

Automated Analysis Software for MALDI-MS

SampleStation and AuraSolution



SampleStation™: simplified sample organization for automated MALDI-MS

The SampleStation software has been designed to facilitate automated analysis on the latest Shimadzu MALDI-TOF MS instruments. Part of the MALDI Solutions™ suite of software, SampleStation allows users to create and manage sample worklists. These are saved in a centralized database which is accessible to multiple users of the system. The simple workflow and data security features make it an ideal solution for both regulated and non-regulated laboratory environments.

Key features:

- Security via individual user login and administrator control
- Flexibility: customizable worklist features to suit different applications
- Simple workflow and intuitive user interface
- Compatible with handheld barcode readers for scanning sample slides and sample vials
- Records chain of data responsibility
- Amenable to regulatory compliance
- Automatically updates worklists following sample analysis
- Can be used with both disposable and reusable FlexiMass™ slides
- Seamless integration with AuraSolution automated acquisition software via the MALDI Solutions database

Flexible sample target options

SampleStation is compatible with the FlexiMass series of microscope slide-format sample targets, providing users with a choice when it comes to sample preparation. The individually barcoded, single-use polymeric FlexiMass-DS slides provide a convenient solution for controlled workflows in regulated laboratories. Alternatively, for users looking for a longer-term, more cost-effective sample preparation solution, the reusable stainless steel FlexiMass-SR slides provide another option.



The SampleStation and AuraSolution software are compatible with the FlexiMass series sample slides (FlexiMass-SR48 (left) and FlexiMass-DS (right) shown)

Workflow designed for sample traceability

Central to each sample worklist is the unique sample slide identifier of the FlexiMass slide used to prepare the samples. The slide identifier (e.g. the FlexiMass-DS slide barcode) provides a link to the sample worklist associated with a given slide, ensuring traceability between sample and result throughout the workflow. Additional checks against duplication of worklists ensure that there is only a single current worklist associated with a given slide.



Data security

Data security in regulated environments is paramount. Access to SampleStation is controlled by password-protected user accounts, ensuring that only permitted users can access the software. The customizable user roles provide the system administrator with an additional means of access control within the software. Each step in the creation of the worklists is recorded, clearly identifying when and by whom changes to worklists were made, providing a chain of data responsibility and traceability.

A simplified workflow enhancing productivity - just scan, select and save!

Creation of a worklist involves 3 simple steps: scan a slide barcode; select sample positions within the graphic and then save. The visual and tabulated worklist provides a simple user interface which helps to reduce the risk of workflow errors.

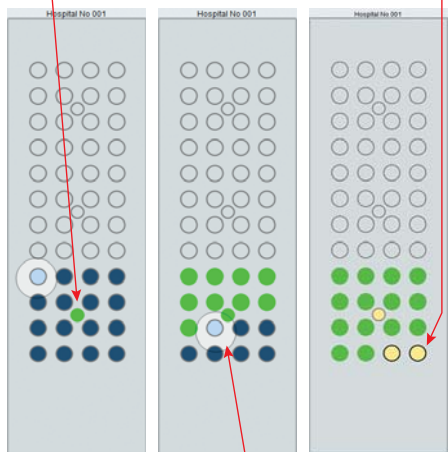
AuraSolution™: confidence during analysis

Data analysis and review

1. Quality assurance: Analysis proceeds to sample spot only if calibration/QC spot passes (green).

3. Flexibility: Samples for reanalysis (yellow).

4. Audit trail window: Records details of all analysis including reanalysis.



View Spectra

Search criteria

Slide filter: 0817202203

Sample ID: [Search]

Export

Results:

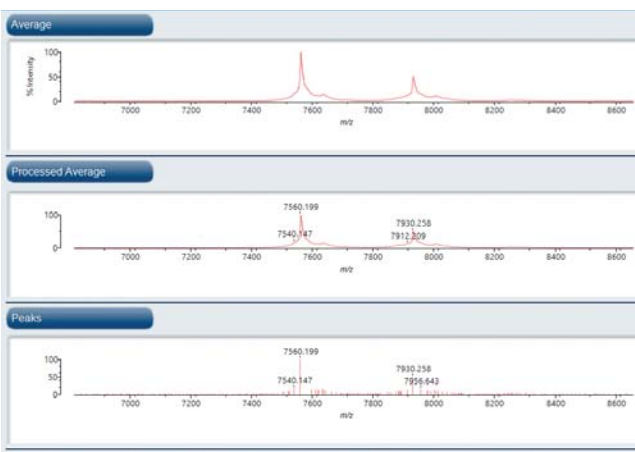
Acquisition Time	Position	User
2012Q18 18:28	L3	Emman
2012Q18 18:34	L4	Emman
2012Q18 18:34	L3	Emman
2012Q18 18:35	L2	Emman
2012Q18 18:35	L1	Emman
2012Q18 18:37	L3	Emman
2012Q18 18:51	K2	Emman
2012Q18 18:51	K1	Emman
2012Q18 18:59	M	Emman
2012Q18 18:59	J3	Emman
2012Q18 18:59	J2	Emman
2012Q18 14:59	J1	Emman
2012Q18 14:59	M	Emman
2012Q18 14:57	J3	Emman
2012Q18 14:58	J2	Emman
2012Q18 14:57	J1	Emman
2012Q18 14:58	K2	Emman
2012Q18 14:58	K1	Emman
2012Q18 14:58	M	Emman

Details:

Profiles passed: 100

Profiles failed: 0

Spectrum Quality: Data Passed

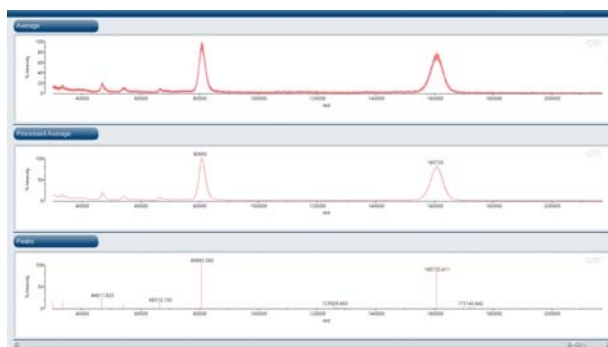


2. Easy data review: Mass spectrum of current sample spot under analysis (pale blue) is shown in the live view. Positions of samples already analyzed (green) or awaiting analysis (dark blue) are easily identifiable.

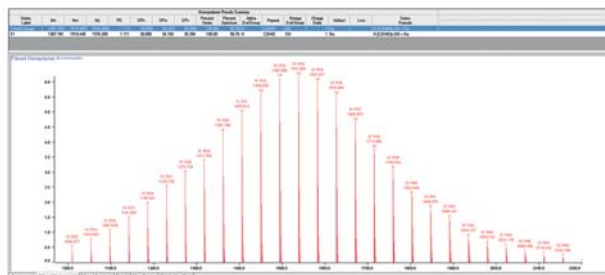
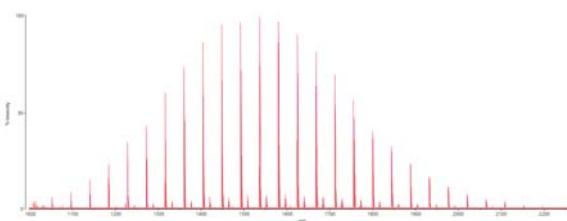
5. Easily retrievable data: Mass spectra of acquired sample spots can be displayed either by clicking on the spot position in the live slide graphic or by selecting the corresponding sample from the results table in the audit window for the given experiment.

Unleash your potential for automated MALDI-MS applications using SampleStation and AuraSolution

The flexibility of SampleStation / AuraSolution allows the software to be integrated into different MALDI-MS workflows, enabling automation of a range of MALDI-based applications. Increase sample throughput and productivity by simply automating the analysis of samples prepared using your existing MALDI sample preparation protocols.



Adaptable to different applications: Analysis of IgA (~160 kDa) using SampleStation and AuraSolution



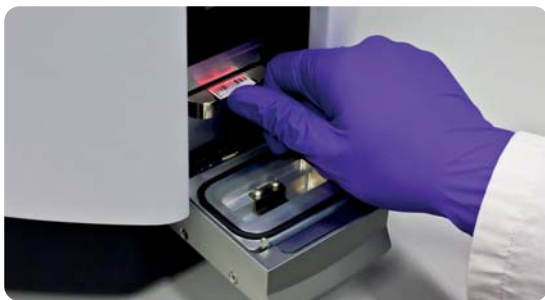
Automated polymer analysis and export to third party data mining software (Polymerix (Sierra Analytics))



AuraSolution and SampleStation are compatible with the Shimadzu MALDI-8020 benchtop linear MALDI-TOF mass spectrometer

Utilizing instrument features to reduce mismatch errors: integrated barcode reader

During insertion of a FlexiMass-DS MALDI slide into the instrument, the AuraSolution software uses the integrated barcode reader in the MALDI-8020 MALDI-TOF mass spectrometer to automatically retrieve and load the corresponding sample worklist. This approach acts as an additional safety mechanism to prevent mismatch errors between sample ID and analyzed results, providing a solution for laboratories where quality assurance is a priority.



Facilitates regulatory compliance

As mass spectrometry moves into clinical laboratories, the data security measures in place come under increased scrutiny from regulatory bodies[†]. As with SampleStation, user access to AuraSolution is password-protected and user accounts are controlled by a system administrator. For each experiment, an audit window indicates when the analysis was performed, which user ran the experiment and whether samples have been reanalyzed. Acquired data is stored in an SQL database and benefits from the associated data security features designed to prevent deletion of data.

[†] SampleStation and AuraSolution are for Research Use Only. Not for use in diagnostic procedures.



Password-protected user login provides peace of mind regarding data security. Only users with the correct permissions can unlock the application, thereby adding another layer of protection. In the example above, the application is locked and is under the ownership of user account 'Technician2'.

Simplifying sample analysis - scan, load and run

The workflow has been designed with regulated laboratories in mind, where 'simple' equates to 'safety'. The barcode of a FlexiMass-DS slide is automatically scanned during insertion into the MALDI-8020 instrument and displays the designated samples for analysis. The user then loads the relevant acquisition parameters and clicks start.

The acquisition parameters are optimized and saved in the MALDI Solutions database via the Data Acquisition software for use by AuraSolution. This integration between the MALDI Solutions database, SampleStation-generated worklists and AuraSolution offers a seamless solution for automated analysis.



Acquisition parameters optimized in MALDI Solutions Data Acquisition software can be directly loaded into AuraSolution.

SampleStation: process simplification, intuitive and secure

The screenshot shows the SampleStation interface with several callouts:

- Unique barcode for worklist:** Points to the slide barcode field (DS171302096).
- User activity monitored and recorded:** Points to the 'Created By' and 'Updated By' fields.
- Current user identified:** Points to the user name 'Hi, Lab user 1' in the top right.
- Save worklist to database and export worklist for records:** Points to the 'Save' and 'Export' buttons.
- Optional customizable sample fields where, for example, barcodes on individual samples can be scanned for additional unique identification:** Points to the 'Sample Fields' column in the table.
- Target slide graphic to 'click and populate' the worklist:** Points to the slide image on the left.
- Seamless integration between SampleStation and the MALDI Solutions database allows differentiation of samples previously acquired using AuraSolution:** Points to the 'Sample Fields' column.

Position	Type	Comment	Sample Fields
x1	Calibration		
A1	Sample	Antibody assay	4803957409
A2	Sample	Antibody assay	6258744815
A3	Sample	Antibody assay	9343988735
A4	Sample	Antibody assay	3378054762
B1	Sample	Antibody assay	3338874825
B2	Sample	Antibody assay	3884145322
B3	Sample	Antibody assay	6284401927
B4	Sample	Antibody assay	6442730925
C1	Sample	Antibody assay	6442730925
C2	Sample	Antibody assay	7013488807
C3	Sample	Antibody assay	305929192
C4	Sample	Antibody assay	6373229962
D1	Sample	Antibody assay	8413778826
D2	Sample	Antibody assay	8907057330
D3	Sample	Antibody assay	1434126481
D4	Sample	Antibody assay	5289297486

AuraSolution: automated high-throughput MALDI-MS acquisition for regulated laboratories

AuraSolution is the second component in the automated MALDI-MS analysis solution provided by Shimadzu. Using sample worklists previously created with SampleStation, the AuraSolution software is used to automate data acquisition and to subsequently review results. The simple 'scan, load and run' workflow and data security features make it an ideal solution for both regulated environments and research laboratories.

Key features:

- Simple workflow – scan slide, load acquisition parameters and start run
- Utilizes the integrated instrument barcode reader (MALDI-8020) as the slides are loaded into the instrument
- Facilitates regulatory compliance through enhanced data security features
- Option of using both disposable and reusable FlexiMass slides
- Fully compatible with the MALDI-8020 mass spectrometer
- Seamless relationship with SampleStation software via the MALDI Solutions database
- Automatically export data as ASCII / mzML formats



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