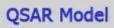
Therapeutic Targets Database





| Target Name | MMP-3 |
|------------------|-----------|
| Target TTD ID | TTDC00105 |

| Target Species | Human |
|-------------------|---|
| Chemical Type | N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives |
| Mode of Action | Inhibitor |
| | $log(10^6/IC_{50}) = -0.042 \times ATS2v - 110.925 \times MATS4m - 55.421 \times MATS8m$ |
| QSAR | $-8.431 \times MATS3v + 2.379 \times GATS6e + 5.227 \times GATS2p + 162.799$ |
| Model 1 | $N = 32;$ $R^2 = 0.808;$ $S = 0.420;$ $p < 10^{-5}$ |
| | $Q_{\text{LOO}}^2 = 0.721$ $S_{\text{CV LOO}} = 0.454$ $Q_{\text{L3O}}^2 = 0.697$ $S_{\text{CV L3O}} = 0.479$ |
| | $\log(10^6/\text{IC}_{50}) = -0.049 \times O[\text{ATS2v}] - 110.925 \times O[\text{MATS4m}] - 32.131 \times O[\text{MATS8m}]$ |
| QSAR | $-2.739 \times O[MATS3v] + 4.427 \times O[GATS6e] + 4.716 \times O[GATS2p]$ |
| Model 2 | + 37.443 |
| | Access the following web-servers to compute molecular descriptors: MoDel and e-dragon |
| | N is the number of compounds included in the models; R^2 are the square of correlation coefficients; S is the standard deviation of the regressions; p is the significance of the variables in the models; Q_{LOO}^2 and $S_{CV,LOO}$ are the correlation coefficients and standard deviations of the LOO cross-validation, |
| Molecular | respectively, and Q_{L30}^2 and S_{CVL30} are the correlation coefficients and standard deviations of the L3O |
| Descriptor | cross-validation, respectively; ${}^{1}\chi^{\nu}$ or log <i>P</i> : hydrophobicity-related descriptors; Descriptors of MMP1 |
| | include ATS2v, MATS5m, MATS7m, GATS1v, GATS1e, GATS4p; Descriptors of MMP2 include |
| | MATS5m, MATS5v, MATS5p, GATS4v, GATS7v, GATS7p; Descriptors of MMP3 include ATS2v, |
| | MATS1m, MATS6m, MATS6e, GATS1v, GATS5v; Descriptors of MMP9 include MATS6m, |
| | MATS2v, MATS1p, GATS3v, GATS7v, GATS8v; Descriptors of MMP13 include ATS2v, |
| | MATS4m, MATS7v, MATS1p, MATS5p, GATS7p; Contribution C_i^{39} of descriptor i is given by: |

| | $C_i = \frac{100 \times \Delta m_i}{\sum \Delta m_i}.$ |
|-----------|--|
| Reference | Linear and nonlinear QSAR study of N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives as |
| | matrix metalloproteinase inhibitors. <i>Bioorganic & Medicinal Chemistry</i> 14 (2006) 4137–4150 |