Target Name	CYP2A6
Target TTD ID	TTDR01443

Target Species	Human
Chemical Type	Naphthalene and non-naphthalene derivatives
Mode of Action	Inhibitor
QSAR Model 1	$\mathrm{pIC_{50(2A6)}} = -0.234(\pm 1.666) - 3.380(\pm 0.847)\mathrm{FPSA\_2} + 0.036(\pm 0.010)\mathrm{COSV} + 0.082(\pm 0.041)\mathrm{Shadow\_YZ}$ $n_{\mathrm{Training}} = 29,\ \mathrm{LOF} = 0.431,\ R^2 = 0.607,\ R^2_{\mathrm{a}} = 0.559,$ $F = 12.84(\mathrm{df}\ 3, 25),\ Q^2 = 0.502,\ \mathrm{PRESS} = 9.950,$ $n_{\mathrm{Test}} = 10,\ R^2_{\mathrm{pred}} = 0.667,\ r^2 = 0.785,\ r^2_0 = 0.648,\ r^2_{\mathrm{m}} = 0.494$
QSAR Model 2	$\mathrm{pIC_{50(2A6)}} = 1.698 + 0.021\mathrm{COSV} + 0.305\mathrm{A\ log\ P} - 0.004\mathrm{PPSA\_2}$ $n_{\mathrm{Training}} = 29,\ \mathrm{LSE} = 0.282,\ R^2 = 0.561,\ R^2_{\mathrm{a}} = 0.508,$ $F = 34.39(\mathrm{df}\ 1, 27),\ Q^2 = 0.489,\ \mathrm{PRESS} = 10.196,$ $n_{\mathrm{Test}} = 10,\ R^2_{\mathrm{pred}} = 0.714,\ r^2 = 0.778,\ r^2_0 = 0.721,\ r^2_{\mathrm{m}} = 0.592$
QSAR Model 3	$\mathrm{pIC_{50(2A6)}} = -4.941(\pm 1.685) + 0.908(\pm 0.148)\mathrm{pIC_{50(2A5)}} - 0.893(\pm 0.498)\mathrm{Density} + 2.742(\pm 0.830)\mathrm{Fo} + 0.500(\pm 0.167)\mathrm{Shadow\_Ylength}$ $n_{\mathrm{Training}} = 29,\ \mathrm{LOF} = 0.320,\ R^2 = 0.757,\ R^2_{\mathrm{a}} = 0.687,$ $F = 18.66(\mathrm{df}\ 4, 24),\ Q^2 = 0.648,\ \mathrm{PRESS} = 7.039,$ $n_{\mathrm{Test}} = 10,\ R^2_{\mathrm{pred}} = 0.869,\ r^2 = 0.842,\ r^2_0 = 0.842,\ r^2_{\mathrm{m}} = 0.842$

QSAR Model 4	$pIC_{50(2A6)} = 0.052 + 0.536pIC_{50(2A5)} + 0.328\ A\ \log P - 0.011NCOSV + 0.158Shadow\_Ylength$ $n_{Training} = 29,\ LSE = 0.192,\ R^2 = 0.679,\ R_a^2 = 0.630,$ $F = 57.07(df\ 1, 27),\ Q^2 = 0.610,\ PRESS = 7.796,$ $n_{Test} = 10,\ R_{pred}^2 = 0.867,\ r^2 = 0.883,\ r_0^2 = 0.866,\ r_m^2 = 0.768$
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