Application Note AN-RS-045

Transition RMID Operations Between Handheld Raman Devices

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.

DATA AND METHOD TRANSFER

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.

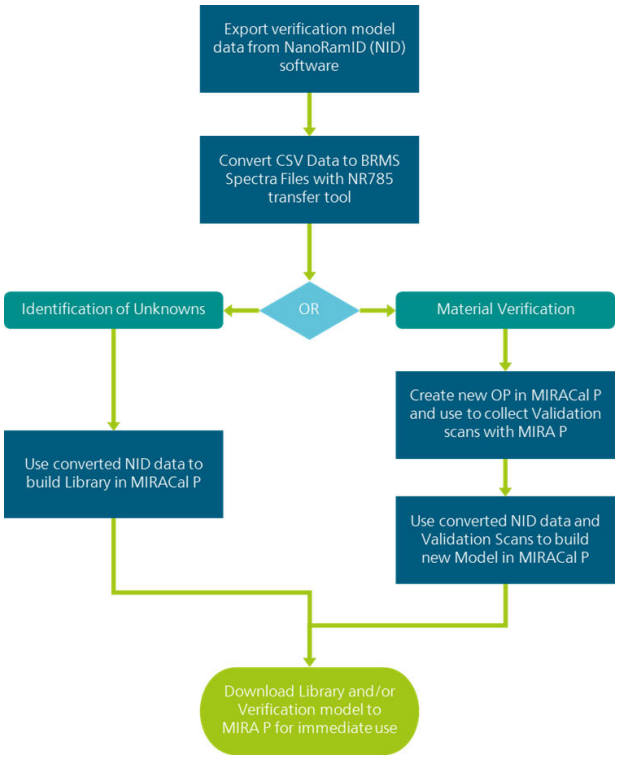
Positive Samples	p-values	Negative Samples	p-values
α-Lactose Monohydrate	0.194	Acetaminophen	0.001
α-Lactose Monohydrate	0.672	Calcium Stearate	0.001
α-Lactose Monohydrate	0.56	Citric Acid	0.001
α-Lactose Monohydrate	0.673	Dextrose	0.001
		α-D-Lactose Monohydrate	0.012
		Lactose Anhydrous	0.001
		Lactose/APAP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



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CONFIGURATION

MIRA P Basic

Le Metrohm Instant Raman Analyzer (MIRA) P est un spectromètre Raman performant et portable destiné à la détermination et la vérification rapides et non destructives de différents types de matériaux, comme les principes actifs et excipients pharmaceutiques. De très petite taille, le Mira P se caractérise pourtant par un design robuste et dispose d'un spectrographe de haute efficacité, équipé de notre technologie « Orbital Raster Scan » (ORS) unique. Le Mira P est parfaitement conforme aux directives de la FDA 21 CFR Part 11.

Le module de base Mira P permet à l'utilisateur d'adapter le Mira P à ses besoins. Le module de base Mira est un module de démarrage qui contient les composants de base nécessaires au fonctionnement du Mira P.

Le module de base contient les accessoires de calibrage/vérification Mira, la bibliothèque USP et la lentille LWD (pour longue distance) destinée aux analyses en flacons ou sachets. Fonctionnement de classe de protection laser 3B.

MIRA P Advanced

Le Metrohm Instant Raman Analyzer (MIRA) P est un spectromètre Raman portable performant qui s'utilise pour les déterminations rapides et non destructives et le contrôle des matériaux les plus divers, comme les principes actifs pharmaceutiques et les excipients. De très petite taille, le MIRA P est pourtant très robuste et dispose d'une structure de spectrographe haute efficacité, équipée de notre technologie « Orbital Raster Scan » (ORS) inédite. MIRA P satisfait aux prescriptions FDA 21 CFR partie 11.

Le Advanced Package comprend une lentille avec laquelle les matériaux peuvent être analysés directement ou dans leur conditionnement (classe de laser 3b), ainsi qu'un support de flacon pour analyser les échantillons dans des flacons en verre (classe de laser 1).

MIRA P Flex

Le MIRA P Flex Package permet à l'utilisateur d'adapter le MIRA P à ses besoins. Le Flex Package comprend tous les composants de base destinés au fonctionnement du MIRA P, sauf les embouts de prélèvement d'échantillons. Un embout de prélèvement d'échantillons est au minimum nécessaire à son fonctionnement. Le MIRA P Flex Package contient la bibliothèque USP, des accessoires de calibrage/vérification et un câble USB. Fonctionnement avec des lasers de classe 3B.