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SUPPLEMENTARY MATERIAL TO

Antithyroid activity of some 6-(alkylsulfanyl)-9*H*-purines

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ANALYTICAL AND SPECTRAL DATA OF THE PREPARED COMPOUNDS

*6-(Methylsulfanyl)-9*H*-purine (**1**)*. Yield: 92 %; m.p. 223 °C (lit.** 218–220 °C[22]). Anal. Calcd. for $C_6H_6N_4S$: C, 43.36; H, 3.64; N, 33.71 %. Found: C, 43.33, H, 3.59, N, 33.69 %. ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 13.48 (1H, *s*, NH imidazole), 8.68 (1H, *s*, CH imidazole), 8.42 (1H, *s*, CH pyrimidine), 2.64 (3H, *s*, CH_3). ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 153.92 (C), 153.41 (C), 151.47 (CH), 143.11 (CH), 129.36 (C), 11.15 (CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 167.0 (M+1) (15.33), 166.0 (M^+) (100.0). UV–Vis (DMSO-d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 280 (39290).

*6-(Ethylsulfanyl)-9*H*-purine (**2**)*. Yield: 89 %; m.p. 196 °C (lit. 196 °C[23]). Anal. Calcd. for $C_7H_8N_4S$: C, 46.65; H, 4.47; N, 31.09 %. Found: C, 46.63; H, 4.43; N, 31.02 %. ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 13.45 (1H, *s*, NH imidazole), 8.67 (1H, *s*, CH imidazole), 8.41 (1H, *s*, CH pyrimidine), 3.27 (2H, *q*, J = 7.20 Hz, CH_2), 1.35 (3H, *t*, J = 7.20 Hz, CH_3). ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 157.95 (C), 151.45 (C), 150.51 (CH), 143.25 (CH), 129.38 (C), 22.41 (CH_2), 14.94 (CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 181 (M+1), (9.99), 180.0 (M^+) (96.64), 164.9 (51.34), 151.9 (47.51), 147.0 (BP), (100). UV–Vis (DMSO-d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 300 (21670).

*6-(Propylsulfanyl)-9*H*-purine (**3**)*. Yield: 94 %; m.p. 182 °C (lit.179 °C[23]). Anal. Calcd. for $C_8H_{10}N_4S$: C, 49.46; H, 5.19; N, 28.84 %. Found: C, 48.95, H, 5.18, N, 28.79 %. ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 13.24 (1H, *s*, NH imidazole), 8.65 (1H, *s*, CH imidazole), 8.40 (1H, *s*, CH pyrimidine), 3.31 (2H, *t*, J = 7.20 Hz, SCH_2,), 1.71 (2H, *sext.*, J = 7.20 Hz, CH_2), 0.99 (3H, *t*, CH_3, J = 7.20 Hz). ^{13}C-NMR (100.6 MHz, DMSO-d_6, δ / ppm): 158.01 (C), 151.34 (C), 150.41 (CH), 143.44 (CH), 129.33 (C), 29.69 (CH_2), 22.61 (CH_2), 13.20

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** Reference numbers hold for the list given in the paper.

(CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 194.0 (M^+) (86.5), 179.0 (76.7), 166.0 (89.9), 165.0 (52.8), 161.0 (48.0), 153.0 (21.5), 152.0 (BP) (100). UV–Vis (DMSO-d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 330 (20910).

*6-(Butylsulfanyl)-9*H*-purine* (**4**). Yield: 95 %; m.p. 152 °C (lit.152 °C[23]). Anal. Calcd. for $C_9H_{12}N_4S$: C, 51.9; H, 5.81; N, 26.90 %. Found: C, 52.1, H, 5.79, N, 26.93 %. ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 13.47 (1H, *s*, NH imidazole), 8.66 (1H, *s*, CH imidazole), 8.41 (1H, *s*, CH pyrimidine), 3.33 (2H, *t*, *J* = 7.20 Hz, SCH_2), 1.67 (2H, *quin*., *J* = 7.20 Hz, $SCH_2C\mathbf{H}_2$), 1.43 (2H, *sext*., *J* = 7.20 Hz, $C\mathbf{H}_2CH_3$), 0.90 (3H, *t*, *J* = 7.20 Hz, CH_3). ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 158.03 (C), 151.44 (C), 150.34 (CH), 143.19 (CH), 129.37 (C), 31.25 (CH_2), 27.48 (CH_2), 21.39 (CH_2), 13.51 (CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 208 (M^+) (43.9), 179.0 (92.5), 175.0 (23.5), 168.0 (10.0), 167.0 (21.1), 166.0 (BP) (100). UV–Vis (DMSO-d_6) (λ_{max} / nm (ε / L mol^{-1} cm^{-1})): 285 (29590).

*6-(Pentylsulfanyl)-9*H*-purine* (***5***). Yield: 94 %; m.p. 117 °C (lit. 115.5 °C[23]). Anal. Calcd. for $C_{10}H_{14}N_4S$: C, 54.03; H, 6.35; N, 25.20%. Found: C, 54.10, H, 6.33, N, 25.18 %. ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 13.51 (1H, *s*, NH imidazole), 8.66 (1H, *s*, CH imidazole), 8.41 (1H, s, CH pyrimidine) 3.32 (2H, *t*, *J* = 7.20 Hz, SCH_2), 1.69 (2H, *quin*., $SCH_2C\mathbf{H}_2$), 1.40 (2H, *quin*., *J* = 7.20 Hz, $SCH_2C\mathbf{H}_2CH_2$), 1.32 (2H, *sext*., *J* = 7.20 Hz, $C\mathbf{H}_2CH_3$), 0.863 (3H, *t*, *J* = = 7.20 Hz, CH_3). ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 157.91 (C), 151.43 (C), 144.46 (CH), 143.18 (CH), 129.31 (C), 30.39 (CH_2), 28.83 (CH_2), 27.74 (CH_2), 21.67 (CH_2), 13.82(CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 222.0 (M^+) 37.2), 189.1 (15.9), 179.0 (62.1), 175.1 (32.1), 168.0 (7.8), 167.0 (15.1), 166.0 (BP) (100). UV–Vis (DMSO-d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 335 (46880).

*6-(Hexylsulfanyl)-9*H*-purine* (***6***). Yield: 78 %; m.p. 79 °C (lit. 77°C[24]). Anal. Calcd. for $C_{11}H_{16}N_4S$: C, 55.90; H, 6.82; N, 23.71 %. Found: C, 55.82, H, 6.77, N, 23.85 %. ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 13.45 (1H, *s*, NH imidazole), 8.66 (1H, *s*, CH imidazole), 8.41 (1H, *s*, CH pyrimidine) 3.32 (2H, *t*, *J* = 7.20 Hz, SCH_2,), 1.68 (2H, *quin*., $SCH_2C\mathbf{H}_2$), 1.39 (2H, *quin*., *J* = 7.20 Hz, $SCH_2CH_2C\mathbf{H}_2$), 1.26 (2H, *quin*., *J* = 7.20 Hz, $C\mathbf{H}_2CH_2CH_3$), 1.23 (2H, *sext*., *J* = = 7.20 Hz, $C\mathbf{H}_2CH_3$), 0.835 (3H, *t*, *J* = 7.20 Hz, CH_3). ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 158.03 (C), 151.42 (C), 150.43 (CH), 143.17 (CH),129.35 (C), 30.75 (CH_2), 29.10 (CH_2), 27.87 (CH_2), 27.78 (CH_2), 21.97 (CH_2), 13.84 (CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 236.1 (M^+) (71.2), 203 (66.6), 189.1 (68.5), 179.0 (75.7), 175.1 (64.9), 167.0 (49.7), 161.0 (49.2), 154.0 (40.9), 152.0 (BP) (100). UV–Vis (DMSO-d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 280 (34580).

*6-(Heptylsulfanyl)-9*H*-purine* (***7***). Yield: 79 %; m.p. 80 °C (lit.79–81 °C[24]). Anal. Calcd. for $C_{12}H_{18}N_4S$: C, 57.57; H, 7.25; N, 22.38 %. Found: C, 57.56,

H,7.20, N, 22.36 %. ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 13.45 (1H, *s*, NH imidazole), 8.64 (1H, *s*, CH imidazole), 8.39 (1H, *s*, CH pyrimidine) 3.32 (2H, *t*, J = 7.20 Hz, SCH_2,), 1.69 (2H, *quin.*, $SCH_2C\mathbf{H}_2$), 1.64–1.24 (8H, *m*, $4CH_2$), 0.842 (3H, *t*, J = 7.20 Hz, CH_3); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 157.91 (C), 151.30 (C), 150.96 (CH), 143.55 (CH), 31.14 (C), 29.17 (CH_2), 28.20 (CH_2), 28.17 (CH_2), 27.80 (CH_2), 22.00 (CH_2), 13.91(CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 249.1 (M^+) (86.1), 235.0 (25.1), 231.7 (48.7), 217.3 (29.5), 203.7 (15.3), 179.0 (47.6), 166.0 (82.3), 152.0 (BP) (100). UV–Vis (DMSO-d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 285 (29240).

*6-(Octylsulfanyl)-9*H*-purine* (***8***). Yield: 94 %; m.p. 84 °C (lit. 78–80 °C[24]). Anal. Calcd. for $C_{13}H_{20}N_4S$: C, 59.06; H, 7.62; N, 21.19 %. Found: C, 59.01, H, 7.58,; N, 21.08 %. ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 13.46 (1H, *s*, NH imidazole), 8.66 (1H, *s*, CH imidazole), 8.41 (1H, *s*, CH pyrimidine) 3.26 (2H, *t*, J = 7.20 Hz, SCH_2), 1.72–1.65 (12H, *m*, $6CH_2$), 0.85 (3H, *t*, J = 7.20 Hz, CH_3). ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 158.02 (C), 151.41 (C), 150.43 (CH), 143.17 (CH), 129.34 (C), 31.18 (CH_2), 29.12 (CH_2), 28.54 (CH_2), 28.48 (CH_2), 28.18 (CH_2), 27.77 (CH_2), 22.04 (CH_2), 13.91 (CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 264.0 (M^+) 82.2), 231.1 (57.6), 217.0 (27.2), 179.0 (48.1), 166.0 (85.2), 151.9 (100.0). UV–Vis (DMSO-d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 285 (32410).

*6-(Nonylsulfanyl)-9*H*-purine* (**9**). Yield: 93 %; m.p. 97 °C. Anal. Calcd. for $C_{14}H_{22}N_4S$: C, 60.40; H, 7.96; N, 20.12 %. Found: C, 60.37, H, 7.89, N, 20.09. ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 13.16 (1H, *s*, NH imidazole), 8.64 (1H, *s*, CH imidazole), 8.39 (1H, *s*, CH pyrimidine), 3.23 (2H, *t*, J = 7.20 Hz, SCH_2), 1.70–1.22 (14H, *m*, $7CH_2$), 0.83 (3H, t, J = 7.20 Hz, CH_3). ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 157.95 (C), 151.27 (C), 150.51 (CH), 143.55 (CH), 129.38 (C), 31.23 (CH_2), 29.14 (CH_2), 28.84 (CH_2), 28.59 (CH_2), 28.53 (CH_2), 28.17 (CH_2), 27.75 (CH_2), 22.05 (CH_2), 13.91(CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 278.1 (M^+) (77.3), 245.1 (47.7), 231.1 (75.8), 221.0 (36.7), 207.0 (17.7), 190.0 (19.3), 179.0 (93.9), 166.0 (100.0). UV–Vis (DMSO--d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 280 (34810).

*6-(Decylsulfanyl)-9*H*-purine* (**10**). Yield: 92 %; m.p. 89 °C (lit. 84–85 °C)[25]. Anal. Calcd. for $C_{15}H_{24}N_4S$: C, 61.61; H, 8.27; N, 19.16; S, 10.96 %. Found: C, 61.53, H, 8.24, N, 19.15 %. ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 13.48 (1H, *s*, NH imidazole), 8.67 (1H, *s*, CH imidazole), 8.42 (1H, s, CH pyrimidine), 3.33 (2H, *t*, J = 7.20 Hz, SCH_2), 1.72 (2H, *quin.*, J = 7.20 Hz, $SCH_2C\mathbf{H}_2$), 1.41–1.23 (14H, *m*, $7CH_2$), 0.84 (3H, *t*, J = 7.20 Hz, CH_3). ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 157.64 (C), 151.39 (C), 150.53 (CH), 143.19 (CH), 129.36 (C), 31.24 (CH_2), 29.09 (CH_2), 28.88 (CH_2), 28.65 (CH_2), 28.59 (CH_2), 28.50 (CH_2), 28.14 (CH_2), 27.73 (CH_2), 22.05 (CH_2), 13.92 (CH_3). EI–MS (*m*/*z*, (relative abundance, %)): 292.1 (M^+) (77.9), 259.1 (74.1), 245.1 (76.1), 231.1 (62.3), 221.1

(68.2), 179.0 (89.0), 152.0 (100.0). UV–Vis (DMSO-d_6) (λ_{max} / nm, (ε / L mol^{-1} cm^{-1})): 280 (34340).

*6-(Benzylsulfanyl)-9*H-*purine* (***11***). Yield 88 %; m.p. 195 °C (lit. 195 °C[25]). Anal. Calcd. for $C_{12}H_{10}N_4S$: C, 59.48; H, 4.16; N, 23.12 %. Found: C, 59.47, H, 4.12, N, 23.14 %. ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 13.12 (1H, *s*, NH imidazole), 8.72 (1H, *s*, CH imidazole), 8.40 (1H, *s*, CH pyrimidine), 7.45–7.21 (5H, *m*, ArH), 4.61 (2H, *s*, CH_2). ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 57.67 (C), 151.38 (C), 150.79 (CH),143.40 (CH), 137.83 (C), 129.46 (C), 128.94 (CH), 128.44 (CH),127.12 (CH), 31.59 (CH_2). EI–MS (*m*/*z*, (relative abundance, %)): 243.0 (M+1) (48.3), 242.0 (M^+) (100.0), 210.0 (36.3), 209.0 (100.0), 208.0 (32.0). UV–Vis (DMSO-d_6) (λ_{max} /nm, (ε / L mol^{-1} cm^{-1})): 285 (29270).