Near infrared: identification of incoming raw materials in a pharmaceutical industry

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Abstract

Near-infrared (NIR) spectroscopy is a technique that is used at CEVA Santé Animale QC Laboratory to identify incoming raw materials. This identification is performed by comparison of the spectrum of the analyzed sample against a database. Identification by NIR is performed on all the containers of a batch and thus avoids doing the identification tests described in the marketing authorization dossier on all the containers: these tests will be carried out on average samples, which are mixtures of several containers of the same batch (sampling according to internal procedures).
Databases were first updated as part of an action to be conducted in the laboratory because of the dysfunction of this method in routine. Thus, for each raw material, 18 spectra from 6 previously analyzed batches were selected from the 25,000 spectra recorded during the last seven years in order to consider the maximum of spectral variability. Then, the identification method for solids was developed: the identification will be carried out using a discriminant analysis with application of two spectral pretreatments which are the Multiplicative Scatter Correction (MSC) and a Savitzky-Golay smoothing. The analysis is restricted to the 7500-4500 cm-1 spectral region using 18 principal components.

A " sub-method " has been developed for povidone raw materials that are not well discriminated using the first method. Analysis mode and spectral pretreatments were unchanged while the spectral region was reduced between 4900 and 4700 cm-1 and only 4 principal components are used.
Both methods had to be validated. An internal validation was carried out with a set of spectra made during the establishment of libraries. Then, according to the European Pharmacopoeia, specificity and robustness had to be validated. Specificity was validated by analyzing raw materials with similar structures and a raw material that is not integrated in the library. For robustness, a design of experiments was performed for the solid identification method. For the povidone identification sub-method, this criterion remains to be validated.

Keywords: near infrared, identification, spectra, discriminant analysis, multiplicative scatter correction, savitzky, golay, principal components, european pharmacopoeia, validation, development, specificity, robustness, design of experiments

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