M+H]^+$, found 256.0532.

[1,3]dioxolo[4,5-j]phenanthridin-6(5H)-one (2C)



Yield 39.2 mg (82%, white solid); ¹H NMR (500 MHz, DMSO-*d*₆) δ 7.97 (s, 1H), 7.78 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.29 (dd, *J* = 7.8, 6.2 Hz, 1H), 7.11 (td, *J* = 7.4, 1.3 Hz, 1H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.91 (d, *J* = 1.7 Hz, 1H), 6.83 (dd, *J* = 8.0, 1.7 Hz, 1H), 6.06 (s, 2H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 153.9, 147.9, 147.1, 136.2, 133.5, 132.8, 130.7, 128.0, 124.2, 124.0, 123.1, 109.9, 109.1, 101.6. HRMS (ESI): m/z calculated for C₁₄H₉NO₃ requires 240.0655 for [M+H]⁺, found 240.0648.

(2-(prop-1-en-2-yl)phenyl)carbamic bromide (I)



white solid; ¹H NMR (500 MHz, DMSO- d_6) δ 8.23 (s, 1H), 7.76 (d, J = 8.2 Hz, 1H), 7.22 (t, J = 7.8 Hz, 1H), 7.14 (d, J = 7.5 Hz, 1H), 7.03 (t, J = 7.5 Hz, 1H), 5.29 (t, J = 1.8 Hz, 1H), 5.01 (d, J = 1.2 Hz, 1H), 2.04 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO- d_6) δ 153.6, 143.5, 135.9, 135.5, 128.7, 127.8, 123.5, 123.4, 117.3, 23.8. LCMS (ESI): m/z calculated for C₁₀H₁₀BrNO requires 240.0019 for [M+H]⁺, found 240.0018.

E. Copies of ¹H, ¹³C and ¹⁹F NMR Spectra for Compounds

¹H NMR spectrum of 2a (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2a (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2b (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2b (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2c (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2c (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2d (500 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2e (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2e (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2f (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2f (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2g (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2g (125 MHz, DMSO-*d*₆)



¹⁹F NMR spectrum of of 2g (125 MHz, DMSO-*d*₆)



0 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 fl (ppm)

¹H NMR spectrum of 2h (500 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2i (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2i (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2j (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2j (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2k (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2k (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2l (500 MHz, DMSO-*d*₆)



S31

¹H NMR spectrum of 2m (500 MHz, DMSO-*d*₆)



¹⁹F NMR spectrum of of 2m (125 MHz, DMSO-*d*₆)



) 10 0 −10 −20 −30 −40 −50 −60 −70 −80 −90 −100 −120 −130 −140 −150 −160 −170 −180 −190 −200 −210 f1 (ppm)

¹H NMR spectrum of 2n (500 MHz, DMSO-*d*₆)



110 100 fl (ppm)

¹H NMR spectrum of 20 (500 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2p (500 MHz, DMSO-*d*₆)



210 200 110 100 90 fl (ppm) ò

¹H NMR spectrum of 2q (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2q (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2r (500 MHz, DMSO-*d*₆)





¹H NMR spectrum of 2s (500 MHz, DMSO-*d*₆)





200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

¹H NMR spectrum of 2t (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2t (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2u (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2u (125 MHz, DMSO-*d*₆)





¹³C{¹H} NMR spectrum of 2v (125 MHz, DMSO-*d*₆)









¹⁹F NMR spectrum of of 2w (125 MHz, DMSO-*d*₆)



10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 fl (com)

¹H NMR spectrum of 2x (500 MHz, DMSO-*d*₆)





¹H NMR spectrum of 2y (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2y (125 MHz, DMSO-*d*₆)







¹H NMR spectrum of 2aa (500 MHz, DMSO-*d*₆)



¹³C{¹H} NMR spectrum of 2aa (125 MHz, DMSO-*d*₆)



¹H NMR spectrum of 2ab (500 MHz, DMSO-*d*₆)



110 100 fl (ppm) -10 Ó



¹³C{¹H} NMR spectrum of 2ah (125 MHz, DMSO-*d*₆)



S50

¹H NMR spectrum of 2ai (500 MHz, DMSO-d₆)



¹H NMR spectrum of 2aj (500 MHz, DMSO-*d*₆)









¹³C{¹H} NMR spectrum of 2A (125 MHz, DMSO-*d*₆)





¹H NMR spectrum of 2B (500 MHz, DMSO-*d*₆)



S56





200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0