Simplified RMID Model Building

Mira Cal P and ModelExpert

Material verification models with complex algorithms such as Principal Component Analysis (PCA), quasi-infinite parameters, and preprocessing options can be incredibly complex. Each model must be rigorously built, evaluated, and validated before it can be put into routine use. Typically, this can take even a highly-trained chemometrician days to complete.

Mira P simplifies material verification for all. With a short, defined user workflow, straightforward results, and a foolproof Operating Procedure-based design,

Mira P is already one of the simplest RMID tools available. ModelExpert, in Mira Cal P, does a chemometrician's work. ModelExpert automatically determines the best model parameters for robust method development. Simply collect Training Set and Validation Set data and ModelExpert will optimize sample analysis. With Mira P and ModelExpert, even non-technical users can achieve better results in a fraction of the time.

Ω Metrohm

INTRODUCTION

ModelExpert is a function integrated into Mira Cal P that optimizes model parameters using Training Set and Validation Set samples provided by the user. This routine iterates 192 combinations of statistical parameters to ensure that optimal model settings are being applied to customer sampling.

DESCRIPTION

ModelExpert leverages the power of receiver operating characteristic (ROC) curves in automated model parameter determination. ROC curves are an integral part of evaluating Machine Learning models. The ROC approach ranks combinations by Area Under the Curve (AUC) score. ModelExpert ranking also includes *a posteriori* knowledge about which combinations perform better than others, in addition to penalizing combinations that produce False Positives/Negatives at the given confidence interval.

METHOD

To use the ModelExpert function, the user first creates a new Training Set in Mira Cal P. ModelExpert is located under Training Sets in the vertical menu. Once ModelExpert is selected, the software automatically runs all possible combinations of model settings (e.g., normalizations, baseline removal, principle components) for the given data while 'Finding Model Settings' is displayed (Figure 1).
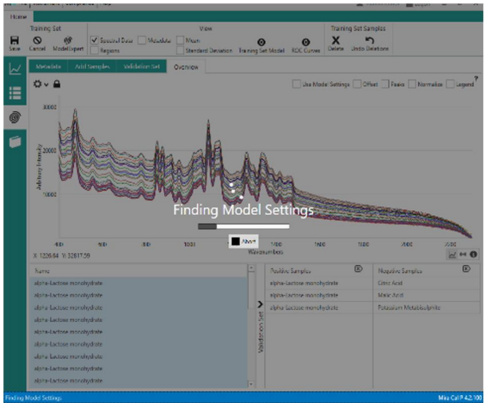

Figure 1. Mira Cal P screenshot during ModelExpert routine.

RESULTS

ModelExpert results appear in a popup window, (Figure 2). This window summarizes the resulting ModelExpert settings. A PDF report containing more information about model settings, ROC curves, and validation samples with associated pvalues may be generated. Once 'Save Training Set' is selected, all optimized model parameters are applied to the associated Training and Validation Sets.
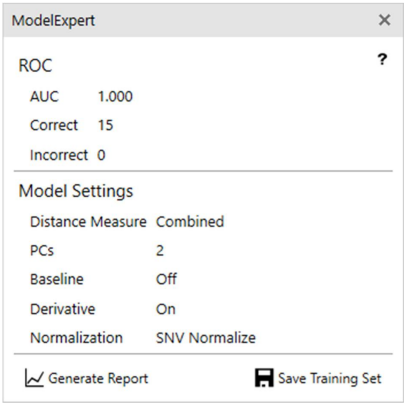

Figure 2. Popup window with ModelExpert Results.

Ω Metrohm

CONCLUSION

Overall, the ModelExpert function is a simple and transparent method of generating optimal parameters and sample data processing using customer data, all with a few simple clicks in Mira Cal P. Metrohm Raman is dedicated to offering the simplest, most efficient and accurate use of Mira P for RMID.

CONTACT

Metrohm Brasil
Rua Minerva, 161
05007-030 São Paulo

metrohm@metrohm.com.br

Ω Metrohm