Target Name	AT_1 Receptor
Target TTD ID	TTDS00267

Target Species	Human
Chemical Type	Triazoline derivatives
Mode of Action	Antagonist
QSAR Model 1	$-\log AT_1 = -0.074\ (\pm 0.015)MR_4 + 0.826\ (\pm 0.157)$ $n = 16,\quad r = 0.800,\quad s = 0.391,\quad F = 24.498$
QSAR Model 2	$-\log AT_1 = 6.800\ (\pm 1.219)\sigma_4 + 0.784\ (\pm 0.137)$ $n = 16,\quad r = 0.830,\quad s = 0.363,\quad F = 31.103$
QSAR Model 3	$-\log IC_{50} = -7.083\ (\text{hydrophobicity at SS1x}) - 3.004\ (\text{hydrophobicity at SS1y}) + 0.827$ $n = 16,\quad r = 0.841,\quad F_{2,13} = 15.701$
QSAR Model 4	$-\log IC_{50} = 0.181\ (\text{refractivity at SS2x}) - 7.355\ (\text{hydrophobicity at SS2y}) + 0.448$ $n = 16,\quad r = 0.864,\quad F_{2,13} = 19.178$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** Hydrophobic (π_s, π_3, π_4, π_5), steric (MR_s, MR_3, MR_4, MR_5) and electronic ($\mathcal{F}_s$, $\mathcal{F}_3$, $\mathcal{F}_4$, $\mathcal{F}_5$,; $\mathcal{R}_s$, $\mathcal{R}_3$, $\mathcal{R}_4$, $\mathcal{R}_5$;σ_s, σ_3, σ_4, σ_5) where the subscript numbers 3, 4 and 5 correspond to the physiochemical parameters of the substituents R_3, R_4, R_5 respectively, while s represents the sum of the physicochemical parameters values at R_1 and R_2 positions. Atomic hydrophobicity indexes at the hydrophobic sites in the vicinity of R_1 substituent (SS1x) and of R_4 substituent (SS1y); atomic hydrophobic index at the hydrophobic site in the vicinity of R_4 substituent (SS2y); Atomic refractivity index at steric site in the vicinity of R_2 substituent (SS2x)

Reference	3-D QSAR Studies of Triazolinone Based Balanced AT_1/AT_2 Receptor Antagonists. Bioorganic & Medicinal Chemistry 9 (2001) 291-300

Target Species	Human
Chemical Type	Benzoyliminothiadiazoline derivatives
Mode of Action	Antagonist
QSAR Model 1	$pKi = 5.173\ (\pm 0.654) + 0.873\ (\pm 0.223)\ L_{1o} \quad (n = 30,\ r^2 = 0.679,\ s = 0.483)$
QSAR Model 2	$pKi = -0.161 + 0.954\ L_{1o} - 0.589\ \pi_1 - 0.329\ (L_2)^2 + 2.677\ L_2 - 0.484\ \sigma_1$ $(\pm 3.409)\ (\pm 0.134)\ (\pm 0.223)\ (\pm 0.158) \quad (\pm 1.441)\ (\pm 0.374)$ $(n = 30,\ r^2 = 0.914,\ s = 0.270,\ F(5/24) = 51.18)$
QSAR Model 3	$pKi = 0.287 + 0.709\ L_{1o} - 0.608\ \pi_1 - 0.337\ (L_2)^2 + 2.731\ L_2 - 0.642\sigma_1 + 1.145\ F_{1o}$ $(\pm 3.040)\ (\pm 0.218)\ (\pm 0.198)\ (\pm 0.140)\ (\pm 1.278)\ (\pm 0.351)\ (\pm 0.854)$ $(n = 30,\ r^2 = 0.936,\ s = 0.239,\ F(6/23) = 55.77)$
QSAR Model 4	$pKi = 0.395 + 0.692\ L_{1o} - 0.344\ (L_2)^2 + 2.813\ L_2 - 0.603\ \pi_1 - 1.295\ F_{1m} - 1.332\ F_{1p}$ $(\pm 2.563)\ (\pm 0.137)\ (\pm 0.118) \quad (\pm 1.077)\ (\pm 0.166)\ (\pm 0.543)\ (\pm 0.543)$ $(n = 30,\ r^2 = 0.955,\ s = 0.201,\ F(6/23) = 79.87,\ L_2opt = 4.089)$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** STERIMOL parameter L_{10} which indicated the steric effect of ortho substituents represented a moderate correlation. Hansch-Fujita substituent constants π_1, Hammett constants σ_1, and STERIMOL parameter L_2 to eq. 1 resulted in eq. 2 with a good correlation. Swain-Lupton field effect parameters F_{10}. Although eq. 3 represented a better correlation, however, it would be noted that the contributions of σ_1 and F_{10} were compensated each other. Therefore, we attempted analyses to use Swain-Lupton F_1 and R_1 (resonance effect) parameters instead of σ_1. As the results of analyses, it was found that there were contributions of neither F_{10} nor R_1 parameter to the binding affinity, and that the following eq.4 using F_{1m} and F_{1p} parameters represented the best correlation.

Reference	Quantitative Structure-Activity Relationships of Benzoyliminothiadiazoline Derivatives as Angiotensin II Receptor Antagonists. *Bioorganic & Medicinal Chemistry Letters*. Vol. 7. No. 4, pp. 385-388, 1997

Target Species	Human
Chemical Type	6-substituted quazinolin-4(3H)-ones
Mode of Action	Antagonist
QSAR Model 1	$$pIC_{50} = 7.63(0.12) + \begin{Bmatrix} -0.782(0.083) & Acid = CO2H \\ +0.782(0.083) & Acid = CN4H \end{Bmatrix} + 0.0113(0.001\beta)V$$ $$- 0.406(0.073)\pi - 1.68(0.35)\sigma_I$$ $$R^2 = 0.82, s = 0.36, n = 41, F = 42.0$$
Molecular Descriptor	R_6-substituent size (*V)*, lipophilicity (π*)*, inductive sigma effect (σ_I), resonance sigma effect (σ_d),l* and sensitivity of σ_d to electronic demand (σ_e).
Reference	Quinazolinones 2: QSAR and In vivo characterization of AT1 selective AII antagonists. *Bioorganic & Medicinal Chemistry Letters*, Vol 3, No. 6, pp. 1299-1304, 1993