



Supporting Information

for

Combining the Ugi-azide multicomponent reaction and rhodium(III)-catalyzed annulation for the synthesis of tetrazole-isoquinolone/pyridone hybrids

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Experimental procedures and compound characterization data

Synthesis and characterization of intermediates and final compounds

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide (1)

TrtNH₂ (2.0 mmol, 519 mg) × 5, (CH₂O)_n (3.0 mmol, 90.1 mg) × 5, CyNC (2.2 mmol, 240 mg, 274 µL) × 5, TMSN₃ (2.2 mmol, 253 mg, 292 µL) × 5, TFA (20.0 mmol, 2.28 g, 1.53 mL), benzoic acid (10 mmol, 1.22 g), TEA (50 mmol, 5.05 g, 6.97 mL), HBTU (10 mmol, 3.79 mg) and DMAP (1.0 mmol, 122 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1a** as a white solid (2.50 g, 88%). R_f = 0.14 (heptane/AcOEt, 1:1); mp 136-138 °C; FT-IR (KBr) ν 3272 (N-H), 1659 (C=O); ¹H NMR (600 MHz, CDCl₃) δ 8.02 (t, *J* = 5.7 Hz, 1H), 7.91 – 7.84 (m, 2H), 7.51 (t, *J* = 7.4 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 4.95 (d, *J* = 5.8 Hz, 2H), 4.62 (tt, *J* = 11.4, 4.2 Hz, 1H), 2.05 – 1.91 (m, 6H), 1.76 (dt, *J* = 13.7, 3.4 Hz, 1H), 1.47 (dddd, *J* = 17.0, 13.2, 8.4, 3.7 Hz, 2H), 1.32 (dddd, *J* = 16.7, 13.1, 8.3, 3.7 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 167.68 (C), 151.78 (C), 132.99 (C), 132.06 (CH), 128.65 (CH), 127.27 (CH), 58.16 (CH), 32.96 (CH₂), 32.53 (CH₂), 25.15 (CH₂), 24.83 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₅H₂₀N₅O 286.1668, Found 286.1662.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-2-methylbenzamide (1b)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 µL), TMSN₃ (2.2 mmol, 253 mg, 292 µL), TFA (4.0 mmol, 456 mg, 306 µL), *o*-methylbenzoic acid (2.0 mmol, 272 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1b** as a light yellow solid (597 mg, 99%). R_f = 0.22 (heptane/AcOEt, 1:1); mp 135-138 °C; FT-IR (KBr) ν 3291 (N-H), 1645 (C=O); ¹H NMR (600 MHz, CDCl₃) δ 7.41 (d, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.25 – 7.18 (m, 2H), 7.08 (t, *J* = 5.8 Hz, 1H), 4.90 (d, *J* = 5.8 Hz, 2H), 4.59 (ddd, *J* = 11.2, 6.8, 4.3 Hz, 1H), 2.44 (s, 3H), 2.09 – 1.95 (m, 6H), 1.83 – 1.78 (m, 1H), 1.56 – 1.46 (m, 2H), 1.39 – 1.30 (m, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 170.09 (C), 151.32 (C), 136.54 (C), 134.58 (C), 131.27 (CH), 130.57 (CH), 126.95 (CH), 125.90 (CH), 58.13 (CH), 32.96 (CH₂), 32.56 (CH₂), 25.19 (CH₂), 24.81 (CH₂); 19.89 (CH₃); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₆H₂₂N₅O 300.1819, Found 300.1819.

2-Bromo-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide, (1c)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μ L), TMSN₃ (2.2 mmol, 253 mg, 292 μ L), TFA (4.0 mmol, 456 mg, 306 μ L), *o*-bromobenzoic acid (2.0 mmol, 330 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1c** as a salmon-colored solid (549 mg, 75%). R_f = 0.28 (heptane/AcOEt, 1:2); mp 164-166 °C; FT-IR (KBr) ν 3249 (N-H), 1659 (C=O); ¹H NMR (600 MHz, CDCl₃) δ 7.60 (d, *J* = 8.0 Hz, 1H), 7.53 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.33 – 7.27 (m, 2H), 4.94 (d, *J* = 5.8 Hz, 2H), 4.62 (tt, *J* = 11.5, 4.1 Hz, 1H), 2.11 – 1.94 (m, 6H), 1.83 – 1.78 (m, 1H), 1.52 (qt, *J* = 13.2, 3.9 Hz, 2H), 1.35 (ddt, *J* = 16.6, 13.1, 6.6 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 167.87 (C), 150.92 (C), 136.34 (C), 133.57 (CH), 131.83 (CH), 129.47 (CH), 127.66 (CH), 119.38 (C), 58.20 (CH), 33.00 (CH₂), 32.62 (CH₂), 25.20 (CH₂), 24.82 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₅H₁₉BrN₅O 364.0768, Found 364.0756.

2-Chloro-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide (1d)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μ L), TMSN₃ (2.2 mmol, 253 mg, 292 μ L), TFA (4.0 mmol, 456 mg, 306 μ L), *o*-chlorobenzoic acid (2.0 mmol, 313 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1d** as a white solid (496 mg, 78%). R_f = 0.28 (heptane/AcOEt, 1:2); mp 161-164 °C; FT-IR (KBr) ν 3253 (N-H), 1661 (C=O); ¹H NMR (600 MHz, CDCl₃) δ 7.64 (d, *J* = 7.6 Hz, 1H), 7.47 – 7.37 (m, 3H), 7.36 – 7.31 (m, 1H), 4.95 (d, *J* = 5.7 Hz, 2H), 4.60 (tt, *J* = 11.4, 4.3 Hz, 1H), 2.10 – 1.93 (m, 6H), 1.82 – 1.30 (m, 1H), 1.51 (dtd, *J* = 17.0, 13.2, 4.1 Hz, 2H), 1.35 (dddd, *J* = 17.0, 13.4, 8.5, 3.8 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 166.80 (C), 150.98 (C), 133.71 (C), 131.89 (CH); 130.90 (C), 130.44 (CH), 129.98 (CH), 127.18 (CH), 58.18 (CH), 32.97 (CH₂), 32.70 (CH₂), 25.19 (CH₂), 24.82 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₅H₁₉ClN₅O 320.1273, Found 320.1267.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-2-methoxybenzamide (1e)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μ L), TMSN₃ (2.2 mmol, 253 mg, 292 μ L), TFA (4.0 mmol, 456 mg, 306 μ L), *o*-anisic acid (2.0 mmol, 304 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound

1e as a white solid (544 mg, 86%). $R_f = 0.24$ (heptane/AcOEt, 1:2); mp 119-122 °C; FT-IR (KBr) ν 3342 (N-H), 1636 (C=O); ^1H NMR (400 MHz, CDCl_3) δ 8.64 (t, $J = 5.9$ Hz, 1H), 8.20 (dd, $J = 7.8, 1.9$ Hz, 1H), 7.57 – 7.40 (m, 1H), 7.09 (t, $J = 7.6$ Hz, 1H), 6.99 (d, $J = 8.4$ Hz, 1H), 4.97 (d, $J = 5.7$ Hz, 2H), 4.66 – 4.52 (m, 1H), 3.98 (s, 3H), 2.05 – 1.87 (m, 6H), 1.75 (dt, $J = 13.0, 3.4$ Hz, 1H), 1.54 – 1.39 (m, 2H), 1.32 (tt, $J = 12.8, 3.4$ Hz, 1H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 165.52 (C), 157.70 (C), 151.70 (C), 133.58 (CH), 132.31 (CH_2), 121.33 (CH), 120.10 (C), 111.44 (CH), 58.00 (CH), 56.07 (CH_3), 32.93 (CH_2), 32.51 (CH_2), 25.18 (CH_2), 24.85 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{22}\text{N}_5\text{O}_2$ 316.1768, Found 316.1773.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-4-methoxybenzamide (1f)

TrtNH_2 (2.0 mmol, 519 mg), $(\text{CH}_2\text{O})_n$ (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN_3 (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), *p*-anisic acid (2.0 mmol, 304 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1f** as a white solid (563 mg, 89%). $R_f = 0.22$ (heptane/AcOEt, 1:2); mp 171-174 °C; FT-IR (KBr) ν 3300 (N-H), 1643 (C=O); ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 7.94 (t, $J = 5.8$ Hz, 1H), 7.85 (d, $J = 8.4$ Hz, 2H), 6.88 (d, $J = 8.5$ Hz, 2H), 4.92 (d, $J = 5.8$ Hz, 2H), 4.61 (tt, $J = 11.1, 4.4$ Hz, 1H), 3.83 (s, 3H), 2.07 – 1.88 (m, 6H), 1.75 (dt, $J = 13.1, 3.5$ Hz, 1H), 1.46 (qt, $J = 12.9, 3.9$ Hz, 2H), 1.31 (tt, $J = 13.1, 3.6$ Hz, 1H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, $\text{DMSO-}d_6$) δ 167.17 (C), 162.62 (C), 151.99 (C), 129.19 (CH), 125.26 (C), 113.84 (CH), 58.14 (CH), 55.41 (CH_3), 32.97 (CH_2), 32.48 (CH_2), 25.16 (CH_2), 24.85 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{22}\text{N}_5\text{O}_2$ 316.1768, Found 316.1763.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-4-methylbenzamide (1g)

TrtNH_2 (4.0 mmol, 1.04 g), $(\text{CH}_2\text{O})_n$ (6.0 mmol, 180 mg), CyNC (4.4 mmol, 480 mg, 548 μL), TMSN_3 (4.4 mmol, 506 mg, 584 μL), TFA (8.0 mmol, 912 mg, 612 μL), *p*-toluic acid (4.0 mmol, 608 mg), TEA (20 mmol, 2.02 g, 2.78 mL), HBTU (4.0 mmol, 1.52 g) and DMAP (0.4 mmol, 48.8 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1g** as a white solid (1.02 g, 85%). $R_f = 0.20$ (heptane/AcOEt, 1:1); mp 172-174 °C; FT-IR (KBr) ν 3356 (N-H), 1650 (C=O); ^1H NMR (400 MHz, CDCl_3) δ 7.89 (t, $J = 5.8$ Hz, 1H), 7.76 (d, $J = 7.9$ Hz, 2H), 7.20 (d, $J = 7.9$ Hz, 2H), 4.93 (d, $J = 5.8$ Hz, 2H), 4.60 (tt, $J = 10.7, 4.5$ Hz, 1H), 2.37 (s, 3H), 2.03 – 1.96 (m, 3H), 1.96 – 1.86 (m, 3H), 1.75 (dt, $J = 13.4, 3.3$ Hz, 1H), 1.46 (qt, $J = 12.8,$

4.0 Hz, 2H), 1.31 (tt, $J = 12.9, 3.5$ Hz, 1H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 167.60 (C), 151.83 (C), 142.59 (C), 130.17 (C), 129.31 (CH), 127.26 (CH), 58.12 (CH), 32.95 (CH_2), 32.48 (CH_2), 25.15 (CH_2), 24.84 (CH_2), 21.47 (CH_3); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{22}\text{N}_5\text{O}$ 300.1819, Found 300.1812.

4-Chloro-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide (1h)

TrtNH_2 (2.0 mmol, 519 mg), $(\text{CH}_2\text{O})_n$ (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN_3 (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), *p*-chlorobenzoic acid (2.0 mmol, 313 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1h** as a white solid (523 mg, 82%). $R_f = 0.24$ (heptane/AcOEt, 1:1); mp 180-182 $^\circ\text{C}$; FT-IR (KBr) ν 3341 (N-H), 1655 (C=O); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 9.37 (t, $J = 5.8$ Hz, 1H), 7.90 (d, $J = 8.1$ Hz, 2H), 7.57 (d, $J = 8.2$ Hz, 2H), 4.83 (d, $J = 5.5$ Hz, 2H), 4.61 (tt, $J = 11.4, 3.9$ Hz, 1H), 1.99 (dt, $J = 9.7, 4.3$ Hz, 2H), 1.79 (qd, $J = 12.0, 11.6, 3.5$ Hz, 4H), 1.67 (d, $J = 12.8$ Hz, 1H), 1.39 (qd, $J = 13.6, 11.9, 6.8$ Hz, 2H), 1.32 – 1.21 (m, 1H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, $\text{DMSO}-d_6$) δ 165.95 (C), 152.77 (C), 137.03 (C), 132.55 (C), 129.68 (CH), 129.04 (CH), 57.18 (CH), 32.92 (CH_2), 32.84 (CH_2), 25.16 (CH_2), 25.00 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{15}\text{H}_{19}\text{ClN}_5\text{O}$ 320.1273, Found 320.1258.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-4-(trifluoromethyl)benzamide (1i)

TrtNH_2 (2.0 mmol, 519 mg), $(\text{CH}_2\text{O})_n$ (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN_3 (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), 4-trifluoromethylbenzoic acid (2.0 mmol, 380 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1i** as a white solid (547 mg, 77%). $R_f = 0.28$ (heptane/AcOEt, 1:1); mp 171-174 $^\circ\text{C}$; FT-IR (KBr) ν 3321 (N-H), 1659 (C=O); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 9.54 (t, $J = 5.6$ Hz, 1H), 8.08 (d, $J = 8.0$ Hz, 2H), 7.88 (d, $J = 8.1$ Hz, 2H), 4.87 (d, $J = 5.6$ Hz, 2H), 4.62 (tt, $J = 11.3, 4.0$ Hz, 1H), 2.06 – 1.96 (m, 2H), 1.89 – 1.74 (m, 4H), 1.71 – 1.63 (m, 1H), 1.39 (qd, $J = 12.0, 10.5, 6.7$ Hz, 2H), 1.26 (tt, $J = 12.5, 2.9$ Hz, 1H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO}-d_6$) δ 165.85 (C), 152.67 (C), 137.55 (C), 132.00 (q, $J = 31.9$ Hz, CF_3), 128.68 (CH), 127.03 (C), 125.97 (q, $J = 3.8$ Hz, CH), 125.22 (C), 123.41 (C), 121.61 (C), 57.19 (CH), 32.91 (CH_2), 25.14 (CH_2),

24.98 (CH₂); ¹⁹F {¹³C} NMR (376 MHz, CDCl₃) δ -56.71; HRMS (ESI/TOF) m/z: [M + H]⁺ Calcd for C₁₆H₁₉F₃N₅O 354.1536, Found 354.1520.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3-methylbenzamide (1j)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN₃ (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), *m*-toluic acid (2.0 mmol, 272 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1j** as a white solid (467 mg, 78%). R_f = 0.24 (heptane/AcOEt, 1:1); mp 122-124 °C; FT-IR (KBr) ν 3276 (N-H), 1635 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 7.94 (t, *J* = 5.8 Hz, 1H), 7.67 (s, 1H), 7.66 – 7.60 (m, 1H), 7.29 (d, *J* = 7.0 Hz, 2H), 4.93 (d, *J* = 5.8 Hz, 2H), 4.61 (tt, *J* = 11.0, 4.5 Hz, 1H), 2.35 (s, 3H), 2.00 (dd, *J* = 11.7, 3.5 Hz, 3H), 1.97 – 1.88 (m, 3H), 1.76 (dt, *J* = 13.2, 3.3 Hz, 1H), 1.47 (qt, *J* = 12.9, 4.0 Hz, 2H), 1.32 (tt, *J* = 12.8, 3.5 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 167.86 (C), 151.78 (C), 138.53 (C), 132.94 (C), 132.81 (CH), 128.53 (CH), 127.93 (CH), 124.25 (CH), 58.15 (CH), 32.96 (CH₂), 32.54 (CH₂), 25.16 (CH₂), 24.84 (CH₂), 21.27 (CH₃); HRMS (ESI/TOF) m/z: [M + H]⁺ Calcd for C₁₆H₂₂N₅O 300.1819, Found 300.1812.

3-Chloro-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide (1k)

TrtNH₂ (4.0 mmol, 1.04 g), (CH₂O)_n (6.0 mmol, 180 mg), CyNC (4.4 mmol, 480 mg, 548 μL), TMSN₃ (4.4 mmol, 506 mg, 584 μL), TFA (8.0 mmol, 912 mg, 612 μL), *m*-chlorobenzoic acid (4.0 mmol, 626 mg), TEA (20 mmol, 2.02 g, 2.78 mL), HBTU (4.0 mmol, 1.52 g) and DMAP (0.4 mmol, 48.8 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1k** as a light yellow solid (1.05 g, 82%). R_f = 0.22 (heptane/AcOEt, 1:1); mp 140-143 °C; FT-IR (KBr) ν 3268 (N-H), 1658 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 8.21 (t, *J* = 5.8 Hz, 1H), 7.85 (d, *J* = 1.9 Hz, 1H), 7.73 (d, *J* = 7.7 Hz, 1H), 7.46 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.33 (t, *J* = 7.9 Hz, 1H), 4.92 (d, *J* = 5.8 Hz, 2H), 4.64 – 4.53 (m, 1H), 2.03 (td, *J* = 11.2, 10.3, 4.5 Hz, 3H), 1.99 – 1.90 (m, 3H), 1.77 (dt, *J* = 13.2, 3.3 Hz, 1H), 1.48 (qt, *J* = 12.8, 4.1 Hz, 2H), 1.33 (tt, *J* = 12.7, 3.4 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 166.36 (C), 151.67 (C), 134.88 (C), 134.64 (C), 132.09 (CH), 129.94 (CH), 127.78 (CH), 125.19 (CH), 58.29 (CH), 32.95 (CH₂), 32.68 (CH₂), 25.17 (CH₂), 24.81 (CH₂); HRMS (ESI/TOF) m/z: [M + H]⁺ Calcd for C₁₅H₁₉ClN₅O 320.1273, Found 320.1266.

3-Bromo-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide (1l)

TrtNH₂ (4.0 mmol, 1.04 g), (CH₂O)_n (6.0 mmol, 180 mg), CyNC (4.4 mmol, 480 mg, 548 µL), TMSN₃ (4.4 mmol, 506 mg, 584 µL), TFA (8.0 mmol, 912 mg, 612 µL), *m*-bromobenzoic acid (4.0 mmol, 804 mg), TEA (20 mmol, 2.02 g, 2.78 mL), HBTU (4.0 mmol, 1.52 g) and DMAP (0.4 mmol, 48.8 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1l** as a light yellow solid (1.20 g, 82%). R_f = 0.22 (heptane/AcOEt, 1:1); mp 131-134 °C; FT-IR (KBr) ν 3237 (N-H), 1636 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 8.23 (t, *J* = 5.8 Hz, 1H), 8.00 (s, 1H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.61 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.26 (t, *J* = 7.9 Hz, 1H), 4.92 (d, *J* = 5.8 Hz, 2H), 4.59 (tt, *J* = 10.4, 4.6 Hz, 1H), 2.07 – 1.92 (m, 6H), 1.77 (dt, *J* = 13.0, 3.5 Hz, 1H), 1.48 (qt, *J* = 12.7, 4.1 Hz, 2H), 1.33 (tt, *J* = 12.8, 3.5 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 166.25 (C), 151.68 (C), 135.00 (CH), 134.81 (C), 130.67 (CH), 130.18 (CH), 125.67 (CH), 122.86 (C), 58.29 (CH), 32.95 (CH₂), 32.67 (CH₂), 25.17 (CH₂), 24.81 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₅H₁₉BrN₅O 364.0768, Found 364.0762.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3-iodobenzamide (**1m**)

TrtNH₂ (4.0 mmol, 1.04 g), (CH₂O)_n (6.0 mmol, 180 mg), CyNC (4.4 mmol, 480 mg, 548 µL), TMSN₃ (4.4 mmol, 506 mg, 584 µL), TFA (8.0 mmol, 912 mg, 612 µL), *m*-iodobenzoic acid (4.0 mmol, 992 mg), TEA (20 mmol, 2.02 g, 2.78 mL), HBTU (4.0 mmol, 1.52 g) and DMAP (0.4 mmol, 48.8 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1m** as a light yellow solid (1.38 g, 84%). R_f = 0.22 (heptane/AcOEt, 1:1); mp 141-146 °C; FT-IR (KBr) ν 3240 (N-H), 1633 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 8.18 (s, 1H), 8.08 (t, *J* = 5.8 Hz, 1H), 7.81 (t, *J* = 8.3 Hz, 2H), 7.13 (t, *J* = 7.8 Hz, 1H), 4.91 (d, *J* = 5.7 Hz, 2H), 4.58 (tt, *J* = 10.2, 4.7 Hz, 1H), 2.11 – 1.90 (m, 6H), 1.80 – 1.74 (m, 1H), 1.48 (dddd, *J* = 16.6, 12.8, 9.9, 4.2 Hz, 2H), 1.34 (tt, *J* = 12.7, 3.4 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 166.11 (C), 151.60 (C), 140.94 (CH), 136.43 (CH), 134.78 (C), 130.28 (CH), 126.25 (CH), 94.34 (C), 58.30 (CH), 32.96 (CH₂), 32.71 (CH₂), 25.18 (CH₂), 24.82 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₅H₁₉IN₅O 411.0631, Found 412.0611.

N-(1-(1-Cyclohexyl-1H-tetrazol-5-yl)-2-methylpropyl)benzamide (**1n**)

TrtNH₂ (2.0 mmol, 519 mg), isobutyraldehyde (3.0 mmol, 216 mg, 274 µL), CyNC (2.2 mmol, 240 mg, 274 µL), TMSN₃ (2.2 mmol, 253 mg, 292 µL), TFA (4.0 mmol, 456 mg, 306 µL), benzoic acid (2.0 mmol, 244 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC

afforded compound **1n** as a white solid (370 mg, 57%). R_f = 0.20 (heptane/AcOEt, 3:1); mp 207–209 °C; FT-IR (KBr) ν 3307 (N-H), 1649 (C=O); ^1H NMR (400 MHz, CDCl_3) δ 7.80 (d, J = 7.6 Hz, 3H), 7.46 (t, J = 7.4 Hz, 1H), 7.36 (t, J = 7.6 Hz, 2H), 5.25 (t, J = 9.1 Hz, 1H), 4.63 (tt, J = 11.7, 4.0 Hz, 1H), 2.42 (dq, J = 9.2, 6.5 Hz, 1H), 2.11 (ddt, J = 12.1, 8.3, 3.9 Hz, 2H), 2.04 – 1.88 (m, 4H), 1.82 – 1.73 (m, 1H), 1.49 (dtp, J = 16.2, 7.8, 3.8 Hz, 2H), 1.35 (tt, J = 12.9, 3.5 Hz, 1H), 1.15 (d, J = 6.7 Hz, 3H), 0.78 (d, J = 6.6 Hz, 3H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 167.54 (C), 154.64 (C), 148.47 (C), 133.29 (C), 133.14 (CH), 131.94 (CH), 130.06 (CH), 128.54 (CH), 128.35 (CH), 128.12 (CH), 127.91 (CH), 127.27 (CH), 126.62 (CH), 58.03 (CH), 49.29 (CH), 33.21 (CH_2), 33.16 (CH_2), 32.40 (CH), 25.33 (CH_2), 25.25 (CH_2), 24.87 (CH_2), 19.50 (CH_3), 19.03 (CH_3); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{18}\text{H}_{26}\text{N}_5\text{O}$ 328.2132, Found 328.2127.

N-(1-(1-Cyclohexyl-1H-tetrazol-5-yl)-2-phenylethyl)benzamide (**1o**)

TrtNH₂ (2.0 mmol, 519 mg), phenylacetaldehyde (3.0 mmol, 360 mg, 348 μL), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN₃ (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), benzoic acid (2.0 mmol, 244 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1o** as a yellow solid (335 mg, 45%). R_f = 0.18 (heptane/AcOEt, 3:1); mp 196–198 °C; FT-IR (KBr) ν 3313 (N-H), 1654 (C=O); ^1H NMR (400 MHz, CDCl_3) δ 8.02 (p, J = 8.6 Hz, 1H), 7.81 (d, J = 7.6 Hz, 2H), 7.50 (t, J = 7.4 Hz, 1H), 7.39 (t, J = 7.6 Hz, 2H), 7.21 – 7.13 (m, 3H), 6.98 – 6.88 (m, 2H), 5.66 (ddd, J = 10.6, 8.2, 5.2 Hz, 1H), 3.96 (tt, J = 8.3, 3.8 Hz, 1H), 3.51 (dd, J = 12.9, 5.3 Hz, 1H), 3.31 (dd, J = 13.0, 10.6 Hz, 1H), 2.05 (d, J = 12.4 Hz, 1H), 1.90 – 1.56 (m, 5H), 1.43 – 1.28 (m, 1H), 1.27 – 1.03 (m, 2H), 0.87 (d, J = 12.4 Hz, 1H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 167.36 (C), 154.50 (C), 135.51 (C), 133.14 (C), 132.02 (CH), 130.10 (CH), 129.26 (CH), 128.84 (CH), 128.61 (CH), 128.40 (CH), 128.12 (CH), 127.90 (CH), 127.40 (CH), 127.36 (CH), 126.60 (CH), 58.06 (CH), 46.18 (CH), 41.11 (CH_2), 32.99 (CH_2), 32.19 (CH_2), 25.22 (CH_2), 24.79 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{22}\text{H}_{26}\text{N}_5\text{O}$ 376.2059, Found 376.2125.

N-((1-Benzyl-1H-tetrazol-5-yl)methyl)benzamide (**1p**)

TrtNH₂ (4.0 mmol, 1.04 g), $(\text{CH}_2\text{O})_n$ (6.0 mmol, 180 mg), BnNC (4.4 mmol, 516 mg, 536 μL), TMSN₃ (4.4 mmol, 506 mg, 584 μL), TFA (8.0 mmol, 912 mg, 612 μL), benzoic acid (4.0 mmol, 488 mg), TEA (20 mmol, 2.02 g, 2.78 mL), HBTU (4.0 mmol, 1.52 g) and DMAP (0.4 mmol,

48.8 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1p** as a light yellow solid (892 mg, 76%). $R_f = 0.20$ (heptane/AcOEt, 1:1); mp 105 °C; FT-IR (KBr) ν 3289 (N-H), 1635 (C=O); ^1H NMR (600 MHz, CDCl_3) δ 8.11 (t, $J = 5.9$ Hz, 1H), 7.82 – 7.78 (m, 2H), 7.51 – 7.46 (m, 1H), 7.37 (t, $J = 7.7$ Hz, 2H), 7.35 – 7.29 (m, 5H), 5.82 (s, 2H), 4.83 (d, $J = 5.9$ Hz, 2H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 167.95 (C), 152.85 (C), 133.55 (C), 132.76 (C), 132.10 (CH), 129.20 (CH), 128.89 (CH), 128.60 (CH), 127.80 (CH), 127.30 (CH), 51.21 (CH_2), 32.41 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{16}\text{H}_{16}\text{N}_5\text{O}$ 294.1349, Found 294.1352.

N-((1-(4-Methoxyphenyl)-1H-tetrazol-5-yl)methyl)benzamide (1q)

TrtNH_2 (4.0 mmol, 1.04 g), $(\text{CH}_2\text{O})_n$ (6.0 mmol, 180 mg), *p*-methoxyphenylisocyanide (4.4 mmol, 586 mg), TMSN_3 (4.4 mmol, 506 mg, 584 μL), TFA (8.0 mmol, 912 mg, 612 μL), benzoic acid (4.0 mmol, 488 mg), TEA (20 mmol, 2.02 g, 2.78 mL), HBTU (4.0 mmol, 1.52 g) and DMAP (0.4 mmol, 48.8 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1q** as a light brown solid (992 mg, 80%). $R_f = 0.24$ (heptane/AcOEt, 1:2); mp 133-134 °C; FT-IR (KBr) ν 3290 (N-H), 1635 (C=O); ^1H NMR (300 MHz, CDCl_3) δ 8.02 (t, $J = 5.5$ Hz, 1H), 7.79 – 7.71 (m, 2H), 7.55 – 7.39 (m, 3H), 7.38 – 7.29 (m, 2H), 7.08 – 7.00 (m, 2H), 4.85 (d, $J = 5.5$ Hz, 2H), 3.86 (s, 3H); ^{13}C $\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 167.68 (C), 161.17 (C), 153.00 (C), 132.83 (C), 131.90 (CH), 128.42 (CH), 127.20 (CH), 126.49 (CH), 125.81 (C), 115.10 (CH), 55.64 (CH_3), 33.88 (CH_2); HRMS (ESI/TOF) m/z : Not found.

N-((1-(tert-Butyl)-1H-tetrazol-5-yl)methyl)benzamide (1r)

TrtNH_2 (2.0 mmol, 519 mg), $(\text{CH}_2\text{O})_n$ (3.0 mmol, 90.1 mg), *t*BuNC (2.2 mmol, 183 mg, 249 μL), TMSN_3 (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), benzoic acid (2.0 mmol, 244 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1r** as a white oil (344 mg, 66%) that solidifies upon standing. $R_f = 0.26$ (heptane/AcOEt, 1:2); mp 80-81 °C; FT-IR (KBr) ν 3265 (N-H), 1656 (C=O); ^1H NMR (400 MHz, CDCl_3) δ 8.00 (t, $J = 5.1$ Hz, 1H), 7.88 – 7.79 (m, 2H), 7.51 – 7.44 (m, 1H), 7.38 (dd, $J = 8.4, 7.0$ Hz, 2H), 5.01 (d, $J = 5.1$ Hz, 2H), 1.77 (s, 9H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 167.56 (C), 151.76 (C), 133.05 (C), 131.95 (CH), 128.58 (CH), 127.23 (CH), 61.57 (C), 35.84 (CH_2), 29.54 (CH_3); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{13}\text{H}_{18}\text{N}_5\text{O}$ 260.1506, Found 260.1514.

Methyl 2-(5-(benzamidomethyl)-1H-tetrazol-1-yl)acetate (1s)

TrtNH₂ (2.0 mmol, 519 mg) × 5, (CH₂O)_n (3.0 mmol, 90.1 mg) × 5, *t*BuNC (2.2 mmol, 183 mg, 249 μL) × 5, TMSN₃ (2.2 mmol, 253 mg, 292 μL) × 5, TFA (20.0 mmol, 2.28 g, 1.53 mL), benzoic acid (10 mmol, 1.22 g), TEA (50 mmol, 5.05 g, 6.97 mL), HBTU (10 mmol, 3.79 g) and DMAP (1.0 mmol, 122 mg) were reacted according to general procedure A. Purification by LCC afforded compound **1s** as a light brown oil (2.10 g, 76%) that solidifies upon standing. *R*_f = 0.24 (heptane/AcOEt, 1:2); mp 119-120 °C; FT-IR (KBr) ν 3286 (N-H), 1750 (C=O), 1632 (C=O); ¹H NMR (300 MHz, CDCl₃) δ 8.29 (t, *J* = 6.1 Hz, 1H), 7.86 – 7.80 (m, 2H), 7.53 – 7.44 (m, 1H), 7.38 (tt, *J* = 6.6, 1.6 Hz, 2H), 5.59 (s, 2H), 4.90 (d, *J* = 6.1 Hz, 2H), 3.71 (s, 3H); ¹³C {¹H} NMR (75 MHz, CDCl₃) δ 168.20 (C), 166.52 (C), 153.97 (C), 132.49 (CH), 128.58 (CH), 127.71 (C), 127.32 (CH), 53.41 (CH₃), 48.47 (CH₂), 32.12 (CH₂); HRMS (ESI/TOF) *m/z*: Not found.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)acrylamide (2a)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN₃ (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), acrylic acid (2.0 mmol, 144 mg, 137 μL), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2a** as a white yellowish solid (117 mg, 25%). *R*_f = 0.16 (heptane/AcOEt, 1:3); mp 128-130 °C; FT-IR (KBr) ν 3326 (N-H), 1661 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 7.73 (t, *J* = 6.1 Hz, 1H), 6.41 – 6.22 (m, 2H), 5.72 (dd, *J* = 9.8, 1.7 Hz, 1H), 4.81 (d, *J* = 5.8 Hz, 2H), 4.55 (tt, *J* = 9.8, 4.8 Hz, 1H), 2.04 – 1.90 (m, 6H), 1.81 – 1.73 (m, 1H), 1.47 (dddd, *J* = 16.0, 12.6, 9.3, 3.3 Hz, 2H), 1.37 – 1.25 (m, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 165.95 (C), 151.63 (C), 129.83 (CH), 127.92 (CH₂), 58.27 (CH), 32.90 (CH₂), 31.96 (CH₂), 25.12 (CH₂), 24.80 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₁H₁₈N₅O 236.1506, Found 236.1516.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)methacrylamide (2b)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN₃ (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), methacrylic acid (2.0 mmol, 172 mg, 170 μL), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2b** as a white sticky solid (391 mg, 78%) that crystallizes upon standing. *R*_f = 0.18 (heptane/AcOEt, 1:2); mp 92-93 °C; FT-IR (KBr) ν 3307 (N-H), 1663 (C=O); ¹H NMR (400 MHz,

CDCl₃) δ 7.51 (s, 1H), 5.85 (s, 1H), 5.42 (s, 1H), 4.80 (s, 2H), 4.53 (s, 1H), 2.14 – 1.67 (m, 10H), 1.54 – 1.25 (m, 3H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 168.48 (C), 151.68 (C), 138.75 (C), 121.21 (CH₂), 58.04 (CH), 32.93 (CH₂), 32.23 (CH₂), 25.13 (CH₂), 24.82 (CH₂), 18.55 (CH₃); HRMS (ESI/TOF) m/z : [M + H]⁺ Calcd for C₁₂H₂₀N₅O 250.1662, Found 250.1665.

(E)-N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-2-methylbut-2-enamide (2c)

TrtNH₂ (4.0 mmol, 1.04 g), (CH₂O)_n (6.0 mmol, 180 mg), CyNC (4.4 mmol, 480 mg, 548 μ L), TMSN₃ (4.4 mmol, 506 mg, 584 μ L), TFA (8.0 mmol, 912 mg, 612 μ L), (E)-2-methylbut-2-enoic acid (4.0 mmol, 400 mg), TEA (20 mmol, 2.02 g, 2.78 mL), HBTU (4.0 mmol, 1.52 g) and DMAP (0.4 mmol, 48.8 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2c** as a light yellow solid (842 mg, 80%). R_f = 0.22 (heptane/AcOEt, 1:2); mp 114-117 °C; FT-IR (KBr) ν 3310 (N-H), 1629 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 7.11 (t, J = 5.8 Hz, 1H), 6.55 (q, J = 7.0 Hz, 1H), 4.79 (d, J = 5.8 Hz, 2H), 4.52 (tt, J = 9.9, 5.4 Hz, 1H), 2.03 – 1.90 (m, 6H), 1.86 (s, 3H), 1.81 – 1.71 (m, 4H (J = 7.2 Hz)), 1.47 (qt, J = 12.9, 3.8 Hz, 2H), 1.33 (tt, J = 12.7, 3.4 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 169.36 (C), 151.74 (C), 132.61 (CH), 130.73 (C), 58.00 (CH), 32.92 (CH₂), 32.36 (CH₂), 25.14 (CH₂), 24.83 (CH₂), 14.04 (CH₃), 12.28 (CH₃); HRMS (ESI/TOF) m/z : [M + H]⁺ Calcd for C₁₃H₂₂N₅O 264.1819, Found 264.1818.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)furan-2-carboxamide (2d)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μ L), TMSN₃ (2.2 mmol, 253 mg, 292 μ L), TFA (4.0 mmol, 456 mg, 306 μ L), 2-furoic acid (2.0 mmol, 224 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2d** as a white solid (377 mg, 69%). R_f = 0.18 (heptane/AcOEt, 1:2); mp 144-146 °C; FT-IR (KBr) ν 3299 (N-H), 1645 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 7.70 (d, J = 6.0 Hz, 1H), 7.44 (d, J = 1.6 Hz, 1H), 7.15 (d, J = 3.5 Hz, 1H), 6.49 (dd, J = 3.6, 1.7 Hz, 1H), 4.92 (d, J = 5.9 Hz, 2H), 4.56 (tt, J = 10.2, 4.8 Hz, 1H), 2.08 – 1.88 (m, 6H), 1.76 (dt, J = 13.1, 3.4 Hz, 1H), 1.47 (qt, J = 12.9, 4.0 Hz, 2H), 1.33 (tt, J = 12.6, 3.4 Hz, 1H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 158.54 (C), 151.50 (C), 146.74 (C), 144.84 (CH), 115.24 (CH), 112.17 (CH), 58.29 (CH), 32.93 (CH₂), 31.76 (CH₂), 25.14 (CH₂), 24.81 (CH₂); HRMS (ESI/TOF) m/z : [M + H]⁺ Calcd for C₁₃H₁₈N₅O₂ 276.1455, Found 276.1577.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)thiophene-2-carboxamide (2e)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 µL), TMSN₃ (2.2 mmol, 253 mg, 292 µL), TFA (4.0 mmol, 456 mg, 306 µL), 2-thiophenecarboxylic acid (2.0 mmol, 256 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2e** as a white solid (463 mg, 79%). R_f = 0.16 (heptane/AcOEt, 1:1); mp 143-144 °C; FT-IR (KBr) ν 3310 (N-H), 1632 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 8.35 (t, *J* = 5.9 Hz, 1H), 7.73 (d, *J* = 3.7 Hz, 1H), 7.48 (d, *J* = 5.3 Hz, 1H), 7.03 (dd, *J* = 5.0, 3.8 Hz, 1H), 4.92 (d, *J* = 5.9 Hz, 2H), 4.62 (tt, *J* = 11.2, 4.2 Hz, 1H), 2.09 – 1.85 (m, 7H), 1.75 (dt, *J* = 13.0, 3.4 Hz, 1H), 1.46 (qt, *J* = 13.0, 3.8 Hz, 2H), 1.31 (dtd, *J* = 18.7, 9.4, 8.1, 4.7 Hz, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 162.31 (C), 151.91 (C), 137.70 (C), 130.97 (CH), 129.05 (CH), 127.94 (CH), 58.23 (CH), 32.97 (CH₂), 32.31 (CH₂), 25.12 (CH₂), 24.84 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₃H₁₈N₅OS 292.1227, Found 292.1228.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-1-methyl-1H-pyrrole-2-carboxamide (2f)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 µL), TMSN₃ (2.2 mmol, 253 mg, 292 µL), TFA (4.0 mmol, 456 mg, 306 µL), 1-methyl-1H-pyrrole-2-carboxylic acid (2.0 mmol, 250 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2f** as a yellow solid (476 mg, 82%). R_f = 0.18 (heptane/AcOEt, 1:1); mp 143-147 °C; FT-IR (KBr) ν 3242 (N-H), 1657 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 7.35 (t, *J* = 6.0 Hz, 1H), 6.77 (dd, *J* = 4.0, 1.7 Hz, 1H), 6.73 (dd, *J* = 2.2, 2.0 Hz, 1H), 6.07 (dd, *J* = 4.0, 2.6 Hz, 1H), 4.86 (d, *J* = 6.0 Hz, 2H), 4.65 – 4.52 (m, 1H), 3.92 (s, 3H), 2.06 – 1.87 (m, 6H), 1.75 (dt, *J* = 13.1, 3.4 Hz, 1H), 1.45 (qt, *J* = 12.5, 4.0 Hz, 2H), 1.32 (tt, *J* = 12.7, 3.3 Hz, 1H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 161.77 (C), 151.93 (C), 128.68 (CH), 124.38 (C), 113.20 (CH), 107.65 (CH), 58.04 (CH), 36.77 (CH₃), 32.94 (CH₂), 31.67 (CH₂), 25.18 (CH₂), 24.84 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₄H₂₁N₆O 289.1771, Found 289.1494.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)benzofuran-2-carboxamide (2g)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 µL), TMSN₃ (2.2 mmol, 253 mg, 292 µL), TFA (4.0 mmol, 456 mg, 306 µL), benzofuran-2-carboxylic acid (2.0 mmol, 324 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC

afforded compound **2g** as a white solid (443 mg, 68%). $R_f = 0.26$ (heptane/AcOEt, 1:1); mp 200-201 °C; FT-IR (KBr) ν 3326 (N-H), 1648 (C=O); ^1H NMR (400 MHz, DMSO- d_6) δ 9.54 (t, $J = 5.8$ Hz, 1H), 7.79 (d, $J = 7.8$ Hz, 1H), 7.67 (d, $J = 8.3$ Hz, 1H), 7.63 (s, 1H), 7.49 (t, $J = 7.7$ Hz, 1H), 7.35 (t, $J = 7.5$ Hz, 1H), 4.85 (d, $J = 5.8$ Hz, 2H), 4.63 (tt, $J = 11.5, 4.0$ Hz, 1H), 2.09 – 1.96 (m, 2H), 1.82 (dd, $J = 13.2, 8.0$ Hz, 4H), 1.70 – 1.62 (m, 1H), 1.40 (dtd, $J = 14.5, 11.1, 10.6, 3.5$ Hz, 2H), 1.26 (tt, $J = 12.7, 3.2$ Hz, 1H); ^{13}C { ^1H } NMR (151 MHz, DMSO- d_6) δ 158.89 (C), 154.80 (C), 152.59 (C), 148.75 (C), 127.59 (CH), 127.46 (C), 124.27 (CH), 123.39 (CH), 112.28 (CH), 110.65 (CH), 57.17 (CH), 32.91 (CH₂), 32.41 (CH₂), 25.14 (CH₂), 25.00 (CH₂); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for C₁₇H₂₀N₅O₂ 326.1611, Found 326.1606.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)benzo[b]thiophene-2-carboxamide (2h)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN₃ (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), thianaphthene-2-carboxylic acid (2.0 mmol, 356 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2h** as a white solid (469 mg, 69%). $R_f = 0.24$ (heptane/AcOEt, 1:1); mp 162-164 °C; FT-IR (KBr) ν 3313 (N-H), 1638 (C=O); ^1H NMR (400 MHz, CDCl₃) δ 8.00 (t, $J = 5.9$ Hz, 1H), 7.90 – 7.82 (m, 2H), 7.54 – 7.46 (m, 1H), 7.45 – 7.36 (m, 2H), 4.94 (d, $J = 5.8$ Hz, 2H), 4.61 (tt, $J = 11.0, 4.5$ Hz, 1H), 2.06 – 1.88 (m, 6H), 1.76 (dt, $J = 13.1, 3.3$ Hz, 1H), 1.47 (qt, $J = 12.8, 4.0$ Hz, 2H), 1.32 (tt, $J = 12.8, 3.4$ Hz, 1H); ^{13}C { ^1H } NMR (151 MHz, DMSO- d_6) δ 162.33 (C), 152.67 (C), 140.79 (C), 139.50 (C), 139.08 (C), 126.93 (CH), 126.06 (CH), 125.84 (CH), 125.47 (CH), 123.30 (CH), 57.25 (CH), 32.94 (CH₂), 32.79 (CH₂), 25.17 (CH₂), 24.99 (CH₂); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for C₁₇H₂₀N₅OS 342.1383, Found 342.1389.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-1-methyl-1H-indole-3-carboxamide (2i)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN₃ (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), 1-methylindole-3-carboxylic acid (2.0 mmol, 356 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2i** as a white solid (330 mg, 49%). $R_f = 0.14$ (heptane/AcOEt, 1:2); mp 203-206 °C; FT-IR (KBr) ν 3282 (N-H), 1619 (C=O); ^1H NMR (400 MHz, CDCl₃) δ 8.66 (t, $J = 5.8$ Hz, 1H), 8.15 (d, $J = 7.8$ Hz, 1H), 8.02 (s, 1H), 7.49 (d, $J = 8.1$ Hz, 1H), 7.20 (dt, $J = 24.9,$

7.3 Hz, 2H), 4.83 (d, J = 5.7 Hz, 2H), 4.76 – 4.64 (m, 1H), 3.83 (s, 3H), 2.07 – 1.94 (m, 2H), 1.87 – 1.72 (m, 4H), 1.65 (d, J = 12.8 Hz, 1H), 1.46 – 1.31 (m, 2H), 1.24 (tt, J = 12.3, 3.3 Hz, 1H); ^{13}C { ^1H } NMR (101 MHz, CDCl_3) δ 169.52 (C), 158.12 (C), 141.92 (C), 137.44 (CH), 131.59 (C), 127.31 (CH), 126.19 (CH), 126.06 (CH), 115.56 (CH), 113.83 (C), 61.88 (CH), 38.27 (CH_3), 37.72 (CH_2), 36.70 (CH_2), 29.93 (CH_2), 29.77 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{18}\text{H}_{23}\text{N}_6\text{O}$ 339.1928, Found 339.1922.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)isonicotinamide (2j)

TrtNH_2 (2.0 mmol, 519 mg), $(\text{CH}_2\text{O})_n$ (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN_3 (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), isonicotinic acid (2.0 mmol, 246 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2j** as a white solid (336 mg, 59%). R_f = 0.20 (AcOEt/MeOH, 20:1); mp 151-152 $^\circ\text{C}$; FT-IR (KBr) ν 3254 (N-H), 1645 (C=O); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 9.60 (t, J = 5.7 Hz, 1H), 8.76 (d, J = 5.1 Hz, 2H), 7.78 (d, J = 5.2 Hz, 1H), 4.87 (d, J = 5.6 Hz, 2H), 4.61 (tt, J = 11.3, 3.9 Hz, 1H), 2.05 – 1.96 (m, 2H), 1.80 (qd, J = 12.0, 11.3, 3.8 Hz, 4H), 1.71 – 1.63 (m, 1H), 1.38 (qd, J = 12.0, 10.4, 6.8 Hz, 2H), 1.31 – 1.21 (m, 1H); ^{13}C { ^1H } NMR (151 MHz, $\text{DMSO}-d_6$) δ 165.52 (C), 152.56 (C), 150.87 (CH), 140.74 (C), 121.63 (CH), 57.21 (CH), 32.91 (CH_2), 32.87 (CH_2), 25.14 (CH_2), 24.99 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{19}\text{N}_6\text{O}$ 287.1615, Found 287.1613.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)thiazole-5-carboxamide (2k)

TrtNH_2 (2.0 mmol, 519 mg), $(\text{CH}_2\text{O})_n$ (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN_3 (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), thiazole-5-carboxylic acid (2.0 mmol, 258 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2k** as a light yellow solid (384 mg, 66%). R_f = 0.20 (heptane/AcOEt, 1:10); mp 159-162 $^\circ\text{C}$; FT-IR (KBr) ν 3235 (N-H), 1632 (C=O); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 9.53 (t, J = 5.7 Hz, 1H), 9.27 (s, 1H), 8.51 (s, 1H), 4.84 (d, J = 5.7 Hz, 2H), 4.58 (tt, J = 11.3, 3.9 Hz, 1H), 1.99 (dt, J = 10.2, 4.4 Hz, 2H), 1.81 (td, J = 10.0, 8.4, 3.6 Hz, 4H), 1.73 – 1.62 (m, 1H), 1.38 (qd, J = 13.3, 11.8, 6.7 Hz, 2H), 1.26 (tt, J = 13.0, 3.2 Hz, 1H); ^{13}C { ^1H } NMR (151 MHz, $\text{DMSO}-d_6$) δ 160.66 (C), 159.01 (CH), 152.57 (C), 144.68 (CH), 134.87 (C), 57.24 (CH), 32.91 (CH_2),

32.65 (CH₂), 25.14 (CH₂), 24.98 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₂H₁₇N₆OS 293.1179, Found 293.1189.

N-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-1-naphthamide (2l)

TrtNH₂ (2.0 mmol, 519 mg), (CH₂O)_n (3.0 mmol, 90.1 mg), CyNC (2.2 mmol, 240 mg, 274 μL), TMSN₃ (2.2 mmol, 253 mg, 292 μL), TFA (4.0 mmol, 456 mg, 306 μL), 1-naphthoic acid (2.0 mmol, 344 mg), TEA (10 mmol, 1.01 g, 1.39 mL), HBTU (2.0 mmol, 758 mg) and DMAP (0.2 mmol, 24.4 mg) were reacted according to general procedure A. Purification by LCC afforded compound **2l** as a white solid (583 mg, 87%). *R*_f = 0.24 (heptane/AcOEt, 1:1); mp 249-250 °C; FT-IR (KBr) ν 3297 (N-H), 1646 (C=O); ¹H NMR (400 MHz, CDCl₃) δ 9.33 (t, *J* = 5.8 Hz, 1H), 8.30 – 8.18 (m, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 8.01 – 7.95 (m, 1H), 7.67 – 7.50 (m, 4H), 4.90 (d, *J* = 5.7 Hz, 2H), 4.68 (tt, *J* = 11.5, 4.0 Hz, 1H), 2.14 – 2.01 (m, 2H), 1.92 – 1.77 (m, 4H), 1.68 (d, *J* = 13.0 Hz, 1H), 1.43 (qt, *J* = 13.1, 2.7 Hz, 2H), 1.28 (tt, *J* = 13.0, 3.4 Hz, 1H); ¹³C {¹H} NMR (151 MHz, DMSO-*d*₆) δ 169.34 (C), 152.81 (C), 133.98 (C), 133.62 (C), 130.79 (CH), 130.17 (C), 128.74 (CH), 127.29 (CH), 126.80 (CH), 125.96 (CH), 125.69 (CH), 125.42 (CH), 57.19 (CH), 32.97 (CH₂), 32.78 (CH₂), 25.18 (CH₂), 25.03 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₁₉H₂₂N₅O 336.1819, Found 336.1828.

Synthesis of tetrazole-isoquinolone/pyridone hybrids

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4a)

Compound **1a** (0.25 mmol, 71.3 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4a** as a white solid (104 mg, 90%). *R*_f = 0.26 (heptane/AcOEt, 2:1); mp 214-219 °C; FT-IR (KBr) ν 1651 (C=O), 1590 (C-H), 704 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.46 (d, *J* = 7.8 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.29 (dt, *J* = 8.6, 3.5 Hz, 2H), 7.24 – 7.05 (m, 9H), 5.22 (s, 2H), 4.19 (ddt, *J* = 10.9, 8.2, 4.4 Hz, 1H), 2.02 – 1.83 (m, 6H), 1.48 – 1.18 (m, 4H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 162.31 (C), 150.84 (C), 140.27 (C), 137.54 (C), 136.10 (C), 134.00 (C), 132.77 (CH), 131.41 (CH), 130.50 (CH), 128.70 (CH), 128.21 (CH), 127.99 (CH), 127.89 (CH), 127.01 (CH), 125.75 (CH), 124.63 (C), 120.12 (C), 58.03 (CH), 39.48 (CH₂), 32.58 (CH₂), 25.18 (CH₂), 24.84 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₂₉H₂₈N₅O 462.2288, Found 462.2270.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-8-methyl-3,4-diphenylisoquinolin-1(2H)-one (4b)

Compound **1b** (0.25 mmol, 74.8 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure II during 24 h. Purification by LCC afforded compound **4b** as a light yellow solid (87 mg, 73%). R_f = 0.33 (heptane/AcOEt, 2:1); mp 192-193 °C; FT-IR (KBr) ν 1641 (C=O), 1595 (C-H), 696 (C-H); ¹H NMR (600 MHz, CDCl₃) δ 7.39 (t, *J* = 7.8 Hz, 1H), 7.29 – 7.26 (m, 1H), 7.26 – 7.23 (m, 2H), 7.22 – 7.15 (m, 6H), 7.13 – 7.08 (m, 2H), 7.00 (d, *J* = 8.1 Hz, 1H), 5.21 (s, 2H), 4.18 (tt, *J* = 9.7, 4.6 Hz, 1H), 2.95 (s, 3H), 1.95 – 1.85 (m, 6H), 1.73 (dd, *J* = 9.6, 6.5 Hz, 1H), 1.42 – 1.29 (m, 3H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 162.88 (C), 150.97 (C), 142.01 (C), 140.17 (C), 139.26 (C), 136.85 (C), 134.28 (C), 131.84 (CH), 131.51 (CH), 130.34 (CH), 130.23 (CH), 128.51 (CH), 128.14 (CH), 127.98 (CH), 126.86 (CH), 124.11 (CH), 123.30 (C), 120.02 (C), 57.93 (CH), 39.29 (CH₂), 32.56 (CH₂), 25.18 (CH₂), 24.84 (CH₂), 24.20 (CH₃); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₃₀H₃₀N₅O 476.2445, Found 476.2427.

8-Bromo-2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4c)

Compound **1c** (0.25 mmol, 91.1 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B during 24 h. Purification by LCC afforded compound **4c** as a yellow solid (49 mg, 36%). R_f = 0.29 (heptane/AcOEt, 1:1); mp 195-197 °C; FT-IR (KBr) ν 1644 (C=O), 1599 (C-H), 697 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.47 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.57 (td, *J* = 8.0, 7.6, 1.5 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.29 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.22 – 7.17 (m, 6H), 7.13 – 7.09 (m, 2H), 5.22 (s, 2H), 4.25 – 4.13 (m, 1H), 1.99 – 1.87 (m, 6H), 1.43 – 1.25 (m, 4H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 162.33 (C), 150.80 (C), 140.23 (C), 137.53 (C), 136.09 (C), 134.00 (C), 132.77 (CH), 131.41 (CH), 130.50 (CH), 128.69 (CH), 128.21 (CH), 127.98 (CH), 127.89 (CH), 127.03 (CH), 126.99 (CH), 125.74 (CH), 124.61 (C), 120.15 (C), 58.04 (CH), 39.45 (CH₂), 32.58 (CH₂), 25.19 (CH₂), 24.83 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₂₉H₂₇BrN₅O 540.1394, Found 540.1405.

8-Chloro-2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4d)

Compound **1d** (0.25 mmol, 80.0 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg)

were reacted according to general procedure B during 24 h. Purification by LCC afforded compound **4d** as a yellow solid (46 mg, 37%). R_f = 0.26 (heptane/AcOEt, 1:1); mp 210-212 °C; FT-IR (KBr) ν 1646 (C=O), 1599 (C-H), 698 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 8.47 (dd, J = 8.0, 1.4 Hz, 1H), 7.60 – 7.54 (m, 1H), 7.50 (t, J = 7.5 Hz, 1H), 7.29 (dd, J = 7.0, 2.8 Hz, 2H), 7.21 – 7.16 (m, 6H), 7.13 – 7.08 (m, 2H), 5.22 (s, 2H), 4.27 – 4.13 (m, 1H), 2.01 – 1.86 (m, 6H), 1.43 – 1.25 (m, 4H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 162.33 (C), 150.80 (C), 140.23 (C), 137.53 (C), 136.10 (C), 134.00 (C), 132.77 (CH), 131.41 (CH), 130.50 (CH), 128.69 (CH), 128.21 (CH), 127.98 (CH), 127.90 (CH), 127.03 (CH), 126.99 (CH), 125.74 (CH), 124.62 (C), 120.15 (C), 58.05 (CH), 39.45 (CH_2), 32.59 (CH_2), 25.20 (CH_2), 24.84 (CH_2); HRMS (ESI/TOF) m/z : Not found.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-8-methoxy-3,4-diphenylisoquinolin-1(2H)-one (4e)

Compound **1e** (0.25 mmol, 78.9 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. The desired product could not be obtained.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-6-methoxy-3,4-diphenylisoquinolin-1(2H)-one (4f)

Compound **1f** (0.25 mmol, 78.9 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4f** as a light yellow solid (107 mg, 87%). R_f = 0.18 (heptane/AcOEt, 2:1); mp 215-216 °C; FT-IR (KBr) ν 1648 (C=O), 1604 (C-H), 714 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 8.39 (d, J = 8.9 Hz, 1H), 7.28 (dd, J = 6.5, 2.8 Hz, 2H), 7.23 – 7.13 (m, 6H), 7.12 – 7.09 (m, 2H), 7.06 (dd, J = 8.9, 2.5 Hz, 1H), 6.53 (d, J = 2.4 Hz, 1H), 5.20 (s, 2H), 4.25 – 4.11 (m, 1H), 3.69 (s, 3H), 2.00 – 1.83 (m, 6H), 1.72 (d, J = 12.0 Hz, 1H), 1.39 – 1.25 (m, 3H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 163.15 (C), 161.95 (C), 150.93 (C), 140.91 (C), 139.70 (C), 136.17 (C), 134.13 (C), 131.36 (CH), 130.42 (CH), 130.11 (CH), 128.64 (CH), 128.18 (CH), 128.01 (CH), 127.00 (CH), 119.83 (C), 118.54 (C), 115.78 (CH), 107.56 (CH), 58.00 (CH), 55.30 (CH_3), 39.27 (CH_2), 32.58 (CH_2), 25.19 (CH_2), 24.84 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{30}\text{H}_{30}\text{N}_5\text{O}_2$ 492.2394, Found 492.2377.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-6-methyl-3,4-diphenylisoquinolin-1(2H)-one (4g)

Compound **1g** (0.25 mmol, 74.8 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg)

were reacted according to general procedure B. Purification by LCC afforded compound **4g** as a light yellow solid (109 mg, 92%). R_f = 0.16 (heptane/AcOEt, 3:1); mp 212-214 °C; FT-IR (KBr) ν 1641 (C=O), 1603 (C-H), 699 (C-H); ^1H NMR (600 MHz, CDCl_3) δ 8.37 (d, J = 8.2 Hz, 1H), 7.34 (dd, J = 8.3, 1.7 Hz, 1H), 7.30 (dd, J = 7.2, 2.4 Hz, 2H), 7.24 – 7.16 (m, 6H), 7.15 – 7.10 (m, 2H), 6.96 (s, 1H), 5.23 (s, 2H), 4.22 (tt, J = 11.1, 4.1 Hz, 1H), 2.37 (s, 3H), 2.01 – 1.88 (m, 6H), 1.76 – 1.72 (m, 1H), 1.39 (qd, J = 13.4, 6.8 Hz, 2H), 1.34 – 1.28 (m, 1H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 162.28 (C), 150.88 (C), 143.50 (C), 140.31 (C), 137.62 (C), 136.24 (C), 134.13 (C), 131.45 (CH), 130.52 (CH), 128.64 (CH), 128.61 (CH), 128.17 (CH), 127.95 (CH), 127.91 (CH), 126.92 (CH), 125.41 (CH), 122.45 (C), 119.99 (C), 58.01 (CH), 39.35 (CH_2), 32.59 (CH_2), 25.20 (CH_2), 24.85 (CH_2), 22.04 (CH_3); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{30}\text{H}_{30}\text{N}_5\text{O}$ 476.2445, Found 476.2425.

6-Chloro-2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4h)

Compound **1h** (0.25 mmol, 79.8 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4h** as a yellow solid (117 mg, 94%). R_f = 0.20 (heptane/AcOEt, 3:1); mp 241-243 °C; FT-IR (KBr) ν 1656 (C=O), 1598 (C-H), 709 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 8.39 (d, J = 8.6 Hz, 1H), 7.44 (dd, J = 8.7, 2.0 Hz, 1H), 7.28 (dd, J = 7.3, 2.4 Hz, 2H), 7.25 – 7.12 (m, 7H), 7.11 – 7.05 (m, 2H), 5.19 (s, 2H), 4.25 – 4.09 (m, 1H), 2.01 – 1.82 (m, 6H), 1.75 – 1.67 (m, 1H), 1.46 – 1.27 (m, 3H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 161.71 (C), 150.61 (C), 141.73 (C), 139.52 (C), 138.89 (C), 135.35 (C), 133.69 (C), 131.29 (CH), 130.29 (CH), 129.74 (CH), 128.86 (CH), 128.28 (CH), 128.20 (CH), 127.56 (CH), 127.31 (CH), 125.08 (CH), 122.96 (C), 119.24 (C), 58.08 (CH), 39.52 (CH_2), 32.56 (CH_2), 25.17 (CH_2), 24.81 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{29}\text{H}_{27}\text{ClN}_5\text{O}$ 496.1899, Found 496.1877.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenyl-6-(trifluoromethyl)isoquinolin-1(2H)-one (4i)

Compound **1i** (0.25 mmol, 88.3 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4i** as a light yellow solid (118 mg, 89%). R_f = 0.20 (heptane/AcOEt, 3:1); mp 165-169 °C; FT-IR (KBr)

ν 1650 (C=O), 693 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 8.58 (d, J = 8.4 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.45 (s, 1H), 7.33 – 7.27 (m, 2H), 7.26 – 7.16 (m, 6H), 7.13 – 7.07 (m, 2H), 5.21 (s, 2H), 4.23 – 4.12 (m, 1H), 2.00 – 1.84 (m, 6H), 1.77 – 1.69 (m, 1H), 1.45 – 1.28 (m, 3H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 161.53 (C), 150.48 (C), 141.90 (C), 137.67 (C), 135.03 (C), 134.36 (q, J = 32.6 Hz, CF_3), 133.53 (C), 131.25 (CH), 130.30 (CH), 129.07 (CH), 128.98 (CH), 128.35 (C), 128.30 (CH), 127.50 (CH), 126.69 (C), 122.96 (q, J = 3.8 Hz, CH), 119.83 (C), 58.15 (CH), 39.69 (CH_2), 32.57 (CH_2), 25.19 (CH_2), 24.81 (CH_2); ^{19}F $\{^{13}\text{C}\}$ NMR (376 MHz, CDCl_3) δ -63.04; HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{30}\text{H}_{27}\text{F}_3\text{N}_5\text{O}$ 530.2162, Found 530.2139.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-7-methyl-3,4-diphenylisoquinolin-1(2H)-one (4j)

Compound **1j** (0.50 mmol, 150 mg), diphenylacetylene (**3a**, 0.750 mmol, 134 mg), $\text{Cu}(\text{OAc})_2$ (1.0 mmol, 182 mg), CsOAc (0.250 mmol, 48.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0250 mmol, 15.4 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4j** as a light yellow solid (219 mg, 92%). R_f = 0.30 (heptane/ AcOEt , 2:1); mp 229-231 $^\circ\text{C}$; FT-IR (KBr) ν 1643 (C=O), 728 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 8.26 (d, J = 1.9 Hz, 1H), 7.38 (dd, J = 8.3, 1.9 Hz, 1H), 7.30 (dd, J = 6.6, 2.8 Hz, 2H), 7.17 (td, J = 8.8, 7.6, 5.4 Hz, 6H), 7.12 – 7.06 (m, 3H), 5.21 (s, 2H), 4.21 (tt, J = 11.2, 4.4 Hz, 1H), 2.47 (s, 3H), 2.02 – 1.85 (m, 6H), 1.73 (d, J = 12.0 Hz, 1H), 1.41 – 1.25 (m, 3H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 162.30 (C), 150.87 (C), 139.27 (C), 137.20 (C), 136.27 (C), 135.24 (C), 134.23 (CH), 134.10 (C), 131.39 (CH), 130.62 (CH), 128.61 (CH), 128.17 (CH), 127.92 (CH), 127.44 (CH), 126.91 (CH), 125.72 (CH), 124.50 (C), 120.10 (C), 58.02 (CH), 39.45 (CH_2), 32.59 (CH_2), 25.20 (CH_2), 24.85 (CH_2), 21.32 (CH_3); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{30}\text{H}_{30}\text{N}_5\text{O}$ 476.2445, Found 476.2430.

7-Chloro-2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4k)

Compound **1k** (0.50 mmol, 160 mg), diphenylacetylene (**3a**, 0.750 mmol, 134 mg), $\text{Cu}(\text{OAc})_2$ (1.0 mmol, 182 mg), CsOAc (0.250 mmol, 48.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0250 mmol, 15.4 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4k** as a light yellow solid (175 mg, 71%). R_f = 0.32 (heptane/ AcOEt , 2:1); mp 107-116 $^\circ\text{C}$; FT-IR (KBr) ν 1648 (C=O), 1596 (C-H), 699 (C-H); ^1H NMR (600 MHz, CDCl_3) δ 8.45 (d, J = 2.3 Hz, 1H), 7.51 (dd, J = 8.8, 2.3 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.25 – 7.18 (m, 6H), 7.15 (d, J = 8.7 Hz, 1H), 7.13 – 7.08 (m, 2H), 5.21 (s, 2H), 4.21 (ddd, J = 11.3, 7.1, 4.3 Hz, 1H), 2.02 – 1.87 (m, 6H), 1.75 (d, J = 12.8 Hz, 1H), 1.45 – 1.35 (m, 2H), 1.32 (tt, J = 13.0, 2.9 Hz, 1H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz,

CDCl₃) δ 161.30 (C), 150.58 (C), 140.60 (C), 135.95 (C), 135.65 (C), 133.69 (C), 133.16 (CH), 131.30 (CH), 130.43 (CH), 128.85 (CH), 128.29 (CH), 128.13 (CH), 127.51 (CH), 127.30 (CH), 127.23 (CH), 125.71 (C), 119.64 (C), 58.12 (CH), 39.60 (CH₂), 32.59 (CH₂), 25.21 (CH₂), 24.83 (CH₂); HRMS (ESI/TOF) m/z : [M + H]⁺ Calcd for C₂₉H₂₇ClN₅O 496.1899, Found 496.1877.

7-Bromo-2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4l)

Compound **1l** (0.50 mmol, 182 mg), diphenylacetylene (**3a**, 0.750 mmol, 134 mg), Cu(OAc)₂ (1.0 mmol, 182 mg), CsOAc (0.250 mmol, 48.0 mg) and [RhCp*Cl₂]₂ (0.0250 mmol, 15.4 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4l** as a light yellow solid (367 mg, 68%). R_f = 0.40 (heptane/AcOEt, 2:1); mp 207-210 °C; FT-IR (KBr) ν 1646 (C=O), 1590 (C-H), 714 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.60 (d, J = 2.1 Hz, 1H), 7.63 (dd, J = 8.7, 2.2 Hz, 1H), 7.29 (dd, J = 7.3, 2.4 Hz, 2H), 7.23 – 7.15 (m, 6H), 7.08 (dd, J = 8.8, 2.8 Hz, 3H), 5.19 (s, 2H), 4.18 (dd, J = 9.9, 5.5 Hz, 1H), 1.99 – 1.85 (m, 6H), 1.78 – 1.70 (m, 1H), 1.43 – 1.26 (m, 3H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 161.16 (C), 150.56 (C), 140.78 (C), 136.27 (C), 135.88 (CH), 135.58 (C), 133.69 (C), 131.29 (CH), 130.43 (CH), 130.38 (CH), 128.85 (CH), 128.28 (CH), 128.12 (CH), 127.61 (CH), 127.22 (CH), 125.94 (C), 121.05 (C), 119.68 (C), 58.11 (CH), 39.60 (CH₂), 32.58 (CH₂), 25.20 (CH₂), 24.82 (CH₂); HRMS (ESI/TOF) m/z : [M + H]⁺ Calcd for C₂₉H₂₇BrN₅O 540.1394, Found 540.1381.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-7-iodo-3,4-diphenylisoquinolin-1(2H)-one (4m)

Compound **1m** (0.50 mmol, 206 mg), diphenylacetylene (**3a**, 0.750 mmol, 134 mg), Cu(OAc)₂ (1.0 mmol, 182 mg), CsOAc (0.250 mmol, 48.0 mg) and [RhCp*Cl₂]₂ (0.0250 mmol, 15.4 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4m** as a light yellow solid (214 mg, 73%). R_f = 0.36 (heptane/AcOEt, 2:1); mp 198-204 °C; FT-IR (KBr) ν 1651 (C=O), 1589 (C-H), 698 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.80 (d, J = 1.7 Hz, 1H), 7.82 (dd, J = 8.6, 1.8 Hz, 1H), 7.33 – 7.27 (m, 2H), 7.23 – 7.13 (m, 6H), 7.10 – 7.05 (m, 2H), 6.91 (d, J = 8.5 Hz, 1H), 5.18 (s, 2H), 4.18 (dd, J = 9.9, 5.6 Hz, 1H), 2.02 – 1.85 (m, 6H), 1.74 (d, J = 11.2 Hz, 1H), 1.44 – 1.27 (m, 3H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 160.94 (C), 150.57 (C), 141.42 (CH), 141.02 (C), 136.65 (CH), 135.52 (C), 133.71 (C), 131.28 (CH), 130.36 (CH), 128.85 (CH), 128.27 (CH), 128.11 (CH), 127.52 (CH), 127.21 (CH), 126.03 (C), 119.73 (C), 92.04 (C), 58.11 (CH), 39.60 (CH₂), 32.58 (CH₂), 25.20 (CH₂), 24.82 (CH₂); HRMS (ESI/TOF) m/z : [M + H]⁺ Calcd for C₂₉H₂₇IN₅O 588.1257, Found 588.1232.

2-(1-(1-Cyclohexyl-1H-tetrazol-5-yl)-2-methylpropyl)-3,4-diphenylisoquinolin-1(2H)-one (4n)

Compound **1n** (0.25 mmol, 81.9 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. The desired product could not be obtained.

2-(1-(1-Cyclohexyl-1H-tetrazol-5-yl)-2-phenylethyl)-3,4-diphenylisoquinolin-1(2H)-one (4o)

Compound **1o** (0.25 mmol, 93.9 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. The desired product could not be obtained.

2-((1-Benzyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4p)

Compound **1p** (0.25 mmol, 73.3 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4p** as a light yellow solid (87 mg, 74%). R_f = 0.18 (heptane/AcOEt, 2:1); mp 199-201 °C; FT-IR (KBr) ν 1637 (C=O), 1594 (C-H), 698 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.46 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.53 (dtd, *J* = 22.5, 7.3, 1.4 Hz, 2H), 7.25 (ddt, *J* = 10.0, 5.4, 2.7 Hz, 5H), 7.21 – 7.12 (m, 7H), 7.12 – 7.08 (m, 2H), 7.07 – 7.02 (m, 2H), 5.67 (s, 2H), 5.05 (s, 2H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 162.40 (C), 151.76 (C), 140.14 (C), 137.49 (C), 136.00 (C), 133.71 (C), 133.49 (C), 132.82 (CH), 131.33 (CH), 130.52 (CH), 129.14 (CH), 128.75 (CH), 128.72 (CH), 128.17 (CH), 127.96 (CH), 127.76 (CH), 127.37 (CH), 127.08 (CH), 126.99 (CH), 125.76 (CH), 124.53 (C), 120.24 (C), 51.03 (CH₂), 39.04 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₃₀H₂₄N₅O 470.1975, Found 470.1955.

2-((1-(4-Methoxyphenyl)-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4q)

Compound **1q** (0.25 mmol, 77.3 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4q** as a yellow solid (80 mg, 66%). R_f = 0.16 (heptane/AcOEt, 2:1); mp 227 °C; FT-IR (KBr) ν 1641 (C=O), 1595 (C-H), 697 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.45 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.60 – 7.47 (m, 2H), 7.35 – 7.29 (m, 2H), 7.27 – 7.23 (m, 2H), 7.18 (td, *J* = 7.4, 5.2 Hz, 7H), 7.13 – 7.08 (m, 2H), 7.00 – 6.95 (m, 2H), 5.19 (s, 2H), 3.84 (s, 3H); ¹³C {¹H} NMR (101 MHz, CDCl₃)

δ 162.32 (C), 161.01 (C), 152.29 (C), 140.12 (C), 137.52 (C), 136.06 (C), 134.02 (C), 132.75 (CH), 131.39 (CH), 130.29 (CH), 128.71 (CH), 128.25 (CH), 127.99 (CH), 127.88 (CH), 127.01 (CH), 126.59 (CH), 125.91 (C), 125.72 (CH), 124.62 (C), 120.10 (C), 114.83 (CH), 55.65 (CH₃), 40.14 (CH₂); HRMS (ESI/TOF) m/z : Not found.

2-((1-(tert-Butyl)-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one (4r)

Compound **1r** (0.25 mmol, 64.8 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4r** as a yellow solid (50 mg, 46%). R_f = 0.33 (heptane/AcOEt, 1:1); mp 269-272 °C; FT-IR (KBr) ν 1650 (C=O), 1601 (C-H), 699 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.51 (dd, J = 8.0, 1.5 Hz, 1H), 7.57 (ddd, J = 8.3, 7.1, 1.6 Hz, 1H), 7.51 (td, J = 7.6, 7.1, 1.3 Hz, 1H), 7.23 – 7.07 (m, 11H), 5.38 (s, 2H), 1.52 (s, 9H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 162.38 (C), 151.31 (C), 140.07 (C), 137.64 (C), 136.12 (C), 134.18 (C), 132.70 (CH), 131.43 (CH), 130.19 (CH), 128.59 (CH), 128.16 (CH), 128.08 (CH), 127.95 (CH), 126.96 (CH), 126.94 (CH), 125.70 (CH), 124.74 (C), 119.97 (C), 60.67 (C), 41.75 (CH₂), 29.24 (CH₃); HRMS (ESI/TOF) m/z : [M + H]⁺ Calcd for C₂₇H₂₆N₅O 436.2132, Found 436.2121.

Methyl 2-(5-((1-oxo-3,4-diphenylisoquinolin-2(1H)-yl)methyl)-1H-tetrazol-1-yl)acetate (4s)

Compound **1s** (0.25 mmol, 68.8 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4s** as a yellow solid (15 mg, 13%). R_f = 0.27 (heptane/AcOEt, 1:1); mp 206-208 °C; FT-IR (KBr) ν 1753 (C=O), 1646 (C=O), 1599 (C-H), 696 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.39 (dd, J = 7.9, 1.5 Hz, 1H), 7.56 (dd, J = 8.0, 1.5 Hz, 1H), 7.53 – 7.47 (m, 1H), 7.41 (dd, J = 6.6, 2.9 Hz, 2H), 7.25 (d, J = 2.1 Hz, 2H), 7.24 – 7.14 (m, 5H), 7.13 – 7.08 (m, 2H), 5.58 (s, 2H), 5.19 (s, 2H), 3.65 (s, 3H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 166.58 (C), 162.51 (C), 152.62 (C), 140.48 (C), 137.56 (C), 136.01 (C), 133.55 (C), 132.94 (CH), 131.35 (CH), 130.84 (CH), 128.94 (CH), 128.32 (CH), 128.02 (CH), 127.56 (CH), 127.13 (CH), 127.07 (CH), 125.85 (CH), 124.26 (C), 120.56 (C), 53.06 (CH₃), 48.34 (CH₂), 38.89 (CH₂); HRMS (ESI/TOF) m/z : Not found.

3,4-Bis(4-bromophenyl)-2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)isoquinolin-1(2H)-one (4t)

Compound **1a** (0.25 mmol, 71.3 mg), 1,2-bis(4-bromophenyl)ethyne (**3b**, 0.375 mmol, 126 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4t** as a yellow solid (154 mg, 99%). R_f = 0.14 (heptane/AcOEt, 3:1); mp 234-235 °C; FT-IR (KBr) ν 1651 (C=O), 1600 (C-H); ¹H NMR (600 MHz, CDCl₃) δ 8.46 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.63 – 7.58 (m, 1H), 7.56 – 7.52 (m, 1H), 7.43 – 7.37 (m, 4H), 7.28 – 7.23 (m, 2H), 7.14 (d, *J* = 8.2 Hz, 1H), 7.01 (d, *J* = 8.3 Hz, 2H), 5.16 (s, 2H), 4.31 (tt, *J* = 11.3, 4.0 Hz, 1H), 2.07 – 2.02 (m, 2H), 2.00 – 1.92 (m, 4H), 1.77 (d, *J* = 13.2 Hz, 1H), 1.49 – 1.39 (m, 2H), 1.37 – 1.31 (m, 1H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 162.13 (C), 150.60 (C), 139.22 (C), 136.98 (C), 134.84 (C), 133.04 (CH), 132.97 (CH), 132.61 (C), 132.12 (CH), 131.75 (CH), 131.54 (CH), 128.00 (CH), 127.45 (CH), 125.48 (CH), 124.66 (C), 123.55 (C), 121.59 (C), 119.11 (C), 58.24 (CH), 39.37 (CH₂), 32.68 (CH₂), 25.24 (CH₂), 24.85 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₂₉H₂₆Br₂N₅O 618.0500, Found 618.0478.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-bis(4-methoxyphenyl)isoquinolin-1(2H)-one (4u)

Compound **1a** (0.25 mmol, 71.3 mg), 1,2-bis(4-methoxyphenyl)ethyne (**3c**, 0.375 mmol, 79.9 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4u** as a yellow solid (68 mg, 58%). R_f = 0.14 (heptane/AcOEt, 2:1); mp 181-184 °C; FT-IR (KBr) ν 1649 (C=O), 1607 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 8.44 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.47 (td, *J* = 7.6, 7.2, 1.2 Hz, 1H), 7.24 – 7.16 (m, 3H), 7.04 – 6.98 (m, 2H), 6.78 – 6.73 (m, 2H), 6.73 – 6.67 (m, 2H), 5.21 (s, 2H), 4.22 (tt, *J* = 11.4, 4.4 Hz, 1H), 3.76 (s, 3H), 3.72 (s, 3H), 2.02 – 1.87 (m, 6H), 1.73 (d, *J* = 12.2 Hz, 1H), 1.46 – 1.29 (m, 3H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 162.41 (C), 159.43 (C), 158.27 (C), 150.94 (C), 140.34 (C), 137.92 (C), 132.66 (CH), 132.41 (CH), 132.21 (CH), 131.74 (CH), 128.50 (C), 127.81 (CH), 126.85 (CH), 126.44 (C), 125.74 (CH), 124.58 (C), 120.06 (C), 115.71 (CH), 113.60 (CH), 113.47 (CH), 58.03 (CH), 55.43 (CH₃), 55.11 (CH₃), 39.40 (CH₂), 32.63 (CH₂), 25.20 (CH₂), 24.85 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₃₁H₃₂N₅O₃ 522.2500, Found 522.2475.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-di(thiophen-2-yl)isoquinolin-1(2H)-one (4v)

Compound **1a** (0.25 mmol, 71.3 mg), 1,2-di(thiophen-2-yl)ethyne **3d** (0.375 mmol, 79.9 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol,

7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **4v** as a brown solid (72 mg, 85%). $R_f = 0.24$ (heptane/AcOEt, 2:1); mp 248-253 °C; FT-IR (KBr) ν 1655 (C=O), 1601 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 8.43 (d, $J = 7.9$ Hz, 1H), 7.68 – 7.59 (m, 1H), 7.53 (t, $J = 7.5$ Hz, 1H), 7.41 (d, $J = 8.1$ Hz, 1H), 7.29 (dd, $J = 10.5, 5.2$ Hz, 2H), 7.17 (d, $J = 3.5$ Hz, 1H), 6.94 (dd, $J = 5.1, 3.6$ Hz, 1H), 6.89 (q, $J = 3.1, 2.6$ Hz, 2H), 5.31 (s, 2H), 4.37 – 4.19 (m, 1H), 2.14 – 1.84 (m, 6H), 1.49 – 1.21 (m, 4H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 162.19 (C), 150.78 (C), 137.40 (C), 136.40 (C), 135.16 (C), 133.55 (C), 133.09 (CH), 131.68 (CH), 129.98 (CH), 128.43 (CH), 127.85 (CH), 127.79 (CH), 126.94 (CH), 126.74 (CH), 126.55 (CH), 125.90 (CH), 124.81 (C), 115.81 (C), 58.16 (CH), 39.63 (CH_2), 32.65 (CH_2), 25.23 (CH_2), 24.84 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{25}\text{H}_{24}\text{N}_5\text{OS}_2$ 474.1417, Found 474.1394.

1-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-5,6-diphenylpyridin-2(1H)-one (5a)

Compound **2a** (0.25 mmol, 55.8 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **5a** as a light yellow solid (52 mg, 50%). $R_f = 0.16$ (heptane/AcOEt, 1:1); mp 230-235 °C; FT-IR (KBr) ν 1666 (C=O), 694 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 7.52 (d, $J = 9.4$ Hz, 1H), 7.43 – 7.36 (m, 2H), 7.28 (d, $J = 8.2$ Hz, 3H), 7.13 (d, $J = 6.4$ Hz, 3H), 6.99 (dd, $J = 7.2, 2.3$ Hz, 2H), 6.67 (d, $J = 9.3$ Hz, 1H), 5.14 (s, 2H), 4.32 (ddd, $J = 11.2, 8.8, 4.4$ Hz, 1H), 2.03 – 1.88 (m, 7H), 1.74 (d, $J = 12.7$ Hz, 1H), 1.42 – 1.30 (m, 3H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 162.13 (C), 150.39 (C), 146.46 (C), 143.01 (CH), 137.96 (C), 133.24 (C), 130.37 (CH), 129.49 (CH), 129.35 (CH), 128.60 (CH), 128.00, 126.74 (CH), 121.61 (C), 119.15 (CH), 58.15 (CH), 39.52 (CH_2), 32.69 (CH_2), 29.70 (CH_2), 25.25 (CH_2), 24.86 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{25}\text{H}_{26}\text{N}_5\text{O}$ 412.2132, Found 412.2115.

1-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3-methyl-5,6-diphenylpyridin-2(1H)-one (5b)

Compound **2b** (0.25 mmol, 62.3 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **5b** as a light yellow solid (94 mg, 89%). $R_f = 0.14$ (heptane/AcOEt, 2:1); mp 122-126 °C; FT-IR (KBr) ν 1637 (C=O), 701 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 7.41 (s, 1H), 7.39 – 7.33 (m, 2H), 7.30 – 7.21 (m, 3H), 7.15 – 7.06 (m, 3H), 6.99 (dd, $J = 7.5, 2.0$ Hz, 2H), 5.16 (s, 2H), 4.26 (tt, $J = 11.7,$

4.3 Hz, 1H), 2.20 (s, 3H), 2.04 – 1.89 (m, 6H), 1.44 – 1.24 (m, 4H). ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 162.43 (C), 150.70 (C), 143.64 (C), 140.38 (CH), 138.29 (C), 133.52 (C), 130.49 (CH), 129.51 (CH), 129.14 (CH), 128.51 (CH), 128.11 (C), 127.89 (CH), 126.54 (CH), 121.10 (C), 58.05 (CH), 39.88 (CH_2), 32.59 (CH_2), 25.18 (CH_2), 24.84 (CH_2), 17.11 (CH_3); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{26}\text{H}_{28}\text{N}_5\text{O}$ 426.2288, Found 426.2273.

1-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-dimethyl-5,6-diphenylpyridin-2(1H)-one (5c)

Compound **2c** (0.25 mmol, 65.9 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **5c** as a light yellow solid (55 mg, 50%). R_f = 0.14 (heptane/ AcOEt , 2:1); mp 175-177 °C; FT-IR (KBr) ν 1644 (C=O), 695 (C-H); ^1H NMR (600 MHz, CDCl_3) δ 7.28 – 7.22 (m, 2H), 7.19 – 7.12 (m, 5H), 7.10 (d, J = 7.2 Hz, 1H), 6.98 (d, J = 7.4 Hz, 2H), 5.12 (s, 2H), 4.24 (tt, J = 11.3, 4.1 Hz, 1H), 2.21 (s, 3H), 2.02 – 1.97 (m, 2H), 1.94 (s, 3H), 1.93 – 1.89 (m, 3H), 1.74 (d, J = 13.5 Hz, 1H), 1.44 – 1.25 (m, 4H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 161.94 (C), 150.81 (C), 146.78 (C), 142.85 (C), 137.64 (C), 133.93 (C), 130.83 (CH), 130.11 (CH), 128.61 (CH), 128.13 (CH), 127.83 (CH), 126.68 (CH), 125.12 (C), 123.25 (C), 58.00 (CH), 39.99 (CH_2), 32.57 (CH_2), 25.18 (CH_2), 24.85 (CH_2), 18.46 (CH_3), 13.40 (CH_3); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{27}\text{H}_{30}\text{N}_5\text{O}$ 440.2445, Found 440.2429.

6-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-4,5-diphenylfuro[2,3-c]pyridin-7(6H)-one (5d)

Compound **2d** (0.25 mmol, 68.8 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B during 24 h. Purification by LCC afforded compound **5d** as a light yellow solid (39 mg, 35%). R_f = 0.22 (heptane/ AcOEt , 1:1); mp 207-210 °C; FT-IR (KBr) ν 1685 (C=O), 703 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 7.75 (d, J = 1.9 Hz, 1H), 7.38 – 7.33 (m, 2H), 7.28 – 7.22 (m, 3H), 7.17 (d, J = 7.4 Hz, 3H), 7.11 – 7.06 (m, 2H), 6.50 (d, J = 1.9 Hz, 1H), 5.26 (s, 2H), 4.27 (ddd, J = 11.2, 6.9, 4.3 Hz, 1H), 2.02 – 1.86 (m, 6H), 1.78 – 1.68 (m, 1H), 1.46 – 1.27 (m, 3H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 152.98 (C), 150.60 (C), 148.72 (CH), 141.78 (C), 140.99 (C), 135.68 (C), 134.63 (C), 133.58 (C), 130.95 (CH), 130.13 (CH), 129.08 (CH), 128.42 (CH), 128.05 (CH), 127.05 (CH), 116.24 (C), 107.68 (CH), 58.14 (CH), 39.15 (CH_2), 32.65 (CH_2), 25.23 (CH_2), 24.86 (CH_2); HRMS (ESI/TOF) m/z : Not found.

*6-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-4,5-diphenylthieno[2,3-*c*]pyridin-7(6H)-one (5e)*

Compound **2e** (0.25 mmol, 72.8 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **5e** as a light yellow solid (112 mg, 96%). R_f = 0.14 (heptane/AcOEt, 2:1); mp 206-208 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.66 (d, *J* = 5.2 Hz, 1H), 7.34 (dd, *J* = 7.4, 2.1 Hz, 2H), 7.26 – 7.14 (m, 6H), 7.14 – 7.08 (m, 2H), 6.92 (d, *J* = 5.2 Hz, 1H), 5.25 (s, 2H), 4.29 – 4.17 (m, 1H), 2.04 – 1.84 (m, 6H), 1.73 (d, *J* = 12.1 Hz, 1H), 1.41 – 1.25 (m, 3H); ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 158.23 (C), 150.70 (C), 146.52 (C), 141.68 (C), 136.48 (C), 133.65 (C), 133.60 (CH), 130.71 (CH), 130.56 (CH), 128.94 (CH), 128.38 (C), 128.32 (CH), 127.98 (CH), 127.06 (CH), 125.09 (CH), 118.89 (C), 58.10 (CH), 39.36 (CH₂), 32.61 (CH₂), 25.20 (CH₂), 24.84 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₂₇H₂₆N₅OS 468.1852, Found 468.1847.

*6-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-1-methyl-4,5-diphenyl-1,6-dihydro-7H-pyrrolo[2,3-*c*]pyridin-7-one (5f)*

Compound **2f** (0.25 mmol, 72.1 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **5f** as a light yellow solid (110 mg, 95%). R_f = 0.22 (heptane/AcOEt, 3:1); mp 223-225 °C; FT-IR (KBr) ν 1654 (C=O), 703 (C-H); ¹H NMR (400 MHz, CDCl₃) δ 7.25 – 7.04 (m, 10H), 7.00 (d, *J* = 2.8 Hz, 1H), 6.04 (d, *J* = 2.8 Hz, 1H), 5.26 (s, 2H), 4.18 (s, 3H), 4.03 (dq, *J* = 9.7, 6.3, 5.2 Hz, 1H), 1.97 – 1.78 (m, 6H), 1.70 (d, *J* = 9.2 Hz, 1H), 1.29 (qt, *J* = 11.2, 7.8, 6.6 Hz, 3H); ¹³C {¹H} NMR (151 MHz, CDCl₃) δ 155.52 (C), 151.29 (C), 136.81 (C), 136.42 (C), 134.54 (C), 132.76 (C), 131.95 (CH), 131.08 (CH), 130.41 (CH), 128.46 (CH), 128.16 (CH), 127.73 (CH), 126.50 (CH), 121.56 (C), 117.60 (C), 102.63 (CH), 57.87 (CH), 38.72 (CH₂), 35.97 (CH₃), 32.50 (CH₂), 25.16 (CH₂), 24.82 (CH₂); HRMS (ESI/TOF) *m/z*: [M + H]⁺ Calcd for C₂₈H₂₉N₆O 465.2397, Found 465.2385.

*2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylbenzofuro[2,3-*c*]pyridin-1(2H)-one (5g)*

Compound **2g** (0.25 mmol, 81.3 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), Cu(OAc)₂ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and [RhCp*Cl₂]₂ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B during 18 h. Purification by LCC afforded

compound **5g** as a white solid (26 mg, 21%). $R_f = 0.12$ (heptane/AcOEt, 2:1); mp 263-265 °C; FT-IR (KBr) ν 1676 (C=O), 706 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 7.65 (d, $J = 8.4$ Hz, 1H), 7.47 (t, $J = 7.9$ Hz, 1H), 7.40 (dd, $J = 6.8, 2.8$ Hz, 2H), 7.28 – 7.19 (m, 8H), 7.09 (t, $J = 7.6$ Hz, 1H), 6.77 (d, $J = 7.9$ Hz, 1H), 5.30 (s, 2H), 4.35 (ddt, $J = 11.9, 9.1, 4.3$ Hz, 1H), 2.06 – 1.89 (m, 8H), 1.74 (d, $J = 12.6$ Hz, 1H), 1.44 – 1.29 (m, 3H); ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 157.23 (C), 153.83 (C), 150.38 (C), 142.45 (C), 141.59 (C), 135.33 (C), 133.16 (C), 130.82 (CH), 130.56 (CH), 129.36 (C), 129.10 (CH), 128.91 (CH), 128.36 (CH), 128.25 (CH), 127.65 (CH), 123.45 (CH), 123.21 (C), 123.15 (CH), 116.93 (C), 112.68 (CH), 58.21 (CH), 39.44 (CH_2), 32.70 (CH_2), 25.26 (CH_2), 24.87 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{31}\text{H}_{28}\text{N}_5\text{O}_2$ 502.2237, Found 502.2219.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylbenzo[4,5]thieno[2,3-c]pyridin-1(2H)-one (5h)

Compound **2h** (0.25 mmol, 85.4 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **5h** as a yellow solid (103 mg, 80%). $R_f = 0.28$ (heptane/AcOEt, 2:1); mp 246-248 °C; FT-IR (KBr) ν 1642 (C=O), 715 (C-H); ^1H NMR (600 MHz, CDCl_3) δ 7.92 (d, $J = 8.1$ Hz, 1H), 7.42 (t, $J = 7.6$ Hz, 1H), 7.35 (dd, $J = 6.6, 2.7$ Hz, 2H), 7.30 – 7.26 (m, 3H), 7.25 – 7.18 (m, 5H), 7.07 (t, $J = 7.8$ Hz, 1H), 6.60 (d, $J = 8.4$ Hz, 1H), 5.30 (s, 2H), 4.28 (tt, $J = 11.7, 4.2$ Hz, 1H), 2.04 – 1.99 (m, 2H), 1.97 – 1.89 (m, 4H), 1.75 (d, $J = 13.1$ Hz, 1H), 1.41 (qt, $J = 13.4, 2.9$ Hz, 2H), 1.34 – 1.27 (m, 1H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 158.47 (C), 150.46 (C), 142.86 (C), 142.76 (C), 140.63 (C), 136.31 (C), 135.58 (C), 133.34 (C), 131.05 (CH), 130.58 (CH), 129.03 (C), 128.91 (CH), 128.40 (CH), 128.24 (CH), 127.69 (CH), 127.56 (CH), 125.95 (CH), 124.39 (CH), 123.25 (CH), 119.38 (C), 58.14 (CH), 39.59 (CH_2), 32.63 (CH_2), 25.20 (CH_2), 24.85 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{31}\text{H}_{28}\text{N}_5\text{OS}$ 518.2009, Found 518.1994.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-5-methyl-3,4-diphenyl-2,5-dihydro-1H-pyrido[4,3-b]indol-1-one (5i)

Compound **2i** (0.25 mmol, 84.6 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **5i** as a

brown solid (20 mg, 16%). R_f = 0.18 (heptane/AcOEt, 2:1); mp 272-274 °C; FT-IR (KBr) ν 1645 (C=O), 708 (C-H); ^1H NMR (400 MHz, CDCl_3) δ 8.44 (d, J = 7.7 Hz, 1H), 7.45 – 7.26 (m, 5H), 7.19 (d, J = 9.4 Hz, 8H), 5.31 (s, 2H), 4.27 (t, J = 4.3 Hz, 1H), 3.15 (s, 3H), 2.00 – 1.84 (m, 6H), 1.45 – 1.22 (m, 4H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 159.12 (C), 151.13 (C), 144.23 (C), 143.24 (C), 140.02 (C), 135.36 (C), 133.99 (C), 131.84 (CH), 130.39 (CH), 128.68 (CH), 128.09 (CH), 128.07 (CH), 127.63 (CH), 124.52 (CH), 124.03 (C), 121.89 (CH), 121.81 (CH), 111.70 (C), 108.90 (CH), 106.86 (C), 57.99 (CH), 38.82 (CH_2), 32.61 (CH_2), 31.85 (CH_3), 25.19 (CH_2), 24.87 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{32}\text{H}_{31}\text{N}_6\text{O}$ 515.2554, Found 515.2540.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenyl-2,6-naphthyridin-1(2H)-one (5j)

Compound **2j** (0.25 mmol, 71.6 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B. Purification by LCC afforded compound **5j** as a white solid (57 mg, 49%). R_f = 0.35 (heptane/AcOEt, 0:1); mp 210-212 °C; FT-IR (KBr) ν 1666 (C=O), 697 (C-H); ^1H NMR (600 MHz, CDCl_3) δ 8.95 – 8.45 (m, 2H), 8.21 (d, J = 5.1 Hz, 1H), 7.36 – 7.29 (m, 2H), 7.22 (dp, J = 8.6, 5.5, 3.6 Hz, 6H), 7.14 (d, J = 7.3 Hz, 2H), 5.22 (s, 2H), 4.17 (ddt, J = 11.0, 8.1, 4.0 Hz, 1H), 1.97 – 1.89 (m, 6H), 1.74 (d, J = 12.9 Hz, 1H), 1.40 – 1.26 (m, 3H); ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) δ 161.25 (C), 150.33 (C), 149.50 (CH), 146.58 (CH), 142.09 (C), 134.25 (C), 133.20 (C), 131.23 (CH), 130.36 (CH), 129.23 (C), 129.09 (CH), 128.39 (CH), 128.25 (CH), 127.52 (CH), 119.63 (CH), 118.40 (C), 58.17 (CH), 39.73 (CH_2), 32.55 (CH_2), 25.17 (CH_2), 24.79 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{28}\text{H}_{27}\text{N}_6\text{O}$ 463.2241, Found 463.2236.

5-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-6,7-diphenylthiazolo[5,4-c]pyridin-4(5H)-one (5k)

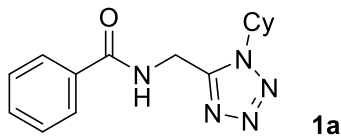
Compound **2k** (0.25 mmol, 73.1 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg) were reacted according to general procedure B during 18 h. The desired product could not be obtained.

2-((1-Cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylbenzo[h]isoquinolin-1(2H)-one (5l)

Compound **2l** (0.25 mmol, 78.9 mg), diphenylacetylene (**3a**, 0.375 mmol, 66.8 mg), $\text{Cu}(\text{OAc})_2$ (0.5 mmol, 90.8 mg), CsOAc (0.125 mmol, 24.0 mg) and $[\text{RhCp}^*\text{Cl}_2]_2$ (0.0125 mmol, 7.7 mg)

were reacted according to general procedure B. Purification by LCC afforded compound **51** as a light yellow solid (94 mg, 73%). $R_f = 0.14$ (heptane/AcOEt, 5:1); mp 203-205 °C; FT-IR (KBr) ν 1640 (C=O), 704 (C-H); ^1H NMR (600 MHz, CDCl_3) δ 10.16 (d, $J = 8.8$ Hz, 1H), 7.94 (d, $J = 8.9$ Hz, 1H), 7.90 (dd, $J = 8.0, 1.4$ Hz, 1H), 7.76 (ddd, $J = 8.6, 6.9, 1.5$ Hz, 1H), 7.63 (ddd, $J = 8.0, 6.9, 1.2$ Hz, 1H), 7.38 (dd, $J = 6.6, 2.9$ Hz, 2H), 7.28 – 7.20 (m, 7H), 7.19 – 7.15 (m, 2H), 5.35 (s, 2H), 4.38 (tt, $J = 11.4, 3.9$ Hz, 1H), 2.10 – 2.04 (m, 2H), 2.02 – 1.94 (m, 4H), 1.81 – 1.74 (m, 1H), 1.50 – 1.40 (m, 2H), 1.35 (tt, $J = 12.7, 3.1$ Hz, 1H); ^{13}C { ^1H } NMR (151 MHz, CDCl_3) δ 162.29 (C), 150.93 (C), 142.25 (C), 139.04 (C), 136.75 (C), 134.24 (C), 134.04 (CH), 132.26 (C), 131.80 (C), 131.69 (CH), 130.33 (CH), 128.73 (CH), 128.61 (CH), 128.27 (CH), 128.23 (CH), 128.10 (CH), 127.44 (CH), 127.06 (CH), 126.57 (CH), 123.55 (CH), 120.32 (C), 118.33 (C), 58.10 (CH), 40.03 (CH_2), 32.70 (CH_2), 25.26 (CH_2), 24.91 (CH_2); HRMS (ESI/TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{33}\text{H}_{30}\text{N}_5\text{O}$ 512.2445, Found 512.2422.

IR and NMR spectra of *N*-acyl aminomethyl tetrazoles



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

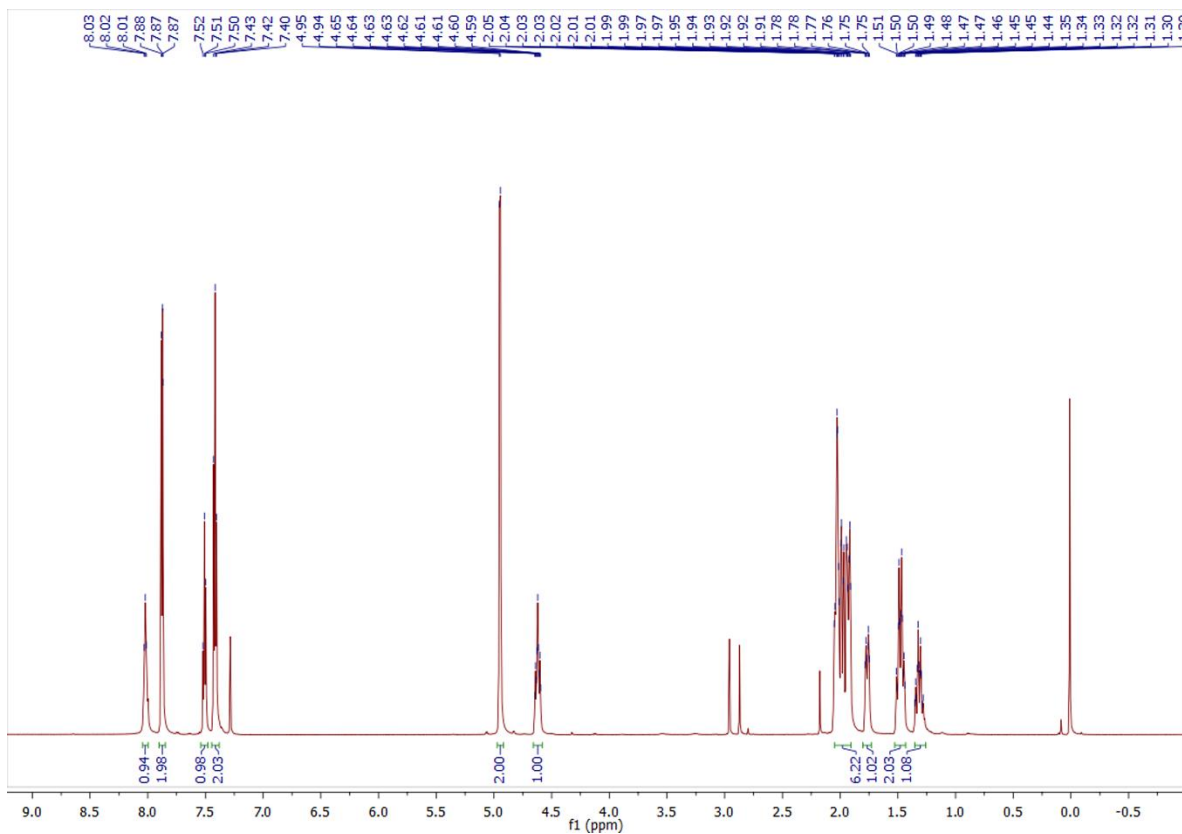
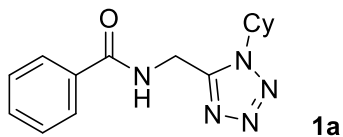


Figure S1. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **1a**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

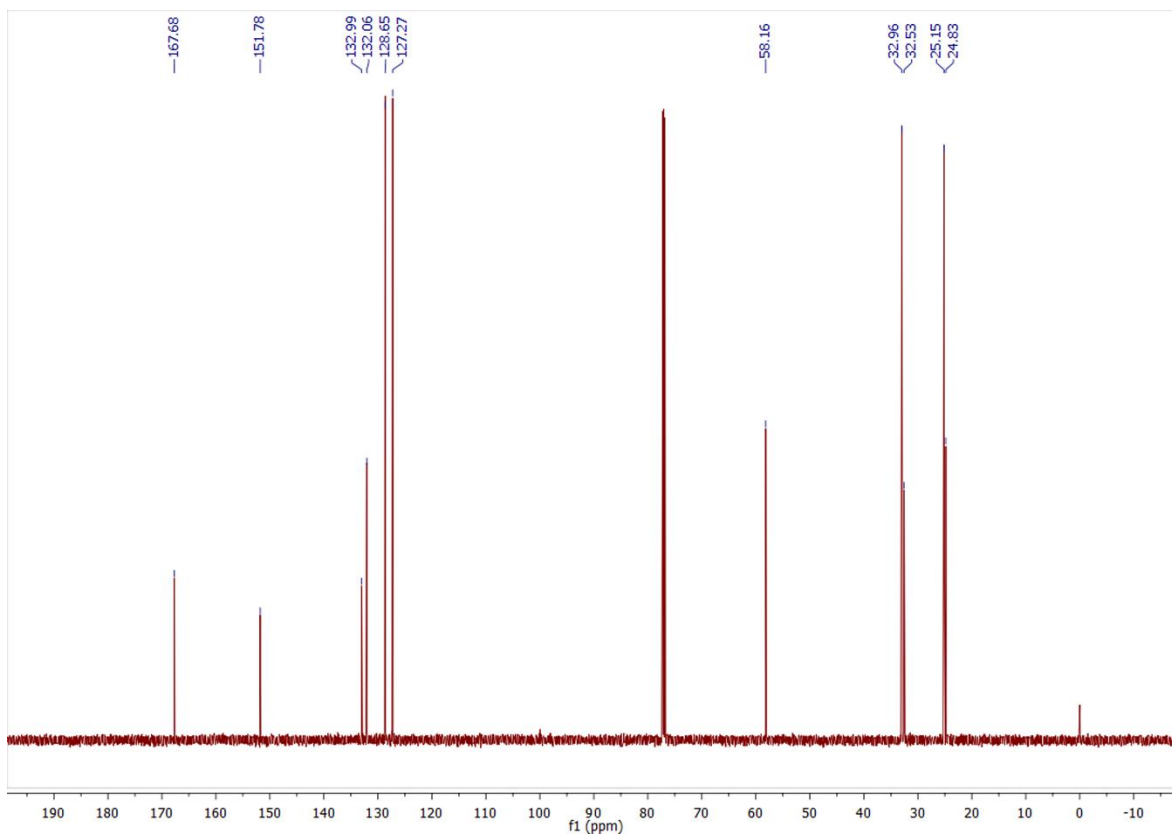
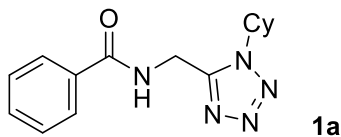
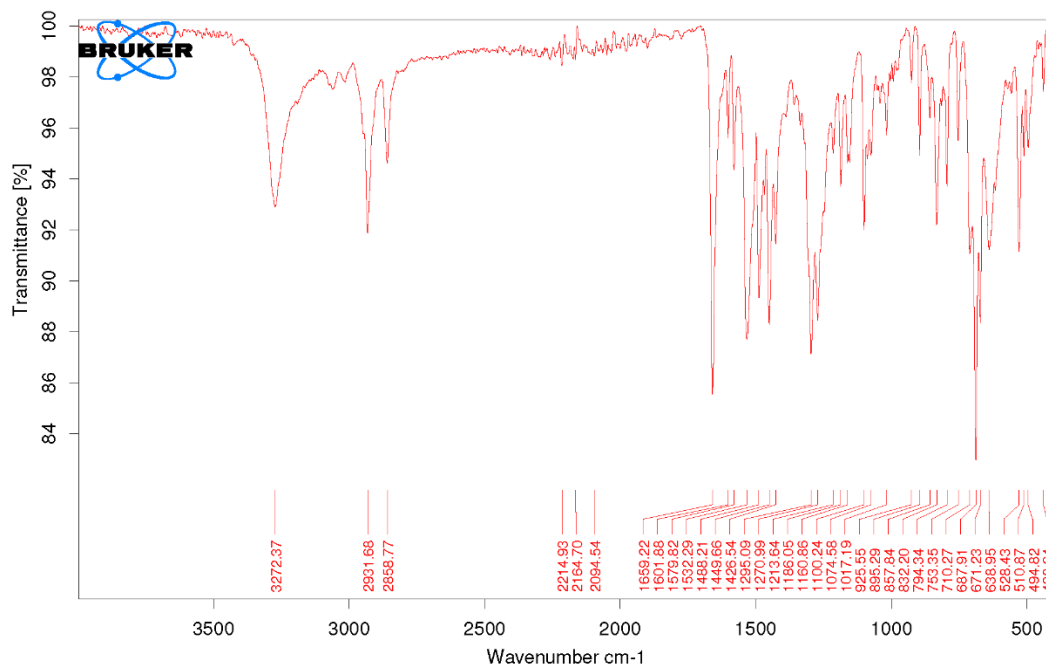


Figure S2. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1a**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide



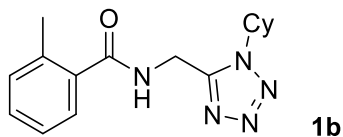
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Figure S3. FT-IR (KBr) spectrum of compound **1a**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-2-methylbenzamide

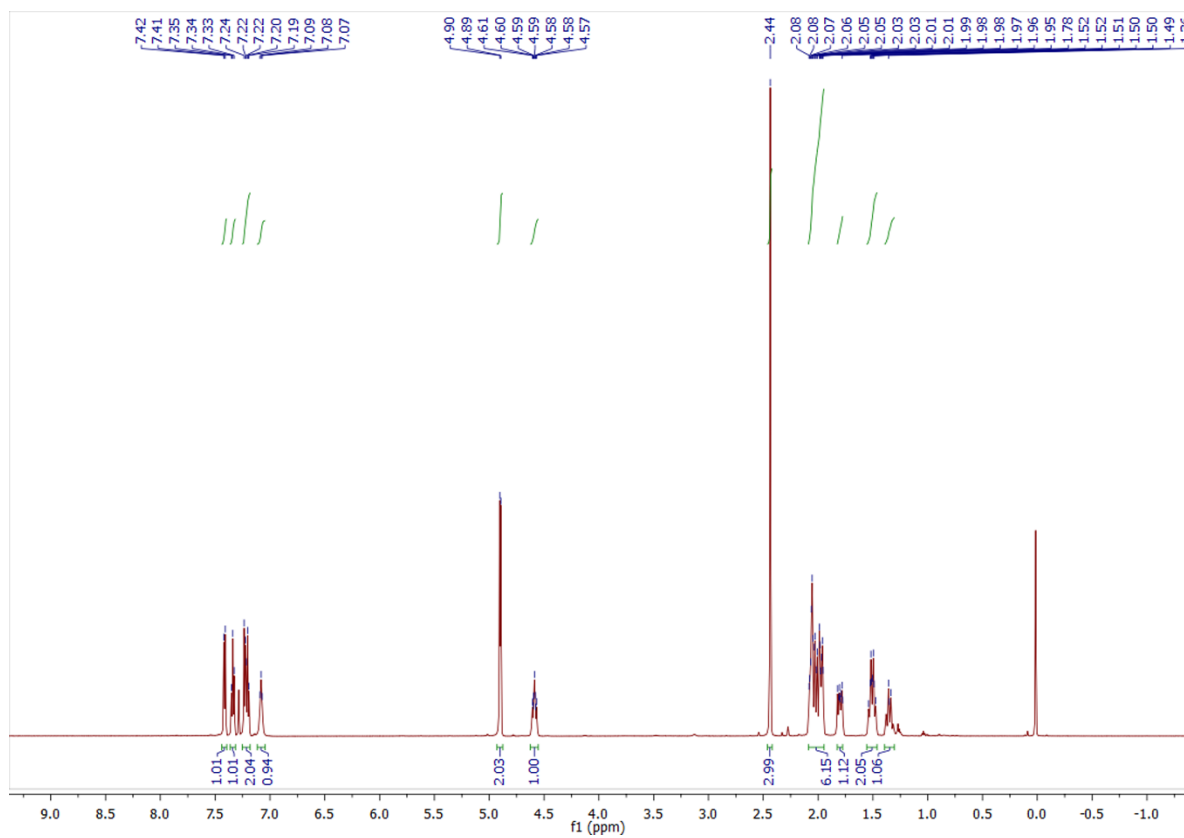
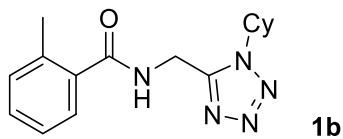


Figure S4. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **1b**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-2-methylbenzamide

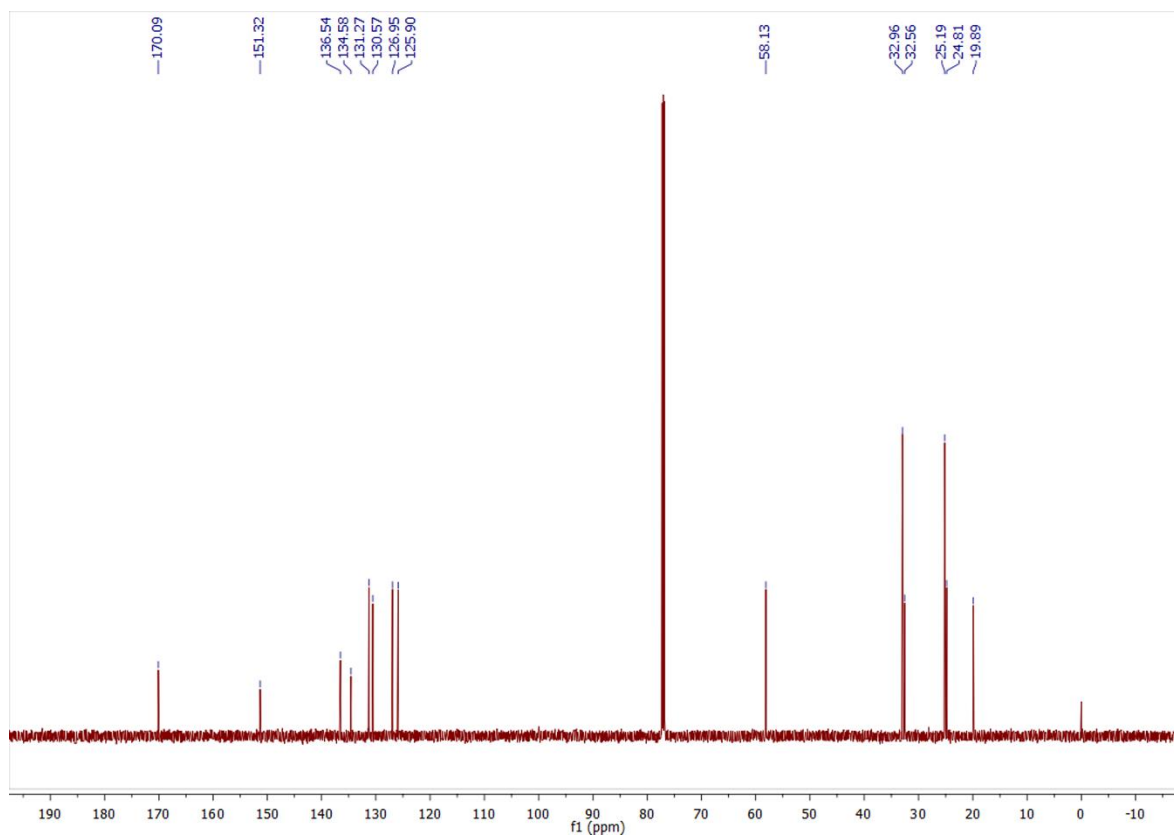
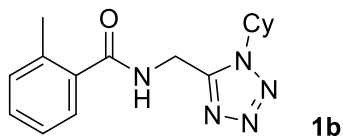
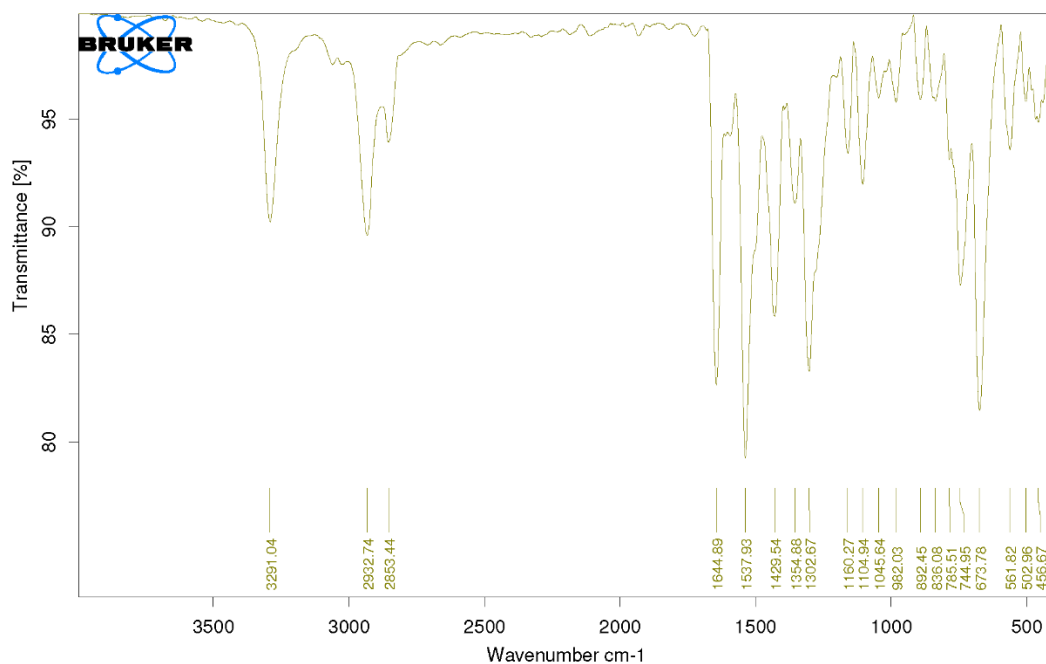


Figure S5. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1b**.



1b
N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-2-methylbenzamide



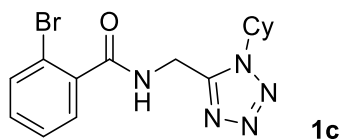
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GM-093

Instrument type and / or accessory

10/12/2018

Figure S6. FT-IR (KBr) spectrum of compound **1b**.



2-bromo-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide

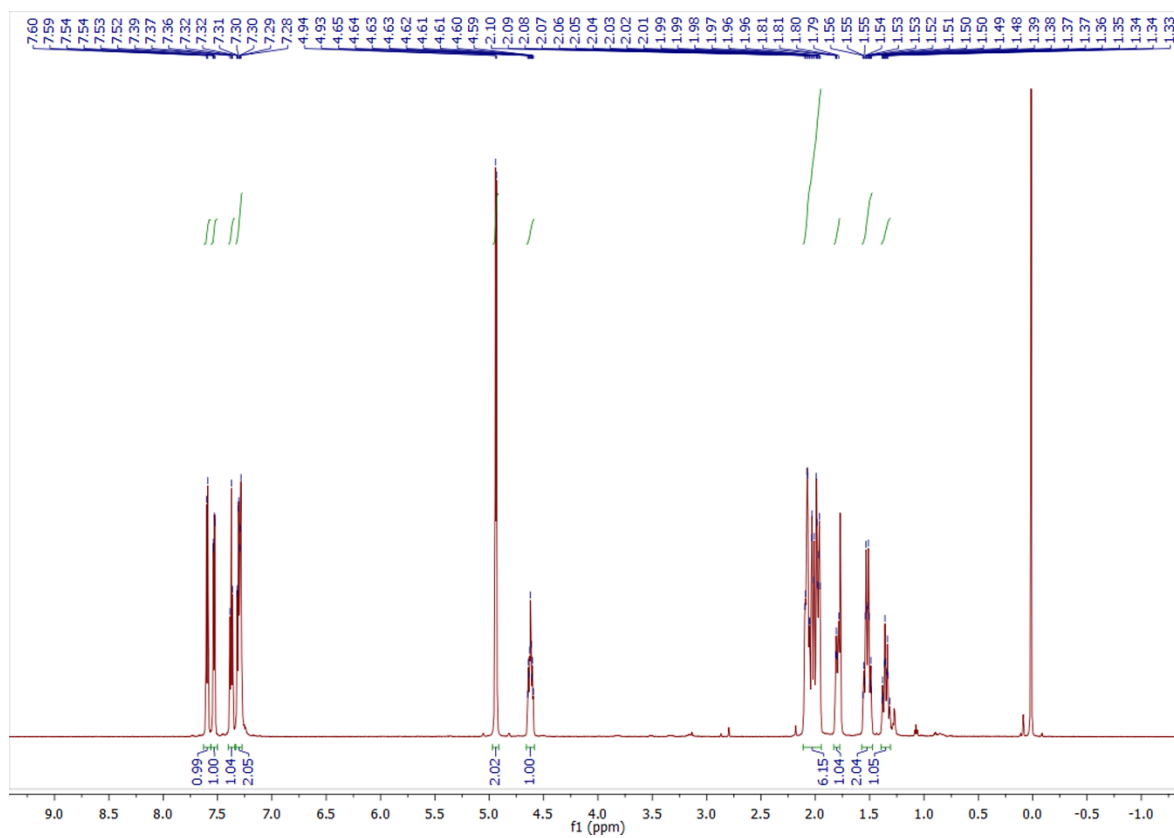
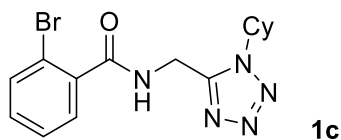


Figure S7. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **1c**.



2-bromo-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

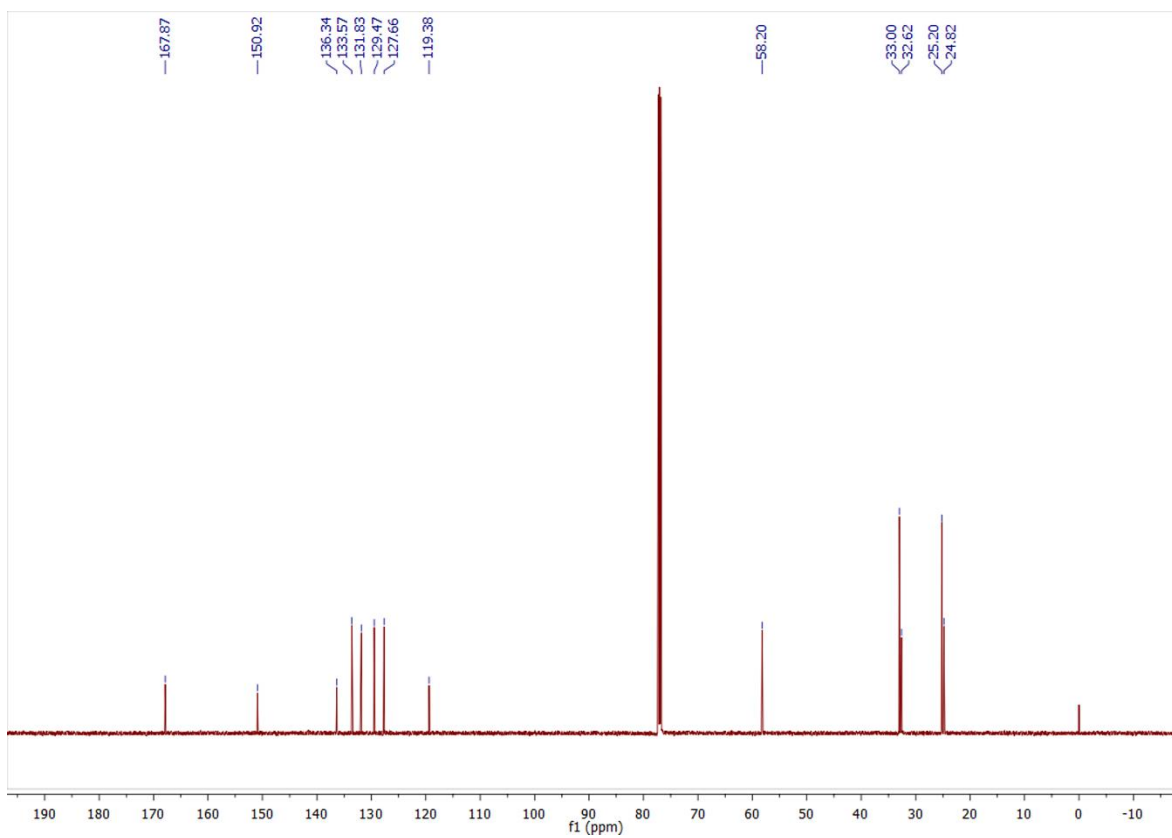
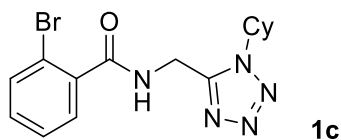
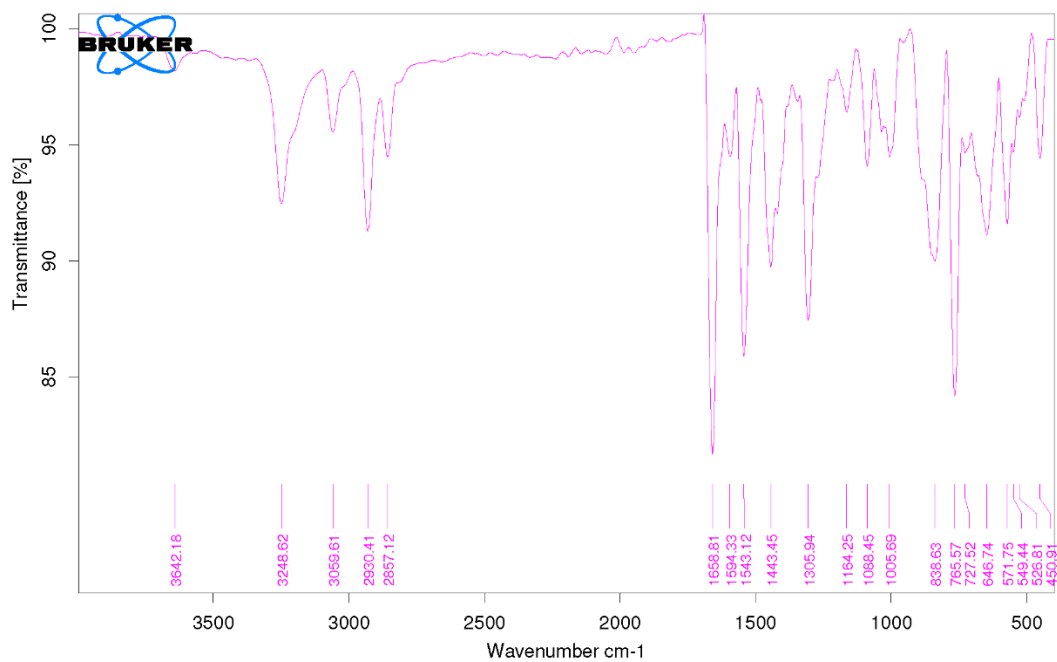


Figure S8. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1c**.



1c
2-bromo-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide



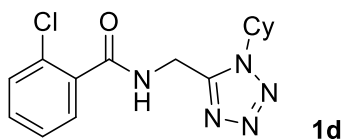
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Instrument type and / or accessory

10/12/2018

Figure S9. FT-IR (KBr) spectrum of compound **1c**.



2-chloro-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide

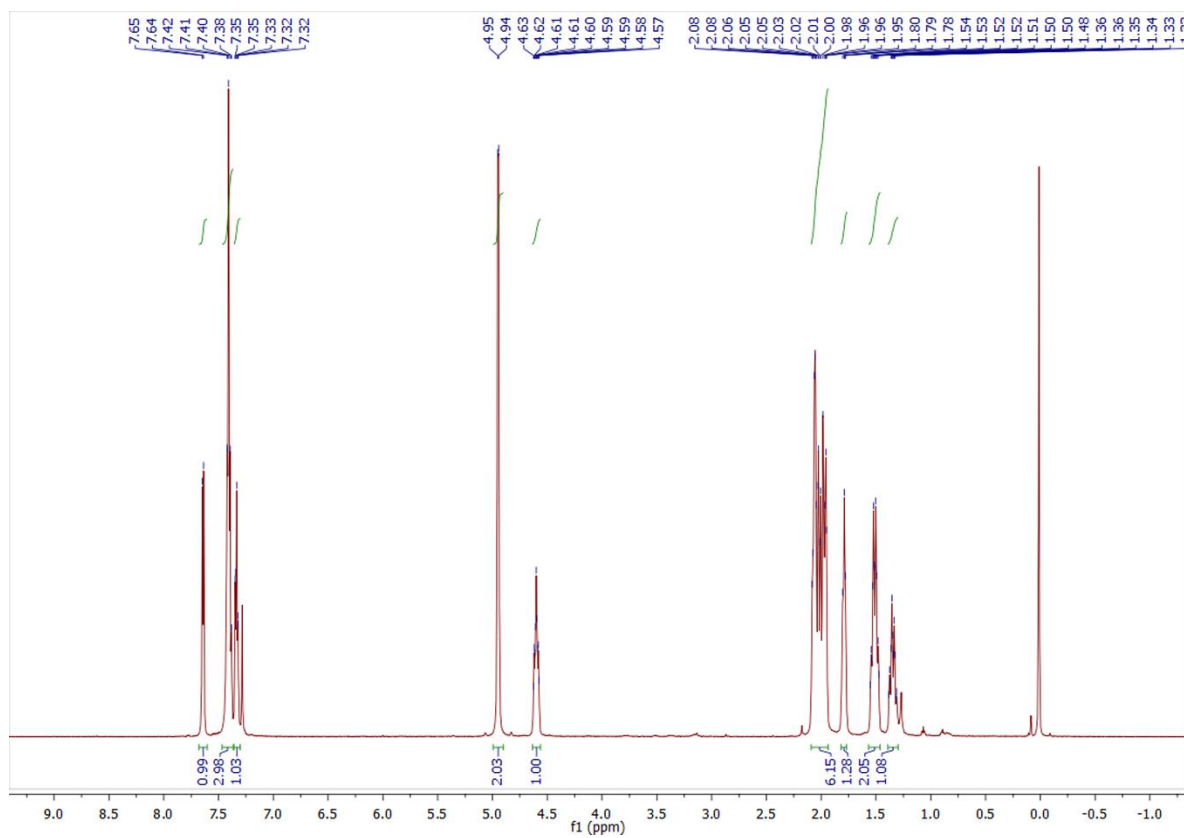
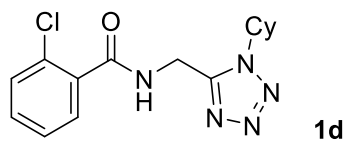


Figure S10. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **1d**.



2-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

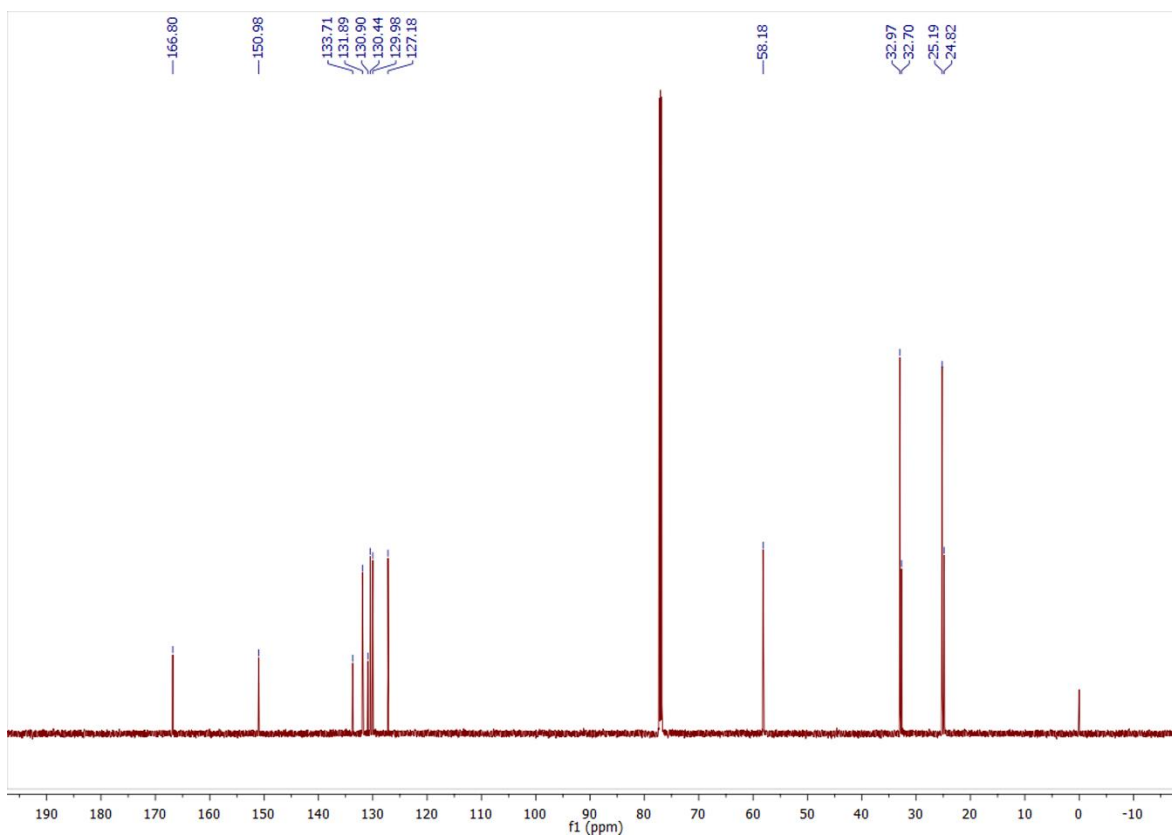
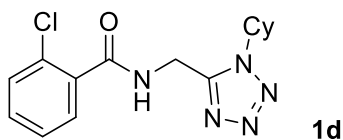
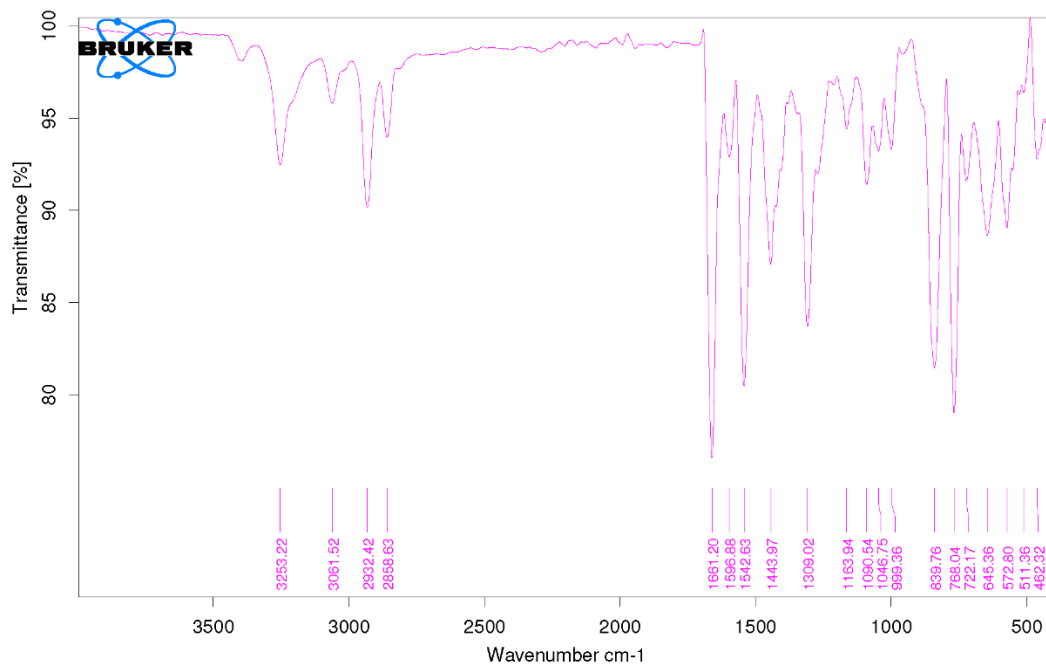


Figure S11. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1d**.



1d
2-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide



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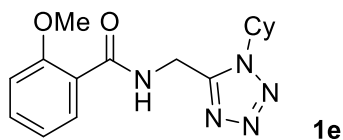
GM-097

Instrument type and / or accessory

10/12/2018

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Figure S12. FT-IR (KBr) spectrum of compound **1d**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-2-methoxybenzamide

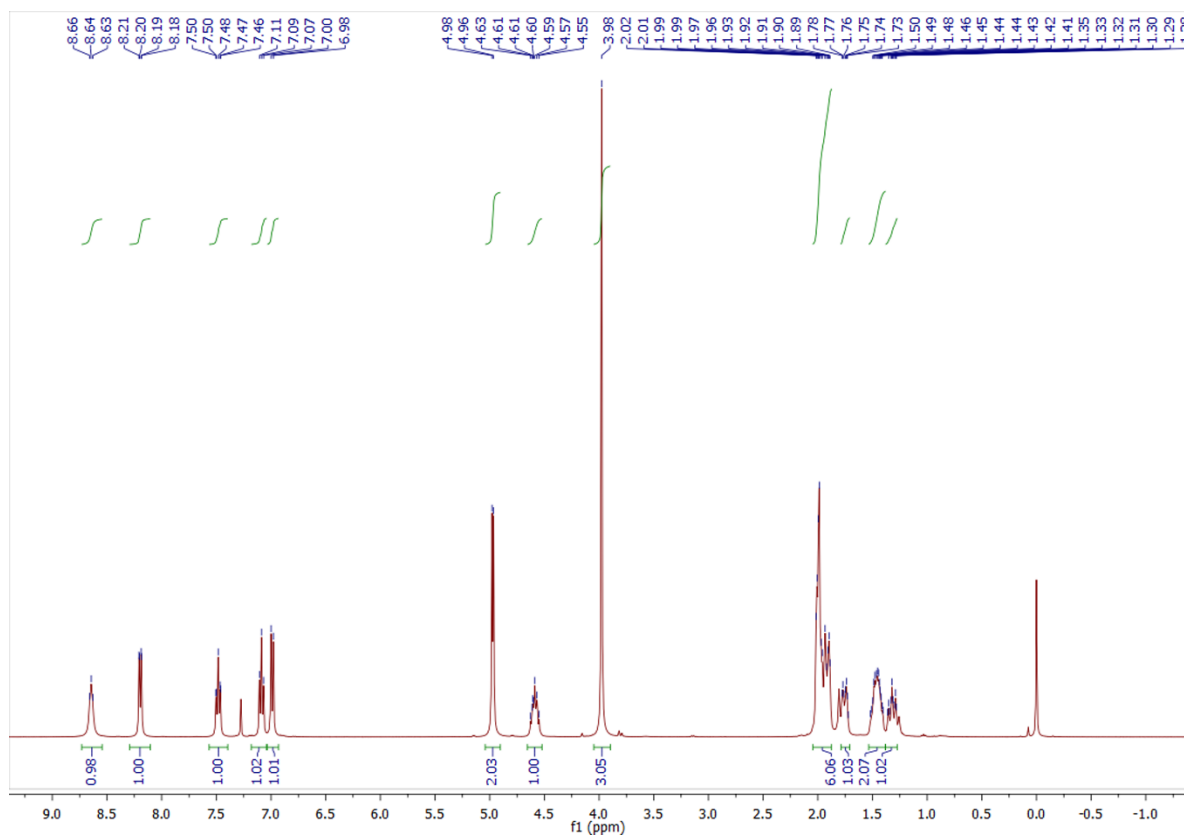
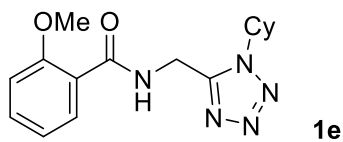


Figure S13. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **1e**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-2-methoxybenzamide

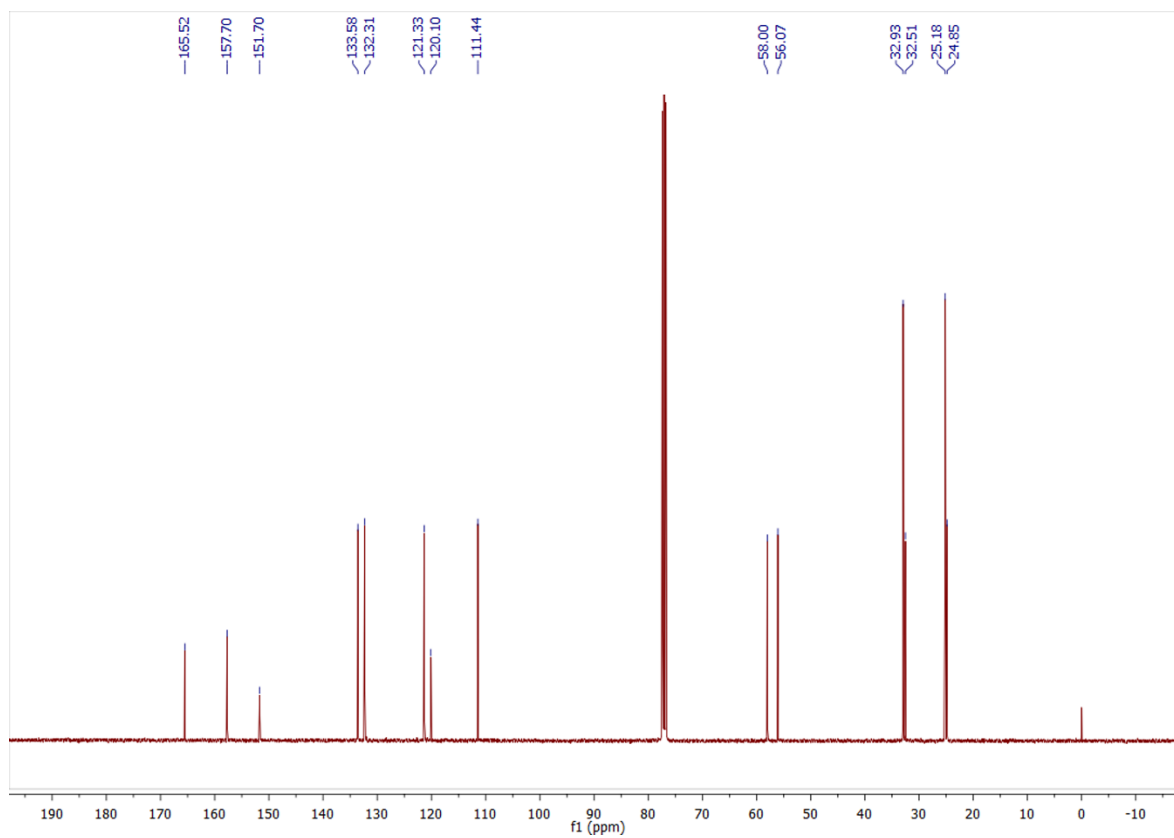
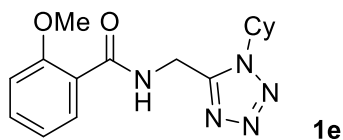
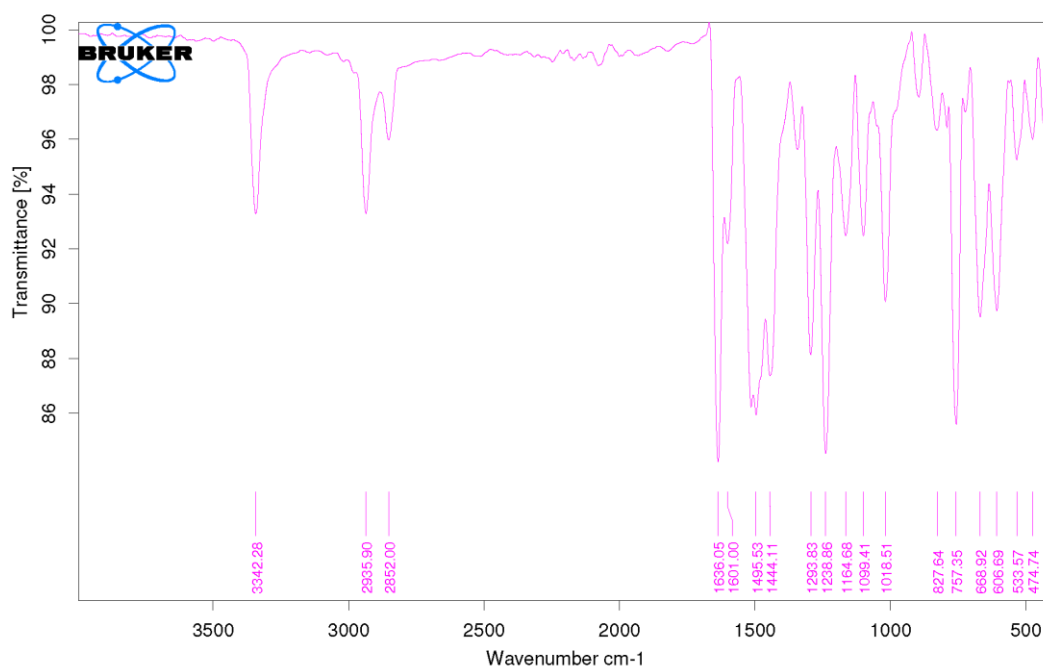


Figure S14. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **1e**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-2-methoxybenzamide



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Instrument type and / or accessory

1/21/2019

Figure S15. FT-IR (KBr) spectrum of compound **1e**.

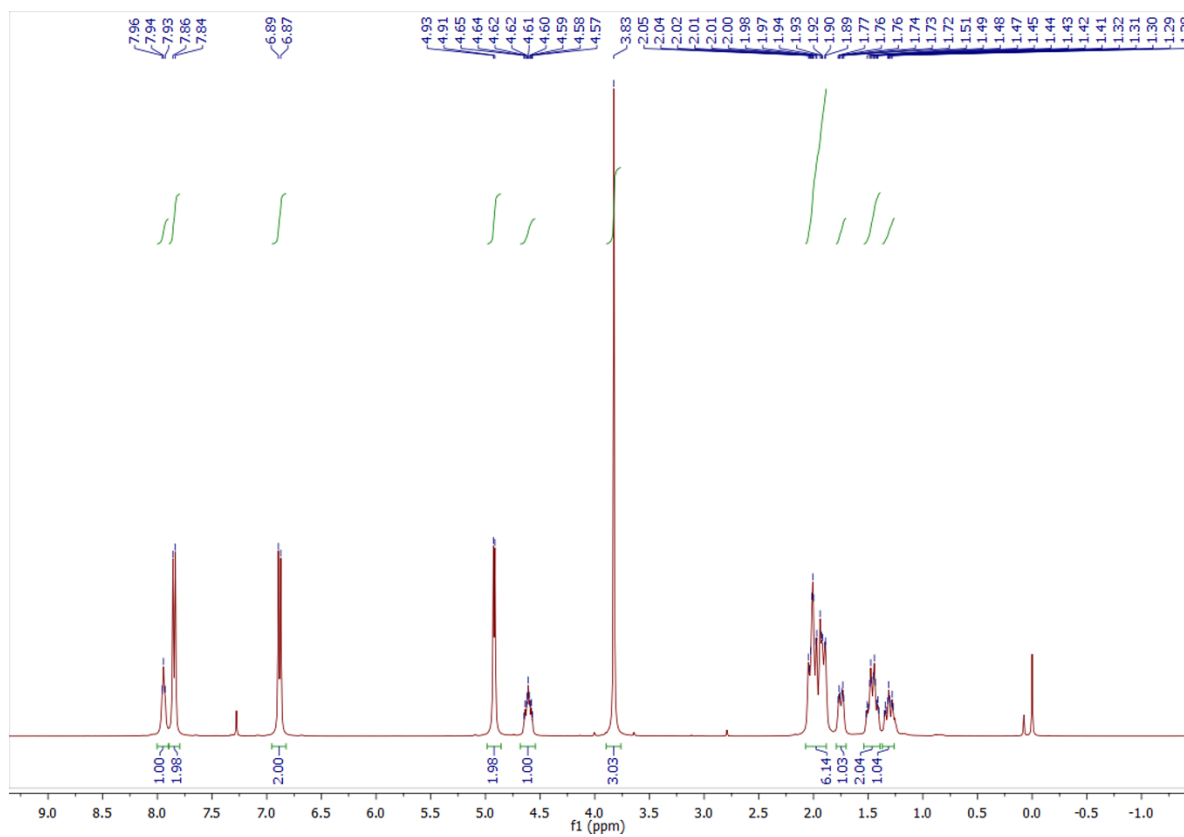
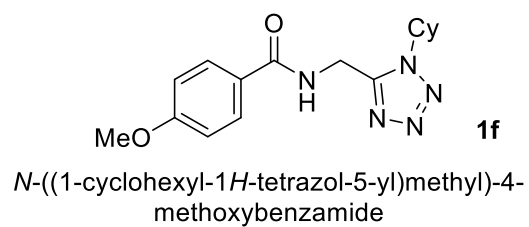


Figure S16. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **1f**.

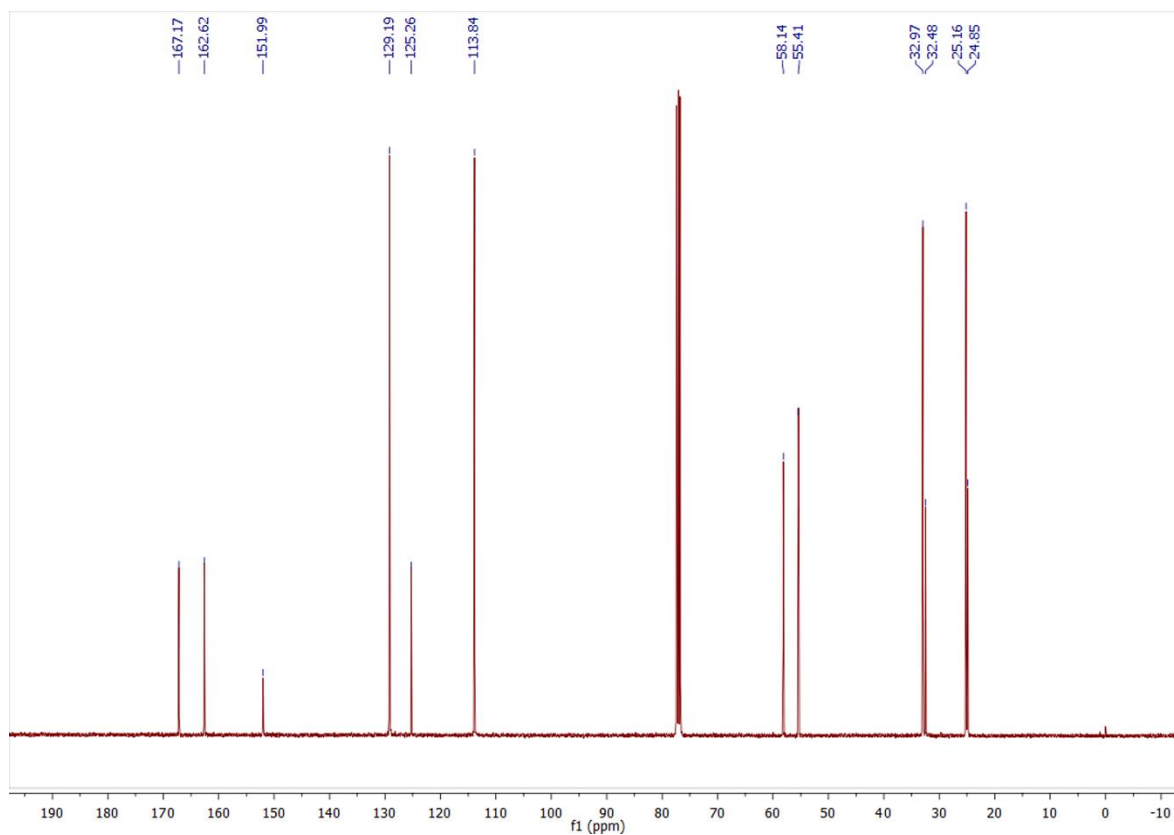
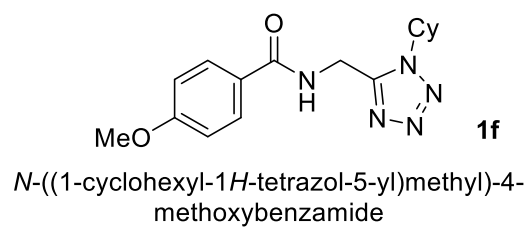
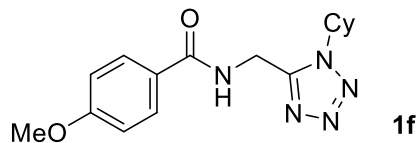
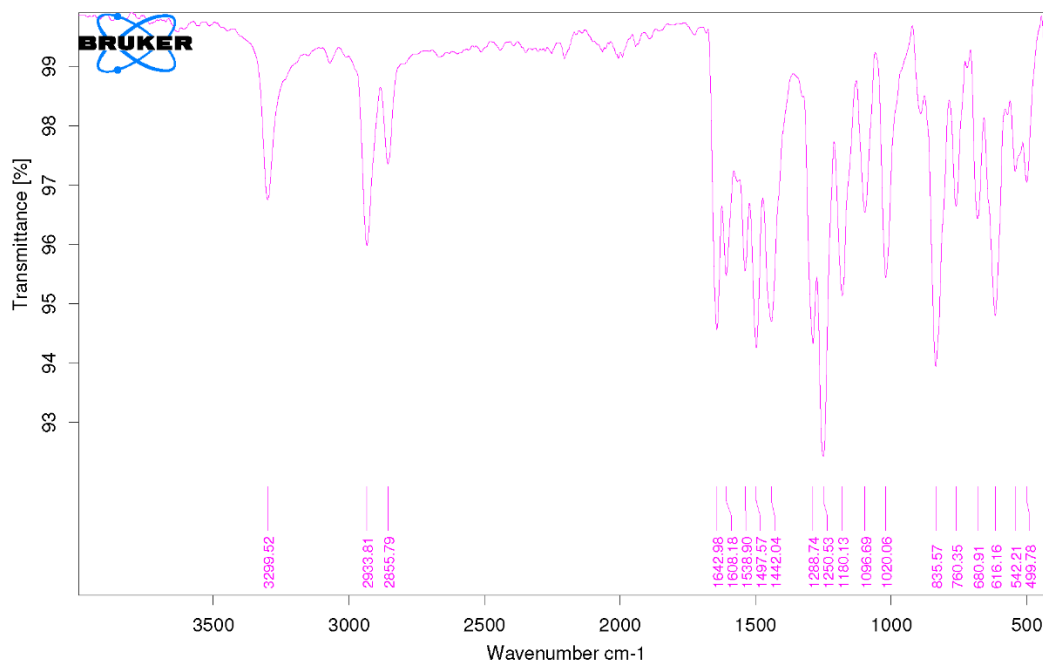


Figure S17. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, $\text{DMSO-}d_6$) spectrum of compound **1f**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-4-methoxybenzamide



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Instrument type and / or accessory

8/24/2018

Figure S18. FT-IR (KBr) spectrum of compound **1f**.

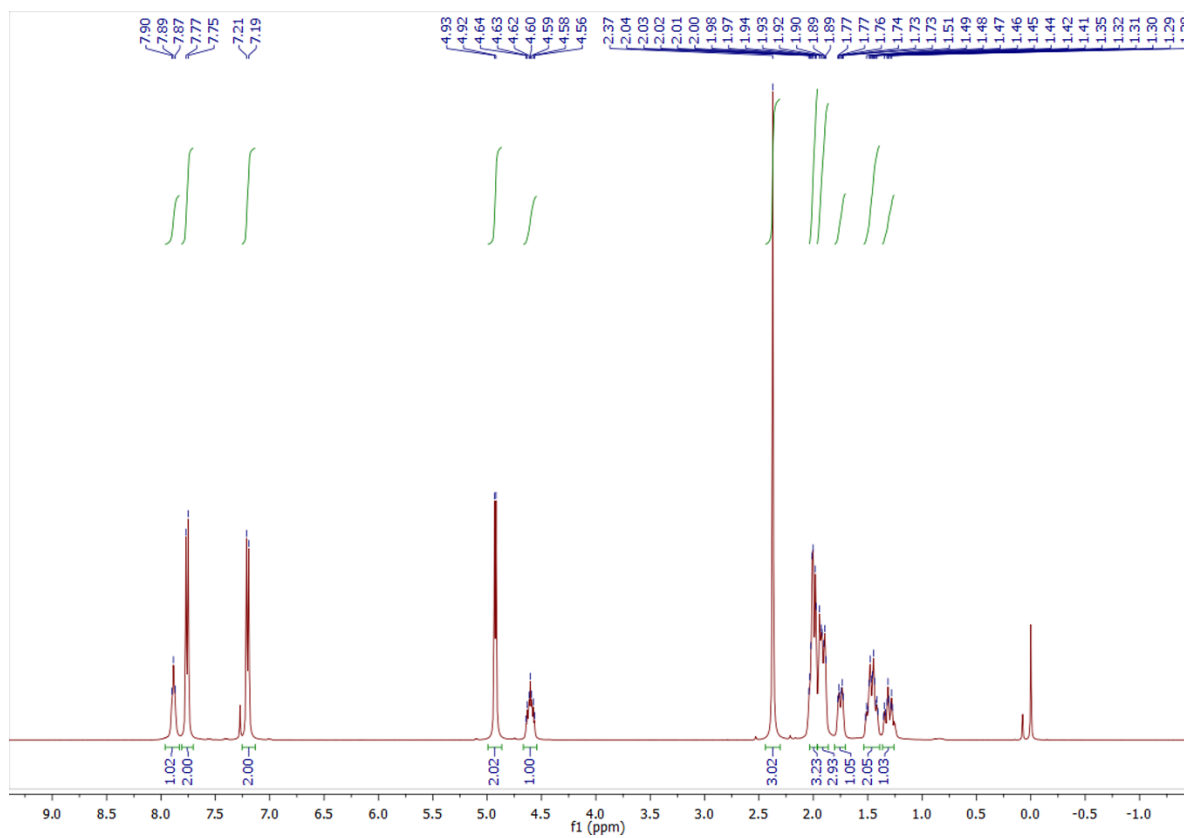
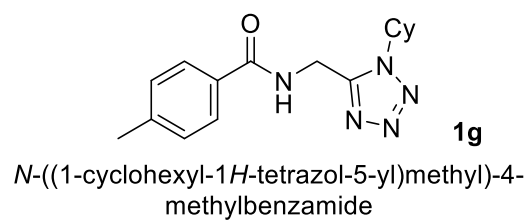


Figure S19. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **1g**.

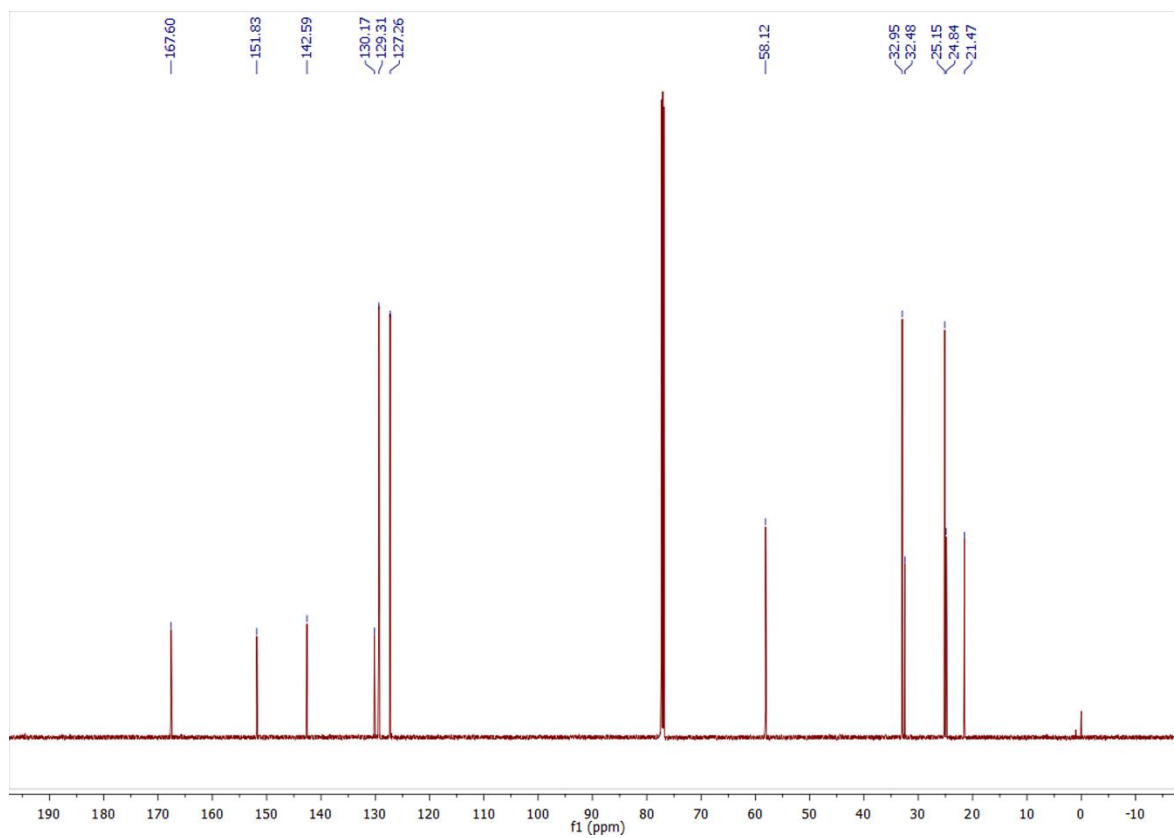
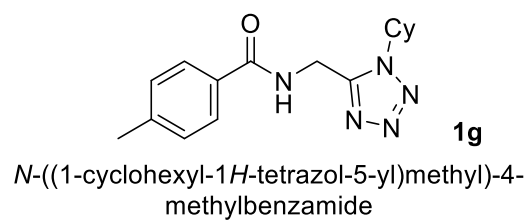
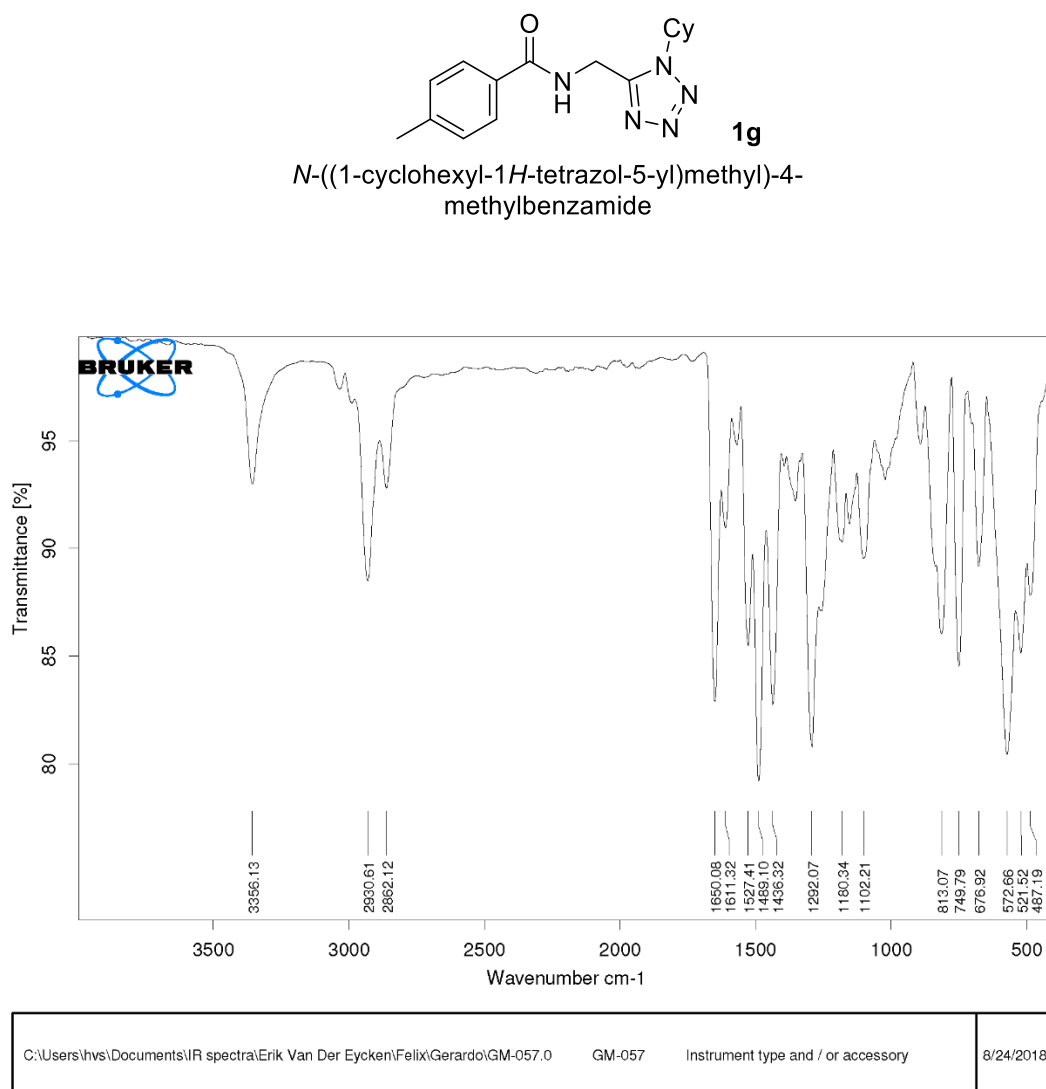
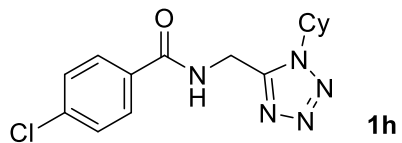


Figure S20. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1g**.



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Figure S21. FT-IR (KBr) spectrum of compound **1g**.



4-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

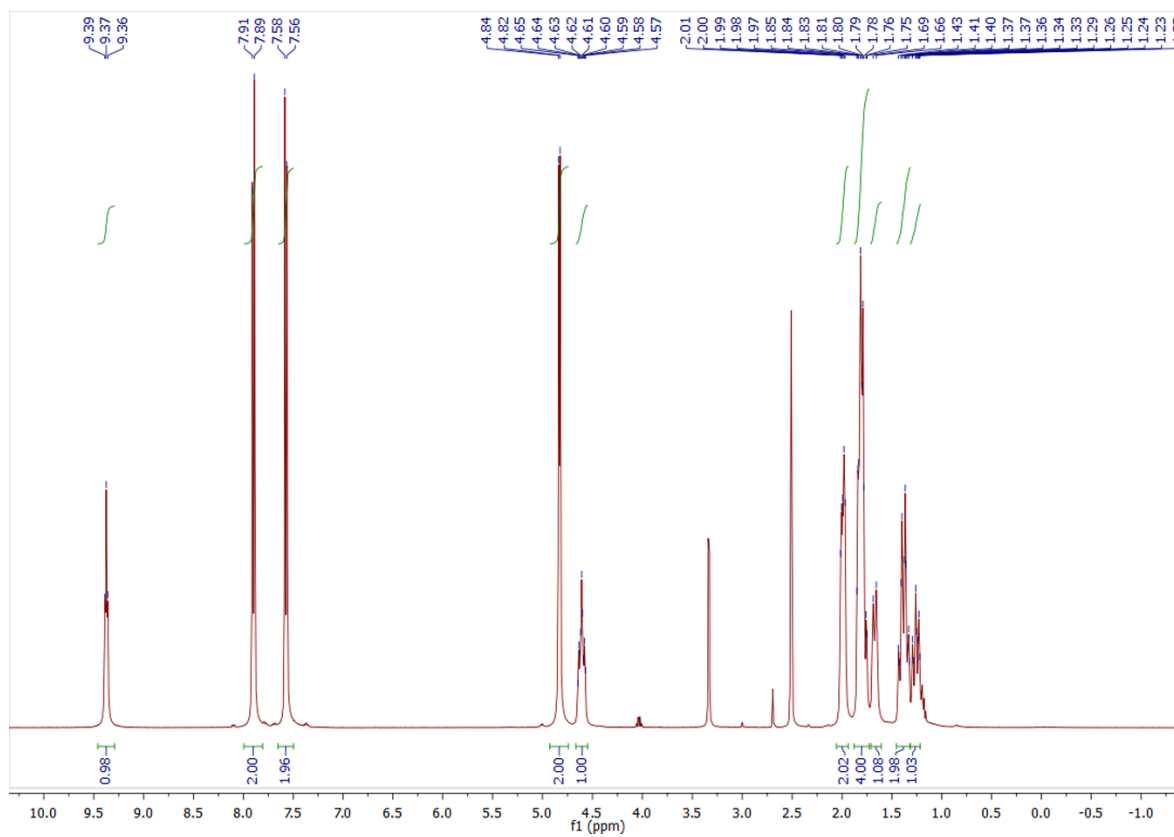
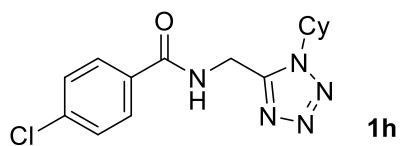


Figure S22. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **1h**.



4-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

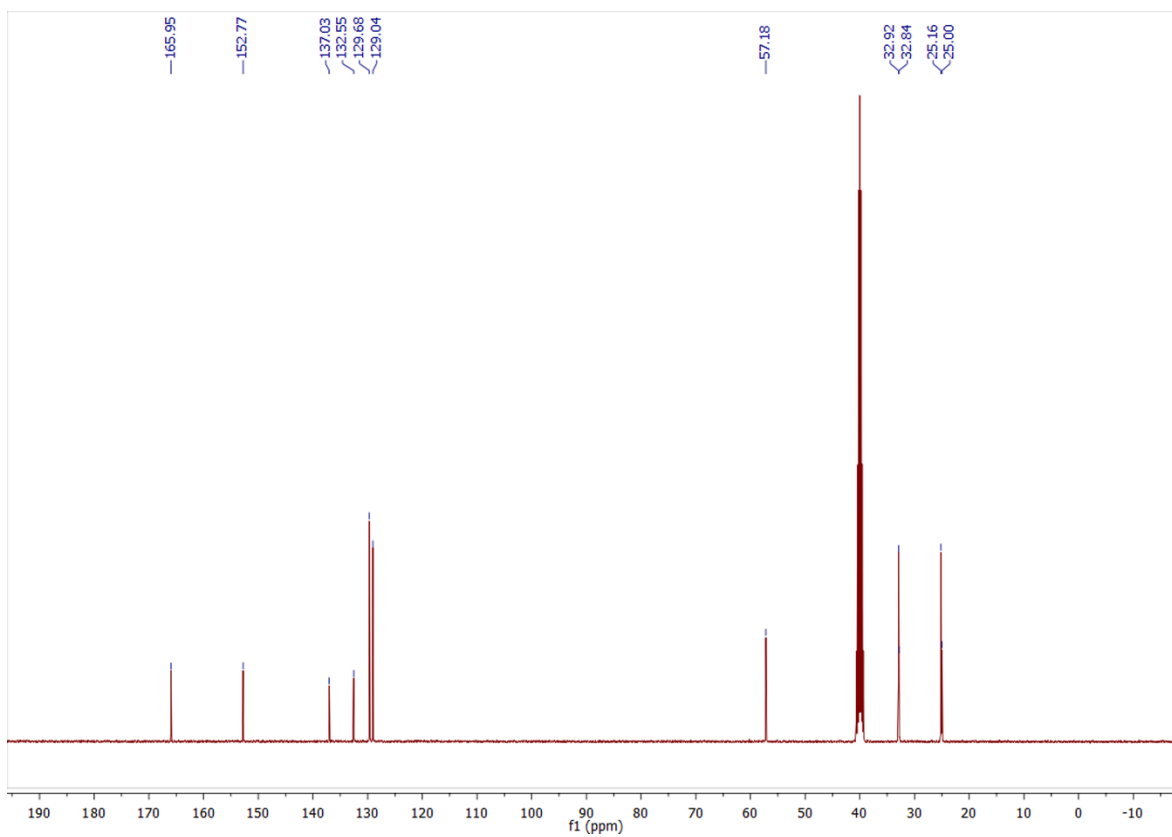
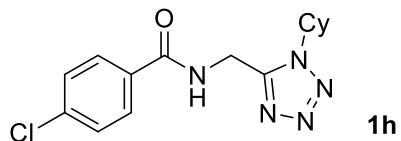
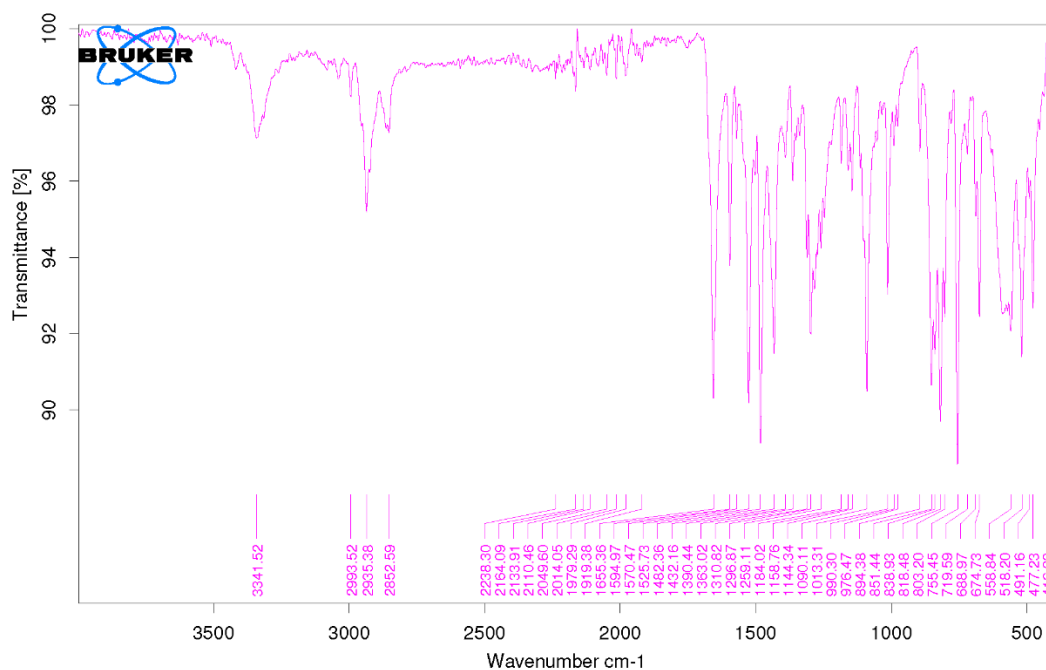


Figure S23. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, $\text{DMSO-}d_6$) spectrum of compound **1h**.



1h
4-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide



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GM-061

Instrument type and / or accessory

8/24/2018

Figure S24. FT-IR (KBr) spectrum of compound **1h**.

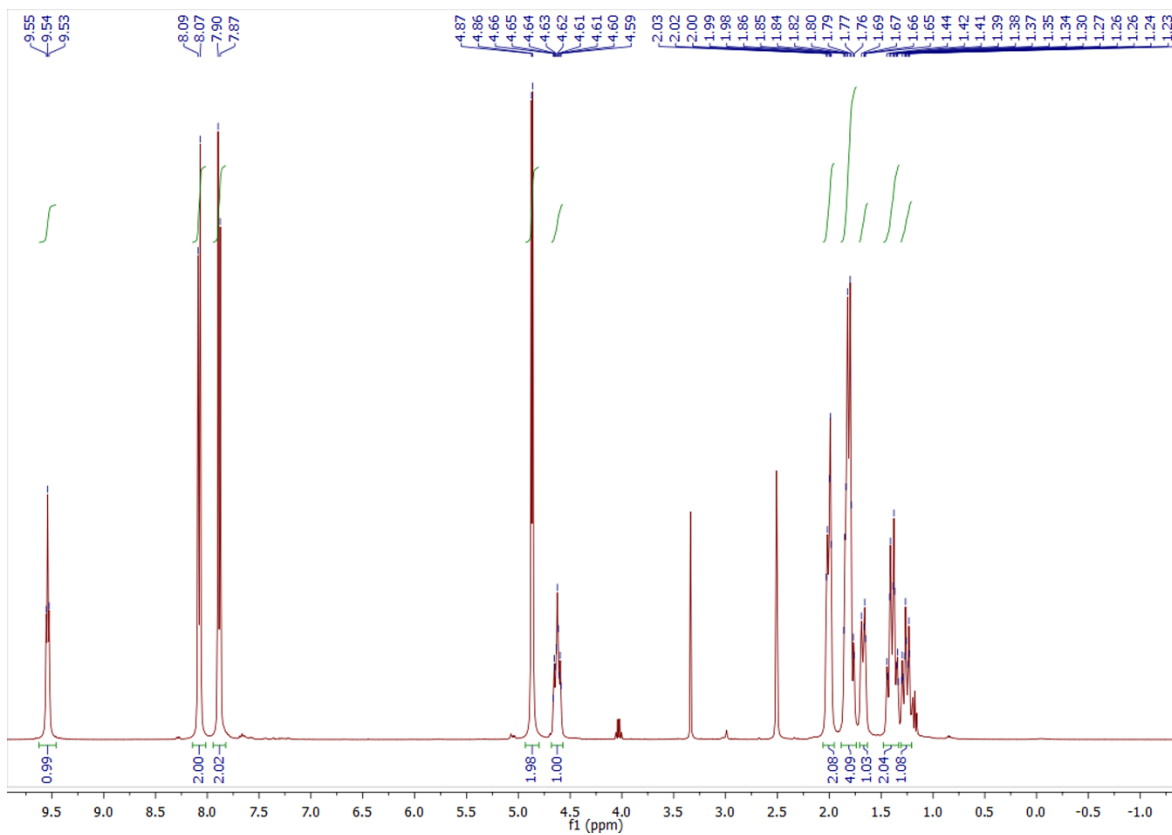
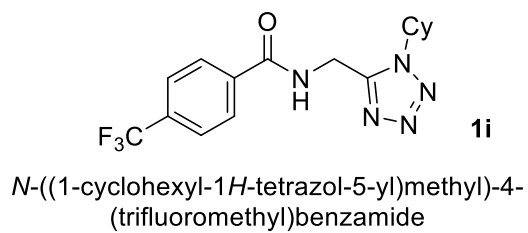


Figure S25. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **1i**.

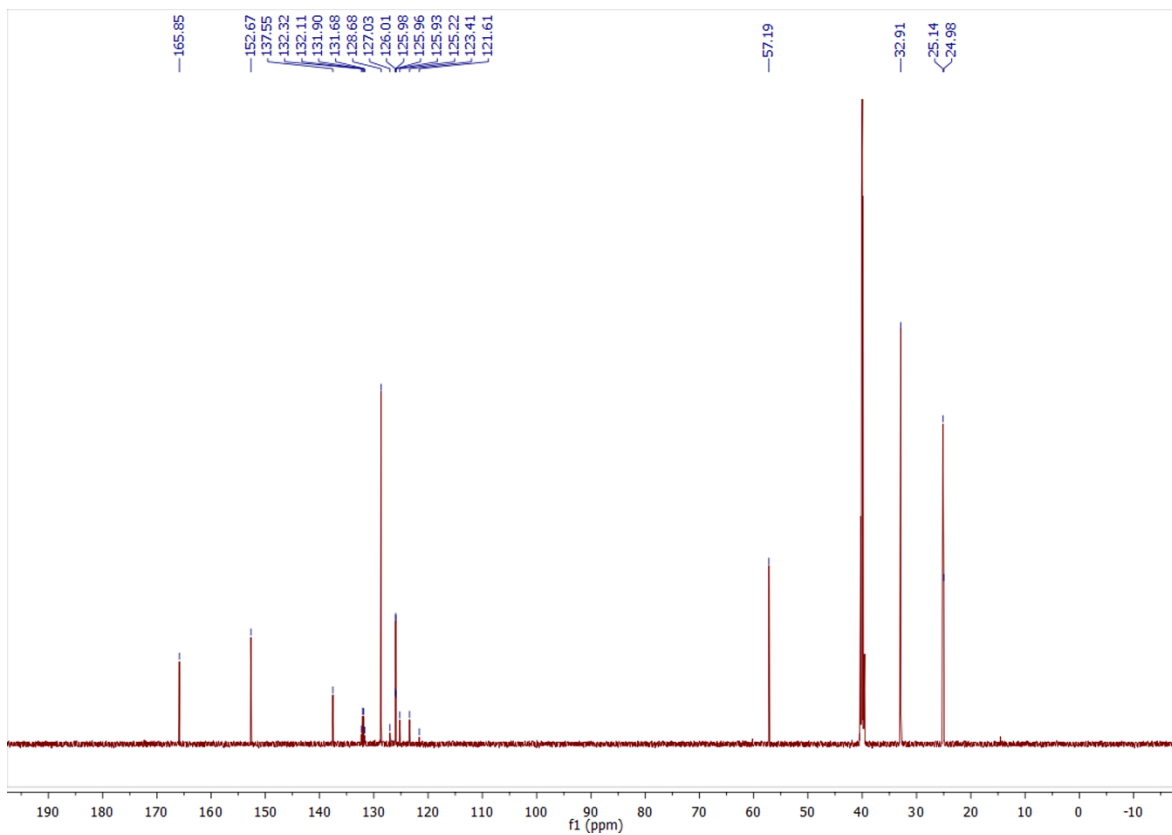
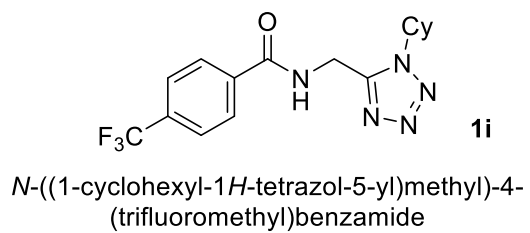


Figure S26. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$) spectrum of compound **1i**.

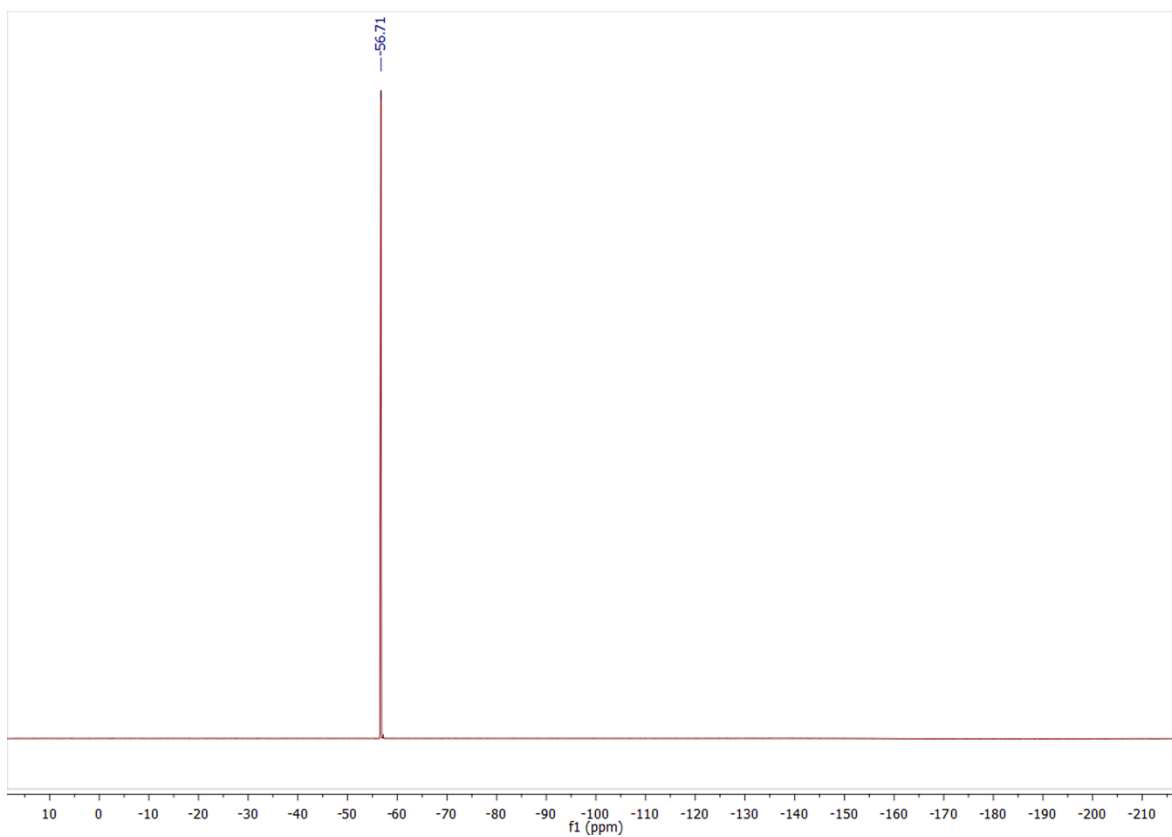
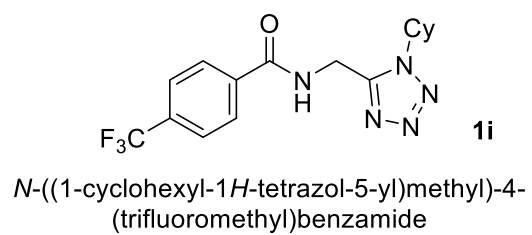
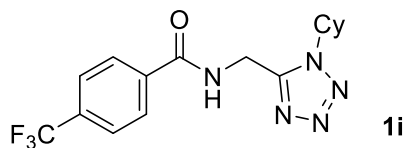
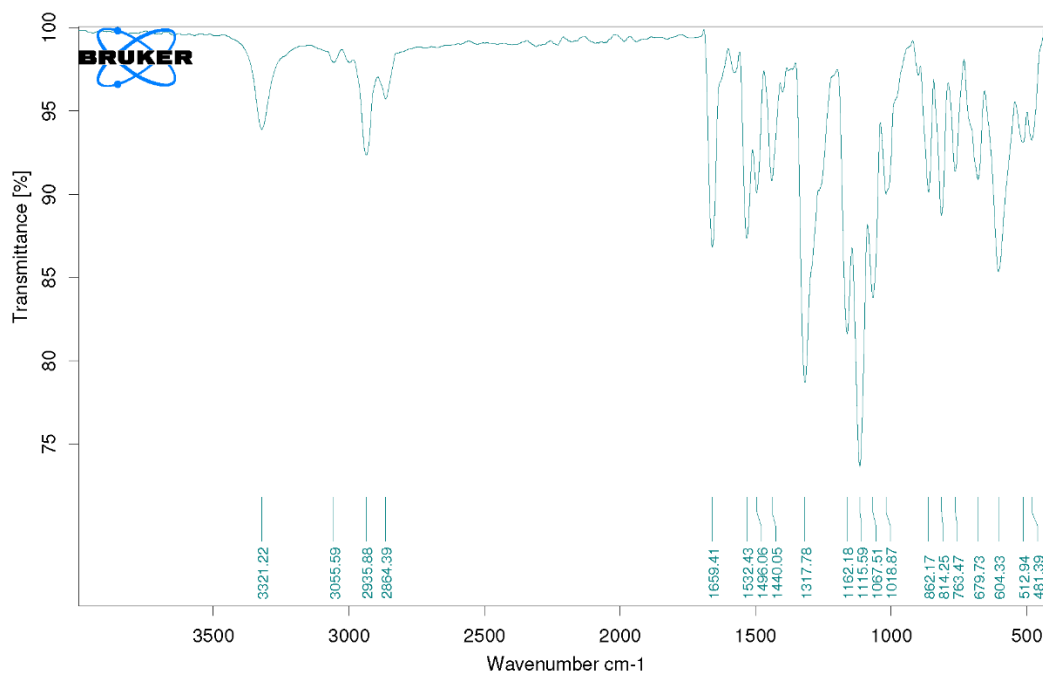


Figure S27. ^{19}F $\{^{13}\text{C}\}$ NMR (376 MHz, CDCl_3) spectrum of compound **1i**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-4-(trifluoromethyl)benzamide



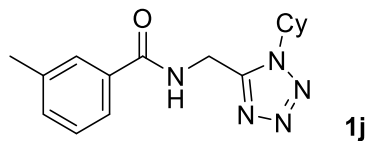
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GM-063

Instrument type and / or accessory

8/24/2018

Figure S28. FT-IR (KBr) spectrum of compound **1i**.



1j
N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3-methylbenzamide

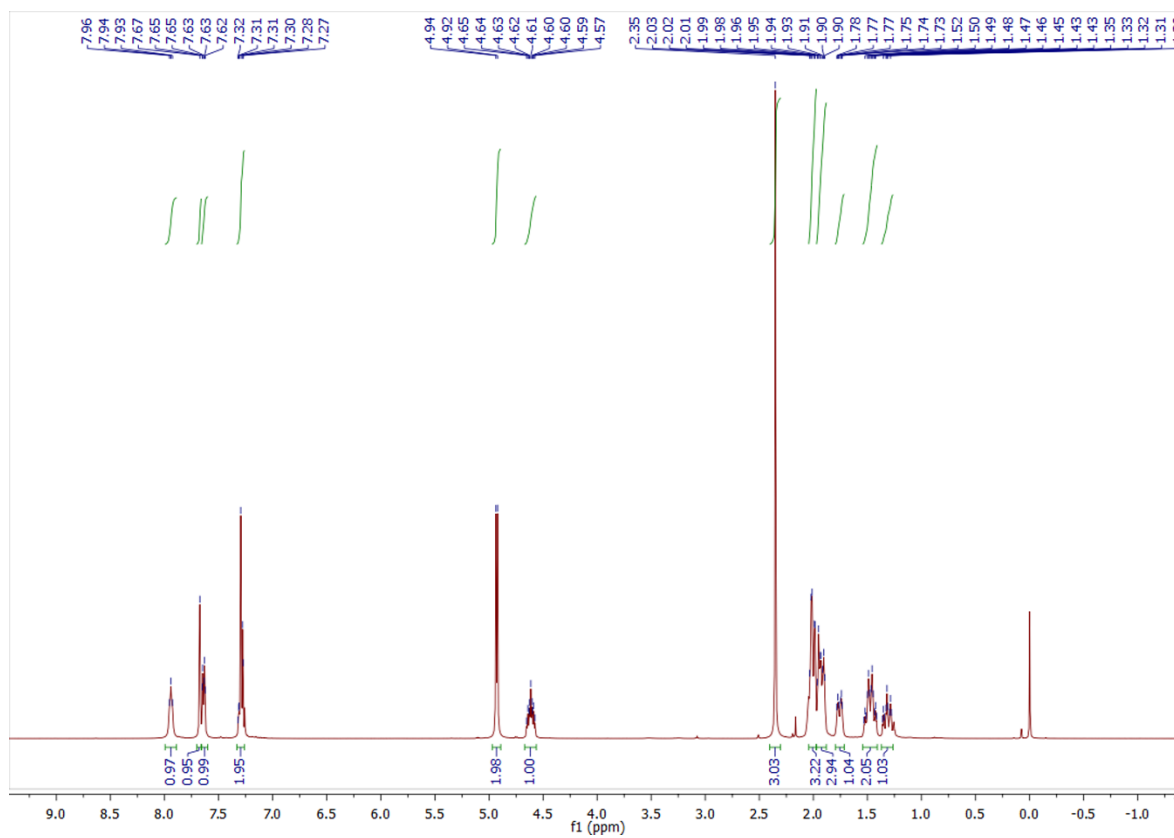
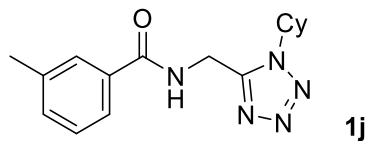


Figure S29. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **1j**.



1j
N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3-methylbenzamide

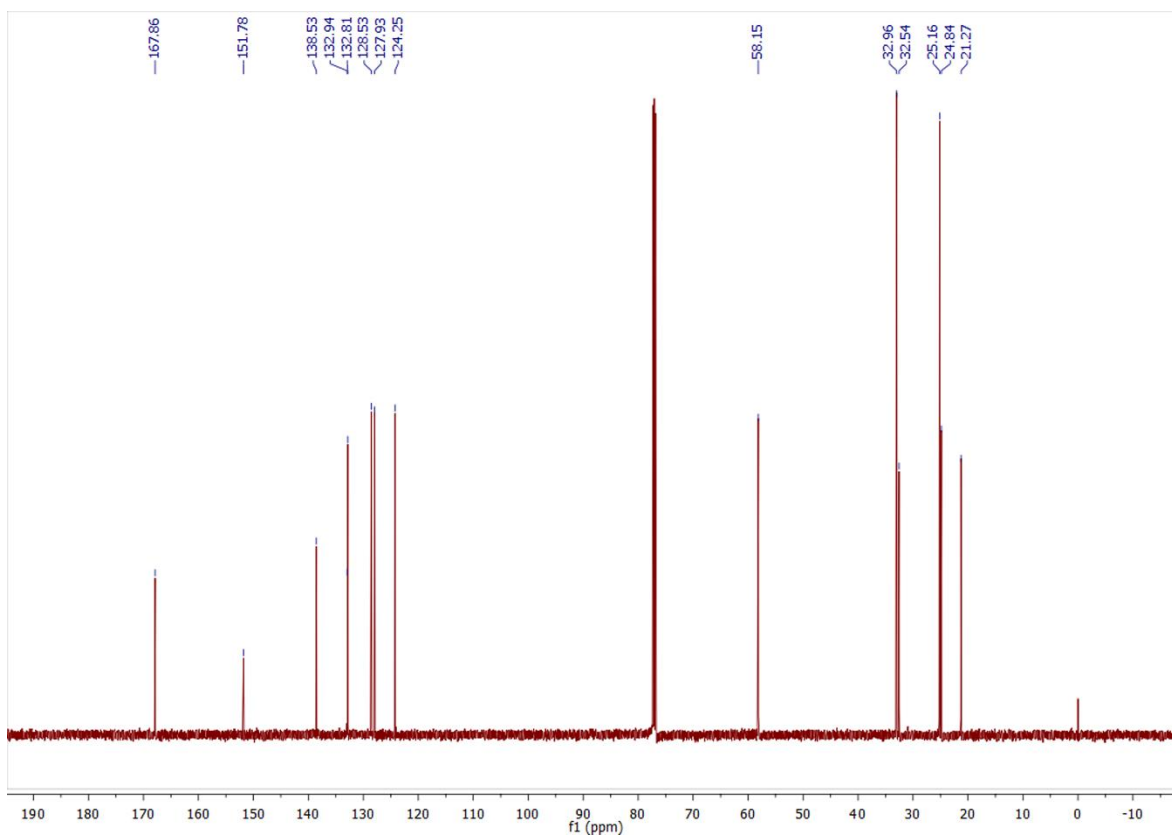
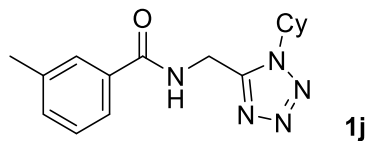
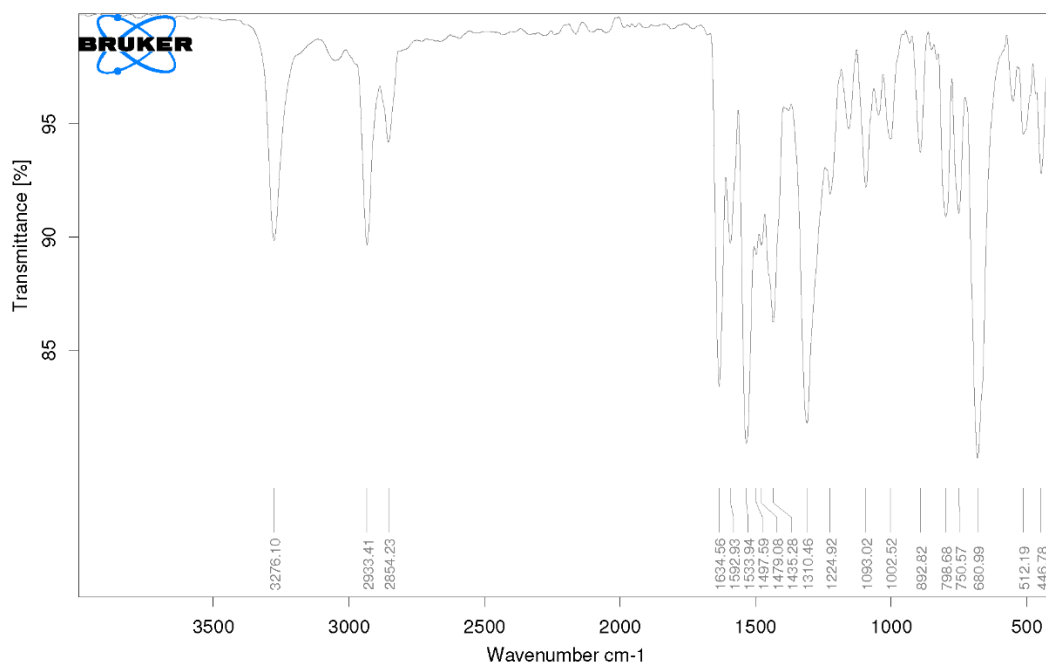


Figure S30. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1j**.



1j
N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3-methylbenzamide



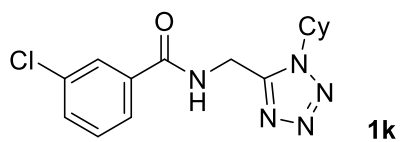
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GM-087

Instrument type and / or accessory

10/12/2018

Figure S31. FT-IR (KBr) spectrum of compound **1j**.



3-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

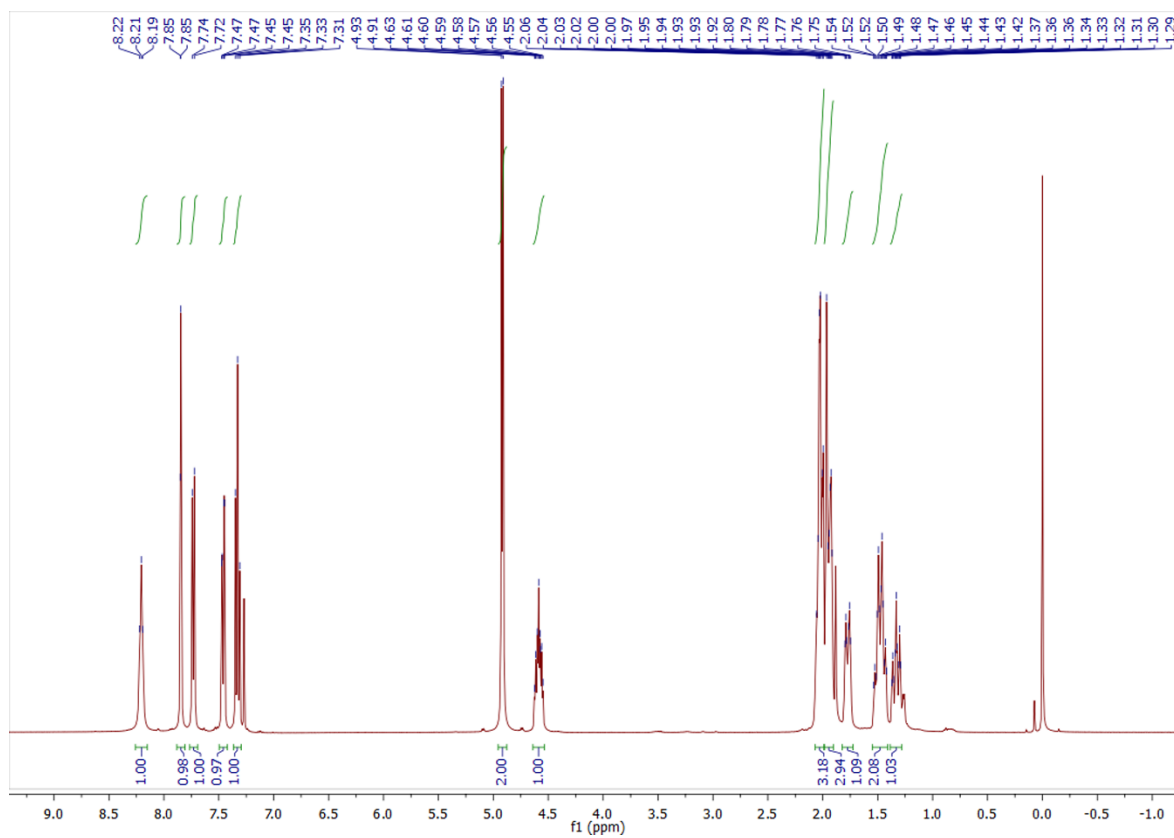
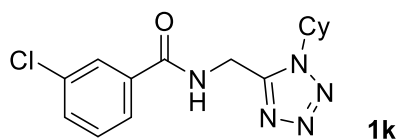


Figure S32. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **1k**.



3-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

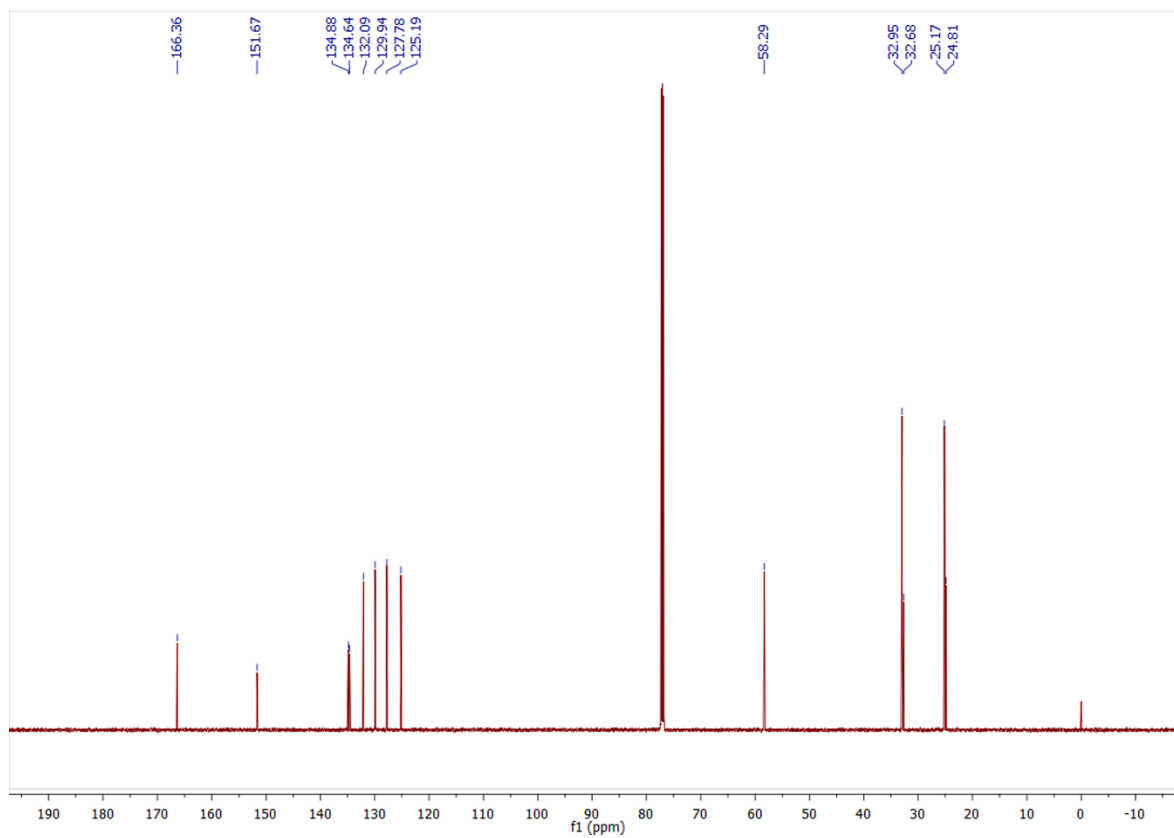
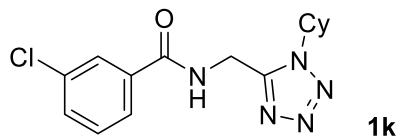
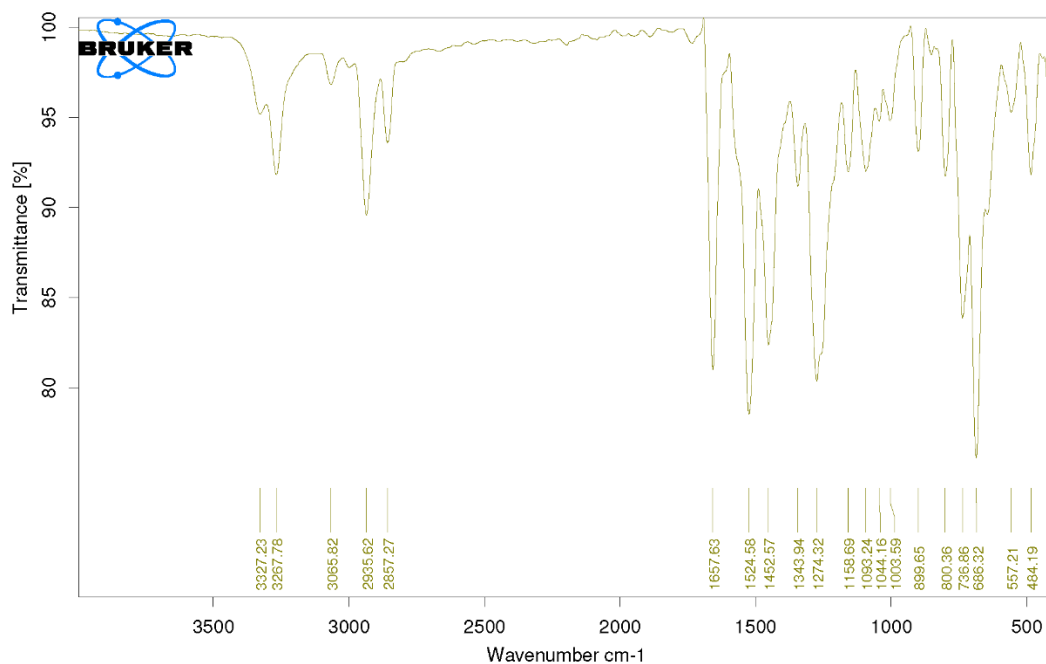


Figure S33. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1k**.



1k
3-chloro-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide



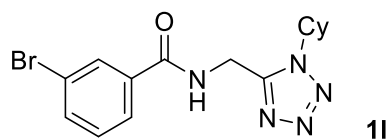
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GM-075

Instrument type and / or accessory

10/12/2018

Figure S34. FT-IR (KBr) spectrum of compound **1k**.



3-bromo-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide

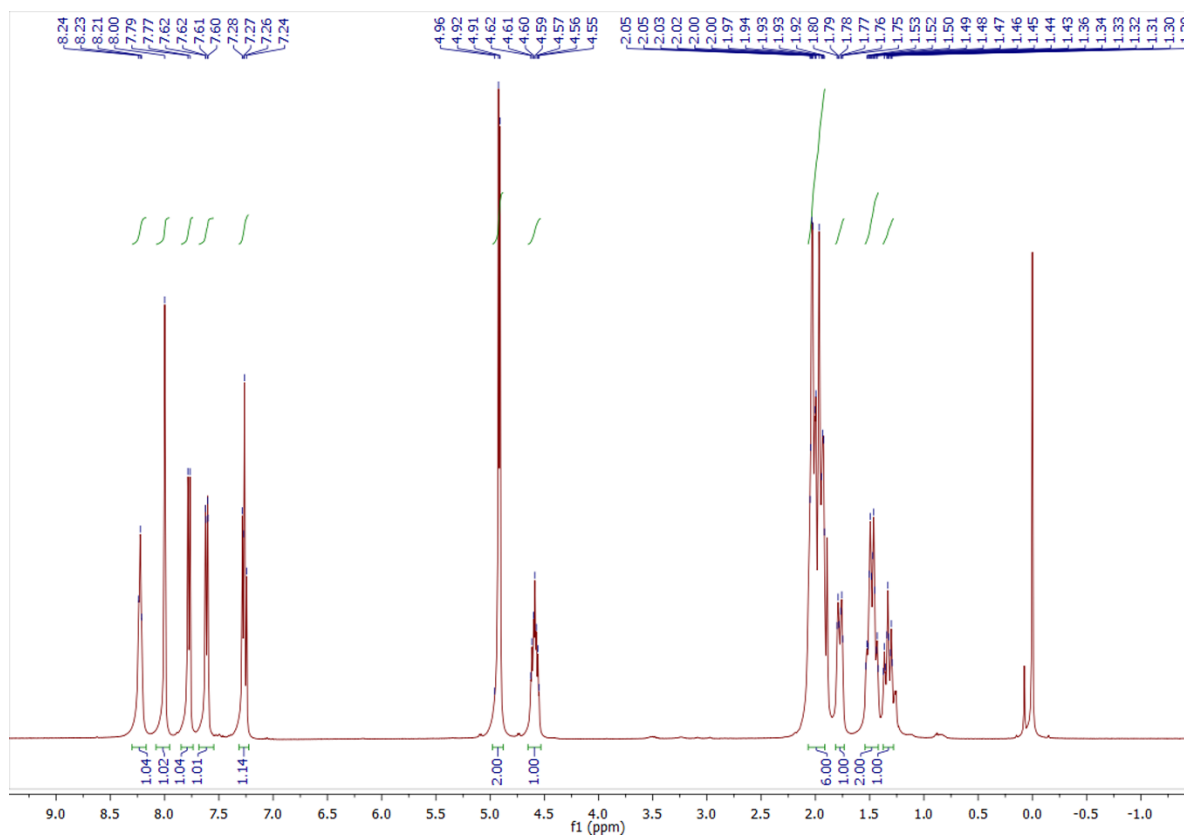
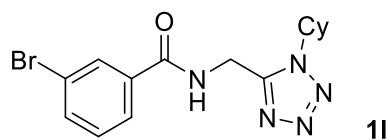


Figure S35. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **11**.



3-bromo-*N*-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzamide

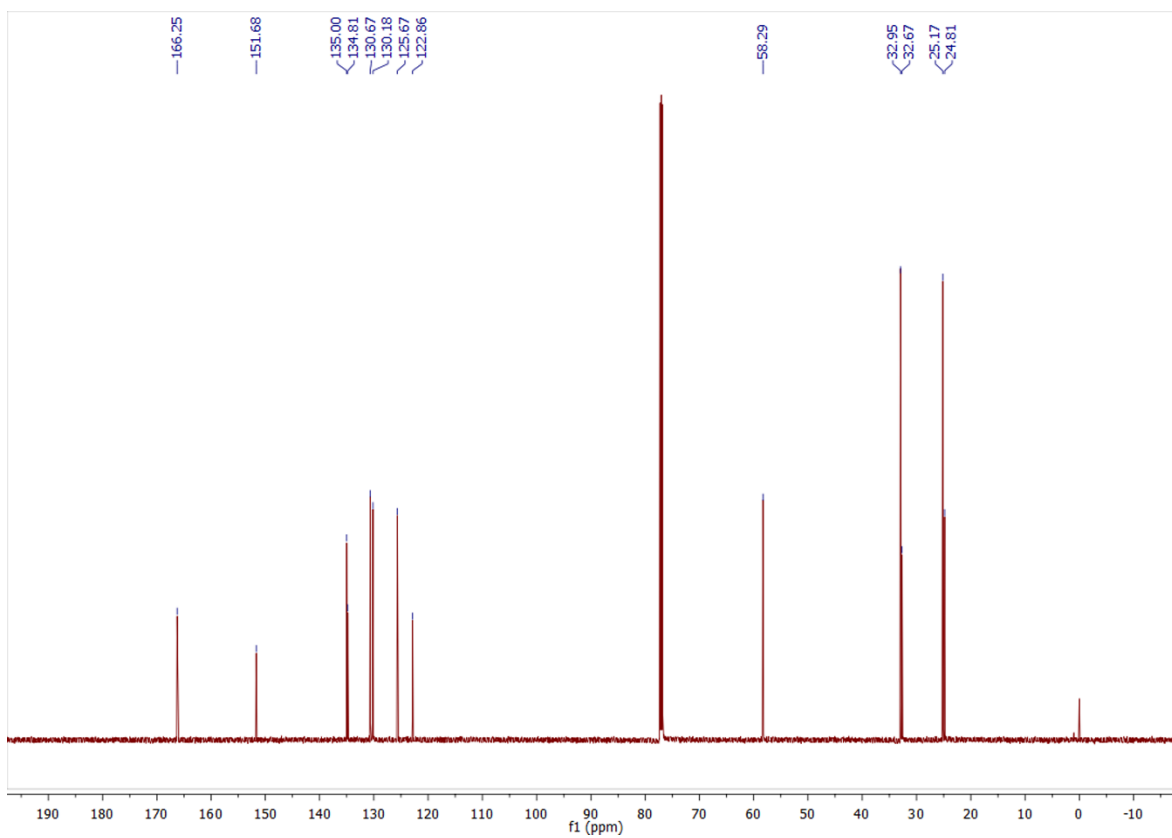
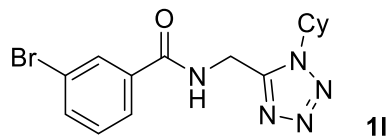
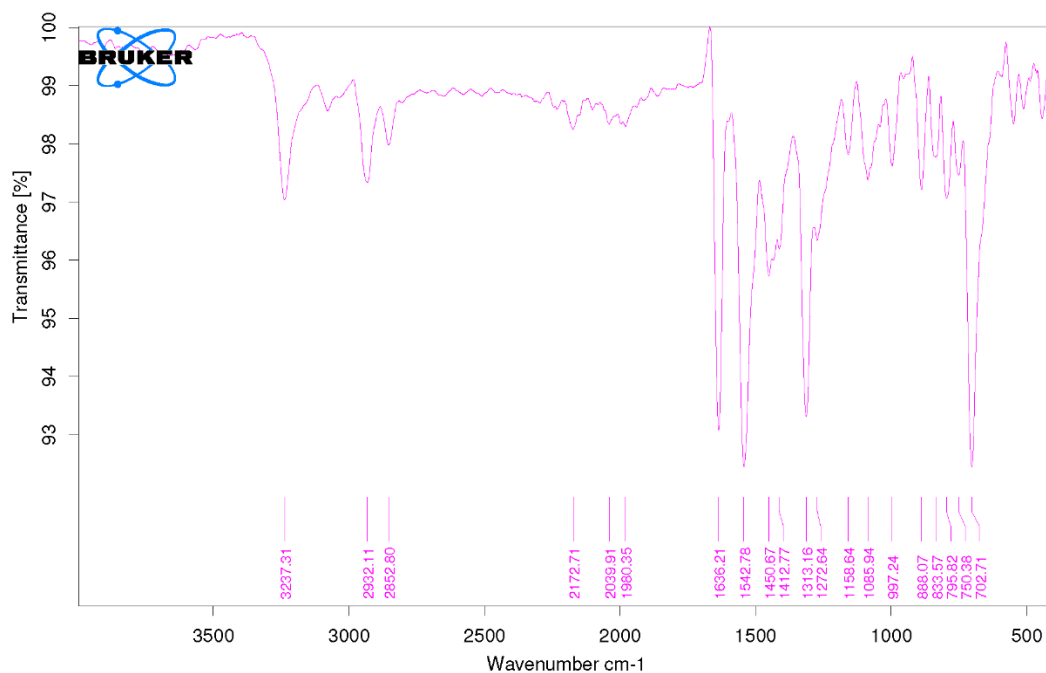


Figure S36. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **11**.



11
3-bromo-N-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)benzamide



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GM-077

Instrument type and / or accessory

10/12/2018

Figure S37. FT-IR (KBr) spectrum of compound **11**.

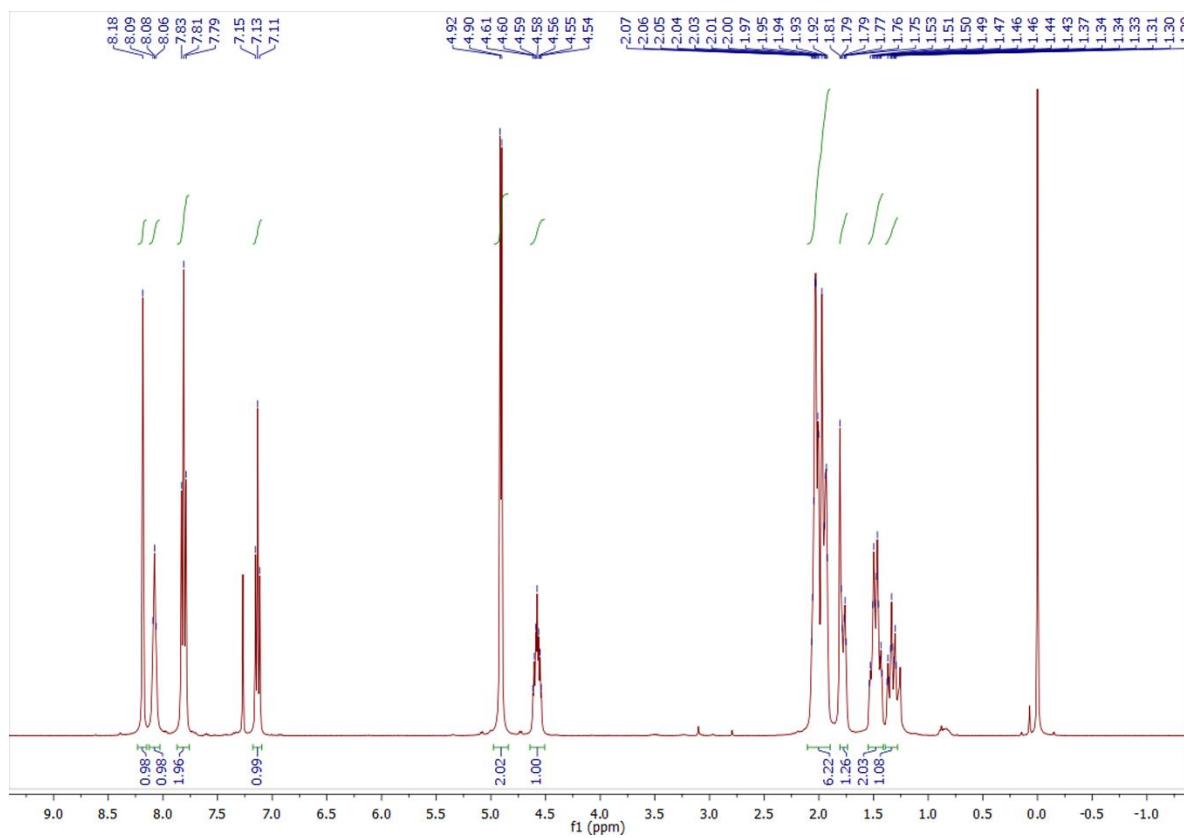
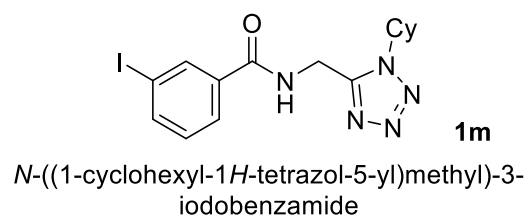


Figure S38. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **1m**.

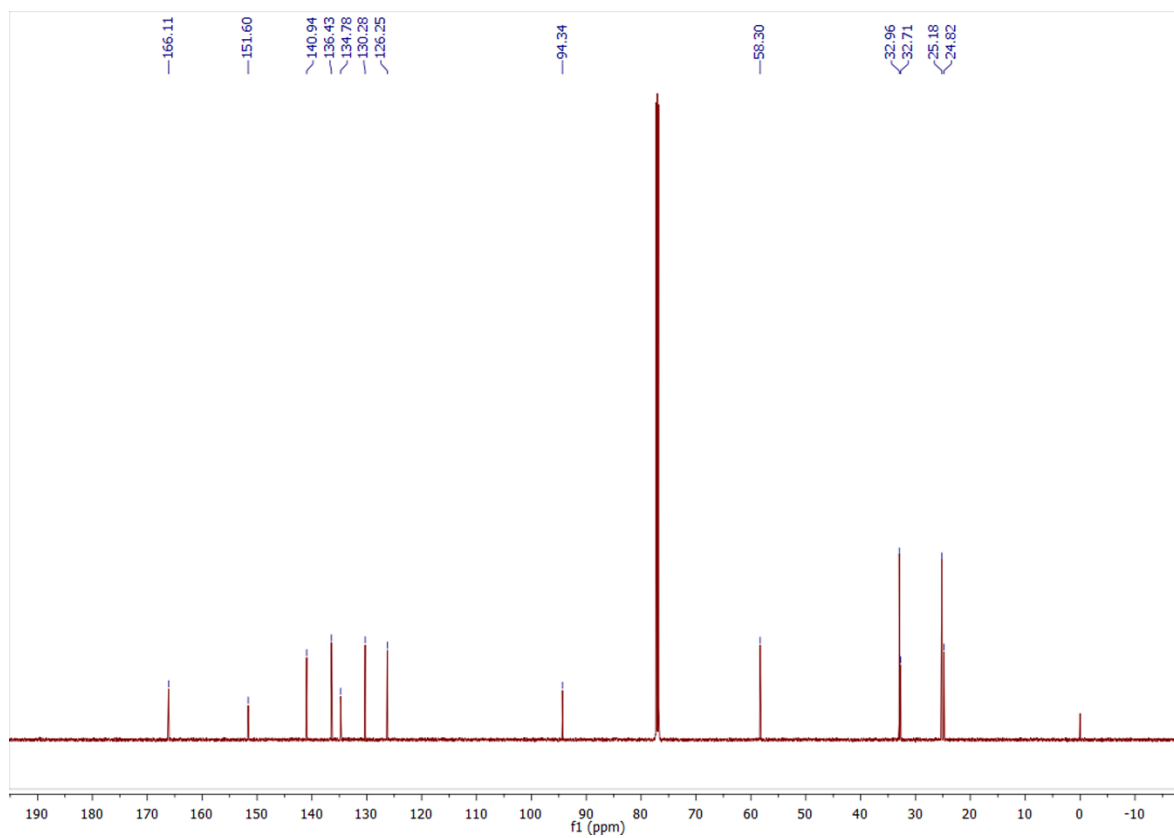
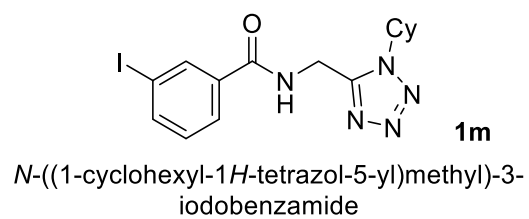


Figure S39. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1m**.

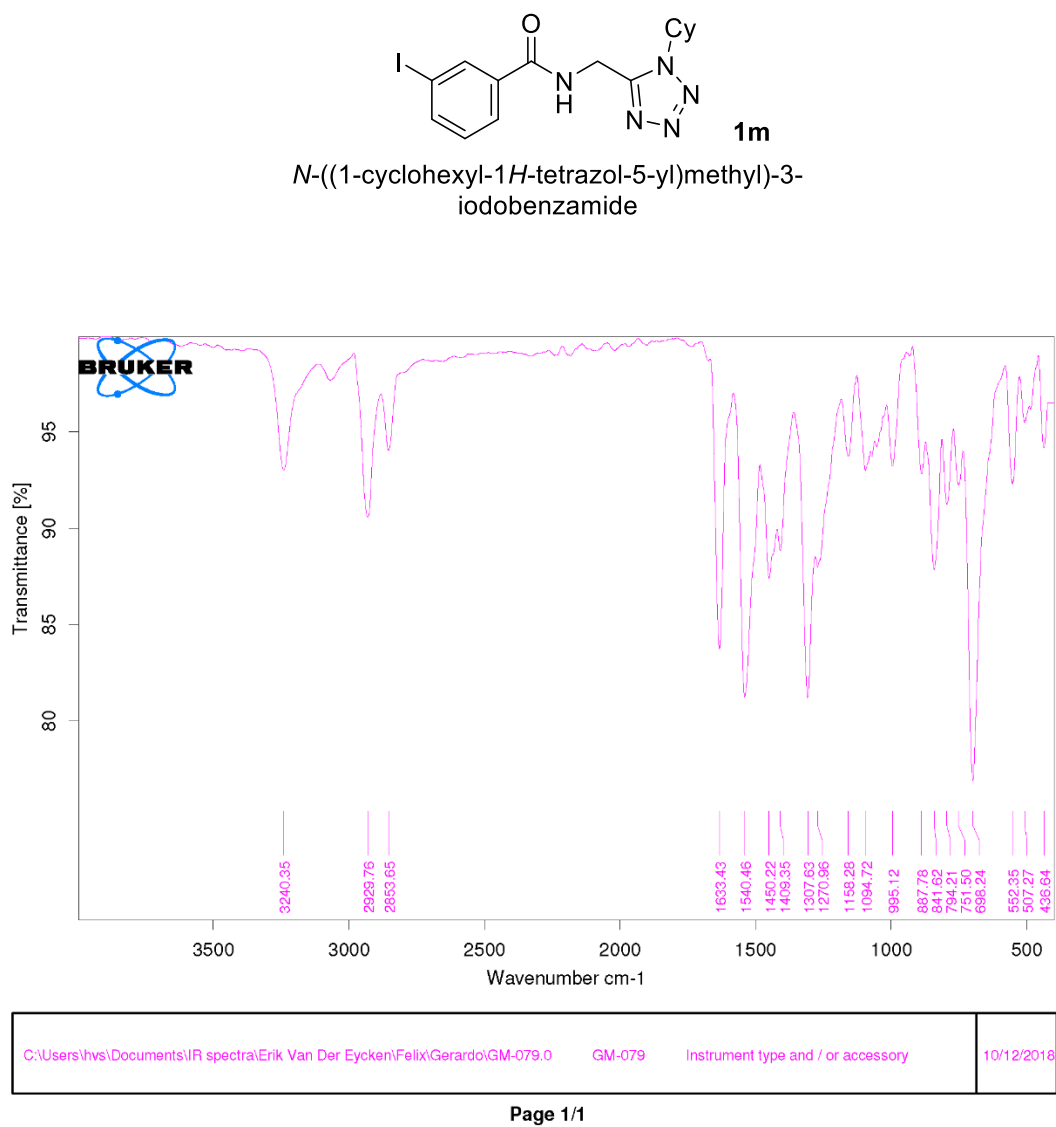
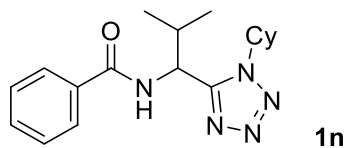


Figure S40. FT-IR (KBr) spectrum of compound **1m**.



N-(1-(1-cyclohexyl-1*H*-tetrazol-5-yl)-2-methylpropyl)benzamide

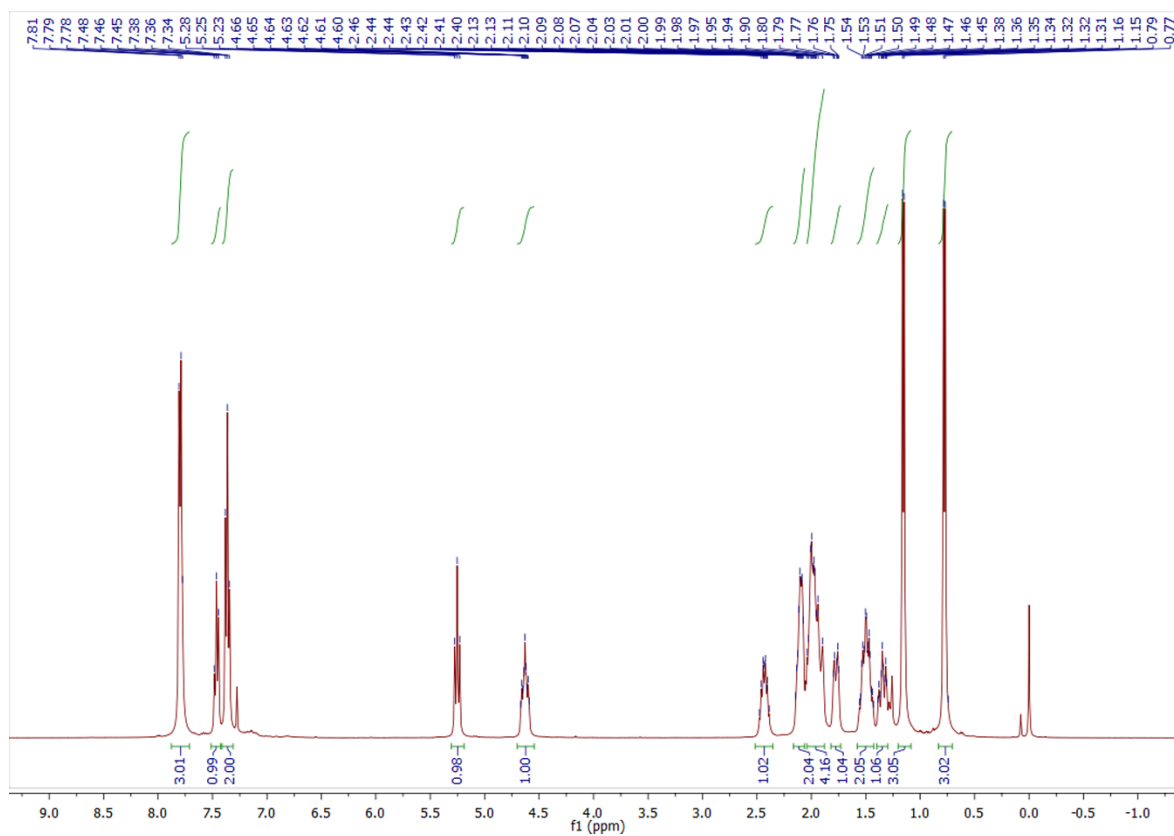
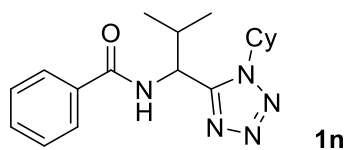


Figure S41. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **1n**.



N-(1-(1-cyclohexyl-1*H*-tetrazol-5-yl)-2-methylpropyl)benzamide

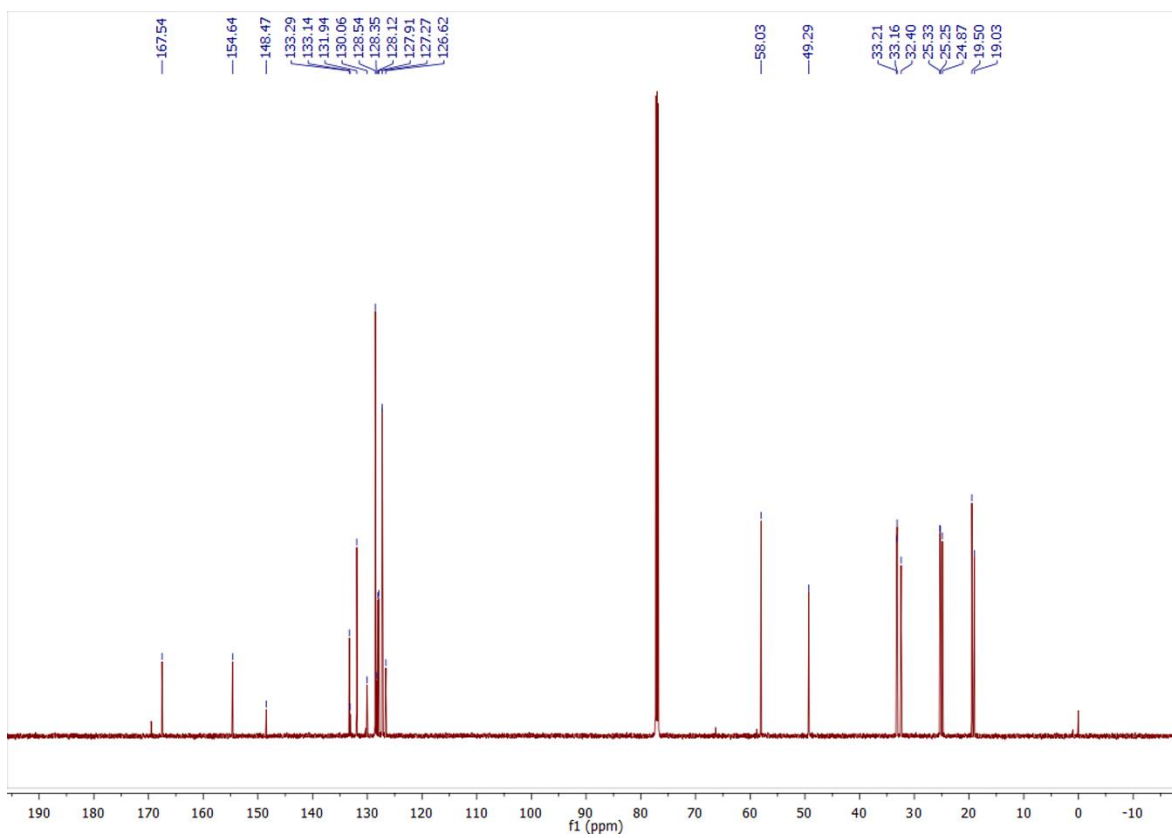
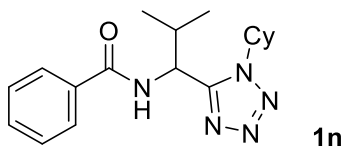
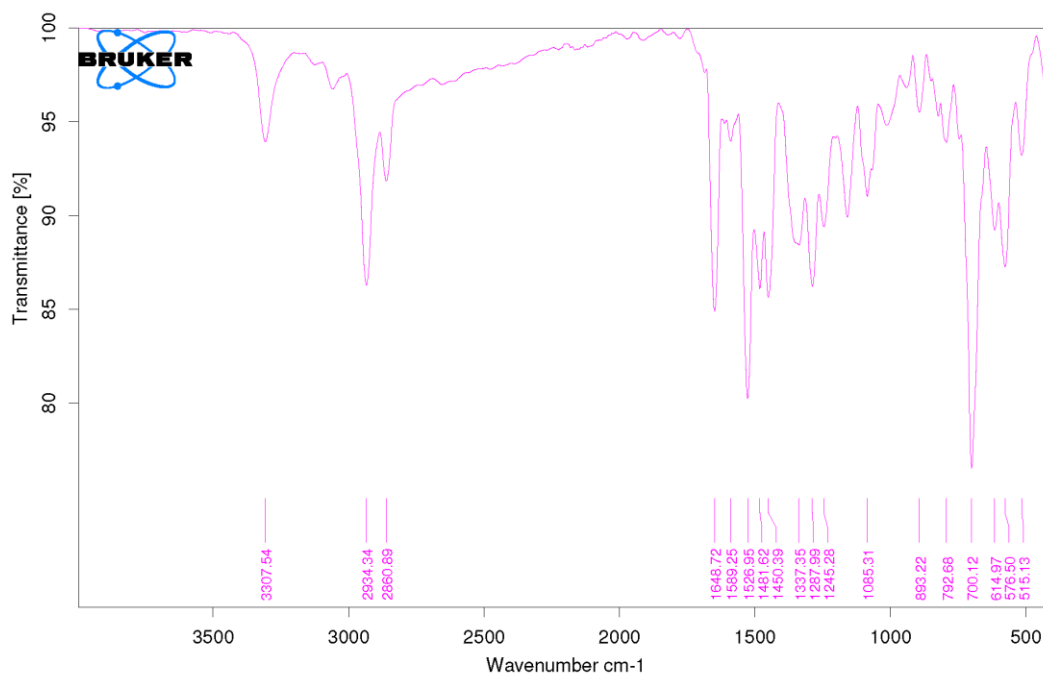


Figure S42. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1n**.



N-(1-(1-cyclohexyl-1*H*-tetrazol-5-yl)-2-methylpropyl)benzamide



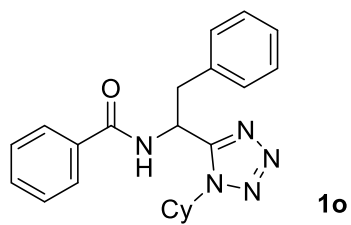
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GM-037

Instrument type and / or accessory

1/21/2019

Figure S43. FT-IR (KBr) spectrum of compound **1n**.



N-(1-(1-cyclohexyl-1*H*-tetrazol-5-yl)-2-phenylethyl)benzamide

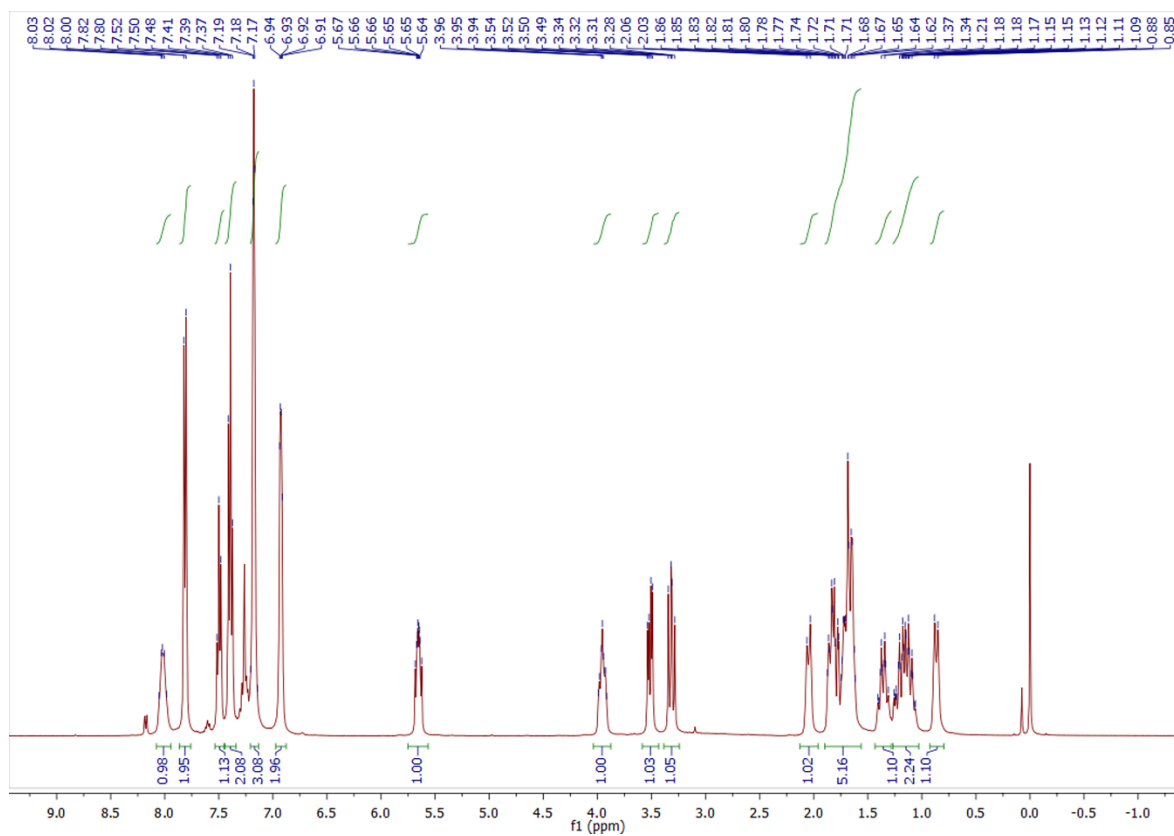
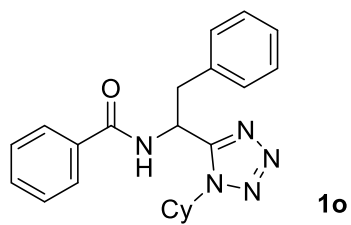


Figure S44. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **1o**.



N-(1-(1-cyclohexyl-1*H*-tetrazol-5-yl)-2-phenylethyl)benzamide

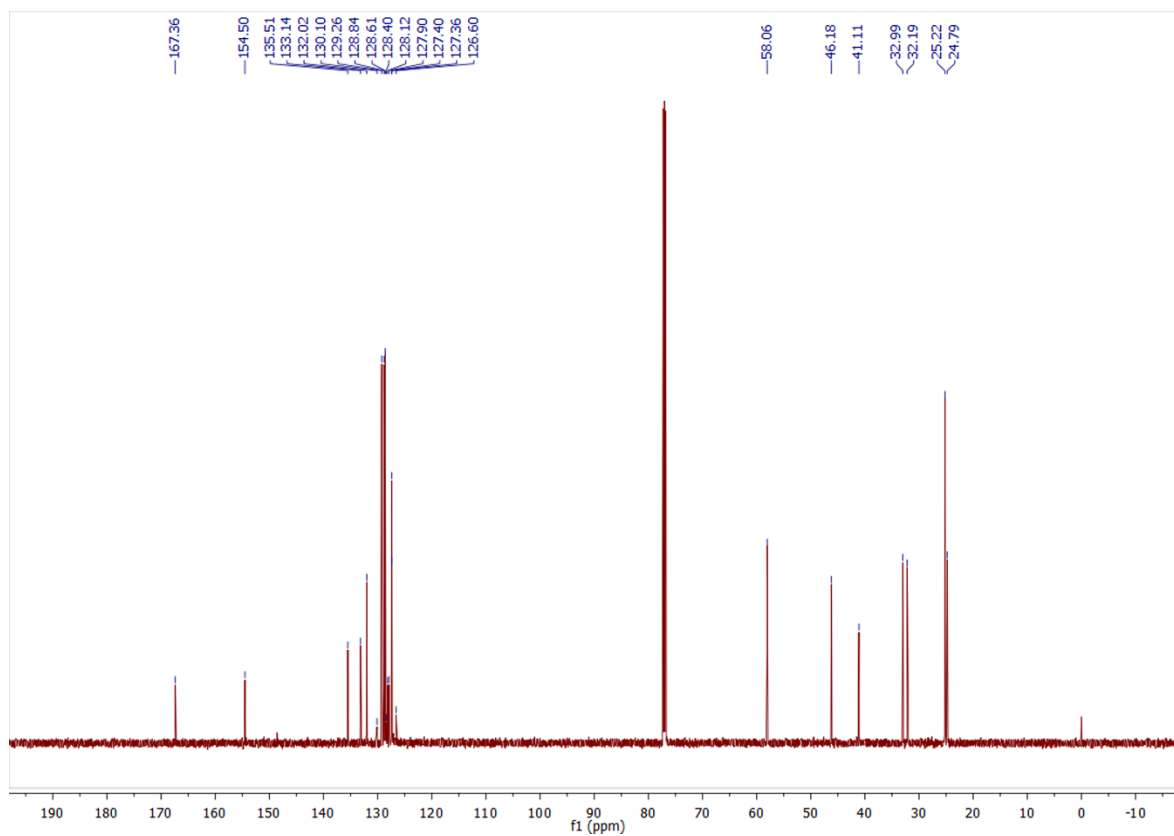
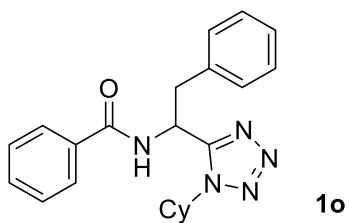
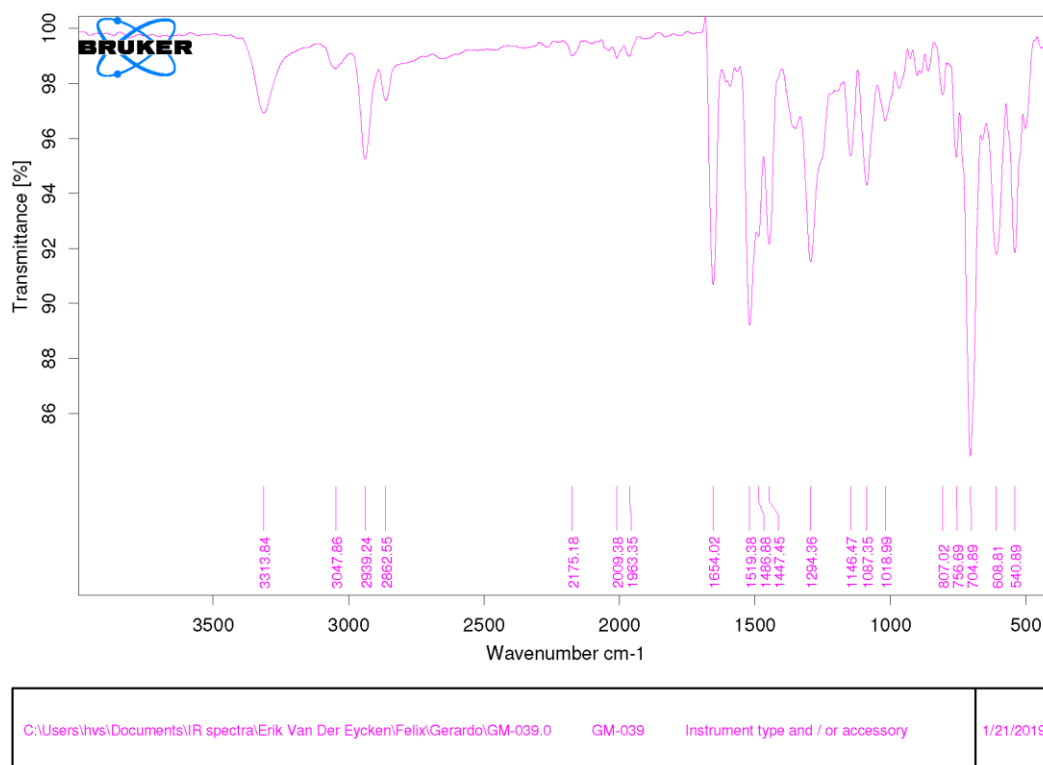


Figure S45. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **1o**.



N-(1-(1-cyclohexyl-1*H*-tetrazol-5-yl)-2-phenylethyl)benzamide



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Figure S46. FT-IR (KBr) spectrum of compound **1o**.

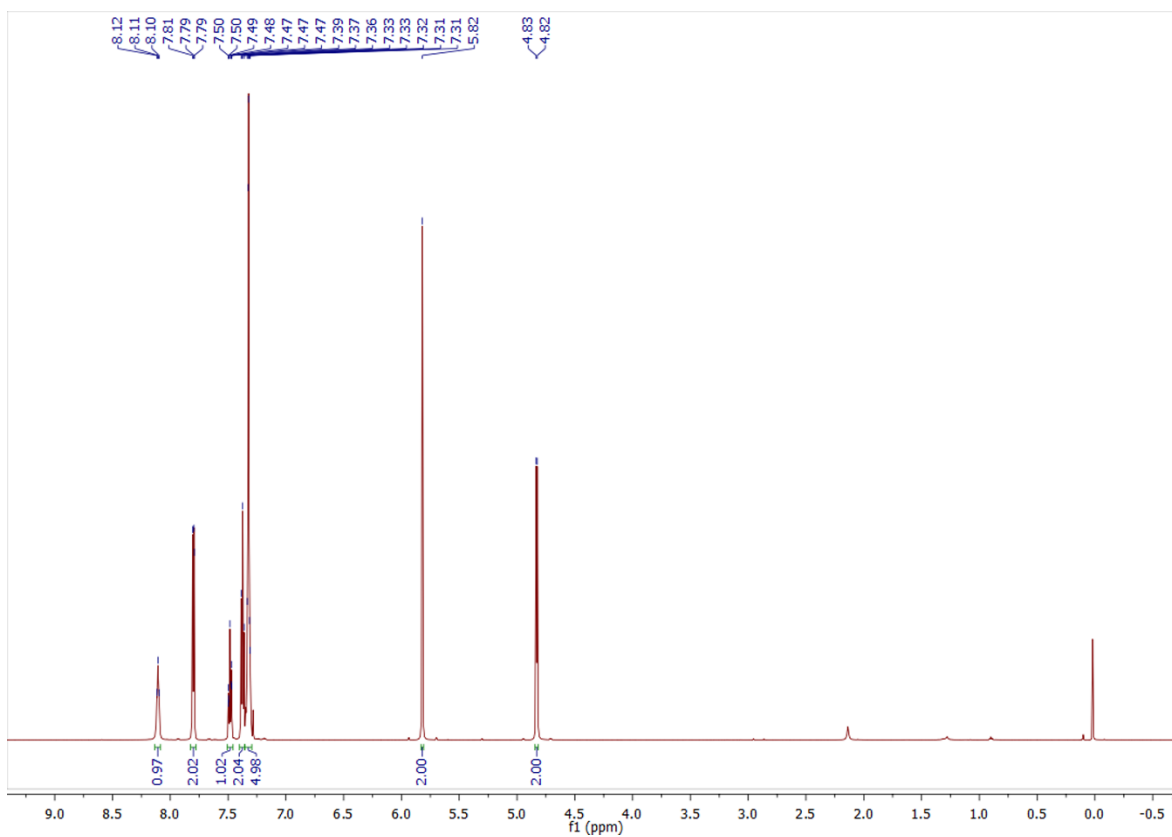
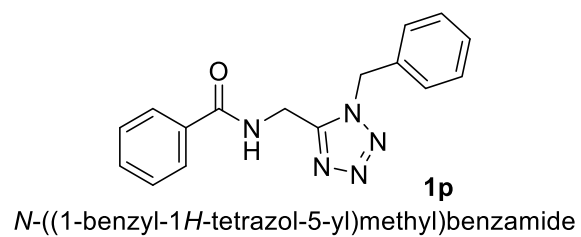


Figure S47. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **1p**.

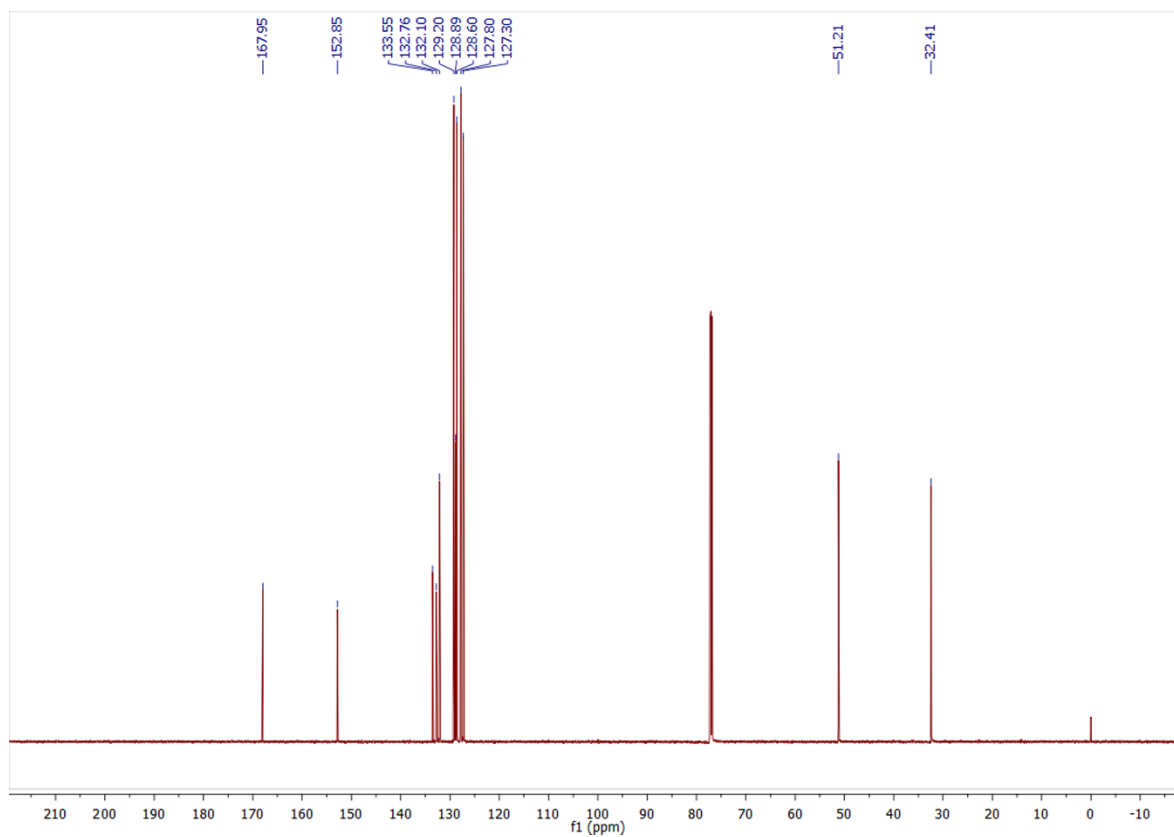
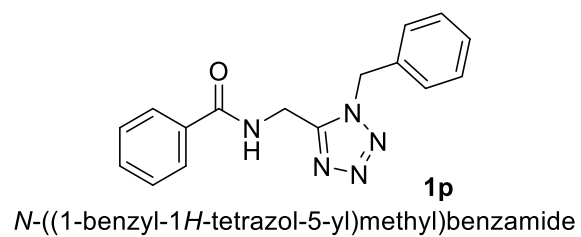
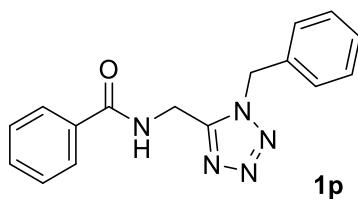
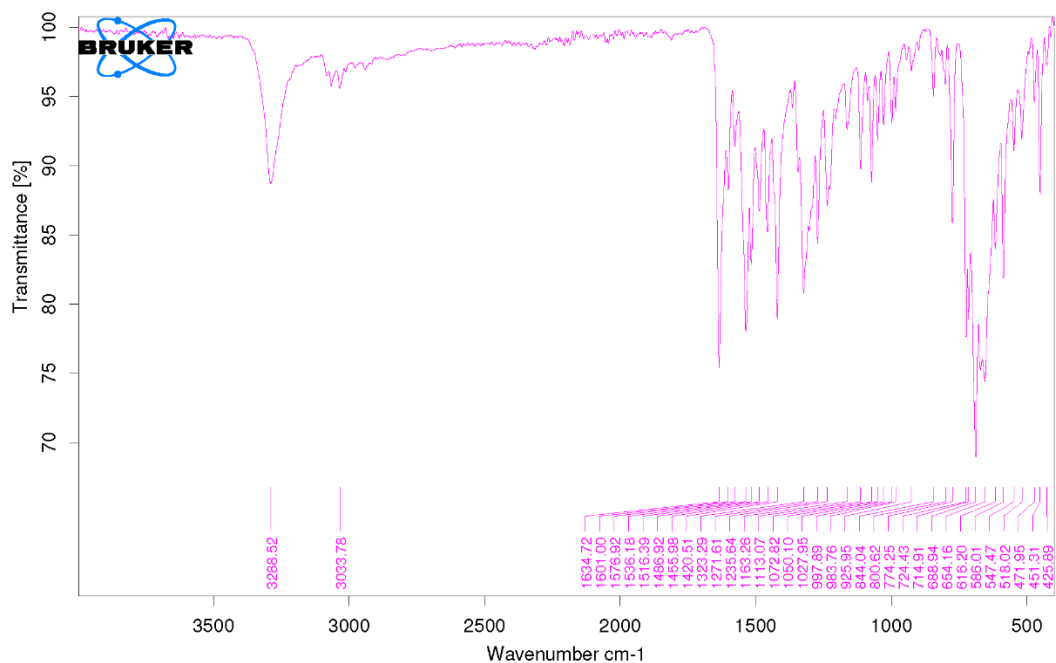


Figure S48. ^{13}C { ^1H } NMR (151 MHz, CDCl_3) spectrum of compound **1p**.



1p
N-((1-benzyl-1H-tetrazol-5-yl)methyl)benzamide



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GM-019

Instrument type and / or accessory

8/24/2018

Figure S49. FT-IR (KBr) spectrum of compound **1p**.

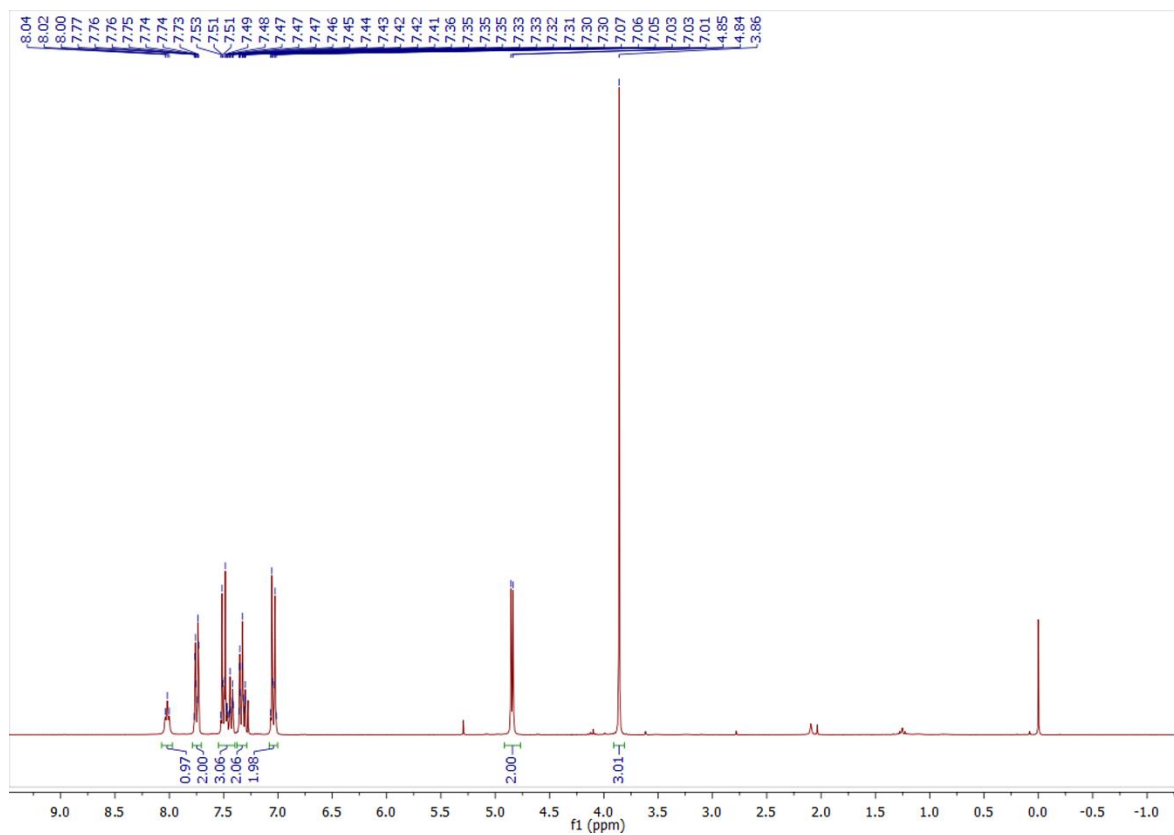
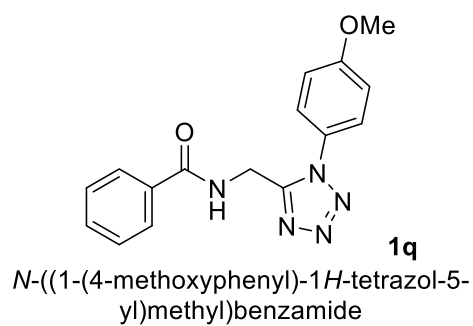


Figure S50. ^1H NMR (300 MHz, CDCl_3) spectrum of compound **1q**.

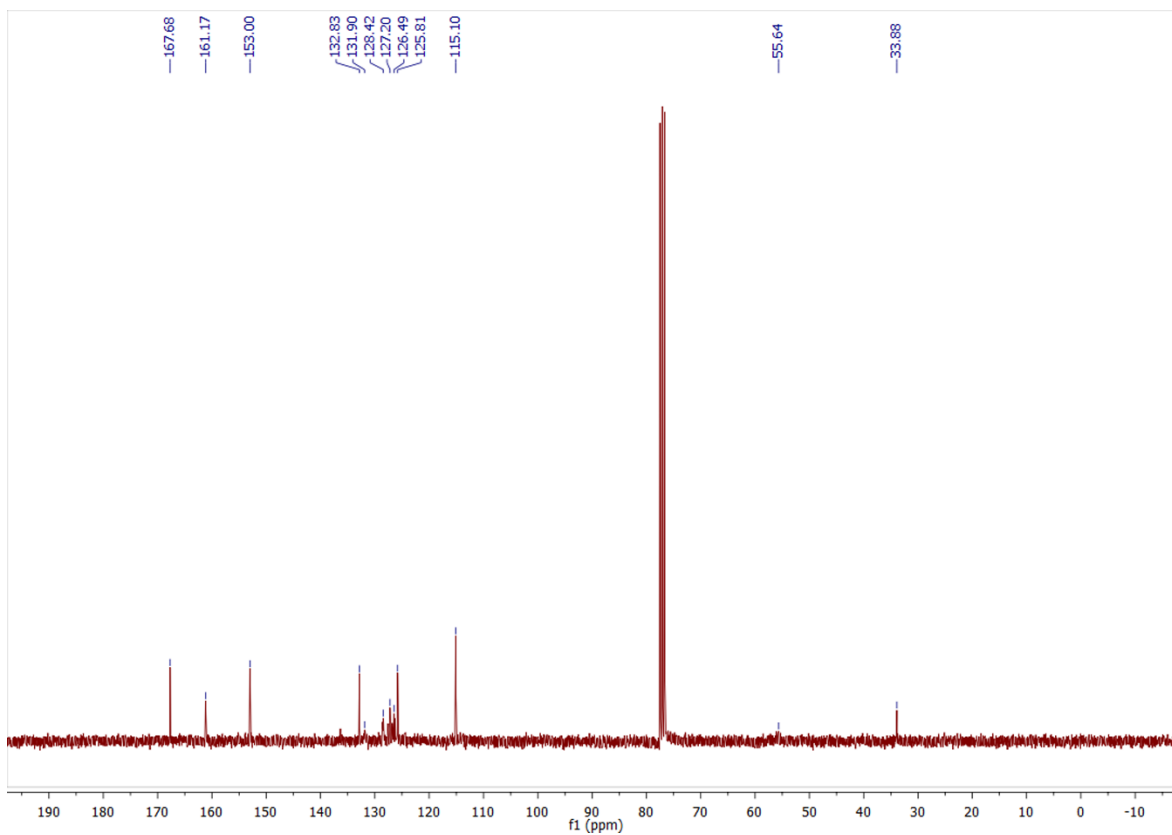
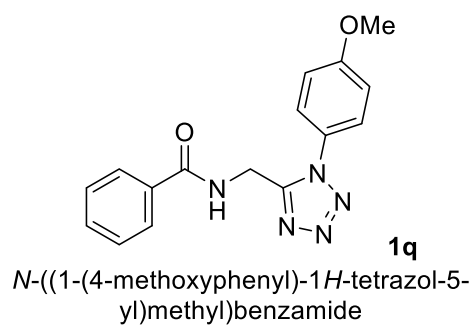
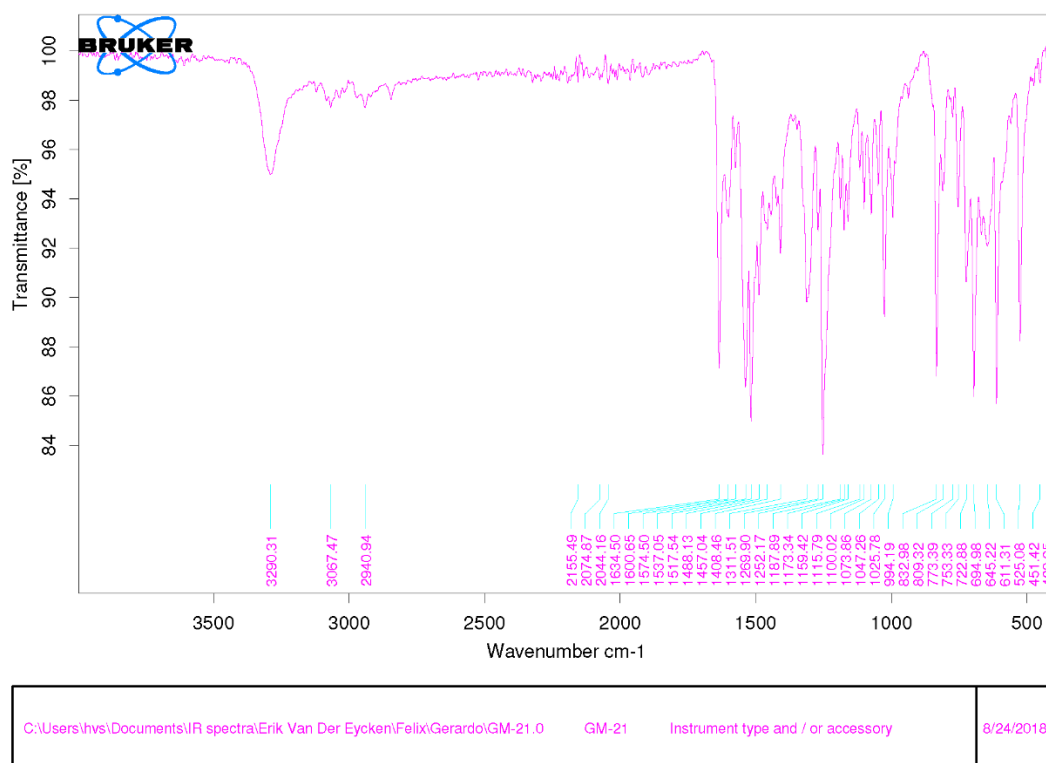
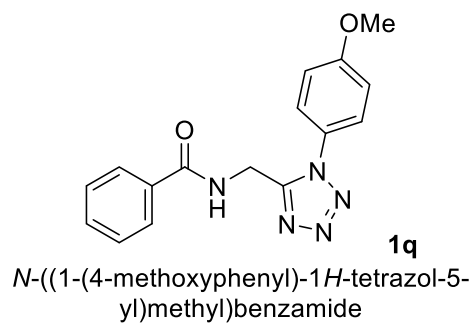


Figure S51. ^{13}C $\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) spectrum of compound **1q**.



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Figure S52. FT-IR (KBr) spectrum of compound **1q**.

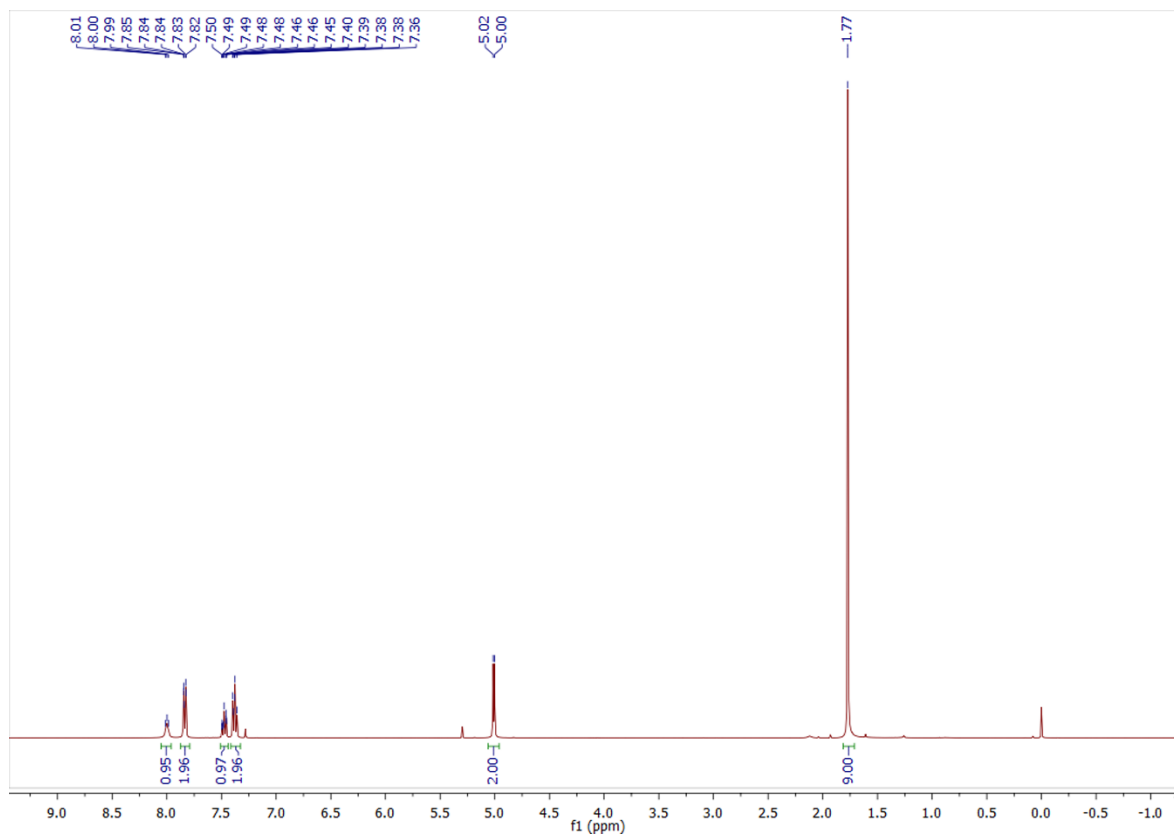
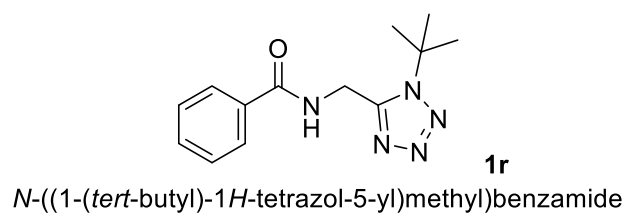
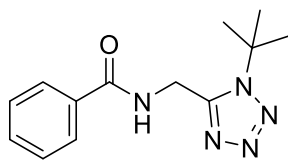


Figure S52. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **1r**.



1r

N-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)methyl)benzamide

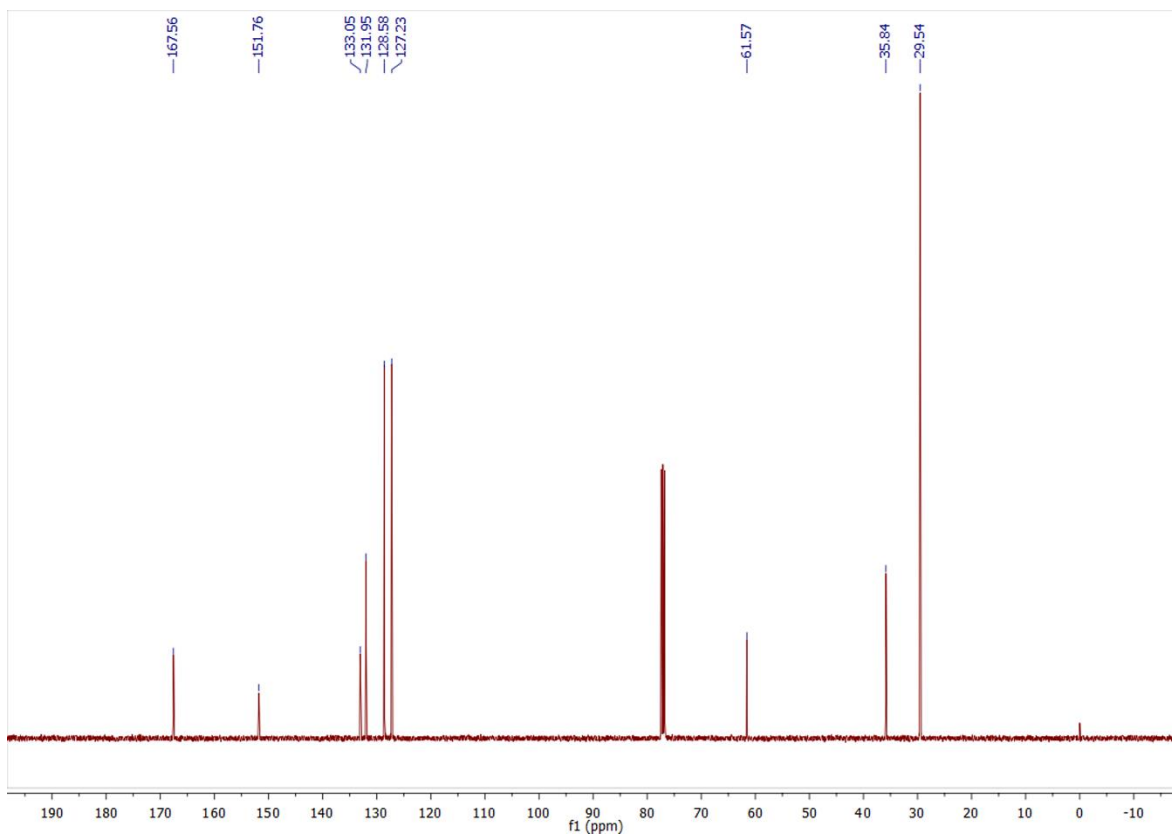
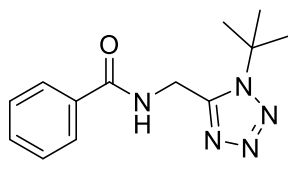
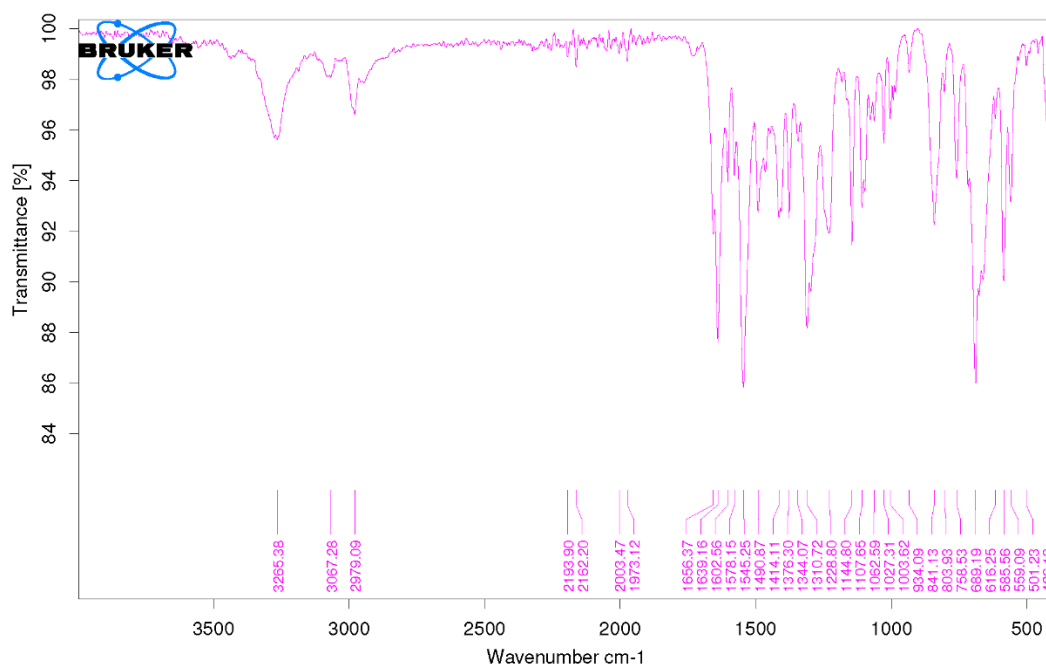


Figure S54. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **1r**.



1r

N-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)methyl)benzamide



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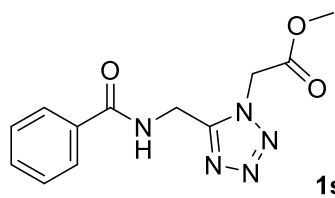
GM-017

Instrument type and / or accessory

8/24/2018

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Figure S55. FT-IR (KBr) spectrum of compound **1r**.



methyl 2-(5-(benzamidomethyl)-1*H*-tetrazol-1-yl)acetate

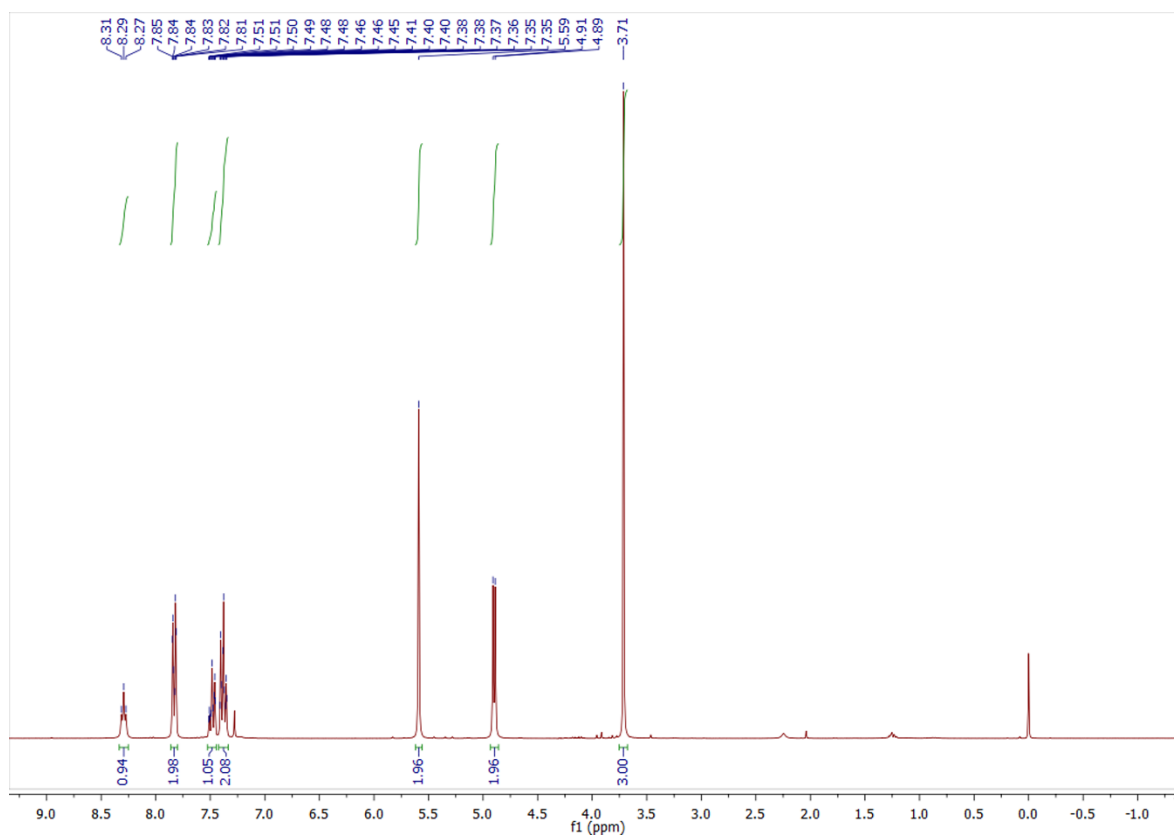
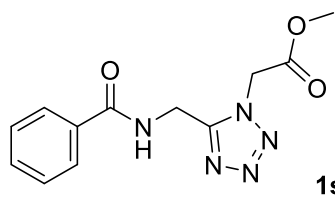


Figure S56. ^1H NMR (300 MHz, CDCl_3) spectrum of compound **1s**.



methyl 2-(5-(benzamidomethyl)-1*H*-tetrazol-1-yl)acetate

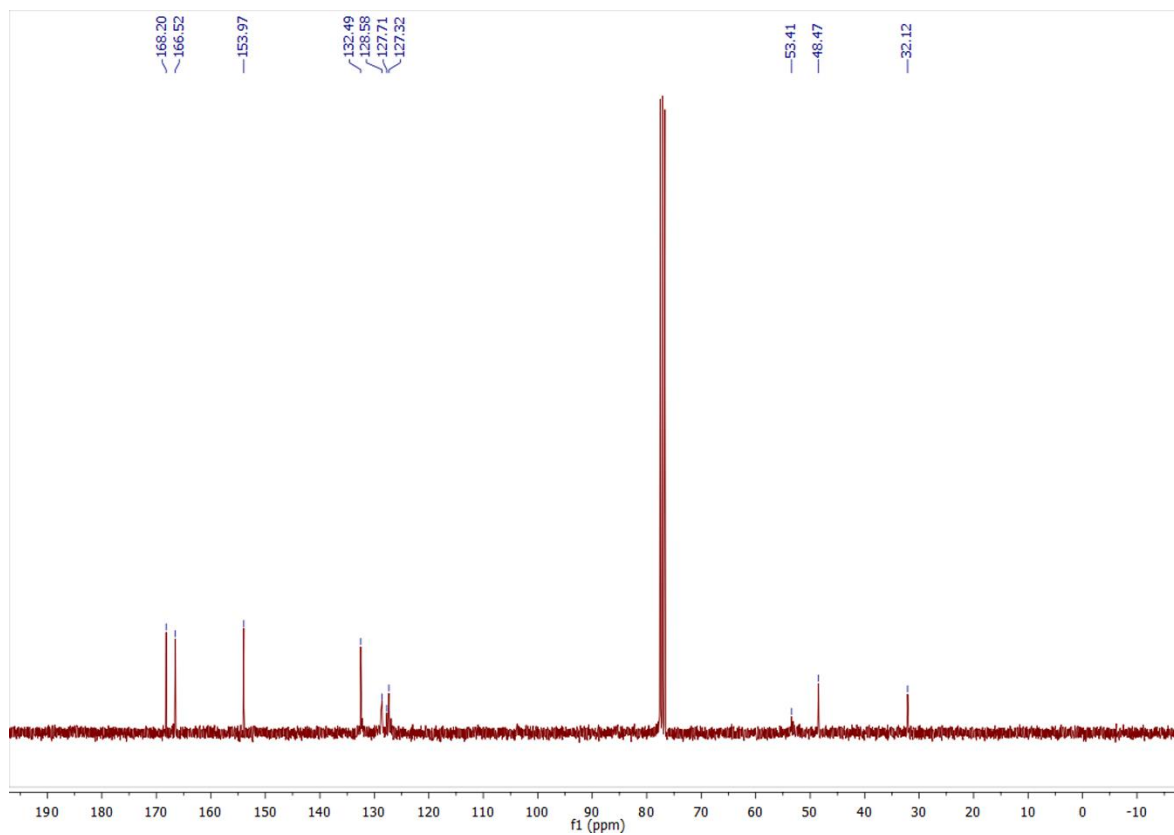
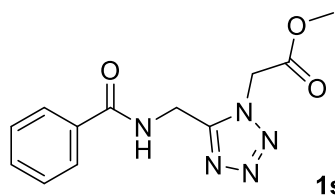
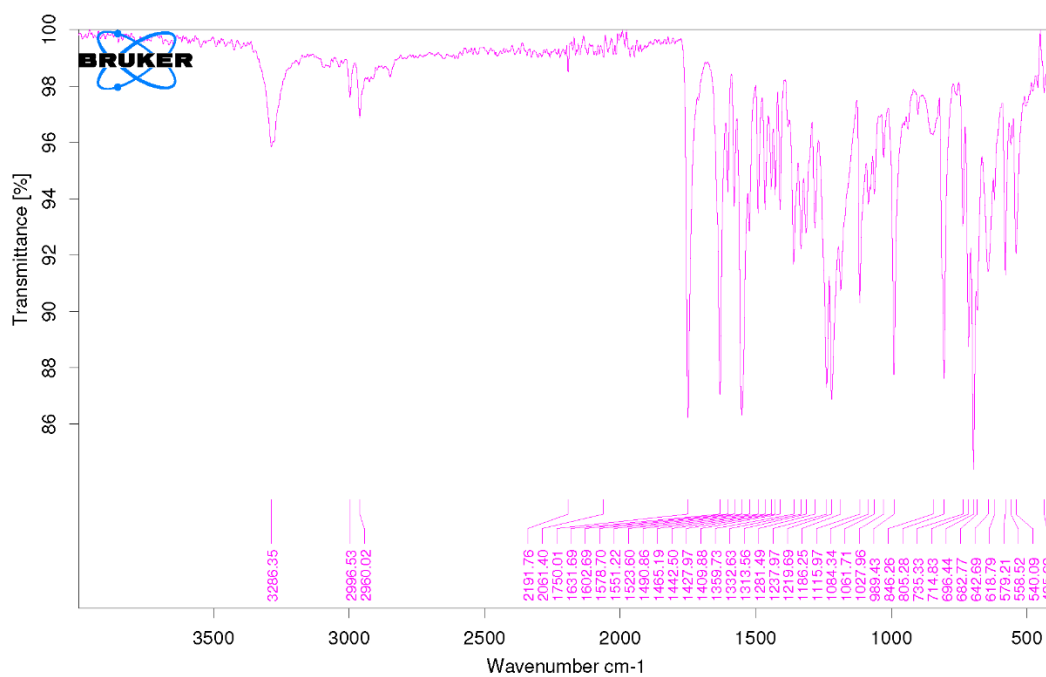


Figure S57. ^{13}C $\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) spectrum of compound **1s**.



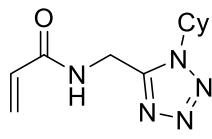
1s

methyl 2-(5-(benzamidomethyl)-1*H*-tetrazol-1-yl)acetate



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Figure S58. FT-IR (KBr) spectrum of compound **1s**.



2a

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)acrylamide

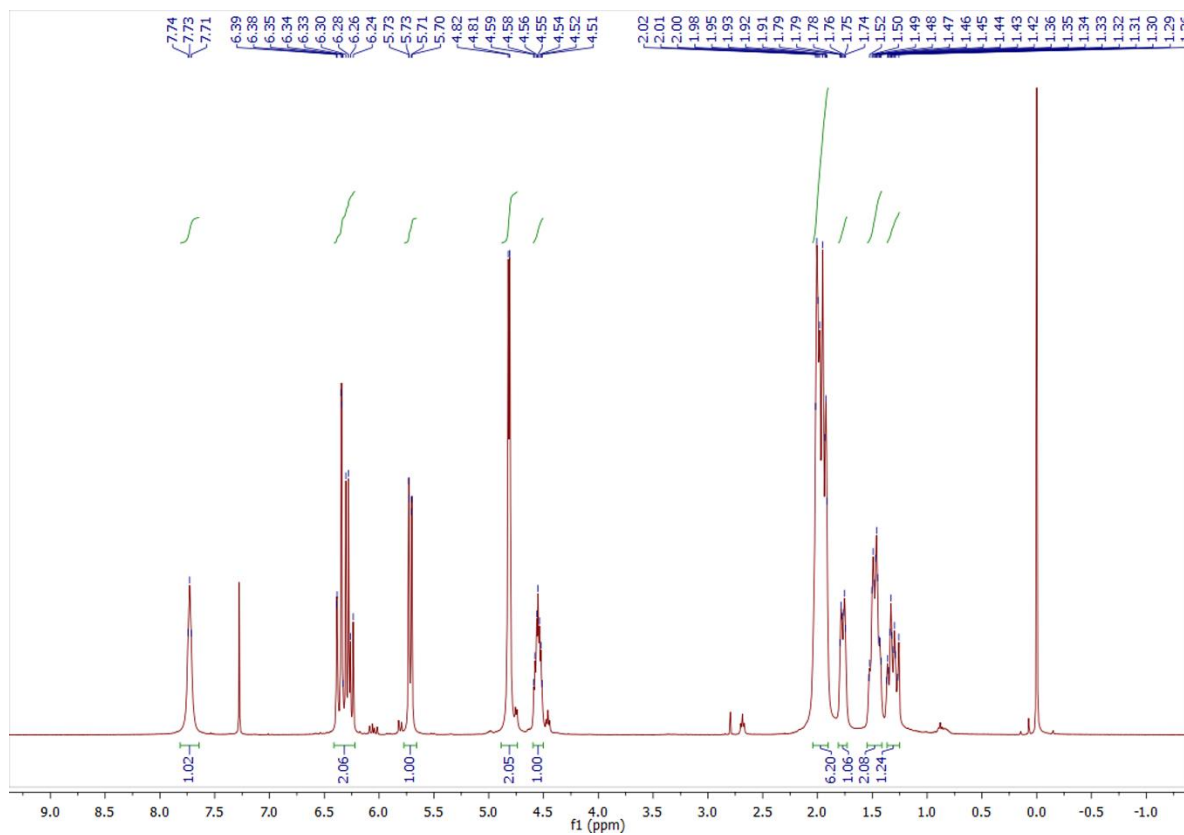
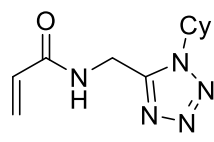


Figure S59. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2a**.



2a

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)acrylamide

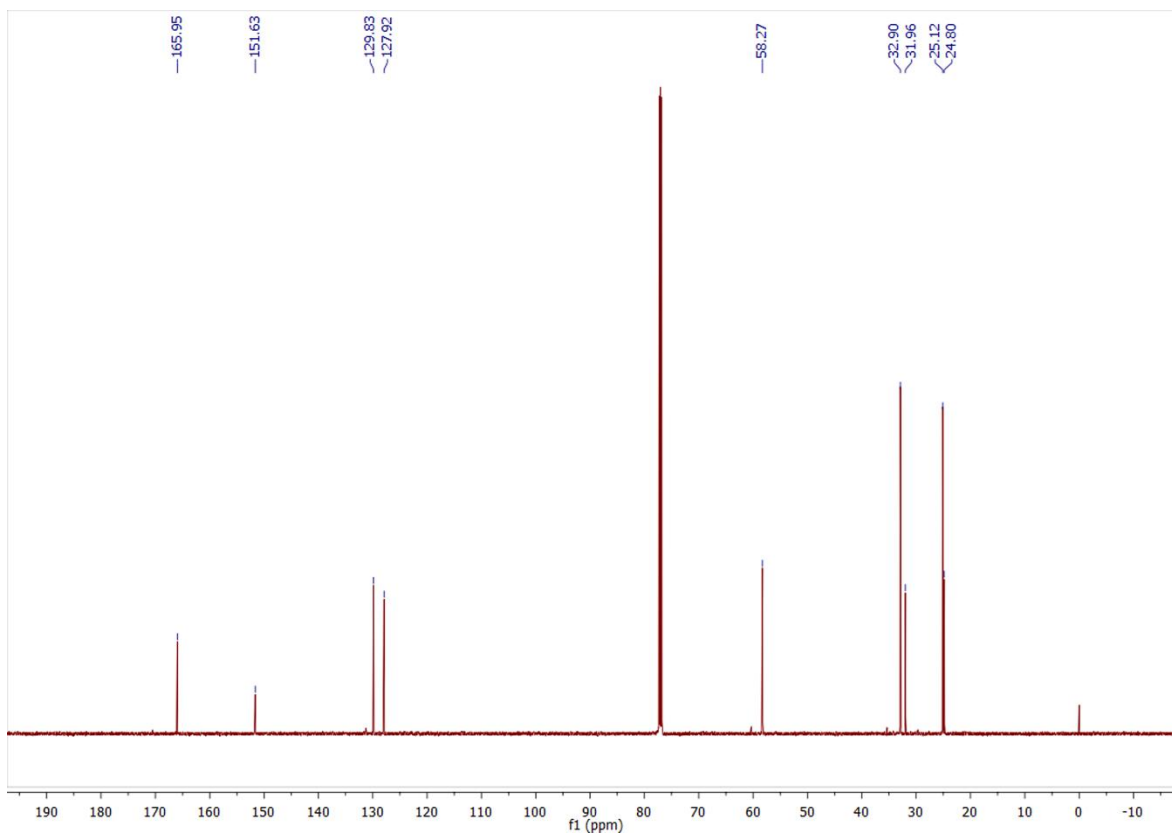
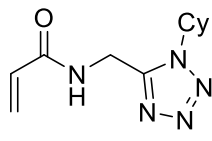
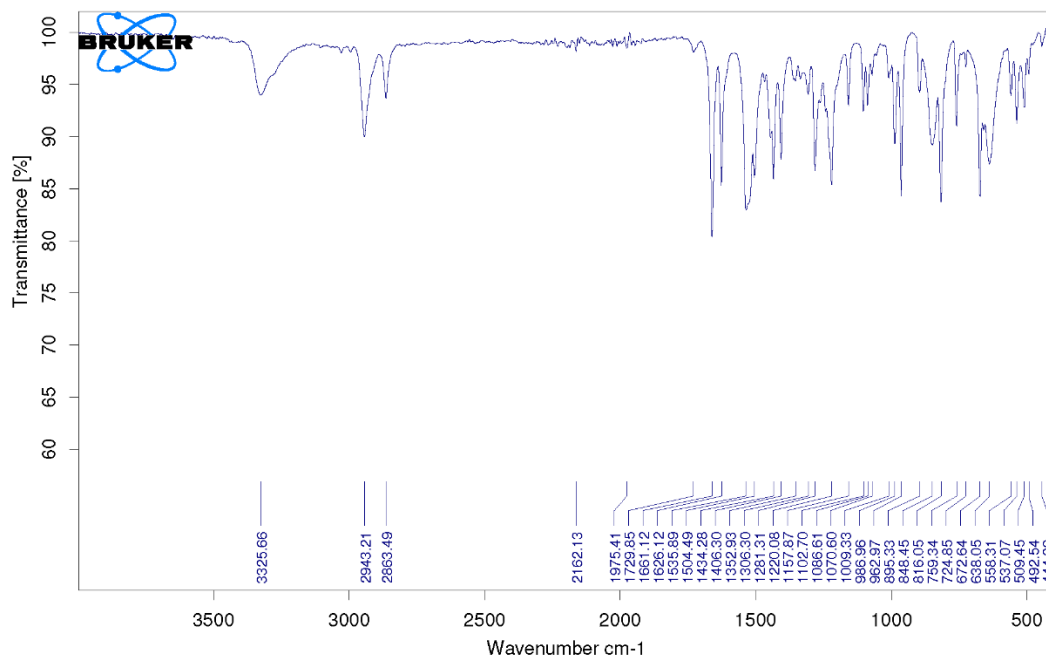


Figure S60. ^{13}C { ^1H } NMR (151 MHz, CDCl_3) spectrum of compound **2a**.



2a

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)acrylamide



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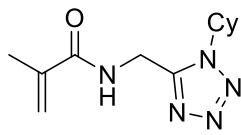
GM-043

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Figure S61. FT-IR (KBr) spectrum of compound **2a**.



2b

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)methacrylamide

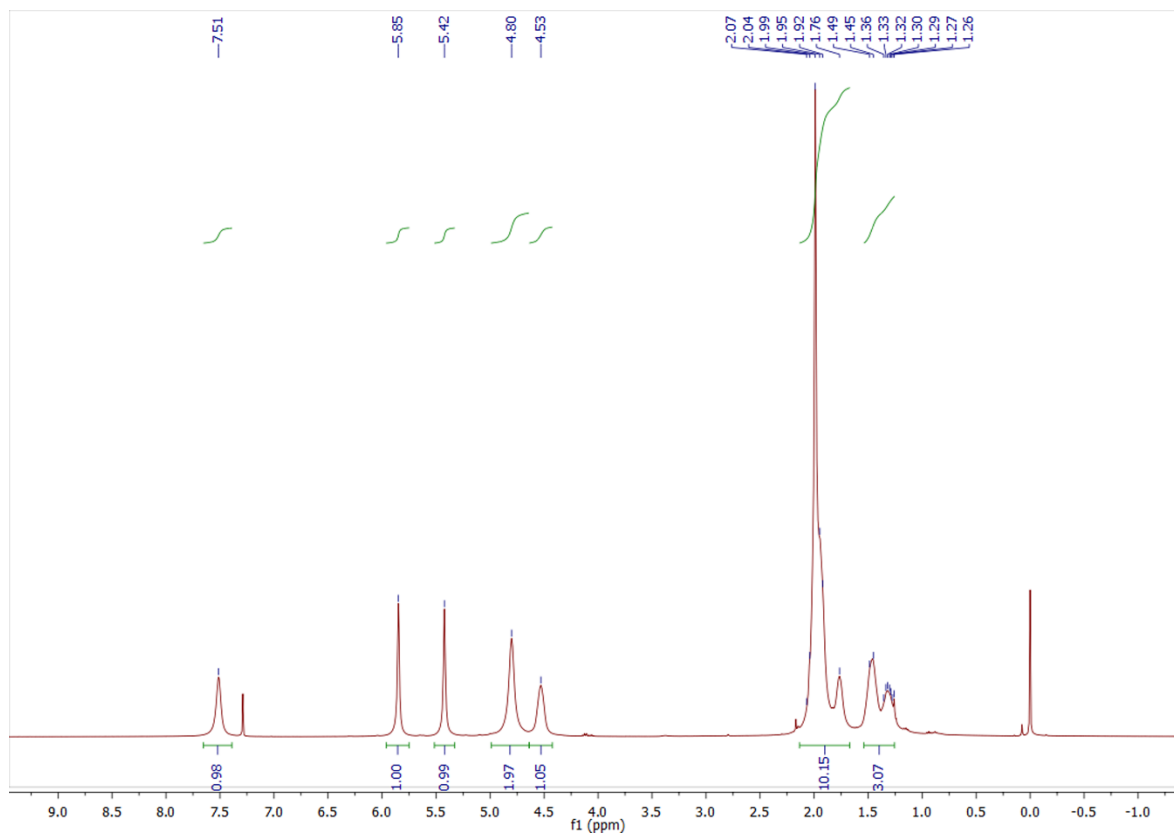
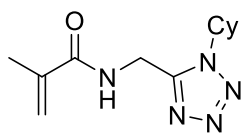


Figure S62. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2b**.



2b

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)methacrylamide

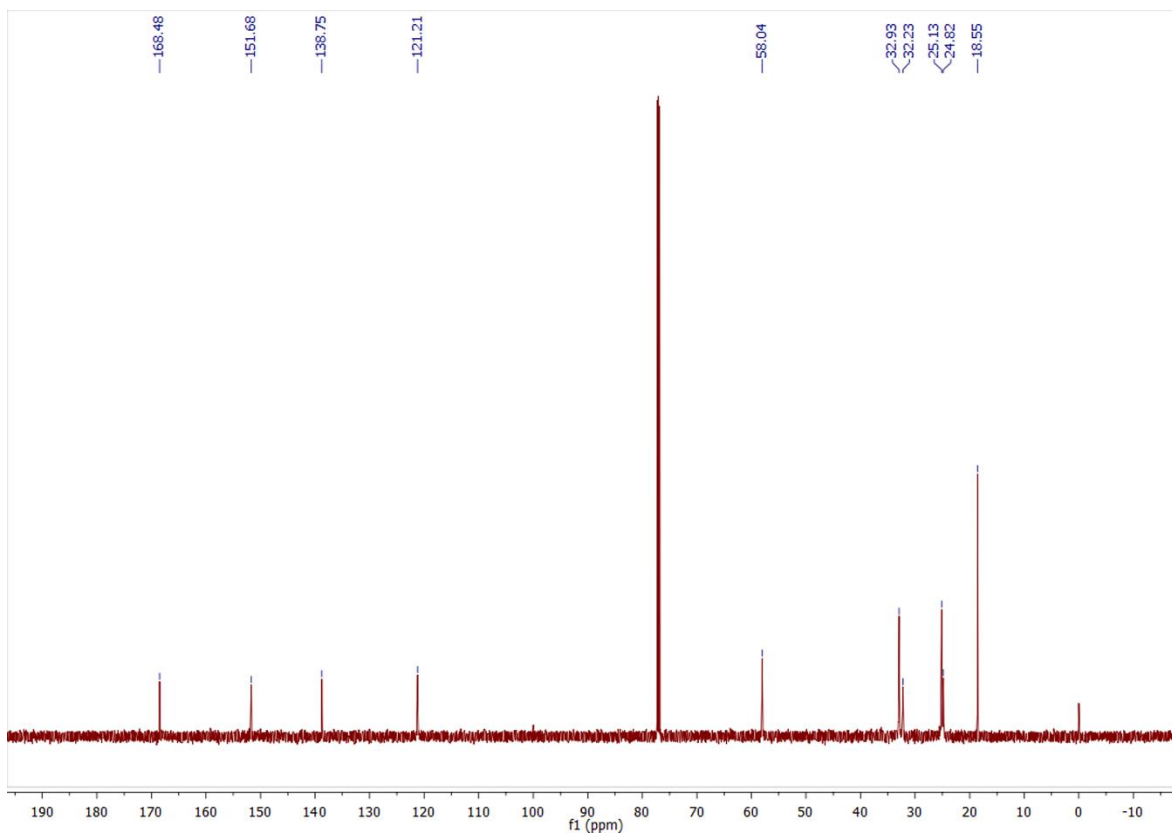
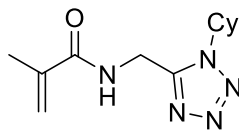
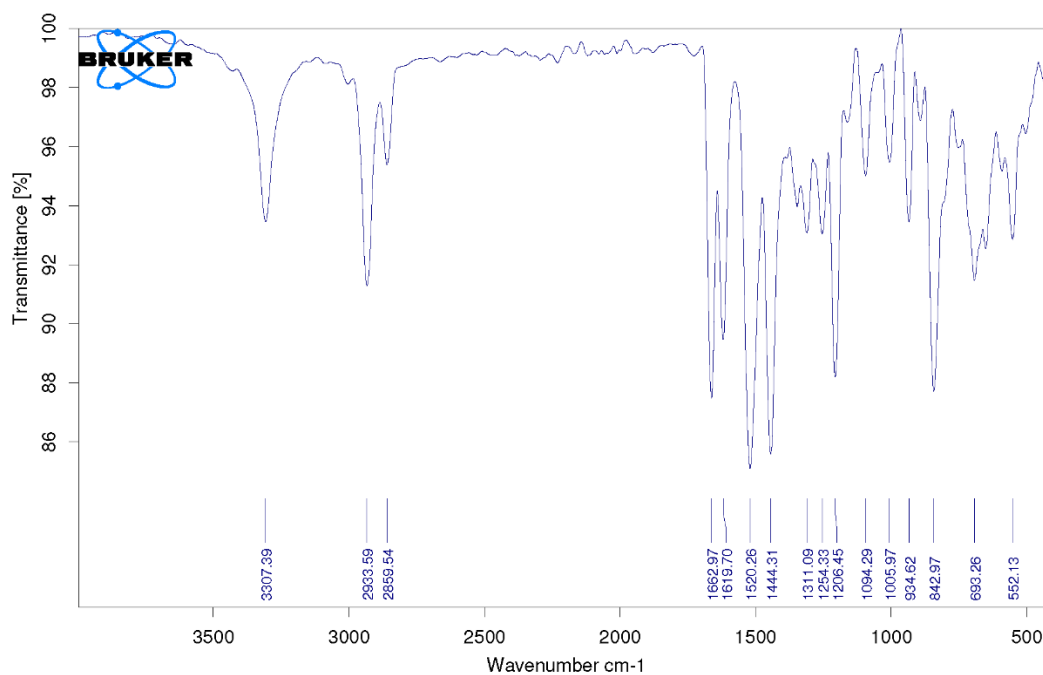


Figure S63. ^{13}C { ^1H } NMR (151 MHz, CDCl_3) spectrum of compound **2b**.



2b

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)methacrylamide



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Figure S64. FT-IR (KBr) spectrum of compound **2b**.

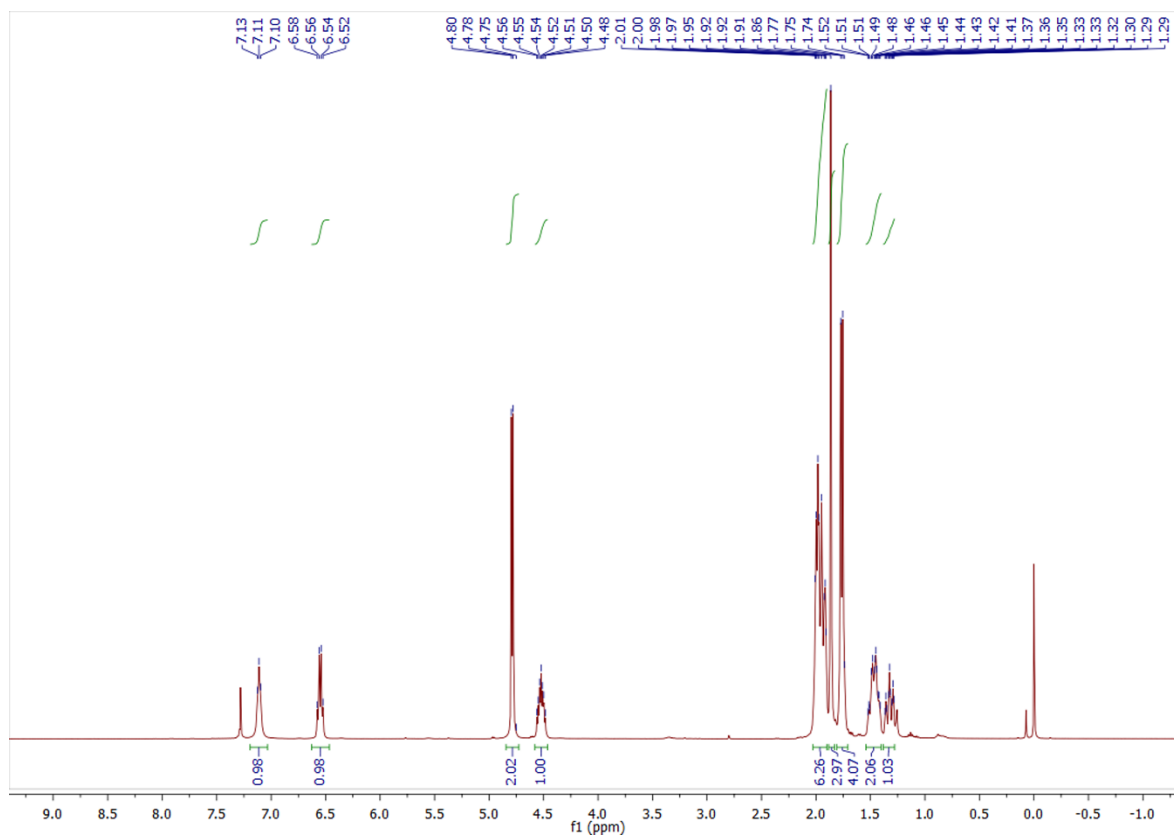
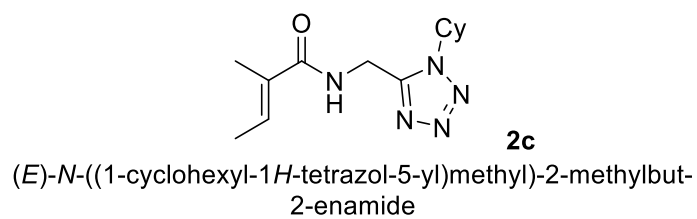


Figure S65. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2c**.

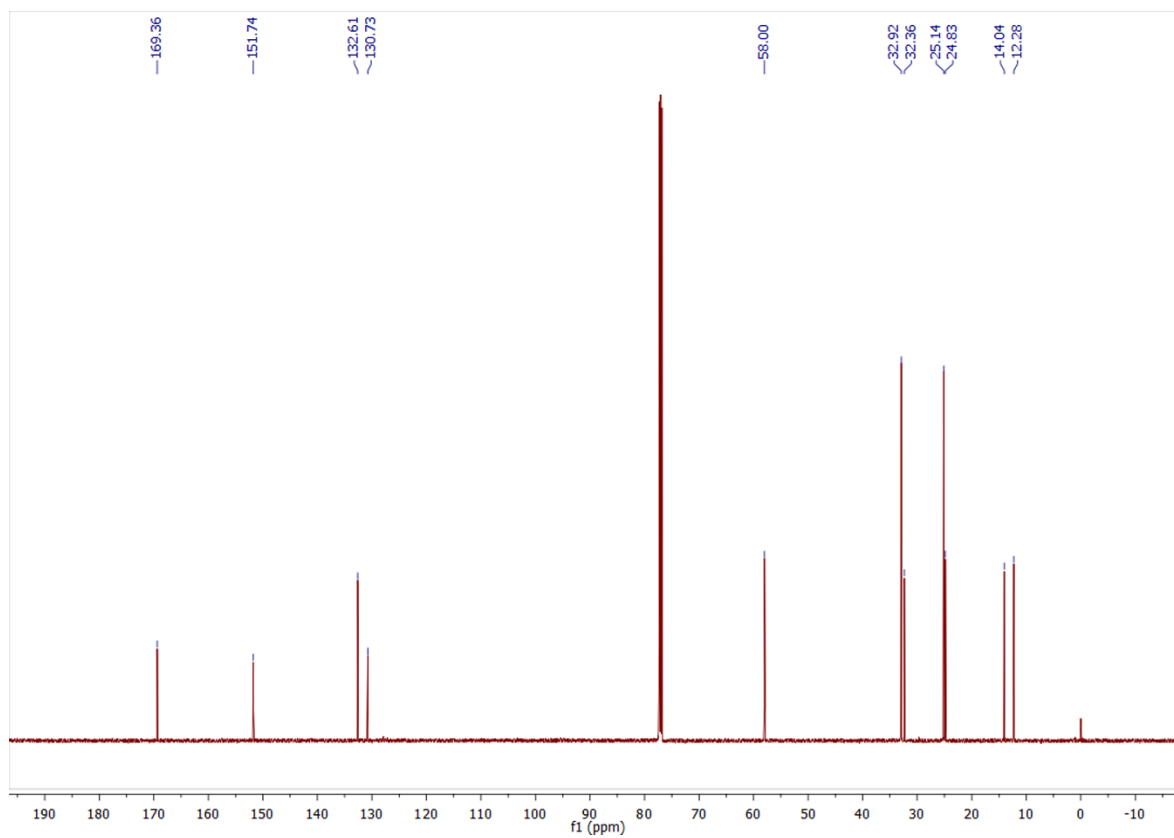
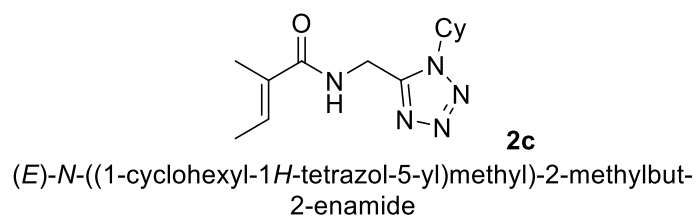
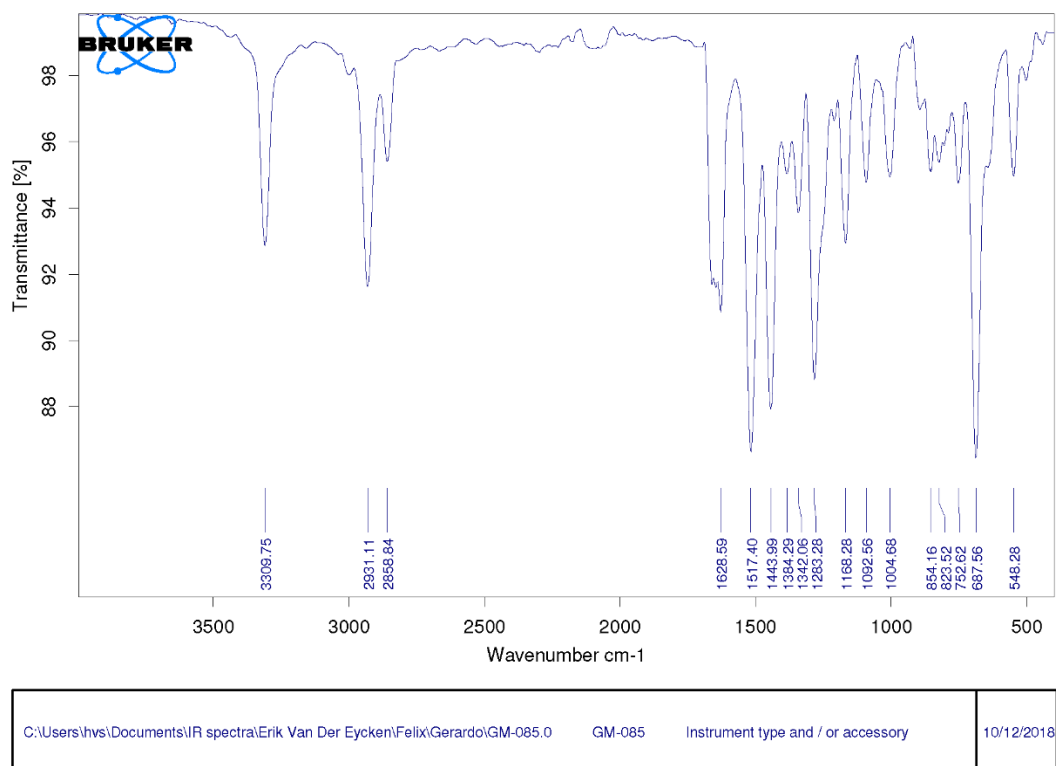
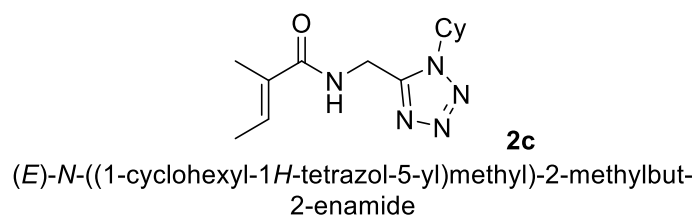
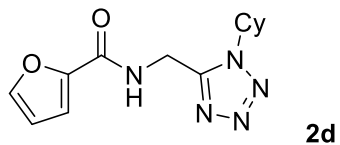


Figure S66. ^{13}C { ^1H } NMR (151 MHz, CDCl_3) spectrum of compound **2c**.



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Figure S67. FT-IR (KBr) spectrum of compound **2c**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)furan-2-carboxamide

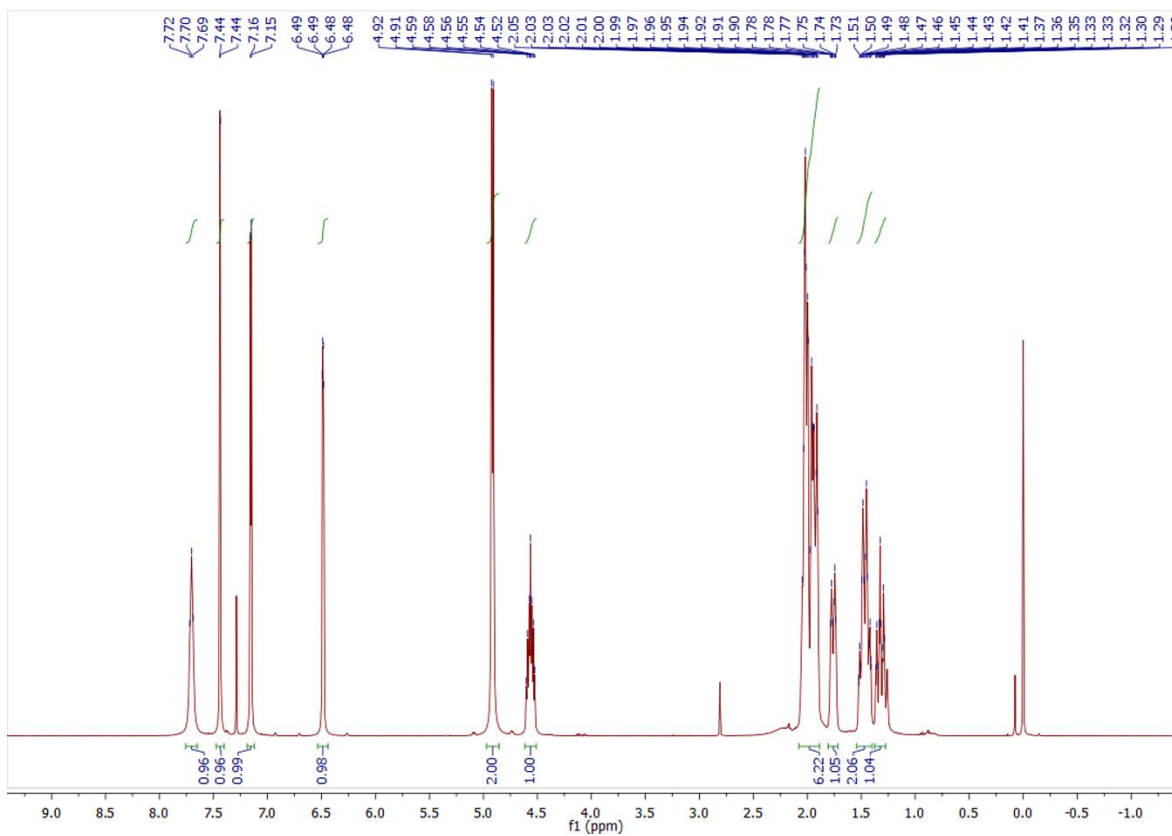
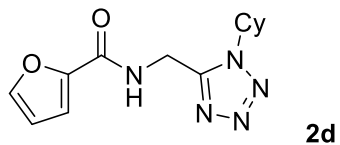


Figure S68. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2d**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)furan-2-carboxamide

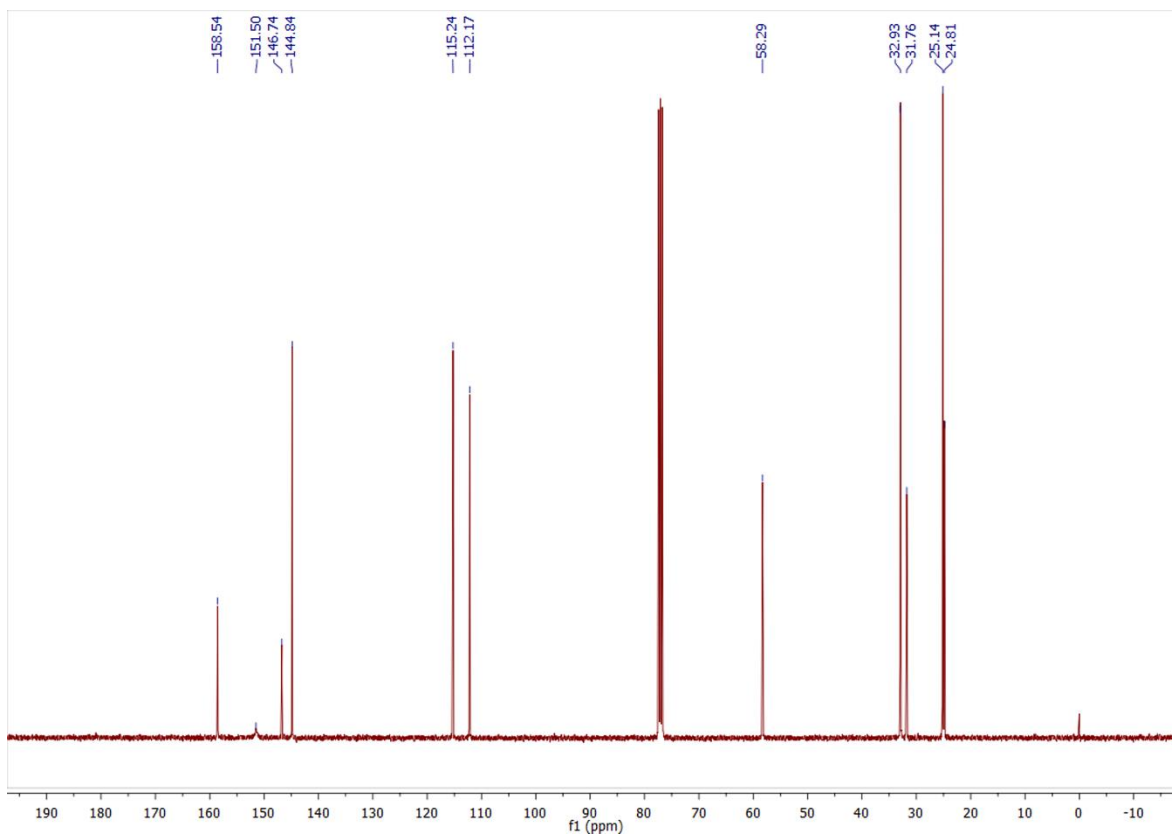
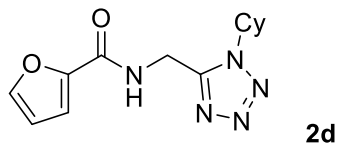
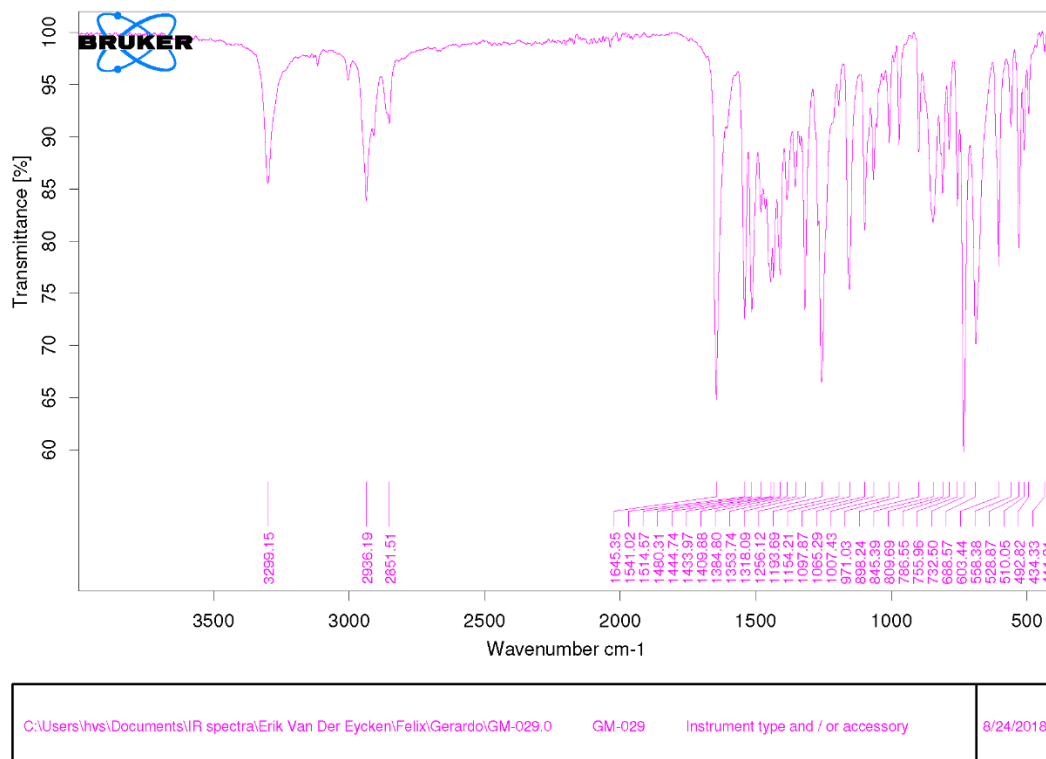


Figure S69. ^{13}C { ^1H } NMR (101 MHz, CDCl_3) spectrum of compound **2d**.

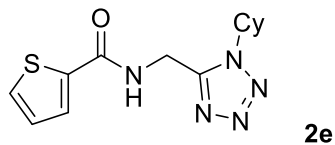


N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)furan-2-carboxamide



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Figure S70. FT-IR (KBr) spectrum of compound **2d**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)thiophene-2-carboxamide

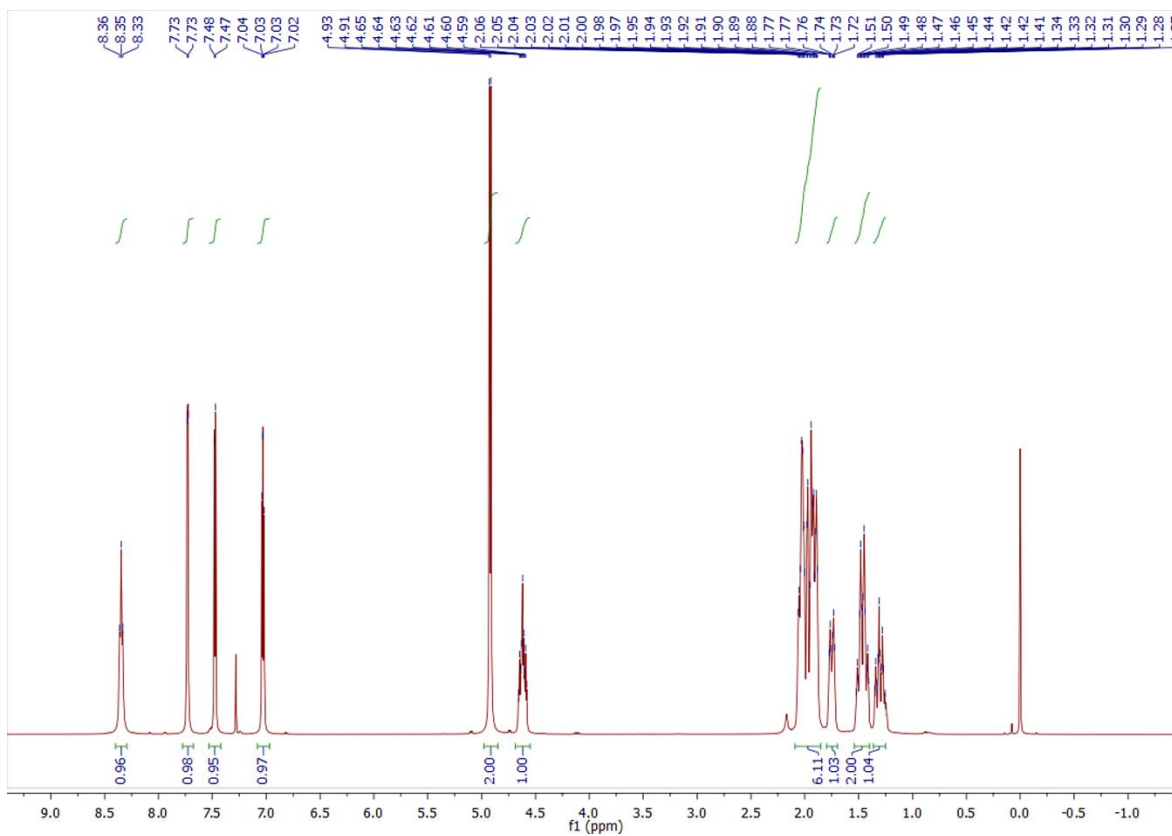
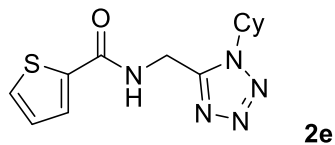


Figure S71. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2e**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)thiophene-2-carboxamide

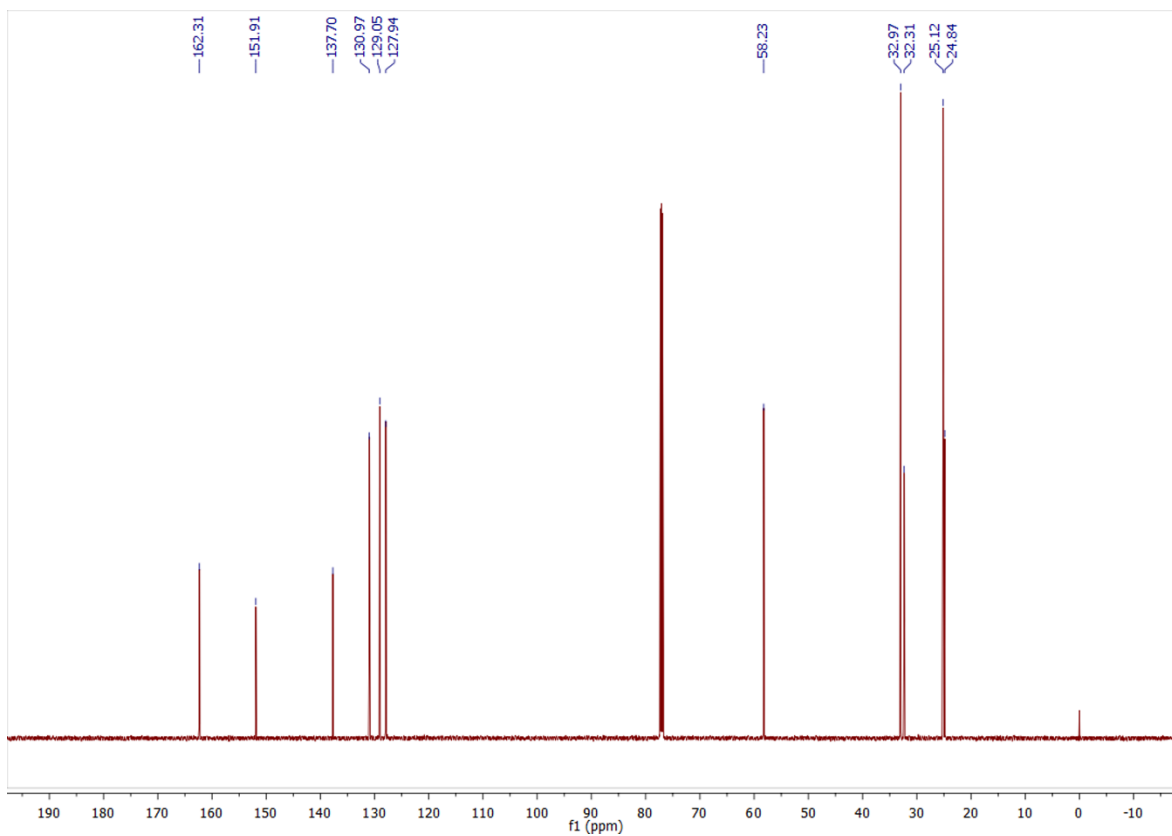
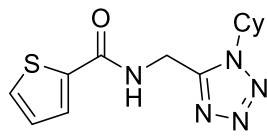
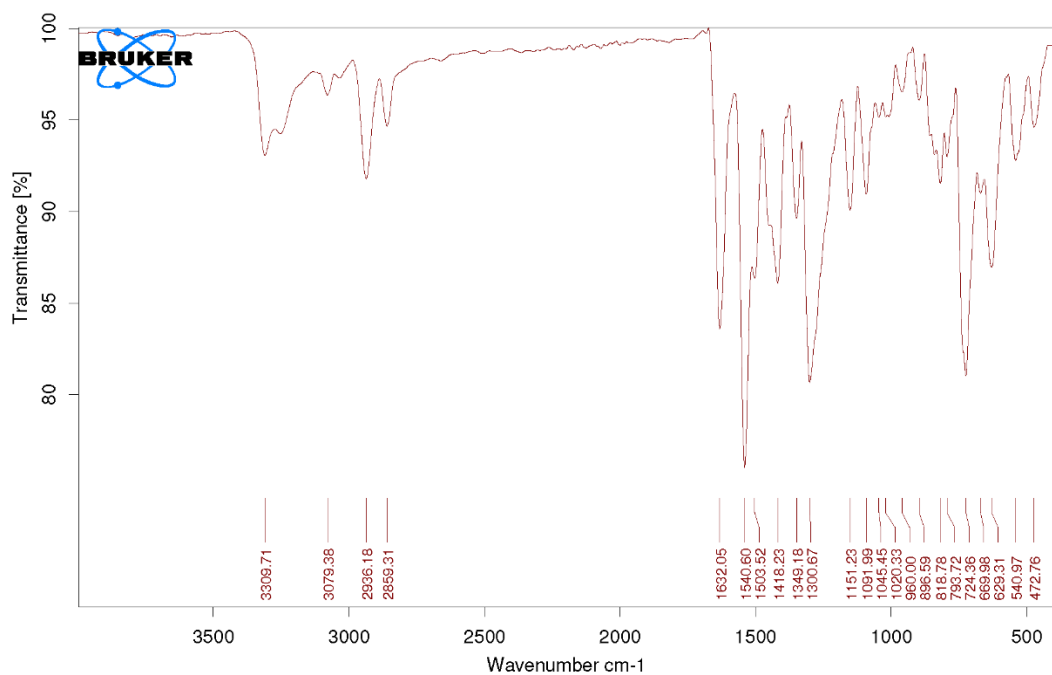


Figure S72. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **2e**.



2e

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)thiophene-2-carboxamide



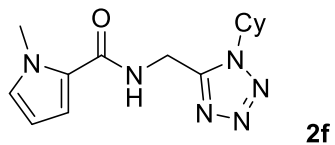
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Figure S73. FT-IR (KBr) spectrum of compound **2e**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-methyl-1*H*-pyrrole-2-carboxamide

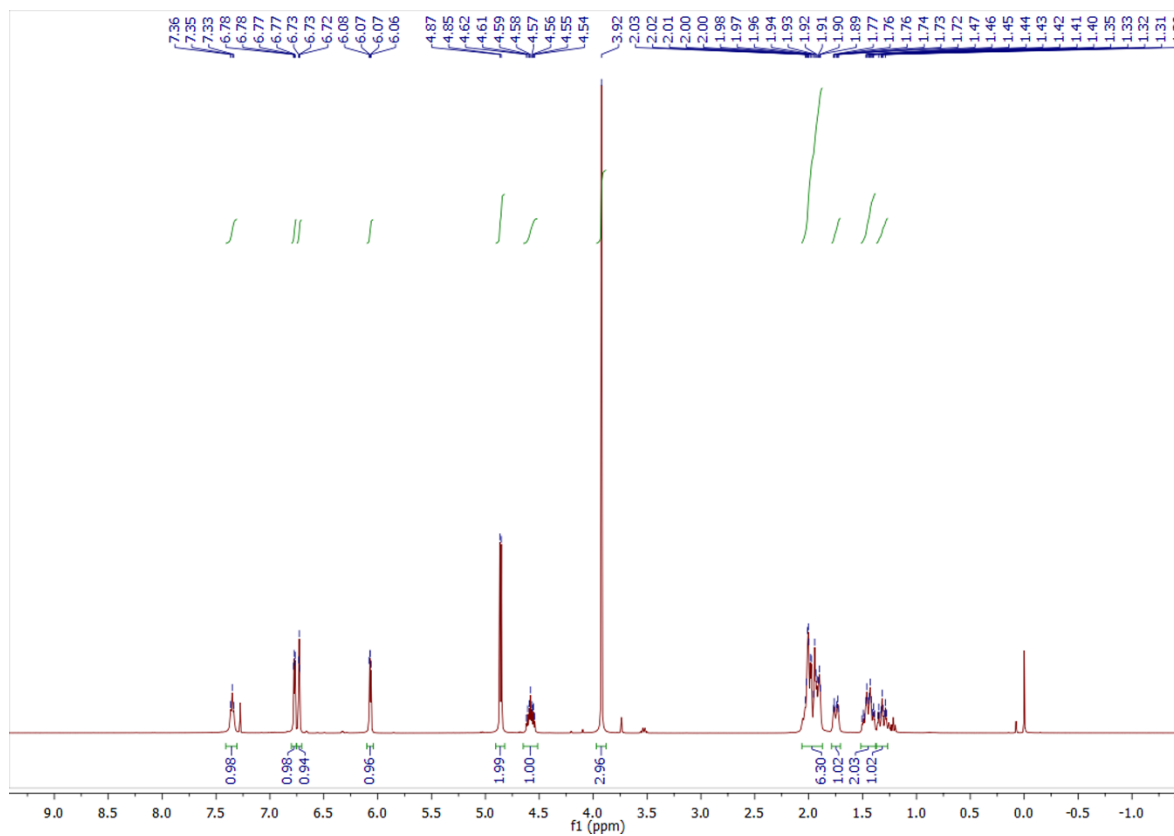
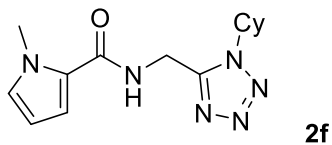


Figure S74. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2f**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-methyl-1*H*-pyrrole-2-carboxamide

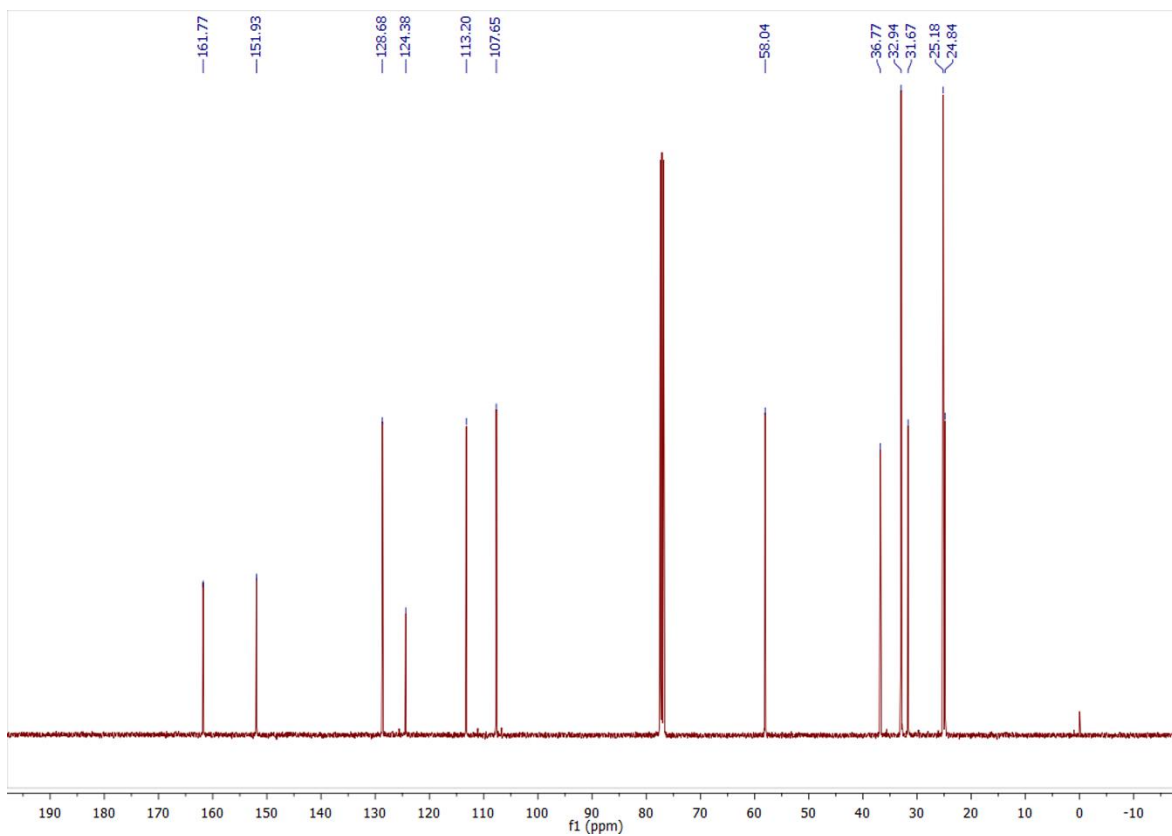
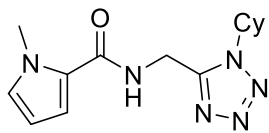
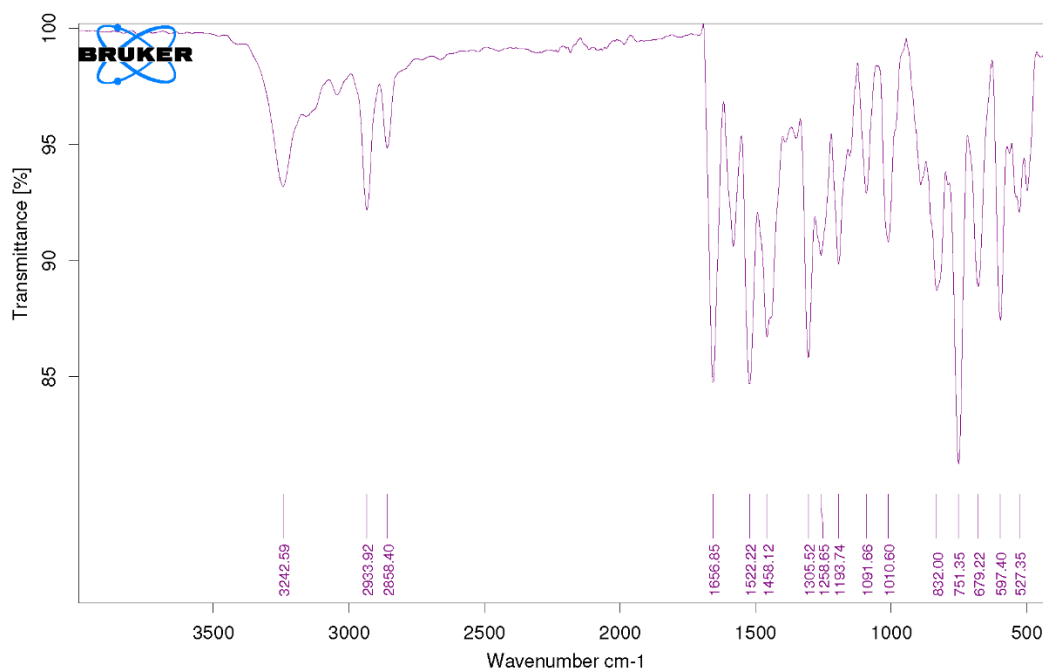


Figure S75. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **2f**.



2f

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-methyl-1*H*-pyrrole-2-carboxamide



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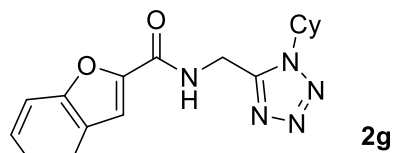
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Figure S76. FT-IR (KBr) spectrum of compound **2f**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzofuran-2-carboxamide

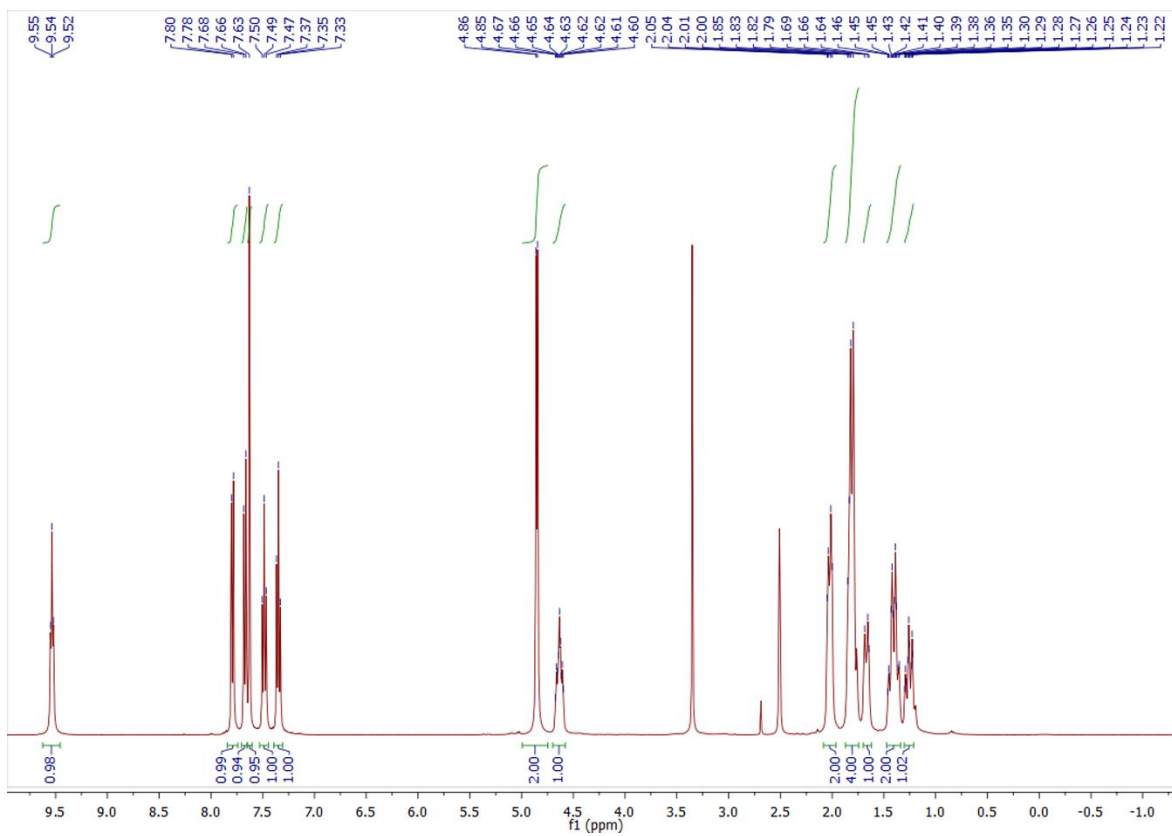


Figure S77. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **2g**.

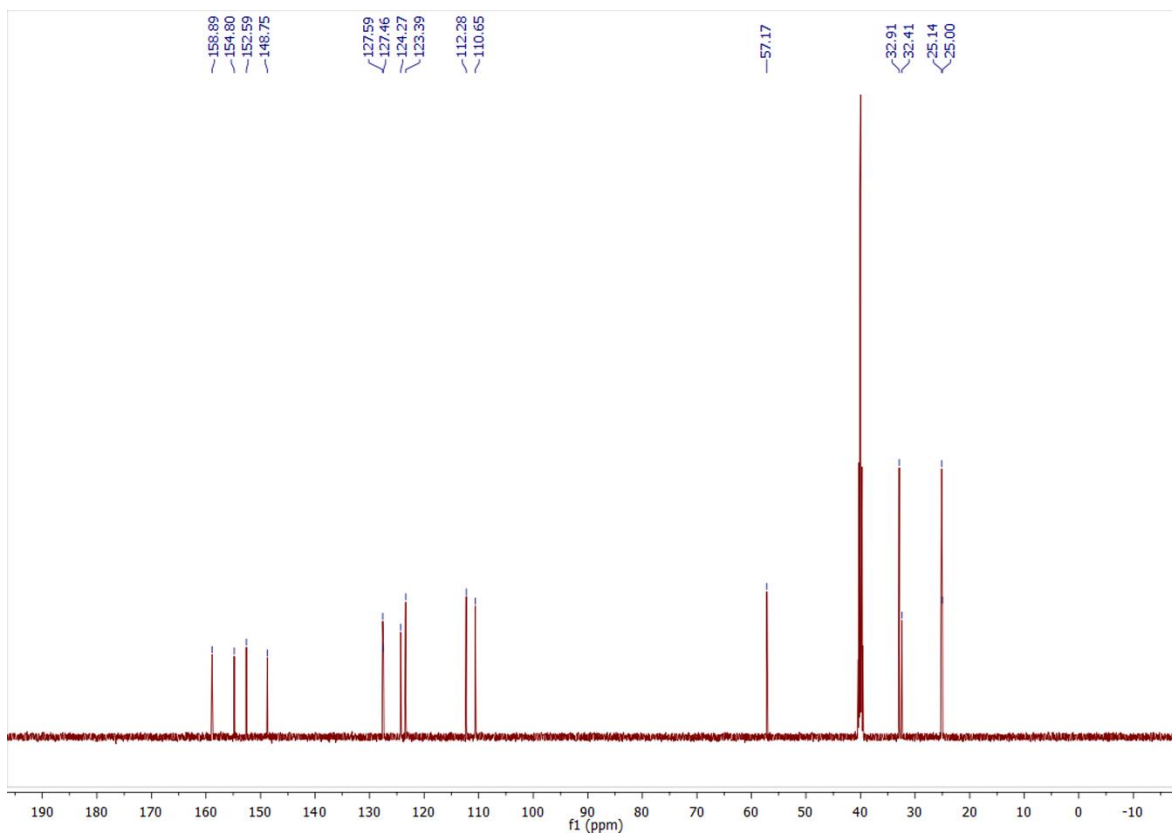
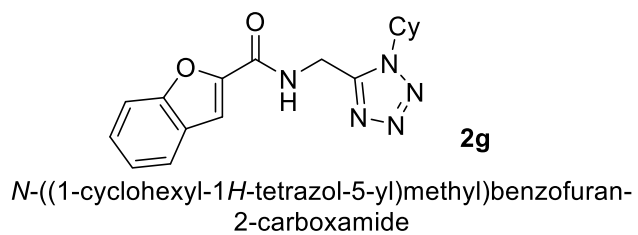
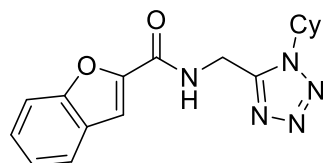
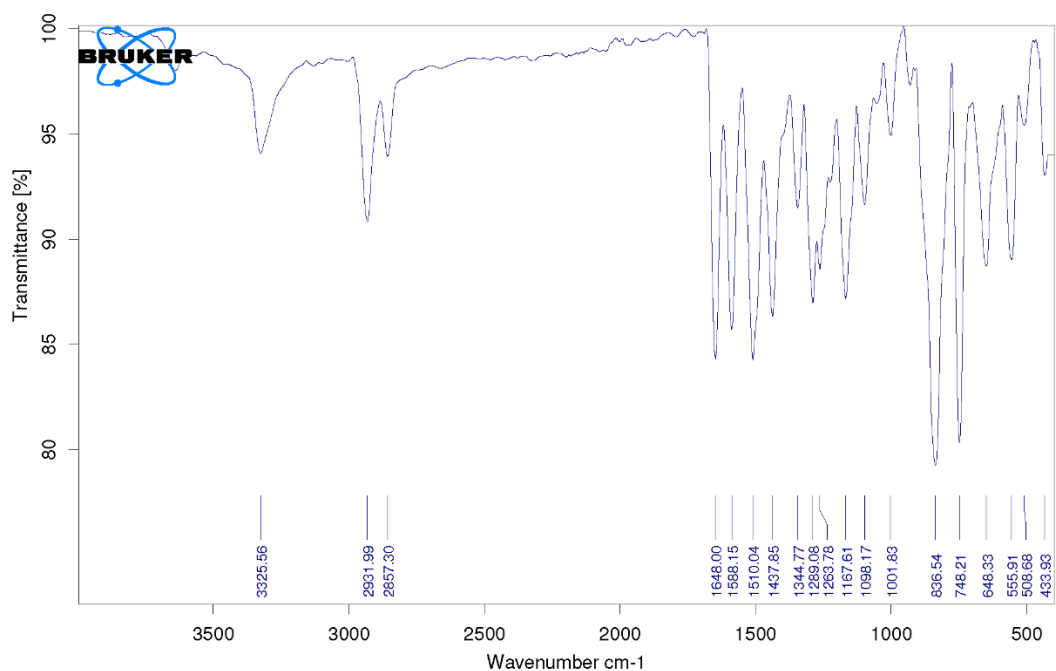


Figure S78. ^{13}C { ^1H } NMR (151 MHz, $\text{DMSO-}d_6$) spectrum of compound **2g**.



2g

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzofuran-2-carboxamide



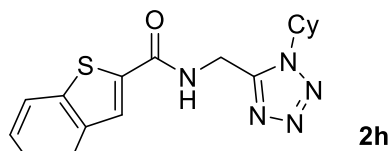
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Instrument type and / or accessory

10/12/2018

Figure S79. FT-IR (KBr) spectrum of compound **2g**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzo[*b*]thiophene-2-carboxamide

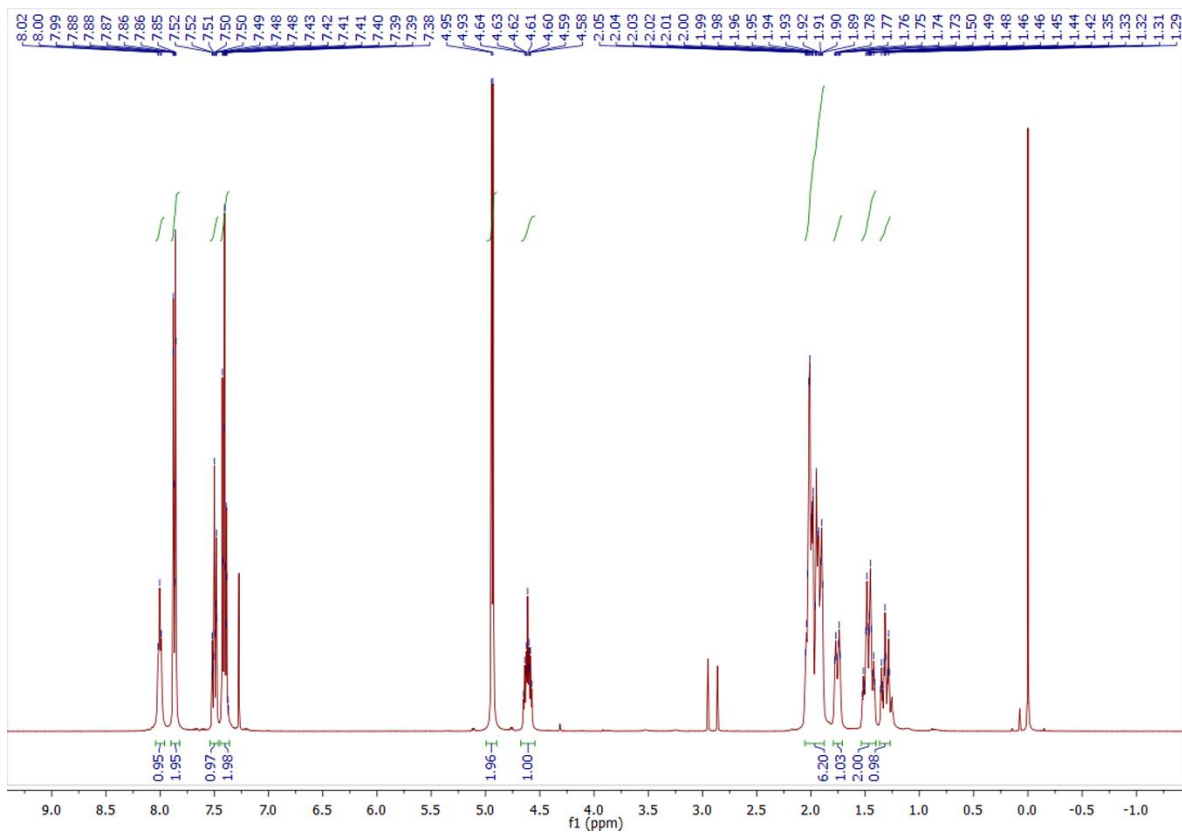
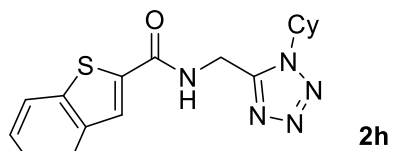


Figure S80. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **2h**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzo[*b*]thiophene-2-carboxamide

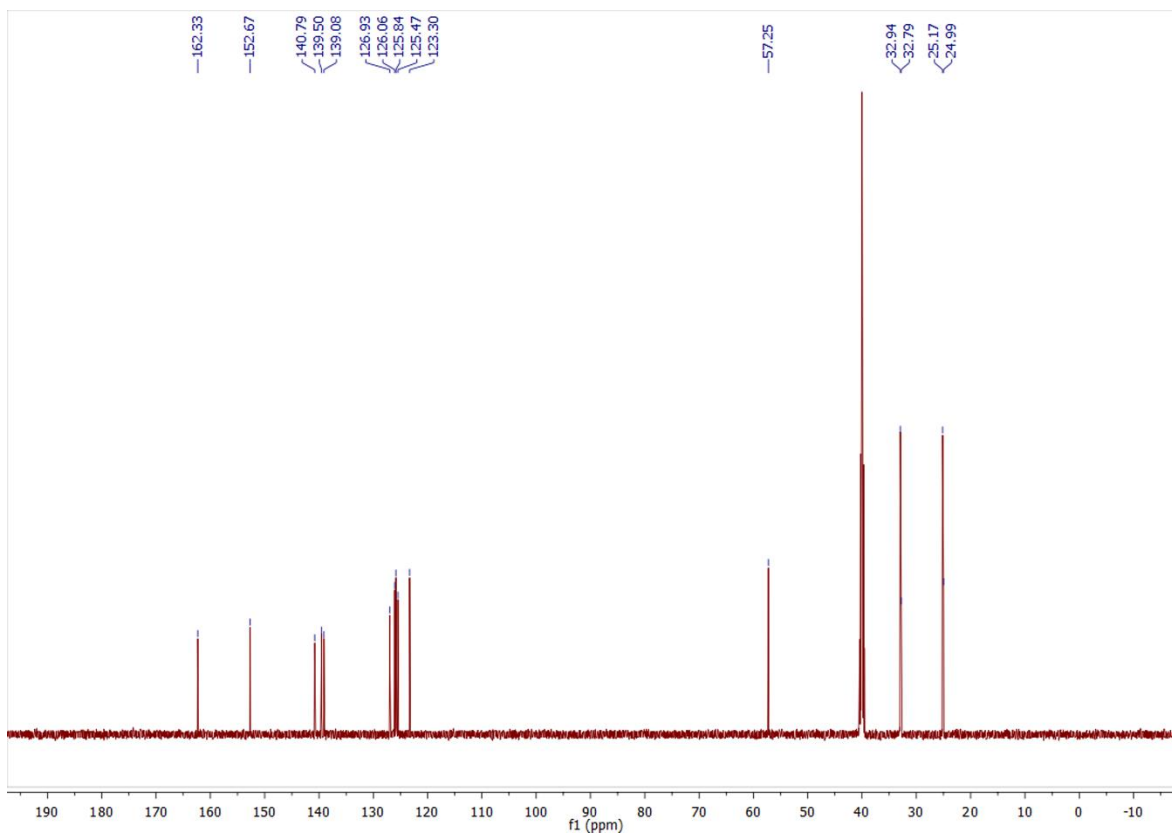
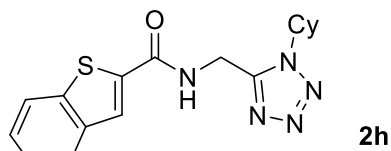
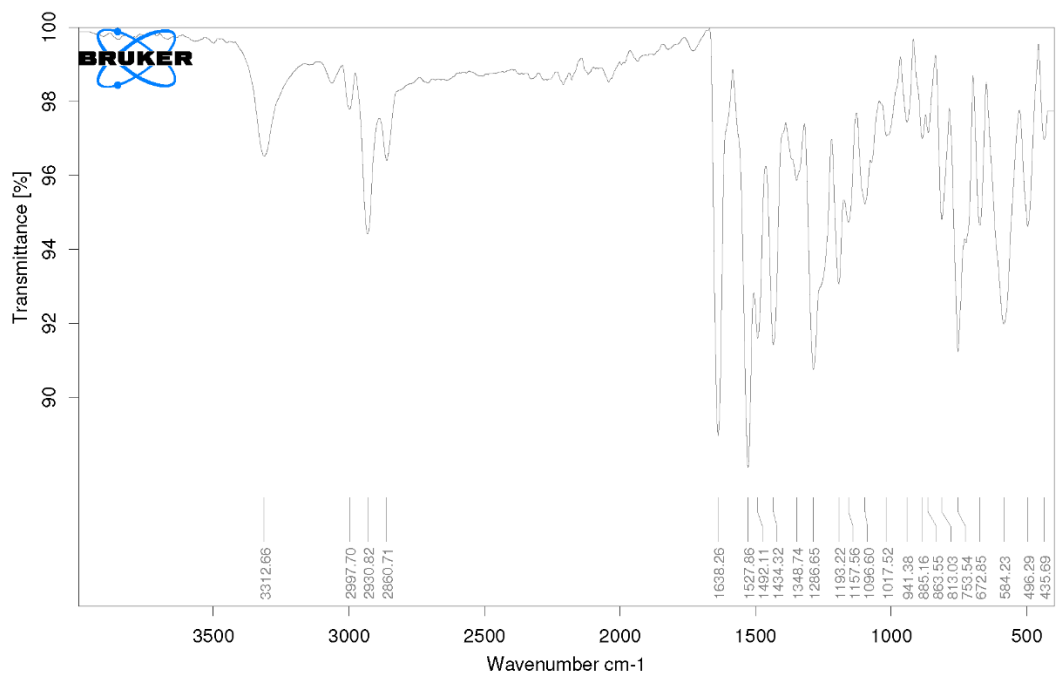


Figure S81. ^{13}C { ^1H } NMR (151 MHz, $\text{DMSO-}d_6$) spectrum of compound **2h**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)benzo[*b*]thiophene-2-carboxamide



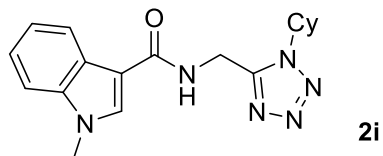
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GM-053

Instrument type and / or accessory

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Figure S82. FT-IR (KBr) spectrum of compound **2h**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-methyl-1*H*-indole-3-carboxamide

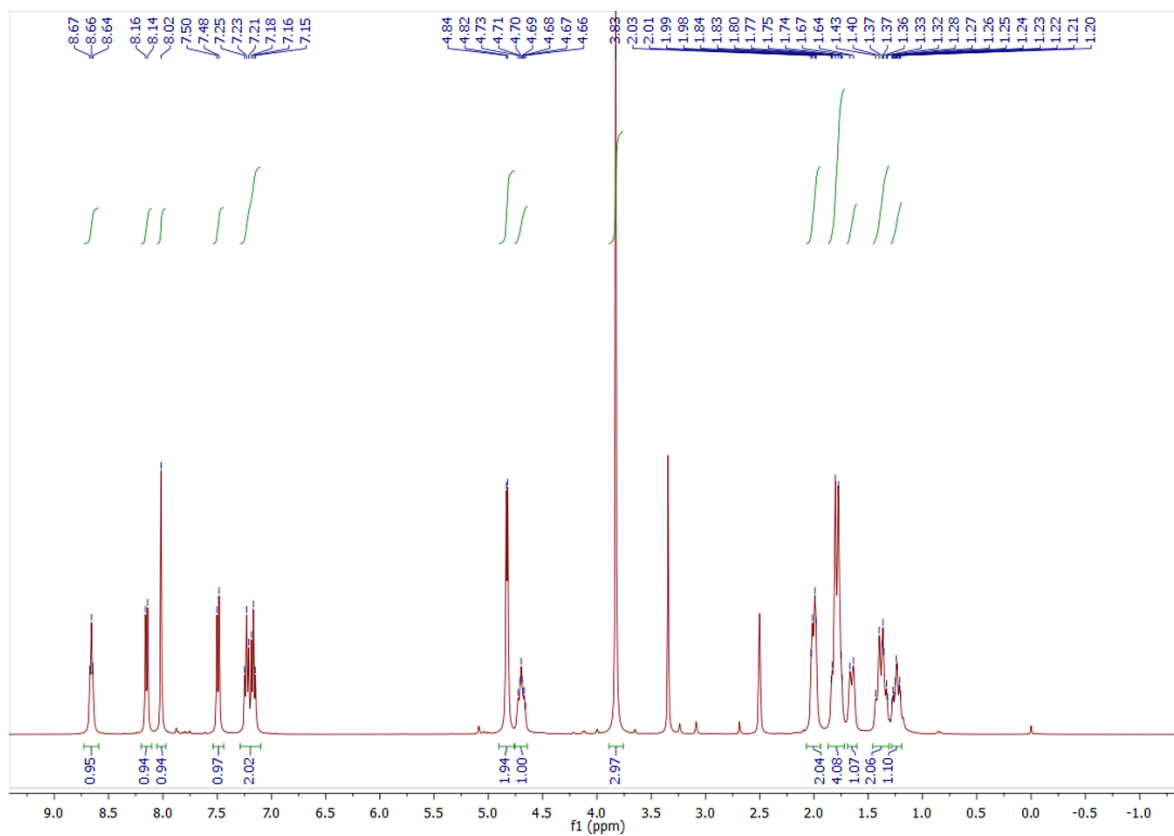
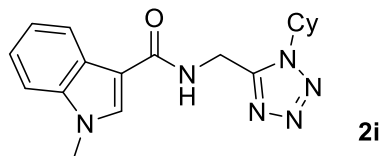


Figure S83. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **2i**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-methyl-1*H*-indole-3-carboxamide

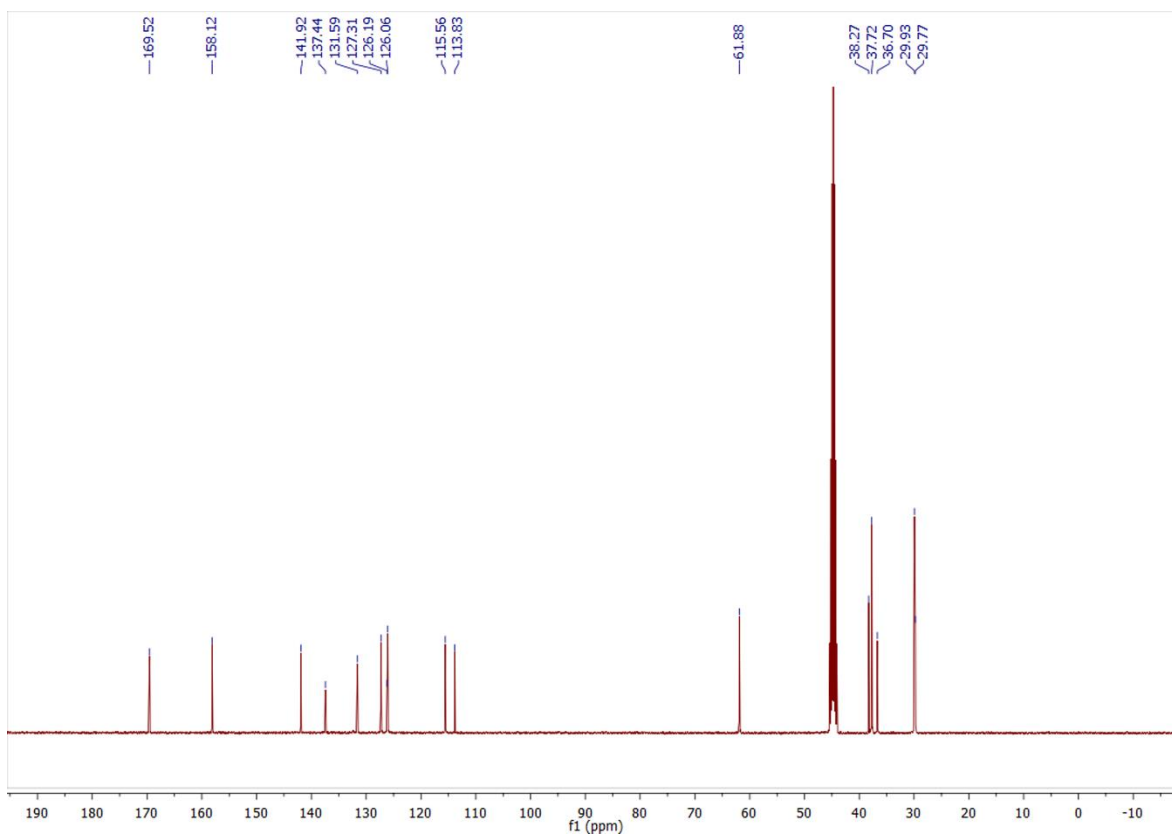
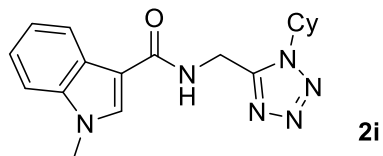
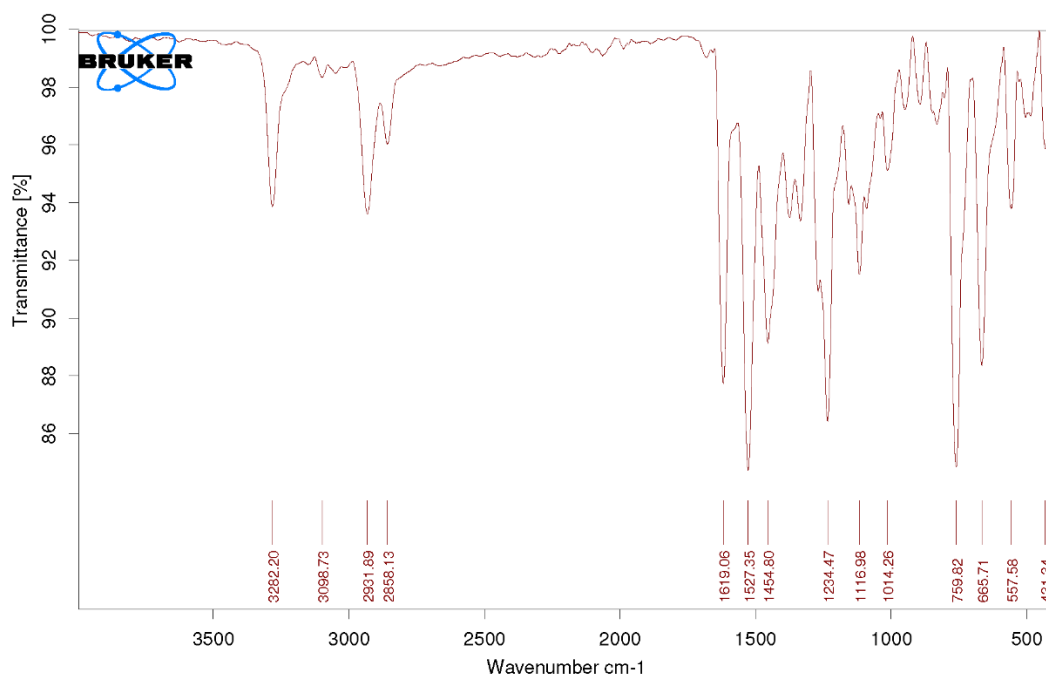


Figure S84. ^{13}C { ^1H } NMR (101 MHz, CDCl_3) spectrum of compound **2i**.



N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-methyl-1*H*-indole-3-carboxamide



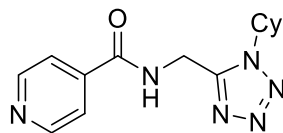
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Instrument type and / or accessory

8/24/2018

Figure S85. FT-IR (KBr) spectrum of compound **2i**.



2j

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)isonicotinamide

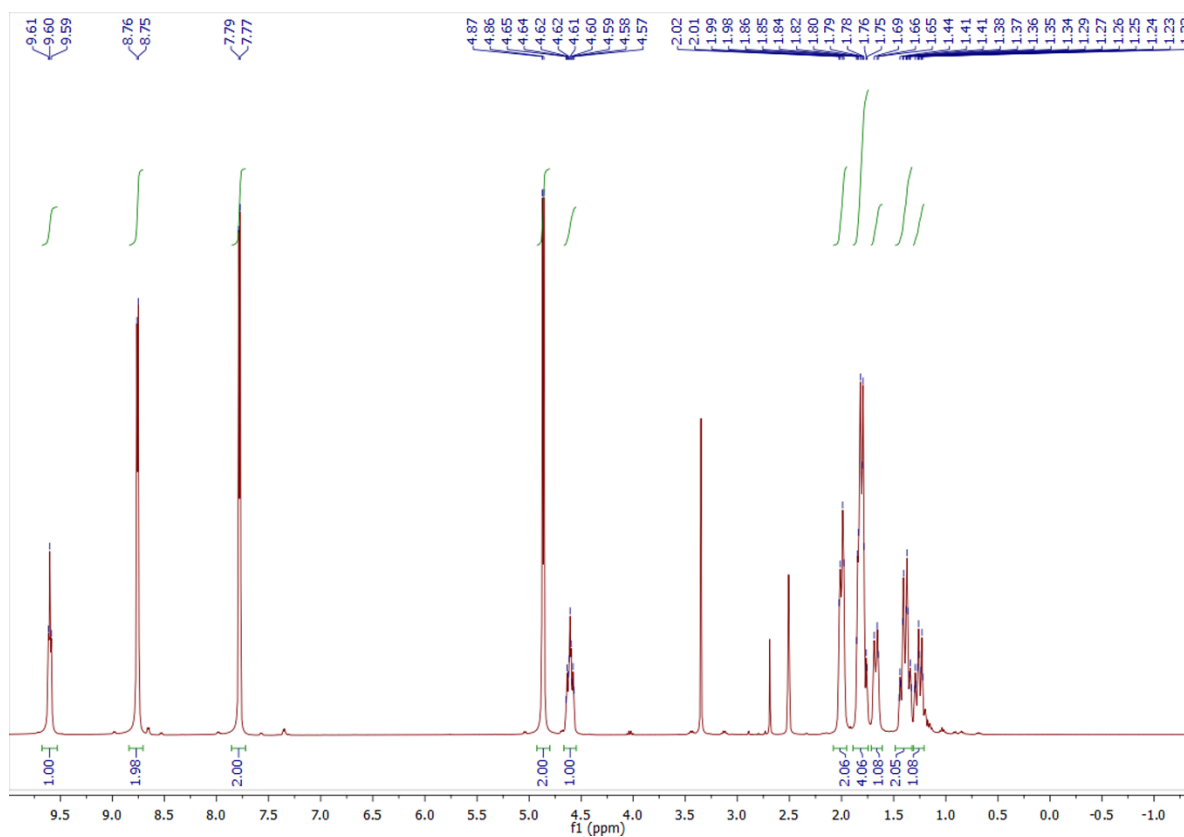
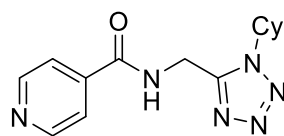


Figure S86. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **2j**.



2j

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)isonicotinamide

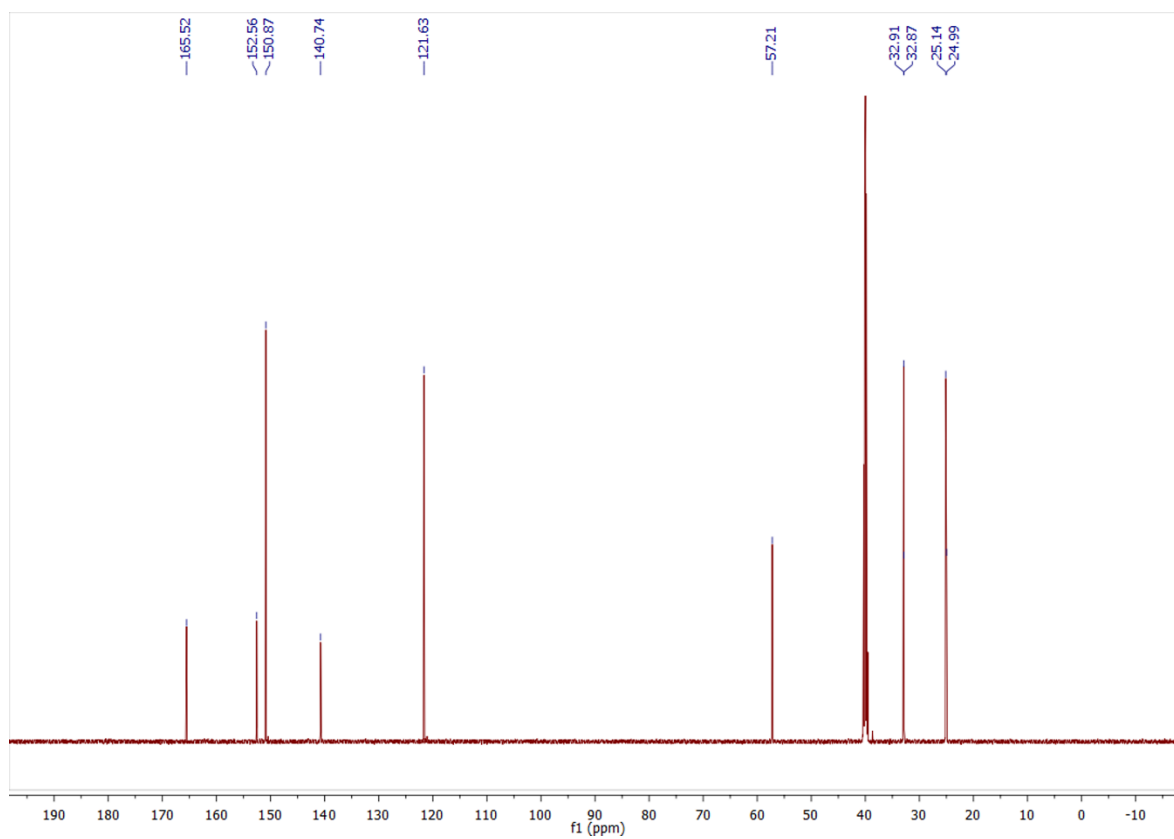
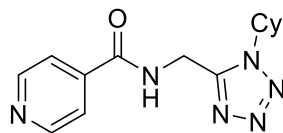
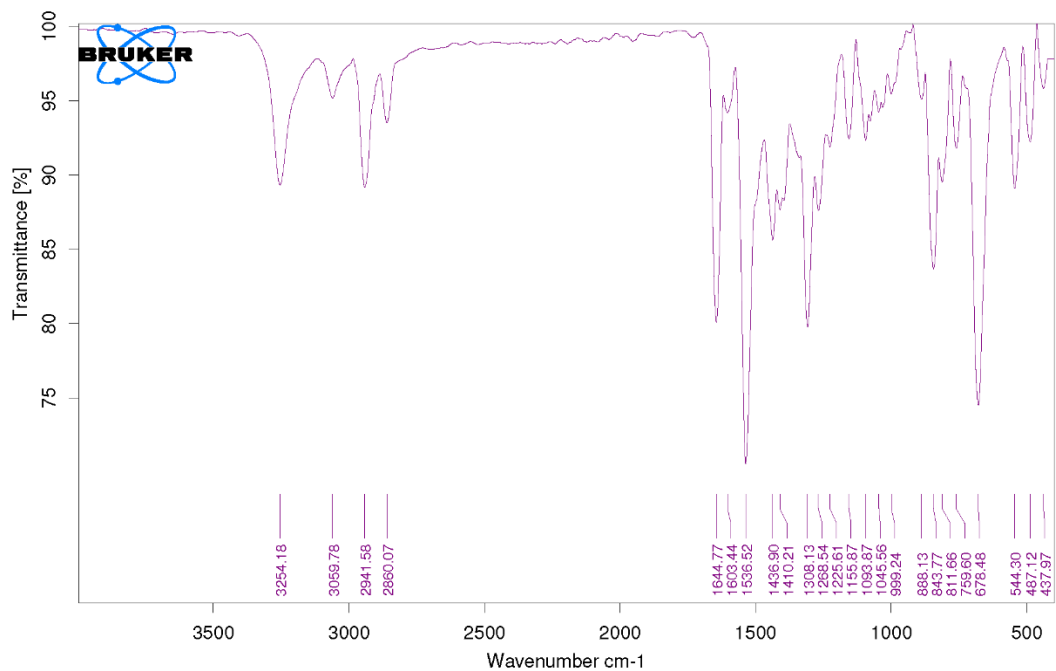


Figure S87. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, DMSO- d_6) spectrum of compound **2j**.



2j

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)isonicotinamide



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Figure S88. FT-IR (KBr) spectrum of compound **2j**.

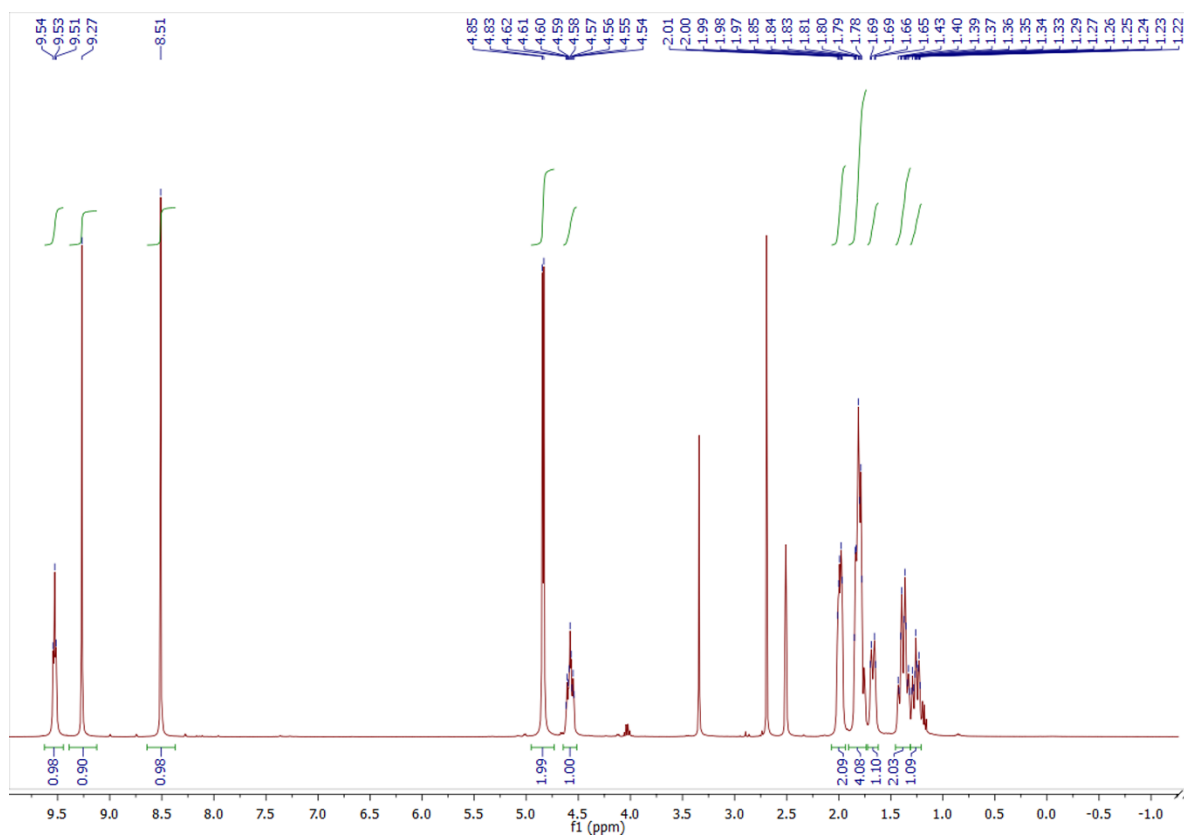
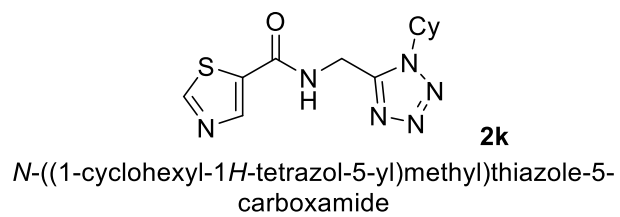
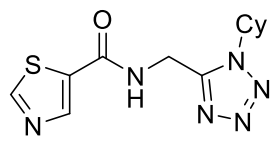


Figure S89. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **2k**.



2k

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)thiazole-5-carboxamide

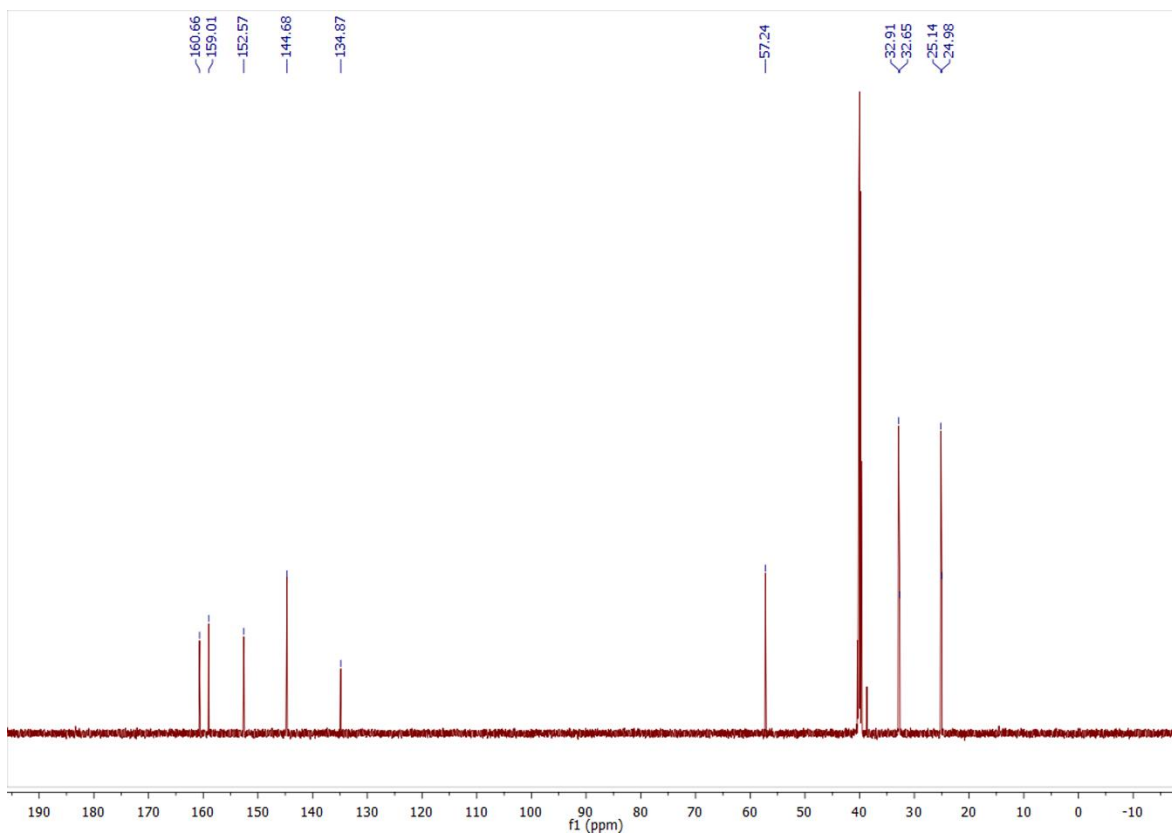
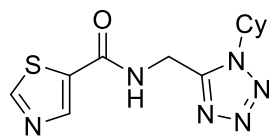
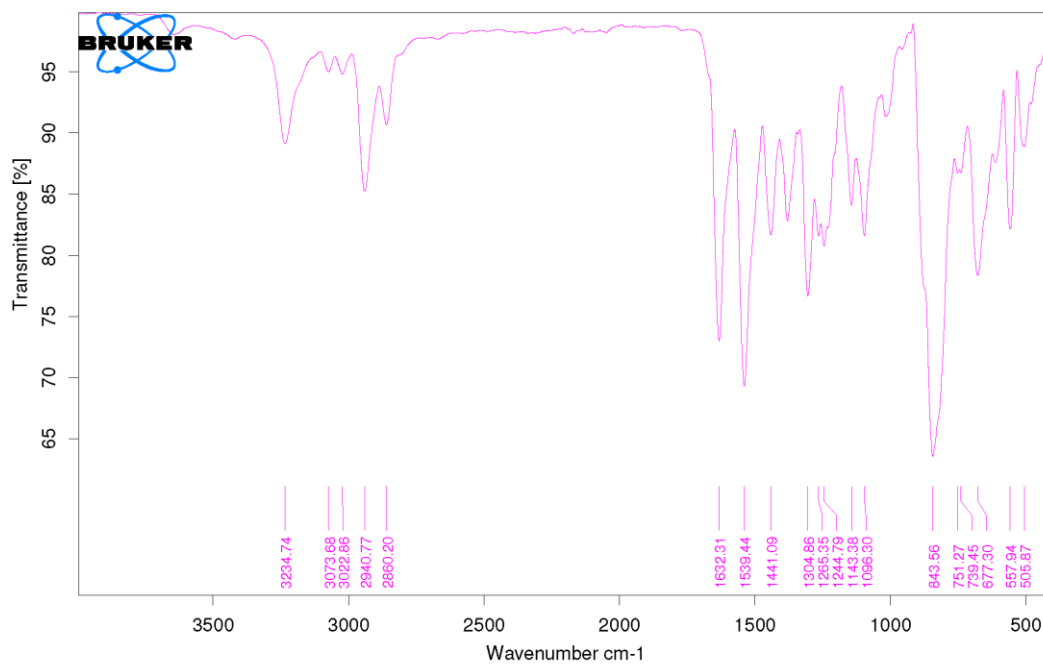


Figure S90. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, DMSO- d_6) spectrum of compound **2k**.



2k

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)thiazole-5-carboxamide



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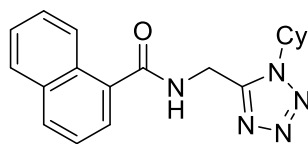
GM-073

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Figure S91. FT-IR (KBr) spectrum of compound **2k**.



21

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-naphthamide

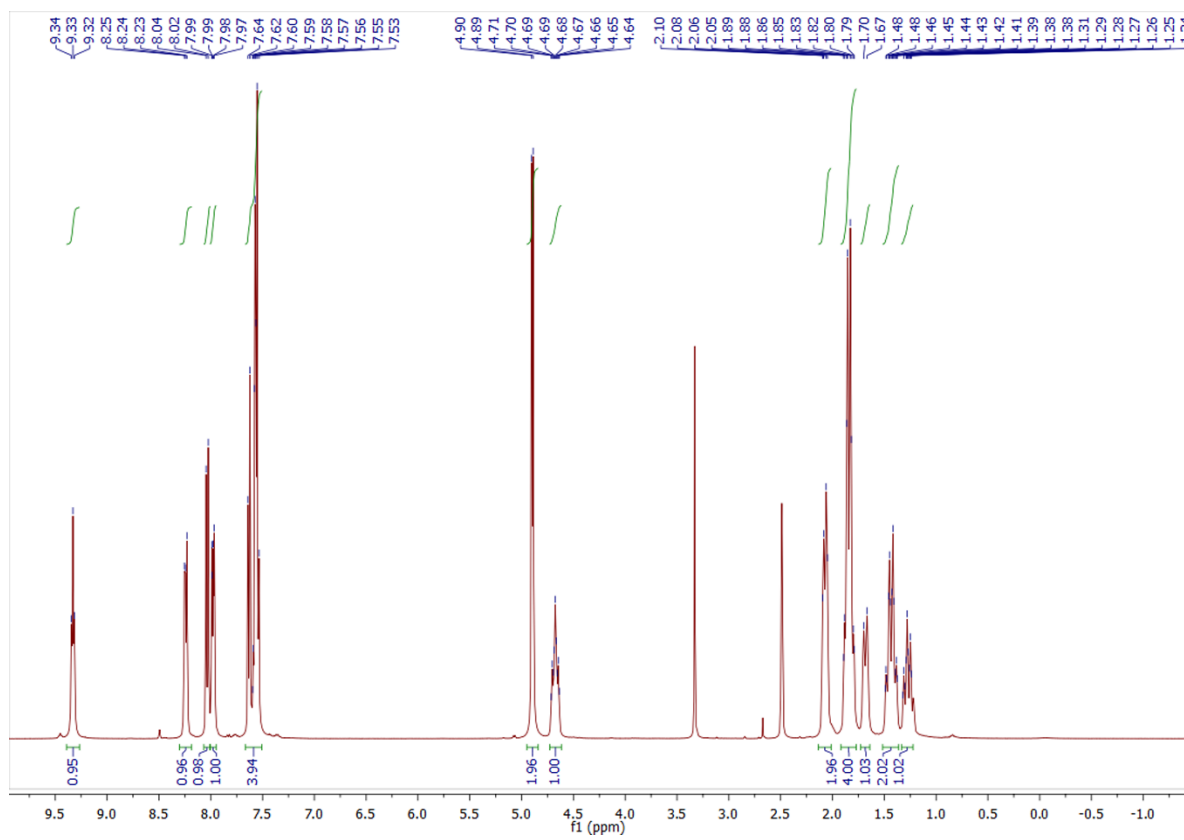
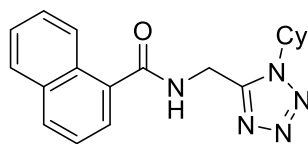


Figure S92. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **21**.



21

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-naphthamide

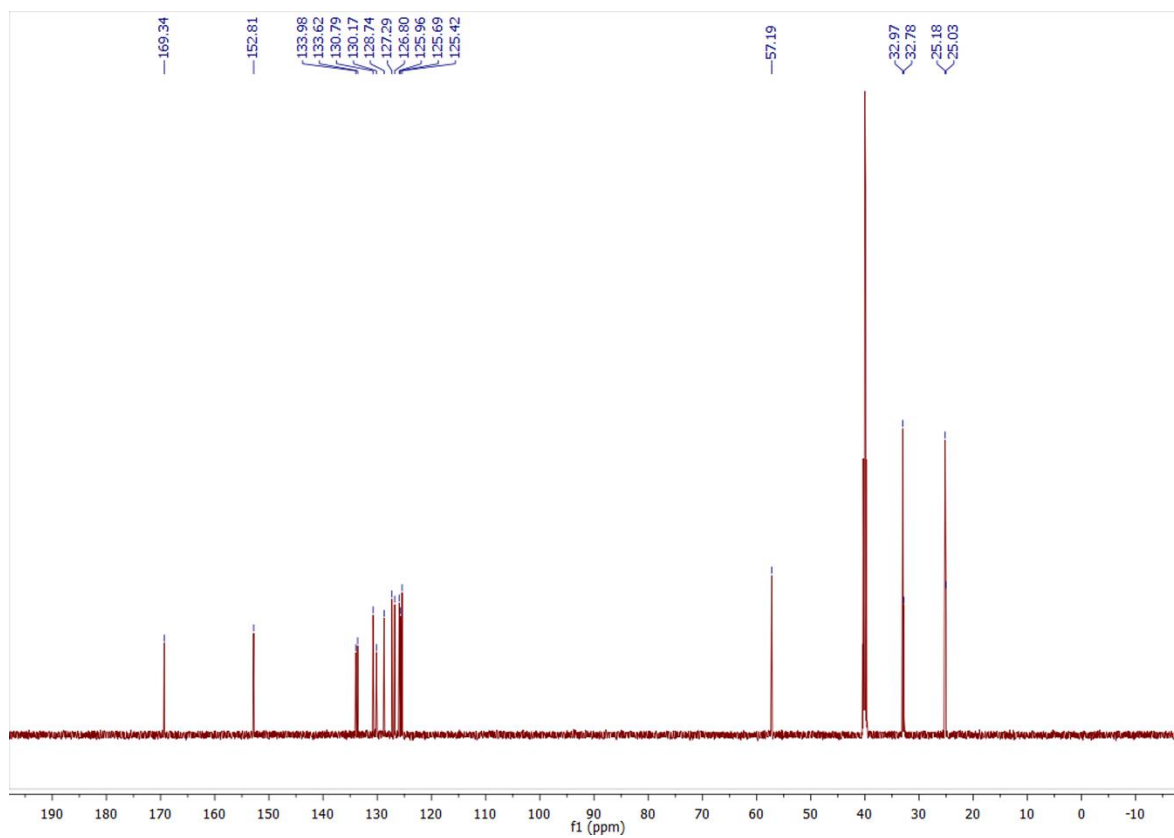
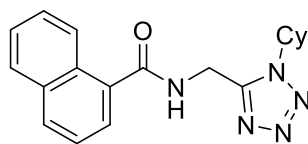
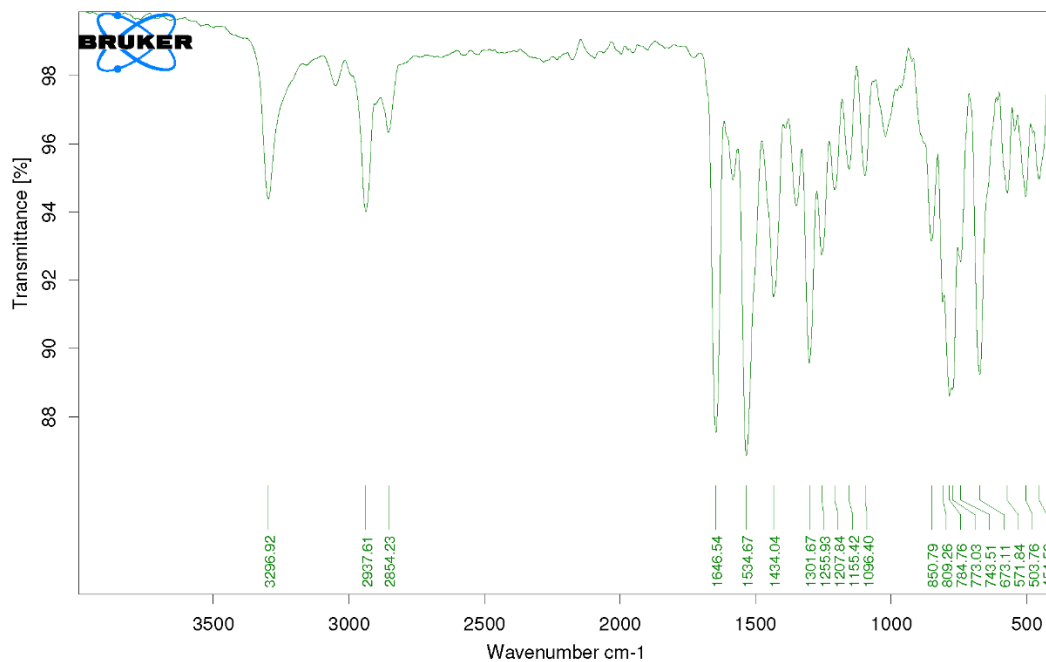


Figure S93. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, $\text{DMSO-}d_6$) spectrum of compound **21**.



21

N-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-naphthamide



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GM-55

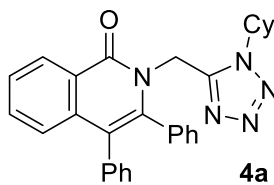
Instrument type and / or accessory

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Figure S94. FT-IR (KBr) spectrum of compound **21**.

IR and NMR spectra of tetrazole-isoquinolone/pyridone hybrids



2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one

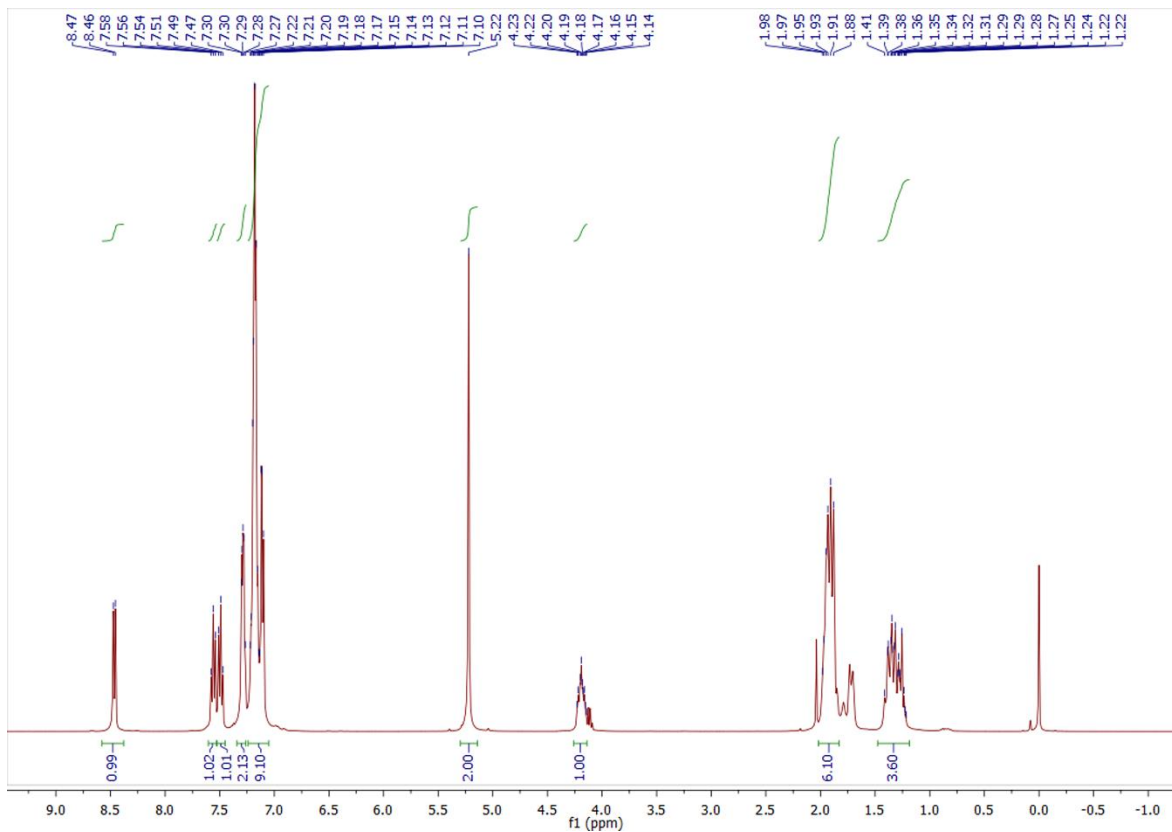
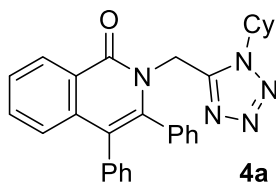


Figure S95. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4a**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

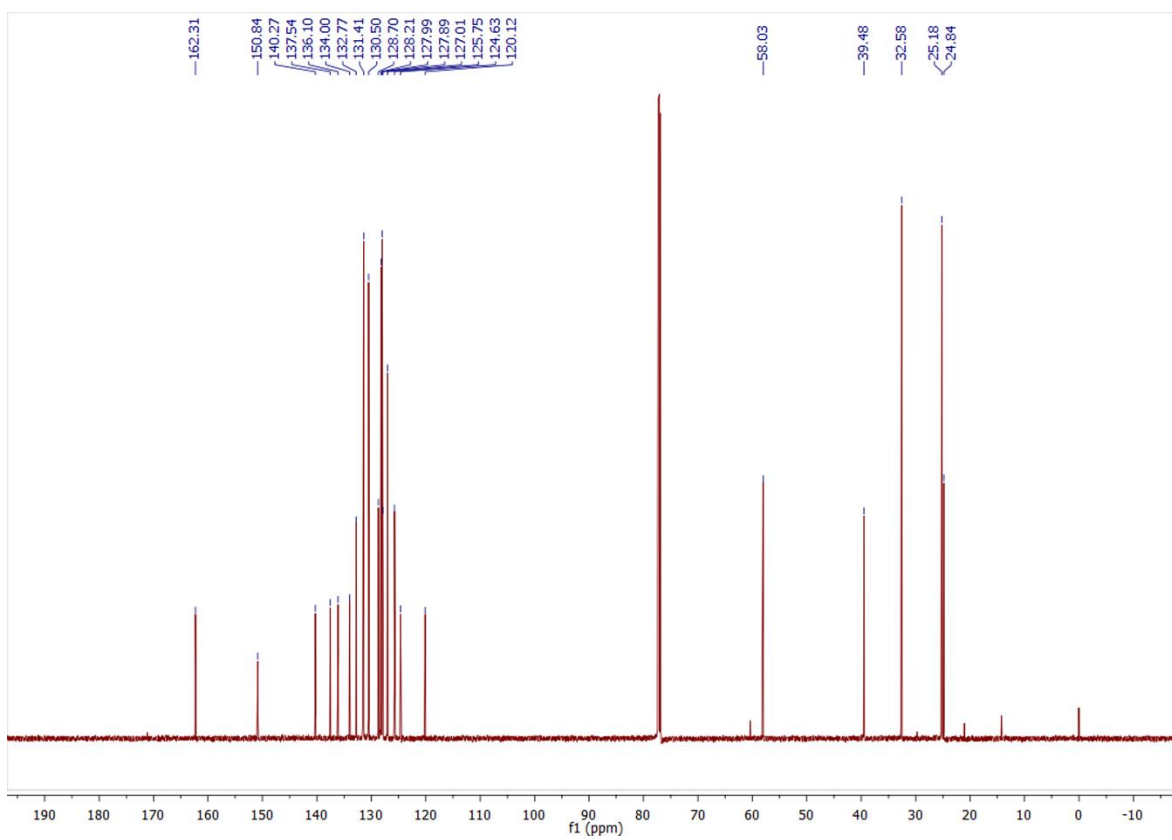
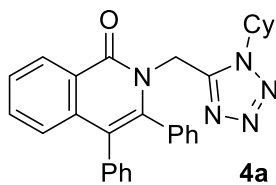
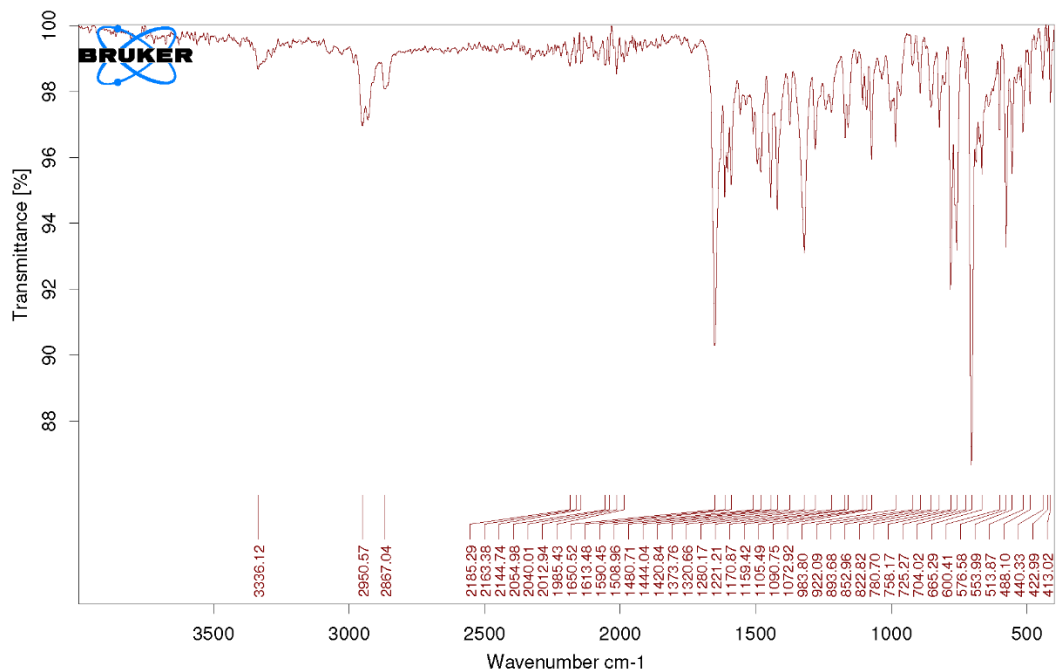


Figure S96. ^{13}C { ^1H } NMR (151 MHz, CDCl_3) spectrum of compound **4a**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one



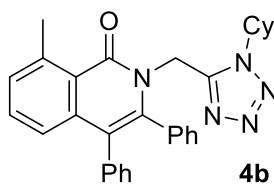
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Figure S97. FT-IR (KBr) spectrum of compound **4a**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-8-methyl-
3,4-diphenylisoquinolin-1(2*H*)-one

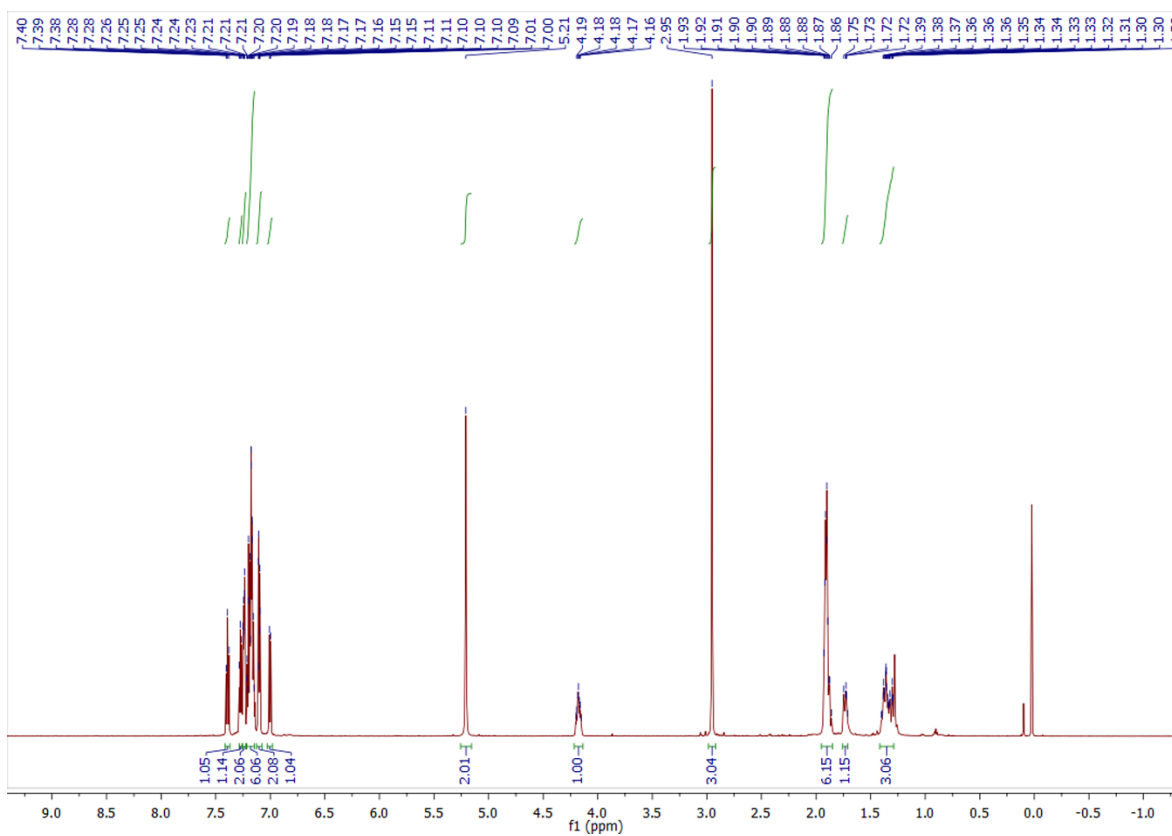
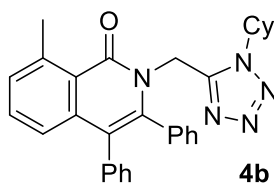


Figure S98. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **4b**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-8-methyl-
3,4-diphenylisoquinolin-1(2*H*)-one

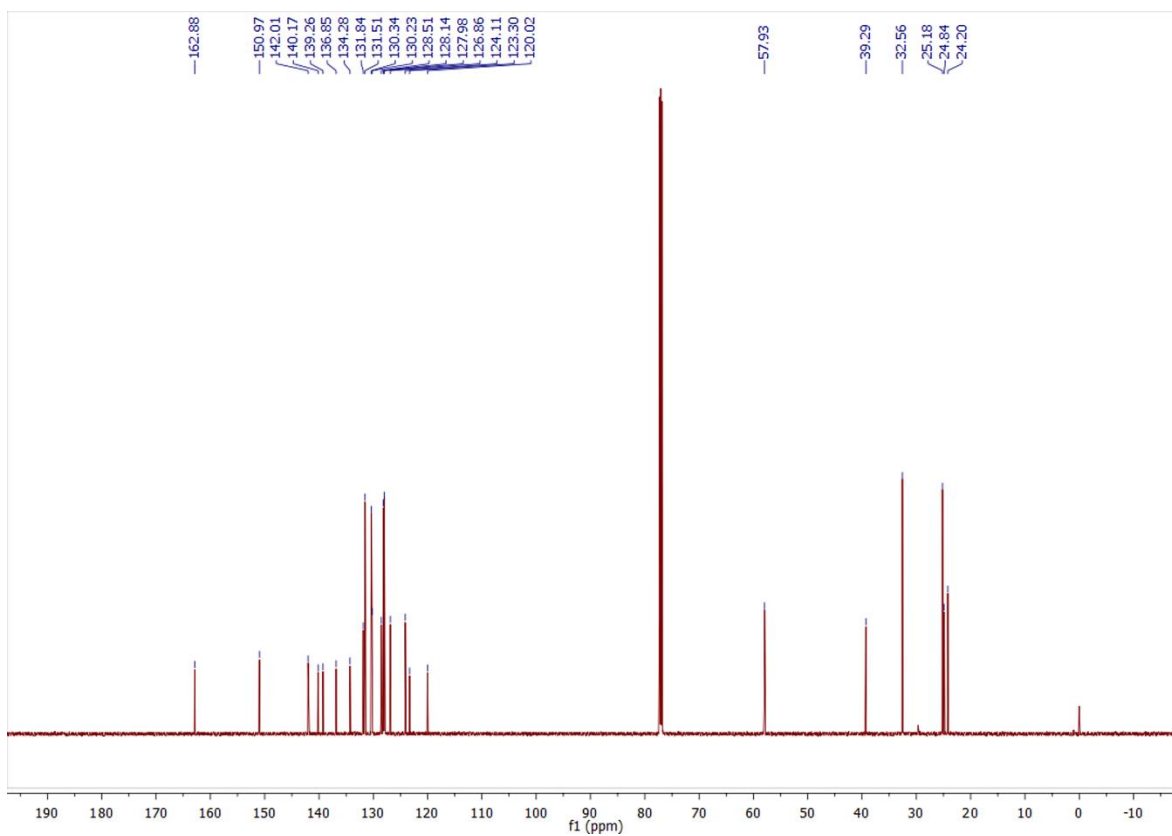
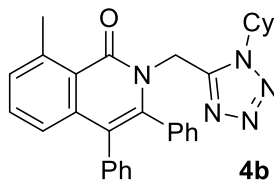
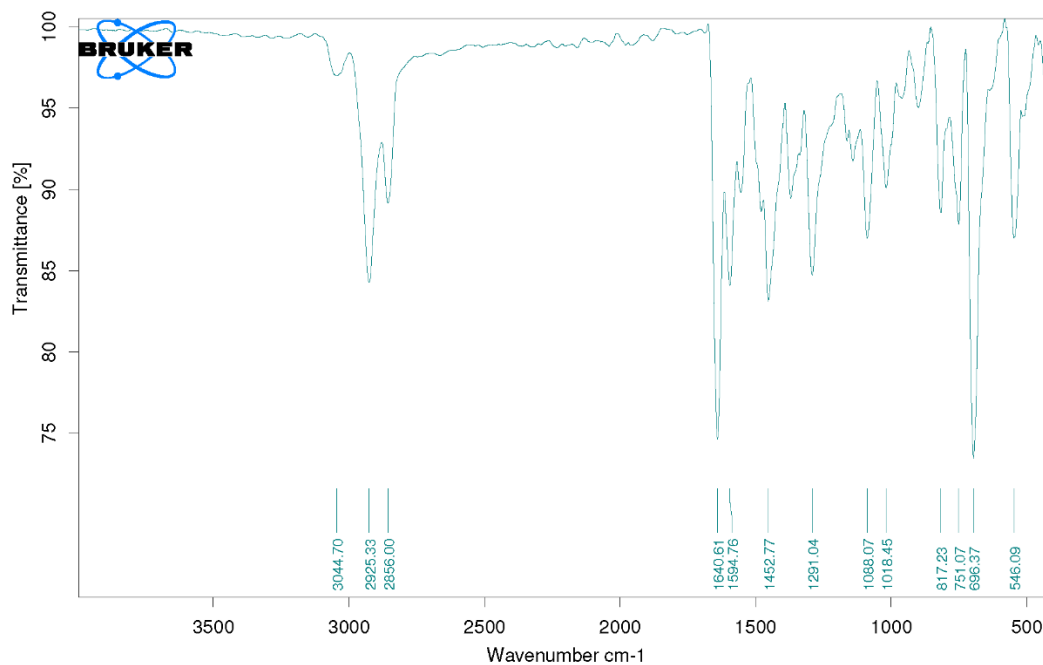


Figure S99. ^{13}C { ^1H } NMR (151 MHz, CDCl_3) spectrum of compound **4b**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-8-methyl-
3,4-diphenylisoquinolin-1(2*H*)-one



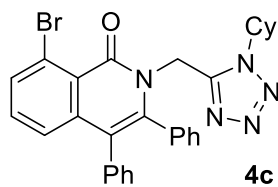
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GM-094-A

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Figure S100. FT-IR (KBr) spectrum of compound **4b**.



8-bromo-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

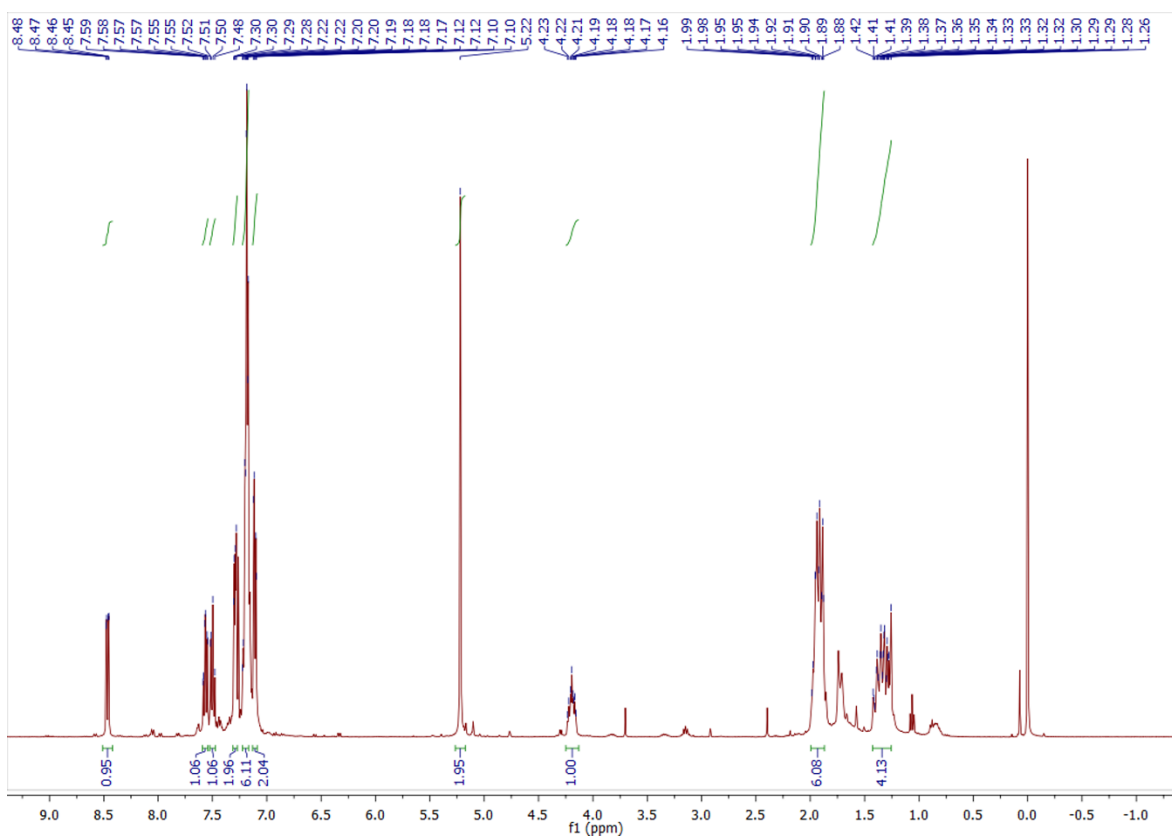
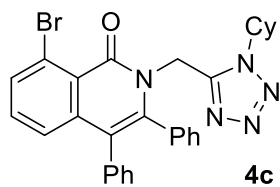


Figure S101. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4c**.



8-bromo-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

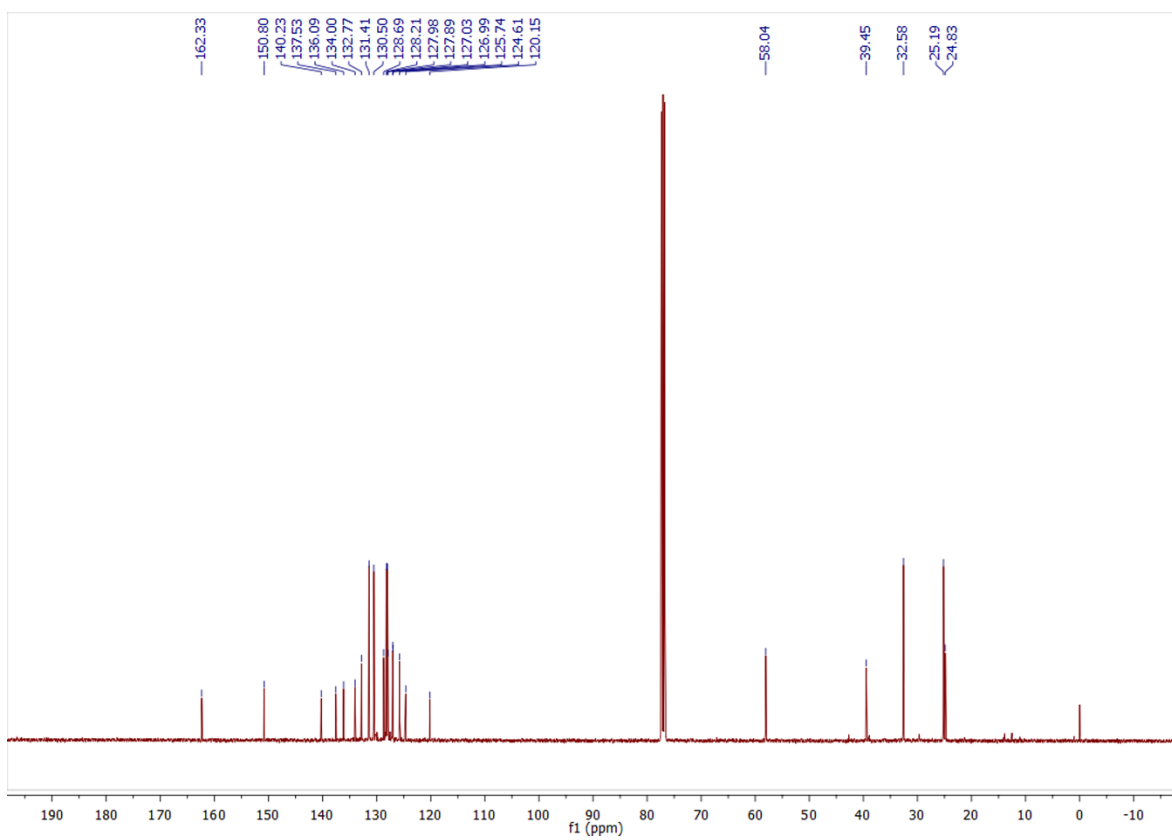
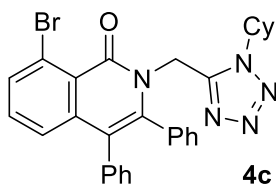
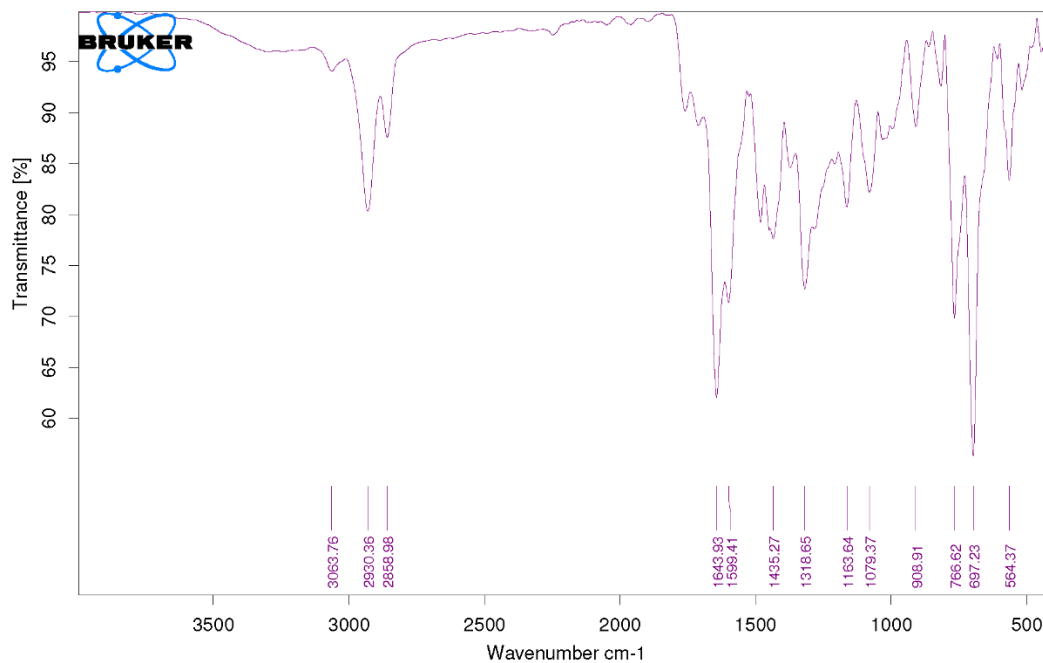


Figure S102. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4c**.



8-bromo-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one



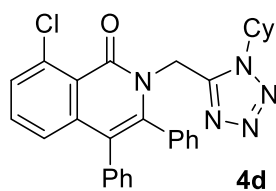
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Figure S103. FT-IR (KBr) spectrum of compound **4c**.



8-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

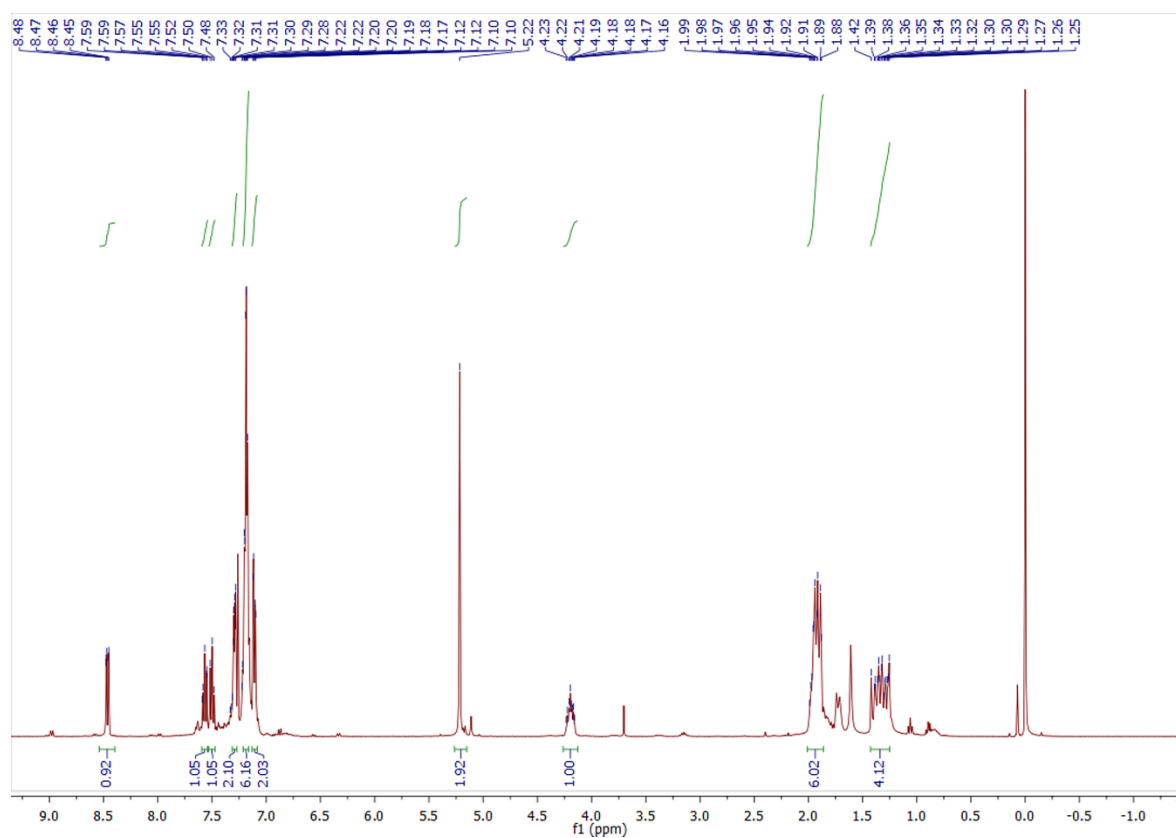
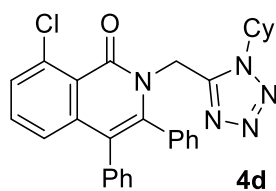


Figure S104. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4d**.



8-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

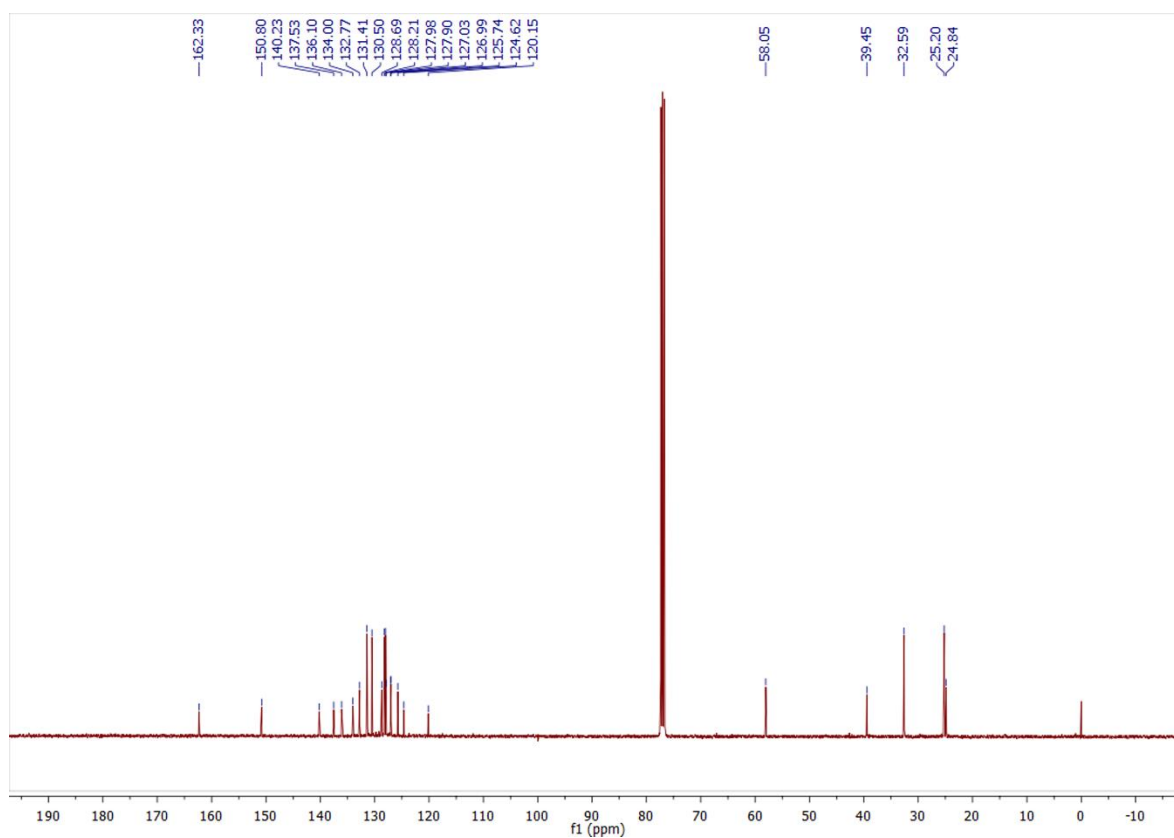
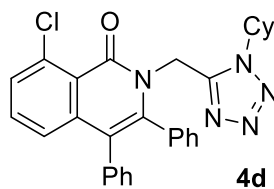
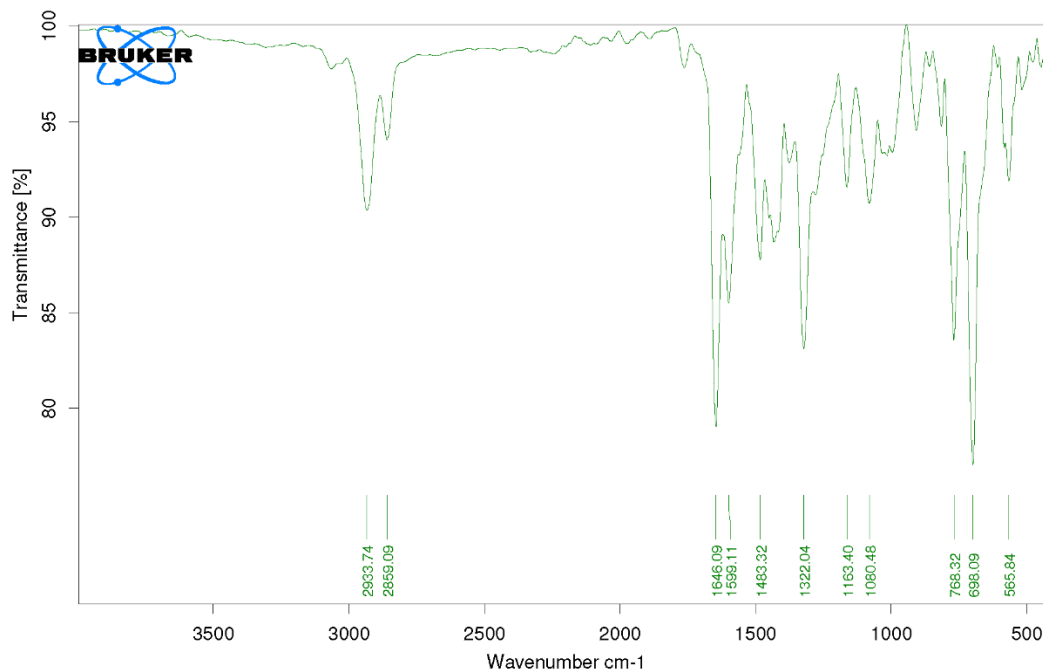


Figure S105. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4d**.



8-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one



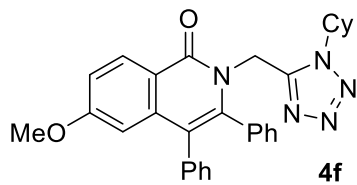
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Instrument type and / or accessory

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Figure S106. FT-IR (KBr) spectrum of compound **4d**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-6-methoxy-3,4-diphenylisoquinolin-1(2*H*)-one

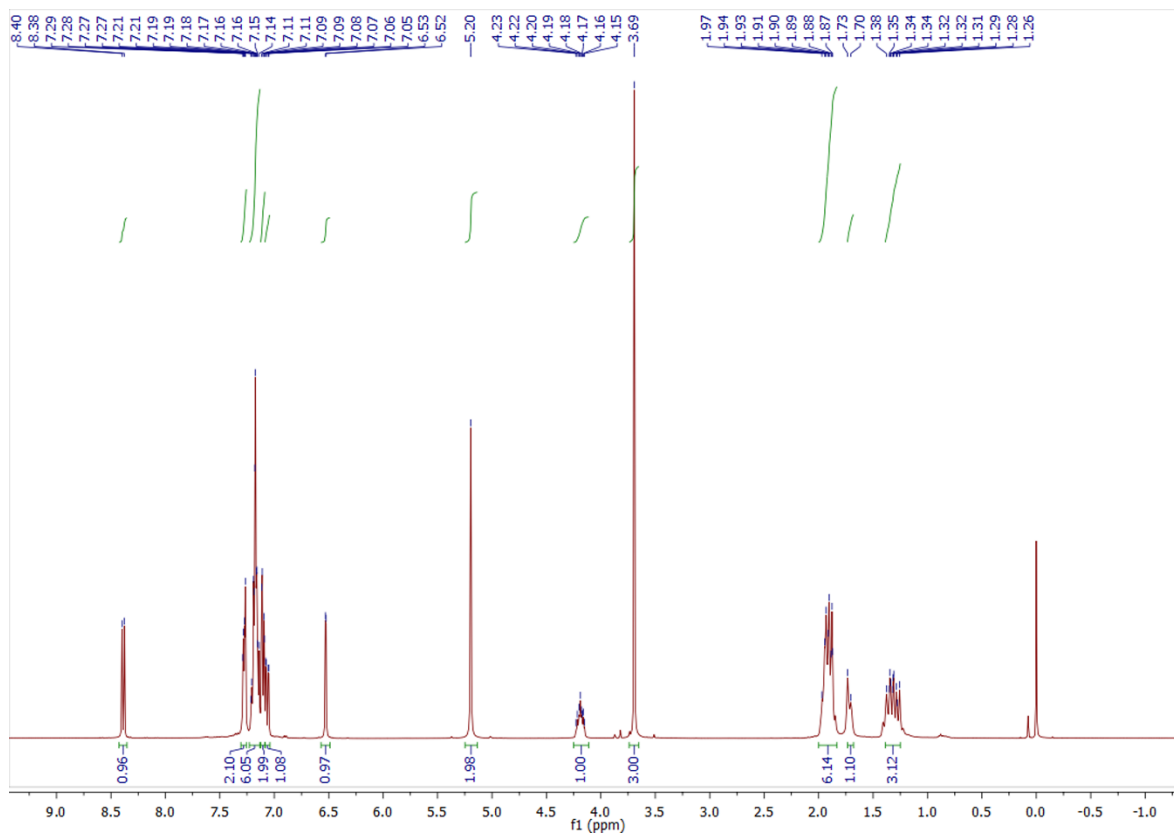
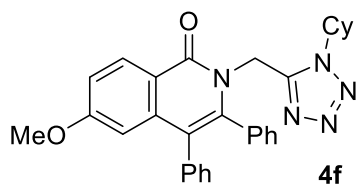


Figure S107. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4f**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-6-methoxy-3,4-diphenylisoquinolin-1(2*H*)-one

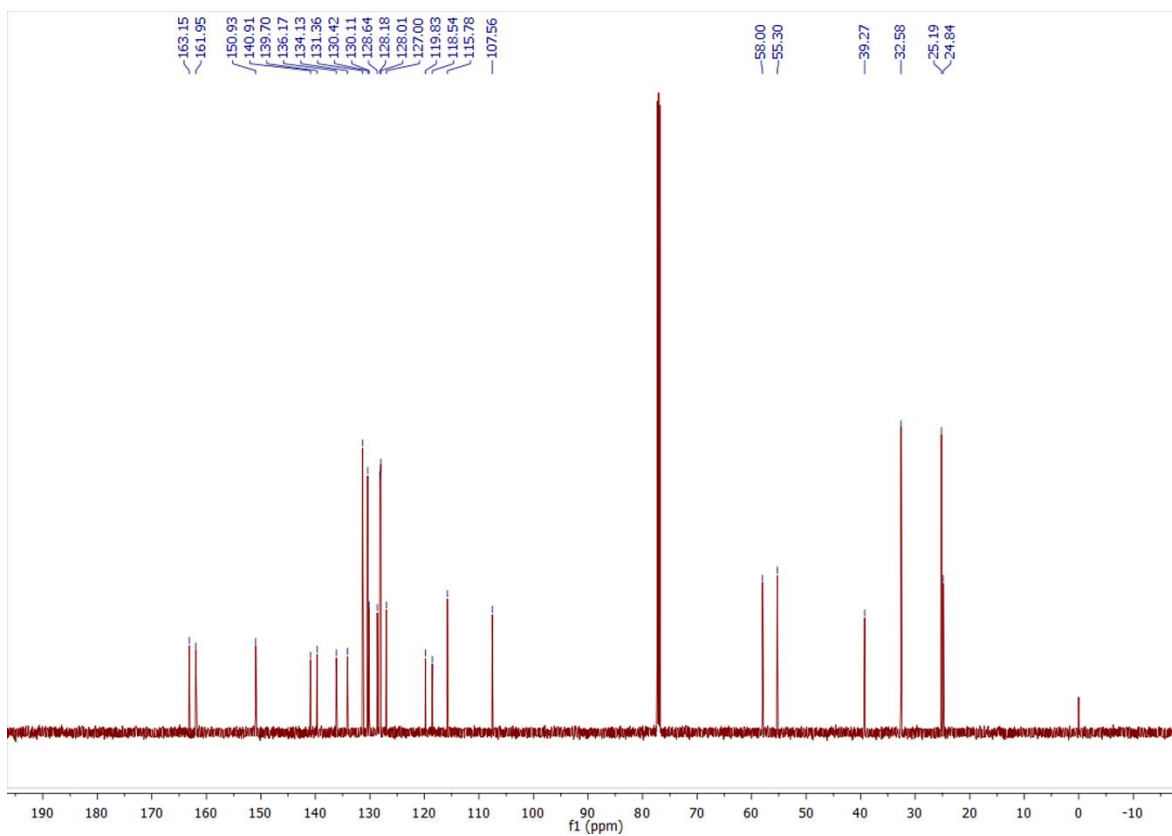
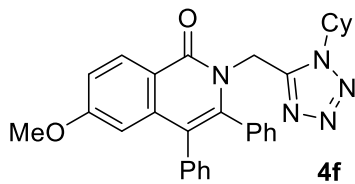
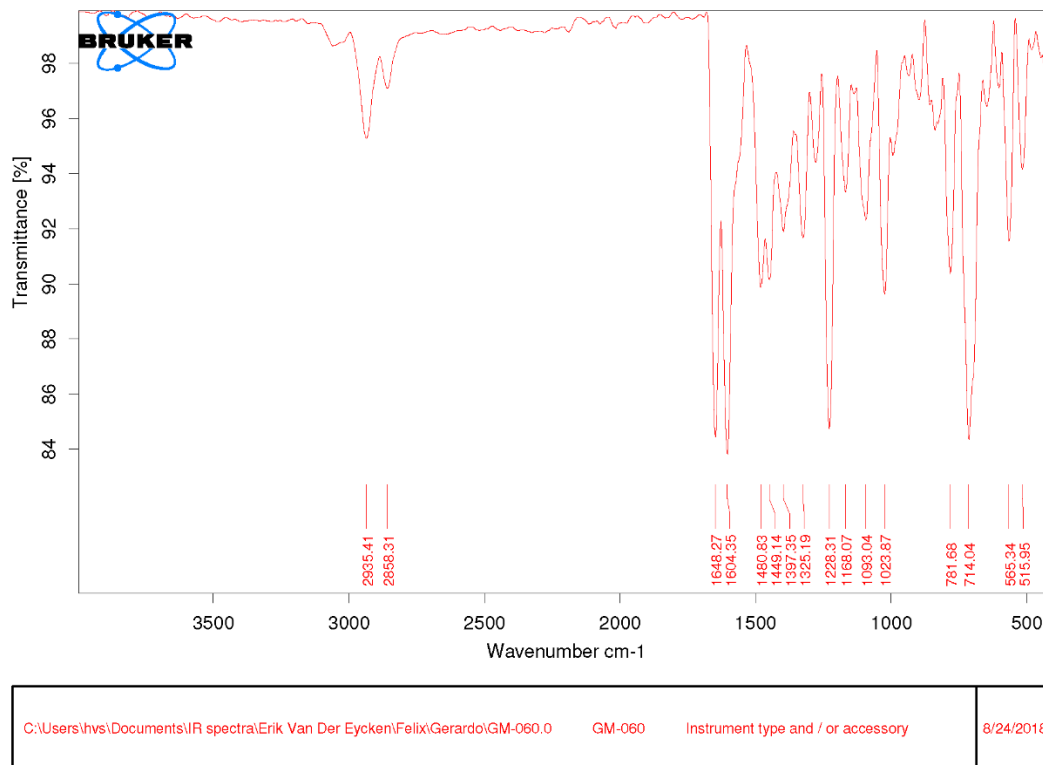


Figure S108. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **4f**.

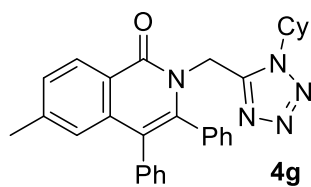


2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-6-methoxy-3,4-diphenylisoquinolin-1(2*H*)-one



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Figure S109. FT-IR (KBr) spectrum of compound **4f**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-6-methyl-
3,4-diphenylisoquinolin-1(2*H*)-one

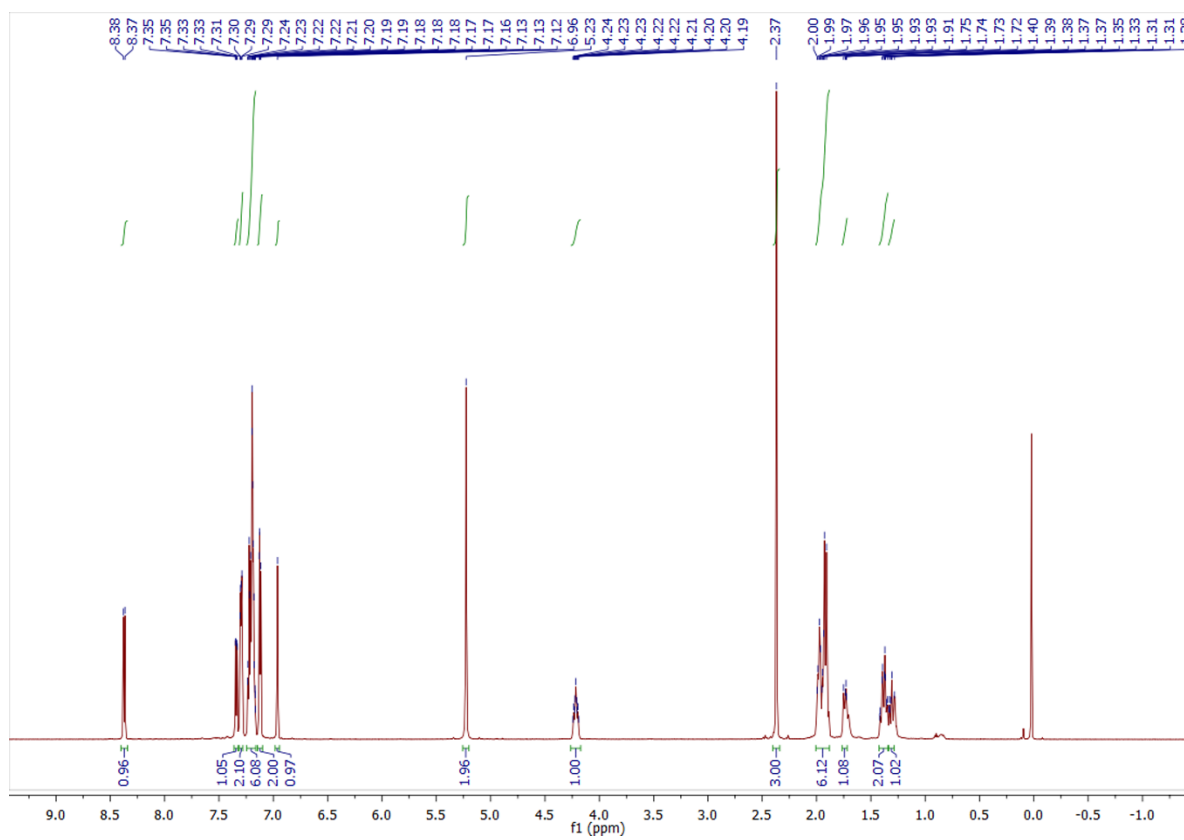
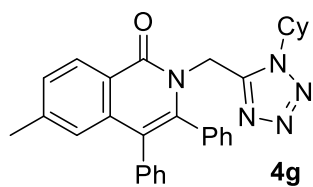


Figure S110. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **4g**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-6-methyl-
3,4-diphenylisoquinolin-1(2*H*)-one

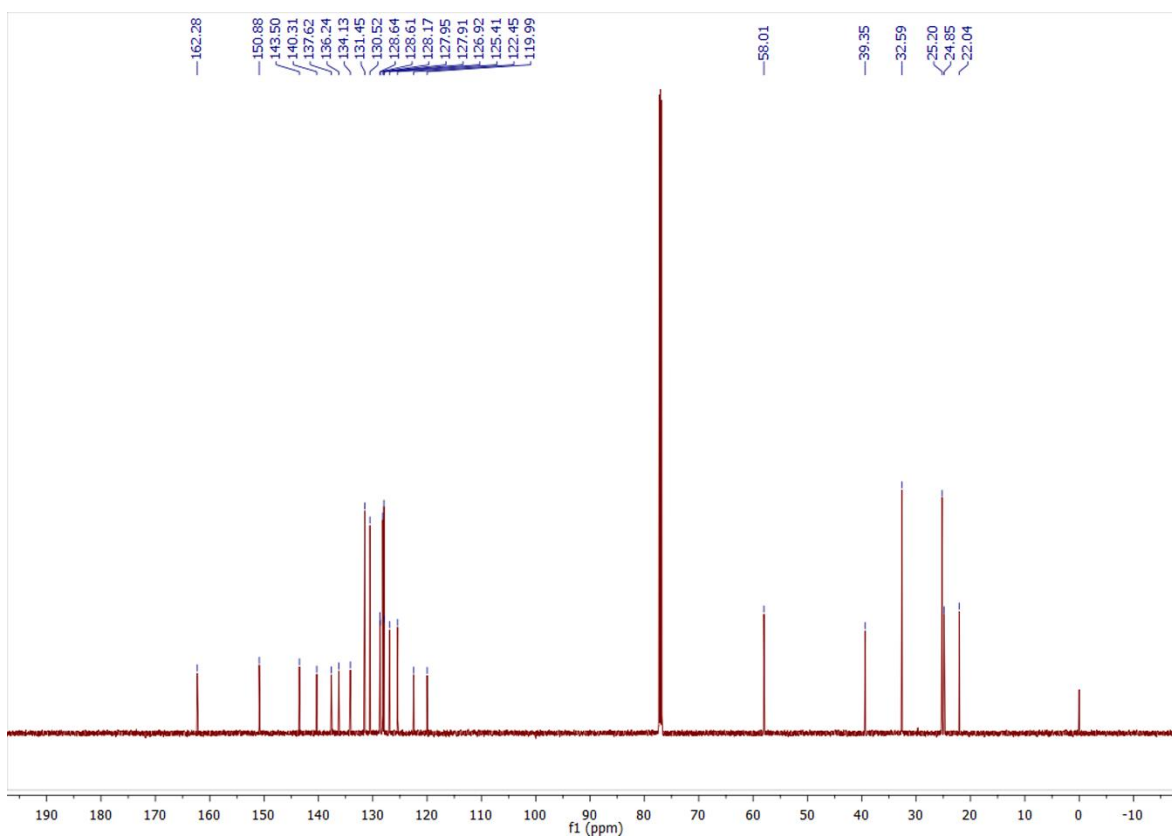
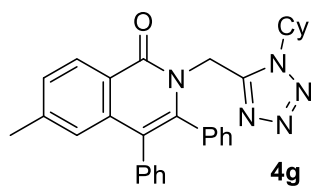
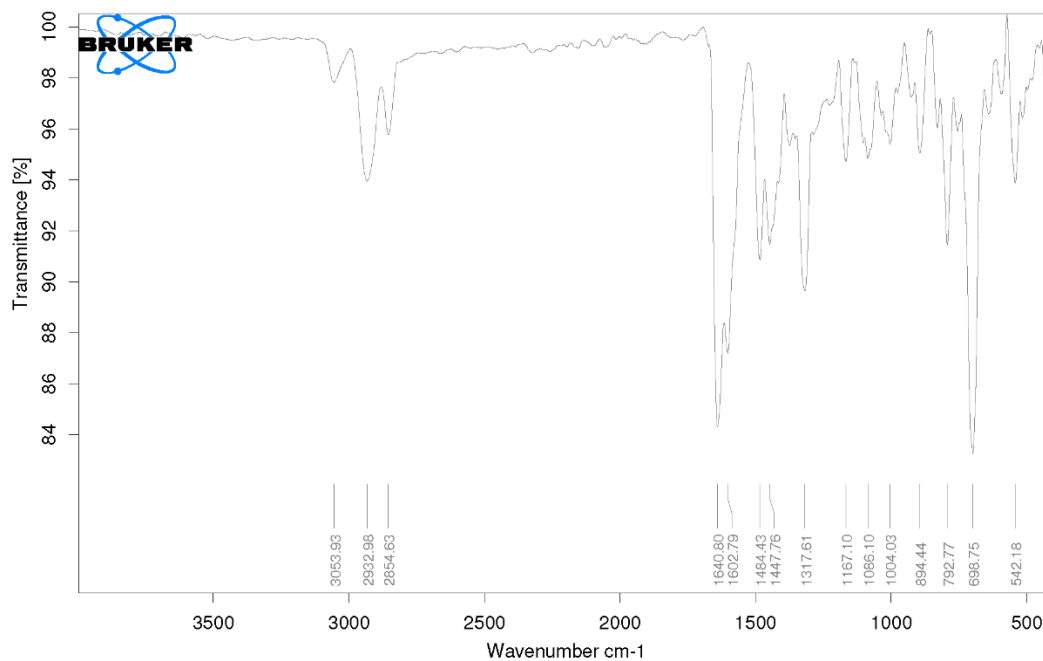


Figure S111. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **4g**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-6-methyl-
3,4-diphenylisoquinolin-1(2*H*)-one



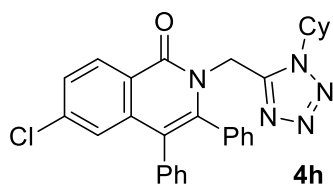
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Instrument type and / or accessory

8/24/2018

Figure S112. FT-IR (KBr) spectrum of compound **4g**.



6-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2*H*)-one

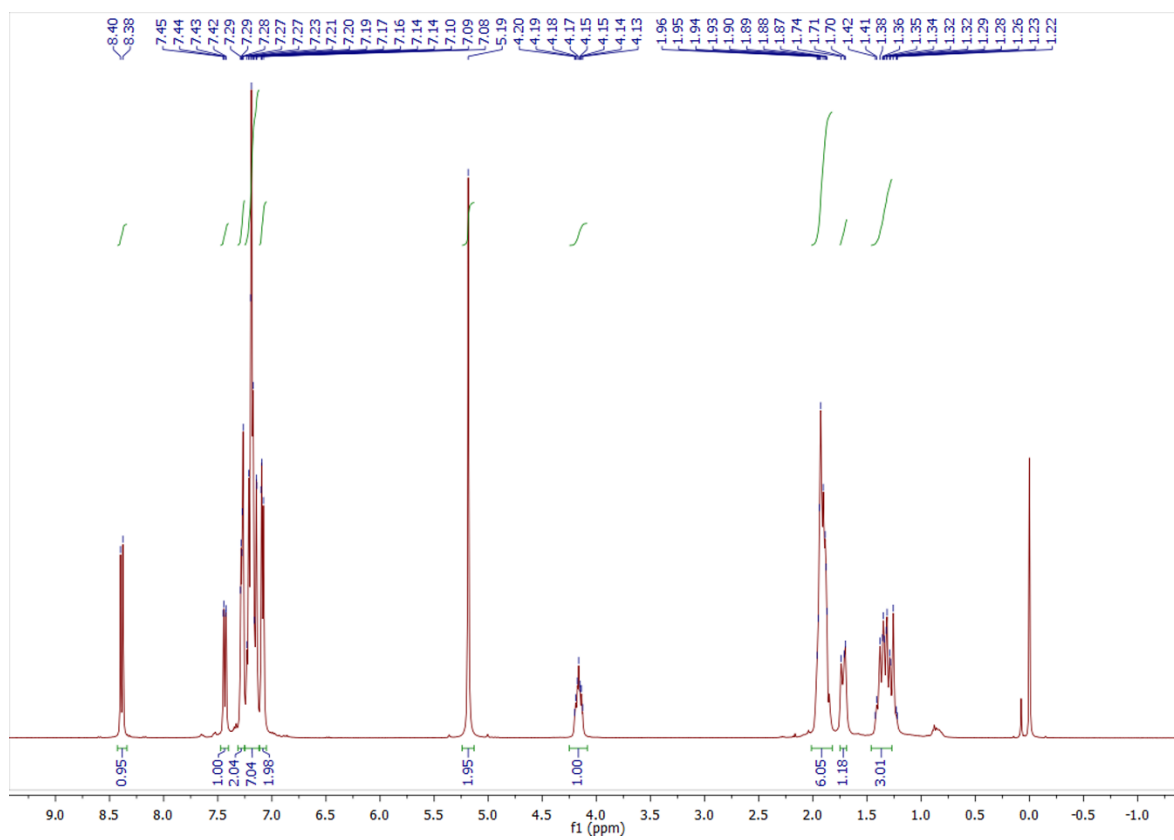
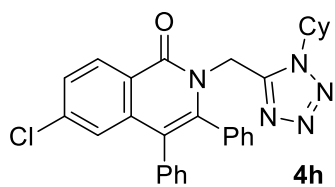


Figure S113. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4h**.



6-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2*H*)-one

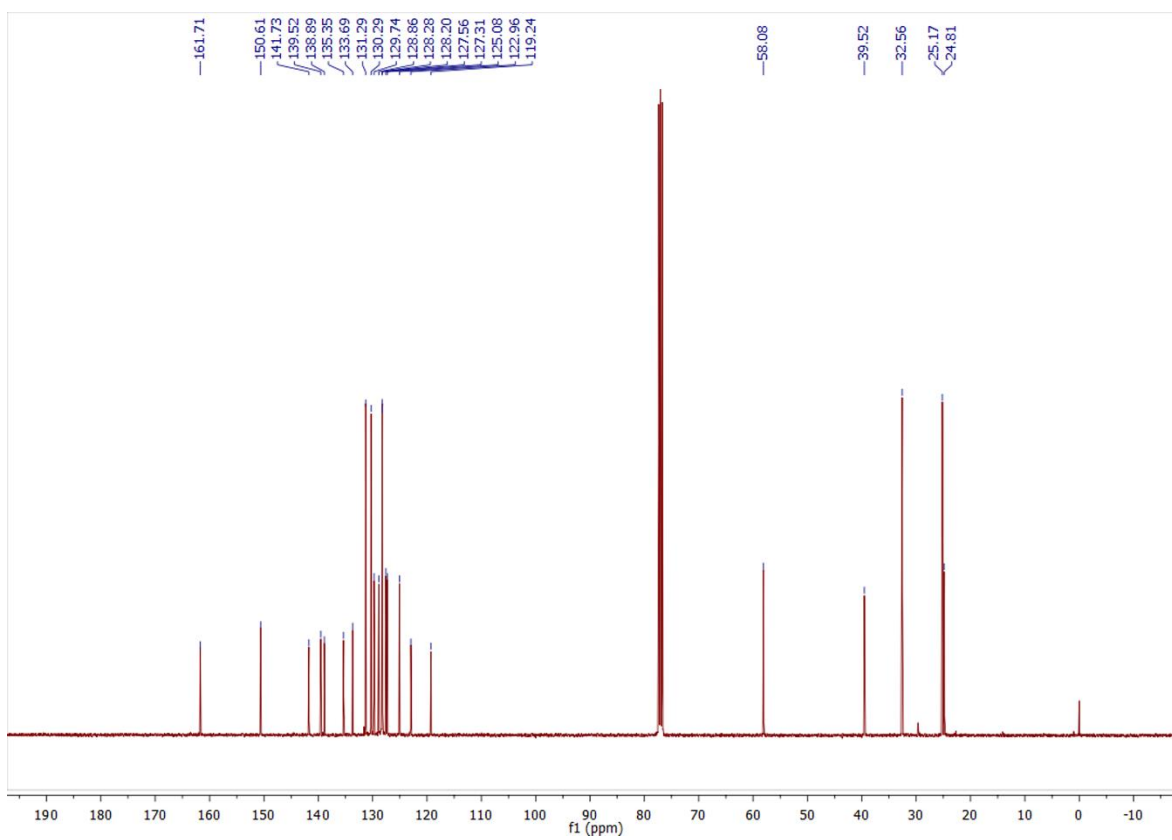
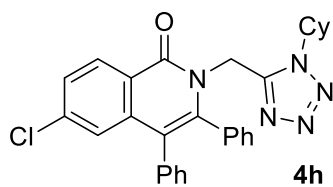
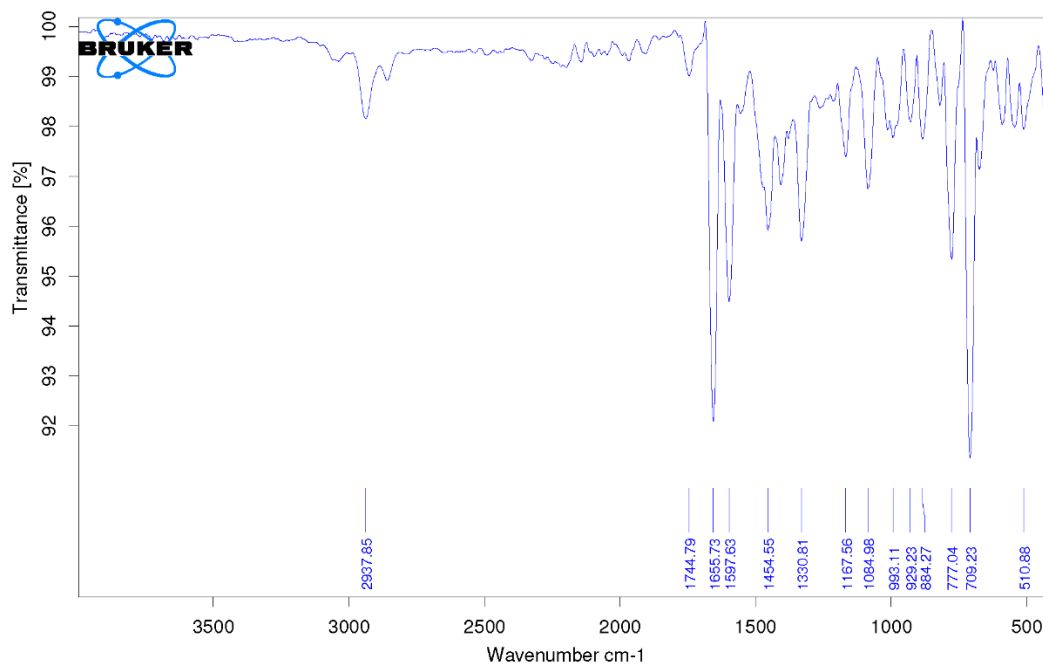


Figure S114. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4h**.



6-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2*H*)-one



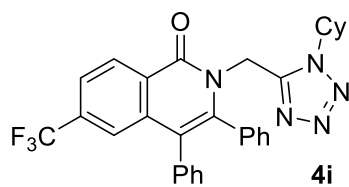
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Instrument type and / or accessory

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Figure S115. FT-IR (KBr) spectrum of compound **4h**.



2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenyl-6-(trifluoromethyl)isoquinolin-1(2H)-one

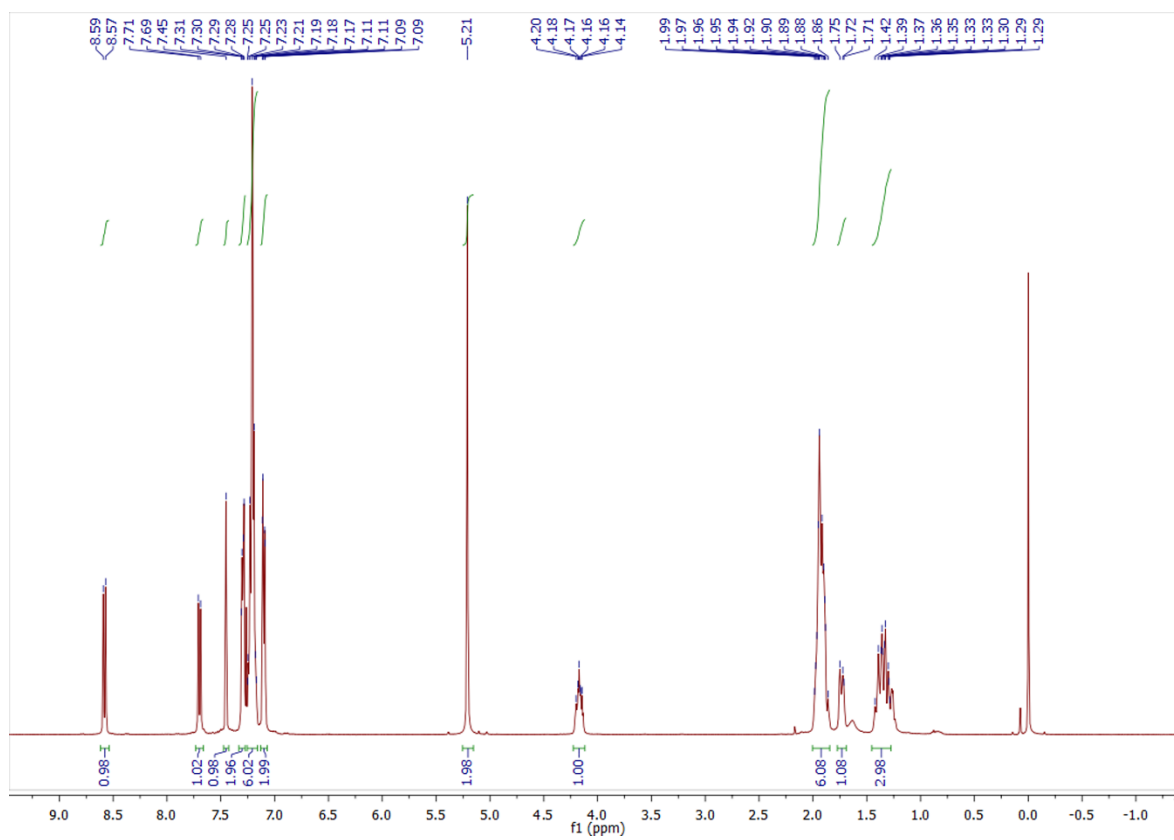
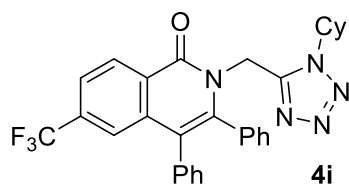


Figure S116. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4i**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenyl-6-(trifluoromethyl)isoquinolin-1(2*H*)-one

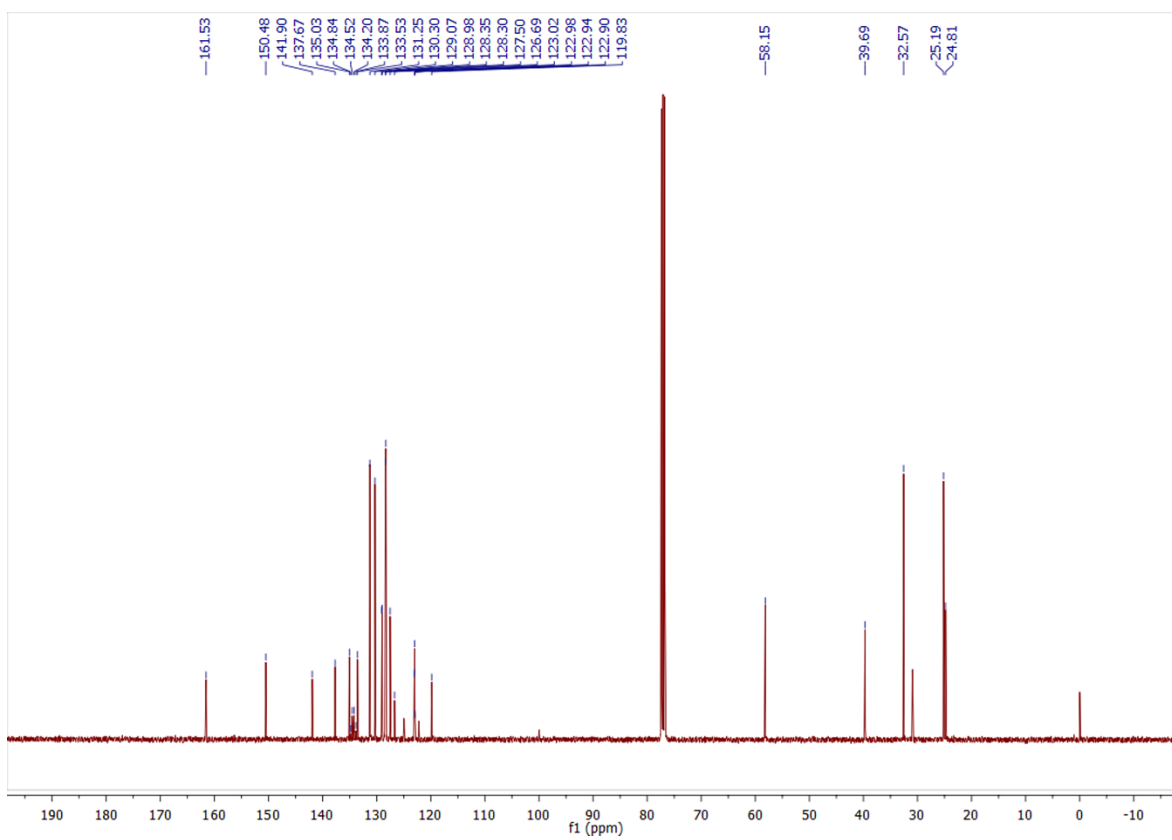
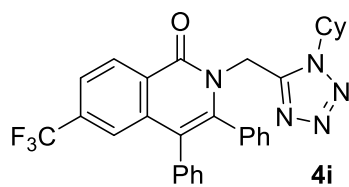


Figure S117. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4i**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenyl-6-(trifluoromethyl)isoquinolin-1(2*H*)-one

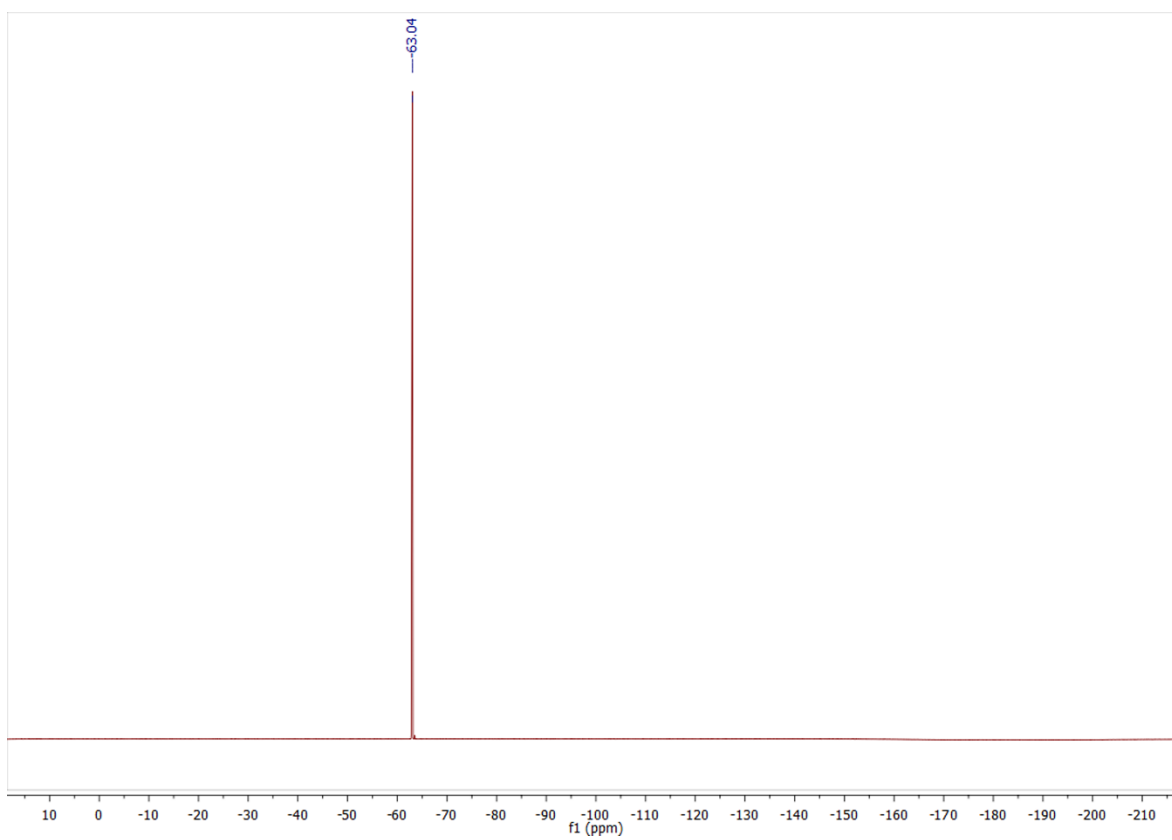
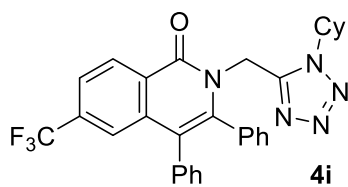
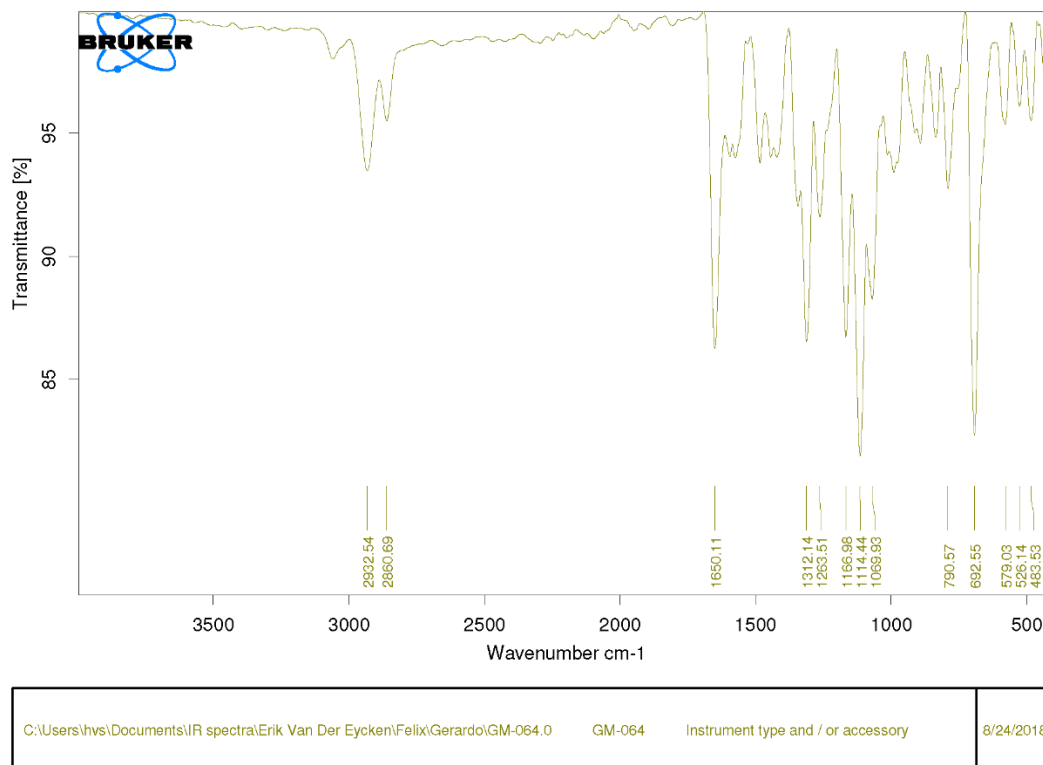


Figure S118. ^{19}F $\{^{13}\text{C}\}$ NMR (376 MHz, CDCl_3) spectrum of compound **4i**.

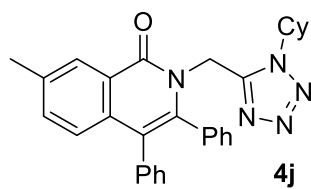


2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenyl-6-(trifluoromethyl)isoquinolin-1(2*H*)-one



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Figure S119. FT-IR (KBr) spectrum of compound **4i**.



2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-7-methyl-
3,4-diphenylisoquinolin-1(2H)-one

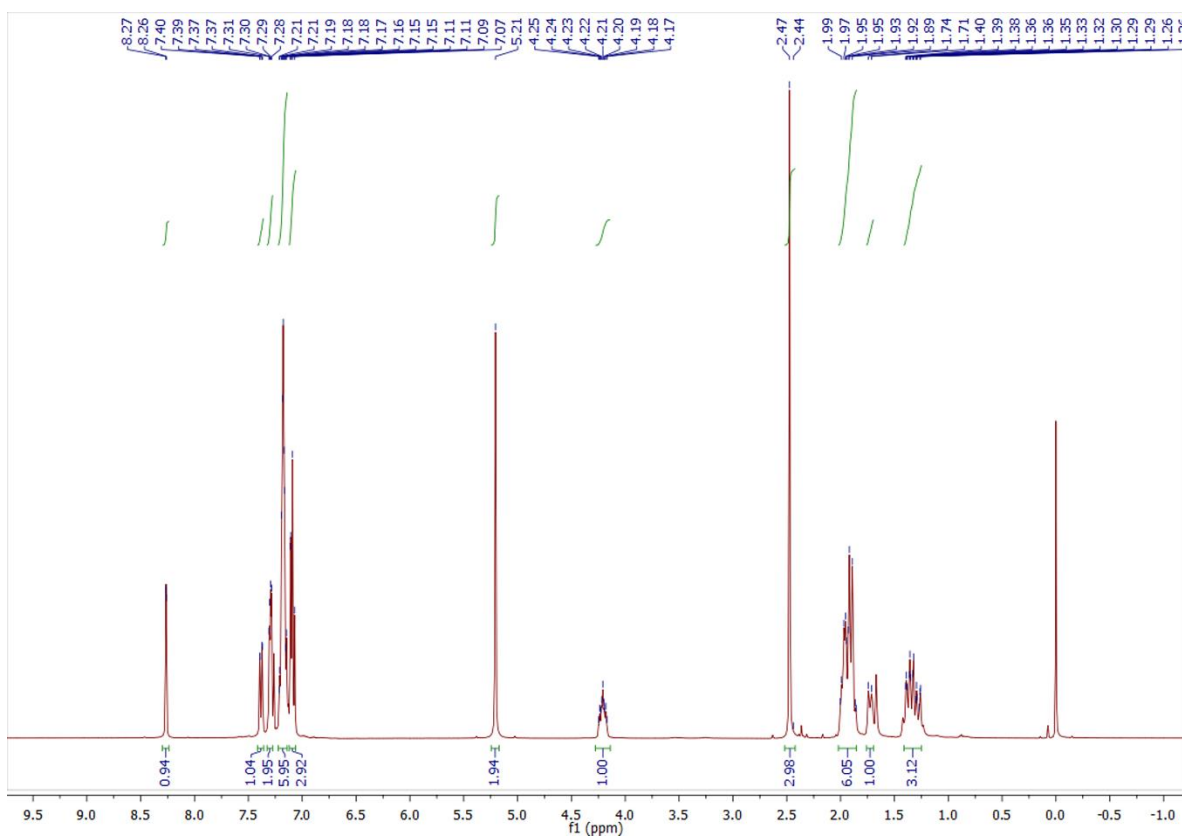
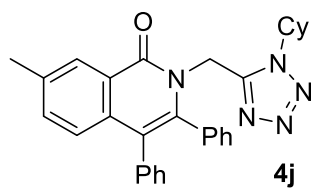


Figure S120. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4j**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-7-methyl-
3,4-diphenylisoquinolin-1(2*H*)-one

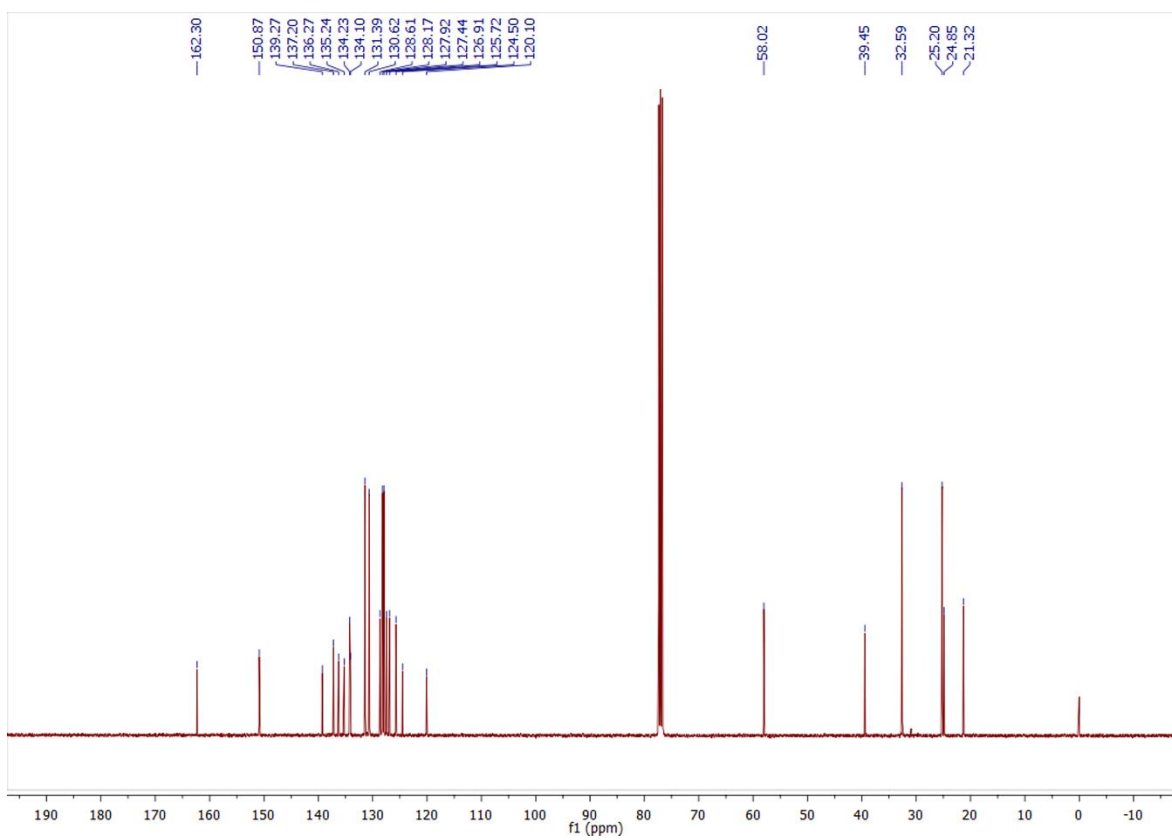
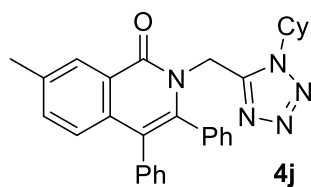
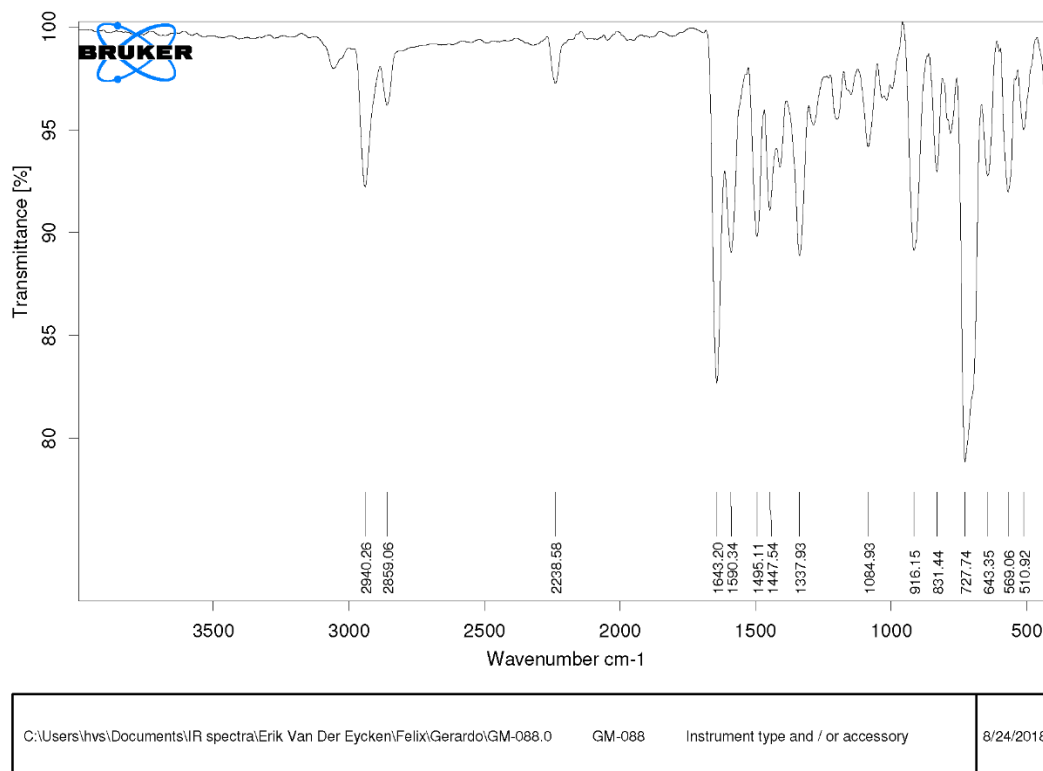


Figure S121. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4j**.

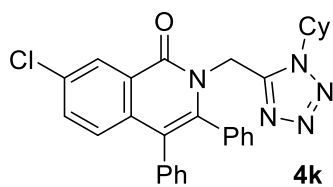


2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-7-methyl-
3,4-diphenylisoquinolin-1(2H)-one



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Figure S122. FT-IR (KBr) spectrum of compound **4j**.



7-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2*H*)-one

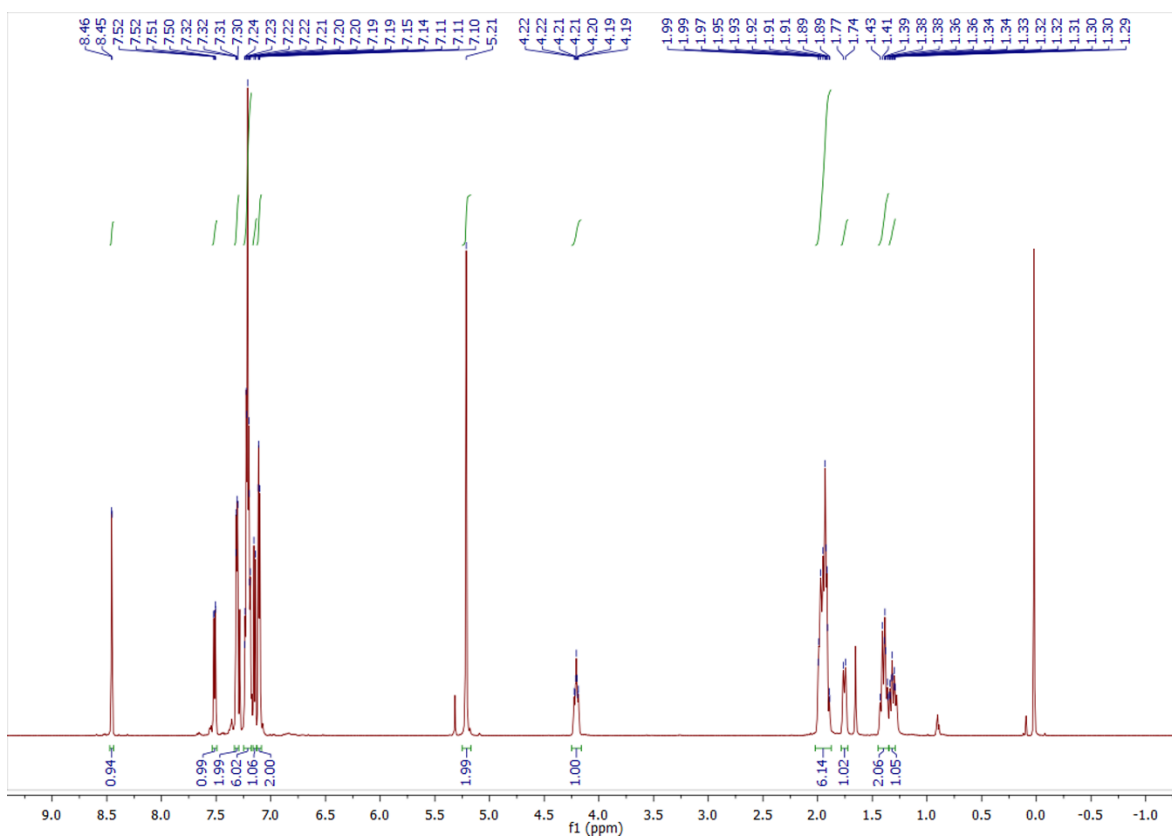
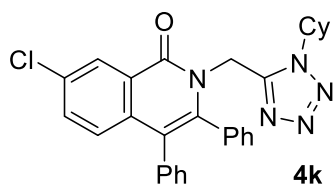


Figure S123. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **4k**.



7-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2*H*)-one

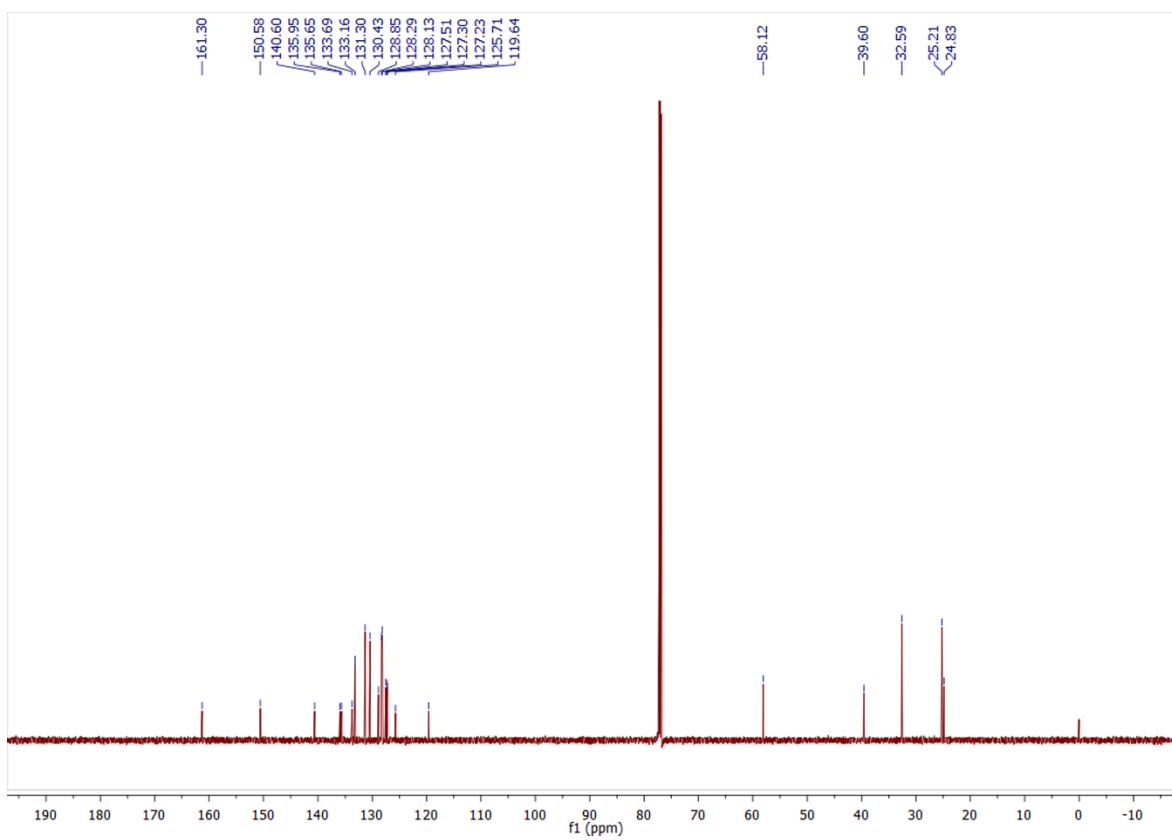
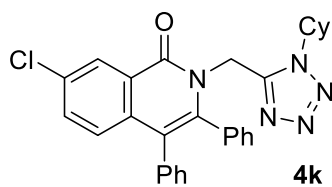
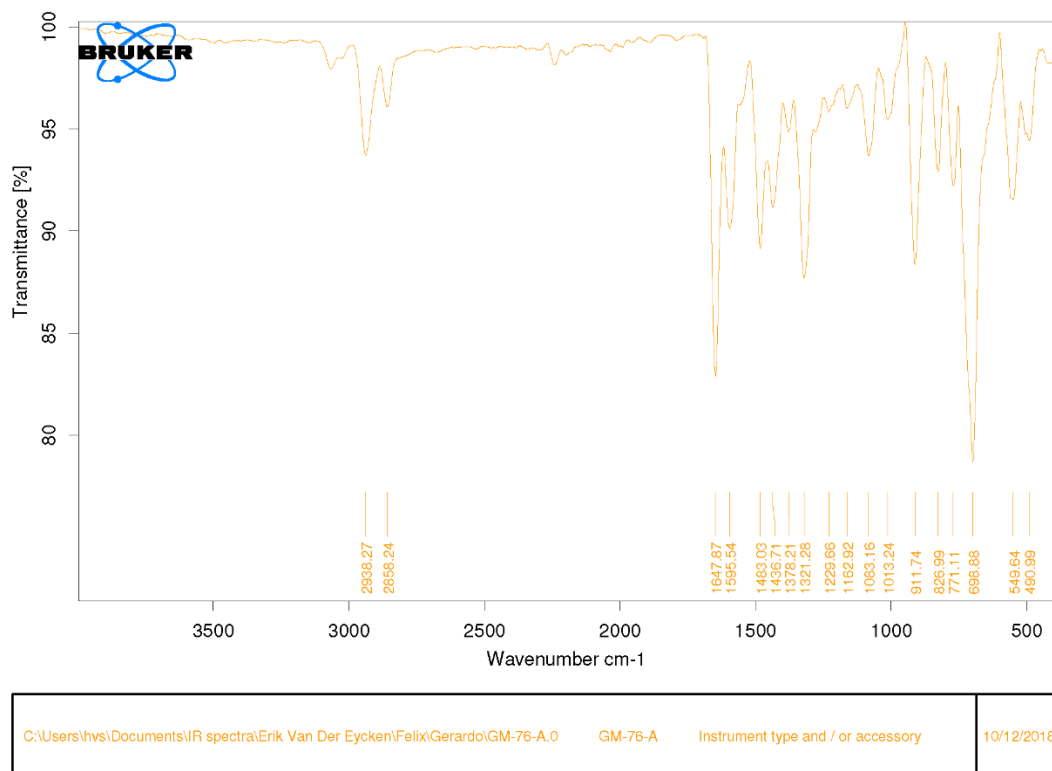


Figure S124. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **4k**.

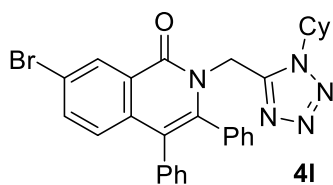


7-chloro-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2*H*)-one



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Figure S125. FT-IR (KBr) spectrum of compound **4k**.



7-bromo-2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2H)-one

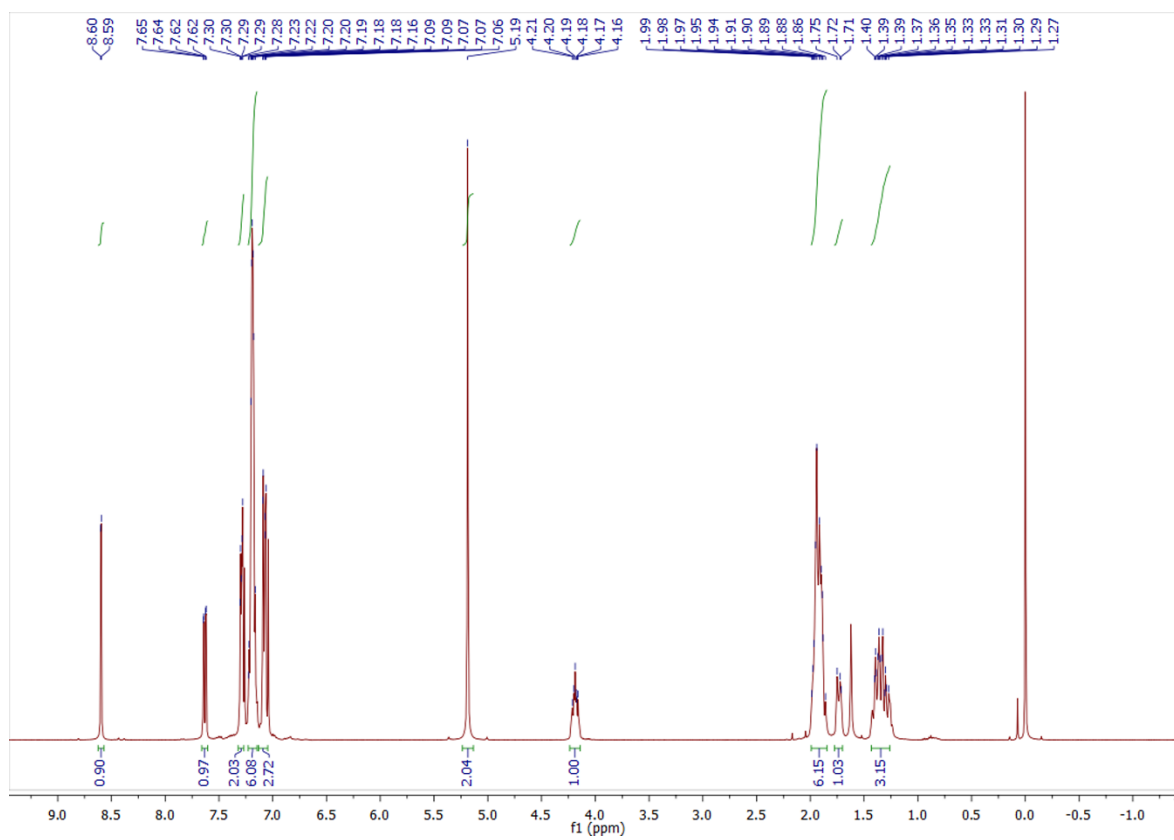
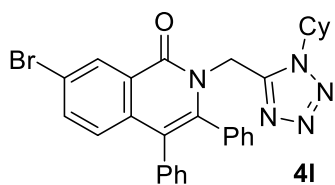


Figure S126. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4l**.



7-bromo-2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2*H*)-one

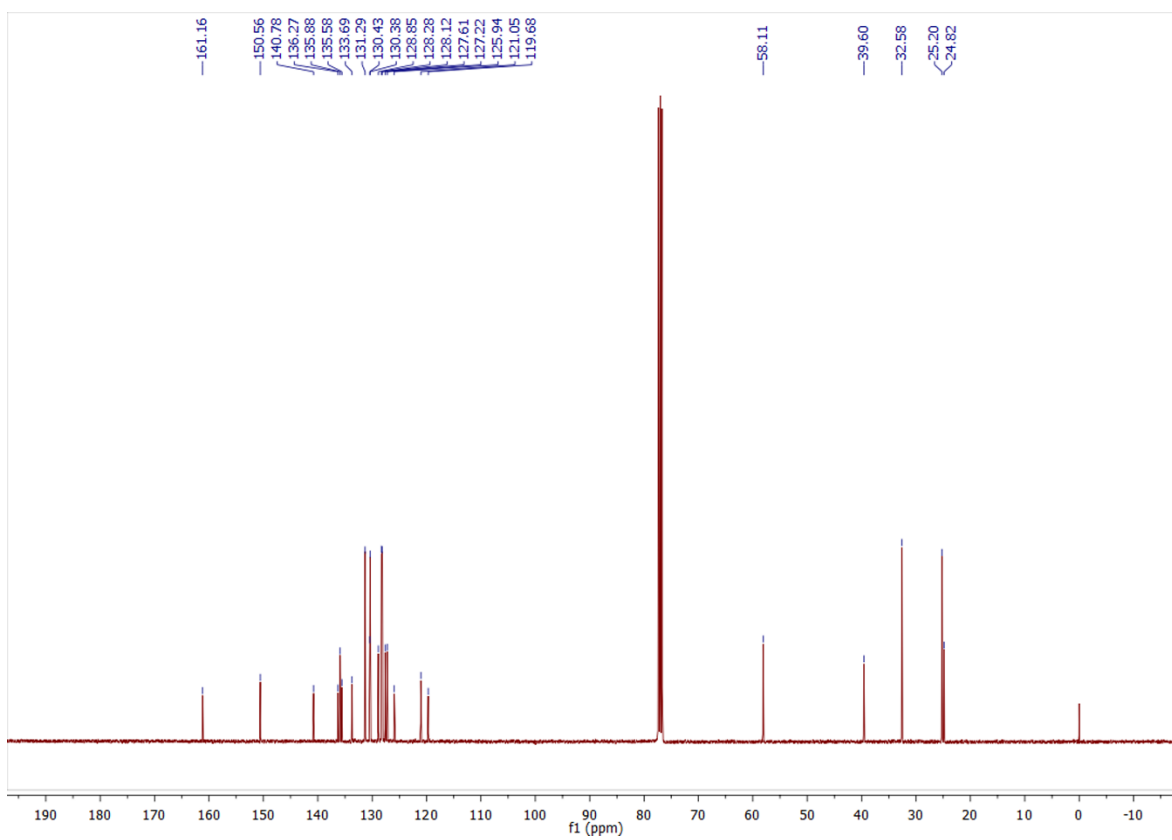
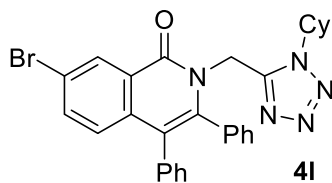
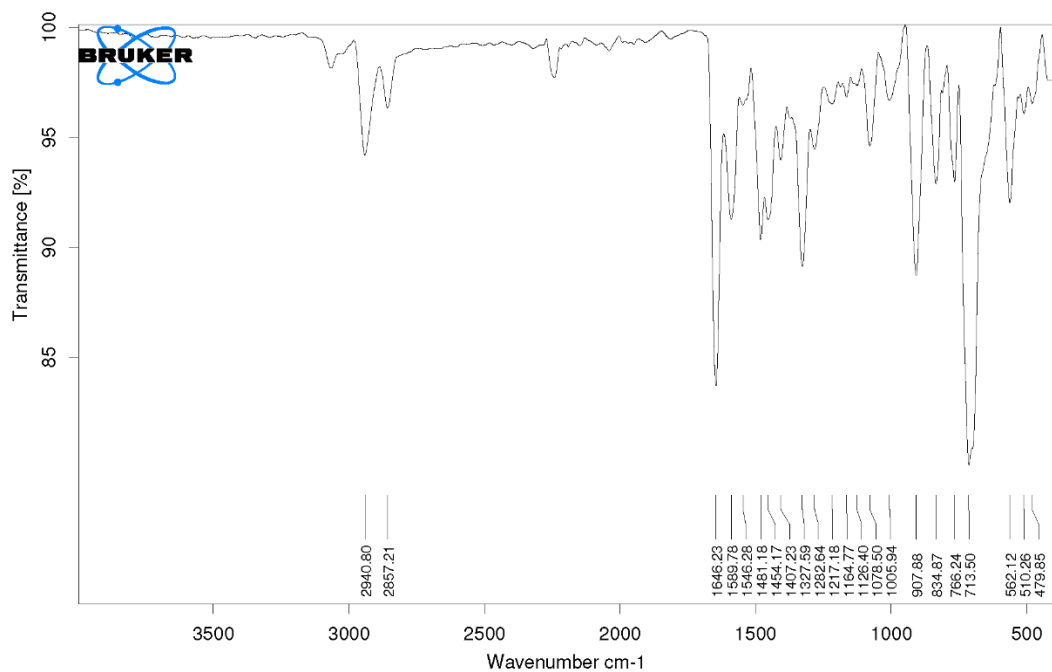


Figure S127. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4l**.

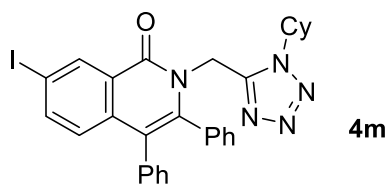


7-bromo-2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-
3,4-diphenylisoquinolin-1(2H)-one



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Figure S128. FT-IR (KBr) spectrum of compound **4I**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-7-iodo-3,4-diphenylisoquinolin-1(2*H*)-one

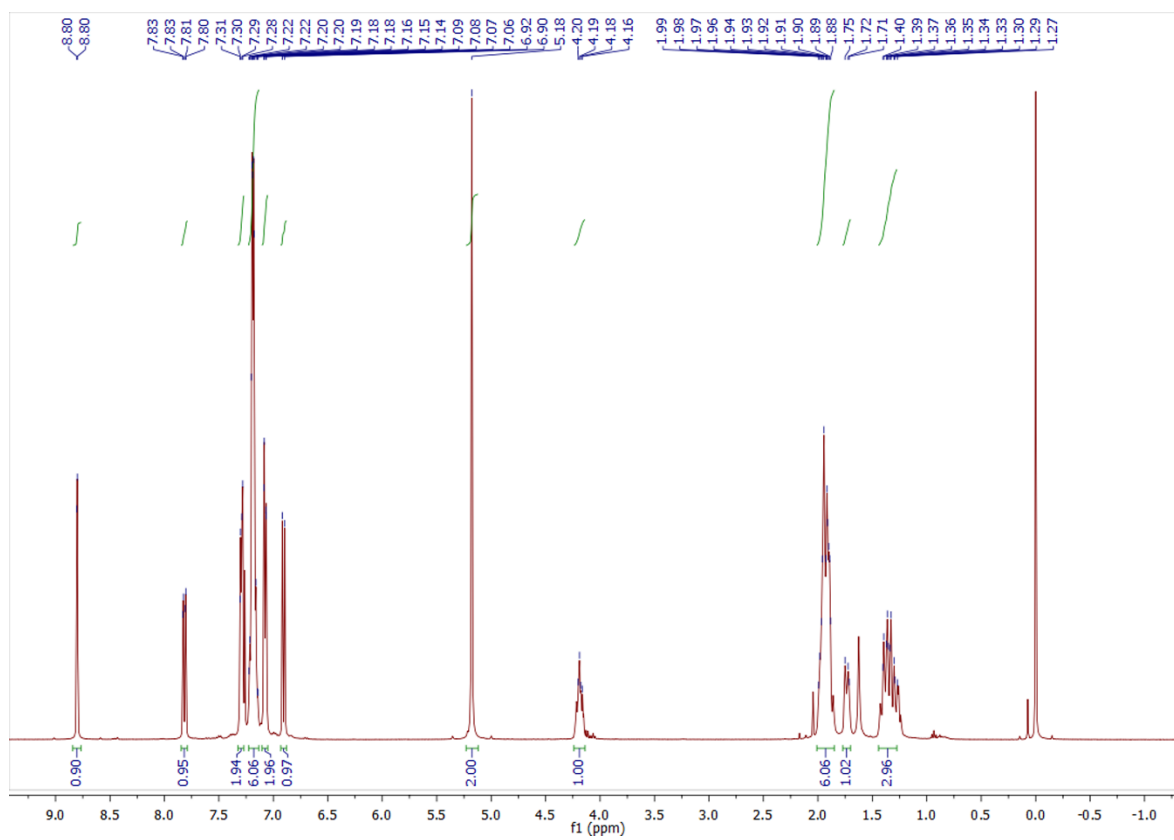
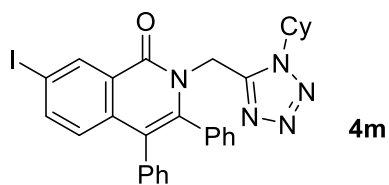


Figure S129. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4m**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-7-iodo-3,4-diphenylisoquinolin-1(2*H*)-one

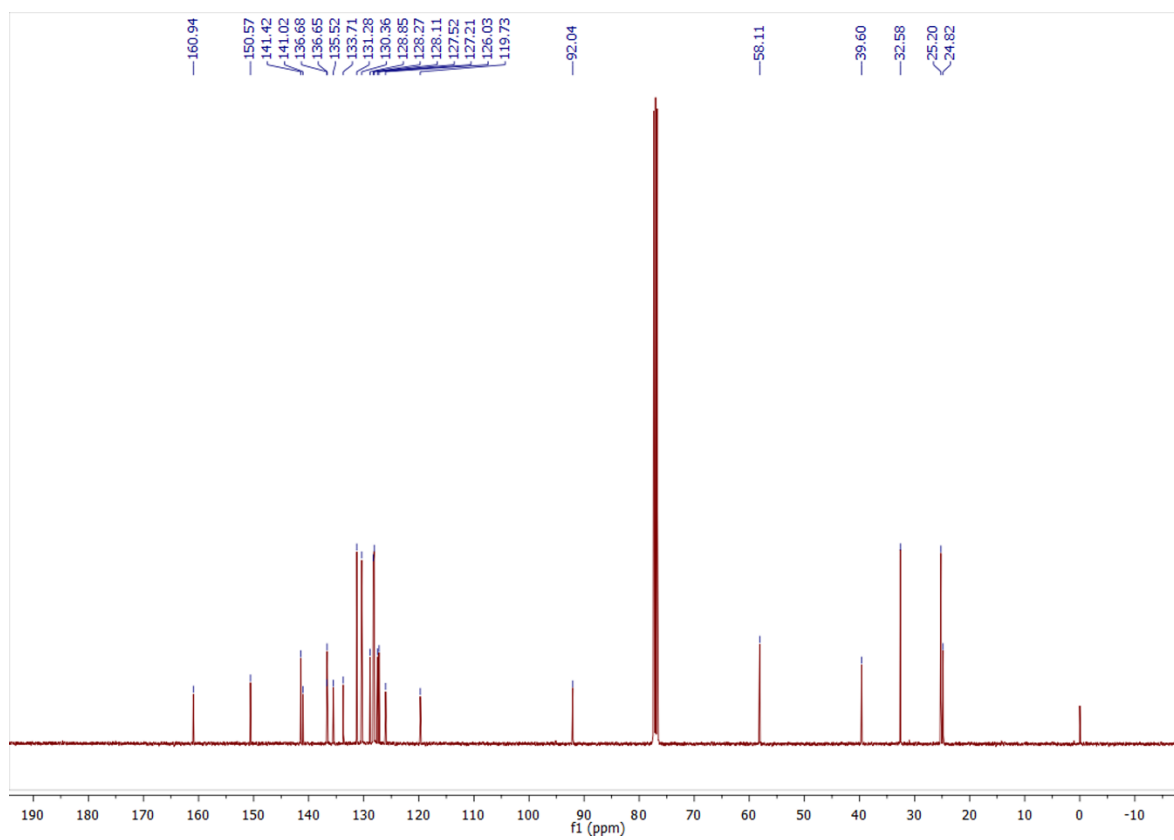
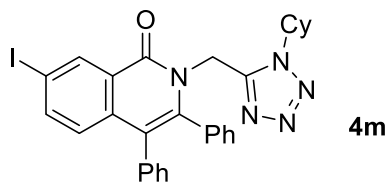
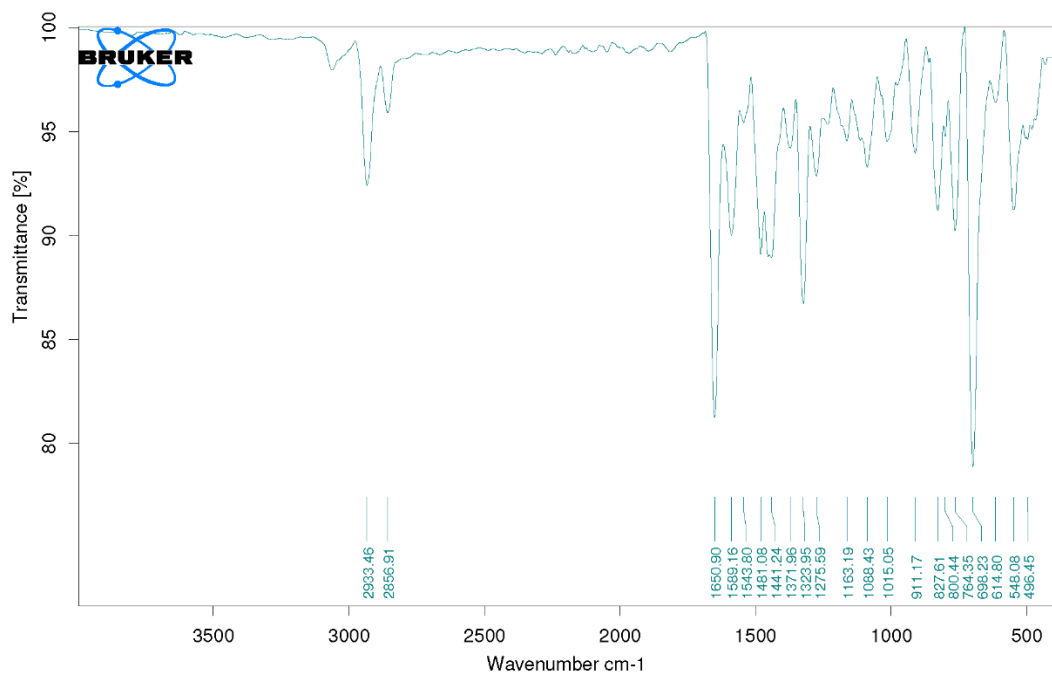


Figure S130. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4m**.

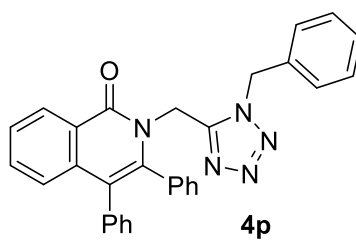


2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-7-iodo-3,4-diphenylisoquinolin-1(2*H*)-one



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Figure S131. FT-IR (KBr) spectrum of compound **4m**.



2-((1-benzyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one

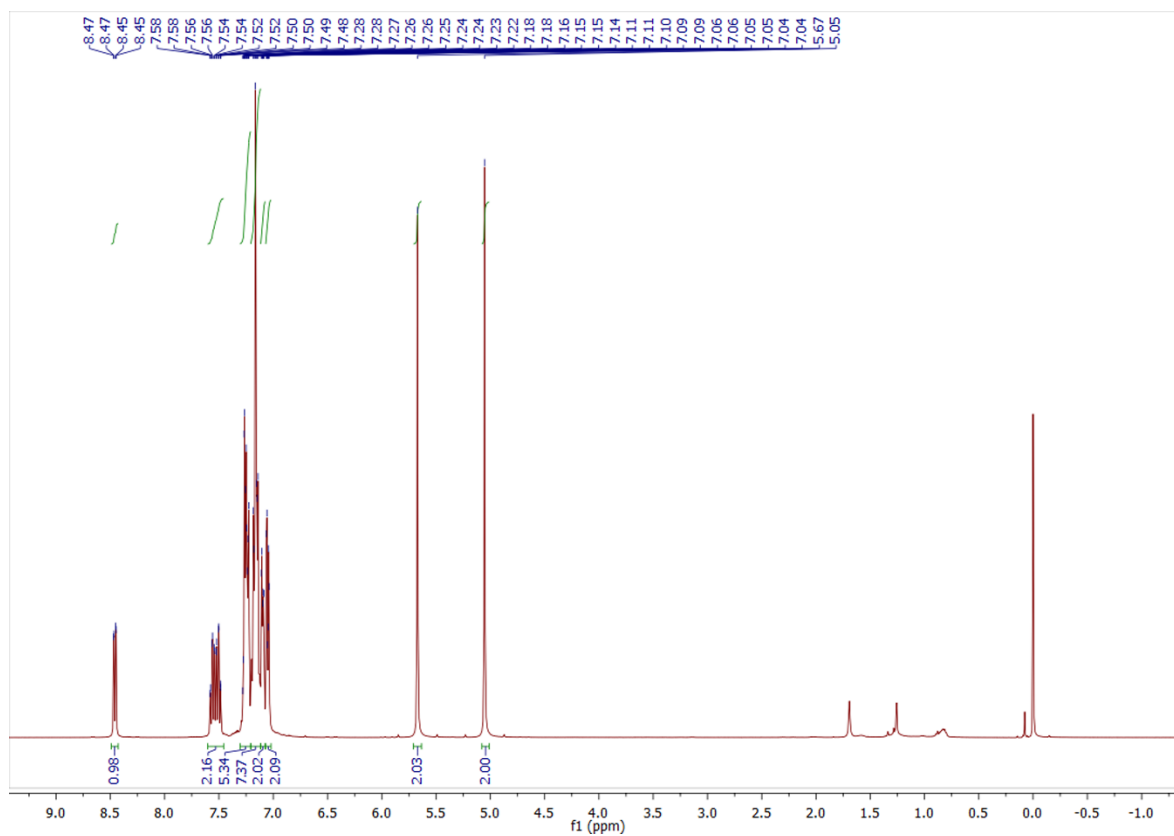
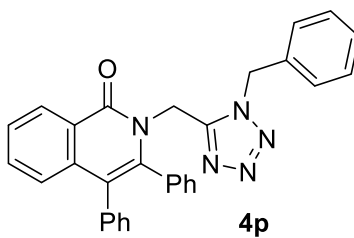


Figure S132. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4p**.



2-((1-benzyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one

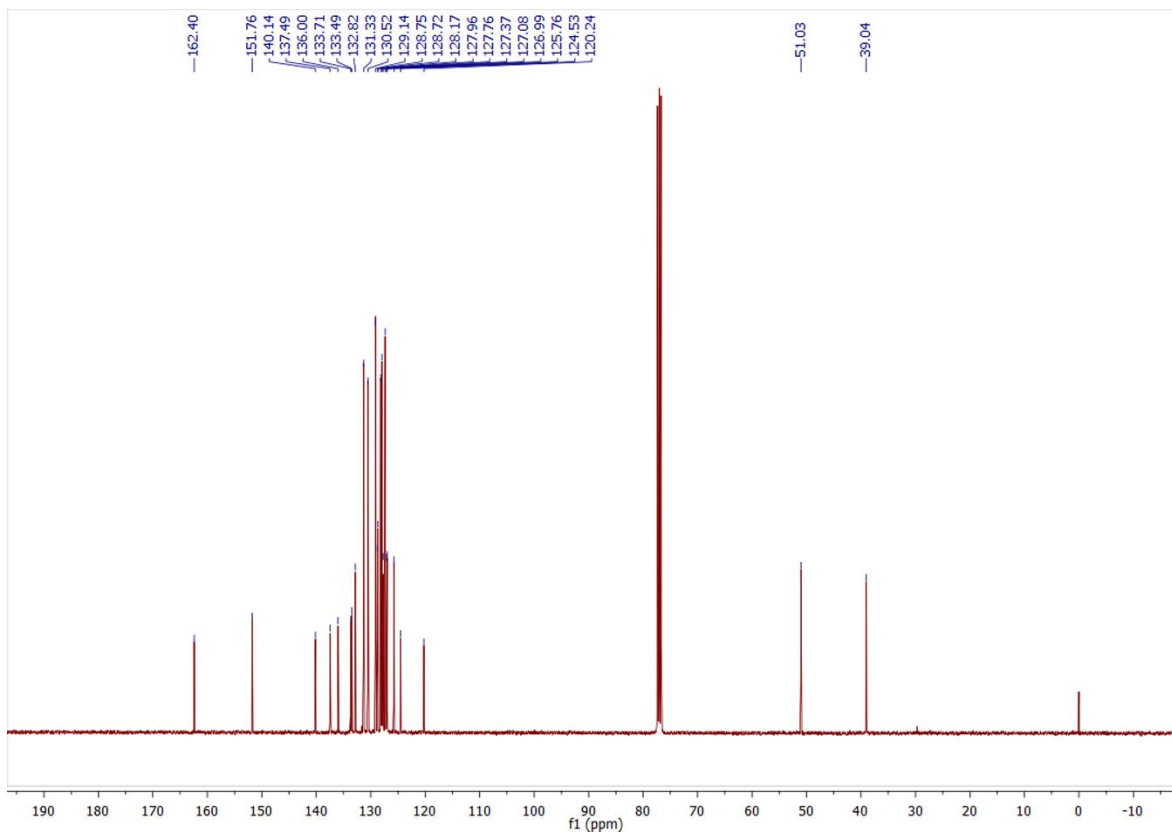
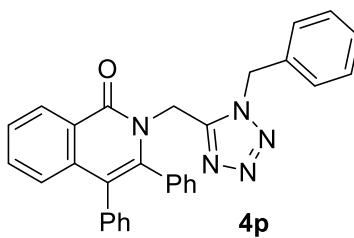
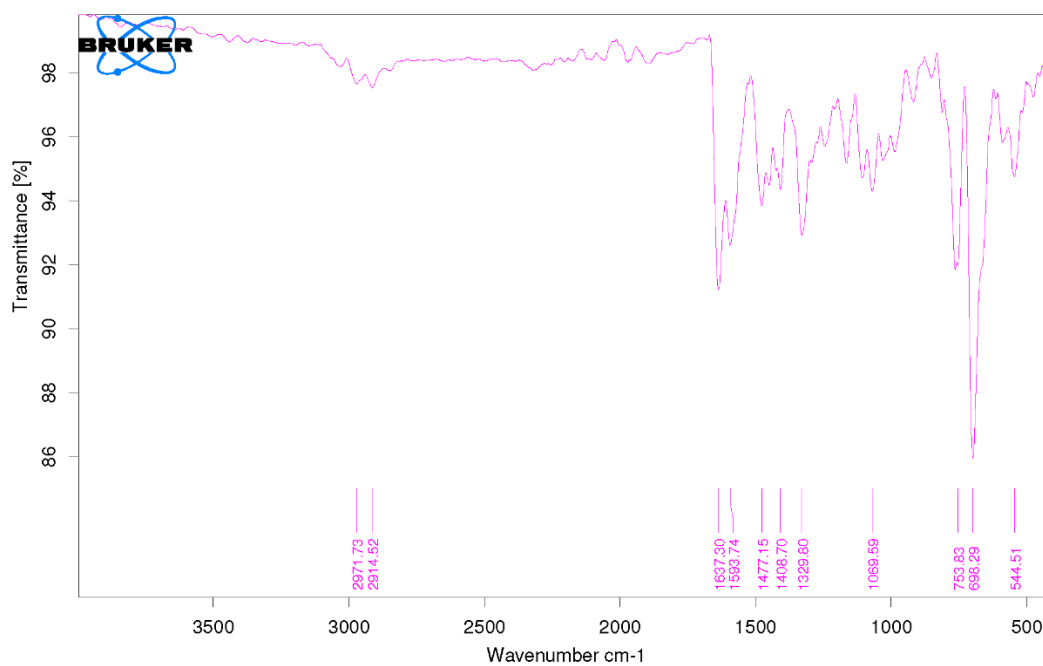


Figure S133. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4p**.



2-((1-benzyl-1H-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2H)-one



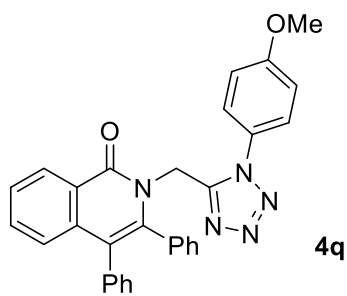
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Figure S134. FT-IR (KBr) spectrum of compound **4p**.



2-((1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

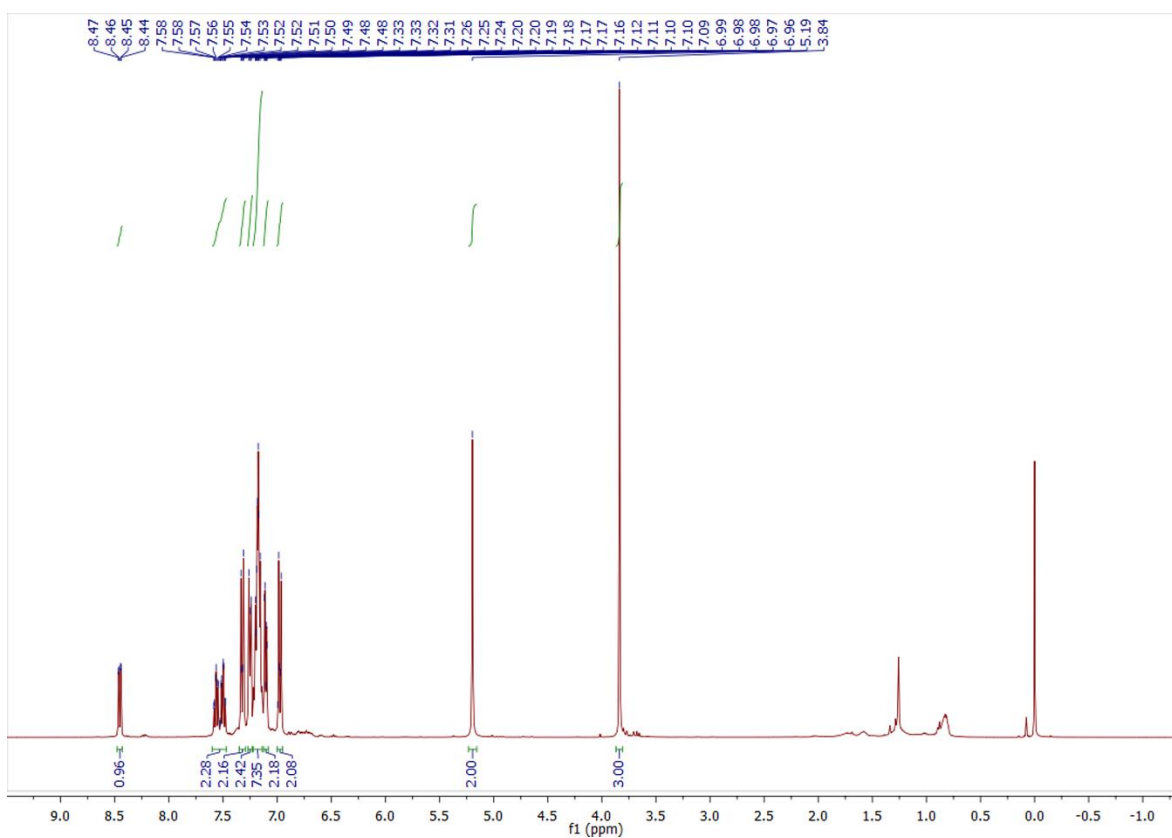
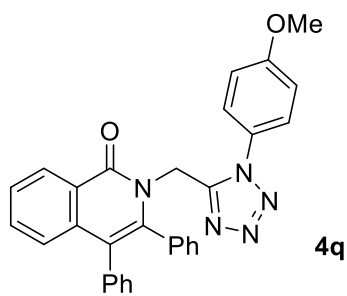


Figure S135. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4q**.



2-((1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

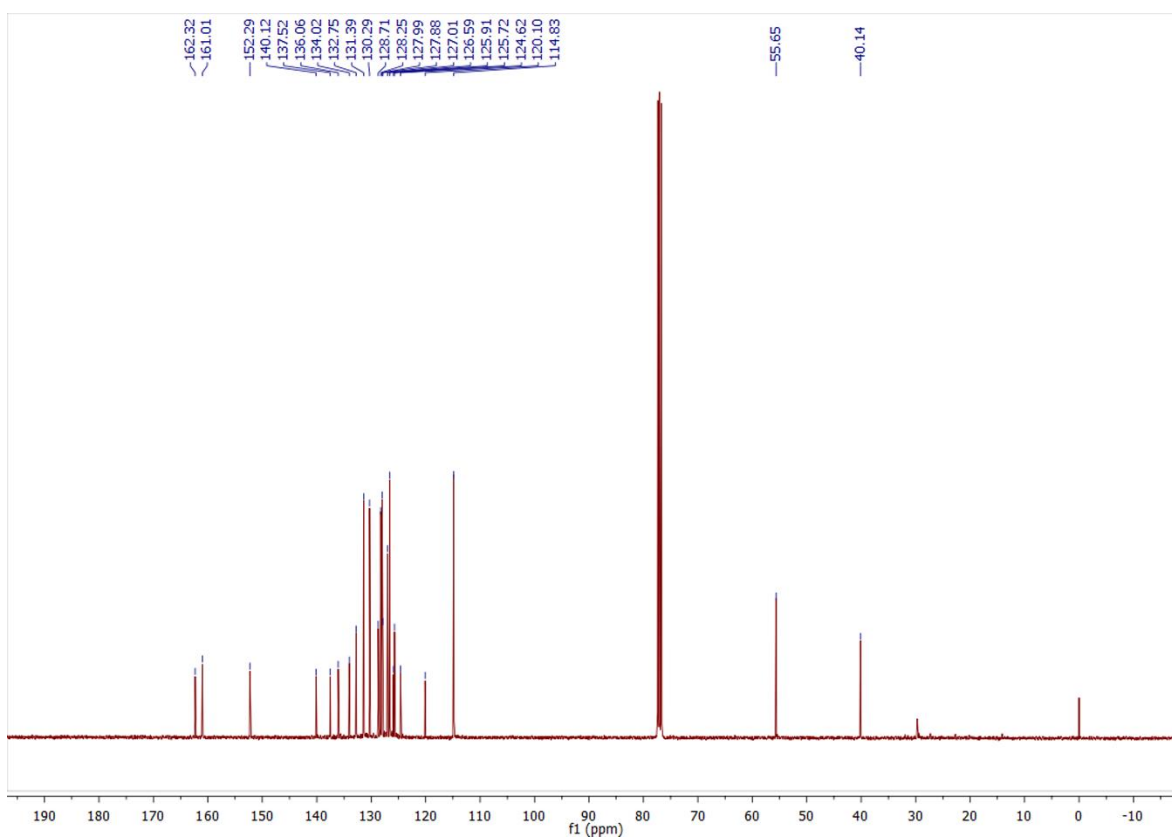
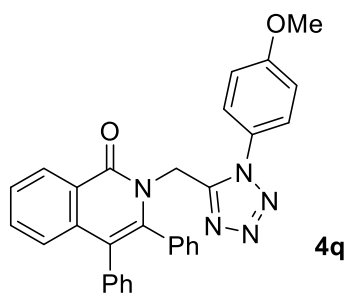
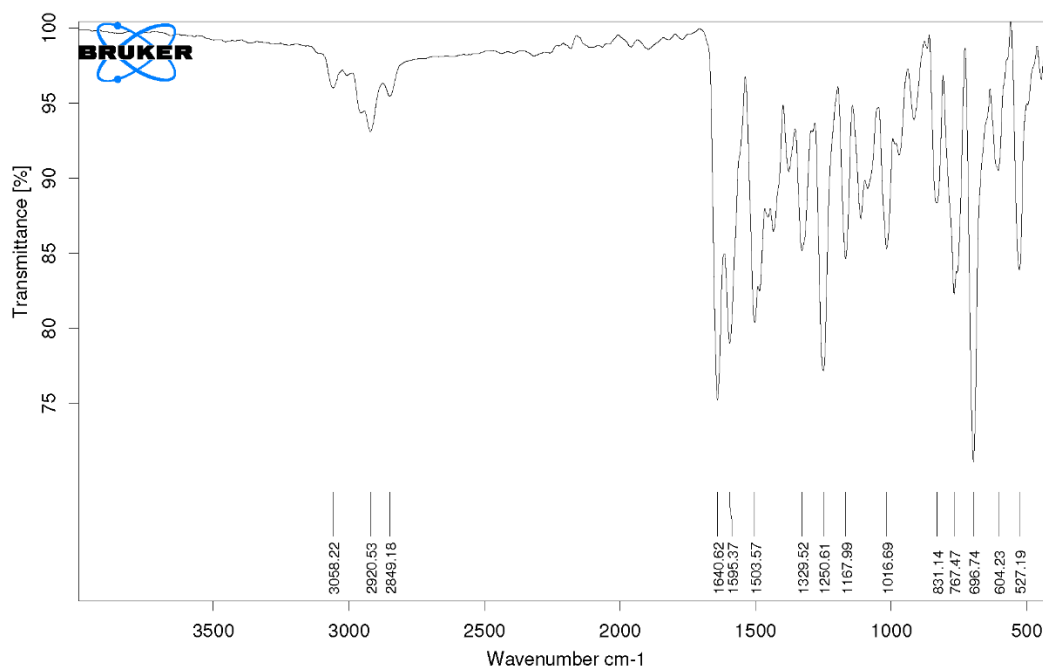


Figure S136. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4q**.



2-((1-(4-methoxyphenyl)-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one



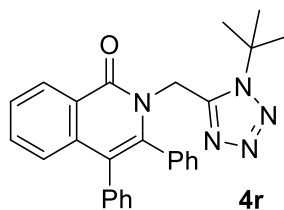
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Figure S137. FT-IR (KBr) spectrum of compound **4q**.



2-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

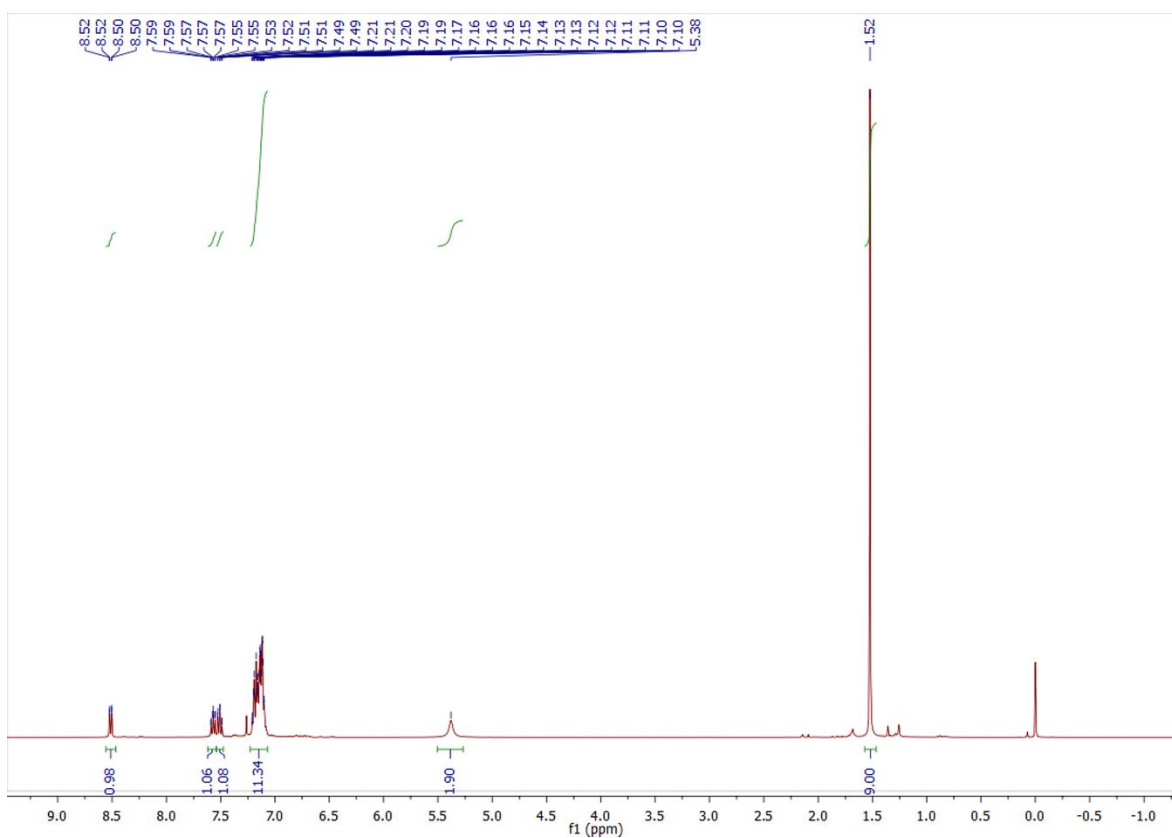
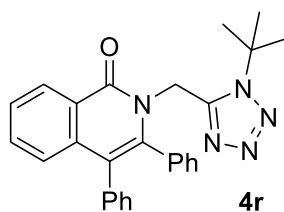


Figure S138. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **4r**.



2-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one

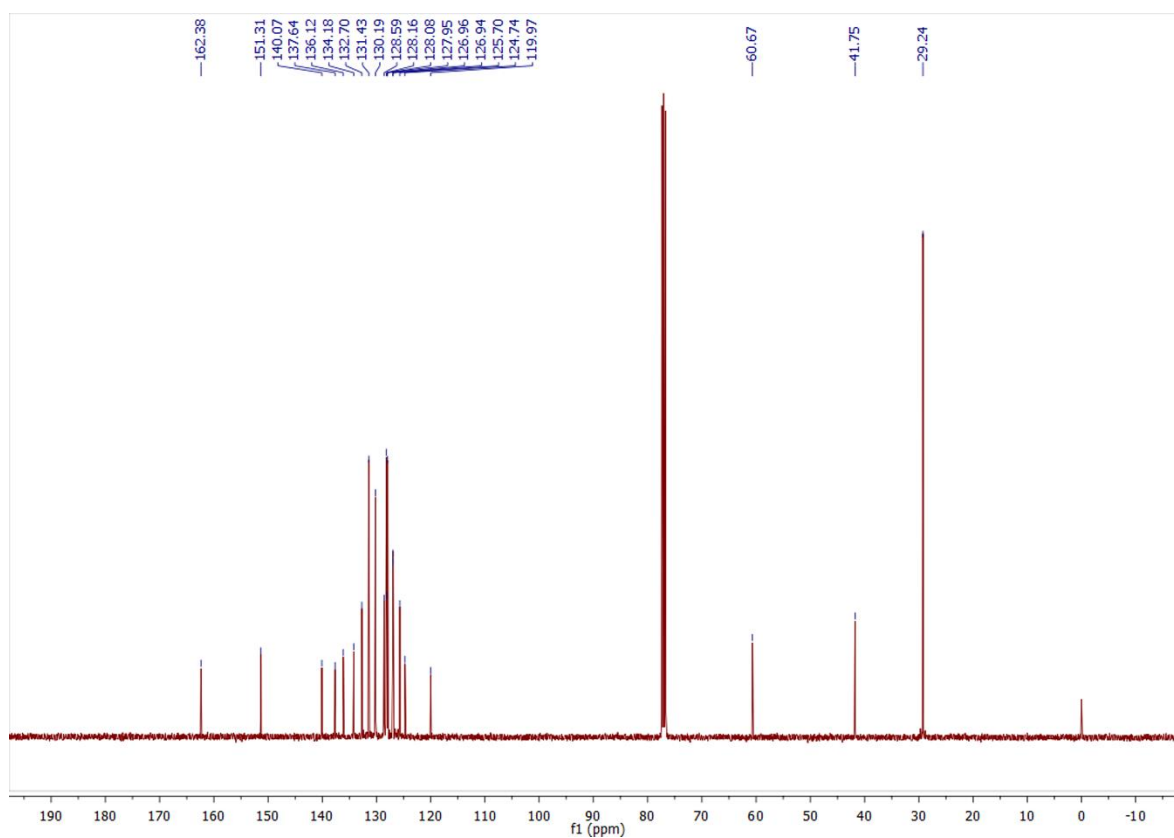
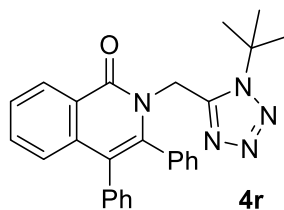
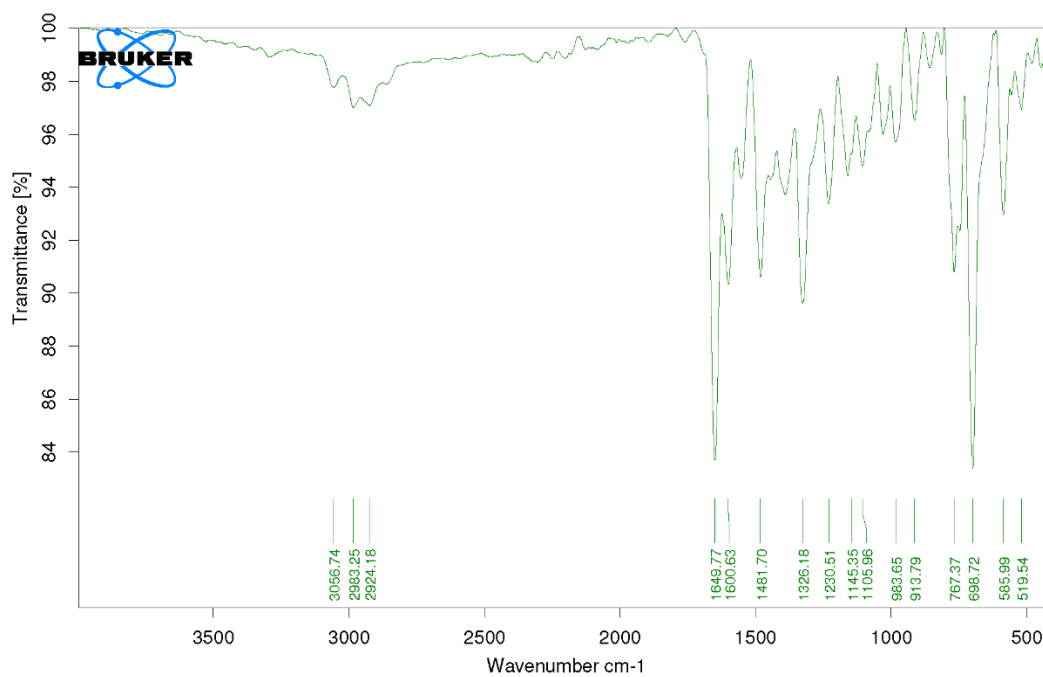


Figure S139. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4r**.



2-((1-(*tert*-butyl)-1*H*-tetrazol-5-yl)methyl)-3,4-diphenylisoquinolin-1(2*H*)-one



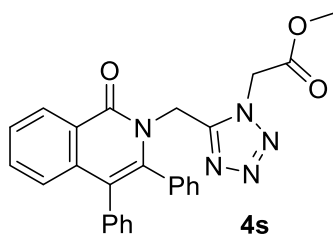
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Figure S140. FT-IR (KBr) spectrum of compound **4r**.



methyl 2-(5-((1-oxo-3,4-diphenylisoquinolin-2(1H)-yl)methyl)-1H-tetrazol-1-yl)acetate

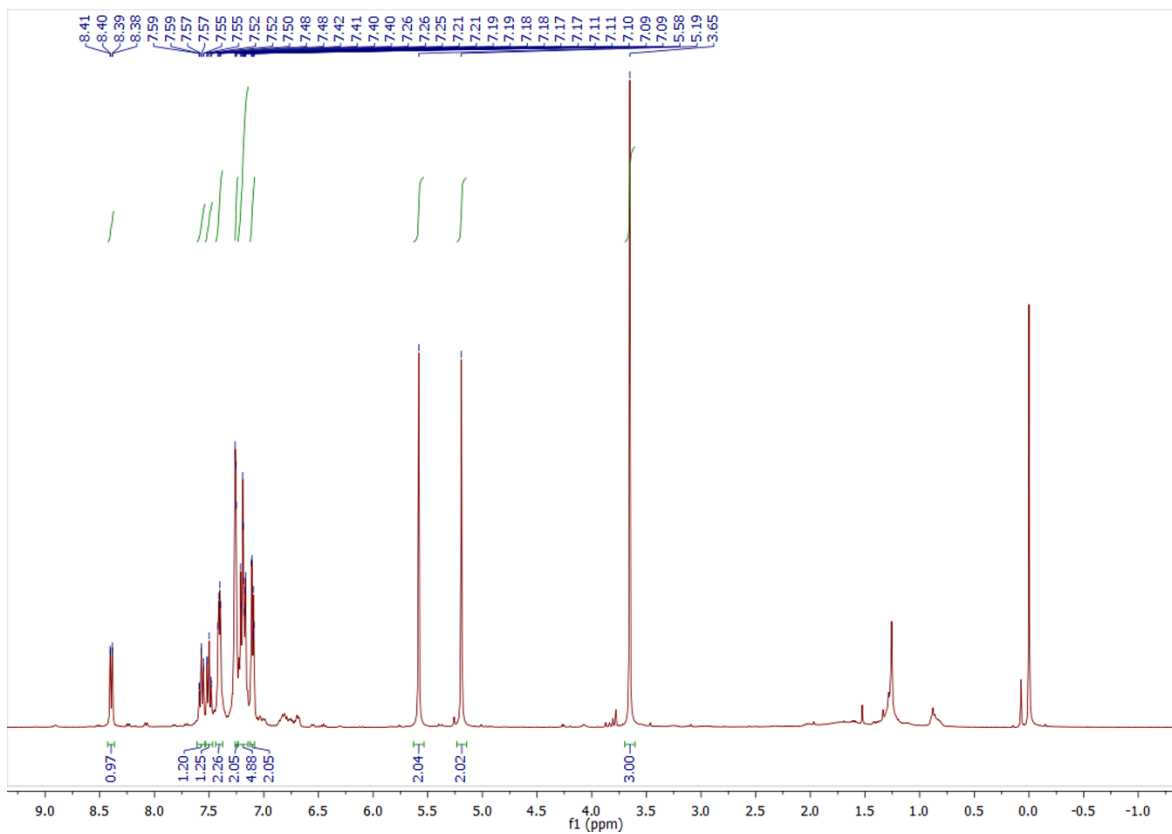
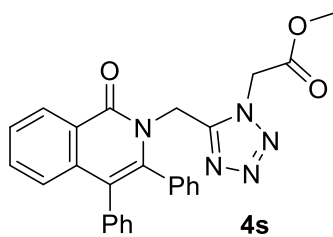


Figure S141 ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4s**.



methyl 2-(5-((1-oxo-3,4-diphenylisoquinolin-2(1*H*)-yl)methyl)-1*H*-tetrazol-1-yl)acetate

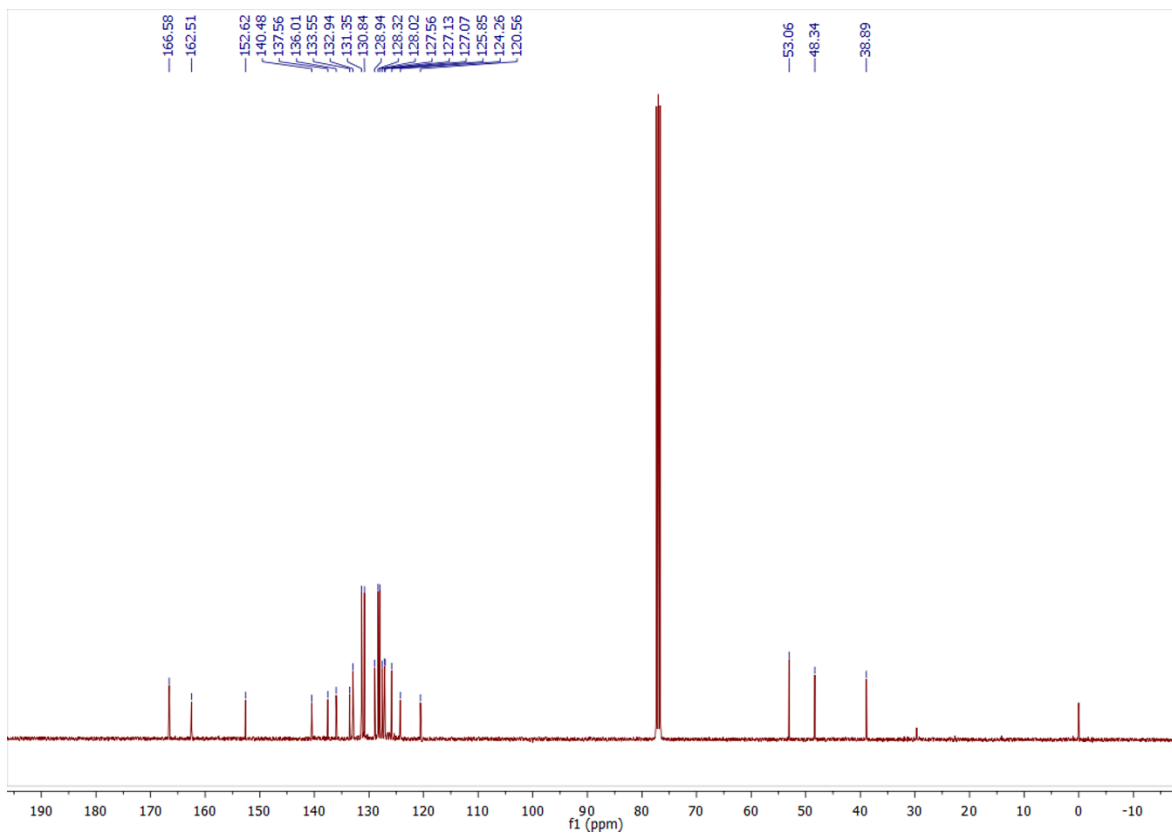
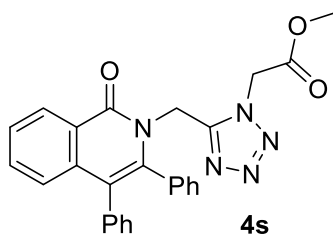
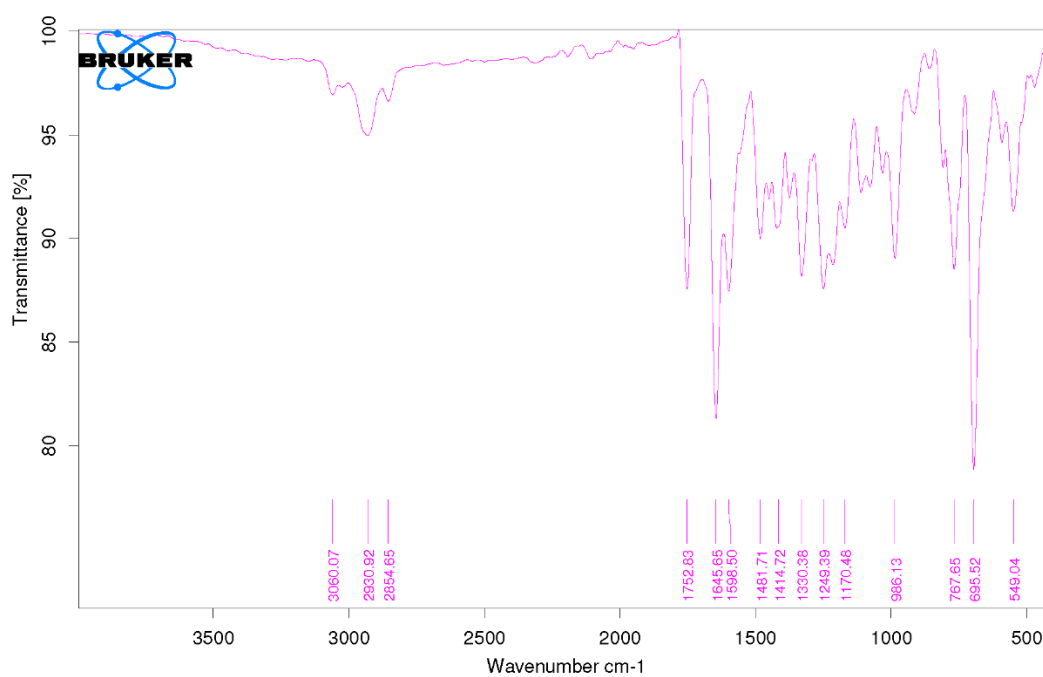


Figure S144. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4s**.



methyl 2-(5-((1-oxo-3,4-diphenylisoquinolin-2(1H)-yl)methyl)-1H-tetrazol-1-yl)acetate



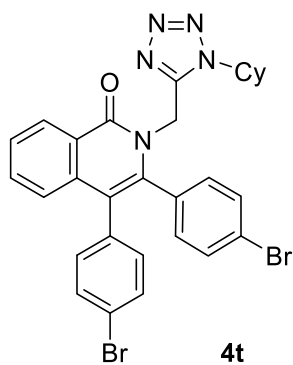
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Figure S143. FT-IR (KBr) spectrum of compound **4s**.



3,4-bis(4-bromophenyl)-2-
((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)isoquinolin-1(2*H*)-one

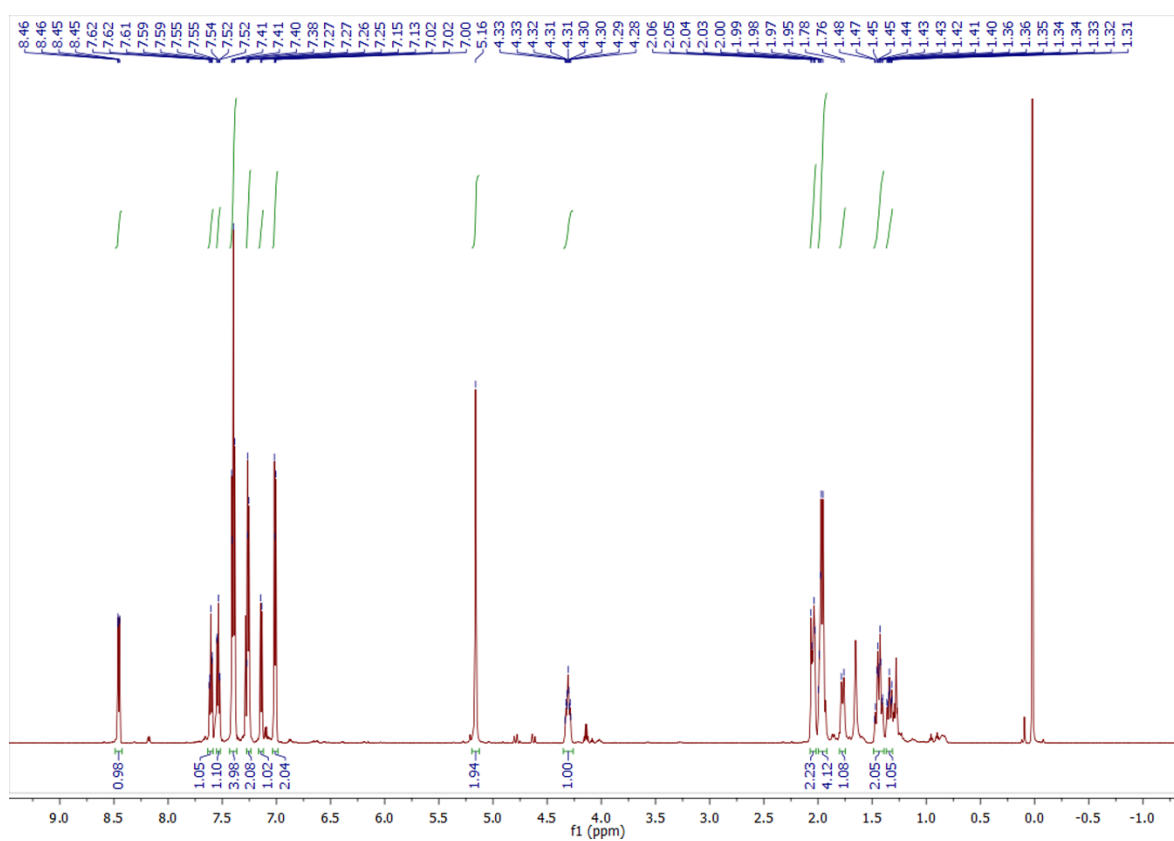
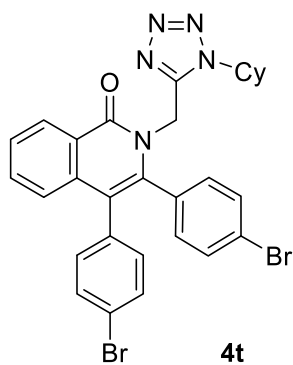


Figure S144. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **4t**.



3,4-bis(4-bromophenyl)-2-
((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)isoquinolin-1(2*H*)-one

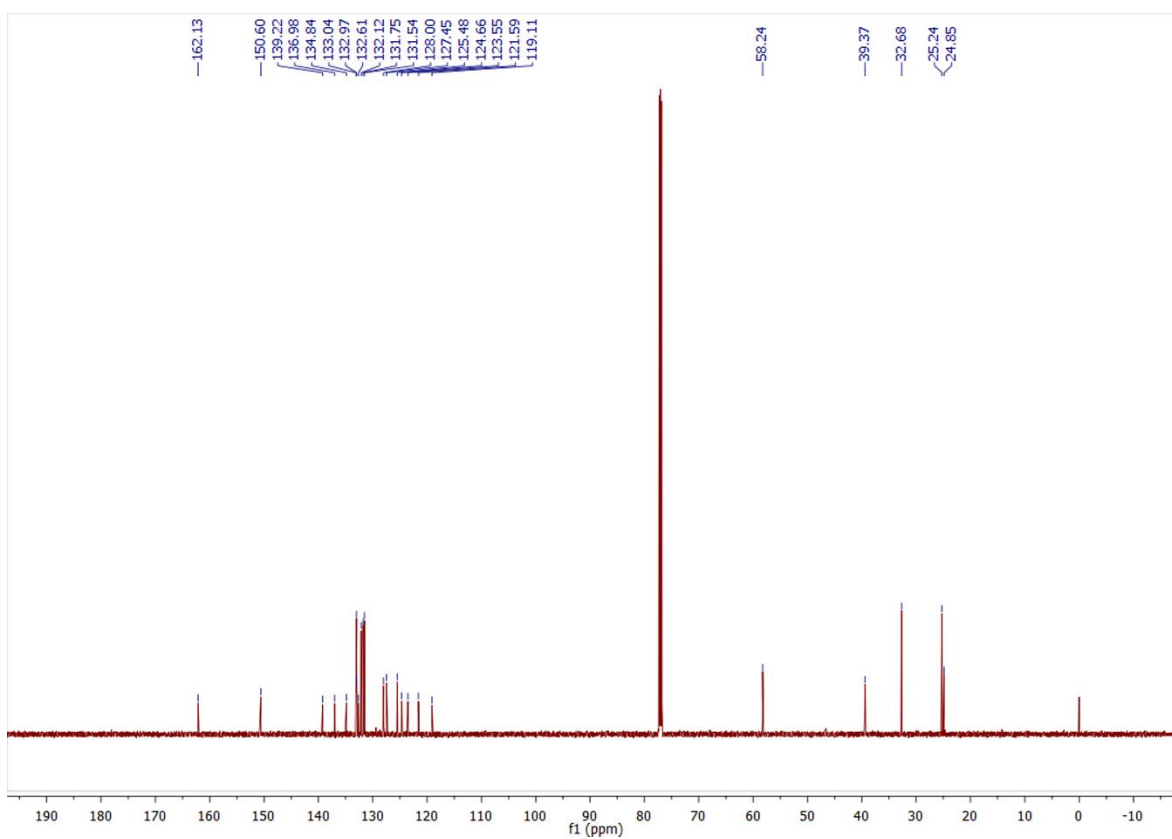
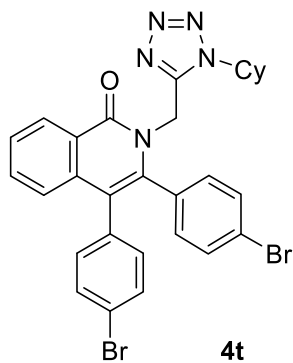
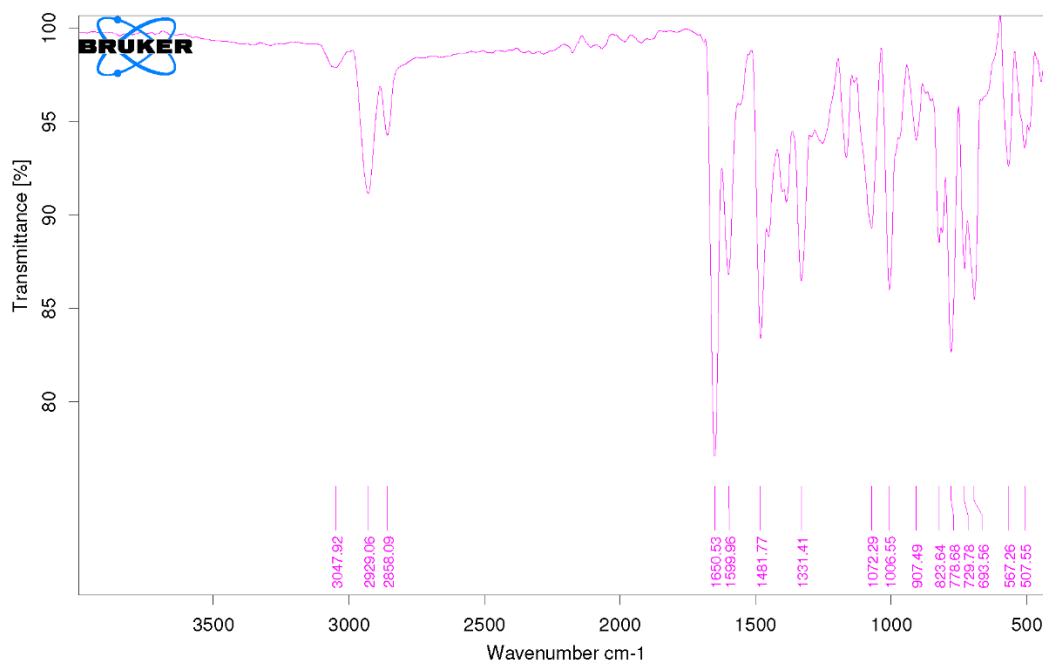


Figure S145. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **4t**.



3,4-bis(4-bromophenyl)-2-
((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)isoquinolin-1(2*H*)-one



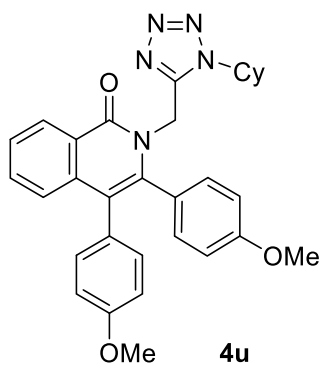
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Figure S146. FT-IR (KBr) spectrum of compound **4t**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-bis(4-methoxyphenyl)isoquinolin-1(2*H*)-one

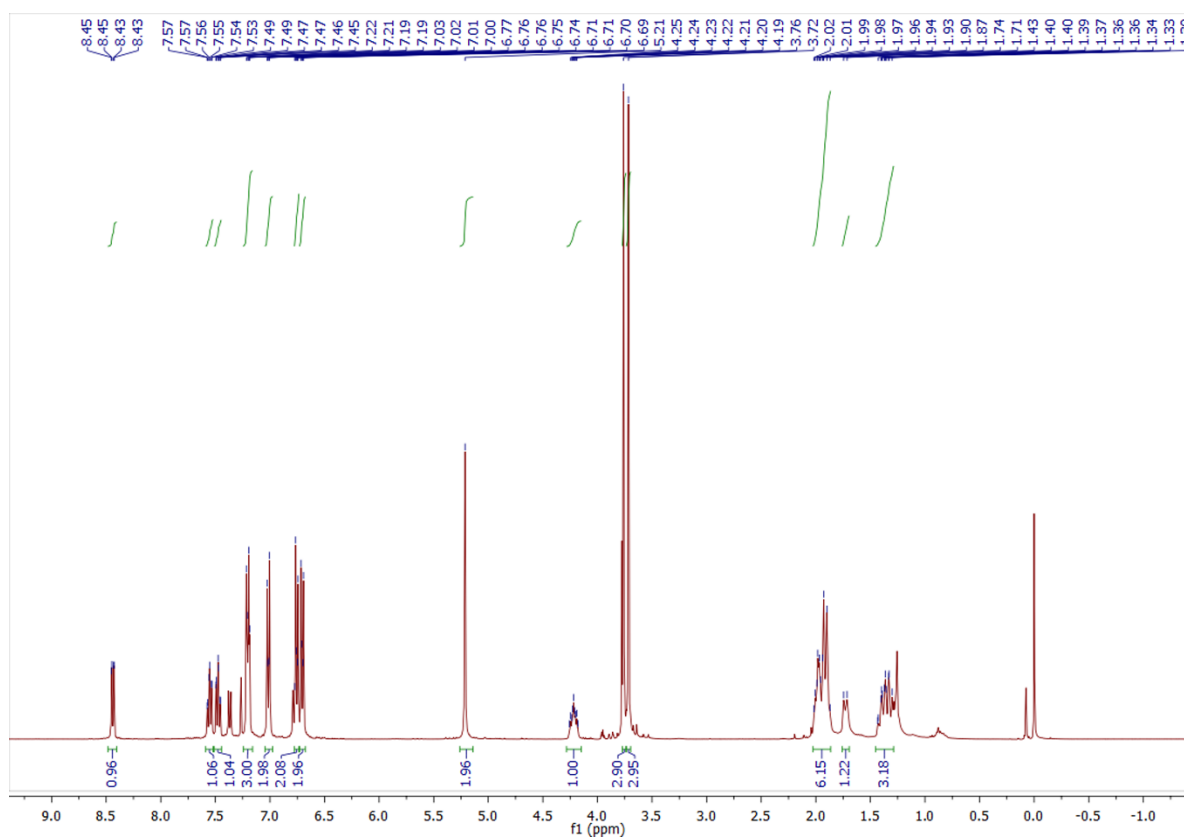
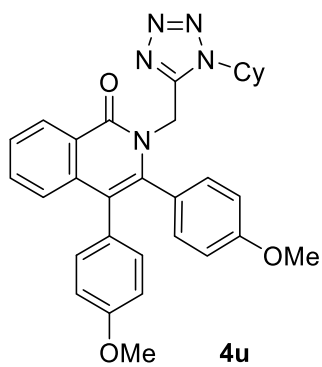


Figure S147. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **4u**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-bis(4-methoxyphenyl)isoquinolin-1(2*H*)-one

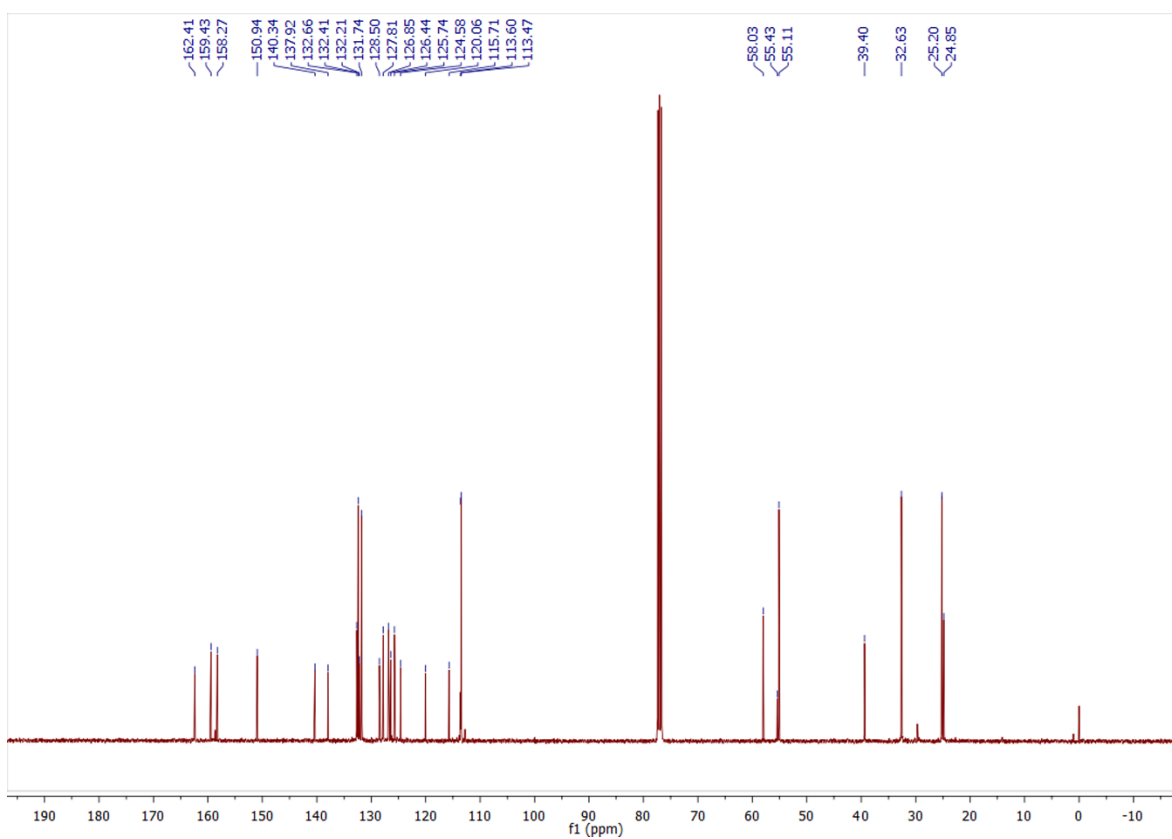
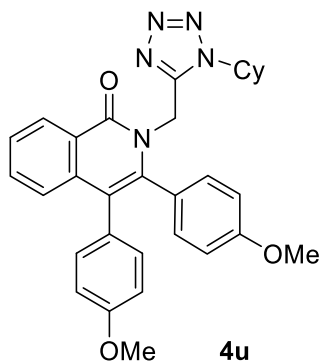
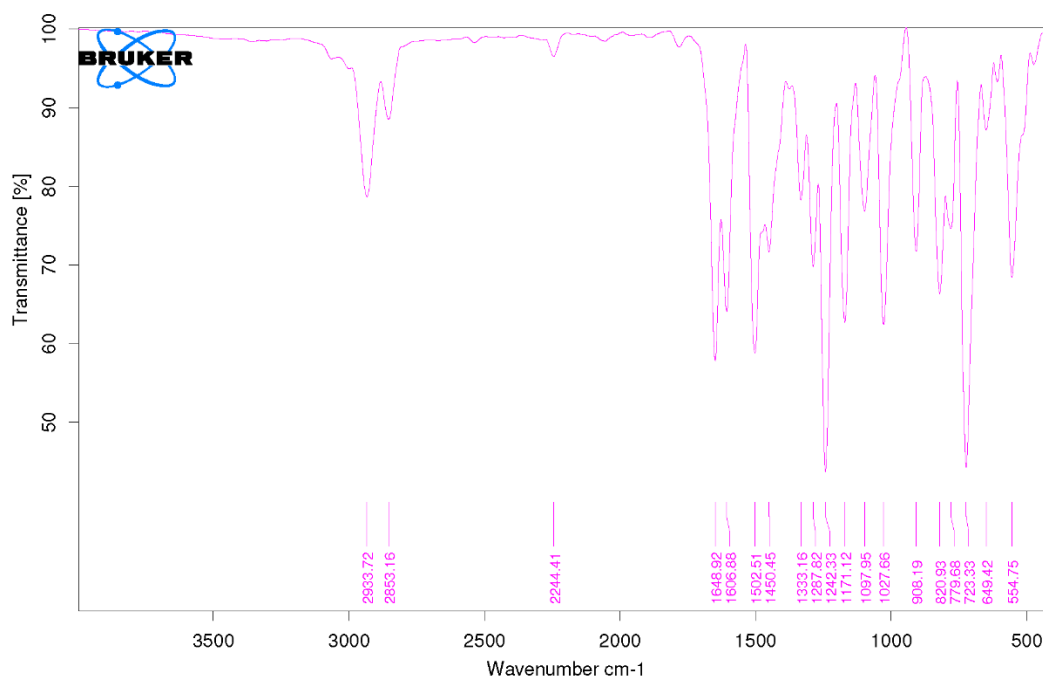


Figure S148. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4u**.



2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-
3,4-bis(4-methoxyphenyl)isoquinolin-1(2H)-one



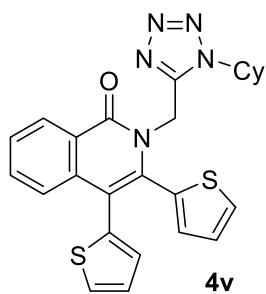
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GM-084

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Figure S149. FT-IR (KBr) spectrum of compound **4u**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-di(thiophen-2-yl)isoquinolin-1(2*H*)-one

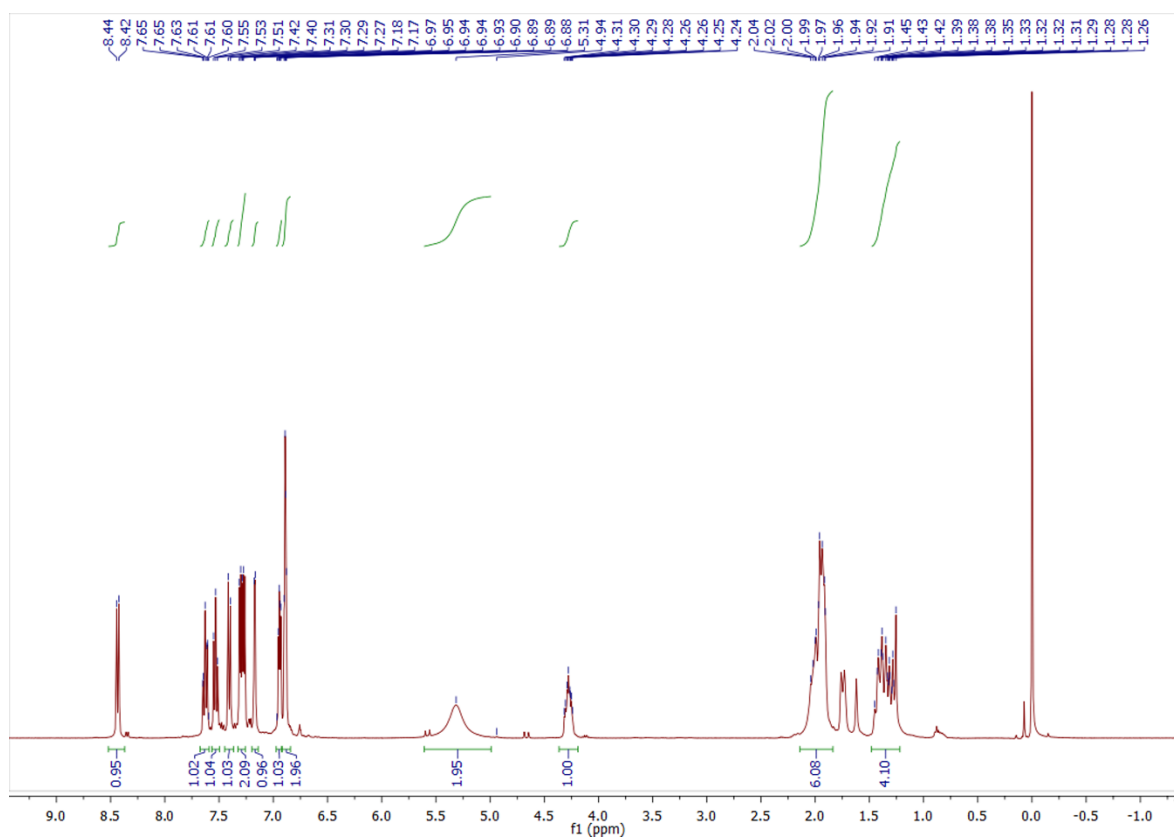
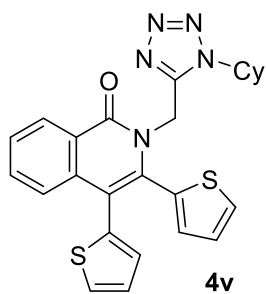


Figure S150. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4v**.



2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-
3,4-di(thiophen-2-yl)isoquinolin-1(2H)-one

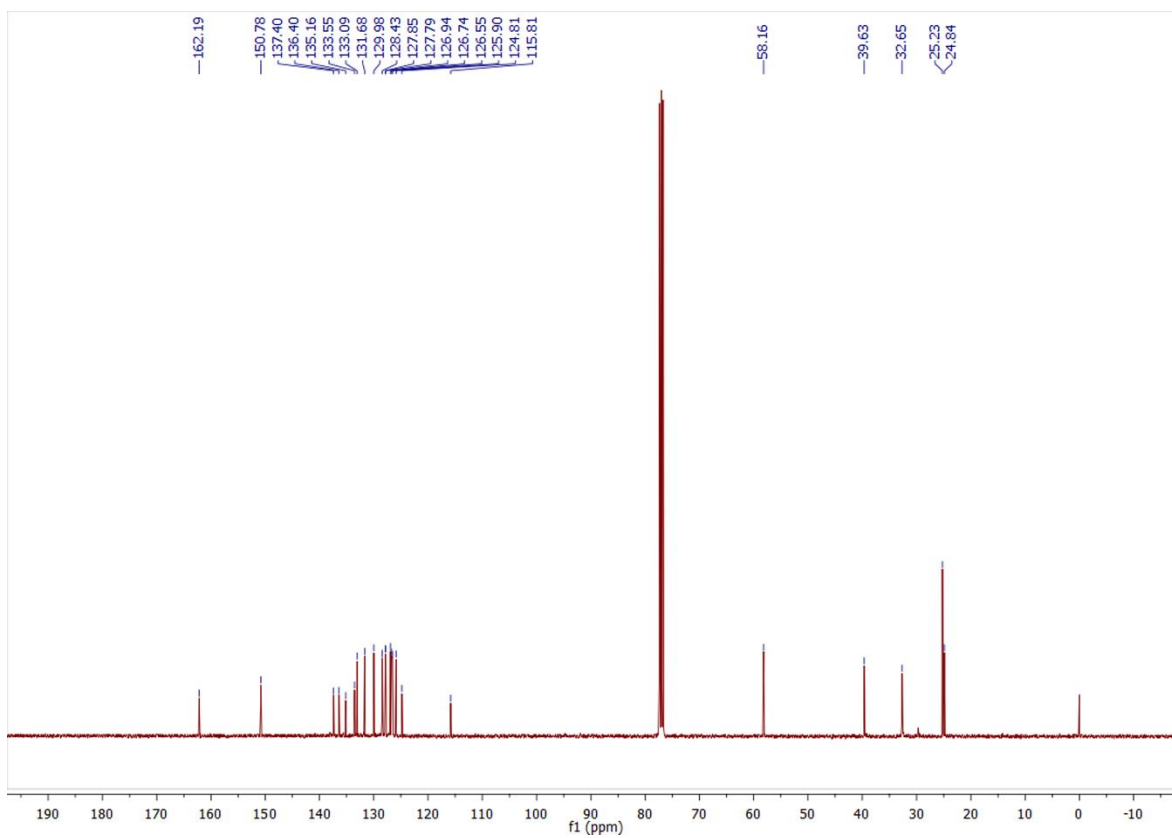
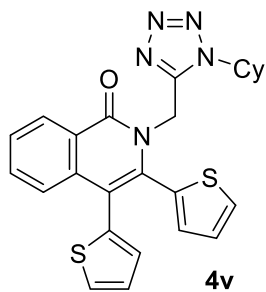
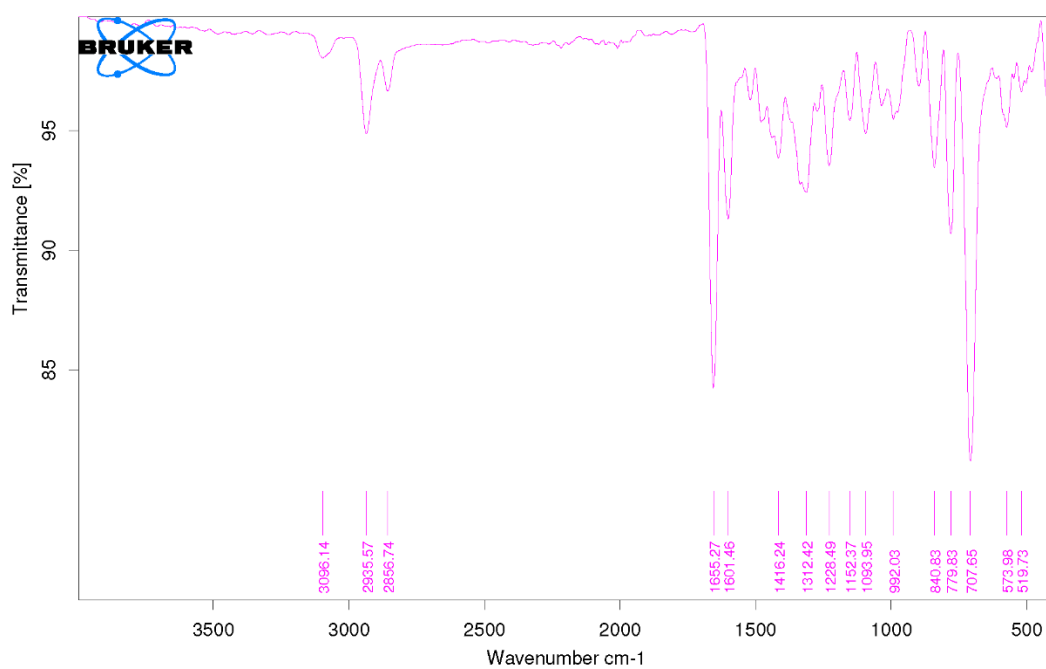


Figure S151. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **4v**.

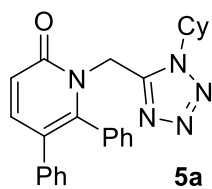


2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-di(thiophen-2-yl)isoquinolin-1(2*H*)-one



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Figure S152. FT-IR (KBr) spectrum of compound **4v**.



1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-5,6-diphenylpyridin-2(1*H*)-one

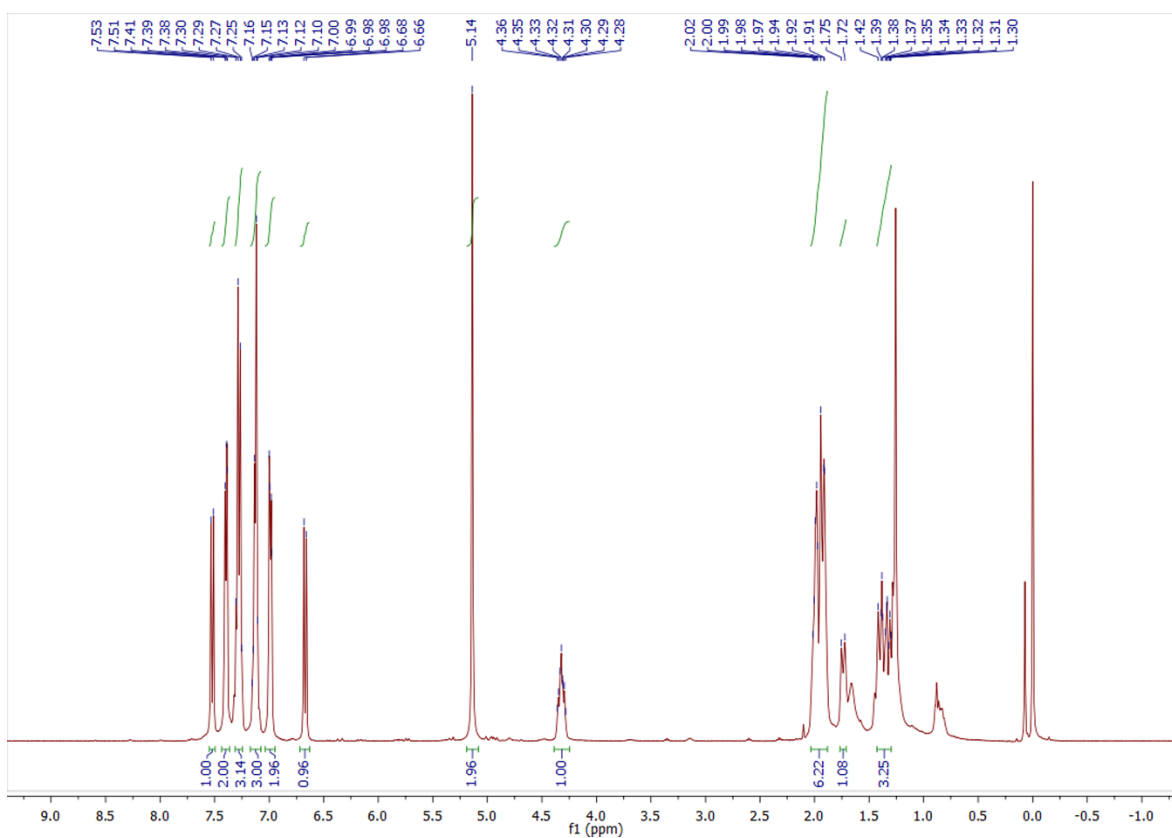
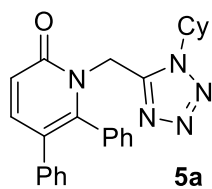


Figure S153. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **5a**.



1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-5,6-diphenylpyridin-2(1*H*)-one

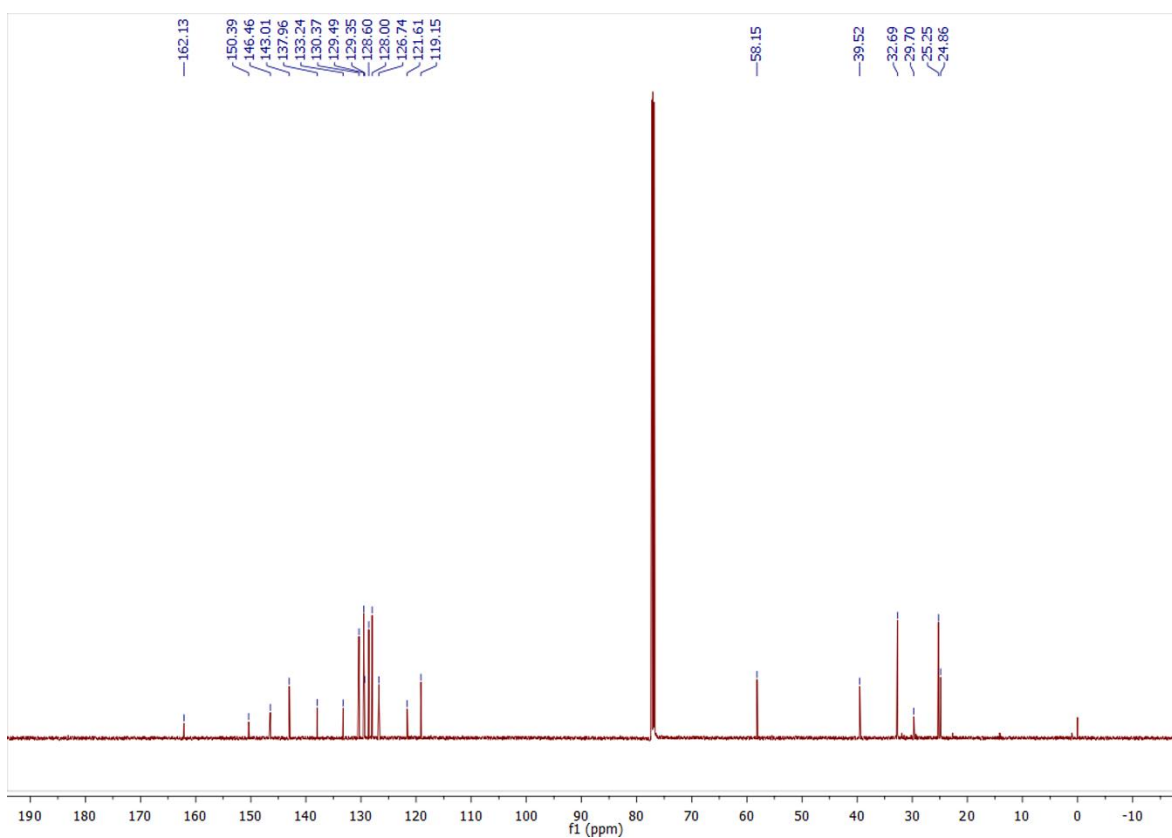
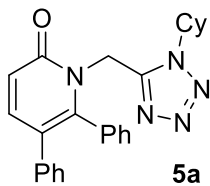
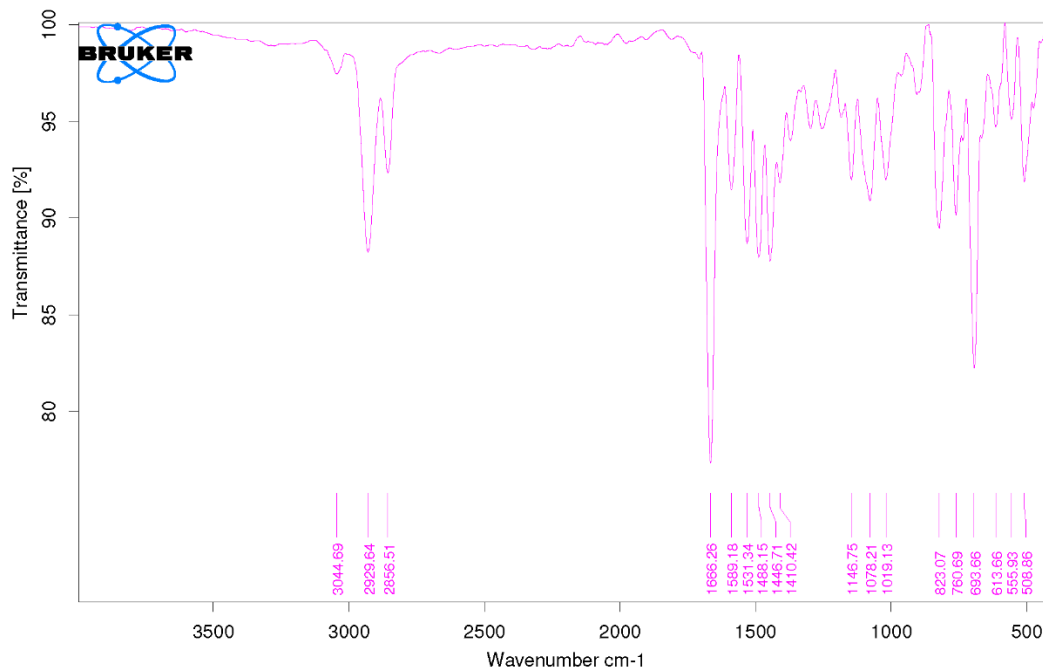


Figure S154. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **5a**.



1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-5,6-diphenylpyridin-2(1*H*)-one



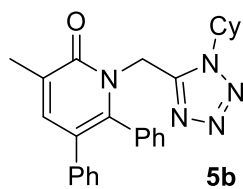
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Figure S155. FT-IR (KBr) spectrum of compound **5a**.



1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3-methyl-5,6-diphenylpyridin-2(1*H*)-one

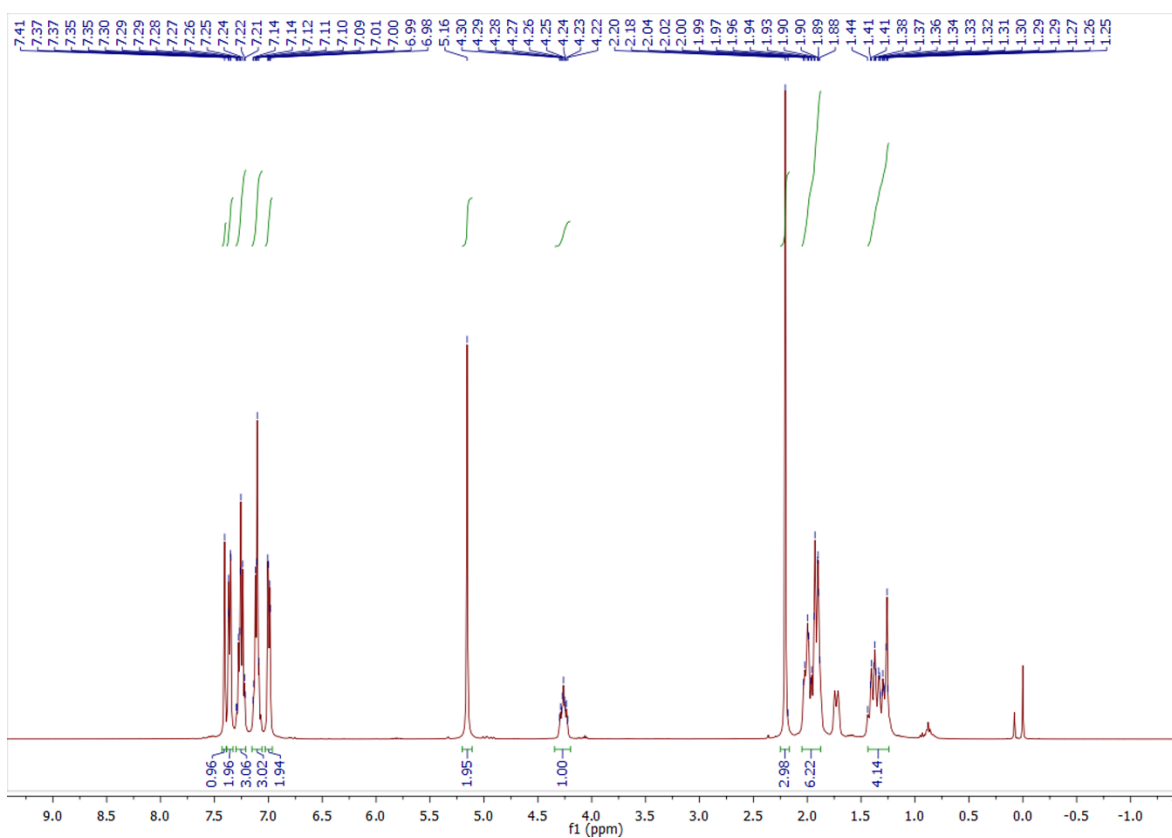
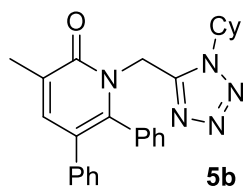


Figure S156. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **5b**.



1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3-methyl-5,6-diphenylpyridin-2(1*H*)-one

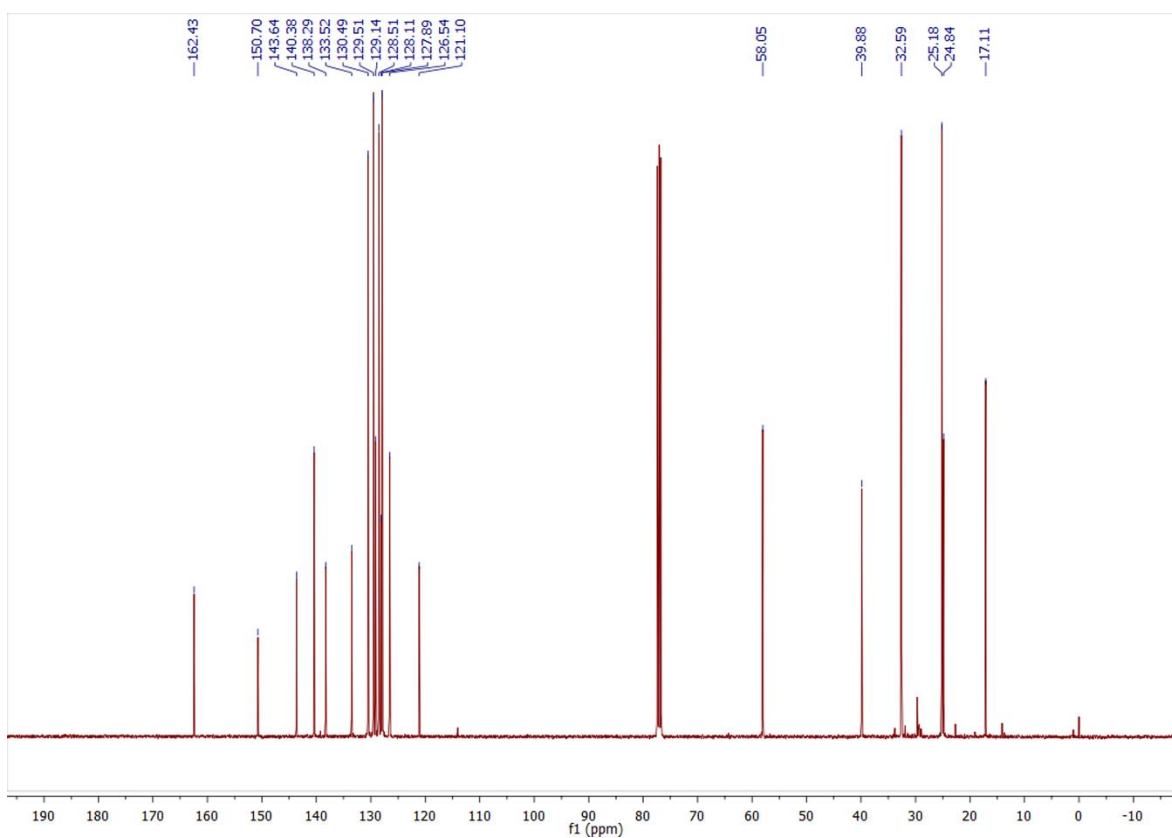
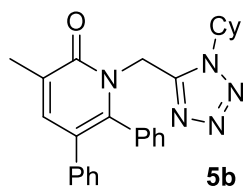
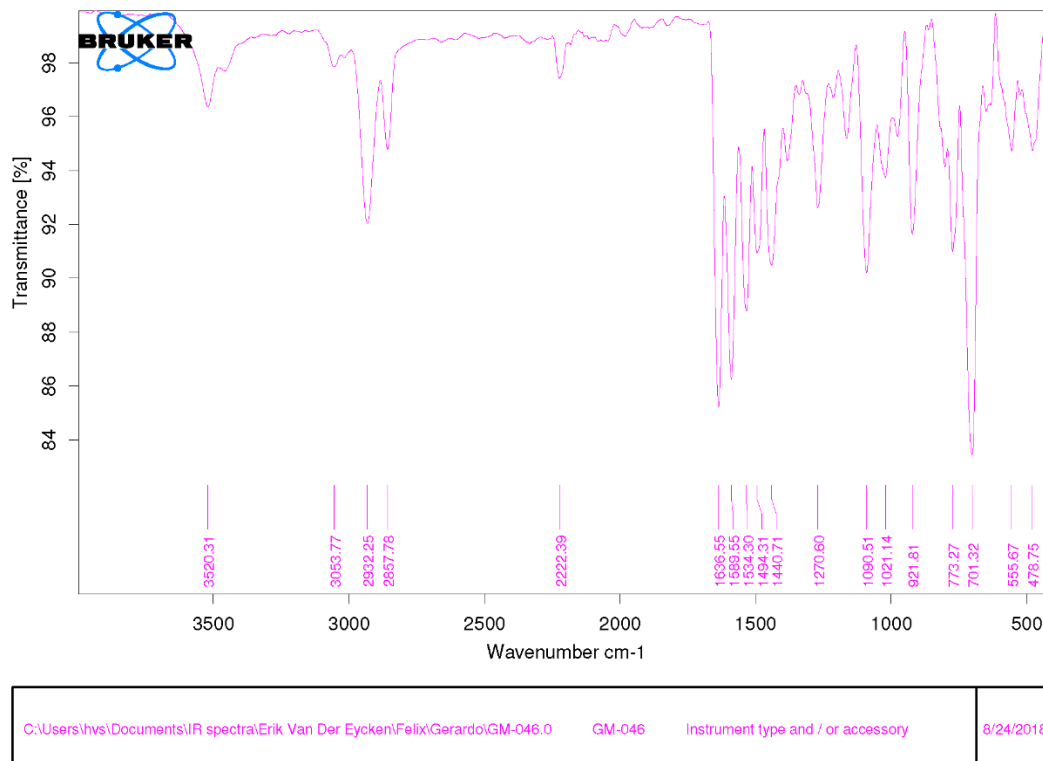


Figure S157. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **5b**.

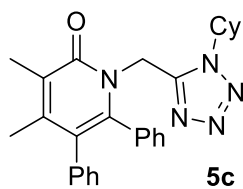


1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3-methyl-5,6-diphenylpyridin-2(1*H*)-one



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Figure S158. FT-IR (KBr) spectrum of compound **5b**.



1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-dimethyl-
5,6-diphenylpyridin-2(1*H*)-one

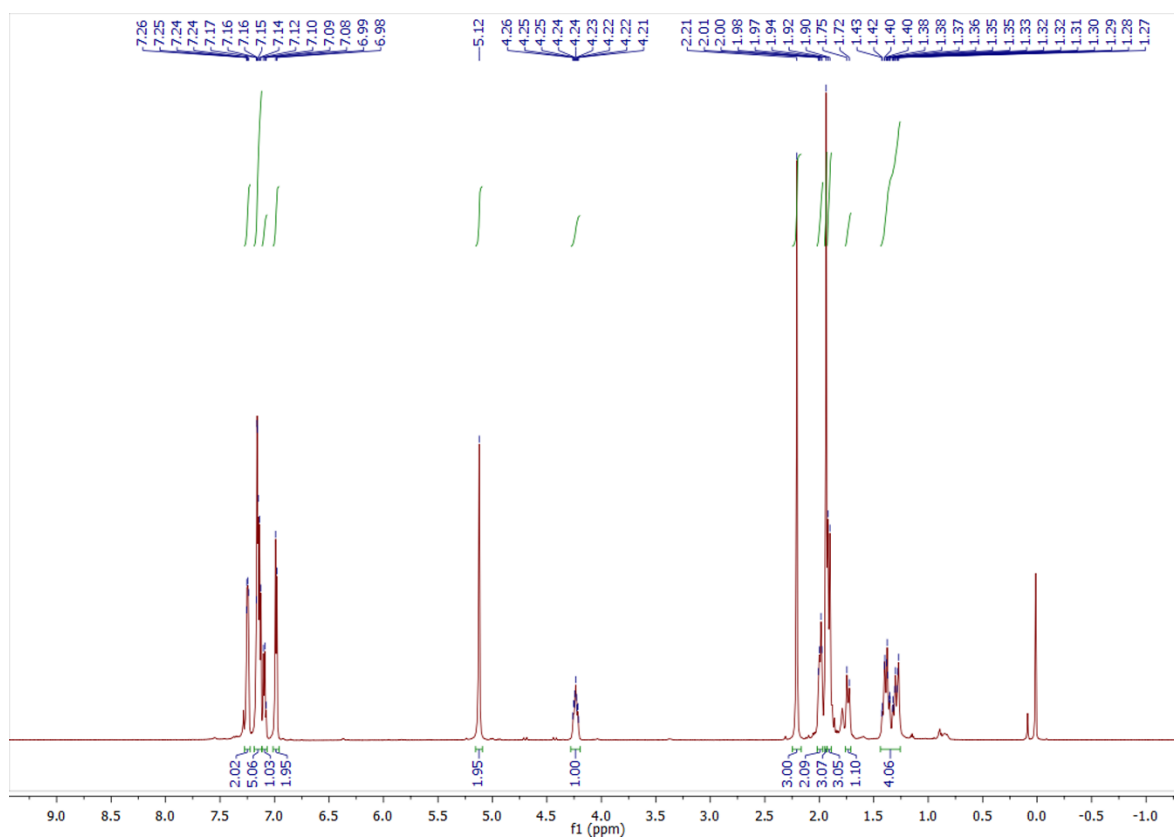
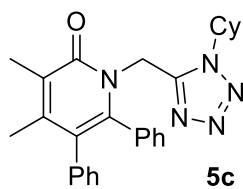


Figure S159. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **5c**.



1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-dimethyl-5,6-diphenylpyridin-2(1*H*)-one

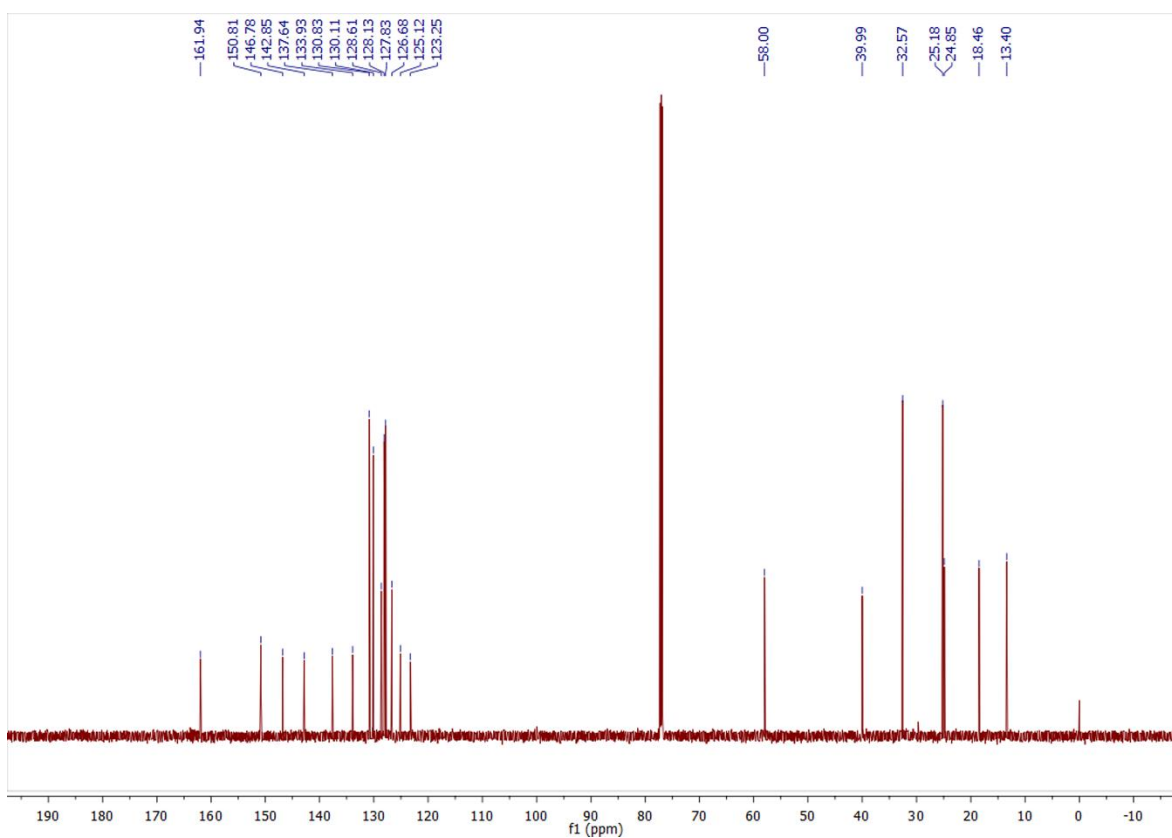
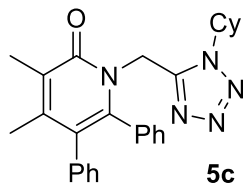
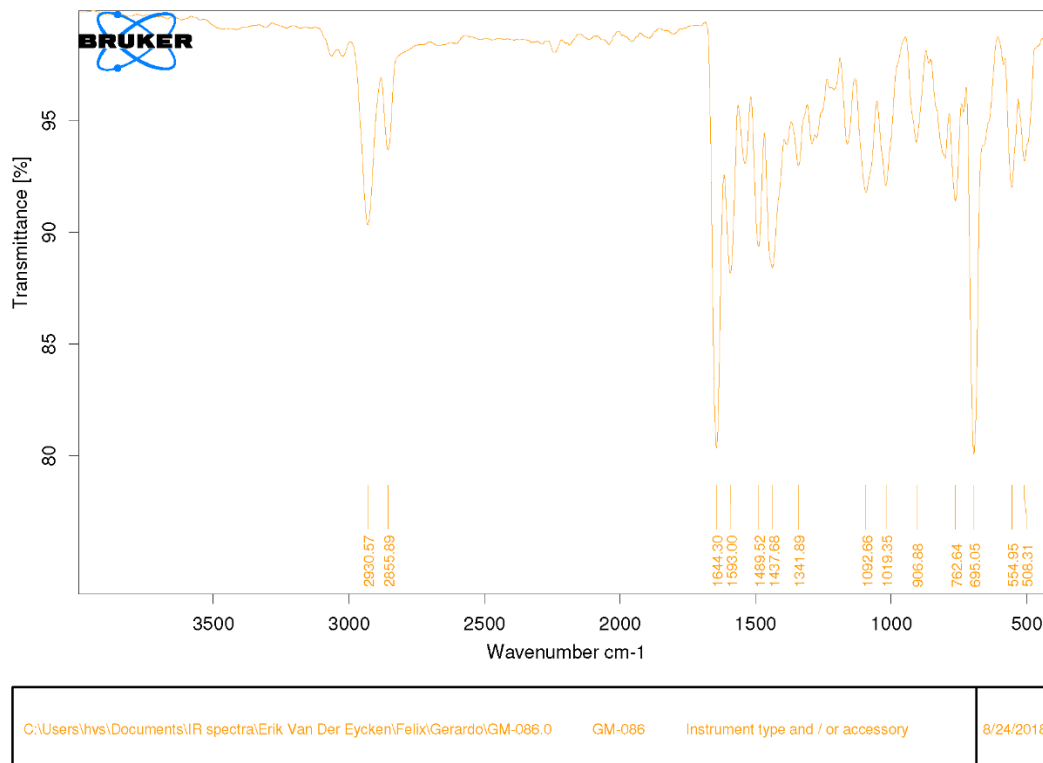


Figure S160. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **5c**.

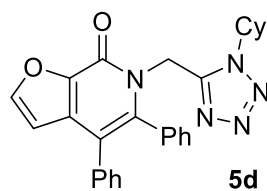


1-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-dimethyl-5,6-diphenylpyridin-2(1*H*)-one



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Figure S161. FT-IR (KBr) spectrum of compound **5c**.



6-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
4,5-diphenylfuro[2,3-*c*]pyridin-7(6*H*)-one

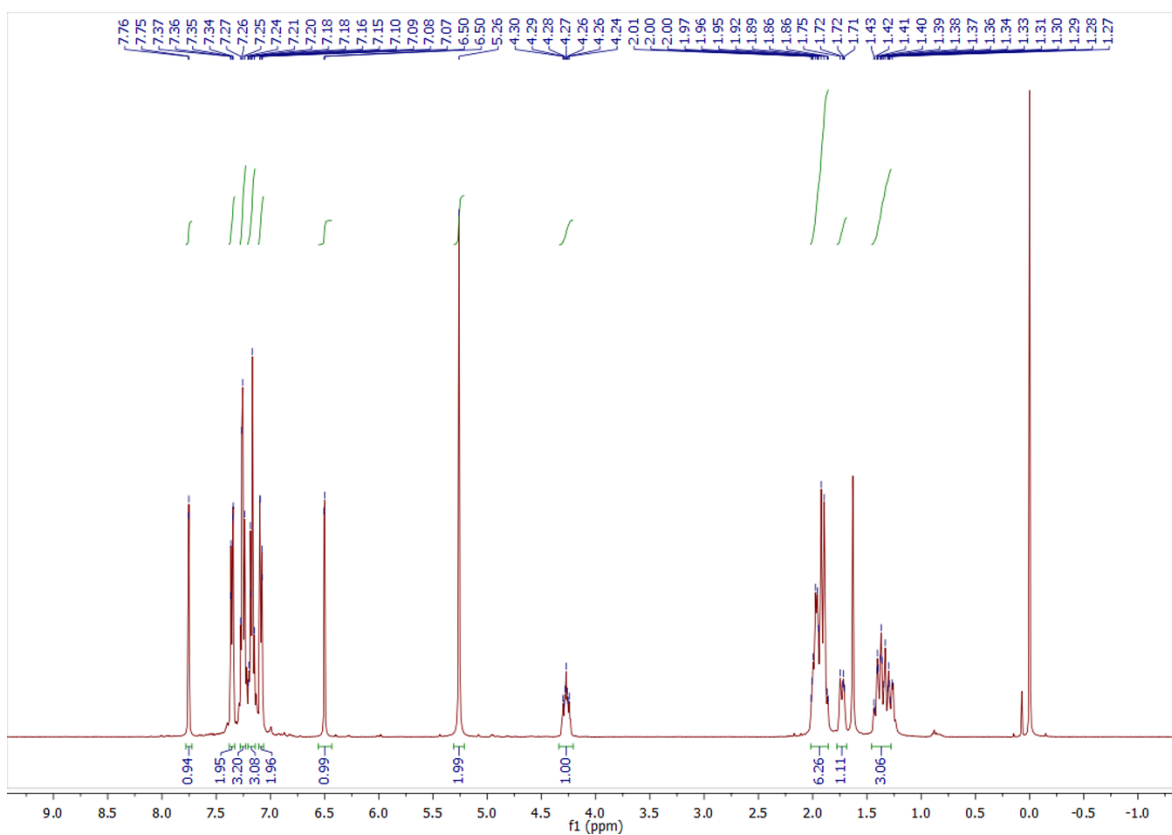
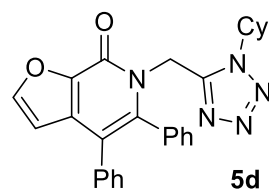


Figure S162. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **5d**.



6-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
4,5-diphenylfuro[2,3-*c*]pyridin-7(6*H*)-one

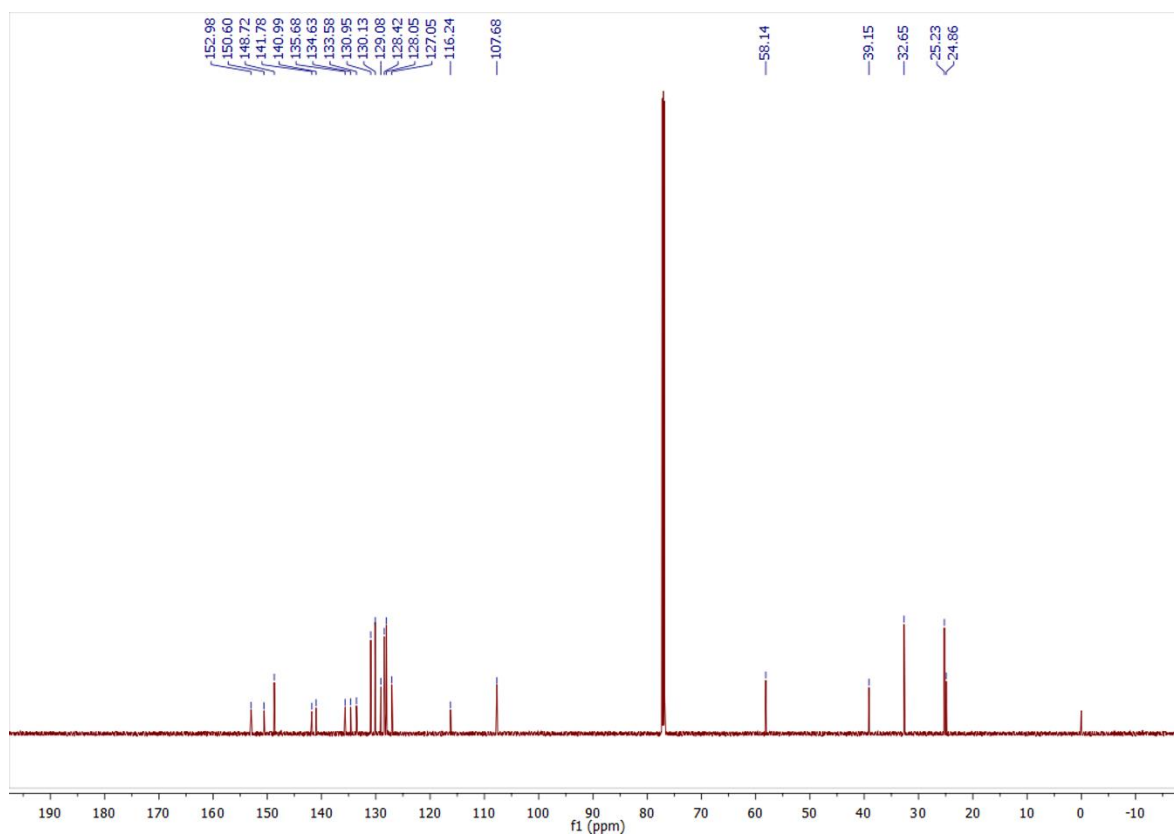
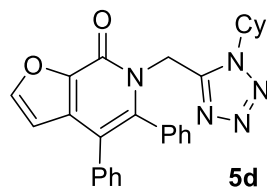
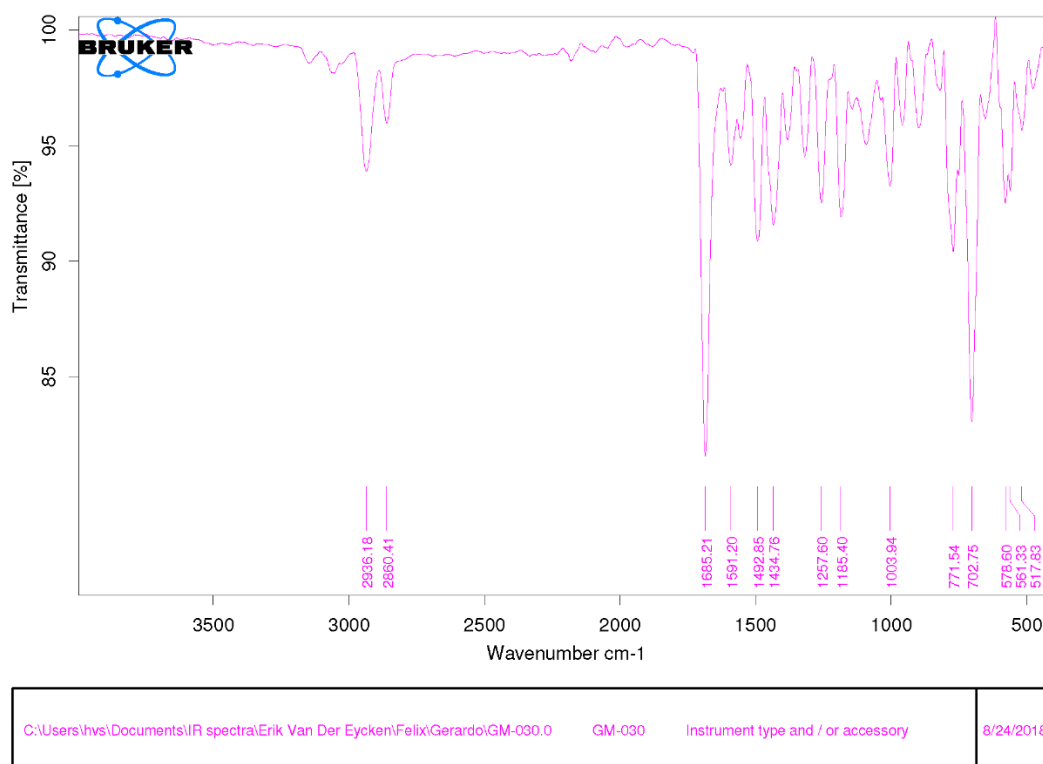


Figure S163. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **5d**.

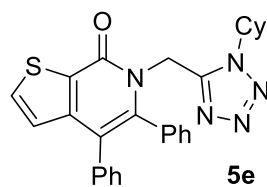


6-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
4,5-diphenylfuro[2,3-*c*]pyridin-7(6*H*)-one



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Figure S164. FT-IR (KBr) spectrum of compound **5d**.



6-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-
4,5-diphenylthieno[2,3-c]pyridin-7(6H)-one

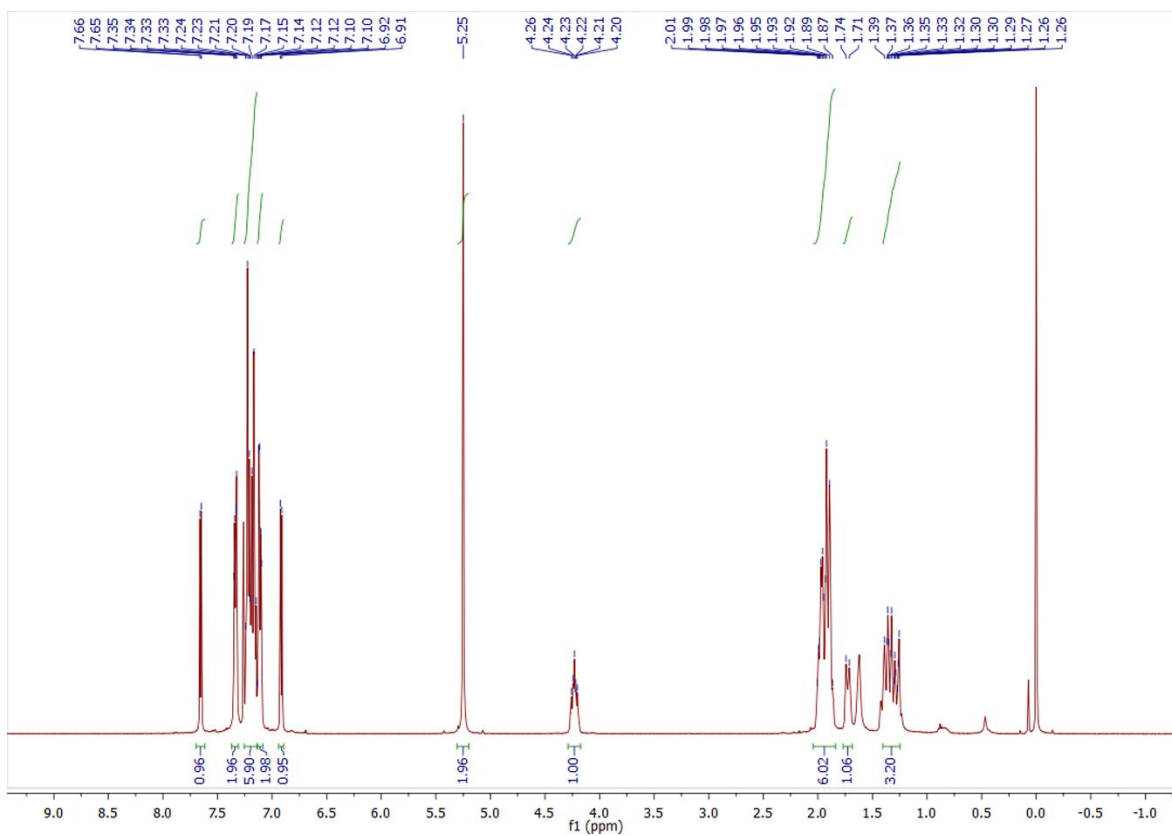
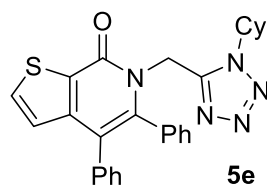


Figure S165. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **5e**.



6-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-
4,5-diphenylthieno[2,3-c]pyridin-7(6H)-one

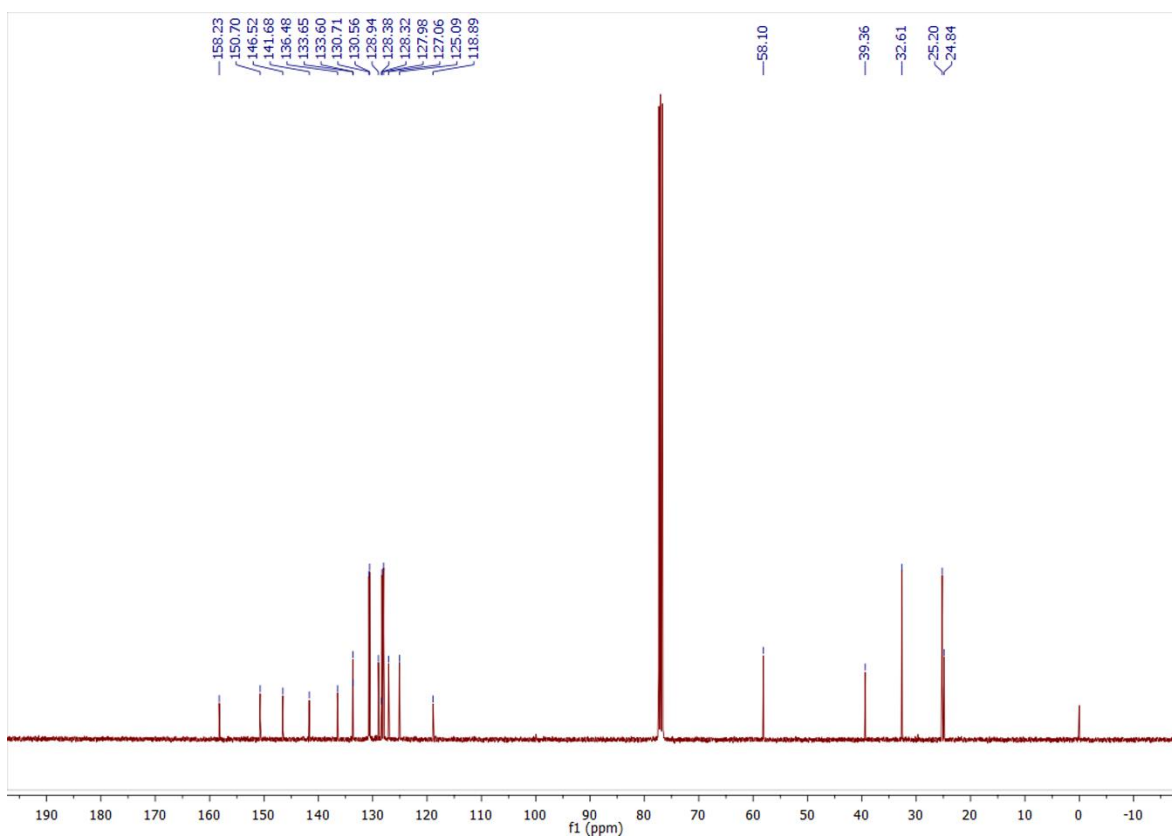
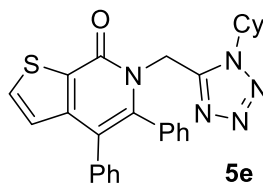
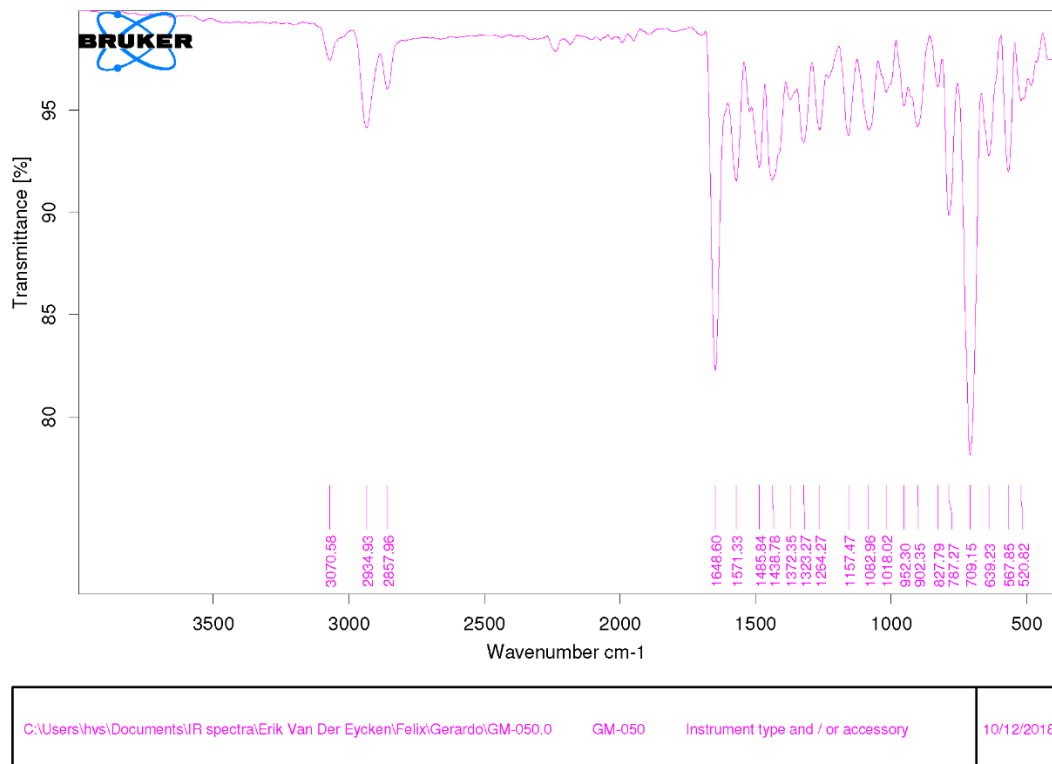


Figure S166. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **5e**.

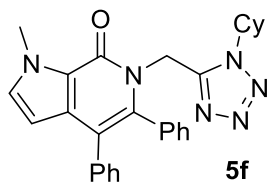


6-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
4,5-diphenylthieno[2,3-*c*]pyridin-7(6*H*)-one



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Figure S167. FT-IR (KBr) spectrum of compound **5e**.



6-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-methyl-
4,5-diphenyl-1,6-dihydro-7*H*-pyrrolo[2,3-*c*]pyridin-7-one

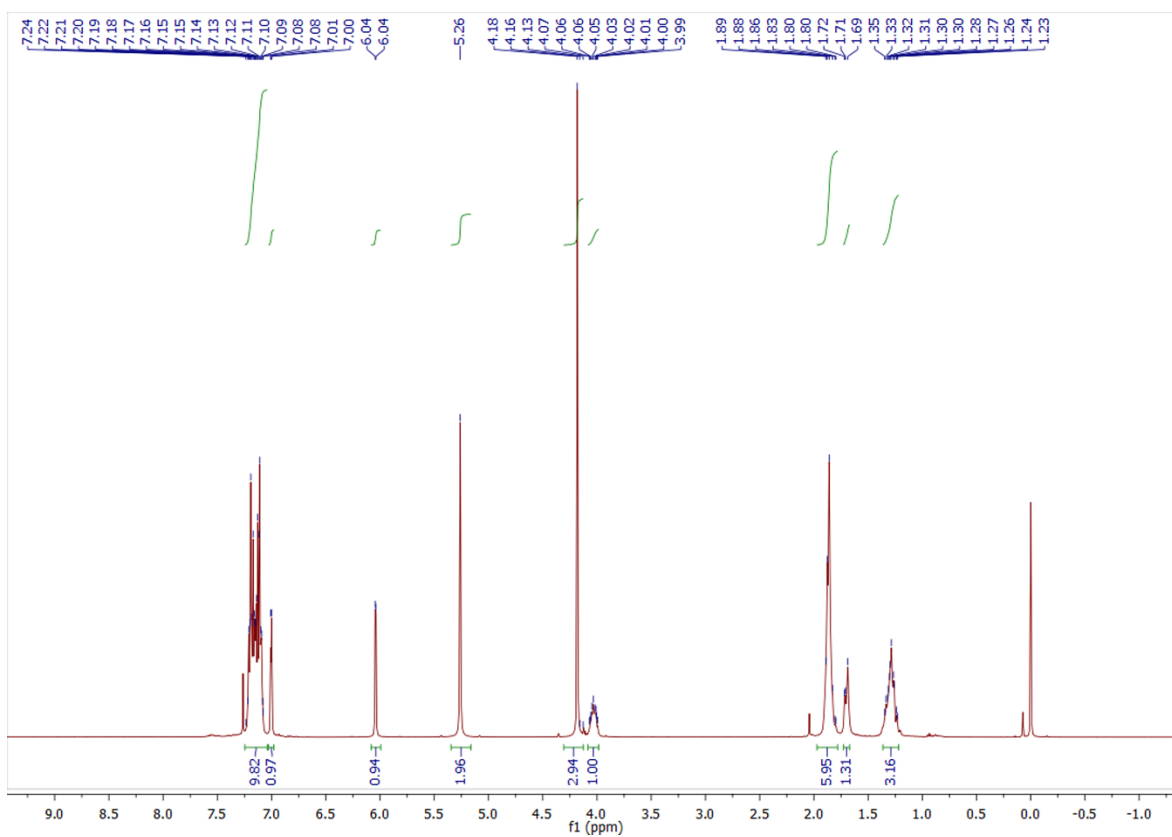
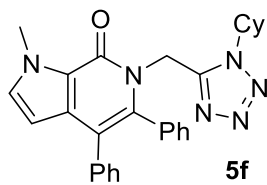


Figure S168. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **5f**.



6-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-1-methyl-4,5-diphenyl-1,6-dihydro-7*H*-pyrrolo[2,3-*c*]pyridin-7-one

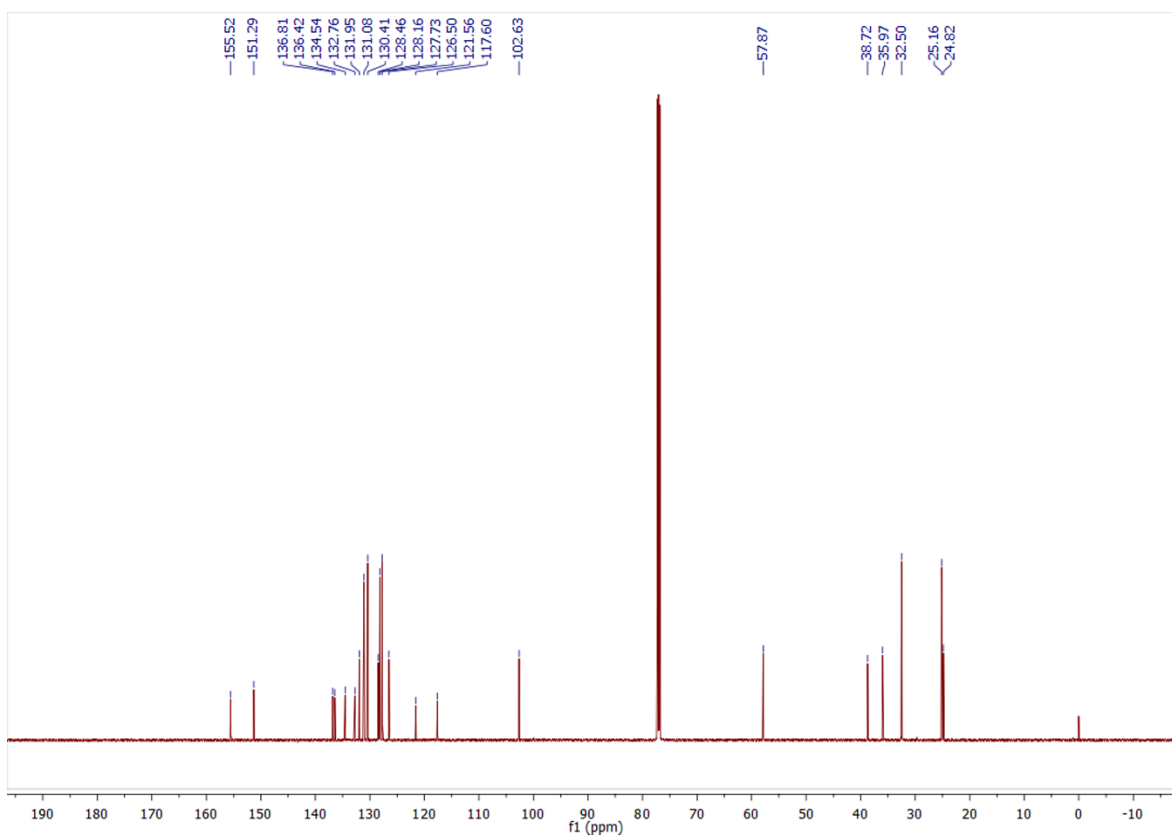
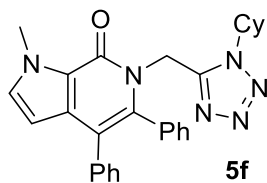
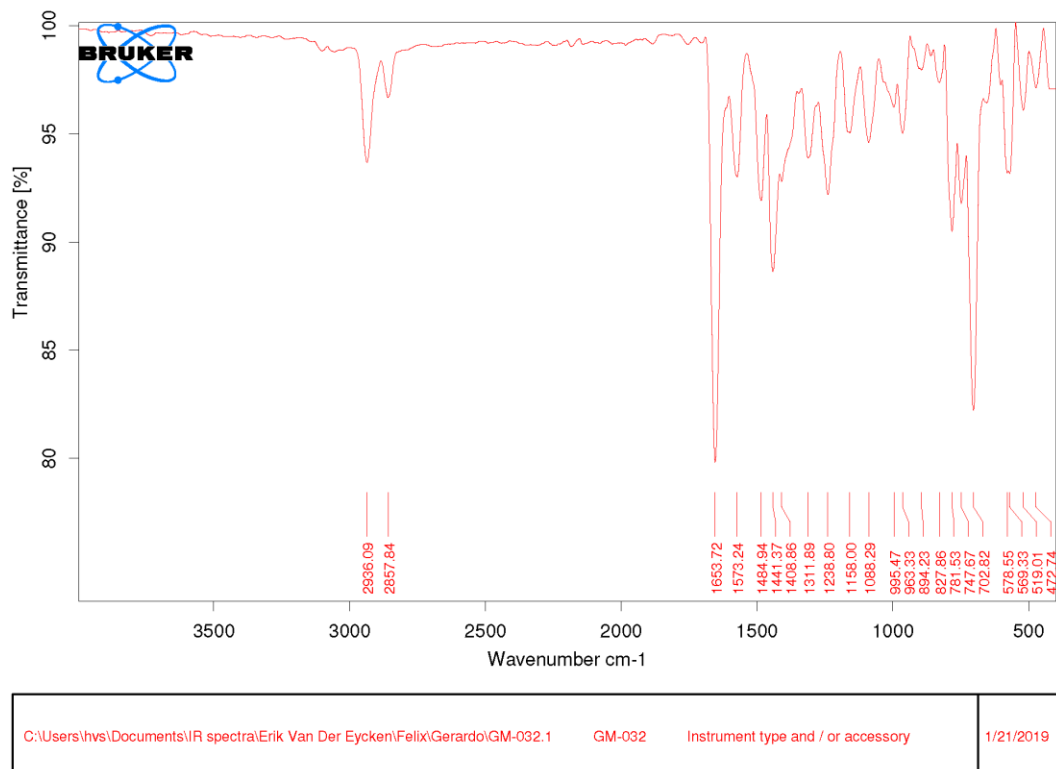


Figure S169. ^{13}C { ^1H } NMR (151 MHz, CDCl_3) spectrum of compound **5f**.

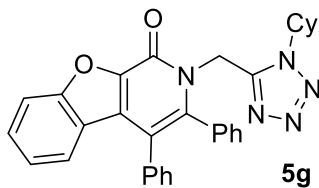


6-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-1-methyl-4,5-diphenyl-1,6-dihydro-7H-pyrrolo[2,3-c]pyridin-7-one



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Figure S170. FT-IR (KBr) spectrum of compound **5f**.



2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-
3,4-diphenylbenzofuro[2,3-c]pyridin-1(2H)-one

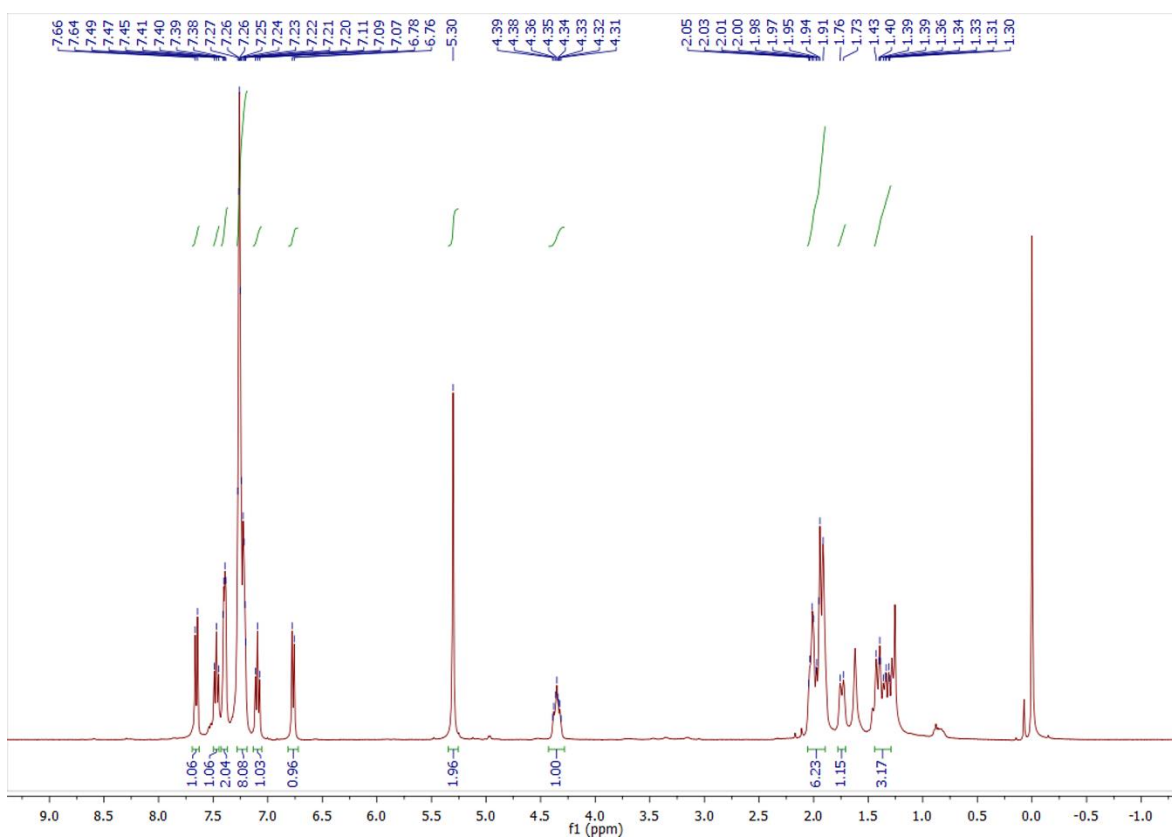
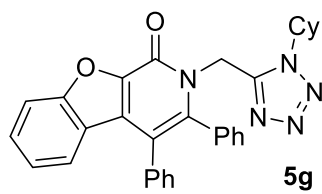


Figure S171. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **5g**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylbenzofuro[2,3-*c*]pyridin-1(2*H*)-one

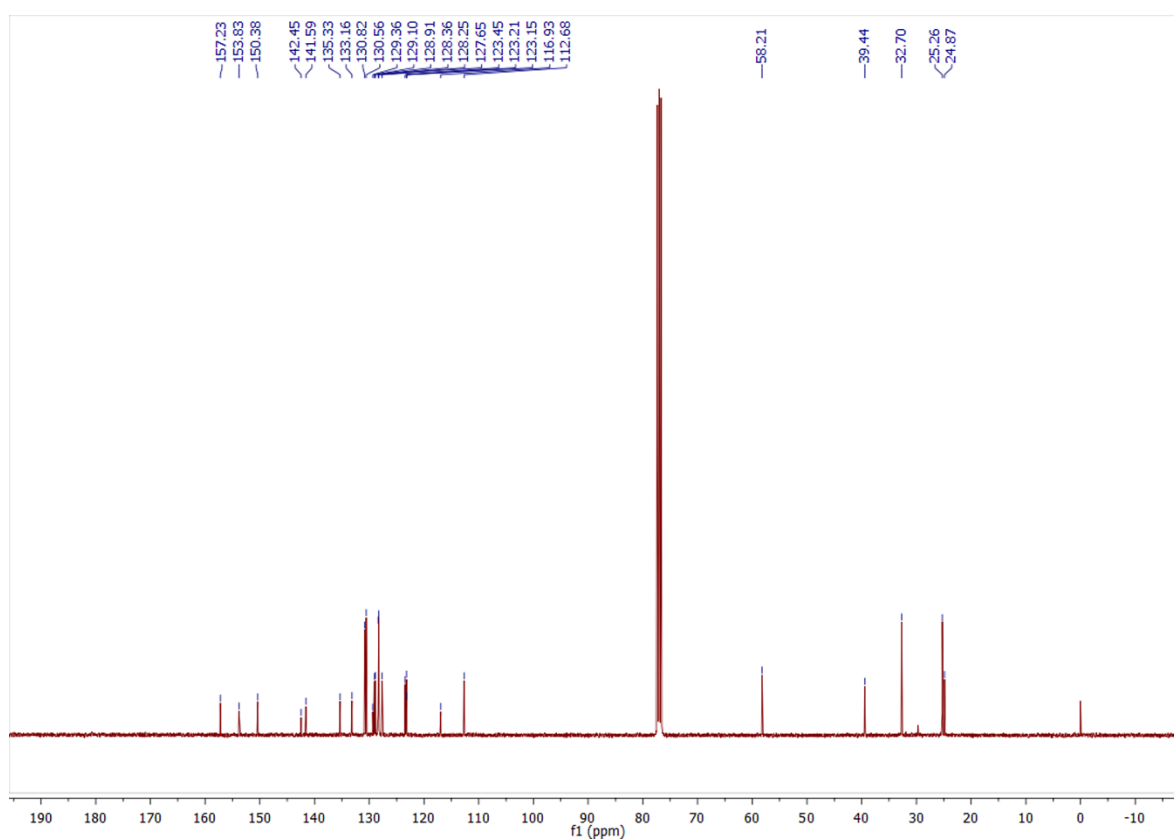
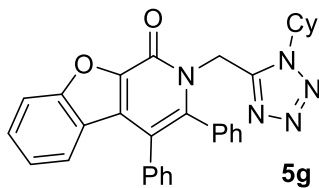
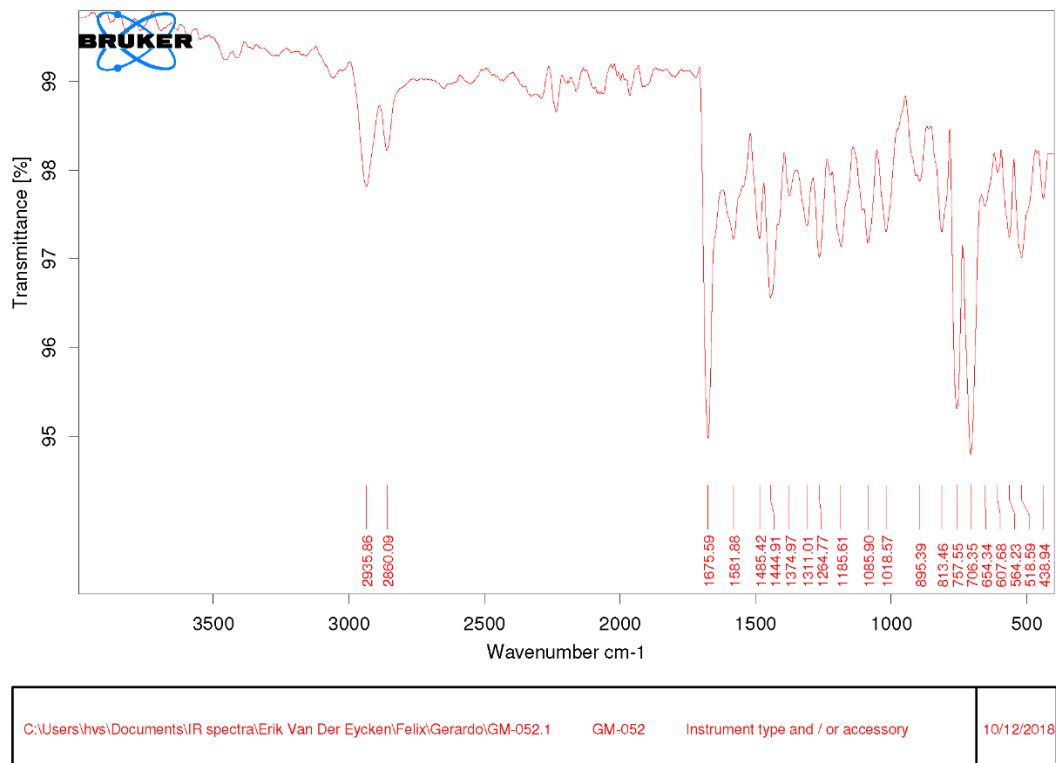


Figure S172. ^{13}C $\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) spectrum of compound **5g**.

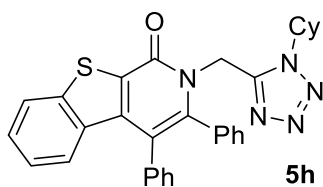


2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylbenzofuro[2,3-*c*]pyridin-1(2*H*)-one



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Figure S173. FT-IR (KBr) spectrum of compound **5g**.



2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-
3,4-diphenylbenzo[4,5]thieno[2,3-c]pyridin-1(2H)-one

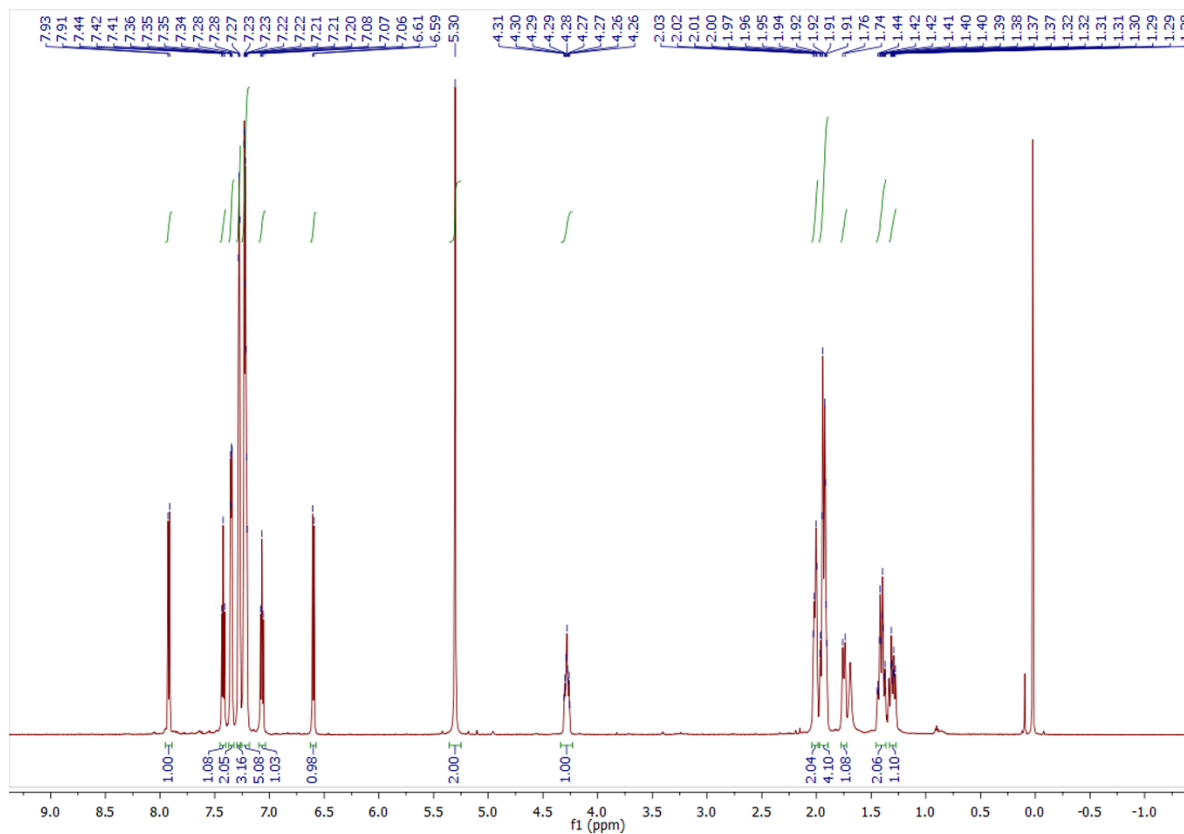
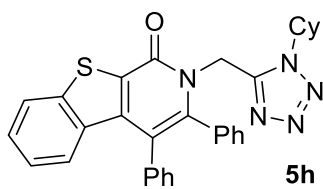


Figure S174. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **5h**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylbenzo[4,5]thieno[2,3-*c*]pyridin-1(2*H*)-one

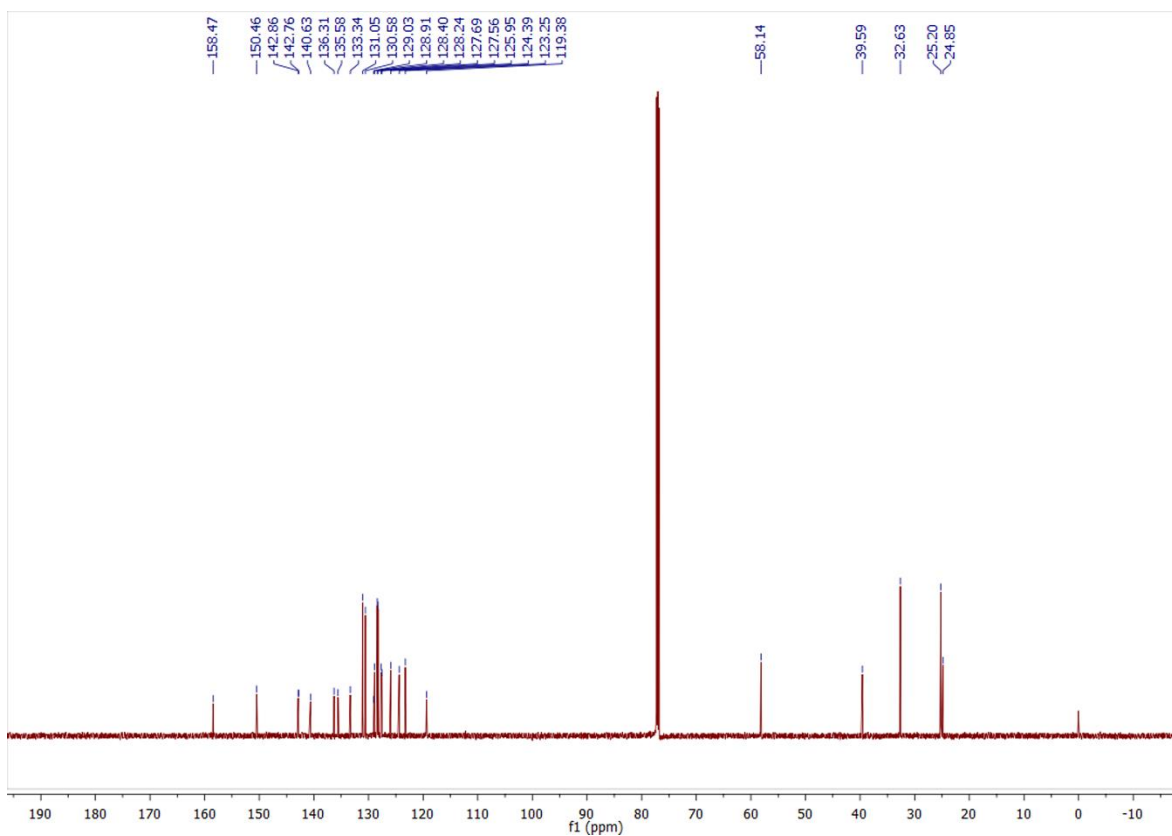
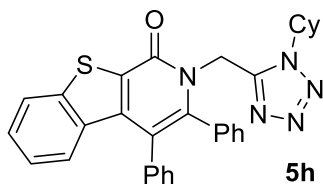


Figure S175. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **5h**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylbenzo[4,5]thieno[2,3-*c*]pyridin-1(2*H*)-one

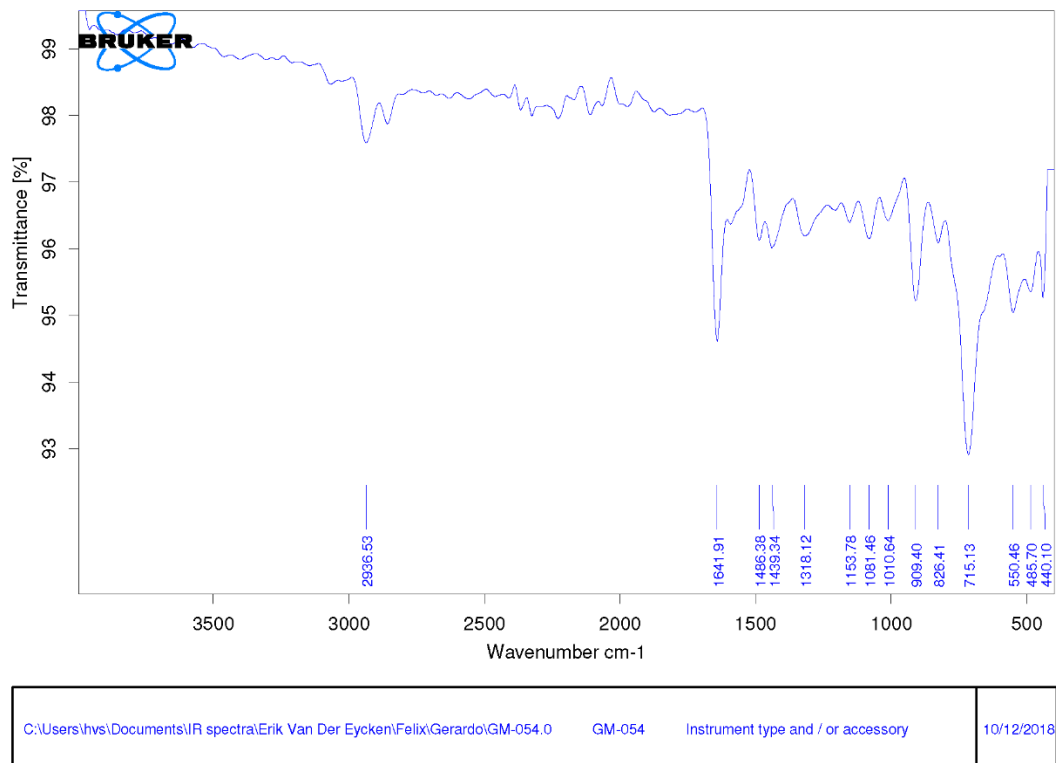
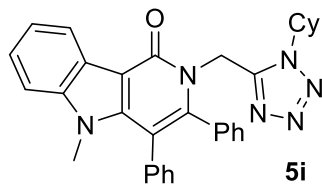


Figure S176. FT-IR (KBr) spectrum of compound **5h**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-5-methyl-3,4-diphenyl-2,5-dihydro-1*H*-pyrido[4,3-*b*]indol-1-one

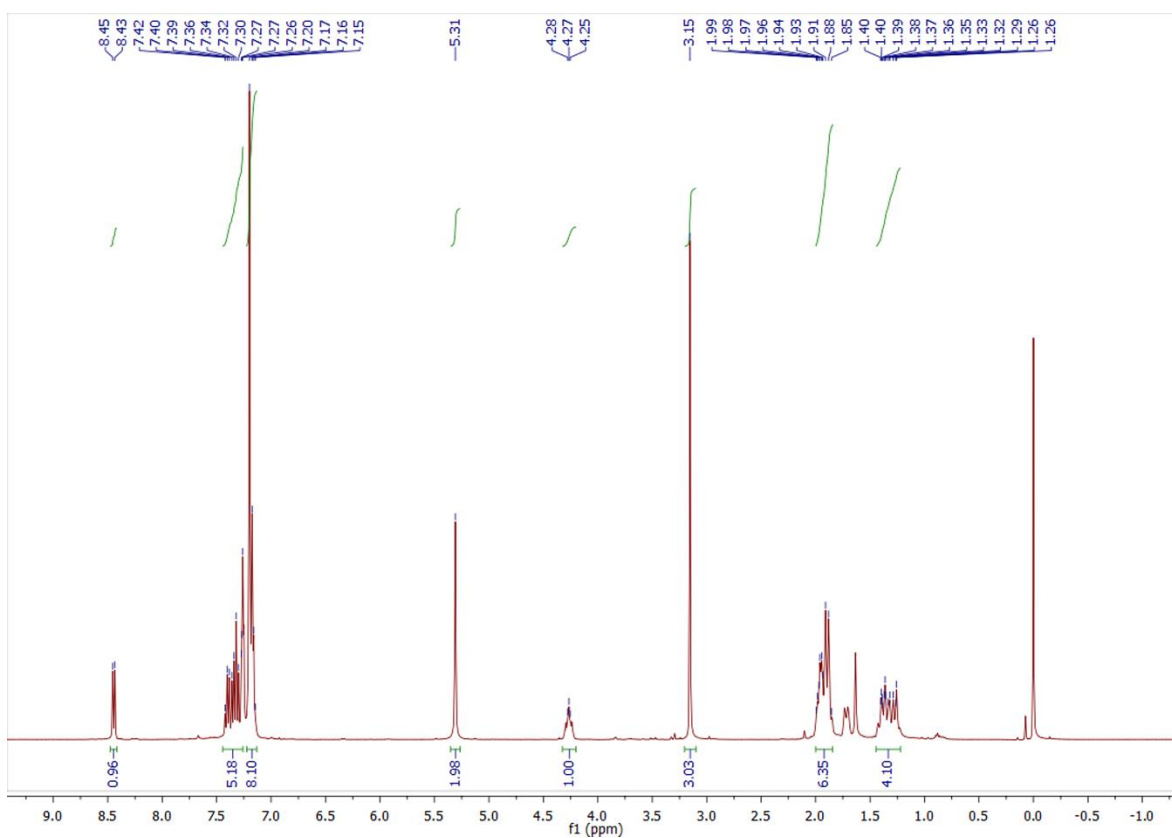
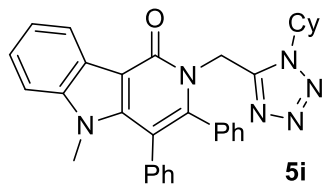


Figure S177. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **5i**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-5-methyl-3,4-diphenyl-2,5-dihydro-1*H*-pyrido[4,3-*b*]indol-1-one

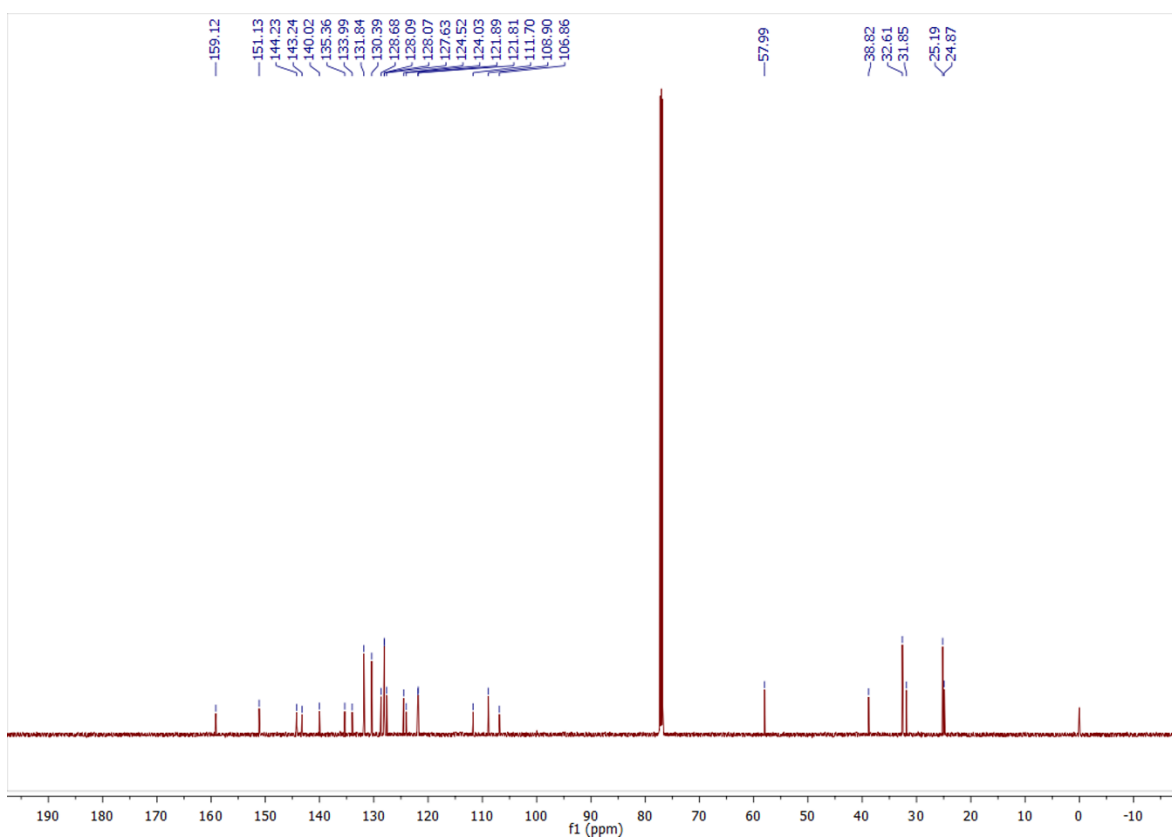
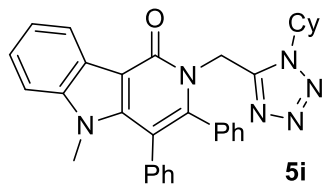
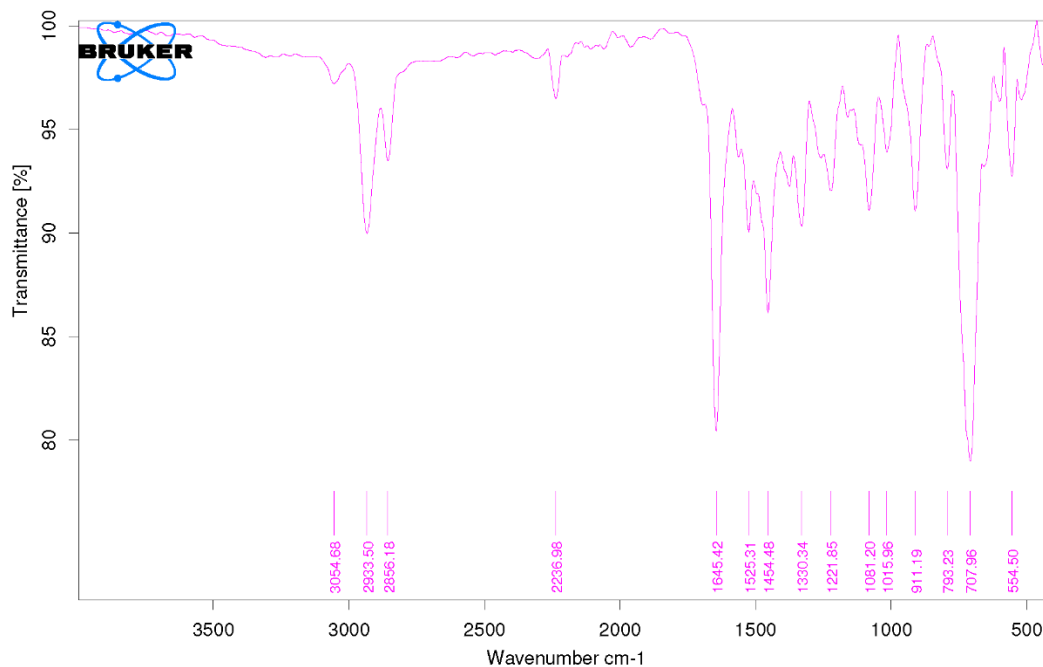


Figure S178. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **5i**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-5-methyl-3,4-diphenyl-2,5-dihydro-1*H*-pyrido[4,3-*b*]indol-1-one



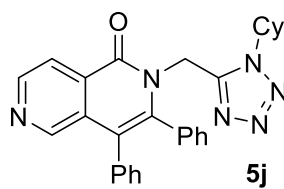
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GM-028

Instrument type and / or accessory

8/24/2018

Figure S179. FT-IR (KBr) spectrum of compound **5i**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenyl-2,6-naphthyridin-1(2*H*)-one

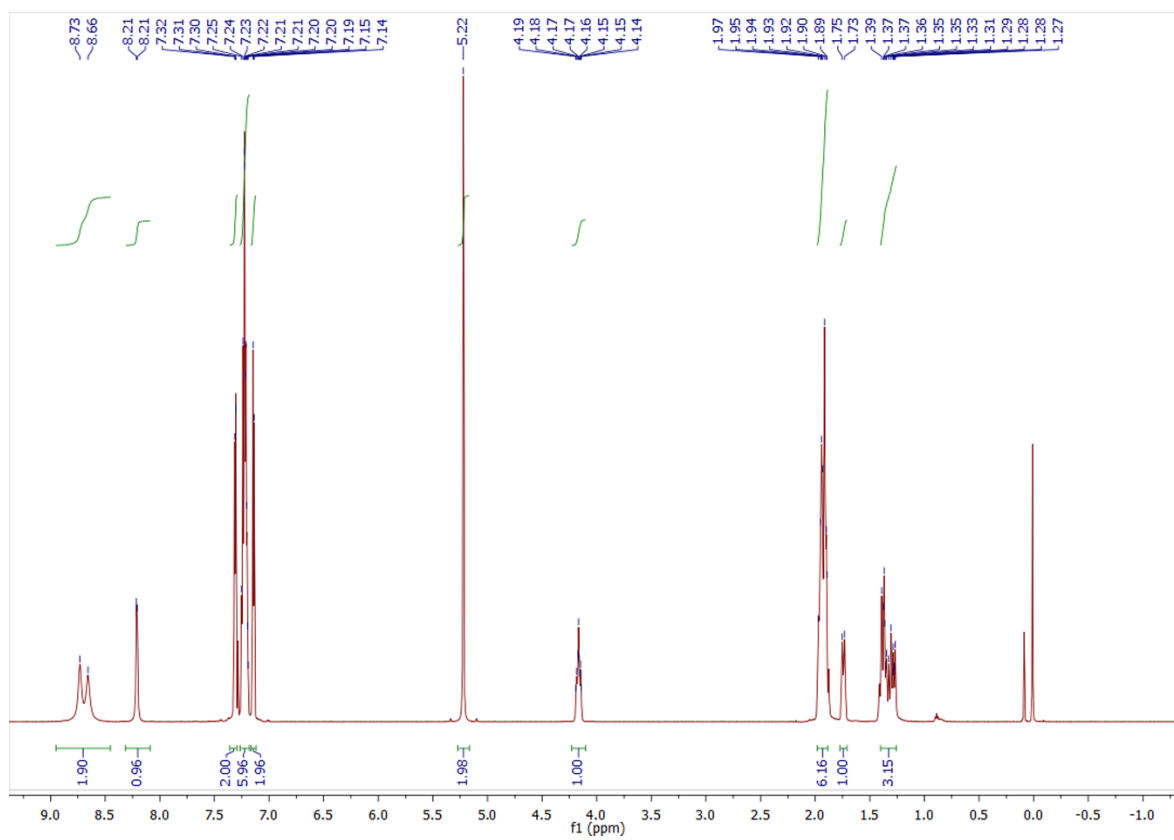
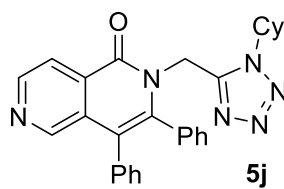


Figure S180. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **5j**.



2-((1-cyclohexyl-1H-tetrazol-5-yl)methyl)-3,4-diphenyl-2,6-naphthyridin-1(2H)-one

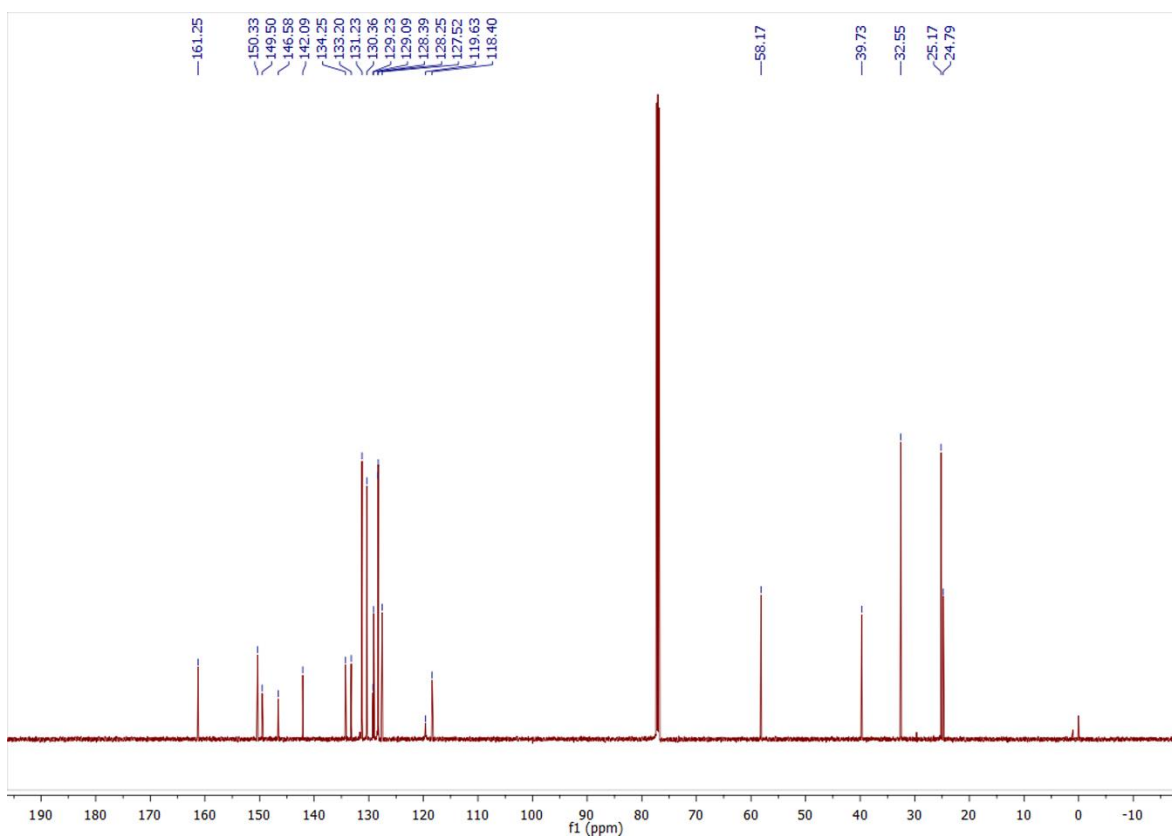
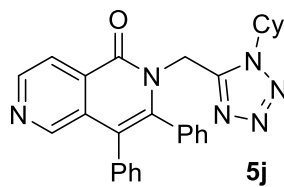
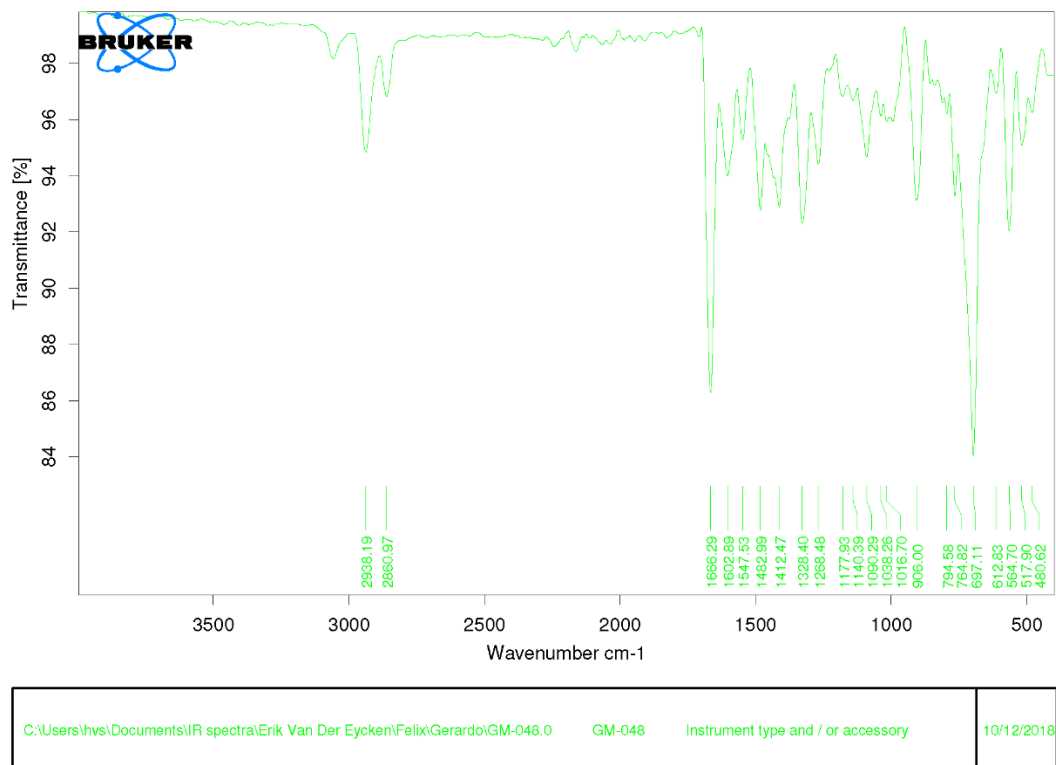


Figure S181. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **5j**.

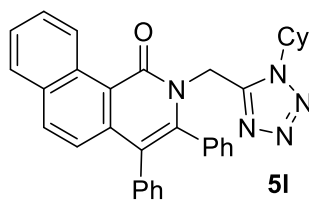


2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-3,4-diphenyl-2,6-naphthyridin-1(2*H*)-one



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Figure S182. FT-IR (KBr) spectrum of compound **5j**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylbenzo[*h*]isoquinolin-1(2*H*)-one

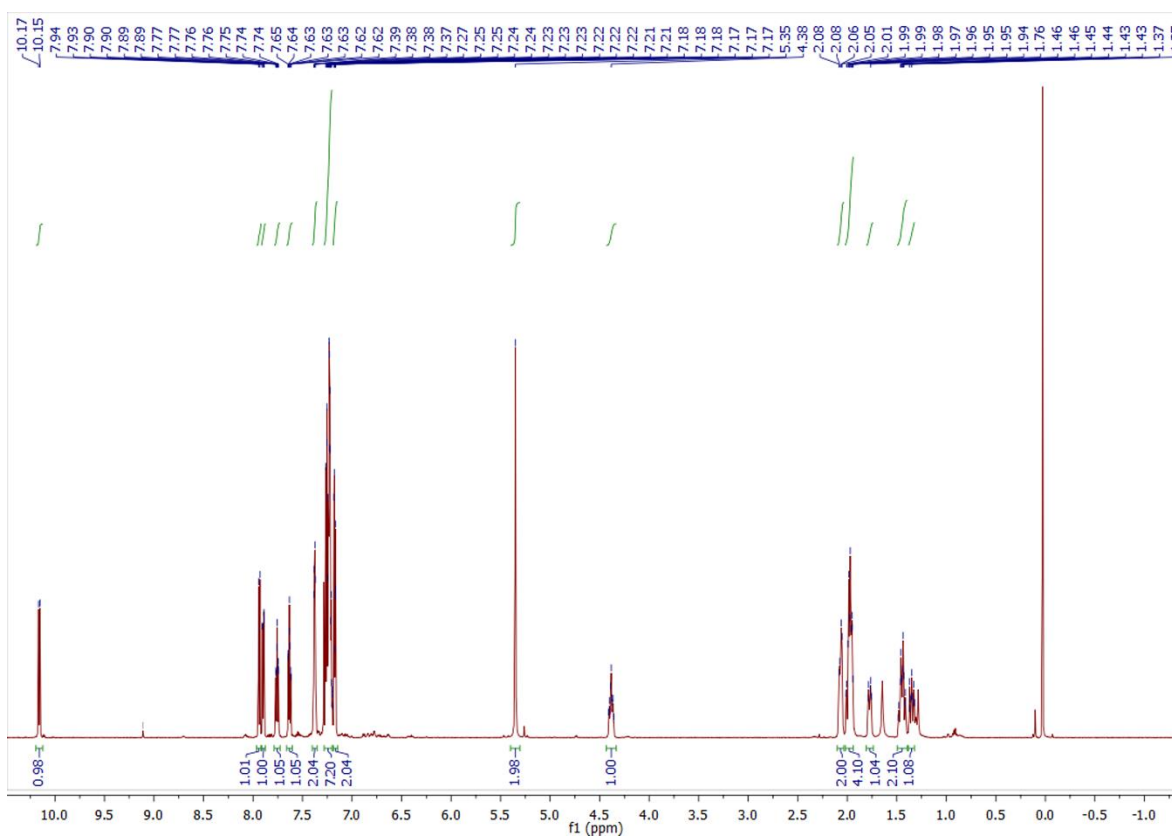
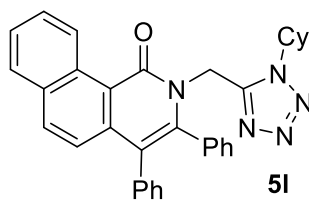


Figure S183. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **5l**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylbenzo[*h*]isoquinolin-1(2*H*)-one

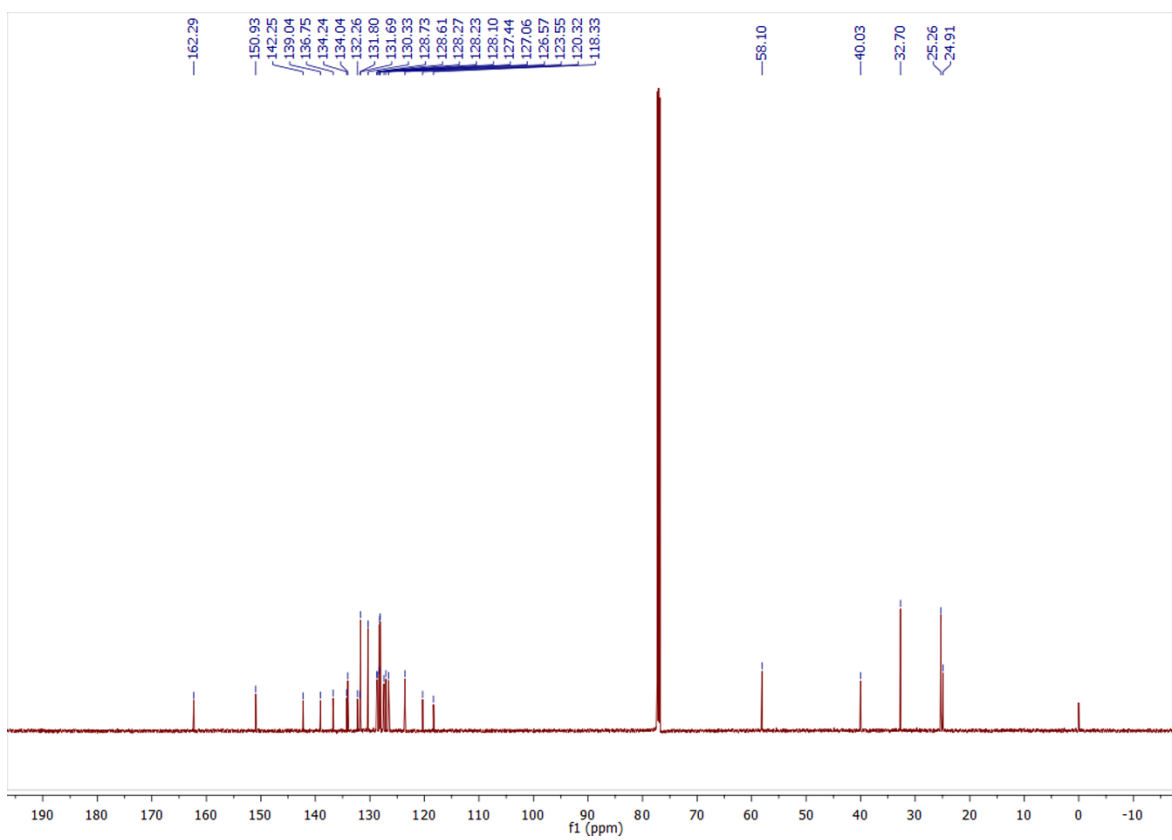
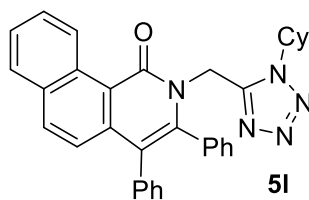
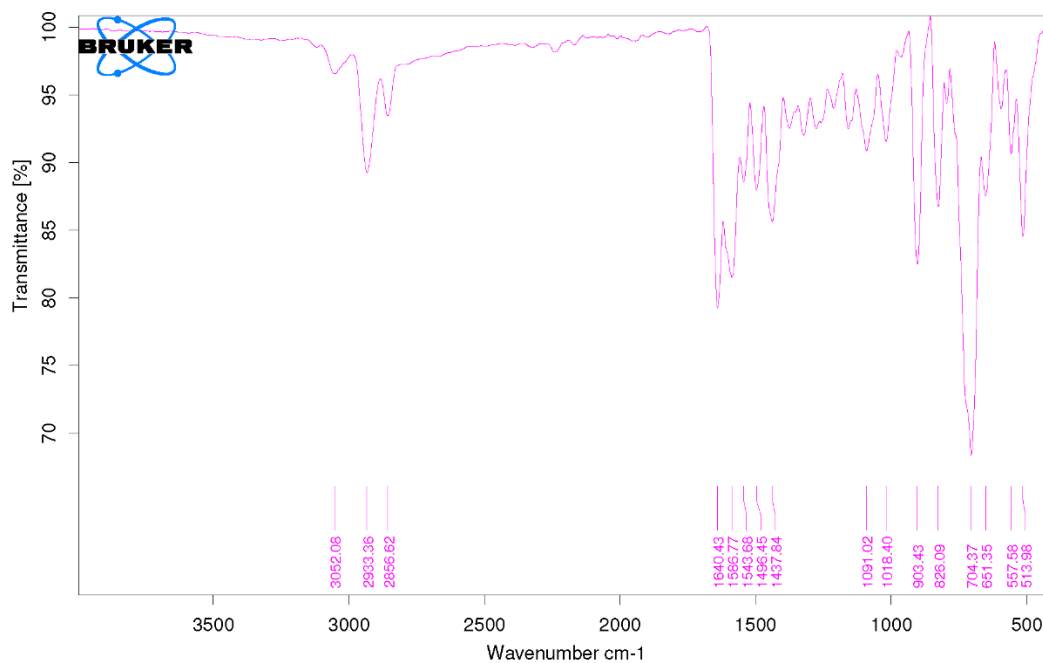


Figure S184. ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, CDCl_3) spectrum of compound **5I**.



2-((1-cyclohexyl-1*H*-tetrazol-5-yl)methyl)-
3,4-diphenylbenzo[*h*]isoquinolin-1(2*H*)-one



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GM-056

Instrument type and / or accessory

8/24/2018

Figure S185. FT-IR (KBr) spectrum of compound **5I**.