
Applications of chemometrics in development and optimization of sample treatment

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Abstract

Sample treatment represents one of the most important steps in the development and optimization of analytical methods. One of the main target of sample treatment is to extract the maximum amount of the analyte of interest from the matrix, meanwhile limiting the co-extraction of potential interfering compounds and obtaining a concentration of the analyte suitable for the chosen instrumental method. Several factors could affect the extraction yield, as the nature of the extracting phase, the duration of the extractive process, the temperature, the addition of salt, the changing of pH....

A chemometric approach can help the researcher to evaluate the actual effects of the considered variables on the response, in order to find the best set of experimental conditions able to maximize extraction recovery.

In general, chemometric techniques allow to obtain greater information on the system under study, at the same time limiting the number of experiment, avoiding waste of resources in terms both of money and working time. Results obtained by the application of chemometric techniques are objective, rational, reproducible and robust. As an example of application of chemometric tools to sample treatment, we can consider the use of ANOVA in selecting the fiber coating in HS-SPME and the use of experimental design in the optimization of equilibration time, extraction time and extraction temperature in HS-SPME.

Keywords: sample treatment, chemometrics, HS, SPME

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