Supplemental Material

Table 1. Effect of geldanamycin derivatives [ref.19] on HSV-2 and cell toxicity inVero cells.

Compounds	CC_{50} (μmol/L)[a]	IC_{50} (μmol/L)[b]	SI[c]
1 (GA)	23.13	0.60	38.6
2a	33.66	5.14	6.5
2b	34.16	2.59	13.2
2c	25.50	2.15	11.9
2d	27.43	2.45	11.2
2e	34.04	1.15	29.6
2f	114.20	2.09	54.6
2g	18.07	2.21	8.2
2h	32.62	1.79	18.2
2i	26.27	3.57	7.4
2j	33.93	8.02	4.2
2k	22.57	>10.43	-
2l	37.28	>10.68	-
3	>286.41	>286.41	-
ACV	>2220.15	112.67	>19.7

[a] 72 hours after treatment, cell toxicity were determined by CPE.

[b] Antiviral activity were determined by CPE.

[c] SI= CC_{50}/IC_{50}

ACV (Acyclovir) were used as positive controls.

Unless otherwise noted, the values represent average ± standard deviation from two separated experiments.

SAR analysis

By examination of the relationships between the structure and the anti-HSV-2 activity of the tested compounds, some general conclusionscan be drawn as follows:

1. The antiviral activity against HSV-2 of 17-substituted GA derivatives decreased compared with GA. And the toxicity of these compounds also decreased slinghtly.
2. Non-cyclic side chain modification could significantly reduce the toxicity.
3. The 17- and 19- bis-substituted derivative lost antiviral activity.
4. The antiviral activity also affected by the 17-substituted group long chain or large volume of space.
5. Introduction of hetero-atom to the 17-substituted cyclic groups was better for antiviral activity.
6. Chirality of 17-substituted side chain could influence the antiviral activity.