Supporting Information

for

New efficient synthesis of polysubstituted 3,4-dihydroquinazolines and 4H-3,1-benzothiazines through a Passerini/Staudinger/aza-Wittig/addition/nucleophilic substitution sequence

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1 Experimental section

1.1 General information
Melting points were determined using an X-4 model apparatus and were uncorrected. $^1$H NMR were recorded in CDCl$_3$ on a Varian Mercury 600 spectrometer and resonances were relative to TMS. $^{13}$C($^1$H) NMR spectra were recorded in CDCl$_3$ on a Varian Mercury 600 (150 MHz) with complete proton decoupling spectrophotometers (CDCl$_3$: 77.0 ppm). HRMS was measured on an Agilent 6224 TOF LC/MS spectrometer. Amines, CS$_2$ and isocyanides were purchased from commercial suppliers and used without further purification. CH$_2$Cl$_2$, toluene and CH$_3$CN were used after drying and distillation. Column chromatography purifications were performed using 400-630 mesh silica gel. Analytical thin-layer chromatography (TLC) was carried out on silica gel 60 F$_{254}$ plates, which were visualized by exposure to ultraviolet light.

1.2 General procedure for preparation of azides 4 via Passerini reaction
To a solution of 2-azidobenzaldehydes 1 (1 mmol) in CH$_2$Cl$_2$ (5 mL) was added sequentially benzoic acid (2) (0.122 g, 1 mmol) and isocyanides 3 (1 mmol) at room temperature. After the reaction mixture was stirred for 48 hours at ambient temperature, the solvent was removed under reduced pressure and the residue was recrystallized from ether/petroleum ether to give azide 4.

1-(2-Azidophenyl)-2-(tert-butylamino)-2-oxoethyl benzoate (4a)
White solid (0.306 g, yield 87%), m.p. 134-136 °C, lit$^{[1]}$ m.p. 136-137 °C, $^1$H NMR (CDCl$_3$, 600 MHz): $\delta$ (ppm) 8.10 (d, $J$ = 7.6 Hz, 2H, Ar-H), 7.60-7.18 (m, 7H, Ar-H), 6.41 (s, 1H, CH), 6.11 (s, 1H, NH), 1.37 (s, 9H, 3CH$_3$).

1-(2-Azidophenyl)-2-(cyclohexylamino)-2-oxoethyl benzoate (4b)
White solid (0.283 g, yield 75%), m.p. 151-153 °C; $^1$H NMR (CDCl$_3$, 600 MHz): $\delta$ (ppm) 8.10 (d, $J$ = 7.2 Hz, 2H, Ar-H), 7.61-7.18 (m, 7H, Ar-H), 6.46 (s, 1H, CH), 6.13 (d, $J$ = 7.2 Hz, 1H, NH), 3.84-3.79 (m, 1H, NCH), 3.00-1.3 (m, 10H, 5CH$_2$); $^{13}$C NMR (CDCl$_3$, 150 MHz): $\delta$ (ppm) 166.8, 165.0, 137.9, 133.5, 130.1, 129.7, 129.4, 129.1, 128.5, 126.9, 125.1, 118.3, 71.2, 48.2, 32.8, 32.6, 25.3, 24.6. HRMS (ESI-TOF) m/z [M+H]$^+$ Calcd for C$_{21}$H$_{23}$N$_3$O$_3$ 379.1765; Found 379.1771.

1-(2-Azido-4-chlorophenyl)-2-(tert-butylamino)-2-oxoethyl benzoate (4c)
White solid (yield 0.309 g, 80%), m.p 168-169 °C; $^1$H NMR (CDCl$_3$, 600 MHz) $\delta$ (ppm) 8.07 (d, $J$ = 7.2 Hz, 2H, Ar-H), 7.61 (t, $J$ = 7.2 Hz, 1H, Ar-H), 7.52 (d, $J$ = 8.4 Hz, 1H, Ar-H), 7.48 (t, $J$ = 7.8 Hz, 2H, Ar-H), 7.19 (s, 1H, Ar-H), 7.16 (d, $J$ = 7.8 Hz, 1H, Ar-H), 6.35 (s, 1H, CH), 6.11 (s, 1H, NH), 1.37 (s, 9H, 3CH$_3$); $^{13}$C NMR (CDCl$_3$, 150 MHz) $\delta$ (ppm) 166.5, 164.9, 139.4, 135.8, 133.7, 130.6, 129.8, 129.1, 128.6, 125.9, 125.5, 118.6, 70.9, 51.7, 28.6. HRMS (ESI-TOF) m/z [M+H]$^+$ Calcd for C$_{19}$H$_{20}$Cl$_2$N$_3$O$_3$ 387.1218; Found 387.1217.

1-(2-Azido-4-chlorophenyl)-2-(butylamino)-2-oxoethyl benzoate (4d)
White solid (yield 0.289 g, 75%), m.p 127-128 °C; $^1$H NMR (CDCl$_3$, 600 MHz) $\delta$ (ppm) 8.08 (d, $J$ = 7.8 Hz, 2H, Ar-H), 7.61 (t, $J$ = 7.2 Hz, 1H, Ar-H), 7.53 (d, $J$ = 7.8 Hz, 1H, Ar-H), 7.48 (t, $J$ = 7.8 Hz, 2H, Ar-H), 7.18 (s, 1H, Ar-H), 7.16 (t, $J$ = 9.0 Hz, 1H, Ar-H), 6.43 (s, 1H, CH), 6.27 (s, 1H, NH), 3.37-3.27 (m, 2H, NCH$_2$), 1.54-1.49
(m, 2H, CH₂), 1.37-1.31 (m, 2H, CH₂), 0.92 (t, J = 7.2 Hz, 3H, CH₃); ¹³C NMR (CDCl₃, 150 MHz) δ (ppm) 167.3, 165.0, 139.3, 135.9, 133.7, 130.6, 129.8, 129.0, 128.6, 125.5, 125.4, 118.5, 70.8, 39.3, 31.5, 19.9, 13.7. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₁₉H₂₅ClN₄O₂⁺ 387.1218; Found 387.1219.

1-(2-Azido-5-methylphenyl)-2-(cyclohexylamino)-2-oxoethyl benzoate (4e)

White solid (yield 0.309 g, 79%), mp 169-171 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.10 (d, J = 7.8 Hz, 2H, Ar-H), 7.60 (t, J = 7.2 Hz, 1H, Ar-H), 7.47 (t, J = 7.8 Hz, 2H, Ar-H), 7.40 (s, 1H, Ar-H), 7.20 (d, J = 7.8 Hz, 1H, Ar-H), 6.41 (s, 1H, CH), 6.12 (d, J = 8.4 Hz, 1H, NH), 3.84-3.79 (m, 1H, NCH₂), 2.34 (s, 3H, CH₃), 2.00-1.12 (m, 10H, 5CH₂); ¹³C NMR (CDCl₃, 150 MHz) δ (ppm) 166.9, 165.1, 135.1, 133.5, 130.9, 130.0, 129.8, 129.4, 128.5, 126.7, 118.3, 71.5, 48.2, 32.9, 32.7, 25.4, 24.6, 20.9. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₂H₃₃N₄O₅⁺ 393.1921; Found 393.1933.

1-(2-Azido-5-methylphenyl)-2-(butylamino)-2-oxoethyl benzoate (4f)

White solid (yield 0.319 g, 87%), mp 135-137 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.11 (d, J = 8.4 Hz, 2H, Ar-H), 7.60 (t, J = 7.8 Hz, 1H, Ar-H), 7.47 (t, J = 7.8 Hz, 2H, Ar-H), 7.40 (s, 1H, Ar-H), 7.20 (d, J = 7.8 Hz, 1H, Ar-H), 6.44 (s, 1H, CH), 6.22 (s, 1H, NH), 3.37-3.25 (m, 2H, NCH₂), 2.35 (s, 3H, CH₃), 1.54-1.50 (m, 2H, CH₂), 1.35-1.31 (m, 2H, CH₂), 0.91 (t, J = 7.2 Hz, 3H, CH₃); ¹³C NMR (CDCl₃, 150 MHz) δ (ppm) 167.8, 165.2, 135.1, 133.5, 130.9, 130.5, 129.9, 129.3, 128.5, 126.6, 118.2, 71.3, 39.3, 31.5, 20.9, 19.9, 13.7. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₀H₂₂N₄O₄⁺ 367.1765; Found 367.1767.

1-(2-Azido-5-methylphenyl)-2-(tert-butyramino)-2-oxoethyl benzoate (4g)

White solid (yield 0.296 g, 81%), mp 145-147 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.10 (d, J = 7.8 Hz, 2H, Ar-H), 7.59 (t, J = 7.2 Hz, 1H, Ar-H), 7.47 (t, J = 7.8 Hz, 2H, Ar-H), 7.39 (s, 1H, Ar-H), 7.20 (d, J = 7.8 Hz, 1H, Ar-H), 7.09 (d, J = 7.8 Hz, 1H, Ar-H), 6.36 (s, 1H, CH), 6.09 (s, 1H, NH), 2.34 (s, 3H, CH₃), 1.37 (s, 9H, 3CH₃); ¹³C NMR (CDCl₃, 150 MHz) δ (ppm) 167.0, 165.1, 135.1, 133.5, 130.8, 129.9, 129.8, 129.4, 128.5, 126.9, 118.3, 71.5, 51.6, 28.7, 20.9. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₀H₂₂N₄O₄⁺ 367.1765; Found 367.1770.

1-(2-Azido-4-chlorophenyl)-2-(cyclohexylamino)-2-oxoethyl benzoate (4h)

White solid (yield 0.347 g, 84%), mp 168-170 °C; ¹H NMR (CDCl₃, 600 MHz) δ (ppm) 8.07 (d, J = 7.2 Hz, 2H, Ar-H), 7.61 (t, J = 7.2 Hz, 1H, Ar-H), 7.53-7.46 (m, 3H, Ar-H), 7.18 (s, 1H, Ar-H), 7.16 (d, J = 8.4 Hz, 1H, Ar-H), 6.40 (s, 1H, CH), 6.12 (d, J = 7.8 Hz, 1H, NH), 3.83-3.79 (m, 1H, NCH₂), 1.99-1.12 (m, 10H, 5CH₂); ¹³C NMR (CDCl₃, 150 MHz) δ (ppm) 166.4, 165.0, 139.4, 135.9, 133.7, 130.7, 129.8, 129.1, 128.6, 125.7, 125.5, 118.6, 70.8, 48.3, 32.9, 32.7, 25.4, 24.6. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₁H₂₂ClN₄O₅⁺ 413.1375; Found 413.1382.

1.3 General procedure for preparation of 3,4-dihydroquinazolines 8

To a stirred solution of azide 4 (1 mmol) in toluene (5 mL) was added dropwise triphenylphosphine (0.26 g, 1 mmol) in toluene (5 mL) at room temperature. After the reaction mixture was stirred for 2-4 h at ambient temperature, isocyanate (1 mmol) was added and the reaction mixture was stirred for 2-8 h at room temperature (for aromatic isocyanate) or 60-80 °C (for aliphatic isocyanate). Then secondary amine (1 mmol) was added and the reaction mixture was stirred for 1-6 h at room temperature. After the addition reaction was completed, the solvent was removed and CH₃CN (5 mL) with K₂CO₃ (0.136 g, 1 mmol) was
added and the mixture was left to stirred at 80 °C for 1–4 h. The solvent was removed under reduced pressure and the residual was purified by column chromatography with EtOAc/ petroleum ether to give 3,4-dihydroquinazolines 8.

**N-tert-Butyl-2-(diethylamino)-3,4-dihydro-3-phenylquinazoline-4-carboxamide (8a)**

White solid (0.317 g, yield 84%), m.p. 118-121 °C; 1H NMR (CDCl3, 600 MHz): δ (ppm) 7.31-6.96 (m, 9H, Ar-H), 5.46 (s, 1H, NH), 4.99 (s, 1H, CH), 3.57-3.55 (m, 2H, NCH2), 3.14-3.08 (m, 2H, NCH2), 1.23 (s, 9H, 3CH3), 1.01 (t, J = 6.6 Hz, 6H, 2CH3); 13C NMR (CDCl3, 150 MHz): δ (ppm) 169.5, 153.2, 146.5, 144.4, 129.1, 128.9, 126.2, 124.2, 123.3, 123.2, 122.1, 67.3, 51.3, 41.6, 41.2, 28.5, 28.1, 12.5, 12.4. Anal. Calcd for C23H23N3O: C, 72.75; H, 7.72; N, 14.67. Found: C, 72.75; H, 7.72; N, 14.67. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C23H23N3O 379.2492; Found 379.2494.

**N-tert-Butyl-3-(4-chloroamino)-2-(diethylamino)-3,4-dihydroquinazoline-4-carboxamide (8b)**

White solid (0.309 g, yield 79%), m.p. 121-123 °C; 1H NMR (CDCl3, 600 MHz): δ (ppm) 7.30-6.95 (m, 7H, Ar-H), 6.89 (d, J = 7.2 Hz, 1H, Ar-H), 5.46 (s, 1H, NH), 4.99 (s, 1H, CH), 3.62-3.56 (m, 2H, NCH2), 3.13-3.07 (m, 2H, NCH2), 2.30 (s, 3H, CH3), 1.23 (s, 9H, 3CH3), 1.01 (t, J = 6.6 Hz, 6H, 2CH3); 13C NMR (CDCl3, 150 MHz): δ (ppm) 169.5, 153.3, 146.5, 144.5, 138.9, 129.1, 128.7, 126.2, 125.0, 123.8, 123.1, 122.2, 121.2, 120.3, 67.3, 51.3, 41.7, 28.4, 21.3, 12.5. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C24H24Cl2N3O 393.2649; Found 393.2650.

**N-tert-Butyl-2-(diethylamino)-3,4-dihydro-3-m-tolyquinazoline-4-carboxamide (8c)**

White solid (0.309 g, yield 79%), m.p. 121-123 °C; 1H NMR (CDCl3, 600 MHz): δ (ppm) 7.30-6.95 (m, 8H, Ar-H), 6.89 (d, J = 7.2 Hz, 1H, Ar-H), 5.46 (s, 1H, NH), 4.95 (s, 1H, CH), 3.60-3.55 (m, 2H, NCH2), 3.12-3.06 (m, 2H, NCH2), 2.29 (s, 3H, CH3), 1.23 (s, 9H, 3CH3), 1.01 (t, J = 6.6 Hz, 6H, 2CH3); 13C NMR (CDCl3, 150 MHz): δ (ppm) 169.5, 153.3, 144.4, 144.0, 133.9, 129.4, 129.1, 126.1, 123.2, 123.1, 123.0, 122.0, 67.4, 51.2, 41.8, 28.7, 28.4, 28.1, 27.8, 21.1, 20.5, 12.7, 12.3. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C25H25N3O 393.2649; Found 393.2649.

**N-tert-Butyl-2-(diethylamino)-3,4-dihydro-3-p-tolyquinazoline-4-carboxamide (8d)**

White solid (0.281 g, yield 72%), m.p. 177-179 °C; 1H NMR (CDCl3, 600 MHz): δ (ppm) 7.28-6.97 (m, 9H, Ar-H), 5.45 (s, 1H, NH), 5.02 (s, 1H, CH), 3.38 (t, J = 7.2 Hz, 4H, 2NCH2), 1.50-1.35 (m, 6H, 3CH3), 1.24 (s, 9H, 3CH3); 13C NMR (CDCl3, 150 MHz): δ (ppm) 169.5, 153.3, 146.1, 144.2, 129.1, 128.9, 126.1, 124.0, 123.1, 122.8, 122.5, 122.2, 66.8, 51.3, 47.4, 28.3, 25.2, 24.6. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C26H25N3O 391.2492; Found 391.2491.

**N-tert-Butyl-3,4-dihydro-3-phenylquinazoline-4-carboxamide (8e)**

White solid (0.281 g, yield 72%), m.p. 177-179 °C; 1H NMR (CDCl3, 600 MHz): δ (ppm) 7.28-6.97 (m, 9H, Ar-H), 5.45 (s, 1H, NH), 5.02 (s, 1H, CH), 3.38 (t, J = 7.2 Hz, 4H, 2NCH2), 1.50-1.35 (m, 6H, 3CH3), 1.24 (s, 9H, 3CH3); 13C NMR (CDCl3, 150 MHz): δ (ppm) 169.5, 153.3, 146.1, 144.2, 129.1, 128.9, 126.1, 124.0, 123.1, 122.8, 122.5, 122.2, 66.8, 51.3, 47.4, 28.3, 25.2, 24.6. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C26H25N3O 391.2492; Found 391.2491.

**N-tert-Butyl-2-(dipropylamino)-3,4-dihydro-3-p-tolyquinazoline-4-carboxamide (8f)**

White solid (0.358 g, yield 85%), m.p. 108-109 °C; 1H NMR (CDCl3, 600 MHz): δ (ppm) 7.30-6.94 (m, 8H, Ar-H), 5.40 (s, 1H, NH), 4.94 (s, 1H, CH), 3.56-3.49 (m, 2H, NCH2), 2.87-2.83 (m, 2H, NCH2), 2.29 (s, 3H,
N-tert-Butyl-2-(dibutylamino)-3,4-dihydro-3-p-tolylquinazoline-4-carboxamide (8g)
White solid (0.309 g, yield 69%); δ (ppm) 7.30-6.95 (m, 8H, Ar-H), 5.40 (s, 1H, NH), 4.94 (s, 1H, CH), 3.62-3.58 (m, 2H, NCH₂), 2.90-2.86 (m, 2H, NCH₂), 2.29 (s, 3H, CH₃), 1.50-1.21 (m, 17H, 4CH₂ and 3CH₃), 0.87 (t, J = 7.2 Hz, 6H, 2CH₃); δ (ppm) 169.5, 153.9, 144.6, 144.3, 134.0, 129.4, 129.1, 126.2, 123.5, 123.1, 122.0, 121.9, 67.6, 51.2, 49.4, 28.3, 20.8, 20.6, 11.5. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₆H₃₃N₃O₂ 421.2961; Found 421.2962.

N-Cyclohexyl-2-(diethylamino)-3,4-dihydro-3-p-tolylquinazoline-4-carboxamide (8h)
White solid (0.296 g, yield 71%); 1H NMR (CDCl₃, 600 MHz): δ (ppm) 7.30-6.95 (m, 8H, Ar-H), 5.51 (d, J = 7.2 Hz, 1H, NH), 5.01 (s, 1H, CH), 3.70-3.65 (m, 1H, NCH), 3.57-3.54 (m, 2H, NCH₂), 3.14-3.08 (m, 2H, NCH₂), 2.30 (s, 3H, CH₃), 1.79-1.08 (m, 10H, 5CH₂), 0.99 (t, J = 6.6 Hz, 6H, 2CH₃); δ (ppm) 169.3, 153.3, 144.5, 144.0, 133.9, 129.4, 129.0, 126.0, 123.3, 123.0, 121.9, 121.7, 66.9, 48.3, 41.8, 32.3, 25.2, 24.3, 20.7, 12.5. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₆H₃₅N₃O₂ 419.2805; Found 419.2804.

N-Cyclohexyl-2-(diethylamino)-3,4-dihydro-3-phenylquinazoline-4-carboxamide (8i)
White solid (0.347 g, yield 86%); 1H NMR (CDCl₃, 600 MHz): δ (ppm) 7.29-6.96 (m, 9H, Ar-H), 5.50 (d, J = 7.8 Hz, 1H, NH), 5.06 (s, 1H, CH), 3.71-3.66 (m, 1H, NCH), 3.57-3.52 (m, 2H, NCH₂), 3.16-3.10 (m, 2H, NCH₂), 1.80-1.10 (m, 10H, 5CH₂), 1.00 (t, J = 6.6 Hz, 6H, 2CH₃); δ (ppm) 169.3, 153.2, 146.5, 144.5, 129.1, 128.9, 126.0, 124.3, 123.3, 123.2, 122.1, 121.9, 66.8, 48.4, 41.9, 32.4, 32.3, 25.3, 24.4, 12.5. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₆H₃₅N₃O₂ 405.2649; Found 405.2647.

3-(4-Chlorophenyl)-N-cyclohexyl-2-(diethylamino)-3,4-dihydroquinazoline-4-carboxamide (8j)
White solid (0.343 g, yield 78%); 1H NMR (CDCl₃, 600 MHz): δ (ppm) 7.32-6.98 (m, 8H, Ar-H), 5.43 (d, J = 7.2 Hz, 1H, NH), 5.00 (s, 1H, CH), 3.69-3.64 (m, 1H, NCH), 3.55-3.51 (m, 2H, NCH₂), 3.13-3.07 (m, 2H, NCH₂), 1.80-1.07 (m, 10H, 5CH₂), 1.01 (t, J = 7.2 Hz, 6H, 2CH₃); δ (ppm) 169.1, 152.9, 145.0, 144.4, 129.6, 129.3, 128.9, 126.0, 124.6, 123.3, 122.4, 121.7, 66.6, 48.5, 42.0, 32.8, 32.3, 24.4, 13.0, 12.2. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₆H₂₆ClN₃O₂ 439.2259; Found 439.2254.

N-Cyclohexyl-2-(diethylamino)-3,4-dihydro-3-(4-(trifluoromethoxy)phenyl)quinazoline-4-carboxamide (8k)
White solid (0.391 g, yield 80%); 1H NMR (CDCl₃, 600 MHz): δ (ppm) 7.35-7.00 (m, 8H, Ar-H), 5.43 (d, J = 7.2 Hz, 1H, NH), 5.02 (s, 1H, CH), 3.70-3.65 (m, 1H, NCH), 3.56-3.49 (m, 2H, NCH₂), 3.15-3.09 (m, 2H, NCH₂), 1.78-1.00 (m, 16H, 5CH₂ and 2CH₃); δ (ppm) 169.0, 152.9, 145.4, 145.0, 144.4, 129.3, 125.9, 124.4, 123.4, 122.4, 122.0 (q, J_F-C = 255.1
Hz), 121.6, 121.5, 66.6, 48.4, 42.0, 32.7, 32.3, 25.3, 24.4, 12.8. HRMS (ESI-TOF) m/z [M+H]^+ Calcd for C_{30}H_{32}F_{3}N_{4}O_{5}^* 489.2472; Found 489.2470.

**N-tert-butyl-3,4-dihydro-2-morpholino-3-p-tolylquinazoline-4-carboxamide (8l)**

White solid (0.284 g, yield 70%), m.p. 138-139 °C; ^1H NMR (CDCl₃, 600 MHz): δ (ppm) 7.52-7.00 (m, 8H, Ar-H), 5.45 (s, 1H, NH), 4.99 (s, 1H, CH), 3.55-3.36 (m, 8H, 2CH₂O and 2CH₂N), 2.31 (s, 3H, CH₃), 1.24 (s, 9H, 3CH₃); ^13C NMR (CDCl₃, 150 MHz): δ (ppm) 169.5, 153.2, 143.8, 143.1, 134.1, 129.6, 129.4, 129.2, 126.0, 123.3, 122.7, 122.6, 66.7, 66.3, 51.3, 46.7, 28.3, 20.7. HRMS (ESI-TOF) m/z [M+H]^+ Calcd for C_{22}H_{31}N_{5}O_{5}^* 407.2442; Found 407.2440.

**N-tert-Butyl-2-(dicyclohexylamino)-3,4-dihydro-3-p-tolylquinazoline-4-carboxamide (8n)**

White solid (0.232 g, yield 57%), m.p. 112-115 °C; ^1H NMR (CDCl₃, 600 MHz): δ (ppm) 7.59-6.91 (m, 8H, Ar-H), 5.88 (s, 0.25H, 0.25NH), 5.67 (s, 0.75H, 0.75NH), 4.82 and 4.79 (ss, 1H, CH), 2.38-2.27 (m, 5H, 2CHN and CH₃), 1.77-0.94 (m, 29H, 10CH₂ and 3CH₃); ^13C NMR (CDCl₃, 150 MHz): δ (ppm) 173.7 (minor), 169.7, 152.9, 145.4 (minor), 144.7, 143.4 (minor), 136.3 (minor), 134.6, 132.2 (minor), 130.5 (minor), 129.4, 128.8, 127.8 (minor), 126.6, 124.8, 123.4, 123.2 (minor), 122.9, 122.2, 121.7 (minor), 118.9 (minor), 71.0 (minor), 68.3, 59.7 (minor), 57.8, 51.2, 51.3, 33.8, 28.7, 28.5, 26.8, 25.7, 20.9. HRMS (ESI-TOF) m/z [M+H]^+ Calcd for C_{32}H_{33}N_{5}O_{5} 501.3586; Found 501.3586.

**7-Chloro-N-cyclohexyl-2-(diisopropylamino)-3-(4-methoxyphenyl)-3,4-dihydroquinazoline-4-carboxamide (8n)**

White solid (yield 0.269 g, 54%), mp 82-84 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.17 (s, 1H, Ar-H), 7.05 (d, J = 7.8 Hz, 2H, Ar-H), 6.92-6.88 (m, 2H, Ar-H), 6.78 (d, J = 8.4 Hz, 2H, Ar-H), 5.68 (d, J = 7.2 Hz, 1H, NH), 4.82-3.69 (m, 6H, OCH₃ and 3NCH); 1.82-1.02 (m, 22H, 5CH₂ and 4CH₃); ^13C NMR (CDCl₃, 150 MHz) δ (ppm) 169.1, 157.2, 153.0, 146.2, 139.9, 134.2, 127.5, 125.9, 122.9, 121.5, 120.2, 114.3, 67.6, 55.4, 48.5, 32.7, 32.6, 25.4, 24.6, 23.2, 19.0. HRMS (ESI-TOF) m/z [M+H]^+ Calcd for C_{32}H_{33}ClN_{5}O_{5} 497.2678; Found 497.2669.

**N,N-Dibutyl-7-chloro-2-(methyl(phenyl)amino)-3,4-dihydroquinazoline-4-carboxamide (8o)**

White solid (yield 0.277 g, 65%), mp 127-129 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.23 (t, J = 7.2 Hz, 2H, Ar-H), 7.17 (d, J = 8.4 Hz, 1H, Ar-H), 7.13 (s, 1H, Ar-H), 7.05 (d, J = 7.8 Hz, 1H, Ar-H), 6.96 (d, J = 7.2 Hz, 2H, Ar-H), 6.84 (t, J = 6.6 Hz, 1H, Ar-H), 5.08 (s, 1H, CH), 3.98 (s, 1H, NH), 3.67-3.33 (m, 4H, 2NCH₂), 2.54 (s, 3H, NCH₃), 1.57-1.06 (m, 8H, 4CH₂), 0.98 (t, J = 7.2 Hz, 3H, CH₃), 0.76 (t, J = 7.2 Hz, 3H, CH₃); ^13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.3, 149.6, 146.6, 146.1, 135.3, 130.8, 128.9, 124.9, 124.9, 123.7, 123.5, 119.5, 116.9, 71.0, 46.6, 41.7, 38.4, 31.3, 29.8, 20.2, 19.7, 13.8, 13.6. HRMS (ESI-TOF) m/z [M+H]^+ Calcd for C_{26}H_{23}ClN_{5}O_{5} 427.2259; Found 427.2261.

**2-(Benzyl(methyl)amino)-N-(tert-butyl)-3-cyclohexyl-6-methyl-3,4-dihydroquinazoline-4-carboxamide (8p)**

White solid (yield 0.329 g, 74%), mp 51-53 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.47-7.11 (m, 8H, Ar-H and NH), 7.03 (d, J = 7.8 Hz, 1H, Ar-H), 4.62 (s, 1H, CH), 3.59-3.47 (m, 3H, NCH₂ and NCH), 2.30 (s, 3H, NCH₃), 2.07 (s, 3H, CH₃), 2.00-1.24 (m, 19H, 5CH₂ and 3CH₃); ^13C NMR (CDCl₃, 150 MHz) δ (ppm) 170.9, 139.3, 137.5, 136.0, 133.9, 130.6, 129.4, 129.3, 128.5, 128.3, 127.0, 123.9, 69.0,
3-Benzyl-7-chloro-N-cyclohexyl-2-(dibenzyramino)-3,4-dihydroquinazoline-4-carboxamide (8q)

White solid (yield 0.385 g, 67%), mp 60-62 °C; $^1$H NMR (CDCl$_3$, 600 MHz) δ (ppm) 7.33-7.18 (m, 15H, Ar-H), 7.07 (d, J = 6.6 Hz, 2H, Ar-H), 6.76 (d, J = 7.8 Hz, 1H, NH), 6.52 (s, 1H, Ar-H), 4.78 (s, 1H, CH), 4.46 (d, J = 15.6 Hz, 1H, NCH$_2$), 4.28 (d, J = 15.6 Hz, 1H, NCH$_3$), 4.23-4.14 (m, 2H, NCH$_2$), 4.14 (t, J = 6.6 Hz, 1H, NCH$_3$), 3.82 (d, J = 13.8 Hz, 1H, NCH$_2$), 3.74-3.69 (m, 1H, NCH), 3.57 (d, J = 14.4 Hz, 1H, NCH$_3$), 1.86-1.02 (m, 10H, 5CH$_2$); $^{13}$C NMR (CDCl$_3$, 150 MHz) δ (ppm) 171.3, 155.0, 151.4, 139.1, 138.6, 137.9, 133.3, 130.7, 128.7, 128.6, 128.2, 127.7, 127.5, 127.4, 127.2, 126.8, 121.5, 120.8, 64.7, 54.8, 52.0, 48.8, 47.6, 33.2, 32.9, 25.5, 24.8. HRMS (ESI-TOF) m/z [M+H]$^+$ Calcd for C$_{38}$H$_{36}$N$_4$O$^+$ 577.2729; Found 577.2725.

3-(tert-Butyl)-N-cyclohexyl-2-(diethylamino)-6-methyl-3,4-dihydroquinazoline-4-carboxamide (8r)

White solid (yield 0.168 g, 42%), mp 51-52 °C; $^1$H NMR (CDCl$_3$, 600 MHz) δ (ppm) 7.53 (d, J = 7.2 Hz, 1H, NH), 7.08 (d, J = 8.4 Hz, 1H, Ar-H), 7.04 (s, 1H, Ar-H), 7.00 (d, J = 7.8 Hz, 1H, Ar-H), 4.80 (s, 1H, CH), 3.84-3.80 (m, 1H, NCH), 2.61-2.58 (m, 2H, NCH$_2$), 2.43-2.39 (m, 2H, NCH$_2$), 2.28 (s, 3H, CH$_3$), 1.90-1.26 (m, 19H, 5CH$_2$ and 3CH$_3$), 1.01 (t, J = 7.2 Hz, 5H, 5CH$_2$); 0.88 (t, J = 6.6 Hz, 1H, 1/6×2CH$_3$); $^{13}$C NMR (CDCl$_3$, 150 MHz) δ (ppm) 171.6, 137.5, 136.4, 133.8, 130.7, 129.8, 129.2, 123.5, 64.8, 57.3 (minor), 47.2 (minor), 43.8, 33.2, 33.0, 31.6, 30.1 (minor), 29.7, 29.3 (minor), 25.6, 24.7, 22.7 (minor), 21.0, 14.1 (minor), 12.5. HRMS (ESI-TOF) m/z [M+H]$^+$ Calcd for C$_{36}$H$_{38}$ClN$_4$O$^+$ 599.3118; Found 599.3110.

1.4 General procedure for preparation of 4H-3,1-benzothiazines 11

To a stirred solution of azide 4 (1 mmol) in CH$_2$Cl$_2$ (3 mL) was added dropwise triphenylphosphine (0.26 g, 1 mmol) in CH$_2$Cl$_2$ (2 mL) at room temperature. After the reaction mixture was stirred for 2–4 h at ambient temperature, CS$_2$ (0.76 g, 10 mmol) was added and the reaction mixture was stirred at 40 °C for 24 h. The solvent and excess CS$_2$ was completely removed and CH$_2$CN (5 mL) was added. Then secondary amine (1 mmol) was added and the reaction mixture was stirred for 1–6 h at room temperature. After the addition reaction was completed, K$_2$CO$_3$ (0.136 g, 1 mmol) was added and the mixture was left to stirred at 80 °C for 1–4 h. The solvent was removed under reduced pressure and the residual was purified by column chromatography with EtOAc/ petroleum ether to give 4H-3,1-benzothiazines 11.

*N-(tert-Butyl)-2-(diethylamino)-4H-3,1-benzothiazine-4-carboxamide (11a)*

White solid (yield 0.262 g, 82%), mp 136-138 °C; $^1$H NMR (CDCl$_3$, 600 MHz) δ (ppm) 7.29 (t, J = 7.2 Hz, 1H, Ar-H), 7.14 (d, J = 7.2 Hz, 2H, Ar-H), 7.01 (t, J = 6.6 Hz, 1H, Ar-H), 5.49 (s, 1H, NH), 4.46 (s, 1H, CH), 3.80-3.50 (m, 4H, 2×NCH$_2$), 1.23 (t, J = 7.2 Hz, 6H, 2CH$_3$), 1.20 (s, 9H, 3CH$_3$); $^{13}$C NMR (CDCl$_3$, 150 MHz) δ (ppm) 168.4, 152.7, 145.7, 129.3, 127.5, 125.2, 122.9, 118.0, 51.4, 48.5, 43.7, 28.3, 14.1. HRMS (ESI-TOF) m/z [M+H]$^+$ Calcd for C$_{17}$H$_{20}$N$_3$S$^+$ 320.1791; Found 320.1785.

*N-(tert-Butyl)-2-(piperidin-1-yl)-4H-3,1-benzothiazine-4-carboxamide (11b)*

White solid (yield 0.274 g, 83%), mp 141-142 °C; $^1$H NMR (CDCl$_3$, 600 MHz) δ (ppm) 7.30 (t, J = 7.8 Hz, 1H, Ar-H), 7.14 (d, J = 7.8 Hz, 2H, Ar-H), 7.04 (t, J = 7.8 Hz, 1H, Ar-H), 5.51 (s, 1H, NH), 4.50 (s, 1H, CH), 3.83-3.73 (m, 4H, 2×NCH$_2$), 1.71-1.59 (m, 6H, 3CH$_2$), 1.22 (s, 9H, 3CH$_3$); $^{13}$C NMR (CDCl$_3$, 150 MHz) δ (ppm) 168.3, 153.7, 145.4,
129.3, 127.5, 125.3, 123.3, 118.1, 51.4, 48.5, 48.0, 28.3, 26.0, 24.9. HRMS (ESI-TOF) m/z [M+H]+ Ccalc for C_{18}H_{26}N_{3}O_{3}S^{+} 332.1791; Found 332.1788.

**N-(tert-Butyl)-2-morpholino-4H-3,1-benzothiazine-4-carboxamide (1c)**

White solid (yield 0.279 g, 84%), mp 157-159 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.32 (t, J = 7.8 Hz, 1H, Ar-H), 7.16 (d, J = 7.8 Hz, 2H, Ar-H), 7.09 (t, J = 7.8 Hz, 1H, Ar-H), 5.43 (s, 1H, NH), 4.52 (s, 1H, CH), 3.83-3.73 (m, 8H, 4CH₂), 1.22 (s, 9H, 3CH₃); ^13C NMR (CDCl₃, 150 MHz) δ (ppm) 167.9, 154.4, 144.8, 129.5, 127.5, 125.5, 124.0, 118.3, 66.7, 51.5, 48.4, 47.4, 28.3. HRMS (ESI-TOF) m/z [M+H]+ Ccalc for C_{17}H_{22}N_{3}O_{3}S^{+} 334.1584; Found 334.1582.

**N-Butyl-2-morpholino-4H-3,1-benzothiazine-4-carboxamide (1d)**

White solid (yield 0.259 g, 78%), mp 123-125 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.34 (t, J = 7.2 Hz, 1H, Ar-H), 7.18-7.15 (m, 2H, Ar-H), 7.10 (t, J = 7.2 Hz, 1H, Ar-H), 5.50 (s, 1H, NH), 4.63 (s, 1H, CH), 3.84-3.73 (m, 8H, 4CH₂), 3.20-3.03 (m, 2H, NCH₂), 1.36-1.32 (m, 2H, CH₂), 1.24-1.19 (m, 2H, CH₂), 0.86 (t, J = 7.8 Hz, 3H, CH₃); ^13C NMR (CDCl₃, 150 MHz) δ (ppm) 169.0, 154.6, 144.9, 129.7, 127.7, 125.6, 124.1, 117.5, 66.6, 47.4, 47.2, 39.6, 31.3, 19.7, 13.7. HRMS (ESI-TOF) m/z [M+H]+ Ccalc for C_{17}H_{22}N_{3}O_{3}S^{+} 334.1584; Found 334.1581.

**N-Cyclohexyl-2-(pyrrolidin-1-yl)-4H-3,1-benzothiazine-4-carboxamide (1e)**

White solid (yield 0.265 g, 77%), mp 148-150 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.30 (t, J = 7.8 Hz, 1H, Ar-H), 7.16 (d, J = 7.8 Hz, 1H, Ar-H), 7.12 (d, J = 7.2 Hz, 1H, Ar-H), 7.01 (t, J = 7.8 Hz, 1H, Ar-H), 5.55 (d, J = 6.6 Hz, 1H, NH), 4.53 (s, 1H, CH), 3.76-3.56 (m, 5H, 2xNCH₂ and NCH), 1.98-1.94 (m, 4H, 2CH₂), 1.71-0.96 (m, 10H, 5CH₂); ^13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.5, 151.9, 145.7, 129.5, 127.7, 125.3, 122.9, 117.2, 48.1, 48.0, 47.6, 32.2, 25.3, 25.0, 24.1. HRMS (ESI-TOF) m/z [M+H]+ Ccalc for C_{19}H_{28}N_{5}O_{5}S^{+} 344.1791; Found 344.1785.

**2-(Benzyl(methylamino)-N-cyclohexyl-4H-3,1-benzothiazine-4-carboxamide (1f)**

White solid (yield 0.311 g, 79%), mp 120-121 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.31-7.15 (m, 8H, Ar-H), 7.06 (t, J = 7.2 Hz, 1H, Ar-H), 5.48 (d, J = 6.6 Hz, 1H, NH), 5.00 (d, J = 15.0 Hz, 1H, NCH₂), 4.73 (d, J = 15.6 Hz, 1H, NCH₂), 4.60 (s, 1H, CH), 3.69-3.64 (m, 1H, NCH), 3.16 (s, 3H, NCH₃), 1.73-0.92 (m, 10H, 5CH₂); ^13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.2, 154.4, 145.6, 137.3, 129.5, 128.6, 127.5, 127.4, 125.5, 123.4, 117.4, 54.2, 48.4, 47.8, 36.5, 32.3, 25.3, 24.3. HRMS (ESI-TOF) m/z [M+H]+ Ccalc for C_{23}H_{38}N_{5}O_{5}S^{+} 394.1948; Found 394.1945.

**N-Cyclohexyl-2-(diethylamino)-6-methyl-4H-3,1-benzothiazine-4-carboxamide (1g)**

White solid (yield 0.258 g, 72%), mp 142-143 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.10 (d, J = 7.8 Hz, 1H, Ar-H), 7.04 (d, J = 8.4 Hz, 1H, Ar-H), 6.94 (s, 1H, Ar-H), 5.52 (d, J = 6.0 Hz, 1H, NH), 4.49 (s, 1H, CH), 3.75-3.48 (m, 5H, 2xNCH₂ and NCH), 2.31 (s, 3H, CH₃), 1.73-1.26 (m, 7H, 7/10x5CH₂), 1.20 (t, J = 7.2 Hz, 6H, 2CH₃), 1.11-0.93 (m, 3H, 3/10x5CH₂); ^13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.6, 152.2, 143.4, 132.6, 130.2, 127.9, 125.1, 117.3, 48.2, 47.7, 43.6, 32.4, 32.3, 25.4, 24.3, 20.8, 14.1. HRMS (ESI-TOF) m/z [M+H]+ Ccalc for C_{25}H_{38}N_{5}O_{5}S^{+} 360.2104; Found 360.2098.

**N-Butyl-6-methyl-2-(piperidin-1-yl)-4H-3,1-benzothiazine-4-carboxamide (1h)**

White solid (yield 0.279 g, 81%), mp 135-136 °C; ^1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.12 (d, J = 7.8 Hz, 1H, Ar-H), 7.05 (d, J = 8.4 Hz, 1H, Ar-H), 6.94 (s, 1H, Ar-H), 5.59 (s, 1H, NH), 4.55 (s, 1H, CH), 3.77-3.71 (m, 4H, 2xNCH₂), 3.27-2.98 (m, 2H, NCH₂), 2.32 (s, 3H, CH₃), 1.68-1.58 (m, 6H, 3CH₂), 1.08-0.92 (m, 2H, 4NCH₂)
N-Cyclohexyl-2-(dibenzylamino)-6-methyl-4H-3,1-benzothiazine-4-carboxamide (11i)

White solid (yield 0.377 g, 78%), mp 156-158 °C; 1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.32-7.25 (m, 10H, Ar-H), 7.14 (d, J = 7.8 Hz, 1H, Ar-H), 7.10 (d, J = 8.4 Hz, 1H, Ar-H), 6.98 (s, 1H, Ar-H), 5.47 (d, J = 7.8 Hz, 1H, NH), 5.10 (s, 2H, NCH₂), 4.57 (s, 1H, CH), 4.54 (d, J = 16.2 Hz, 2H, NCH₂), 3.69-3.65 (m, 1H, NCH), 2.34 (s, 3H, CH₃), 1.78-0.92 (m, 10H, 5CH₂); 13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.4, 154.0, 143.1, 137.5, 133.3, 130.3, 128.5, 128.0, 127.7, 127.3, 125.7, 117.3, 51.1, 48.6, 48.0, 32.5, 32.4, 25.3, 24.5, 20.9. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₉₁H₂₈N₂O₅S+ 346.1948; Found 346.1945.

N-(tert-Butyl)-2-(dipropylamino)-6-methyl-4H-3,1-benzothiazine-4-carboxamide (11j)

White solid (yield 0.271 g, 75%), mp 156-157 °C; 1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.09 (d, J = 7.8 Hz, 1H, Ar-H), 7.02 (d, J = 7.8 Hz, 1H, Ar-H), 6.93 (s, 1H, Ar-H), 5.50 (s, 1H, NH), 4.41 (s, 1H, CH), 3.67-3.62 (m, 2H, NCH₂), 3.40-3.36 (m, 2H, NCH₂), 2.31 (s, 3H, CH₃), 1.69-1.62 (m, 4H, 2CH₂), 1.20 (s, 9H, 3CH₃), 0.93 (t, J = 7.2 Hz, 6H, 2CH₃); 13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.6, 152.6, 143.2, 132.5, 130.0, 127.9, 125.1, 117.6, 51.3, 51.1, 48.6, 48.0, 32.5, 32.4, 25.3, 24.5, 20.9. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₀H₂₃N₂O₅S+ 484.2417; Found 484.2411.

7-Chloro-N-cyclohexyl-2-(diethylamino)-4H-3,1-benzothiazine-4-carboxamide (11k)

White solid (yield 0.315 g, 83%), mp 162-164 °C; 1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.15 (s, 1H, Ar-H), 7.06 (d, J = 8.4 Hz, 1H, Ar-H), 6.98 (d, J = 7.8 Hz, 1H, Ar-H), 5.49 (d, J = 6.0 Hz, 1H, NH), 4.53 (s, 1H, CH), 3.74-3.48 (m, 5H, 2×NCH₂ and NCH), 1.74-1.29 (m, 7H, 7/10×5CH₂), 1.21 (t, J = 7.2 Hz, 6H, 2CH₃), 1.12-0.94 (m, 3H, 3/10×5CH₂); 13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.0, 153.5, 147.1, 134.7, 128.4, 125.0, 122.7, 116.0, 48.4, 47.1, 43.9, 32.4, 32.3, 25.3, 24.3, 14.0. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₁₉₂H₂₇ClN₂O₅S+ 380.1558; Found 380.1554.

N-(tert-Butyl)-7-chloro-2-(dicyclohexylamino)-4H-3,1-benzothiazine-4-carboxamide (11l)

White solid (yield 0.249 g, 54%), mp 118-120 °C; 1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.12 (s, 1H, Ar-H), 7.05 (d, J = 7.8 Hz, 1H, Ar-H), 6.97 (d, J = 7.8 Hz, 1H, Ar-H), 5.58 (s, 1H, NH), 4.41 (s, 1H, CH), 3.80-3.67 (m, 2H, 2CH₂), 2.21-1.15 (m, 29H, 10CH₂ and 3CH₃); 13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.2, 152.5, 146.6, 134.4, 128.4, 124.6, 122.6, 116.6, 59.1, 51.5, 48.3, 32.0, 30.7, 28.4, 26.3, 26.2, 25.4. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₅H₂₃ClN₂O₅S+ 462.2340; Found 462.2336.

N-Cyclohexyl-2-(diisopropylamino)-6-methyl-4H-3,1-benzothiazine-4-carboxamide (11m)

White solid (yield 0.186 g, 48%), mp 168-169 °C; 1H NMR (CDCl₃, 600 MHz) δ (ppm) 7.09 (d, J = 7.8 Hz, 1H, Ar-H), 7.03 (d, J = 8.4 Hz, 1H, Ar-H), 6.92 (s, 1H, Ar-H), 5.61 (d, J = 6.6 Hz, 1H, NH), 4.48 (s, 1H, CH), 4.23-4.18 (m, 2H, 2CH₂), 3.69-3.64 (m, 1H, NCH), 2.31 (s, 3H, CH₃), 1.78-0.94 (m, 22H, 5CH₂ and 4CH₂); 13C NMR (CDCl₃, 150 MHz) δ (ppm) 168.8, 150.9, 143.0, 132.6, 130.0, 127.8, 125.0, 117.5, 49.0, 48.2, 48.0, 32.5, 32.3, 25.4, 24.3, 22.1, 20.8. HRMS (ESI-TOF) m/z [M+H]+ Calcd for C₂₂H₃₄N₂O₅S+ 388.2417; Found 388.2412.
**N-Cyclohexyl-2-(methyl(phenyl)amino)-4H-3,1-benzothiazine-4-carboxamide (11n)**

White solid (yield 0.212 g, 56%), mp 194-196 °C; $^1$H NMR (CDCl$_3$, 600 MHz) $\delta$ (ppm) 7.41 (t, $J$ = 7.8 Hz, 2H, Ar-H), 7.34 (t, $J$ = 7.8 Hz, 2H, Ar-H), 7.25-7.10 (m, 3H, Ar-H), 7.17 (d, $J$ = 7.2 Hz, 1H, Ar-H), 7.09 (t, $J$ = 7.2 Hz, 1H, Ar-H), 5.64 (d, $J$ = 6.0 Hz, 1H, NH), 4.47 (s, 1H, CH), 3.70-3.66 (m, 1H, NCH), 3.56 (s, 3H, NCH$_3$), 1.81-0.99 (m, 10H, 5CH$_2$); $^{13}$C NMR (CDCl$_3$, 150 MHz) $\delta$ (ppm) 167.9, 153.2, 144.9, 144.0, 129.3, 128.6, 127.8, 127.6, 125.5, 123.9, 118.2, 48.3, 48.0, 39.7, 32.4, 25.4, 24.3. HRMS (ESI-TOF) m/z [M+H]$^+$ Calcd for C$_{22}$H$_{26}$N$_3$OS$^+$ 380.1791; Found 380.1785.

**N-Cyclohexyl-6-methyl-2-(methyl(phenyl)amino)-4H-3,1-benzothiazine-4-carboxamide (11o)**

White solid (yield 0.201 g, 51%), mp 207-208 °C; $^1$H NMR (CDCl$_3$, 600 MHz) $\delta$ (ppm) 7.40 (t, $J$ = 7.2 Hz, 2H, Ar-H), 7.32 (t, $J$ = 7.2 Hz, 1H, Ar-H), 7.22-7.14 (m, 4H, Ar-H), 6.97 (s, 1H, Ar-H), 5.69 (d, $J$ = 5.4 Hz, 1H, NH), 4.41 (s, 1H, CH), 3.70-3.66 (m, 1H, NCH), 3.54 (s, 3H, NCH$_3$), 2.33 (s, 3H, CH$_3$), 1.81-1.01 (m, 10H, 5CH$_2$); $^{13}$C NMR (CDCl$_3$, 150 MHz) $\delta$ (ppm) 168.0, 152.5, 144.1, 142.5, 133.6, 130.1, 129.3, 128.3, 127.6, 127.4, 125.3, 117.9, 48.3, 48.1, 39.7, 32.4, 25.4, 24.3, 20.8. HRMS (ESI-TOF) m/z [M+H]$^+$ Calcd for C$_{23}$H$_{28}$N$_3$OS$^+$ 394.1948; Found 394.1942.

1.5 Reference

2. Copies of $^1$H and $^{13}$C NMR spectrum of compound 4, 8 and 11

![NMR Spectra](image)

**CDCl$_3$, 600 MHz**

**CDCl$_3$, 150 MHz**
\[\text{CDCl}_3, 600 \text{ MHz}\]

\[\text{CDCl}_3, 150 \text{ MHz}\]
The image contains detailed spectra data for two different spectrometers: CDCl₃, 600 MHz and CDCl₃, 150 MHz. The spectra include peak positions in ppm and chemical shifts. The structures labeled as 8h are shown on the left side of the spectra, indicating the positions of the protons or other nuclei in the molecule.
**11a**

CDCl$_3$, 600 MHz

![NMR Spectra](image)

**11a**

CDCl$_3$, 150 MHz

![NMR Spectra](image)
CDCl₃, 600 MHz

CDCl₃, 150 MHz
CDCl₃, 600 MHz

CDCl₃, 150 MHz