Supporting Information

9-(2-*C*-Cyano-2-deoxy-β-D-*arabino*-pentofuranosyl)guanine, a Potential Antitumor Agent against B-Lymphoma Infected with Kaposi's Sarcoma-associated Herpesvirus

Masaki Ohtawa,[a] Satoshi Ichikawa,[a] Yasuhiro Teishikata,[b] Masahiro Fujimuro,[b] Hideyoshi Yokosawa,[b] and Akira Matsuda.[a]

Department of Medicinal Chemistry[a] and Biological Chemistry,[b] Faculty of Pharmaceutical Sciences, Hokkaido University, Kita-ku, Kita-12, Nishi-6, Sapporo 060-0812, Japan.

9-(2-*C*-Cyano-2-deoxy-β-D-*arabino*-pentofuranosyl)guanine (CNDAG), a Potential Antitumor Agent against B-Lymphoma Infected with Kaposi's Sarcoma-associated Herpesvirus (KSHV).

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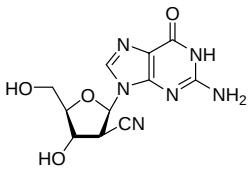

CNDAG

General

NMR spectra were obtained on a JEOL AL400 or Bruker ARX-500 and were reported in parts per million (δ) relative to tetramethylsilane (0.00 ppm) as an internal standard otherwise noted. Coupling constant (*J*) was reported in herz (Hz). Abbreviations of multiplicity were as follows; s: singlet, d; doublet, t: triplet, q: quatlet, m: multiplet, br: broad. Data were presented as follows; chemical shift (multiplicity, integration, coupling constant). Assignment was based on ^{1}H-^{1}H COSY, HMBC and HMQC NMR spectra. FAB-MS data were obtained on a JEOL JMS-HX101 or JEOL JMS-700TZ. Analytical thin layer chromatography (TLC) was performed on Merck silica gel $60F_{254}$ plates. Normal-phase column chromatography was performed on Merck silica gel 5715 or Kanto Chemical silica gel 60N (neutral). Flash column chromatography was performed on Merck silica gel 60. Dichloromethane was distilled from P_2O_5 and then CaH_2. Methanol was distilled from sodium metal or directly used HPLC grade solvent from Kanto Chemical Co., Inc. Toluene was distilled from sodium metal/benzophenone ketyl. *N*,*N*-Dimethylformamide was distilled from CaH_2 under reduced pressure or purchased dehydrated solvent from Kishida Chemical Co., Ltd. Tetrahydrofuran was purchased dehydrated stabilizer free solvent from Kanto Chemical Co., Inc.

9-[2-*C*-Cyano-2-deoxy-3,5-*O*-(tetraisopropyldisiloxane-1,3-diyl)-β-D-*arabino*-pentofuranosyl]-6-methoxypurine (14). A mixture of CrO_3 (2.00 g, 19.5 mmol), MS4A (5.5 g) and pyridine (3.10 mL, 38.9 mmol) in CH_2Cl_2 (30 mL) was stirred at 0 ˚C for 0.5 h. Ac_2O (3.70 mL, 38.9 mmol) was added to the mixture, which was further stirred at 0 ˚C for 20 min. 9-[3,5-*O*-(tetraisopropyldisiloxane-1,3-diyl)-β-D-ribofuranosyl]-6-methoxypurine **8** (3.00 g, 5.56 mmol) in CH_2Cl_2 (10 mL) was added to the above mixture, and the solution was stirred at 0 ˚C for 15 min. The reaction mixture was poured into Et_2O (80 mL), and the resulting insoluble was filtered off through Celite and Florisil pad. The filtrate was washed with 1 M aqueous HCl, saturated aqueous $NaHCO_3$ and brine, dried (Na_2SO_4), filtered, and concentrated in *vacuo*. The residue in CH_2Cl_2 (50 mL) was treated with Bu_4NCN (2.70 g, 10.0 mmol) at 0 ˚C, and the mixture was stirred for 15 min. The reaction mixture was diluted with Et_2O (100 mL), washed with brine, dried (Na_2SO_4), filtered, and concentrated in *vacuo*. The residue in CH_2Cl_2 (50 mL) was treated with DMAP (1.02 g, 8.34 mmol), PhOC(S)Cl (1.15 mL, 8.34 mmol) and Et_3N (1.16 mL, 8.34 mmol) at 0 ˚C, and the mixture was stirred for 15 min. Saturated aqueous $NaHCO_3$ was added, and the resulting biphasic layers were vigorously stirred at room temperature for 10 min. The organic layer was washed with saturated aqueous $NaHCO_3$, dried (Na_2SO_4), filtered, and concentrated in *vacuo*. The residue was semi-purified by silica gel column chromatography (5×12 cm, hexane:EtOAc = 3:1-2:1) to afford the crude thionocarbonate **11** as a pale yellow foam. A solution of thionocarbonate **11** in

toluene (16 mL) was treated with AIBN (400 mg, 2.44 mmol) and Bu_3SnH (0.57 mL, 2.44 mmol), and the reaction mixture was heated at 100 ˚C for 15 min, which was then allowed to room temperature. The mixture was concentrated in *vacuo*. The residue was purified by flash silica gel column chromatography (3×15 cm, hexane:EtOAc = 2:1-3:2) to afford **14** (685 mg, 4 steps 22%) as a white foam: ^{1}H NMR ($CDCl_3$, 500 MHz) 7.90 (s, 1H, H-8), 6.35 (d, 1H, H-1', $J_{1',2'}$ = 7.3 Hz), 5.07 (t, 1H, H-3', $J_{3',2'} = J_{3',4'}$ = 8.5 Hz), 4.87 (br s, 2H, NH_2), 4.15 (dd, 1H, H-5'a, $J_{5'a,4'}$ = 3.7, $J_{5'a,5'b}$ = 12.0 Hz), 4.10-4.05 (m, 4H, H-5'b, OMe), 3.87 (ddd, 1H, H-4', $J_{4',3'}$ = 8.5, $J_{4',5'a} = J_{4',5'b}$ = 3.7 Hz), 3.70 (dd, 1H, H-2', $J_{2',1'}$ = 7.3, $J_{2',3'}$ = 8.5 Hz), 1.18-0.98 (m, 28H, isopropyl × 4); ^{13}C NMR ($CDCl_3$, 125 MHz) 161.71, 159.44, 153.04, 136.50, 115.84, 115.27, 84.09, 80.78, 73.11, 60.07, 53.91, 42.90. 17.41, 17.31, 17.26, 17.24, 16.98, 16.89, 16.83, 13.40, 12.99, 12.41; FAB-LRMS *m/z* 549.4 (MH^+); FAB-HRMS ($CHCl_3$) calcd for $C_{24}H_{40}N_6O_5Si_2$ 548.2600, found 549.2673 (MH^+); IR ($CHCl_3$) 2260 cm^{-1}.

9-[2-*C*-Cyano-2-deoxy-3,5-*O*-(tetraisopropyldisiloxane-1,3-diyl)-β-D-*arabino*-pentofuranosyl]-2,6-diaminopurine (15). Compound **15** was prepared from 9-[3,5-*O*-(tetraisopropyldisiloxane-1,3-diyl)-β-D-ribofuranosyl]-2,6-diaminopurine **9** (2.62 g, 5.00 mmol) as described above for the synthesis of **14**. Purification by silica gel column chromatography (3×15 cm, hexane:EtOAc = 1:1-1:2-1:3) gave **15** (800 mg, 4 steps 30%) as a white foam: ^{1}H NMR ($CDCl_3$, 500 MHz) 7.81 (s, 1H, H-8), 6.34 (d, 1H, H-1', $J_{1',2'}$ = 7.5 Hz), 5.65 (br s, 2H, NH_2), 5.03 (t, 1H, H-3', $J_{3',2'} = J_{3',4'}$ = 8.5 Hz), 4.81 (br s, 2H, NH_2), 4.14 (dd, 1H, H-5'a, $J_{5'a,4'}$ = 3.8, $J_{5'a,5'b}$ = 13.0 Hz), 4.06 (dd, 1H, H-5'b, $J_{5'b,4'}$ = 3.8, $J_{5'b,5'a}$ = 13.0 Hz), 3.85 (ddd, 1H, $J_{4',3'}$ = 8.5, $J_{4',5'a} = J_{4',5'b}$ = 3.8 Hz), 3.70 (dd, 1H, H-2', $J_{2',1'}$ = 7.5, $J_{2',3'}$ = 8.5 Hz), 1.18-0.98 (m, 28H, isopropyl × 4); ^{13}C NMR ($CDCl_3$, 125 MHz) 161.54, 157.55, 152.95, 136.81, 117.10, 115.93, 85.62, 82.24, 74.99, 62.39, 44.53, 18.99, 18.91, 18.87, 18.82, 18.61, 18.52, 18.49, 18.43, 15.03, 14.59, 14.52, 14.01; FAB-LRMS *m/z* 534.4 (MH^+); FAB-HRMS ($CHCl_3$) calcd for $C_{23}H_{39}N_7O_4Si_2$ 533.2600, found 534.2682 (MH^+); IR ($CHCl_3$) 2260 cm^{-1}.

2-Amino-6-chloro-9-[2-*C*-cyano-2-deoxy-3,5-*O*-(tetraisopropyldisiloxane-1,3-diyl)-β-D-*arabino*-pentofuranosyl]purine (16). Compound **16** was prepared from 2-amino-6-chloro-9-[3,5-*O*-(tetraisopropyldisiloxane-1,3-diyl)-β-D-ribofuranosyl]purine **10** (380 mg, 0.70 mmol) as described above for the synthesis of **14**. Purification by silica gel column chromatography (3×8 cm, hexane:EtOAc = 5:1-2:1) gave **16** (126 mg, 4 steps 33%) as a white foam: ^{1}H NMR ($CDCl_3$, 500 MHz) 8.07 (s, 1H, H-8), 6.37 (d, 1H, H-1', $J_{1',2'}$ = 7.5 Hz), 5.09 (br s, 2H, NH_2), 5.02 (t, 1H, H-3', $J_{3',2'} = J_{3',4'}$ = 9.0 Hz), 4.16 (dd, 1H, H-5'a, $J_{5'a,4'}$=3.0, $J_{5'a,5'b}$=13.1 Hz), 4.08 (dd, 1H, H-5'b, $J_{5'b,4'}$ = 3.0, $J_{5'b,5'a}$= 13.1 Hz), 3.89 (ddd, 1H, $J_{4',3'}$ = 9.0, $J_{4',5'a} = J_{4',5'b}$ = 3.0 Hz), 3.72 (dd, 1H, H-2', $J_{2',1'}$ = 7.5, $J_{2',3'}$ = 9.0 Hz),

1.18-0.94 (m, 28H, isopropyl × 4); ^{13}C NMR ($CDCl_3$, 125 MHz) 160.14, 153.86, 152.58, 140.13, 126.02, 115.90, 84.63, 81.36, 72.97, 60.56, 42.85, 17.56, 17.42, 17.38, 17.31, 17.25, 16.99, 16.91, 16.85, 13.58, 13.44, 12.95, 12.65; FAB-LRMS *m/z* 553.4 (MH^+); FAB-HRMS ($CHCl_3$) calcd for $C_{23}H_{37}ClN_6O_4Si_2$ 553.2100, found 553.2178 (MH^+); IR ($CHCl_3$) 2260 cm^{-1}.

9-(2-*C*-Cyano-2-deoxy-β-D-*arabino*-pentofuranosyl)-6-methoxypurine (4). A solution of **14** (200 mg, 0.37 mmol) in THF (4 mL) was treated with AcOH (42 μL, 0.73 mmol) and Bu_4NF (0.73 mL of 1 M solution in THF, 0.73 mmol) at 0 ˚C, and the resulting mixture was stirred at 0 ˚C for 1 h. After the mixture was concentrated in *vacuo*, the residue was purified by silica gel column chromatography (2×7 cm, $CHCl_3$:MeOH = 15:1), and triturated by $CHCl_3$ to afford **4** (81 mg, 73%) as a white solid: ^{1}H NMR (DMSO-d_6, 500 MHz) 8.14 (s, 1H, H-8), 6.52 (br s, 2H, NH_2), 6.35 (d, 1H, H-1', $J_{1',2'}$ = 7.5 Hz), 6.25 (br d, 1H, OH-3', $J_{OH\text{-}3',\,3'}$ = 5.8 Hz), 5.14 (br t, 1H, OH-5', $J_{OH\text{-}5',\,5'a} = J_{OH\text{-}5',\,5'b}$ = 5.3 Hz), 4.76 (ddd, 1H, H-3', $J_{3',2'}$ = 8.4, $J_{3',4'}$ = 6.5, $J_{3',\,OH\text{-}3'}$ = 5.8 Hz), 4.03 (dd, 1H, H-2', $J_{2',\,1'}$ = 7.5, $J_{2',3'}$ = 8.4 Hz), 3.81–3.78 (m, 1H, H-4'), 3.77-3.73 (m, 1H, H-5'a), 3.69-3.65 (m, 1H, H-5'b); ^{13}C NMR (DMSO-d_6, 125 MHz) 160.67, 159.90, 153.36, 137.94, 117.05, 113.58, 113.49, 85.35, 84.89, 81.25, 80.20, 79.91, 71.17; FAB-LRMS *m/z* 307.1 (MH^+); FAB-HRMS (DMSO) calcd for $C_{12}H_{14}N_6O_4$ 306.108, found 307.1152 (MH^+); IR (DMSO) 2250 cm^{-1}; Anal. Calcd for $C_{12}H_{14}N_6O_4 \cdot 1.2\ H_2O$: C, 43.06; H, 5.04; N, 25.63. Found: C, 44.22; H, 4.79; O, 25.48.

9-(2-*C*-Cyano-2-deoxy-β-D-*arabino*-pentofuranosyl)-2,6-diaminopurine (5). Compound **5** was prepared from **15** (53 mg, 0.10 mmol) as described above for the synthesis of **4**. After purification by silica gel column chromatography (2×7 cm, $CHCl_3$:MeOH = 10:1), the residue was crystallized from EtOH to afford **5** (18 mg, 64%, mp 221 ˚C, decomp.): ^{1}H NMR (DMSO-d_6, 500 MHz) 7.96 (s, 1H, H-8), 6.76 (br s, 2H, NH_2), 6.29 (d, 1H, H-1', $J_{1',2'}$ = 7.4 Hz), 6.23 (br d, 1H, OH-3', $J_{OH\text{-}3',\,3'}$ = 5.8 Hz), 5.81 (br s, 2H, NH_2), 5.18 (br t, 1H, OH-5', $J_{OH\text{-}5',\,5'a} = J_{OH\text{-}5',\,5'b}$ = 5.3 Hz), 4.77 (dd, 1H, H-3', $J_{3',2'}$ = 8.4, $J_{3',\,4'}$ = 5.3 Hz), 3.99 (t, 1H, H-2', $J_{2',\,1'} = J_{2',3'}$ = 7.4 Hz), 3.95-3.76 (m, 1H, H-4'), 3.73-3.23 (m, 1H, H-5'a), 3.68-3.63 (m, 1H, H-5'b); ^{13}C NMR (DMSO-d_6, 125 MHz) 160.29, 156.17, 151.12, 135.79, 134.12, 117.19, 112.91, 85.23, 84.79, 81.08, 79.76, 71.71, 71.19; FAB-LRMS *m/z* 292.1 (MH^+); FAB-HRMS (DMSO) calcd for $C_{11}H_{13}N_7O_3$ 291.108, found 292.1154 (MH^+); Anal. Calcd for $C_{11}H_{13}N_7O_3 \cdot 0.1\ H_2O$: C, 45.08; H, 4.54; N, 33.46. Found: C, 45.23; H, 4.41; O, 33.27; IR (DMSO) 2245 cm^{-1}.

2-Amino-6-chloro-9-(2-*C*-cyano-2-deoxy-β-D-*arabino*-pentofuranosyl)purine (6). Compound **6** was prepared from **16** (271 mg, 0.50 mmol) as described above for the synthesis of **4**. After purification by silica

gel column chromatography (2×7 cm, $CHCl_3$:MeOH = 10:1), the residue was crystallized from EtOH to afford **6** (110 mg, 73%) as a colorless needle (mp 192 ˚C, decomp.); ^{1}H NMR (DMSO-d_6, 500 MHz) 8.41 (s, 1H, H-8), 7.04 (br s, 2H, NH_2), 6.38 (d, 1H, H-1', $J_{1',2'}$ = 7.4 Hz), 6.31 (br d, 1H, OH-3', $J_{OH\text{-}3',3'}$ = 3.7 Hz), 5.18 (br s, 1H, OH-5'), 4.77 (dd, 1H, H-3', $J_{3',2'}$ = 7.4, $J_{3',4'}$ = 3.8 Hz), 4.08 (t, 1H, H-2', $J_{2',1'} = J_{2',3'}$ = 7.4 Hz), 3.82-3.80 (m, 1H, H-4'), 3.77-3.74 (m, 1H, H-5'a), 3.69-3.65 (m, 1H, H-5'b); ^{13}C NMR (DMSO-d_6, 125 MHz) 159.85, 153.21, 149.72, 141.31, 139.68, 123.19, 123.10, 117.01, 86.06, 81.37, 80.55, 71.32; FAB-LRMS *m/z* 311.1 (MH^+); FAB-HRMS (DMSO) calcd for $C_{11}H_{11}ClN_6O_3$ 310.058, found 311.0633 (MH^+); Anal. Calcd for $C_{11}H_{11}ClN_6O_3 \cdot 0.3H_2O$: C, 41.80; H, 3.70; N, 26.59. Found: C, 41.95; H, 3.40; O, 26.62; IR (DMSO) 2221 cm^{-1}.

9-(2-*C*-Cyano-2-deoxy-β-D-*arabino*-pentofuranosyl)guanine (3) and **9-(2-*C*-cyano-2-deoxy-1-β-D-*ribo*-pentofuranosyl)guanine (17).** A solution of **4** (150 mg, 0.49 mmol) in phosphate buffer (0.1 M, pH 7.0, 30 mL) was treated with bovine adenosine deaminase (150 unit, Sigma) at 37 ˚C for 20 h. Charcoal (Wako chemical) was added until the UV absorption of the solution was disappeared. The suspension was mounted on a column, which was washed with H_2O and eluted with MeOH. The UV positive fractions were collected and concentrated in *vacuo*, and the residue was further purified by C18 HPLC (YMC-Pack D-ODS-5-A, 250×20 mm, 5% MeCN, 0.1% AcOH in H_2O) to afford **3** (22 mg, 18%) and **17** (59 mg, 42%) as a white solid: Data for **3**; retention time; 7.2 min; ^{1}H NMR (DMSO-d_6, 400 MHz) 10.64 (br s, 1H, NH), 7.98 (s, 1H, H-8), 6.53 (br s, 2H, NH_2), 6.27 (d, 1H, OH-3', $J_{OH\text{-}3',3'}$ = 5.5 Hz), 6.23 (d, 1H, H-1', $J_{1',2'}$ = 7.5 Hz), 5.14 (t, 1H, OH-5', $J_{OH\text{-}5',5'a'} = J_{OH\text{-}5',5'b'}$ = 5.3 Hz), 4.70 (ddd, 1H, H-3', $J_{3',2'}$ = 8.8, $J_{3',4'}$ = 8.5, $J_{3',OH\text{-}3'}$ = 5.5 Hz), 4.01 (dd, 1H, H-2', $J_{2',1'}$ = 7.5, $J_{2',3'}$ = 8.8 Hz), 3.78–3.61 (m, 3H, H-4'. H-5'); ^{13}C NMR (DMSO-d_6, 100 MHz) 153.77, 150.58, 134.86, 117.01, 116.37, 85.06, 80.50, 71.22, 59.37, 42.44, 40.41, 40.12; FAB-LRMS *m/z* 293.1 (MH^+); FAB-HRMS (MeOH) calcd for $C_{11}H_{12}N_6O_4$ 292.092, found 293.1002 (MH^+); IR (DMSO) 2251 cm^{-1}; Anal. Calcd for $C_{11}H_{12}N_6O_4 \cdot 1.2$ H_2O: C, 42.05; H, 4.63; N, 26.74. Found: C, 42.32; H, 4.33; O, 26.43. Data for **17**; retention time; 15.9 min; ^{1}H NMR (DMSO-d_6, 400 MHz) 10.78 (br s, 1H, NH), 8.05 (s, 1H, H-8), 6.63 (br s, 2H, NH_2), 6.46 (d, 1H, OH-3', $J_{OH\text{-}3',3'}$ = 5.1 Hz), 6.24 (d, 1H, H-1', $J_{1',2'}$ = 8.8 Hz), 5.21 (t, 1H, OH-5', $J_{OH\text{-}5',5'a'} = J_{OH\text{-}5',5'b'}$ = 5.4 Hz), 4.56 (m, 1H, H-3'), 4.30 (dd, 1H, H-2', $J_{2',1'}$ = 8.8, $J_{2',3'}$ = 5.2 Hz), 4.04 (m, 1H, H-4'), 3.62 – 3.61 (m, 2H, H-5'); ^{13}C NMR (DMSO-d_6, 100 MHz) 156.39, 153.81, 150.98, 135.02, 116.46, 116.08, 87.46, 83.16, 71.25, 60.93, 40.52; FAB-LRMS *m/z* 293.1 (MH^+); FAB-HRMS (MeOH) calcd for $C_{11}H_{12}N_6O_4$ 292.092, found 293.0991 (MH^+); IR (DMSO) 2250 cm^{-1}; Anal. Calcd for $C_{11}H_{12}N_6O_4 \cdot 0.5$ H_2O: C, 43.86; H, 4.35; N, 27.9. Found: C, 44.12; H, 4.14; O, 27.89.

2-Amino-9-(2-*C*-cyano-2-deoxy-β-D-*arabino*-pentofuranosyl)purine (7). A mixture of **6** (80 mg, 0.26 mmol) and 10% Pd/C (80 mg) in MeOH (25 mL) was vigorously stirred under an H_2 atmosphere at room temperature for 6 h. The catalyst was filtered off through Celite pad, and the filtrate was concentrated in *vacuo*. The residue was purified by flash silica gel column chromatography (1×5 cm, $CHCl_3$:MeOH = 10:1-8:1), and triturated by EtOH to afford **6** (30 mg, 42%) as a white solid: ^{1}H NMR (DMSO-d_6, 500 MHz) 7.96 (s, 1H, H-8), 6.76 (br s, 2H, NH_2), 6.29 (d, 1H, H-1', $J_{1',2'}$ = 7.4 Hz), 6.23 (br d, 1H, OH-3', $J_{OH\text{-}3',3'}$ = 5.8 Hz), 5.81 (br s, 2H, NH_2), 5.18 (br t, 1H, OH-5', $J_{OH\text{-}5',5'a} = J_{OH\text{-}5',5'b}$ = 5.3 Hz), 4.77 (dd, 1H, H-3', $J_{3',2'}$ = 8.4, $J_{3',4'}$= 5.3 Hz), 3.99 (t, 1H, H-2', $J_{2',1'} = J_{2',3'}$ = 7.4 Hz), 3.95-3.76 (m, 1H, H-4'), 3.73-3.23 (m, 1H, H-5'a), 3.68-3.63 (m, 1H, H-5'b); ^{13}C NMR (DMSO-d_6, 125 MHz) 160.29, 156.17, 151.12, 135.79, 134.12, 117.19, 112.91, 85.23, 84.79, 81.08, 79.76, 71.71, 71.19; FAB-LRMS *m/z* 277.1 (MH^+); FAB-HRMS (DMSO) calcd for $C_{11}H_{13}N_7O_3$ 276.097, found 277.1055 (MH^+); Anal. Calcd for $C_{11}H_{11}N_6O_3$□0.33EtOH: C, 48.05; H, 4.83; N, 28.83. Found: C, 47.76; H, 4.53; O, 28.45; IR (DMSO) 2221 cm^{-1}.

Cell lines and culture

KSHV-mediated primary effusion lymphoma (PEL) cells (KSHV-positive, EBV-negative BC3 cells and KSHV-positive, EBV-negative BC2 cells) and herpesvirus-negative Burkitt's lymphoma cells (DG75 cells) were grown in 10% FBS RPMI medium 1640 at 37 ^oC.

Cell viability assay[24]

Cells were seeded to 96-well plates at 1.5×10^4 cells/well in 200 μL of the growth medium with and without various concentrations of nucleoside analogues, and were incubated at 37 °C for 4 days in a humidified CO_2-controlled atmosphere. Cytotoxic effects of the test compounds, the test compounds and adenosine deaminase inhibitor (10 μM), or the test compounds and competitor nucleoside (50 μM) were assessed by colorimetric MTT [3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl tetrazolium bromide] dye reduction assay using a cell counting kit-8 (Dojindo). MTT is converted into a purple formazan product with an absorbance at 560 nm through the actions of mitochondrial enzymes. The optical density in ACV/GCV-treated cells was measured at 560 nm with a microplate spectrophotometer and expressed as percentage to the value in untreated cells (defined as 100%). The value of IC_{50}, a 50% cytotoxic concentration of drug, was calculated from the plot of drug concentration versus the percentage of live cells. Data are shown as the mean value ± S.E.M. of three independent experiments.

Table S1. Elemental analysis data for target compounds

compound	elemental analysis	
	calculated	found
3		
$C_{11}H_{12}N_6O_4$□0.5 H_2O	C, 43.86; H, 4.35; N, 27.90	C, 44.12; H, 4.14; O, 27.89
4		
$C_{12}H_{14}N_6O_4$□1.2 H_2O	C, 43.06; H, 5.04; N, 25.63	C, 44.22; H, 4.79; O, 25.48
5		
$C_{11}H_{13}N_7O_3$□0.1 H_2O	C, 45.08; H, 4.54; N, 33.46	C, 45.23; H, 4.41; O, 33.27
6		
$C_{11}H_{11}ClN_6O_3$□0.3H_2O	C, 41.80; H, 3.70; N, 26.59	C, 41.95; H, 3.40; O, 26.62
7		
$C_{11}H_{11}N_6O_3$□0.33EtOH	C, 48.05; H, 4.83; N, 28.83	C, 47.76; H, 4.53; O, 28.45