

**Table S1.** Thymine-related structures were used in the study.

Structures	PubChem ID
Cidofovir (Standard)	60613
(1)	65049
(2)	11243988
(3)	123370001
(4)	129802452
(5)	154137224
(6)	191372
(7)	21308117
(8)	451892
(9)	59119818
(10)	90413362
(11)	90413364
(12)	1135
(13)	566009
(14)	78957
(15)	667607
(16)	330104
(17)	78112
(18)	3385
(19)	348851
(20)	69672
(21)	163114065

**Table S2.** Generated pharmacophore models with scores

Pharmacophore models	Score (0-1)
Model-1	0.8320
Model-2	0.8163
Model-3	0.8064
Model-4	0.8033
Model-5	0.7995
Model-6	0.7994
Model-7	0.7909
Model-8	0.7908
Model-9	0.7850
Model-10	0.7722