Prediction of flexural strength of polymer using QSPR method

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The flexural strength is one of the important properties in the mechanical properties of a material, and it measures the change in stress and fracture that appear while applying the flexural force to warp the material. Plastic polymers need to have appropriate flexural strength depending on their use, so it takes a lot of time and cost for polymer synthesis and testing to develop suitable materials. In this study, we developed a QSPR model that predicts the flexural modulus from the chemical structure of polymers, to promote the prioritization of polymer synthesis and experiments. The prediction model was developed with MLR and SVM algorithms by applying forward selection and genetic algorithms as feature selection methods. The developed model was verified through the performance of the external set not used for training and the y-scrambling method. The reliability of the predicted value of the model can be checked by whether it exists in the applicability domain. The developed predictive model predicts the flexural strength of polymers, saving time and cost in developing new polymer materials.