

Prediction of tensile strength of polymer using QSPR method

김예슬, 신동렬, 이성광[†]
한남대학교

The tensile strength is one of the important mechanical properties of polymer materials, the force showing the strength of the material, which is the largest force of force applied until cut when attracting the material. Polymer material with high tensile strength increase the loads that be processed and can withstand deformation without material breaking. In this study, we developed a tensile strength prediction model using the QSPR (Quantitative Structure-Property Relationship) method. Tensile strength data were collected in NIMS[1], and molecular descriptor was calculated from the chemical structures using the PreADMET program. The prediction model is applied to the forward selection and general algorithms as feature selection methods using multiple linear regression (MLR) and support vector machine (SVM) algorithms. The developed predictive model predicts the tensile strength of polymers, reducing time and cost in developing new polymer materials, and is expected to be useful for studies on the deformation process and stress/strength of materials.