

QC Reporter



QC Reporter™: mass confirmation and quality assessment with confidence

Within a given manufacturing process, quality control (QC) plays a fundamental role in guaranteeing the supply of a high quality product. QC Reporter is an automated analysis and reporting software solution for QC environments. Compatible with the MALDI-8020 benchtop linear MALDI-TOF mass spectrometer, this software provides a simple and secure platform for typical QC workflows.

QC Reporter

QC Reporter is a fully automated software application designed for high-throughput quality control analysis using MALDI-TOF MS. The acquisition, calibration, processing, quality assessment and reporting processes are performed automatically within a single platform and a simple, intuitive workflow design. Using QC Reporter, a typical QC experiment can be performed with a few simple steps:

- defining the acquisition and quality assessment criteria settings
- importing samples for analysis using a predefined sample worklist
- viewing and/or exporting the results

The quality criteria (detection of the target mass and amount of permitted adducts/impurities) are applied on the fly for each acquired sample and are presented in a colour-coded manner providing an at a glance summary for easy reading. The option to subsequently export a summary of the entire experiment or to generate individual sample reports provides the user with options for different workflows.

QC criteria

A wide selection of user-defined parameters can be configured as acceptance criteria for the QC assay, providing flexibility for the user to customize each type of experiment for a given application. These include:

- mass tolerance (compared with the expected mass)
- signal-to-noise threshold
- minimum resolution of the target mass
- acceptable limits for adducts
- acceptable limits for impurity levels

Set the parameters which are appropriate for your experiment.

QC Criteria

Select the criteria that constitutes a QC test. A QC test is marked as Pass if none of the Fail or Query criteria are met

Include in test	Criteria	Value	Measure	Fail	Query	Special Condit..
Absolute Criteria						
<input type="checkbox"/>	Mass tolerance is greater than	2	Da	<input checked="" type="radio"/>	<input type="radio"/>	<input type="radio"/>
<input checked="" type="checkbox"/>	S/N threshold is less than	5		<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>
<input checked="" type="checkbox"/>	Minimum resolution	1000		<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>
<input checked="" type="checkbox"/>	Sum of adducts is greater than	50	%Area	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>
<input checked="" type="checkbox"/>	Maximum impurity level	40	%Area	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>
Range Criteria						
<input type="checkbox"/>	S/N is within range			<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
<input type="checkbox"/>	Sum of adducts is within range	Apex(mV)		<input type="radio"/>	<input type="radio"/>	<input type="radio"/>
<input type="checkbox"/>	Min > max acceptable impurity level	%Area		<input type="radio"/>	<input type="radio"/>	<input type="radio"/>

Special Conditions - Optional additional specific criteria that may be applied

Mass NOT within tolerance but Adducts found: ☒ Fail ☐ Query

Define the Mass calculation Type: ☒ Monoisotopic ☐ Average

Define Adducts... 2 selected
Define Amino Acids... 0 selected
Define Matrix Ions... 0 selected
Define Impurities... 0 selected

Absolute Criteria: Set the target mass tolerance, S/N and resolution thresholds

Absolute Criteria: Specify the permitted levels of adducts and/or impurities relative to the intensity or the area of the target mass

Range Criteria: Set a range of values for criteria applied to the target mass and adducts/impurities

Result: Decide whether the sample is reported as Fail or Query if the quality criteria are not achieved

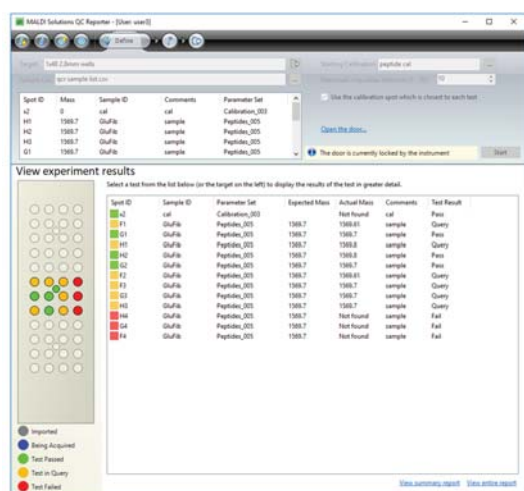
Define the Adducts and Impurities: Link to the (editable) database of adducts, matrix ions and impurities

Quality criteria parameters for the target mass, adducts, matrix ions and impurities.

Acquisition

The information regarding each sample is provided via a simple .csv spreadsheet containing:

- sample location on the MALDI target
- sample identifier/sample name
- expected molecular weight
- acquisition/calibration sample analysis methods (parameter sets)
- additional comments (optional)



Results window in QC Reporter showing the colour-coded, tabulated experiment results (Red = 'Fail'; Green = 'Pass'; Yellow = 'Query').

The acquisition, calibration and data processing methods are created and saved in the MALDI Solutions™ Data Acquisition application and can be retrieved via the seamless integration with the shared SQL MALDI Solutions database.

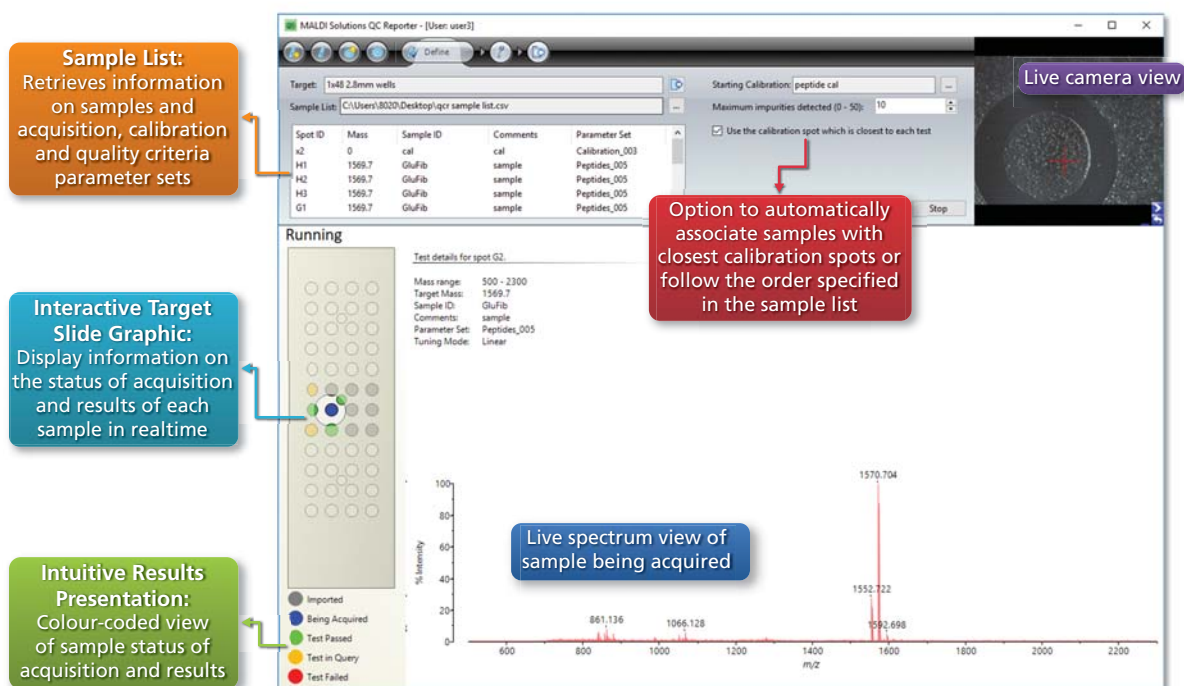
Experiments and results are stored in the SQL database and benefit from the database security features designed to limit access to data/results and prevent unauthorized deletion of data.

The data for each sample is evaluated and compared against the QC criteria, specified in the acquisition parameter set, in realtime. As the experiment progresses, the target slide graphic is updated with a colour-coded indication of the obtained results:

Green = Pass: the expected mass has been found within the given tolerance and all other specified criteria are within the acceptable limits

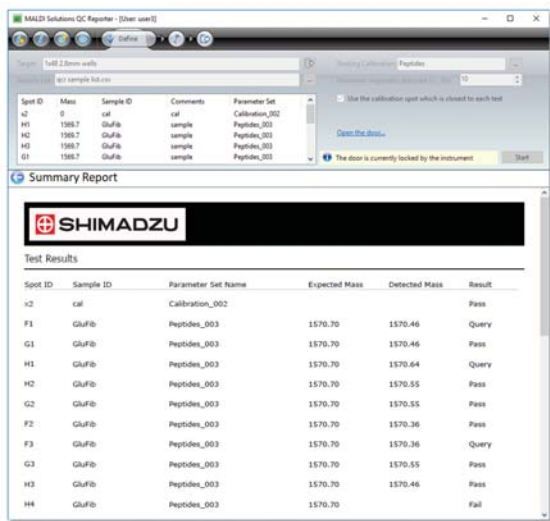
Red = Fail: the expected mass has not been found within the given tolerance or other specified criteria were set to trigger a 'Fail' result

Yellow = Query: the expected mass has been found but it does not meet the absolute criteria (e.g. signal-to-noise, resolution) or high level of impurities/adducts have been detected



Main QC Reporter window showing the progress of the QC experiment. The quality criteria specified in the parameter set are applied to each sample analyzed. The target slide graphic is updated with the colour-coded results in realtime.

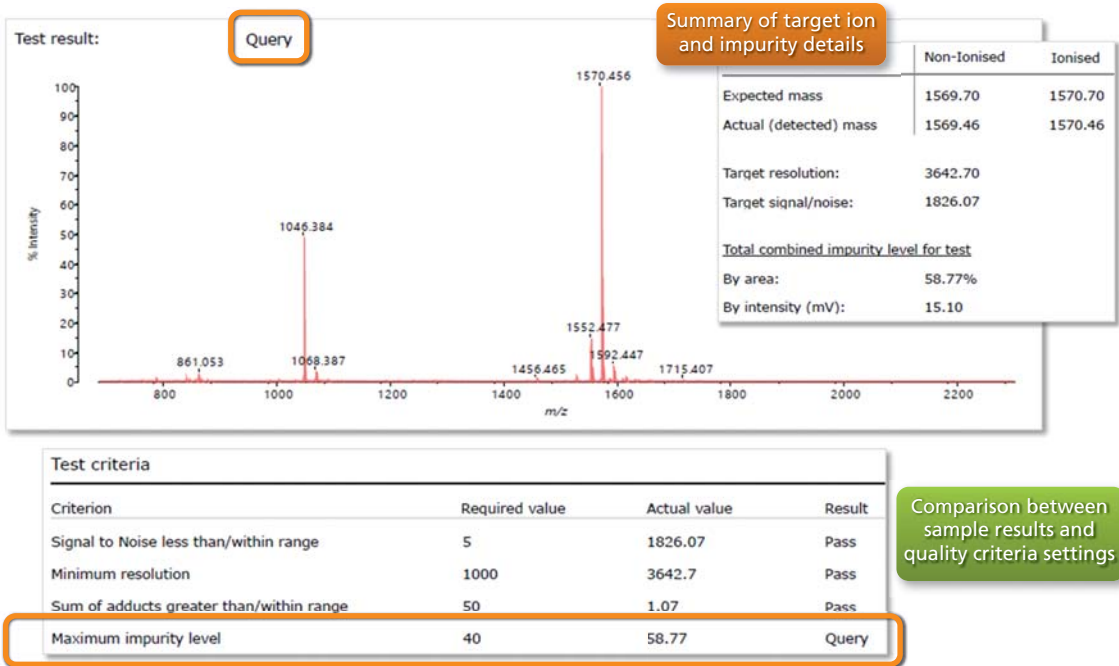
Reporting



Overview report of the QC experiment results which may be customized and exported as a PDF.

During an experiment, the acquired spectrum and result for each analyzed sample are displayed in realtime on the target slide graphic using the colour-coded results reporting schema. At the end of the experiment, the results are presented as a tabulated, colour-coded summary report in the main results window. From this view, the user can further interrogate individual sample results.

After reviewing the results, these can be exported as PDF printable reports for the experiment summary, all samples or selected individual samples. These can be used to report the results back to customers or kept as records of the sample analysis jobs.



A detailed report for each individual sample can be generated, where information on the sample acquisition, target mass and levels of adducts/impurities is provided. In this example, the overall test result is reported as 'Query' due to the detected sum impurity level (% Area) exceeding the user-specified threshold.

Key features:

- Security via individual user login and Administrator control of user roles and permissions
- Flexibility: applicable to different applications (peptides, proteins, oligonucleotides and small molecules)
- Fully compatible with the MALDI-8020 mass spectrometer
- Simple operation: set the acquisition and criteria parameter sets, run the samples and view the results!
- Intuitive user-interface: colour-coded results providing an at a glance summary of the QC experiment. Review individual results via the interactive slide graphic
- Comprehensive reporting: all relevant information is presented in exportable sample reports
- Seamless relationship with MALDI Solutions Data Acquisition software via the MALDI Solutions database

Data security

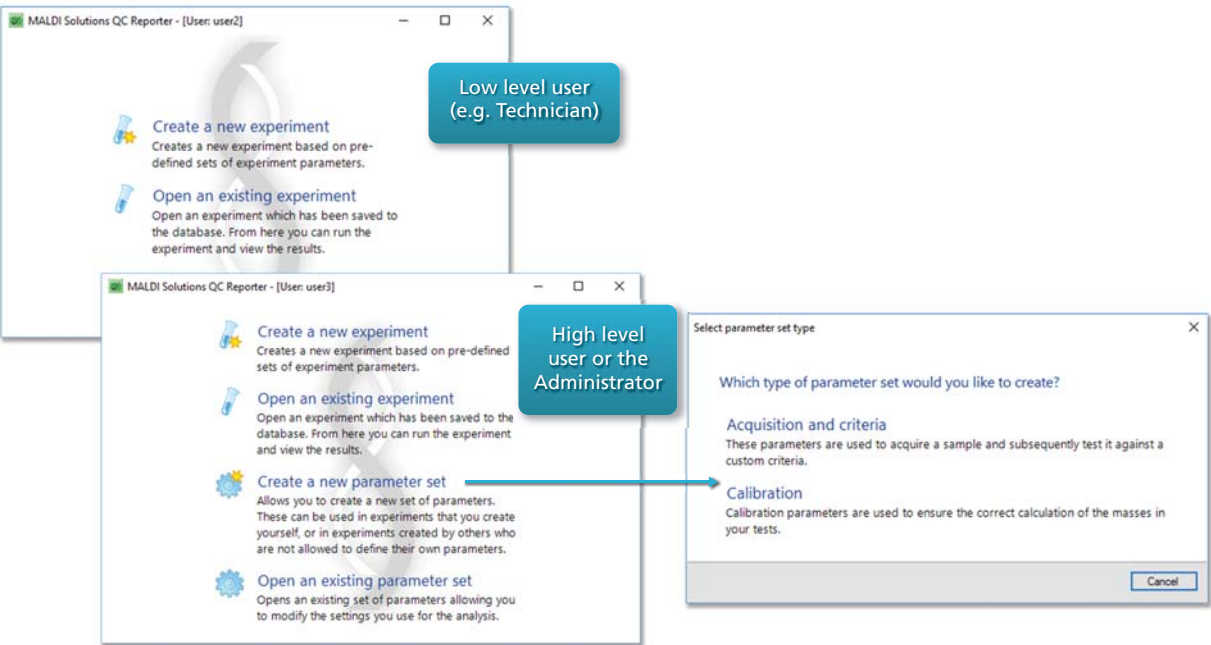
User-access to QC Reporter is via password-protected login and is controlled by a System Administrator who manages access within the application. The Administrator is able to control access to features within the software via various roles which can be applied to individual user accounts.

For example, the acquisition, calibration and data processing methods are created and/or edited by the Administrator or by users who have been granted this permission. This protects the acquisition methods against unpermitted changes and provides peace of mind in regulated environments.



- ✓ Create/edit/delete users
- ✓ Define roles and permissions

Password-protected user login generated by the Administrator. Only those users with the correct permissions can unlock the application.



Defined options for creating/loading parameter sets and QC experiments. Only those users who have been granted the permission to create parameter sets (methods) are able to see these options.



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