Supporting Information

Selective Oxidative Cleavage of 3-Methylindoles with Primary Amines Affording Quinazolinones

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1. General Information

The reactions were carried out in schlenk tubes of 25 mL under N₂ atmosphere. All solvents and reagents were used as commercially supplied without further purification unless otherwise stated. Column chromatography was performed using Silica Gel 60 (300–400 mesh). The reactions were monitored by GC and GC-MS. GC-MS results were recorded on GC-MS QP2010, and GC analysis was performed on GC 2014 plus. The ¹H, ¹³C NMR and ¹⁹F NMR spectra were recorded on a Brucker ADVANCE III spectrometer at 400 MHz, 100 MHz and 376 MHz respectively, and chemical shifts were reported in parts per million (ppm). The ionization method of the HRMS was electron ionization (EI) or electrospray ionization (ESI), and the mass analyzer type was TOF for ESI and Double focusing mass analyzer for EI. The single-crystal X-ray diffraction was conducted in the X-ray and Spectral Center at Zhejiang University, China. All solvents and reagents were purchased from Energy Chemical, Alfa, Aesar, and Aladdin.

2. General Experimental Procedure

2.1 General experimental procedure for the synthesis of quinazolin-4(3H)-ones

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with 3-methyl indole (1, 0.2 mmol), TBAI (20 mol %), was evacuated and backfilled with N₂ three times. A premixed solution of CH₂CN and H₂O (1.5 mL, CH₂CN/H₂O = 2:1), amines (2, 0.4 mmol) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 12 h and monitored by GC or GC-MS. Upon completion, the reaction mixture was cooled to room temperature, then washed with H₂O, and extracted with ethyl acetate. The organic layer was dried over anhydrous Na₂SO₄ and was concentrated under vacuum. The residue was purified by column chromatography on silica gel and eluted with petroleum/ethyl acetate to afford the desired product 3.

2.2 Gram-Scale synthesis of 3-benzylquinazolin-4(3H)-one (3a)

An oven-dried 100-mL Schlenk tube, equipped with a magnetic stir bar and charged with 3-methyl indole (1a, 6 mmol), TBAI (20 mol %) was evacuated and backfilled with N₂ three times. A premixed solution of CH₂CN and H₂O (45 mL, CH₂CN/H₂O = 2:1), benzylamine (2a, 2.0 equiv) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 24 h. After completion of the reaction, the reaction mixture was cooled to room temperature. Then washed with H₂O (25 mL), and extracted with ethyl acetate (3 × 25 mL), and the organic layer was dried over anhydrous Na₂SO₄ and was concentrated under vacuum. The residue was purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford 3a in a 72% yield (1.01 g).

2.3 Preparation of substrates

Compounds 1a, 2a–2zi were commercially available. Other reagents such as indoles 1zl–1zt, compound 7, 8, 9 and 3-phenylindole 10 were prepared in accordance to methods described in the references.

General procedure for the synthesis of 3-methyl indoles 1zj–1zqi:

Under an open-air atmosphere, an oven-dried 25-mL Schlenk tube was added starting indoles (1.0 mmol), [Cp*IrCl₂]₂ (0.01 mmol, 1 mol %), KOtBu (1.0 mmol, 1 equiv.), and methanol (3 mL). The tube was sealed with a PFTE septa screw-cap and stirred at 140 °C in IKA for 24 h. After cooled to ambient temperature, the reaction mixture was concentrated in vacuo and purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the corresponding products in 30–80% yields.

Typical procedure for the synthesis of 5-fluoro-3-methyl-1H-indole (1zp) as the representative example:
Under an open-air atmosphere, an oven-dried 25-mL Schlenk tube was added starting 5-fluoro-1H-indole (1.0 mmol), [Cp*IrCl₂]₂ (0.01 mmol, 1 mol %), KOTBu (1.0 mmol, 1 equiv.), and methanol (3 mL). The tube was sealed with a PTFE septa screw-cap and stirred at 140 °C in IKA for 24 h. After cooled to ambient temperature, the reaction mixture was concentrated in vacuo and purified by column chromatography on silica gel with petroleum ether /ethylacetate (20/1) to afford the corresponding products in 70% yield (31.3 mg).

3,7-dimethyl-1H-indole (1zl)

Brown solid, 113.0 mg, 78%. ¹H NMR (400 MHz, CDCl₃): δ 7.80 (s, 1H), 7.44 (d, J = 7.8 Hz, 1H), 7.06 (t, J = 7.4 Hz, 1H), 7.02–6.96 (m, 2H), 2.48 (s, 3H), 2.34 (d, J = 0.9 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 135.8, 127.8, 122.3, 121.2, 120.0, 119.3, 116.5, 112.2, 16.5, 9.7.

3,5-dimethyl-1H-indole (1zm)

Brown solid, 116.1 mg, 80%. ¹H NMR (400 MHz, CDCl₃): δ 7.73 (s, 1H), 7.36 (s, 1H), 7.21 (d, J = 8.3 Hz, 1H), 7.01 (dd, J = 8.2, 1.1 Hz, 1H), 6.91 (s, 1H), 2.46 (s, 3H), 2.30 (d, J = 0.9 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 134.5, 128.4, 128.2, 123.4, 121.6, 118.4, 111.1, 110.5, 21.4, 9.6.

3,4-dimethyl-1H-indole (1zn)

Brown solid, 72.5 mg, 50%. ¹H NMR (400 MHz, CDCl₃): δ 7.81 (s, 1H), 7.16 (d, J = 8.1 Hz, 1H), 7.04 (d, J = 7.2 Hz, 1H), 6.90 (d, J = 1.0 Hz, 1H), 6.82 (d, J = 7.1 Hz, 1H), 2.73 (s, 3H), 2.52 (d, J = 1.0 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 136.8, 131.2, 126.5, 122.0, 121.7, 120.5, 112.6, 108.9, 20.0, 13.0.

5-methoxy-3-methyl-1H-indole (1zo)

White solid, 127.3 mg, 79%. ¹H NMR (400 MHz, CDCl₃): δ 7.94 (s, 1H), 7.26 (d, J = 8.7 Hz, 1H), 7.13 (d, J = 2.0 Hz, 1H), 6.96 (dd, J = 8.9, 2.4 Hz, 2H), 3.97 (s, 3H), 2.40 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 153.6, 131.3, 128.4, 122.5, 111.8, 111.6, 111.1, 100.6, 55.8, 9.6.

5-fluoro-3-methyl-1H-indole (1zp)
Brown solid, 104.0 mg, 70% 1H NMR (400 MHz, CDCl3): δ 7.88 (s, 1H), 7.25–7.18 (m, 2H), 7.07–6.99 (m, 2H), 2.28 (s, 3H); 13C NMR (100 MHz, CDCl3): δ 157.6 (d, J = 233.8 Hz), 132.7, 128.6 (d, J = 9.6 Hz), 123.4, 111.7 (d, J = 4.7 Hz), 111.5 (d, J = 9.7 Hz), 110.0 (d, J = 26.4 Hz), 103.6 (d, J = 23.1 Hz), 9.5.

5-chloro-3-methyl-1H-indole (1zq)

Brown solid, 132.0 mg, 80% 1H NMR (400 MHz, CDCl3): δ 7.89 (s, 1H), 7.53 (d, J = 1.9 Hz, 1H), 7.24 (d, J = 8.5 Hz, 1H), 7.13 (dd, J = 8.6, 2.0 Hz, 1H), 6.98 (s, 1H), 2.29 (d, J = 1.0 Hz, 3H); 13C NMR (100 MHz, CDCl3): δ 134.5, 129.4, 124.8, 122.9, 122.1, 118.3, 111.8, 111.5. 9.5.

5-bromo-3-methyl-1H-indole (1zr)

Brown solid, 156.7 mg, 75% 1H NMR (400 MHz, CDCl3): δ 7.90 (s, 1H), 7.69 (d, J = 1.8 Hz, 1H), 7.26 (dd, J = 8.5, 1.9 Hz, 1H), 7.20 (d, J = 8.6 Hz, 1H), 6.96 (s, 1H), 2.28 (d, J = 1.0 Hz, 3H); 13C NMR (100 MHz, CDCl3): δ 134.8, 130.0, 124.6, 122.7, 121.5, 112.3, 112.3, 111.4, 9.5.

3-methyl-5-(trifluoromethyl)-1H-indole (1zs)

Yellow liquid, 59.1 mg, 30%. 1H NMR (400 MHz, CDCl3): δ 8.04 (s, 1H), 7.91 (s, 1H), 7.47–7.37 (m, 2H), 7.06 (s, 1H), 2.37 (s, 3H); 13C NMR (100 MHz, CDCl3): δ 137.5, 127.6, 125.5 (d, J = 271.3 Hz), 123.2, 121.5 (q, J = 31.7 Hz), 118.5 (q, J = 3.4 Hz), 116.5 (q, J = 4.3 Hz), 112.7, 111.1, 9.3. HRMS (EI) m/z: [M]+ calcd. for C10H8F3N 199.0609; found 199.0607

3-methyl-1H-pyrrolo[2,3-c]pyridine (1zt)

White solid, 54.1 mg, 41%. mp 128–130 °C. 1H NMR (400 MHz, CDCl3): δ 11.60 (s, 1H), 8.86 (s, 1H), 8.07 (d, J = 5.7 Hz, 1H), 7.49 (d, J = 5.7 Hz, 1H), 7.29 (s, 1H), 2.29 (s, 3H); 13C NMR (100 MHz, CDCl3): δ 133.9, 133.4, 133.3, 131.6, 129.4, 113.8, 110.9, 9.1. HRMS (EI) m/z: [M]+ calcd. for C8H8N2 132.0687; found 132.0689.

The procedure for the synthesis of compound 7:

4
Under an open-air atmosphere, a solution of 3-methyl indole (0.396 g, 3.2 mmol) in methanol (10 mL) was added to a solution of sodium periodate (1.34 g, 6.26 mmol) in water (10 mL) at room temperature for 24 h. The sodium iodate was filtered off, the filtrate was washed with H₂O (25 mL) and extracted with methylene chloride (3 × 25 mL). The organic layer was dried over anhydrous Na₂SO₄ and concentrated under vacuum. The residue was purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford compound 7 in 75% yield (391 mg). ¹H NMR (400 MHz, CDCl₃): δ 11.61 (s, 1H), 8.75 (d, J = 8.4 Hz, 1H), 8.50 (s, 1H), 7.92 (dd, J = 8.0, 1.3 Hz, 1H), 7.57 (t, J = 7.7 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 2.68 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 202.6, 159.8, 139.7, 135.0, 131.5, 122.9, 121.8, 121.4, 28.4.

General procedure for the synthesis of compounds 8³ and 9³:

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<td>150°C, 3 or 24 h, toluene</td>
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To a mixture of the corresponding indole (1 mmol) and KOH (1.3 mmol), was added the benzyl alcohol (3 mmol), toluene (2 mL). The resulting mixture was stirred at 150 °C during 3 h (R = H) or 24 h (R = Ph). The resulting mixture was quenched with H₂O (5.0 mL) and extracted with ethyl acetate (3 × 5 mL). The organic layer was dried over anhydrous Na₂SO₄ and was concentrated under vacuum. The residue was purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (10/1) to afford a white solid 8 in 85% yield (176 mg). ¹H NMR (400 MHz, CDCl₃): δ 7.94 (s, 1H), 7.52 (d, J = 7.9 Hz, 1H), 7.35 (d, J = 8.1 Hz, 1H), 7.29–7.26 (m, 4H), 7.22–7.14 (m, 2H), 7.10–7.05 (m, 1H), 6.94–6.89 (m, 1H), 4.12 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 141.1, 136.4, 128.6, 128.2, 127.4, 125.8, 122.2, 122.0, 119.3, 119.1, 115.8, 111.0, 31.5. and a brown solid 9 in 80% yield (226 mg). ¹H NMR (400 MHz, CDCl₃): δ 7.91 (s, 1H), 7.45–7.30 (m, 13H), 6.95 (t, J = 7.4 Hz, 1H), 6.43 (s, 1H), 5.63 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 143.9, 136.6, 128.9, 128.2, 126.9, 126.1, 124.0, 122.0, 119.8, 119.7, 119.3, 111.0.

The procedure for the synthesis of 3-phenylindole 10³:

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A mixture of phenyl hydrazines.HCl (1 mmol), phenylacetaldehyde (1 mmol) and cyanuric chloride (TCT) (0.1 mmol) in distilled ethanol (2 mL) was heated to 80 °C. After 2 h, the starting material was absent as monitored by TLC. The reaction mixture was cooled to ambient temperature and diluted with water. The product was extracted into ethyl acetate (5 x 3 mL). The combined organic layer was dried over anhydrous Na₂SO₄ and concentrated to residue. The residue was purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a white solid 10 in 80% yield (153 mg). ¹H NMR (400 MHz, CDCl₃): δ 8.18 (s, 1H), 7.95 (d, J = 7.9 Hz, 1H), 7.70–7.64 (m, 2H), 7.48–7.38 (m, 3H), 7.33 (d, J = 2.5 Hz, 1H), 7.31–7.17 (m, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 136.6, 135.5, 128.7, 127.4, 125.9, 125.7, 122.3, 121.7, 120.2, 119.7, 118.3, 111.3.
The procedure for the scheme 3:

1) The procedure for the synthesis of compound 5:

An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with 3zr (0.2 mmol), Pd(PPh₃)₂Cl₂ (10 mol %) and CuI (10 mol %). After charging nitrogen for three times, phenylacetylene (4) (0.24 mmol, 1.2 eq) and triethylamine (1 mL) was added under nitrogen atmosphere, and the reaction mixture was stirred at 100 °C in IKA for 16 h. The precipitate was removed by filtration and washed with EtOAc, and the filtrate was washed with brine, dried over Na₂SO₄ and then concentrated under vacuum. The title compound was purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 86% yield (57.8 mg). mp 198‒200 °C; H NMR (400 MHz, CDCl₃): δ 8.48 (d, J = 1.6 Hz, 1H), 8.09 (s, 1H), 7.85 (dd, J = 8.4, 1.7 Hz, 1H), 7.67 (d, J = 8.4 Hz, 1H), 7.59‒7.51 (m, 2H), 7.39‒7.32 (m, 8H), 5.20 (s, 2H). 13C NMR (100 MHz, CDCl₃) δ 160.4, 147.5, 146.7, 136.9, 135.5, 131.7, 130.1, 129.1, 128.6, 128.4, 128.0, 127.7, 122.7, 122.6, 122.2, 91.2, 88.3, 49.6. HRMS (EI) m/z: [M]+ calcd. for C₂₃H₁₆N₂O 336.1263; found 336.1265.

2) The procedure for the synthesis of compound 6:

An oven dried Schlenk tube of 25 mL equipped with a magnetic stir bar was charged with 3j (0.2 mmol), Pd(PPh₃)₂Cl₂ (10 mol %) and CuI (10 mol %). After charging nitrogen for three times, phenylacetylene (4) (0.24 mmol, 1.2 eq.), diisopropylmine (0.4 mmol, 2.0 equiv.) and THF (1 mL) was added under nitrogen atmosphere, and the reaction mixture was stirred at 100 °C in IKA for 16 h. After cooling down to room temperature, the precipitate was removed by filtration and washed with EtOAc, and the filtrate was washed with brine, dried over Na₂SO₄ and then concentrated under vacuum. The title compound was purified by column chromatography on silica gel eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 94% yield (63.2 mg). mp 194‒196 °C; H NMR (400 MHz, CDCl₃): δ 8.33 (dd, J = 8.1, 1.1 Hz, 1H), 8.10 (s, 1H), 7.79‒7.69 (m, 2H), 7.54‒7.48 (m, 5H), 7.36‒7.30 (m, 5H), 5.19 (s, 2H); 13C NMR (100 MHz, CDCl₃): δ 161.0, 148.0, 146.1, 135.6, 134.3, 132.1, 131.5, 128.3, 128.3, 127.9, 127.5, 127.4, 126.8, 123.4, 122.9, 122.1, 90.1, 88.6, 49.3. HRMS (ESI) m/z: [M+H]⁺ calcd. for C₂₃H₁₇N₂O 337.1335; found 337.1338.
The procedure for the scheme 4:

1) scheme 4, eq 1

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with 3-methyl indole (1a, 0.2 mmol), TBAI (20 mol %), BHT (4.0 equiv, 0.8 mmol) was evacuated and backfilled with N₂ three times. A premixed solution of CH₃CN and H₂O (1.5 mL, CH₃CN/H₂O = 2:1), benzylamine (2a, 0.4 mmol) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 12 h and monitored by GC or GC-MS. Upon completion, the reaction mixture was cooled to room temperature, then washed with H₂O, and extracted with ethyl acetate. The organic layer dried over anhydrous Na₂SO₄ then analyzed by GC-MS.

2) scheme 4, eq 2

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with 3-methyl indole (1a, 0.2 mmol), TBAI (20 mol %), was evacuated and backfilled with N₂ three times. A premixed solution of CH₃CN and H₂O (1.5 mL, CH₃CN/H₂O = 2:1), benzylamine (2a, 0.4 mmol) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 12 h and monitored by GC or GC-MS. Upon completion, the reaction mixture was cooled to room temperature and diluted with 5ml of dichloromethane. The mixture then dried over anhydrous Na₂SO₄ and analyzed by GC-MS. Then concentrated under vacuum and the residue was purified by column chromatography on silica gel and eluted with petroleum/ethyl acetate to afford the desired product 3a in 68%.

3) scheme 4, eq 3

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with 3-methyl indole
7.31 (m, 2H), 7.02 (t, room temperature, then washed with H2O, and extracted with ethyl acetate. The organic layer was dried over anhydrous Na2SO4 and then analyzed by GC or GC-MS. Upon completion, the reaction mixture was cooled to room temperature, then washed with H2O, and extracted with ethyl acetate. The organic layer was dried over anhydrous Na2SO4 and was concentrated under vacuum. The residue was purified by column chromatography on silica gel and eluted with petroleum/ethyl acetate to afford the desired product 7 in a 20% yield. 1H NMR (400 MHz, CDCl3): δ 11.61 (s, 1H), 8.75 (d, J = 8.4 Hz, 1H), 8.50 (s, 1H), 7.92 (dd, J = 8.0, 1.3 Hz, 1H), 7.57 (t, J = 7.7 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 2.68 (s, 3H); 13C NMR (100 MHz, CDCl3): δ 202.6, 159.8, 139.7, 135.0, 131.5, 122.9, 121.8, 121.4, 28.4.

4) scheme 4, eq 4

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with N-(2-acylphenyl)formamide (7, 0.2 mmol), TBAI (20 mol %), was evacuated and backfilled with N2 three times. A premixed solution of CH3CN and H2O (1.5 mL, CH3CN/H2O = 2:1), benzylamine (2a, 0.4 mmol) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 12 h and monitored by GC or GC-MS. Upon completion, the reaction mixture was cooled to room temperature, then washed with H2O, and extracted with ethyl acetate. The organic layer was dried over anhydrous Na2SO4 and was concentrated under vacuum. The residue was purified by column chromatography on silica gel and eluted with petroleum/ethyl acetate to afford the desired product 3a in 7% yield.

5) scheme 4, eq 5

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with 3-benzyl indole (8, 0.2 mmol), TBAI (20 mol %), was evacuated and backfilled with N2 three times. A premixed solution of CH3CN and H2O (1.5 mL, CH3CN/H2O = 2:1), 4-fluorobenzylamine (2e, 0.4 mmol) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 12 h and monitored by GC or GC-MS. Upon completion, the reaction mixture was cooled to room temperature, then washed with H2O, and extracted with ethyl acetate. The organic layer was dried over anhydrous Na2SO4 and was concentrated under vacuum. The residue was purified by column chromatography on silica gel and eluted with petroleum/ethyl acetate to afford the desired product 3e in 66% yield (33.5mg). 1H NMR (400 MHz, CDCl3): δ 8.30 (d, J = 7.9 Hz, 1H), 8.10 (s, 1H), 7.79–7.65 (m, 2H), 7.50 (t, J = 7.3 Hz, 1H), 7.39–7.31 (m, 2H), 7.02 (t, J = 8.3 Hz, 2H), 5.15 (s, 2H); 13C NMR (100 MHz, CDCl3): δ 162.5 (d, J = 247.5 Hz), 160.9, 147.9, 146.0, 134.3, 131.5 (d, J = 3.2 Hz), 129.9, 129.8, 127.4 (d, J = 4.2 Hz), 126.8, 122.1, 115.9 (d, J = 21.7 Hz), 49.0. 19F NMR (376 MHz, CDCl3): δ -113.4. and benzaldehyde in 50% yield (10.3mg). 1H NMR (400 MHz, CDCl3): δ 10.01 (s, 1H), 7.88 (d, J = 7.4 Hz, 2H), 7.63 (t, J = 7.4 Hz, 1H), 7.53 (t, J = 7.5 Hz, 2H), 13C NMR (100 MHz, CDCl3): δ 192.3, 136.3, 134.4, 129.6, 128.9.

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with 3-diphenylmethylindole (9, 0.2 mmol), TBAI (20 mol %), was evacuated and backfilled with N2 three times. A premixed solution of CH3CN and H2O (1.5 mL, CH3CN/H2O = 2:1), 4-fluorobenzylamine (2e, 0.4 mmol) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 12 h and monitored by GC or GC-MS. Upon completion, the reaction mixture was cooled to room temperature, then washed with H2O, and extracted with ethyl acetate. The organic layer was dried over anhydrous Na2SO4 and was concentrated under vacuum. The residue was purified by column chromatography on silica gel and eluted with petroleum/ethyl acetate to afford the desired product 3f in 15% yield (33.5mg), and benzophenone in 10% yield (4.0 mg). 1H NMR (400 MHz, CDCl3): δ 7.80 (d, J = 7.3 Hz, 4H), 7.58 (t, J = 7.4 Hz, 2H), 7.48 (t, J = 7.6 Hz, 4H); 13C NMR (100 MHz, CDCl3): δ 196.6, 137.5, 132.3, 129.9, 128.2.

6) scheme 4, eq 6

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with indole or 3-phenylindole (0.2 mmol), TBAI (20 mol %), was evacuated and backfilled with N2 three times. A premixed solution of CH3CN and H2O (1.5 mL, CH3CN/H2O = 2:1), benzylamine (2a, 0.4 mmol) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 12 h and monitored by GC or GC-MS. Upon completion, the reaction mixture was cooled to room temperature, then washed with H2O, and extracted with ethyl acetate. The organic layer was dried over anhydrous Na2SO4 and then analyzed by GC-MS and GC-MS.

7) scheme 4, eq 7

An oven-dried 25-mL Schlenk tube, equipped with a magnetic stir bar and charged with 3-methyl indole (1a, 0.2 mmol), TBAI (20 mol %), was evacuated and backfilled with N2 three times. A premixed solution of CH3CN and H2O (1.5 mL, CH3CN/H2O = 2:1), n-butylamine (2r, 0.4 mmol) and TBHP (6.0 equiv, 70% in water) were then added. The reaction mixture was stirred at 100 °C in IKA (RCT basic) for 10min and then
BHT (4 equiv, 0.8 mmol) was added under N₂ and then stirred for 3 h. Upon completion, the reaction mixture was cooled to room temperature, then washed with H₂O, and extracted with ethyl acetate. The organic layer was dried over anhydrous Na₂SO₄ and was concentrated under vacuum. The organic layer dried over anhydrous Na₂SO₄ and then analyzed by GC-MS and GC-MS.

2.4 Optimization of conditions

Table S1. Optimization of reaction Parameters

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a Reaction conditions: 1a (0.2 mmol), 2a (0.4 mmol), catalyst (20 mol %), and TBHP (70% in H₂O, 6.0 equiv) in solvent (1.5 mL) at 100 °C under N₂ for 12 h. GC yield using n-tridecane as an internal standard. n-Bu₄NI (30 mol %). TBHP (4.0 equiv). TBHP (8.0 equiv). 80 °C, 120 °C. Under air.

The unsuccessful substrates:
3. Investigations of the Reaction Mechanism

3.1 Radical trapping experiments.

When TEMPO or BHT (4.0 equiv) was added to the system, the reaction was completely suppressed, and a radical adduct \( C' \) could be observed by the radical inhibitor BHT (Scheme S1, eq 1), which indicated that the reaction involved radical processes. Radical adduct \( C' \) was also obtained by the direct reaction of \( 1a \) with BHT (Scheme S1, eq 2). When 3-methylindole (\( 1a \)) and \( n \)-butylamine (\( 2t \)) were reacted under standard conditions, the reaction was completely inhibited, and a O-radical adduct \( G' \) was observed (Scheme S1, eq 3).

Scheme S1. Radical trapping experiment.
Figure S1. The GC-MS charts of the crude reaction mixture of eq 1, among a, b, c, d, were irrelevant.
Figure S2. The GC-MS charts of the crude reaction mixture of eq 2, among e, f, g, h, i were irrelevant compound.
Figure S3. The GC-MS charts of the crude reaction mixture of eq 3. among j, k, l, m, n were irrelevant compound.
3.2 $^{18}$O-labling experiments.

When the reaction was carried out with anhydrous CH$_3$CN and anhydrous TBHP, 3a was isolated in 48% yield (Scheme S2, eq 6), and when the reaction was carried out with anhydrous CH$_3$CN and anhydrous TBHP in the presence of H$_2^{18}$O, 3a was isolated in 68% yield (Scheme S2, eq 5), without observation of $^{18}$O-labeled product. In contrast to the standard conditions, no reaction occurred when O$_2$ was used instead of TBHP (Scheme S2, eqs 4 and 7). These results indicated that the carbonyl oxygen atom of the product came from TBHP.

Scheme S2. $^{18}$O-labling experiment.
Figure S4. The GC-MS charts of the crude reaction mixture of eq 4.

Figure S5. The GC-MS charts of the crude reaction mixture of eq 5.
3.3 Transformation of sp³C-H bonds of indoles

The reaction of 3-benzyl indole (8) or 3-diphenylmethylindole (9) with 4-fluorobenzylamine (2e) could produce the desired products (3e, 66% or 15% yield) with the concomitant generation of benzaldehyde (50% yield) or diphenyl ketone (11% yield) in similar yields, respectively (Scheme S3, eqs 8 and 9). These results demonstrated that the sp³C-H bonds of indoles were oxygenated in the reaction.

**Scheme S3. Transformation of sp³C-H bonds of indoles**

**Figure S6. The GC-MS charts of the crude reaction mixture of eq 8.**
Figure S7. The GC-MS charts of the crude reaction mixture of eq 9.
3.4 The order of cleavage of C2–C3 double bonds and nitrogenation of C2 atoms of indoles

It is reported that indoles could be oxidized to N-(2-acetylphenyl)formamide (7). We assumed that 7 probably was the reaction intermediate via cleavage of oxidative C2–C3 double bonds of indoles. A 20% yield of 7 was obtained by the treatment of 1a under the standard conditions (Scheme S4, eq 10). The reaction of 7 with 2a only gave the desired product 3a in 7% yield under the standard conditions, and 8% yield of the product was obtained by the treatment of 7 even with 10 equiv of 2a (Scheme S4, eq 11). A 90% yield of 7 could be recovered by treatment of it under the oxidative conditions without addition of 2a (Scheme S4, eq 12), 3a was not produced when compound 4 with 2a only in CH3CN/H2O solvent in the absence of TBAI/TBHP (Scheme S4, eq. 13), which demonstrated that 7 was stable under the oxidative conditions. The above results suggested that compound 7 was not the reaction intermediate, i.e. nitrogenation of C2 atoms was prior to the oxidative cleavage of C2–C3 bonds.

In addition, the replacement of 1a with indole or 3-phenylindole without sp3C–H bond did not give the desired product at all (Scheme S4, eq 14). This result suggested that a sp3C–H bond on C3 positions of indoles was essential, and the oxidative cleavage of C3-sp3C bond resulted in the formation of C=O double bonds.

Scheme S4. Control experiments for the order of cleavage of C2–C3 double bonds and nitrogenation of C2 atoms of indoles.
Figure S8. The GC charts of the crude reaction mixture of eq 10

Figure S9. The GC-MS charts of the crude reaction mixture of eq 10.
Figure S10. The GC charts of the crude reaction mixture of eq 11a.

Figure S11. The GC-MS charts of the crude reaction mixture of eq 11a.
Figure S12. The GC charts of the crude reaction mixture of eq 11b.
Figure S13. The GC-MS charts of the crude reaction mixture of eq 11b.

Figure S14. The GC charts of the crude reaction mixture of eq 12.
4. X-ray crystallographic data of 3a

![X-ray crystal structure of compound 3a (CCDC number: 1938061). Thermal ellipsoids are drawn at 50% probability.](image)

1. The preparation of 3a:

20 Mg of 3a was dissolved in 1 mL of dichloromethane, it was filtered through a plug of silica gel. The filtrate was transferred to a tube (diameter, 0.6 cm), and 2 mL of petroleum ether was slowly added. Yellow crystals were grown from standing it for a week.

2. Crystal structure determination of 3a:
Crystal Data for C15H12N2O (M=236.27 g/mol): triclinic, space group P-1 (no. 2), a = 6.4647(8) Å, b = 8.1397(9) Å, c = 11.5509(13) Å, α = 91.733(9), β = 99.055(10), γ = 98.579(10), V = 592.63(13) Å³, Z = 2, T = 293.15K, μ(MoKα) = 0.085 mm⁻¹, Dcalc = 1.324 g/cm³, 3595 reflections measured (6.042 ≤ 2Θ ≤ 50.696), 2166 unique (Rint = 0.0246, Rsigma = 0.0424) which were used in all calculations. The final R₁ was 0.0519 (I > 2σ(I)) and wR₂ was 0.1390 (all data).

Table S2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for 3a (CCDC number: 1938061). Ueq is defined as 1/3 of of the trace of the orthogonalised U₁₁ tensor.

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Table S3 Anisotropic Displacement Parameters (Å²×10³) for 3a (CCDC number: 1938061). The Anisotropic displacement factor exponent takes the form: -2π²[h²a*²U₁₁+2hka*b*U₁₂+2ka*c*U₁₃+2h*b*a*U₂₂+2k*b*c*U₂₃+2k*c*a*U₃₃+2l*a*c*U₃₁+2l*b*c*U₃₂+2l*c*a*U₃₃].

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Table S5 Bond Angles for 3a (CCDC number: 1938061).

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<td>C1</td>
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<td>C15</td>
<td>C14</td>
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Table S6 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 3a (CCDC number: 1938061).

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<td>3730.43</td>
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</table>

Figure S17. Molecular structure of compound 3a (CCDC number: 1938061). Thermal ellipsoids are drawn at 50% probability. H atoms are omitted for clarity.
Table S7. Summary of X-ray crystallographic data for compound 3a.

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<td><strong>R1, wR2 [I &gt; 2σ(I)]</strong></td>
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<td><strong>R1, wR2 (all data)</strong></td>
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</tbody>
</table>

5. Characterization Data for the Products

3-benzylquinazolin-4(3H)-one (3a)

![Structure of 3-benzylquinazolin-4(3H)-one (3a)](image)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 87% yield (41.0 mg). mp 105–107 °C (lit. 106–109 °C). ^1H NMR (400 MHz, CDCl₃): δ 8.32 (d, J = 7.9 Hz, 1H), 8.10 (s, 1H), 7.80–7.63 (m, 2H), 7.50 (t, J = 7.3 Hz, 1H), 7.39–7.28 (m, 5H), 5.19 (s, 2H). ^13C NMR (100 MHz, CDCl₃): δ 161.0, 147.9, 146.3, 135.6, 134.2, 128.9, 128.2, 127.9, 127.4, 127.3, 126.8, 122.1, 49.5.

3-(4-methylbenzyl)quinazolin-4(3H)-one (3b)

![Structure of 3-(4-methylbenzyl)quinazolin-4(3H)-one (3b)](image)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 70% yield (35.0 mg).
mp 118–120 °C (lit.6 119–121 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ 8.33 (d, J = 7.9 Hz, 1H), 8.10 (s, 1H), 7.80–7.64 (m, 2H), 7.50 (t, J = 7.4 Hz, 1H), 7.25 (d, J = 7.1 Hz, 2H), 7.15 (d, J = 7.7 Hz, 2H), 5.16 (s, 2H), 2.32 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): δ 161.0, 148.0, 146.3, 138.1 (s), 134.2, 132.7, 129.6, 128.0, 127.4, 127.2, 126.8, 122.2, 49.3, 21.08.

3-(4-(tert-butyl)benzyl)quinazolin-4(3H)-one (3c)\(^7\)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 80% yield (46.7 mg).

mp 128–130 °C. \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ 8.33 (d, J = 8.0 Hz, 1H), 8.11 (s, 1H), 7.77–7.67 (m, 2H), 7.50 (t, J = 7.4 Hz, 1H), 7.37 (d, J = 8.2 Hz, 2H), 7.29 (d, J = 8.2 Hz, 2H), 5.17 (s, 2H), 1.29 (s, 9H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): δ 161.0, 151.3, 148.0, 146.3, 134.2, 132.6, 127.8, 127.4, 126.8, 125.9, 122.2, 34.5, 31.2.

3-(4-methoxybenzyl)quinazolin-4(3H)-one (3d)\(^6\)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 71% yield (37.7 mg).

mp 122–124 °C (lit.15 123–125 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ 8.31 (d, J = 8.0 Hz, 1H), 8.10 (s, 1H), 7.78–7.64 (m, 2H), 7.49 (t, J = 7.4 Hz, 1H), 7.30 (d, J = 8.1 Hz, 2H), 6.86 (d, J = 8.1 Hz, 2H), 5.12 (s, 2H), 3.77 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): δ 161.0, 159.5, 147.9, 146.2, 134.2, 129.5, 127.8, 127.4, 127.2, 126.8, 125.9, 122.2, 49.3, 21.08.

3-benzyl-6-fluoroquinazolin-4(3H)-one (3e)\(^7\)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 90% yield (45.7 mg).

mp 110–112 °C (lit.10 112–114 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): δ 8.30 (d, J = 7.9 Hz, 1H), 8.10 (s, 1H), 7.79–7.65 (m, 2H), 7.50 (t, J = 7.3 Hz, 1H), 7.39–7.31 (m, 2H), 7.02 (t, J = 8.3 Hz, 2H), 5.15 (s, 2H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): δ 162.5 (d, J = 247.5 Hz), 160.9, 147.9, 146.0, 134.3, 131.5 (d, J = 3.2 Hz), 129.9, 129.8, 127.4 (d, J = 4.2 Hz), 126.8, 122.1, 115.9 (d, J = 21.7 Hz), 49.0. \(^{19}\)F NMR (376 MHz, CDCl\(_3\)): δ -113.4.

3-(4-chlorobenzyl)quinazolin-4(3H)-one (3f)\(^7\)
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 79% yield (42.6 mg). mp 130–132 °C. \( ^1 \text{H NMR (400 MHz, CDCl}_3 \):} \( \delta \) 8.30 (d, \( J = 8.0 \text{ Hz, 1H} \), 8.09 (s, 1H), 7.78–7.68 (m, 2H), 7.51 (t, \( J = 7.5 \text{ Hz, 1H} \), 7.33–7.27 (m, 4H), 5.15 (s, 2H); \( ^{13} \text{C NMR (100 MHz, CDCl}_3 \):} \( \delta \) 160.9, 147.9, 146.0, 134.4, 134.2, 134.1, 129.3, 129.1, 127.5, 127.4, 126.8, 122.1, 49.0.

3-(3-chlorobenzyl)quinazolin-4(3H)-one (3g)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 76% yield (41.0 mg). mp 140–142 °C. \( ^1 \text{H NMR (400 MHz, CDCl}_3 \):} \( \delta \) 8.31 (d, \( J = 8.0 \text{ Hz, 1H} \), 8.11 (s, 1H), 7.79–7.69 (m, 2H), 7.51 (t, \( J = 7.4 \text{ Hz, 1H} \), 7.34 (s, 1H), 7.30–7.25 (m, 2H), 7.24–7.21 (m, 1H), 5.16 (s, 2H); \( ^{13} \text{C NMR (100 MHz, CDCl}_3 \):} \( \delta \) 160.8, 147.9, 146.0, 137.6, 134.7, 134.3, 130.1, 128.4, 127.9, 127.4, 126.7, 125.9, 122.0, 48.9.

3-(2-chlorobenzyl)quinazolin-4(3H)-one (3h)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 70% yield (37.8 mg). mp 114–116 °C \( ^1 \text{H NMR (400 MHz, CDCl}_3 \):} \( \delta \) 8.20 (d, \( J = 8.0 \text{ Hz, 1H} \), 8.07 (s, 1H), 7.67–7.57 (m, 2H), 7.39 (t, \( J = 7.4 \text{ Hz, 1H} \), 7.28 (t, \( J = 7.8 \text{ Hz, 2H} \), 7.17–7.09 (m, 2H), 5.18 (s, 2H); \( ^{13} \text{C NMR (100 MHz, CDCl}_3 \):} \( \delta \) 161.1, 147.9, 146.5, 134.3, 133.4, 132.9, 130.5, 129.7, 129.6, 127.4, 127.3, 126.7, 125.9, 122.0, 47.4.

3-(4-bromobenzyl)quinazolin-4(3H)-one (3i)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 86% yield (54.2 mg). mp 154–156 °C \( \text{lit.}^6 155–157 ^\circ \text{C} \). \( ^1 \text{H NMR (400 MHz, CDCl}_3 \):} \( \delta \) 8.30 (d, \( J = 8.0 \text{ Hz, 1H} \), 8.08 (s, 1H), 7.77–7.67 (m, 2H), 7.53–7.43 (m, 3H), 7.23 (d, \( J = 8.2 \text{ Hz, 2H} \), 5.12 (s, 2H); \( ^{13} \text{C NMR (100 MHz, CDCl}_3 \):} \( \delta \) 160.9, 147.9, 145.9, 134.7, 134.3, 132.1, 129.6, 127.5, 127.4, 126.8, 122.3, 122.0, 49.1.

3-(4-iodobenzyl)quinazolin-4(3H)-one (3j)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 86% yield (54.2 mg). mp 154–156 °C \( \text{lit.}^6 155–157 ^\circ \text{C} \). \( ^1 \text{H NMR (400 MHz, CDCl}_3 \):} \( \delta \) 8.30 (d, \( J = 8.0 \text{ Hz, 1H} \), 8.08 (s, 1H), 7.77–7.67 (m, 2H), 7.53–7.43 (m, 3H), 7.23 (d, \( J = 8.2 \text{ Hz, 2H} \), 5.12 (s, 2H); \( ^{13} \text{C NMR (100 MHz, CDCl}_3 \):} \( \delta \) 160.9, 147.9, 145.9, 134.7, 134.3, 132.1, 129.6, 127.5, 127.4, 126.8, 122.3, 122.0, 49.1.
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 75% yield (48.3 mg). mp 163–165 °C; 1H NMR (400 MHz, CDCl3): δ 8.29 (d, J = 7.9 Hz, 1H), 8.09 (s, 1H), 7.76–7.62 (m, 4H), 7.50 (t, J = 7.3 Hz, 1H), 7.09 (d, J = 7.7 Hz, 2H), 5.11 (s, 2H); 13C NMR (100 MHz, CDCl3): δ 160.9, 147.9, 146.0, 138.0, 135.3, 134.4, 129.7, 127.4, 126.8, 93.9, 49.2. HRMS (ESI) m/z: [M+H]+ calcd. for C15H12IN2O 362.9989; found 362.9993.

3-benzyl-6-fluoroquinazolin-4(3H)-one (3k)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 70% yield (40.3 mg). mp 142–144 °C; 1H NMR (400 MHz, CDCl3): δ 8.33 (dd, J = 8.0, 0.9 Hz, 1H), 8.12 (s, 1H), 7.82–7.72 (m, 2H), 7.58–7.51 (m, 1H), 7.45 (dd, J = 6.8, 2.1 Hz, 1H), 7.32–7.25 (m, 1H), 7.13 (t, J = 8.6 Hz, 1H), 5.15 (s, 2H); 13C NMR (100 MHz, CDCl3): δ 160.9, 157.9 (d, J = 250.3 Hz), 148.0, 145.8, 134.5, 132.81 (d, J = 4.1 Hz), 130.3, 127.9 (d, J = 7.5 Hz), 127.6, 126.8, 122.0, 121.67 (d, J = 18.1 Hz), 117.2, 117.0. 19F NMR (376 MHz, CDCl3): δ -115.5. HRMS (ESI) m/z: [M+H]+ calcd. for C15H11ClFN2O 289.0538; found 289.0544.

3-(4-(trifluoromethyl)benzyl)quinazolin-4(3H)-one (3l)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 92% yield (55.9 mg). mp 175–177 °C; 1H NMR (400 MHz, CDCl3): δ 8.30 (d, J = 7.9 Hz, 1H), 8.11 (s, 1H), 7.82–7.76 (m, 2H), 7.59 (d, J = 7.7 Hz, 2H), 7.55–7.42 (m, 3H), 5.23 (s, 2H); 13C NMR (100 MHz, CDCl3): δ 160.9, 147.9, 145.9, 139.5, 134.5, 130.5 (d, J = 32.7 Hz), 128.1, 127.5 (d, J = 0.9 Hz), 126.8, 125.9 (q, J = 7.4, 3.7 Hz), 125.1, 122.4, 122.0, 49.2. 19F NMR (376 MHz, CDCl3): δ -62.7.

3-(naphthalen-1-ylmethyl)quinazolin-4(3H)-one (3m)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale white solid in 91% yield (52.0 mg). mp 176–178 °C; NMR (400 MHz, CDCl3): δ 8.40 (d, J = 7.9 Hz, 1H), 8.05–7.84 (m, 4H), 7.79–7.67 (m, 2H), 7.62–7.48 (m, 3H), 7.31–7.18 (m, 2H), 6.73–6.59 (m, 1H), 5.26 (s, 2H); 13C NMR (100 MHz, CDCl3): δ 148.5, 141.8, 139.5, 130.8, 129.1, 127.8, 126.9, 125.4 (t, J = 53.1 Hz), 124.7, 123.3 (d, J = 23.9 Hz), 115.8, 115.3, 113.7, 109.4, 109.3, 49.1. 15N NMR (150 MHz, CDCl3): δ 36.8. HRMS (ESI) m/z: [M+H]+ calcd. for C24H16IN3O2 433.9640; found 433.9641.
7.58–7.34 (m, 5H), 5.68 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 161.0, 147.7, 145.8, 134.3, 133.8, 130.9, 130.7, 129.3, 128.9, 127.4, 127.3, 127.1, 126.9, 126.9, 126.2, 125.3, 122.9, 121.9, 46.6. HRMS (ESI) m/z: [M+H]$^+$ calcd. for C$_{19}$H$_{15}$N$_2$O 287.1179; found 287.1180.

3-(thiophen-2-ylmethyl)quinazolin-4(3H)-one (3n)$^6$

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale red solid in 78% yield (37.7 mg). mp 121–123 °C. $^1$H NMR (400 MHz, CDCl$_3$): δ 8.33 (d, $J = 7.9$ Hz, 1H), 8.15 (s, 1H), 7.78–7.67 (m, 2H), 7.50 (t, $J = 7.4$ Hz, 1H), 7.27 (s, 1H), 7.15 (s, 1H), 6.97 (s, 1H), 5.35 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 160.6, 147.8, 145.7, 137.4, 137.7, 127.7, 127.3, 127.0, 126.7, 126.5, 121.9, 44.2.

3-(pyridin-3-ylmethyl)quinazolin-4(3H)-one (3o)$^7$

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale white solid in 79% yield (37.4 mg). mp 125–127 °C. $^1$H NMR (400 MHz, CDCl$_3$): δ 8.64 (s, 1H), 8.53 (s, 1H), 8.27 (d, $J = 7.9$ Hz, 1H), 8.10 (s, 1H), 7.76–7.65 (m, 3H), 7.48 (t, $J = 7.3$ Hz, 1H), 7.23 (s, 1H), 5.16 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 160.9, 149.7, 149.2, 147.9, 145.7, 135.8, 134.5, 131.4, 127.5, 126.7, 123.7, 122.0, 47.4.

3-(1-phenylethyl)quinazolin-4(3H)-one (3p)$^6$

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow oil in 62% yield (31.0 mg). $^1$H NMR (400 MHz, CDCl$_3$): δ 8.33 (d, $J = 7.9$ Hz, 1H), 7.93 (s, 1H), 7.77–7.62 (m, 2H), 7.48 (t, $J = 7.4$ Hz, 1H), 7.39–7.27 (m, 5H), 6.35 (q, $J = 6.9$ Hz, 1H), 1.82 (d, $J = 7.1$ Hz, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$): δ 160.6, 147.4, 144.3, 139.3, 134.1, 128.9, 128.1, 127.2, 127.1, 126.8, 121.7, 51.6, 19.0.

3-benzhydrylquinazolin-4(3H)-one (3q)
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow oil in 50% yield (31.2 mg). 1H NMR (400 MHz, CDCl₃): δ 8.34 (d, J = 8.0 Hz, 1H), 7.98 (s, 1H), 7.79–7.67 (m, 2H), 7.50 (t, J = 7.5 Hz, 1H), 7.46 (s, 1H), 7.41–7.30 (m, 6H), 7.22 (d, J = 7.2 Hz, 4H); 13C NMR (100 MHz, CDCl₃): δ 160.8, 147.5, 145.3, 137.9, 134.3, 128.9, 128.5, 128.3, 127.4, 127.3, 127.0, 121.7, 60.6. HRMS (EI) m/z: [M]⁺ calcd. for C₂₁H₁₆N₂O 312.1263; found 312.1261.

3-butylquinazolin-4(3H)-one (3r)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 78% yield (31.5 mg). mp 69–71 °C (lit. 70–72 °C). 1H NMR (400 MHz, CDCl₃): δ 8.30 (d, J = 8.0 Hz, 1H), 8.01 (s, 1H), 7.80–7.63 (m, 2H), 7.48 (t, J = 7.4 Hz, 1H), 3.99 (t, J = 7.3 Hz, 2H), 1.82–1.71 (m, 2H), 1.46–1.34 (m, 2H), 0.96 (t, J = 7.3 Hz, 3H); 13C NMR (100 MHz, CDCl₃): δ 161.0, 148.0, 146.5, 134.0, 127.3, 127.1, 126.6, 122.1, 46.7, 31.3, 19.8, 13.5.

3-hexylquinazolin-4(3H)-one (3s)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (20/1) to afford a pale yellow solid in 84% yield (38.6 mg). mp 65–67 °C. 1H NMR (400 MHz, CDCl₃): δ 8.30 (d, J = 8.0 Hz, 1H), 8.01 (s, 1H), 7.76–7.67 (m, 2H), 7.48 (t, J = 7.4 Hz, 1H), 3.98 (t, J = 7.3 Hz, 2H), 1.82–1.73 (m, 2H), 1.36–1.26 (m, 6H), 0.87 (t, J = 6.3 Hz, 3H); 13C NMR (100 MHz, CDCl₃): δ 161.0, 148.1, 146.5, 134.0, 127.3, 127.1, 126.6, 122.1, 47.0, 31.2, 29.3, 26.2, 22.4, 13.9.

3-hexadecylquinazolin-4(3H)-one (3t)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 90% yield (66.6 mg). mp 64–66 °C. 1H NMR (400 MHz, CDCl₃): δ 8.29 (d, J = 7.9 Hz, 1H), 8.01 (s, 1H), 7.76–7.66 (m, 2H), 7.48 (t, J = 7.2 Hz, 1H), 3.97 (t, J = 7.1 Hz, 2H), 1.23 (s, 28H), 0.85 (t, J = 6.0 Hz, 3H); 13C NMR (100 MHz, CDCl₃): δ 161.0, 148.0, 146.5, 134.0, 127.3, 127.1, 126.6, 122.1, 47.0, 31.8, 29.6, 29.6, 29.5, 29.4, 29.3, 29.2, 26.6, 22.6, 14.0. HRMS (ESI) m/z: [M+H]⁺ calcd. for C₂₄H₃₉N₂O 371.3057; found 371.3062.

3-(3-phenylpropyl)quinazolin-4(3H)-one (3u)
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 91% yield (48.1 mg). mp 90–92 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.30 (d, $J = 8.0$ Hz, 1H), 7.95 (s, 1H), 7.76–7.66 (m, 2H), 7.51–7.45 (m, 1H), 7.31–7.24 (m, 2H), 7.21–7.15 (m, 3H), 3.99 (t, $J = 7.2$ Hz, 2H), 2.71 (t, $J = 7.6$ Hz, 2H), 2.20–2.08 (m, 2H). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 160.9, 147.9, 146.3, 140.2, 134.0, 128.4, 128.1, 127.2, 127.0, 126.5, 126.1, 121.9, 46.4, 32.5, 30.2. HRMS (EI) m/z: [M]$^+$ calcd. for C$_{17}$H$_{16}$N$_2$O 264.1263; found 264.1263.

3-(2-ethylhexyl)quinazolin-4(3H)-one (3v)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow oil in 94% yield (48.5 mg). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.28 (d, $J = 8.0$ Hz, 1H), 7.97 (s, 1H), 7.75–7.65 (m, 2H), 7.47 (t, $J = 7.4$ Hz, 1H), 3.88–3.84 (d, $J = 8.0$ Hz, 2H), 1.82–1.84 (m, 1H), 1.37–1.23 (m, 8H), 0.93–0.83 (m, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 161.1, 147.9, 146.9, 134.0, 127.3, 127.1, 126.6, 122.1, 50.5, 38.5, 30.1, 28.3, 23.4, 22.8, 13.9, 10.3. HRMS (EI) m/z: [M]$^+$ calcd. for C$_{16}$H$_{22}$N$_2$O 258.1732; found 258.1730.

3-(cyclopropylmethyl)quinazolin-4(3H)-one (3w)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow oil in 87% yield (34.8 mg). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.28 (d, $J = 7.9$ Hz, 1H), 8.08 (s, 1H), 7.75–7.64 (m, 2H), 7.46 (t, $J = 8.0$ Hz, 1H), 3.84 (d, $J = 7.1$ Hz, 2H), 1.32–1.19 (m, 1H), 0.60 (d, $J = 6.3$ Hz, 2H), 0.39 (s, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 161.0, 148.0, 146.2, 134.0, 127.2, 127.0, 126.6, 122.1, 50.9, 10.7, 4.0.

3-isobutylquinazolin-4(3H)-one (3x)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 89% yield (35.9 mg). mp 90–94 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.28 (d, $J = 7.1$ Hz, 1H), 7.96 (s, 1H), 7.75–7.63 (m, 2H), 7.50–7.43 (m, 1H), 3.78 (d, $J = 5.5$ Hz, 2H), 2.22–2.14 (m, 1H), 0.95 (d, $J = 3.2$ Hz, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 161.1, 147.9, 146.8, 134.0, 127.2, 127.1, 126.6, 122.0, 54.0, 28.0, 19.8.

3-isopropylquinazolin-4(3H)-one (3y)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 89% yield (35.9 mg). mp 90–94 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.28 (d, $J = 7.1$ Hz, 1H), 7.96 (s, 1H), 7.75–7.63 (m, 2H), 7.50–7.43 (m, 1H), 3.78 (d, $J = 5.5$ Hz, 2H), 2.22–2.14 (m, 1H), 0.95 (d, $J = 3.2$ Hz, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 161.1, 147.9, 146.8, 134.0, 127.2, 127.1, 126.6, 122.0, 54.0, 28.0, 19.8.
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale white solid in 65% yield (24.4 mg). mp 90–92 °C (lit.13 91–93 °C). ¹H NMR (400 MHz, CDCl₃): δ 8.28 (d, J = 7.9 Hz, 1H), 8.09 (s, 1H), 7.75–7.63 (m, 2H), 7.46 (t, J = 7.3 Hz, 1H), 5.23–5.10 (m, 1H) 1.46 (d, J = 6.9 Hz, 6H); ¹³C NMR (100 MHz, CDCl₃): δ 160.6, 147.4, 143.5, 134.0, 127.1, 127.0, 126.7, 121.8, 45.9, 21.9.

3-neopentylquinazolin-4(3H)-one (3za)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow oil in 60% yield (25.9 mg). ¹H NMR (400 MHz, CDCl₃): δ 8.29 (d, J = 7.3 Hz, 1H), 7.98 (s, 1H), 7.77–7.64 (m, 2H), 7.47 (s, 1H), 3.86 (s, 2H), 1.00 (s, 9H); ¹³C NMR (100 MHz, CDCl₃): δ 161.4, 147.8, 147.5, 134.0, 127.2, 127.0, 126.9, 122.1, 56.3, 33.7, 27.6.

3-cyclopropylquinazolin-4(3H)-one (3zb)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow oil in 58% yield (21.5 mg). ¹H NMR (400 MHz, CDCl₃): δ 8.29 (d, J = 8.0 Hz, 1H), 7.98 (s, 1H), 7.76–7.64 (m, 2H), 7.48 (t, J = 7.5 Hz, 1H), 3.27–3.20 (m, 1H), 1.20 (q, J = 6.7 Hz, 2H), 0.92 (q, J = 6.7 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 162.2, 147.5, 146.7, 134.1, 127.2, 127.2, 126.5, 121.7, 29.2, 6.4.

3-cyclohexylquinazolin-4(3H)-one (3zc)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow oil in 90% yield (41.0 mg). ¹H NMR (400 MHz, CDCl₃): δ 8.28 (d, J = 8.0 Hz, 1H), 8.10 (s, 1H), 7.75–7.63 (m, 2H), 7.46 (t, J = 7.4 Hz, 1H), 4.83–4.73 (m, 1H), 2.85–2.02 (m, 4H), 1.78–1.70 (m, 1H), 1.68–1.43 (m, 4H), 1.28–1.18 (m, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 160.5, 147.3, 143.8, 134.0, 127.1, 127.0, 126.8, 121.8, 53.3, 32.5, 25.8, 25.1.

3-((tetrahydro-2H-pyran-4-yl)methyl)quinazolin-4(3H)-one (3zd)
The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a pale yellow oil in 91% yield (44.4 mg). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.28 (d, $J$ = 7.9 Hz, 1H), 7.95 (s, 1H), 7.76–7.65 (m, 2H), 7.48 (t, $J$ = 7.4 Hz, 1H), 3.98–3.91 (m, 2H), 3.85 (d, $J$ = 7.2 Hz, 2H), 3.36–3.27 (m, 2H), 2.21–2.06 (m, 1H), 1.64–1.52 (m, 2H), 1.45–1.33 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 161.1, 147.9, 146.6, 134.2, 127.3, 127.2, 126.6, 122.0, 67.2, 52.5, 34.5, 30.3. HRMS (EI) m/z: [M]$^+$ calcd. for C$_{14}$H$_{16}$N$_2$O$_2$ 244.1212; found 244.1214.

3-((tetrahydrofuran-2-yl)methyl)quinazolin-4(3H)-one (3ze) $^{10}$

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a pale yellow oil in 78% yield (35.8 mg). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.27 (d, $J$ = 8.0 Hz, 1H), 8.12 (s, 1H), 7.74–7.66 (m, 2H), 7.46 (t, $J$ = 7.4 Hz, 1H), 4.34–4.28 (m, 1H), 4.22–4.15 (m, 1H), 3.89–3.60 (m, 2H), 3.75–3.68 (m, 1H), 2.09–2.03 (m, 1H), 1.91–1.80 (m, 2H), 1.62–1.52 (m, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 161.2, 148.0, 147.4, 134.1, 127.3, 126.9, 126.6, 121.9, 76.7, 68.0, 49.4, 28.7, 25.7.

3-(3-methoxypropyl)quinazolin-4(3H)-one (3zf) $^6$

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale white oil in 82% yield (35.7 mg). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.29 (d, $J$ = 8.0 Hz, 1H), 8.04 (s, 1H), 7.76–7.66 (m, 2H), 7.48 (t, $J$ = 7.4 Hz, 1H), 4.10 (t, $J$ = 6.7 Hz, 2H), 3.38 (t, $J$ = 5.7 Hz, 2H), 3.32 (s, 3H), 2.09–2.01 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 161.1, 148.1, 147.0, 134.1, 127.3, 126.5, 122.1, 68.6, 58.6, 44.2, 28.5.

3-(2-(cyclohex-1-en-1-yl)ethyl)quinazolin-4(3H)-one (3zg)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow oil in 92% yield (46.7 mg). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.28 (d, $J$ = 7.9 Hz, 1H), 7.92 (s, 1H), 7.74–7.65 (m, 2H), 7.47 (t, $J$ = 7.3 Hz, 1H), 5.34 (s, 1H), 4.04 (t, $J$ = 7.0 Hz, 2H), 2.36 (t, $J$ = 6.7 Hz, 2H), 1.98 (s, 2H), 1.88 (s, 2H), 1.64–1.57 (m, 2H), 1.54–1.46 (m, 2H); $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 160.8, 147.9, 146.6, 134.0, 133.0, 127.2, 127.0, 126.6, 125.1, 122.0, 45.3, 37.2, 28.1, 25.1, 22.7, 22.0. HRMS (EI) m/z: [M]$^+$ calcd. for C$_{16}$H$_{18}$N$_2$O 254.1419; found 254.1419.
3-(prop-2-yn-1-yl)quinazolin-4(3H)-one (3zh)\textsuperscript{15}

\[
\text{\begin{tikzpicture}
\draw (-0.5,0) -- (0.5,0) -- (0,0.5) -- (-0.5,0);
\end{tikzpicture}}
\]

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a yellow solid in 60% yield (21.9 mg). mp 113–115 °C (lit.\textsuperscript{15} 114–115 °C), \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}): \(\delta\) 8.29–8.25 (m, 2H), 7.76–7.67 (m, 2H), 7.48 (t, \(J = 7.5\) Hz, 1H), 4.80–4.78 (m, 1H), 2.50–2.46 (m, 1H); \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}): \(\delta\) 160.2, 147.8, 144.9, 134.4, 127.4, 126.6, 121.6, 76.3, 75.0, 35.1.

3-(2-hydroxyethy)quinazolin-4(3H)-one (3zi)\textsuperscript{15}

\[
\text{\begin{tikzpicture}
\draw (-0.5,0) -- (0.5,0) -- (0,0.5) -- (-0.5,0);
\end{tikzpicture}}
\]

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (1/1) to afford a yellow solid in 67% yield (28.3 mg). mp 156–158 °C (lit.\textsuperscript{15} 154–155 °C), \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}): \(\delta\) 8.12 (d, \(J = 8.0\) Hz, 1H), 8.06 (s, 1H), 7.56 (d, \(J = 8.2\) Hz, 1H), 7.40 (t, \(J = 7.6\) Hz, 1H), 4.13 (t, \(J = 9.2\) Hz, 2H), 4.00 (t, \(J = 9.6\) Hz, 2H), 3.48 (s, 1H); \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}): \(\delta\) 161.4, 147.7, 147.3, 134.3, 127.2, 127.1, 126.4, 121.7, 60.5, 49.6.

3-(2,2,2-trifluoroethyl)quinazolin-4(3H)-one (3zj)\textsuperscript{14}

\[
\text{\begin{tikzpicture}
\draw (-0.5,0) -- (0.5,0) -- (0,0.5) -- (-0.5,0);
\end{tikzpicture}}
\]

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (2/1) to afford a pale yellow oil in 45% yield (20.5 mg). \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}): \(\delta\) 8.33 (d, \(J = 8.0\) Hz, 1H), 8.03 (s, 1H), 7.81 (t, \(J = 7.6\) Hz, 1H), 7.48 (t, \(J = 7.5\) Hz, 1H), 4.68 (q, \(J = 8.5\) Hz, 2H); \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}): \(\delta\) 160.4, 147.5, 145.2, 135.0, 128.0, 127.8, 127.1, 123.2 (q, \(J = 278.0\) Hz), 121.6 (s), 45.47 (q, \(J = 35.6\) Hz). \textsuperscript{19}F NMR (376 MHz, CDCl\textsubscript{3}) \(\delta\): -70.83.

3-phenylquinazolin-4(3H)-one (3zk)\textsuperscript{7}

\[
\text{\begin{tikzpicture}
\draw (-0.5,0) -- (0.5,0) -- (0,0.5) -- (-0.5,0);
\end{tikzpicture}}
\]

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale brown solid in 35% yield (15.5 mg). mp 141–143 °C (lit.\textsuperscript{10} 138–140 °C), \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}): \(\delta\) 8.36 (d, \(J = 7.9\) Hz, 1H), 8.12 (s, 1H), 7.78 (q, \(J = 7.8\) Hz, 2H), 7.58–7.47 (m, 4H), 7.42 (d, \(J = 7.5\) Hz, 2H); \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}): \(\delta\) 160.7, 147.8, 146.0, 137.4, 134.5, 129.6, 129.0, 127.6, 127.5, 127.1, 126.9, 122.3.
3-benzyl-8-methylquinazolin-4(3H)-one (3zl)\(^6\)

![3-benzyl-8-methylquinazolin-4(3H)-one (3zl)](image)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a white solid in 86% yield (43.0 mg). mp 132–134 °C (lit.\(^6\) 133–135 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 8.17 (d, \(J =\) 8.0 Hz, 1H), 8.11 (s, 1H), 7.57 (d, \(J =\) 7.2 Hz, 1H), 7.41–7.27 (m, 6H), 5.18 (s, 2H), 2.59 (s, 3H); \(^1\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 161.3, 146.6, 145.0, 135.9, 135.7, 134.9, 128.9, 128.2, 128.0, 126.9, 124.5, 122.1, 49.5, 17.3

3-benzyl-6-methylquinazolin-4(3H)-one (3zm)\(^6\)

![3-benzyl-6-methylquinazolin-4(3H)-one (3zm)](image)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 81% yield (40.5 mg). mp 120–122 °C (lit.\(^6\) 119–121 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 8.11 (s, 1H), 8.06 (s, 1H), 7.63–7.53 (m, 2H), 7.38–7.28 (m, 5H), 5.19 (s, 2H), 2.48 (s, 3H); \(^1\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 160.9, 145.8, 145.5, 137.5, 135.7, 135.6, 128.8, 128.1, 127.8, 127.1, 126.2, 121.7, 49.4, 21.2.

3,5-dimethyl-1H-indole (3zn)\(^6\)

![3,5-dimethyl-1H-indole (3zn)](image)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 60% yield (30.0 mg). mp 150–152 °C (lit.\(^6\) 150–153 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 8.07 (s, 1H), 7.63–7.52 (m, 2H), 7.41–7.27 (m, 6H), 5.17 (s, 2H), 2.91 (s, 3H); \(^1\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 161.5 149.6, 146.1, 141.4, 135.9, 133.4, 129.9, 128.9, 128.1, 127.8, 125.7, 120.7, 49.4, 23.2.

3-benzyl-6-methoxyquinazolin-4(3H)-one (3zo)\(^6\)

![3-benzyl-6-methoxyquinazolin-4(3H)-one (3zo)](image)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 72% yield (38.3 mg). mp 88–90 °C (lit.\(^6\) 85–87 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) 8.01 (s, 1H), 7.67 (d, \(J =\) 2.9 Hz, 1H), 7.62 (d, \(J =\) 8.9 Hz, 1H), 7.36–7.28 (m, 6H), 5.18 (s, 2H), 3.89 (s, 3H); \(^1\)C NMR (100 MHz, CDCl\(_3\)): \(\delta\) 160.8, 158.7, 144.1, 142.5, 135.7, 128.9, 128.9, 128.1, 127.9, 124.4, 122.9, 106.1, 55.7, 49.6.
3-benzyl-6-fluoroquinazolin-4(3H)-one (3zp)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 83% yield (42.1 mg). mp 127–129 °C; ¹H NMR (400 MHz, CDCl₃): δ 8.06 (s, 1H), 7.94 (d, J = 8.4 Hz, 1H), 7.70 (dd, J = 8.6, 4.9 Hz, 1H), 7.46 (t, J = 8.5 Hz, 1H), 7.38–7.31 (m, 5H), 5.19 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 161.1 (d, J = 247.6 Hz), 160.3 (d, J = 3.5 Hz), 145.5 (d, J = 2.2 Hz), 144.6, 135.4, 129.9 (d, J = 8.3 Hz), 129.0, 128.3, 127.9, 123.4 (d, J = 8.7 Hz), 122.8 (d, J = 24.2 Hz), 111.7 (d, J = 23.7 Hz), 49.6. ¹⁹F NMR (376 MHz, CDCl₃): δ -115.5. HRMS (ESI) m/z: [M+H]⁺ calcd. for C₁₅H₁₂FN₂O 255.0928; found 255.0931.

3-benzyl-6-chloroquinazolin-4(3H)-one (3zq)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 70% yield (37.8 mg). mp 120–122 °C (lit.⁶ 120–124 °C). ¹H NMR (400 MHz, CDCl₃): δ 8.27 (s, 1H), 8.08 (s, 1H), 7.65 (q, J = 8.7 Hz, 2H), 7.37–7.30 (m, 5H), 5.18 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 159.9, 146.4, 146.4, 135.3, 134.6, 133.1, 129.1, 129.0, 128.4, 127.9, 126.2, 123.1, 49.6.

3-benzyl-6-bromoquinazolin-4(3H)-one (3zr)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (5/1) to afford a pale yellow solid in 89% yield (55.8 mg). mp 113–115 °C (lit.⁶ 112–115 °C). ¹H NMR (400 MHz, CDCl₃): δ 8.44 (s, 1H), 8.09 (s, 1H), 7.80 (d, J = 8.6 Hz, 1H), 7.56 (d, J = 8.6 Hz, 1H), 7.35–7.31 (m, 5H), 5.18 (s, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 159.8, 146.8, 146.5, 137.4, 135.3, 129.4, 129.2, 129.0, 128.4, 127.9, 123.5, 120.9, 49.7.

3-benzyl-6-(trifluoromethyl)quinazolin-4(3H)-one (3zs)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (1/5) to afford a pale yellow oil in 65% yield (39.5 mg). ¹H
NMR (400 MHz, CDCl3): δ 8.60 (s, 1H), 8.18 (s, 1H), 7.92 (dd, J = 8.6, 1.4 Hz, 1H), 7.79 (d, J = 8.5 Hz, 1H), 7.39–7.28 (m, 5H), 5.20 (s, 2H); 13C NMR (100 MHz, CDCl3): δ 160.2, 150.0, 148.0, 135.1, 130.3 (q, J = 3.2 Hz), 129.0, 128.5, 128.4, 128.0, 124.7 (q, J = 4.1 Hz), 122.0, 49.7. 19F NMR (376 MHz, CDCl3): δ -82.4. HRMS (EI) m/z: [M]+ calcd. for C16H11F3N2O 304.0823; found 304.0825

3-benzylpyrido[3,4-d]pyrimidin-4(3H)-one (3zt)

The title compound was prepared according to the general procedure and purified by column chromatography on silica gel and eluted with petroleum ether/ethyl acetate (1/2) to afford a pale yellow solid in 28% yield (13.3 mg). mp 124–126 °C (lit.13 125–127 °C). 1H NMR (400 MHz, CDCl3): δ 9.13 (s, 1H), 8.70 (d, J = 5.2 Hz, 1H), 8.17 (s, 1H), 8.07 (d, J = 5.2 Hz, 1H), 7.37–7.31 (m, 5H), 5.19 (s, 2H); 13C NMR (100 MHz, CDCl3): δ 159.9, 151.2, 147.9, 146.9, 142.5, 134.9, 129.1, 128.6, 127.1, 118.6, 49.9.

6. References

7. Copies of $^1$H, $^{13}$C and $^{19}$F NMR Spectra of the Products

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3a
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3a

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3b
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3b

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3c
$1^3$C NMR (100 MHz, CDCl$_3$) Spectra of 3c

$1^H$ NMR (400 MHz, CDCl$_3$) Spectra of 3d
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3d

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3e
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectra of 3e

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3e
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3f

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3f
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3g

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3g
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3h

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3h
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3i

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3i
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3j

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3j
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3k

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3k
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectra of 3k

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3l
\[ ^{13}\text{C NMR (100 MHz, CDCl}_3\text{) Spectra of 3I} \]
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectra of 3l

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3m

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3m
\(^1\)H NMR (400 MHz, CDCl\(_3\)) Spectra of \(3n\)

\(^{13}\)C NMR (100 MHz, CDCl\(_3\)) Spectra of \(3n\)
^1H NMR (400 MHz, CDCl3) Spectra of 3o

^13C NMR (100 MHz, CDCl3) Spectra of 3o
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3p

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3p
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3q

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3q
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3r

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3r
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3s

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3s
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3t

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3t
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3u

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3u
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3v

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3v
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3w

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3w
$^{1}$H NMR (400 MHz, CDCl$_3$) Spectra of 3x

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3x
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3y

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3y
\[^1\text{H} \text{NMR} \ (400 \text{ MHz, } \text{CDCl}_3) \text{ Spectra of 3za}\]

\[^{13}\text{C} \text{ NMR} \ (100 \text{ MHz, } \text{CDCl}_3) \text{ Spectra of 3za}\]
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zb

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zb
\(^1\)H NMR (400 MHz, CDCl\(_3\)) Spectra of 3zc

\(^{13}\)C NMR (100 MHz, CDCl\(_3\)) Spectra of 3ze
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zd

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zd
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3ze

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3ze
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zf

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zf
$\text{H NMR (400 MHz, CDCl}_3\text{) Spectra of } 3\text{zg}$

$\text{C NMR (100 MHz, CDCl}_3\text{) Spectra of } 3\text{zg}$
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zh

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zh
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zi

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zi
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zj

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zj
\(^{19}\text{F} \) NMR (376 MHz, CDCl\(_3\)) Spectra of 3zj
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zk

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zk

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zl
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zl

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zm
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zm

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zn
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zo
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zo

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zp
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zp

$^{19}$F NMR (376 MHz, CDCl$_3$) Spectra of 3zp
\[ ^1H \text{ NMR (400 MHz, CDCl}_3\text{) Spectra of 3zq} \]

\[ ^13C \text{ NMR (100 MHz, CDCl}_3\text{) Spectra of 3zq} \]
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zr

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zr
$^1$H NMR (400 MHz, CDCl₃) Spectra of 3zs

$^{13}$C NMR (100 MHz, CDCl₃) Spectra of 3zs
$^{19}$F NMR (376 MHz, CDCl$_3$) Spectra of 3zs

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 3zt
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 3zt

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 1zl
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 1zl

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 1zm
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 1zn

$^1$C NMR (100 MHz, CDCl$_3$) Spectra of 1zm
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 1zn

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 1zo
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 1zo

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 1zp
\textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}) Spectra of 1zp

\textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}) Spectra of 1zq
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 1zq

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 1zr
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 1zr

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 1zs
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 1zs

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 1zt
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 1zt

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 5
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 5

$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 6
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 6
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 7

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 7
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 8

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 8
$^1$H NMR (400 MHz, CDCl₃) Spectra of 9

$^{13}$C NMR (100 MHz, CDCl₃) Spectra of 9
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of benzaldehyde

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of benzaldehyde
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of diphenyl ketone

$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of diphenyl ketone
$^1$H NMR (400 MHz, CDCl$_3$) Spectra of 10
$^{13}$C NMR (100 MHz, CDCl$_3$) Spectra of 10