Concentration prediction of imidacloprid in water through the combination of Fourier transform infrared spectral data and 1DCNN with multilevel feature fusion

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ABSTRACT

The Fourier transform infrared (FTIR) spectra combined with one-dimensional convolutional neural network (1DCNN) based on multi-level feature fusion, that is, MLF-1DCNN, were used to determine the concentration of imidacloprid in water. The FTIR spectra of imidacloprid water solutions with different concentrations (0–0.41 g/L) in 700–4,000 cm^{-1} were measured and the corresponding dataset was constructed, and the concentrations were predicted by the MLF-1DCNN. The effect of the spectral data preprocessing by multivariate scattering correction (MSC) and standard normal variate (SNV) transformation on improving the concentration prediction accuracy was studied. The result shows that the SNV preprocessing has the better prediction effect. The comparison of our model with partial least squares (PLS), support vector regression (SVR) and multiple linear regression (MLR) shows that our model can effectively predict the imidacloprid concentrations with a higher prediction accuracy than the other comparative models. The results obtained in this study demonstrate the analytical potential of applying this method to rapidly predict imidacloprid concentration in water.

Keywords: Concentration prediction; Convolutional neural network; Fourier transform infrared (FTIR) spectra

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