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Application of third-order multivariate calibration algorithms to the determination of carbaryl, naphthol and propoxur by kinetic spectroscopic measurements.

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Abstract

In the present work a new application of third-order multivariate calibration algorithms is presented, in order to quantify carbaryl, naphthol and propoxur using kinetic spectroscopic data. The time evolution of fluorescence data matrices was measured, in order to follow the alkaline hydrolysis of the pesticides mentioned above. This experimental system has the additional complexity that one of the analytes is the reaction product of another analyte, and this fact generates linear dependency problems between concentration profiles. The data were analyzed by three different methods: parallel factor analysis (PARAFAC), unfolded partial least-squares (U-PLS) and multi-dimensional partial least-squares (N-PLS); these last two methods were assisted with residual trilinearization (RTL) to model the presence of unexpected signals not included in the calibration step. The ability of the different algorithms to predict analyte concentrations was checked with Download English Version:

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