Supplement information

Spectroscopic data of isolated compounds

1,9-dimethylguanine (**1**) ^{1}H-NMR (DMSO-d_6, 300MHz): δ 7.64 (1H, s, H-8), 7.01 (2H, s, NH_2), 3.53 (3H, s, N-CH_3), 3.30 (3H, s, N-CH_3); ^{13}C-NMR (DMSO-d_6, 75 MHz) : δ 156.4 (C-2), 154.1 (C-6), 149.5 (C-4), 138.1 (C-8), 115.5 (C-5), 29.0 (N-CH_3), 27.9 (N-CH_3); UV (MeOH) λ_{max}, nm (log ε) : 206 (4.20), 257 (4.05); EI-MS *m/z* 179 $[M]^+$ (100), 163 $[M-NH_2]^+$ (20); mp 286.2˚C.

Adenosine (**2**) ^{1}H-NMR (DMSO-d_6, 300 MHz) δ 8.34 (1H, s, H-2), 8.13 (1H, s, H-8), 7.32 (2H, s, NH_2), 5.88 (1H, d, *J* = 6 Hz), 5.41 (2H, s, 2 x OH), 5.19 (1H, s, OH), 4.5 ~ 3.5 (m, ribose); ^{13}C-NMR (DMSO-d_6, 75 MHz) δ 156.25 (C-6), 152.50 (C-2), 149.12 (C-4), 140.06 (C-8), 119.43 (C-5), 88.01, 86.02, 73.55, 70.77, 61.77 (ribose carbons); UV (MeOH) λ_{max}, nm (log ε): 210 (4.29), 260 (4.18); EI-MS *m/z* 267 $[M]^+$ (5); mp 231.0˚C.

Uridine (**3**) ^{1}H-NMR (DMSO-d_6, 300 MHz) δ 11.3 (1H, s, NH), 7.89 (1H, d, *J* = 8.1 Hz, H-6), 5.77 (1H, d, anomeric proton), 5.65 (1H, d, *J* = 8.1 Hz, H-5), 5.43 (1H, s, OH), 5.13 (2H, s, 2 x OH); ^{13}C-NMR (DMSO-d_6, 75 MHz) δ 163.5 (C-4), 151.2 (C-2), 141.2 (C-6), 102.2 (C-5), 88.2, 85.3, 73.9, 70.3, 61.3 (ribose carbons); UV (MeOH) λ_{max}, nm (log ε): 206 (3.96), 262 (4.00); EI-MS *m/z* 226 $[M]^+$ (20), 113 $[M\text{-ribose}]^+$ (100); mp 167.7˚C.

Nicotinamide (**4**) ^{1}H-NMR (DMSO-d_6, 300 MHz) δ 9.02 (1H, d, *J* = 2.0 Hz, H-2), 8.69 (1H, dd, *J* = 4.7, 1.5 Hz, H-6), 8.19 (1H, ddd, *J* = 8.0, 2.0, 1.5 Hz, H-4), 8.12 (1H, br s, NH_{2b}), 7.54 (1H, br s, NH_{2a}), 7.49 (1H, ddd, *J* = 8.0, 4.7, 0.9 Hz, H-5); ^{13}C-NMR (DMSO-d_6, 75 MHz) δ 166.5 (C-7), 151.8 (C-2), 148.6 (C-6), 135.1 (C-4), 129.7 (C-3), 123.3 (C-5); UV (MeOH) λ_{max}, nm (log ε): 214 (3.91), 262 (3.43); EI-MS *m/z* 122 $[M]^+$ (100), 106 $[M-NH_2]^+$ (80); mp 131.2˚C.

3-Methyluracil (**5**) ^{1}H-NMR (DMSO-d_6, 600 MHz) δ 7.41 (1H, d, *J* = 7.8 Hz, H-5), 5.58 (1H, d, *J* = 7.8 Hz, H-6), 3.11 (3H, s, N-CH_3); ^{13}C-NMR (DMSO-d_6, 150 MHz) δ 163.24 (C-4), 151.52 (C-2), 140.26 (C-5), 99.50 (C-6), 26.32 (N-$\underline{C}H_3$); UV (MeOH) λ_{max}, nm (log ε) : 206 (3.77), 258 (3.71); EI-MS *m/z* 126 $[M]^+$ (100), 69 $[M\text{-CO-}NH_3]^+$ (60).

1,7-Dimethylxanthine (**6**) ^{1}H-NMR (DMSO-d_6, 300 MHz) δ 7.62 (1H, s, H-8), 3.51 (3H, s, O-CH_3), 3.30 (3H, s, N-CH_3); ^{13}C-NMR (DMSO-d_6, 75 MHz) δ 157.48 (C-2), 153.44 (C-6), 151.7 (C-8), 138.87 (C-4), 116.34 (C-5), 29.05 (N-$\underline{C}H_3$), 27.82 (N-$\underline{C}H_3$); UV (MeOH) λ_{max}, nm (log ε): 206 (4.23), 254 (4.13); EI-MS *m/z* 179 $[M-H]^+$ (100), 149 $[M-H-2xCH_3]^+$ (20); mp 288.6˚C.

Nudifloric acid (**7**) ^{1}H-NMR (DMSO-d_6, 300 MHz) δ 8.44 (1H , s, H-6), 7.77 (1H, d, *J* = 9.6 Hz, H-3), 6.39 (1H, d, *J* = 9.6 Hz, H-4), 3.17 (3H, s, N-CH_3); ^{13}C-NMR (DMSO-d_6, 75 MHz) δ 165.6 (C-7), 162.25 (C-2), 144.96 (C-6), 139.09 (C-4), 118.23 (C-3), 109.56 (C-5), 48.82 (N-$\underline{C}H_3$); HMBC (H→C) : H-6→ C-5, C-4, C-2, COOH, and N-$\underline{C}H_3$, H-4→ C-2, C-6, and $\underline{C}$OOH, H-3 → C-5, and C-2, N-C$\underline{H}_3$ → C-2 and C-6; UV (MeOH) λ_{max}, nm (log ε): 206 (4.04), 259 (4.14); EI-MS *m/z* 153 $[M]^+$ (100), 136 $[M\text{-}OH]^+$ (5), 108 $[M\text{-}COOH]^+$ (50) ; mp 241.5˚C.

Mannitol (8) ^{13}C-NMR (D_2O, 75 MHz) δ 73.5 (C-2 and C-5), 71.9 (C-3 and C-4), and 65.9 (C-1 and C-6).

Supplement Fig. 1. Schematic isolation procedure of chemical ingredients