Supporting Information

Photogenerated chlorine radical activates C(sp³)-H bonds of

alkylbenzenes to access quinazolinones

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I. General information

NMR spectra were obtained on a BRUKER Ascend 500. Chemical shifts were recorded in parts per million (ppm, δ) relative to tetramethylsilane (δ 0.00). 1H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublets); m (multiplets), and etc. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). The ¹H NMR (500 MHz) chemical shifts were measured relative to CDCl₃ or DMSO-d₆ as the internal reference (CDCl₃: δ = 7.26 ppm; DMSO-d₆: δ = 2.50 ppm). The ¹³C NMR (125 MHz) chemical shifts were given using CDCl₃ or DMSO-d₆ the internal standard (CDCl₃: δ = 77.00 ppm; DMSO-d₆: δ = 39.52 ppm). Highresolution mass spectra (HR-MS) were obtained with a BRUKER solanX 70 FT-MS (ESI⁺). Flash chromatography was performed using Qingdao Haiyang silica gel 300-400 with distilled solvents. Visualization was performed using a UV lamp. UV–vis absorption spectra were measured in the wavelength range of 250–800 nm using a Perkin-Elmer Lambda 750 UV/Visible Spectrometer.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification.

Photoreactor configuration:

The 25 W 450-460 nm LED lamps were purchased from FacaiLEDzhaoming (https://shop358870690.taobao.com/index.htm?spm=2013.1.w5002-

15754154505.2.1ef84d30UkiJ8U). Reactions were irradiated by using a simple photoreactor consisting of two 25 W 450-460 nm LED lamps with a magnetic stirrer. The distance between blue lamp and the reaction tube was 8 cm.

Manufacturer: Xuzhou Aijia Electronic Technology Co., Ltd

Wavelength of peak intensity: 450-460 nm

Material of the irradiation vessel (15 mL Schlenk tubes): borosilicate glass.

Distance of the irradiation vessel from the light source: approximately 8 cm.

No use any filters.

Reaction Setup:



II. Additional Optimization Experiments

General Procedure for optimization of catalyst:

To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), and catalyst (0.02 mmol, 10 mol%), then a mixture solvent of toluene (1 mL) and CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at 65 °C. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a**.

Table S1.	Optimization	of catalyst.
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NH ₂ +	CH ₃ Catalyst, S blue LED	olvent, Temperature s 450-460 nm × 2
1a 	2a	3a
Entry	Catalyst	Yield/%
1	Dy(NO ₃) ₃	30
2	CuI	0
3	Sc(CF ₃ SO ₃) ₃	0
4	CeCl ₃ •7H ₂ O	35
5	Ce(NO ₃) ₃ •6H ₂ O	30
6	$Ce(SO_4)_2 \cdot 4H_2O$	10
7	Ce(OTf) ₃	50
8°	HC1	45%
9°	CF ₃ CH ₂ OH	5%
10 ^c	CF ₃ SO ₃ H	26%

11^d FeCl₃•6H₂O 83%

^aReactions conditions: **1a** (0.2 mmol), **2a** (1 mL), cat. (10 mol%), air atmosphere, in CH₃CN (1 mL) at 65 °C under irradiation of 25 W blue LEDs \times 2 for 12 h. ^bIsolated yield. ^c1 eq. Lewis acid was used. ^dAnhydrous toluene and ultra-dry acetonitrile are used for the reaction.

General Procedure for optimization of additive:

To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), additive (1 eq.) and FeCl₃ (0.02 mmol, 10 mol%), then a mixture solvent of toluene (1 mL) and CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at 65 °C. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a**.

Table S2. Optimization of additive.

	NH ₂ +	CH ₃ Catalyst, blue LE	Solvent, Temperature Ds 450-460 nm × 2	NH NH
1a		2a		3a 🦷
Entry	Catalyst	Solvent	Additive	Yield/%
1	FeCl ₃	CH ₃ CN	<i>n</i> Bu ₄ NCl	45
2	FeCl ₃	CH ₃ CN	NH ₄ Cl	30
3	FeCl ₃	CH ₃ CN	NaCl	10
aReactio	ons conditions:	1a (0.2 mmol), 2a (1 m	mL), FeCl ₃ (10 mol%), a	dditive (1 eq.) air

atmosphere, in CH₃CN (1 mL) at 65 °C under irradiation of 25 W blue LEDs \times 2 for 12 h. ^bIsolated yield.

General Procedure for optimization of solvent:

To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), **2a** (1 mL), and FeCl₃ (0.02 mmol, 10 mol%), then solvent was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at 65 °C. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a**.

Table S3. Optimization of solvent.



3	FeCl ₃	DCM	20
4	FeCl ₃	DMSO	50
5	FeCl ₃	CH ₃ OH	40
6	FeCl ₃	1,4-dioxane	5
7	FeCl ₃	DMF	0
8	FeCl ₃	H_2O	30
9°	FeCl ₃	CH ₃ CN	20
10 ^d	FeCl ₃	CH ₃ CN	68
11 ^e	FeCl ₃	CH ₃ CN	69
12 ^f	FeCl ₃	CH ₃ CN	10
^a Reactions conditions: 1a (0.2 mmol), 2a (1 mL), FeCl ₃ (10 mol%), air atmosphere, in solvent			
(1 mL) at 65 °C under irradiation of 25 W blue LEDs \times 2 for 12 h. ^b Isolated yield. ^c A mixture			

solvent of toluene (0.5 mL) and CH ₃ CN (1 mL) was used. ^d A mixture solvent of toluene (1.5
mL) and CH ₃ CN (1 mL) was used. ^e A mixture solvent of toluene (2 mL) and CH ₃ CN (1 mL)
was used. ^f A mixture solvent of toluene (10 eq., 0.21 mL) and CH ₃ CN (1 mL) was used.

III. General Procedure for Oxidative Synthesis of Quinazolin-4(3H)-

ones



To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1** (27.2 mg, 0.2 mmol), **2** (1 mL) or **4** (1.2 eq.), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 5-12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-ones **3**.

General procedure for Oxidative Synthesis of Quinazolin-4(3H)-ones in large-scale.



To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (1.3606 g, 10 mmol), **2** (10 mL), and FeCl₃ (1 mmol, 10 mol%), then CH₃CN (10 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 24 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a** in yield of 75%.

IV. Controlled experiments

To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), **5a** (1.2 eq.), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 5-12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a** in yield of 90%.

To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), and **5a** (1.2 eq.), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 5-12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a** in yield of 90%.



To a 15 mL silica tube containing a magnetic stir bar, was added 2-(benzylamino)benzamide **6a** (45.2 mg, 0.2 mmol), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a** in yield of 90%.

To a 15 mL silica tube containing a magnetic stir bar, was added 2-amino-Nbenzylbenzamide **6b** (45.2 mg, 0.2 mmol), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a** in yield of 0%.



To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), **2a** (1 mL), 2,2,6,6-tetramethyl-1-piperinedinyloxy (TEMPO) (0.4 mmol), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a** in yield of 0%, and **7a** was detected by HRMS.

To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), **2a** (1 mL), ethene-1,1-diyldibenzene (0.4 mmol), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a** in trace yield.





7c, detected by HRMS $[M+H]^+$ calcd. for $C_9H_{19}NOCI$ 192.1150 found 192.1155

To a 15 mL silica tube containing a magnetic stir bar, was added 2a (1 mL), 2,2,6,6-tetramethyl-1-piperinedinyloxy (TEMPO) (0.4 mmol), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at room temperature. **7a** and **7c** were found in the reaction mixture by HRMS.



To a 15 mL silica tube containing a magnetic stir bar, was added 2a (1 mL), ethene-1,1-diyldibenzene (0.4 mmol), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at room temperature. **7b** and **7d** were found in the reaction mixture by GCMS.

To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), **2a** (1 mL), activated molecular sieves (powder, 4Å) (0.7 g), and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3*H*)-one **3a** in yield of 0.



To a 15 mL silica tube containing a magnetic stir bar, was added 2-aminobenzamide **1a** (27.2 mg, 0.2 mmol), **2a** (1 mL), benzoquinone(43 mg, 0.4 mmol) and FeCl₃ (0.02 mmol, 10 mol%), then CH₃CN (1 mL) was added under atmosphere of air. The mixture was stirred at 1400 RPM for 12 h under irradiation by blue LEDs at room temperature. The reaction mixture was concentrated under reduced pressure and purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford quinazolin-4(3H)-one **3a** in trace yield.

UV-vis studies

Sample preparation

FeCl₃ (6.48 mg, 0.04 mmol) was dissolved in 2.0 mL of acetonitrile.

FeCl₃ (6.48 mg, 0.04 mmol) was dissolved in 1 mL of 2a and 1.0 mL of acetonitrile.

1a (27.2 mg, 0.2 mmol) was dissolved in 2.0 mL of acetonitrile.

FeCl₃ (6.48 mg, 0.04 mmol) and 1a (27.2 mg, 0.2 mmol) were dissolved in 2.0 mL of acetonitrile.

FeCl₃ (6.48 mg, 0.04 mmol) and 1a (27.2 mg, 0.2 mmol) were dissolved in 1 mL of 2a and 1.0 mL of acetonitrile.

1a (27.2 mg, 0.2 mmol) was dissolved in 1 mL of 2a and 1.0 mL of acetonitrile.

The resultant solution was stirred for 15 minutes, and a 2.0 mL aliquot was drawn and added in a quartz cuvette.



 λ/nm

V. Characterizations of Products



2-Phenylquinazolin-4(3H)-one (3a)^[1]:

Following the general procedure, compound **3a** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 35.5 mg, 80% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.54 (s, 1H), 8.17 (dd, *J* = 12.8, 7.7 Hz, 3H), 7.83 (t, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.55 (ddt, *J* = 21.6, 14.8, 7.2 Hz, 4H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.7, 152.8, 149.3, 135.1, 133.2, 131.9, 129.1, 128.3, 128.0, 127.1, 126.3, 121.5 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₄H₁₁N₂O 223.0866; found 223.0868.



6-Fluoro-2-phenylquinazolin-4(*3H*)-one (**3b**)^[2]:

Following the general procedure, compound **3b** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 42.3 mg, 88% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.66 (s, 1H), 8.20 – 8.11 (m, 2H), 7.81 (dt, J = 8.2, 3.8 Hz, 2H), 7.71 (td, J = 8.8, 2.9 Hz, 1H), 7.56 (dt, J = 15.0, 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.2 (d, J = 3.5 Hz), 160.5 (d, J = 245.5 Hz), 152.4, 146.2, 133.1, 132.0, 130.9 (d, J = 8.6 Hz), 129.2, 128.3, 123.6 (d, J = 24.1 Hz), 122.7 (d, J = 8.7 Hz), 111.1 (d, J = 23.1 Hz) ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₄H₉FN₂O 241.0772; found 241.0775.



6-Chloro-2-phenylquinazolin-4(*3H*)-one (**3c**)^[1]:

Following the general procedure, compound 3c was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 44.0 mg, 86% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.72 (s, 1H), 8.17 (d, *J* = 6.9 Hz, 2H), 8.09 (s, 1H), 7.87 (d, *J* = 8.7 Hz, 1H), 7.77 (d, *J* = 8.7 Hz, 1H), 7.57 (dt, *J* = 15.1, 7.3 Hz, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.9, 153.4, 148.0, 135.3, 133.0, 132.1, 131.3,

130.3, 129.2, 128.4, 125.4, 122.8 ppm. HRMS (ESI-TOF) $[M+H]^+$ calcd. for $C_{14}H_{10}ClN_2O$ 257.0476; found 257.0475.



6-Bromo-2-phenylquinazolin-4(*3H*)-one (**3d**)^[1]:

Following the general procedure, compound **3d** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 53.4 mg, 89% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.72 (s, 1H), 8.23 (s, 1H), 8.17 (d, *J* = 6.7 Hz, 2H), 7.98 (d, *J* = 11.1 Hz, 1H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.57 (dt, *J* = 14.9, 7.2 Hz, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.7, 153.5, 148.3, 138.0, 133.0, 132.2, 130.4, 129.2, 128.5, 128.4, 123.1, 119.5 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₄H₁₀BrN₂O 300.9971; found 300.9975.



7-Methyl-2-phenylquinazolin-4(3H)-one (**3e**)^[1]:

Following the general procedure, compound 3e was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 38.2 mg, 81% yield, yellow solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.43 (s, 1H), 8.16 (d, *J* = 7.2 Hz, 2H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.61 – 7.49 (m, 4H), 7.32 (d, *J* = 8.1 Hz, 1H), 2.45 (s, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.6, 152.8, 149.3, 145.6, 133.2, 131.8, 129.1, 128.5, 128.2, 127.6, 126.2, 119.0, 21.8 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₅H₁₃N₂O 237.1022; found 237.1032.



3-Methyl-2-phenylquinazolin-4(*3H*)-one (**3f**)^[1]:

Following the general procedure, compound **3f** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 41.6 mg, 88% yield, white solid.

¹H NMR (500 MHz, CDCl₃) δ 8.33 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 7.1 Hz, 2H), 7.61 – 7.44 (m, 6H), 3.49 (s, 3H) ppm. ¹³C{¹H} NMR (125 MHz, CDCl₃) δ 162.7, 156.1, 147.3, 135.4, 134.3, 130.1, 128.9, 128.0, 127.5, 127.0, 126.7, 120.5, 34.2 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₅H₁₃N₂O 237.1022; found 237.1031.



3-Phenyl-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (**3g**)^[3]:

Following the general procedure, compound 3g was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 40.3 mg, 78% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.21 (s, 1H), 8.04 (d, *J* = 7.6 Hz, 2H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.72 (dt, *J* = 15.8, 7.6 Hz, 2H), 7.64 (d, *J* = 7.6 Hz, 3H), 7.51 (t, *J* = 7.6 Hz, 1H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 155.4, 136.0, 133.7, 133.4, 132.4, 129.4, 128.8, 127.3, 123.9, 122.0, 119.0 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₃H₁₁N₂O₂S 259.0536; found 259.0532.



3-(4-Chlorophenyl)-2*H*-benzo[e][1,2,4]thiadiazine 1,1-dioxide (**3h**)^[3]:

Following the general procedure, compound **3h** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 23.3 mg, 40% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.26 (s, 1H), 8.13 – 8.03 (m, 2H), 7.91 – 7.83 (m, 1H), 7.78 – 7.68 (m, 3H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.52 (t, *J* = 7.7 Hz, 1H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 154.2, 138.3, 135.9, 133.7, 131.1, 130.7, 129.5, 127.4, 123.9, 122.0, 119.0 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₃H₁₀ClN₂O₂S 293.0146; found 293.0150.



3-(4-Fluorophenyl)-3,4-dihydro-2*H*-benzo[*e*][1,2,4]thiadiazine 1,1-dioxide (**3i**)^[4]: Following the general procedure, compound **3i** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 28.5 mg, 52.2% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 7.92 (d, J = 11.7 Hz, 1H), 7.77 – 7.64 (m, 2H), 7.53 (d, J = 7.9 Hz, 1H), 7.40 (s, 1H), 7.30 (t, J = 8.8 Hz, 3H), 6.90 (d, J = 8.3 Hz, 1H), 6.77 (t, J = 7.5 Hz, 1H), 5.80 (d, J = 11.5 Hz, 1H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.87 (d, J = 245.2 Hz), 145.06, 134.14 (d, J = 3.0 Hz), 133.37, 130.32 (d, J = 8.4 Hz), 124.23, 122.74, 117.32, 116.84, 115.80 (d, J = 21.5 Hz), 67.50. HRMS (ESI-TOF) m/z: [M+H]⁺ Calcd for C₁₃H₁₁FN₂O₂S 279.0582; Found 279.0598.



3-(4-Methoxyphenyl)-3,4-dihydro-2*H*-benzo[*e*][1,2,4]thiadiazine 1,1-dioxide (**3j**)^[4]: Following the general procedure, compound **3j** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 24 mg, 41.4% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 7.87 (d, *J* = 11.1 Hz, 1H), 7.52 (s, 1H), 7.37 (s, 2H), 7.29 (s, 2H), 7.21 (s, 1H), 6.99 (s, 1H), 6.90 (s, 1H), 6.76 (s, 1H), 5.74 (d, *J* = 10.5 Hz, 1H), 3.78 (s, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 159.8, 144.3, 139.2, 130.1, 122.0, 120.3, 117.2, 116.8, 115.4, 113.3, 68.8, 55.7 ppm. HRMS (ESI-TOF) m/z: [M+H]⁺ Calcd for C₁₄H₁₄N₂O₃S 291.0782; Found 291.0798.



 $3-(p-\text{Tolyl})-3,4-\text{dihydro}-2H-\text{benzo}[e][1,2,4]\text{thiadiazine}1,1-\text{dioxide}(3\mathbf{k})^{[4]}$:

Following the general procedure, compound **3k** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 27.4 mg, 50% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 7.83 (d, *J* = 11.4 Hz, 1H), 7.60 – 7.44 (m, 3H), 7.38 – 7.18 (m, 4H), 6.89 (d, *J* = 7.9 Hz, 1H), 6.75 (t, *J* = 7.3 Hz, 1H), 5.72 (d, *J* = 12.1 Hz, 1H), 2.33 (s, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 144.4, 138.1, 134.9, 133.3, 130.0, 127.9, 124.2, 122.3, 117.1, 116.8, 68.7, 21.3 ppm. HRMS (ESI-TOF) m/z: [M+H]⁺ Calcd for C₁₄H₁₄N₂O₂S 275.0836; Found 275.0849.



2-(*o*-Tolyl)quinazolin-4(*3H*)-one (**3l**)^[1]:

Following the general procedure, compound **3l** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 28.3 mg, 60% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.44 (s, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 7.86 – 7.80 (m, 1H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.57 – 7.48 (m, 2H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.38 – 7.30 (m, 2H), 2.38 (s, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.3, 154.9, 149.3, 136.6, 135.0, 134.6, 131.1, 130.4, 129.7, 127.9, 127.2, 126.31, 126.23, 121.5, 20.1 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₅H₁₃N₂O 237.1022; found 237.1028.



2-(m-Tolyl)quinazolin-4(3H)-one $(3m)^{[5]}$:

Following the general procedure, compound **3m** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 24.6 mg, 52% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.47 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 8.02 (s, 1H), 7.97 (d, *J* = 7.5 Hz, 1H), 7.83 (t, *J* = 7.7 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.41 (dt, *J* = 13.5, 7.6 Hz, 2H), 2.40 (s, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.7, 152.9, 149.3, 138.5, 135.1, 133.2, 132.5, 129.0, 128.8, 128.0, 127.1, 126.4, 125.4, 121.5, 21.5 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₅H₁₃N₂O 237.1022; found 237.1029.



2-(*p*-Tolyl)quinazolin-4(*3H*)-one (**3n**)^[1]:

Following the general procedure, compound **3n** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 24.6 mg, 52% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.48 (s, 1H), 8.14 (d, *J* = 6.3 Hz, 1H), 8.09 (d, *J* = 6.5 Hz, 2H), 7.87 – 7.79 (m, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.57 – 7.45 (m, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.39 (s, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO) δ 162.8, 152.8, 149.3, 142.0, 135.1, 130.4, 129.7, 128.2, 127.9, 126.9, 126.4, 121.4, 21.5 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₅H₁₃N₂O 237.1022; found 237.1023.



2-(2-Methoxyphenyl)quinazolin-4-(3H)-one (**3o**)^[6]:

Following the general procedure, compound **30** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 26.2 mg, 52% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.12 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.83 (t, *J* = 7.7 Hz, 1H), 7.70 (d, *J* = 7.7 Hz, 2H), 7.53 (s, 2H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 3.86 (s, 3H).¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 161.9, 157.7, 152.9, 149.6, 135.1, 132.8, 131.0, 128.0, 127.2, 126.4, 123.2, 121.6, 121.0, 112.5, 56.4 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₅H₁₃N₂O₂ 253.0972; found 253.0975.



2-(3-Methoxyphenyl)quinazolin-4(3H)-one (**3p**)^[2]:

Following the general procedure, compound **3p** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 35.8 mg, 71% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.55 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.86 – 7.81 (m, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 2H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.14 (d, *J* = 8.4 Hz, 1H), 3.86 (s, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.8, 159.9, 152.6, 149.2, 135.2, 134.5, 130.3, 128.1, 127.2, 126.4, 121.5, 120.7, 118.1, 113.0, 55.9, ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₅H₁₃N₂O₂ 253.0972; found 253.0974.



2-(4-Methoxyphenyl)quinazolin-4-(*3H*)-one (**3q**)^[1]:

Following the general procedure, compound 3q was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 34.8 mg, 69% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.42 (s, 1H), 8.19 (d, *J* = 8.9 Hz, 2H), 8.13 (d, *J* = 7.9 Hz, 1H), 7.85 – 7.77 (m, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 9.0 Hz, 2H), 3.85 (s, 3H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.9, 162.4, 152.4, 149.4, 135.1, 130.0, 127.8, 126.7, 126.4, 125.3, 121.2, 114.5, 56.0 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₅H₁₃N₂O₂ 253.0972; found 253.0975.



2-(4-Fluorophenyl)quinazolin-4(3H)-one (**3r**)^[1]:

Following the general procedure, compound $3\mathbf{r}$ was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 32.2 mg, 67% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.56 (s, 1H), 8.28 – 8.20 (m, 2H), 8.15 (d, *J* = 8.0 Hz, 1H), 7.83 (t, *J* = 8.4 Hz, 1H), 7.73 (d, *J* = 8.2 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.39 (d, *J* = 8.6 Hz, 2H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO) δ 164.6 (d, *J* = 249.8 Hz), 162.8, 151.9, 149.2, 135.2, 130.9 (d, *J* = 9.1 Hz), 129.8 (d, *J* = 3.0 Hz), 128.0, 127.2, 126.4, 121.4, 116.2 (d, *J* = 22.0 Hz) ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₄H₁₀FN₂O 241.0772; found 241.0780.



2-(4-Chlorophenyl)quinazolin-4(3*H*)-one (3s)^[1]:

Following the general procedure, compound **3s** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 35.8 mg, 70% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.61 (s, 1H), 8.17 (dd, *J* = 23.3, 8.5 Hz, 3H), 7.84 (t, *J* = 7.9 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.53 (t, *J* = 7.6 Hz, 1H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 163.8, 156.5, 151.9, 136.8, 135.2, 132.1, 130.1, 129.2, 128.0, 127.3, 126.4, 121.5 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₄H₉ClN₂O 257.0476; found 257.0480.



2-(4-Bromophenyl)quinazolin-4(3*H*)-one (**3t**)^[1]:

Following the general procedure, compound **3t** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 43.8 mg, 73% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.62 (s, 1H), 8.17 – 8.08 (m, 3H), 7.84 (t, *J* = 7.7 Hz, 1H), 7.74 (t, *J* = 8.9 Hz, 3H), 7.53 (t, *J* = 7.6 Hz, 1H) ppm. ¹³C NMR (125 MHz, DMSO-*d*₆) δ 162.8, 152.1, 145.8, 135.2, 132.4, 132.1, 130.3, 128.0, 127.3, 126.4, 125.9, 121.8 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₄H₉BrN₂O 300.9971; found 300.9975.



2-(4-Isopropylphenyl)quinazolin-4(3H)-one (**3u**)^[7]:

Following the general procedure, compound 3u was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 26.4 mg, 50% yield, white solid.

¹H NMR (500 MHz, CDCl₃) δ 11.84 (s, 1H), 8.34 (d, J = 8.4 Hz, 1H), 8.21 (d, J = 8.2 Hz, 2H), 7.81 (dd, J = 14.1, 8.5 Hz, 2H), 7.50 (t, J = 7.4 Hz, 1H), 7.43 (d, J = 8.3 Hz, 2H), 3.02 (p, J = 6.8 Hz, 1H), 1.32 (d, J = 7.0 Hz, 6H) ppm. ¹³C{¹H} NMR (125 MHz, CDCl₃) δ 164.2, 152.9, 152.0, 149.6, 134.8, 130.2, 127.8, 127.6, 127.0, 126.5, 126.3, 120.7, 34.1, 23.7 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₇H₁₇N₂O 265.1335; found 265.1340.



2-(Naphthalen-2-yl)quinazolin-4(3H)-one (3v)^[1]:

Following the general procedure, compound 3v was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 28.3 mg, 52% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.67 (s, 1H), 8.81 (s, 1H), 8.30 (d, J = 8.6 Hz, 1H), 8.18 (d, J = 7.9 Hz, 1H), 8.06 (t, J = 7.4 Hz, 2H), 8.01 (d, J = 7.0 Hz, 1H), 7.90 – 7.82 (m, 1H), 7.80 (d, J = 8.1 Hz, 1H), 7.68 – 7.59 (m, 2H), 7.57 – 7.50 (m, 1H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.8, 152.8, 149.3, 135.2, 134.7, 132.8, 130.5, 129.5, 128.7, 128.6, 128.4, 128.2, 128.1, 127.4, 127.2, 126.4, 125.0, 121.6 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₈H₁₃N₂O 273.1022; found 273.1025.



2-(Thiophen-2-yl)quinazolin-4(*3H*)-one (**3w**)^[1]:

Following the general procedure, compound 3w was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 19.6 mg, 43% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.65 (s, 1H), 8.23 (d, *J* = 3.7 Hz, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.86 (d, *J* = 5.0 Hz, 1H), 7.82 – 7.76 (m, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.48 (t, *J* = 7.5 Hz, 1H), 7.23 (t, *J* = 4.4 Hz, 1H) ppm. ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.3, 149.2, 148.4, 137.9, 135.2, 132.7, 129.9, 129.1, 127.5, 126.9, 126.5, 121.4 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₂H₉N₂OS 229.0430; found 229.0432.



2-propylquinazolin-4(3*H*)-one (**3aa**)^[9]:

Following the general procedure, compound **3aa** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 24.2 mg, 64.3% yield, white solid.

¹H NMR (500 MHz, DMSO-*d*₆) δ 12.17 (s, 1H), 8.06 (d, J = 7.7 Hz, 1H), 7.75 (t, J = 7.2 Hz, 1H), 7.58 (d, J = 8.1 Hz, 1H), 7.44 (t, J = 7.5 Hz, 1H), 2.56 (t, J = 7.6 Hz, 2H), 1.72 (q, J = 7.4 Hz, 2H), 0.91 (t, J = 7.3 Hz, 3H). ¹³C{¹H} NMR (125 MHz, DMSO-*d*₆) δ 162.3, 157.8, 149.4, 134.8, 127.3, 126.4, 126.1, 121.2, 36.8, 20.7, 14.0 ppm. HRMS (ESI-TOF) m/z: [M+H]⁺ Calcd for C₁₁H₁₂N₂O 189.1022; Found 189.1009.



2-Amino-*N*-benzylbenzamide (**6b**)^[8]:

Following the general procedure, compound **6b** was obtained by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 5:1, v/v), 22.6 mg, 50% yield, white solid.

¹H NMR (500 MHz, CDCl₃) δ 7.41 – 7.27 (m, 6H), 7.23 – 7.17 (m, 1H), 6.68 (d, J = 8.2 Hz, 1H), 6.62 (t, J = 7.5 Hz, 1H), 6.41 (s, 1H), 5.55 (s, 2H), 4.59 (d, J = 5.7 Hz, 2H) ppm. ¹³C{¹H} NMR (125 MHz, CDCl₃) δ 169.1, 148.8, 138.2, 132.3, 128.7, 127.7, 127.5, 127.1, 117.3, 116.5, 115.7, 43.6 ppm. HRMS (ESI-TOF) [M+H]⁺ calcd. for C₁₄H₁₅N₂O 227.1179; found 227.1180.

VI. References

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VII. ¹H NMR and ¹³C NMR Spectra





¹H NMR (DMSO-*d*₆) spectra of compound 3c



iiil f1 (ppm) -1

¹H NMR (DMSO-d₆) spectra of compound 3d



100 90 f1 (ppm) -10



¹H NMR (CDCl₃) spectra of compound 3f





210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

¹H NMR (DMSO-*d*₆) spectra of compound 3h







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



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

¹H NMR (DMSO-*d*₆) spectra of compound 31





¹H NMR (DMSO-*d*₆) spectra of compound 3n







¹H NMR (DMSO-*d*₆) spectra of compound 3q





¹H NMR (DMSO-*d*₆) spectra of compound 3s



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 f1 (ppm)

110 100 f1 (ppm)

¹H NMR (DMSO-*d*₆) spectra of compound 3aa

- r (Phi