Target Name	TrpV1
Target TTD ID	TTDC00049

Target Species	Human
Chemical Type	Heteroaromatic urea
Mode of Action	Antagonist
QSAR Model 1	$Y = -2.51332 + 0.03079 \times (X_2 - 205.585) + 0.887655 \times (5.08034 - X_1) + 1.5287 \times (6.23382 - X_3)$ N = 70, LOF = 0.6765, r^2 = 0.7652, q^2 = 0.7362
QSAR Model 2	$Y = -2.76309 + 0.0320076 \times (X_2 - 205.585) + 0.90919 \times (5.24822 - X_1) + 1.55305 \times (6.23382 - X_3)$ N = 70, LOF = 0.6784, r^2 = 0.7646, q^2 = 0.7341
QSAR Model 3	$Y = -2.799 + 0.0315143 \times (X_2 - 206.149) + 0.906525 \times (5.12872 - X_1) + 1.51339 \times (6.39084 - X_3)$ N = 70, LOF = 0.6808, r^2 = 0.7637, q^2 = 0.7333
QSAR Model 4	$Y = -2.03973 + 0.0279783 \times (X_2 - 205.585) + 0.814747 \times (5.02866 - X_1) + 1.51257 \times (6.07399 - X_3)$ N = 70, LOF = 0.6837, r^2 = 0.7627, q^2 = 0.7324
QSAR Model 5	$Y = -2.93228 + 0.0326323 \times (X_2 - 206.149) + 0.910343 \times (5.4187 - X_1) + 1.56003 \times (6.23382 - X_3)$ N = 70, LOF = 0.6849, r^2 = 0.7624, q^2 = 0.7301
QSAR Model 6	$Y = -3.11736 + 0.0329731 \times (X_2 - 206.541) + 0.926299 \times (5.36845 - X_1) + 1.53829 \times (6.39084 - X_3)$ N = 70, LOF = 0.6854, r^2 = 0.7621, q^2 = 0.7289
QSAR Model 7	$Y = -2.20791 + 0.0287627 \times (X_2 - 206.149) + 0.823367 \times (5.19232 - X_1) + 1.52281 \times (6.07399 - X_3)$ N = 70, LOF = 0.6874, r^2 = 0.7615, q^2 = 0.7292
QSAR Model 8	$Y = 6.7769 - 1.49565 \times X_3 + 0.0315796 \times (X_2 - 206.541) + 0.909073 \times (5.14921 - X_1)$

	N = 70, LOF = 0.6879, r^2 = 0.7613, q^2 = 0.7297
QSAR Model 9	$Y = 1.65316 + 0.0315449 \times (X_2 - 206.541) - 1.49524 \times (X_3 - 3.4271) + 0.90807 \times (5.14921 - X_1)$ N = 70, LOF = 0.6885, r^2 = 0.7611, q^2 = 0.7294
QSAR Model 10	$Y = 6.85434 - 1.4682 \times X_3 + 0.0301838 \times (X_2 - 206.541) + 0.882324 \times (4.99746 - X_1)$ N = 70, LOF = 0.6895, r^2 = 0.7607, q^2 = 0.7304
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** X_1, base rings defined as the number of rings in the smallest set of smallest rings; X_2, 3D volume for each molecule using the current 3D coordinates; X_3, Kappa shape indices (molecular flexibility); N, number of samples; LOF, Friedman's lack-of-fit score; r^2 is squared correlation coefficient; q^2, square of the correlation coefficient of the cross-validation
Reference	QSAR Approach to Correlate TRPV1 Antagonist Activity for a Series of Heteroaromatic Urea. *QSAR Comb. Sci.* 28, 2009, No. 10, 1098 – 1111