Target Name	CYP2A5
Target TTD ID	TTDR01445

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

QSAR Model 4	$pIC_{50(2A5)} = -1.994 + 0.427pIC_{50(2A6)} + 0.166Shadow\_Zlength + 3.850FNSA\_1 + 0.394Shadow\_Xlength + 0.012PNSA\_2 - 0.355Sr$ $n_{Training} = 29,\ LSE = 0.061,\ R^2 = 0.859,\ R^2_a = 0.794,$ $F = 36.67(df\ 4,24),\ Q^2 = 0.746,\ PRESS = 3.168,$ $n_{Test} = 10,\ R^2_{pred} = 0.902,\ r^2 = 0.903,\ r^0_2 = 0.881,\ r^2_m = 0.769$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** **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 **Shape**-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