Target Name	CYP3A4
Target TTD ID	TTDS00418

Target Species	Human
Chemical Type	Azole compounds
Mode of Action	Inhibitor
QSAR Model 1	Human CYP3A4: $$\mathrm{pIC_{50}(Inhibitory\ activity)} = 1.37(\pm0.34)\log P - 2.31(\pm0.79)\log(\beta P + 1) - 1.59(\pm0.77)I_{\mathrm{OH}} + 2.45(\pm0.83)$$ $n = 17,\ r = 0.927,\ s = 0.609,\ F = 26.7,\ \log\beta = -3.87,\ \log P_{\mathrm{opt}} = 4.03,$ Outlier = flusilazole (**6**)
QSAR Model 2	Human CYP3A4: $$\mathrm{pIC_{50}(Inhibitory)} = 1.35(\pm0.41)\mathrm{pIC_{50}\,(Binding)} - 1.07(\pm0.82)I_{\mathrm{OH}} - 1.79(\pm2.21)$$ $n = 18,\ r = 0.875,\ s = 0.744,\ F = 24.4$
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 –

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Target Species	Rat
Chemical Type	Azole compounds
Mode of Action	Inhibitor
QSAR Model 1	Rat CYP3A: $\mathrm{pIC_{50}(Binding)} = 1.07(\pm0.11)\log P - 1.34(\pm0.19)\log(\beta P + 1) + 0.23(\pm0.20)I_{\mathrm{azole}} + 2.90(\pm0.29)$ $n = 18,\ r = 0.985,\ s = 0.185,\ F = 157,\ \log\beta = -3.12,\ \log P_{\mathrm{opt}} = 3.73$
QSAR Model 2	Rat CYP3A: $\mathrm{pIC_{50}(Binding)} = 1.01(\pm0.11)\log P - 1.25(\pm0.19)\log(\beta P + 1) + 7.03(\pm5.29)E_{\mathrm{HOMO}} + 5.48(\pm1.85)$ $n = 18,\ r = 0.987,\ s = 0.179,\ F = 169,\ \log\beta = -3.15,\ \log P_{\mathrm{opt}} = 3.76$
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