Synthesis of Quinazolinones via Radical Cyclization of α-Azidyl Benzamides

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Supplementary Information

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General methods

The $^1$H and $^{13}$C NMR spectra were recorded on a Bruker AM-400 MHz spectrometer or a Bruker AM-300 MHz spectrometer with CDCl$_3$ or d$_6$-DMSO as the solvent. In CDCl$_3$, the chemical shifts in $^1$H NMR spectra were determined with Si(CH$_3$)$_4$ as the internal standard ($\delta = 0.00$ ppm); the chemical shifts in $^{13}$C NMR spectra were determined based on the chemical shift of CDCl$_3$ ($\delta = 77.00$ ppm). In d$_6$-DMSO, the chemical shifts in $^1$H NMR and $^{13}$C NMR spectra were determined based on those of DMSO ($\delta = 2.54$ ppm and 40.45 ppm, respectively). The EI-MS spectra were measured on an HP 5988A spectrometer by direct inlet at 70 eV. The high resolution mass spectra (HRMS) were measured on a Bruker micrOTOF QII by ESI. The Fourier transformation infrared spectra (FT-IR) were measured on a NEXUS 670 spectrometer. Melting points were measured on an XT-4 melting point apparatus and were uncorrected. The iminyl radical was calculated by Gauss 09W and GaussView 5.0. Flash column chromatography was carried out on silica gel (200-300 mesh). Dichloromethane was distilled from P$_2$O$_5$. N-bromosuccimide (NBS) was purchased from Tianjin Guangfu Chemical Factory and used as received.

General experimental procedures

General procedure for the preparation of compounds 1, 5, 6 and 10

To a stirred solution of amine (15 mmol) and triethylamine (25 mmol, 3.50 mL) in 30 mL CH$_2$Cl$_2$ (held in a 100 mL flask immersed in an ice bath) was added over 5 min a solution of benzoyl chloride derivative (15 mmol) in 10 mL CH$_2$Cl$_2$. The mixture was stirred at room temperature for 12h. After that, the mixture was poured into a saturated aqueous NaHCO$_3$ solution (50 mL), and the aqueous phase was extracted with CH$_2$Cl$_2$ (3×30 mL). The combined organic phases were washed with brine, dried over anhydrous Na$_2$SO$_4$, and evaporated under reduced pressure on a rotary evaporator to give the crude amide product. A solution of the crude amide (5 mmol) and iodobenzene diacetate (10 mmol, 3.22 g) in 50
mL of CH₃CN was cooled in an ice-salt bath under an argon atmosphere. Into it under stirring was injected TMSN₃ (20 mmol, 2.70 mL) with a syringe. The mixture was slowly warmed to room temperature, and the stirring was continued until no gas was generated. The solvent was then removed under reduced pressure on a rotary evaporator. The thus obtained crude product was purified by column chromatography on silica gel (Petroleum ether:ethyl acetate, 5:1, v/v) to give compounds 1, 5, 6 and 10.

**General procedure for the preparation of compounds 7a-7c**

\[ \text{R} = \text{Me, n-Pr, n-Bu} \]

**Scheme 2**

A suspension of amide (10 mmol) and paraformaldehyde (5.55 mmol, 0.5 g) in TMSCl (25 mL) was refluxed for 3h. The low volatile components were then evaporated under reduced pressure on a rotary evaporator. The residual was dissolved in DMSO (50 mL) along with NaN₃ (15 mmol, 0.98 g), and the solution was stirred overnight at room temperature. After that, the mixture was poured into a saturated aqueous NaHCO₃ solution (50 mL), and product was extracted with ethyl acetate (3× 50 mL). The combined organic phases were washed with brine (6×100 mL), dried over anhydrous Na₂SO₄, and concentrated under reduced pressure on a rotary evaporator. The residual was treated with silica gel column chromatography (petroleum ether:ethyl acetate, 5:1, v/v) to yield 7.

**General procedure for the preparation of 12 and 14**

**Scheme 3**

A solution of benzamide (5.0 mmol) and 50% ethyl glyoxyate (10 mmol, 2.04 g) in toluene (20 mL) was refluxed for 12h and then cooled to room temperature. Into it was next added thionyl chloride (10 mmol, 1.19 g), and mixture was stirred at 60 °C for 4h followed by refluxing for 3h. The low volatile components were removed under reduced pressure on a rotary evaporator. The residual was dissolved in DMSO (50 mL) along with NaN₃ (15 mmol, 0.98 g), and the solution was stirred overnight at room temperature. After that, the reaction mixture was poured into a saturated aqueous NaHCO₃ solution (50 mL), and was extracted with ethyl acetate (3×50 mL). The combined organic phases were washed with brine (6×100 mL), dried over anhydrous Na₂SO₄, and then concentrated under reduced pressure on a rotary evaporator. The residual was treated with silica gel column chromatography (petroleum ether:ethyl acetate, 3:1, v/v) to yield 12 or 14.

**General procedure for the NBS-mediated reaction of α-azidyl benzamides under visible light irradiation**
A solution of a α-azidyl benzamide substrate (0.5 mmol) and NBS (1.0 mmol, 178 mg) in 25 mL of anhydrous CH₂Cl₂ (bubbled with argon for 30 min before use) contained in a 50 mL Pyrex round bottom flask was irradiated with a 25 W fluorescent lamp under an argon atmosphere for 2 h. The mixture was then poured into a saturated aqueous NaHCO₃ solution (25 mL), and the aqueous phase was extracted with CH₂Cl₂ (3 × 10 mL). The combined organic phases were washed with brine, dried over anhydrous Na₂SO₄, and concentrated under reduced pressure on a rotary evaporator. The residual was treated with silica gel column chromatography (petroleum ether:ethyl acetate, 2:1, v/v) to yield the quinazolinone product.

O¹⁸-Isotope labeling for 3a
A solution of 1a (0.5 mmol, 108 mg), H₂O¹⁸ (20 uL) and NBS (1.0 mmol, 178 mg) in 25 mL of anhydrous CH₂Cl₂ (bubbled with argon for 30 min before use) contained in a 50 mL Pyrex round bottom flask was irradiated with a 25 W fluorescent lamp under an argon atmosphere for 2 h. The mixture was then poured into a saturated aqueous NaHCO₃ solution (25 mL), and the aqueous phase was extracted with CH₂Cl₂ (3 × 10 mL). The combined organic phases were washed with brine, dried over anhydrous Na₂SO₄, and concentrated under reduced pressure on a rotary evaporator. The residual was treated with silica gel column chromatography (petroleum ether:ethyl acetate, 2:1, v/v) to yield 2a and 3a. The appearance of O¹⁸ in 3a was identified with EI-MS.

Characterization data for the substrates

![Chemical structure of 1a](image)

(2-Azidopyrrolidin-1-yl)(phenyl)methanone (1a)
Pale yellow syrup (799 mg, 74%); Rf = 0.35 (petroleum ether: EtOAc, 3:1, v/v); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.56–7.54 (m, 2.0 H), 7.45–7.41 (m, 3.0 H), 5.91 (br, s, 0.7 H), 5.18 (br, s, 0.3 H), 3.72–3.41 (m, 2.0 H), 2.08 (br, 3.0 H), 1.88 (br, 1.0 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 170.8, 135.7, 131.0, 130.2, 128.5, 128.2, 127.2, 126.9, 75.4, 73.6, 49.0, 45.8, 35.8, 31.7, 23.7, 21.2; FT-IR (KBr, cm⁻¹): 2110.3; ESI-HRMS: m/z calcd for C₁₁H₁₂N₂O⁺H⁺: 217.1084, found: 217.1081.

![Chemical structure of 1b](image)

(2-Azidopyrrolidin-1-yl)(4-fluorophenyl)methanone (1b)
Pale yellow syrup (679 mg, 58%); Rf = 0.35 (petroleum ether: EtOAc, 3:1, v/v); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.60 (t, J = 6.4 Hz, 2.0 H), 7.11 (t, J = 8.0 Hz, 2.0 H), 5.92 (br, s, 0.7 H), 5.17 (br, s, 0.3 H), 3.64–3.45 (br, m, 2.0 H), 2.11–1.91 (m, 4.0 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 169.9, 163.7 (d, J = 249 Hz), 131.8, 129.6, 129.5, 115.5, 115.3, 73.9, 49.2, 46.0, 33.2, 31.8, 29.6, 23.9, 21.3; FT-IR (KBr, cm⁻¹): 2109.2; ESI-HRMS: m/z calcd for C₁₁H₁₂FN₂O⁺H⁺: 235.0990, found: 235.0986.
(2-Azidopyrrolidin-1-yl)(4-chlorophenyl)methanone (1c)
Pale yellow syrup (775 mg, 62%); Rf = 0.37 (Petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl3, 400 MHz, δ ppm): 7.51 (br, 2 H), 7.39 (d, J = 5.6 Hz, 2 H), 5.88 (br, s, 0.6 H), 5.14 (br, s, 0.4 H), 3.69–3.39 (m, 2 H), 2.09–1.88 (m, 4 H); 13C NMR (CDCl3, 100 MHz, δ ppm): 169.6, 136.3, 133.9, 128.5, 128.4, 75.3, 73.7, 49.0, 45.9, 33.0, 31.6, 23.7, 21.1; FT-IR (KBr, cm⁻¹): 2113.0; ESI-HRMS: m/z calcd for C11H11ClN4O+H+: 251.0694, found: 251.0698.

2-Azidopyrrolidin-1-yl)(4-bromophenyl)methanone (1d)
Pale yellow syrup (679 mg, 46%); Rf = 0.37 (petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl3, 400 MHz, δ ppm): 7.56 (d, J = 8.4 Hz, 2 H), 7.45 (d, J = 8.0 Hz, 2 H), 5.88 (br, s, 0.7 H), 5.14 (br, s, 0.3 H), 3.70–3.40 (m, 2 H), 2.10–2.00 (br, m, 2 H), 1.89 (br, s, 1 H); 13C NMR (CDCl3, 100 MHz, δ ppm): 169.7, 134.5, 131.5, 128.8, 124.7, 75.4, 73.8, 49.0, 46.0, 33.1, 31.7, 23.8, 21.1; FT-IR (KBr, cm⁻¹): 2110.9; ESI-HRMS: m/z calcd for C11H11BrN4O+H+: 295.0189, found: 295.0192.

4-(2-Azidopyrrolidine-1-carbonyl)benzonitrile (1e)
Pale yellow syrup (711 mg, 59%); Rf = 0.16 (petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl3, 400 MHz, δ ppm): 7.77 (d, J = 6.8 Hz, 2 H), 7.68 (d, J = 7.6 Hz, 2 H), 5.90 (br, s, 0.7 H), 5.10 (br, s, 0.3 H), 3.74–3.57 (m, 1.3 H), 3.40–3.36 (m, 0.7 H), 2.14–2.04 (m, 2.7 H), 1.94–1.93 (m, 1.3 H); 13C NMR (CDCl3, 100 MHz, δ ppm): 168.8, 139.8, 132.1, 127.6, 117.7, 113.8, 75.1, 73.7, 48.8, 46.0, 32.9, 31.6, 23.6, 21.0; FT-IR (KBr, cm⁻¹): 2108.6; ESI-HRMS: m/z calcd for C12H11N5O+H+: 242.1036, found 242.1038.

(2-Azidopyrrolidin-1-yl)(4-nitrophenyl)methanone (1f)
Pale yellow syrup (665 mg, 51%); Rf = 0.20 (petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl3, 400 MHz, δ ppm): 8.30 (d, J = 7.6 Hz, 2 H), 7.75 (d, J = 7.2 Hz, 2 H), 5.92 (br, s, 0.7 H), 5.10 (br, s, 0.3 H), 3.77–3.56 (m, 1.4 H), 3.39–3.37 (m, 0.6 H), 2.16–2.05 (m, 2.7 H), 1.96 (br, 1.3 H); 13C NMR (CDCl3, 100 MHz, δ ppm): 168.8, 168.3, 148.6, 141.6, 128.2, 123.7, 73.9, 49.0, 31.8, 23.8; FT-IR (KBr, cm⁻¹): 2111.2; ESI-HRMS: m/z calcd for C11H11N5O3+H+: 262.0935, found: 262.0934.
2-Azidopyrrolidin-1-yl)(4-(trifluoromethyl)phenyl)methanone (1g)
Pale yellow syrup (753 mg, 53%); R_f = 0.68 (petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl_3, 400 MHz, δ ppm): 7.70 (br, 5.0 H), 5.92 (br, 0.7 H), 5.11 (br, s, 0.3 H), 3.75–3.39 (m, 2.0 H), 2.13–2.04 (m, 2.8 H), 1.92 (br, 1.2 H); 13C NMR (CDCl_3, 100 MHz, δ ppm): 169.5, 132.1 (q, J = 32 Hz), 130.2, 127.7, 127.6, 127.5, 125.4, 124.9, 122.2, 119.5, 75.3, 73.8, 49.0, 46.0, 33.1, 31.8, 23.8, 21.2; FT-IR (KBr, cm⁻¹): 2108.9; ESI-HRMS: m/z calcd for C_{12}H_{11}F_{3}N_{4}O+Na+: 307.0777, found 307.0780.

(2-Azidopyrrolidin-1-yl)(ρ-tolyl)methanone (1h)
Pale yellow syrup (747 mg, 65%); R_f = 0.42 (Petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl_3, 400 MHz, δ ppm): 7.47 (d, J = 8.0 Hz, 2.0 H), 7.22 (d, J = 7.6 Hz, 2.0 H), 5.92 (br, s, 0.7 H), 5.20 (br, s, 0.3 H), 3.45 (br, 1.40 H), 3.64 (br, s, 0.6 H), 2.38 (s, 3H), 2.08–1.83 (m, 4.0 H); 13C NMR (CDCl_3, 100 MHz, δ ppm): 171.0, 140.6, 132.8, 128.8, 127.2, 73.8, 49.1, 45.8, 33.2, 31.7, 23.9, 21.3; FT-IR (KBr, cm⁻¹): 2107.3; ESI-HRMS: m/z calcd for C_{12}H_{14}NO+H+: 231.1240, found: 231.1244.

(2-Azidopyrrolidin-1-yl)(4-methoxyphenyl)methanone (1i)
Pale yellow syrup (738 mg, 60%); R_f = 0.26 (Petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl_3, 400 MHz, δ ppm): 7.57 (d, J = 8.8 Hz, 2.0 H), 6.92 (d, J = 8.4 Hz, 2.0 H), 5.90 (br, s, 0.7 H), 5.29 (br, s, 0.3 H), 3.83 (s, 3.0 H), 3.67–3.54 (m, 2.0 H), 2.07–1.92 (m, 4.0 H); 13C NMR (CDCl_3, 100 MHz, δ ppm): 170.5, 161.2, 129.3, 127.8, 113.5, 74.0, 55.2, 49.3, 31.9, 23.7; FT-IR (KBr, cm⁻¹): 2109.9; ESI-HRMS: m/z calcd for C_{12}H_{14}NO_{2}+H+: 247.1190, found: 247.1188.

2-Azidopyrrolidin-1-yl)(3-fluorophenyl)methanone (1j)
Pale yellow syrup (503 mg, 43%); R_f = 0.42 (Petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl_3, 400 MHz, δ ppm): 7.42–7.40 (m, 2.0 H), 7.30 (d, J = 9.6 Hz, 1.0 H), 7.16 (t, J = 7.6 Hz, 1.0 H), 5.91 (br, s, 0.7 H), 5.17 (br, s, 0.3 H), 3.72–3.42 (m, 2.0 H), 2.11 (br, s, 2.7 H), 1.91 (br, s, 1.3 H); 13C NMR (CDCl_3, 100 MHz, δ ppm): 169.4, 162.2 (d, J = 247 Hz), 137.7, 137.6, 130.1, 129.8, 129.8, 125.5, 122.7, 117.4, 117.2, 116.7, 114.4, 114.2, 75.4, 73.8, 49.0, 45.9, 33.2, 31.7, 23.7, 21.1; FT-IR (KBr, cm⁻¹): 2109.7; ESI-HRMS: m/z calcd for C_{11}H_{11}FN_{4}O+H+: 235.0990, found: 235.0984.
2-Azidopyrrolidin-1-yl)(3-(trifluoromethyl)phenyl)methanone (1k)
Pale yellow syrup (738 mg, 52%); R<sub>f</sub> = 0.53 (petroleum ether: EtOAc, 3:1, v/v); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, δ ppm): 7.85 (s, 1.0 H), 7.76 (d, J = 6.0 Hz, 1.0 H), 7.73 (d, J = 8.0 Hz, 1.0 H), 7.56 (t, J = 7.6 Hz, 1.0 H), 5.92 (br, s, 0.7 H), 5.11 (br, s, 0.3 H), 3.74 − 3.42 (m, 2.0 H), 2.13 (br, s, 2.7 H), 1.92 (br, s, 1.3 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, δ ppm): 169.3, 136.6, 131.0, 130.7, 130.4, 129.0, 127.6, 127.0, 127.0, 124.9, 124.2, 124.2, 124.2, 124.1, 122.2, 119.5, 73.9, 49.1, 46.1, 33.2, 31.8, 23.8, 21.3; FT-IR (KBr, cm<sup>-1</sup>): 2108.7; ESI-HRMS: m/z calcd for C<sub>12</sub>H<sub>11</sub>F<sub>3</sub>N<sub>4</sub>O +Na<sup>+</sup>: 307.0777, found: 307.0779.

(2-Azidopyrrolidin-1-yl)(3,5-dinitrophenyl)methanone (1l)
Pale yellow syrup (704 mg, 46%); R<sub>f</sub> = 0.38 (petroleum ether: EtOAc, 3:1, v/v); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, δ ppm): 9.11 (s, 1.0 H), 8.84 − 8.77 (m, 2.0 H), 5.92 (br, s, 0.7 H), 5.15 (br, s, 0.3 H), 3.82 − 3.53 (m, 2.0 H), 2.23 − 2.02 (m, 4.0 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, δ ppm): 165.8, 148.2, 138.8, 127.5, 120.1, 74.8, 74.4, 49.1, 46.7, 32.7, 31.6, 23.8, 21.6; FT-IR (KBr, cm<sup>-1</sup>): 2112.4; ESI-HRMS: m/z calcd for C<sub>11</sub>H<sub>10</sub>N<sub>6</sub>O<sub>5</sub> +H<sup>+</sup>: 307.0785, found: 307.0786.

(2-Azidopyrrolidin-1-yl)(2-chlorophenyl)methanone (1m)
Pale yellow syrup (663 mg, 53%); R<sub>f</sub> = 0.44 (petroleum ether: EtOAc, 3:1, v/v); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, δ ppm): 7.44 − 7.32 (m, 4.0 H), 5.94 (d, J = 4.8 Hz, 0.6 H), 5.04 (d, J = 3.6 Hz, 0.4 H), 3.79 − 3.67 (m, 1.0 H), 3.40 − 3.36 (m, 0.5 H), 3.23 − 3.16 (m, 0.5 H), 2.11 − 1.88 (m, 4.0 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, δ ppm): 165.8, 148.2, 138.8, 127.5, 120.1, 74.8, 74.4, 49.1, 46.7, 32.7, 31.6, 23.8, 21.6; FT-IR (KBr, cm<sup>-1</sup>): 2114.6; ESI-HRMS: m/z calcd for C<sub>11</sub>H<sub>11</sub>ClN<sub>4</sub>O +H<sup>+</sup>: 251.0694, found: 251.0698.

(2-Azidopyrrolidin-1-yl)(2-bromophenyl)methanone (1n)
Pale yellow syrup (590 mg, 40%); R<sub>f</sub> = 0.38 (Petroleum ether: EtOAc, 3:1, v/v); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, δ ppm): 7.60 − 7.58 (m, 1.0 H), 7.45 − 7.26 (m, 3.0 H), 5.94 (d, J = 4.8 Hz, 0.6 H), 5.04 (d, J = 3.6 Hz, 0.4 H), 3.79 − 3.67 (m, 1.0 H), 3.40 − 3.36 (m, 0.5 H), 3.23 − 3.16 (m, 0.5 H), 2.11 − 1.88 (m, 4.0 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, δ ppm): 168.2, 167.4, 136.1, 136.7, 130.8, 130.5, 129.7, 127.5, 127.2, 75.4, 72.8, 47.4, 33.6, 32.0, 23.3, 21.6; FT-IR (KBr, cm<sup>-1</sup>): 2112.4; ESI-HRMS: m/z calcd for C<sub>11</sub>H<sub>11</sub>BrN<sub>4</sub>O +H<sup>+</sup>: 295.0189, found: 295.0196.
(2-azidopiperidin-1-yl)(phenyl)methanone (5)
Pale yellow syrup (271 mg, 24%); R_f = 0.40 (petroleum ether: EtOAc, 3:1, v/v); ^1H NMR (CDCl_3, 400 MHz, δ ppm): 7.48–7.40 (m, 5.00 H), 6.44 (d, J = 8.0 Hz, 0.50 H), 5.23 (s, 0.15 H), 4.84 (s, 0.35 H), 3.84 (br, s, 1.0 H), 3.55 (br, s, 0.30 H), 3.16 (br, s, 0.70 H), 2.14–2.10 (m, 1.00 H), 1.95 (br, s, 0.75 H), 1.86–1.78 (m, 1.00 H), 1.75–1.68 (m, 2.50 H), 1.52–1.49 (m, 0.75 H); ^13C NMR (CDCl_3, 100 MHz, δ ppm): 135.1, 130.1, 128.6, 128.3, 127.4, 127.0, 107.4, 41.0, 29.5, 24.9, 21.8, 21.6, 18.7; FT-IR (KBr, cm^-1): 2110.1; ESI-HRMS: m/z calcd for C_{12}H_{14}N_4O^+: 230.1168, found: 230.1171.

(2-azidoazepan-1-yl)(phenyl)methanone (6)
Pale yellow syrup (976 mg, 74%); R_f = 0.35 (petroleum ether: EtOAc, 3:1, v/v); ^1H NMR (CDCl_3, 400 MHz, δ ppm): 7.42 (br, 5.00 H), 6.27–6.23 (m, 0.40 H), 5.18–5.14 (m, 0.60 H), 4.33 (d, J = 14.4 Hz, 0.60 H), 3.54 (d, J = 14.4 Hz, 0.40 H), 3.23 (t, J = 12.0 Hz, 0.40 H), 3.01 (t, J = 12.0 Hz, 0.60 H), 2.26–2.19 (m, 1.00 H), 1.97–1.56 (m, 5.00 H), 1.30–1.22 (m, 2.00 H); ^13C NMR (CDCl_3, 100 MHz, δ ppm): 173.8, 171.5, 136.0, 135.5, 129.4, 128.5, 128.3, 126.6, 126.2, 74.1, 69.8, 44.1, 33.1, 27.2, 23.0, 22.6; FT-IR (KBr, cm^-1): 2100.0; ESI-HRMS: m/z calcd for C_{13}H_{16}N_4O^+: 244.1324, found: 244.1326.

N-(azidomethyl)-N-methylbenzamide (7a)
Pale yellow syrup (779 mg, 82%); R_f = 0.56 (petroleum ether: EtOAc, 3:1, v/v); ^1H NMR (CDCl_3, 400 MHz, δ ppm): 7.47–7.40 (m, 5 H), 4.90 (br, s, 1 H), 4.74 (br, s, 1 H), 1.13 (br, s, 3 H); ^13C NMR (CDCl_3, 100 MHz, δ ppm): 134.7, 130.3, 128.5, 127.2; FT-IR (KBr, cm^-1): 2108.4; ESI-HRMS: m/z calcd for C_{9}H_{10}N_4O^+: 213.0747, found: 213.0750.

N-(azidomethyl)-N-propylbenzamide (7b)
Pale yellow syrup (937 mg, 86%); R_f = 0.68 (petroleum ether: EtOAc, 3:1, v/v); ^1H NMR (CDCl_3, 400 MHz, δ ppm): 7.46–7.39 (m, 5 H), 4.78 (br, 2 H), 3.55 (br, s, 1 H), 3.34 (br, s, 1 H), 1.66 (br, 2 H), 0.88 (br, s, 3 H); ^13C NMR (CDCl_3, 100 MHz, δ ppm): 135.2, 129.9, 128.4, 128.2, 126.8, 11.0; FT-IR (KBr, cm^-1): 2109.8; ESI-HRMS: m/z calcd for C_{11}H_{14}N_4O^+: 241.1060, found: 241.1058.

N-(azidomethyl)-N-butylbenzamide (7c)
Pale yellow syrup (916 mg, 79%); R_f = 0.75 (petroleum ether: EtOAc, 3:1, v/v); ^1H NMR
(CDCl$_3$, 400 MHz, δ ppm): 7.45–7.39 (m, 5 H), 4.84 (br, 2 H), 3.54 (br, s, 1 H), 3.35 (br, s, 1 H), 1.61 (br, 2 H), 1.34 (br, 2 H), 0.88 (br, s, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 135.5, 130.0, 128.5, 127.0, 126.9, 9.6; FT-IR (KBr, cm$^{-1}$): 2108.7; ESI-HRMS: m/z calcd for C$_{12}$H$_{16}$N$_{4}$O$^{+}$Na$: 255.1216, found 255.1219.

N-(1-azidoethyl)-N-ethylbenzamide (9)
Pale yellow syrup (297 mg, 27%); R$_f$ = 0.63 (petroleum ether: EtOAc, 3:1, v/v); $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 7.44–7.42 (m, 3 H), 7.39 (br, 2 H), 5.65 (br, 1 H), 3.53–3.42 (m, 2 H), 1.42 (d, $J$ = 6.4 Hz, 3 H), 1.26 (br, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 135.9, 129.6, 128.6, 126.5, 36.2, 19.0, 14.8; FT-IR (KBr, cm$^{-1}$): 2108.4; ESI-HRMS: m/z calcd for C$_{11}$H$_{14}$N$_{4}$O$^{+}$H$: 219.1246, found 219.1250.

N-(azidomethyl)benzamide (10a)
White solid (484 mg, 55%); m.p. = 62–63 °C (recrystallized from petroleum ether and CH$_2$Cl$_2$); $^1$H NMR (CDCl$_3$, 300 MHz, δ ppm): 8.15 (br, s, 1 H), 7.84–7.81 (m, 2 H), 7.53–7.48 (m, 1 H), 5.61–5.54 (m, 1 H), 1.80–1.69 (m, 2 H), 1.01 (t, $J$ = 7.5 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 75 MHz, δ ppm): 167.9, 133.1, 132.0, 128.5, 127.1, 68.4, 27.6, 9.6; FT-IR (KBr, cm$^{-1}$): 2110.3; ESI-HRMS: m/z (rel.int., %): 176 (M$^+$, 3.86), 175 (20.85), 105 (100.00), 77 (30.78).

N-(1-azidopropyl)benzamide (10b)
White solid (469 mg, 46%); m.p. = 60–61 °C (recrystallized from petroleum ether and CH$_2$Cl$_2$); $^1$H NMR (CDCl$_3$, 300 MHz, δ ppm): 7.81 (d, $J$ = 7.2 Hz, 2 H), 7.53–7.48 (m, 1 H), 7.42–7.37 (m, 2 H), 7.21–7.18 (m, 1 H), 5.61–5.54 (m, 1 H), 1.77–1.63 (m, 2 H), 1.53–1.41 (m, 2 H), 0.96 (t, $J$ = 7.2 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 75 MHz, δ ppm): 167.6, 133.2, 132.1, 128.6, 127.1, 66.9, 36.5, 18.4, 13.4; FT-IR (KBr, cm$^{-1}$): 2108.0; ESI-HRMS: m/z calcd for C$_{11}$H$_{14}$N$_{4}$O$^{+}$Na$: 241.1060, found: 241.1058.
**N-(azido(phenyl)methyl)benzamide (10d)**

White solid (916 mg, 39%); m.p. = 98–99 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.82–7.80 (m, 2 H), 7.57 -7.53 (m, 1 H), 7.50–7.39 (m, 7 H), 6.82 (m, 2 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 167.3, 136.9, 132.8, 132.3, 129.2, 129.0, 128.7, 127.2, 126.3, 68.3; FT-IR (KBr, cm⁻¹): 2104.1; ESI-HRMS: m/z Calcd for C₁₄H₁₁N₄O⁺Na⁺: 275.0909, found: 275.0912.

**Ethyl 2-azido-2-benzamidoacetate (12a)**

White solid (918 mg, 74%); m.p. = 64–65 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.86–7.80 (m, 3 H), 7.51–7.50 (m, 1 H), 7.42–7.40 (m, 2 H), 6.00 (d, J = 7.6 Hz, 1 H), 4.27 (q, J = 7.2 Hz, 2 H), 1.30 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 167.3, 166.6, 132.2, 132.2, 128.3, 127.2, 64.9, 62.8, 13.7; FT-IR (KBr, cm⁻¹): 2115.9; ESI-HRMS: m/z Calcd for C₁₁H₁₂FN₄O₃⁺H⁺: 249.0988, found: 249.0992.

**Ethyl 2-azido-2-(4-fluorobenzamido)acetate (12b)**

White solid (811 mg, 61%); m.p. = 77–78 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.89–7.85 (m, 2 H), 7.27–7.26 (m, 1 H), 7.16 (t, J = 8.4 Hz, 2 H), 5.98 (d, J = 8.0 Hz, 1 H), 4.35 (q, J = 7.2 Hz, 2 H), 1.38 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 166.9, 166.1, 162.6 (d, J = 253 Hz), 129.8 (d, J = 9 Hz), 128.7 (d, J = 3 Hz), 115.9 (d, J = 11 Hz), 65.2, 63.3, 14.0; FT-IR (KBr, cm⁻¹): 2118.1; ESI-HRMS: m/z Calcd for C₁₁H₁₁FN₄O₃⁺Na⁺: 289.0707, found: 289.0708.

**Ethyl 2-azido-2-(4-chlorobenzamido)acetate (12c)**

White solid (635 mg, 45%); m.p. = 85–86 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.78 (d, J = 8.4 Hz, 2 H), 7.47–7.42 (m, 3 H), 5.98 (d, J = 8.0 Hz, 1 H), 4.33 (q, J = 7.2 Hz, 2 H), 1.36 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 166.8, 166.2, 138.9, 130.8, 129.0, 128.8, 65.1, 63.2, 14.0; FT-IR (KBr, cm⁻¹): 2115.9; ESI-HRMS: m/z Calcd for C₁₁H₁₁ClN₄O₃⁺Na⁺: 305.0412, found: 305.0417.

**Ethyl 2-azido-2-(4-bromobenzamido)acetate (12d)**
White solid (717 mg, 44%); m.p. = 101–102 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.71 (d, J = 8.0 Hz, 2 H), 7.59 (d, J = 8.0 Hz, 2 H), 7.44 (d, J = 7.2 Hz, 1 H), 5.98 (d, J = 8.0 Hz, 1 H), 4.34 (q, J = 7.2 Hz, 2 H), 1.36 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 166.8, 166.3, 131.9, 131.3, 128.9, 127.4, 65.1, 63.2, 14.0; FT-IR (KBr, cm⁻¹): 2107.3; ESI-HRMS: m/z Calcd for C₁₁H₁₁BrN₄O₃Na⁺: 348.9907, found: 348.9904.

**Ethyl 2-azido-2-(4-cyanobenzamido)acetate (12e)**

Yellow solid (764 mg, 56%); m.p. = 113–114 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.96 (d, J = 8.4 Hz, 2 H), 7.79 (d, J = 8.4 Hz, 2 H), 7.46 (br, d, J = 8.4 Hz, 1 H), 5.97 (d, J = 8.0 Hz, 1 H), 4.36 (q, J = 7.2 Hz, 2 H), 1.38 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 166.6, 165.5, 136.3, 132.6, 128.0, 117.7, 116.1, 65.1, 63.4, 14.0; FT-IR (KBr, cm⁻¹): 2117.9; ESI-HRMS: m/z calcd for C₁₂H₁₁N₅O₃Na⁺: 296.0760, found: 296.0763.

**Ethyl 2-azido-2-(4-nitrobenzamido)acetate (12f)**

Yellow solid (1011 mg, 69 %); m.p. = 98–99 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 8.31 (d, J = 8.4 Hz, 2 H), 8.04 (d, J = 8.8 Hz, 2 H), 7.59 (d, J = 7.6 Hz, 1 H), 5.99 (d, J = 8.0 Hz, 1 H), 4.36 (q, J = 7.2 Hz, 2 H), 1.38 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 166.6, 165.4, 150.1, 137.9, 128.6, 123.9, 65.1, 63.4, 14.0; FT-IR (KBr, cm⁻¹): 2108.8; ESI-HRMS: m/z calcd for C₁₁H₁₁N₅O₅Na⁺: 316.0658, found: 316.0662.

**Ethyl 2-azido-2-(4-(trifluoromethyl)benzamido)acetate (12g)**

White solid (774 mg, 49%); m.p. = 75–76 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.96 (d, J = 8.0 Hz, 2.0 H), 7.59 (d, J = 7.6 Hz, 2.0 H), 7.55 (br, 1.0 H), 6.01 (d, J = 8.0 Hz, 1.0 H), 4.35 (q, J = 7.2 Hz, 2.0 H), 1.37 (t, J = 7.2 Hz, 3.0 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 166.7, 166.1, 135.7, 134.1 (q, J = 32 Hz), 129.1, 127.8, 125.8, 125.7, 124.8, 122.1, 119.4, 65.1, 63.3, 13.9; FT-IR (KBr, cm⁻¹): 2109.6; ESI-HRMS: m/z calcd for C₁₂H₁₁F₃N₄O₃Na⁺: 339.0675, found: 339.0680.

**Ethyl 2-azido-2-(4-methylbenzamido)acetate (12h)**

White solid (550 mg, 42%); m.p. = 58–59 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 300 MHz, δ ppm): 7.74 (d, J = 10.8 Hz, 2 H), 7.42 (d, J = 10.8 Hz, 1 H), 7.24 (d, J = 10.4 Hz, 2 H), 5.99 (d, J = 8.0 Hz, 1 H), 4.32 (q, J = 7.2 Hz, 2 H), 2.40 (s, 3 H), 1.38–1.33 (m, 3 H); ¹³C NMR (CDCl₃, 75 MHz, δ ppm): 167.1, 166.9, 143.1, 129.6,
Ethyl 2-azido-2-(4-methoxybenzamido)acetate (12i)
White solid (1000 mg, 72%); m.p. = 50–51 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 300 MHz, δ ppm): 7.84–7.81 (m, 2 H), 7.36 (br, 1 H), 6.95–6.92 (m, 2 H), 6.00 (d, J = 8.1 Hz, 1 H), 4.34 (q, J = 7.2 Hz, 2 H), 3.85 (s, 3 H), 1.36 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 75 MHz, δ ppm): 166.9, 166.7, 162.9, 129.5, 129.3, 129.0, 124.3, 114.0, 113.8, 113.7, 65.1, 63.1, 55.4, 14.0; FT-IR (KBr, cm⁻¹): 2116.1; ESI-HRMS: m/z calcd for C₁₁H₁₄N₄O₃⁺Na⁺: 285.0958, found: 285.0962.

Ethyl 2-azido-2-(3-fluorobenzamido)acetate (12j)
Yellow solid (718 mg, 54%); m.p. = 49–50 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.63–7.56 (m, 2 H), 7.46–7.40 (m, 1 H), 7.29–7.23 (m, 1 H), 5.99 (d, J = 8.0 Hz, 1 H), 4.33 (q, J = 7.2 Hz, 2 H), 1.36 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 166.7, 166.0 (d, J = 3 Hz), 162.6 (d, J = 247 Hz), 134.6 (d, J = 7 Hz), 130.0 (d, J = 8 Hz), 122.7 (d, J = 7 Hz), 119.4 (d, J = 11 Hz), 114.7 (d, J = 23 Hz), 65.1, 63.2, 13.9; FT-IR (KBr, cm⁻¹): 2116.6; ESI-HRMS: m/z calcd for C₁₁H₁₁FN₄O₃⁺Na⁺: 289.0707, found: 289.0704.

Ethyl 2-azido-2-(3-(trifluoromethyl)benzamido)acetate (12k)
White solid (822 mg, 52%); m.p. = 39–40 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 8.13 (s, 1 H), 8.03 (d, J = 7.6 Hz, 1 H), 7.80 (d, J = 7.6 Hz, 1 H), 7.72 (d, J = 8.0 Hz, 1 H), 7.60 (t, J = 7.6 Hz, 1 H), 6.02 (d, J = 7.6 Hz, 1 H), 4.33 (q, J = 7.2 Hz, 2 H), 1.36 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 166.7, 166.3, 133.3, 131.2 (q, J = 32 Hz), 130.5, 129.3, 129.0, 128.9, 127.5, 124.8, 124.5 (q, J = 32 Hz), 122.1, 119.4, 65.2, 63.3, 13.9; FT-IR (KBr, cm⁻¹): 2111.4; ESI-HRMS: m/z calcd for C₁₂H₁₁F₃N₄O₃⁺H⁺: 317.0856, found: 317.0860.

Ethyl 2-azido-2-(3-methylbenzamido)acetate (12l)
White solid (721 mg, 55%); m.p. = 52–53 °C (recrystallized from petroleum ether and CH₂Cl₂); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.66 (s, 1 H), 7.62 (d, J = 7.2 Hz, 1 H), 7.44 (d, J = 7.2 Hz, 1 H), 7.37–7.31 (m, 2 H), 6.00 (d, J = 8.0 Hz, 1 H), 4.33 (q, J = 7.2 Hz, 2 H), 1.29, 1.27, 1.65, 1.63, 1.21, 1.39; FT-IR (KBr, cm⁻¹): 2115.1; ESI-HRMS: m/z calcd for C₁₁H₁₄N₄O₃⁺Na⁺: 285.0958, found: 285.0962.
2.39 (s, 3 H), 1.36 (t, J = 7.2 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 167.4, 166.8, 138.6, 133.2, 132.4, 128.5, 128.0, 124.3, 65.1, 63.1, 21.2, 13.9; FT-IR (KBr, cm$^{-1}$): 2108.3; 
ESI-HRMS: m/z calcd for C$_{12}$H$_{14}$N$_4$O$_3$+Na$^+$: 285.0958, found: 285.0960.

Ethyl 2-azido-2-(2-chlorobenzamido)acetate (12m)
White solid (916 mg, 65%); m.p. = 72–73 °C (recrystallized from petroleum ether and CH$_2$Cl$_2$); $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 7.73–7.67 (m, 2 H), 7.40–7.39 (m, 2 H), 7.34–7.30 (m, 1 H), 5.93 (d, $J$ = 8.0 Hz, 1 H), 4.31 (q, $J$ = 7.2 Hz, 2 H), 1.34 (t, $J$ = 7.2 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 166.2, 166.2, 132.8, 132.1, 130.8, 130.3, 127.0, 64.9, 63.0, 13.8; FT-IR (KBr, cm$^{-1}$): 2114.9; ESI-HRMS: m/z calcd for C$_{11}$H$_{11}$ClN$_4$O$_3$+Na$^+$: 305.0412, found: 305.0409.

Ethyl 2-azido-2-(2-bromobenzamido)acetate (12n)
White solid (834 mg, 51 %); m.p. = 92–94 °C (recrystallized from petroleum ether and CH$_2$Cl$_2$); $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 7.64–7.57 (m, 2 H), 7.44–7.33 (m, 3 H), 5.98–5.93 (m, 1 H), 4.35–4.29 (m, 2 H), 1.39–1.34 (m, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 167.2, 166.3, 135.6, 133.6, 133.6, 132.1, 132.0, 130.0, 129.9, 127.6, 127.5, 119.2, 64.8, 63.1, 13.9; FT-IR (KBr, cm$^{-1}$): 2115.4; ESI-HRMS: m/z calcd for C$_{11}$H$_{11}$BrN$_4$O$_3$+Na$^+$: 348.9907, found: 348.9911.

Ethyl 2-azido-2-($N$-methylbenzamido)acetate (14a)
Pale yellow syrup (603 mg, 46%); R$_f$ = 0.53 (petroleum ether: EtOAc, 3:1, v/v); $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 7.84–7.81 (m, 2 H), 7.32 (d, $J$ = 8.0 Hz, 1 H), 6.96–6.94 (m, 2 H), 5.99 (d, $J$ = 8.0 Hz, 1 H), 4.39 (q, $J$ = 7.2 Hz, 2 H), 3.86 (s, 3 H), 1.36 (t, $J$ = 7.2 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 166.9, 166.6, 135.6, 133.6, 133.6, 132.1, 132.0, 130.0, 129.9, 127.6, 127.5, 119.2, 64.8, 63.1, 13.9; FT-IR (KBr, cm$^{-1}$): 2115.3; ESI-HRMS: m/z Calcd for C$_{12}$H$_{14}$N$_4$O$_3$+H$^+$: 263.1144, found: 263.1147.

Ethyl 2-azido-2-($N$-phenylbenzamido)acetate (14b)
Pale yellow syrup (680 mg, 42%); R$_f$ = 0.53 (petroleum ether: EtOAc, 3:1, v/v); Unstable compound; $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 7.87 (d, $J$ = 7.2 Hz, 0.3 H), 7.66 (d, $J$ = 8.0 Hz, 0.3 H), 7.56–7.37 (m, 1.2 H), 7.34–7.33 (m, 2.0 H), 7.26–7.21 (m, 4.0 H), 5.81 (s, 1.0 H), 5.04 (s, 0.1 H), 4.32–4.25 (m, 2.6 H), 1.34 (t, $J$ = 7.2 Hz, 0.9 H), 1.28 (t, $J$ = 7.2 Hz, 3.0 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 170.9, 165.6, 165.0, 141.1, 138.0, 134.9, 133.8, 131.6, 131.2, 130.4, 130.0, 129.8, 129.3, 128.9, 128.8, 128.7, 128.6,
128.1, 127.9, 127.8, 127.0, 125.2, 124.3, 120.2, 85.2, 73.7, 62.6, 13.9; FT-IR (KBr, cm$^{-1}$): 2113.6; ESI-HRMS: m/z calcd for C$_{17}$H$_{16}$N$_4$O$_3$+$\text{Na}^+$: 347.1115, found: 347.1120.

Characterization data for products

2,3-Dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2a)
White solid (52.1 mg, 56%); m.p. = 102–103 $^\circ$C; $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 8.25 (dd, $J = 8.0, 1.2$ Hz, 1 H), 7.71 (td, $J = 8.4, 1.2$ Hz, 1 H), 7.61 (d, $J = 8.0$ Hz, 1 H), 7.45–7.41 (m, 1 H), 4.19 (t, $J = 7.2$ Hz, 2 H), 3.16 (t, $J = 8.0$ Hz, 2 H), 2.32–2.24 (m, 2 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 160.7, 159.3, 148.9, 133.9, 126.6, 126.1, 126.0, 120.3, 46.3, 32.3, 19.3; ESI-HRMS: m/z calcd for C$_{11}$H$_{10}$N$_2$O+H$: 187.0866, found: 187.0864.

5-Azido-1-benzoylpyrrolidin-2-one (3a)
Pale yellow syrup (16.1 mg, 14%); R$_f$ = 0.32 (petroleum ether: EtOAc, 3:1, v/v); $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 7.63 (d, $J = 7.2$ Hz, 2 H), 7.36 (d, $J = 7.2$ Hz, 1 H), 7.43 (t, $J = 7.6$ Hz, 2 H), 6.00 (dd, $J = 6.4$ Hz, 1 H), 2.83–2.74 (m, 1 H), 2.57–2.49 (m, 1 H), 2.43–2.34 (m, 1 H), 2.13–2.06 (m, 1 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 172.9, 170.6, 133.3, 132.6, 129.1, 127.9, 74.4, 30.7, 25.9; ESI-HRMS: m/z calcd for C$_{11}$H$_{10}$N$_4$O$_2$+H$: 231.0877, found: 231.0879; EI-MS: m/z (rel.int., %) for C$_{11}$H$_{10}$N$_4$O$_2$: 230 (M$^+$, 1.1), 188 (26.1), 105 (100.0), 77 (25.6); EI-Ms: m/z (rel.int., %) for C$_{11}$H$_{10}$N$_4$O$_2$O$_2$: 232 (M$^+$, 0.97), 190 (19.4), 105 (100.0), 77 (26.9).

6-Fluoro-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2b)
White solid (16.3 mg, 54%); m.p. = 130–131 $^\circ$C; $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 8.23 (dd, $J = 8.8, 6.0$ Hz, 1 H), 7.24 (dd, $J = 9.6, 2.4$ Hz, 1 H), 7.13 (td, $J = 8.8, 2.4$ Hz, 1 H), 4.19 (t, $J = 7.6$ Hz, 2 H), 3.17 (t, $J = 8.0$ Hz, 2 H), 2.34–2.26 (m, 2 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 167.4, 164.9, 160.7, 160.0, 151.3, 151.1, 128.8, 128.7, 117.1, 117.1, 114.8, 114.6, 112.1, 111.8, 46.4, 32.4, 19.3; ESI-HRMS: m/z calcd for C$_{11}$H$_{9}$FN$_2$O+H$: 205.0772, found: 205.0775.

5-Azido-1-(3-fluorobenzoyl)pyrrolidin-2-one (3b)
Pale yellow syrup (13.6 mg, 11%); R$_f$ = 0.20 (petroleum ether: EtOAc, 3:1, v/v); $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 7.70–7.66 (m, 2 H), 7.11 (t, $J = 8.8$ Hz, 2 H), 5.99 (dd, $J = 6.8, 2.0$ Hz, 1 H), 2.83–2.57 (m, 1H), 2.50–2.56 (m, 1 H), 2.44–2.34 (m, 1 H), 2.13–2.06 (m, 1 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 173.0, 169.4, 166.7, 164.1, 132.0, 129.4, 115.2, 74.5, 30.8, 25.9; ESI-HRMS: m/z calcd for C$_{11}$H$_9$FN$_2$O$_2$+H$: 249.0782, found: 249.0784.
6-Chloro-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2c)
White solid (58.6 mg, 54%); m.p. = 190–191 °C; ¹H NMR (CDCl₃, 400 MHz, δ ppm): 8.19 (d, J = 8.8 Hz, 1 H), 7.63 (d, J = 2.0 Hz, 1 H), 7.39 (dd, J = 8.4, 2.0 Hz 1 H), 4.20 (t, J = 7.6 Hz, 2 H), 3.18 (t, J = 8.0 Hz, 2 H), 2.34–2.26 (m, 2 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 160.8, 160.3, 150.1, 140.3, 127.8, 126.8, 126.4, 119.0, 46.6, 33.0, 19.4; ESI-HRMS: m/z Calcd for C₁₁H₉ClN₂O+: 221.0476, found: 221.0481.

5-Azido-1-(4-chlorobenzoyl)pyrrolidin-2-one (3c)
Pale yellow syrup (19.8 mg, 15%); Rᵥ = 0.29 (petroleum ether: EtOAc, 3:1, v/v); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.60–7.56 (m, 2 H), 7.42–7.40 (m, 2 H), 5.99 (dd, J = 2.4, 6.8 Hz, 1 H), 2.83–2.74 (m, 1 H), 2.57–2.50 (m, 1 H), 2.44–2.34 (m, 1 H), 2.13–2.06 (m, 1 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 172.9, 169.6, 139.0, 131.6, 130.6, 128.3, 74.4, 30.7, 25.9; ESI-HRMS: m/z calcd for C₁₁H₉ClN₄O₂+: 265.0487, found: 265.0482.

6-Bromo-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2d)
White solid (64.9 mg, 49%); m.p. = 219–220 °C; ¹H NMR (CDCl₃, 400 MHz, δ ppm): 8.06 (d, J = 8.4 Hz, 1 H), 7.77 (d, J = 1.6 Hz, 1 H), 7.51 (dd, J = 8.4, 2.0 Hz, 1 H), 4.19 (t, J = 8.4 Hz, 2 H), 3.18 (t, J = 8.0 Hz, 2 H), 2.34–2.26 (m, 2 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 160.7, 160.2, 149.9, 129.4, 129.3, 128.6, 127.6, 119.2, 46.5, 32.5, 19.3; ESI-HRMS: m/z calcd for C₁₁H₉BrN₂O+: 264.9971, found: 264.9973.

5-Azido-1-(4-bromobenzoyl)pyrrolidin-2-one (3d)
Pale yellow syrup (29.4 mg, 19%); Rᵥ = 0.27 (petroleum ether: EtOAc, 3:1, v/v); ¹H NMR (CDCl₃, 400 MHz, δ ppm): 7.58–7.56 (m, 2 H), 7.51–7.49 (m, 2 H), 5.98 (dd, J = 2.0, 6.4 Hz, 1 H), 2.82–2.73 (m, 1 H), 2.56–2.48 (m, 1 H), 2.42–2.35 (m, 1 H), 2.11–2.06 (m, 1 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 172.9, 169.6, 132.0, 131.2, 130.7, 127.5, 74.4, 30.7, 25.9; ESI-HRMS: m/z calcd for C₁₁H₉BrN₂O₂+: 308.9982, found: 308.9979.

9-Oxo-1,2,3,9-tetrahydropyrrolo[2,1-b]quinazoline-6-carbonitrile (2e)
White solid (66.5 mg, 63%); m.p. = 204–205 °C; ¹H NMR (CDCl₃, 400 MHz, δ ppm): 8.31 (d, J = 8.4 Hz, 1 H), 7.90 (d, J = 8.0 Hz, 1 H), 7.61 (dd, J = 8.4, 1.2 Hz, 1 H), 4.24 (t, J = 7.6 Hz, 2 H), 3.24 (t, J = 8.0 Hz, 2 H), 2.39–2.32 (m, 2 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm):
4-(2-Azido-5-oxopyrrolidine-1-carbonyl)benzonitrile (3e)
Pale yellow syrup (7.7 mg, 6%); R_{f} = 0.20 (petroleum ether: EtOAc, 3:1, v/v); ^1H NMR (CDCl\textsubscript{3}, 400 MHz, \delta ppm): 7.74–7.72 (m, 2 H), 7.69–7.67 (m, 2 H), 6.04–6.02 (m, 1 H), 2.84–2.75 (m, 1 H), 2.58–2.50 (m, 1 H), 2.47–2.37 (m, 1 H), 2.16–2.10 (m, 1 H); ^13C NMR (CDCl\textsubscript{3}, 100 MHz, \delta ppm): 172.9, 169.0, 137.5, 131.7, 129.3, 127.8, 115.6, 74.1, 30.6, 25.9; ESI-HRMS: m/z calcd for C\textsubscript{12}H\textsubscript{9}N\textsubscript{3}O\textsubscript{2}+H\textsuperscript{+}: 256.0829, found: 256.0827.

6-Nitro-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2f)
White solid (78.5 mg, 68%); m.p. = 202–203 °C; ^1H NMR (CDCl\textsubscript{3}, 400 MHz, \delta ppm): 8.40 (dd, J = 8.4, 2.4 Hz, 1 H), 8.38 (s, 1 H), 8.16 (dd, J = 8.8, 2.4 Hz, 1 H), 4.25 (t, J = 7.6 Hz, 2 H), 3.25 (t, J = 8.0 Hz, 2 H), 2.41–2.34 (m, 2 H); ^13C NMR (CDCl\textsubscript{3}, 100 MHz, \delta ppm): 161.9, 159.5, 151.2, 149.5, 128.1, 124.5, 122.3, 119.7, 46.8, 32.5, 19.3; ESI-HRMS: m/z calcd for C\textsubscript{11}H\textsubscript{9}N\textsubscript{3}O\textsubscript{3}+H\textsuperscript{+}: 232.0717, found: 232.0718.

6-(Trifluoromethyl)-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2g)
White solid (66.0 mg, 52%); m.p. = 143–144 °C; ^1H NMR (CDCl\textsubscript{3}, 400 MHz, \delta ppm): 8.36 (d, J = 8.4, 1 H), 7.90 (s, 1 H), 7.63 (d, J = 8.0 Hz, 1 H), 4.23 (t, J = 7.6 Hz, 2 H), 3.21 (t, J = 8.0 Hz, 2 H), 2.37–2.30 (m, 2 H); ^13C NMR (CDCl\textsubscript{3}, 100 MHz, \delta ppm): 160.9, 160.0, 149.0, 135.6 (q, J = 32 Hz), 127.4, 124.7, 124.3, 124.3, 122.7, 122.1, 122.0, 46.6, 32.5, 19.4; EI-MS: m/z (rel.int., %): 255 (M\textsuperscript{+}, 9.2), 254 (67.6), 253 (100.0), 235 (5.6), 170 (5.0).

6-(Bromomethyl)-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2h)
White solid (43.1 mg, 31%); m.p. = 141–142 °C; ^1H NMR (CDCl\textsubscript{3}, 300 MHz, \delta ppm): 8.24 (d, J = 7.8 Hz, 1 H), 7.63 (d, J = 1.5 Hz, 1 H), 7.45 (dd, J = 7.8, 1.5 Hz, 1 H), 4.56 (s, 2 H), 4.20 (t, J = 7.2 Hz, 2 H), 3.17 (t, J = 7.2 Hz, 2 H), 2.35–2.24 (m, 2 H); ^13C NMR (CDCl\textsubscript{3}, 75 MHz, \delta ppm): 160.4, 160.1, 149.3, 143.9, 126.8, 127.0, 126.9, 120.1, 46.5, 32.5, 32.1, 19.4; ESI-HRMS: m/z calcd for C\textsubscript{12}H\textsubscript{11}BrN\textsubscript{2}O\textsuperscript{+}: 279.1033, found: 279.1035.
5-Azido-1-(4-(bromomethyl)benzoyl)pyrrolidin-2-one (3h)
Pale yellow syrup (21.0 mg, 13%); Rf = 0.31 (petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl3, 400 MHz, δ ppm): 7.62–7.60 (m, 2.5 H), 7.44 (d, J = 8.4 Hz, 1.5 H), 6.00–5.98 (m, 1.0 H), 4.49 (s, 2.0 H), 2.83–2.73 (m, 1.0 H), 2.56–2.48 (m, 1.0 H), 2.42–2.33 (m, 1.0 H), 2.12–2.06 (m, 1.0 H); 13C NMR (CDCl3, 100 MHz, δ ppm): 172.9, 169.9, 142.1, 133.2, 129.6, 128.5, 74.4, 32.2, 30.7, 25.9; ESI-HRMS: m/z calcd for C12H11BrN4O2+H+: 323.0138, found: 323.0139.

5-Bromo-6-methoxy-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2i)
White solid (33.9 mg, 23%); m.p. = 268–269 °C; 1H NMR (CDCl3, 400 MHz, δ ppm): 8.21 (d, J = 8.8 Hz, 1 H), 7.06 (d, J = 8.8 Hz, 1 H), 4.18 (t, J = 7.2 Hz, 2 H), 4.04 (s, 3 H), 3.26 (t, J = 7.6 Hz, 2 H), 2.32–2.25 (m, 2 H); 13C NMR (CDCl3, 100 MHz, δ ppm): 161.2, 160.6, 160.2, 148.4, 126.9, 115.4, 110.5, 108.8, 56.7, 46.4, 33.0, 19.5; ESI-HRMS: m/z calcd for C12H11BrN2O2+H+: 295.0082, found: 295.0086.

5-Azido-1-(4-methoxybenzoyl)pyrrolidin-2-one (3i)
Pale yellow syrup (11.7 mg, 9%); Rf = 0.24 (petroleum ether: EtOAc, 3:1, v/v); 1H NMR (CDCl3, 400 MHz, δ ppm): 7.67 (dd, J = 6.8, 2.0 Hz, 2 H), 6.90 (dd, J = 6.8, 2.0 Hz, 2 H), 5.96 (dd, J = 6.8, 2.4 Hz, 1 H), 3.86 (s, 1 H), 2.82–2.73 (m, 1 H), 2.56–2.42 (m, 1 H), 2.42–2.32 (m, 1 H), 2.10–2.03 (m, 1 H); 13C NMR (CDCl3, 100 MHz, δ ppm): 173.0, 169.8, 163.5, 132.0, 125.3, 113.3, 74.7, 55.4, 30.9, 26.0; ESI-HRMS: m/z calcd for C12H12N4O3+H+: 261.0982, found: 261.0979.

5-Fluoro-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2j-1)
White solid (33.7 mg, 33%); m.p. = 158–160 ºC; 1H NMR (CDCl3, 400 MHz, δ ppm): 8.03 (d, J = 8.0 Hz, 1 H), 7.45 (dt, J = 1.2, 8.0 Hz, 1 H), 7.40–7.34 (m, 1 H), 4.22 (t, J = 7.6 Hz, 2 H), 3.17 (t, J = 8.0 Hz, 2 H), 2.34–2.26 (m, 2 H); 13C NMR (CDCl3, 100 MHz, δ ppm): 160.2, 160.0 (d, J = 3 Hz), 156.7 (d, J = 253 Hz), 122.5, 121.8 (d, J = 3 Hz), 119.5 (d, J = 19 Hz), 46.6, 32.7, 19.4; ESI-HRMS: m/z calcd for C11H8FN2O+H+: 205.0772, found: 205.0773.

7-Fluoro-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2j-2)
White solid (55.1 mg, 54%); m.p. = 172–174 ºC; 1H NMR (CDCl3, 400 MHz, δ ppm): 7.91
(dd, J = 8.4, 2.8 Hz, 1 H), 7.65 (dd, J = 9.2, 4.8 Hz, 1 H), 7.45 (td, J = 4.8, 8.4 Hz, 1 H), 4.21 (t, J = 7.6 Hz, 2 H), 3.18 (t, J = 8.0 Hz, 2 H), 2.34–2.26 (m, 2 H); ^13^C NMR (CDCl₃, 100 MHz, δ ppm): 161.8, 159.3, 158.8, 145.8, 129.1, 129.0, 122.8, 122.5, 121.8, 111.4, 111.2, 46.5, 32.4, 19.6; ESI-HRMS: m/z calcd for C₁₁H₉FN₂O⁺H⁺: 205.0772, found: 205.0770.

5-(Trifluoromethyl)-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2k-1)
White solid (39.4 mg, 31%); m.p. = 134–135 °C; ^1^H NMR (CDCl₃, 400 MHz, δ ppm): 8.47 (d, J = 8.0 Hz, 1 H), 8.04 (d, J = 7.6 Hz, 1 H), 7.49 (t, J = 8.0 Hz, 1 H), 4.22 (t, J = 7.6 Hz, 2 H), 3.25 (t, J = 8.0 Hz, 2 H), 2.35–2.27 (m, 2 H); ^13^C NMR (CDCl₃, 100 MHz, δ ppm): 160.6, 160.2, 147.0, 131.8, 131.7, 126.3, 126.0, 125.0, 124.9, 122.2, 121.7, 46.6, 32.9, 19.5; ESI-HRMS: m/z calcd for C₁₂H₉FN₂O⁺H⁺: 255.0740, found 255.0743.

7-(Trifluoromethyl)-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2k-2)
White solid (30.5 mg, 24%); m.p. = 142–144 °C; ^1^H NMR (CDCl₃, 400 MHz, δ ppm): 8.56 (s, 1 H), 7.91 (dd, J = 8.4, 1.6 Hz, 1 H), 7.74 (d, J = 8.8 Hz, 1 H), 4.24 (t, J = 7.6 Hz, 2 H), 3.22 (t, J = 8.0 Hz, 2 H), 2.35–2.27 (m, 2 H); ^13^C NMR (CDCl₃, 100 MHz, δ ppm): 161.7, 160.2, 151.3, 130.3, 130.3, 128.3, 128.0, 127.8, 125.1, 124.4, 124.3, 122.4, 120.4, 46.7, 32.7, 19.4; ESI-HRMS: m/z calcd for C₁₂H₉FN₂O⁺H⁺: 255.0740, found 255.0742.

5,7-Dinitro-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (2l)
White solid (62.1 mg, 45%); m.p. = 260–261 °C; ^1^H NMR (CDCl₃, 400 MHz, δ ppm): 9.29 (d, J = 2.8 Hz, 1 H), 8.81 (d, J = 2.4 Hz, 1 H), 4.29 (t, J = 7.6 Hz, 2 H), 3.32 (t, J = 8.0 Hz, 2 H), 2.43–2.35 (m, 2 H); ^13^C NMR (CDCl₃, 100 MHz, δ ppm): 166.1, 158.2, 146.5, 145.6, 143.5, 125.8, 122.7, 122.7, 47.4, 33.4, 19.2; ESI-HRMS: m/z calcd for C₁₁H₈N₄O₅⁺H⁺: 277.0567, found: 277.0571.

3-Bromo-5,7-dinitro-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one (4l)
White solid (40.8 mg, 23%); m.p. = 300 °C; ^1^H NMR (CDCl₃, 400 MHz, δ ppm): 9.30 (d, J = 2.8 Hz, 1 H), 8.84 (d, J = 2.4 Hz, 1 H), 5.31 (dd, J = 6.4, 1.2 Hz, 1 H), 4.51–4.46 (m, 1 H), 4.34–4.26 (m, 1 H), 2.92–2.82 (m, 1 H), 2.72–2.66 (m, 1 H); ^13^C NMR (CDCl₃, 100 MHz, δ ppm): 163.4, 157.8, 146.9, 145.4, 144.3, 125.8, 123.1, 123.0, 45.3, 44.7, 31.7; ESI-HRMS: m/z calcd for C₁₁H₇BrN₄O₅⁺H⁺: 354.9673, found: 354.9677.
3-Methylquinazolin-4(3H)-one (8a)\(^7\)
White solid (42.4 mg, 53%); m.p. = 88–89 °C; \(^1\)H NMR (CDCl\(_3\), 400 MHz, \(\delta\) ppm): 8.31 (d, \(J = 8.0\) Hz, 1 H), 8.06 (s, 1 H), 7.77–7.69 (m, 2 H), 7.50 (dt, \(J = 1.2\) Hz, 8.0 Hz, 1 H), 3.95 (s, 3 H); \(^{13}\)C NMR (CDCl\(_3\), 100 MHz, \(\delta\) ppm): 161.4, 148.1, 146.7, 134.0, 127.3, 127.2, 126.4, 121.8, 33.9; EI-MS: m/z (rel.int., %): 160 (M\(^+\), 100), 159 (19.2), 131 (14.0), 119 (19.5).

3-Propylquinazolin-4(3H)-one (8b)\(^4\)
White solid (38.5 mg, 41%); mp = 73–74 °C; \(^1\)H NMR (CDCl\(_3\), 400 MHz, \(\delta\) ppm): 8.32 (d, \(J = 8.0\) Hz, 1 H), 8.04 (s, 1 H), 7.78–7.72 (m, 2 H), 7.51 (t, \(J = 8.0\) Hz,, 1 H), 3.98 (t, \(J = 8.0\) Hz, 2 H), 1.87–1.70 (m, 2 H), 1.01 (t, \(J = 8.0\) Hz, 3 H); \(^{13}\)C NMR (CDCl\(_3\), 100 MHz, \(\delta\) ppm): 161.0, 148.1, 146.7, 134.1, 127.4, 127.2, 126.7, 122.2, 48.6, 22.6, 11.1; EI-MS: m/z (rel.int., %): 188 (M\(^+\), 41.99), 160 (10.37), 146 (100.00), 129 (25.17), 118 (18.14).

3-Butylquinazolin-4(3H)-one (8c)\(^8\)
White solid (43.4 mg, 43%); mp = 66–68 °C; \(^1\)H NMR (CDCl\(_3\), 400 MHz, \(\delta\) ppm): 8.32 (d, \(J = 8.0\) Hz, 1 H), 8.07 (s, 1 H), 7.76–7.71 (m, 2 H), 7.51 (t, \(J = 8.0\) Hz, 1 H), 4.02 (t, \(J = 8.0\) Hz, 2 H), 1.83–1.75 (m, 2 H), 1.47–1.38 (m, 2 H), 0.98 (t, \(J = 8.0\) Hz, 3 H); \(^{13}\)C NMR (CDCl\(_3\), 100 MHz, \(\delta\) ppm): 161.0, 147.9, 146.6, 134.1, 127.3, 127.2, 126.7, 122.7, 46.8, 31.4, 19.9, 13.6; EI-MS: m/z (rel.int., %): 202 (M\(^+\), 41.7), 185 (19.2), 173 (13.2), 160 (73.8), 146 (100.0), 118 (17.7).

2-Phenylquinazolin-4(3H)-one (11d)\(^9\)
White solid (65.5 mg, 59%); m.p. = 216–218 °C; \(^1\)H NMR (d6-DMSO, 300 MHz, \(\delta\) ppm): 12.55 (br, s, 1 H), 8.20–8.14 (m, 3 H), 7.86–7.80 (m, 1 H), 7.79–7.73 (m, 1 H), 7.61–7.49 (m, 4 H); \(^{13}\)C NMR (d6-DMSO, 100 MHz, \(\delta\) ppm): 162.3, 153.1, 148.7, 135.1, 132.9, 132.0, 129.1, 129.0, 128.3, 127.5, 127.1, 126.4, 121.4; EI-MS: m/z (rel.int., %): 222 (M\(^+\), 94.4), 221 (4.7), 119 (100.0), 111 (6.9).

Ethyl 4-oxo-3,4-dihydroquinazoline-2-carboxylate (13a)\(^10\)
White solid (86.7 mg, 74%); m.p. = 188–190 °C; \(^1\)H NMR (CDCl\(_3\), 400 MHz, \(\delta\) ppm): 10.85 (s, 1 H), 8.38 (dd, \(J = 2.4\) Hz, 10.4 Hz, 1 H), 7.80 (d, \(J = 2.4\) Hz, 1 H), 7.78–7.72 (m, 1 H),
7.66–7.61 (m, 1 H), 4.69 (q, J = 9.6 Hz, 2 H), 1.51 (t, J = 9.6 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 75 MHz, δ ppm): 161.3, 160.5, 147.5, 141.7, 135.0, 129.2, 129.1, 126.7, 123.0, 64.1, 14.1; EI-MS: m/z (rel.int., %): 218 (M$^+$, 19.8), 147 (21.1), 146 (100.0), 145 (21.0), 119 (63.18), 90 (29.1).

**Ethyl 7-fluoro-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13b)**

White solid (98.0 mg, 83%); m.p. = 175–177 °C; $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 10.75 (s, 1 H), 8.39 (dd, J = 8.8 Hz, 6.0 Hz, 1 H), 7.62 (dd, J = 8.8 Hz, 6.0 Hz, 1 H), 7.57 (dt, J = 8.4 Hz, 2.4 Hz, 1 H), 4.59 (q, J = 7.2 Hz, 2 H), 1.51 (t, J = 7.2 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 167.9, 165.4, 160.4 (d, J = 17 Hz), 149.8 (d, J = 11 Hz), 142.9, 129.4 (d, J = 10 Hz), 119.8, 117.8 (d, J = 23 Hz), 114.7 (d, J = 23 Hz), 64.3, 14.1; EI-MS: m/z (rel.int., %): 236 (M$^+$, 16.1), 164 (100.0), 137 (66.7), 108 (43.0).

**Ethyl 7-chloro-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13c)**

White solid (82.1 mg, 65%); m.p. = 179–180 °C; $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 11.03 (s, 1 H), 8.29 (d, J = 8.8 Hz, 1 H), 7.95 (s, 1 H), 7.57 (dt, J = 8.4 Hz, 2.4 Hz, 1 H), 4.59 (q, J = 7.2 Hz, 2 H), 1.51 (t, J = 7.2 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 160.7, 160.2, 148.5, 142.9, 141.3, 129.6, 128.6, 128.1, 121.4, 64.2, 14.1; EI-MS: m/z (rel.int., %): 254 (M$^+$+2, 5.2), 252 (M$^+$, 15.0), 182 (31.2), 180 (100.0), 155 (18.2), 153 (56.8), 124 (31.2).

**Ethyl 7-bromo-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13d)**

White solid (85.1 mg, 61%); m.p. = 184–185 °C; $^1$H NMR (CDCl$_3$, 400 MHz, δ ppm): 11.13 (s, 1 H), 8.21 (d, J = 8.0 Hz, 1 H), 8.13 (s, 1 H), 7.72 (d, J = 8.0 Hz, 1 H), 4.58 (q, J = 7.2 Hz, 2 H), 1.51 (t, J = 7.2 Hz, 3 H); $^{13}$C NMR (CDCl$_3$, 100 MHz, δ ppm): 160.9, 160.2, 148.5, 142.8, 132.4, 131.8, 129.7, 128.0, 121.8, 64.1, 14.1; EI-MS: m/z (rel.int., %): 298 (M$^+$+2, 12.9), 296 (M$^+$, 15.0), 226 (96.1), 224 (100.0), 199 (45.2), 197 (49.0), 170 (30.6), 168 (28.4).

**Ethyl 7-cyano-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13e) and succinimide**

White solid (158.4 mg, 81%, NMR yield); $^1$H NMR (CDCl$_3$, 300 MHz, δ ppm): 11.23 (br, s, 1.0 H), 9.35 (br, s, 1.5 H), 8.46 (dd, J = 8.1 Hz, 1.5 Hz, 1.0 H), 8.27 (s, 1.0 H), 7.86–7.82 (m, 1.0 H), 4.60 (qt, J = 7.1 Hz, 1.8 Hz, 1.0 H), 2.78 (t, J = 1.5 Hz, 6.0 Hz), 1.51 (tt, J = 7.1 Hz, 1.5 Hz, 3.0 H); $^{13}$C NMR (CDCl$_3$, 75 MHz, δ ppm): 178.3, 160.4, 160.0, 147.5, 143.3, 133.4, 20
Ethyl 7-nitro-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13f)\textsuperscript{11}

Yellow solid (97.3 mg, 74%); m.p. = 187–189 °C; \textsuperscript{1}H NMR (d\textsubscript{6}-DMSO, 400 MHz, δ ppm): 11.07 (br, s, 3.4 H (incorporating water peak)), 8.50 (s, 1 H), 8.39–8.32 (m, 2 H), 4.32 (q, J = 7.2 Hz, 2 H), 1.39 (t, J = 7.2 Hz, 3 H); \textsuperscript{13}C NMR (d\textsubscript{6}-DMSO, 100 MHz, δ ppm): 179.5, 160.3, 159.8, 151.3, 147.7, 145.5, 128.3, 127.3, 123.3, 122.1, 63.0, 14.1; EI-MS: m/z (rel.int., %): 263 (M\textsuperscript{+}, 9.66), 191 (100.00), 164 (53.94), 129 (20.62).

Ethyl 4-oxo-7-(trifluoromethyl)-3,4-dihydroquinazoline-2-carboxylate (13g)\textsuperscript{11}

White solid (105.8 mg, 74%); m.p. = 154–156 °C; \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 400 MHz, δ ppm): 10.97 (s, 1 H), 8.50 (d, J = 8.0 Hz, 1 H), 8.26 (s, 1 H), 7.83 (dd, J = 8.0 Hz, 1.6 Hz, 1 H), 4.61 (q, J = 7.2 Hz, 2 H), 1.52 (t, J = 7.2 Hz, 3 H); \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 100 MHz, δ ppm): 160.5, 160.2, 147.6, 142.9, 127.9, 126.7, 126.6, 126.6, 125.4, 125.2, 125.1, 124.4, 121.7, 64.4, 14.1; EI-MS: m/z (rel.int., %): 286 (M\textsuperscript{+}, 11.6), 214 (100.0), 187 (77.6), 158 (16.4), 138 (13.8).

Ethyl 7-(dibromomethyl)-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13h)

White solid (95.6 mg, 49%); m.p. = 180–181 °C; \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 400 MHz, δ ppm): 10.73 (s, 1 H), 8.39 (d, J = 8.0 Hz, 1 H), 8.13 (d, J = 1.6 Hz, 1 H), 7.83 (dd, J = 8.4 Hz, 1.6 Hz, 1 H), 6.74 (s, 1 H), 4.60 (q, J = 7.2 Hz, 2 H), 1.52 (t, J = 7.2 Hz, 3 H); \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 100 MHz, δ ppm): 160.3, 148.2, 147.6, 142.6, 127.7, 126.9, 126.3, 64.3, 38.8, 14.1; ESI-HRMS: m/z calcd for C\textsubscript{12}H\textsubscript{10}Br\textsubscript{2}N\textsubscript{2}O\textsubscript{3}H\textsuperscript{+}: 390.9110, found: 390.9117.

Ethyl 7-methoxy-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13i)\textsuperscript{12}

White solid (98.0 mg, 79%); m.p. = 206–208 °C; \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 400 MHz, δ ppm): 10.73 (s, 1 H), 8.26 (d, J = 8.8 Hz, 1 H), 7.36 (d, J = 2.0 Hz, 1 H), 7.18 (dd, J = 8.8, 2.0 Hz, 1 H), 4.59 (q, J = 7.2 Hz, 2 H), 3.94 (s, 3 H), 1.51 (t, J = 7.2 Hz, 3 H); \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 100 MHz, δ ppm): 132.4, 131.0, 128.0, 125.9, 118.5, 117.1, 64.4, 29.5, 14.0; EI-MS: m/z (rel.int., %): 243 (M\textsuperscript{+}, 11.65), 172 (29.03), 171 (100.00), 144 (50.78), 143 (14.94).
δ ppm): 164.9, 160.8, 160.5, 150.0, 142.4, 128.1, 119.1, 116.4, 109.9, 64.0, 55.8, 14.1; EI-MS: m/z (rel.int., %): 248 (M+, 23.1), 176 (100.0), 149 (69.0), 120 (19.0).

**Ethyl 8-fluoro-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13j)**

White solid (79.1 mg, 67%); m.p. = 190-191 °C; ¹H NMR (CDCl₃, 400 MHz, δ ppm): 10.49 (s, 1 H), 8.17-8.14 (m, 1 H), 8.02 – 7.97 (m, 1 H), 7.60 – 7.54 (m, 2 H), 4.61 – 4.55 (m, 2 H), 1.50 (t, J = 7.2 Hz, 3 H); ¹H NMR (d6-DMSO, 400 MHz, δ ppm): 12.81 (br, s, 1.0 H), 7.96 (d, J = 8.0 Hz, 0.7 H), 7.91 – 7.87 (m, 0.3 H), 7.83 – 7.81 (m, 0.3 H), 7.77 – 7.72 (m, 1.0 H), 7.64 – 7.59 (m, 0.7 H), 4.42 – 4.37 (m, 2.0 H), 1.37 – 1.33 (m, 3.0 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 160.9, 160.6, 160.5, 160.3, 158.8, 156.3, 144.5, 143.4, 137.0, 129.6, 129.5, 125.4, 123.8, 123.5, 122.3, 122.3, 120.9, 120.7, 111.5, 111.3, 63.3, 63.2, 14.3; EI-MS: m/z (rel.int., %): 236 (M+, 21.8), 164 (100.0), 137 (59.2), 108 (38.6).

**Ethyl 4-oxo-8-(trifluoromethyl)-3,4-dihydroquinazoline-2-carboxylate (13k)**

White solid (55.6 mg, 39%); m.p. = 190-192 °C; ¹H NMR (CDCl₃, 400 MHz, δ ppm): 10.54 (s, 1 H), 8.56 (d, J = 7.2 Hz, 1 H), 8.16 (d, J = 7.6 Hz, 1 H), 7.68 (t, J = 8.0 Hz, 1 H), 4.55 (q, J = 7.2 Hz, 2 H), 1.50 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 160.9, 160.6, 160.5, 160.3, 158.8, 156.3, 144.5, 143.4, 137.0, 129.6, 129.5, 125.4, 123.8, 123.5, 122.3, 122.3, 120.9, 120.7, 111.5, 111.3, 63.3, 63.2, 14.3; ESI-HRMS: m/z calcd for C₁₁H₉F₃N₂O₃+: 309.0457, found: 309.0460.

**Ethyl 8-(dibromomethyl)-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13l-1)**

White solid (72.2 mg, 37%); m.p. = 208-210 °C; ¹H NMR (d-DMSO, 400 MHz, δ ppm): 12.89 (s, 1 H), 8.39 (dd, J = 7.2 Hz, 1.2 Hz, 1 H), 8.20 (dd, J = 7.2 Hz, 1.2 Hz, 1 H), 7.76 (t, J = 8.0 Hz, 1 H), 4.42 (q, J = 7.2 Hz, 2 H), 1.38 (t, J = 7.2 Hz, 3 H); ¹³C NMR (d-DMSO, 100 MHz, δ ppm): 160.4, 159.7, 143.9, 141.3, 138.9, 135.2, 129.0, 127.9, 122.7, 62.9, 35.4, 13.9; ESI-HRMS: m/z calcd for C₁₂H₁₀Br₂N₂O₃+: 390.9110, found: 390.9115.

**Ethyl 6-(dibromomethyl)-4-oxo-3,4-dihydroquinazoline-2-carboxylate (13l-2)**

White solid (76.1 mg, 39%); m.p. = 175-176 °C; ¹H NMR (CDCl₃, 400 MHz, δ ppm): 10.60 (s, 1 H), 8.44 (d, J = 3.2 Hz, 1 H), 8.16-8.13 (m, 1 H), 8.02-7.99 (m, 1 H), 6.78 (s, 1 H), 4.60 (q, J = 7.2 Hz, 2 H), 1.52 (t, J = 7.2 Hz, 3 H); ¹³C NMR (CDCl₃, 100 MHz, δ ppm): 160.4, 160.3, 148.3, 142.6, 142.5, 133.9, 130.3, 123.9, 122.7, 64.4, 38.9, 14.2; ESI-HRMS:
m/z calcd for C_{12}H_{10}Br_{2}N_{2}O_{3}+H^{+}: 390.9110, found: 390.9113.

Ethyl 3-methyl-4-oxo-3,4-dihydroquinazoline-2-carboxylate (15a)\textsuperscript{14}

Pale yellow syrup (22.0 mg, 19\%); R\textsubscript{f} = 0.31 (petroleum ether:EtOAc, 3:1, v/v); Unstable compound; \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 400 MHz, \textdelta ppm): 8.32–8.30 (m, 1 H), 7.77–7.76 (m, 2 H), 7.57–7.54 (m, 1 H), 4.52 (q, \textit{J} = 7.2 Hz, 2 H), 3.64 (s, 3 H), 1.42 (t, \textit{J} = 7.2 Hz, 3 H); \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 75 MHz, \textdelta ppm): 161.3, 161.3, 147.0, 146.3, 134.4, 128.2, 127.9, 126.8, 121.7, 63.2, 32.0, 14.0; EI-MS: m/z (rel.int., %): 232 (M\textsuperscript{+}, 25.23), 203 (13.66), 160 (100.00), 159 (28.37), 119 (40.97).

References

Copies of $^1$H NMR and $^{13}$C NMR spectra of substrates

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1i (in CDCl₃)

[Chemical structures and NMR spectra images]

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![Chemical Structure](image)
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[Chemical Structures]
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13f (in d$_6$-DMSO + a drop of D$_2$O)
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Computational studies of iminyl radical intermediates R-5, R-6 and R-7

The geometries of all the structures were fully optimized by hybrid density functional theory (DFT) using the Gaussian 09W programs. For DFT calculations, we used the hybrid gradient corrected exchange functional of Lee, Yang, and Parr. A standardized 6-31G basis set was used together with polarization (d and p) functions. The spin unrestricted (UB3LYP) formalism was used for open-shell (doublet) species. Vibrational frequency calculations at the B3LYP/6-31G (d, p) level were used to characterize all stationary points as minima or transition states. The relative energies are, thus, corrected for vibrational zero-point energies.

**Figure 1** Conformation of iminyl radical intermediates R-5, R-6 and R-7 as calculated by hybrid density functional theory (DFT)/B3LYP/6-31G

### R-5

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