Therapeutic Targets Database

QSAR Model



| Target Name | Pseudomonas aeruginosa Deacetylase LpxC | | | | |
|------------------|---|--|--|--|--|
| Target TTD ID | TTDR00865 | | | | |

| Target Species | Human | | | | | |
|-------------------------|---|--|--|--|--|--|
| Chemical Type | 2-Aryloxazolines | | | | | |
| Mode of Action | Inhibitor | | | | | |
| QSAR Model 1 | $\log (1/IC_{50}) = 5.155 65 - 1.596 14 \text{mor} 14 \text{v} - 0.9239 < 2.485 - \text{H2U} > \\ + 1.7411 < \text{mor} 24 \text{U} - 0.104 > - 3.1202 < \text{mor} 24 \text{U} - 0.505 > \\ + 81.1483 < 0.101 - \text{HATS2p} > - 5.09371 < \text{mor} 26 \text{p} + 0.157 > \\ I = 34, \text{LOF} = 0.347, \ r^2 = 0.813, \ r^2 \text{adj} = 0.771, \ \text{F-test} = 17.515, \ \text{LSE} = 0.087, \\ I = 0.732, \ \text{Bsr}^2 = 0.813, \ \text{Bsr}^2 \ \text{error} = 0.004, \ r^2_{\text{pred}} = 0.857$ | | | | | |
| 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 <i>Pseudomonas aeruginosa</i> Deacetylase LpxC Inhibitory Activity of Dual PDE4-TNFr Inhibitors: A Multiscreening Approach. <i>J. Chem. Inf. Model.</i> 2007, 47, 1188-1195 | | | | | |

| Target | Human | |
|--------|-------|--|
|--------|-------|--|

| Species | |
|-------------------------|---|
| Chemical Type | Aroylserines |
| Mode of Action | Inhibitors |
| QSAR Model 1 | $\begin{split} \text{Log (1/IC}_{50}) &= 5.155\ 65 - 1.596\ 14\text{mor}14\text{v} - 0.9239 < 2.485 - \text{H2U}> \\ & + 1.7411 < \text{mor}24\text{U} - 0.104> - 3.1202 < \text{mor}24\text{U} - 0.505> \\ & + 81.1483 < 0.101 - \text{HATS2p}> - 5.09371 < \text{mor}26\text{p} + 0.157> \\ N &= 34, \text{LOF} = 0.347, \ r^2 = 0.813, \ r^2 \text{adj} = 0.771, \ \text{F-test} = 17.515, \ \text{LSE} = 0.087, \\ q^2 &= 0.732, \ \text{Bsr}^2 = 0.813, \ \text{Bsr}^2 \ \text{error} = 0.004, \ r^2_{\text{pred}} = 0.857 \end{split}$ |
| 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_{adj}^2 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_{pred}^2 is the predicted correlation coefficient calculated from the predicted activity of the test set compound. Morse descriptors (mor14v, mor24U, and mor26p). |
| Reference | Evaluation of <i>Pseudomonas aeruginosa</i> Deacetylase LpxC Inhibitory Activity of Dual PDE4-TNFr Inhibitors: A Multiscreening Approach. <i>J. Chem. Inf. Model.</i> 2007, 47, 1188-1195 |

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

| | $Log (1/IC_{50}) = 5.155 65 - 1.596 14mor14v - 0.9239 < 2.485 - H2U>$ |
|-------------------------|---|
| QSAR Model 1 | + 1.7411 < mor24U - 0.104 > - 3.1202 < mor24U - 0.505 > |
| | +81.1483 < 0.101 - HATS2p > -5.09371 < mor26p + 0.157 > |
| Wiodei i | $N = 34$, LOF = 0.347, $r^2 = 0.813$, $r^2 \text{adj} = 0.771$, F-test = 17.515, LSE = 0.087, |
| | $q^2 = 0.732$, Bsr ² = 0.813, Bsr ² error = 0.004, $r_{\text{pred}}^2 = 0.857$ |
| | Access the following web-servers to compute molecular descriptors: MoDel and e-dragon |
| Molecular Descriptor | N is number of compounds in the training set; LOF is the lack of fit; r^2 is the squared correlation coefficient; r_{adj}^2 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_{pred}^2 is the predicted correlation coefficient calculated from the predicted activity of the test set compound. Morse descriptors (mor14v, mor24U, and mor26p). |
| Reference | Evaluation of <i>Pseudomonas aeruginosa</i> Deacetylase LpxC Inhibitory Activity of Dual PDE4-TNFr Inhibitors: A Multiscreening Approach. <i>J. Chem. Inf. Model.</i> 2007, 47, 1188-1195 |

| Target Species | Pseudomonas aeruginosa | | | | | |
|-------------------|--|--|--|--|--|--|
| Chemical Type | 2-Aryloxazolines | | | | | |
| Mode of Action | Inhibitor | | | | | |
| QSAR Model 1 | $\log(1/\text{IC}_{50}) = -7.04877 + 43.526 \times \text{mats} 1\text{v}^2 + 3.48946 \times \text{VEA1} \\ -1.75733 \times \text{SPP}^2 - 0.1086 \times \text{X4V}^2 - 0.0232 \times \langle \text{D/Dr}05 - 88.418 \rangle$ $N = 37, \text{ LOF} = 0.314, \ r^2 = 0.703, \ r_{\text{adi}}^2 = 0.655, \ F\text{-test} = 14.698,$ $\text{LSE} = 0.155, \ r = 0.839, \ \vec{q}^2 = 0.584, \ \text{BS} r^2 \pm \text{SD} = 0.704 \pm .006, r_{\text{pred}}^2 = 0.107$ | | | | | |

| QSAR Model 3 $\log(1/\Gamma C_{50}) = 3.9227 + 165.06 \times MATS1P^{\circ}2 + 0.0048 \times MDDD^{\circ}2$ $+ 2.1208 \times \langle -0.023 - MATS8m \rangle - 53.057 \times (0.223 - VEP2)$ $N = 17$, LOF = 0.163, $r^{2} = 0.944$, $q^{2} = 0.926$, $BSr^{2} \pm SD = 0.904 \pm 0.00$, $r_{pred}^{2} = 0.608$. 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} asj is square of adjusted correlation coefficient. S.No. Descriptors Symbol Descriptors' meaning Moran autocorrelation lag one weighted by van der Waals volume Descriptor Mats1v (I(d)) Moran autocorrelation lag one weighted by atomic masses 4 GATS5m (C(d)) Geary autocorrelation lag one weighted by atomic masses 5 SPP A Submolecular polarity parameter 6 X4V $^{m}X_{q}^{p}$ Valence connectivity index chi-4 VEA1 λ_{1}^{A} Eigenvector coefficient sum from adjacency matrix 8 | QSAR Model 2 | $\log(1/\text{IC}_{50}) = 5.3512 + 0.0795 \times \text{MAXDP}^{2} + 16.6973 \times \langle 1.961 - \text{JHETE} \rangle$ $-1.755 \times \text{GATS5m}^{2} - 2.8359 \times \langle \text{vez1} - 4.509 \rangle$ $N = 20, \text{ LOF} = 0.170, \ r^{2} = 0.904, \ r_{\text{adj}}^{2} = 0.878, \ F\text{-test} = 35.126,$ $\text{LSE} = 0.042, \ r = 0.951, \ q^{2} = 0.805, \ \text{BS}r^{2} \pm \text{SD} = 0.904 \pm 0.003, \ r_{\text{pred}}^{2} = 0.598.$ | | | |
|--|-----------------|---|--|--|--|
| 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 A Submolecular polarity parameter 6 X4V ${}^mX_q^p$ Valence connectivity index chi-4 7 VEA1 λ_i^A Eigenvector coefficient sum from adjacency matrix Eigenvector coefficient sum from z weighted distance matrix (Barysz matrix) | - | $+ 2.1208 \times \langle -0.023 - MATS8m \rangle - 53.057 \times \langle 0.223 - VEP2 \rangle$ | | | |
| (Barysz matrix) | | Mats1v (Waals vo sum from X4V (co descripto N is the r squared o S. No. 1 2 3 4 5 6 7 | a 2D-autocorre folumes; VEA (an adjacency mannectivity descriptor) which is a discorrelation coeff Descriptors Mats1v Mats1p Mats8m GATS5m SPP X4V VEA1 | elation descriptor an eigenvaluntrix; SPP (a riptor) which istance/deto ecules in transficient, and Symbol $(I(d))$ $(I(d))$ $(I(d))$ $(C(d))$ Δ mX_q^v λ_i^A | riptor) which is Moran autocorrelation lag one weighted by van der ne-based indices descriptor) which is an Eigenvector coefficient a charge descriptor) which is a sub-molecular polarity parameter; the is a valence connectivity index chi-4; D/Dr05 (a topological pur ring index of order 5. Inning set, LOF is lack of fit score that resists overfitting, r² is lar² adj is square of adjusted correlation coefficient. Descriptors' meaning Moran autocorrelation lag one weighted by van der Waals volume Moran autocorrelation lag one weighted by atomic polarizability Moran autocorrelation lag one weighted by atomic masses Geary autocorrelation lag one weighted by atomic masses Submolecular polarity parameter Valence connectivity index chi-4 Eigenvector coefficient sum from adjacency matrix |
| | | | | $rac{\lambda_i^D}{T_lpha^E}$ | (Barysz matrix) |

| | 10 | MDDD | Δσ | Mean distance degree deviation | |
|-----------|---|-------------------|------------------------|--|--|
| | 11 | D/Dr05 | $[D/\!\varDelta]_{ij}$ | Distance/detour ring index of order 5 | |
| | 12 | JHETE | J^{x} | Balaban type index from electronegativity weighted distance matrix | |
| | 13 | VEP2 | λ_i^{lpha} | Average coefficient sum from polarizability weighted distance matrix | |
| | MAXDP, maximal electrotopological positive variation, which is connectivity indices descrip | | | | |
| | 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. | | | | |
| | | | | | |
| | MATS | P, Moran auto | correlation la | ag 1/weighted by atomic polarizability, which is 2D- | |
| | autocor | relation descrip | tor; MDDD | which is connectivity based indices descriptor; MATS8m, Moran | |
| | autocor | relation - 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. | | | | |
| | Cluster | analysis and | two-dimens | ional quantitative structure-activity relationship (2D-QSAR) of | |
| Reference | 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 | $\log(1/\text{IC}_{50}) = -7.04877 + 43.526 \times \text{mats} 1\text{v}^2 + 3.48946 \times \text{VEA1} \\ -1.75733 \times \text{SPP}^2 - 0.1086 \times \text{X4V}^2 - 0.0232 \times \langle \text{D/Dr}05 - 88.418 \rangle$ $N = 37, \text{ LOF} = 0.314, \ r^2 = 0.703, \ r_{\text{adi}}^2 = 0.655, \ F\text{-test} = 14.698,$ $\text{LSE} = 0.155, \ r = 0.839, \ \vec{q}^2 = 0.584, \ \text{BS} r^2 \pm \text{SD} = 0.704 \pm .006, r_{\text{pred}}^2 = 0.107$ | | | | | |

| QSAR Model 2 | $\log(1/\text{IC}_{50}) = 5.3512 + 0.0795 \times \text{MAXDP}^2 + 16.6973 \times \langle 1.961 - \text{JHETE} \rangle \\ -1.755 \times \text{GATS5m}^2 - 2.8359 \times \langle \text{vez1} - 4.509 \rangle \\ N = 20, \text{ LOF} = 0.170, \ r^2 = 0.904, \ r_{\text{adj}}^2 = 0.878, \ F\text{-test} = 35.126, \\ \text{LSE} = 0.042, \ r = 0.951, \ q^2 = 0.805, \ \text{BS} r^2 \pm \text{SD} = 0.904 \pm 0.003, \ r_{\text{pred}}^2 = 0.598.$ | | | | |
|-----------------|--|-----------------|--------------------------|---|--|
| QSAR Model 3 | $\begin{split} \log(1/\text{IC}_{50}) = & 3.9227 + 165.06 \times \text{MATS1P}^2 + 0.0048 \times \text{MDDD}^2 \\ & + 2.1208 \times \langle -0.023 - \text{MATS8m} \rangle - 53.057 \times \langle 0.223 - \text{VEP2} \rangle \\ N = & 17, \text{ LOF} = 0.163, \ r^2 = 0.944, \ r_{\text{adj}}^2 = 0.925, \ F\text{-test} = 50.359, \\ \text{LSE} = & 0.028, \ r = 0.944, \ q^2 = 0.906, \ \text{BS} \\ r^2 \pm \text{ SD} = 0.904 \pm 0.00, \ r_{\text{pred}}^2 = 0.608. \end{split}$ | | | | |
| | Access th | he following wo | eb-servers t | o 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. | | | | |
| | | | | uning set, LOF is lack of fit score that resists overfitting, r^2 is r^2_{adj} is square of adjusted correlation coefficient. | |
| | S. No. | Descriptors | Symbol | Descriptors' meaning | |
| Molecular | 1 | Mats1v | (I(d)) | Moran autocorrelation lag one weighted by van der Waals volume | |
| Descriptor | 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 | (<i>C</i> (<i>d</i>)) | Geary autocorrelation lag one weighted by atomic masses | |
| | 5 | SPP | Δ | Submolecular polarity parameter | |
| | 6 | X4V | $^mX_q^v$ | 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 | Δσ | 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^{lpha} | Average coefficient sum from polarizability weighted distance matrix | |
| | MAXDP, maximal electrotopological positive variation, which is connectivity indices descrip | | | | |
| | 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. | | | | |
| | | | | | |
| | MATS | P, Moran auto | correlation la | ag 1/weighted by atomic polarizability, which is 2D- | |
| | autocor | relation descrip | tor; MDDD | which is connectivity based indices descriptor; MATS8m, Moran | |
| | autocor | relation - 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. | | | | |
| | Cluster | analysis and | two-dimens | ional quantitative structure-activity relationship (2D-QSAR) of | |
| Reference | Pseudomonas aeruginosa deacetylase LpxC inhibitors. Bioorganic & Medicinal Chemistry Letters 16 | | | | |
| | (2006) | 5136–5143 | | | |

| Target Species | Pseudomonas aeruginosa | | | | |
|-------------------|--|--|--|--|--|
| Chemical Type | 2-Arylthiazolines | | | | |
| Mode of Action | Inhibitor | | | | |
| QSAR Model 1 | $\log(1/\text{IC}_{50}) = -7.04877 + 43.526 \times \text{mats} 1\text{v}^2 + 3.48946 \times \text{VEA1} \\ -1.75733 \times \text{SPP}^2 - 0.1086 \times \text{X4V}^2 - 0.0232 \times \langle \text{D/Dr}05 - 88.418 \rangle$ $N = 37, \text{ LOF} = 0.314, \ r^2 = 0.703, \ r_{\text{adi}}^2 = 0.655, \ F\text{-test} = 14.698,$ $\text{LSE} = 0.155, \ r = 0.839, \ \vec{q}^2 = 0.584, \ \text{BS} r^2 \pm \text{SD} = 0.704 \pm .006, r_{\text{pred}}^2 = 0.107$ | | | | |

| QSAR Model 2 | $\begin{split} \log(1/\text{IC}_{50}) &= 5.3512 + 0.0795 \times \text{MAXDP}^{\wedge}2 + 16.6973 \times \langle 1.961 - \text{JHETE} \rangle \\ &- 1.755 \times \text{GATS5m}^{\wedge}2 - 2.8359 \times \langle \text{vez1} - 4.509 \rangle \\ N &= 20, \text{ LOF} = 0.170, \ r^2 = 0.904, \ r_{\text{adj}}^2 = 0.878, \ F\text{-test} = 35.126, \\ \text{LSE} &= 0.042, \ r = 0.951, \ q^2 = 0.805, \ \text{BS} \\ r^2 \pm \text{SD} &= 0.904 \pm 0.003, \ r_{\text{pred}}^2 = 0.598. \end{split}$ | | | | | |
|-------------------------|---|--|--|---|--|--|
| QSAR Model 3 | $\begin{aligned} \log(1/\text{IC}_{50}) = & 3.9227 + 165.06 \times \text{MATS1P}^{\wedge}2 + 0.0048 \times \text{MDDD}^{\wedge}2 \\ & + 2.1208 \times \langle -0.023 - \text{MATS8m} \rangle - 53.057 \times \langle 0.223 - \text{VEP2} \rangle \\ N = & 17, \text{ LOF} = 0.163, \ r^2 = 0.944, \ r_{\text{adj}}^2 = 0.925, \ F\text{-test} = 50.359, \\ \text{LSE} = & 0.028, \ r = 0.944, \ q^2 = 0.906, \ \text{BS}r^2 \pm \text{SD} = 0.904 \pm 0.00, \ r_{\text{pred}}^2 = 0.608. \end{aligned}$ | | | | | |
| Molecular Descriptor | Mats1v (Waals vo sum from X4V (co descripto N is the | (a 2D-autocorrection of a 2D-autocorrection o | elation described an eigenvaluntrix; SPP (a riptor) which istance/detorules in tra | riptor) which is Moran autocorrelation lag one weighted by van der ue-based indices descriptor) which is an Eigenvector coefficient a charge descriptor) which is a sub-molecular polarity parameter; the is a valence connectivity index chi-4; D/Dr05 (a topological our ring index of order 5. In ining set, LOF is lack of fit score that resists overfitting, r² is lar² adj is square of adjusted correlation coefficient. Descriptors' meaning Moran autocorrelation lag one weighted by van der Waals volume Moran autocorrelation lag one weighted by atomic polarizability Moran autocorrelation lag one weighted by atomic masses Geary autocorrelation lag one weighted by atomic masses Submolecular polarity parameter Valence connectivity index chi-4 Eigenvector coefficient sum from adjacency matrix Eigenvector coefficient sum from z weighted distance matrix (Barysz matrix) | | |
| | 9 | MAXDP | T^E_{lpha} | Maximal electrotopological positive variation | | |

| | 10 | MDDD | Δσ | Mean distance degree deviation | | | |
|-----------|---|--------|---------------------|--|--|--|--|
| | 11 | D/Dr05 | [D/Δ] _{ij} | Distance/detour ring index of order 5 | | | |
| | 12 | JHETE | $J^{^{\chi}}$ | Balaban type index from electronegativity weighted distance matrix | | | |
| | 13 | VEP2 | λ_i^{lpha} | 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. <i>Bioorganic & Medicinal Chemistry Letters</i> 16 (2006) 5136–5143 | | | | | | |