

Target Name	Prostacyclin receptor
Target TTD ID	TTDS00170

Target Species	Mice
Chemical Type	1-hydroxyl-2-substituted phenyl-4,4,5,5-tetramethylimidazolines
Mode of Action	Antagonist
QSAR Model 1	$PTV_{90} = -1424.11(\pm 240.56) + 795.06(\pm 126.04) \times IDET - 20.92(\pm 3.71) \times Mor07e$ $+ 20.49(\pm 5.13) \times JGI1 - 10.26(\pm 2.65) \times MATS6v$ <p> <math>N = 20, R = 0.94, S = 4.47, \bar{e} = 3.84, R_{LOO} = 0.88, S_{LOO} = 6.06, \bar{e}_{LOO} = 5.22,</math>  <math>F = 27.75, p &lt; 10^{-5}, AIC = 44.40, FIT = 3.05</math> </p>
Molecular Descriptor	<p>Access the following web-servers to compute molecular descriptors: <a href="#">MoDel</a> and <a href="#">e-dragon</a></p> <p>N is the number of compounds; PTV90 (i.e. the PTV value measured at 90 min) is considered as the analgesic activity of a compound; IDET, IDET, Mor07e, Mor13e and MATS6v, descriptors selected from e-dragon server; R, the regression coefficient and F, F-ratio.</p>
Reference	A new class of analgesic agents toward prostacyclin receptor inhibition: Synthesis, biological studies and QSAR analysis of 1-hydroxyl-2-substituted phenyl-4,4,5,5-tetramethylimidazolines. <i>European Journal of Medicinal Chemistry</i> 43 (2008) 1048-1058