Target Name	Telomerase
Target TTD ID	TTDC00195

Target Species	Human
Chemical Type	Acridinic derivatives
Mode of Action	Inhibitor
QSAR Model 1	$IC_{50} = -10.40 + 4.11nArNHR + 1.42nCar - 1.90nCbH$ $N = 75, \lambda = 0.58, D_2 = 2.75, F(3,71) = 16.62, p < 0.001$
QSAR Model 2	$IC_{50} = 0.091 + 1.71^{1}\Omega(nArNHR) + 0.66^{2}\Omega(nCar) - 1.11^{3}\Omega(nCbH)$ $N = 75, \lambda = 0.58, D^2 = 2.75, F(3,71) = 16.62, p < 0.001$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** nArNHR, number of secondary amines (aromatic); nCar, number of aromatic C(sp2); nCbH, number of unsubstituted benzene C(sp2) ; *N*, number of samples; D_2, square of Mahalanobis distance; *F*, Fisher ratio; *p*, the corresponding p-level. Count descriptors directly encode particular features of molecular structure and are simply obtained from the chemical structure of molecules by counting defined elements such as atoms (nAT), bonds (nBT), rings (nCIC), H-bond acceptor (nHA) and H-bond donor (nHD) atoms, path counts, walk counts and so on. If atomtypes are considered, atom-type counts are obtained such as number of carbon atoms (nC), number of halogens (nX), number of oxygen atoms (nO), etc. Analogously, functional group counts and fragment counts are calculated such as number of hydroxyl-groups (nOH), number of nitro-groups (nNO), number of amino-groups (nNH2), etc.
Reference	Prediction of telomerase inhibitory activity for acridinic derivatives based on chemical structure. *European Journal of Medicinal Chemistry* 44 (2009) 4826–4840