



## Application Note AN-RS-045

# 在不同手持拉曼设备之间的RMID(原材料鉴定)操作过渡

## 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

| Identificat<br>ion | 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.** Validation test results with passing

**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.

(green) and failing (red) p-values.

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

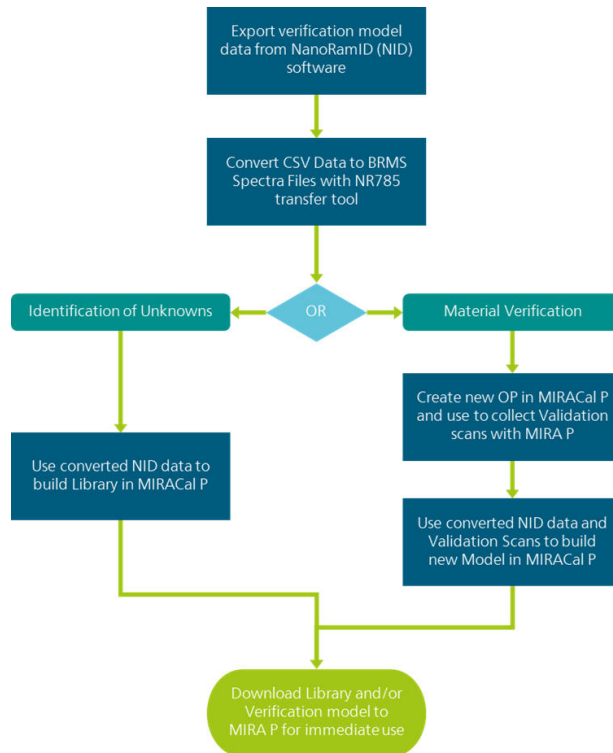
## CONCLUSION

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

Metrohm Taiwan Ltd.  
開封街二段 46 號 5 樓  
108 台北市

[info@metrohm.com.tw](mailto:info@metrohm.com.tw)

## CONFIGURATION



### MIRA P Basic

瑞士万通快速拉曼分析仪 (MIRA) P 是一款性能强大的便携式拉曼光谱仪,可用于各种材料类型的快速无损测定和验证,例如药物有效成分和辅助材料。尽管 MIRA P 体积很小,但是其采用了坚固的设计,并且具 ORS 特色技术。MIRA P 符合 FDA 21 CFR 第 11 部分的准则要求。

使用 MIRA P Basic-Paket,用户可以根据其需求对 MIRA P 进行调整。MIRA Basic-Paket 是一款入门级套装,其包含了运行 MIRA DS 所需的基本组件。

基本套餐包含了 MIRA 校正/验证配件、USP 功能库和用来在瓶子或袋子里进行分析的 LWD 附件。激光防护等级 3B 的使用。



### MIRA P Advanced

瑞士万通快速拉曼分析仪 (MIRA) P 是一款性能强大的手持式拉曼光谱仪,可用于各种材料的快速无损测定和验证,例如药物有效成分和赋形剂。MIRA P 小而坚固,配备了瑞士万通的 ORS 技术。MIRA P 符合 FDA 联邦法规 21 章第 11 款的规定

。Advanced Package 包含一个附加透镜,可用它直接分析材料或者在材料容器中分析(3b 级激光器),还有一个小管支架套筒用于分析玻璃小管中的样本(1 级激光器)。



### MIRA P Flex

使用 MIRA P Flex Package,用户可以根据其需求对 MIRA P 进行调整。Flex Package 包括了用来运行 MIRA P 的所有基本组件,无需采样用附件。运行需要一个采样用附件。MIRA P Flex Package 包括了 USP 功能库,用于校正/验证的附件和一根 USB 电缆。以 3B 级投入使用。