Target Name	*Pseudomonas aeruginosa* Deacetylase LpxC
Target TTD ID	TTDR00865

Target Species	Human
Chemical Type	2-Aryloxazolines
Mode of Action	Inhibitor
QSAR Model 1	$\text{Log}\ (1/IC_{50}) = 5.155\ 65 - 1.596\ 14\text{mor14v} - 0.9239 < 2.485 - \text{H2U} > + 1.7411 < \text{mor24U} - 0.104 > - 3.1202 < \text{mor24U} - 0.505 > + 81.1483 < 0.101 - \text{HATS2p} > - 5.09371 < \text{mor26p} + 0.157 >$ $N = 34$, LOF $= 0.347$, $r^2 = 0.813$, $r^2\text{adj} = 0.771$, F-test $= 17.515$, LSE $= 0.087$, $q^2 = 0.732$, $\text{Bsr}^2 = 0.813$, Bsr^2 error $= 0.004$, $r^2_{\text{pred}} = 0.857$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** N is number of compounds in the training set; LOF is the lack of fit; r^2 is the squared correlation coefficient; r^2_{adj} is the square of the adjusted correlation coefficient; F-test is a variance-related statistic that compares two models differing by one or more variable to see if the more complex model is more reliable than the less complex one; LSE is the least-square error; q^2 is the square of the correlation coefficient of the cross-validation; r^2_{pred} is the predicted correlation coefficient calculated from the predicted activity of the test set compound. Morse descriptors (mor14v, mor24U, and mor26p).
Reference	Evaluation of *Pseudomonas aeruginosa* Deacetylase LpxC Inhibitory Activity of Dual PDE4-TNFr Inhibitors: A Multiscreening Approach. *J. Chem. Inf. Model.* 2007, 47, 1188-1195

Target	Human

Species	
Chemical Type	Aroylserines
Mode of Action	Inhibitors
QSAR Model 1	$\text{Log}\ (1/IC_{50}) = 5.155\ 65 - 1.596\ 14\text{mor14v} - 0.9239 < 2.485 - \text{H2U} > + 1.7411 < \text{mor24U} - 0.104 > - 3.1202 < \text{mor24U} - 0.505 > + 81.1483 < 0.101 - \text{HATS2p} > - 5.09371 < \text{mor26p} + 0.157 >$ $N = 34,\ \text{LOF} = 0.347,\ r^2 = 0.813,\ r^2\text{adj} = 0.771,\ \text{F-test} = 17.515,\ \text{LSE} = 0.087,$ $q^2 = 0.732,\ \text{Bsr}^2 = 0.813,\ \text{Bsr}^2\ \text{error} = 0.004,\ r^2_{\text{pred}} = 0.857$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** N is number of compounds in the training set; LOF is the lack of fit; r^2 is the squared correlation coefficient; r^2_{adj} is the square of the adjusted correlation coefficient; F-test is a variance-related statistic that compares two models differing by one or more variable to see if the more complex model is more reliable than the less complex one; LSE is the least-square error; q^2 is the square of the correlation coefficient of the cross-validation; r^2_{pred} is the predicted correlation coefficient calculated from the predicted activity of the test set compound. Morse descriptors (mor14v, mor24U, and mor26p).
Reference	Evaluation of *Pseudomonas aeruginosa* Deacetylase LpxC Inhibitory Activity of Dual PDE4-TNFr Inhibitors: A Multiscreening Approach. *J. Chem. Inf. Model.* 2007, 47, 1188-1195

Target Species	Human
Chemical Type	2- Arylthiazolines
Mode of Action	Inhibitors

QSAR Model 1	$\text{Log}\ (1/IC_{50}) = 5.155\ 65 - 1.596\ 14\text{mor14v} - 0.9239 < 2.485 - \text{H2U} > + 1.7411 < \text{mor24U} - 0.104 > - 3.1202 < \text{mor24U} - 0.505 > + 81.1483 < 0.101 - \text{HATS2p} > - 5.09371 < \text{mor26p} + 0.157 >$ $N = 34,\ \text{LOF} = 0.347,\ r^2 = 0.813,\ r^2\text{adj} = 0.771,\ \text{F-test} = 17.515,\ \text{LSE} = 0.087,$ $q^2 = 0.732,\ \text{Bsr}^2 = 0.813,\ \text{Bsr}^2\ \text{error} = 0.004,\ r^2_{\text{pred}} = 0.857$
Molecular Descriptor	Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon** *N* is number of compounds in the training set; LOF is the lack of fit; r^2 is the squared correlation coefficient; r^2_{adj} is the square of the adjusted correlation coefficient; F-test is a variance-related statistic that compares two models differing by one or more variable to see if the more complex model is more reliable than the less complex one; LSE is the least-square error; q^2 is the square of the correlation coefficient of the cross-validation; r^2_{pred} is the predicted correlation coefficient calculated from the predicted activity of the test set compound. Morse descriptors (mor14v, mor24U, and mor26p).
Reference	Evaluation of *Pseudomonas aeruginosa* Deacetylase LpxC Inhibitory Activity of Dual PDE4-TNFr Inhibitors: A Multiscreening Approach. *J. Chem. Inf. Model.* 2007, 47, 1188-1195

Target Species	Pseudomonas aeruginosa
Chemical Type	2-Aryloxazolines
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/IC_{50}) = -7.04877 + 43.526 \times \text{mats1v\^2} + 3.48946 \times \text{VEA1} - 1.75733 \times \text{SPP\^2} - 0.1086 \times \text{X4V\^2} - 0.0232 \times \langle \text{D/Dr05} - 88.418 \rangle$ $N = 37,\ \text{LOF} = 0.314,\ r^2 = 0.703,\ r^2_{\text{adj}} = 0.655,\ F\text{-test} = 14.698,$ $\text{LSE} = 0.155,\ \ r = 0.839,\ \ \bar{q}^2 = 0.584,\ \ \text{BS}r^2 \pm \text{SD} = 0.704 \pm .006,\ r^2_{\text{pred}} = 0.107$

QSAR Model 2

$$\log(1/IC_{50}) = 5.3512 + 0.0795 \times MAXDP\text{^}2 + 16.6973 \times \langle 1.961 - JHETE\rangle - 1.755 \times GATS5m\text{^}2 - 2.8359 \times \langle vez1 - 4.509\rangle$$

$N = 20,\ LOF = 0.170,\ r^2 = 0.904,\ r^2_{adj} = 0.878,\ F\text{-test} = 35.126,$
$LSE = 0.042,\ \ r = 0.951,\ \ q^2 = 0.805,\ \ BSr^2 \pm SD = 0.904 \pm 0.003,\ r^2_{pred} = 0.598.$

QSAR Model 3

$$\log(1/IC_{50}) = 3.9227 + 165.06 \times MATS1P\text{^}2 + 0.0048 \times MDDD\text{^}2 + 2.1208 \times \langle -0.023 - MATS8m\rangle - 53.057 \times \langle 0.223 - VEP2\rangle$$

$N = 17,\ LOF = 0.163,\ r^2 = 0.944,\ r^2_{adj} = 0.925,\ F\text{-test} = 50.359,$
$LSE = 0.028,\ \ r = 0.944,\ \ q^2 = 0.906,\ \ BSr^2 \pm SD = 0.904 \pm 0.00,\ r^2_{pred} = 0.608.$

Molecular Descriptor

Access the following web-servers to compute molecular descriptors: **MoDel** and **e-dragon**

Mats1v (a 2D-autocorrelation descriptor) which is Moran autocorrelation lag one weighted by van der Waals volumes; VEA (an eigenvalue-based indices descriptor) which is an Eigenvector coefficient sum from adjacency matrix; SPP (a charge descriptor) which is a sub-molecular polarity parameter; X4V (connectivity descriptor) which is a valence connectivity index chi-4; D/Dr05 (a topological descriptor) which is a distance/detour ring index of order 5.

N is the number of molecules in training set, LOF is lack of fit score that resists overfitting, r^2 is squared correlation coefficient, and r^2_{adj} is square of adjusted correlation coefficient.

S. No.	Descriptors	Symbol	Descriptors' meaning
1	Mats1v	*(I(d))*	Moran autocorrelation lag one weighted by van der Waals volume
2	Mats1p	*(I(d))*	Moran autocorrelation lag one weighted by atomic polarizability
3	Mats8m	*(I(d))*	Moran autocorrelation lag one weighted by atomic masses
4	GATS5m	*(C(d))*	Geary autocorrelation lag one weighted by atomic masses
5	SPP	Δ	Submolecular polarity parameter
6	X4V	${}^{m}X_q^v$	Valence connectivity index chi-4
7	VEA1	λ_i^A	Eigenvector coefficient sum from adjacency matrix
8	VEZ1	λ_i^D	Eigenvector coefficient sum from z weighted distance matrix (Barysz matrix)
9	MAXDP	T_α^E	Maximal electrotopological positive variation

	10	MDDD	$\Delta\sigma$	Mean distance degree deviation
	11	D/Dr05	$[D/\Delta]_{ij}$	Distance/detour ring index of order 5
	12	JHETE	J^{x}	Balaban type index from electronegativity weighted distance matrix
	13	VEP2	λ_i^{α}	Average coefficient sum from polarizability weighted distance matrix
	MAXDP, maximal electrotopological positive variation, which is connectivity indices descriptor; JHETE, Balaban-type index from electronegativity weighted distance matrix, which is eigenvalue-based indices descriptor; GATS5m, Geary autocorrelationlag 5/weighted by atomic masses, which is 2D-autocorrelation descriptor; vez1, Eigenvector coefficient sum from z-weighted distance matrix, which is eigenvalue-based descriptor. MATS1P, Moran autocorrelation lag 1/weighted by atomic polarizability, which is 2D-autocorrelation descriptor; MDDD which is connectivity based indices descriptor; MATS8m, Moran autocorrelation - lag 8/weighted by atomic masses, which is 2D-autocorrelation descriptor; VEP2, average eigenvector coefficient sum from polarizability weighted distance matrix, which is eigenvalue-based descriptor.			
Reference	Cluster analysis and two-dimensional quantitative structure–activity relationship (2D-QSAR) of Pseudomonas aeruginosa deacetylase LpxC inhibitors. *Bioorganic & Medicinal Chemistry Letters* 16 (2006) 5136–5143			

Target Species	Pseudomonas aeruginosa
Chemical Type	Aroylserines
Mode of Action	Inhibitor
QSAR Model 1	$\log(1/\mathrm{IC}_{50}) = -7.04877 + 43.526 \times \mathrm{mats1v\text{^}2} + 3.48946 \times \mathrm{VEA1} - 1.75733 \times \mathrm{SPP\text{^}2} - 0.1086 \times \mathrm{X4V\text{^}2} - 0.0232 \times \langle \mathrm{D/Dr05} - 88.418 \rangle$ $N = 37,\ \mathrm{LOF} = 0.314,\ r^2 = 0.703,\ r^2_{\mathrm{adj}} = 0.655,\ F\text{-test} = 14.698,$ $\mathrm{LSE} = 0.155,\ \ r = 0.839,\ \ \bar{q}^2 = 0.584,\ \ \mathrm{BS}r^2 \pm \mathrm{SD} = 0.704 \pm .006,\ r^2_{\mathrm{pred}} = 0.107$

QSAR Model 2

$$\log(1/IC_{50}) = 5.3512 + 0.0795 \times MAXDP\text{^}2 + 16.6973 \times \langle 1.961 - JHETE\rangle - 1.755 \times GATS5m\text{^}2 - 2.8359 \times \langle vez1 - 4.509\rangle$$

$N = 20,\ LOF = 0.170,\ r^2 = 0.904,\ r^2_{adj} = 0.878,\ F\text{-test} = 35.126,$
$LSE = 0.042,\ \ r = 0.951,\ \ q^2 = 0.805,\ \ BSr^2 \pm SD = 0.904 \pm 0.003,\ r^2_{pred} = 0.598.$

QSAR Model 3

$$\log(1/IC_{50}) = 3.9227 + 165.06 \times MATS1P\text{^}2 + 0.0048 \times MDDD\text{^}2 + 2.1208 \times \langle -0.023 - MATS8m\rangle - 53.057 \times \langle 0.223 - VEP2\rangle$$

$N = 17,\ LOF = 0.163,\ r^2 = 0.944,\ r^2_{adj} = 0.925,\ F\text{-test} = 50.359,$
$LSE = 0.028,\ \ r = 0.944,\ \ q^2 = 0.906,\ \ BSr^2 \pm SD = 0.904 \pm 0.00,\ r^2_{pred} = 0.608.$

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