

Target Name	AT ₂ Receptor
Target TTD ID	TTDS00525

Target Species	Human
Chemical Type	Triazoline derivatives
Mode of Action	Antagonist
QSAR Model 1	$-\log AT_2 = 7.081 (\pm 1.319)\pi_3 - 1.726 (\pm 0.308)\mathcal{R}_s - 1.109 (\pm 0.130)$ $n = 16, r = 0.908, s = 0.563, F = 9.224$
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: MoDel and e-dragon</p> <p>Hydrophobic ($\pi_s, \pi_3, \pi_4, \pi_5$), steric ($MR_s, MR_3, MR_4, MR_5$) and electronic ($\mathcal{F}_s, \mathcal{F}_3, \mathcal{F}_4, \mathcal{F}_5; \mathcal{R}_s, \mathcal{R}_3, \mathcal{R}_4, \mathcal{R}_5; \sigma_s, \sigma_3, \sigma_4, \sigma_5$) where the subscript numbers 3, 4 and 5 correspond to the physicochemical parameters of the substituents R₃, R₄, R₅ respectively, while s represents the sum of the physicochemical parameters values at R₁ and R₂ positions.</p> <p>Atomic hydrophobicity indexes at the hydrophobic sites in the vicinity of R₁ substituent (SS1x) and of R₄ substituent (SS1y); atomic hydrophobic index at the hydrophobic site in the vicinity of R₄ substituent (SS2y)</p> <p>Atomic refractivity index at steric site in the vicinity of R₂ substituent (SS2x)</p>
Reference	3-D QSAR Studies of Triazolinone Based Balanced AT ₁ /AT ₂ Receptor Antagonists. Bioorganic & Medicinal Chemistry 9 (2001) 291-300