Supporting Information

External Photocatalysts-free Visible Light Induced Aerobic Oxidation and 1, 4-

Bisfunctionalization of N-Alkyl isoquinolinium/quinolinium Salts

Youkang Zhou^a, Wei Liu^{a,b}, Zhiming Xing^a, Jiali Guan^a, Zhibin Song^{a,*}, and Yiyuan

Peng^a

^a Key Laboratory of Functional Small Organic Molecules, Ministry of Education,

College of Chemistry and Chemical Engineering, Jiangxi Normal University,

Nanchang 330022, China; E-mail: zbsong@jxnu.edu.cn; djtao@jxnu.edu.cn

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Gram scale: 1aa (7 mmol, 1.898 g), base. (10.5 mmol, 3.421g), solvent (175 mL), AT: ambient temperature (\approx 40 $^{\circ}C$)

| Figure | S1. A | Apparatus | and s | scalable | visible | light | induced | synthesis | of isoc | minolo | one 3 | a |
|----------|-------|-----------|-------|----------|---------|--------|---------|-------------|---------|--------|--------------|---|
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| N ⁺ I | RT, Cs ₂ (Solv | CO ₃ , Air, I ₂ √ent | N O 5a |
|---------------------|-------------------------------|---|--------------|
| Entry | Solvent | Cs ₂ CO ₃ | Yield |
| | | (eq) | a |
| 1 ^b | THF | 1.5 | 57% |
| 2 | THF | 1.5 | 35% |
| 3 | THF | 2 | 36% |
| 4 | THF | 4 | 45% |
| 5 | THF | 6 | 56% |
| 6 | THF | 8 | 62% |
| 7 | CH ₃ CN | 8 | 42% |
| 8 | Toluen | 8 | 59% |
| | e | | |
| 9 | DCE | 8 | 68% |
| 10 ^{с,е} | DCE | 8 | 74% |
| 11 ^d | DCE | 8 | 69% |
| 12 ^{b,c} | DCE | 1.5 | 74% |

Table S1. Optimization of the reaction conditions for synthesis of benzimidazole.^a

Reaction conditions: 1aa (0.2 mmol), Cs_2CO_3 (1.5 - 8 equiv.), I_2 (0.6 mmol, 3 equiv.), Solvent (5.0 mL), Reaction time: 5 hours under daylight and air atmosphere, RT: room temperature (\approx 25 °C) ^a Isolated yield. ^b Radiation for 5 hours under 20 W Blue LEDs and air atmosphere, AT: ambient temperature (\approx 50 °C). ^c DCE (2.0 mL). ^d Gram scale: 1aa (5 mmol, 1.356 g), Cs_2CO_3 (40 mmol, 13.032g), I_2 (15 mmol, 3.807g), DCE (50 mL), Yield=69% (0.983 g). ^e no light.



Figure S2 ESI-MS spectrum of 3a from the reaction in presence of H₂O¹⁸



Figure S3 ESI-MS spectrum of 5a from the reaction in presence of H₂O¹⁸

| N ⁺ Br [−] | + NBS | AT, B Solv | Br O So | |
|-----------------------------------|--------|---------------|---------------------------------|-------|
| Entry | Solven | NBS | Cs ₂ CO ₃ | Yield |
| | t | (eq.) | (eq.) | а |
| 1 | THF | 1.5 | 1.5 | 17% |
| 2 | DCE | 1.5 | 1.5 | 12% |
| 3 | MeCN | 1.5 | 1.5 | Trace |
| 4 | THF | 2 | 1.5 | 19% |
| 5 | THF | 3 | 1.5 | 19% |
| 6 | THF | 3 | 2 | 20% |
| 7 | THF | 3 | 4 | 26% |
| 8 ^b | THF | | 4 | Trace |
| 9 | THF | 3 | 6 | 23% |
| 10 | THF | 3 | 8 | 25% |
| 11° | THF | 3 | 8 | Trace |

Table S2. Optimization of the reaction conditions for synthesis of 4-bromo-2-propylisoquinolin-1(2H)-one (**5q**).^a

Reaction conditions: 1r (0.2 mmol), Cs_2CO_3 (1.5-8 equiv.), Solvent (5.0 mL), Radiation for 5 hours under 20 W Blue LEDs and air atmosphere, AT: ambient temperature (\approx 50 °C); ^a Isolated yield. ^bBr₂(3 eq.) replaces NBS. ^c Under no-light conditions.



Figure S4. The absorption spectra of isoquinolinium salt 1aa (10 μ M) in THF



Figure S5. The emission spectrum of **1aa** in THF (10 μ M, λ_{Ex} = 450 nm);



Figure S6. The absorption spectra of isoquinolinium salt **1aa** (10 μ M) and PDI (10 μ M) in THF under visible light irradiation (blue LED 20W)

General methods

All reagents were purchased from standard suppliers (Sigma-Aldrich, Alfa Aesar, or TCI) and were used without further purification. THF was distilled over sodium. Column chromatography was conducted with silica gel (mesh 200-300) from the Qingdao Ocean Chemicals. The ESI-MS spectra were recorded by a Finnigan 8230 instrument. High resolution mass spectrometry (HRMS) spectra analysis was performed by electrospray ionization (ESI-microTOF). Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance 400 spectrometer at 25 °C operating at 400 MHz for ¹H-NMR and 100 MHz for ¹³C-NMR by using CDCl₃ or DMSO-*d*₆ as solvents and TMS as an internal standard. Data are reported as following: chemical shift, multiplicity (s = singlet, d = doublet, m = multiplet, br = broad signal), coupling constant (Hz), and integration. The UV-Vis Spectra has been recorded on a Shimadazu UV 3100 UV-Vis spectrometer. The steady fluorescence spectra have been recorded on a Horiba FluoMax-plus spectrometer. Electron paramagnetic resonance (EPR) spectra were recorded on a Bruker EMXplus-9.5/12 spectrometer under visible light irradiation using mercury lamp.

Experimental Procedures

General procedure for the preparation of isoquinolinium iodide or bromide salts



Using **1aa** as example, isoquinoline (5 mmol, 645.7 mg), CH_3I (10 mmol, 2.0 eq.) and CH_3CN (15 mL) were added to a pressure round-bottom flask. The reaction mixture was stirred at 90 °C with oil bath for 12 hours. After cooled to room temperature, the isoquinoline salt was precipitated by adding ethyl acetate. The pure product was obtained through filtration, washing with ethyl acetate and drying.

General procedure for the preparation of isoquinolinium tetrafluoroborate salts (1ab and 2fb)

The round-bottom flask was charged with iodide salt **1aa** (1 mmol, 271.1 mg) or **2aa** (1 mmol, 397.3 mg), $AgBF_4$ (1 mmol, 194.7 mg) and ethanol (10 ml). The reaction mixture was stirred at room temperature for 30 min. After filtering out the precipitate, the filtrate was collected. The pure product was obtained by drying under vacuum.

General procedure for the preparation of isoquinolones and quinolones





Reaction conditions: 1 or 2 (0.2 mmol), Cs_2CO_3 (0.3 mmol, 1.5 equiv.), THF (5.0 mL), Radiation for 5-12 hours under 20 W Blue LEDs and air atmosphere, ambient temperature (\approx 50 °C), Isolated yield.

Using **3a** as example, a 50 ml test tube was charged with **1aa** (0.2 mmol, 54.3 mg), Cs_2CO_3 (0.3 mmol, 97.8 mg, 1.5 eq) and THF (5 mL) with light irradiation by blue LEDs (20 W). The reaction mixture was stirred for 5 h under air. When the reaction was complete, the reaction mixture was filtered. The filtrate was collected. The pure product was obtained by column chromatography on silica gel (petroleum ether/ethyl acetate).

General procedure for the preparation of 4-iodoisoquinolinones 5



Using **5a** as example, a 10 ml test tube was charged with **1aa** (0.2 mmol, 54.3 mg), I_2 (0.6 mmol, 152.3 mg, 3 eq.), Cs_2CO_3 (1.6 mmol, 521.3 mg, 8 eq) and DCE (2 mL). The reaction mixture was stirred for 5 h under air. When the reaction was complete, the reaction mixture was poured into the saturated solution of $Na_2S_2O_3$ (15 ml) and allowed to stir for 15 min. Then, the reaction mixture was extracted with ethyl acetate for three times. The combined organic phase was dried with anhydrous MgSO₄. The pure product was obtained by column chromatography on silica gel (petroleum ether/ethyl acetate).

Procedure for the preparation of 4-iodoisoquinolinones 5q from isoquinolinium bromide salt 1r



A 50 ml test tube was charged with 1r (0.2 mmol, 50.5 mg), *N*-Bromosuccinimide (0.6 mmol, 106.8 mg, 3 eq.), Cs₂CO₃ (0.8 mmol, 260.6 mg, 4 eq) and THF (5 mL) with light irradiation by blue LEDs (20 W). The reaction mixture was stirred for 5 h under air. When the reaction was complete, the reaction mixture was filtered. The filtrate was collected. The pure product was obtained by column chromatography on silica gel (petroleum ether/ethyl acetate).

NMR data for isoquinolinium/quinolinium salts and products 2-methylisoquinolin-2-ium iodide (1aa)



Yellow solid; 1.220 g in 5 mmol scale, 90 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.06 (s, 1 H), 8.73 (dd, J = 6.8, 1.1 Hz, 1 H), 8.60 (d, J = 6.8 Hz, 1 H), 8.50 (d, J = 8.3 Hz, 1 H), 8.37 (d, J

= 8.3 Hz, 1 H), 8.32-8.20 (m, 1 H), 8.15-8.00 (m, 1 H), 4.50 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.1, 137.2, 137.1, 136.4, 131.6, 130.6, 127.7, 127.5, 125.9, 48.4 ppm; HRMS [M+H]⁺ calculated for C₁₀H₁₀N⁺: 140.0808, found: 140.0808.

2-methylisoquinolin-2-ium tetrafluoroborate (1ab)



Grey solid; 0.189 g in 1 mmol scale, 82 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.97 (s, 1 H), 8.69 (d, J = 6.7 Hz, 1 H), 8.56 (d, J = 6.8 Hz, 1 H), 8.47 (d, J = 8.3 Hz, 1 H), 8.34 (d, J =

8.3 Hz, 1 H), 8.25 (t, J = 7.3 Hz, 1 H), 8.07 (t, J = 7.6 Hz, 1 H), 4.48 (s, 3H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 151.1$, 137.2, 137.1, 136.3, 131.6, 130.6, 127.7, 127.5, 125.9, 48.4 ppm; HRMS [M+H]⁺ calculated for C₁₀H₁₀N⁺: 140.0808, found: 140.0807.

6-methoxy-2-methylisoquinolin-2-ium iodide (1b)



Light yellow solid;1.309 g in 5 mmol scale, 87 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.78 (s, 1 H), 8.57 (d, *J* = 6.7 Hz, 1 H), 8.36 (dd, *J* = 11.0, 8.1 Hz, 2 H), 7.76 (d, *J* = 2.1 Hz, 1 H), 7.66 (dd, *J* = 9.1, 2.3 Hz, 1 H), 4.39 (s, 3 H), 4.06 (s, 3 H) ppm; ¹³C

NMR (100 MHz, DMSO- d_{δ}) δ = 165.8, 149.2, 140.1, 136.6, 132.5, 124.4, 124.0, 122.9, 106.3, 57.1, 47.7 ppm; HRMS [M+H]⁺ calculated for C₁₁H₁₂ON⁺: 174.0913, found: 174.0913.

6-chloro-2-methylisoquinolin-2-ium iodide (1c)



Yellow solid; 1.360 g in 5 mmol scale, 89 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.06 (s, 1 H), 8.76 (d, J = 6.8 Hz, 1 H), 8.52 (dd, J = 7.6, 4.0 Hz, 3 H), 8.11 (dd, J = 8.9, 1.7 Hz, 1 H), 4.48 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.2,

142.2, 138.0, 137.5, 132.8, 132.3, 126.8, 126.1, 125.0, 48.6 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_9ClN^+$: 178.0418, found: 178.0419.

6-bromo-2-methylisoquinolin-2-ium iodide (1d)



Yellow solid; 1.523 g in 5 mmol scale, 87 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.05 (s, 1 H), 8.75 (d, J = 6.8 Hz, 1 H), 8.70 (s, 1 H), 8.50 (d, J = 6.8 Hz, 1 H), 8.43 (d, J = 8.8 Hz, 1 H), 8.23-8.21 (m, 1 H), 4.46 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.4, 138.0, 137.5, 134.9, 132.5, 131.8, 130.0,

126.3, 124.9, 48.6 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_9BrN^+$: 221.9913, found: 221.9911.

2-benzylisoquinolin-2-ium bromide (1e)



White solid; 1.260 g in 5 mmol scale, 84 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.41 (s, 1 H), 8.89 (d, J = 6.8 Hz, 1 H), 8.63 (d, J = 6.8 Hz, 1 H), 8.56 (d, J = 8.3 Hz, 1 H), 8.38 (d, J = 8.3 Hz, 1 H), 8.29 (t, J = 7.6 Hz, 1 H), 8.10

(t, J = 7.6 Hz, 1 H), 7.63 (d, J = 6.4 Hz, 2 H), 7.49-7.43 (m, 3 H), 6.03 (s, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 150.7$, 137.6, 137.6, 135.3, 134.8, 131.8, 131.1, 129.8, 129.6, 129.4, 127.9, 127.8,126.8, 63.8 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₄N⁺: 220.1121, found: 220.1123.

2-butylisoquinolin-2-ium iodide (1f)



Yellow solid; 1.393 g in 5 mmol scale, 89 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.17 (s, 1H), 8.85 (d, J = 6.7 Hz, 1 H), 8.64 (d, J = 6.8 Hz, 1 H), 8.52 (d, J = 8.3 Hz, 1 H), 8.38 (d, J = 8.3 Hz, 1 H), 8.28 (t, J = 7.5 Hz, 1H), 8.10 (t,

J = 7.6 Hz, 1 H), 4.76 (t, J = 7.4 Hz, 2 H), 2.07-2.00 (m, 2 H), 1.42-1.32 (m, 2 H), 0.95 (t, J = 7.4 Hz, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 150.4$, 137.4, 137.3, 135.4, 131.7, 130.8, 127.8, 127.7, 126.3, 61.0, 32.9, 19.3, 13.9 ppm; HRMS [M+H]⁺ calculated for C₁₃H₁₆N⁺: 186,1277, found: 186,1278.

2-(naphthalen-1-ylmethyl)isoquinolin-2-ium bromide (1g)



White solid; 1.365 g in 5 mmol scale, 78 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.35 (s, 1 H), 8.86 (dd, J = 6.8, 1.1 Hz, 1 H), 8.64 (d, J = 6.8 Hz, 1 H), 8.58 (d, J= 8.3 Hz, 1H), 8.39 (d, J = 8.3 Hz, 1 H), 8.31-8.27 (m, 1 H), 8.23 (d, J = 7.9 Hz, 1 H), 8.08 (td, J = 8.3, 1.3 Hz, 3

H), 7.67-7.59 (m, 4 H), 6.58 (s, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 150.7, 137.7, 137.7, 135.4, 134.0, 131.8, 131.2, 131.0, 130.6, 130.0, 129.5, 129.0, 128.0, 127.8, 127.8, 127.1, 126.7, 126.2, 123.4, 61.6 ppm; HRMS [M+H]⁺ calculated for C₂₀H₁₆N⁺: 270.1277, found: 270.1273.

2-(4-nitrobenzyl)isoquinolin-2-ium bromide (1h)



White solid; 1.466 g in 5 mmol scale, 85 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.46 (s, 1 H), 8.93 (dd, J = 6.8, 1.2 Hz, 1 H), 8.69 (d, J = 6.8 Hz, 1 H), 8.58 (d, J = 8.3 Hz, 1 H), 8.41 (d, J = 8.2 Hz, 1 H), 8.34-8.29 (m,

3 H), 8.13 (dd, J = 11.3, 4.0 Hz, 1 H), 7.90 (d, J = 8.7 Hz, 2 H), 6.24 (s, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 151.3$, 148.4, 141.8, 137.8, 137.7, 135.4, 131.9, 131.2, 130.7, 127.9, 127.8, 126.9, 124.6, 62.5 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₃O₂N₂⁺: 265.0972, found: 265.0973.

2-methyl-6-phenylisoquinolin-2-ium iodide (1i)



Yellow solid; 1.492 g in 5 mmol scale, 86 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.02 (s, 1 H), 8.72-8.68 (m, 2 H), 8.56 (dd, J = 7.7, 4.2 Hz, 2 H), 8.42 (dd, J = 8.7, 1.6 Hz, 1H), 7.99-7.97 (m, 2H), 7.63 (dd, J = 10.0, 4.6 Hz, 2 H), 7.58-7.55 (m, 1 H), 4.50 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 150.6, 147.9, 138.1, 137.7, 136.7, 131.3, 130.6, 130.2,

129.9, 128.3, 126.6, 125.9, 124.7, 48.4 ppm; HRMS $[M+H]^+$ calculated for $C_{16}H_{14}N^+$: 220.1121, found: 220.1124.

2-(4-bromobenzyl)isoquinolin-2-ium bromide (1j)



White solid; 1.497 g in 5 mmol scale, 79 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ 10.38 (s, 1 H), 8.88 (dd, J = 6.8, 1.2 Hz, 1 H), 8.64 (d, J = 6.8 Hz, 1 H), 8.56 (d, J = 8.3 Hz, 1 H), 8.38 (d, J = 8.3 Hz, 1 H), 8.31-8.27 (m, 1 H),

8.11 (t, J = 7.6 Hz, 1 H), 7.73-7.64 (m, 2 H), 7.61 (d, J = 8.5 Hz, 2 H), 6.03 (s, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ 150.8, 137.7, 137.6, 135.3, 134.1, 132.6, 131.8, 131.7, 131.1, 127.9, 127.8, 126.8, 123.3, 62.9 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₃BrN⁺: 298.0226, found: 298.0231.

2-(3-chlorobenzyl)isoquinolin-2-ium bromide (1k)



White solid; 1.236 g in 5 mmol scale, 74 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.46 (s, 1 H), 8.93 (dd, J = 6.8, 1.3 Hz, 1 H), 8.66 (d, J = 6.8 Hz, 1 H), 8.57 (d, J = 8.3 Hz, 1 H), 8.39 (d, J = 8.2 Hz, 1 H), 8.34-8.25 (m, 1

H), 8.14-8.10 (m, 1 H), 7.84 (s, 1 H), 7.66-7.63 (m, 1 H), 7.53-7.48 (m, 2 H), 6.08 (s, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.0, 137.7, 137.6, 136.9, 135.2, 134.1, 131.8, 131.5, 131.2, 129.8, 129.5, 128.3, 127.8, 126.8, 62.8 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₃ClN⁺: 254.0731, found: 254.0729.

2-(2-bromobenzyl)isoquinolin-2-ium bromide (11)



White solid; 1.440 g in 5 mmol scale, 76 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.28 (s, 1 H), 8.79 (dd, J = 6.8, 1.3 Hz, 1 H), 8.68 (d, J = 6.8 Hz, 1 H), 8.61 (d, J = 8.3 Hz, 1 H), 8.42 (d, J = 8.2 Hz, 1 H), 8.34-8.30 (m, 1 H), 8.14-8.10 (m, 1 H), 7.79 (dd, J = 7.8, 0.8 Hz, 1 H), 7.54-7.42 (m, 3 H),

6.15 (s, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.3, 137.9, 137.8, 135.5, 133.9, 133.6, 132.1, 132.0, 131.9, 131.3, 129.2, 127.9, 127.7, 126.7, 124.0, 63.8 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₃BrN⁺: 298.0226, found: 298.0222.

2,2'-(butane-1,4-diyl)bis(isoquinolin-2-ium) iodide (1m)



Light yellow solid; 1.789 g in 5 mmol scale, 63 % yield; ¹H NMR (400 MHz, DMSO- d_{δ}) δ = 10.15 (s, 1 H), 8.82 (dd, J = 6.8, 1.0 Hz, 1 H), 8.63 (d, J = 6.8 Hz, 1 H), 8.49 (d, J = 8.2 Hz, 1 H), 8.37 (d, J = 8.2 Hz, 1

H), 8.30-8.26 (m, 1 H), 8.11-8.07 (m, 1 H), 4.79 (d, J = 23.4 Hz, 2 H), 2.12 (d, J = 27.8 Hz, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 150.6$, 137.5, 137.4, 135.4, 131.7, 130.9, 127.8, 127.7, 126.4, 60.5, 27.5 ppm; HRMS [M+H]⁺ calculated for $C_{22}H_{22}N_2^{2+}$: 314.1772, found: 314.1773.

2-(4-(tert-butyl)benzyl)isoquinolin-2-ium bromide (1n)



White solid; 1.317 g in 5 mmol scale, 74 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.43 (s, 1 H), 8.91 (dd, J = 6.8, 1.1 Hz, 1 H), 8.63 (d, J = 6.8 Hz, 1 H), 8.57 (d, J = 8.3 Hz, 1 H), 8.37 (d, J = 8.3 Hz, 1 H), 8.29 (dd, J = 11.2, 4.0 Hz, 1 H), 8.10 (t, J = 7.6 Hz, 1

H), 7.58 (d, J = 8.3 Hz, 2 H), 7.47 (d, J = 8.3 Hz, 2 H), 6.00 (s, 2 H), 1.26 (s, 9 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 152.4$, 150.6, 137.6, 137.5, 135.3, 132.0, 131.8, 131.1, 129.2, 127.9, 127.8, 126.8, 126.4, 63.5, 34.9, 31.4 ppm; HRMS [M+H]⁺ calculated for C₂₀H₂₂N⁺: 276.1747, found: 276.1748.

2-(3-phenylpropyl)isoquinolin-2-ium bromide (10)



Light yellow oil; 1.115 g in 5 mmol scale, 68 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.28 (s, 1 H), 8.92 (dd, J = 6.8, 1.2 Hz, 1 H), 8.63 (d, J = 6.8 Hz, 1 H), 8.52 (d, J = 8.2 Hz, 1 H), 8.38 (d, J = 8.3 Hz, 1 H),

8.29-8.25 (m, 1 H), 8.11-8.07 (m, 1 H), 7.25 (s, 4 H), 7.18-7.13 (m, 1 H), 4.86 (t, J = 7.3 Hz, 2 H), 2.77-2.73 (m, 2 H), 2.53-2.37 (m, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta =$ 150.6, 140.8, 137.4, 137.2, 135.4, 131.5, 130.8, 128.8, 128.7, 127.7, 127.6, 126.5, 126.3, 61.0, 32.3, 32.2 ppm; HRMS [M+H]⁺ calculated for C₁₈H₁₈N⁺: 248.1434, found: 248.1430.

4-bromo-2-methylisoquinolin-2-ium iodide (1p)



Yellow solid; 1.540 g in 5 mmol scale, 88 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.12 (s, 1 H), 9.24 (s, 1 H), 8.57 (d, J = 8.2 Hz, 1 H), 8.44-8.37 (m, 2 H), 8.18 (t, J = 7.4 Hz, 1 H), 4.47 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.2, 139.0, 137.7, 135.9, 132.5, 131.8, 127.7, 126.3, 121.4, 48.4 ppm; HRMS [M+H]⁺

calculated for C₁₀H₉BrN⁺: 221.9913, found: 221.9913.

2-methyl-4-phenylisoquinolin-2-ium iodide (1q)



Yellow solid; 1.388 g in 5 mmol scale, 80 % yield; ¹H NMR (400 MHz, DMSO- d_6) $\delta = 10.08$ (s, 1 H), 8.80 (d, J = 1.1 Hz, 1 H), 8.59 (d, J = 8.2 Hz, 1 H), 8.26 (ddd, J = 8.3, 7.1, 1.2 Hz, 1 H), 8.11 (dd, J = 15.8, 7.8 Hz, 2 H), 7.72-7.64 (m, 5 H), 4.54 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 150.1$, 137.9, 137.7, 135.7, 135.5, 133.5, 131.5, 131.4, 130.5, 130.1, 129.7, 127.9, 125.4, 48.4 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₄N⁺: 220.1121, found:

220.1118.

2-propylisoquinolin-2-ium bromide (1r)



Light yellow solid; 0.932 g in 5 mmol scale, 74 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.29 (s, 1 H), 8.89 (d, J = 6.8 Hz, 1 H), 8.64 (d, J = 6.8 Hz, 1 H), 8.51 (d, J = 8.3 Hz, 1 H), 8.37 (d, J = 8.3 Hz, 1 H), 8.25 (t, J = 7.6 Hz, 1 H), 8.07 (t, J = 7.6 Hz, 1 H), 4.74 (t, J = 7.3 Hz, 2 H), 2.05 (dd, J = 14.6,

7.3 Hz, 2 H), 0.92 (t, J = 7.4 Hz, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 150.5$, 137.4, 137.3, 135.4, 131.6, 130.9, 127.8, 127.7, 126.3, 62.4, 24.4, 10.8 ppm; HRMS [M+H]⁺ calculated for C₁₂H₁₄N⁺: 172.1121, found: 172.1123.

2-pentylisoquinolin-2-ium bromide (1s)



Yellow solid; 1.078 g in 5 mmol scale, 77 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.28 (s, 1 H), 8.91 (dd, J = 6.8, 1.0 Hz, 1 H), 8.66 (d, J = 6.8 Hz, 1 H), 8.54 (d, J= 8.3 Hz, 1 H), 8.40 (d, J = 8.3 Hz, 1 H), 8.31-8.27 (m, 1 H), 8.10 (t, J = 7.6 Hz, 1 H), 4.78 (t, J = 7.4 Hz, 2 H),

2.09-2.02 (m, 2 H), 1.38-1.30 (m, 4 H), 0.88 (t, J = 6.9 Hz, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 150.4$, 137.4, 137.3, 135.4, 131.6, 130.8, 127.8, 127.7, 126.3, 61.1, 30.7, 28.1, 22.1, 14.2 ppm; HRMS [M+H]⁺ calculated for C₁₄H₁₈N⁺: 200.1434, found: 200.1439.

1-methylquinolin-1-ium iodide (2a)



Yellow solid; 1.192 g in 5 mmol scale, 88 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.05 (s, 1 H), 8.72 (d, J = 6.7 Hz, 1 H), 8.59 (d, J = 6.7 Hz, 1 H), 8.49 (d, J = 8.3 Hz, 1 H), 8.36 (d, J = 8.3 Hz, 1 H), 8.26 (t, J = 7.6 Hz, 1 H), 8.08 (t, J = 7.6 Hz, 1 H), 4.50 (s, 3 H) ppm; ¹³C

NMR (100 MHz, DMSO- d_6) $\delta = 151.1$, 137.2, 137.1, 136.4, 131.6, 130.6, 127.7, 127.5,125.9, 48.5 ppm; HRMS [M+H]⁺ calculated for C₁₀H₁₀N⁺: 140.0808, found: 140.0810.

6-bromo-1-methylquinolin-1-ium iodide (2b)



Yellow solid; 1.505 g in 5 mmol scale, 86 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.55 (d, J = 5.6 Hz, 1 H), 9.21 (d, J = 8.4 Hz, 1 H), 8.82 (d, J = 1.3 Hz, 1 H), 8.45 (dt, J = 9.4, 5.6 Hz, 2 H), 8.23 (dd, J = 8.3, 5.8 Hz, 1 H), 4.64 (s, 3 H) ppm; ¹³C

NMR (100 MHz, DMSO- d_6) δ = 151.2, 146.5, 138.3, 137.8, 132.5, 130.9, 123.7, 123.6, 122.0, 46.1 ppm; HRMS [M+H]⁺ calculated for C₁₀H₉BrN⁺: 221.9913, found: 221.9913.

6-methoxy-1-methylquinolin-1-ium iodide (2c)



Yellow solid; 1.204 g in 5 mmol scale, 80 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.33 (d, J = 5.6 Hz, 1 H), 9.12 (d, J = 8.4 Hz, 1 H), 8.44 (d, J = 10.4 Hz, 1 H), 8.11 (dd, J = 8.3, 5.9 Hz, 1 H), 7.92 (d, J = 7.1 Hz, 2 H), 4.62 (s, 3 H), 4.02 (s, 3 H)

ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 159.7, 147.7, 145.6, 134.6, 131.7, 127.9, 122.9, 121.3, 108.5, 56.9, 46.0 ppm; HRMS [M+H]⁺ calculated for C₁₁H₁₂ON⁺: 174.0913, found: 174.0912.

6-chloro-1-methylquinolin-1-ium iodide (2d)



Yellow solid; 1.265 g in 5 mmol scale, 83 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.55 (d, J = 5.6 Hz, 1 H), 9.22 (d, J = 8.4 Hz, 1 H), 8.68 (d, J = 1.9 Hz, 1 H), 8.57 (d, J = 9.4 Hz, 1 H), 8.34 (dd, J = 9.4, 2.1 Hz, 1 H), 8.24 (dd, J = 8.3, 5.8 Hz, 1 H), 4.65 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.2,

146.7, 137.6, 135.8, 134.9, 130.6, 129.2, 123.8, 122.2, 46.2 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_9CIN^+$: 178.0418, found: 178.0419.

1-(3-phenylpropyl)quinolin-1-ium bromide (2e)



Brown oil; 1.164 g in 5 mmol scale, 71 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.80 (dd, J = 5.8, 1.0 Hz, 1 H), 9.36 (d, J = 8.3 Hz, 1 H), 8.69 (d, J = 9.0 Hz, 1H), 8.60-8.49 (m, 1 H), 8.29 (ddd, J = 8.7, 7.1, 1.3 Hz, 1 H), 8.22 (dd, J = 8.3, 5.8 Hz, 1 H), 8.07 (t, J = 7.6 Hz, 1 H), 7.28-7.23 (m, 4 H), 7.19-7.16

(m, 1 H), 5.23 (t, J = 7.5 Hz, 2 H), 2.90-2.78 (m, 2H), 2.33 (dq, J = 15.4, 7.8 Hz, 2 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 150.3$, 147.9, 140.9, 137.9, 136.1, 131.2, 130.3, 130.2, 128.8, 128.7, 126.5, 122.6, 119.4, 57.5, 32.2, 31.5 ppm; HRMS [M+H]⁺ calculated for C₁₈H₁₈N⁺: 248.1434, found: 248.1434.

1-methyl-3-(naphthalen-1-yl)quinolin-1-ium iodide (2fa)



Yellow solid; 1.548 g in 5 mmol scale, 78 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.83 (d, J = 0.9 Hz, 1 H), 9.47 (s, 1 H), 8.61 (d, J = 8.9 Hz, 1 H), 8.54 (d, J = 7.9 Hz, 1 H), 8.38-8.33 (m, 1 H), 8.19 (dd, J = 6.0, 3.4 Hz, 1 H), 8.13 (t, J = 7.6 Hz, 2 H), 7.95 (d, J = 8.3 Hz, 1 H), 7.77 (q, J = 3.1 Hz, 2 H), 7.69-7.60 (m, 2 H), 4.73 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.6, 147.1, 138.1, 135.9, 133.9, 133.8, 132.8, 131.1, 131.0,

130.7, 130.4, 129.7, 129.4, 129.1, 128.0, 127.2, 126.1, 125.2, 119.5, 45.9 ppm; HRMS $[M+H]^+$ calculated for $C_{20}H_{16}N^+$: 270.1277, found: 270.1277.

1-methyl-3-(naphthalen-1-yl)quinolin-1-ium tetrafluoroborate (2fb)



Yellow solid; 0.286 g in 1 mmol scale, 80 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.83 (s, 1 H), 9.46 (s, 1 H), 8.61 (d, J = 8.9 Hz, 1 H), 8.53 (d, J = 8.0 Hz, 1 H), 8.35 (t, J = 7.7 Hz, 1 H), 8.16 (dt, J = 15.4, 6.0 Hz, 3 H), 7.95 (d, J = 8.2 Hz, 1 H), 7.78-7.75 (m, 2 H), 7.65 (dt, J = 14.5, 6.9 Hz, 2 H), 4.72 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 151.6, 147.1, 138.1, 135.9,

134.0, 133.9, 132.8, 131.1, 131.0, 130.7, 130.4, 129.7, 129.3, 129.1, 128.0, 127.2, 126.1, 125.2, 119.4, 45.8 ppm; HRMS $[M+H]^+$ calculated for $C_{20}H_{16}N^+$: 270.1277, found: 270.1279.

1-methyl-6-phenylquinolin-1-ium iodide (2g)



Yellow solid; 1.422 g in 5 mmol scale, 82 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.51 (d, J = 5.5 Hz, 1 H), 9.31 (d, J = 8.4 Hz, 1 H), 8.83 (d, J = 1.9 Hz, 1 H), 8.63 (dt, J = 19.3, 5.6 Hz, 2 H), 8.21 (dd, J = 8.4, 5.7 Hz, 1 H), 7.97-7.95 (m, 2H), 7.62 (dd, J = 10.2, 4.7 Hz, 2 H), 7.55-.51 (m, 1 H), 4.69 (s, 3 H) ppm;

¹³C NMR (100 MHz, DMSO- d_6) δ = 150.3, 147.5, 141.5, 138.2, 137.7, 134.6, 130.2, 129.9, 129.6, 127.9, 127.5, 122.9, 120.4), 45.9 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₄N⁺: 220.1121, found: 220.1124.

1-(3-methylbenzyl)quinolin-1-ium bromide (2h)



White solid; 1.114g in 5 mmol scale, 71 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 9.84 (dd, J = 5.8, 1.1 Hz, 1 H), 9.42 (d, J = 8.3 Hz, 1 H), 8.55 (d, J = 8.6 Hz, 2 H), 8.32 (dd, J = 8.4, 5.8 Hz, 1 H), 8.23 (ddd, J = 8.7, 7.1, 1.4 Hz, 1 H), 8.04 (t, J = 7.7 Hz, 1 H), 7.30-7.27 (m, 2 H), 7.22-7.17 (m, 2 H), 6.39 (s, 2 H), 2.27 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 150.9, 148.6,

139.0, 138.0, 136.2, 134.3, 131.3, 130.5, 130.4, 129.9, 129.5, 128.3, 124.9, 123.0, 119.8, 60.4, 21.4 ppm; HRMS $[M+H]^+$ calculated for $C_{17}H_{16}N^+$: 234.1277, found: 234.1281.

1-methyl-3-phenylquinolin-1-ium iodide (2i)



Yellow solid; 1.441 g in 5 mmol scale, 83 % yield; ¹H NMR (400 MHz, DMSO- d_6) δ = 10.00 (s, 1 H), 9.66 (s, 1 H), 8.53 (t, J = 7.8 Hz, 2 H), 8.28 (ddd, J = 8.7, 7.1, 1.3 Hz, 1 H), 8.08 (dd, J = 14.9, 7.5 Hz, 3 H), 7.67 (dd, J = 10.2, 4.7 Hz, 2 H), 7.61-7.57 (m, 1 H), 4.74 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 149.7, 143.3, 137.7, 135.6, 134.0, 133.8, 131.0,

130.7, 130.3, 123.0, 129.7, 127.9, 119.4, 46.0 ppm; HRMS $[M+H]^+$ calculated for $C_{16}H_{14}N^+$: 220.1121, found: 220.1123.

3-bromo-1-methylquinolin-1-ium iodide (2j)



Yellow solid; 1.470 g in 5 mmol scale, 84 % yield; ¹H NMR (400 MHz, DMSO- d_6) $\delta = 9.91$ (d, J = 1.6 Hz, 1 H), 9.65 (d, J = 1.5 Hz, 1 H), 8.51 (d, J = 8.9 Hz, 1 H), 8.41 (dd, J = 8.3, 1.0 Hz, 1 H), 8.31 (ddd, J = 8.8, 7.0, 1.4 Hz, 1 H), 8.10 (t, J = 7.6 Hz, 1 H), 4.63 (s, 3)

H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 151.8$, 148.6, 137.7, 136.1, 131.3, 130.1, 130.0, 119.7, 115.0, 45.8 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_9BrN^+$: 221.9913, found: 221.9914.

1-(naphthalen-1-ylmethyl)quinolin-1-ium bromide (2k)



White solid; 1.190 g in 5 mmol scale, 68 % yield; ¹H NMR (400 MHz, DMSO- d_6) $\delta = 9.56$ (dd, J = 5.8, 1.1 Hz, 1 H), 9.50 (d, J =8.3 Hz, 1 H), 8.62 (dd, J = 8.2, 1.1 Hz, 1 H), 8.44 (d, J = 8.9 Hz, 1 H), 8.29 (dd, J = 8.3, 5.8 Hz, 1 H), 8.25-8.19 (m, 2 H), 8.08 (t, J =7.7 Hz, 2 H), 8.01 (d, J = 8.3 Hz, 1 H), 7.75-7.67 (m, 2 H), 7.42-7.39 (m, 1 H), 6.94 (s, 2 H), 6.81 (d, J = 7.1 Hz, 1 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) δ = 150.5, 148.9, 138.7, 136.4, 133.8,

131.4, 130.6, 130.4, 130.3, 129.8, 129.7, 129.4, 127.8, 127.2, 126.1, 125.4, 123.5, 123.1, 119.7, 58.4 ppm; HRMS $[M+H]^+$ calculated for $C_{20}H_{16}N^+$: 270.1277, found: 270.1276.

1-methylpyridin-1-ium iodide (21)



Light yellow solid; 0.950 g in 5 mmol scale, 86 % yield; ¹H NMR (400 MHz, DMSO- d_6) $\delta = 9.02$ (d, J = 5.8 Hz, 2 H), 8.60 (t, J = 7.8 Hz, 1 H), 8.15 (t, J = 7.0 Hz, 2 H), 4.38 (s, 3 H) ppm; ¹³C NMR (100 MHz, DMSO- d_6) $\delta = 146.0, 145.6, 128.2, 48.5 \text{ ppm}; \text{HRMS } [\text{M+H}]^+ \text{ calculated}$ for C₆H₈N⁺: 94.0651, found: 94.0653.

2-methylisoquinolin-1(2*H*)-one (3a)



Light yellow oil; 28 mg in 0.2 mmol scale, 86% yield from iodide salt; 25 mg in 0.2 mmol scale, 78% yield from tetrafluoroborate salt; ¹H NMR (400 MHz, CDCl₃) δ = 8.42 (d, J = 8.1 Hz, 1 H), 7.60 (t, J = 7.5 Hz, 1H), 7.46 (dd, J = 13.7, 7.7 Hz, 2 H), 7.04 (d, J = 7.3 Hz,

1 H), 6.45 (d, J = 7.3 Hz, 1 H), 3.58 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta =$ 162.6, 137.1, 132.4, 132.0, 127.6, 126.8, 126.1, 125.9, 106.0, 37.0 ppm; HRMS $[M+H]^+$ calculated for C₁₀H₁₀ON⁺: 160.0757, found: 160.0758.

6-methoxy-2-methylisoquinolin-1(2*H*)-one (3b)



Light yellow solid; 34 mg in 0.2 mmol scale, 90% yield; m. p. 90-91 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.33 (d, J = 8.9 Hz, 1 H), 7.04 (dd, J = 6.7, 3.6 Hz, 2 H), 6.84 (s, 1 H), 6.39 (d, J =7.3 Hz, 1 H), 3.89 (s, 3 H), 3.57 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 162.6$, 162.4, 139.2, 133.1, 129.7, 120.0,

116.3 106.7, 105.7, 55.4, 36.8 ppm; HRMS $[M+H]^+$ calculated for $C_{11}H_{12}O_2N^+$: 190.0863, found: 190.0862.

6-chloro-2-methylisoquinolin-1(2H)-one (3c)



White solid; 33 mg in 0.2 mmol scale, 85% yield; m. p. 132-133 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.34 (d, *J* = 8.6 Hz, 1 H), 7.47 (d, *J* = 1.7 Hz, 1 H), 7.40 (dd, *J* = 8.6, 1.8 Hz, 1 H), 7.08 (d, *J* = 7.3 Hz, 1 H), 6.38 (d, *J* = 7.3 Hz, 1 H), 3.58 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.0, 138.5, 138.4, 133.8,

129.5, 127.3, 125.1, 124.4, 104.9, 37.0 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_9OCIN^+$: 194.0367, found: 194.0368.

6-bromo-2-methylisoquinolin-1(2H)-one (3d)



White solid; 41 mg in 0.2 mmol scale, 86% yield; m. p. 146-147 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.26 (d, *J* = 8.6 Hz, 1 H), 7.64 (s, 1 H), 7.55 (dd, *J* = 8.6, 1.6 Hz, 1 H), 7.08 (d, *J* = 7.3 Hz, 1 H), 6.37 (d, *J* = 7.3 Hz, 1 H), 3.58 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.1, 138.6, 133.8, 130.0, 129.6, 128.3,

127.1, 124.8, 104.8, 37.1 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_9OBrN^+$: 237.9862, found: 237.9864.

2-benzylisoquinolin-1(2*H*)-one (3e)



Light yellow oil; 35 mg in 0.2 mmol scale, 74% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.46 (d, *J* = 7.7 Hz, 1 H), 7.65-7.61 (m, 1 H), 7.51-7.47 (m, 2 H), 7.35 - 7.31 (m, 4 H), 7.28 (dd, *J* = 9.8, 5.6 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H),

6.48 (d, J = 7.4 Hz, 1 H), 5.22 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 162.3$, 137.0, 136.9, 132.2, 131.3, 128.8, 128.1, 128.0, 127.8, 126.9, 126.4, 125.9, 106.5, 51.7 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₄ON⁺: 236.1070, found: 236.1069.

2-butylisoquinolin-1(2*H*)-one (3f)



Light yellow oil; 31 mg in 0.2 mmol scale, 78% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.43 (d, *J* = 8.0 Hz, 1 H), 7.61 (dd, *J* = 10.9, 4.1 Hz, 1 H), 7.48 (dd, *J* = 14.5, 7.6 Hz, 2 H), 7.06 (d, *J* = 7.3 Hz, 1 H), 6.48 (d, *J* = 7.3 Hz, 1 H), 4.02-

3.98 (m, 2 H), 1.77 (dt, J = 15.1, 7.5 Hz, 2 H), 1.41 (dq, J = 14.7, 7.4 Hz, 2 H), 0.96 (t, J = 7.4 Hz, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 162.1$, 137.0, 132.0, 131.7, 127.8, 126.7, 126.4, 125.8, 105.9, 49.1, 31.4, 20.0, 13.7 ppm; HRMS [M+H]⁺ calculated for C₁₃H₁₆ON⁺: 202.1226, found: 202.1224.

2-(naphthalen-1-ylmethyl)isoquinolin-1(2H)-one (3g)



White solid; 36 mg in 0.2 mmol scale, 63% yield; m. p. 122-123 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.53 (d, *J* = 8.0 Hz, 1 H), 8.07-8.05 (m, 1 H), 7.87-7.82 (m, 2H), 7.64-7.60 (m, 1 H), 7.52-7.48 (m, 3 H), 7.43 (dd, *J* = 15.4, 8.1

Hz, 2 H), 7.33 (d, J = 7.0 Hz, 1 H), 6.96 (d, J = 7.4 Hz, 1 H), 6.38 (d, J = 7.4 Hz, 1 H), 5.68 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 162.2$, 136.9, 133.9, 132.3, 132.2, 131.4, 130.4, 129.0, 128.8, 128.2, 127.1, 126.9, 126.2, 126.1, 126.0, 125.3, 123.5, 106.4, 48.8 ppm; HRMS [M+H]⁺ calculated for C₂₀H₁₆ON⁺: 286.1226, found: 286.1226.

2-(4-nitrobenzyl)isoquinolin-1(2H)-one (3h)



Brown solid; 17 mg in 0.2 mmol scale, 30% yield; m. p. 153-154 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.44 (d, J = 7.9 Hz, 1 H), 8.18 (d, J = 8.4 Hz, 2 H), 7.67 (t, J = 7.5 Hz, 1H), 7.55-7.46 (m, 4 H), 7.09 (d, J = 7.3 Hz, 1 H), 6.56 (d, J = 7.3 Hz, 1 H), 5.30 (s, 2 H) ppm; ¹³C NMR

 $(100 \text{ MHz}, \text{CDCl}_3) \delta = 162.2, 144.2, 137.0, 132.6, 131.0, 128.5, 128.1, 127.3, 126.2, 126.1, 124.0, 107.1, 51.6 \text{ ppm}; \text{HRMS } [M+H]^+ \text{ calculated for } C_{16}H_{13}O_3N_2^+: 281.0921, found: 281.0920.$

2-methyl-6-phenylisoquinolin-1(2*H*)-one (3i)



White solid; 22 mg in 0.2 mmol scale, 47% yield; m. p. 139-140 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.48 (d, *J* = 8.3 Hz, 1 H), 7.72-7.65 (m, 4 H), 7.49-7.45 (m, 2 H), 7.42-7.38 (m, 1 H), 7.08 (d, *J* = 7.3 Hz, 1 H), 6.52 (d, *J* = 7.3 Hz, 1 H), 3.61 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.5, 144.8, 140.5, 137.6, 132.8, 128.9, 128.3, 128.1, 127.5, 126.1, 125.0,

124.0, 106.1, 37.0 ppm; HRMS $[M+H]^+$ calculated for $C_{16}H_{14}ON^+$: 236.1070, found: 236.1073.

2-(4-bromobenzyl)isoquinolin-1(2*H*)-one (3j)



White solid; 42 mg in 0.2 mmol scale, 67% yield; m. p. 159-160 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.49-8.40 (m, 1 H), 7.66-7.61 (m, 1 H), 7.51-7.43 (m, 4 H), 7.20 (d, J = 8.4 Hz, 2 H), 7.05 (d, J = 7.4 Hz, 1 H), 6.49 (d, J = 7.4 Hz, 1 H), 5.15 (s, 2 H) ppm; ¹³C NMR (100 MHz,

CDCl₃) δ = 162.2, 129.7, 128.1, 127.1, 126.3, 126.0, 121.9, 106.7, 51.3 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₃BrON⁺: 314.0175, found: 314.0172.

2-(3-chlorobenzyl)isoquinolin-1(2H)-one (3k)



White solid; 41 mg in 0.2 mmol scale, 76% yield; m. p. 95-96 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.37 (d, *J* = 8.0 Hz, 1 H), 7.56 (t, *J* = 7.5 Hz, 1 H), 7.41 (t, *J* = 7.5 Hz, 2 H), 7.22 (s, 1 H), 7.14 (dt, *J* = 8.9, 4.7 Hz, 3 H), 6.98 (d,

J = 7.4 Hz, 1 H), 6.42 (d, J = 7.4 Hz, 1 H), 5.10 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 162.2$, 139.0, 137.0, 134.7, 132.4, 131.1, 130.1, 128.1, 128.0, 127.9, 127.1, 126.3, 126.1, 126.0, 106.7, 51.3 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₃ClON⁺: 270.0680, found: 270.0687.

2-(2-bromobenzyl)isoquinolin-1(2H)-one (3l)



Light yellow solid; 33 mg in 0.2 mmol scale, 53% yield; m. p. 87-88 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.47 (d, *J* = 8.0 Hz, 1 H), 7.67-7.63 (m, 1 H), 7.59 (d, *J* = 8.0 Hz, 1 H), 7.53-7.48 (m, 2 H), 7.23 (dd, *J* = 11.9, 5.3 Hz, 1 H), 7.18-7.07 (m, 3 H), 6.51 (d, *J* = 7.4 Hz, 1 H), 5.33 (s, 2 H) ppm;

¹³C NMR (100 MHz, CDCl₃) δ = 162.4, 137.1, 136.0, 133.0, 132.4, 131.5, 129.5, 129.3, 128.1, 127.9, 127.0, 126.3, 126.0, 123.4, 106.5, 51.7 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₃BrON⁺: 314.0175, found: 314.0175.

2,2'-(butane-1,4-diyl)bis(isoquinolin-1(2H)-one) (3m)



White solid; 18 mg in 0.1 mmol scale, 51% yield; m. p. 185-186 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.34 (d, *J* = 8.0 Hz, 2 H), 7.53 (t, *J* = 7.5 Hz, 2 H), 7.41-7.37 (m, 4 H), 6.98 (d, *J* = 7.3 Hz, 2 H), 6.39

(d, J = 7.2 Hz, 2H), 3.98 (s, 4 H), 1.78 (s, 4 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.2, 137.1, 132.1, 131.7, 127.8, 126.8, 126.2, 125.9, 106.2, 48.6, 26.3 ppm; HRMS [M+H]⁺ calculated for C₂₂H₂₁O₂N₂⁺: 345.1598, found: 345.1597.

2-(4-(tert-butyl)benzyl)isoquinolin-1(2H)-one (3n)



Light yellow oil; 33 mg in 0.2 mmol scale, 57% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.39 (d, *J* = 7.7 Hz, 1 H), 7.56-7.52 (m, 1 H), 7.40 (dd, *J* = 11.3, 4.3 Hz, 2 H), 7.28-7.26 (m, 2 H), 7.20-7.17 (m, 2 H), 7.02 (d, *J* = 7.4 Hz, 1 H), 6.40 (d, *J* = 7.4 Hz, 1 H), 5.11 (s, 2 H), 1.21 (s,

9 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.3, 150.8, 137.0, 133.9, 132.2, 131.4, 128.1, 127.8, 126.9, 126.4, 125.9, 125.7, 106.3, 51.5, 34.5, 31.3 ppm; HRMS [M+H]⁺ calculated for C₂₀H₂₂ON⁺: 292.1696, found: 292.1694.

2-(3-phenylpropyl)isoquinolin-1(2*H*)-one (30)



Light yellow oil; 18 mg in 0.2 mmol scale, 34% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.44 (d, *J* = 8.0 Hz, 1 H), 7.61 (dd, *J* = 10.5, 4.5 Hz, 1 H), 7.50-7.45 (m, 2 H), 7.27 (dd, *J* = 12.7, 5.5 Hz, 2 H), 7.19 (dd, *J* = 10.3, 7.5

Hz, 3 H), 6.99 (d, J = 7.3 Hz, 1 H), 6.47 (d, J = 7.3 Hz, 1 H), 4.04-4.00 (m, 2 H), 2.73-2.69 (m, 2 H), 2.13 (dt, J = 14.9, 7.6 Hz, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 162.2$, 141.0, 137.0 132.1, 131.6, 128.5, 128.4, 127.9, 126.8, 126.4, 126.1, 125.9, 106.0, 49.0, 32.9, 30.6 ppm; HRMS [M+H]⁺ calculated for C₁₈H₁₈ON⁺: 264.1383, found: 264.1382.

4-bromo-2-methylisoquinolin-1(2*H*)-one (3p)



White solid; 41 mg in 0.2 mmol scale, 88% yield; m. p. 127-128 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.34 (d, *J* = 8.0 Hz, 1 H), 7.70 (d, *J* = 8.0 Hz, 1 H), 7.63 (t, *J* = 7.6 Hz, 1 H), 7.45 (t, *J* = 7.5 Hz, 1 H), 7.26 (s, 1 H), 3.50 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.7, 135.5, 133.0, 132.8, 128.1, 127.8, 126.3, 125.8, 99.5, 36.9 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_9BrON^+$: 237.9862, found: 237.9861.

2-methyl-4-phenylisoquinolin-1(2H)-one (3q)



White solid; 25 mg in 0.2 mmol scale, 53% yield; m. p. 174-175 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.53 (d, *J* = 7.9 Hz, 1H), 7.59-7.50 (m, 3 H), 7.43 (dd, *J* = 20.5, 6.9 Hz, 5 H), 7.04 (s, 1 H), 3.65 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.2, 136.4, 136.3, 132.0, 131.5, 130.0, 128.7, 128.1, 127.7, 126.9, 125.9, 124.6, 119.6, 37.0 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₄ON⁺: 236.1070, found: 236.1072.

2-propylisoquinolin-1(2*H*)-one (3r)



Colorless oil; 24 mg in 0.2 mmol scale, 65% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.44 (d, *J* = 8.0 Hz, 1 H), 7.61 (dd, *J* = 11.0, 3.9 Hz, 1 H), 7.48 (dd, *J* = 14.7, 7.5 Hz, 2 H), 7.06 (d, *J* = 7.3 Hz, 1 H), 6.48 (d, *J* = 7.3 Hz, 1 H), 3,99-3.95 (m, 2 H), 1.82 (dd, *J* = 14.7, 7.4 Hz, 2 H), 0.98 (t, *J* = 7.4 Hz, 3 H) ppm;

¹³C NMR (100 MHz, CDCl₃) δ 162.1, 137.0, 132.0, 131.8, 127.9, 126.7, 126.4, 125.8, 105.8, 51.0, 22.6, 11.2 ppm; HRMS [M+H]⁺ calculated for $C_{12}H_{14}ON^+$: 188.1070, found: 188.1074.

2-pentylisoquinolin-1(2*H*)-one (3s)



Light yellow oil; 22 mg in 0.2 mmol scale, 50% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.44 (d, *J* = 8.0 Hz, 1 H), 7.66-7.57 (m, 1 H), 7.48 (dd, *J* = 14.6, 7.4 Hz, 2 H), 7.06 (d, *J* = 7.3 Hz, 1 H), 6.48 (d, *J* = 7.3 Hz, 1 H), 4.00-3.97 (m, 2 H), 1.81-1.74 (m, 2 H), 1.39-1.33 (m, 4 H), 0.90 (t,

J = 6.8 Hz, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 162.1$, 137.0, 132.0, 131.7, 127.8, 126.7, 126.3, 125.8, 105.9, 49.4, 29.0, 28.9, 22.4, 14.0 ppm; HRMS [M+H]⁺ calculated for C₁₄H₁₈ON⁺: 216.1383, found: 216.1381.

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



Light yellow oil; 25 mg in 0.2 mmol scale, 78% yield; ¹H NMR (400 MHz, CDCl₃) δ = 7.67 (d, *J* = 9.5 Hz, 1 H), 7.58 (dd, *J* = 12.7, 4.4 Hz, 2 H), 7.37 (d, *J* = 8.4 Hz, 1 H), 7.27-7.22 (m, 1 H), 6.72 (d, *J* = 9.5 Hz, 1 H), 3.72 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ

= 162.4, 140.1, 139.0, 130.6, 128.8, 122.1, 121.7, 120.7, 114.1, 29.4 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_{10}ON^+$: 160.0757, found: 160.0758.

6-bromo-1-methylquinolin-2(1*H*)-one (4b)



White solid; 36 mg in 0.2 mmol scale, 77% yield; m. p. 141-142 °C; ¹H NMR (400 MHz, CDCl₃) δ = 7.67-7.61 (m, 2 H), 7.57 (d, J = 9.5 Hz, 1 H), 7.23 (d, J = 8.9 Hz, 1 H), 6.72 (d, J = 9.5 Hz, 1 H), 3.68 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 161.8$, 139.0, 137.7, 133.3, 130.8, 123.0, 122.1, 115.8, 114.9, 29.5 ppm; HRMS [M+H]⁺ calculated for C₁₀H₉OBrN⁺: 237.9862, found: 237.9861.

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



Light yellow solid; 33 mg in 0.2 mmol scale, 89% yield; m. p. 70-71 °C; ¹H NMR (400 MHz, CDCl₃) δ = 7.61 (d, *J* = 9.4 Hz, 1 H), 7.29 (t, *J* = 7.4 Hz, 1 H), 7.19 (dd, *J* = 9.2, 2.5 Hz, 1 H), 7.00 (d, *J* = 2.4 Hz, 1 H), 6.72 (d, *J* = 9.4 Hz, 1 H), 3.87 (s, 3

H), 3.71 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.0, 154.7, 138.4, 134.6, 122.3, 121.4, 119.2, 115.4, 110.5, 55.7, 29.5 ppm; HRMS [M+H]⁺ calculated for C₁₁H₁₂O₂N⁺: 190.0863, found: 190.0864.

6-chloro-1-methylquinolin-2(1*H*)-one (4d)



Off-white solid; 31 mg in 0.2 mmol scale, 80% yield; m. p. 145-146 °C; ¹H NMR (400 MHz, CDCl₃) δ = 7.58 (d, *J* = 9.5 Hz, 1 H), 7.51 (d, *J* = 10.4 Hz, 2 H), 7.29 (d, *J* = 8.6 Hz, 1 H), 6.73 (d, *J* = 9.5 Hz, 1 H), 3.69 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.9, 138.6, 137.8, 130.6, 127.8, 127.6,

123.1, 121.7, 115.6, 29.6 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_9OCIN^+$: 194.0367, found: 194.0367.

1-(3-phenylpropyl)quinolin-2(1*H*)-one (4e)



Yellow oil; 19 mg in 0.2 mmol scale, 36% yield; ¹H NMR (400 MHz, CDCl₃) δ = 7.64 (d, *J* = 9.4 Hz, 1 H), 7.54 (d, *J* = 7.7 Hz, 1 H), 7.47 (dd, *J* = 8.5, 7.3 Hz, 1 H), 7.30-7.29 (m, 2 H), 7.25-7.17 (m, 4 H), 7.12 (d, *J* = 8.6 Hz, 1 H), 6.69 (d, *J* = 9.4 Hz, 1 H), 4.33-4.29 (m, 2 H), 2.80 (t, *J* = 7.6 Hz, 2 H), 2.12-2.04 (m, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.1, 141.2, 139.2, 139.0, 130.5, 129.0, 128.5, 128.4, 126.1, 121.9, 121.8, 121.0, 114.0, 41.8, 33.2, 28.8 ppm; HRMS [M+H]⁺ calculated for C₁₈H₁₈ON⁺: 264.1383,

found: 264.1375.

1-methyl-3-(naphthalen-1-yl)quinolin-2(1H)-one (4f)



Yellow solid; 50 mg in 0.2 mmol scale, 88% yield from iodide salt; 46 mg in 0.2 mmol scale, 81% yield from tetrafluoroborate salt; m. p. 161-162 °C; ¹H NMR (400 MHz, CDCl₃) δ = 7.85 (d, J = 7.7 Hz, 2 H), 7.75-7.72 (m, 2 H), 7.58-7.50 (m, 3 H), 7.45 (ddd, J = 6.1, 4.8, 2.5 Hz, 2 H), 7.42-7.37 (m, 2 H), 7.24-7.19 (m, 1 H), 3.78 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.9, 140.1, 139.1, 135.2, 133.7, 132.8, 132.1, 130.6, 128.9, 128.7,

128.4, 127.5, 126.2, 125.8, 125.4, 122.3, 120.6, 114.2, 30.1 ppm; HRMS $[M+H]^+$ calculated for $C_{20}H_{16}ON^+$: 286.1226, found: 286.1227.

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



Grey solid; 20 mg in 0.2 mmol scale, 43% yield; m. p. 136-137 °C; ¹H NMR (400 MHz, CDCl₃) δ = 7.73 (dd, *J* = 8.7, 2.0 Hz, 1 H), 7.66 (dd, *J* = 13.3, 5.7 Hz, 2 H), 7.54 (d, *J* = 7.5 Hz, 2 H), 7.35 (ddd, *J* = 25.7, 14.9, 7.4 Hz, 4 H), 6.67 (d, *J* = 9.5 Hz, 1 H), 3.67 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ =

162.3, 139.7, 139.4, 139.0, 135.2, 129.6, 129.0, 127.5, 126.9, 126.8, 122.2, 121.0, 114.6, 29.5 ppm; HRMS $[M+H]^+$ calculated for $C_{16}H_{14}ON^+$: 236.1070, found: 236.1064.

1-(3-methylbenzyl)quinolin-2(1H)-one (4h)



Light yellow oil; 32 mg in 0.2 mmol scale, 64% yield; ¹H NMR (400 MHz, CDCl₃) δ = 7.73 (d, *J* = 9.5 Hz, 1 H), 7.55 (d, *J* = 7.7 Hz, 1H), 7.41 (t, *J* = 7.9 Hz, 1 H), 7.27 (d, *J* = 8.6 Hz, 1 H), 7.17 (t, *J* = 7.6 Hz, 2 H), 7.02 (t, *J* = 8.0 Hz, 3 H), 6.80 (d, *J* = 9.5 Hz, 1 H), 5.52 (s, 2 H), 2.28 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.5, 139.6, 139.5, 138.5, 136.3, 130.6, 128.8, 128.7, 128.1, 127.2, 123.7, 122.2, 121.7, 121.0, 115.1, 46.0, 21.4 ppm;

HRMS [M+H]⁺ calculated for C₁₇H₁₆ON⁺: 250.1226, found: 250.1224.

1-methyl-3-phenylquinolin-2(1*H*)-one (4i)



Yellow solid; 29 mg in 0.2 mmol scale, 62% yield; m. p. 127-128 °C; ¹H NMR (400 MHz, CDCl₃) δ = 7.79 (s, 1 H), 7.72-7.70 (m, 2 H), 7.61-7.57 (m, 1 H), 7.56-7.54 (m, 1 H), 7.45-7.41 (m, 2 H), 7.38-7.34 (m, 2 H), 7.26-7.22 (m, 1 H), 3.79 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.6, 139.7, 136.8, 136.7, 132.5, 130.3, 129.0, 128.9, 128.2, 128.1, 122.2,

120.8, 114.0, 30.0 ppm; HRMS $[M+H]^+$ calculated for $C_{16}H_{14}ON^+$: 236.1070, found: 236.1074.

3-bromo-1-methylquinolin-2(1*H*)-one (4j)



White solid; 27 mg in 0.2 mmol scale, 58% yield; m. p. 144-145 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.12 (s, 1 H), 7.60 (ddd, *J* = 8.6, 7.3, 1.5 Hz, 1 H), 7.52 (dd, *J* = 7.8, 1.2 Hz, 1 H), 7.36 (d, *J* = 8.5 Hz, 1 H), 7.26 (dd, *J* = 8.8, 6.2 Hz, 1 H), 3.80 (s, 3 H) ppm; ¹³C

NMR (100 MHz, CDCl₃) δ = 158.5, 140.6, 139.4, 130.9, 128.1, 122.7, 120.5, 117.6, 114.4, 31.1 ppm; HRMS [M+H]⁺ calculated for C₁₀H₉BrON⁺: 237.9862, found: 237.9864.

1-(naphthalen-1-ylmethyl)quinolin-2(1*H*)-one (4k)



Grey solid; 43 mg in 0.2 mmol scale, 75% yield; m. p. 186-187 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.14 (d, *J* = 8.3 Hz, 1 H), 7.90 (d, *J* = 8.1 Hz, 1 H), 7.80-7.78 (m, 1 H), 7.72 (d, *J* = 8.1 Hz, 1 H), 7.64-7.53 (m, 3 H), 7.31-7.21 (m, 2 H), 7.16 (t, *J* = 7.5 Hz, 1 H), 7.02 (d, *J* = 8.4 Hz, 1 H), 6.84 (dd, *J* = 9.5, 2.1 Hz, 1 H), 6.78 (d, *J* = 7.1 Hz, 1 H), 5.99 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 162.5, 139.7, 139.6, 133.9, 130.8, 130.7, 130.6, 129.1, 128.8, 127.7, 126.5, 125.9, 125.6, 122.4, 122.3, 121.7, 121.0,

115.3, 43.9 ppm; HRMS $[M+H]^+$ calculated for $C_{20}H_{16}ON^+$: 286.1226, found: 286.1219.

4-iodo-2-methylisoquinolin-1(2H)-one (5a)



White solid; 42 mg in 0.2 mmol scale, 74% yield; 45 mg in 0.2 mmol scale, 79% yield from tetrafluoroborate salt; m. p. 123-124 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.37 (d, *J* = 8.0 Hz, 1 H), 7.69 (t, *J* = 7.5 Hz, 1 H), 7.62 (d, *J* = 8.0 Hz, 1 H), 7.52-7.49 (m, 2 H), 3.58 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 161.9, 138.7, 137.2, 133.1, 130.3, 128.0, 127.8, 126.4, 71.4, 36.8 ppm; HRMS

[M+H]⁺ calculated for C₁₀H₉OIN⁺: 285.9723, found: 285.9725.

4-iodo-6-methoxy-2-methylisoquinolin-1(2*H*)-one (5b)



White solid; 44 mg in 0.2 mmol scale, 70% yield; m. p. 177-178 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.31 (d, *J* = 8.8 Hz, 1 H), 7.51 (s, 1 H), 7.07-7.03 (m, 2 H), 3.95 (s, 3 H), 3.57 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 163.5, 161.6, 139.4, 139.3, 130.4, 120.2, 116.8, 112.1, 71.0, 55.6, 36.6 ppm; HRMS [M+H]⁺ calculated for C₁₁H₁₁O₂IN⁺: 315.9829, found: 315.9829.

6-chloro-4-iodo-2-methylisoquinolin-1(2H)-one (5c)



White solid; 50 mg in 0.2 mmol scale, 78% yield; m. p. 213-214 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.31 (d, *J* = 8.6 Hz, 1 H), 7.64 (d, *J* = 1.9 Hz, 1 H), 7.54 (s, 1H), 7.44 (dd, *J* = 8.6, 2.0 Hz, 1 H), 3.58 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.3, 140.0, 139.9, 138.7, 130.0, 129.8, 128.3, 124.7, 69.3, 36.9 ppm;

HRMS $[M+H]^+$ calculated for $C_{10}H_8CIOIN^+$: 319.9334, found: 319.9336.

6-bromo-4-iodo-2-methylisoquinolin-1(2*H*)-one (5d)



White solid; 53 mg in 0.2 mmol scale, 73% yield; m. p. 208-209 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.24 (d, *J* = 8.5 Hz, 1 H), 7.83 (d, *J* = 1.6 Hz, 1 H), 7.61 (dd, *J* = 8.5, 1.6 Hz, 1 H), 7.55 (s, 1 H), 3.59 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.5, 139.9, 138.8, 133.0, 131.2, 130.0, 128.7, 125.1, 69.2,

36.9 ppm; HRMS $[M+H]^+$ calculated for $C_{10}H_8BrOIN^+$: 363.8828, found: 363.8831.

2-benzyl-4-iodoisoquinolin-1(2H)-one (5e)



Light yellow solid; 50 mg in 0.2 mmol scale, 69% yield; m. p. 91-92 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.42 (dd, *J* = 8.0, 0.5 Hz, 1 H), 7.71-7.62 (m, 2 H), 7.53-7.49 (m, 2 H), 7.34-7.28 (m, 5 H), 5.18 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.6, 137.6, 137.1, 136.4, 133.3, 130.5, 129.0, 128.5, 128.1, 128.0, 127.9, 126.7, 72.1, 51.7 ppm; HRMS [M+H]⁺

calculated for C₁₆H₁₃OIN⁺: 362.0036, found: 362.0037.

2-butyl-4-iodoisoquinolin-1(2H)-one (5f)



Light yellow oil; 52 mg in 0.2 mmol scale, 80% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.32 (d, *J* = 8.0 Hz, 1 H), 7.65-7.57 (m, 2 H), 7.46-7.42 (m, 2 H), 3.90 (t, *J* = 7.4 Hz, 2 H), 1.68 (dt, *J* = 15.1, 7.5 Hz, 2 H), 1.33 (dq, *J* = 14.8, 7.4 Hz, 2 H), 0.89 (t, *J* = 7.4 Hz, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ =

161.5, 138.0, 137.1, 133.1, 130.3, 128.2, 127.7, 126.7, 71.4, 49.1, 31.5, 20.0, 13.7 ppm; HRMS $[M+H]^+$ calculated for $C_{13}H_{15}OIN^+$: 328.0193, found: 328.0189.

4-iodo-2-(naphthalen-1-ylmethyl)isoquinolin-1(2H)-one (5g)



Off-white solid; 48 mg in 0.2 mmol scale, 58% yield; m. p. 137-138 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.41 (dd, J = 8.0, 0.7 Hz, 1 H), 7.99-7.94 (m, 1 H), 7.79-7.71 (m, 2 H), 7.63-7.57 (m, 1 H), 7.52 (d, J = 7.6 Hz, 1 H), 7.46-7.39 (m, 3 H), 7.36-7.32 (m, 2 H), 7.24 (d, J = 6.9 Hz, 1 H), 5.56 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ =

161.5, 137.1, 136.8, 134.0, 133.4, 131.6, 131.3, 130.5, 129.3, 128.9, 128.6, 127.9, 127.2, 127.1, 126.6, 126.3, 125.4, 123.3, 72.4, 48.7 ppm; HRMS $[M+H]^+$ calculated for $C_{20}H_{15}OIN^+$: 412.0193, found: 412.0194.

4-iodo-2-(4-nitrobenzyl)isoquinolin-1(2H)-one (5h)



Yellow solid; 39 mg in 0.2 mmol scale, 48% yield; m. p. 166-167 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.40 (d, J = 8.0 Hz, 1 H), 8.18 (d, J = 8.6 Hz, 2 H), 7.75 (t, J = 7.6 Hz, 1 H), 7.68 (d, J = 7.9 Hz, 1 H), 7.58-7.55 (m, 2 H), 7.48 (d, J = 8.6 Hz, 2 H), 5.26 (s, 2 H) ppm; ¹³C

NMR (100 MHz, CDCl₃) δ = 161.5, 155.6, 147.7, 143.6, 137.1, 133.7, 130.7, 128.6, 128.4, 128.3, 126.4, 124.1, 72.9, 51.4 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₂O₃IN₂⁺: 406.9887, found: 406.9893.

4-iodo-2-methyl-6-phenylisoquinolin-1(2H)-one (5i)

Orange solid; 55 mg in 0.2 mmol scale, 76% yield; m. p. 170-171 °C; ¹H NMR (400



MHz, CDCl₃) δ = 8.42 (d, *J* = 8.3 Hz, 1 H), 7.80 (d, *J* = 1.5 Hz, 1 H), 7.70 (ddd, *J* = 8.6, 7.8, 3.5 Hz, 3 H), 7.52-7.47 (m, 3H), 7.42 (ddd, *J* = 7.3, 3.7, 1.1 Hz, 1 H), 3.58 (s, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.8, 145.9, 139.8, 139.1, 137.5, 129.0, 128.8, 128.6, 128.4, 127.6, 126.9, 125.3, 71.6, 36.8 ppm; HRMS [M+H]⁺ calculated for C₁₆H₁₃OIN⁺:

362.0036, found: 362.0034.

2-(4-bromobenzyl)-4-iodoisoquinolin-1(2H)-one (5j)



White solid; 67 mg in 0.2 mmol scale, 76% yield; m. p. 114-115 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.41 (dd, *J* = 8.0, 0.8 Hz, 1H), 7.74-7.69 (m, 1 H), 7.65 (d, *J* = 7.4 Hz, 1 H), 7.55-7.50 (m, 2 H), 7.47-7.44 (m, 2 H), 7.21 (d, *J* = 8.4 Hz, 2 H), 5.12 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.6, 137.3, 137.1, 135.4, 133.4,

132.1, 130.6, 129.7, 128.4, 128.1, 126.6, 122.2, 72.4, 51.3 ppm; HRMS $[M+H]^+$ calculated for $C_{16}H_{12}BrOIN^+$: 439.9141, found: 439.9149.

2-(3-chlorobenzyl)-4-iodoisoquinolin-1(2H)-one (5k)



Off-white solid; 43 mg in 0.2 mmol scale, 54% yield; m. p. 97-98 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.42 (d, J = 8.0 Hz, 1 H), 7.74-7.70 (m, 1 H), 7.65 (d, J = 8.0 Hz, 1H), 7.55-7.51 (m, 2 H), 7.32 (s, 1 H), 7.26 (d, J = 5.2 Hz, 2 H), 7.21 (dd, J = 8.8, 3.5 Hz, 1 H), 5.14 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.6, 138.4,

137.3, 137.1, 134.8, 133.5, 130.6, 130.2, 128.5, 128.4, 128.1, 128.0, 126.6 126.1, 72.5, 51.3 ppm; HRMS $[M+H]^+$ calculated for $C_{16}H_{12}CIOIN^+$: 395.9647, found: 395.9654.

2-(2-bromobenzyl)-4-iodoisoquinolin-1(2H)-one (5l)



Grey solid; 43 mg in 0.2 mmol scale, 49% yield; m. p. 169-170 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.43 (dd, *J* = 8.0, 0.8 Hz, 1 H), 7.72 (ddd, *J* = 19.2, 13.1, 4.3 Hz, 2 H), 7.61-7.52 (m, 3 H), 7.28-7.24 (m, 1 H), 7.19-7.14 (m, 2 H), 5.30 (s, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.7, 137.7, 137.2, 135.4, 133.4, 133.1, 130.6, 129.6, 129.5, 128.5, 128.0, 126.6,

123.3, 72.2, 51.6 ppm; HRMS $[M+H]^+$ calculated for $C_{16}H_{12}BrOIN^+$: 439.9141, found: 439.9142.

2,2'-(butane-1,4-diyl)bis(4-iodoisoquinolin-1(2*H*)-one) (5m)

Light yellow solid; 14 mg in 0.1 mmol scale, 23% yield; m. p. 237-238 °C; ¹H NMR



(400 MHz, CDCl₃) $\delta = 8.41$ (d, J = 8.0 Hz, 1 H), 7.72 (t, J = 7.5 Hz, 1 H), 7.66 (d, J = 8.0 Hz, 1 H), 7.58-7.51 (m, 2 H), 4.08 (t, J = 6.0 Hz, 2 H), 1.86 (t, J = 6.4 Hz, 2 H) ppm; ¹³C NMR (100 MHz, CDCl₃) $\delta = 161.6$, 137.8, 137.1, 133.2, 130.4, 128.2, 127.9, 126.6, 71.9, 48.3, 26.3 ppm; HRMS [M+H]⁺ calculated for C₂₂H₁₉O₂I₂N₂⁺:

596.9530, found: 596.9526.

2-(4-(tert-butyl)benzyl)-4-iodoisoquinolin-1(2H)-one (5n)



White solid; 56 mg in 0.2 mmol scale, 67% yield; m. p. 176-177 °C; ¹H NMR (400 MHz, CDCl₃) δ = 8.43 (d, *J* = 8.0 Hz, 1 H), 7.71-7.67 (m, 1 H), 7.63 (d, *J* = 7.6 Hz, 1 H), 7.52 (dd, *J* = 14.2, 6.3 Hz, 2 H), 7.36 (d, *J* = 8.4 Hz, 2 H), 7.28-7.24 (m, 2 H), 5.15 (s, 2 H), 1.29 (s, 9 H) ppm;

¹³C NMR (100 MHz, CDCl₃) δ = 161.6, 151.1, 137.7, 137.1, 133.4, 133.2, 130.4, 128.5, 127.9, 127.8, 126.8, 125.9, 72.0, 51.5, 34.6, 31.3 ppm; HRMS [M+H]⁺ calculated for C₂₀H₂₁OIN⁺: 418.0662, found: 418.0665.

4-iodo-2-(3-phenylpropyl)isoquinolin-1(2H)-one (50)



yellow oil; 51 mg in 0.2 mmol scale, 66% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.39 (d, *J* = 8.0 Hz, 1 H), 7.70-7.62 (m, 2 H), 7.50 (t, *J* = 7.4 Hz, 1 H), 7.41 (s, 1 H), 7.27 (t, *J* = 7.4 Hz, 2 H), 7.19 (d, *J* = 7.3 Hz, 3 H), 3.98 (t, *J* = 7.3 Hz, 2 H), 2.70 (t, *J* = 7.6 Hz, 2 H), 2.15-2.08 (m, 2 H)

ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 161.5, 140.7, 138.0, 137.1, 133.1, 130.3, 128.6, 128.4, 128.2, 127.8, 126.7, 126.2, 71.5, 49.0, 32.9, 30.5 ppm; HRMS [M+H]⁺ calculated for C₁₈H₁₇OIN⁺: 390.0349, found: 390.0349.

4-bromo-2-propylisoquinolin-1(2H)-one (5q)



Colorless liquid; 14 mg in 0.2 mmol scale, 26% yield; ¹H NMR (400 MHz, CDCl₃) δ = 8.46-8.44 (m, 1 H), 7.81 (d, *J* = 7.8 Hz, 1 H), 7.76-7.72 (m, 1 H), 7.57-7.53 (m, 1 H), 7.35 (s, 1 H), 3.98-3.94 (m, 2 H), 1.82 (dd, *J* = 14.8, 7.4 Hz, 2 H), 0.99 (t, *J* = 7.4 Hz, 3 H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ 161.2, 135.4, 132.8, 132.3, 128.3, 127.7, 126.6, 125.8, 99.6, 51.0,

22.6, 11.2 ppm; HRMS $[M+Na]^+$ calculated for $C_{12}H_{13}^{79}BrNNaO^+$: 287.9994 and $C_{12}H_{13}^{81}BrNNaO^+$: 289.9979 found: 287.9994 and 289.9974.

1,2-phenylenebis(phenylmethanone)



yellow solid; ¹H NMR (400 MHz, CDCl₃) δ = 7.70 (d, *J* = 7.7 Hz, 4 H), 7.61 (s, 4 H), 7.50 (t, *J* = 7.4 Hz, 2 H), 7.36 (t, *J* = 7.7 Hz, 4H) ppm; ¹³C NMR (100 MHz, CDCl₃) δ = 196.6, 140.1, 137.2, 133.0, 130.4, 129.8, 129.7, 128.3 ppm; HRMS [M+H]⁺ calculated for C₂₀H₁₅O₂⁺: 287.1067, found: 287.1070.

NMR spectra of all compounds The ¹H NMR and ¹³C NMR spectra of 1aa



The ¹H NMR and ¹³C NMR spectra of 1ab



The ¹H NMR and ¹³C NMR spectra of 1b



The ¹H NMR and ¹³C NMR spectra of 1c



The ¹H NMR and ¹³C NMR spectra of 1d



The ¹H NMR and ¹³C NMR spectra of 1e



The ¹H NMR and ¹³C NMR spectra of 1f



The ¹H NMR and ¹³C NMR spectra of 1g



The ¹H NMR and ¹³C NMR spectra of 1h



The ¹H NMR and ¹³C NMR spectra of 1i


The ¹H NMR and ¹³C NMR spectra of 1j



The ¹H NMR and ¹³C NMR spectra of 1k



The ¹H NMR and ¹³C NMR spectra of 11



The ¹H NMR and ¹³C NMR spectra of 1m



The ¹H NMR and ¹³C NMR spectra of 1n





The ¹H NMR and ¹³C NMR spectra of 10



The ¹H NMR and ¹³C NMR spectra of 1p



The ¹H NMR and ¹³C NMR spectra of 1q



The ¹H NMR and ¹³C NMR spectra of 1r



The ¹H NMR and ¹³C NMR spectra of 1s



The ¹H NMR and ¹³C NMR spectra of 2a





The ¹H NMR and ¹³C NMR spectra of 2b



The ¹H NMR and ¹³C NMR spectra of 2c



The ¹H NMR and ¹³C NMR spectra of 2d



The ¹H NMR and ¹³C NMR spectra of 2e



The ¹H NMR and ¹³C NMR spectra of 2fa



The ¹H NMR and ¹³C NMR spectra of 2fb



The ¹H NMR and ¹³C NMR spectra of 2g



The ¹H NMR and ¹³C NMR spectra of 2h



The ¹H NMR and ¹³C NMR spectra of 2i



The ¹H NMR and ¹³C NMR spectra of 2j



The ¹H NMR and ¹³C NMR spectra of 2k



The ¹H NMR and ¹³C NMR spectra of 2l



The ¹H NMR and ¹³C NMR spectra of 3a



The ¹H NMR and ¹³C NMR spectra of 3b



The ¹H NMR and ¹³C NMR spectra of 3c



The ¹H NMR and ¹³C NMR spectra of 3d



The ¹H NMR and ¹³C NMR spectra of 3e



The ¹H NMR and ¹³C NMR spectra of 3f



The ¹H NMR and ¹³C NMR spectra of 3g



The ¹H NMR and ¹³C NMR spectra of 3h



The ¹H NMR and ¹³C NMR spectra of 3i



The ¹H NMR and ¹³C NMR spectra of 3j



The ¹H NMR and ¹³C NMR spectra of 3k



The ¹H NMR and ¹³C NMR spectra of 31



The ¹H NMR and ¹³C NMR spectra of 3m


The ¹H NMR and ¹³C NMR spectra of 3n



The ¹H NMR and ¹³C NMR spectra of 30



The ¹H NMR and ¹³C NMR spectra of 3p



The ¹H NMR and ¹³C NMR spectra of 3q



The ¹H NMR and ¹³C NMR spectra of 3r



The ¹H NMR and ¹³C NMR spectra of 3s



The ¹H NMR and ¹³C NMR spectra of 4a



The ¹H NMR and ¹³C NMR spectra of 4b



The ¹H NMR and ¹³C NMR spectra of 4c



The ¹H NMR and ¹³C NMR spectra of 4d



The ¹H NMR and ¹³C NMR spectra of 4e









SI-85



90 80 f1 (ppm) -100











The ¹H NMR and ¹³C NMR spectra of 4k

SI-89



The ¹H NMR and ¹³C NMR spectra of 5a



The ¹H NMR and ¹³C NMR spectra of 5b



The ¹H NMR and ¹³C NMR spectra of 5c



The ¹H NMR and ¹³C NMR spectra of 5d



The ¹H NMR and ¹³C NMR spectra of 5e



The ¹H NMR and ¹³C NMR spectra of 5f



The ¹H NMR and ¹³C NMR spectra of 5g



The ¹H NMR and ¹³C NMR spectra of 5h



The ¹H NMR and ¹³C NMR spectra of 5i



The ¹H NMR and ¹³C NMR spectra of 5j



The ¹H NMR and ¹³C NMR spectra of 5k



The ¹H NMR and ¹³C NMR spectra of 5l



The ¹H NMR and ¹³C NMR spectra of 5m



The ¹H NMR and ¹³C NMR spectra of 5n



The ¹H NMR and ¹³C NMR spectra of 50



The ¹H NMR and ¹³C NMR spectra of 5q



The ¹H NMR and ¹³C NMR spectra of 1, 2-dibenzoylbenzene

