Reductive Cyclizations of Amidines involving Aminal Radicals

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General experimental

All experiments were performed under nitrogen atmosphere unless stated otherwise. All solvents were purchased at the highest commercial grade and used as received or after purification by passing through activated alumina columns or distillation from sodium/benzophenone under nitrogen. All other chemicals were purchased at the highest commercial grade and used as received. $^1$H NMR spectra were recorded on NMR spectrometers at 400 MHz and 500 MHz and $^{13}$C NMR at 100 MHz and 126 MHz. $^{19}$F NMR spectra were obtained at 376 MHz. $^1$H NMR chemical shifts ($\delta_{\text{H}}$) and $^{13}$C NMR chemical shifts ($\delta_{\text{C}}$) are quoted in parts per million (ppm) downfield from trimethylsilane (TMS) and coupling constants ($J$) are quoted in Hertz (Hz). Abbreviations for NMR data are s (singlet), d (doublet), t (triplet), q (quartet), quin (quinet), sxt (sextet). Infrared (IR) spectra were recorded on a FTIR spectrometer and mass spectra were obtained using positive or negative electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), electron impact ionization (EI) or chemical ionization (CI) techniques. $^1$H NMR and $^{13}$C NMR spectra were assigned with the aid of COSY, HSQC, HMBC, DEPT 135 and nOe NMR techniques and stereochemistry assigned with the aid of X-ray crystallography. Chromatography was carried out using silica gel 60 Angstrom (Å), 240 – 400 mesh. Thin layer chromatography (TLC) was performed on aluminium sheets pre-coated with silica gel, 0.20 mm (Macherey-Nagel, Polygram$^\text{®}$ Sil G/UV254). TLC plates were visualised by UV absorption, phosphomolybdic acid, vanillin or potassium permanganate solution and heating. Diiodoethane was washed with diethyl ether and sodium thiosulfate before use.
Preparation of samarium diiodide (SmI$_2$)

An oven-dried flask, equipped with a dry stirrer bar, was flushed with a strong flow of N$_2$ for 30 minutes and loaded with samarium metal (-40 mesh, 1.4 equiv) and washed diiodoethane (1 equiv). The flask was flushed for another 30 minutes, after which, freshly distilled and degassed THF (0.1 M) was added with stirring. Stirring was continued under a positive pressure of N$_2$ overnight at room temperature. The mixture was allowed to settle for one hour and titrated prior to use.$^{[1-5]}$
Preparation of starting materials

General procedure A: formation of the cyclization substrates by Mitsunobu reaction\textsuperscript{[6,7]}

To a solution of the amidine (1.0 mmol, 1.0 equiv), alcohol (1.1 mmol, 1.1 equiv) and PPh\textsubscript{3} (1.5 mmol, 1.5 equiv) in anhydrous CH\textsubscript{2}Cl\textsubscript{2} (10 mL) was added DIAD (diisopropyl azodicarboxylate) (1.5 mmol, 1.5 equiv) dropwise at 0 °C. The mixture was warmed to room temperature and stirred under a N\textsubscript{2} atmosphere for 12 h, then concentrated \textit{in vacuo} to give the crude product, which after purification by chromatography on silica gel, gave the desired product (1).

\textbf{(E)-3-(4-Phenylbut-3-en-1-yl)quinazolin-4(3H)-one (1a)}

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-phenylbut-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh\textsubscript{3} (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH\textsubscript{2}Cl\textsubscript{2} (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1a (0.186 g, 0.674 mmol, 67\%) as a white solid. M.p. = 135-137 °C.

\textbf{\textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3})}: \(\delta\) ppm 8.34 (1 H, dt, \(J = 8.0, 0.8\) Hz, ArH), 8.03 (1 H, s, N=CH), 7.65 - 7.83 (2 H, m, ArH), 7.48 - 7.58 (1 H, m, ArH), 7.29 - 7.35 (4 H, m, ArH), 7.24 (1 H, m, ArH), 6.47 (1 H, d, \(J = 15.8\) Hz, ArCH=CH), 6.11 - 6.26 (1 H, m, ArCH=CH), 4.15 (2 H, t, \(J = 7.0\) Hz, NCH\textsubscript{2}CH\textsubscript{2}), 2.74 (2 H, qd, \(J = 7.2, 1.1\) Hz, NCH\textsubscript{2}CH\textsubscript{2}). \textbf{\textsuperscript{13}C NMR (101 MHz, CDCl\textsubscript{3})}: \(\delta\) ppm 161.1 (C=O), 148.2 (ArC\textsuperscript{\textalpha}), 146.5 (N=CH), 136.8 (ArC\textsuperscript{\textalpha}), 134.2
(ArCH), 133.7 (ArCH=CH), 128.6 (2 × ArCH), 127.6 (ArCH), 127.5 (ArCH), 126.7 (ArCH), 126.2 (2 × ArCH), 124.9 (ArCH=CH), 122.2 (ArC), 46.9 (NCH₂CH₂), 32.7 (NCH₂CH₂). IR (neat, cm⁻¹): 2935, 1690, 1395, 1259, 1135, 900, 749, 665. MS (ESI⁺) m/z (%): 277.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₆H₁₄N₂O (M + H⁺): 277.1335. Found: 277.1336.

(E)-3-(4-(O-Tolyl)but-3-en-1-yl)quinazolin-4(3H)-one (1b)

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-((o-tolyl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1b (0.158 g, 0.543 mmol, 54%) as a white solid. M.p. = 104-106.5 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.34 (1 H, dd, J = 8.0, 1.3 Hz, ArH), 8.04 (1 H, s, N=CH), 7.65 - 7.80 (2 H, m, ArH), 7.42 - 7.59 (1 H, m, ArH), 7.32 - 7.42 (1 H, m, ArH), 7.04 - 7.19 (3 H, m, ArH), 6.63 (1 H, d, J = 15.6 Hz, ArCH=CH), 5.98 - 6.13 (1 H, m, ArCH=CH), 4.16 (2 H, t, J = 6.9 Hz, NCH₂CH₂), 2.76 (2 H, q, J = 7.0 Hz, NCH₂CH₂), 2.21 (3 H, s, CH₃).

¹³C NMR (101 MHz, CDCl₃): δ ppm 161.1 (C=O), 148.2 (ArC), 146.6 (N=CH), 136.1 (ArC), 135.2 (ArC), 134.2 (ArCH), 131.8 (ArCH=CH), 130.2 (ArCH), 127.5 (ArCH), 127.3 (ArCH), 126.7 (ArCH), 126.3 (ArCH=CH), 126.1 (ArCH), 125.7 (ArCH), 122.2 (ArC), 46.9 (NCH₂CH₂), 32.9 (NCH₂CH₂), 19.6 (CH₃). IR (neat, cm⁻¹): 3019, 1673, 1610, 1474, 1374, 1215, 752, 668. MS (ESI⁺) m/z (%): 291.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₉N₂O (M + H⁺): 291.1492. Found: 291.1484.

(E)-3-(4-(3-Methoxyphenyl)but-3-en-1-yl)quinazolin-4(3H)-one (1c)

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv),
(E)-4-(3-methoxyphenyl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1c (0.267 g, 0.873 mmol, 87%) as a white solid. M.p. = 87-89.5 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.16 - 8.40 (1 H, m, ArH), 8.03 (1 H, s, N=CH), 7.61 - 7.82 (2 H, m, ArH), 7.52 (1 H, t, J = 7.4 Hz, ArH), 7.21 (1 H, t, J = 7.9 Hz, ArH), 6.91 (1 H, d, J = 7.8 Hz, ArH), 6.74 - 6.87 (2 H, m, ArH), 6.44 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.09 - 6.25 (1 H, m, ArCH=CH), 4.1 (2 H, t, J = 7.2 Hz, NCH₂CH₃), 3.81 (3 H, s, OCH₃), 2.73 (2 H, q, J = 7.1 Hz, NCH₂CH₃). ¹³C NMR (101 MHz, CDCl₃): δ ppm 161.1 (C=O), 159.8 (ArC=O), 148.2 (ArC=O), 146.5 (N=CH), 138.3 (ArC=O), 134.2 (ArCH), 133.6 (ArCH=CH), 129.6 (ArCH), 127.5 (ArCH), 127.3 (ArCH), 126.7 (ArCH), 125.2 (ArCH=CH), 122.2 (ArC=O), 118.8 (ArCH), 113.1 (ArCH), 111.6 (ArCH), 55.2 (OCH₃), 46.9 (NCH₂CH₃), 32.7 (NCH₂CH₃). IR (neat, cm⁻¹): 3014, 1671, 1474, 1374, 1216, 1156, 1045, 731, 698. MS (ESI⁺) m/z (%): 307.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₉N₂O₂ (M + H⁺): 307.1441. Found: 307.1434.

(E)-3-(4-(4-Methoxyphenyl)but-3-en-1-yl)quinazolin-4(3H)-one (1d)

![Diagram](https://example.com/diagram.png)

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-(4-methoxyphenyl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1d (0.186 g, 0.608 mmol, 61%) as a white solid. M.p. = 89-92 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.34 (1 H, dd, J = 7.8, 1.3 Hz, ArH), 8.03 (1 H, s, N=CH), 7.61 - 7.85 (2 H, m, ArH), 7.41 - 7.61 (1 H, m, ArH), 7.25 (2 H, d, J = 8.8 Hz, ArH), 6.75 - 6.92 (2 H, m, ArH), 6.40 (1 H, d, J = 15.8 Hz, ArCH=CH), 5.98 - 6.10 (1 H, m, ArCH=CH), 4.13 (2 H, t, J = 7.0 Hz, NCH₂CH₃), 3.80 (3 H, s, OCH₃), 2.70 (2 H, q, J = 6.7 Hz, NCH₂CH₃). ¹³C NMR (101 MHz, CDCl₃): δ ppm 161.1 (C=O), 159.2 (ArC=O), 137.4 (ArC=O), 134.2 (ArCH), 133.6 (ArCH=CH), 129.6 (ArCH), 127.5 (ArCH), 127.3 (ArCH), 126.7 (ArCH), 125.2 (ArCH=CH), 122.2 (ArC=O), 118.8 (ArCH), 113.1 (ArCH), 111.6 (ArCH), 55.2 (OCH₃), 46.9 (NCH₂CH₃), 32.7 (NCH₂CH₃).
148.2 (ArC\(^6\)), 146.5 (N=CH), 134.2 (ArCH), 133.1 (ArCH=CH), 129.7 (ArC\(^6\)), 127.5 (ArCH), 127.3 (2× ArCH), 127.2 (ArCH), 126.7 (ArCH), 122.6 (ArCH=CH), 122.2 (ArC\(^6\)), 114.0 (2× ArCH), 55.3 (OCH\(_3\)), 47.0 (NCH\(_2\)CH\(_2\)), 32.7 (NCH\(_2\)CH\(_2\)). IR (neat, cm\(^{-1}\)): 3016, 1739, 1673, 1609, 1511, 1374, 1248, 1217, 763. MS (ESI\(^+\)) m/z (%): 307.2 (M + H\(^+)\); HRMS (ESI\(^+\)): calcd. for C\(_{19}\)H\(_{16}\)N\(_2\)O\(_2\) (M + H\(^+)\): 307.1441. Found: 307.1435.

\((E)-3-(4-(4-Bromophenyl)but-3-en-1-yl)quinazolin-4(3H)-one\) (1e)

![Diagram of quinazolin-4(3H)-one](image)

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-(4-bromophenyl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh\(_3\) (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH\(_2\)Cl\(_2\) (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1e (0.239 g, 0.675 mmol, 68%) as a white solid. M.p. = 171.8-172.9 \({}^\circ\text{C}\). \(^{1}\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) ppm 8.33 (1 H, dd, \(J = 8.0, 1.0\) Hz, ArH), 8.02 (1 H, s, N=CH), 7.67 - 7.83 (2 H, m, ArH), 7.47 - 7.58 (1 H, m, ArH), 7.38 - 7.45 (2 H, m, ArH), 7.17 (2 H, m, \(J = 8.3\) Hz, ArH), 6.39 (1 H, d, \(J = 15.8\) Hz, ArCH=CH), 6.08 - 6.24 (1 H, m, ArCH=CH), 4.14 (2 H, t, \(J = 7.0\) Hz, NCH\(_2\)CH\(_2\)), 2.57 - 2.77 (2 H, m, NCH\(_2\)CH\(_2\)). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) ppm 161.1 (C=O), 148.1 (ArC\(^6\)), 146.4 (N=CH), 135.8 (ArC\(^6\)), 134.3 (ArCH), 132.5 (ArCH=CH), 131.7 (2× ArCH), 127.7 (2× ArCH), 127.5 (ArCH), 127.3 (ArCH), 126.7 (ArCH), 125.8 (ArCH=CH), 122.1 (ArC\(^5\)), 121.3 (ArC\(^6\)), 46.7 (NCH\(_2\)CH\(_2\)), 32.7 (NCH\(_2\)CH\(_2\)). IR (neat, cm\(^{-1}\)): 2970, 1740, 1671, 1615, 1474, 1365, 1218, 1156, 1071, 974, 877, 774. MS (ESI\(^+\)) m/z (%): 355.1 (M + H\(^+)\); HRMS (ESI\(^+\)): calcd. for C\(_{18}\)H\(_{16}\)N\(_2\)OBr (M + H\(^+)\): 355.0441. Found: 355.0433.

\((E)-3-(4-(4-(Trifluoromethyl)phenyl)but-3-en-1-yl)quinazolin-4(3H)-one\) (1f)

![Diagram of quinazolin-4(3H)-one](image)

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv),
(E)-4-(4-(trifluoromethyl)phenyl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1f (0.204 g, 0.593 mmol, 59%) as a white solid. M.p. = 162.9-164 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.34 (1 H, dd, J = 8.0, 1.3 Hz, ArH), 8.03 (1 H, s, N=CH), 7.74 - 7.83 (1 H, m, ArH), 7.66 - 7.74 (1 H, m, ArH), 7.49 - 7.58 (3 H, m, ArH), 7.40 (2 H, d, J = 8.0 Hz, ArH), 6.49 (1 H, d, J = 16.1 Hz, ArCH=CH), 6.31 (1 H, dd, J = 15.1, 7.8 Hz, ArCH=CH), 4.17 (2 H, t, J = 7.0 Hz, NCH₂CH₃), 2.77 (2 H, q, J = 6.7 Hz, NCH₂CH₃). ¹³C NMR (101 MHz, CDCl₃): δ ppm 161.1 (C=O), 148.1 (ArC=), 146.3 (N=CH), 140.2 (ArC=), 134.3 (ArCH), 132.4 (ArCH=CH), 129.4 (q, J = 32.3 Hz, ArC=), 127.8 (ArCH=CH), 127.5 (ArCH), 127.4 (ArCH), 126.7 (ArCH), 126.3 (2 × ArCH), 125.5 (q, J = 3.0 Hz, 2 × ArCH), 124.0 (q, J = 238.4 Hz, CF₃), 122.1 (ArC=), 46.6 (NCH₂CH₃), 32.8 (NCH₂CH₃). IR (neat, cm⁻¹): 2800, 1739, 1665, 1365, 1217, 1158, 1106, 771, 699. MS (ESI⁺) m/z (%): 345.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₆N₂O₃F (M + H⁺): 345.1204. Found: 345.1204.

(E)-3-(4-(Benzo[d][1,3]dioxol-5-yl)but-3-en-1-yl)quinazolin-4(3H)-one (1g)

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-(benzo[d][1,3]dioxol-5-yl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1g (0.130 g, 0.406 mmol, 41%) as a white solid. M.p. = 177-179 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.34 (1 H, dd, J = 8.0, 1.3 Hz, ArH), 8.02 (1 H, s, N=CH), 7.67 - 7.80 (2 H, m, ArH), 7.46 - 7.58 (1 H, m, ArH), 6.86 (1 H, s, ArH), 6.73 (2 H, s, ArH), 6.36 (1 H, d, J = 15.8 Hz, ArCH=CH), 5.98 - 6.06 (1 H, m, ArCH=CH), 5.95 (2 H, s, OCH₂O), 4.13 (2 H, t, J = 7.0 Hz, NCH₂CH₃), 2.70 (2 H, q, J = 7.0 Hz, NCH₂CH₃). ¹³C NMR (101 MHz, CDCl₃): δ ppm 161.1 (C=O), 148.2 (ArC=), 148.0 (ArC=), 147.2 (ArC=), 146.5 (N=CH), 134.2 (ArCH), 129.4 (ArC=), 127.8 (ArCH=CH), 127.5 (ArCH), 127.4 (ArCH), 126.7 (ArCH), 126.3 (2 × ArCH), 125.5 (q, J = 3.0 Hz, 2 × ArCH), 124.0 (q, J = 238.4 Hz, CF₃), 122.1 (ArC=), 46.6 (NCH₂CH₃), 32.8 (NCH₂CH₃). IR (neat, cm⁻¹): 2800, 1739, 1665, 1365, 1217, 1158, 1106, 771, 699. MS (ESI⁺) m/z (%): 345.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₆N₂O₃F (M + H⁺): 345.1204. Found: 345.1204.
133.2 \text{ (ArCH=CH)}, 131.3 \text{ (ArC\textsuperscript{6})}, 127.5 \text{ (ArCH)}, 127.3 \text{ (ArCH)}, 126.7 \text{ (ArCH)}, 123.0 \text{ (ArCH=CH)}, 122.2 \text{ (ArC\textsuperscript{6})}, 120.8 \text{ (ArCH)}, 108.3 \text{ (ArCH)}, 105.5 \text{ (ArCH)}, 101.1 \text{ (OCH\textsubscript{2}O)}, 47.0 \text{ (NCH\textsubscript{2}CH\textsubscript{2})}, 32.6 \text{ (NCH\textsubscript{2}CH\textsubscript{2})}. \text{ IR (neat, cm}^{-1})\text{: } 2898, 1679, 1609, 1473, 1444, 1371, 1249, 1037, 929, 775. \text{ MS (ESI\textsuperscript{*}) } m/z \text{ (%): } 321.2 \text{ (M + H\textsuperscript{+})}; \text{ HRMS (ESI\textsuperscript{*})}: \text{ calcd. for C}_{19}H_{17}N\textsubscript{2}O_{3} \text{ (M + H\textsuperscript{+})}: 321.1234. \text{ Found: } 321.1232.

\textit{(E)-3-((2,4-Dichlorophenyl)but-3-en-1-yl)quinazolin-4(3H)-one (1h)}

![Image of (E)-3-((2,4-Dichlorophenyl)but-3-en-1-yl)quinazolin-4(3H)-one (1h)]

General procedure A was followed: using quinazolin-4(3H)-one \text{(1.0 mmol, 1.0 equiv)}, \text{(E)-4-((2,4-dichlorophenyl)but-3-en-1-ol} \text{ (1.1 mmol, 1.1 equiv), PPh\textsubscript{3} (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH\textsubscript{2}Cl\textsubscript{2} (10 mL) for 12 h. The mixture was purified by chromatography (40\% EtOAc/hexanes) and gave \textbf{1h} \text{(0.242 g, 0.703 mmol, 70\%)} as a white solid. M.p. = 152.5-154 °C. \text{ ^1H NMR (400 MHz, CDCl}_3\text{): } \delta \text{ ppm 8.33 (1 H, dd, } J = 8.0, 1.3 \text{ Hz, ArH}), 8.03 \text{ (1 H, s, N=CH)}, 7.66 - 7.82 \text{ (2 H, m, ArH)}, 7.47 - 7.58 \text{ (1 H, m, ArH)}, 7.39 \text{ (1 H, d, } J = 8.3 \text{ Hz, ArH}), 7.33 \text{ (1 H, d, } J = 2.0 \text{ Hz, ArH}), 7.18 \text{ (1 H, dd, } J = 8.3, 2.0 \text{ Hz, ArH}), 6.72 \text{ (1 H, d, } J = 15.8 \text{ Hz, ArCH=CH}), 6.16 \text{ (1 H, dt, } J = 15.7, 7.3 \text{ Hz, ArCH=CH}), 4.17 \text{ (2 H, t, } J = 7.0 \text{ Hz, NCH\textsubscript{2}CH\textsubscript{2})}, 2.78 \text{ (2 H, qd, } J = 7.0, 1.3 \text{ Hz, NCH\textsubscript{2}CH\textsubscript{2})}. \text{ ^13C NMR (101 MHz, CDCl}_3\text{): } \delta \text{ ppm 161.1 (C=O), 148.2 (ArC\textsuperscript{6}), 146.3 (N=CH), 134.3 (ArCH), 133.7 (ArC\textsuperscript{6}), 133.6 (ArC\textsuperscript{6}), 133.3 (ArC\textsuperscript{6}), 129.4 (ArCH), 128.9 (ArCH=CH), 128.6 (ArCH=CH), 127.6 (ArCH), 127.5 (ArCH), 127.4 (ArCH), 127.3 (ArCH), 126.7 (ArCH), 122.1 (ArC\textsuperscript{6}), 46.5 \text{ (NCH\textsubscript{2}CH\textsubscript{2})}, 32.9 \text{ (NCH\textsubscript{2}CH\textsubscript{2})}. \text{ IR (neat, cm}^{-1})\text{: } 3027, 1679, 1401, 1216, 750, 691. \text{ MS (ESI\textsuperscript{*}) } m/z \text{ (%): } 345.1 \text{ (M + H\textsuperscript{+})}; \text{ HRMS (ESI\textsuperscript{*})}: \text{ calcd. for C}_{18}H_{18}N\textsubscript{2}OCl\textsubscript{2} \text{ (M + H\textsuperscript{+})}: 345.0556. \text{ Found: } 345.0550.

\textit{(E)-3-((Naphthalen-1-yl)but-3-en-1-yl)quinazolin-4(3H)-one (1i)}

![Image of (E)-3-((Naphthalen-1-yl)but-3-en-1-yl)quinazolin-4(3H)-one (1i)]

General procedure A was followed: using
quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-(naphthalen-1-yl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1i (0.150 g, 0.460 mmol, 46%) as a white solid. M.p. = 114.5-116 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.37 (1 H, dd, J = 7.9, 1.1 Hz, ArH), 8.07 (1 H, s, N=CH), 7.67 - 7.94 (5 H, m, ArH), 7.35 - 7.58 (5 H, m, ArH), 7.15 (1 H, d, J = 15.6 Hz, ArCH=CH), 6.05 - 6.26 (1 H, m, ArCH=CH), 4.22 (2 H, t, J = 6.9 Hz, NCH₂CH₂), 2.86 (2 H, qd, J = 7.0, 1.3 Hz, NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 161.2 (C=O), 148.2 (ArC⁰), 146.6 (N=CH), 134.7 (ArC⁰), 134.2 (ArCH), 133.5 (ArC⁰), 131.3 (ArCH=CH), 131.0 (ArC⁰), 128.5 (ArCH), 128.2 (ArCH=CH), 127.9 (ArCH), 127.5 (ArCH), 127.3 (ArCH), 126.7 (ArCH), 126.0 (ArCH), 125.7 (ArCH), 125.6 (ArCH), 123.9 (ArCH), 123.7 (ArCH), 122.2 (ArC⁰), 46.9 (NCH₂CH₂), 33.0 (NCH₂CH₂). IR (neat, cm⁻¹): 3014, 1671, 1474, 1374, 1215, 968, 743, 668. MS (ESI⁺) m/z (%): 327.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₂₂H₁₉N₂O (M + H⁺): 327.1492. Found: 327.1485.

3-(4,4-Diphenylbut-3-en-1-yl)quinazolin-4(3H)-one (1j)

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), 4,4-diphenylbut-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1j (0.215 g, 0.611 mmol, 61%) as a white solid. M.p. = 99-101 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.27 (1 H, dd, J = 8.0, 1.0 Hz, ArH), 7.89 (1 H, s, N=CH), 7.74 (1 H, dd, J=7.0, 1.5 Hz, ArH), 7.64 - 7.72 (1 H, m, ArH), 7.46 - 7.57 (1 H, m, ArH), 7.17 - 7.29 (8 H, m, ArH), 6.90 - 7.01 (2 H, m, ArH), 6.10 (1 H, t, J = 7.7 Hz, C=CH), 4.07 (2 H, t, J = 6.9 Hz, NCH₂CH₂), 2.64 (2 H, q, J = 7.0 Hz, NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 160.9 (C=O), 148.1 (ArC⁰), 146.4 (N=CH), 145.5 (ArC⁰), 141.8 (C⁰),

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139.2 (ArC6), 134.1 (ArCH), 129.4 (2 × ArCH), 128.3 (2 × ArCH), 128.2 (2 × ArCH), 127.4 (2 × ArCH), 127.3 (ArCH), 127.2 (2 × ArCH), 127.2 (ArCH), 126.7 (ArCH), 123.5 (C=CH), 122.2 (ArC6), 46.5 (NCH2CH3), 29.4 (NCH2CH3). IR (neat, cm⁻¹): 2970, 1739,1365, 1228, 1217, 754. MS (ESI⁺) m/z (%): 353.2 (M + H⁺); HRMS (ESI⁺): calcd. for C24H20N2O (M + Na⁺): 375.1468. Found: 375.1463.

(E)-3-(4-(1-Methyl-1H-indol-2-yl)but-3-en-1-yl)quinazolin-4(3H)-one (1k)

General procedure A was followed: using quinzolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-(1-methyl-1H-indol-2-yl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh3 (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH2Cl2 (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1k (0.179 g, 0.544 mmol, 54%) as a white solid. M.p. = 150-152 °C. ¹H NMR (500 MHz, CDCl₃): δ ppm 8.26 - 8.39 (1 H, m, ArH), 8.04 (1 H, s, N=CH), 7.75 - 7.83 (1 H, m, ArH), 7.66 - 7.75 (1 H, m, ArH), 7.49 - 7.60 (2 H, m, ArH), 7.25 (1 H, d, J = 8.4 Hz, ArH), 7.15 - 7.21 (1 H, m, ArH), 7.02 - 7.13 (1 H, m, ArH), 6.60 (1 H, s, ArH), 6.51 (1 H, d, J = 15.7 Hz, ArCH=CH), 6.12 - 6.32 (1 H, m, ArCH=CH), 4.18 (2 H, t, J = 6.9 Hz, NCH2CH3), 3.62 (3 H, s, NCH3), 2.79 (2 H, q, J = 6.9 Hz, NCH2CH3). ¹³C NMR (126 MHz, CDCl₃): δ ppm 161.1 (C=O), 148.2 (ArC6), 146.5 (N=CH), 137.7 (ArC6), 137.5 (ArC6), 134.3 (ArCH), 127.8 (ArCH=CH), 127.7 (ArC6), 127.5 (ArCH), 127.4 (ArCH), 126.7 (ArCH), 122.8 (ArCH=CH), 122.1 (ArC6), 121.6 (ArCH), 120.3 (ArCH), 119.8 (ArCH), 109.1 (ArCH), 98.8 (ArCH), 46.7 (NCH2CH3), 33.0 (NCH2CH3), 29.8 (NCH3). IR (neat, cm⁻¹): 3014, 2346, 1736, 1670, 1611, 1474, 1370, 1216, 749, 700, 668. MS (ESI⁺) m/z (%): 330.2 (M + H⁺); HRMS (ESI⁺): calcd. for C21H20N3O (M + H⁺): 330.1601. Found: 330.1596.

(E)-3-(4-(Benzo[b]thiophen-3-yl)but-3-en-1-yl)quinazolin-4(3H)-one (1l)
General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-(benzo[b]thiophen-3-yl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1I (0.122 g, 0.367 mmol, 37%) as a light yellow oil. \(^1\)H NMR (400 MHz, CDCl₃): δ ppm 8.30 - 8.40 (1 H, m, ArH), 8.06 (1 H, s, N=CH), 7.80 - 7.90 (1 H, m, ArH), 7.66 - 7.80 (3 H, m, ArH), 7.46 - 7.57 (1 H, m, ArH), 7.32 - 7.42 (3 H, m, ArH), 6.70 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.13 - 6.34 (1 H, m, ArCH=CH), 4.19 (2 H, t, J = 7.0 Hz, NCH₂CH₂), 2.74 - 2.85 (2 H, m, NCH₂CH₂). \(^13\)C NMR (101 MHz, CDCl₃): δ ppm 161.1 (C=O), 148.2 (ArC⁰), 146.5 (N=CH), 140.4 (ArC⁰), 137.5 (ArC⁰), 134.3 (ArCH), 133.6 (ArC⁰), 127.5 (ArCH), 127.3 (ArCH), 126.8 (ArCH=CH), 126.7 (ArCH), 126.0 (ArCH=CH), 124.4 (ArCH), 124.2 (ArCH), 122.9 (ArCH), 122.2 (ArC⁰), 121.9 (ArCH), 121.8 (ArCH), 46.8 (NCH₂CH₂), 33.1 (NCH₂CH₂). IR (neat, cm⁻¹): 1671, 1609, 1473, 1374, 1155, 908, 731, 698. MS (ESI⁺) m/z (%): 333.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₂₀H₁₅N₂O₂S (M + H⁺): 333.1056. Found: 333.1053.

(E)-3-(4-(Benzo[b]thiophen-2-yl)but-3-en-1-yl)quinazolin-4(3H)-one (1m)

General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-(benzo[b]thiophen-2-yl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1m (0.167 g, 0.503 mmol, 50%) as a light yellow solid. M.p. = 172.6-174 °C. \(^1\)H NMR (400 MHz, CDCl₃): δ ppm 8.33 - 8.40 (1 H, m, ArH), 8.04 (1 H, s, N=CH), 7.68 - 7.83 (3 H, m, ArH), 7.64 - 7.68 (1 H, m, ArH), 7.46 - 7.58 (1 H, m, ArH), 7.28 - 7.34 (2 H, m, ArH), 7.06 (1 H, s, ArH), 6.68 (1 H, d, J = 15.6 Hz, 1291.5035).
ArCH=CH), 6.04 - 6.20 (1 H, m, ArCH=CH), 4.16 (2 H, t, J = 7.0 Hz, NCH₂CH₂), 2.76 (2 H, d, J = 7.0 Hz, NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 161.1 (C=O), 148.2 (ArC⁶), 146.4 (N=CH), 141.9 (ArC⁶), 140.0 (ArC⁶), 138.7 (ArC⁶), 134.3 (ArCH), 127.6 (ArCH), 127.5 (ArCH=CH), 127.3 (ArCH and ArCH=CH), 126.7 (ArCH), 124.7 (ArCH), 124.4 (ArCH), 123.4 (ArCH), 122.5 (ArCH), 122.2 (ArC⁶), 46.7 (NCH₂CH₂), 32.6 (NCH₂CH₂). IR (neat, cm⁻¹): 2969, 1737, 1666, 1609, 1472, 1365, 1224, 955, 772, 737, 697. MS (ESI⁺) m/z (%): 333.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₂₀H₁₇N₂OS (M + H⁺): 333.1056. Found: 333.1056.

*(E)-3-(4-(Thiophen-2-yl)but-3-en-1-yl)quinazolin-4(3H)-one (1n)*

**General procedure A** was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-(thiophen-2-yl)but-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1n (0.114 g, 0.404 mmol, 40%) as a light yellow solid. M.p. = 103.1-105 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.35 (1 H, dd, J = 7.9, 1.1 Hz, ArH), 8.04 (1 H, s, N=CH), 7.68 - 7.82 (2 H, m, ArH), 7.47 - 7.59 (1 H, m, ArH), 7.14 (1 H, d, J = 5.3 Hz, ArH), 6.95 (1 H, dd, J = 5.3, 3.5 Hz, ArH), 6.89 (1 H, d, J = 3.3 Hz, ArH), 6.60 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.0 - 6.1 (1 H, m, ArCH=CH), 4.14 (2 H, t, J = 7.2 Hz, NCH₂CH₂), 2.71 (2 H, dd, J = 7.3, 1.0 Hz, NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 161.1 (C=O), 148.2 (ArC⁶), 146.4 (N=CH), 141.8 (ArC⁶), 134.2 (ArCH), 127.5 (ArCH), 127.3 (ArCH), 127.3 (ArCH), 126.8 (ArCH=CH), 126.7 (ArCH), 125.4 (ArCH), 124.5 (ArCH=CH), 124.1 (ArCH), 122.2 (ArC⁶), 46.9 (NCH₂CH₂), 32.5 (NCH₂CH₂). IR (neat, cm⁻¹): 3013, 1670, 1610, 1474, 1375, 1323, 1217, 1105, 959, 753, 698. MS (ESI⁺) m/z (%): 283.1 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₆H₁₅N₂OS (M + H⁺): 283.0900. Found: 283.0893.
(E)-7-Bromo-3-(4-phenylbut-3-en-1-yl)quinazolin-4(3H)-one (1o)

General procedure A was followed: using 7-bromoquinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-phenylbut-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh3 (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH2Cl2 (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1o (0.200 g, 0.563 mmol, 56%) as a white solid. M.p. = 155-156.8 °C. 1H NMR (400 MHz, CDCl3): δ ppm 8.19 (1 H, d, J = 8.5 Hz, ArH), 8.03 (1 H, s, N=CH), 7.89 (1 H, d, J = 1.8 Hz, ArH), 7.63 (1 H, dd, J = 8.5, 1.8 Hz, ArH), 7.30 - 7.35 (4 H, m, ArH), 7.59 - 7.27 (1 H, m, ArH), 6.46 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.13 - 6.24 (1 H, m, ArCH=CH), 4.14 (2 H, t, J = 8.5 Hz, NCH2), 1.5 mmol, 1.5 equiv

13C NMR (101 MHz, CDCl3): δ ppm 160.6 (C=O), 149.2 (ArC6), 147.6 (N=CH), 136.7 (ArC6), 133.9 (ArCH=CH), 130.7 (ArCH), 130.3 (ArCH), 129.0 (ArC6), 128.6 (2 × ArCH), 128.2 (ArCH), 127.6 (ArCH), 126.2 (2 × ArCH), 124.6 (ArCH=CH), 121.0 (ArC6), 47.0 (NCH2CH3), 32.6 (NCH2CH3). IR (neat, cm⁻¹): 2969, 2346, 1736, 1664, 1365, 1228, 882, 775, 663. MS (ESI⁺) m/z (%): 356.3 (M + H⁺); HRMS (ESI⁺): calcd. for C19H16N3OBr (M + H⁺): 355.0441. Found: 355.0432.

(E)-6-Bromo-3-(4-phenylbut-3-en-1-yl)quinazolin-4(3H)-one (1p)

General procedure A was followed: using 6-bromoquinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-phenylbut-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh3 (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH2Cl2 (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1p (0.231 g, 0.651 mmol, 65%) as a white solid. M.p. = 97-98.5 °C. 1H NMR (400 MHz, CDCl3): δ ppm 8.46 (1 H, d, J = 2.3 Hz, ArH), 8.02 (1 H, s, N=CH), 7.83 (1 H, dd, J = 8.5, 2.3 Hz, ArH), 7.58 (1 H, d, J = 8.8 Hz, ArH), 7.29 - 7.35 (4 H, m, ArH), 7.13 - 7.25 (1 H, m, ArH), 6.45 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.02 - 6.25 (1 H, m,
ArCH=CH), 4.14 (2 H, t, J = 7.0 Hz, NCH2CH2), 2.72 (2 H, q, J = 7.2 Hz, NCH2CH2). 13C NMR (101 MHz, CDCl3): δ ppm 159.9 (C=O), 147.0 (ArC=), 146.8 (N=CH), 137.4 (ArCH), 136.7 (ArC), 133.9 (ArCH=CH), 129.3 (ArCH), 129.3 (ArCH), 128.6 (2 × ArCH), 127.6 (ArCH), 126.2 (2 × ArCH), 124.6 (ArCH=CH), 123.5 (ArC=), 120.9 (ArC=), 47.0 (NCH2CH2), 32.6 (NCH2CH2). IR (neat, cm⁻¹): 2970, 1739, 1365, 1228, 1217, 754. MS (ESI⁺) m/z (%): 355.1 (M⁺); HRMS (ESI⁺): calcd. for C18H16N2OBr (M + H⁺): 355.0441. Found: 355.0430.

(E)-6-Fluoro-3-(4-phenylbut-3-en-1-yl)quinazolin-4(3H)-one (1q)

General procedure A was followed: using 6-fluoroquinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-phenylbut-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh3 (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH2Cl2 (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1q (0.230 g, 0.782 mmol, 78%) as a white solid. M.p. = 121-123.3 °C. 1H NMR (400 MHz, CDCl3): δ ppm 7.92 - 8.04 (2 H, m, N=CH and ArH), 7.72 (1 H, dd, J = 8.9, 4.9 Hz, ArH), 7.48 (1 H, td, J = 8.5, 3.0 Hz, ArH), 7.28 - 7.35 (4 H, m, ArH), 7.19 - 7.26 (1 H, m, ArH), 6.46 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.10 - 6.24 (1 H, m, ArCH=CH), 4.15 (2 H, t, J = 7.0 Hz, NCH2CH2), 2.73 (2 H, qd, J = 7.1, 1.0 Hz, NCH2CH2). 13C NMR (101 MHz, CDCl3): δ ppm 161.2 (d, J = 249.5 Hz, CF), 160.4 (C=O), 145.7 (N=CH), 144.8 (ArC=), 136.8 (ArC=), 133.8 (ArCH=CH), 130.0 (d, J = 8.1 Hz, ArCH), 128.6 (2 × ArCH), 127.6 (ArCH), 126.2 (2 × ArCH), 124.7 (ArCH=CH), 123.5 (d, J = 8.1 Hz, ArC=), 122.8 (d, J = 24.2 Hz, ArCH), 111.6 (d, J = 24.2 Hz, ArCH), 47.0 (NCH2CH2), 32.7 (NCH2CH2). IR (neat, cm⁻¹): 3024, 1739, 1674, 1607, 1486, 1374, 1269, 1216, 966, 836, 749. MS (ESI⁺) m/z (%): 295.2 (M + H⁺); HRMS (ESI⁺): calcd. for C18H16N2OF (M + H⁺): 295.1241. Found: 295.1235.

(E)-7-Fluoro-3-(4-phenylbut-3-en-1-yl)quinazolin-4(3H)-one (1r)
General procedure A was followed: using 7-fluoroquinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-phenylbut-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1r (0.203 g, 0.690 mmol, 69%) as a white solid. M.p. = 143.7-144.5 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.34 (1 H, dd, J = 8.9, 6.1 Hz, ArH), 8.03 (1 H, s, N=CH), 7.28 - 7.37 (5 H, m, ArH), 6.46 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.09 - 6.24 (1 H, m, ArCH=CH), 4.14 (2 H, t, J = 7.0 Hz, NCH₂CH₂), 2.73 (2 H, q, J = 6.7 Hz, NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 166.4 (d, J = 255.5 Hz, CF), 160.4 (C=O), 150.3 (d, J = 13.1 Hz, ArC⁶), 147.7 (N=CH), 136.8 (ArC⁶), 133.8 (ArCH=CH), 129.5 (d, J = 11.1 Hz, ArCH), 128.6 (2 × ArCH), 127.6 (ArCH), 126.2 (2 × ArCH), 124.7 (ArCH=CH), 118.9 (d, J = 2.0 Hz, ArC⁶), 116.1 (d, J = 23.2 Hz, ArCH), 112.9 (d, J = 21.2 Hz, ArCH), 46.9 (NCH₂CH₂), 32.7 (NCH₂CH₂). IR (neat, cm⁻¹): 3016, 1676, 1606, 1477, 1373, 1216, 1126, 960, 870, 753. MS (ESI⁺) m/z (%): 295.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₆H₁₆N₂O₂F (M + H⁺): 295.1241. Found: 295.1235.

(E)-6,7-Dimethoxy-3-(4-phenylbut-3-en-1-yl)quinazolin-4(3H)-one (1s)

General procedure A was followed: using 6,7-dimethoxyquinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-phenylbut-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1s (0.217 g, 0.646 mmol, 65%) as a white solid. M.p. = 111-112.3 °C. ¹H NMR (500 MHz, CDCl₃): δ ppm 7.95 (1 H, s, N=CH), 7.65 (1 H, s, ArH), 7.29 - 7.36 (4 H, m, ArH), 7.20 - 7.26 (1 H, m, ArH), 7.10 (1 H, s, ArH), 6.46 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.10 - 6.24 (1 H, m, ArCH=CH), 4.14 (2 H, t, J = 6.9 Hz,
NCH₂CH₂), 4.02 (3 H, s, CH₃), 4.00 (3 H, s, CH₃), 2.73 (2 H, q, J = 6.9 Hz, NCH₂CH₂). ¹³C NMR (126 MHz, CDCl₃): δ ppm 160.5 (C=O), 154.9 (ArC⁰), 149.4 (ArC⁰), 145.3 (N=CH), 144.5 (ArC⁰), 136.9 (ArC⁰), 133.6 (ArCH=CH), 128.6 (2 × ArCH), 127.5 (ArCH), 126.2 (2 × ArCH), 125.0 (ArCH=CH), 115.6 (ArC⁰), 107.9 (ArCH), 105.6 (ArCH), 56.3 (2 × CH₃), 46.9 (NCH₂CH₂), 32.8 (NCH₂CH₂). IR (neat, cm⁻¹): 3024, 2969, 2249, 1661, 1610, 1499, 1376, 1270, 1217, 1123, 1017, 968, 729. MS (ESI⁺) m/z (%): 337.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₂₀H₂₁N₂O₃ (M + H⁺): 337.1547. Found: 337.1537.

(E)-2-Methyl-3-(4-phenylbut-3-en-1-yl)quinazolin-4(3H)-one (1t)

![Chemical Structure](image)

General procedure A was followed: using 2-methylquinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-4-phenylbut-3-en-1-ol (1.1 mmol, 1.1 equiv), PPh₃ (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH₂Cl₂ (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1t (0.158 g, 0.545 mmol, 55%) as a white solid. M.p. = 69-71.1 °C.

¹H NMR (400 MHz, CDCl₃): δ ppm 8.27 (1 H, dd, J = 8.0, 1.3 Hz, ArH), 7.68 - 7.82 (1 H, m, ArH), 7.59 - 7.65 (1 H, m, ArH), 7.40 - 7.50 (1 H, m, ArH), 7.29 - 7.37 (4 H, m, ArH), 7.20 - 7.27 (1 H, m, ArH), 6.50 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.24 (1 H, dt, J = 15.8, 7.3 Hz, ArCH=CH), 4.17 - 4.29 (2 H, m, NCH₂CH₂), 2.63 - 2.73 (5 H, m, NCH₂CH₂ and CH₃). ¹³C NMR (101 MHz, CDCl₃): δ ppm 162.0 (C=O), 153.9 (ArC⁰), 147.3 (ArC⁰), 136.9 (ArC⁰), 134.3 (ArCH), 133.0 (ArCH=CH), 128.6 (2 × ArCH), 127.5 (ArCH), 126.8 (ArCH), 126.7 (ArCH), 126.4 (ArCH), 126.1 (2 × ArCH), 125.3 (ArCH=CH), 120.5 (ArC⁰), 44.4 (NCH₂CH₂), 32.1 (NCH₂CH₂), 23.4 (CH₃). IR (neat, cm⁻¹): 2970, 1738, 1690, 1608, 1472, 1373, 920, 773, 698. MS (ESI⁺) m/z (%): 291.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₅N₂O (M + H⁺): 291.1492. Found: 291.1492.

(E)-3-(5-Phenylpent-4-en-1-yl)quinazolin-4(3H)-one (1u)

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General procedure A was followed: using quinazolin-4(3H)-one (1.0 mmol, 1.0 equiv), (E)-5-phenylpent-4-en-1-ol (1.1 mmol, 1.1 equiv), PPh3 (1.5 mmol, 1.5 equiv) and DIAD (1.5 mmol, 1.5 equiv) in anhydrous CH2Cl2 (10 mL) for 12 h. The mixture was purified by chromatography (40% EtOAc/hexanes) and gave 1u (0.192 g, 0.662 mmol, 66%) as a white solid. M.p. = 115-117 °C. 1H NMR (500 MHz, CDCl3): δ ppm 8.33 (1 H, dd, J = 8.0, 1.4 Hz, ArH), 8.05 (1 H, s, N=CH), 7.70 - 7.80 (2 H, m, ArH), 7.47 - 7.55 (1 H, m, ArH), 7.27 - 7.37 (4 H, m, ArH), 7.15 - 7.24 (1 H, m, ArH), 6.46 (1 H, d, J = 15.8 Hz, ArCH=CH), 6.21 (1 H, dt, J = 15.8, 6.9 Hz, ArCH=CH), 4.02 - 4.12 (2 H, m, NCH2CH2), 2.27 - 2.40 (2 H, m, ArCH=CH2CH2), 2.03 (2 H, quin, J = 7.3 Hz, NCH2CH2). 13C NMR (126 MHz, CDCl3): δ ppm 161.1 (C=O), 148.2 (ArC=), 146.6 (N=CH), 137.2 (ArC=), 134.2 (ArCH), 131.3 (ArCH=CH), 128.5 (2 × ArCH), 127.5 (ArCH), 127.3 (2 × ArCH), 127.2 (ArCH), 126.7 (ArCH=CH), 126.0 (2 × ArCH), 122.2 (ArC=), 46.6 (NCH2CH2), 29.9 (ArCH=CHCH2), 28.6 (NCH2CH2). IR (neat, cm⁻¹): 2970, 1738, 1670, 1608, 1365, 1217, 773. MS (ESI+) m/z (%): 313.1 (M + Na⁺); HRMS (ESI+): calcd. for C19H18N2OK (M + K⁺): 329.1051. Found: 329.1045.
Reductive Cyclizations of Amidines involving Aminal Radicals

**General procedure B: SmI₂ mediated radical cyclization to give bicyclic products**

(2)

An oven-dried vial containing a stirrer bar was charged with the substrate 1 (0.1 mmol, 1 equiv) and NH₄Cl (0.3 mmol, 3 equiv), then placed under a positive pressure of nitrogen. THF (0.05 M, typically, 2.0 mL) was added, followed by addition of the fresh SmI₂ solution slowly over 1 h. After the specified time (typically, 1 h), the reaction was quenched by bubbling air through the mixture before dilution with CH₂Cl₂ (30 mL) and aqueous HCl (0.1 M, 20 mL). The aqueous layer was extracted with CH₂Cl₂ (3 × 20 mL) and the combined organic phases were dried over MgSO₄, filtered and concentrated. The crude product was purified by chromatography on silica gel.

![Chemical structure of 1a and 2a](image)

(35,3aR)-3-Benzyl-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2a).

According to the general procedure B, using 1a (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2a (22.5 mg, 0.0809 mmol, 81%, >95:5 dr) as a white solid. M.p. = 244-246 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 7.92 (1 H, dd, J = 7.8, 1.3 Hz, ArH), 7.17 - 7.38 (6 H, m, ArH), 6.83 - 6.93 (1 H, m, ArH), 6.67 (1 H, d, J = 8.0 Hz, ArH), 5.18 (1 H, d, J = 5.3 Hz, NHCH), 4.31 (1 H, s, NH), 3.85 (1 H, dt, J = 11.9, 7.7 Hz, 1 H from NCH₂CH₂), 3.61 (1 H, ddd, J = 12.2, 8.1, 4.5 Hz, 1 H from NCH₂CH₂), 3.10 (1 H, dd, J = 13.8, 5.5 Hz, 1 H from ArCH₂CH), 2.70 -
2.80 (1 H, m, ArCH₂CH), 2.65 (dd, J = 13.8, 9.8 Hz, 1 H from ArCH₂CH), 1.87 - 1.96 (1 H, m, 1 H from NCH₂CH₂), 1.77 - 1.87 (1 H, m, 1 H from NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 162.5 (C=O), 147.5 (ArC⁰), 139.7 (ArC⁰), 133.0 (ArCH), 128.9 (2 × ArCH), 128.7 (2 × ArCH), 128.3 (ArCH), 126.5 (ArCH), 119.7 (ArCH), 117.6 (ArC⁰), 114.9 (ArCH), 71.9 (NHCH), 43.4 (ArCH₂CH), 42.8 (NCH₂CH₂), 33.8 (ArCH₂CH), 26.8 (NCH₂CH₂). IR (neat, cm⁻¹): 3269, 2945, 1736, 1671, 1618, 1450, 1216, 752, 690. MS (ESI⁺) m/z (%): 279.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₉N₂O (M + H⁺): 279.1492. Found: 279.1496.

(35,3ₐR)-3-(2-Methylbenzyl)-2,3,3ₐ,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2b).
According to the general procedure B, using 1b (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2b (18.0 mg, 0.0616 mmol, 62%, >95:5 dr) as a colorless oil. ¹H NMR (400 MHz, CDCl₃): δ ppm 7.92 (1 H, d, J = 7.8 Hz, ArH), 7.27 - 7.32 (1 H, m, ArH), 7.13 - 7.23 (4 H, m, ArH), 6.89 (1 H, t, J = 7.5 Hz, ArH), 6.68 (1 H, d, J = 8.0 Hz, ArH), 5.21 (1 H, d, J = 5.3 Hz, NHCH), 4.33 (1 H, s, NH), 3.75 - 3.94 (1 H, m, 1 H from NCH₂CH₂), 3.64 (1 H, ddd, J = 12.2, 8.2, 4.3 Hz, 1 H from NCH₂CH₂), 3.11 (1 H, dd, J = 14.3, 5.3 Hz, 1 H from ArCH₂CH), 2.76 (1 H, dd, J = 10.3, 4.8 Hz, ArCH₂CH), 2.56 - 2.70 (1 H, m, 1 H from ArCH₂CH), 2.36 (3 H, s, CH₃), 1.76 - 1.97 (2 H, m, NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 162.5 (C=O), 147.5 (ArC⁰), 137.9 (ArC⁰), 136.4 (ArC⁰), 133.0 (ArCH), 130.6 (ArCH), 129.2 (ArCH), 128.3 (ArCH), 126.5 (ArCH), 126.2 (ArCH), 119.7 (ArCH), 117.6 (ArC⁰), 114.9 (ArCH), 72.1 (NHCH), 42.8 (NCH₂CH₂), 42.1 (ArCH₂CH), 30.7 (ArCH₂CH), 26.8 (NCH₂CH₂), 19.7 (CH₃). IR (neat, cm⁻¹): 2969, 2346, 1736, 1671, 1618, 1450, 1216, 752, 690. MS (ESI⁺) m/z (%):
293.2 (M + H'); **HRMS (ESI)**: calcd. for C_{19}H_{21}N_{2}O (M + H^+): 293.1648. Found: 293.1635.

(3S,3aR)-3-(3-Methoxybenzyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2c). According to the general procedure B, using 1c (0.10 mmol), SmI\(_2\) (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH\(_4\)Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2c (24.3 mg, 0.0789 mmol, 79%, >95:5 dr) as a white solid. M.p. = 172-174 °C. **\(^1\)H NMR (400 MHz, CDCl\(_3\))**: \(\delta\) ppm 7.86 - 7.95 (1 H, m, ArH), 7.21 - 7.32 (2 H, m, ArH), 6.84 - 6.92 (1 H, m, ArH), 6.73 - 6.84 (3 H, m, ArH), 6.73 - 6.84 (3 H, m, ArH), 6.66 (1 H, d, \(J = 8.0\) Hz, ArH), 5.17 (1 H, d, \(J = 5.5\) Hz, NHCH\(_2\)), 4.31 (1 H, s, NH), 3.83 - 3.89 (1 H, m, 1 H from NC\(_2\)H\(_2\)CH\(_2\)), 3.81 (3 H, s, OCH\(_3\)), 3.60 (1 H, ddd, \(J = 12.2, 8.1, 4.5\) Hz, 1 H from NCH\(_2\)CH\(_2\)), 3.07 (1 H, dd, \(J = 13.9, 5.9\) Hz, 1 H from ArCH\(_3\)CH), 2.69 - 2.80 (1 H, m, ArCH\(_3\)CH), 2.55 - 2.69 (1 H, m, 1 H from ArCH\(_2\)CH), 1.86 - 1.97 (1 H, m, 1 H from NCH\(_2\)CH\(_2\)), 1.67 - 1.86 (1 H, m, 1 H from NCH\(_2\)CH\(_2\)). **\(^{13}\)C NMR (101 MHz, CDCl\(_3\))**: \(\delta\) ppm 162.5 (C=O), 159.9 (ArC\(^6\)), 147.5 (ArC\(^6\)), 141.3 (ArC\(^6\)), 133.0 (ArCH), 129.7 (ArCH), 128.3 (ArCH), 121.2 (ArCH), 119.7 (ArCH), 117.6 (ArC\(^6\)), 114.9 (ArCH), 114.8 (ArCH), 111.5 (ArCH), 71.9 (NHCH), 55.2 (OCH\(_3\)), 43.3 (ArCH\(_2\)CH), 42.8 (NCH\(_2\)CH\(_2\)), 33.8 (ArCH\(_2\)CH), 26.8 (NCH\(_2\)CH\(_2\)). **IR (neat, cm\(^{-1}\))**: 3284, 3004, 1739, 1633, 1485, 1434, 1365, 1217, 754. **MS (ESI)** \(m/z\) (%): 309.2 (M + H\(^+\)); **HRMS (ESI)**: calcd. for C_{19}H_{21}N_{2}O (M + H\(^+\)) 309.1598. Found: 309.1588.
(35,3aR)-3-(4-Methoxybenzyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2d). According to the general procedure B, using 1d (0.10 mmol), SmI$_2$ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH$_4$Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2d (14.8 mg, 0.0481 mmol, 48%, >95:5 dr) as a white solid. M.p. = 187-191.2 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ ppm 7.88 - 7.94 (1 H, m, ArH), 7.26 (1 H, d, $J$ = 1.5 Hz, ArH), 7.15 (2 H, d, $J$ = 8.8 Hz, ArH), 6.86 - 6.91 (3 H, m, ArH), 6.65 (1 H, d, $J$ = 8.0 Hz, ArH), 5.16 (1 H, d, $J$ = 5.3 Hz, NHC$_H$), 4.20 (1 H, s, NH), 3.78 - 3.88 (4 H, m, 1 H from NC$_H$$_2$CH$_2$ and OCH$_3$), 3.60 (1 H, ddd, $J$ = 12.2, 8.0, 4.6 Hz, 1 H from NCH$_2$CH$_2$ and OCH$_3$), 3.03 (1 H, dd, $J$ = 12.2, 8.0, 4.6 Hz, 1 H from NCH$_2$CH$_2$), 2.71 (1 H, dd, $J$ = 10.3, 5.0 Hz, ArCH$_2$CH), 2.57 - 2.67 (1 H, m, 1 H from ArCH$_2$CH), 1.86 - 1.97 (1 H, m, 1 H from NCH$_2$CH$_2$), 1.76 - 1.86 (1 H, m, 1 H from NCH$_2$CH$_2$). $^{13}$C NMR (101 MHz, CDCl$_3$): $\delta$ ppm 162.5 (C=O), 158.2 (ArC$^9$), 147.4 (ArC$^9$), 132.9 (ArCH), 131.5 (ArC$^9$), 129.8 (2 $\times$ ArCH), 128.3 (ArCH), 119.8 (ArCH), 117.7 (ArC$^9$), 114.9 (ArCH), 114.1 (2 $\times$ ArCH), 71.8 (NHCH), 55.3 (OCH$_3$), 43.6 (ArCH$_2$CH), 42.8 (NCH$_2$CH$_2$), 32.9 (ArCH$_2$CH), 26.9 (NCH$_2$CH$_2$). IR (neat, cm$^{-1}$): 3738, 2966, 2331, 1736, 1639, 1512, 1436, 1216, 763. MS (ESI$^+$) $m/z$ (%): 309.2 (M + H$^+$); HRMS (ESI$^+$): calcd. for C$_{19}$H$_{21}$N$_2$O$_2$ (M + H$^+$): 309.1598. Found: 309.1591.
According to the general procedure B, using 1e (0.10 mmol), SmI$_2$ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH$_4$Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2e (26.7 mg, 0.0748 mmol, 75%, >95:5 dr) as a white solid. M.p. = 126-127.3 °C. $^1$H NMR (400 MHz, CDCl$_3$): δ ppm 7.87 - 7.95 (1 H, m, ArH), 7.45 (2 H, m, $J = 8.3$ Hz, ArH), 7.27 - 7.33 (1 H, m, ArH), 7.09 (2 H, m, $J = 8.3$ Hz, ArH), 6.88 (1 H, t, $J = 7.4$ Hz, ArH), 6.67 (1 H, d, $J = 8.0$ Hz, ArH), 5.19 (1 H, d, $J = 5.3$ Hz, NHCH), 4.32 (1 H, s, NH), 3.79 (1 H, dt, $J = 12.0$, 8.0 Hz, 1 H from NC$_2$H$_2$CH$_2$), 3.62 (1 H, ddd, $J = 12.1$, 8.5, 3.8 Hz, 1 H from NC$_2$H$_2$CH$_2$), 3.06 (1 H, dd, $J = 13.9$, 5.4 Hz, 1 H from ArCH$_2$CH), 2.69 (1 H, dd, $J = 9.4$, 5.4 Hz, ArCH$_2$CH), 2.51 - 2.63 (1 H, m, 1 H from ArCH$_2$CH), 1.83 - 1.96 (1 H, m, 1 H from NCH$_2$C$_2$H), 1.71 - 1.83 (1 H, m, 1 H from NCH$_2$C$_2$H). $^{13}$C NMR (101 MHz, CDCl$_3$): δ ppm 162.5 (C=O), 147.4 (ArC$^6$), 138.7 (ArC$^6$), 133.1 (ArCH), 131.8 (2 × ArCH), 130.7 (2 × ArCH), 128.2 (ArCH), 120.3 (ArC$^6$), 119.8 (ArCH), 117.5 (ArC$^6$), 114.9 (ArCH), 71.9 (NHCH), 43.3 (ArCH$_2$CH), 42.6 (NCH$_2$C$_2$H), 33.2 (ArCH$_2$CH), 26.4 (NCH$_2$C$_2$H). IR (neat, cm$^{-1}$): 2966, 2247, 1667, 1620, 1487, 1467, 1383, 1071, 1011, 907, 773. MS (ESI$^+$) $m$/z (%): 357.1 (M$^+$); HRMS (ESI$^+$): calcd. for C$_{18}$H$_{18}$N$_2$OBr (M + H$^+$): 357.0597. Found: 357.0595.

(35,3aR)-3-(4-(Trifluoromethyl)benzyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1 H)-one (2f). According to the general procedure B, using 1f (0.10 mmol), SmI$_2$ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH$_4$Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2f (28.0 mg, 0.0809 mmol, 81%, >95:5 dr) as a white solid. M.p. = 193.4-195 °C. $^1$H NMR (400 MHz, CDCl$_3$): δ ppm 7.91 (1 H, dd, $J = 7.8$, 1.5 Hz, ArH), 7.58
(2 H, d, J = 8.0 Hz, ArH), 7.28 - 7.37 (3 H, m, ArH), 6.82 - 6.94 (1 H, m, ArH), 6.69 (1 H, d, J = 7.8 Hz, ArH), 5.22 (1 H, d, J = 5.0 Hz, NHCH), 4.41 (1 H, s, NH), 3.73 - 3.88 (1 H, m, 1 H from NCH₂CH₃), 3.65 (1 H, ddd, J = 12.0, 8.5, 3.8 Hz, 1 H from NCH₂CH₃), 3.18 (1 H, dd, J = 13.4, 4.6 Hz, 1 H from ArCH₂CH₂), 2.57 - 2.82 (2 H, m, ArCH₂CH and 1 H from ArCH₂CH), 1.83 - 1.99 (1 H, m, 1 H from NCH₂CH₃), 1.65 - 1.83 (1 H, m, 1 H from NCH₂CH₃). ¹³C NMR (101 MHz, CDCl₃): δ ppm 162.5 (C=O), 147.4 (ArC), 144.0 (ArC), 133.1 (ArCH), 129.3 (2 × ArCH), 128.9 (q, J = 32.3 Hz, ArC), 128.2 (ArCH), 125.6 (q, J = 4.0 Hz, 2 × ArCH), 124.2 (q, J = 272.7 Hz, CF₃), 119.8 (ArCH), 117.4 (ArC), 114.9 (ArCH), 72.0 (NHCH), 43.3 (ArCH₂CH), 42.5 (NCH₂CH₃), 33.5 (ArCH₂CH), 26.2 (NCH₂CH₃). IR (neat, cm⁻¹): 3269, 3004, 1739, 1633, 1483, 1435, 1324, 1216, 1122, 1067, 743. MS (ESI⁺) m/z (%): 347.2 (M⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₅N₂O₃ (M + H⁺): 347.1366. Found: 347.1361.

(3S,3aR)-3-(Benzo[d][1,3]dioxol-5-ylmethyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2g). According to the general procedure B, using 1g (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2g (23.9 mg, 0.0742 mmol, 74%, >95:5 dr) as a white solid. M.p. = 223-224.5 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 7.91 (1 H, d, J = 7.5 Hz, ArH), 7.30 (1 H, d, J = 1.5 Hz, ArH), 6.88 (1 H, t, J = 7.4 Hz, ArH), 6.78 (1 H, d, J = 7.8 Hz, ArH), 6.62 - 6.74 (3 H, m, ArH), 5.96 (2 H, s, OCH₃O), 5.16 (1 H, d, J = 5.5 Hz, NHCH), 4.26 (1 H, s, NH), 3.83 (1 H, dt, J = 12.0, 7.7 Hz, 1 H from NCH₂CH₃), 3.60 (1 H, ddd, J = 12.2, 8.0, 4.6 Hz, 1 H from NCH₂CH₃), 3.01 (1 H, dd, J = 13.9, 5.6 Hz, 1 H from ArCH₂CH₂), 2.68 (1 H, dd, J =
10.5, 5.0 Hz, ArCH₂CH), 2.50 - 2.63 (1 H, m, 1 H from ArCH₂CH), 1.86 - 1.96 (1 H, m, 1 H from NCH₂CH₂), 1.73 - 1.86 (1 H, m, 1 H from NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 162.5 (C=O), 148.0 (ArC⁰), 147.4 (ArC⁰), 146.2 (ArC⁰), 133.3 (ArC⁰), 133.0 (ArCH), 128.3 (ArCH), 121.7 (ArCH), 119.8 (ArCH), 117.7 (ArC⁰), 114.9 (ArCH), 109.0 (ArCH), 108.4 (ArCH), 101.0 (OCH₃), 71.8 (NHCH), 43.5 (ArCH₂CH), 42.8 (NCH₂CH₂), 33.5 (ArCH₂CH), 26.7 (NCH₂CH₂). IR (neat, cm⁻¹): 3291, 2924, 1635, 1487, 1442, 1215, 1039, 757. MS (ESI⁺) m/z (%): 323.3 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₉N₂O₃ (M + H⁺): 323.1390. Found: 323.1386.

(3S,3aR)-3-(2,4-Dichlorobenzyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2h). According to the general procedure B, using 1h (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2h (32.0 mg, 0.0922 mmol, 92%, >95:5 dr) as a white solid. M.p. = 218.4-220 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 7.93 (1 H, d, J = 7.8 Hz, ArH), 7.43 (1 H, d, J = 2.0 Hz, ArH), 7.29 - 7.35 (1 H, m, ArH), 7.14 - 7.25 (2 H, m, ArH), 6.91 (1 H, t, J = 7.5 Hz, ArH), 6.72 (1 H, d, J = 8.0 Hz, ArH), 5.23 (1 H, d, J = 5.0 Hz, NHCH), 4.23 (1 H, s, NH), 3.76 - 3.91 (1 H, m, 1 H from NCH₂CH₂), 3.60 - 3.71 (1 H, m, 1 H from NCH₂CH₂), 3.24 (1 H, dd, J = 13.9, 4.4 Hz, 1 H from ArCH₂CH₂), 2.71 - 2.82 (1 H, m, ArCH₂CH), 2.57 - 2.71 (1 H, m, 1 H from ArCH₂CH), 1.84 - 1.96 (1 H, m, 1 H from NCH₂CH₂), 1.80 (1 H, dd, J = 7.0, 3.5 Hz, 1 H from NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 162.4 (C=O), 147.2 (ArC⁰), 136.1 (ArC⁰), 134.9 (ArC⁰), 133.1 (ArCH), 133.1 (ArC⁰), 132.1 (ArCH), 129.6 (ArCH), 128.3 (ArCH), 127.2 (ArCH), 119.9 (ArCH), 117.5 (ArC⁰), 114.8 (ArCH), 72.1
(NHCH), 42.5 (NCH₂CH₂), 41.7 (ArCH₂CH), 30.9 (ArCH₂CH), 25.9 (NCH₂CH₂). IR (neat, cm⁻¹): 3229, 2970, 1739, 1625, 1435, 1365, 1216, 769. MS (ESI⁺) m/z (%): 347.1 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₈H₁₇N₂OCl₂ (M + H⁺): 347.0712. Found: 347.0706.

(35,3aR)-3-(Naphthalen-1-ylmethyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2i). According to the general procedure B, using 1i (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2i (31.9 mg, 0.0972 mmol, 97%, >95:5 dr) as a light yellow solid. M.p. = 202.6-203.4 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 8.03 - 8.11 (1 H, m, ArH), 7.87 - 7.97 (2 H, m, ArH), 7.79 (1 H, d, J = 8.0 Hz, ArH), 7.49 - 7.57 (2 H, m, ArH), 7.41 - 7.48 (1 H, m, ArH), 7.34 - 7.40 (1 H, m, ArH), 7.28 - 7.33 (1 H, m, ArH), 6.84 - 6.95 (1 H, m, ArH), 6.71 (1 H, d, J = 8.0 Hz, ArH), 5.26 (1 H, d, J = 5.0 Hz, NHCH), 4.47 (1 H, s, NH), 3.94 (1 H, dt, J = 12.0, 7.9 Hz, 1 H from NCH₂CH₂), 3.54 - 3.68 (2 H, m, 1 H from NCH₂CH₂ and 1 H from ArCH₂CH), 2.99 - 3.07 (1 H, m, 1 H from ArCH₂CH), 2.94 (1 H, dd, J = 10.0, 5.0 Hz, ArCH₂CH), 1.79 - 1.92 (2 H, m, NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 162.6 (C=O), 147.5 (ArC⁰), 135.7 (ArC⁰), 134.1 (ArC⁰), 133.1 (ArCH), 131.9 (ArC⁰), 129.1 (ArCH), 128.3 (ArCH), 127.4 (ArCH), 126.9 (ArCH), 126.1 (ArCH), 125.8 (ArCH), 125.5 (ArCH), 123.5 (ArCH), 119.8 (ArCH), 117.6 (ArC⁰), 115.0 (ArCH), 72.1 (NHCH), 42.8 (NCH₂CH₂), 42.5 (ArCH₂CH), 30.5 (ArCH₂CH), 26.9 (NCH₂CH₂). νmax (thin film/cm⁻¹): 3268, 2945, 1629, 1482, 1434, 1216, 1029, 791, 763. MS (ESI⁺) m/z (%): 329.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₂₂H₁₇N₂O (M + H⁺): 329.1648. Found: 329.1641.
According to the general procedure B, using 1j (0.10 mmol), SmI$_2$ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH$_4$Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2j (30.0 mg, 0.0847 mmol, 85%, >95:5 dr) as a white solid. M.p. = 186-187.8 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ ppm 7.76 - 7.86 (1 H, m, ArH), 7.46 (2 H, d, $J = 7.3$ Hz, ArH), 7.31 - 7.41 (2 H, m, ArH), 7.21 - 7.29 (5 H, m, ArH), 7.11 - 7.21 (2 H, m, ArH), 6.75 - 6.87 (1 H, m, ArH), 6.30 (1 H, d, $J = 7.8$ Hz, ArH), 5.08 (1 H, d, $J = 7.0$ Hz, NHCH), 4.16 (1 H, d, $J = 11.8$ Hz, Ph$_2$CHCH), 4.05 (1 H, s, ArH), 3.29 - 3.41 (1 H, m, Ph$_2$CHCH), 3.26 (1 H, ddd, $J = 11.7$, 9.8, 6.7 Hz, 1 H from NCH$_2$CH), 1.60 - 1.78 (2 H, m, NCH$_2$CH). $^{13}$C NMR (101 MHz, CDCl$_3$): $\delta$ ppm 162.1 (C=O), 147.5 (ArC$^6$), 143.1 (ArC$^6$), 142.3 (ArC$^6$), 132.7 (ArCH), 129.6 (2 $\times$ ArCH), 128.9 (2 $\times$ ArCH), 128.4 (ArCH), 127.6 (2 $\times$ ArCH), 127.5 (ArCH), 127.4 (2 $\times$ ArCH), 126.9 (ArCH), 120.0 (ArCH), 117.9 (ArC$^6$), 115.1 (ArCH), 70.5 (NHCH), 51.8 (Ph$_2$CHCH), 47.1 (Ph$_2$CHCH), 44.5 (NCH$_2$CH$_2$), 29.7 (NCH$_2$CH$_2$). IR (neat, cm$^{-1}$): 3358, 2970, 1739, 1652, 1427, 1365, 1217, 772. MS (ESI$^+$) $m/z$ (%): 355.2 (M + H$^+$); HRMS (ESI$^+$): calcd. for C$_{24}$H$_{23}$N$_2$O (M + H$^+$): 355.1805. Found: 355.1800.
(3R,3aR)-3-((1-Methyl-1H-indol-2-yl)methyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2k). According to the general procedure B, using 1k (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2k (26.8 mg, 0.0810 mmol, 81%, >95:5 dr) as a white solid. M.p. = 200-201.9 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 7.92 (1 H, dd, J = 7.8, 1.3 Hz, ArH), 7.58 (1 H, d, J = 7.8 Hz, ArH), 7.28 - 7.36 (1 H, m, ArH), 7.18 - 7.27 (2 H, m, ArH), 7.10 - 7.17 (1 H, m, ArH), 6.82 - 6.92 (1 H, m, ArH), 6.60 (1 H, d, J = 8.0 Hz, ArH), 6.33 (1 H, s, ArH), 5.26 (1 H, d, J = 5.5 Hz, NHCH), 4.43 (1 H, s, NH), 3.83 - 3.91 (1 H, m, 1 H from NCH₂CH₂), 3.68 - 3.71 (3 H, m, CH₃), 3.61 - 3.68 (1 H, m, 1 H from NCH₂CH₂), 3.24 (1 H, dd, J = 15.9, 7.2 Hz, 1 H from ArCH₂CH), 2.95 (1 H, td, J = 5.9, 4.5 Hz, ArCH₂CH), 2.80 (1 H, dd, J = 16.1, 7.5 Hz, 1 H from ArCH₂CH), 2.04 - 2.17 (1 H, m, 1 H from NCH₂CH₂), 1.93 - 2.03 (1 H, m, 1 H from NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 162.5 (C=O), 147.4 (ArC⁶), 138.8 (ArC⁶), 137.5 (ArC⁵), 133.1 (ArCH), 128.2 (ArCH), 127.7 (ArC⁶), 121.2 (ArCH), 119.9 (ArCH), 119.7 (ArCH), 119.7 (ArCH), 117.3 (ArC⁵), 115.0 (ArCH), 109.0 (ArCH), 99.2 (ArCH), 71.8 (NHCH), 42.7 (NCH₂CH₂), 41.0 (ArCH₂CH), 29.7 (CH₃), 27.8 (NCH₂CH₂), 25.5 (ArCH₂CH). IR (neat, cm⁻¹): 3293, 2927, 1634, 1467, 1432, 1334, 1217, 749. MS (ESI⁺) m/z (%): 332.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₂₁H₂₂N₂O (M + H⁺): 332.1757. Found: 332.1746.

(35,3aR)-3-(Benzo[b]thiophen-3-ylmethyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2l). According to the general procedure B, using 1l (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1
h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2l (21.5 mg, 0.0644 mmol, 64%, >95:5 dr) as a light yellow solid. M.p. = 275-276.3 °C. 

**1H NMR (500 MHz, CDCl₃)**: δ ppm 7.87 - 7.99 (2 H, m, ArH), 7.73 - 7.82 (1 H, m, ArH), 7.33 - 7.47 (2 H, m, ArH), 7.27 - 7.31 (1 H, m, ArH), 7.17 (1 H, s, ArH), 6.89 (1 H, t, J = 7.4 Hz, ArH), 6.66 (1 H, d, J = 7.9 Hz, ArH), 5.24 (1 H, d, J = 5.0 Hz, NHCH), 4.41 (1 H, s, NH), 3.88 (1 H, dt, J = 12.0, 7.9 Hz, 1 H from NHCH₂CH₂), 3.64 (1 H, ddd, J = 12.2, 8.3, 4.4 Hz, 1 H from NHCH₂CH₂), 3.23 - 3.39 (1 H, m, 1 H from ArCH₂CCH), 3.21 - 3.39 (1 H, m, 1 H from ArCH₂CCH), 2.82 - 2.99 (2 H, m, ArCH₂CH and 1 H from ArCH₂CH), 1.94 - 2.04 (1 H, m, 1 H from NHCH₂CH₂), 1.85 - 1.93 (1 H, m, 1 H from NHCH₂CH₂). 

**13C NMR (126 MHz, CDCl₃)**: δ ppm 162.5 (C=O), 147.4 (ArC), 140.6 (ArC), 138.8 (ArC), 134.2 (ArC), 133.1 (ArC), 128.3 (ArC), 124.6 (ArCH), 124.2 (ArCH), 123.1 (ArCH), 122.3 (ArCH), 121.6 (ArCH), 119.8 (ArCH), 117.5 (ArC), 115.0 (ArCH), 71.9 (NHCH), 42.7 (NHCH₂CH₂), 41.7 (ArCH₂CH), 27.3 (NHCH₂CH₂), 26.7 (ArCH₂CH). 

**IR (neat, cm⁻¹):** 3295, 2928, 1667, 1611, 1467, 1383, 1334, 907, 727, 695. 

**MS (ESI⁺) m/z (%):** 335.2 (M + H⁺); **HRMS (ESI⁺):** calcd. for C₂₀H₁₉N₂O₃S (M + H⁺): 335.1213. Found: 335.1208.

(3R,3aR)-3-(Benzo[b]thiophen-2-ylmethyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2m). According to the general procedure B, using 1m (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2m (25.0 mg, 0.0748 mmol, 75%, >95:5 dr) as a light yellow solid. M.p. = 232.1-234 °C. 

**1H NMR (500 MHz, CDCl₃):** δ ppm 7.92 (1 H, d, J = 7.6 Hz, ArH), 7.80 (1 H, d, J = 7.9 Hz, ArH), 7.71 (1 H, d, J = 7.9 Hz, ArH), 7.28 - 7.42 (3 H, m, ArH), 7.10
N

2

Ar

Ar

Ar

H

NH

ArCH

NCH

Ar

Ar

Ar

Ar

H

Ar

Ar

Ar

3.30 (1 H, dd, 12.0, 7.8 Hz)

d, 7.21 (1 H, m

NMR (400 MHz, CDCl₃), gave

stirring

equiv,

(3

HRMS (neat

71.7 (C=O), 143.4 (ArC⁵),

140.0 (ArC³), 139.4 (ArC⁵), 133.1 (ArCH), 128.3 (ArCH), 124.4 (ArCH), 124.0 (ArCH),

123.0 (ArCH), 122.2 (ArCH), 122.1 (ArCH), 119.9 (ArCH), 117.5 (ArC⁵), 114.9 (ArCH),

71.7 (NHCH), 43.5 (ArCH₂), 42.6 (NCH₂CH₃), 29.2 (ArCH₃CH), 26.9 (NCH₂CH₃). IR

(neat, cm⁻¹): 3297, 2932, 1638, 1482, 905, 712, 649. MS (ESI⁺) m/z (%): 335.2 (M + H⁺);


(3R,3aR)-3-(Thiophen-2-ylmethyl)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2n). According to the general procedure B, using 1n (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2n (15.1 mg, 0.0532 mmol, 53%, >95:5 dr) as a light yellow oil. ¹H NMR (400 MHz, CDCl₃): δ ppm 7.84 - 7.94 (1 H, m, ArH), 7.26 - 7.31 (1 H, m, ArH), 7.17 - 7.21 (1 H, m, ArH), 6.97 (1 H, dd, J = 5.0, 3.5 Hz, ArH), 6.86 - 6.92 (2 H, m, ArH), 6.66 (1 H, d, J = 7.8 Hz, ArH), 5.19 (1 H, d, J = 5.5 Hz, NHCH), 4.31 (1 H, s, NH), 3.83 (1 H, dt, J = 12.0, 7.8 Hz, 1 H from NCH₂CH₃), 3.61 (1 H, ddd, J = 12.2, 8.1, 4.5 Hz, 1 H from NCH₂CH₃), 3.30 (1 H, dd, J = 15.3, 6.5 Hz, 1 H from ArCH₂CH), 2.87 - 3.02 (1 H, m, 1 H from ArCH₂CH), 2.62 - 2.82 (1 H, m, ArCH₂CH), 1.80 - 2.10 (2 H, m, NCH₂CH₃). ¹³C NMR (101
**MHZ, CDCl₃**: δ ppm 162.4 (C=O), 147.4 (ArC), 142.3 (ArC), 133.0 (ArCH), 128.3 (ArCH), 127.1 (ArCH), 125.5 (ArCH), 124.0 (ArCH), 119.8 (ArCH), 117.5 (ArC), 114.9 (ArCH), 71.6 (NHCH), 44.0 (ArCH₂), 42.7 (NCH₂CH₂), 28.3 (ArCH₂CH), 27.1 (NCH₂CH₂). **IR (neat, cm⁻¹)**: 2969, 2346, 1678, 1612, 1467, 1386, 1217, 753, 695. **MS (ESI⁺) m/z (%)**: 285.1 (M + H⁺); **HRMS (ESI⁺)**: calcd. for C₁₆H₁₇N₂O₃ (M + H⁺): 285.1056. Found: 285.1048.

(35,3aR)-3-Benzyl-6-bromo-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2o). According to the general procedure B, using 1o (0.10 mmol), Sml₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2o (15.3 mg, 0.0430 mmol, 43%, >95:5 dr) as a white solid. M.p. = 200-202 °C. **¹H NMR (400 MHZ, CDCl₃)**: δ ppm 7.92 (1 H, d, J = 7.0 Hz, ArH), 7.29 - 7.37 (2 H, m, ArH), 7.21 - 7.26 (3 H, m, ArH), 6.88 (1 H, t, J = 7.5 Hz, ArH), 6.66 (1 H, d, J = 8.0 Hz, ArH), 5.18 (1 H, d, J = 5.5 Hz, NHCH), 4.28 (1 H, s, NH), 3.85 (1 H, dt, J = 12.0, 7.8 Hz, 1 H from NCH₂CH₂), 3.61 (1 H, ddd, J = 12.0, 8.0, 4.5 Hz, 1 H from NCH₂CH₂), 3.10 (1 H, dd, J = 13.6, 5.5 Hz, 1 H from ArCH₂CH), 2.72 - 2.84 (1 H, m, ArCH₂CH), 2.55 - 2.72 (1 H, m, 1 H from ArCH₂CH), 1.87 - 1.97 (1 H, m, 1 H from NCH₂CH₂), 1.77 - 1.87 (1 H, m, 1 H from NCH₂CH₂). **¹³C NMR (101 MHZ, CDCl₃)**: δ ppm 162.5 (C=O), 147.4 (ArC), 139.7 (ArC), 133.0 (ArCH), 128.9 (2 × ArCH), 128.7 (ArC and ArCH), 128.3 (ArCH), 126.5 (ArCH), 119.7 (ArCH), 117.6 (ArC), 114.9 (ArCH), 71.9 (NHCH), 43.4 (ArCH₂CH), 42.8 (NCH₂CH₂), 33.8 (ArCH₂CH), 26.8 (NCH₂CH₂). **IR (neat, cm⁻¹)**: 3274, 3025, 2944. 1629, 1483, 1434, 907, 729, 697. **MS (ESI⁺) m/z (%)**: 357.2 (M + H⁺); **HRMS (ESI⁺)**: calcd. for C₁₈H₁₆N₂OBr (M +
According to the general procedure B, using 1p (0.10 mmol), SmI$_2$ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH$_4$Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2p (20.0 mg, 0.0562 mmol, 56%, >95:5 dr) as a white solid. M.p. = 213.4-215 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ ppm 8.01 (1 H, d, $J$ = 2.3 Hz, ArH), 7.30 - 7.38 (3 H, m, ArH), 7.19 - 7.26 (3 H, m, ArH), 6.55 (1 H, d, $J$ = 8.5 Hz, ArH), 5.15 (1 H, d, $J$ = 5.5 Hz, NHCH), 4.35 (1 H, s, NH), 3.82 (1 H, dt, $J$ = 12.0, 8.0 Hz, 1 H from NCH$_2$CH$_2$), 3.60 (1 H, ddd, $J$ = 12.2, 8.1, 4.5 Hz, 1 H from NCH$_2$CH$_2$), 3.07 (1 H, dd, $J$ = 13.9, 5.9 Hz, 1 H from ArCH$_2$CH), 2.71 - 2.81 (1 H, m, ArCH$_2$CH), 2.60 - 2.70 (1 H, m, 1 H from ArCH$_2$CH), 1.86 - 1.98 (1 H, m, 1 H from NCH$_2$CH$_2$), 1.77 - 1.86 (1 H, m, 1 H from NCH$_2$CH$_2$). $^{13}$C NMR (101 MHz, CDCl$_3$): $\delta$ ppm 161.2 (C=O), 146.3 (ArC$^\alpha$), 139.4 (ArC$^\alpha$), 135.6 (ArCH), 130.8 (ArCH), 128.8 (2 x ArCH), 128.8 (2 x ArCH), 126.6 (ArCH), 119.2 (ArC$^\alpha$), 116.6 (ArCH), 111.8 (ArC$^\alpha$), 71.9 (NHCH), 43.3 (ArCH$_2$CH), 42.9 (NCH$_2$CH$_2$), 33.8 (ArCH$_2$CH), 26.8 (NCH$_2$CH$_2$). IR (neat, cm$^{-1}$): 3265, 3001, 2346, 1735, 1634, 1492, 1450, 1365, 1216, 752, 662. MS (ESI$^+$) m/z (%): 357.2 (M + H$^+$); HRMS (ESI$^+$): calcd. for C$_{18}$H$_{18}$N$_2$OBr (M + H$^+$): 357.0597. Found: 357.0590.
(3S,3aR)-3-Benzyl-7-fluoro-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2q).

According to the general procedure B, using 1q (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₂Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2q (20.0 mg, 0.0676 mmol, 68%, >95:5 dr) as a white solid. M.p. = 175.1-176 °C. ¹H NMR (400 MHz, CDCl₃): δ ppm 7.61 (1 H, dd, J = 8.8, 3.0 Hz, ArH), 7.31 - 7.40 (2 H, m, ArH), 7.21 - 7.26 (3 H, m, ArH), 7.01 (1 H, td, J = 8.4, 2.8 Hz, ArH), 6.63 (1 H, dd, J = 8.7, 4.1 Hz, ArH), 5.14 (1 H, d, J = 5.5 Hz, NHCH), 4.15 (1 H, s, NH), 3.84 (1 H, dt, J = 12.0, 7.7 Hz, 1 H from NCH₂CH₂), 3.60 (1 H, ddd, J = 12.2, 8.0, 4.6 Hz, 1 H from NCH₂CH₂), 3.08 (1 H, dd, J = 13.8, 5.8 Hz, 1 H from ArCH₂CH), 2.72 - 2.82 (1 H, m, ArCH₃CH), 2.62 - 2.71 (1 H, m, 1 H from ArCH₃CH), 1.87 - 1.98 (1 H, m, 1 H from NCH₂CH₂), 1.77 - 1.87 (1 H, m, 1 H from NCH₂CH₂). ¹³C NMR (101 MHz, CDCl₃): δ ppm 161.5 (C=O), 156.9 (d, J = 239.4 Hz, CF), 143.6 (d, J = 2.0 Hz, ArC⁰), 139.5 (ArC⁰), 128.8 (2 × ArCH), 128.8 (2 × ArCH), 126.6 (ArCH), 120.2 (d, J = 24.2 Hz, ArCH), 119.0 (d, J = 7.0 Hz, ArC⁰), 116.3 (d, J = 7.1 Hz, ArCH), 114.3 (d, J = 25.3 Hz, ArCH), 72.1 (NHCH), 43.3 (ArCH₂CH), 42.9 (NCH₂CH₂), 33.8 (ArCH₃CH), 27.0 (NCH₂CH₂). IR (neat, cm⁻¹): 3271, 2944, 1634, 1494, 1451, 1252, 1193, 908, 732. MS (ESI⁺) m/z (%): 297.2 (M + H⁺); HRMS (ESI⁺): calcd. for C₁₉H₁₈N₂OF (M + H⁺): 297.1398. Found: 297.1387.

(3S,3aR)-3-Benzyl-6-fluoro-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2r).

According to the general procedure B, using 1r (0.10 mmol), SmI₂ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH₂Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2r
(20.1 mg, 0.0679 mmol, 68%, >95:5 dr) as a colorless oil. \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta\) ppm 7.89 (1 H, dd, \(J = 8.5, 6.5\) Hz, Ar\(H\)), 7.31 - 7.38 (2 H, m, Ar\(H\)), 7.18 - 7.27 (3 H, m, Ar\(H\)), 6.55 (1 H, td, \(J = 8.7, 2.3\) Hz, Ar\(H\)), 6.35 (1 H, dd, \(J = 10.0, 2.3\) Hz, Ar\(H\)), 5.19 (1 H, d, \(J = 5.3\) Hz, NH\(C\(H\)), 4.55 (1 H, s, NH), 3.82 (1 H, dt, \(J = 11.9, 8.0\) Hz, 1 H from NCH\(_2\)CH\(_2\)), 3.60 (1 H, ddd, \(J = 12.1, 8.2, 4.3\) Hz, 1 H from NCH\(_2\)CH\(_2\)), 3.08 (1 H, dd, \(J = 14.1, 5.8\) Hz, 1 H from Ar\(CH\(_2\)CH\)), 2.69 - 2.81 (1 H, m, Ar\(CH\(_2\)CH\)), 2.56 - 2.69 (1 H, m, 1 H from Ar\(CH\(_2\)CH\)), 1.88 - 1.97 (1 H, m, 1 H from NCH\(_2\)CH\(_2\)), 1.75 - 1.88 (1 H, m, 1 H from NCH\(_2\)CH\(_2\)). \(^{13}\)C NMR (101 MHz, CDCl\(_3\)): \(\delta\) ppm 166.0 (d, \(J = 252.5\) Hz, CF), 161.9 (C=O), 149.4 (d, \(J = 12.1\) Hz, Ar\(C\)), 139.5 (Ar\(C\)), 130.7 (d, \(J = 11.1\) Hz, Ar\(CH\)), 128.9 (2 × Ar\(CH\)), 128.8 (2 × Ar\(CH\)), 126.5 (Ar\(CH\)), 113.8 (d, \(J = 2.0\) Hz, Ar\(C\)), 107.1 (d, \(J = 24.2\) Hz, Ar\(CH\)), 101.4 (d, \(J = 25.3\) Hz, Ar\(CH\)), 72.0 (NH\(CH\)), 43.3 (Ar\(CH\(_2\)CH\)), 42.7 (NCH\(_2\)CH\(_2\)), 33.7 (Ar\(CH\(_2\)CH\)), 26.7 (NCH\(_2\)CH\(_2\)). IR (neat, cm\(^{-1}\)): 3026, 2360, 2249, 1673, 1612, 1478, 1442, 1281, 1144, 908, 776. MS (ESI\(^+\)) \(m/z\) (%): 297.2 (M + H\(^+\)); HRMS (ESI\(^+\)): calcd. for C\(_{18}\)H\(_{18}\)N\(_2\)OF (M + H\(^+\)): 297.1398. Found: 297.1386.

(3S,3aR)-3-Benzyl-6,7-dimethoxy-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2s). According to the general procedure B, using 1s (0.10 mmol), Sml\(_2\) (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH\(_4\)Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2s (27.6 mg, 0.0817 mmol, 82%, >95:5 dr) as a white solid. M.p. = 169.4-170.2 °C. \(^1\)H NMR (500 MHz, CDCl\(_3\)): \(\delta\) ppm 7.40 (1 H, s, Ar\(H\)), 7.30 - 7.36 (2 H, m, Ar\(H\)), 7.15 - 7.26 (3 H, m, Ar\(H\)), 6.21 (1 H, s, Ar\(H\)), 5.11 (1 H, d, \(J = 5.4\) Hz, NHCH\(_3\)), 4.14 (1 H, s, NH), 3.86 (3 H, s, CH\(_3\)), 3.85 (3 H, s, CH\(_3\)), 3.75 - 3.83 (1 H, m, 1 H from NCH\(_2\)CH\(_2\)),
3.58 (1 H, ddd, J = 12.2, 8.0, 4.7 Hz, 1 H from NCH$_2$CH$_2$), 3.08 (1 H, dd, J = 13.7, 5.5 Hz, 1 H from ArCH$_2$CH), 2.73 (1 H, dd, J = 10.2, 5.2 Hz, ArCH$_2$CH), 2.59 - 2.69 (1 H, m, 1 H from ArCH$_2$CH), 1.85 - 1.93 (1 H, m, 1 H from NCH$_2$CH$_2$), 1.74 - 1.84 (1 H, m, 1 H from NCH$_2$CH$_2$). $^{13}$C NMR (126 MHz, CDCl$_3$): $\delta$ ppm 162.6 (C=O), 153.4 (ArC$^6$), 143.4 (ArC$^6$), 142.7 (ArC$^6$), 139.7 (ArC$^6$), 128.8 (2 × ArCH), 128.7 (2 × ArCH), 126.5 (ArCH), 110.0 (ArCH), 109.9 (ArC$^6$), 98.8 (ArCH), 72.3 (NHCH), 56.3 (OCH$_3$), 56.0 (OCH$_3$), 43.4 (ArCH$_2$CH), 42.7 (NCH$_2$CH$_2$), 33.8 (ArCH$_2$CH), 27.0 (NCH$_2$CH$_2$). IR (neat, cm$^{-1}$): 3256, 2936, 1611, 1451, 1265, 1223, 1114, 1014, 910, 727, 645. MS (ESI$^+$) m/z (%): 339.2 (M + H$^+$); HRMS (ESI$^+$): calcd. for C$_{20}$H$_{15}$N$_2$O$_3$ (M + H$^+$): 339.1703. Found: 339.1691.

(3S,3aR)-3-Benzyl-3a-methyl-2,3,3a,4-tetrahydropyrrrolo[2,1-b]quinazolin-9(1H)-one (2t).

According to the general procedure B, using 1t (0.10 mmol), SmI$_2$ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and NH$_4$Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2t (13.5 mg, 0.0462 mmol, 46%, 69:31 dr) as a white solid. M.p. = 221-223 °C. $^1$H NMR (500 MHz, CDCl$_3$): $\delta$ ppm 7.91 (1 H, d, J = 7.6 Hz, ArH), 7.28 - 7.36 (3 H, m, ArH), 7.19 - 7.26 (3 H, m, ArH), 6.85 (1 H, t, J = 7.6 Hz, ArH), 6.62 (1 H, d, J = 7.9 Hz, ArH), 4.13 (1 H, s, NH), 3.92 (1 H, dt, J = 12.3, 7.7 Hz, 1 H from NCH$_2$CH$_2$), 3.55 (1 H, ddd, J = 12.5, 8.4, 4.7 Hz, 1 H from NCH$_2$CH$_2$), 3.12 (1 H, dd, J = 13.1, 4.9 Hz, 1 H from ArCH$_2$CH), 2.51 - 2.64 (2 H, m, 1 H from ArCH$_2$CH and ArCH$_2$CH), 1.95 - 2.04 (1 H, m, 1 H from NCH$_2$CH$_2$), 1.74 - 1.80 (1 H, m, 1 H from NCH$_2$CH$_2$), 1.48 (3 H, s, CH$_3$). $^{13}$C NMR (126 MHz, CDCl$_3$): $\delta$ ppm 161.5 (C=O), 145.8 (ArC$^6$), 140.0 (ArC$^6$), 133.1 (ArCH), 129.0 (2 × ArCH), 128.7 (2 × ArCH), 128.2 (ArCH), 126.4 (ArCH), 119.1 (ArCH), 116.1 (ArC$^6$), 114.9 (ArCH), 77.5 (C$^6$),
50.5 (ArCH₂CH), 42.7 (NCH₂CH₂), 35.6 (ArCH₂CH), 26.9 (CH₃), 26.8 (NCH₂CH₂). **IR (neat, cm⁻¹):** 3269, 2970, 1612, 1484, 1417, 1217, 750. **MS (ESI⁺) m/z (%):** 293.2 (M + H⁺); **HRMS (ESI⁺):** calcd. for C₁₉H₁₉N₂O (M + H⁺): 293.1648. Found: 293.1646.

(5αR,6S)-6-Benzyl-5,5a,6,7,8,9-hexahydro-11H-pyrido[2,1-b]quinazolin-11-one (2u).

According to the general procedure B, using 1u (0.10 mmol), SmI₂ (0.50 mmol, 5 equiv, 5.0 mL, 0.10 M) and NH₄Cl (16 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2u (12.9 mg, 0.0442 mmol, 44%, 79:21 dr) as a colorless oil. **¹H NMR (500 MHz, CDCl₃):** (major diastereomer only) δ ppm 7.83 - 7.92 (1 H, ArH), 7.30 - 7.39 (2 H, ArH), 7.23 - 7.28 (2 H, ArH), 7.14 - 7.23 (2 H, ArH), 6.75 - 6.82 (1 H, m, ArH), 6.18 (1 H, d, J = 7.9 Hz, ArH), 4.69 (1 H, ddt, J = 13.5, 4.3, 2.0, 2.0 Hz, 1 H from NCH₂), 4.55 (1 H, d, J = 9.3 Hz, NHCH), 4.17 (1 H, s, NH), 2.83 (1 H, dd, J = 13.7, 6.8 Hz, 1 H from ArCH₂CH), 2.51 - 2.68 (2 H, m, 1 H from ArCH₂CH and 1 H from NCH₂), 2.15 - 2.25 (1 H, m, ArCH₂CH), 1.83 - 1.92 (1 H, m, 1 H from NCH₂CH₂CH₂), 1.66 - 1.74 (1 H, m, 1 H from NCH₂CH₂CH₂), 1.50 - 1.59 (1 H, m, 1 H from NCH₂CH₂CH₂). **¹³C NMR (126 MHz, CDCl₃):** (major diastereomer only) δ ppm 163.6 (C=O), 145.1 (ArC⁶), 139.2 (ArC⁶), 133.3 (ArCH), 128.97 (2 × ArCH), 128.87 (2 × ArCH), 128.4 (ArCH), 126.6 (ArCH), 118.8 (ArCH), 115.1 (ArC⁶), 114.1 (ArCH), 74.3 (NHCH), 43.14 (NCH₂), 43.10 (ArCH₂CH), 39.4 (ArCH₂CH), 30.1 (NCH₂CH₂CH₂), 24.1 (NCH₂CH₂CH₂). **IR (neat, cm⁻¹):** 3303, 2940, 1738, 1612, 1365, 1229, 750. **MS (ESI⁺) m/z (%):** 311.1 (M + K⁺); **HRMS (ESI⁺):** calcd. for C₁₉H₁₅N₂O (M + H⁺): 293.1648. Found: 293.1644.
Deuterium Labelling Experiment

(3S,3aR)-3-(Phenylmethyl-d)-2,3,3a,4-tetrahydropyrrolo[2,1-b]quinazolin-9(1H)-one (2a-D). According to the general procedure B, using 1a (0.10 mmol), SmI$_2$ (0.30 mmol, 3 equiv, 3.0 mL, 0.10 M) and ND$_4$Cl (18 mg, 0.3 mmol, 3 equiv) with a slow addition over 1 h, stirring at room temperature for 1 h and purification by chromatography (50% EtOAc/hexanes), gave 2a-D (22.3 mg, 0.0799 mmol, 80%, 83:17 dr) as a yellow solid. M.p. = 165-167 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ ppm 7.92 (1 H, dd, $J = 7.8, 1.3$ Hz, ArH), 7.17 - 7.38 (6 H, m, ArH), 6.83 - 6.93 (1 H, m, ArH), 6.67 (1 H, d, $J = 8.0$ Hz, ArH), 5.18 (1 H, d, $J = 5.3$ Hz, NHCH$_3$), 4.31 (1 H, s, NH), 3.85 (1 H, dt, $J = 11.9, 7.7$ Hz, 1 H from NCH$_2$CH$_2$), 3.61 (1 H, ddd, $J = 12.2, 8.1, 4.5$ Hz, 1 H from NCH$_2$CH$_2$), 2.70 - 2.80 (1 H, m, ArCH$_2$CH$_2$), 2.66 (d, $J = 9.9$ Hz, 1 H from ArCHDCH), 1.87 - 1.96 (1 H, m, 1 H from NCH$_2$CH$_2$), 1.77 - 1.87 (1 H, m, 1 H from NCH$_2$CH$_2$). $^{13}$C NMR (101 MHz, CDCl$_3$): $\delta$ ppm 162.5 (C=O), 147.5 (ArC$_6$), 139.7 (ArC$_6$), 133.0 (ArCH), 128.9 (2 × ArCH), 128.7 (2 × ArCH), 128.3 (ArCH), 126.5 (ArCH), 119.7 (ArCH), 117.6 (ArC$_6$), 114.9 (ArCH), 71.9 (NHCH), 43.4 (ArCHDCH), 42.8 (NCH$_2$CH$_2$), 33.5 (t, $J = 19.2$ Hz, ArCHDCH), 26.8 (NCH$_2$CH$_2$). IR (neat, cm$^{-1}$): 3268, 2970, 1738, 1632, 1435, 1365, 1217, 758. MS (ESI$^+$) $m/z$ (%): 318.1 (M + K$^+$); HRMS (ESI$^+$): calcd. for C$_{18}$H$_{17}$DN$_2$OK (M + K$^+$): 318.1113. Found: 318.1107.
NOE Study for 2u

\[ \text{2u} : \text{2u'} = 79:21 \text{ dr} \]

NHCH in the minor isomer

Irradiation at CHCH\(_2\)Ph in the minor isomer
When we irraditated the CHCH$_2$Ph in the minor isomer, we observed the NOE peak (2%) of the NHCH in the minor isomer. However, when we irradiated the NHCH in the major isomer, we did not observe any NOE peak for the CHCH$_2$Ph in the major isomer. So we propose the following stereochemistry:

![Proposed major isomer (2u)](image1)

![Proposed minor isomer (2u')] (image2)
Proposed Stereochemistry of 2u

From the $^1$H NMR spectra, the $J$ value coupling constant of $H_a$ in the major isomer is 9.3 Hz, the $J$ value coupling constant of $H_a$ in the minor isomer is 3.1 Hz.

The 3D chemical structures of the major and minor isomers for 2u were calculated using MM2 minimization in Chem3D (version 16.0.1.4, Perkin Elmer) and the 3D mol files exported to MSpin (version 2.3.2-694, MestReLab Research S. L.). $^3J_{H_a,H_b}$ coupling values were calculated using the Karplus option in the JCoupling tool of MSpin. When $H_a$ and $H_b$ are anti, $J$ value coupling constant is calculated as 9.3 Hz which matches the major isomer ($J = 9.3$ Hz), see Figure S 1. When $H_a$ and $H_b$ are syn, $J$ value coupling constant is calculated as 4.9 Hz which matches the minor isomer ($J = 3.1$ Hz), see Figure S 2.

We therefore propose the following stereochemistry and it matches the results we observe from NOE study:

- **2u**: Proposed major isomer
- **2u'**: Proposed Minor isomer
**Figure S1.** Calculated $J$ value coupling constant when the $H_a$ and $H_b$ are *anti*.

**Figure S2.** Calculated $J$ value coupling constant when the $H_a$ and $H_b$ are *syn*.
X-ray structure of 2a

**Table S1. Crystal data and details of data collection and refinement for compound 2a**

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X-ray structure of 2g

CCDC 1846531

![2g Chemical Structure](image)

![2g Crystal Structure](image)

**Table S2.** Crystal data and details of data collection and refinement for compound 2g

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X-ray structure of 2t

CCDC 1846532

![Structure of 2t](image)

**Table S3.** Crystal data and details of data collection and refinement for compound 2t

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References


$^1$H and $^{13}$C NMR Spectra of Compounds

$^1$H NMR (400 MHz, CDCl$_3$)

![$^1$H NMR spectrum](image)

$^{13}$C NMR (101 MHz, CDCl$_3$)

![$^{13}$C NMR spectrum](image)
$^1$H NMR (400 MHz, CDCl$_3$)

![NMR Spectrum](image)

$^{13}$C NMR (101 MHz, CDCl$_3$)

![NMR Spectrum](image)
$^1$H NMR (400 MHz, CDCl$_3$)

![NMR Spectrum Image]

Chemical shift (ppm)

$^1$C NMR (101 MHz, CDCl$_3$)

![NMR Spectrum Image]

Chemical shift (ppm)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^1$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (500 MHz, CDCl$_3$)

$^13$C NMR (126 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^1$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
1H NMR (400 MHz, CDCl₃)

13C NMR (101 MHz, CDCl₃)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^1$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (500 MHz, CDCl$_3$)

$^{13}$C NMR (126 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (500 MHz, CDCl$_3$)

$^{13}$C NMR (126 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)

S 70
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)

S 71
$^1$H NMR (400 MHz, CDCl$_3$)

$^1$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^1$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
**H NMR (500 MHz, CDCl₃)**

![1H NMR spectrum](image)

**C NMR (126 MHz, CDCl₃)**

![13C NMR spectrum](image)
$^1$H NMR (500 MHz, CDCl$_3$)

13C NMR (126 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^1$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^{1}$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (101 MHz, CDCl$_3$)
$^1$H NMR (500 MHz, CDCl$_3$)

$^{13}$C NMR (126 MHz, CDCl$_3$)
$^1$H NMR (500 MHz, CDCl$_3$)

$^{13}$C NMR (126 MHz, CDCl$_3$)
$^1$H NMR (500 MHz, CDCl$_3$)

$^13$C NMR (126 MHz, CDCl$_3$)
$^1$H NMR (400 MHz, CDCl$_3$)

$^{13}$C NMR (126 MHz, CDCl$_3$)