Target Name	N-type calcium channel
Target TTD ID	TTDS00529

Target Species	Human
Chemical Type	Phenylalanine derivatives
Mode of Action	Blocker
QSAR Model 1	$pIC_{50} = 6.04274 - 0.325494 * \text{"ADME\_Solubility"} + 0.118937 * \text{"Atype\_C\_24"} + 0.369743 * \text{"Rotlbonds"} - 0.266013 * \text{"Atype\_N\_68"} + 0.125834 * \text{"S\_sssN"}$ $N = 83; LOF = 0.048; r^2 = 0.798; r^2_{adj} = 0.785; F - test = 62.27; LSE = 0.038; r = 0.893; q^2 = 0.769$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *N* is the number of molecules in the training set; LOF is lack of fit score; r^2 is the squared correlation coefficient; r^2_{adj} is the square of adjusted correlation coefficient; *F*-test is a variance-related statistic that compares two models differing by one or more variables to see if the more complex model is more reliable than the less complex one.
Reference	Molecular modelling and QSAR analysis of some structurally diverse N-type calcium channel blockers. *J Mol Model* (2010) 16:629–644

Target Species	Human
Chemical Type	N-Dialkyldipeptidylamines
Mode of Action	Blocker

QSAR Model 1	$pIC_{50} = 6.04274 - 0.325494 * \text{"ADME\_Solubility"} + 0.118937 * \text{"Atype\_C\_24"} + 0.369743 * \text{"Rotlbonds"} - 0.266013 * \text{"Atype\_N\_68"} + 0.125834 * \text{"S\_sssN"}$ $N = 83; LOF = 0.048; r^2 = 0.798; r^2_{adj} = 0.785; F - test = 62.27; LSE = 0.038; r = 0.893; q^2 = 0.769$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *N* is the number of molecules in the training set; LOF is lack of fit score; r^2 is the squared correlation coefficient; r^2_{adj} is the square of adjusted correlation coefficient; *F*-test is a variance-related statistic that compares two models differing by one or more variables to see if the more complex model is more reliable than the less complex one.
Reference	Molecular modelling and QSAR analysis of some structurally diverse N-type calcium channel blockers. *J Mol Model* (2010) 16:629–644

Target Species	Human
Chemical Type	N-methyl-N-aralkyl-peptidylamines
Mode of Action	Blocker
QSAR Model 1	$pIC_{50} = 6.04274 - 0.325494 * \text{"ADME\_Solubility"} + 0.118937 * \text{"Atype\_C\_24"} + 0.369743 * \text{"Rotlbonds"} - 0.266013 * \text{"Atype\_N\_68"} + 0.125834 * \text{"S\_sssN"}$ $N = 83; LOF = 0.048; r^2 = 0.798; r^2_{adj} = 0.785; F - test = 62.27; LSE = 0.038; r = 0.893; q^2 = 0.769$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *N* is the number of molecules in the training set; LOF is lack of fit score; r^2 is the squared correlation coefficient; r^2_{adj} is the square of adjusted correlation coefficient; *F*-test is a variance-related statistic that compares two models differing by one or more variables to see if the more complex model is more reliable than the less complex one.
Reference	Molecular modelling and QSAR analysis of some structurally diverse N-type calcium channel blockers. *J Mol Model* (2010) 16:629–644