Application Note AN-RS-045

在不同手持拉曼之的RMID(原材料定)操作渡

Library and Model Transfer from NanoRam 785 to MIRA P

For lab-quality results in non-traditional testing scenarios such as materials inspection at the point of receipt, Raman spectroscopy surpasses traditional raw material identification and verification (RMID) methods. Handheld Raman devices streamline RMID processes and efficiently verify a material's quality and consistency. This efficiency helps manufacturers save time and resources, ensuring more reliable and cost-effective operations.

Verification models are key to RMID with Raman spectroscopy. It is possible to transfer established and validated verification models already in routine use from one Raman product from Metrohm to another. For example, though NanoRam 785 may no longer be sold, existing customers can easily transition their RMID operations to MIRA P. This Application Note describes user/custom library and model transfer from NanoRam 785 to MIRA P for the smoothest transition possible. Transferring models between MIRA P instruments is discussed in a separate Application Note (AN-RS-044).

INTRODUCTION

NanoRam 785 (NR785) users can find model building basics for MIRA P on the Metrohm website [**1**].

Readers of this application are assumed to be NR785 users that are familiar with RMID basics and are already working with established models.

Transferring models between NR785 and MIRA P is simply a matter of changing file formats and reassembling the NR785 model for MIRA P. New users will find that quality testing with MIRA P and its software, MIRA Cal P, is streamlined and intuitive.

TERMINOLOGY

Software terminology differs between NanoRam ID (NID) and MIRA Cal P. Terms are defined in **Table 1**.

Table 1. Relevant terms used in NID and MIRA Cal P.

Software	**NanoRam ID**	**MIRA Cal P**
Data Collection	Operating Preset	Operating Procedure (OP)
Verification Parameters	Method	Training Set Model
Data File Format	CSV	BRMS
ROC Curve	An analytical method used to evaluate the performance of a model at various thresholds.	

IDENTIFICATION VS. VERIFICATION

Identification methods measure spectral similarity between an unknown sample and a collection of library spectra. Identification can be performed with a custom-built library or a library of standards like the Metrohm Comprehensive USP Library.

Unlike identification, **verification** detects very slight spectral differences for high specificity. Each sample spectrum is projected onto a training set (i.e., a collection of spectra representing the target substance) to see how well it matches the model's criteria. This process can discriminate between very similar samples (e.g., the same chemical from two different producers) for strict adherence to verification standards.

The type of transfer depends on the type of test-library transfer for identification and method/model transfer for verification.

Step 1. Data export

Identification	Verification
Library data are exported out of B&W Tek NID software as CSV files	Method data are exported out of B&W Tek NID software as CSV files

Step 2. Convert data format

Identification	Verification
For both types of transfer, exported CSV files are converted to the binary BRMS format for use by MIRA P. Metrohm provides a software conversion tool for this process.	

Step 3. Configure MIRA Cal P software

Identification	Verification
The conversion tool creates a folder containing converted library data which is imported into MIRA Cal P. A new library is built and synchronized to the device for immediate use. This is a very straightforward process.	Metrohm provides a simple verification SOP. A new OP is created for each material in MIRA Cal P, synchronized to the device, and used to collect validation scans.

Step 4. New model in MIRA Cal P

Identification	Verification
—	Import the converted data from NR785 into corresponding folders in MIRA Cal P. Create a training set with the transfer samples. Create a validation set. Generate All ROC curves, then select the best curve and save. Add the validated model to the OP. Synchronize MIRA P and the model is ready for use.

After transfer and ROC optimization, model settings for a lactose example are listed in **Table 2** below.

Table 2. ROC-optimized model settings.

PCS	3
Pretreatment	Mean Center
Distance Measure	Combined
Confidence Interval	0.95
Normalization	Min/Max Normalize
Smooth	YES
Points	13
Poly Order	3
Baseline	NO
Derivative	YES
IVC	YES

VALIDATION WITH P-VALUES

Validation of a model demonstrates that the model adequately assesses a material on a new instrument. In other words, validation data serves as a «diagnosis» of how the model performs on the new unit.

Validation is an assessment of a method using test samples:

- that are expected to PASS (positive samples). These are samples of the target material that are different than the samples used to build the Training Set.
- that are expected to FAIL (negative samples). These can be dissimilar materials or similar but different materials. This ensures the specificity of a model.

Table 3 shows validation test results for a lactose model, after transfer. Lactose is an excellent indicator of transfer success because it is a particularly challenging material for 785 nm Raman due to fluorescence.

Model robustness and specificity are quite high after transfer. This was tested by including different types of lactose (with unique CAS numbers) in the negative validation set and confirming that they failed appropriately.

Table 3. Validation test results with passing (green) and failing (red) p-values.

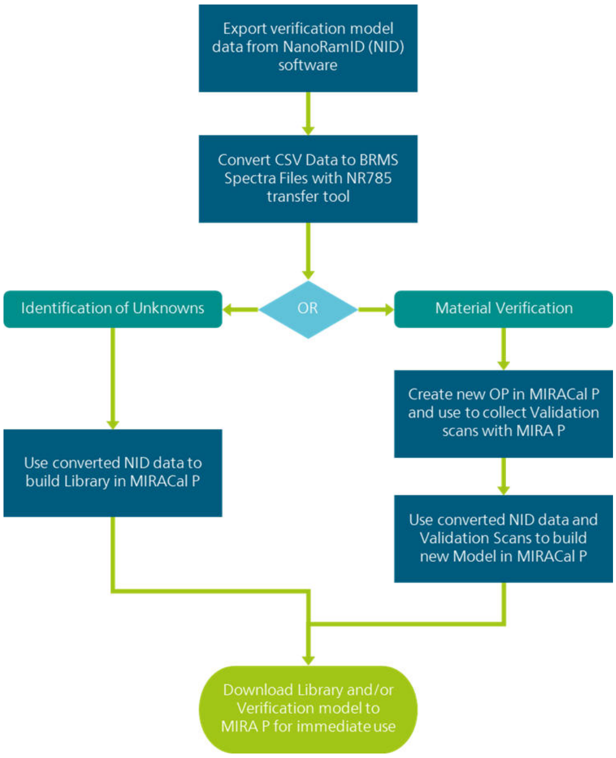
Positive Samples	p-values	Negative Samples	p-values
α-Lactose Monohydrate	0.194	Acetaminophen	0.001
α-Lactose Monohydrate	0.672	Calcium Stearate	0.001
α-Lactose Monohydrate	0.56	Citric Acid	0.001
α-Lactose Monohydrate	0.673	Dextrose	0.001
		α-D-Lactose Monohydrate	0.012
		Lactose Anhydrous	0.001
		Lactose/APAP	0.001
		L-Thyroxine	0.001
		Sucrose	0.001
		Theophylline	0.001

CONCLUSION

NanoRam 785 to MIRA P library and model transfer is a simple procedure that enables a fast and efficient transition. Leverage Metrohm’s Raman portfolio for the best possible RMID experience.

REFERENCES

1. Gelwicks, M. J. Real World Raman:
   Simplifying Incoming Raw Material Inspection.
   Analyze This – The Metrohm Blog, 2021



CONTACT

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CONFIGURATION

MIRA P Basic

(MIRA) P ,, MIRA P ,,ORSMIRA P FDA 21 CFR 11

MIRA P Basic-Paket, MIRA P MIRA Basic-Paket , MIRA DS

MIRA /USP LWD 3B

MIRA P Advanced

(MIRA) P ,,MIRA P ,ORSMIRA P FDA 21 11

Advanced Package ,(3b),(1)

MIRA P Flex

MIRA P Flex Package, MIRA P Flex Package MIRA P ,MIRA P Flex Package USP ,/ USB 3B