Target Name	Thymidine kinase
Target TTD ID	TTDR00500

Target Species	Herpes simplex virus (HSV)
Chemical Type	N^2-phenylguanines
Mode of Action	Inhibitor
QSAR Model 1	$log(1/C_{HSV1\ TK}) = 0.594(\pm 0.229)\pi_m - 0.414(\pm 0.200) \times \pi_p + 1.048(\pm 0.746)\sigma_m + 2.381(\pm 0.871)\Re_p + 5.077(\pm 0.244)$ $n = 34;\ r = 0.897;\ s = 0.399;\ F = 29.767;\ Q^2 = 0.741;\ s_{PRESS} = 0.459$
QSAR Model 2	$\log(1/C_{HSV2\ TK}) = 0.424(\pm 0.239)\pi_m - 0.496(\pm 0.221) \times \pi_p + 2.055(\pm 0.771)\sigma_n + 1.468(\pm 0.898)\Re_p + 5.238(\pm 0.253)$ $n = 33;\ r = 0.896;\ s = 0.410;\ F = 28.431;\ Q^2 = 0.736;\ s_{PRESS} = 0.474$
QSAR Model 3	$\log(1/C_{HSV1\ TK}) = 1.28(\pm 0.77)\pi_{3,4} - 2.22(\pm 1.17) \times \log(\beta \cdot 10^{\pi 3,4} + 1) + 3.20(\pm 0.86) - 1.42(\pm 0.82)\mathcal{T} + 1.79(\pm 0.59) \times B_{1-3}$ $n = 30;\ r = 0.831;\ s = 0.530;\ F = 10.74;\ \pi_o = 0.53;\ \log\beta = -0{,}401$
QSAR Model 4	$\log(1/C_{HSV1\ TK}) = 0.486(\pm 0.160)\pi_m + 8.201 \times (\pm 3.000)F_2^{(e)} - 6.180(\pm 4.230)$ $n = 13;\ r = 0.953;\ s = 0.209;\ F_{(2,10)} = 49.057;\ Q^2 = 0.805;\ s_{PRESS} = 0.303$
QSAR Model 5	$\log(1/C_{HSV2\ TK}) = 0.292(\pm 0.096)\pi_m - 0.205 \times (\pm 0.030)F_1{}'^{(n)} - 0.922(\pm 0.370)B_{1m} + 2.067(\pm 0.570)$ $n = 13;\ 4 = 0.988;s = 0.117;\ F_{(3,9)} = 120.946;\ Q^2 = 0.952;\ s_{PRESS} = 0.166$
Molecular	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**

Descriptor	$C_{HSV1\ TK}$ and $C_{HSV2\ TK}$ are the PHG molar concentrations that provide 50% of HSV1 TK and HSV2 TK inhibition, respectively; π is the Hansch lipophilic substituent constant; σ is the Hammett electronic substituent constant; $\mathcal{R}$ is the Swain-Lupton resonance parameter; subscripts m and p stand for meta and para positions of the phenyl ring of the PHG derivative molecule, respectively; n is the number of compounds included in the models; r is the correlation coefficient; s is the overall standard deviation; F is the Fischer variance ratio; Q is the cross validation correlation coefficient; and S_{PRESS} is the cross validation standard deviation. The numbers in parentheses are the 95% confidence interval of the respective regression coefficients; $\pi_{3,4}$ is the sum of the π constant of the substituents attached to meta and para positions of the phenyl ring of PHG derivatives, β is the bilinear constant, B_{1-3} is the Sterimol parameter B_1, which is a measure of the width of the substituent, on the meta position, $\mathfrak{I}$ is the Swain-Lupton field substituent parameter, and π_o is the optimum $\pi_{3,4}$ value. The atomic frontier electron density $F_n^{(e)}$ is a property that denotes the electron density in the HOMO of a given atom in a molecule.
Reference	QSAR and molecular graphics analysis of N^2-phenylguanines as inhibitors of herpes simplex virus thymidine kinases. *Journal of Molecular Graphics and Modelling* 18, 33–41, 2000