

### Technical Report

# **MALDI EasyCare**: Automated detector tuning to maintain instrument performance for demanding applications

Caroline J. Jones<sup>1</sup>, Simona Salivo<sup>1</sup>

#### Abstract:

The MALDI EasyCare systems have been designed to facilitate routine user maintenance to help retain optimal instrument performance for high-throughput or high-laser-shot-number MALDI-TOF MS applications. All MALDI-TOF instruments are prone to fouling of the ion optics positioned close to the sample, or detector wear, and this can lead to reduced instrument performance e.g., reduced sensitivity and resolution. With the MALDI EasyCare systems, end users can easily perform maintenance tasks without the need for an expensive service engineer visit. A software wizard guides the user through the entire process. Here, we provide an example showing how the performance of an instrument used for MALDI imaging was recovered by this simple user maintenance procedure.

Keywords: detector tuning, MALDI EasyCare, MALDI-TOF, user maintenance

#### Introduction

Matrix assisted laser desorption ionization (MALDI) is a fast and highly sensitive ionization technique capable of generating ions from biological samples such as peptides, proteins, oligonucleotides, lipids and carbohydrates. Often coupled with a time-of-flight (TOF) analyser, MALDI-TOF stands out for its simplicity, robustness and speed of analysis. Among the various mass spectrometry applications, MALDI imaging is one of the fastest-growing in recent years. In this technique, a target species is measured directly from the surface of the sample (e.g., a tissue) after appropriate coating with a MALDI matrix. The distribution of the species is then visualised in the form of a 2D map by using dedicated software. During the MALDI process, the matrix absorbs the laser energy and is ablated from the target along with the sample ions of interest. During this process, some of the ablated material will deposit on the ion optics, resulting in contamination over time. The wide bore of the extraction lens on the Shimadzu MALDI-TOF instruments provides some protection against the effects of contamination of the ion optics, however this will, alongside wear of the detector from

ion bombardment, ultimately lead to a deterioration of instrument performance. In the majority of cases, the instrument performance can be recovered simply by tuning the detector, a job often reserved for trained service engineers. With the introduction of MALDI EasyCare (Figure 1a), this routine maintenance task can now be safely performed by instrument operators.

## Loss of performance through extended use and detector wear

To demonstrate the effectiveness of the MALDI EasyCare functionality to recover performance after detector wear, MALDI imaging was used as an example of an intensive, high-laser-shot-number MALDI-TOF MS application. Fingermarks were used as sample and prepared for the imaging analysis by depositing 2,5-dihydroxybenzoic acid (DHB) matrix via sublimation using the Shimadzu iMLayer™ sublimator device.

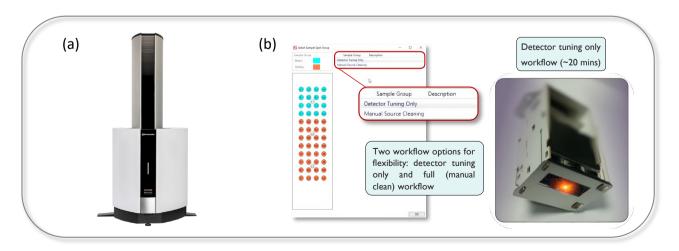


Figure 1: (a) MALDI EasyCare instrument (MALDI-8030 in this picture). (b) MALDI EasyCare provides two workflow options: full manual source clean and detector tuning only. The latter takes about 20 minutes.

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Prior to starting the series of imaging acquisitions, the instrument underwent the full MALDI EasyCare workflow to ensure optimal performance i.e., ion optics were manually cleaned and detector voltage was automatically optimised. The instrument performance was checked as per sensitivity test described in the customer QC tests. A fingermark sample was run at 30 µm pixel size demonstrating typical performance on a working instrument. Figure 2a shows the overlaid MALDI image of a triacylglycerol (TAG) species in the ridges (m/z 841; red), an endogenous species localised in the sweat pores (m/z 422; green), and a matrix ion (m/z 417; blue). The corresponding pixel spectrum extracted from the ridges displaying a good quality TAG profile, is shown in Figure 3a. Figure 2b shows the overlaid MALDI image of the same species as Figure 2a obtained after multiple intensive imaging experiments resulted in detector wear. It can be clearly observed how the structures of the ridges and sweat pores are lost due to poor spectral signals. This is confirmed in the pixel spectrum shown in Figure 3b where the poor signal and signal-tonoise of the TAG species clearly demonstrates a deterioration in performance. The loss in performance was also confirmed with the sensitivity test described in the customer QC test.

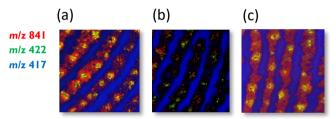


Figure 2: overlaid MALDI images of a TAG species in the ridges (*m/z* 841; red), an endogenous species in the sweat pores (*m/z* 422; green), and a matrix ion (*m/z* 417; blue). (a) First imaging run. (b) After running multiple imaging experiments. (c) After MALDI EasyCare detector tuning to recover instrument performance.

#### Performance recovery using MALDI EasyCare

Using the software wizard, the operator is presented with two workflow options: full (manual source clean) workflow and detector tuning only (Figure 1b). To recover performance after detector wear, the automated detector tuning only option can be used. The detector tuning workflow can be conveniently performed without breaking the vacuum and removing any parts from instruments, and the whole procedure takes about 20 minutes. After tuning, the instrument performance recovery was confirmed with the sensitivity test described in the customer QC test (data not shown) and subsequent MALDI imaging analysis of another fingermark sample. Figure 2c shows the overlaid MALDI image of the TAG species at m/z 841 in the ridges (red), the endogenous species at m/z 422 in the sweat pores (green), and the matrix ion at m/z 417 (blue).

All the main fingermark features are clearly visible demonstrating instrument performance recovery, as confirmed by the pixel spectrum in Figure 3c that shows full signal and signal-to-noise recovery.

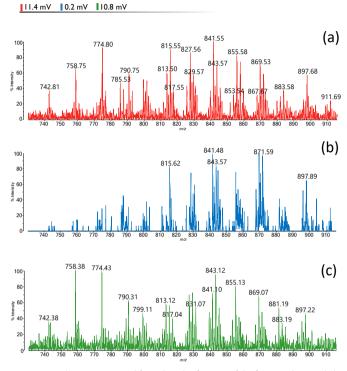


Figure 3: Pixel spectra extracted from the ridge features of the fingermark expanded in the TAG region. (a) First imaging run. (b) After running multiple imaging experiments. (c) After MALDI EasyCare detector tuning to recover instrument performance.

#### Conclusion

The MALDI EasyCare systems have been designed to facilitate routine user maintenance to help retain optimal instrument performance for intensive, high-laser-shot-number MALDI-TOF MS applications. It provides the user with two workflow options: full (manual source clean) workflow and detector tuning only. Depending on the application and matrix, there may be some instances where the application might benefit from the full workflow including ion optics cleaning. This could potentially reduce the voltage gain required on the detector and prolong the longevity.

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