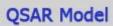
## **Therapeutic Targets Database**





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	$pIC_{50} = -7.65701 - 0.984981 * Atype\_N\_72 - 2.8118 * Atype\_O\_60 \\ + 0.768097 * Atype\_C\_26 + 0.638227 * CHI - 2$
	$N = 19$ , LOF = 0.381, $r^2 = 0.874$ , $r_{\text{adj.}}^2 = 0.838$ , $F$ -test = 24.283, LSE = 0.128, $r = 0.935$ , $q^2 = 0.772$ , $r_{\text{pred}}^2 = 0.505$
QSAR Model 2	$\begin{aligned} & pIC_{50} = -3.55704 + 1.75378 * Radius \ of \ gyration - 1.52078 \\ & * Atype\_S\_107 + 0.662542 * S\_aaaC - 0.055225 * MR \end{aligned}$
	$N = 45$ , LOF = 0.459, $r^2 = 0.850$ , $r_{\text{adj.}}^2 = 0.831$ , $F$ -test = 44.148, LSE = 0.278, $r = 0.922$ $q^2 = 0.793$ , $r_{\text{pred}}^2 = 0.879$
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, $r^2  ext{ is squared correlation coefficient,}$
	r <sup>2</sup> <sub>adj</sub> . 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<sup>2</sup> 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 Amatrix, 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