Target Name	Neuropeptide Y (NPY) Y5 receptor
Target TTD ID	TTDC00089

Target Species	Human
Chemical Type	Arylsulfonamidomethylcyclohexyl derivatives
Mode of Action	Inhibitor
QSAR Model 1	$pIC_{50} = -7.65701 - 0.984981 * \text{Atype\_N\_72} - 2.8118 * \text{Atype\_O\_60} + 0.768097 * \text{Atype\_C\_26} + 0.638227 * \text{CHI} - 2$ $N = 19,\ \text{LOF} = 0.381,\ r^2 = 0.874,\ r^2_{\text{adj.}} = 0.838,\ F\text{-test} = 24.283,$ $\text{LSE} = 0.128,\ r = 0.935,\ q^2 = 0.772,\ r^2_{\text{pred}} = 0.505$
QSAR Model 2	$pIC_{50} = -3.55704 + 1.75378 * \text{Radius of gyration} - 1.52078 * \text{Atype\_S\_107} + 0.662542 * \text{S\_aaaC} - 0.055225 * \text{MR}$ $N = 45,\ \text{LOF} = 0.459,\ r^2 = 0.850,\ r^2_{\text{adj.}} = 0.831,\ F\text{-test} = 44.148,$ $\text{LSE} = 0.278,\ r = 0.922\ \ q^2 = 0.793,\ r^2_{\text{pred}} = 0.879$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** N is the number of compounds in training set, LOF is lack of fit, r^2 is squared correlation coefficient, r^2_{adj}. is the square of adjusted correlation coefficient, F-test is a statistical parameter which compares 2 models differing by 1 or more variables to see if the more complex model is more reliable than the less complex one. LSE is least-square error, r is correlation coefficient,

	q^2 is the square of the correlation coefficient of the cross validation r^2_{pred}. is the square of redicted correlation coefficient calculated from the predicted activity of test set compounds. Atype_N_72, Atype_O_60 and Atype_C_26 are atom-type based AlogP descriptors. Each AlogP98 atom-type value represents the number of atoms of that type in the molecule. CHI-2 is the Kier and Hall connectivity index of order 2. Description of the parameters used in the study **Type** : Descriptors **E-state indices** : Electrotopological-state indices **Electronic** : Sum of partial charges, sum of formal charges, dipole moment, energy of the highest occupied orbital, energy of the lowest unoccupied orbital **Information content** : Information of atomic composition index, information indices based on the A-matrix, information indices based on the D-matrix, multigraph information content indices **Spatial** : Radius of gyration, Jurs descriptors, shadow indices, area, density, PMI, Vm **Structural** : Number of chiral centers, molecular weight, number of rotatable bonds, number of hydrogen-bond acceptors, number of hydrogen-bond donors **Thermodynamic** : Log of the partition coefficient, log of the partition coefficient atom-type value, desolvation free energy of water, desolvation free energy of octanol, heat of formation, molar refractivity **Topological** : Wiener index, Zagreb index, Hosoya index, Kier and Hall molecular connectivity index, Balaban indices
Reference	A novel range based QSAR study of human neuropeptide Y (NPY) Y5 receptor inhibitors. *European Journal of Medicinal Chemistry* 42 (2007) 463e470