

Supporting Information

Copper-catalyzed C5-selective thio/selenocyanation of 8-aminoquinolines

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Materials and Methods

1. General

All reactions were carried out in oven-dried glassware. Melting points (m.p.) were taken on an XT-4 micro melting point apparatus and uncorrected. IR spectra were recorded in KBr on a Nicolet Impact 410 grating infrared spectrophotometer (ν_{\max} in cm^{-1}). ^1H NMR and ^{13}C NMR spectra were recorded on Bruker-300 spectrometers, and were referenced to the residual peaks of CDCl_3 at 7.26 ppm or $\text{DMSO}-d_6$ at 2.50 ppm (^1H NMR) and CDCl_3 at 77.0 ppm or $\text{DMSO}-d_6$ at 39.5 ppm (^{13}C NMR). Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, brs = broad singlet, m = multiplet), coupling constant (Hz), and integration. High Resolution Mass measurement was performed on Agilent QTOF 6520 mass spectrometer with electron spray ionization (ESI) as the ion source. Flash column chromatography was carried out using commercially available 200-300 mesh under pressure.

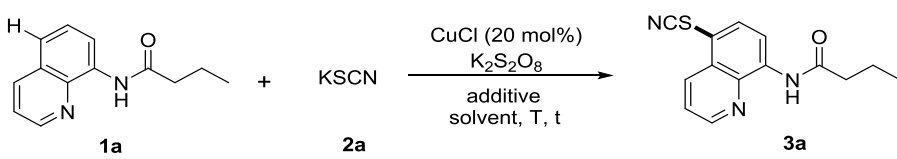
2. Materials

Unless otherwise indicated, all reagents were obtained from commercial suppliers used without further purification. PE refers to petroleum ether (b.p. 60-90 °C) and EA refers to ethyl acetate, and all reaction solvents were freshly distilled prior to use.

Preparation of Substrates

All substrates were synthesized according to the literature procedures and the ^1H NMR spectrum data for them showed good agreement with the literature data.¹

Table S1 Optimization of Reaction Conditions^a



Entry	$\text{K}_2\text{S}_2\text{O}_8$ (equiv.)	Solvent	Additive (mol%)	T (°C)	t (h)	Yield ^b (%)
1	$\text{K}_2\text{S}_2\text{O}_8$ (1.0)	DCE	/	120	24	36
2	$\text{K}_2\text{S}_2\text{O}_8$ (1.5)	DCE	/	120	24	54
3	$\text{K}_2\text{S}_2\text{O}_8$ (2.0)	DCE	/	120	24	65
4	$\text{K}_2\text{S}_2\text{O}_8$ (3.0)	DCE	/	120	24	64
5	$\text{K}_2\text{S}_2\text{O}_8$ (2.0)	CHCl_3	/	120	24	58
6	$\text{K}_2\text{S}_2\text{O}_8$ (2.0)	THF	/	120	24	0

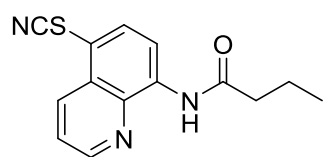
7	K ₂ S ₂ O ₈ (2.0)	CH ₃ CN	/	120	24	0
8	K ₂ S ₂ O ₈ (2.0)	dioxane	/	120	24	0
9	K ₂ S ₂ O ₈ (2.0)	toluene	/	120	24	trace
10	K ₂ S ₂ O ₈ (2.0)	chlorobenzene	/	120	24	trace
11	K ₂ S ₂ O ₈ (2.0)	DMF	/	120	24	0
12	K ₂ S ₂ O ₈ (2.0)	DMSO	/	120	24	0
13	K ₂ S ₂ O ₈ (2.0)	DCE	TBAI (5)	120	24	61
14	K ₂ S ₂ O ₈ (2.0)	DCE	TBAI (10)	120	24	73
15	K ₂ S ₂ O ₈ (2.0)	DCE	TBAI (20)	120	24	56
16	K ₂ S ₂ O ₈ (2.0)	DCE	TBAI (50)	120	24	34
17	K ₂ S ₂ O ₈ (2.0)	DCE	TBAI (10)	100	24	39
18	K ₂ S ₂ O ₈ (2.0)	DCE	TBAI (10)	140	24	71
19	K ₂ S ₂ O ₈ (2.0)	DCE	TBAI (10)	120	18	55
20	K ₂ S ₂ O ₈ (2.0)	DCE	TBAI (10)	120	36	75

^a Reaction conditions: **1a** (0.2 mmol), **2a** (0.4 mmol), CuCl (20 mol%), K₂S₂O₈, TBAI, solvent (2 mL). Isolated yield.

General Procedure for thio/selenocyanation of Quinolines

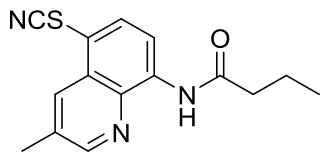
To a 15 mL sealed tube with a magnetic stirring bar were added aminoquinolines derivatives (**1**, 0.2 mmol), KSCN/SeCN (**2**, 0.4 mmol), CuCl (20 mol%), K₂S₂O₈ (0.4 mmol), TBAI (10 mol%) and DCE (2 mL). The reaction mixture was placed in an oil bath at 120 °C and vigorously stirred for 24 h. Afterward it was cooled to ambient temperature, filtered through a pad of celite and then washed with CH₂Cl₂ (3 × 5 mL). The solvents were removed under reduced pressure and the crude reaction mixture was purified by flash chromatography using *PE/EA* = 30:1 ~ 15:1 as an eluent to obtain the desired product.

Analytical Data for the Products



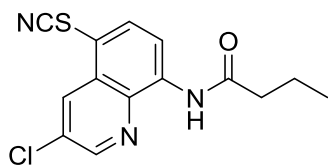
N-(quinolin-5-thiocyanate-8-yl)butanamide (**3a**)

Obtained as a white solid (39.6 mg, 73%); m.p. 99 – 101 °C; IR (KBr), cm⁻¹: 3332, 2960, 2921, 2152, 1691, 1514, 1479, 1451, 1382, 1315, 1178, 1149, 862, 815, 792, 693; ¹H NMR (300 MHz, CDCl₃) δ 9.93 (s, 1H), 8.89 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.81 (d, *J* = 8.3 Hz, 1H), 8.66 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.68 (dd, *J* = 8.5, 4.2 Hz, 1H), 2.57 (t, *J* = 7.5 Hz, 2H), 1.92 – 1.78 (m, 2H), 1.06 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 171.78, 148.62, 138.48, 137.79, 136.01, 133.25, 127.83, 123.09, 115.59, 111.24, 110.42, 39.79, 18.67, 13.56; HRMS (ESI) calculated for C₁₄H₁₄N₃OS [M + H]⁺ 272.0852, found 272.0853.



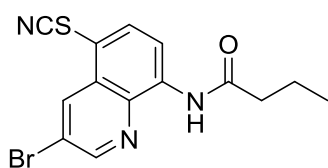
***N*-(3-methylquinolin-5-thiocyanate-8-yl)butanamide (3b)**

Obtained as a white solid (48.5 mg, 85%); m.p. 104 – 106 °C; IR (KBr), cm^{-1} : 3337, 3310, 2962, 2925, 2872, 2849, 2154, 1686, 1565, 1513, 1466, 1369, 1321, 1192, 1172, 880, 855, 764, 750; ^1H NMR (300 MHz, CDCl_3) δ 9.89 (s, 1H), 8.75 (d, $J = 8.3$ Hz, 2H), 8.45 – 8.38 (m, 1H), 7.94 (d, $J = 8.3$ Hz, 1H), 2.64 (s, 3H), 2.56 (t, $J = 7.5$ Hz, 2H), 1.92 – 1.76 (m, 2H), 1.06 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (75 MHz, CDCl_3) δ 171.89, 150.58, 137.90, 136.95, 136.28, 133.35, 132.12, 127.94, 114.92, 110.69, 110.63, 39.94, 18.89, 18.80, 13.65; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{16}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 286.1009, found 286.1013.



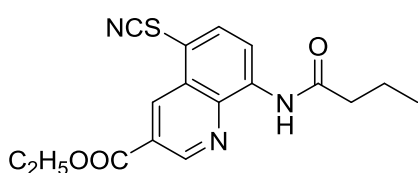
***N*-(3-chloroquinolin-5-thiocyanate-8-yl)butanamide (3c)**

Obtained as a slight yellow solid (38.5 mg, 63%); m.p. 140 – 142 °C. IR (KBr), cm^{-1} : 3314, 2955, 2921, 2851, 2156, 1692, 1560, 1522, 1465, 1364, 1316, 1276, 1261, 1178, 1107, 858, 764, 750; ^1H NMR (300 MHz, CDCl_3) δ 9.76 (s, 1H), 8.84 (d, $J = 8.3$ Hz, 1H), 8.81 (d, $J = 2.2$ Hz, 1H), 8.66 (d, $J = 2.2$ Hz, 1H), 8.03 (d, $J = 8.3$ Hz, 1H), 2.57 (t, $J = 7.5$ Hz, 2H), 1.92 – 1.76 (m, 2H), 1.06 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.95, 148.26, 138.32, 137.90, 136.78, 131.92, 131.61, 128.84, 116.23, 110.07, 40.04, 18.83, 13.67; HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{13}\text{ClN}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 306.0462, found 306.0467.



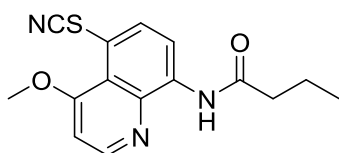
***N*-(3-bromoquinolin-5-thiocyanate-8-yl)butanamide (3d)**

Obtained as a slight yellow solid (42.7 mg, 61%); m.p. 134 – 136 °C; IR (KBr), cm^{-1} : 3316, 2958, 2924, 2851, 2156, 1692, 1655, 1557, 1523, 1460, 1385, 1314, 1178, 1101, 967, 895, 869, 843, 719, 637; ^1H NMR (300 MHz, CDCl_3) δ 9.75 (s, 1H), 8.89 (d, $J = 2.1$ Hz, 1H), 8.86 (d, $J = 8.3$ Hz, 1H), 8.82 (d, $J = 2.1$ Hz, 1H), 8.02 (d, $J = 8.3$ Hz, 1H), 2.57 (t, $J = 7.5$ Hz, 2H), 1.92 – 1.77 (m, 2H), 1.06 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.96, 150.00, 138.28, 137.75, 136.80, 135.01, 129.23, 120.26, 116.24, 110.46, 110.10, 39.95, 18.77, 13.66; HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{12}\text{BrN}_3\text{NaOS}$ $[\text{M}+\text{Na}]^+$ 371.9777, found 371.9786.



***N*-(3-ethoxycarbonyl-5-thiocyanate-8-yl)butanamide (3e)**

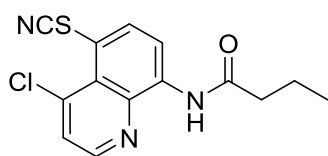
Obtained as a white solid (33.0 mg, 48%); m.p. 160 – 162 °C; IR (KBr), cm^{-1} : 3333, 2959, 2924, 2867, 2837, 2155, 1717, 1693, 1607, 1521, 1471, 1400, 1388, 1320, 1278, 1234, 1175, 1112, 1020, 860, 767, 750, 708; ^1H NMR (300 MHz, CDCl_3) δ 9.88 (s, 1H), 9.42 (d, $J = 1.8$ Hz, 1H), 9.28 (d, $J = 1.8$ Hz, 1H), 8.94 (d, $J = 8.3$ Hz, 1H), 8.06 (d, $J = 8.3$ Hz, 1H), 4.54 (q, $J = 7.1$ Hz, 2H), 2.58 (t, $J = 7.4$ Hz, 2H), 1.92 – 1.80 (m, 2H), 1.50 (t, $J = 7.1$ Hz, 3H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.11, 164.44, 148.84, 140.38, 138.16, 137.21, 135.77, 127.25, 125.60, 117.97, 113.03, 110.20, 62.13, 40.10, 18.88, 14.31, 13.72; HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{17}\text{NaN}_3\text{O}_3\text{S}$ $[\text{M}+\text{Na}]^+$ 366.0883, found 366.0898.



***N*-(4-methoxyquinolin-5-thiocyanate-8-yl)butanamide (3g)**

Obtained as a white solid (47.0 mg, 78%); m.p. 168 – 170 °C; IR (KBr), cm^{-1} : 3333, 2964, 2920, 2849, 2152, 1683, 1596, 1530, 1485, 1455, 1371, 1322, 1179, 1035, 967, 820, 692; ^1H NMR (300

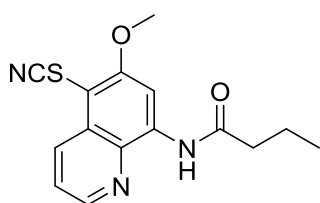
MHz, CDCl₃) δ 9.80 (s, 1H), 8.80 (d, J = 8.6 Hz, 1H), 8.66 (d, J = 5.2 Hz, 1H), 7.82 (d, J = 8.6 Hz, 1H), 6.84 (d, J = 5.2 Hz, 1H), 4.08 (s, 3H), 2.53 (t, J = 7.5 Hz, 2H), 1.91 – 1.76 (m, 2H), 1.05 (t, J = 7.4 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 171.67, 162.17, 149.62, 140.07, 134.23, 126.23, 118.02, 116.62, 112.91, 111.66, 101.79, 55.87, 40.01, 18.90, 13.73; HRMS (ESI) calculated for C₁₅H₁₆N₃O₂S [M+H]⁺ 302.0958, found 302.0965.



***N*-(4-chloroquinolin-5-thiocyanate-8-yl)butanamide (3h)**

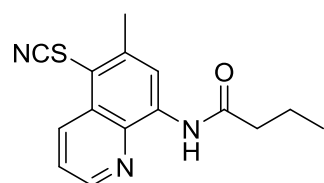
Obtained as a slight yellow solid (43.4 mg, 71%); m.p. 140 – 142 °C; IR (KBr), cm⁻¹: 3336, 3302, 2960, 2926, 2869, 2152, 1692, 1578, 1517, 1478, 1414, 1358, 1316, 1178, 1135, 909, 793, 735, 696; ¹H NMR (300 MHz, CDCl₃) δ 9.90 (s, 1H), 8.88 (d, J = 8.5 Hz, 1H),

8.69 (d, J = 4.7 Hz, 1H), 8.06 (d, J = 8.6 Hz, 1H), 7.63 (d, J = 4.6 Hz, 1H), 2.55 (t, J = 7.5 Hz, 2H), 1.92 – 1.76 (m, 2H), 1.06 (t, J = 7.4 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 171.88, 147.70, 141.40, 140.55, 136.73, 134.56, 125.05, 120.80, 116.85, 112.39, 111.15, 40.08, 18.85, 13.71; HRMS (ESI) calculated for C₁₄H₁₃ClN₃OS [M+H]⁺ 306.0462, found 306.0469.



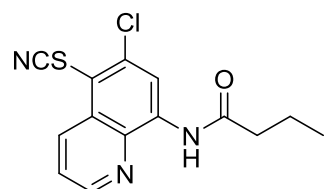
***N*-(6-methoxyquinolin-5-thiocyanate-8-yl)butanamide (3i)**

Obtained as a white solid (53.0 mg, 88%); m.p. 122-124 °C; IR (KBr), cm⁻¹: 3335, 3317, 2964, 2941, 2873, 2156, 1691, 1612, 1587, 1561, 1526, 1459, 1397, 1334, 1205, 1171, 1085, 903, 858, 803, 782, 716; ¹H NMR (300 MHz, CDCl₃) δ 9.99 (s, 1H), 8.86 (s, 1H), 8.71 (dd, J = 4.2, 1.2 Hz, 1H), 8.64 (dd, J = 8.6, 1.2 Hz, 1H), 7.61 (dd, J = 8.6, 4.2 Hz, 1H), 4.14 (s, 3H), 2.59 (t, J = 7.4 Hz, 2H), 1.93 – 1.77 (m, 2H), 1.07 (t, J = 7.4 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 172.30, 160.29, 146.04, 139.43, 134.36, 132.46, 129.59, 123.70, 110.84, 103.14, 94.22, 56.92, 39.94, 18.67, 13.65; HRMS (ESI) calculated for C₁₅H₁₆N₃O₂S [M+H]⁺ 302.0958, found 302.0959.



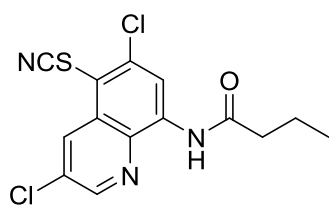
***N*-(6-methylquinolin-5-thiocyanate-8-yl)butanamide (3j)**

Obtained as a slight yellow solid (46.2 mg, 81%); m.p. 120 – 122 °C; IR (KBr), cm⁻¹: 3350, 3312, 2964, 2923, 2851, 2154, 1689, 1661, 1520, 1467, 1397, 1365, 1326, 1179, 886, 784, 749; ¹H NMR (300 MHz, CDCl₃) δ 9.90 (s, 1H), 8.85 (s, 1H), 8.83 (dd, J = 4.2, 1.5 Hz, 1H), 8.77 (dd, J = 8.6, 1.5 Hz, 1H), 7.66 (dd, J = 8.6, 4.2 Hz, 1H), 2.84 (s, 3H), 2.57 (t, J = 7.5 Hz, 2H), 1.93 – 1.79 (m, 2H), 1.07 (t, J = 7.4 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 171.96, 147.66, 145.48, 137.66, 137.31, 133.49, 129.04, 123.21, 118.62, 110.23, 109.75, 39.91, 22.66, 18.78, 13.62; HRMS (ESI) calculated for C₁₅H₁₆N₃OS [M+H]⁺ 286.1009, found 286.1007.



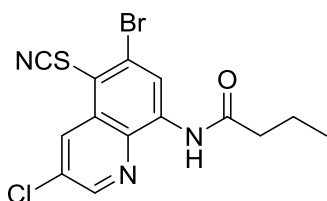
***N*-(6-chloroquinolin-5-thiocyanate-8-yl)butanamide (3k)**

Obtained as a slight yellow solid (41.0 mg, 67%); m.p. 155 – 157 °C; IR (KBr), cm⁻¹: 3316, 2964, 2920, 2849, 2160, 1699, 1559, 1507, 1460, 1363, 1348, 1315, 1174, 1149, 871, 809, 783, 720; ¹H NMR (300 MHz, CDCl₃) δ 9.93 (s, 1H), 9.04 (s, 1H), 8.88 (d, J = 4.2 Hz, 1H), 8.76 (d, J = 8.6 Hz, 1H), 7.72 (dd, J = 8.6, 4.3 Hz, 1H), 2.58 (t, J = 7.4 Hz, 2H), 1.92 – 1.79 (m, 2H), 1.07 (t, J = 7.4 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 172.03, 148.52, 141.89, 138.49, 137.29, 134.07, 129.41, 124.13, 117.36, 109.73, 109.28, 39.88, 18.71, 13.64; HRMS (ESI) calculated for C₁₄H₁₃ClN₃OS [M+H]⁺ 306.0462, found 306.0469.



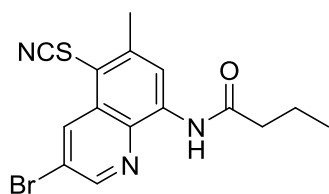
***N*-(3,6-dichloroquinolin-5-thiocyanate-8-yl)butanamide (3l)**

Obtained as a slight yellow solid (38.8 mg, 52%); m.p. 133 – 135 °C; IR (KBr), cm^{-1} : 3351, 2963, 2921, 2851, 2156, 1704, 1598, 1552, 1509, 1455, 1361, 1309, 1174, 1143, 982, 918, 881, 657; ^1H NMR (300 MHz, CDCl_3) δ 9.73 (s, 1H), 9.04 (s, 1H), 8.77 (d, $J = 2.2$ Hz, 1H), 8.72 (d, $J = 2.2$ Hz, 1H), 2.57 (t, $J = 7.4$ Hz, 2H), 1.91 – 1.79 (m, 2H), 1.06 (d, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.09, 147.97, 143.67, 138.69, 135.37, 132.52($\times 2$), 130.19, 117.79, 109.02, 108.90, 39.97, 18.74, 13.67; HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{12}\text{Cl}_2\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 340.0073, found 340.0071.



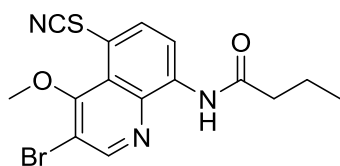
***N*-(3-chloro-6-bromoquinolin-5-thiocyanate-8-yl)butanamide (3m)**

Obtained as a slight yellow solid (40.0 mg, 52%); m.p. 154 – 156 °C; IR (KBr), cm^{-1} : 3347, 2962, 2922, 2853, 2154, 1705, 1596, 1556, 1517, 1458, 1362, 1309, 1182, 1101, 977, 907, 881, 764, 749; ^1H NMR (300 MHz, CDCl_3) δ 9.71 (s, 1H), 9.20 (s, 1H), 8.78 (d, $J = 2.2$ Hz, 1H), 8.74 (d, $J = 2.2$ Hz, 1H), 2.57 (t, $J = 7.4$ Hz, 2H), 1.91 – 1.77 (m, 2H), 1.06 (d, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.04, 147.98, 138.41, 135.54, 134.95, 132.83, 132.50, 132.42, 130.23, 120.62, 117.67, 111.47, 108.92, 39.89, 18.68, 13.65; HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{12}\text{BrClN}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 383.9567, found 383.9571.



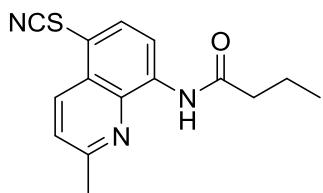
***N*-(6-methyl-3-bromoquinolin-5-thiocyanate-8-yl)butanamide (3n)**

Obtained as a slight yellow solid (53.2 mg, 73%); m.p. 140 – 142 °C; IR (KBr), cm^{-1} : 3358, 2961, 2922, 2850, 2155, 2155, 1698, 1606, 1553, 1517, 1457, 1394, 1310, 1180, 955, 892; ^1H NMR (300 MHz, CDCl_3) δ 9.70 (s, 1H), 8.89 (d, $J = 2.0$ Hz, 1H), 8.85 (s, 1H), 8.80 (d, $J = 1.9$ Hz, 1H), 2.84 (s, 3H), 2.56 (t, $J = 7.4$ Hz, 2H), 1.91 – 1.77 (m, 2H), 1.06 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.14, 149.01, 147.36, 137.69, 135.97, 135.26, 130.41, 120.36, 119.19, 109.91, 108.99, 40.05, 22.96, 18.86, 13.71; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{15}\text{BrN}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 364.0114, found 364.0124.



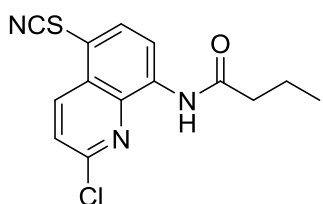
***N*-(4-methoxy-3-bromoquinolin-5-thiocyanate-8-yl)butanamide (3o)**

Obtained as a white solid (51.7 mg, 68%); m.p. 127 – 129 °C; IR (KBr), cm^{-1} : 3357, 2962, 2929, 2872, 2153, 1694, 1570, 1512, 1472, 1447, 1352, 1333, 1276, 1260, 1177, 966, 830, 764, 750; ^1H NMR (300 MHz, CDCl_3) δ 9.61 (s, 1H), 8.86 (d, $J = 8.6$ Hz, 1H), 8.81 (s, 1H), 7.91 (d, $J = 8.6$ Hz, 1H), 4.16 (s, 3H), 2.54 (t, $J = 7.5$ Hz, 2H), 1.90 – 1.76 (m, 2H), 1.05 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.75, 160.00, 151.96, 139.44, 134.88, 128.08, 121.97, 117.33, 112.12, 111.12, 110.20, 62.09, 40.03, 18.89, 13.73; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{14}\text{BrN}_3\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 380.0063, found 380.0070.



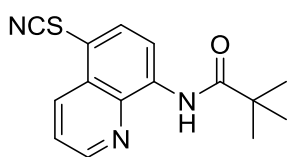
***N*-(2-methylquinolin-5-thiocyanate-8-yl)butanamide (3p)**

Obtained as a slight yellow solid (13.7 mg, 24%); m.p. 106 – 108 °C; IR (KBr), cm^{-1} : 3316, 2959, 2922, 2845, 2153, 1687, 1655, 1561, 1526, 1489, 1458, 1375, 1328, 1275, 1261, 857, 764, 750; ^1H NMR (300 MHz, CDCl_3) δ 9.98 (s, 1H), 8.79 (d, $J = 8.2$ Hz, 1H), 8.55 (d, $J = 8.7$ Hz, 1H), 7.89 (d, $J = 8.3$ Hz, 1H), 7.55 (d, $J = 8.7$ Hz, 1H), 2.80 (s, 3H), 2.58 (t, $J = 7.5$ Hz, 2H), 1.93 – 1.79 (m, 2H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.99, 158.37, 137.46, 138.35, 135.27, 133.66, 126.48, 124.23, 115.99, 111.43, 110.78, 40.07, 25.11, 18.85, 13.75; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{16}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 286.1009, found 286.1013.



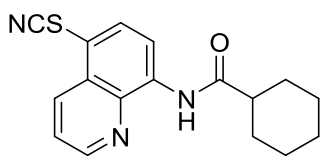
***N*-(2-chloroquinolin-5-thiocyanate-8-yl)butanamide (3q)**

Obtained as a slight yellow solid (6.7 mg, 11%); m.p. 130 – 132 °C; IR (KBr), cm^{-1} : 3313, 2957, 2921, 2851, 2160, 1693, 1655, 1631, 1524, 1477, 1320, 1275, 1179, 1156, 1144, 1109, 853, 826, 764, 750, 715; ^1H NMR (300 MHz, CDCl_3) δ 9.53 (s, 1H), 8.89 (d, $J = 8.4$ Hz, 1H), 8.64 (d, $J = 8.8$ Hz, 1H), 7.98 (d, $J = 8.3$ Hz, 1H), 7.66 (d, $J = 8.8$ Hz, 1H), 2.59 (t, $J = 7.5$ Hz, 2H), 1.92 – 1.79 (m, 2H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.13, 150.50, 138.59, 137.38, 136.69, 129.90, 127.16, 124.79, 117.41, 111.82, 110.26, 40.03, 18.80, 13.72; HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{13}\text{ClN}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 306.0462, found 306.0469.



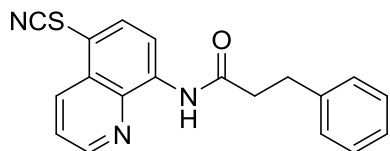
***N*-(quinolin-5-thiocyanate-8-yl)pivalamide (4a)**

Obtained as a white solid (35.4 mg, 62%); m.p. 123-125 °C; IR (KBr), cm^{-1} : 3366, 3344, 2963, 2919, 2871, 2155, 1686, 1569, 1516, 1482, 1451, 1396, 1376, 1365, 1318, 1171, 1140, 841, 791, 675; ^1H NMR (300 MHz, CDCl_3) δ 10.40 (s, 1H), 8.93 (dd, $J = 4.2, 1.3$ Hz, 1H), 8.83 (d, $J = 8.3$ Hz, 1H), 8.68 (dd, $J = 8.5, 1.1$ Hz, 1H), 7.98 (d, $J = 8.3$ Hz, 1H), 7.70 (dd, $J = 8.5, 4.2$ Hz, 1H), 1.43 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 177.41, 148.89, 139.16, 138.15, 136.27, 133.47, 128.04, 123.21, 115.64, 111.32, 110.53, 40.36, 27.46 ($\times 3$); HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{16}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 286.1009, found 286.1015.



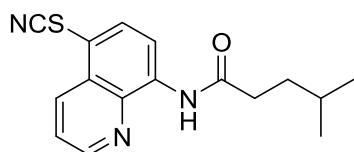
***N*-(quinolin-5-thiocyanate-8-yl)cyclohexanecarboxamide (4b)**

Obtained as a white solid (40.5 mg, 65%); m.p. 130 – 132 °C; IR (KBr), cm^{-1} : 3348, 2925, 2851, 2151, 1693, 1586, 1516, 1480, 1450, 1380, 1368, 1319, 1149, 1128, 838, 812, 795, 653; ^1H NMR (300 MHz, CDCl_3) δ 10.03 (s, 1H), 8.93 (d, $J = 3.2$ Hz, 1H), 8.84 (d, $J = 8.2$ Hz, 1H), 8.69 (d, $J = 8.3$ Hz, 1H), 7.98 (d, $J = 8.2$ Hz, 1H), 7.71 (dd, $J = 8.4, 4.1$ Hz, 1H), 2.50 (t, $J = 11.6$ Hz, 1H), 2.09 (d, $J = 11.9$ Hz, 2H), 1.89 (d, $J = 12.0$ Hz, 2H), 1.73 – 1.58 (m, 3H), 1.46 – 1.27 (m, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 175.12, 148.86, 139.05, 138.25, 136.45, 133.64, 128.22, 123.30, 115.96, 111.41, 110.62, 46.79, 29.56 ($\times 2$), 25.59 ($\times 3$); HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{18}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 312.1165, found 312.1167.



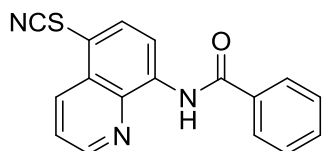
***N*-(quinolin-5-thiocyanate-8-yl)phenylpropanamide (4c)**

Obtained as a white solid (50.0 mg, 75%); m.p. 122 – 124 °C; IR (KBr), cm^{-1} : 3310, 3055, 3029, 2923, 2853, 2161, 1683, 1517, 1477, 1453, 1382, 1363, 1316, 1199, 1178, 1141, 1076, 856, 787, 748, 702, 654; ^1H NMR (300 MHz, CDCl_3) δ 9.90 (s, 1H), 8.92 – 8.86 (m, 1H), 8.83 (d, $J = 8.3$ Hz, 1H), 8.67 (dd, $J = 8.5, 1.3$ Hz, 1H), 7.98 (d, $J = 8.3$ Hz, 1H), 7.68 (dd, $J = 8.5, 4.2$ Hz, 1H), 7.33 – 7.28 (t, $J = 6.7$ Hz, 4H), 7.25 – 7.17 (m, 1H), 3.15 (t, $J = 7.7$ Hz, 2H), 2.92 (t, $J = 7.8$ Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.02, 148.76, 140.29, 138.71, 137.85, 136.23, 133.50, 128.52($\times 2$), 128.28 ($\times 2$), 128.08, 126.28, 123.26, 115.95, 111.67, 110.51, 39.57, 31.12; HRMS (ESI) calculated for $\text{C}_{19}\text{H}_{16}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 334.1009, found 334.1013.



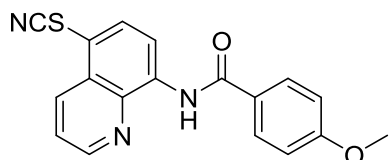
4-methyl-*N*-(quinolin-5-thiocyanate-8-yl)pentanamide (4d)

Obtained as a white solid (45.5 mg, 76%); m.p. 92 – 94 °C; IR (KBr), cm^{-1} : 3341, 2957, 2931, 2869, 2360, 2342, 2152, 1698, 1568, 1518, 1479, 1451, 1383, 1317, 1176, 1146, 836, 812, 794, 749; ^1H NMR (300 MHz, CDCl_3) δ 9.95 (s, 1H), 8.93 (d, $J = 4.1$ Hz, 1H), 8.83 (d, $J = 8.3$ Hz, 1H), 8.70 (d, $J = 8.5$ Hz, 1H), 7.99 (d, $J = 8.3$ Hz, 1H), 7.71 (dd, $J = 8.5, 4.2$ Hz, 1H), 2.59 (t, $J = 7.5$ Hz, 2H), 1.74 – 1.67 (m, 3H), 0.98 (d, $J = 6.1$ Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.28, 148.81, 138.79, 138.06, 136.31, 133.54, 128.13, 123.26, 115.87, 111.46, 110.52, 36.13, 34.08, 27.67, 22.26 ($\times 2$); HRMS (ESI) calculated for $\text{C}_{16}\text{H}_{18}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 300.1165, found 300.1170.



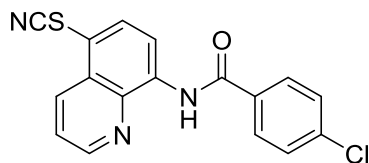
***N*-(quinolin-5-thiocyanate-8-yl)benzamide (4e)**

Obtained as a slight yellow solid (40.9 mg, 67%); m.p. 164 – 165 °C; IR (KBr), cm^{-1} : 3366, 2920, 2850, 2154, 1678, 1581, 1532, 1480, 1382, 1366, 1327, 1201, 1157, 852, 791, 701, 687, 645; ^1H NMR (300 MHz, CDCl_3) δ 10.89 (s, 1H), 9.02 – 8.95 (m, 2H), 8.73 (dd, $J = 8.5, 1.4$ Hz, 1H), 8.13 – 8.03 (m, 3H), 7.74 (dd, $J = 8.5, 4.2$ Hz, 1H), 7.68 – 7.53 (m, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.39, 149.01, 139.19, 138.02, 136.28, 134.19, 133.62, 132.30, 128.85 ($\times 2$), 128.17, 127.24 ($\times 2$), 123.40, 116.00, 111.92, 110.55; HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{12}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 306.0696, found 306.0699.



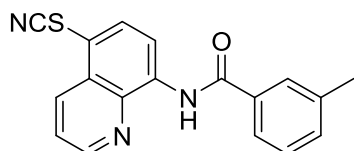
4-methoxy-*N*-(quinolin-5-thiocyanate-8-yl)benzamide (4f)

Obtained as a slight yellow solid (47.6 mg, 71%); m.p. 180 – 182 °C; IR (KBr), cm^{-1} : 3340, 2920, 2849, 2150, 1670, 1606, 1529, 1508, 1480, 1379, 1310, 1264, 1186, 1122, 1099, 1021, 842, 815, 787, 757, 641; ^1H NMR (300 MHz, CDCl_3) δ 10.81 (s, 1H), 9.01 – 8.93 (m, 2H), 8.72 (dd, $J = 8.5, 1.5$ Hz, 1H), 8.09 – 8.01 (m, 3H), 7.73 (dd, $J = 8.5, 4.2$ Hz, 1H), 7.10 – 7.01 (m, 2H), 3.91 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 164.81, 162.80, 148.88, 139.15, 138.22, 136.31, 133.55, 129.18 ($\times 2$), 128.14, 126.41, 123.31, 115.77 ($\times 2$), 114.01, 111.45, 110.61, 55.42; HRMS (ESI) calculated for $\text{C}_{18}\text{H}_{14}\text{N}_3\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 336.0801, found 336.0812.



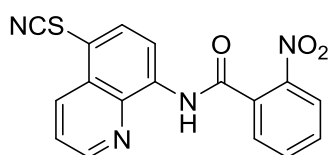
4-chloro-*N*-(quinolin-5-thiocyanate-8-yl)benzamide(4g)

Obtained as a slight yellow solid (43.5 mg, 64%); m.p. 214 – 216 °C; IR (KBr), cm^{-1} : 3330, 2152, 1676, 1595, 1522, 1475, 1379, 1319, 1258, 1102, 1007, 896, 833, 790, 748, 652; ^1H NMR (300 MHz, CDCl_3) δ 10.83 (s, 1H), 8.99 – 8.94 (m, 2H), 8.73 (dd, $J = 8.5, 1.4$ Hz, 1H), 8.03 (t, $J = 8.6$ Hz, 3H), 7.73 (dd, $J = 8.5, 4.2$ Hz, 1H), 7.54 (d, $J = 8.6$ Hz, 2H). ^{13}C NMR (75 MHz, CDCl_3) δ 164.46, 149.16, 139.30, 138.72, 137.92, 136.35, 133.83, 132.74, 129.21 ($\times 2$), 128.76 ($\times 2$), 128.31, 123.55, 116.23, 112.40, 110.49; HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{11}\text{ClN}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 340.0306, found 340.0310.



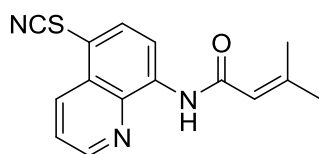
3-methyl-*N*-(quinolin-5-thiocyanate-8-yl)benzamide (4h)

Obtained as a slight yellow solid (46.0 mg, 72%); m.p. 174 – 176 °C; IR (KBr), cm^{-1} : 3368, 2918, 2849, 2152, 1677, 1587, 1530, 1482, 1382, 1325, 1270, 852, 810, 791, 727, 684, 650; ^1H NMR (300 MHz, CDCl_3) δ 10.84 (s, 1H), 9.02 – 8.96 (m, 2H), 8.72 (dd, $J = 8.5, 1.5$ Hz, 1H), 8.05 (d, $J = 8.3$ Hz, 1H), 7.89 – 7.83 (m, 2H), 7.73 (dd, $J = 8.5, 4.2$ Hz, 1H), 7.51 – 7.40 (m, 2H), 2.50 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.71, 149.03, 139.30, 138.81, 138.19, 136.36, 134.29, 133.67, 133.08, 128.72, 128.24, 128.05, 124.21, 123.40, 116.08, 111.88, 110.55, 21.43; HRMS (ESI) calculated for $\text{C}_{18}\text{H}_{14}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 320.0852, found 320.0848.



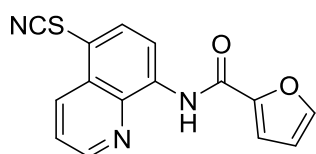
2-nitro-*N*-(quinolin-5-thiocyanate-8-yl)benzamide (4i)

Obtained as a slight yellow solid (42.0 mg, 60%); m.p. 182 – 184 °C; IR (KBr), cm^{-1} : 3392, 2923, 2853, 2160, 1683, 1586, 1514, 1483, 1442, 1381, 1356, 1317, 1131, 1079, 938, 899, 854, 842, 776, 720; ^1H NMR (300 MHz, CDCl_3) δ 10.29 (s, 1H), 8.94 (d, $J = 8.2$ Hz, 1H), 8.87 (dd, $J = 4.2, 1.5$ Hz, 1H), 8.72 (dd, $J = 8.6, 1.5$ Hz, 1H), 8.17 (dd, $J = 8.1, 0.7$ Hz, 1H), 8.07 (d, $J = 8.2$ Hz, 1H), 7.85 – 7.68 (m, 4H); ^{13}C NMR (75 MHz, CDCl_3) δ 164.52, 149.11, 146.38, 138.78, 137.55, 135.96, 133.91, 133.61, 132.24, 131.07, 128.37, 128.08, 124.68, 123.51, 116.57, 113.09, 110.39; HRMS (ESI) calculated for $\text{C}_{17}\text{H}_{11}\text{N}_4\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$ 351.0546, found 351.0554.



3-methyl-*N*-(quinolin-5-thiocyanate-8-yl)but-2-enamide (4j)

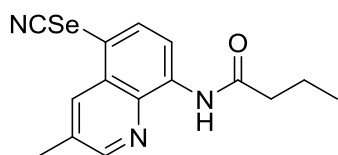
Obtained as a slight yellow solid (41.9 mg, 74%); m.p. 179 – 181 °C; IR (KBr), cm^{-1} : 3304, 3006, 2984, 2914, 2840, 2155, 1673, 1640, 1518, 1369, 1318, 1276, 1261, 1139, 847, 764, 750; ^1H NMR (300 MHz, CDCl_3) δ 9.86 (s, 1H), 8.95 – 8.85 (m, 2H), 8.68 (dd, $J = 8.5, 1.5$ Hz, 1H), 7.98 (d, $J = 8.3$ Hz, 1H), 7.69 (dd, $J = 8.5, 4.2$ Hz, 1H), 5.99 (t, $J = 1.2$ Hz, 1H), 2.30 (d, $J = 0.9$ Hz, 3H), 1.99 (d, $J = 0.9$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.15, 155.32, 148.63, 138.82, 138.55, 136.37, 133.49, 128.14, 123.20, 118.66, 115.52, 110.96, 110.66, 27.53, 20.06; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{14}\text{N}_3\text{OS}$ $[\text{M}+\text{H}]^+$ 284.0852, found 284.0858.



***N*-(quinolin-5-thiocyanate-8-yl)furan-2-carboxamide(4k)**

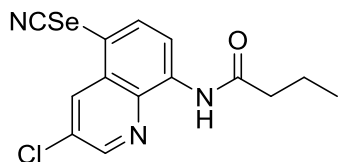
Obtained as a slight yellow solid (33.1 mg, 56%); m.p. 180 – 182 °C; IR (KBr), cm^{-1} : 3349, 2921, 2850, 2152, 1681, 1646, 1588, 1570, 1532, 1488, 1474, 1453, 1324, 1273, 1167, 1012, 812, 850, 791, 763, 676, 639, 596; ^1H NMR (300 MHz, CDCl_3) δ 10.89 (s, 1H), 9.00 (dd, $J = 4.2, 1.4$ Hz, 1H), 8.92 (d, $J = 8.3$ Hz, 1H), 8.70 (dd, $J = 8.5, 1.4$ Hz, 1H), 8.02 (d, $J = 8.3$ Hz,

1H), 7.73 (dd, $J = 8.5, 4.2$ Hz, 1H), 7.66 (d, $J = 0.7$ Hz, 1H), 7.35 (d, $J = 3.2$ Hz, 1H), 6.62 (dd, $J = 3.4, 1.7$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 156.33, 149.13, 147.69, 144.92, 139.11, 137.74, 136.17, 133.55, 128.22, 123.43, 116.10, 115.96, 112.66, 112.12, 110.53; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{10}\text{N}_3\text{O}_2\text{S}$ $[\text{M}+\text{H}]^+$ 296.0488, found 296.0495.



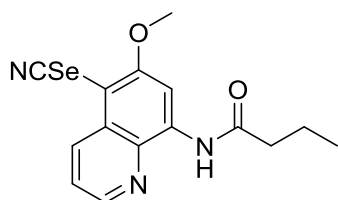
***N*-(3-methylquinolin-5-selenocyanate-8-yl)butanamide (5a)**

Obtained as a slight yellow solid (49.8 mg, 75%); m.p. 128 – 130 °C; IR (KBr), cm^{-1} : 3312, 2957, 2925, 2873, 2152, 1686, 1564, 1523, 1467, 1367, 1320, 1196, 1176, 885, 853, 721, 638; ^1H NMR (300 MHz, CDCl_3) δ 9.89 (s, 1H), 8.71 (dd, $J = 5.0, 3.1$ Hz, 2H), 8.37 (s, 1H), 8.02 (d, $J = 8.2$ Hz, 1H), 2.64 (s, 3H), 2.56 (t, $J = 7.5$ Hz, 2H), 1.92 – 1.79 (m, 2H), 1.06 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.88, 150.50, 137.82 ($\times 2$), 136.96, 134.48, 133.36, 128.69, 115.11, 110.43, 101.02, 39.93, 18.81 ($\times 2$), 13.65; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{16}\text{N}_3\text{OSe}$ $[\text{M}+\text{H}]^+$ 334.0453, found 334.0460.



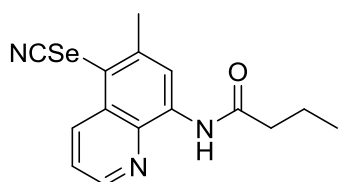
***N*-(3-chloroquinolin-5-selenocyanate-8-yl)butanamide (5b)**

Obtained as a slight yellow solid (40.9 mg, 58%); m.p. 158 – 160 °C; IR (KBr), cm^{-1} : 3308, 2959, 2921, 2850, 2154, 1684, 1632, 1556, 1522, 1460, 1361, 1316, 1180, 1105, 965, 896, 855, 723, 636; ^1H NMR (300 MHz, CDCl_3) δ 9.76 (s, 1H), 8.83 – 8.78 (m, 2H), 8.63 (d, $J = 2.2$ Hz, 1H), 8.11 (d, $J = 8.2$ Hz, 1H), 2.57 (t, $J = 7.5$ Hz, 2H), 1.92 – 1.78 (m, 2H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.06, 148.24, 139.65, 138.33, 136.86, 134.36, 131.66, 129.74, 116.46, 110.07, 100.46; HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{13}\text{ClN}_3\text{OSe}$ $[\text{M}+\text{H}]^+$ 353.9907, found 353.9915.



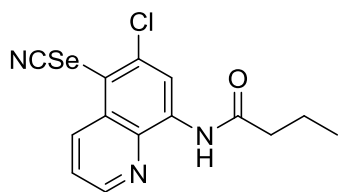
***N*-(6-methoxyquinolin-5-selenocyanate-8-yl)butanamide (5c)**

Obtained as a slight yellow solid (57.8 mg, 83%); m.p. 122 – 124 °C; IR (KBr), cm^{-1} : 3319, 2963, 2921, 2851, 2152, 1689, 1613, 1587, 1562, 1519, 1459, 1394, 1332, 1203, 1172, 1138, 1081, 899, 855, 779, 716; ^1H NMR (300 MHz, CDCl_3) δ 9.99 (s, 1H), 8.87 (s, 1H), 8.69 (dd, $J = 4.2, 1.4$ Hz, 1H), 8.60 (dd, $J = 8.6, 1.4$ Hz, 1H), 7.59 (dd, $J = 8.6, 4.2$ Hz, 1H), 4.11 (s, 3H), 2.58 (t, $J = 7.4$ Hz, 2H), 1.93 – 1.80 (m, 2H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.14, 159.40, 145.89, 139.04, 134.48, 134.30, 129.79, 123.52, 102.88, 101.14, 95.29, 56.83, 39.80, 18.57, 13.57; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{16}\text{N}_3\text{O}_2\text{Se}$ $[\text{M}+\text{H}]^+$ 350.0402, found 350.0409.



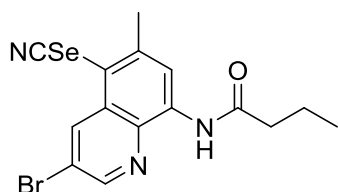
***N*-(6-methylquinolin-5-selenocyanate-8-yl)butanamide (5d)**

Obtained as a slight yellow solid (53.8 mg, 81%); m.p. 100 – 102 °C; IR (KBr), cm^{-1} : 3346, 2963, 2927, 2873, 2151, 1691, 1561, 1522, 1467, 1395, 1366, 1182, 885, 788, 750; ^1H NMR (300 MHz, CDCl_3) δ 9.89 (s, 1H), 8.86 (s, 1H), 8.80 (dd, $J = 4.2, 1.4$ Hz, 1H), 8.74 (dd, $J = 8.6, 1.4$ Hz, 1H), 7.63 (dd, $J = 8.6, 4.2$ Hz, 1H), 2.87 (s, 3H), 2.57 (t, $J = 7.5$ Hz, 2H), 1.92 – 1.79 (m, 2H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.90, 147.56, 145.26, 137.44, 137.03, 135.82, 129.56, 123.15, 118.33, 111.52, 100.69, 39.85, 25.14, 18.75, 13.59; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{16}\text{N}_3\text{OSe}$ $[\text{M}+\text{H}]^+$ 334.0453, found 334.0455.



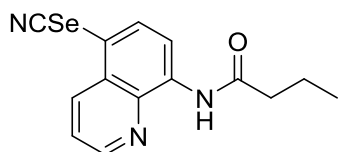
***N*-(6-chloroquinolin-5-selenocyanate-8-yl)butanamide (5e)**

Obtained as a slight yellow solid (38.8 mg, 55%); m.p. 156 – 158 °C; IR (KBr), cm^{-1} : 3314, 2962, 2921, 2851, 2155, 1698, 1557, 1509, 1460, 1378, 1358, 1344, 1312, 1176, 1150, 1077, 864, 808, 782, 717, 631; ^1H NMR (300 MHz, CDCl_3) δ 9.91 (s, 1H), 9.03 (s, 1H), 8.85 (dd, $J = 4.2, 1.5$ Hz, 1H), 8.71 (dd, $J = 8.6, 1.5$ Hz, 1H), 7.69 (dd, $J = 8.6, 4.2$ Hz, 1H), 2.58 (t, $J = 7.5$ Hz, 2H), 1.92 – 1.79 (m, 2H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.09, 148.50, 141.94, 138.41, 137.39, 136.73, 130.15, 124.19, 117.34, 111.13, 100.09, 39.99, 18.81, 13.70; HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{13}\text{ClN}_3\text{OSe}$ $[\text{M}+\text{H}]^+$ 353.9907, found 353.9913.



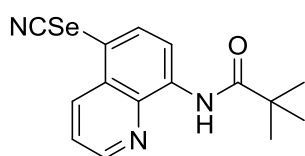
***N*-(6-methyl-3-bromoquinolin-5-selenocyanate-8-yl)butanamide (5f)**

Obtained as a slight yellow solid (52.6 mg, 64%); m.p. 130 – 132 °C; IR (KBr), cm^{-1} : 3354, 2962, 2928, 2872, 2151, 1695, 1606, 1516, 1456, 1393, 1368, 1307, 1182, 951, 928, 893, 750; ^1H NMR (300 MHz, CDCl_3) δ 9.69 (s, 1H), 8.89 (d, $J = 2.0$ Hz, 1H), 8.88 (s, 1H), 8.78 (d, $J = 2.0$ Hz, 1H), 2.88 (s, 3H), 2.56 (t, $J = 7.4$ Hz, 2H), 1.91 – 1.78 (m, 2H), 1.06 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 172.08, 148.86, 147.24, 137.55, 137.48, 135.78, 130.98, 120.25, 118.92, 110.48, 100.28, 40.02, 25.50, 18.85, 13.70; HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{15}\text{BrN}_3\text{OSe}$ $[\text{M}+\text{H}]^+$ 411.9558, found 411.9552.



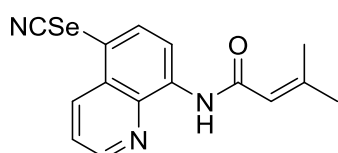
***N*-(quinolin-5-selenocyanate-8-yl)butanamide (5g)**

Obtained as a slight yellow solid (40.7 mg, 64%); m.p. 112 – 114 °C; IR (KBr), cm^{-1} : 3336, 2960, 2923, 2851, 2150, 1686, 1564, 1515, 1477, 1380, 1361, 1316, 1179, 1149, 1086, 842, 790, 750; ^1H NMR (300 MHz, CDCl_3) δ 9.95 (s, 1H), 8.90 (dd, $J = 4.2, 1.5$ Hz, 1H), 8.81 (d, $J = 8.2$ Hz, 1H), 8.65 (dd, $J = 8.5, 1.5$ Hz, 1H), 8.08 (d, $J = 8.2$ Hz, 1H), 7.69 (dd, $J = 8.5, 4.2$ Hz, 1H), 2.58 (t, $J = 7.5$ Hz, 2H), 1.93 – 1.80 (m, 2H), 1.07 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 171.95, 148.73, 138.77, 137.96, 137.86, 135.90, 128.88, 123.32, 116.02, 111.14, 100.88, 39.98, 18.83, 13.67; HRMS (ESI) calculated for $\text{C}_{14}\text{H}_{14}\text{N}_3\text{OSe}$ $[\text{M}+\text{H}]^+$ 320.0297, found 320.0302.



***N*-(quinolin-5-selenocyanate-8-yl)pivalamide (5h)**

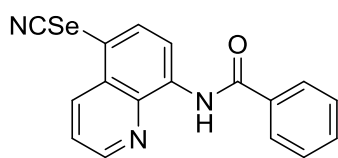
Obtained as a slight yellow solid (40.5 mg, 61%); m.p. 110 – 112 °C; IR (KBr), cm^{-1} : 3361, 3344, 2960, 2920, 2850, 2149, 1675, 1647, 1515, 1480, 1448, 1395, 1361, 1315, 1173, 1141, 933, 851, 839, 789, 682; ^1H NMR (300 MHz, CDCl_3) δ 10.39 (s, 1H), 8.90 (dd, $J = 4.1, 1.3$ Hz, 1H), 8.79 (d, $J = 8.2$ Hz, 1H), 8.63 (dd, $J = 8.5, 1.3$ Hz, 1H), 8.05 (d, $J = 8.2$ Hz, 1H), 7.67 (dd, $J = 8.5, 4.2$ Hz, 1H), 1.43 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 177.56, 148.93, 139.38, 138.29, 138.05, 136.02, 129.02, 123.38, 116.01, 111.09, 100.88, 27.57 ($\times 3$); HRMS (ESI) calculated for $\text{C}_{15}\text{H}_{16}\text{N}_3\text{OSe}$ $[\text{M}+\text{H}]^+$ 334.0453, found 334.0447.



3-methyl-*N*-(quinolin-5-selenocyanate-8-yl)but-2-enamide (5i)

Obtained as a slight yellow solid (41.6 mg, 63%); m.p. 178 – 180 °C; IR (KBr), cm^{-1} : 3340, 3302, 2920, 2850, 2149, 1681, 1670, 1642, 1526, 1479, 1369, 1317, 1161, 1143, 847, 832, 790, 663; ^1H

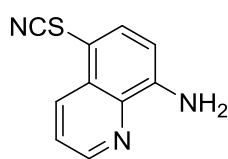
NMR (300 MHz, CDCl₃) δ 9.87 (s, 1H), 8.91 – 8.79 (m, 2H), 8.64 (dd, J = 8.5, 1.5 Hz, 1H), 8.06 (d, J = 8.3 Hz, 1H), 7.67 (dd, J = 8.5, 4.2 Hz, 1H), 5.99 (d, J = 1.2 Hz, 1H), 2.30 (d, J = 0.9 Hz, 3H), 1.98 (d, J = 0.9 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 165.33, 155.22, 148.70, 139.05, 138.69, 138.15, 136.07, 129.11, 123.40, 118.81, 115.90, 110.78, 100.94, 27.60, 20.13; HRMS (ESI) calculated for C₁₅H₁₄N₃OSe [M+H]⁺ 332.0297, found 334.0307.



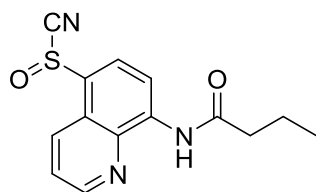
N-(quinolin-5-selenocyanate-8-yl)benzamide (5j)

Obtained as a slight yellow solid (41.6 mg, 63%); m.p. 194 – 196 °C; IR (KBr), cm⁻¹: 3364, 2921, 2851, 2150, 1669, 1581, 1531, 1480, 1382, 1367, 1363, 1324, 1261, 851, 790, 701 688, 643; ¹H NMR (300 MHz, CDCl₃) δ 10.89 (s, 1H), 8.99 – 8.93 (m, 2H), 8.69 (dd, J = 8.5, 1.5 Hz, 1H), 8.15 (d, J = 8.2 Hz, 1H), 8.12 – 8.06 (m, 2H), 7.72 (dd, J = 8.5, 4.2 Hz, 1H), 7.67 – 7.54 (m, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 165.51, 149.00, 139.31, 138.10, 137.98, 136.09, 134.35, 132.30, 129.06, 128.90 (\times 2), 127.31 (\times 2), 123.53, 116.29, 111.64, 100.86; HRMS (ESI) calculated for C₁₇H₁₂N₃OSe [M+H]⁺ 354.0140, found 354.0138.

Synthetic Applications of 3a

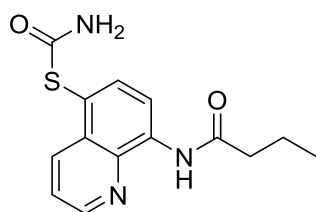


Quinolin-5-selenocyanate-8-amine (6)^{1d} To a solution of **3a** (0.2 mmol) in EtOH (2 mL), 0.5 mL of concentrated hydrochloric acid (10 M) was added. The mixture was refluxed for 1 h and then concentrated under reduced pressure. The residue was dissolved in CH₂Cl₂ (10.0 mL), washed by saturated NaHCO₃ aqueous solution (5 mL \times 2), brine (5 \times 2 mL), and dried over Na₂SO₄. The organic solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel using *PE/EA* = 10 : 1 as an eluent to give the title product as a slight yellow solid (36.6 mg, 91%); m.p. 90 – 91 °C; IR (KBr), cm⁻¹: 3474, 3363, 2920, 2851, 2150, 1610, 1591, 1503, 1468, 1363, 1340, 812, 789, 669, 650; ¹H NMR (300 MHz, DMSO-*d*₆) δ 8.86 (dd, J = 4.1, 1.5 Hz, 1H), 8.57 (dd, J = 8.5, 1.6 Hz, 1H), 7.82 (d, J = 8.2 Hz, 1H), 7.76 (dd, J = 8.6, 4.2 Hz, 1H), 6.90 (d, J = 8.3 Hz, 1H), 6.80 (s, 2H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 149.59, 147.57, 137.90, 137.74, 132.82, 129.18, 123.60, 112.65, 108.14, 99.45; HRMS (ESI) calculated for C₁₀H₈N₃S [M+H]⁺ 202.0433, found 202.0438.

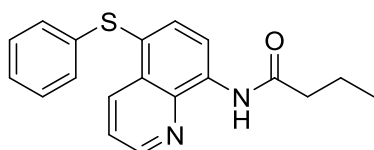


N-(quinolin-5-sulfinylcyanide-8-yl)butanamide (7)² To a solution of **3a** (0.2 mmol) in CHCl₃ (2 mL), 99 mg (70%, 0.6 mmol) of metachloroperbenzoic acid was added. The mixture was refluxed for 6 h, then diluted with 10 mL of CHCl₃, washed by saturated NaHCO₃ aqueous solution (5 mL \times 2), brine (5 mL \times 2), and dried over Na₂SO₄. The organic solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel using *PE/EA* = 8:1 as an eluent to give the title product as a slight yellow solid (47.0 mg, 86%); m.p. 154 – 156 °C; IR (KBr), cm⁻¹: 3359, 2958, 2921, 2851, 2153, 1687, 1584, 1531, 1494, 1395, 1331, 1260, 1196, 1151, 857, 807, 752; ¹H NMR (300 MHz, CDCl₃) δ 14.37 (s, 1H), 9.15 (d, J = 8.7 Hz, 1H), 8.48 (dd, J = 6.1, 0.9 Hz, 1H), 8.35 (dd, J = 8.8, 0.9 Hz, 1H), 8.02 (d, J = 8.7 Hz, 1H), 7.53 (dd, J = 8.8, 6.1 Hz, 1H), 2.49 (t, J = 7.5 Hz, 2H), 1.89 – 1.75 (m, 2H), 1.03 (t, J = 7.4 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 172.57,

138.37, 138.27, 138.02, 132.63, 132.06, 125.58, 122.46, 118.16, 111.90, 109.75, 40.97, 18.74, 13.67; HRMS (ESI) calculated for C₁₄H₁₄N₃O₂S [M+H]⁺ 288.0801, found 288.0803.



***N*-(quinolin-5-thiocarbamate-8-yl)butanamide (8)**³ To a solution of **3a** (0.2 mmol) in CH₂Cl₂ (2 mL), 0.1 mL of concentrated sulfuric acid (18 M) was added. The mixture was stirred under the ice bath condition for 4 h, then diluted with 10 mL of CH₂Cl₂, washed by saturated NaHCO₃ aqueous solution (5 mL × 3), brine (5 mL × 2), and dried over Na₂SO₄. The organic solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel using *PE/EA* = 1 : 1 as an eluent to obtain the title product as a slight yellow solid (47.5 mg, 82%); m.p. 154 – 155 °C; IR (KBr), cm⁻¹: 3374, 3325, 3253, 3191, 2960, 2923, 2845, 2359, 2343, 1659, 1614, 1530, 1481, 1384, 1321, 1149, 846, 792, 726, 619, 597; ¹H NMR (300 MHz, DMSO-*d*₆) δ 10.21 (s, 1H), 8.98 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.66 (d, *J* = 8.1 Hz, 1H), 8.58 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.92 (brs, 1H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.75 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.60 (brs, 1H), 2.59 (t, *J* = 7.3 Hz, 2H), 1.75 – 1.62 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 171.94, 165.03, 148.82, 138.48, 136.84, 136.50, 134.76, 129.93, 122.86, 119.21, 115.86, 38.66, 18.64, 13.60; HRMS (ESI) calculated for C₁₄H₁₆N₃O₂S [M+H]⁺ 290.0958, found 290.0960.



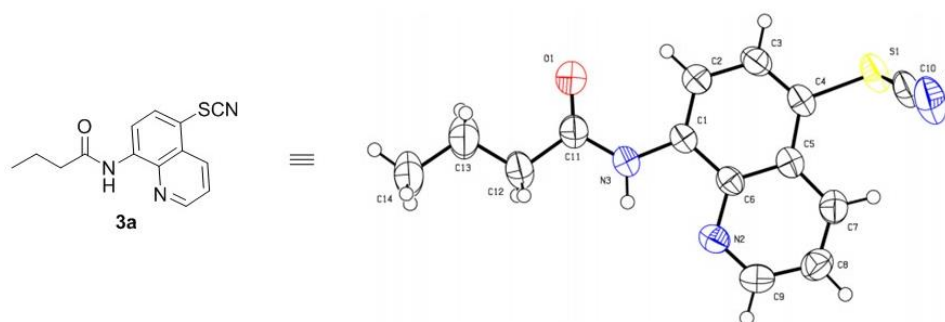
***N*-(quinolin-5-phenylthio-8-yl)butanamide (9)**⁴ To a solution of **3a** (0.2 mmol) in H₂O (2 mL), iodobenzene (2.0 mmol), CuI (10 mol %), 1,10-phenanthroline (10 mol %), TBAB (10 mol %), NaHCO₃ (0.4 mmol) were added. The reaction mixture was placed in an oil bath at 100 °C and vigorously stirred for 10 h. Afterward it was cooled to ambient temperature, diluted with 10 mL of CH₂Cl₂, washed brine (5 mL × 2), and dried over Na₂SO₄. The organic solvent was removed under reduced pressure and the residue was purified by flash chromatography on silica gel using *PE/EA* = 30 : 1 as an eluent to give the title product as a slight yellow solid (46.4 mg, 72%); m.p. 133 – 135 °C; IR (KBr), cm⁻¹: 3341, 2958, 2924, 2871, 1689, 1581, 1519, 1477, 1455, 1376, 1362, 1312, 1184, 1147, 1083, 1023, 866, 817, 795, 746, 690; ¹H NMR (300 MHz, CDCl₃) δ 9.93 (s, 1H), 8.80 (dd, *J* = 4.9, 3.3 Hz, 2H), 8.67 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.46 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.22–7.02 (m, 5H), 2.57 (t, *J* = 7.5 Hz, 2H), 1.87 (dd, *J* = 14.9, 7.4 Hz, 2H), 1.06 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 171.88, 148.29, 139.07, 137.78, 136.20, 136.02, 134.93, 129.30, 129.01(×2), 127.38 (×2), 125.71, 122.52, 122.36, 116.20, 40.15, 19.06, 13.79. HRMS (ESI) calculated for C₁₉H₁₉N₂O₂S [M+H]⁺ 323.1213, found 323.1214.

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Single-crystal X-ray data for compound 3a



Bond precision: C-C = 0.0033 Å

Wavelength=0.71073

Cell: a=7.680 (5) b=8.494 (5) c=11.449 (7)
 alpha=85.960 (7) beta=77.314 (7) gamma=66.467 (7)
 Temperature: 296 K

	Calculated	Reported
Volume	667.9 (7)	667.9 (7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H13 N3 O S	?
Sum formula	C14 H13 N3 O S	C14 H13 N3 O S
Mr	271.33	271.33
Dx, g cm ⁻³	1.349	1.349
Z	2	2
Mu (mm ⁻¹)	0.237	0.237
F000	284.0	284.0
F000'	284.34	
h, k, lmax	9, 10, 14	9, 10, 14
Nref	2861	2544
Tmin, Tmax	0.977, 0.986	
Tmin'	0.977	

Correction method= Not given

Data completeness= 0.889

Theta (max)= 26.766

R(reflections)= 0.0458 (1906)

wR2(reflections)= 0.1661 (2544)

S = 0.986

Npar= 174

Copies of ^1H and ^{13}C NMR spectra for the title compounds

