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Dual inhibitors of α-amylase and α-glucosidase for the diabetes treatment: A fuzzy rules and machine learning approach.

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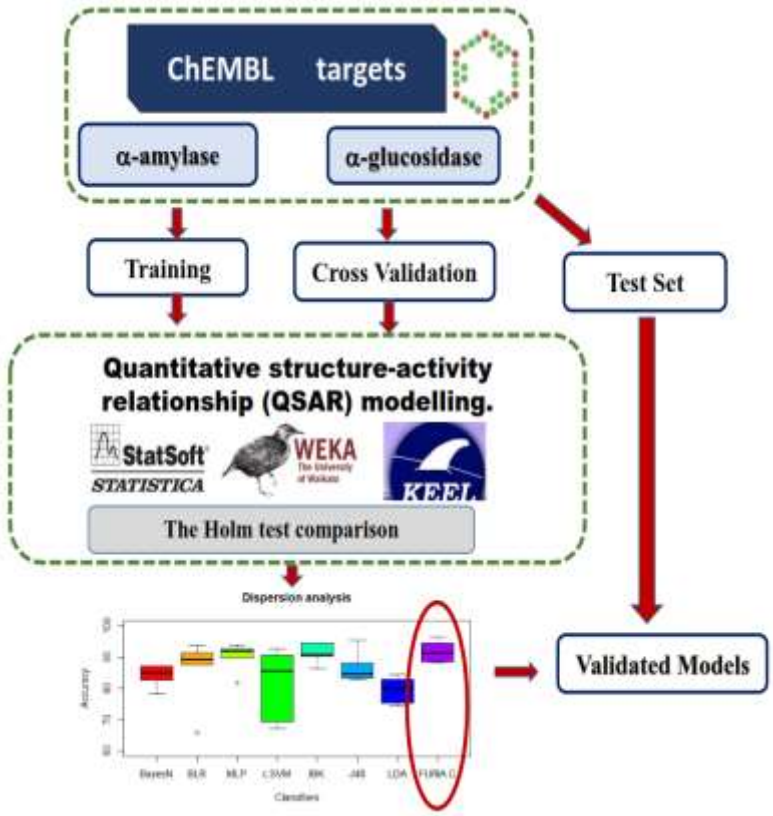
Graphical Abstract



Abstract.

In this report, we propose the Machine Learning FURIA-C as a cutting-edge to classify drug-like compounds with anti-diabetic inhibitory ability toward the main two pharmacological targets α-amylase, and α-glucosidase. This model was tested for its classification capability over each repository, achieving the satisfactory accuracy scores of 94.5% and 96.5%, respectively. Another important outcome was to achieve various α-amylase and α-glucosidase fuzzy rules with a high Certainty Factor values. Some of the rules derived from the training series and active classification rules were interpreted. An important external validation step, comparing our method with the ones already reported, was included as well. The Holm test comparison showed significant differences (p-value<0.05) between Furia C versus Linear Discriminating Analysis (LDA) and Bayes Network, the former beating the last two ones. According to the relative ranking score, the out-performing technique is FURIA-C. Our analysis suggests that Furia-C could be used as a cutting-edge technique to predict (classify or screen), the α-amylase and α-glucosidase inhibitory activity, leading to the discovery of potent antidiabetic agents.

Keywords: Anti-diabetic Agents; induction rule; FURIA-C, QSAR; Machine-learning techniques

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