Target Name	VCAM-1
Target TTD ID	TTDR00453

Target Species	Human
Chemical Type	Piperazinyl phenylalanine derivatives
Mode of Action	Inhibitor
QSAR Model 1	$-\log IC_{50}$= [2.93] + SaaNEindex [-0.037] + SsClcount [0.77] + 4path count [0.064] + SlogP [-0.69] n=21, r=0.93, r^2=0.8567, r^2 se=0.25, F=33.89, F tabulated=7.46, q^2=0.76, q^2_se=0.33, pred_r^2=0.42, pred_r^2 se=0.24, degree of freedom=17
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** SaaNEindex, electro-topological state indices for number of nitrogen atoms connected with two aromatic double bonds; SsClcount, electro-topological parameter defining total number of chlorine atoms connected with one single bond; 4pathcount, topological parameter signifying total number of fragments of fourth order (four bond path) in compound; SlogP, signify log of the octanol/water partition coefficient; n, number of samples, r, correlation coefficient; r^2 se, standard error of squared correlation coefficient; F, F-ratio; F tabulated, tabulated F-ratio; q^2, square of the correlation coefficient; q^2 se, standard error of square of the correlation coefficient; pred r^2, predicted squared correlation coefficient; pred r^2 se, standard error of predicted squared correlation coefficient
Reference	Quantitative Structure Activity Relationship Studies of Piperazinyl Phenylalanine Derivatives as VLA-4/VCAM-1 Inhibitors. *Medicinal Chemistry*, 2009, *5*, 446-454