Target Name	Renin
Target TTD ID	TTDS00451

Target Species	Human
Chemical Type	6-ethyl-2, 4-diaminopyrimidine-based
Mode of Action	Inhibitor
QSAR Model 1	$\frac{\log(1/IC_{50})}{MW} = +3.15 \times 10^{-4}(\text{Hypo1/5}) + 2.68 \times 10^{-4}(\text{Hypo1/7}) - 1.39 \times 10^{-3}(\text{ShadowNU}) - 2.327 \times 10^{-3}({}^{1}\chi^{v}) + 1.94 \times 10^{-3}({}^{0}\chi^{v}) - 4.45 \times 10^{-4}\,(\text{ADME\_Absorption\_Level\_2D}) - 1.52 \times 10^{-2}$ $n = 96, r^2_{96} = 0.75, r^2_{BS} = 0.746, r^2_{LOO} = 0.697, r^2_{L25\%O} = 0.717, F = 43.52, r^2_{PRESS} = 0.527$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** n is the number of training compounds; $r^2_{96,}$ the correlation coefficient against 96 training compounds; r^2_{LOO} , the leave-one-out cross-validation correlation coefficient; , $r^2_{L25\%}O$, the leave 25% out cross-validation correlation coefficient; r^2_{BS} , the bootstrapping regression coefficient; r^2_{PRESS}, the predictive r2 determined for 23 randomly selected test compounds; Hypo1/5 and Hypo1/7, fit values of the training compounds against the 1st pharmacophore models in 5th and 7th automatic runs. ShadowNU, the ratio between the largest to smallest X, Y and Z dimensions of the molecule and ADME Absorption Level 2D, a categorical descriptor related to the distance of a particular molecule from the centre of the chemical space defined by well-absorbed compounds on the scatter plot constructed between Log P (Atom-based Log P) versus polar surface area (PSA).
Reference	Discovery of new renin inhibitory leads via sequential pharmacophore modeling, QSAR analysis, in silico screening and in vitro evaluation. *Journal of Molecular Graphics and Modelling* 29 (2011) 843–864

Target Species	Human
Chemical Type	Amino-aryl-piperidine-based
Mode of Action	Inhibitor
QSAR Model 1	$\frac{\log(1/IC_{50})}{MW} = +3.15 \times 10^{-4}(\text{Hypo1/5}) + 2.68 \times 10^{-4}(\text{Hypo1/7}) - 1.39 \times 10^{-3}(\text{ShadowNU}) - 2.327 \times 10^{-3}({}^{1}\chi^{v}) + 1.94 \times 10^{-3}({}^{0}\chi^{v}) - 4.45 \times 10^{-4}\,(\text{ADME\_Absorption\_Level\_2D}) - 1.52 \times 10^{-2}$ $n = 96, r^2_{96} = 0.75, r^2_{BS} = 0.746, r^2_{LOO} = 0.697, r^2_{L25\%O} = 0.717, F = 43.52, r^2_{PRESS} = 0.527$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** n is the number of training compounds; $r^2_{96,}$ the correlation coefficient against 96 training compounds; r^2_{LOO} , the leave-one-out cross-validation correlation coefficient; , $r^2_{L25\%}O$, the leave 25% out cross-validation correlation coefficient; r^2_{BS} , the bootstrapping regression coefficient; r^2_{PRESS}, the predictive r2 determined for 23 randomly selected test compounds; Hypo1/5 and Hypo1/7, fit values of the training compounds against the 1st pharmacophore models in 5th and 7th automatic runs. ShadowNU, the ratio between the largest to smallest X, Y and Z dimensions of the molecule and ADME Absorption Level 2D, a categorical descriptor related to the distance of a particular molecule from the centre of the chemical space defined by well-absorbed compounds on the scatter plot constructed between Log P (Atom-based Log P) versus polar surface area (PSA).
Reference	Discovery of new renin inhibitory leads via sequential pharmacophore modeling, QSAR analysis, in silico screening and in vitro evaluation. *Journal of Molecular Graphics and Modelling* 29 (2011) 843–864

Target Species	Human
Chemical Type	6-(24 diaminopyrimidinyl)-1,4-benzoxazin-3-ones
Mode of	Inhibitor

Action	
QSAR Model 1	$\frac{\log(1/IC_{50})}{MW} = +3.15 \times 10^{-4}(\text{Hypo1/5}) + 2.68 \times 10^{-4}(\text{Hypo1/7}) - 1.39 \times 10^{-3}(\text{ShadowNU}) - 2.327 \times 10^{-3}({}^{1}\chi^{v}) + 1.94 \times 10^{-3}({}^{0}\chi^{v}) - 4.45 \times 10^{-4}\,(\text{ADME\_Absorption\_Level\_2D}) - 1.52 \times 10^{-2}$ $n = 96, r^2_{96} = 0.75, r^2_{BS} = 0.746, r^2_{LOO} = 0.697, r^2_{L25\%O} = 0.717, F = 43.52, r^2_{PRESS} = 0.527$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** n is the number of training compounds; $r^2_{96,}$ the correlation coefficient against 96 training compounds; r^2_{LOO} , the leave-one-out cross-validation correlation coefficient; , $r^2_{L25\%}O$, the leave 25% out cross-validation correlation coefficient; r^2_{BS} , the bootstrapping regression coefficient; r^2_{PRESS}, the predictive r2 determined for 23 randomly selected test compounds; Hypo1/5 and Hypo1/7, fit values of the training compounds against the 1st pharmacophore models in 5th and 7th automatic runs. ShadowNU, the ratio between the largest to smallest X, Y and Z dimensions of the molecule and ADME Absorption Level 2D, a categorical descriptor related to the distance of a particular molecule from the centre of the chemical space defined by well-absorbed compounds on the scatter plot constructed between Log P (Atom-based Log P) versus polar surface area (PSA).
Reference	Discovery of new renin inhibitory leads via sequential pharmacophore modeling, QSAR analysis, in silico screening and in vitro evaluation. *Journal of Molecular Graphics and Modelling* 29 (2011) 843–864

Target Species	Human
Chemical Type	Ketopiperazine-based
Mode of Action	Inhibitor
QSAR Model 1	$\frac{\log(1/IC_{50})}{MW} = +3.15 \times 10^{-4}(\text{Hypo1/5}) + 2.68 \times 10^{-4}(\text{Hypo1/7}) - 1.39 \times 10^{-3}(\text{ShadowNU}) - 2.327 \times 10^{-3}({}^{1}\chi^{v}) + 1.94 \times 10^{-3}({}^{0}\chi^{v}) - 4.45 \times 10^{-4}\,(\text{ADME\_Absorption\_Level\_2D}) - 1.52 \times 10^{-2}$ $n = 96, r^2_{96} = 0.75, r^2_{BS} = 0.746, r^2_{LOO} = 0.697, r^2_{L25\%O} = 0.717, F = 43.52, r^2_{PRESS} = 0.527$

Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** n is the number of training compounds; $r^2_{96,}$ the correlation coefficient against 96 training compounds; r^2_{LOO} , the leave-one-out cross-validation correlation coefficient; , $r^2_{L25\%}O$, the leave 25% out cross-validation correlation coefficient; r^2_{BS} , the bootstrapping regression coefficient; r^2_{PRESS}, the predictive r2 determined for 23 randomly selected test compounds; Hypo1/5 and Hypo1/7, fit values of the training compounds against the 1^{st} pharmacophore models in 5^{th} and 7^{th} automatic runs. ShadowNU, the ratio between the largest to smallest X, Y and Z dimensions of the molecule and ADME Absorption Level 2D, a categorical descriptor related to the distance of a particular molecule from the centre of the chemical space defined by well-absorbed compounds on the scatter plot constructed between Log P (Atom-based Log P) versus polar surface area (PSA).
Reference	Discovery of new renin inhibitory leads via sequential pharmacophore modeling, QSAR analysis, in silico screening and in vitro evaluation. *Journal of Molecular Graphics and Modelling* 29 (2011) 843–864