

References to synthesis of starting materials

All 6-chloropurines **1** and **3** used in the syntheses of compounds **2**, **4** and **5** were available by literature methods:

6-Chloro-1*H*-purine **1a**,¹⁹ 6-chloro-9-methyl-9*H*-purine **1b**,²⁰ 6-chloro-9-(2-propen-1-yl)-9*H*-purine **1c**,²¹ 9-benzyl-6-chloro-9*H*-purine **1d**,¹⁶ 9-benzyl-2,6-dichloro-9*H*-purine **1e**,^{6a} 6-chloro-9-(cyclohexylmethyl)-9*H*-purine **1f**,²² 6-chloro-9-(2-phenylethyl)-9*H*-purine **1g**,²³ 6-chloro-9-tetrahydropyranyl-9*H*-purine **1h**,²⁴ 2,6-dichloro-9-tetrahydropyranyl-9*H*-purine **1i**,²⁵ 6-chloro-9-(2,3,5-tri-*O*-acetyl-β-D-ribofuranosyl)-9*H*-purine **3a**,²⁶ 6-chloro-9-(2,3,5-tri-*O*-*tert*-butyldimethylsilyl-β-D-ribofuranosyl)-9*H*-purine **3b**,²⁷ and 2,6-dichloro-9-(2,3,5-tri-*O*-acetyl-β-D-ribofuranosyl)-9*H*-purine **3c**.²⁸

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Detailed information on synthesis and characterization of novel compounds

6-(2-Furyl)-1*H*-purine (2b). EtOH-CHCl₃ (1:9) was used for flash chromatography; off-white microcrystalline solid, yield 53%, mp ca. 280 °C (subl.). ¹H NMR (200 MHz, DMSO-d₆): δ 6.81 (m, 1H, furyl), 7.74 (m, 1H, furyl), 8.05 (m, 1H, furyl), 8.61 (s, 1H, H-8), 8.86 (s, 1H, H-2); MS EI m/z (rel. %): 186 (100, M⁺), 158 (24), 157 (9), 131 (7), 130 (9), 104 (10), 103 (4), 93 (4), 77 (8) 76 (6). Anal. (C₉H₆N₄O) C, H, N.

6-(2-Furyl)-9-methyl-9*H*-purine (2c). EtOAc-EtOH (20:1) was used for flash chromatography; off-white small needles, yield 88%, mp 191-193 °C. ¹H NMR (200 MHz, CDCl₃): δ 3.91 (s, 3H, CH₃), 6.65 (dd, *J* = 3.6 Hz and 1.6 Hz, 1H, furyl), 7.75 (m, 1H, furyl), 7.82 (br d, *J* = 3.6 Hz, 1H, furyl), 8.06 (s, 1H, H-8), 8.95 (s, 1H, H-2); ¹³C NMR (50 MHz, CDCl₃): δ 29.7 (CH₃), 112.5 (CH in furyl), 117.1 (CH in furyl), 128.2 (C-5), 144.9 (CH in furyl / C-8), 145.7 (CH in furyl / C-8), 149.6 (C in furyl and C-6), 152.4 (C-4), 152.3 (C-2); MS EI m/z (rel. %): 200 (100, M⁺), 172 (32), 171 (12), 157 (3), 144 (5), 130 (7), 118 (2), 117 (3), 104 (3), 100 (4). HRMS: Found 200.0698, calcd. for C₁₀H₈N₄O 200.0706. Anal. Found: C, 59.24; H, 3.83. C₁₀H₈N₄O requires C, 60.00; H, 4.03%. Anal. (C₁₀H₈N₄O) C, H, N.

6-(2-Furyl)-9-(2-propen-1-yl)-9*H*-purine (2d). EtOAc-hexane (2:1) was used for flash chromatography; yellow needles, yield 68%, mp 126-128 °C. ¹H NMR (200 MHz, CDCl₃): δ 4.85-4.89 (m, 2H, CH₂), 5.16-5.33 (m, 2H, CH₂=), 5.96-6.10 (m, 1H, CH=), 6.63 (dd, *J* = 3.4 Hz and 1.6 Hz, 1H, furyl), 7.73 (m, 1H, furyl), 7.81 (dd, *J* = 3.4 and 0.6 Hz, 1H, furyl), 8.06 (s, 1H, H-8), 8.91 (s, 1H, H-2); ¹³C NMR (50 MHz, CDCl₃): δ 45.4 (CH₂), 112.3 (CH in furyl), 117.0 (CH in furyl), 119.0 (CH₂=), 128.3 (C-5), 131.2 (CH=), 144.1 (CH in furyl / C-8), 145.5 (CH in furyl / C-8), 149.5 (C in furyl and C-6), 151.6 (C-4), 152.3 (C-2); MS EI m/z (rel. %): 226 (100, M⁺), 199 (13), 198 (7), 197 (5), 186 (9), 171 (4), 158 (2), 143 (2), 106 (3), 99 (2). Anal. (C₁₂H₁₀N₄O) C, H, N.

6-(2-Furyl)-9-(phenylmethyl)-9*H*-purine (2i). EtOAc-acetone-hexane (1:2:5) was used for flash chromatography; colorless crystals, yield 93%, mp 223-225 °C. ¹H NMR (300 MHz, CDCl₃): δ 5.50 (s, 2H, CH₂), 6.69 (dd, *J* = 3.4 and 1.7 Hz, 1H, furyl), 7.33-7.37 (m, 5H, Ph), 7.79 (m, 1H, furyl), 7.87 (br d, *J* = 3.4 Hz, 1H, furyl), 8.10 (s, 1H, H-8), 9.01 (s, 1H, H-2); ¹³C NMR (75 MHz,

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 CDCl_3): δ 47.2 (CH_2), 112.6 (CH in furyl), 117.3 (CH in furyl), 127.7 (CH in Ph), 128.2 (C-5), 128.5 (CH in Ph), 129.1 (CH in Ph), 135.1 (C in Ph), 144.3 (CH in furyl / C-8), 145.8 (CH in furyl / C-8), 145.9 (C in furyl), 149.7 (C-6), 152.0 (C-4), 152.8 (C-2); MS EI m/z (rel. %): 276 (100, M^+), 275 (79), 248 (7), 247 (15), 223 (8), 199 (8), 181 (13), 92 (7), 91 (88), 65 (18). HRMS: Found 276.1008, calcd. for $\text{C}_{16}\text{H}_{12}\text{N}_4\text{O}$ 276.1011. Anal. ($\text{C}_{16}\text{H}_{12}\text{N}_4\text{O}$) Found: C, 69.06 H, 4.51, N, 20.00. $\text{C}_{16}\text{H}_{12}\text{N}_4\text{O}$ requires C, 69.55 H, 4.38; N, 20.28%.

9-(Cyclohexylmethyl)-6-(2-furyl)-9*H*-purine (2k). EtOAc-hexane (1:1) was used for flash chromatography; off-white microcrystalline solid, yield 89%, mp 198-200 °C. ^1H NMR (200 MHz, CDCl_3): δ 0.98- 1.23 (m, 5H, cyclohexyl), 1.59-1.68 (m, 5H, cyclohexyl), 1.93 (m, 5H, cyclohexyl), 4.11 (d, $J = 7.0$ Hz, 2H, CH_2N), 6.65 (dd, $J = 3.6$ and 1.6 Hz, 1H, furyl), 7.75 (m, 1H, furyl), 7.82 (br d, $J = 3.6$ Hz, 1H, furyl), 8.03 (s, 1H, H-8), 8.94 (s, 1H, H-2); ^{13}C NMR (50 MHz, CDCl_3): δ 25.4 (cyclohexyl), 26.0 (cyclohexyl), 30.5 (cyclohexyl), 38.1 (cyclohexyl), 50.0 (CH_2N), 112.5 (CH in furyl), 117.1 (CH in furyl), 128.2 (C-5), 144.9 (CH in furyl / C-8), 145.7 (CH in furyl / C-8), 149.8 (C in furyl and C-6), 152.2 (C-4), 152.5 (C-2); MS EI m/z (rel. %): 282 (86, M^+), 253 (15), 239 (7), 227 (6), 225 (7), 200 (67), 199 (85), 186 (100), 171 (10), 158 (15). Anal. ($\text{C}_{16}\text{H}_{18}\text{N}_4\text{O}$) C, H, N.

6-(2-Furyl)-9-(2-phenylethyl)-9*H*-purine (2l). EtOAc-hexane (2:1) was used for flash chromatography; off-white microcrystalline solid, yield 88%, mp 119-120 °C. ^1H NMR (200 MHz, CDCl_3): δ 3.23 (t, $J = 6.9$ Hz, 2H, CH_2), 4.56 (t, $J = 6.9$ Hz, 2H, CH_2N), 6.68 (dd, $J = 3.6$ and 1.6 Hz, 1H, furyl), 7.05-7.10 (m, 2H, Ph), 7.24-7.30 (m, 3H, Ph), 7.71 (s, 1H, H-8), 7.75 (dd, $J = 1.6$ and 0.8 Hz, 1H, furyl), 7.83 (dd, $J = 3.6$ and 0.8 Hz, 1H, furyl), 8.99 (s, 1H, H-2); ^{13}C NMR (50 MHz, CDCl_3): δ 36.0 (CH_2), 45.4 (CH_2), 112.5 (CH in furyl), 117.1 (CH in furyl), 127.0 (CH in Ph), 128.5 (CH in Ph), 128.8 (CH in Ph), 132.0 (C-5), 137.0 (C in Ph), 144.5 (CH in furyl / C-8), 145.7 (CH in furyl / C-8), 149.7 (C-6), 151.8 (C-4), 152.4 (C-2) one signal was hidden; MS EI m/z (rel. %): 290 (23, M^+), 199 (6), 186 (93), 170 (11), 158 (22), 117 (12), 104 (48), 91 (100), 77 (32), 65 (31). Anal. ($\text{C}_{17}\text{H}_{14}\text{N}_4\text{O}$) C, H, N.

9-(Tetrahydro-2*H*-pyran-2-yl)-6-(2-thienyl)-9*H*-purine (2n). EtOAc-hexane (1:2) was used for flash chromatography; off-white crystals, yield 93%, mp 139-140 °C. ^1H NMR (200 MHz, CDCl_3): δ 1.66-1.80 (m, 3H, THP), 2.03-2.13 (m, 3H, THP), 3.72-3.85 (m, 1H, THP), 4.15-4.22 (m, 1H, THP), 5.81 (dd, $J = 9.4$ and 3.4 Hz, 1H, THP), 7.21-7.27 (m, 1H, thienyl), 7.59 (dd, $J = 5.0$

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and 1.2 Hz, 1H, thienyl), 8.29 (s, 1H, H-8), 8.67 (dd, J = 3.8 and 1.2 Hz, 1H, thienyl), 8.88 (s, 1H,
H-2); ^{13}C NMR (50 MHz, CDCl_3): δ 22.4 (THP), 24.5 (THP), 31.3 (THP), 68.4 (THP), 81.6 (THP),
128.3 (CH in thienyl), 128.5 (C-5), 130.3 (CH in thienyl), 132.4 (CH in thienyl), 139.7 (C in
Thienyl), 141.8 (C-8), 149.6 (C-4/C-6), 150.9 (C-4/C-6), 152.0 (C-2); MS EI m/z (rel. %): 286 (10,
 M^+), 258 (1), 204 (6), 203 (17), 202 (100), 201 (5), 175 (10), 158 (3), 148 (3), 84 (12). Anal.
($\text{C}_{14}\text{H}_{14}\text{N}_4\text{OS}$) C, H, N.

2-Chloro-9-(tetrahydro-2*H*-pyran-2-yl)-6-(2-thienyl)-9*H*-purine (2o). EtOAc-hexane (3:7)
was used for flash chromatography; yellow crystals, yield 58%, mp 143-144 °C. ^1H NMR (200
MHz, CDCl_3): δ 1.54-2.17 (m, 6H, THP), 3.71-3.84 (m, 1H, THP), 4.14-4.19 (m, 1H, THP), 5.78
(dd, J = 9.8 and 2.2 Hz, 1H THP), 7.25-7.30 (m, 1H, thienyl), 7.64 (dd, J = 5.0 and 1.2 Hz, 1H,
thienyl), 8.26 (s, 1H, H-8), 8.64 (dd, J = 3.8 and 1.2 Hz, 1H, thienyl); ^{13}C NMR (50 MHz, CDCl_3):
 δ 22.5 (THP), 24.6 (THP), 31.8 (THP), 68.7 (THP), 81.7 (THP), 127.7 (C-5), 131.9 (CH in thienyl),
133.4 (2xCH in thienyl), 138.3 (C in thienyl), 142.4 (C-8), 151.5 (C-2/C-4/C-6), 152.5 (C-2/C-4/C-
6), 153.8 (C-2/C-4/C-6); MS EI m/z (rel. %): 322/320 (5/14, M^+), 239 (8), 238 (38), 237 (25), 236
(100), 209 (3), 201 (8), 174 (3), 147 (3), 85 (9). HRMS: Found 320.320.0490, calcd. for
 $\text{C}_{14}\text{H}_{13}\text{ClN}_4\text{OS}$ 320.0489. Anal. ($\text{C}_{14}\text{H}_{13}\text{ClN}_4\text{OS}$) Found: C, 52.73; H, 4.08; N, 16.97.
 $\text{C}_{14}\text{H}_{13}\text{ClN}_4\text{OS}$ requires C, 52.42; H, 4.08; N, 17.47%

6-(2-Furyl)-9-(tetrahydro-2*H*-pyran-2-yl)-9*H*-purine (2p). EtOAc-hexane (1:1) was used for
flash chromatography; colorless crystals, yield 90%, mp 133-134 °C. ^1H NMR (200 MHz, CDCl_3):
 δ 1.67-1.82 (m, 3H, THP), 2.02-2.11 (m, 3H, THP), 3.71-3.84 (m, 1H, THP), 4.14-4.21 (m, 1H,
THP), 5.80 (dd, J = 9.4 and 3.4 Hz, 1H, THP), 6.63-6.65 (m, 1H, furyl), 7.74 (br s, 1H, furyl), 7.82
(br d, J = 3.6 Hz, 1H, furyl), 8.29 (s, 1H, H-8), 8.92 (s, 1H, H-2); ^{13}C NMR (50 MHz, CDCl_3):
 δ 22.6 (THP), 24.7 (THP), 31.7 (THP), 68.7 (THP), 81.8 (THP), 112.5 (CH in furyl), 117.2 (CH in
furyl), 123.8 (C-5), 142.2 (CH in furyl / C-8), 145.7 (CH in furyl / C-8), 149.6 (C in furyl and C-6),
151.1 (C-4), 152.5 (C-2); MS EI m/z (rel. %): 270 (20, M^+), 242 (4), 213 (2), 201 (2), 199 (2), 187
(33), 186 (100), 184 (11), 158 (11), 85 (7). Anal. ($\text{C}_{14}\text{H}_{14}\text{N}_4\text{O}_2$) C, H, N.

2-Chloro-6-(2-furyl)-9-(tetrahydro-2*H*-pyran-2-yl)-9*H*-purine (2q). EtOAc-hexane (2:3) was
used for flash chromatography; off-white crystals, yield 86%, mp 138-140 °C. ^1H NMR (200 MHz,
 CDCl_3): δ 1.54-2.15 (m, 6H, THP), 3.73-3.82 (m, 1H, THP), 4.14-4.20 (m, 1H, THP), 5.78 (dd J =
10.0 and 2.2 Hz, 1H, THP), 6.65 (m, 1H, furyl), 7.77 (br s, 1H, furyl), 7.86 (br d, J = 3.0 Hz, 1H,

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furyl), 8.27 (s, 1H, H-8); ^{13}C NMR (50 MHz, CDCl_3): δ 22.5 (THP), 24.7 (THP), 32.0 (THP), 68.8
(THP), 81.8 (THP), 112.7 (CH in furyl), 118.7 (CH in furyl), 127.2 (C-5), 142.8 (CH in furyl / C-
8), 146.6 (CH in furyl / C-8), 147.2 (C in furyl / C-6), 148.7 (C in furyl / C-6), 152.7 (C-2 / C-4),
154.2 (C-2 / C-4); MS EI m/z (rel. %): 306/304 (5/15, M^+), 223 (13), 222 (33), 221 (42), 220 (100),
219 (9), 192 (9), 105 (8), 85 (14), 84 (10). Anal. ($\text{C}_{14}\text{H}_{13}\text{ClN}_4\text{O}_2$) C, H, N.

9-(β -D-Ribofuranosyl)-6-(2-thienyl)-9*H*-purine (5b). MeOH- CH_2Cl_2 (1:20) was used for flash chromatography; microcrystalline solid, yield 87%, mp 128-130 °C (lit.¹² 126-129 °C). ^1H NMR (200 MHz, DMSO- d_6): δ 3.58-3.73 (m, 2H, H-5'), 3.99 (br d, J = 3.8 Hz, 1H, H-4'), 4.20 (br d, J = 3.6 Hz, 1H, H-3'), 4.52-4.65 (m, 1H, H-2'), 5.12 (t, J = 5.6 Hz, 1H, OH), 5.23 (d, J = 5.0 Hz, 1H, OH), 5.55 (d, J = 6.0 Hz, 1H, OH), 6.05 (d, J = 5.4 Hz, 1H, H-1'), 7.34 (dd, J = 4.8 and 4.0 Hz, 1H, thienyl), 7.97 (br d, J = 5.0 Hz, 1H, thienyl), 8.63 (br d, J = 3.6 Hz, 1H, thienyl), 8.86 (s, 1H, H-8), 8.89 (s, 1H, H-2); ^{13}C NMR (50 MHz, DMSO- d_6): δ 61.2 (C-5), 70.3 (C-3'), 73.8 (C-2'), 85.7 (C-4'), 87.8 (C-1'), 128.6 (C-5), 129.1 (CH in thienyl), 131.8 (CH in thienyl), 132.5 (CH in thienyl), 139.6 (C in thienyl), 145.0 (C-8), 148.8 (C-6), 151.6 (C-4), 152.0 (C-2); MS EI m/z (rel. %): 334 (18, M^+), 304 (6), 245 (21), 231 (40), 215 (15), 210 (17), 203 (46), 202 (100), 169 (12), 166 (10).

6-(2-Furyl)-9-(β -D-ribofuranosyl)-9*H*-purine (5c). MeOH- CHCl_3 (1:10) was used for flash chromatography; microcrystalline solid, yield 92%, mp 171-173 °C (lit.¹² 165-168 °C). ^1H NMR (200 MHz, DMSO- d_6): δ 3.57-3.73 (m, 2H, H-5'), 3.98 (br d, J = 3.7 Hz, 1H, H-4'), 4.20 (br d, J = 3.6 Hz, 1H, H-3'), 4.58-4.63 (m, 1H, H-2'), 5.13 (br t, J = 5.3 Hz, 1H, OH), 5.24 (br d, J = 4.8, 1H, OH), 5.55 (br d, J = 5.4 Hz, 1H, OH), 6.05 (d, J = 5.0 Hz, 1H, H-1'), 6.82 (br s, 1H, furyl), 7.85 (br d, J = 2.6 Hz, 1H, furyl), 8.07 (br s, 1H, furyl), 8.87 (s, 1H, H-8), 8.90 (s, 1H, H-2); MS EI m/z (rel. %): 318 (4, M^+), 229 ((6), 215 (15), 187 (26), 186 (100), 158 (18), 142 (5), 130 (7), 104 (8), 77 (7).

2-Chloro-6-(2-furyl)-9-(β -D-ribofuranosyl)-9*H*-purine (5d). MeOH-EtOAc (2:3) was used for flash chromatography; yellow crystals, yield 49%, mp 151-153 °C. ^1H NMR (200 MHz, DMSO- d_6): δ 3.78-4.01 (m, 4H, ribose), 4.35 (br s, 1H, ribose), 4.46-4.48 (m, 1H, ribose), 5.03-5.08 (m, 2H, ribose), 5.86 (d, J = 7.2 Hz, 1H, H-1'), 6.67 (m, 1H, furyl), 7.76 (br s, 1H, furyl), 7.83 (br d, J = 3.4 Hz, 1H, furyl), 8.11 (s, 1H, H-8); ^{13}C NMR (50 MHz, DMSO- d_6): δ 60.9 (C-5'), 70.0 (C-3'), 73.8 (C-2'), 85.6 (C-4'), 87.6 (C-1'), 113.2 (CH in furyl), 119.0 (CH in furyl), 127.3 (C-5), 145.4 (CH in furyl / C-8), 146.0 (C in furyl / C-6), 147.4 (CH in furyl / C-8), 147.7 (C in furyl / C-6), 152.6 (C-2 / C-4), 153.1 (C-2 / C-4); MS EI m/z (rel. %): 354/352 (2/6, M^+), 315 (7), 313 (10), 269

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(26), 249 (15), 222 (36), 220 (100), 192 (20), 186 (60), 158 (21). HRMS: Found 352.0560, calcd.
for $C_{14}H_{13}ClN_4O_5$ 352.0574. Anal. ($C_{14}H_{13}ClN_4O_5 \times 1H_2O$) Found: C, 44.88; H, 3.60.
 $C_{14}H_{13}ClN_4O_5 \times 1H_2O$ requires C, 45.35; H, 4.08; N, 17.47%

Elemental Analysis of Novel Compounds

6-(2-Furyl)-1*H*-purine (2b).

Elementanal: Found: C, 57.98; H, 3.37; N, 29.92. C₉H₆N₄O requires C, 58.06; H, 3.25; N, 30.09%

6-(2-Furyl)-9-methyl-9*H*-purine (2c).

Elementanal: Found: C, 59.83; H, 4.06; N, 27.87. C₁₀H₈N₄O requires C, 60.00; H, 4.03; N, 27.99%

6-(2-Furyl)-9-(2-propen-1-yl)-9*H*-purine (2d).

Elementanal: Found: C, 63.40; H, 4.46; N, 24.74. C₁₂H₁₀N₄O requires C, 63.37; H, 4.46; N, 24.77%

9-Benzyl-6-(2-Furyl)-9*H*-purine (2i).

Elementanal: Found: C, 69.02 H, 4.51, N, 20.00. C₁₆H₁₂N₄O requires C, 69.55 H, 4.38; N, 20.28%

9-(Cyclohexylmethyl)-6-(2-furyl)-9*H*-purine (2k).

Elementanal: Found: C, 67.78; H, 6.39; N, 19.72. C₁₆H₁₈N₄O requires C, 68.06; H, 6.42; N, 19.84%

6-(2-Furyl)-9-(2-phenylethyl)-9*H*-purine (2l).

Elementanal: Found: C, 70.14; H, 4.99; N, 19.32. C₁₇H₁₄N₄O requires C, 70.33; H, 4.86; N, 19.30%

9-(Tetrahydro-2*H*-pyran-2-yl)-6-(2-thienyl)-9*H*-purine (2n).

Elementanal: Found: C, 58.82; H, 4.91; N, 19.72. C₁₄H₁₄N₄OS requires C, 58.72 H, 4.93; N, 19.57%

286 (10, M⁺), 258 (1), 204 (6), 203 (17), 202 (100), 201 (5), 175 (10), 158 (3), 148 (3), 84 (12).

2-Chloro-9-(tetrahydro-2*H*-pyran-2-yl)-6-(2-thienyl)-9*H*-purine (2o).

Elementanal: Found: C, 52.73; H, 4.08; N, 16.97. C₁₄H₁₃ClN₄OS requires C, 52.42; H, 4.08; N, 17.47%

6-(2-Furyl)-9-(tetrahydro-2*H*-pyran-2-yl)-9*H*-purine (2p).

Elementanal: Found: C, 69.06 H, 4.51, N, 20.00. C₁₆H₁₂N₄O requires C, 69.55 H, 4.38; N, 20.28%

2-Chloro-6-(2-furyl)-9-(tetrahydro-2*H*-pyran-2-yl)-9*H*-purine (2q).

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Elementanal: Found: C, 55.53; H, 4.30; N, 18.18. $C_{14}H_{13}ClN_4O_2$ requires C, 55.18; H, 4.30; N,
18.39%

2-Chloro-6-(2-furyl)-9-(β -D-ribofuranosyl)-9*H*-purine (5d)

Elementanal: Found: C, 44.88; H, 3.60; $C_{14}H_{13}ClN_4O_5 \times 1H_2O$ requires C, 45.35; H, 4.08%