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Chemometric modeling of refractive index of polymers using 2D descriptors: A QSPR approach

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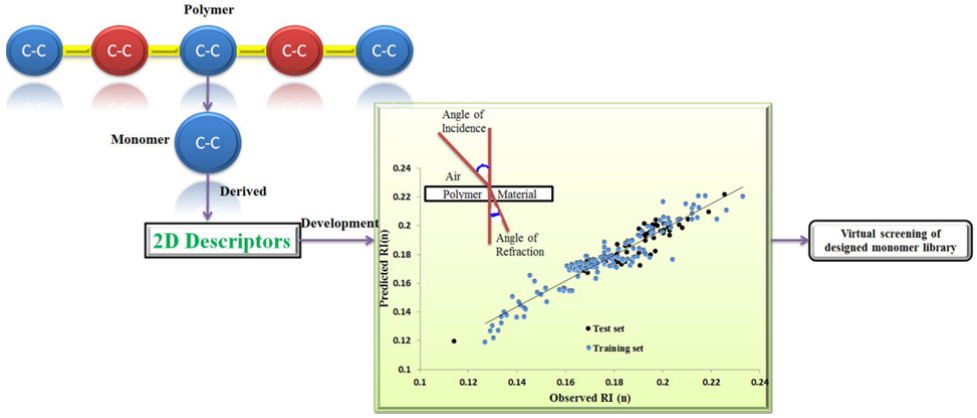
Graphical Abstract



Abstract

In recent years, an increased attention has been paid towards the use of chemometric modeling tools in predicting properties of various synthetic organic materials including polymers. In silico tools such as quantitative structure-property relationships (QSPRs) have become very much popular in designing organic molecules with desired physicochemical properties. These approaches save man power, cost of instrumentation, time and chemical wastages. In the current work, predictive QSPR models have been developed for predicting refractive index (RI) of a set of 221 diverse organic polymers by using theoretical 2D molecular descriptors computed from the monomer units of the polymers. Double cross-validation (DCV) followed by partial least squares (PLS) regression methodology was adopted for the generation of QSPR models using genetic algorithm (GA) as the descriptor selection technique. The

	predictive performance of models was judged by using cross-validation (leave-one-out or LOO), Y randomization, prediction for a test set and applicability domain analysis followed by comparison with the quality of previously reported QSPR models. Presence of polarizability, aromatic ring and different functional groups were the main contributing factors that influence the change of refractive index. An "Intelligent consensus predictor" (http://teqip.jdvu.ac.in/QSAR_Tools/DTCLab/) was employed on the final models to improve the quality of predictions for the external dataset. We have used the final selected models for the prediction of the refractive index of five small virtual libraries of monomers recently reported (Computational Materials Science, 2017, 137:215-224), and finally the predicted values were compared with the previous model derived predictions. Additionally, a true external data set of 98 diverse monomer units with the experimental RI values of the corresponding polymers were used to check the predictability of the obtained QSPR models. The good predictive ability of the derived QSPR models was also reflected from very good external predicted variance for the true external set.

References

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