Target Name	CYP2B6
Target TTD ID	TTDR01444

Target Species	Human
Chemical Type	Azole compounds
Mode of Action	Inhibitor
QSAR Model 1	Human CYP2B6: $pIC_{50}(\text{Inhibitory activity}) = 1.48(\pm0.43)\log P - 1.64(\pm0.76)\log(\beta P + 1) - 0.98(\pm0.82)I_{OH} + 2.20(\pm0.86)$ $n = 15,\ r = 0.936,\ s = 0.589,\ F = 26.0,\ \log\beta = -3.0,\ \log P_{opt} = 3.97,$ Outliers = ketoconazole (**13**), [triadimenol (**8**) and fluconazole (**9**)]
QSAR Model 2	Human CYP2B6: $pIC_{50}(\text{Inhibitory}) = 1.30(\pm0.43)pIC_{50}(\text{Binding}) - 1.04(\pm0.98)I_{OH} - 1.42(\pm2.24)$ $n = 15,\ r = 0.886,\ s = 0.727,\ F = 21.9,$ Outliers = hexaconazole (**5**), [triadimenol (**8**) and fluconazole (**9**)]
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **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. *QSAR Comb. Sci.* 28, 2009, No. 6-7, 629 – 636