Table S1: Twenty-six reference compounds identified from the literature. These compounds have shown activity against HPV-positive cells in *in vitro* assays, and/or against E6 protein in *in silico* approaches.

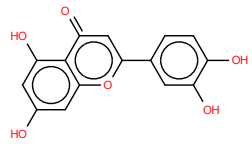
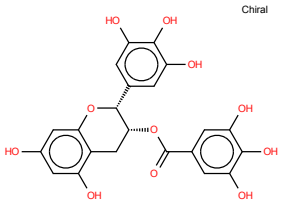
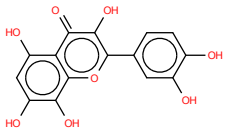
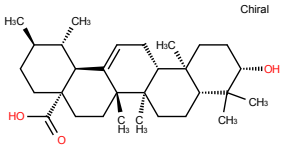
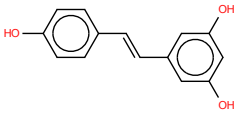
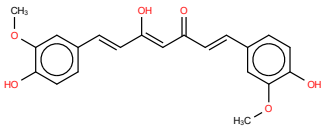
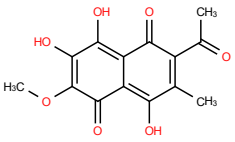
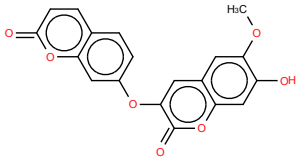
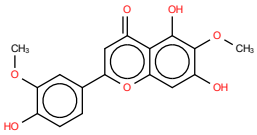
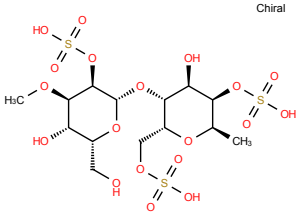
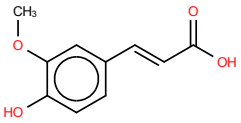
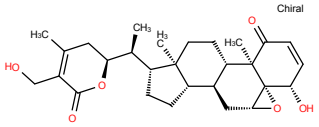
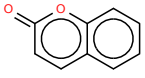
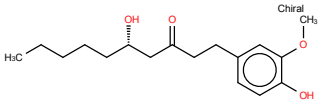
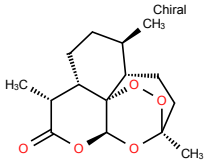
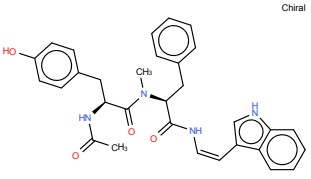
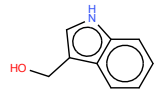
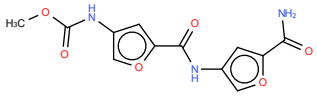
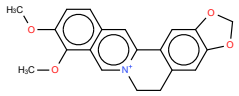
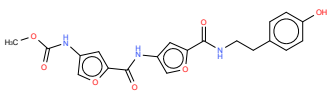
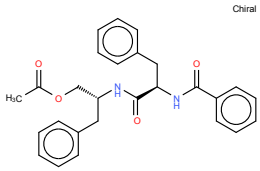
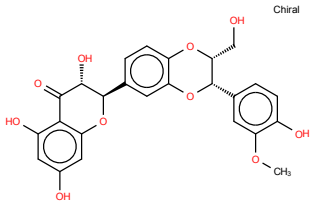
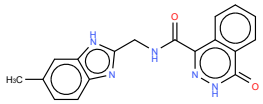
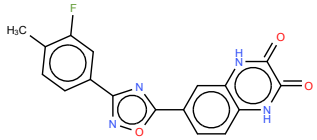
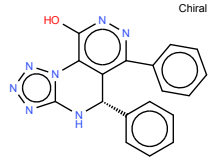
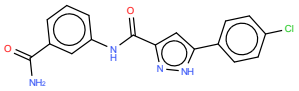
Structure	Name	Structure	Name
	Luteolin ZINC000018185774 [1–4]		Egcg ZINC000003870412 [5–7]
	Gossypetin ZINC000006525297 [1]		Ursolic-acid ZINC000003978827 [8–10]
	Resveratrol ZINC000000006787 [5,10]		Curcumin ZINC000100067274 [11–15]
	Celiptium ZINC000100089149 [15,16]		Daphnoretin ZINC000000689683 [15]
	Jaceosidin ZINC000014779854 [4,7,17]		Carrageenan ZINC000064373300 [18]
	Ferulate ZINC000000058258 [16,19]		Withaferin-A ZINC000064373300 [10,20,21]
	Coumarin ZINC000000074709 [22,23]		Gingerol ZINC000001531846 [7,24]
	Artemisinin ZINC000008681831 [7,25]		Miyakamide-A ZINC000014594537 [26]

Table S1: Twenty-six reference compounds identified from the literature. These compounds have shown activity against HPV-positive cells in *in vitro* assays, and/or against E6 protein in *in silico* approaches.

Structure	Name	Structure	Name
	Indol-3-carbinol ZINC000000158743 [27]		Proximicine-A ZINC000043073751 [26]
	Berberine ZINC000003779067 [28]		Proximicine-B ZINC000043078506 [26]
	Aurantiamide acetate ZINC000013374322 [26]		Silibinin ZINC000002033588 [29–31]
	C1-a ZINC000000100126 [10]		C1-b ZINC000009679272 [10]
	C1-c ZINC000000100126 [10]		C1-d ZINC000009679272 [10]

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