In Silico Multivariate Regression Analysis and Validation Studies on Selective MMP-13 Inhibitors

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Abstract

QSAR(Quantitative Structure Activity Relationship) studies were carried out on a set of 72 α-sulfone hydroxamates as Matrix Metalloproteinase-13 (MMP-13) inhibitors using multiple regression procedure. Outliers were removed based on Relative Error calculation and Extent of Extrapolation. The activity contributions of these compounds were determined from regression equation and the validation procedures such as external set cross-validation r2, (R2cv, ext) and the regression of observed activities versus predicted activities and vice versa for validation set was described to analyze the predictive ability of the QSAR model. Parameters concerning predictive ability of QSAR model and Y-randomization tests were found to be within the limits. From a set of 5 models, an accurate and reliable QSAR model involving six descriptors was chosen based on the FIT Kubinyi function, which defines the statistical quality of the model. The generated model could be useful in designing more potent inhibitors of MMP-13.

References

Index Terms

Computer Science
Circuits and Systems

Keywords

α-sulfone hydroxamates, QSAR, Multiple regression, Cross validation, Outliers, FIT Kubinyi, descriptors, MMP-13.