Novel Synthesis and Reactions of 5,7-Dialkyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carbonitrile and 6-Methyl-4-oxo-4*H*-1-aza-5-oxa-2-thiaindene-3-carbonitriles

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Supporting Information

5-Ethyl-7-methyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carbonitrile (**4b**).

From the reaction of **1** (165 mg, 0.79 mmol), 6-amino-3-ethyl-1-methyluracil (65 mg, 0.39 mmol) and pyridine (98 mg, 1.24 mmol) for 1 day was obtained **4b** (68 mg, 74%): mp 160–161 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 2960, 2224, 1712, 1674, 1648, 1437, 1363, 1325, 1261, 1229, 1213, 1178, 1088, 997, 774, 742 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.28 (t, *J* = 7.1 Hz, 3H), 3.68 (s, 3H), 4.10 (q, *J* = 7.1 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 13.0, 30.8, 37.6, 108.5, 120.0, 138.0, 150.1, 154.7, 157.1. Anal. Calcd for C₉H₈N₄O₂S: C, 45.75; H, 3.41; N, 23.71; S, 13.57. Found: C, 45.68; H, 3.37; N, 23.88; S, 13.69.

5-Isopropyl-7-methyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carbonitrile

(**4c**). From the reaction of **1** (240 mg, 1.15 mmol), 6-amino-3-isopropyl-1-methyluracil (106 mg, 0.58 mmol) and pyridine (196 mg, 2.48 mmol) for 1 day was obtained **4c** (118 mg, 81%): mp 117–118 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 2960, 2204, 1722, 1661, 1574, 1504, 1446, 1347, 1261, 1229, 1206, 1158, 1088, 1002, 874, 718, 742 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.48 (d, *J* = 6.5 Hz, 6H), 3.62 (s, 3H), 5.19–5.26 (m, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 19.3, 30.7, 47.4, 108.7, 120.3, 138.0, 150.2, 155.1, 157.2. Anal. Calcd for C₁₀H₁₀N₄O₂S: C, 47.99; H, 4.03; N, 22.39; S,

12.81. Found: C, 48.12; H, 4.00; N, 22.45; S, 12.70.

5-*n*-Butyl-7-methyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carbonitrile

(4d). From the reaction of **1** (150 mg, 0.72 mmol), 6-amino-3-*n*-butyl-1-methyluracil (69 mg, 0.35 mmol) and pyridine (127 mg, 1.60 mmol) for 1 day was obtained **4d** (54 mg, 57%): mp 110–112 °C (MeOH); IR (KBr): 2944, 2208, 1712, 1664, 1568, 1501, 1421, 1331, 1267, 1181, 742 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 0.97 (t, *J* = 7.3 Hz, 3H), 1.37–1.44 (m, 2H), 1.62–1.68 (m, 2H), 3.65 (s, 3H), 4.03 (t, *J* = 7.6 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 14.1, 20.6, 30.2, 31.2, 42.6, 108.9, 120.4, 138.5, 150.7, 155.2, 157.5. Anal. Calcd for C₁₁H₁₂N₄O₂S: C, 49.99; H, 4.58; N, 21.20; S, 12.13. Found: C, 50.08; H, 4.55; N, 21.35; S, 12.20.

5-Allyl-7-methyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carbonitrile (4e).

From the reaction of **1** (255 mg, 1.22 mmol), 3-allyl-6-amino-1-methyluracil (103 mg, 0.57 mmol) and pyridine (176 mg, 2.23 mmol) for 1 day was obtained **4e** (66 mg, 47%): mp 129–130 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 2224, 1715, 1667, 1571, 1504, 1421, 1373, 1318, 1267, 1235, 1184, 928, 861, 778, 742 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 3.66 (s, 3H), 4.63 (d, *J* = 6.1 Hz, 2H), 5.25 (d, *J* = 10.1 Hz, 1H), 5.35 (d, *J* = 17.0 Hz, 1H), 5.83–5.96 (m, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 30.9, 44.2, 108.4, 119.4, 119.8, 130.8, 138.3, 150.0, 154.5, 157.1. Anal. Calcd for C₁₀H₈N₄O₂S: C, 48.38; H, 3.25; N, 22.57; S, 12.92. Found: C, 48.30; H, 3.27; N, 22.39; S, 12.78.

5-(3-Butenyl)-7-methyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-

carbonitrile (4f). From the reaction of **1** (242 mg, 1.16 mmol), 6-amino-3-(3-butenyl)-1-methyluracil (100 mg, 0.56 mmol) and pyridine (196 mg, 2.48 mmol) for 1 day was obtained **4f** (69 mg, 47%): mp 93–94 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 2224, 1715, 1661, 1568, 1424, 1350, 1328, 1267, 1235, 1181, 1104, 912, 864, 781 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 2.41–2.48 (m, 2H), 3.67 (s, 3H), 4.11 (t, *J* = 7.2 Hz, 2H), 5.03 (d, *J* = 9.0 Hz, 1H), 5.07 (d, *J* = 16.0 Hz, 1H), 5.76–5.89 (m, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 30.8, 32.1, 41.5, 108.5, 117.6, 119.8, 134.2, 138.2, 150.2, 154.8, 157.1. Anal. Calcd for C₁₁H₁₀N₄O₂S: C, 50.37; H, 3.84; N, 21.36; S, 12.23. Found: C, 50.43; H, 3.87; N, 21.29; S, 12.41.

7-Methyl-5-(4-pentenyl)-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-

carbonitrile (4g). From the reaction of **1** (270 mg, 1.29 mmol), 6-amino-1-methyl-3-(4-

pentenyl)uracil (120 mg, 0.57 mmol) and pyridine (147 mg, 1.86 mmol) for 1 day was obtained **4g** (55 mg, 35%): mp 66–67 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 2224, 1715, 1667, 1574, 1498, 1421, 1354, 1331, 1264, 1229, 1174, 1001, 989, 909, 778, 742 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.75–1.83 (m, 2H), 2.15 (q, *J* = 7.5 Hz, 2H), 3.67 (s, 3H), 4.04 (t, *J* = 7.5 Hz, 2H), 4.99 (d, *J* = 10.2 Hz, 1H), 5.07 (d, *J* = 17.1 Hz, 1H), 5.76–5.89 (m, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 27.1, 31.2, 31.4, 42.4, 108.9, 115.7, 120.3, 137.7, 138.5, 150.6, 155.2, 157.5. Anal. Calcd for C₁₂H₁₂N₄O₂S: C, 52.16; H, 4.38; N, 20.28; S, 11.60. Found: C, 52.00; H, 4.36; N, 20.43; S, 11.42.

7-Methyl-5-(4-pentynyl)-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-

carbonitrile (4h). From the reaction of **1** (640 mg, 3.07 mmol), 6-amino-1-methyl-3-(4-pentynyl)uracil (317 mg, 1.53 mmol) and pyridine (489 mg, 6.18 mmol) for 1 day was obtained **4h** (57 mg, 14%): mp 131–132 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3248, 2224, 1706, 1664, 1506, 1504, 1418, 1382, 1357, 1331, 1264, 1232, 1181, 1153, 1062, 992, 870, 774, 691, 672 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.87–1.97 (m, 3H), 2.28–2.34 (m, 2H), 3.70 (s, 3H), 4.15 (t, *J* = 7.3 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 16.3, 26.3, 30.8, 41.5, 69.0, 82.9, 108.5, 119.8, 138.2, 150.3, 154.9, 157.1. Anal. Calcd for C₁₂H₁₀N₄O₂S: C, 52.54; H, 3.67; N, 20.43; S, 11.69. Found: C, 52.74; H, 3.62; N, 20.58; S, 11.81.

5-Benzyl-7-methyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carbonitrile

(4i). From the reaction of **1** (358 mg, 1.72 mmol), 6-amino-3-benzyl-1-methyluracil (199 mg, 0.86 mmol) and pyridine (245 mg, 3.08 mmol) for 1 day was obtained **4i** (200 mg, 78%): mp 140–142 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 2224, 1709, 1664, 1571, 1504, 1421, 1376, 1328, 1261, 1229, 1146, 1072, 1024, 861, 742, 698 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 3.64 (s, 3H), 5.17 (s, 2H), 7.24–7.32 (m, 3H), 7.49–7.52 (m, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 31.3, 45.7, 108.9, 120.3, 128.5, 129.0, 129.8, 136.3, 138.7, 150.7, 155.2, 157.5. Anal. Calcd for C₁₄H₁₀N₄O₂S: C, 56.37; H, 3.38; N, 18.78; S, 10.75. Found: C, 56.41; H, 3.38; N, 18.69; S, 10.83.

General procedure for the reactions of 5,7-dimethyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carbonitrile (4a) with alkylamines. To a solution of **4a** (0.37–0.80 mmol) in DMF (5 mL) was added alkyl amine (0.73–1.99 mmol). The mixture was stirred at reflux temperature for 1 h. After removal of the solvent *in vacuo*, the residue was chromatographed on a silica gel (70–230 mesh, 2 x 10 cm). Elution with a mixture of *n*-hexane and

EtOAc (3:1) gave 5,7-dimethyl-3-alkylamino-7*H*-isothiazolo[3,4-*d*]pyrimidine-4,6-diones (**5a-c**).

5,7-Dimethyl-3-*n*-propylamino-7*H*-isothiazolo[3,4-*d*]pyrimidine-4,6-dione (5a**).** From the reaction of **4a** (82 mg, 0.37 mmol) and *n*-propylamine (74 mg, 0.73 mmol) for 1 h was obtained **5a** (91 mg, 97%): mp 160–161 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 3312, 2944, 1690, 1642, 1584, 1539, 1501, 1443, 1261, 1245, 1098, 1062, 771 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.03 (t, *J* = 7.4 Hz, 3H), 1.70–1.82 (m, 2H), 3.17–3.24 (m, 2H), 3.34 (s, 3H), 3.51 (s, 3H), 7.45 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 11.3, 22.2, 27.3, 29.3, 49.7, 94.7, 151.7, 155.7, 160.1, 177.7. Anal. Calcd for C₁₀H₁₄N₄O₂S: C, 47.23; H, 5.55; N, 22.03; S, 12.61. Found: C, 47.09; H, 5.53; N, 22.21; S, 12.79.

3-Allylamino-5,7-dimethyl-7*H*-isothiazolo[3,4-*d*]pyrimidine-4,6-dione (5b**).** From the reaction of **4a** (178 mg, 0.80 mmol) and allylamine (114 mg, 1.99 mmol) for 1 h was obtained **5b** (190 mg, 94%): mp 146–147 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 3296, 1693, 1645, 1574, 1504, 1427, 1353, 1267, 1235, 1091, 1069, 979, 925, 771, 742 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 3.32 (s, 3H), 3.49 (s, 3H), 3.87–3.91 (m, 2H), 5.33 (d, *J* = 10.2 Hz, 1H), 5.40 (d, *J* = 17.0 Hz, 1H), 5.83–5.94 (m, 1H), 7.67 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 27.3, 29.3, 49.8, 95.1, 119.1, 131.1, 151.6, 155.4, 159.9, 177.5. Anal. Calcd for C₁₀H₁₂N₄O₂S: C, 47.61; H, 4.79; N, 22.21; S, 12.71. Found: C, 47.63; H, 4.79; N, 22.11; S, 12.90.

3-[2-(1*H*-Indol-3-yl)ethyl]amino-5,7-dimethyl-7*H*-isothiazolo[3,4-*d*]pyrimidine-4,6-dione (5c**).** From the reaction of **4a** (77 mg, 0.35 mmol) and tryptamine (90 mg, 0.56 mmol) for 5 h was obtained **5c** (93 mg, 74%): mp 178–179 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 3360, 3312, 1690, 1632, 1504, 1446, 1331, 1261, 1101, 1062, 771, 733 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 3.19 (t, *J* = 6.8 Hz, 2H), 3.32 (s, 3H), 3.50 (s, 3H), 3.50–3.57 (m, 2H), 7.11–7.26 (m, 3H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.54 (s, br, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 8.31 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 25.3, 29.7, 48.3, 51.2, 95.2, 111.7, 111.9, 118.7, 120.1, 122.8, 122.9, 127.2, 136.9, 152.1, 156.0, 160.3, 177.9. Anal. Calcd for C₁₇H₁₇N₅O₂S: C, 57.45; H, 4.82; N, 19.70; S, 9.02. Found: C, 57.32; H, 4.88; N, 19.86; S, 9.21.

3-Ethylsulfanyl-5,7-dimethyl-7*H*-isothiazolo[3,4-*d*]pyrimidine-4,6-dione (5d**).** To a solution of NaH (50 mg, 1.25 mmol) and ethanethiol (84 mg, 1.35 mmol) in THF (10 mL) was added **4a** (94

mg, 0.42 mmol). The mixture was stirred at rt for 3 h. Water (30 mL) was added and after removal of THF *in vacuo*, the mixture was extracted with CH₂Cl₂ (25 mL x 3). The combined extracts were dried over MgSO₄, followed by evaporation of the solvent. The residue was chromatographed on a silica gel (70–230 mesh, 2 x 10 cm). Elution with a mixture of *n*-hexane and EtOAc (3:1) gave **5d** (100 mg, 92%): mp 164–166 °C (CH₂Cl₂ –*n*-hexane); IR (KBr) 1696, 1648, 1539, 1498, 1418, 1350, 1270, 1235, 1069, 1011, 835, 768, 742 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.53 (t, *J* = 7.4 Hz, 3H), 3.11 (q, *J* = 7.4 Hz, 2H), 3.38 (s, 3H), 3.58 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 13.4, 27.9, 28.8, 30.1, 110.6, 151.3, 157.3, 157.7, 175.0. Anal. Calcd for C₉H₁₁N₃O₂S₂: C, 42.01; H, 4.31; N, 16.33; S, 24.92. Found: C, 41.89; H, 4.37; N, 16.21; S, 25.11.

5,7-Dimethyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carboxylic amide (5e). To a solution of NaOH (42 mg, 1.05 mmol) in THF/H₂O (10/2 mL) was added **4a** (79 mg, 0.36 mmol). The mixture was stirred at rt for 1 h. Water (30 mL) was added and after removal of THF *in vacuo*, the residue was filtered and recrystallized from MeOH to give **5e** (45 mg, 53%): mp >300 °C (MeOH); IR (KBr) 3216, 3120, 1696, 1651, 1562, 1491, 1434, 1366, 1286, 1238, 1088, 986, 787, 746, 707 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 3.04 (s, 3H), 3.28 (s, 3H), 8.32 (s, br, 1H), 9.51 (s, br, 1H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 29.4, 31.1, 112.2, 150.9, 159.5, 159.5, 159.7, 171.3. Anal. Calcd for C₈H₈N₄O₃S: C, 40.00; H, 3.36; N, 23.32; S, 13.35. Found: C, 39.91; H, 3.38; N, 23.47; S, 13.51.

5,7-Dimethyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carbothioic amide (5f). To a solution of **4a** (109 mg, 0.49 mmol) in DMF (5 mL) was added NaSH·xH₂O (126 mg). The mixture was stirred at rt for 1 h. After removal of the solvent *in vacuo*, the residue was chromatographed on a silica gel (70–230 mesh, 2 x 10 cm). Elution with a mixture of *n*-hexane and EtOAc (3:1) gave **5f** (40 mg, 33%): mp 225–227 °C (CH₂Cl₂); IR (KBr) 3296, 3216, 1699, 1651, 1613, 1549, 1491, 1418, 1398, 1363, 1283, 1232, 1146, 1088, 954, 851, 736 cm⁻¹; ¹H NMR (300 MHz, DMSO-*d*₆) δ 3.41 (s, 3H), 3.62 (s, 3H), 7.95 (s, br, 1H), 15.05 (s, br, 1H); ¹³C NMR (75 MHz, DMSO-*d*₆) δ 29.6, 31.0, 109.5, 150.8, 159.8, 160.0, 175.6, 184.9. Anal. Calcd for C₈H₈N₄O₂S₂: C, 37.49; H, 3.15; N, 21.86; S, 25.02. Found: C, 37.34; H, 3.18; N, 21.78; S, 25.24.

5,7-Dimethyl-3-(2*H*-tetrazol-5-yl)-7*H*-isothiazolo[3,4-*d*]pyrimidine-4,6-dione (5g)

To a solution of **4a** (81 mg, 0.36 mmol) in DMF (5 mL) was added NaN₃ (64 mg, 0.98 mmol). The

mixture was stirred at reflux for 1 h. After removal of DMF *in vacuo*, 5% aq HCl (30 mL) was added and the residue was filtered and recrystallized from MeOH to give **5g** (78 mg, 81%): mp 210–212 °C (MeOH); IR (KBr) 3184, 1709, 1648, 1594, 1530, 1418, 1364, 1277, 1235, 1197, 1146, 1043, 784, 736, 502 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 3.55 (s, 3H), 3.74 (s, 3H), 15.60 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 29.2, 31.0, 112.5, 146.2, 150.1, 154.0, 157.9, 159.1. Anal. Calcd for C₈H₇N₇O₂S: C, 36.22; H, 2.66; N, 36.96; S, 12.09. Found: C, 36.36; H, 2.61; N, 36.79; S, 12.23.

5,7-Dimethyl-4,6-dioxo-4,5,6,7-tetrahydroisothiazolo[3,4-*d*]pyrimidine-3-carboximidic ethyl ester (5h). To a solution of Na (23 mg, 1.00 mmol) in EtOH (10 mL) was added **4a** (105 mg, 0.47 mmol). The mixture was stirred at rt for 24 h. Water (30 mL) was added and after removal of EtOH *in vacuo*, the mixture was extracted with CH₂Cl₂ (25 mL x 3). The combined extracts were dried over MgSO₄, followed by evaporation of the solvent. The residue was recrystallized from CH₂Cl₂ and *n*-hexane to give **5h** (102 mg, 80%): mp 160–161 °C (CH₂Cl₂ – *n*-hexane); IR (KBr): 3200, 2976, 1702, 1651, 1558, 1488, 1421, 1357, 1315, 1274, 1168, 1098, 1082, 1037, 1018, 925, 883 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.39 (t, *J* = 7.1 Hz, 3H), 3.44 (s, 3H), 3.64 (s, 3H), 4.35 (q, *J* = 7.1 Hz, 2H), 10.89 (s, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 14.4, 29.2, 30.9, 62.8, 113.4, 150.8, 154.2, 156.0, 158.4, 165.2. Anal. Calcd for C₁₀H₁₂N₄O₃S: C, 44.77; H, 4.51; N, 20.88; S, 11.95. Found: C, 44.58; H, 4.53; N, 20.95; S, 11.78.

6-Methyl-4-oxo-4*H*-1-aza-5-oxa-2-thiaindene-3-carbontirile (8). To a suspension of 4-chloro-5*H*-1,2,3-dithiazolium chloride (**1**) (684 mg, 3.28 mmol) in CH₂Cl₂ (30 mL) was added 4-amino-6-methylpyran-2-one (209 mg, 1.67 mmol), followed by dropwise addition of pyridine (538 mg, 6.80 mmol). The mixture was stirred for 24 h at rt. Water (30 mL) was added and the mixture was extracted with CH₂Cl₂ (25 mL x 3). The combined extracts were dried over MgSO₄, followed by evaporation of the solvent. The residue was chromatographed on a silica gel (70–230 mesh, 2 x 10 cm). Elution with *n*-hexane gave sulfur. Subsequent elution with a mixture of *n*-hexane and EtOAc (5:1) gave 4-chloro-5*H*-1,2,3-dithiazole-5-thione (144 mg, 26%). Subsequent elution with a mixture of *n*-hexane and EtOAc (3:1) gave **8** (160 mg, 50%): mp 185–186 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 2224, 1741, 1635, 1520, 1424, 1280, 1235, 1156, 1104, 1069, 976, 810 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 2.35 (s, 3H), 6.56 (s, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 19.9, 100.7, 108.6, 125.0, 139.6, 155.3, 160.7, 163.9. Anal. Calcd for C₈H₄N₂O₂S: C, 49.99; H, 2.10; N, 14.58; S, 16.68. Found: C, 50.13; H, 2.04; N, 14.69; S, 16.72.

4-Oxo-4H-chromeno[4,3-c]isothiazole-3-carbonitrile (9). To a suspension of 4-chloro-5H-1,2,3-dithiazolium chloride (**1**) (971 mg, 4.66 mmol) in CH₂Cl₂ (30 mL) was added 4-aminochromen-2-one (375 mg, 2.33 mmol), followed by dropwise addition of pyridine (489 mg, 6.18 mmol). The mixture was stirred for 24 h at rt. Water (30 mL) was added and the mixture was extracted with CH₂Cl₂ (25 mL x 3). The combined extracts were dried over MgSO₄, followed by evaporation of the solvent. The residue was chromatographed on a silica gel (70–230 mesh, 2 x 10 cm). Elution with *n*-hexane gave sulfur. Subsequent elution with a mixture of *n*-hexane and EtOAc (5:1) gave 4-chloro-5H-1,2,3-dithiazole-5-thione (32 mg, 4%). Subsequent elution with a mixture of *n*-hexane and EtOAc (3:1) gave **9** (349 mg, 66%): mp (dec) 260–263 °C (CHCl₃); IR (KBr) 2208, 1734, 1600, 1581, 1530, 1450, 1270, 1245, 1190, 1146, 1146, 1114, 1094, 947, 899, 765 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 7.46–7.55 (m, 2H), 7.69–7.75 (m, 1H), 8.23 (d, *J* = 7.8 Hz, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 110.6, 117.0, 118.2, 124.8, 126.3, 128.3, 133.9, 140.1, 153.3, 155.5, 161.6; MS (*m/z*): 228 (M⁺, 100%), 200 (9), 171 (2). Anal. Calcd for C₁₁H₄N₂O₂S: C, 57.89; H, 1.77; N, 12.27; S, 14.05. Found: C, 57.67; H, 1.74; N, 12.41; S, 14.23.

General procedure for the reactions of 6-methyl-4-oxo-4H-1-aza-5-oxa-2-thiaindene-3-carbonitrile (8) with alkylamines.

To a solution of 6-methyl-4-oxo-4H-1-aza-5-oxa-2-thiaindene-3-carbonitrile (**8**) (0.20–0.47 mmol) in DMF (5 mL) was added alkylamine (0.38–1.37 mmol). The mixture was stirred for 0.5–2 h at 50 °C. After removal of the solvent *in vacuo*, the residue was chromatographed on a silica gel (70–230 mesh, 2 x 10 cm). Elution with a mixture of *n*-hexane and EtOAc (3:1) gave **11**.

5-Cyano-3-(2-oxopropyl)isothiazole-4-carboxylic acid *n*-propylamide (11a). From the reaction of **8** (91 mg, 0.47 mmol) and *n*-propylamine (72 mg, 1.22 mmol) for 1 h was obtained **11a** (82 mg, 70%): mp 146–147 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3280, 2960, 2224, 1706, 1632, 1549, 1418, 1386, 1354, 1293, 1162, 800 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.00 (t, *J* = 7.4 Hz, 3H), 1.58–1.67 (m, 2H), 2.31 (s, 3H), 3.34–3.42 (m, 2H), 4.29 (s, 2H), 6.67 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 11.3, 22.5, 30.2, 42.1, 46.8, 110.2, 132.1, 139.5, 160.2, 164.4, 203.9. Anal. Calcd for C₁₁H₁₃N₃O₂S: C, 52.57; H, 5.21; N, 16.72; S, 12.76. Found: C, 52.73; H, 5.24; N, 16.72; S, 12.58.

5-Cyano-3-(2-oxopropyl)isothiazole-4-carboxylic acid isopropylamide (11b). From the reaction

of **8** (70 mg, 0.36 mmol) and isopropylamine (69 mg, 1.17 mmol) for 0.5 h was obtained **11b** (63 mg, 70%): mp 154–156 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3248, 2974, 2208, 1715, 1648, 1682, 1558, 1418, 1382, 1350, 1315, 1162, 1123, 784 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.27 (d, *J* = 6.5 Hz, 6H), 2.31 (s, 3H), 4.14–4.26 (m, 1H), 4.29 (s, 2H), 6.40 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 22.7, 30.6, 43.1, 47.1, 110.5, 132.5, 140.0, 159.8, 164.7, 204.2. Anal. Calcd for C₁₁H₁₃N₃O₂S: C, 52.57; H, 5.21; N, 16.72; S, 12.76. Found: C, 52.73; H, 5.22; N, 16.69; S, 12.80.

5-Cyano-3-(2-oxopropyl)isothiazole-4-carboxylic acid benzylamide (11c). From the reaction of **8** (70 mg, 0.36 mmol) and benzylamine (147 mg, 1.37 mmol) for 0.5 h was obtained **11c** (57 mg, 53%): mp 136–138 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3248, 2224, 1706, 1632, 1539, 1446, 1424, 1379, 1357, 1315, 1274, 1162, 736 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 2.25 (s, 3H), 4.30 (s, 2H), 4.62 (d, *J* = 5.5 Hz, 2H), 6.90 (s, br, 1H), 7.21–7.47 (m, 5H); ¹³C NMR (75 MHz, CDCl₃) δ 30.6, 44.8, 47.2, 110.5, 128.2, 128.3, 129.3, 132.8, 137.2, 139.3, 160.2, 164.8, 204.4. Anal. Calcd for C₁₅H₁₃N₃O₂S: C, 60.18; H, 4.38; N, 14.04; S, 10.71. Found: C, 60.15; H, 4.38; N, 14.06; S, 10.77.

5-Cyano-3-(2-oxopropyl)isothiazole-4-carboxylic acid allylamide (11d). From the reaction of **8** (70 mg, 0.36 mmol) and allylamine (38 mg, 0.67 mmol) for 1.5 h was obtained **11d** (63 mg, 70%): mp 142–144 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3264, 3072, 2224, 1706, 1635, 1546, 1418, 1386, 1354, 1296, 1162, 982, 803 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 2.31 (s, 3H), 4.03–4.07 (m, 2H), 4.30 (s, 2H), 5.23 (d, *J* = 10.4 Hz, 1H), 5.32 (d, *J* = 15.7 Hz, 1H), 5.85–5.90 (m, 1H), 6.71 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 30.3, 42.6, 46.8, 110.1, 117.4, 132.3, 132.7, 139.1, 160.1, 164.5, 203.9. Anal. Calcd for C₁₁H₁₁N₃O₂S: C, 53.00; H, 4.45; N, 16.86; S, 12.86. Found: C, 53.12; H, 4.43; N, 16.77; S, 12.99.

5-Cyano-3-(2-oxopropyl)isothiazole-4-carboxylic acid *tert*-butylamide (11e). From the reaction of **8** (70 mg, 0.36 mmol) and *t*-butylamine (89 mg, 1.20 mmol) for 2 h was obtained **11e** (61 mg, 64%): mp 144–146 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3344, 3248, 2960, 2224, 1709, 1654, 1632, 1542, 1446, 1414, 1382, 1357, 1312, 1286, 1216, 1158, 813 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.38 (s, 9H), 2.31 (s, 3H), 4.28 (s, 2H), 6.33 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 28.8, 30.6, 47.0, 53.2, 110.5, 132.1, 140.8, 160.6, 164.7, 204.8. Anal. Calcd for C₁₂H₁₅N₃O₂S: C, 54.32; H, 5.70; N, 15.84; S, 12.09. Found: C, 54.40; H, 5.71; N, 15.82; S, 12.12.

5-Cyano-3-(2-oxopropyl)isothiazole-4-carboxylic acid *n*-pentylamide (11f). From the reaction of **8** (76 mg, 0.40 mmol) and *n*-pentylamine (75 mg, 0.86 mmol) for 0.5 h was obtained **11f** (80 mg, 73%): mp 123–124 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3280, 2944, 2224, 1706, 1638, 1552, 1421, 1386, 1354, 1315, 1165, 800, 691 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 0.92 (t, *J* = 7.1 Hz, 3H), 1.35–1.40 (m, 4H), 1.59–1.65 (m, 2H), 2.31 (s, 3H), 3.38–3.48 (m, 2H), 4.30 (s, 2H), 6.56 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 14.4, 22.7, 29.2, 29.3, 30.7, 40.8, 47.2, 110.6, 132.5, 139.8, 160.5, 164.8, 204.1. Anal. Calcd for C₁₃H₁₇N₃O₂S: C, 55.89; H, 6.13; N, 15.04; S, 11.48. Found: C, 55.92; H, 6.12; N, 15.11; S, 11.27.

5-Cyano-3-(2-oxopropyl)isothiazole-4-carboxylic acid *n*-hexylamide (11g). From the reaction of **8** (39 mg, 0.20 mmol) and *n*-hexylamine (38 mg, 0.38 mmol) for 0.5 h was obtained **11g** (40 mg, 67%): mp 108–109 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3264, 2912, 2224, 1715, 1642, 1622, 1555, 1459, 1418, 1379, 1315, 1197, 1155, 794 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 0.90 (t, *J* = 6.7 Hz, 3H), 1.32–1.40 (m, 6H), 1.59–1.64 (m, 2H), 2.31 (s, 3H), 3.42 (q, *J* = 5.9 Hz, 2H), 4.30 (s, 2H), 6.49 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 14.0, 22.5, 26.5, 29.4, 30.3, 31.4, 40.4, 46.8, 110.2, 132.1, 139.2, 160.1, 164.5, 203.8. Anal. Calcd for C₁₄H₁₉N₃O₂S: C, 57.31; H, 6.53; N, 14.32; S, 10.93. Found: C, 57.18; H, 6.55; N, 14.46; S, 11.12.

5-Cyano-3-(2-oxopropyl)isothiazole-4-carboxylic acid [2-(1*H*-indol-3-yl)ethyl]amide (11h). From the reaction of **8** (70 mg, 0.36 mmol) and tryptamine (100 mg, 0.62 mmol) for 1 h was obtained **11h** (83 mg, 66%): mp 151–152 °C (CH₂Cl₂ – *n*-hexane); IR (KBr) 3392, 3264, 2224, 1699, 1629, 1539, 1450, 1421, 1386, 1309, 1162, 806, 733 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 2.20 (s, 3H), 3.07 (t, *J* = 6.6 Hz, 2H), 3.73–3.79 (m, 2H), 4.14 (s, 2H), 6.62 (s, br, 1H), 7.08–7.25 (m, 3H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 8.18 (s, br, 1H); ¹³C NMR (75 MHz, CDCl₃) δ 25.3, 30.6, 40.7, 47.0, 110.5, 111.8, 112.4, 119.0, 120.0, 122.7, 123.2, 127.5, 132.7, 136.9, 139.6, 160.6, 164.6, 204.6. Anal. Calcd for C₁₈H₁₆N₄O₂S: C, 61.35; H, 4.58; N, 15.90; S, 9.10. Found: C, 61.49; H, 4.52; N, 15.72; S, 9.23.

3-(2-Oxopropyl)-6,7,8-trihydro-4*H*-1-thia-2,5,9-triazacyclopentacyclononane-4,10-dione (12). IR (neat) 3472, 2944, 1715, 1651, 1570, 1446, 1395, 1354, 1315, 1274, 1236, 1162, 1088, 982 cm⁻¹; ¹H NMR (300 MHz, CDCl₃) δ 1.90–1.97 (m, 2H), 2.28 (s, 3H), 3.68 (t, *J* = 5.9 Hz, 2H), 3.77 (t, *J* = 5.6 Hz, 2H), 4.11 (s, 2H), 4.68 (s, br, 1H); one NH proton is invisible; ¹³C NMR (75 MHz, CDCl₃)

δ 20.4, 30.5, 38.1, 45.8, 46.9, 138.1, 145.3, 157.1, 160.5, 167.0, 202.7. HRMS ($M^+ + 1$) m/z calcd for $C_{11}H_{13}N_3O_3S$ 267.0756 found 268.0762.

(2-([5-Cyano-3-(2-oxopropyl)isothiazole-4-carbonyl]amino)ethyl)carbamic acid *tert*-butyl ester (13a). From the reaction of **8** (103 mg, 0.54 mmol), ethylenediamine (45 mg, 0.75 mmol) and $(BOC)_2O$ (400 mg, 1.83 mmol) for 10 min was obtained **13a** (127 mg, 68%): mp 150–151 °C ($CH_2Cl_2 - n$ -hexane); IR (KBr) 3360, 3264, 2224, 1709, 1680, 1635, 1552, 1523, 1386, 1360, 1270, 1162, 973 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$) δ 1.43 (s, 9H), 2.31 (s, 3H), 3.34–3.36 (m, 2H), 3.51–3.56 (m, 2H), 4.29 (s, 2H), 5.14 (s, br, 1H), 7.16 (s, br, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 28.6, 28.8, 30.7, 40.4, 47.0, 80.2, 110.4, 132.7, 140.0, 156.9, 161.4, 164.5, 204.6. Anal. Calcd for $C_{15}H_{20}N_4O_4S$: C, 51.12; H, 5.72; N, 15.90; S, 9.10. Found: C, 51.30; H, 5.76; N, 15.79; S, 9.16.

(2-([5-Cyano-3-(2-oxopropyl)isothiazole-4-carbonyl]amino)propyl)carbamic acid *tert*-butyl ester (13b). mp 129–130 °C ($CH_2Cl_2 - n$ -hexane): IR (KBr) 3344, 3296, 2976, 2224, 1706, 1680, 1638, 1526, 1382, 1357, 1274, 1248, 1165 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$) δ 1.44 (s, 9H), 1.69–1.73 (m, 2H), 2.29 (s, 3H), 3.23–3.27 (m, 2H), 3.40–3.49 (m, 2H), 4.28 (s, 2H), 4.94 (s, br, 1H), 7.51 (s, br, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 28.7, 28.8, 30.2, 37.4, 43.3, 47.1, 80.0, 110.4, 132.7, 140.0, 157.2, 161.0, 164.7, 204.0. Anal. Calcd for $C_{16}H_{22}N_4O_4S$: C, 52.44; H, 6.05; N, 15.29; S, 8.75. Found: C, 52.38; H, 6.03; N, 15.36; S, 8.86.

(2-([5-Cyano-3-(2-oxopropyl)isothiazole-4-carbonyl]amino)butyl)carbamic acid *tert*-butyl ester (13c). From the reaction of **8** (118 mg, 0.61 mmol), 1,4-diaminobutane (70 mg, 0.79 mmol) and $(BOC)_2O$ (400 mg, 1.83 mmol) for 10 min was obtained **13c** (141 mg, 61%): mp 128–129 °C ($CH_2Cl_2 - n$ -hexane); IR (KBr) 3312, 3298, 2944, 2224, 1709, 1680, 1632, 1542, 1520, 1440, 1382, 1353, 1309, 1274, 1248, 1165, 1011, 801 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$) δ 1.43 (s, 9H), 1.59–1.62 (m, 4H), 2.31 (s, 3H), 3.14–3.17 (m, 2H), 3.41–3.46 (m, 2H), 4.29 (s, 2H), 5.30 (s, br, 1H), 6.97 (s, br, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 26.1, 26.1, 27.4, 28.4, 30.3, 39.9, 46.7, 79.30, 110.2, 132.1, 139.5, 156.2, 160.4, 164.3, 203.9. Anal. Calcd for $C_{17}H_{24}N_4O_4S$: C, 53.67; H, 6.36; N, 14.73; S, 8.43. Found: C, 53.70; H, 6.33; N, 14.70; S, 8.51.

3-(3-Cyano-6-methyl-4-oxo-4*H*-isothiazolo[4,3-*c*]pyridin-5-yl)carbamic acid *tert*-butyl ester (16). mp 134–135 °C ($CH_2Cl_2 - n$ -hexane): IR (KBr) 3379, 2976, 2224, 1699, 1651, 1606, 1510,

1446, 1389, 1357, 1312, 1251, 1171, 1085, 835 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 1.46 (s, 9H), 1.87–1.96 (m, 2H), 2.48 (s, 3H), 3.21–3.25 (m, 2H), 4.13 (t, J = 7.3 Hz, 2H), 5.13 (s, br, 1H), 6.58 (s, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 21.4, 28.8, 29.8, 38.1, 41.8, 79.8, 102.7, 109.7, 129.8, 137.4, 145.4, 156.6, 158.4, 163.5. Anal. Calcd for $\text{C}_{16}\text{H}_{20}\text{N}_4\text{O}_3\text{S}$: C, 55.15; H, 5.79; N, 16.08; S, 9.20. Found: C, 55.21; H, 5.73; N, 16.20; S, 9.32.

Typical Procedure: To a solution of 6-methyl-4-oxo-4*H*-1-aza-5-oxa-2-thiaindene-3-carbonitrile (**8**) (100 mg, 0.52 mmol) in DMF (5 mL) was added *p*-anisidine (130 mg, 1.05 mmol). The mixture was stirred for 14 h at reflux. After removal of the solvent *in vacuo*, the residue was chromatographed on a silica gel (70–230 mesh, 2 x 10 cm). Elution with a mixture of *n*-hexane and EtOAc (3:1) gave 5-(4-methoxyphenyl)-6-methyl-4-oxo-4,5-dihydroisothiazolo[4,3-*c*]pyridine-3-carbonitrile (**17a**) (71mg, 46%): mp 158–160 °C (CH_2Cl_2 – *n*-hexane): IR (KBr) 3088, 2224, 1734, 1661, 1610, 1504, 1463, 1434, 1389, 1322, 1290, 1270, 1245, 1197, 1168, 1139, 1104, 1020, 832 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 2.06 (s, 3H), 3.88 (s, 3H), 6.64 (s, 1H), 7.05 (d, J = 8.9 Hz, 2H), 7.16 (d, J = 8.9 Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 22.3, 55.6, 101.4, 109.4, 115.1, 129.4, 129.6, 129.9, 137.4, 146.3, 158.1, 159.9, 163.6. Anal. Calcd for $\text{C}_{15}\text{H}_{11}\text{N}_3\text{O}_2\text{S}$: C, 60.59; H, 3.73; N, 14.13; S, 10.78. Found: C, 60.44; H, 3.72; N, 14.21; S, 10.59.

5-(4-Chlorophenyl)-6-methyl-4-oxo-4,5-dihydroisothiazolo[4,3-*c*]pyridine-3-carbonitrile

(**17b**). From the reaction of **8** (85 mg, 0.44 mmol) and *p*-chloroaniline (113 mg, 0.88 mmol) for 24 h was obtained **17b** (37 mg, 28%): mp 152–154 °C (CH_2Cl_2 – *n*-hexane); IR (KBr) 2208, 1661, 1613, 1482, 1318, 1267, 1197, 1085, 1011, 829, 771, 720 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 2.04 (s, 3H), 6.65 (s, 1H), 7.19 (d, J = 8.6 Hz, 2H), 7.52 (d, J = 8.9 Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 22.6, 102.2, 109.7, 130.0, 130.2, 130.6, 135.9, 136.0, 138.0, 145.7, 158.2, 163.8. Anal. Calcd for $\text{C}_{14}\text{H}_8\text{ClN}_3\text{OS}$: C, 55.72; H, 2.67; N, 13.93; S, 10.63. Found: C, 55.68; H, 2.65; N, 13.72; S, 10.85.

6-Methyl-5-(4-methylphenyl)-4-oxo-4,5-dihydroisothiazolo[4,3-*c*]pyridine-3-carbonitriles

(**17c**). From the reaction of **8** (77 mg, 0.40 mmol) and *p*-toluidine (138 mg, 1.29 mmol) for 24 h was obtained **17c** (54 mg, 48%): mp 178–179 °C (CH_2Cl_2 – *n*-hexane); IR (KBr) 2208, 1661, 1610, 1504, 1453, 1427, 1382, 1318, 1267, 1197, 826, 736 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 2.04 (s, 3H), 2.43 (s, 3H), 6.62 (s, 1H), 7.10 (d, J = 8.2 Hz, 2H), 7.33 (d, J = 8.2 Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 21.6, 22.6, 101.8, 109.7, 128.5, 130.3, 130.9, 134.9, 137.9, 139.8, 146.4, 158.3,

164.0. Anal. Calcd for $C_{15}H_{11}N_3OS$: C, 64.04; H, 3.94; N, 14.94; S, 11.40. Found: C, 64.21; H, 3.98; N, 14.88; S, 11.25.

5-(3,5-Dimethoxyphenyl)-6-methyl-4-oxo-4,5-dihydroisothiazolo[4,3,-c]pyridine-3-

carbontitriles (17d). From the reaction of **8** (82 mg, 0.43 mmol) and 3,5-dimethoxyaniline (232 mg, 1.51 mmol) for 48 h was obtained **17d** (57 mg, 41%): mp 205–206 °C (CH_2Cl_2 – *n*-hexane); IR (KBr) 3072, 2208, 1658, 1606, 1578, 1507, 1459, 1421, 1299, 1251, 1194, 1149, 1056, 854, 806, 710 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$) δ 2.12 (s, 3H), 3.75 (s, 6H), 6.37 (s, 2H), 6.57 (s, 1H), 6.62 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 22.1, 55.9, 101.7, 101.8, 107.1, 107.1, 109.7, 130.2, 139.1, 146.2, 158.0, 162.1, 163.9. Anal. Calcd for $C_{16}H_{13}N_3O_3S$: C, 58.70; H, 4.00; N, 12.84; S, 9.80. Found: C, 58.68; H, 4.01; N, 12.89; S, 9.73.

5-(2,5-Dimethoxyphenyl)-6-methyl-4-oxo-4,5-dihydroisothiazolo[4,3,-c]pyridine-3-

carbontitriles (17e). From the reaction of **8** (56 mg, 0.29 mmol) and 2,5-dimethoxyaniline (128 mg, 0.84 mmol) for 48 h was obtained **17e** (17 mg, 18%): mp 208–210 °C (CH_2Cl_2 – *n*-hexane); IR (KBr) 2208, 1661, 1613, 1498, 1453, 1424, 1321, 1277, 1219, 1200, 1178, 1149, 1123, 1034, 1011, 826 cm^{-1} ; 1H NMR (300 MHz, $CDCl_3$) δ 2.03 (s, 3H), 3.76 (s, 3H), 3.79 (s, 3H), 6.62 (s, 1H), 6.77 (s, 1H), 6.99–7.03 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.3, 55.9, 56.2, 101.1, 109.5, 113.0, 115.5, 115.8, 125.9, 129.9, 137.3, 146.5, 149.1, 153.9, 157.4, 163.8. Anal. Calcd for $C_{16}H_{13}N_3O_3S$: C, 58.70; H, 4.00; N, 12.84; S, 9.80. Found: C, 58.62; H, 4.03; N, 12.92; S, 9.99.