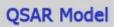
Therapeutic Targets Database





Target Name	CYP2B6
Target TTD ID	TTDR01444

Target Species	Human					
Chemical Type	Azole compounds					
Mode of Action	Inhibitor					
QSAR Model 1	Human CYP2B6: $pIC_{50}(\text{Inhibitory activity}) = 1.48(\pm 0.43)\log P - 1.64(\pm 0.76)\log (\beta P + 1) \\ -0.98(\pm 0.82)I_{\text{OH}} + 2.20(\pm 0.86) \\ n = 15, r = 0.936, s = 0.589, F = 26.0, \log \beta = -3.0, \log P_{\text{opt}} = 3.97, \\ \text{Outliers} = \text{ketoconazole} \ (\textbf{13}), [\text{triadimenol} \ (\textbf{8}) \text{ and fluconazole} \ (\textbf{9})]$					
QSAR Model 2	Human CYP2B6: $pIC_{50}(Inhibitory) = 1.30(\pm 0.43)pIC_{50} (Binding) - 1.04(\pm 0.98)I_{OH} - 1.42(\pm 2.24)$ $n = 15, \ r = 0.886, \ s = 0.727, \ F = 21.9,$ Outliers = hexaconazole (5), [triadimenol (8) and fluconazole (9)]					
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: $\underline{\text{MoDel}}$ and $\underline{\text{e-dragon}}$ P is the 1-octanol-water partition coefficient; β is the value related to the location of the optimum log P value. X is an indicator variable taking the value of unity for the presence and zero for the absence of certain structural features. E_{HOMO} is the energy level of HOMO. I_{azole} is the indicator variable for unity for imidazoles and zero for triazoles. I_{OH} is the indicator variable taking unity and zero for compounds with and without a hydroxyl group in the molecule.					
Reference	Quantitative Structure – Activity Relationship for Inhibition of CYP2B6 and CYP3A4 by Azole Compounds – Comparison with Their Binding Affinity. <i>QSAR Comb. Sci.</i> 28, 2009, No. 6-7, 629 – 636					