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Prediction of the Refractive Index of Polymers Using QSAR

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Polymers are a wide group of materials that have quite a wide range of applications due to their diverse properties. Their properties depend on their chemical structure, morphology, method of synthesis and processing. Since there are many variables that affect their characteristics, the characterization of these materials can be lengthy process.

In order to overcome this problem, quantitative structure–activity relationships (QSAR) modeling is a convenient tool for predicting the properties of polymeric materials.

Within this research, QSAR models were prepared for prediction of the refractive index of 100 polymers using theoretical descriptors. Descriptors were generated based on the monomer units of an appropriate number of polymers.

XLSTAT software packaging and several variable selection methods: stepwise, forward and best model with 2, 3 and 4 descriptors were used for model development. Several statistical parameters were used to test the quality of the developed QSAR models.

The correlation coefficients (R^2) and adjusted coefficient of correlation ($R^2_{adj.}$) for all QSAR models are > 0.9; mean squared error (MSE) < 0.0007; root mean square error (RMSE) < 0,003 and Fischer test (F-test)> 400, indicating that all models are statistically significant.

Keywords: QSAR, polymers, refractive index, descriptors