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Intelligent consensus predictor: Towards more precise predictions for external set compounds

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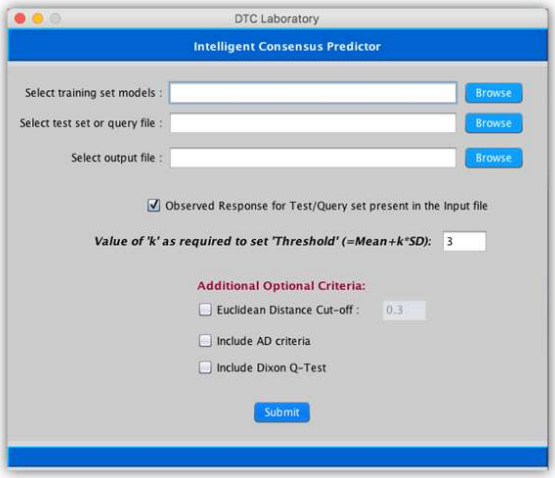
Graphical Abstract



Abstract

Quantitative structure-activity relationship (QSAR) modeling has travelled a long journey in drug discovery process as well as in prediction of property and/or toxicity data of diverse chemicals in order to fill the data gaps. The goodness-of-fit and quality of a model and its prediction capability for untested compounds are assessed through diverse validation metrics. There is a constant endeavor among QSAR researchers to get better the quality of predictions for lowering the predicted residuals for external compounds. The objective of the present study has been to improve the prediction quality for external compounds with implication of "intelligent" consensus modeling approach.Three different forms of consensus models were developed for six different datasets to explore their prediction capability on query chemicals. The types are average of predictions from all qualifying individual models (CM1), weighted average predictions from all qualifying individual models (CM2), and best selection of predictions (compound-wise) from individual models (CM3). Among three consensus models, newer strategies like CM2 and CM3 are evolved as the "winners" considering prediction errors of query compounds for the studied six data sets irrespective of diverse responses, number of data points as well as dissimilar modeling algorithm. We have also developed a tool named "Intelligent Consensus Predictor" which is freely accessible via the web http://teqip.jdvu.ac.in/QSAR_Tools/ and http://dtclab.webs.com/software-tools.The details of this work have been presented in *Conferentia Chemometrica*http://cc2017.ttk.mta.hu/ in Hungary during September 3-6, 2017.

References

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