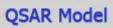
## Therapeutic Targets Database





Target Name	CYP2A5
Target TTD ID	TTDR01445

Target Species	Rat
Chemical Type	Naphthalene and non-naphthalene derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\begin{split} \text{pIC}_{50(2\text{A5})} &= 2.682(\pm 0.858) - 0.316(\pm 0.134) \text{Sr} + 0.728(\pm 0.105) \text{Shadow\_Xlength} \\ &- 7.569(\pm 0.915) \text{FPSA\_2} - 0.067(\pm 0.010) \text{WNSA\_1} \\ &- 2.497(\pm 0.619) \text{RNCG} - 0.141(\pm 0.030) \text{PNSA\_3} \\ n_{\text{Training}} &= 31, \text{ LOF} = 0.253, \ R^2 = 0.796, \ R_{\text{a}}^2 = 0.745, \ \ F = 15.64(\text{df } 6,24), \ Q^2 = 0.686, \\ \text{PRESS} &= 4.533, \ \ n_{\text{Test}} = 11, \ R_{\text{pred}}^2 = 0.707, \ r^2 = 0.734, \ r_0^2 = 0.732, \ r_{\text{m}}^2 = 0.701 \end{split}$
QSAR Model 2	$\begin{aligned} \text{pIC}_{50(2\text{A5})} &= 2.225 - 0.780 \text{RNCG} + 0.647 \text{Shadow\_Xlength} - 0.0003 \text{Apol} - 0.439 \text{Sr} \\ &- 0.005 \text{PMI} + 0.014 \text{RPCS} + 3.131 \text{FNSA\_1} - 51.603 \text{FPSA\_3} \\ n_{\text{Training}} &= 31, \text{ LSE} = 0.091, \ R^2 = 0.779, \ R_{\text{a}}^2 = 0.726, \ F = 22.88 (\text{df 4,26}), \ Q^2 = 0.575, \\ \text{PRESS} &= 6.140, \ n_{\text{Test}} = 11, \ R_{\text{pred}}^2 = 0.615, \ r^2 = 0.679, \ r_0^2 = 0.639, \ r_{\text{m}}^2 = 0.543 \end{aligned}$
QSAR Model 3	$\begin{aligned} \text{pIC}_{50(2\text{A5})} &= 2.989(\pm 0.727) + 0.334(\pm 0.071) \text{pIC}_{50(2\text{A6})} + 0.422(\pm 0.076) \text{Shadow\_Xlength} \\ &- 0.367(\pm 0.118) \text{Sr} - 43.219(\pm 8.814) \text{FPSA\_3} - 0.058(\pm 0.014) \text{Molref} \\ &+ 0.236(\pm 0.095) \text{ A log P98} \\ n_{\text{Training}} &= 29, \text{ LOF} &= 0.128, R^2 &= 0.898, R_{\text{a}}^2 &= 0.870, \\ F &= 32.36(\text{df } 6,22), Q^2 &= 0.814, \text{ PRESS} &= 2.321, \\ n_{\text{Test}} &= 10, R_{\text{pred}}^2 &= 0.914, r^2 &= 0.905, r_0^2 &= 0.904, r_{\text{m}}^2 &= 0.876 \end{aligned}$

QSAR Model 4	$plC_{50(2A5)} = -1.994 + 0.427 plC_{50(2A6)} + 0.166 Shadow\_Zlength + 3.850 FNSA\_1$
	$+0.394$ Shadow_Xlength $+0.012$ PNSA_2 $-0.355$ Sr
	$n_{\text{Training}} = 29$ , LSE = 0.061, $R^2 = 0.859$ , $R_a^2 = 0.794$ ,
	$F = 36.67(df 4, 24), Q^2 = 0.746, PRESS = 3.168,$
	$n_{\text{Test}} = 10, R_{\text{pred}}^2 = 0.902, r^2 = 0.903, r_2^0 = 0.881, r_{\text{m}}^2 = 0.769$
	Access the following web-servers to compute molecular descriptors: MoDel and e-dragon
Molecular Descriptor	Type of descriptor-Descriptor name: Definition
	Electronic-Apol: Sum of atomic polarizabilities; Dipole: Dipole moment; HOMO: Highest occupied
	molecular orbital energy; LUMO: Lowest unoccupied molecular orbital energy; Sr
	Superdelocalizability
	<b>Shape</b> -DIFFV: The difference between the volume of the individual molecule and the volume of the
	shape reference compound; COSV The common volume between each individual molecule and the
	molecule selected as the reference compound; Fo: The common overlap steric volume descriptor
	(COSV, see above) divided by the volume of the individual molecule; NCOSV: The difference
	between the volume of the individual molecule and the common overlap steric volume (COSV);
	ShapeRMS: Root mean square (RMS) deviation between the individual molecule and the shape
	reference compound; SRVolume: The volume of the shape reference compound
	Spatial-RadOfGyration: ; Density: The ratio of molecular weight to molecular volume; PMI-mag: It
	calculates the principal moments of inertia about the principal axes of a molecule; Vm: Molecular
	volume inside the contact surface; Area: van der Waals area of a molecule; Jurs descriptors: These are
	calculated by mapping atomic partial charges on solvent-accessible surface areas of individual atoms;
	Shadow indices: This set of geometric descriptors helps to characterize the shape of the molecules
	Thermodynamic-AlogP: Log of the partition coefficient; Molref: Molar refractivity; AlogP98: Log
	of partition coefficient
Reference	Exploring QSAR and QAAR for inhibitors of cytochrome P450 2A6 and 2A5 enzymes using GFA
	and G/PLS techniques. European Journal of Medicinal Chemistry 44 (2009) 1941–1951