

## DEVELOPMENT OF NEAR INFRARED SPECTROSCOPIC METHODS USING DESIRABILITY INDEXES: HOW TO SELECT THE MOST APPROPRIATE CALIBRATION MODEL

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In the last decade, considerable research and developments dealing with near infrared spectroscopy (NIRS) have taken place in industrial field, especially in pharmaceutical industry. This enthusiasm can be explained by the fact that NIRS is regarded as promising and attractive tool in Process Analytical Technology (PAT) and Green Chemistry frameworks. Taking into account its non-invasive, non-destructive character, fast data acquisition and the use of probes in on-line, in-line and at-lines, this technique is expected to reach the aims of the latter.

However, the development of a NIR quantitative method is not straightforward in comparison with conventional analytical techniques. Its development requires time-consuming reference methods, chemometrics and iterative heuristic approaches to build a model allowing the prediction of the analyte of interest according to the acceptance criteria consistent with the intended use of the method.

Facing to the lack of objective decision rule of the traditional chemometric criteria such as  $R^2$ , RMSEC, RMSECV and RMSEP, it is essential to develop innovative approaches for the selection of the most appropriate calibration model from a models plurality.

In this context, a methodology using desirability indexes, such as the Fitting Model Index (FMI), based on tolerance intervals was developed in order to increase significantly the objectivity of the decision process. This latter allows to reduce dramatically the development and the validation steps and thus could ease the implementation of NIR spectroscopy in pharmaceutical industry.