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A Simple Method to Classification α-Amylase and α-Glucosidase Inhibitors Using LDA and Decision Trees

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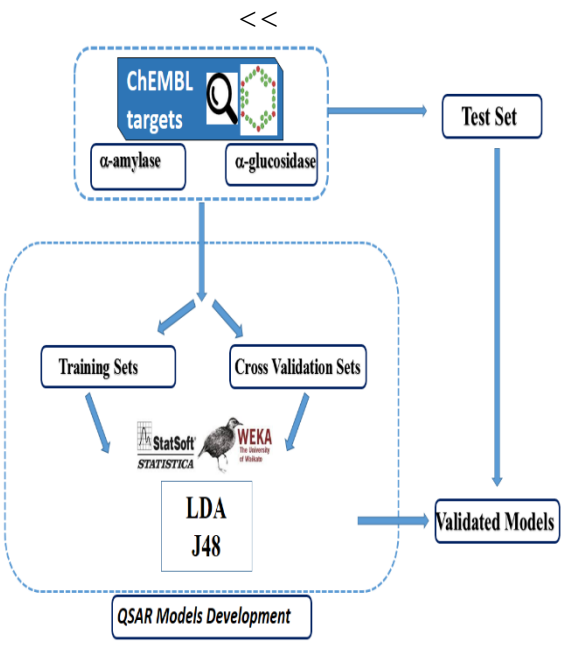
.Graphical Abstract



Abstract.

In this report are used two datasets involving the main antidiabetic enzymes targets α-amylase and α-glucosidase. The prediction of α-amylase and α -glucosidase inhibitory activity as Antidiabetic Agents is carried out using LDA and classification trees (CT). A large data set of 640 compounds for α-amylase and 1546 compounds in the case of α-glucosidase are selected to develop the tree model. In the case of CT-J48 have the better classification model performances for both targets with values above 80- 90% for the training and prediction sets, correspondingly. The best model shows an accuracy higher than 95% for training set; the model was also validated using 10-fold cross-validation procedure and through a test set achieving accuracies values of 85.32% and 86.80%, correspondingly. The main descriptors that influence the inhibitory activity of the antidiabetic enzymes are interpreted. Additionally, the obtained model is compared with other approaches previously published in the international literature showing better or goodness results. Finally, we can say that, the present results provided a double target approach for increasing the estimation of antidiabetic chemicals identification aimed by double-way workflow in virtual screenings pipelines.>>

References

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