Base-promoted ring opening of 3-chlorooxindoles for the construction of 2-aminoarylthioates and their transformation to quinazolin-4(3H)-ones

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Optimization of the reaction conditions for the formation of quinazolin-4(3H)-ones

Table S1. Optimization of the reaction conditions for the formation of 11a

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Catalysts (10 mol%)</th>
<th>Solvents</th>
<th>Condition</th>
<th>Yield (%)</th>
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<td>1</td>
<td>-</td>
<td>Toluene</td>
<td>12h, Reflux</td>
<td>-</td>
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<tr>
<td>2</td>
<td>In(OTf)₃</td>
<td>Toluene</td>
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<td>Au(PPh₃)CH₃</td>
<td>Toluene</td>
<td>12h, 80 °C</td>
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<tr>
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<td>Toluene</td>
<td>12h, Reflux</td>
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<td>Cu(OTf)₂</td>
<td>THF</td>
<td>12h, 80 °C</td>
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</table>

[a] Reaction conditions: 3a (0.27 mmol), 10a (0.27 mmol), and catalyst (10 mol%) in 3 mL solvent were stirred under nitrogen gas protection.

Characterization data of substrates (1a-1e)

3-Chloroindolin-2-one (1a): ¹H NMR (300 MHz, DMSO-d₆) δ 10.79 (1H, s), 7.36 (1H, d, J = 7.4 Hz), 7.29 (1H, t, J = 7.7 Hz), 7.03 (1H, t, J = 7.5 Hz), 6.87 (1H, d, J = 7.8 Hz), 5.57 (1H, s); ¹³C NMR (75 MHz, DMSO-d₆) δ 173.2, 142.4, 130.3, 126.5, 125.6, 122.3, 110.1, 52.2; ATR-IR (neat) 3351, 3150, 1685, 1618, 1466, 1165, 743, 674 cm⁻¹.

3-Chloro-5-methoxyindolin-2-one (1b): ¹H NMR (300 MHz, CDCl₃) δ 9.11 (1H, s), 6.97 (1H, s), 6.80 (1H, s), 5.11 (1H, s), 3.77 (3H, s); ¹³C NMR (75 MHz, CDCl₃) δ 174.6, 156.3, 134.2, 127.2, 115.5, 112.2, 111.2, 55.8, 52.3; ATR-IR (neat) 3151, 3148, 3148, 1684, 1473, 1177, 823, 675, 561 cm⁻¹.

3,5-Dichloroindolin-2-one (1c): ¹H NMR (300 MHz, DMSO-d₆) δ 10.91 (1H, s), 7.43 (1H, s), 7.35 (1H, dd, J = 8.3, 2.1 Hz), 6.88 (1H, d, J = 8.3 Hz), 5.58 (1H, s); ¹³C NMR (75 MHz, DMSO-d₆) δ 173.7, 142.1, 130.9, 129.3, 127.0, 126.5, 112.4, 52.5; ATR-IR (neat) 3148, 2098, 1739, 1684, 1473, 1177, 823, 675, 561 cm⁻¹.

3-Chloro-5-fluoroindolin-2-one (1d): ¹H NMR (300 MHz, DMSO-d₆) δ 10.81 (1H, s), 7.29 (1H, dd, J = 8.0, 2.1 Hz), 7.18-7.11 (1H, m), 6.89-6.85 (1H, m), 5.59 (1H, s); ¹³C NMR (75 MHz, DMSO-d₆) δ 173.1, 158.1 (J = 236.2 Hz), 138.6, 128.1 (J = 8.7 Hz), 116.7 (J = 23.2 Hz), 113.38 (J = 25.5 Hz), 111.1 (J = 8.2 Hz), 52.0; ATR-IR (neat) 3166, 1685, 1398, 1479, 1177, 757, 690, 540 cm⁻¹.
3-Chloro-5-nitroindolin-2-one (1e): $^1$H NMR (300 MHz, DMSO-$d_6$) $\delta$ 11.45 (1H, s), 8.21-8.16 (2H, m), 7.04 (1H, d, $J = 8.5$ Hz), 5.66 (1H, s); $^{13}$C NMR (75 MHz, DMSO-$d_6$) $\delta$ 173.5, 148.7, 142.4, 127.5, 127.2, 121.2, 110.4, 51.1; ATR-IR (neat) 3308, 1741, 1615, 1327, 1192, 1069, 835, 661 cm$^{-1}$.

Characterization data of the synthesized compounds

**S-Ethyl 2-aminobenzothioate (3a):** Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and ethanethiol 2a (31 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (65 mg, 72%). $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.81 (1H, d, $J = 8.4$ Hz), 7.20–7.15 (1H, m), 6.61–6.56 (2H, m), 5.70 (2H, s), 2.93 (2H, q, $J = 7.5$ Hz), 1.25 (3H, t, $J = 7.5$ Hz); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 193.3, 147.7, 234.1, 130.1, 118.5, 117.1, 116.3, 23.1, 14.8; ATR-IR (neat) 3478, 3364, 2967, 2928, 1613, 1579, 1200, 911, 812, 742, 681 cm$^{-1}$; HRMS $m/z$ (M$^+$) calcd for C$_{9}$H$_{11}$NOS: 181.0561. Found: 181.0558.

**S-Propyl 2-aminobenzothioate (3b):** Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and propane-1-thiol 2b (38 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (73 mg, 75%); $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.86 (1H, d, $J = 8.4$ Hz), 7.23–7.18 (1H, m), 6.65–6.60 (2H, m), 5.89 (2H, s), 2.93 (2H, t, $J = 7.5$ Hz), 1.69–1.56 (2H, m), 0.97 (3H, t, $J = 7.2$ Hz); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 193.4, 147.2, 134.1, 130.1, 118.9, 117.3, 116.7, 30.7, 23.0, 13.5; ATR-IR (neat) 3478, 3364, 2962, 2926, 1613, 1579, 1199, 911, 812, 742, 681 cm$^{-1}$; HRMS $m/z$ (M$^+$) calcd for C$_{10}$H$_{13}$NOS: 195.0718. Found: 195.0718.

**S-Butyl 2-aminobenzothioate (3c):** Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and butane-1-thiol 2c (45 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (74 mg, 71%); $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.82 (1H, dd, $J = 8.7, 1.8$ Hz), 7.17 (1H, t, $J = 7.2$ Hz), 6.59–6.54 (2H, m), 5.75 (2H, s), 2.92 (2H, t, $J = 7.2$ Hz), 1.58–1.53 (2H, m), 1.40–1.33 (2H, m), 0.86 (3H, t, $J = 7.5$ Hz); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 193.3, 147.7, 134.0, 130.0, 118.5, 117.0, 116.3, 31.6, 28.4, 22.0, 13.6; ATR-IR (neat) 3479, 3365, 2957, 1613, 1578, 1199, 1158, 910, 741, 681 cm$^{-1}$; HRMS $m/z$ (M$^+$) calcd for C$_{11}$H$_{15}$NOS: 209.0874. Found: 209.0876.

**S-Isopropyl 2-aminobenzothioate (3d):** Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and propane-2-thiol 2d (38 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (68 mg, 70%); $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.75 (1H, dd, $J = 8.7, 1.5$ Hz), 7.16–7.10 (1H, m), 6.56–6.50 (2H, m), 5.71 (2H, s), 3.75–3.61 (1H, m), 1.29 (6H, d, $J = 6.9$ Hz); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 193.3, 147.8, 134.0, 130.0, 118.4, 116.9, 116.1, 34.3, 23.0; ATR-IR (neat) 3477, 3356, 2950, 1612, 1190, 1145, 942, 742, 645 cm$^{-1}$; HRMS $m/z$ (M$^+$) calcd for C$_{10}$H$_{13}$NOS: 209.0874. Found: 209.0876.

**S-(Tert-butyl) 2-aminobenzothioate (3e):** Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and 2-methylpropane-2-thiol 2e (45 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (54 mg, 52%); $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 7.79 (1H, d, $J = 8.4$ Hz), 7.15 (1H, t, $J = 7.2$ Hz), 6.57–6.52 (2H, m), 5.64 (2H, s), 1.49 (9H, s); $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 194.7, 147.6, 133.8, 130.0, 119.5, 117.2, 116.3, 47.8, 30.0; ATR-IR (neat) 3472, 3358,
2952, 1614, 1468, 1189, 930, 742, 647 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₁H₁₅NOS: 209.0874. Found: 209.0875.

**S-Ethyl 2-amino-5-methoxybenzothioate (3f):** Prepared from 3-chloro-5-methoxyindolin-2-one 1b (99 mg, 0.5 mmol) and ethanethiol 2a (31 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (76 mg, 72%); ¹H NMR (300 MHz, CDCl₃) δ 7.33 (1H, d, J = 2.7 Hz), 6.92 (1H, dd, J = 8.7, 2.7 Hz), 6.59 (1H, d, J = 9.0 Hz), 5.53 (2H, s), 3.75 (3H, s), 2.98 (2H, q, J = 7.2 Hz), 1.31 (3H, t, J = 7.5 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 192.8, 150.5, 142.4, 123.2, 118.6, 118.4, 112.0, 55.8, 23.3, 14.7; ATR-IR (neat) 3476, 3365, 2930, 1583, 1556, 1167, 949, 838, 677 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₀H₁₃NO₂S: 211.0667. Found: 211.0667.

**S-Butyl 2-amino-5-methoxybenzothioate (3g):** Prepared from 3-chloro-5-methoxyindolin-2-one 1b (99 mg, 0.5 mmol) and butane-1-thiol 2c (45 mg, 0.5 mmol) over 14 h according to the general procedure. The product was obtained as a liquid (81 mg, 68%). ¹H NMR (300 MHz, CDCl₃) δ 7.37 (1H, d, J = 2.7 Hz), 6.93 (1H, dd, J = 9.0, 2.7 Hz), 6.61 (1H, d, J = 9.0 Hz), 5.53 (2H, s), 3.76 (3H, s), 3.01 (2H, t, J = 7.5 Hz), 1.66–1.61 (2H, m), 1.48–1.41 (2H, m), 0.93 (3H, t, J = 7.2 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 192.9, 150.8, 142.2, 123.2, 118.9, 118.7, 112.5, 55.9, 31.7, 28.7, 22.0, 13.5; ATR-IR (neat) 3483, 3367, 2927, 1584, 1556, 1492, 1241, 1168, 950, 838 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₂H₂₇NO₂S: 239.0980. Found: 239.0982.

**S-Isopropyl 2-amino-5-methoxybenzothioate (3h):** Prepared from 3-chloro-5-methoxyindolin-2-one 1b (99 mg, 0.5 mmol) and propane-2-thiol 2d (38 mg, 0.5 mmol) over 14 h according to the general procedure. The product was obtained as a liquid (61 mg, 54%); ¹H NMR (300 MHz, CDCl₃) δ 7.32 (1H, d, J = 2.7 Hz), 6.92 (1H, dd, J = 8.7, 2.7 Hz), 6.60 (1H, d, J = 9.0 Hz), 5.32 (2H, s), 3.84–3.70 (4H, m), 1.38 (6H, d, J = 6.9 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 193.0, 162.3, 150.8, 142.3, 123.2, 118.9, 118.7, 112.4, 55.9, 34.7, 23.1; ATR-IR (neat) 3478, 3366, 2961, 2924, 2859, 1584, 1492, 1169, 1042, 950, 839 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₁H₁₅NO₂S: 225.0823. Found: 225.0826.

**S-Ethyl 2-amino-5-chlorobenzothioate (3i):** Prepared from 3,5-dichloroindolin-2-one 1c (101 mg, 0.5 mmol) and ethanethiol 2a (31 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (78 mg, 72%); ¹H NMR (300 MHz, CDCl₃) δ 7.82 (1H, d, J = 1.8 Hz), 7.18 (1H, dd, J = 8.7, 2.1 Hz), 6.50 (1H, d, J = 8.7 Hz), 5.77 (2H, s), 2.99 (2H, q, J = 7.2 Hz), 1.30 (3H, t, J = 7.2 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 192.5, 146.2, 134.1, 129.1, 120.7, 119.1, 118.5, 23.4, 14.7; ATR-IR (neat) 3478, 3366, 2960, 2872, 1577, 1188, 32, 818, 647 cm⁻¹; HRMS m/z (M⁺) calcd for C₉H₁₀ClNOS: 215.0172. Found: 215.0174.

**S-Propyl 2-amino-5-chlorobenzothioate (3j):** Prepared from 3,5-dichloroindolin-2-one 1c (101 mg, 0.5 mmol) and propane-1-thiol 2b (38 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (75 mg, 65%); ¹H NMR (300 MHz, CDCl₃) δ 7.82 (1H, d, J = 2.4 Hz), 7.18 (1H, dd, J = 8.7, 2.4 Hz), 6.58 (1H, d, J = 8.7 Hz), 5.80 (2H, s), 2.97 (2H, t, J = 7.2 Hz), 1.72–1.60 (2H, m), 1.00 (3H, t, J = 7.2 Hz); ¹³C NMR (75 MHz, CDCl₃) δ 192.5, 146.1, 134.0, 129.2, 120.8, 119.2, 118.5, 30.8, 22.9, 13.4; ATR-IR (neat) 3480, 3364, 2963, 2930, 1613, 1576, 1480, 1186, 930, 816, 741, 517 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₀H₁₂ClNOS: 229.0328. Found: 229.0326.
**S-Isopropyl 2-amino-5-chlorobenzothioate (3k):** Prepared from 3,5-dichloroindolin-2-one 1c (101 mg, 0.5 mmol) and propane-2-thiol 2d (38 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a solid (71 mg, 62%); \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 7.80 (1H, d, \(J = 2.4\) Hz), 7.16 (1H, dd, \(J = 9.0, 2.4\) Hz), 6.56 (1H, d, \(J = 9.0\) Hz), 5.80 (2H, s), 3.78–3.72 (1H, m), 1.37 (6H, d, \(J = 6.9\) Hz); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 192.6, 146.3, 134.0, 129.2, 120.7, 119.3, 118.5, 34.8, 23.0; ATR-IR (neat) 3454, 3349, 2968, 2926, 2868, 1613, 1544, 1189, 1154, 929, 819, 742, 508 cm\(^{-1}\); HRMS \(m/z\) (M\(^{+}\)) calcd for \(\text{C}_{10}\text{H}_{12}\text{ClNOS}\): 229.0328. Found: 229.0326.

**S-(Tert-butyl) 2-amino-5-chlorobenzothioate (3l):** Prepared from 3,5-dichloroindolin-2-one 1c (101 mg, 0.5 mmol) and 2-methylpropane-2-thiol 2e (45 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (61 mg, 50%); \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 7.81 (1H, d, \(J = 2.4\) Hz), 7.15 (1H, dd, \(J = 8.7, 2.4\) Hz), 6.57 (1H, d, \(J = 8.7\) Hz), 5.68 (2H, s), 1.54 (9H, s); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 193.8, 146.0, 133.7, 129.2, 120.6, 120.1, 118.6, 48.3, 29.9; ATR-IR (neat) 3426, 3320, 2959, 2921, 1612, 1580, 1468, 1152, 924, 815, 742, 519 cm\(^{-1}\); HRMS \(m/z\) (M\(^{+}\)) calcd for \(\text{C}_{11}\text{H}_{14}\text{NOS}\): 243.0485. Found: 243.0488.

**S-Ethyl 2-amino-5-fluorobenzothioate (3m):** Prepared from 3-chloro-5-fluorourindolin-2-one 1d (93 mg, 0.5 mmol) and ethanethiol 2a (31 mg, 0.5 mmol) over 8 h according to the general procedure. The product was obtained as a liquid (69 mg, 74%); \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 7.54 (1H, d, \(J = 9.6, 2.7\) Hz), 7.03–6.97 (1H, m), 6.61–6.56 (1H, m), 5.67 (2H, s), 2.98 (2H, q, \(J = 7.2\) Hz), 1.03 (3H, t, \(J = 7.5\) Hz); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 192.5 (\(J = 3.0\) Hz), 153.7 (\(J = 234.0\) Hz), 144.2, 122.1 (\(J = 23.2\) Hz), 118.3 (\(J = 7.5\) Hz), 118.1 (\(J = 6.0\) Hz), 114.8 (\(J = 22.5\) Hz), 23.4, 14.7; ATR-IR (neat) 3452, 3349, 2965, 1618, 1559, 1486, 1230, 1148, 850, 827, 685 cm\(^{-1}\); HRMS \(m/z\) (M\(^{+}\)) calcd for \(\text{C}_{9}\text{H}_{10}\text{FNOS}\): 199.0467. Found: 199.0468.

**S-Propyl 2-amino-5-fluorobenzothioate (3n):** Prepared from 3-chloro-5-fluorourindolin-2-one 1d (93 mg, 0.5 mmol) and propane-1-thiol 2b (38 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (75 mg, 70%); \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 7.57 (1H, dd, \(J = 9.9, 3.0\) Hz), 7.02–6.96 (1H, m), 6.59–6.55 (1H, m), 5.65 (2H, s), 2.96 (2H, t, \(J = 6.9\) Hz), 1.71–1.59 (2H, m), 0.99 (3H, t, \(J = 7.5\) Hz); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 192.5 (\(J = 3.0\) Hz), 153.6 (\(J = 234.0\) Hz), 144.3 (\(J = 1.5\) Hz), 122.1 (\(J = 23.2\) Hz), 118.3 (\(J = 7.5\) Hz), 118.1 (\(J = 5.2\) Hz), 114.8 (\(J = 23.2\) Hz), 30.8, 22.9, 13.3; ATR-IR (neat) 3480, 3368, 2964, 2873, 1588, 1557, 1488, 1229, 1146, 965, 842, 524 cm\(^{-1}\); HRMS \(m/z\) (M\(^{+}\)) calcd for \(\text{C}_{10}\text{H}_{12}\text{FNOS}\): 213.0624. Found: 213.0620.

**S-Butyl 2-amino-5-fluorobenzothioate (3o):** Prepared from 3-chloro-5-fluorourindolin-2-one 1d (93 mg, 0.5 mmol) and butane-1-thiol 2c (45 mg, 0.5 mmol) over 8 h according to the general procedure. The product was obtained as a liquid (77 mg, 68%); \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 7.57 (1H, dd, \(J = 9.9, 3.0\) Hz), 7.01–7.00 (1H, m), 6.62–6.57 (1H, m), 5.66 (2H, s), 2.99 (2H, t, \(J = 7.5\) Hz), 1.64–1.56 (2H, m), 1.46–1.38 (2H, m), 0.92 (3H, t, \(J = 7.2\) Hz); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 192.6 (\(J = 3.0\) Hz), 153.7 (\(J = 234.0\) Hz), 144.2 (\(J = 0.75\) Hz), 122.1 (\(J = 23.2\) Hz), 118.4 (\(J = 6.7\) Hz), 118.2 (\(J = 6.0\) Hz), 114.9 (\(J = 23.2\) Hz), 31.5, 28.7, 22.0, 13.6; ATR-IR (neat) 3481, 3369, 2958, 2929, 1588, 1557, 1231, 1147, 966, 844, 865, 525 cm\(^{-1}\); HRMS \(m/z\) (M\(^{+}\)) calcd for \(\text{C}_{11}\text{H}_{14}\text{FNOS}\): 227.0780. Found: 227.0782.
S-Propyl 2-amino-5-nitrobenzothioate (3p): Prepared from 3-chloro-5-nitroindolin-2-one 1e (106 mg, 0.5 mmol) and propane-1-thiol 2b (38 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a solid (94 mg, 78%), mp: 92–94 °C; \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 8.80 (1H, d, \(J = 2.4\) Hz), 8.04 (1H, dd, \(J = 9.3, 2.7\) Hz), 6.66–6.63 (3H, m), 2.97 (2H, t, \(J = 7.2\) Hz), 1.71–1.59 (2H, m), 0.98 (3H, t, \(J = 7.2\) Hz); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 192.8, 152.5, 136.7, 128.8, 127.4, 116.8, 116.5, 31.0, 22.7, 13.3; ATR-IR (neat) 3450, 3338, 1609, 1482, 1312, 1201, 1104, 942, 747, 637 cm\(^{-1}\); HRMS \(m/z\) (M\(^+\)) calcd for C\(_{10}\)H\(_{12}\)N\(_2\)O\(_3\)S: 240.0569. Found: 240.0567.

S-Cyclopentyl 2-aminobenzothioate (4a): Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and cyclopentanethiol 2f (51 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (68 mg, 62%); \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 7.84 (1H, dd, \(J = 8.4, 1.5\) Hz), 7.25–7.19 (1H, m), 6.65–6.59 (2H, m), 5.89 (2H, s), 3.85–2.18 (1H, m), 2.18–2.11 (2H, m), 1.76–1.60 (6H, m); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 194.0, 147.6, 133.9, 130.1, 118.5, 117.0, 116.2, 42.2, 33.2, 24.7; ATR-IR (neat) 3477, 3362, 2955, 2866, 1612, 1578, 1199, 1157, 741, 683 cm\(^{-1}\); HRMS \(m/z\) (M\(^+\)) calcd for C\(_{12}\)H\(_{15}\)NOS: 221.0874. Found: 221.0877.

S-Cyclohexyl 2-aminobenzothioate (4b): Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and cyclohexanethiol 2g (58 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (71 mg, 60%); \(^1\)H NMR (600 MHz, CDCl\(_3\)) \(\delta\) 7.81 (1H, d, \(J = 8.4\) Hz), 7.18 (1H, t, \(J = 7.8\) Hz), 6.60–6.57 (2H, m), 5.96 (2H, s), 3.59–3.55 (1H, m), 1.94–1.91 (2H, m), 1.70–1.68 (2H, m), 1.56–1.54 (1H, m), 1.46–1.37 (4H, m), 1.27–1.24 (1H, m); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 193.3, 147.5, 134.0, 130.1, 119.0, 117.3, 116.6, 42.2, 33.2, 26.1, 25.6; ATR-IR (neat) 3478, 3363, 2927, 2851, 1612, 1578, 1196, 1157, 741, 683 cm\(^{-1}\); HRMS \(m/z\) (M\(^+\)) calcd for C\(_{13}\)H\(_{17}\)NOS: 235.1031. Found: 235.1029.

S-Cyclopentyl 2-amino-5-methoxybenzothioate (4c): Prepared from 3-chloro-5-methoxyindolin-2-one 1b (99 mg, 0.5 mmol) and cyclopentanethiol 2f (51 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (82 mg, 65%); \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 7.30 (1H, d, \(J = 3.0\) Hz), 6.91 (1H, dd, \(J = 9.0, 2.7\) Hz), 6.61 (1H, d, \(J = 9.0\) Hz), 5.49 (2H, s), 3.87–3.77 (1H, m), 3.75 (3H, s), 2.18–2.08 (2H, m), 1.76–1.65 (6H, m); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 193.7, 150.5, 142.1, 123.2, 118.8, 118.6, 111.9, 55.8, 42.4, 33.2, 24.7; ATR-IR (neat) 3463, 3360, 2962, 2860, 1586, 1556, 1489, 1164, 1040, 823, 677 cm\(^{-1}\); HRMS \(m/z\) (M\(^+\)) calcd for C\(_{13}\)H\(_{17}\)NO\(_2\)S: 251.0980. Found: 251.0982.

S-Cyclopentyl 2-amino-5-chlorobenzothioate (4d): Prepared from 3,5-dichloroindolin-2-one 1c (101 mg, 0.5 mmol) and cyclopentanethiol 2f (51 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (87.68%); \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 7.30 (1H, d, \(J = 3.0\) Hz), 6.91 (1H, dd, \(J = 9.0, 2.7\) Hz), 6.61 (1H, d, \(J = 9.0\) Hz), 5.49 (2H, s), 3.87–3.77 (1H, m), 3.75 (3H, s), 2.18–2.08 (2H, m), 1.76–1.65 (6H, m); \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 193.7, 150.5, 142.1, 123.2, 118.8, 118.6, 111.9, 55.8, 42.4, 33.2, 24.7; ATR-IR (neat) 3463, 3360, 2962, 2860, 1586, 1556, 1489, 1164, 1040, 823, 677 cm\(^{-1}\); HRMS \(m/z\) (M\(^+\)) calcd for C\(_{12}\)H\(_{14}\)ClNO\(_2\)S: 255.0485. Found: 255.0487.

S-Cyclohexyl 2-amino-5-chlorobenzothioate (4e): Prepared from 3,5-dichloroindolin-2-one 1c (101 mg, 0.5 mmol) and cyclohexanethiol 2g (58 mg, 0.5 mmol) over 12 h according to the general
procedure. The product was obtained as a liquid (72 mg, 60%); ^1H NMR (600 MHz, CDCl₃) δ 7.83 (1H, d, J = 1.8 Hz), 7.17 (1H, dd, J = 8.4, 2.4 Hz), 6.58 (1H, d, J = 8.4 Hz), 5.88 (2H, s), 3.64–3.61 (1H, m), 1.99–1.97 (2H, m), 1.75–1.73 (2H, m), 1.61–1.59 (1H, m), 1.52–1.42 (4H, m), 1.33–1.28 (1H, m); ^13C NMR (150 MHz, CDCl₃) δ 192.5, 146.2, 134.0, 129.3, 120.8, 119.5, 118.5, 42.5, 33.1, 26.0, 25.6; ATR-IR (neat) 3423, 3325, 2961, 2919, 1614, 1579, 1452, 1160, 918, 817, 738 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₃H₁₆ClNOS: 269.0641. Found: 269.0639.

S-Cyclopentyl 2-amino-5-fluorobenzothioate (4f): Prepared from 3-chloro-5-fluoroindolin-2-one 1d (93 mg, 0.5 mmol) and cyclopentanethiol 2f (51 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (94 mg, 70%); ^1H NMR (300 MHz, CDCl₃) δ 7.52 (1H, dd, J = 9.9, 3.0 Hz), 7.03–6.96 (1H, m), 6.62–6.57 (1H, m), 5.67 (2H, s), 3.84–3.77 (1H, m), 2.20–2.10 (2H, m), 1.76–1.55 (6H, m); ^13C NMR (75 MHz, CDCl₃) δ 193.4 (J = 3.0 Hz), 153.7 (J = 234.0 Hz), 144.1, 122.0 (J = 24.0 Hz), 118.4, 118.3, 115.0 (J = 23.2 Hz), 42.6, 33.1, 24.7; ATR-IR (neat) 3480, 3366, 2957, 2868, 1588, 1557, 1230, 1147, 966, 845, 686 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₂H₁₄FNOS: 239.0780. Found: 239.0782.

S-Cyclohexyl 2-amino-5-fluorobenzothioate (4g): Prepared from 3-chloro-5-fluoroindolin-2-one 1d (93 mg, 0.5 mmol) and cyclohexanethiol 2g (58 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (83 mg, 65%); ^1H NMR (600 MHz, CDCl₃) δ 7.55 (1H, dd, J = 10.2, 3.0 Hz), 7.02–6.98 (1H, m), 6.62–6.60 (1H, m), 5.75 (2H, s), 3.64–3.61 (1H, m), 2.02–1.95 (2H, m), 1.75–1.73 (2H, m), 1.61–1.59 (1H, m), 1.52–1.44 (4H, m), 1.33–1.27 (1H, m); ^13C NMR (150 MHz, CDCl₃) δ 192.6 (J = 2.0 Hz), 153.9 (J = 234.4 Hz), 143.9, 122.0 (J = 23.1 Hz), 118.7, 118.5 (J = 6.9 Hz), 115.0 (J = 22.9 Hz), 42.6, 33.1, 26.0, 25.5; ATR-IR (neat) 3479, 3367, 2928, 2852, 1556, 1487, 1229, 1145, 964, 841, 685 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₃H₁₆FNOS: 253.0937. Found: 253.0934.

S-Benzyl 2-aminobenzothioate (5a): Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and phenylmethanethiol 2h (62 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (83 mg, 65%); ^1H NMR (300 MHz, CDCl₃) δ 7.79 (1H, d, J = 7.8 Hz), 7.31–7.28 (2H, m), 7.25–7.14 (4H, m), 6.59–6.54 (2H, m), 5.83 (2H, s), 4.18 (2H, s); ^13C NMR (75 Hz, CDCl₃) δ 192.2, 147.8, 137.7, 134.3, 130.1, 128.9, 128.5, 127.1, 118.1, 117.0, 116.4, 33.0; ATR-IR (neat) 3481, 3366, 3027, 1612, 1578, 1550, 1200, 1157, 908, 680 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₄H₁₃NOS: 243.0718. Found: 243.0718.

S-(4-(Tert-butyl)benzyl) 2-aminobenzothioate (5b): Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and (4-(tert-butyl)phenyl)methanethiol 2i (90 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a liquid (97 mg, 65%); ^1H NMR (300 MHz, CDCl₃) δ 7.94 (1H, dd, J = 8.4, 1.5 Hz), 7.42–7.36 (4H, m), 7.36–7.27 (1H, m), 6.72–6.67 (2H, m), 5.82 (2H, s), 4.31 (2H, s), 1.38 (9H, s); ^13C NMR (75 MHz, CDCl₃) δ 192.3, 147.8, 137.7, 134.3, 130.1, 128.9, 128.5, 127.1, 118.1, 117.1, 116.4, 33.0; ATR-IR (neat) 3483, 3366, 3027, 1612, 1578, 1550, 1200, 1157, 908, 680 cm⁻¹; HRMS m/z (M⁺) calcd for C₁₈H₂₁NOS: 299.1344. Found: 299.1346.

S-(2-chlorobenzyl) 2-aminobenzothioate (5c): Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and (2-chlorophenyl)methanethiol 2j (79 mg, 0.5 mmol) over 12 h according to the general procedure. The product was obtained as a solid (97 mg, 70%), mp: 56–58 °C; ^1H NMR
(400 MHz, CDCl$_3$) δ 7.88 (1H, dd, $J = 8.4, 1.6$ Hz), 7.55–7.53 (1H, m), 7.40–7.38 (1H, m), 7.29–7.25 (1H, m), 7.23–7.20 (2H, m), 6.67–6.63 (2H, m), 5.86 (2H, s), 4.39 (2H, s). $^{13}$C NMR (100 MHz, CDCl$_3$) δ 191.9, 148.1, 135.6, 134.4, 134.2, 131.1, 130.1, 129.5, 128.6, 126.9, 117.9, 117.0, 116.3, 30.8; ATR-IR (neat) 3476, 3356, 1613, 1573, 1549, 1202, 1157, 906, 734 cm$^{-1}$; HRMS m/z (M$^+$) calcd for C$_{14}$H$_{12}$ClNO: 277.0328. Found: 277.0327.

S-(4-Chlorobenzyl) 2-aminobenzothioate (5d): Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and (4-chlorophenyl)methanethiol 2k (79 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a solid (66 mg, 58%), mp: 71–73 °C; $^1$H NMR (600 MHz, DMSO-$d_6$) δ 7.72 (1H, dd, $J = 8.2, 1.3$ Hz), 7.39–7.34 (4H, m), 7.28–7.25 (1H, m), 6.92 (2H, s), 6.81 (1H, dd, $J = 8.4, 0.7$ Hz), 6.56–6.53 (1H, m), 4.23 (2H, s); $^{13}$C NMR (150 MHz, DMSO-$d_6$) δ 190.4, 149.3, 137.2, 134.5, 131.6, 130.6, 129.4, 128.3, 117.0, 115.8, 114.9, 31.2; ATR-IR (neat) 3488, 3367, 3034, 1634, 1576, 1548, 1205, 1160, 912, 844, 510 cm$^{-1}$; HRMS m/z (M$^+$) calcd for C$_{14}$H$_{12}$ClNO: 277.0328. Found: 277.0331.

S-Benzy 2-aminobenzothioate (5e): Prepared from 3-chlorooxindolin-2-one 1b (99 mg, 0.5 mmol) and phenylmethanethiol 2h (62 mg, 0.5 mmol) over 14 h according to the general procedure. The product was obtained as a liquid (82 mg, 60%); $^1$H NMR (300 MHz, CDCl$_3$) δ 7.30–7.13 (6H, m), 6.85 (1H, dd, $J = 9.0, 2.7$ Hz), 6.52 (1H, d, $J = 9.0$ Hz), 5.45 (2H, s), 4.17 (2H, s), 3.64 (3H, s); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 191.7, 150.5, 142.5, 137.6, 128.9, 128.5, 127.1, 123.6, 118.7, 117.8, 111.7, 55.7, 33.1; ATR-IR (neat) 3475, 3362, 2924, 1579, 1489, 1237, 1154, 909, 833, 697 cm$^{-1}$; HRMS m/z (M$^+$) calcd for C$_{15}$H$_{15}$NO$_2$: 273.0823. Found: 273.0822.

S-Benzy 2-aminobenzothioate (5f): Prepared from 3,5-dichlorooxindolin-2-one 1c (101 mg, 0.5 mmol) and phenylmethanethiol 2h (62 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (90 mg, 65%); $^1$H NMR (300 MHz, CDCl$_3$) δ 7.74 (1H, d, $J = 2.4$ Hz), 7.30–7.17 (5H, m), 7.11 (1H, dd, $J = 8.7, 2.4$ Hz), 6.51 (1H, d, $J = 8.7$ Hz), 5.75 (2H, s), 4.18 (2H, s); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 191.4, 146.3, 137.3, 134.3, 129.2, 128.9, 128.6, 127.3, 120.8, 118.6, 118.5, 33.2; ATR-IR (neat) 3483, 3365, 3029, 1612, 1576, 1185, 929, 814, 699, 515 cm$^{-1}$; HRMS m/z (M$^+$) calcd for C$_{14}$H$_{12}$ClNO: 277.0328. Found: 277.0331.

S-(4-(Tert-butyl)benzyl) 2-aminobenzothioate (5g): Prepared from 3,5-dichlorooxindolin-2-one 1c (101 mg, 0.5 mmol) and (4-(tert-butyl)phenyl)methanethiol 2i (90 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a liquid (114 mg, 68%); $^1$H NMR (300 MHz, CDCl$_3$) δ 7.82 (1H, d, $J = 2.1$ Hz), 7.34–7.27 (4H, m), 7.18 (1H, dd, $J = 8.7, 2.4$ Hz), 6.60 (1H, d, $J = 8.7$ Hz), 5.76 (2H, s), 4.23 (2H, s), 1.29 (9H, s); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 191.1, 150.3, 146.2, 134.2, 134.1, 129.3, 128.6, 125.5, 121.0, 118.9, 118.6, 34.4, 32.9, 31.3; ATR-IR (neat) 3484, 3367, 2959, 2924, 1577, 1544, 1185, 929, 814, 741 cm$^{-1}$; HRMS m/z (M$^+$) calcd for C$_{18}$H$_{20}$ClNO$_2$: 333.0954. Found: 333.0952. 

S-(4-Chlorobenzyl) 2-aminobenzothioate (5h): Prepared from 3,5-dichlorooxindolin-2-one 1c (101 mg, 0.5 mmol) and (4-chlorophenyl)methanethiol 2k (79 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a solid (109 mg, 70%); mp: 108–110 °C; $^1$H NMR (300 MHz, CDCl$_3$) δ 7.70 (1H, d, $J = 2.4$ Hz), 7.30–7.26 (4H, m), 7.18 (1H, dd, $J = 9.0, 2.4$ Hz), 6.59 (1H, d, $J = 9.0$ Hz), 5.72 (2H, s), 4.19 (2H, s); $^{13}$C NMR (75 MHz, CDCl$_3$) δ 191.1, 146.5, 136.0, 134.4, 133.0, 130.2, 129.2, 128.7, 120.8, 118.6, 118.5, 32.5; ATR-IR (neat) 3474, 3365,
S-(4-(Tert-butyl)benzyl) 2-amino-5-fluorobenzothioate (5i): Prepared from 3-chloro-5-fluoroindolin-2-one 1d (93 mg, 0.5 mmol) and (4-(tert-butyl)phenyl)methanethiol 2i (90 mg, 0.5 mmol) over 10 h according to the general procedure. The product was obtained as a solid (108 mg, 68%), mp: 52–54 °C; 1H NMR (300 MHz, CDCl3) δ 7.54 (1H, dd, J = 9.9, 3.0 Hz), 7.34–7.27 (4H, m), 7.05–6.99 (1H, m), 6.64–6.60 (1H, m), 5.66 (2H, s), 4.23 (2H, s), 1.29 (9H, s); 13C NMR (75 MHz, CDCl3) δ 191.7 (J = 3.0 Hz), 153.8 (J = 234.7 Hz), 150.2, 144.1, 134.1, 128.5, 125.5, 122.3 (J = 23.2 Hz), 118.5 (J = 7.5 Hz), 117.9 (J = 6.0 Hz), 114.9 (J = 23.2 Hz), 34.4, 32.9, 31.2; ATR-IR (neat) 3485, 3454, 3377, 2959, 1585, 1553, 1147, 968, 806, 685 cm⁻¹; HRMS m/z (M⁺) calcd for C18H20FNOS: 317.1250. Found: 317.1252.

3-(Ethylthio)indolin-2-one (6): Prepared from 3-chlorooxindole 1a (84 mg, 0.5 mmol) and ethanethiol 2a (31 mg, 0.5 mmol) over 4 h under an argon atmosphere. The product was obtained as a sticky liquid (31 mg, 32%). 1H NMR (600 MHz, CDCl3) δ 9.71 (1H, s), 7.33 (1H, d, J = 7.8 Hz), 7.20 (1H, t, J = 7.8 Hz), 7.03 (1H, t, J = 6.6 Hz), 6.2 (1H, d, J = 7.8 Hz), 4.29 (1H, s), 2.68–2.63 (1H, m), 2.48–2.42 (1H, m), 1.17 (3H, t, J = 7.8 Hz); 13C NMR (150 MHz, CDCl3) δ 178.7, 141.3, 128.8, 126.7, 125.0, 122.7, 110.2, 45.6, 23.6, 14.0; ATR-IR (neat) 3209, 2924, 1698, 1616, 1467, 1325, 1229, 745, 678 cm⁻¹.

3-(Tert-butyl)quinazolin-4(3H)-one (11a): Prepared from S-ethyl 2-aminobenzothioate 3a (50 mg, 0.27 mmol) and 2-isocyano-2-methylpropane 10a (23 mg, 0.27 mmol) over 12 h according to the general procedure. The product was obtained as a solid (47 mg, 86%), mp: 76–78 °C; 1H NMR (600 MHz, CDCl3) δ 8.27 (1H, s), 8.24 (1H, dd, J = 6.0, 2.1 Hz), 7.69–7.66 (1H, m), 7.63–7.61 (1H, m), 7.43–7.41 (1H, m), 1.71 (9H, s); 13C NMR (150 MHz, CDCl3) δ 161.9, 147.2, 143.9, 133.8, 126.8, 126.6, 126.6, 123.0, 60.7, 28.6; ATR-IR (neat) 3013, 1674, 1598, 1472, 1365, 1311, 1188, 1126, 924, 764, 696 cm⁻¹; HRMS m/z (M⁺) calcd for C12H14N2O: 202.1106. Found: 202.1107.

3-Cyclohexylquinazolin-4(3H)-one (11b): Prepared from S-ethyl 2-aminobenzothioate 3a (50 mg, 0.27 mmol) and isocyanocyclohexane 10b (30 mg, 0.27 mmol) over 10 h according to the general procedure. The product was obtained as a solid (50 mg, 82%), mp: 104–106 °C; 1H NMR (300 MHz, CDCl3) δ 8.28 (1H, d, J = 8.1 Hz), 8.11 (1H, s), 7.74–7.66 (2H, m), 7.46 (1H, t, J = 7.8 Hz), 4.83–4.73 (1H, m), 1.99–1.89 (4H, m), 1.78–1.73 (1H, m), 1.68–1.42 (4H, m), 1.31–1.16 (1H, m); 13C NMR (75 MHz, CDCl3) δ 160.5, 147.2, 143.8, 134.1, 127.1, 127.0, 126.9, 121.5, 53.3, 32.5, 25.8, 25.2; ATR-IR (neat) 3065, 2925, 2853, 1662, 1559, 1473, 1328, 1130, 770, 697 cm⁻¹; HRMS m/z (M⁺) calcd for C14H16N2O: 228.1263. Found: 228.1263.

3-(Tert-butyl)-6-methoxyquinazolin-4(3H)-one (11c): Prepared from S-ethyl 2-amino-5-methoxybenzothioate 3f (57 mg, 0.27 mmol) and 2-isocyano-2-methylpropane 10a (23 mg, 0.27 mmol) over 12 h according to the general procedure. The product was obtained as a solid (52 mg, 83%), mp: 106–108 °C; 1H NMR (600 MHz, CDCl3) δ 8.19 (1H, s), 7.62 (1H, d, J = 2.4 Hz), 7.56 (1H, d, J = 9.0 Hz), 7.28 (1H, dd, J = 9.0, 3.0 Hz), 3.87 (3H, s), 1.72 (9H, s); 13C NMR (150 MHz, CDCl3) δ 161.7, 158.5, 141.8, 141.7, 128.2, 124.3, 105.7, 60.7, 55.7, 28.6; ATR-IR (neat) 3099, 2923, 1651, 1491, 1358, 1301, 1217, 1028, 837, 736, 554 cm⁻¹; HRMS m/z (M⁺) calcd for C13H16N2O2: 232.1212. Found: 232.1209.
3-(Tert-butyl)-6-chloroquinazolin-4(3H)-one (11d): Prepared from S-ethyl 2-amino-5-chlorobenzothioate (3i) (58 mg, 0.27 mmol) and 2-isocyano-2-methylpropane **10a** (23 mg, 0.27 mmol) over 10 h according to the general procedure. The product was obtained as a solid (50 mg, 78%), mp: 120–122 °C; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) \( \delta \) 8.29 (1H, s), 8.22 (1H, s), 7.64–7.59 (2H, m), 1.72 (9H, s); \textsuperscript{13}C NMR (150 MHz, CDCl\textsubscript{3}) \( \delta \) 160.7, 145.3, 144.2, 134.4, 132.8, 128.2, 126.1, 124.0, 61.3, 28.5; ATR-IR (neat) 2922, 2853, 1672, 1597, 1378, 1315, 1254, 1094, 930, 828 cm\(^{-1}\); HRMS \textit{m/z} (M\(^{+}\)) calced for C\textsubscript{12}H\textsubscript{13}ClN\textsubscript{2}O: 236.0716. Found: 236.0719.

6-Chloro-3-cyclohexylquinazolin-4(3H)-one (11e): Prepared from S-ethyl 2-amino-5-chlorobenzothioate (3i) (58 mg, 0.27 mmol) and isocyanocyclohexane **10b** (30 mg, 0.27 mmol) over 10 h according to the general procedure. The product was obtained as a solid (50 mg, 70%), mp: 110–112 °C; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) \( \delta \) 8.24 (1H, d, \( J = 1.8 \) Hz), 8.08 (1H, s), 7.65–7.60 (2H, m), 4.78–4.74 (1H, m), 1.98–1.91 (4H, m), 1.78–1.75 (1H, m), 1.64–1.57 (2H, m), 1.52–1.46 (2H, m), 1.26–1.20 (1H, m); \textsuperscript{13}C NMR (150 MHz, CDCl\textsubscript{3}) \( \delta \) 15.6, 145.9, 144.0, 134.5, 132.9, 128.8, 126.3, 122.9, 53.6, 32.5, 25.8, 25.2; ATR-IR (neat) 2935, 2853, 1672, 1600, 1472, 1255, 825, 647, 518 cm\(^{-1}\); HRMS \textit{m/z} (M\(^{+}\)) calcd for C\textsubscript{14}H\textsubscript{15}ClN\textsubscript{2}O: 262.0873. Found: 262.0870.

3-(Tert-butyl)-6-fluoroquinazolin-4(3H)-one (11f): Prepared from S-ethyl 2-amino-5-fluorobenzothioate (3m) (54 mg, 0.27 mmol) and 2-isocyano-2-methylpropane **10a** (23 mg, 0.27 mmol) over 10 h according to the general procedure. The product was obtained as a solid (48 mg, 80%), mp: 105–107 °C; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) \( \delta \) 8.27 (1H, s), 7.88 (1H, dd, \( J = 8.4, 2.4 \) Hz), 7.67–7.65 (1H, m), 7.44–7.40 (1H, m), 1.73 (9H, s); \textsuperscript{13}C NMR (150 MHz, CDCl\textsubscript{3}) \( \delta \) 161.1, 161.0 (d, \( J = 247.0 \) Hz), 143.6, 143.2 (d, \( J = 2.4 \) Hz), 128.9 (d, \( J = 8.1 \) Hz), 124.3, 122.6 (d, \( J = 24.1 \) Hz), 111.5 (d, \( J = 22.9 \) Hz), 61.1, 28.5, 25.8, 25.2; ATR-IR (neat) 2924, 2853, 1672, 1600, 1472, 1255, 825, 647, 518 cm\(^{-1}\); HRMS \textit{m/z} (M\(^{+}\)) calcd for C\textsubscript{12}H\textsubscript{13}FN\textsubscript{2}O: 220.1012. Found: 220.1012.

6-Chloro-3-cyclohexylquinazolin-4(3H)-one (11g): Prepared from S-ethyl 2-amino-5-chlorobenzothioate (3i) (58 mg, 0.27 mmol) and isocyanocyclohexane **10b** (30 mg, 0.27 mmol) over 10 h according to the general procedure. The product was obtained as a solid (50 mg, 75%), mp: 106–108 °C; \textsuperscript{1}H NMR (600 MHz, CDCl\textsubscript{3}) \( \delta \) 8.27 (1H, s), 7.88 (1H, dd, \( J = 9.0, 3.0 \) Hz), 7.66–7.63 (1H, m), 7.41–7.38 (1H, m), 4.78–4.70 (1H, m), 1.73–1.71 (4H, m), 1.61–1.54 (2H, m), 1.49–1.41 (2H, m), 1.23–1.15 (1H, m); \textsuperscript{13}C NMR (150 MHz, CDCl\textsubscript{3}) \( \delta \) 161.1 (d, \( J = 252.4 \) Hz), 160.2, 143.8, 143.2, 129.5 (d, \( J = 8.1 \) Hz), 122.7 (d, \( J = 24.1 \) Hz), 111.9, 111.7, 53.6, 32.5, 25.8, 25.2; ATR-IR (neat) 3075, 2928, 2855, 1672, 1483, 1259, 1124, 891, 831, 723, 630 cm\(^{-1}\); HRMS \textit{m/z} (M\(^{+}\)) calcd for C\textsubscript{14}H\textsubscript{15}FN\textsubscript{2}O: 246.1168. Found: 246.1166.
Copies of NMR spectra of substrates (1a-1e)

$^1$H NMR of 1a
(300 MHz, DMSO-$d_6$)

$^{13}$C NMR of 1a
(75 MHz, DMSO-$d_6$)
$^1$H NMR of 1b  
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 1b  
(75 MHz, CDCl$_3$)
$^1$H NMR of 1c
(300 MHz, DMSO-d$_6$)

$^{13}$C NMR of 1c
(75 MHz, DMSO-d$_6$)
$^1$H NMR of 1d
(300 MHz, DMSO-$d_6$)

$^{13}$C NMR of 1d
(75 MHz, DMSO-$d_6$)
\( ^1 \text{H NMR of 1e} \)

\( 300 \text{ MHz, DMSO}\text{-d}_6 \)

\[ \begin{array}{c}
\text{Spectrum Image}
\end{array} \]

\( ^{13} \text{C NMR of 1e} \)

\( 75 \text{ MHz, DMSO-d}_6 \)

\[ \begin{array}{c}
\text{Spectrum Image}
\end{array} \]
Copies of NMR spectra of synthesized compounds (3, 4, 5, 6 and 11)
$^1$H NMR of 3b
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 3b
(75 MHz, CDCl$_3$)
$^1$H NMR of 3c
(300 MHz, CDCl₃)

$^{13}$C NMR of 3c
(75 MHz, CDCl₃)
$^1$H NMR of 3d
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 3d
(75 MHz, CDCl$_3$)
$$^{1}H\text{ NMR of }3e$$

(300 MHz, CDCl$_3$)

$$^{13}C\text{ NMR of }3e$$

(75 MHz, CDCl$_3$)
$^1$H NMR of 3f (300 MHz, CDCl$_3$)

$^{13}$C NMR of 3f (75 MHz, CDCl$_3$)
H NMR of 3g (300 MHz, CDCl₃)

C NMR of 3g (75 MHz, CDCl₃)
$^1$H NMR of 3h (300 MHz, CDCl$_3$)

$^{13}$C NMR of 3h (75 MHz, CDCl$_3$)
\( \text{H NMR of 3i} \)

(300 MHz, CDCl\(_3\))

\( \text{C NMR of 3i} \)

(75 MHz, CDCl\(_3\))

\( \text{S O NH}_2 \text{Cl} \)
$^1$H NMR of 3j
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 3j
(75 MHz, CDCl$_3$)
$^1$H NMR of 3k
(600 MHz, CDCl$_3$)

$^{13}$C NMR of 3k
(150 MHz, CDCl$_3$)
$^1$H NMR of 3l
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 3l
(75 MHz, CDCl$_3$)
$^1$H NMR of 3m
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 3m
(75 MHz, CDCl$_3$)
$^1$H NMR of 3n
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 3n
(75 MHz, CDCl$_3$)
$^1$H NMR of 3o
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 3o
(75 MHz, CDCl$_3$)
\[ \text{H NMR of } 3p \] 
(300 MHz, CDCl\textsubscript{3})

\[ \text{\textsuperscript{13}C NMR of } 3p \] 
(75 MHz, CDCl\textsubscript{3})

\[ \text{O}_2\text{N} - \text{S} - \text{NH}_2 \]
$^1$H NMR of 4a
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 4a
(75 MHz, CDCl$_3$)
$^1$H NMR of 4b
(600 MHz, CDCl$_3$)

$^{13}$C NMR of 4b
(150 MHz, CDCl$_3$)
$\text{H NMR of 4c (300 MHz, CDCl$_3$)}$

$\text{\textsuperscript{13}C NMR of 4c (75 MHz, CDCl$_3$)}$
$^1$H NMR of 4d (600 MHz, CDCl$_3$)

$^{13}$C NMR of 4d (150 MHz, CDCl$_3$)
**1H NMR of 4e**

(600 MHz, CDCl₃)

**13C NMR of 4e**

(150 MHz, CDCl₃)
\[ \text{1H NMR of 4f} \\
(300 MHz, CDCl}_3) \]

\[ \text{13C NMR of 4f} \\
(75 MHz, CDCl}_3) \]
$^1$H NMR of 4g (600 MHz, CDCl$_3$)

$^{13}$C NMR of 4g (150 MHz, CDCl$_3$)
$^1$H NMR of 5a (300 MHz, CDCl$_3$)

$^{13}$C NMR of 5a (75 MHz, CDCl$_3$)
$^1$H NMR of 5b
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 5b
(75 MHz, CDCl$_3$)
$^1$H NMR of 5c
(400 MHz, CDCl$_3$)

$^{13}$C NMR of 5c
(100 MHz, CDCl$_3$)
$^1\text{H NMR of 5d} (600 \text{ MHz, DMSO-$d_6$})$

$^{13}\text{C NMR of 5d} (150 \text{ MHz, DMSO-$d_6$})$
$^1$H NMR of 5e
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 5e
(75 MHz, CDCl$_3$)
$^1$H NMR of 5f
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 5f
(75 MHz, CDCl$_3$)
$^1$H NMR of 5g
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 5g
(75 MHz, CDCl$_3$)
$^1$H NMR of 5h
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 5h
(75 MHz, CDCl$_3$)
$^{1}$H NMR of 5i
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 5i
(75 MHz, CDCl$_3$)
$^1$H NMR of 6 (600 MHz, CDCl$_3$)

$^{13}$C NMR of 6 (150 MHz, CDCl$_3$)
$^1$H NMR of 11a
(600 MHz, CDCl$_3$)

$^{13}$C NMR of 11a
(150 MHz, CDCl$_3$)
$^1$H NMR of 11b
(300 MHz, CDCl$_3$)

$^{13}$C NMR of 11b
(150 MHz, CDCl$_3$)
$^1$H NMR of 11c  
(600 MHz, CDCl$_3$)

$^{13}$C NMR of 11c  
(150 MHz, CDCl$_3$)
$^1$H NMR of 11d
(600 MHz, CDCl$_3$)

$^{13}$C NMR of 11d
(150 MHz, CDCl$_3$)
$^1$H NMR of 11e  
(600 MHz, CDCl$_3$)

$^{13}$C NMR of 11e  
(150 MHz, CDCl$_3$)
$^1$H NMR of 11f
(600 MHz, CDCl$_3$)

$^1$C NMR of 11f
(150 MHz, CDCl$_3$)
Experimental section for fluorescence sensing

Fluorescence sensing of Fe$^{3+}$ ions

The fluorescent spectra of nine of the synthesized compounds (0.001 M) were measured in acetonitrile at room temperature, upon excitation wavelength at 360 nm. Then, 0.50 mL of compound $3n$ (0.001 M) in acetonitrile was taken in a 4 mL quartz cuvette as a fluorescent probe and was titrated with 50 µM of various metal ions in acetonitrile for selectivity studies. Further, the fluorescent sensitivity of compound $3n$ (0.001 M) was studied towards different concentrations of Fe$^{3+}$ in acetonitrile. All the fluorescent (Hitachi-7000 F) measurements were carried out at room temperature at 360 nm (excitation wavelength).