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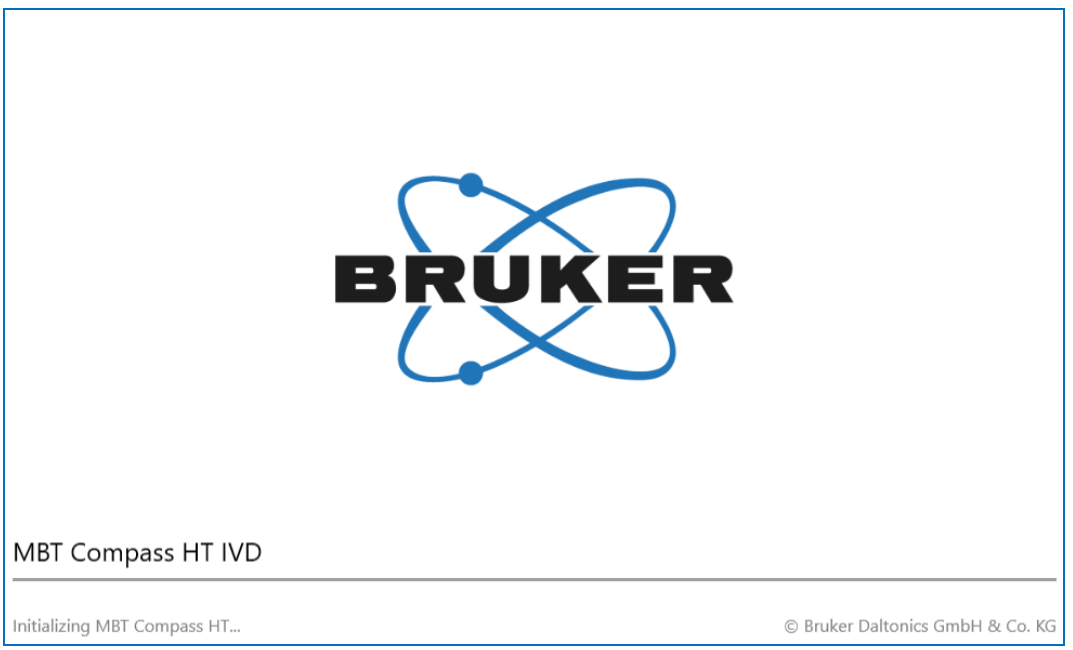
MBT Compass HT IVD
User Manual



IVD CE

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Document history

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The following table describes changes from the previous version C of this document.

Version	Section	Changes
E	-	"score value" replaced by "log(score)", "Id" replaced by "identifier"
E	6.3.2, 6.4, B 2.1, B 2.2, B 2.3	"Caution" message added
E	Symbols	two symbols added

Table of contents

Legal and regulatory notices ... **2**
Manufacturer ... **3**
Document history ... **4**
1 Intended purpose ... **9**
2 Precautions and warnings ... **10**
2.1 Safety instructions ... 10
2.2 General precautions and warnings ... 10
2.3 Data safety and cybersecurity ... 11
2.3.1 Backing up data ... 11
3 Product description ... **12**
3.1 Test principle ... 12
3.1.1 Sample preparation and processing ... 12
3.1.2 Generating a 'molecular fingerprint' ... 13
3.1.3 Calculating a log(score) value ... 13
3.1.4 MBT Compass HT IVD workflow ... 14
3.2 Limitations ... 15
3.2.1 Limitations of use ... 15
3.2.2 Limitations of method ... 15
3.3 Performance characteristics ... 16
3.3.1 Clinical performance data ... 16
3.3.2 Analytical performance data (Precision – Reproducibility/Repeatability) ... 18
3.4 Scope of supply ... 19
3.5 Materials required ... 20
4 Installing and licensing of the software ... **21**
4.1 System requirements ... 21
4.2 Installing MBT Compass HT IVD software ... 22
4.3 Licensing MBT Compass HT IVD software ... 22
4.4 Uninstalling MBT Compass HT IVD software ... 23
5 Calibrating the software ... **24**
5.1 Mass spectrometer pre-check ... 24

6 Using the software 25
6.1 Starting MBT Compass HT IVD 25
6.2 MBT Compass HT IVD Home view 27
6.2.1 MBT Compass HT IVD online help 28
6.2.2 PREPARED TARGETS list 28
6.2.3 LATEST ID RUNS list 29
6.3 Creating an identification run 31
6.3.1 Assigning sample positions 35
6.3.2 Assigning BTS Quality Control positions 35
6.3.3 Changing or adding positions to an identification run 36
6.3.4 Reviewing identification run status 36
6.4 Starting acquisition 37
6.5 Monitoring acquisition of an identification run 39
6.6 Stopping acquisition of an identification run 43
6.7 Generating a report 44
6.7.1 Structure of the report 44
6.7.1.1 Header and footer 45
6.7.1.2 Report Info 45
6.7.1.3 Run Info 46
6.7.1.4 Result overview table 47
6.7.1.5 Detailed Results 47
6.7.1.6 Matching Hints 47
6.7.1.7 Meaning of Consistency Categories (A–C) 48
6.7.1.8 Meaning of log(score) Values 51
6.8 Viewing and exporting results 51
6.8.1 Checkbox for report selection 51
6.8.2 log(score) indicator 52
6.8.3 Position, Sample identifier, Name, Sample type 52
6.8.4 Detected species 52
6.8.5 Comment 52
6.8.6 Consistency 53
6.8.7 Export Time 53
6.8.8 Spectrum 53

6.8.9 Score ... 54
6.8.10 Preparation Protocol ... 54
6.8.11 Isolate identifier ... 54
6.8.12 Description ... 54
6.8.13 Exporting results ... 55
6.8.14 Filtering results ... 55
7 Evaluating IVD MALDI Biotyper results ... 56
7.1 Definition of false positive and false negative identifications ... 56
7.2 Possible causes of incorrect identification results ... 57
7.3 Possible causes of ambiguous identification results ... 58
7.4 Possible causes of a delayed or lost identification, or no identification ... 59
8 Troubleshooting MBT Compass HT IVD identification runs ... 61
8.1 Error messages ... 62
9 Administration ... 65
9.1 Configuration ... 65
9.1.1 Views ... 65
9.1.2 Imports ... 66
9.1.3 Exports ... 66
9.1.4 Msp abbreviations ... 66
9.1.5 Acquisition ... 66
9.1.6 Modules ... 66
9.1.7 Global ... 67
9.2 Maintenance ... 67
9.2.1 E-Log book ... 67
9.2.2 Consumables registration ... 67
9.2.3 Runs administration ... 68
9.2.4 Troubleshooting ... 69
10 Symbols ... 70
11 Glossary ... 71
Appendix A — Sample preparation ... 76
A.1 Warnings and cautions ... 76
A.2 Precautions ... 77
A.3 Reagents and chemicals ... 77

A.4 Handling MALDI target plates ... 79
A.5 Tracking MALDI target plates ... 79
A.6 Cleaning and storing reusable MALDI target plates ... 80
A.7 Storing cleaned MALDI target plates ... 82
A.8 Testing reusable MALDI target plates ... 82
A.8.1 Test procedure for new MALDI target plates ... 83
A.8.2 Test procedure for used MALDI target plates ... 84
A.9 Checking disposable MALDI target plates ... 85
A.9.1 New disposable MALDI target plates ... 85
A.9.2 Partially used disposable MALDI target plates ... 86
A.10 General recommendations ... 86
A.10.1 Culturing samples ... 88
A.10.1.1 Culture media ... 88
A.10.1.2 Culturing bacteria ... 89
A.10.1.3 Culturing yeasts ... 89
Appendix B — Sample preparation guide ... 90
B.1 Sample preparation ... 91
B.1.1 Reusable MALDI target plate cleaning procedures ... 91
B.2 Sample preparation procedures ... 93
B.2.1 Direct transfer sample preparation procedure ... 93
B.2.2 Extended direct transfer sample preparation procedure ... 94
B.2.3 Extraction sample preparation procedure ... 96
Appendix C — User management ... 99
C.1 Default mapping of MBT Compass HT IVD user roles to Windows groups ... 99
C.2 User group rights ... 100
Appendix D — Sample report ... 109
Index ... 110

1 Intended purpose

MBT Compass HT IVD software is an *in vitro* diagnostic software for use with a Bruker IVD MALDI-TOF mass spectrometer for the automatic qualitative calculation of the similarity of a mass spectrometry-based pattern profile of unknown microorganisms sub-cultured from human specimens compared to mass spectrometry-based pattern profiles of characterized strains stored in a reference library. This allows identification of unknown microorganisms (bacteria and yeasts) at the species level after standardized sample preparation procedures. MBT Compass HT IVD provides an aid to diagnosis and is for professional use only.

2 Precautions and warnings

All users must read this manual before using the IVD MALDI Biotyper System and MBT Compass HT IVD. Do not attempt to operate the IVD MALDI Biotyper until you thoroughly understand all instructions and procedures in this manual. Failure to comply with these instructions may compromise the performance and reliability of the IVD MALDI Biotyper.

CAUTION Do not use the IVD MALDI Biotyper until it has been installed by a Bruker Service Representative and laboratory staff have been trained by a Bruker representative.

2.1 Safety instructions

This document uses the following safety instructions:

Note *Includes additional information about using the software.*

2.2 General precautions and warnings

Use the software only as specified by Bruker and as described in this user manual. If the operator does not follow the instructions given in this user manual, or if the operator uses the software for other than the intended purpose, Bruker accepts no responsibility for erroneous results.

2.3 Data safety and cybersecurity

Cybersecurity

The MALDI Biotyper data system comes with an activated Windows Update feature in order to automatically install (cyber) security related updates. This setting must not be changed – especially if the data system is to be connected to the Internet.

The MALDI Biotyper data system comes with an activated default Windows antivirus software. Before connection of the MALDI Biotyper data system to a network, we strongly recommend to contact your local IT specialists about their preferred antivirus software, and, if needed, to install it and make sure that it is kept up-to-date. It is the customer's responsibility to ensure that their system is effectively protected against cyber-attack.

We strongly suggest separating the subnet with the MALDI Biotyper data system (including its clients, if any) from the rest of your network by a firewall that only allows the inbound traffic you want and need. The MALDI Biotyper data system itself does not need to be accessed from outside its subnet. Contact your local IT specialists for further planning of your network structure.

Make sure that all local Windows users on the MALDI Biotyper data system that were created by Bruker are either deleted or the password is changed according to your IT's password policy.

Antivirus software configuration

Contact the MALDI Biotyper Hotline for a current list of MBT Compass HT IVD resources to exclude from antivirus software.

2.3.1 Backing up data

The user is responsible for backing up the raw data (spectra). The MBT Compass HT IVD database can be configured to automatically write daily, monthly, and yearly backups to a defined local or remote folder. Contact your local Bruker Service department for help in configuring and validating the MBT Compass HT IVD backup procedure.

3 Product description

MBT Compass HT IVD software together with a Bruker IVD MALDI-TOF mass spectrometer, consumables and defined workflows allows the identification of unknown microorganisms (bacteria and yeasts) in samples sub-cultured from human specimens.

3.1 Test principle

3.1.1 Sample preparation and processing

Microorganisms to be identified using the IVD MALDI Biotyper are isolated by streaking a microbial culture onto an agar plate. Selective media can be used to facilitate isolation of selected microorganisms. The tested sample — either an individual colony from a culture plate or a cell extract — is transferred to a selected position on a MALDI target plate.

The MALDI target plate is air-dried and matrix is added (for more information on processing samples, see Appendix A). The standard solvent in the matrix solution extracts proteins from the microorganisms. The extracted proteins are mainly ribosomal proteins, which are present in high concentrations in microorganisms. When the matrix has crystallized and is completely dry, the prepared MALDI target plate is ready to be analyzed using MBT Compass HT IVD.

Samples are analyzed using MALDI (matrix-assisted laser desorption/ionization) TOF (time-of-flight) mass spectrometry. A laser in the MALDI-TOF mass spectrometer irradiates the dried matrix spot with a focused, intense burst of UV light. This causes rapid evaporation of the matrix and proteins, resulting in the release of intact, positively charged proteins and peptides (a so-called "soft" ionization technique).

These ions are electrostatically accelerated over a short distance and arrive in the flight tube at a mass-dependent speed. Because different proteins/peptides have different masses, ions arrive at the detector at different times (time of flight). The mass spectrometer measures the time (in the microsecond range) between pulsed acceleration and the corresponding detector signal, and the speed is converted into an exact molecular mass.

3.1.2 Generating a 'molecular fingerprint'

The highly abundant microbial ribosomal proteins result in a mass spectrum with a characteristic mass and intensity distribution pattern. For many microorganisms, this pattern is species-specific and can be used as a 'molecular fingerprint' to identify the sample.

3.1.3 Calculating a log(score) value

Data acquisition is controlled using MBT Compass HT IVD software. The spectrum of the unknown sample is first transformed into a peak list. Using a biostatistical algorithm, this peak list is compared to reference peak lists of organisms in the reference library database and a log(score) between 0.00 and 3.00 is generated.

The higher the log(score), the higher the degree of similarity between the pattern for the unknown peak list and the peak list for the entry in the reference library. A log(score) greater than or equal to 2.00 is considered an acceptable probability for sample identification at the species level (*High confidence species identification*).

If the log(score) is less than 2.00 (*Low confidence species identification* or even *No organism identification possible*) after initial analysis, samples can be processed using an alternative sample preparation procedure and the analysis repeated. For more information on alternative sample preparation procedures, see Appendix A.

The log(score) ranges defined in MBT Compass HT IVD reflect the probability of organism identification. Results should be reviewed by a trained clinical microbiologist and final organism identification should be based on all relevant information available. This information includes but is not limited to: Gram staining, colony morphology, growth characteristics, and sample matrix.

The software uses the following log(score) ranges, interpretations as confidence levels, confidence symbols and confidence colors, see table 3-1.

Table 3-1 Score ranges and their interpretation and visualization

Score range	Interpretation	Symbols	Color
2,00–3,00	High confidence species identification	(+++)	**Green**
1,70–1,99	Low confidence species identification	(+)	**Yellow**
0,00–1,69	No organism identification possible	(-)	**Red**

3.1.4 MBT Compass HT IVD workflow

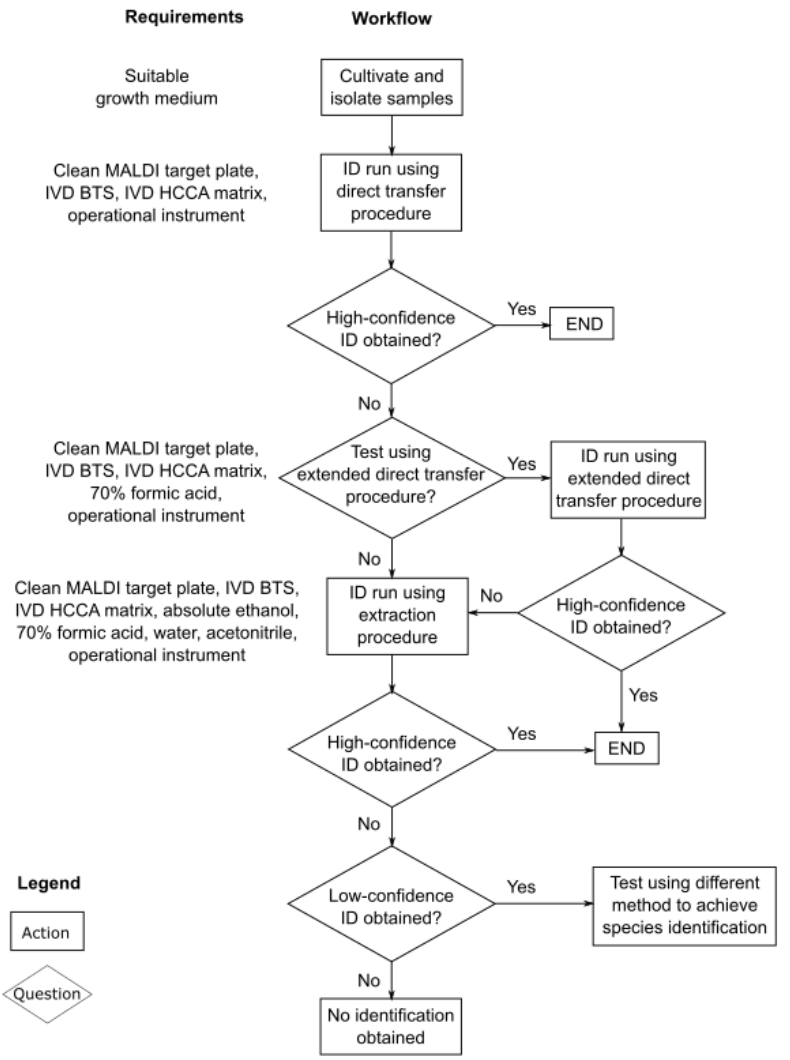

Figure 3-1 Software perspective of the MBT Compass HT IVD workflow

3.2 Limitations

3.2.1 Limitations of use

Use of MBT Compass HT IVD is limited to users trained in the procedure. Training is provided by a person authorized by Bruker when performing the initial startup.

MBT Compass HT IVD may only be used in combination with a Bruker IVD MALDI Biotyper System and consumables and further products of the Bruker IVD MALDI Biotyper System portfolio, see section 3.5.

3.2.2 Limitations of method

MBT Compass HT IVD may only be used to identify organisms included in the released and distributed reference library.

Unless a suitable Bruker IVD product is available, MBT Compass HT IVD may not be used for:

- Identification of filamentous fungi and mycobacteria
- Direct analysis of patient samples, that is, without preparing a subculture
- Analysis of mixed cultures
- Identification of organisms from liquid cultures
- Identification of Biosafety Level 3/4 organisms
- Identification of organisms for which no reference pattern is contained in the IVD MALDI Biotyper reference library
- Identification of viruses
- Identification of serotypes

Certain microorganisms (for example, *Salmonella*) may only be identified at the genus level and not at the species level.

3.3 Performance characteristics

3.3.1 Clinical performance data

The clinical performance of MBT Compass HT IVD was demonstrated in a performance evaluation study. The results obtained were compared with biochemical identification results. Where deviations occurred, identifications were confirmed using 16S rRNA gene sequencing.

Clinical spectra were reanalyzed *in silico* with MBT Compass HT IVD and the reference library 11.0 to confirm identity of results with previously generated data obtained with MBT Compass IVD, see Table 3-2.

Table 3-2 Results of the *in silico* analysis of clinical spectra with MBT Compass HT IVD

17448 clinical spectra	**IVD 11.0 (2021)**			
	confidence			
	high	**low**	**high & low**	**no ID**
ALL	17448			
	14819	1875	16694	754[1]
	84.9%	10.7%	95.7%	4.3%
Gram-	9874			
	9156	714	9870	4
	92.7%	7.2%	99.96%	0.04%
Gram+	5512			
	4475	1027	5502	10
	81.2%	18.6%	99.82%	0.18%
Yeast	1322			
	1188	134	1322	0
	89.9%	10.1%	100%	0%
Anaerobes	818			
	727	91	818	0
	88.9%	11.1%	100%	0%
Staphylococcus sp.	3635			
	2878	757	3635	0
	79.2%	20.8%	100%	0%

[1] *740 samples could not be identified because applicable reference mass spectra were not included in the current library or spectra quality was insufficient for successful identification.*

17448 clinical spectra	IVD 11.0 (2021)			
	confidence			
	high	low	high & low	no ID
Enterobacteriaceae	7535			
	7045	489	7534	1
	93.5%	6.5%	99.99%	0.01%
Non-fermenters	8235			
	7675	558	8233	2
	93.2%	6.8%	99.98%	0.02%

3.3.2 Analytical performance data (Precision – Reproducibility/Repeatability)

For the precision test, 20 different species covering 5 different organism groups of relevant microorganisms were selected, see Table 3-3.

Table 3-3 Species selected for precision test

Microorganism group	Species
Non-fermenting gram-negative bacteria	*Acinetobacter baumannii*, *Stenotrophomonas maltophilia*
Enterobacteriacea	*Leclercia adecarboxylata*, *Proteus vulgaris*, *Enterobacter cloacae*
Other gram-negative bacteria	*Ochrobactrum anthropi*, *Brevundimonas diminuta*, *Sphingobacterium spiritivorum*
Gram-positive bacteria	*Kocuria kristinae*, *Streptococcus equi*, *S. pyogenes*, *Staphylococcus lugdunensis*, *S. sciuri*
Yeasts	*Saccharomyces cerevisiae*, *Yarrowia lipolytica*, *Candida tropicalis*, *C. albicans*, *C. parapsilosis*, *C. glabrata*, *Clavispora lusitaniae*

This selection of microorganisms represents a real challenge set in a routine environment, both from the mass spectrometry point of view as well as in clinical microbiology. The precision test was conducted at three sites. The 20 samples were prepared and measured 3 times at the same day, this was repeated the following day and the day after. In this way, inter-day reproducibility was evaluated.

Results

The mean of the precision study results over all three sites was 94.1%.

3.4 Scope of supply

The standard MBT Compass HT IVD package contains the following components:

- MBT Compass HT IVD / MBT Compass HT IVD Library
- MBT IVD Library Extension[1]
- User Manuals and Release Notes
- License for MBT Compass HT IVD (delivered by e-mail)

Additional software modules are available to extend the range of IVD MALDI Biotyper applications.

For more information on MBT Compass HT IVD software modules, refer to the release notes or respective module documentation or visit www.bruker.com/mbt.

[1] *Libraries might be delivered separately due to technical or logistics reasons.*

3.5 Materials required

The following consumables and reagents are required in order to use the product as intended, and can be ordered separately:

Product	Part number
IVD Matrix HCCA-portioned	8290200
IVD Bacterial Test Standard	8290190

Depending on your workflow, the following MALDI target plates are compatible:

Product	Part number
MBT Biotarget 96 IVD	1839298
MSP 48 target polished steel BC	8281817
MSP 96 target polished steel BC	8280800

4 Installing and licensing of the software

MBT Compass HT IVD software supports Windows 10 English Version. For details on the required service packs, see the Release Notes contained in the installation package.

MBT Compass HT IVD must be licensed, see section 4.3. If it does not find a valid license when it is started, an error message will be displayed.

4.1 System requirements

For detailed information, refer to the Release Notes.

The minimum requirements for a computer running both server and client applications are listed below:

- CPU: Multicore processor, for example, Intel Core or Intel Xeon
- Hard disk: At least 100 GB of free disk space
- Main memory: 6 GB RAM or more for workstations, 16 GB RAM or more for the server
- Operating system: Windows 10
- Graphic resolution: 1280 × 1024 pixels, 32-bit colors or higher (for instance, 1680 × 1050)
- CD-ROM / DVD drive (for installation)
- Web browser: Edge 98 or Firefox 97
- Microsoft .NET Runtime 4.8
- PDF viewer

4.2 Installing MBT Compass HT IVD software

MBT Compass HT IVD software uses a client/server architecture. There are two main installation packages: the client package (MBT Compass HT IVD Client) and the server package (MBT Compass HT IVD Server). Because the server is responsible for data management, the server package is installed only on one computer (central server). The client package can be installed on different computers (each installation requires a separate license). All IVD MALDI Biotyper clients can access the data on the central server.

Client and server installation are initiated by double clicking the setup in the Client respective Server folder of the installation medium.

For information on how to upgrade from an older IVD MALDI Biotyper or MBT Compass IVD software version, contact Bruker.

MBT Compass IVD software connects data acquisition (flexControl) to identification. If this package is not installed on an acquisition system (no flexControl), then it must operate in a mode used for defining runs and retrieving results only (localhost-noFC). This mode is automatically activated when MBT Compass HT IVD is running on a computer without flexControl.

4.3 Licensing MBT Compass HT IVD software

MBT Compass HT IVD must be licensed before it can be used. Upon delivery of the ordered components, an e-mail is sent to the customer with a link to the Bruker license portal.

Refer to the `BDAL License Activation Instructions.pdf` document for details on how to activate, deactivate or transfer licenses.

In case of a real client-server installation (MBT Compass HT IVD Server and MBT Compass HT IVD Client on different PCs), we suggest installing all licenses on the server PC and configure it as license server. See the referenced document for instructions.

4.4 Uninstalling MBT Compass HT IVD software

►► To uninstall MBT Compass HT IVD Client/Server

1. Open the Windows menu.
2. Start typing “Add or remove programs”.
3. Click on "Add or remove programs".
4. Select the MBT Compass HT IVD software from the list of installed programs.
5. Click **Uninstall**.
6. Confirm the request to remove the software.

5 Calibrating the software

5.1 Mass spectrometer pre-check

The IVD MALDI Biotyper mass spectrometer is automatically checked before each run to confirm that the mass spectrometer settings are appropriate.

The check requires that IVD Bacterial Test Standard (IVD BTS) is spotted on the MALDI target plate at one or more BTS quality control (**BTS QC**) positions.

The **BTS QC** position is automatically measured multiple times before the run proceeds. The following parameters are checked:

- Calibration peaks (*m/z*, width, height)
- Spectrum baseline

The parameters are combined to provide an overall quality value from which the final **BTS QC** outcome is determined.

If the check fails, the run is stopped and the message "**FAILED**" will be displayed in the **QC Status** section of the MBT Compass HT IVD Run View.

Users can define a MALDI target plate position on which an automatic BTS QC procedure will be performed before starting an identification run. The BTS QC is performed on a MALDI target plate position containing a sample of IVD Bacterial Test Standard (IVD BTS, Bruker part no. # 8290190). This standard is essentially a preparation of *E. coli* DH5 α that has been spiked with two additional proteins in the upper mass range, enabling calibration over a mass range of 4 to 17 kDa.

6 Using the software

6.1 Starting MBT Compass HT IVD

1. Log on to the MBT Compass HT IVD computer using the user name **tof-user** (or the user name provided by your system administrator).
2. Start MBT Compass HT IVD by double-clicking the **MBT Compass HT IVD Client** shortcut on the desktop.

   Alternatively, MBT Compass HT IVD can be started by selecting **Start > All Programs > Bruker > MBT Compass HT IVD Client**.

Figure 6-1 MBT Compass HT IVD desktop shortcut

After starting, MBT Compass HT IVD will ask for a login (username and password). Depending on the role of the user used for login, some functionality will not be available. See Appendix C for details on which role can use which functionality.

During startup, the software will indicate successful connection to the server and instrument and check the contents of the IVD library.

If no connection can be made, an error view opens enabling users to connect to a different server, see figure 6-2.

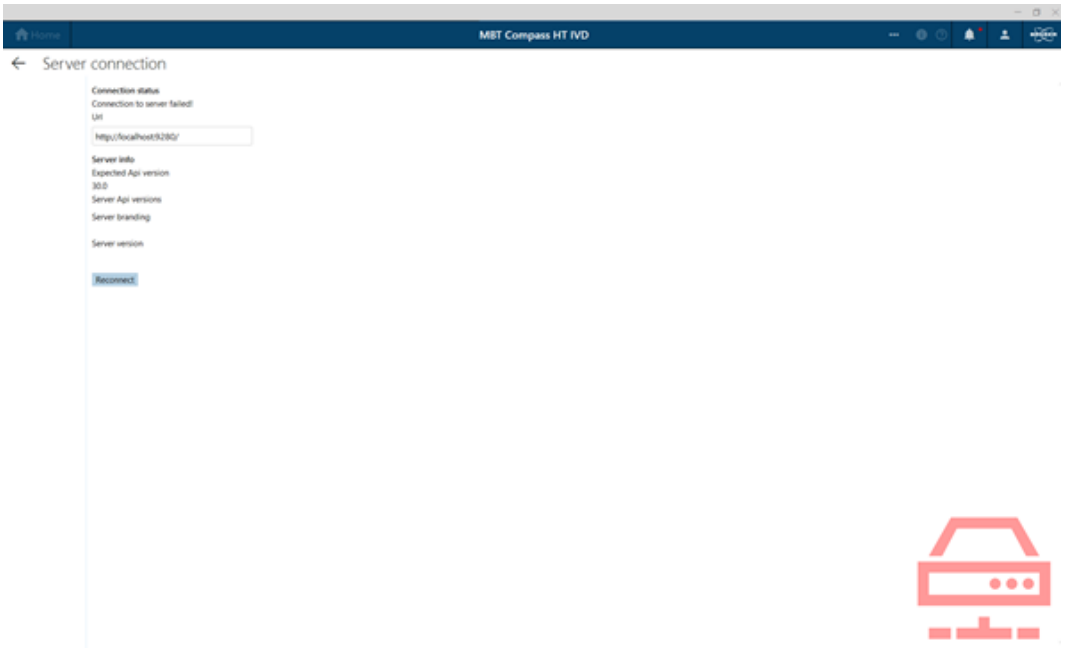

Figure 6-2 Select different server after connection failure. The shown versions might differ.

3. After successful startup, the MBT Compass HT IVD Home view is displayed, see figure 6-3.

   It is the starting point for all MBT Compass HT IVD identification workflows.

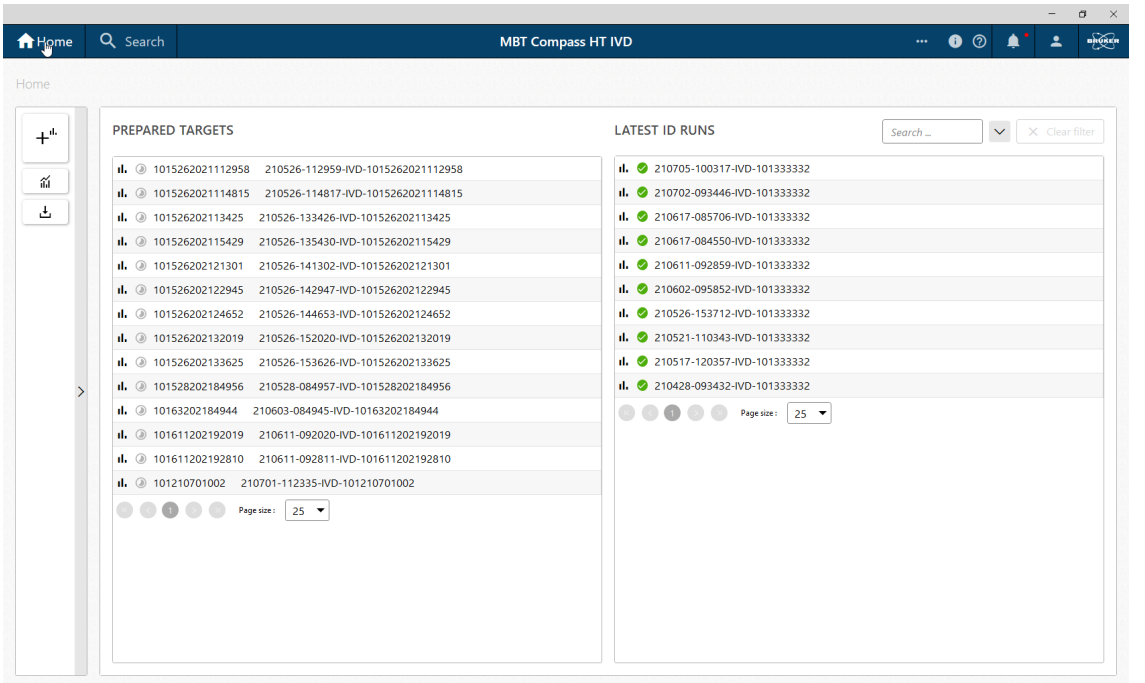

Figure 6-3 MBT Compass HT IVD Home view

6.2 MBT Compass HT IVD Home view

The MBT Compass HT IVD **Home view** contains the following main control elements:

- A ribbon bar (permanently visible on all views) with the following buttons:
  - **Home**
  - **Search**
  - **Show more** — when clicked, a popup window opens with the following options:
    - **Configuration**
    - **Maintenance**
    - **Server connection** status
    - **Instrument connection** status
  - **Show about**
  - **Show help**

- **Message(s)** — the icon contains a red dot in case a message is available
- Information about the user and its roles

- The view bar area containing the name of the view (and a left arrow if not on the MBT Compass HT IVD **Home view** to go to the previous view)
- The function area on the left side with action buttons to
  - **Create a new ID run**
  - **Display statistics**
  - **Import run**

  Note *The number of buttons may vary depending on further licensed MBT software modules.*

- **PREPARED TARGETS** — a list of prepared MALDI targets plates.
- **LATEST ID RUNS** — a list of recent identification runs.

6.2.1 MBT Compass HT IVD online help

Online support is provided for MBT Compass HT IVD. Help can be launched directly from the MBT Compass HT IVD computer interface by clicking the **Show help** button in the ribbon bar.

6.2.2 PREPARED TARGETS list

The **PREPARED TARGETS** list in the MBT Compass HT IVD **Home view** displays a chronological list of prepared runs in the order that they were submitted, with the oldest pending measurement at the top. This order reflects the order in which the MALDI target plates should be measured. By default, the 25 oldest prepared targets are displayed. It is possible to jump to further pages so that all prepared targets can be viewed.

Each preparation is represented by a single line starting with a spectrum symbol , followed by the run state symbol and the MALDI target plate serial number (target identifier) the **Run Name**, see figure 6-4. The first three digits of the target identifier indicate the type of MALDI target plate, see 3.5.

The **Run Name** always contains a timestamp from when the run was created in the format YYMMDD-hhmmss followed by IVD and the target identifier. For example, a run with the **Run Name** `201006-1549-101333332` was created on 6 October 2020 at 15:49 using the MALDI target plate with the serial number 101333332.

Figure 6-4 PREPARED TARGETS list of pending runs

Moving the mouse pointer over an entry in the **PREPARED TARGETS** list displays the following options:

- **Open this run** — opens the run in the MBT Compass HT IVD **Run view** where measurement can be started by clicking **Start acquisition**.
- **Edit this run** — opens the run in the MBT Compass HT IVD **Run editor** where the run can be modified and where the measurement can be started by clicking **Start acquisition**. This option is not available if the run was already started and aborted in the past.
- **Show run info** — displays a small popup with some information about the run like who created it when.
- **Create target layout** — creates a PDF document showing the MALDI target plate layout with the appropriate sample identifiers at the prepared positions.
- **Show run log** — shows a popup window with information about the evolution of the run.
- **Hide this run**— removes the run from the list.

CAUTION Care must be taken by the end user to define a procedure which prevents incorrect sample placement and identification during this process.

6.2.3 LATEST ID RUNS list

The **LATEST ID RUNS** list in the MBT Compass HT IVD **Home view** displays a list of measured identification runs in reverse chronological order with the most recent measurement at the top, see figure 6-5.

The **LATEST ID RUNS** list gives an overview of the (by default) 25 most recent runs. It is possible to jump to further pages so that all runs can be viewed.

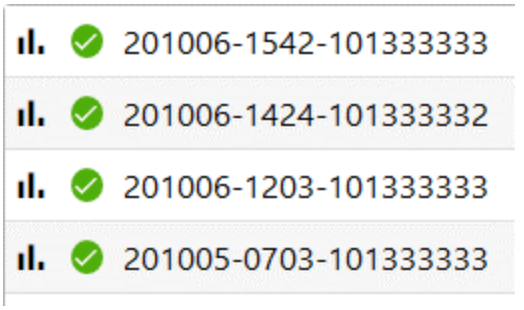

Figure 6-5 LATEST ID RUNS list of measured identification runs

The color of the symbols indicates the progress of the relevant procedure, see table 6-1.

Table 6-1 Identification run progress indicators

Symbol	Color	Status
	Green	Complete
	Red	Aborted
	Gray	Not started
	Yellow	In progress

Moving the mouse pointer over an entry in the **LATEST ID RUNS** list displays the following options:

- **Open this run** — opens the run in the MBT Compass HT IVD **Run view** where an interrupted measurement can be resumed, results can be exported to a laboratory information management system (LIMS), or reports can be generated.
- **Show run info** — displays a small popup with some information about the run like who created it when.
- **Show run log** — shows a popup window with information about the evolution of the run.
- **Hide this run** — hides the run from the list.

6.3 Creating an identification run

1. On the MBT Compass HT IVD **Home view**, press the **Create a new ID run** button +. The **Create new run** view is displayed, see figure 6-6.
2. Scan the MALDI target plate serial number (target identifier) into the **Target identifier** entry field of the **Create new run** view using a CCD barcode scanner*. The barcode on the MALDI target plate consists of a ten-digit number: the first three digits indicate the MALDI target plate type and the last seven digits constitute a unique serial number.

   Alternatively, type the unique ten-digit MALDI target plate identifier into the **Target identifier** entry field and press the Enter key.

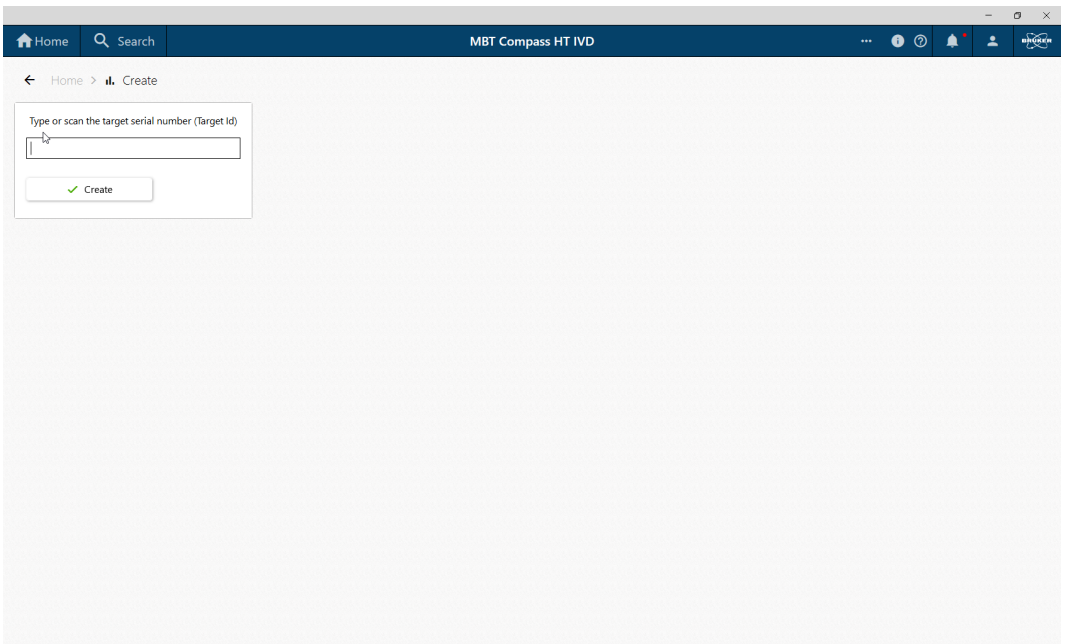

Figure 6-6 Create new run view

3. After the MALDI target plate identifier has been entered, the **Run editor** will open, see figure 6-7.

Scan barcodes using the Hand-held CCD scanner [P/N: 8268821]. Other CCD barcode scanners may be able to read the barcode, but Bruker does not guarantee that all CCD scanners are compatible with Bruker MALDI target plates. Laser barcode scanners cannot be used to read the barcode on MALDI target plates.

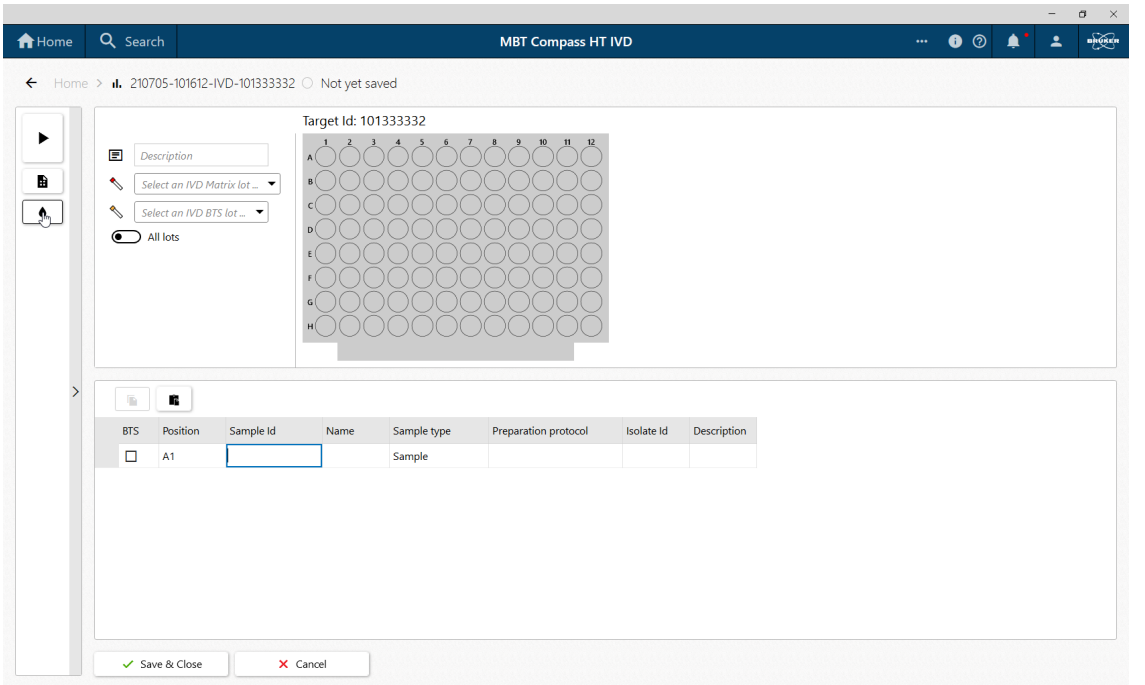

Figure 6-7 MBT Compass HT IVD Run editor

CAUTION Care must be taken by the end user to define a procedure which prevents incorrect sample placement and identification during this process.

4. Complete the run definition by typing a description of the identification run in the **Description** field, see figure 6-7.

   An entry in the **Description** field (indicated by the symbol) is optional but recommended.

   The **Run Name** visible in the view header is generated automatically.

   The **Run Name** always contains a timestamp from when the run was created in the format YYMMDD-hhmmss followed by IVD and the target identifier. It is possible to customize the string added to the **Run Name** after the date. Contact Bruker for more information.

   An optional IVD Matrix lot and an IVD BTS lot can be selected. These lots are defined under **Maintenance > Consumables registration**.

When the lots are selected, either all lots  or only unexpired lots  can be shown using the toggle button.

5. Select the sample and **BTS QC** positions on the MALDI target plate that will be used in the run (that is, all positions where either samples or IVD BTS were or will be applied).

   a. Highlight MALDI target plate positions by:

      - Dragging a rectangle around the positions
      - Selecting individual positions (press Ctrl to select multiple positions)

   Selected positions will be surrounded by a light-blue circle, see figure 6-8.

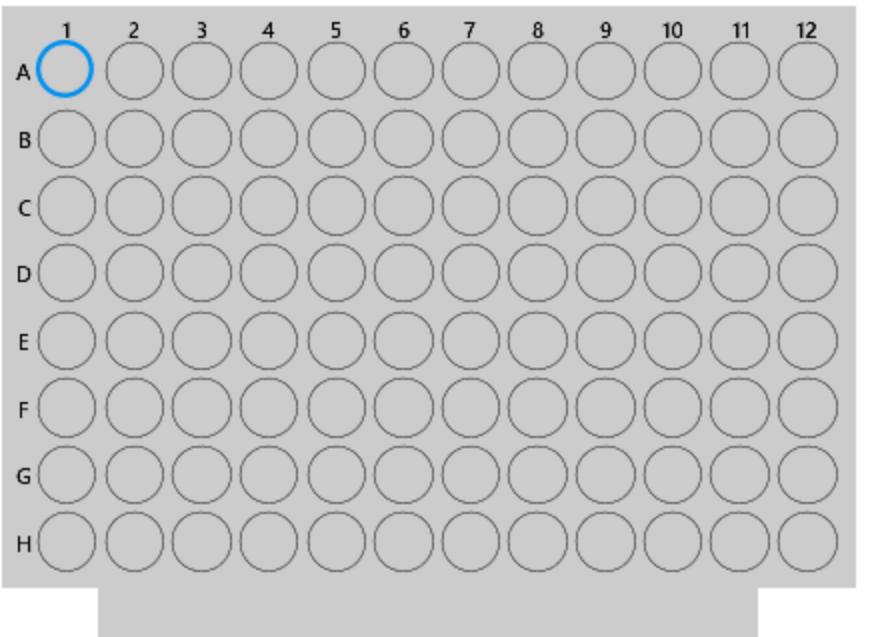

Figure 6-8 Position A1 is selected

6. Activate the selected sample and **BTS QC** positions on the MALDI target plate that will be used for the run (that is, all positions where either samples or IVD BTS were or will be applied).

   a. Activate selected MALDI target plate positions by:

      - Pressing the Insert key
      - Right-clicking the MALDI target plate display and selecting **Add**

      Active positions are displayed in yellow and added to the sample list below the MALDI target plate display, see figure 6-9. Positions used for previous runs are displayed in gray, see figure 6-10.

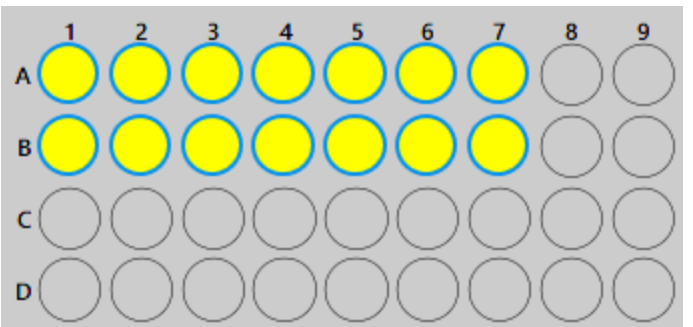

Figure 6-9 Active MALDI target plate positions

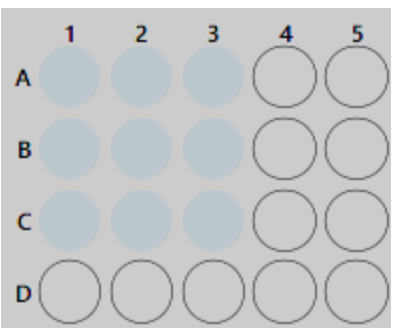

Figure 6-10 MALDI target plate positions used for previous runs

7. Assign active positions as sample positions or **BTS QC** positions, see sections 6.3.1 and 6.3.2.

MBT Compass HT IVD keeps track of which positions on a given MALDI target plate have been used for previous runs. These positions are unavailable (colored gray) when a new run is defined for the MALDI target plate, see figure 6-10. If a reusable MALDI target plate has been cleaned since its last use, click **Reset target** to make previously processed positions available and reset the start position to A1.

6.3.1 Assigning sample positions

Assign sample positions by scanning sample position identifier using a CCD barcode scanner*. Active sample positions will be defined from left to right and from top to bottom (for example, for a 48-spot MALDI target plate A1 to A8, B1 to B8, and so on).

Alternatively, type a valid sample identifier (sometimes called a sample accession number) into the **Sample identifier** column and an optional description into the **Description** column of the sample.

Note

- *After an active sample position has been assigned , press the Enter key to proceed to the next available sample position (sequential insert mode).*
- *To change the assignment of a sample position, click in the relevant cell of the sample list and make the necessary changes.*
- *All assigned positions must contain a valid identifier before the run can proceed.*

6.3.2 Assigning BTS Quality Control positions

After all sample positions have been assigned, at least one **BTS QC** position must be assigned.

Clicking **Save & Close** or **Start acquisition** before a **BTS QC** position has been assigned will generate a warning message **Assign BTS QC position to proceed.**

1. Type an optional name and description into the **Name** and **Description** columns of the **BTS QC** sample row.

Scan barcodes using the Hand-held CCD scanner (8268821, Bruker). Other CCD barcode scanners may be able to read the barcode, but Bruker does not guarantee that all CCD scanners are compatible with Bruker MALDI target plates. Laser barcode scanners cannot be used to read the barcode on MALDI target plates.

2. Select the **BTS** check box in the sample rows that correspond to the **BTS QC** position(s) where IVD BTS was spotted onto the MALDI target plate.

   The **Sample identifier** will be automatically changed to **BTS**.

   Alternatively, a **BTS QC** position can be assigned by typing the string "**BTS**" into the **Sample identifier** column of the appropriate row.

3. Click **Save & Close** to complete creation of the identification run

   or

   click **Start acquisition** to save the run and start data acquisition.

CAUTION Before starting acquisition, double check that the target identifier of the target inserted into the IVD MALDI Biotyper instrument and the target identifier of the run are identical. Using a wrong target or run will cause wrong results and patient harm.

Note *If the measurement has not yet started, existing sample positions or BTS QC definitions can be changed and new positions can be added by selecting the **Edit this run** option in the **PREPARED TARGETS** list of the MBT Compass HT IVD Home view.*

6.3.3 Changing or adding positions to an identification run

To change sample or **BTS QC** position assignments, select the **Edit this run** option in the **PREPARED TARGETS** list of the MBT Compass HT IVD Home view and make the necessary changes or additions.

Note *Changes can be made to existing sample or **BTS QC** position assignments as long as the **BTS QC** is not passed.*

6.3.4 Reviewing identification run status

Identification runs are saved in the MBT Compass HT IVD database and can be accessed at any time before, during, or after a run.

►► To review identification run status

Go to the MBT Compass HT IVD Home view.

- Runs where data acquisition has not started or was aborted will be listed under **PREPARED TARGETS**.
- Runs where data acquisition is in progress or is complete will be listed under **LATEST ID RUNS**, see figure 6-11.
  - The symbol to the left of the run name indicates the status of the run measurement and export, see figure 6-11. The visibility of the export symbol depends on your configuration.
  - The color of the circle indicates the progress of the relevant procedure, see 6.1.
  - To view the identification run results in the MBT Compass HT IVD Run view, select the relevant run and click **Open this run** .
  - The **LATEST ID RUNS** list gives an overview of all runs.

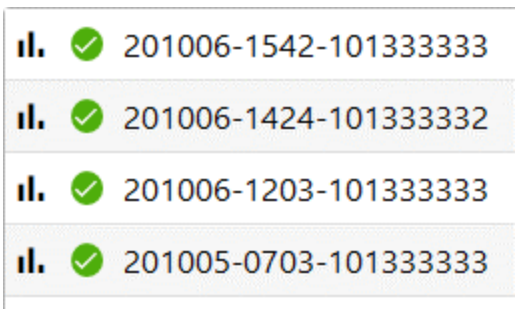

Figure 6-11 LATEST ID RUNS list (most recent on top)

6.4 Starting acquisition

Changes can be made to existing sample or **BTS QC** position assignments as long as the BTS QC is not passed, see section 6.3.3.

To start measurement of the MALDI target plate, EITHER:

- Click **Start acquisition** in the MBT Compass HT IVD Run editor

  OR

- Select the run in the **PREPARED TARGETS** list, select the **Open this run** option ( ), and click **Start acquisition** the MBT Compass HT IVD Run view.

CAUTION Before starting acquisition, double check that the target identifier of the target inserted into the IVD MALDI Biotyper instrument and the target identifier of the run are identical. Using a wrong target or run will cause wrong results and patient harm.

The measurement will start with a BTS QC on the first **BTS QC** position defined in the sample list.

The status and progress of the BTS QC are displayed in the right part of the MBT Compass HT IVD Acquisition view, see figure 6-12.

The first step in the BTS QC is an automatic calibration. After this is completed, the BTS QC will proceed with a validation step.

During the BTS QC validation step, eight BTS spectra are measured with fixed laser settings. The progress of these measurements is indicated by the **QC Status** progress bar.

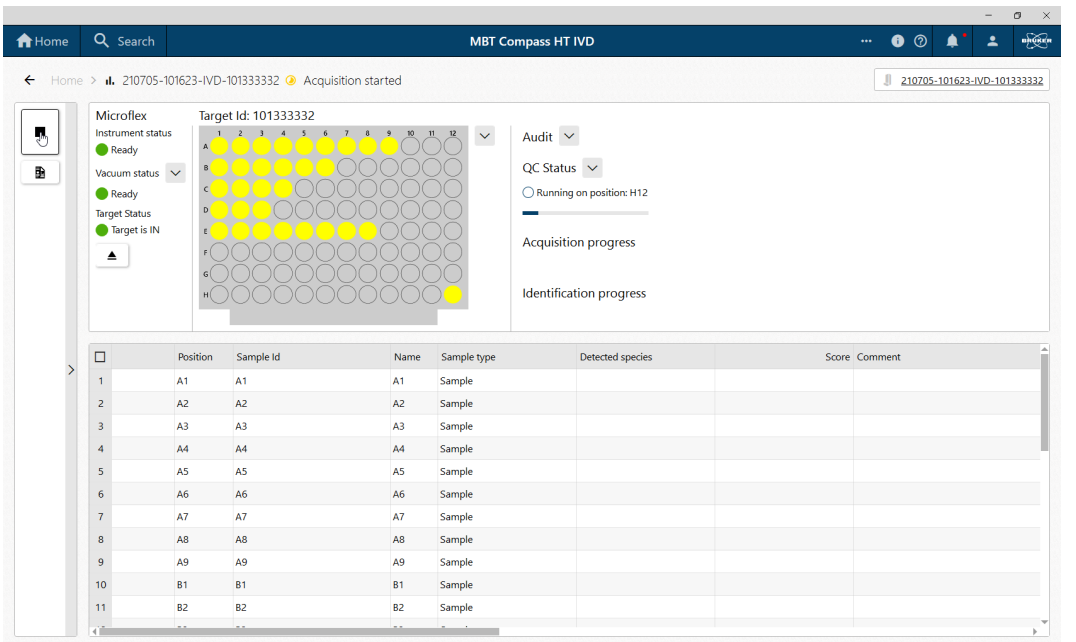

Figure 6-12 Progress of the BTS QC

After the BTS QC of a **BTS QC** position is successfully completed, sample positions are measured. The **Acquisition progress** bar represents the number of measured positions and the **Identification progress** bar represents the number of identified sample positions, see figure 6-13.

If the BTS QC fails, the identification of sample positions will not proceed.

- Repeat the run using the same MALDI target plate used for initial identification and a new (unused) **BTS QC** position for the run.
- Add a new **BTS QC** position to the plate layout by selecting **Edit this run** in the **PREPARED TARGETS** list of the MBT Compass HT IVD Home view.
- If the BTS QC using a second **BTS QC** position fails, repeat the run. If the BTS QC fails again, contact Bruker Technical Support.

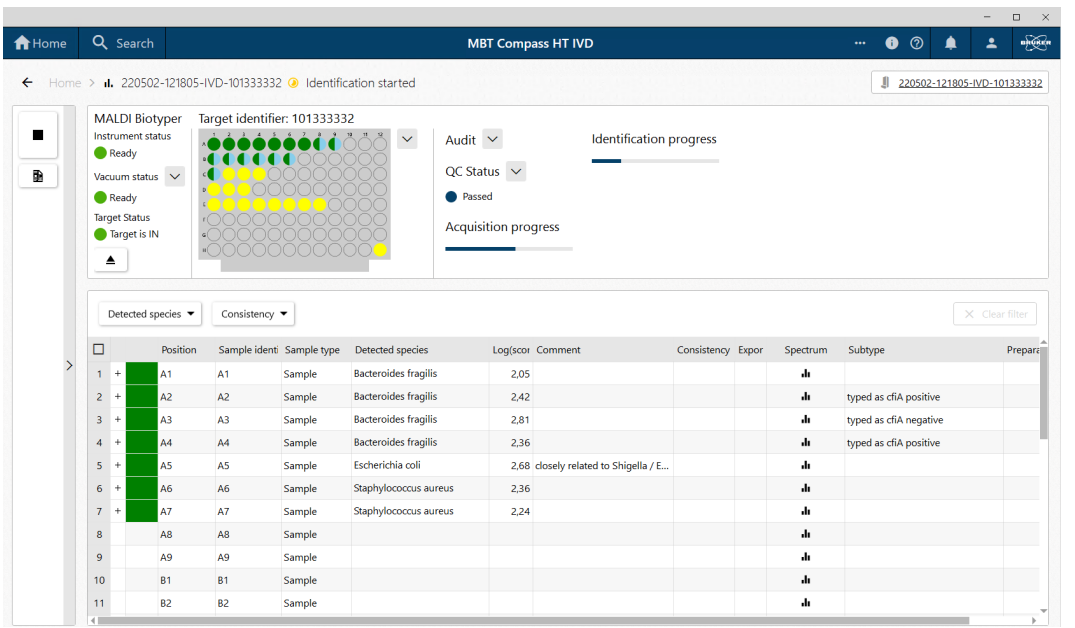

Figure 6-13 Measurement status

6.5 Monitoring acquisition of an identification run

MBT Compass HT IVD processing consists of two steps, which are performed on each sample and BTS QC position:

- A mass spectrum is acquired from the sample or **BTS QC** position (measurement step).
- The resulting mass spectrum is processed, and the resulting peak pattern is matched against reference patterns in the MBT Compass HT IVD Library (identification step).

The identification step is started immediately after the associated measurement step has been completed and a mass spectrum is available.

When the identification run is started, the MALDI target plate positions to be measured appear as yellow circles in the MALDI target plate display, see figure 6-14.

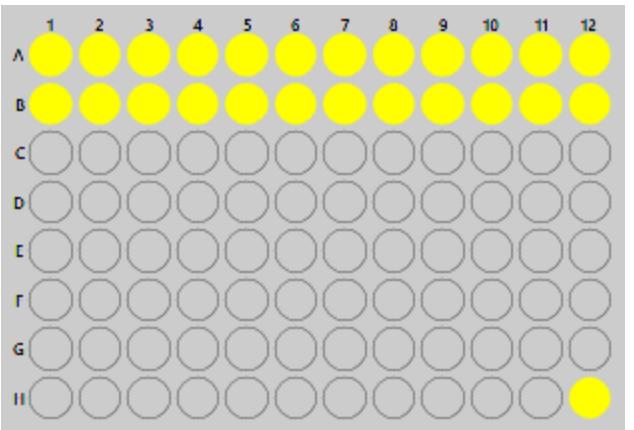

Figure 6-14 MALDI target plate positions to be measured appear as yellow circles in the MALDI target plate display

During the run, the appearance of the sample and **BTS QC** positions in the MALDI target plate display reflects the success of the measurement and identification process at each position.

If spectrum measurement is successfully completed, the left half of the sample position is colored green. If measurement fails, the left half of the sample position is colored orange, see figure 6-15.

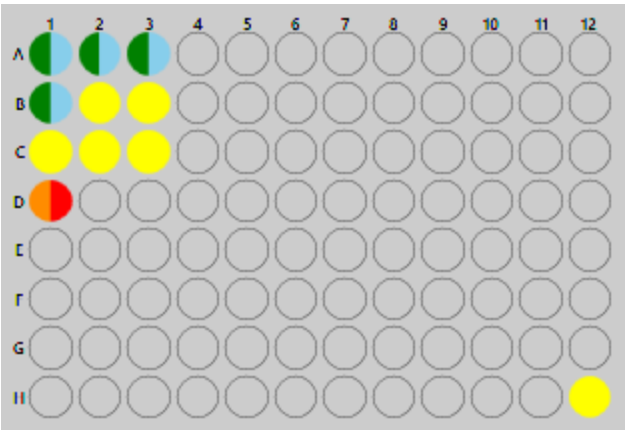

Figure 6-15 Identification run in progress

The coloring of the right half of the sample position indicates the score value of the identification, see section 6.7.1.7. The legend display explains the color-coding used to indicate the status of sample positions in the MALDI target plate display.

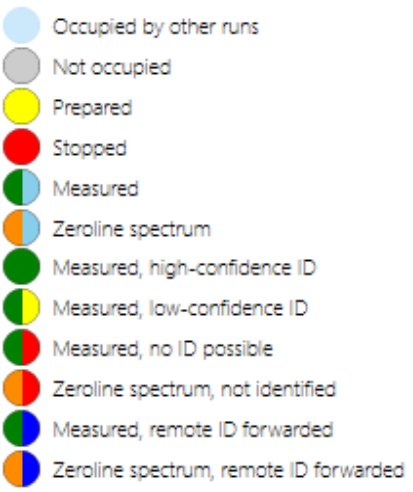

Figure 6-16 Color-coding used to indicate the status of sample positions in the MALDI target plate display

Tip *Point to the drop-down triangle ⌄ next to the top-right corner of the MALDI target plate display in the MBT Compass HT IVD Run view to show the color-coding legend, see figure 6-17.*

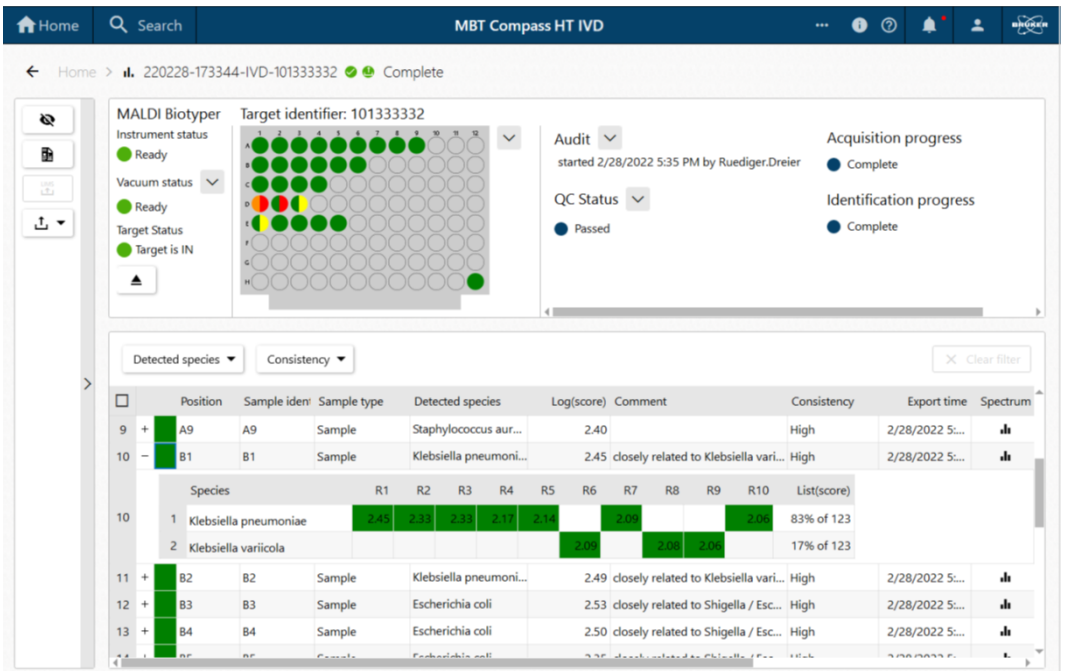

Figure 6-17 Completed run

When the identification of a sample position is completed, the respective identification result is entered in the sample table.

The sample table of the MBT Compass HT IVD Run view gives a real-time overview of the identification results for the active run. This table shows the best-matching reference pattern for each sample position and is a summary of the complete Result Report.

Each row (except those for lines with "no peaks found") shows a + sign at the beginning of the row. Clicking on this + sign will insert an additional small table between this row and the next row. This table shows the ten best matches grouped by species, their log (score) and their ratio of the list(score) compared to the sum of list(score) of this sample.

The list(score) is calculated as follows: the log(score) is multiplied by a weighting factor - the best match has the factor 10, the second best the factor 9 and the 10th match has the factor 1. The calculation uses the internal representation of the log(score), not the rounded value shown, so a best match with log(score) 2.50 might have a value of 24.96. The sum of all these values for a species is the list(score) of the species [the "species list(score)"].

The GUI displays the list(score) in the form "p% of n" where n is the sum of list(score) values for this sample [the "sample list(score)"] and p is the ratio of the list(score) of the species compared to the sum of list(score) values for the sample. Both values are rounded to no decimal values, therefore the sum of the percentage values might not be 100.
For red results, list(score) values are not calculated/displayed. Each log(score) value in the table has a tool-tip with more information about the match.

Tip *If a column in the sample table is too narrow to display all its content, move the mouse pointer over the relevant cell to show the content in a tooltip.*

A PDF result report can be generated at any time by clicking **Show run report**.

When measurement and identification of all sample positions has been completed, the additional information area in the right part of the MBT Compass HT IVD Acquisition view will show *Complete* for the **Acquisition progress** and **Identification progress**.

Clicking on the drop-down triangle ⌄ next to **QC Status** in the upper middle of the MBT Compass HT IVD Run view opens a window that displays information about the eight spectra acquired as quality check including their spectrum.

6.6 Stopping acquisition of an identification run

An identification run can be stopped manually by clicking **Stop acquisition** ▪. The run will be stopped without notification.

Measurement can be resumed by clicking **Start acquisition** ▸.

Before measurement continues, the IVD MALDI Biotyper will perform a check on the first **BTS QC** position defined in the sample list, see section 6.3.2.

An aborted identification run can be finalized by clicking **Finalize this run** ⊘. A finalized run is shown in the **LATEST ID RUNS** list and it is not possible to continue acquisition and/or identification of this run.

Although an Uninterruptible Power Supply (UPS) is recommended as part of the MBT Compass HT IVD, an identification run may be unintentionally interrupted, for example, because of a long-term power outage in the laboratory.

Note

- *Stopping an identification run stops the measurement of sample positions and the identification of measured sample positions. After stopping an identification run, the remaining unmeasured positions will be colored red in the MALDI target plate display, the unidentified positions are colored as unidentified positions (usually left side green, right side light blue).*
- *Finalizing an aborted identification run marks all unmeasured positions yellow and moves the run from the **PREPARED TARGETS** list to the **LATEST ID RUNS** list.*
- *Unmeasured or incompletely measured runs can be hidden from the Home view.*
- *If an unintended or unexpected interruption of MBT Compass HT IVD occurs, reopen the identification run and restart measurement, see section 6.4.*

6.7 Generating a report

After the acquisition of the MALDI target plate has been completed, click **Show run report**  to generate a PDF report.

6.7.1 Structure of the report

See Appendix D for a sample report.

A Result Report consists of the following sections:

- Header and footer
- **Report Info**
- **Run Info**
- **Result Overview**
- Detailed Results
- **Matching Hints**
- **Meaning of Consistency Categories (A–C)**
- **Meaning of Score Values**

6.7.1.1 Header and footer

The report header and footer contain the following information: **Run Identifier** and **Run Creation Date/Time** (header), Report **Creation Date/Time**, Project Type, page x of y (footer).

6.7.1.2 Report Info

The **Report Info** section appears directly below the report header and contains the following information:

Category	Comment
Created by	Name of the user who created the report
Creation Date/Time	Date and time of the creation of the report
Tests coverage	Number of sample positions in the report and total number of sample positions in the identification run

6.7.1.3 Run Info

The **Run Info** section appears directly below the **Report Info** section and contains the following information:

Category	Comment
Run Identifier	Name of the identification run
Comment	Description of the identification run (if specified)
Created by	Name of the creator of the identification run
Run Creation Date/Time	Identification run creation timestamp
Number of Tests	Number of sample positions in this report of the identification run
BTS QC	Result of **BTS QC** quality control (`passed` or `failed`)
BTS QC Position	Position where the **BTS QC** quality control was performed
Instrument Identifier	Instrument on which the run was done
Server Version	Build information of the MBT Compass HT IVD Server
BTS / Matrix Lot Numbers	Lots of BTS and HCCA used for preparation of the target

6.7.1.4 Result overview table

The **Result overview table** lists the best match found for each sample and contains the following columns:

Column	Comment
Sample identifier	Identifier of the sample in the **Sample identifier** column of the Run editor
Target Pos.	Target position of the sample
Organism (best match)	Organism whose reference pattern has the highest score value. A hyperlinked entry indicates that a matching hint is available for this identification, see section 6.7.1.6.
log(score) **(Conf.)**	log(score) value of the best match. Confidence value of the best match.
Organism (second best match)	Organism whose reference pattern has the second highest score value. A hyperlinked entry indicates that a matching hint is available for this identification , see section 6.7.1.6.
log(score) **(Conf.)**	log(score) value of the second-best match. Confidence value of the second-best match.

The color coding, score value ranges, and scoring symbols used in the **Result Overview** are explained in the **Meaning of Score Values** section, see section 6.7.1.8.

6.7.1.5 Detailed Results

For each Sample identifier, meta information (like Sample Name, methods used, library used) and the ten best matches (and the list(score) as in the GUI) are displayed.

6.7.1.6 Matching Hints

Matching hints provide additional information that may be useful to achieve a greater level of confidence in an identification.

Matching hints consist of two parts, the matched reference pattern name and a corresponding comment.

The **Matching Hints** table contains the following columns:

Column	Comment
Matched Species	Name of matched reference pattern (complete strain designation).
Comment	Comment available for this reference pattern (matching hint).

6.7.1.7 Meaning of Consistency Categories (A–C)

The **Meaning of Consistency Categories (A–C)** section provides the corresponding interpretation for the letter in parentheses (A, B, or C) in the **Consistency** column of the **Result Overview**. The consistency category is based on the confidence level of the best and second-best matches.

Table 6-2 Identification consistency category descriptions

Results table consistency category	Results report consistency category	Description
High	A	The best match is a high- confidence identification. The second-best match is: • a high-confidence identification in which the species is identical to the best match • a low-confidence identification in which the genus is identical to the best match • a non-identification

Results table consistency category	Results report consistency category	Description
Low	B	The requirements for high consistency are not met. The best match is a high- or low-confidence identification. The second-best match is: • a high- or low-confidence identification in which the genus is identical to the best match • a non-identification
None	C	The requirements for high or low consistency are not met.

IMPORTANT Results with a consistency category of B (= low consistency) or C (= none) must be reviewed carefully by a trained clinical microbiologist.

Table 6-3 Consistency category table

Best match	Example	Second-best match	Example	Consistency category
High-confidence ID: Genus A, Species A	*Escherichia coli*	High-confidence ID: Genus A, Species A	*Escherichia coli*	High-consistency = A
High-confidence ID: Genus A, Species A	*Escherichia coli*	High-confidence ID: Genus A, Species B	*Escherichia fergusonii*	Low-consistency = B

Best match	Example	Second-best match	Example	Consistency category
High-confidence ID: Genus A, Species A	*Escherichia coli*	High-confidence ID: Genus B, Species B	*Gardnerella vaginalis*	None = C
High-confidence ID: Genus A, Species A	*Escherichia coli*	Low-confidence ID: Genus A, Species A	*Escherichia coli*	High-consistency = A
High-confidence ID: Genus A, Species A	*Escherichia coli*	Low-confidence ID: Genus A, Species B	*Escherichia fergusonii*	High-consistency = A
High-confidence ID: Genus A, Species A	*Escherichia coli*	Low-confidence ID: Genus B, Species B	*Gardnerella vaginalis*	None = C
High-confidence ID: Genus A, Species A	*Escherichia coli*	No identification		High-consistency = A
Low-confidence ID: Genus A, Species A	*Escherichia coli*	Low-confidence ID: Genus A, Species A	*Escherichia coli*	Low-consistency B
Low-confidence ID: Genus A, Species A	*Escherichia coli*	Low-confidence ID: Genus A, Species B	*Escherichia fergusonii*	Low-consistency = B

Best match	Example	Second-best match	Example	Consistency category
Low-confidence ID: Genus A, Species A	*Escherichia coli*	Low-confidence ID: Genus B, Species B	*Gardnerella vaginalis*	None = C
Low-confidence ID: Genus A, Species A	*Escherichia coli*	No identification		Low-consistency = B
No identification		No identification		None = C

6.7.1.8 Meaning of log(score) Values

The **Meaning of log(score) Values** section explains the meaning of the color codes and log(score) ranges used in the **Result Overview**. log(score) value ranges and interpretations are listed for each type of sample tested (for example, **Standard Sample** or **Sepsityper Sample**).

6.8 Viewing and exporting results

Identification results are displayed in the results table. The results table contains the following elements.

Note *Further columns might be displayed depending on the installed/licensed modules.*

6.8.1 Checkbox for report selection

Checkbox to select if a Sample identifier should be part of a report or not. If no Sample identifier is checked, all entries of the results table are reported, otherwise only the selected ones are reported.

6.8.2 log(score) indicator

A colored box indicates the confidence level of the detected species identification.

Indicator	Color	Symbols	Interpretation
	Green	(+++)	High confidence species identification
	Yellow	(+)	Low confidence species identification
	Red	(-)	No organism identification possible

6.8.3 Position, Sample identifier, Name, Sample type

Information about the sample as entered in the Run editor during creation of the identification run.

6.8.4 Detected species

Organism whose reference pattern has the highest log(score).

6.8.5 Comment

Additional information that may be useful to achieve a greater level of confidence in an identification. The same information is provided in the **Matching Hints** section of the results report.

6.8.6 Consistency

This additional information may be useful to achieve a greater overall level of confidence in the identification.

Different from the confidence classification (green, yellow, red) which is done for a single MSP match of the unknown spectrum (according to an appropriate lookup table), the consistency classification takes the N best MSP matches into account (N = 2 for MBT-Compass). It indicates whether these N best matching MSPs have a consistent name pattern, like showing the same species names (high consistency) or the same genus names (low consistency) or none of these (no consistency).

Exemplary combinations of results that generate each consistency category are listed in section 6.7.1.7.

The determined consistency is only displayed, you cannot change it.

6.8.7 Export Time

If the information for a Sample identifier was exported, this field shows the date/time when this export was done.

6.8.8 Spectrum

Contains a spectrum symbol. Double-clicking on this symbol opens a popup window that displays the mass spectrum of the Sample identifier that was used for identification, see figure 6-18.

In this spectrum window, the spectrum is displayed as intensity (y-axis)/mass (x-axis) graph. Moving the mouse over the spectrum displays the exact values (x/y) at the mouse position. Marking a range in the spectrum zooms into this range. Double-clicking into the zoomed spectrum resets zooming to show the full spectrum. Clicking the X symbol (top right) closes the popup window.

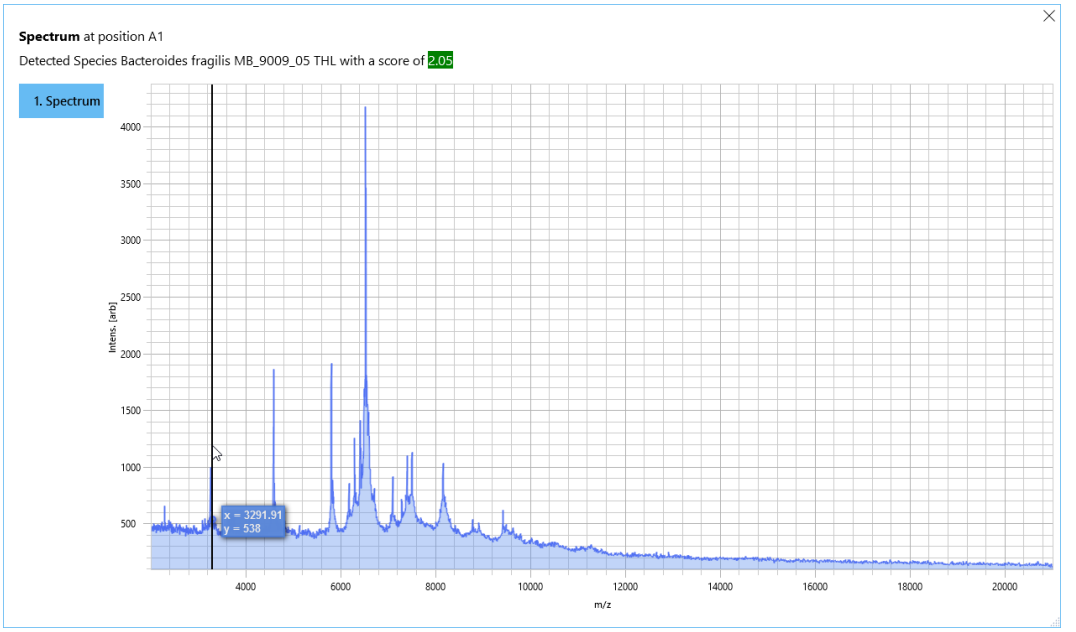

Figure 6-18 Spectrum window

6.8.9 Score

log(score) value of the identification.

6.8.10 Preparation Protocol

Contains the preparation protocol if it was entered in the Run editor during creation of the identification run.

6.8.11 Isolate identifier

The isolate identifier as it was entered in the Run editor during creation of the identification run.

6.8.12 Description

Description entered into the Run editor during creation of the identification run.

6.8.13 Exporting results

By default, result export is disabled.

Results can be exported for external processing (for example, in a laboratory management system = LIMS).

Note *For IVD systems, the LIMS integration must be validated after activation and configuration. Bruker can usually assist you in validating your system. Contact the Bruker Service Department for more information.*

Once LIMS export has been enabled under **Configuration > Exports**, results are exported automatically after every run.

You can select results for reexport by selecting the check boxes in the first column of the result table and clicking the **LIMS export** button LIMS .

6.8.14 Filtering results

The sample table contains a functionality to filter by detected species and consistency level.

For filtering, click on the buttons above the table to show a selection of entries.

The **Detected species** drop down box Detected species contains a list of all detected species in that run (so the content might vary from run to run). By clicking on one of the species, the content of the result table is limited to those Sample identifiers where the best match is the selected species.

The **Consistency** drop down box Consistency contains the consistency levels “High”, “Low”, “No”. By clicking on one of them, the result table is limited to those Sample identifiers where the consistency is high, low, or no organism identification is possible.

To clear all filters, click on the **Clear filter** button × Clear filter above the result table on the right side.

7 Evaluating IVD MALDI Biotyper results

Despite extreme diligence, an incorrect result in analytic tests can never be completely excluded. Therefore, the final results must be assessed by a professional experienced in clinical microbiology. Where the identification results do not correlate with additional sample or patient information (for example, sample origin or medical history), then another identification method — such as Gram staining, colony morphology, or growth characteristics — should be considered to secure an accurate identification.

7.1 Definition of false positive and false negative identifications

False positive identifications

A false positive identification is generated if the patient sample contains no microorganisms but the IVD MALDI Biotyper identifies an organism in the sample. This may lead to unnecessary additional testing that may delay appropriate treatment.

IMPORTANT Because a prerequisite for IVD MALDI Biotyper analysis is a microbial colony cultured from a patient sample, in principle, it is impossible to obtain a false positive result using the IVD MALDI Biotyper.

False negative identifications

A false negative identification is generated if the patient sample contains microorganisms but the IVD MALDI Biotyper does not identify any organisms in the sample. This may lead to unnecessary additional testing that may delay appropriate treatment.

IMPORTANT In principle, it is impossible to obtain a false negative result using the IVD MALDI Biotyper. In samples where microorganisms are present, IVD MALDI Biotyper analysis always delivers an identification or the result **No identification possible**. It should be noted that this result does not represent an unequivocal identification of the microorganism, and in cases where the confidence level falls below the high-confidence threshold, different microbiological methods must be used for identification.

7.2 Possible causes of incorrect identification results

Incorrect identifications using the IVD MALDI Biotyper — where the organism identified is not that present in the sample — cannot be completely ruled out. Such results may lead to inappropriate treatment of the patient and side effects that may adversely affect the patient's health.

The main risk factors for an incorrect identification are cross- contamination and transposition of samples. In addition, a microorganism that is not contained in the IVD MALDI Biotyper reference library but is closely related to a microorganism that is contained in the IVD MALDI Biotyper reference library, could possibly be falsely identified as this closely related microorganism.

To minimize the risk of an incorrect identification, we strongly recommend taking the following precautions:

- **To avoid cross-contamination of samples:**
  - Make sure that reusable MALDI target plates are cleaned and tested or checked before use, see Appendix A.
  - Make sure that disposable MALDI target plates are checked before use, see Appendix A.
  - Make sure that the surface of the MALDI target plate is not damaged during preparation, and do not touch the upper surface of a prepared MALDI target plate.
  - Use a new pipette tip for application of each sample and for matrix application on different samples, and make sure that samples do not bleed into neighboring MALDI target plate positions.

- **To avoid transposition of samples:**
  - Make sure all sample containers are clearly labeled before and after cultivation and during processing.
  - Do not confuse samples during application to the MALDI target plate (when using a robot, this procedure must be validated by the customer).
  - Do not confuse samples when assigning samples to sample positions in an identification run. This can lead to dislocation between the sample and the result. This step is highly dependent on local personnel, data organization, and peripheral hardware and software (for example, barcode label printers). It is the customer's responsibility to assure the accuracy and correctness of sample assignment.
  - Do not mix up MALDI target plates.

Incorrect identifications cannot be retrospectively detected on the basis of measurement results. Therefore, meticulous sample preparation is essential to avoid incorrect identifications.

7.3 Possible causes of ambiguous identification results

Ambiguous identifications are results in which several, different organisms are identified with high confidence in a single sample.

The main risk factors for an ambiguous identification are errors during sample preparation.

To minimize the risk of an ambiguous identification, we strongly recommend taking the following precautions:

- Do not test samples directly obtained from liquid cultures.
- Make sure that the sample tested derives from a taxonomically pure, single colony.
- Use a new pipette tip for application of each sample and for matrix application on different samples.
- Make sure that the recommended conditions are used for sample culture growth and storage. Growth or storage of cultures under inappropriate conditions may lead to changes in mass spectra.

- Measure the MALDI target plate as quickly as possible after preparation. Prepared MALDI target plates must be measured within 24 hours of preparation. If more than 24 hours have elapsed since preparation, the sample preparation procedure must be repeated on unused positions or on a new MALDI target plate. In case of reusable MALDI target plates, repeat the sample preparation procedure on a cleaned MALDI target plate.

Ambiguous identifications may also be obtained due to the similarity of reference patterns between different species or strains of a single species.

The IVD MALDI Biotyper provides additional information to aid interpretation of ambiguous results.

Consistency category

Each identification result is assigned a consistency category (A = high, B = low, or C = none) that reflects the overall level of confidence in the identification result, see table 6-2.

Matching hints

Matching hints provide additional information that may be useful to achieve a greater level of confidence in an identification, see section 6.7.1.6.

7.4 Possible causes of a delayed or lost identification, or no identification

Delayed identifications using the IVD MALDI Biotyper are results that are not obtained directly after measurement.

Lost identifications are results that are generated but not delivered to the user.

No identification is obtained if the log(score) of the sample falls below the low-confidence identification threshold.

The consequences of delayed or lost identifications or no identification can be a late or no diagnosis. Such results may lead to late or no treatment, which may adversely affect the patient's health.

The main risk factors for delayed or lost identifications or no identification are errors during sample preparation or the use of reagents, materials, or instruments other than those specified.

To minimize the risk of delayed or lost identifications or no identification, we strongly recommend taking the following precautions:

- Make sure that you apply an appropriate amount of biological material to the MALDI target plate and that you follow the sample preparation procedures rigorously.
- Make sure that you use the correct reagents, that the reagents have the required purity, and that all solutions are prepared as described in the relevant procedure.
- Avoid contamination of the sample with polymers by using the specified plastic consumables.
- Make sure that your MALDI target plates are suitable for use with the IVD MALDI Biotyper and are cleaned and tested or checked before use.
- Make sure that your mass spectrometer is suitable for use with the IVD MALDI Biotyper, see section 1.
- Connect the mass spectrometer to an uninterruptible power supply (UPS) and back up your data regularly.
- Make sure that all connected peripherals are validated for use with the IVD MALDI Biotyper.

Delayed or lost identifications or no identification may also be caused by the following:

- Inefficient extraction of proteins from microorganisms with very rigid cell walls.
- Absence of the microorganism from the IVD MALDI Biotyper reference library.
- Use of the Bruker MALDI- TOF mass spectrometer outside of its analytical specifications.
- Technical failure of the Bruker MALDI-TOF mass spectrometer or the software. If a software or mass spectrometer error message appears, contact Bruker.

Results with a log(score) below the low-confidence threshold are listed in the results report as **No identification possible**. In this case, use an alternative IVD MALDI Biotyper sample preparation method or an alternative analysis method to obtain an identification.

A result of **No peaks found** indicates that no spectrum is available. Testing should be repeated, ensuring that sufficient material is deposited onto the MALDI target plate.

8 Troubleshooting MBT Compass HT IVD identification runs

Potential problems are listed according to their relevance.

Scenario A: Low log(score) values

Potential cause	Recommended action
Suboptimal sample preparation	Too little or too much material may have been used, see Figure A-1. Make sure that all required steps in the testing procedure were performed and none (for example, matrix addition) were accidentally omitted. The sample may have been contaminated with traces of polymers from plastic consumables. Make sure that materials used for IVD MALDI Biotyper procedures meet the criteria in section A.3. Incorrect reagents may have been used. Make sure that reagents used for IVD MALDI Biotyper procedures meet the criteria in section 3.5.
MALDI target plate was not cleaned or was cleaned incorrectly.	Reusable MALDI target plates should be cleaned before each use using one of the procedures in section A.6. Incorrect cleaning of a MALDI target plate may cause cross-contamination. If this is suspected, repeat the MALDI target plate cleaning procedure and sample preparation.
Sample not included in the reference library.	The sample may not be included in the reference library and therefore cannot be identified. See product insert for reference library information.
Unsuitable or stale reagents	Always use the highest quality reagents available. Where possible, use freshly prepared reagents. Do not use reagents that have passed their expiration date.
Unsuitable starting material	Make sure that sample material was correctly cultured, see section A.10.1.

Scenario B: Automatic measurement is interrupted

Potential cause	Recommended action
Power outage in the laboratory.	Contact Bruker for help with restarting the MS instrument and the computer and resuming the interrupted identification run and obtaining the remaining results.

Scenario C: The MALDI target plate display shows that the final sample position was measured but not classified.

Potential cause	Recommended action
The identification result message generated by the server is not displayed in the MBT Compass IVD Run editor.	No data is lost. The PDF report will contain the positions missing in the MALDI target plate display. Reload the identification run or use the **Report** function to generate a report.

8.1 Error messages

Error message: Error! Please call service!

Cause 1: Every unexpected internal error causes the display of this error message.

Recommended action: Contact Bruker.

Cause 2: The identification run may have been started without a MALDI target plate loaded in the mass spectrometer.

Recommended action: Click **OK**, insert and load the MALDI target plate, and restart the identification run.

Error message: Connection to flexControl failed, make sure flexControl has been started.

Cause: While starting MBT Compass IVD the connection to the flexControl software could not be made. In most cases, this is due to a problem with the initial software installation process.

Recommended action: Contact Bruker.

Error message: Error!

Cause: An unexpected event occurred.

Recommended action: Repeat the last command and/or action.

If the message persists, restart MBT Compass HT IVD and repeat the last command and/or action.

If the message persists, restart the computer and MBT Compass HT IVD. Repeat the last command and/or action.

If this message still persists, contact Bruker.

Error message: Initializing MBT Compass HT IVD failed!

Cause: MBT Compass HT IVD could not be started.

Recommended action: Contact Bruker.

Error message: QC on position <X> failed!

Cause: Spectra quality from the prepared IVD Bacterial Test Standard spot was insufficient.

Recommended action: Make sure that IVD BTS was prepared at the selected **BTS QC** position. Repeat the measurement by reloading and restarting the identification run (this helps if the MALDI target plate **BTS QC** position was overloaded).

If this message persists, contact Bruker.

In the event of any of the following:

- The error message "**Error! Please call service.**" is displayed.
- An error not covered in the preceding table occurs.

contact Bruker, see Manufacturer section.

9 Administration

The following sections describe the views for configuration and maintenance. Note that not every view is visible or editable for every user – this depends on the roles of the logged-in user. See Appendix C for details who can see/modify which setting.

9.1 Configuration

9.1.1 Views

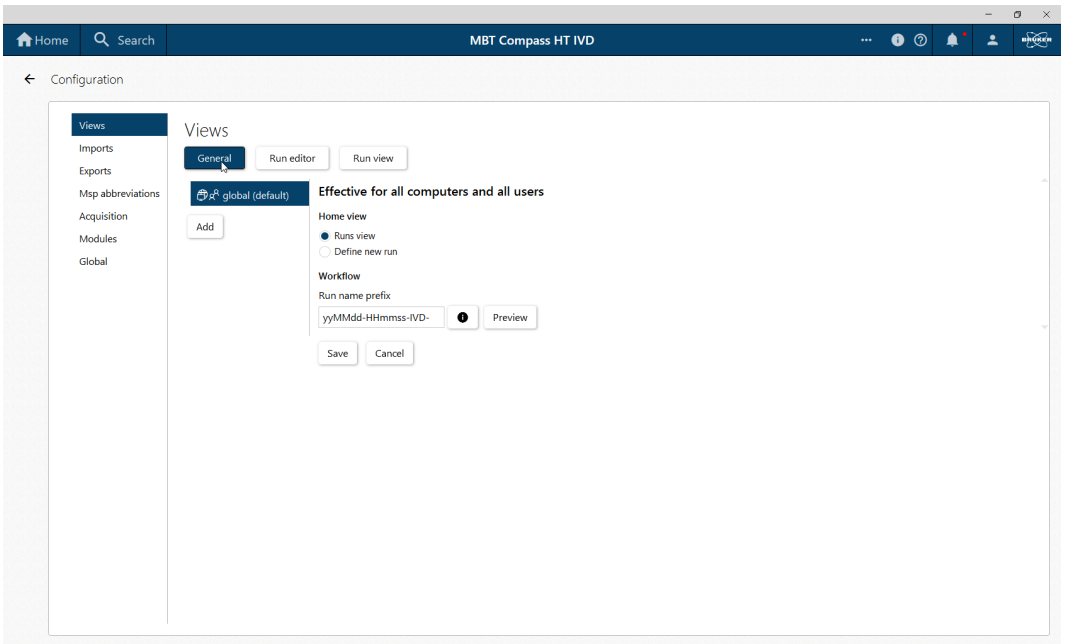

Figure 9-1 Views configuration settings

In the **General** tab of the **Views** configuration, see figure 9-1, you can define:

- if you want to have the usual Home view or only the possibility to define new runs
- the name prefix for run names

In the **Run editor** tab, you can define:

- the column separator for pasting CSV files to the editor
- if you want to be able to select the preparation protocol
- which sample types should be available in the Run editor

In the **Run view** tab, you can select which columns are visible in the Run view.

9.1.2 Imports

- On the **LIMS** tab, you can activate and configure LIMS integration of MBT Compass HT IVD. Contact Bruker support for details and support.
- On the **CSV** tab, you can activate and configure CSV import. Imported runs are displayed in the **Create new run** view and can be selected there.

9.1.3 Exports

Here you can configure automatic exports of runs, e.g. into CSV files.

9.1.4 Msp abbreviations

Here you can define/configure MSP aliases to make sure that the names used/exported by MBT Compass HT IVD conform to those used in your LIMS system.

9.1.5 Acquisition

Here you can view and configure acquisition related parameters. For MBT Compass HT IVD, most settings are fixed (e.g. quality check settings). You can define a folder for automatic spectrum export and activate/deactivate it.

9.1.6 Modules

In this view, you can see and uninstall your installed modules and install additional modules.

9.1.7 Global

- In the **Appearance** tab, you can activate dark mode (background uses a dark color while text is bright) or classic mode (bright background and dark text). You can also activate ColorADD® to make sure that people having problems to distinguish red/yellow/green can identify the colors used for result encoding.
- In the **Region & language** tab, you can select the language used for the GUI and report of MBT Compass HT IVD and the date and number format.
- In the **Licenses** tab is a link to open the website of your locally running WIBU Codemeter service.

9.2 Maintenance

9.2.1 E-Log book

In this view, you can look at the manual and system log book entries (incl. filtering and searching) and add manual entries.

9.2.2 Consumables registration

In this view, you can register your BTS and matrix lots (serial number and expiration date). These consumables can then be selected when creating a new run.

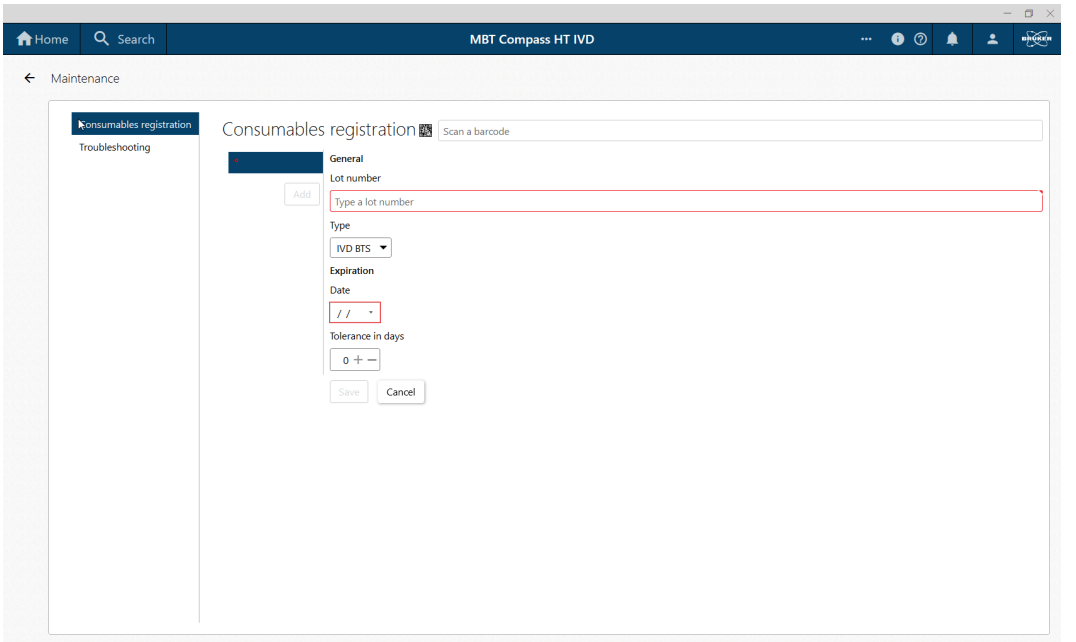

Figure 9-2 Consumables registration settings

9.2.3 Runs administration

In this view, you can administrate your runs:

- **Archive**: displays all runs that can be archived (or that are archived when you activate the **Archived** toggle). Select one or multiple runs and click on the **Archive** button at the bottom (only visible when at least one entry is selected). The run is then archived to the folder entered in the **Archive folder** field.
- **Hide**: displays all runs that can be hidden from the lists in the Home view. Select one or multiple and click the **Hide** button.
- **Unhide**: displays all runs that were hidden before. Select one or more and click **Unhide** to show them again in the lists in the Home view.
- **Unlock**: as soon as someone starts editing a run, it is internally locked to avoid parallel modifications. When the edit session ends, the lock is removed. If, for any reason like crashes, the lock state of a run persists, you can use this list to remove it manually.

- **Cleanup**: displays a list with all archived runs. Select one or multiple and click **Delete** to remove the run(s) permanently from the database.
- **Restore**: displays a list with all deleted runs (see above). You can restore them by using the archived copy of it.

9.2.4 Troubleshooting

- **Create status report...** creates a file with several log files (client+server) that can be used in communication with Bruker software support.
- **Enable service access** activates a special service account for 24 hours. When activated, a count down timer is displayed and you can immediately disable the account again.

10 Symbols

The following symbols are used in the labeling:

	Catalog number
	CE mark
	*In vitro* diagnostic medical device
	Manufacturer
	Batch code
	Consult User Manual
	Biological risks
	Highly flammable chemicals
	Corrosive chemicals
	Harmful chemicals

11 Glossary

A

Active (MALDI target plate) position
MALDI target plate position selected for sample data entry. Indicated by a light-blue circle in the MALDI target plate display of the MBT Compass HT IVD Run editor.

Assigned sample position
MALDI target plate position with associated sample data. Indicated by a yellow circle in the MALDI target plate display of the MBT Compass HT IVD Run editor.

B

BDAL
Bruker Daltonics

BTS quality control (BTS QC) position
Positions on a MALDI target plate where BTS is spotted for instrument calibration and validation.

F

flexControl
The software that controls and runs the mass spectrometer and facilitates data acquisition.

Fume hood
A device used to safely extract chemical fumes from the laboratory, for example, through an exhaust or by absorption using charcoal filters. NOTE: Not to be confused with a laminar air bench used for cell culture techniques. These devices only remove particles, they do not remove reagents.

H

HCCA
See α-cyano-4-hydroxycinnamic acid.

I

Identification
The process of comparing the peak pattern of an unknown spectrum with all (or a subset of) reference patterns in the MALDI Biotyper database. Depending on the log(score) of the best match(es), the identification is deemed to be successful or unsuccessful.

Identification results
Results of an identification run in tabular form.

Identification run
The container for all data related to the identification of samples on a MALDI target plate measured in one batch.

IVD Bacterial Test Standard (IVD BTS)
A preparation of bacterial proteins used to calibrate and validate the IVD MALDI Biotyper system.

L

Library
Reference entries of microorganism protein mass signatures in a database-like structure.

LIMS
Laboratory Information Management System

LIS
Laboratory Information System (synonym of LIMS)

log(score) value
A biostatistical parameter that reflects the reliability of the match between the sample pattern and a reference pattern. The higher the log(score), the better the match.

M

MALDI
The acronym for Matrix Assisted Laser Desorption/Ionization.

MALDI Biotyper Reference Library
Collection of reference spectra against which sample spectra are compared to find the best match.

MALDI target plate
Sample carrier used for MALDI Biotyper procedures, usually in the form of a steel plate.

Matching hint
Additional information that may be useful to achieve a greater level of confidence in an identification.

Matrix (MALDI matrix)
A reagent that absorbs UV light and transfers protons to other molecules. Essential in MALDI-TOF mass spectrometry.

MBT
MALDI Biotyper

MBT Compass HT IVD Software
Software used to define, acquire, and review IVD MALDI Biotyper identification runs.

MBT preprocessing method
Set of parameters used for creating a peak list from a (calibrated) raw spectrum.

MBT Satellite IVD Module
Used for efficient paperless setup of IVD MALDI Biotyper projects.

MSP
Main spectrum (reference pattern used in the MBT pattern matching approach)

MSP identification method
A set of parameters used to match the peak list (of an unknown spectrum) against a reference pattern from the pattern repository (library).

P

Polymer signals
Traces of polymers leached from plastic disposables. Visible as a characteristic pattern of numerous repeating peaks separated by small, equal distances in the x-axis (m/z-range).

R

Realtime identification
Combined sample measurement and identification.

Run editor
Page in MBT Compass HT IVD software used to enter and display sample data and position, start measurement, view results, and generate reports.

S

Sample
Organism to be analyzed (defined, measured, and classified) in the IVD MALDI Biotyper identification run.

Sample position
MALDI target plate position with associated analyte data. Indicated by a white circle in the target display. Geometric position containing sample to be analyzed. Location of sample on a MALDI target plate, for example, A1, B5, etc.

Selected (MALDI target plate) position
MALDI target plate position selected for sample or BTS placement in the MALDI target plate display of the MBT Compass HT IVD Run editor. Indicated by a blue square.

Spot
Dried sample or droplet of liquid applied to a MALDI target plate.

T

Target position
Geometric location on a MALDI target plate, for example, A1, B5.

A

α-Cyano-4-hydroxycinnamic acid (HCCA)
Matrix used for IVD MALDI Biotyper measurements.

Appendix A — Sample preparation

A.1 Warnings and cautions

WARNING — BIOLOGICAL RISKS: The IVD MALDI Biotyper system deals with potentially dangerous biological material. All patient samples and cultures should be handled as potentially infectious material.

WARNING — HIGHLY FLAMMABLE CHEMICALS: Some of the chemicals used in IVD MALDI Biotyper procedures are highly flammable. Read the relevant Material Safety Data Sheet(s) provided by the reagent supplier.

WARNING — CORROSIVE CHEMICALS: Some of the chemicals used in IVD MALDI Biotyper procedures are corrosive. Read the relevant Material Safety Data Sheet(s) provided by the reagent supplier.

WARNING — HARMFUL CHEMICALS: Some of the chemicals used in IVD MALDI Biotyper procedures are harmful. Read the relevant Material Safety Data Sheet(s) provided by the reagent supplier.

A.2 Precautions

We strongly recommend taking the following precautions during IVD MALDI Biotyper sample preparation and measurement:

- Bruker instruments are designed for use in laboratories designated as Biosafety Level 1 or Biosafety Level 2.
- When handling patient samples, microbial cultures, or chemicals, wear personal protective equipment (lab coats, safety glasses, and gloves) in accordance with the defined laboratory safety procedures. Work inside a fume hood if recommended by the reagent supplier.
- Use only the recommended chemicals and reagents and take special care not to contaminate reagents.
- Handle and dispose of biological material and waste chemicals in accordance with the defined laboratory safety procedures.
- Handle and decontaminate or dispose of all accessories and consumables in accordance with the defined laboratory procedures.
- When cleaning MALDI target plates, ensure adequate ventilation.
- Do not forcibly open mass spectrometer protective covers and never operate the mass spectrometer if the protective covers are not in place.

A.3 Reagents and chemicals

The following reagents and chemicals are required to perform the mass spectrometry measurement. For best results, use freshly prepared solutions and chemicals of the highest purity available (for example, CHROMASOLV LC-MS solvents).

- IVD Matrix HCCA-portioned (IVD HCCA, # 8290200, Bruker Daltonics GmbH & Co. KG) and IVD Bacterial Test Standard (IVD BTS, # 8290190, Bruker Daltonics GmbH & Co. KG)
- Standard solvent (Acetonitrile 50%, water 47.5% and trifluoroacetic acid 2.5%)[1].
- Acetonitrile

[1] *Standard solvent (Acetonitrile 50%, water 47.5% and trifluoroacetic acid 2.5%) from Sigma-Aldrich (Bruker standard solvent, 900666), Honeywell Riedel-de Haen (Acetonitrile 50%, Water 47.5% and Trifluoroacetic acid 2.5%, 19182), or VWR International (SOLUTION OS, # PRLS89449.230) which have been tested by Bruker Daltonics GmbH & Co. KG and are recommended for dissolution of IVD BTS and IVD HCCA.*

- HPLC-grade water
- Formic acid
- Absolute ethanol
- Trifluoroacetic acid
- Guanidine hydrochloride
- Culture media for microorganisms

Consumables

- Sample applicators (for example, inoculation loops or pipette tips)
- High-quality pipette tips 0.5–20 µL, 2–200 µL, 50–1000 µL
- Suitable pipettes for volumes from 1 µL to 1000 µL
- Eppendorf plastic tubes , 1.5 mL (Eppendorf AG[1])
- Eppendorf micropestles (Eppendorf AG[1])
- Screw-cap micro tubes and screw caps (Sarstedt[1])
- Plastic centrifuge tubes, 50 mL
- Paper towels

Standard laboratory equipment

- Bench-top microcentrifuge capable of 13,000 to 15,000 rpm
- Vortex mixer
- Beaker, 250 mL
- Glass dish or stainless steel basin of sufficient size for MALDI target plate cleaning
- Graduated cylinder, 100 mL

[1] *Recommended vendor. Other vendors may be used, but Bruker does not guarantee the suitability of consumables sourced from alternative vendors.*

A.4 Handling MALDI target plates

In IVD MALDI Biotyper procedures, reusable and disposable MALDI target plates are handled differently.

Reusable MALDI target plates

- Before each use, reusable MALDI target plates must be cleaned using one of the procedures in section A.6.
- Before its first use, each reusable MALDI target plate must be tested using the procedure in section A.8.1.
- If deep scratches develop on the surface of a reusable MALDI target plate, it must be tested using the procedure in section A.8.2.

Disposable MALDI target plates

- Before use, disposable MALDI target plates must be checked using one of the procedures in section A.9.

A.5 Tracking MALDI target plates

To avoid cross-contamination, it is very important not to mix up cleaned MALDI target plates with MALDI target plates that have not been properly cleaned. We strongly recommend that laboratories use a tracking system based on MALDI target plate serial numbers.

The barcode on the MALDI target plate consists of a ten-digit number: the first three digits indicate the MALDI target plate type and the last seven digits constitute a unique serial number.

For MALDI target plates without a barcode, the first five digits indicate the MALDI target plate type and the last five digits constitute a unique serial number.

A.6 Cleaning and storing reusable MALDI target plates

Ideally, reusable MALDI target plates should be cleaned before each use. In practice, unused positions on a MALDI target plate that has already been measured can generally be used for subsequent analyses without cleaning the MALDI target plate beforehand. However, if all positions on a MALDI target plate have been used, the MALDI target plate must be cleaned before being used again.

Either of the following procedures can be used for cleaning the surface of reusable MALDI target plates:

- **Trifluoroacetic acid procedure**, which uses 80% aqueous trifluoroacetic acid to clean the surface of the MALDI target plate.

WARNING — CORROSIVE CHEMICALS: The trifluoroacetic acid procedure uses highly corrosive chemicals and requires access to a fume hood.

- **Guanidine hydrochloride procedure**, which uses 4 M guanidine hydrochloride to clean the surface of the MALDI target plate.

Both procedures eliminate memory effects from the MALDI target plate surface.

IMPORTANT The cleaning procedures described here are valid for the reusable MALDI target plates listed in section 3.5. No other reusable MALDI target plates or cleaning procedures may be used.

Note

- Always wear chemical protective gloves when preparing cleaning solutions or cleaning MALDI target plates.
- Do not soak reusable MALDI target plates in any organic solvent for longer than 20 minutes.
- It is the customer's responsibility to choose the MALDI target plate cleaning procedure appropriate for their laboratory.

The solutions required for cleaning reusable MALDI target plates must be prepared as follows:

►► Preparation of 70% aqueous ethanol (100 mL)

1. Measure 30 mL of HPLC-grade water into a graduated 100 mL cylinder.
2. Transfer the contents of the cylinder into a beaker.
3. Add 70 mL absolute ethanol to the contents of the beaker.

   Use a graduated 100 mL cylinder to measure the volume.

4. Mix by transferring the ethanol solution from the beaker into the graduated cylinder and back again five times.

   The solution is ready for use.

►► Preparation of 80% aqueous trifluoroacetic acid (1 mL)

1. Transfer 200 µL of HPLC-grade water into a 1.5 mL Eppendorf plastic tube.
2. Carefully add 800 µL 100% trifluoroacetic acid.
3. Close the tube tightly.
4. Mix by inverting the tube five times.

   The solution is ready for use.

►► Preparation of 4 M aqueous guanidine hydrochloride (30 mL)

Best results are obtained using freshly prepared 4 M guanidine hydrochloride solutions.

1. Weigh 11.5 g guanidine hydrochloride into a 50 mL graduated tube.
2. Add 30 mL HPLC-grade water and shake the tube until the guanidine hydrochloride is completely dissolved.

   The solution is ready for use.

►► Reusable MALDI target plate cleaning procedures

See section B.1.1.

A.7 Storing cleaned MALDI target plates

Store cleaned MALDI target plates in a dry place at room temperature in the supplied container. Avoid exposing cleaned MALDI target plates to potential sources of contamination (for example, dust) or corrosive atmospheres.

After cleaning, do not touch the upper surface of the MALDI target plate.

Note *Do not place any adhesive labels on the MALDI target plate. Do not drop or scratch the MALDI target plate.*

A.8 Testing reusable MALDI target plates

Before its first use, each reusable MALDI target plate must be tested using the procedure in section A.8.1.

If deep scratches develop on the surface of a reusable MALDI target plate, it must be tested using the procedure in section A.8.2.

Required reagents

- Dissolved IVD Bacterial Test Standard (IVD BTS, # 8290190)[1]
- Dissolved IVD Matrix HCCA-portioned (IVD HCCA, # 8290200)[2]

[1] *Preparation must be performed as described in the latest Instructions for Use IVD Bacterial Test Standard.*
[2] *Preparation must be performed as described in the latest Instructions for Use IVD Matrix HCCA-portioned.*

A.8.1 Test procedure for new MALDI target plates

►► To test the suitability of new MALDI target plates for IVD MALDI Biotyper applications

1. Clean the MALDI target plate using one of the procedures in section B.1.1.
2. Deposit 1 µL IVD BTS solution onto five well-separated MALDI target plate positions and air-dry the spots at room temperature.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

3. Overlay each position with 1 µL IVD HCCA matrix solution.
4. Dry the spots at room temperature.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

5. Carefully inspect the MALDI target plate and make sure that spots are well-separated from each other and that none of the spots has bled into a neighboring position.
   - If all spots are well-separated from each other and none of the spots has bled into a neighboring position, the MALDI target plate is suitable for use in IVD MALDI Biotyper applications.
   - If a spot has bled into a neighboring position, repeat steps (1) to (5) of this procedure. If any spot bleeds into a neighboring position after repeating this procedure, the MALDI target plate is unsuitable for IVD MALDI Biotyper applications. Contact your local Bruker Service Department to arrange return of the MALDI target plate.

   Note *Before using it to identify samples, clean the MALDI target plate using one of the procedures in section B.1.1.*

Store cleaned MALDI target plates in the supplied container. Cleaned MALDI target plates can be stored before use in a dry place at room temperature. Avoid exposing cleaned MALDI target plates to potential sources of contamination (for example, dust) or corrosive atmospheres.

A.8.2 Test procedure for used MALDI target plates

Over time, MALDI target plates may develop scratches on their surface. Use the following procedure to test the suitability of used MALDI target plates for IVD MALDI Biotyper applications.

►► To test the suitability of used MALDI target plates for IVD MALDI Biotyper applications

1. Clean the MALDI target plate using one of the procedures in section B.1.1.
2. Deposit 1 µL IVD BTS solution onto MALDI target plate positions that are affected by scratches.
3. Carefully inspect the MALDI target plate and make sure that spots are well-separated from each other and that none of the spots has bled into a neighboring position.
   - If a spot has bled into a neighboring position, the MALDI target plate is unsuitable for IVD MALDI Biotyper applications and should be disposed of.
   - If all spots are well-separated from each other, proceed to step (4).
4. Air-dry the IVD BTS spots at room temperature and overlay each position with 1 µL IVD HCCA matrix solution.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

   To minimize solvent evaporation, make sure that the screw cap tube containing IVD HCCA is tightly closed after use.

CAUTION If IVD HCCA matrix solution is not added to samples within 30 minutes after they have dried, these positions cannot be tested.

5. Dry the spots at room temperature.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

6. Carefully inspect the MALDI target plate and make sure that spots are well-separated from each other and that none of the spots has bled into a neighboring position.
   - If a spot has bled into a neighboring position, the MALDI target plate is unsuitable for IVD MALDI Biotyper applications and should be disposed of.
   - If all spots are well-separated from each other, load the MALDI target plate into the mass spectrometer and measure the **BTS QC** positions. High-confidence *Escherichia coli* identifications with a log(score) ≥2.0 should be obtained.
   - If the expected high-confidence *Escherichia coli* identifications are not obtained, repeat steps (1)–(6) until high-confidence identifications are obtained.

A.9 Checking disposable MALDI target plates

IMPORTANT The checking procedure described here is valid for the disposable MALDI target plates listed in section 3.5. No other disposable MALDI target plates or checking procedures may be used.

►► To test the suitability of disposable MALDI target plates for IVD MALDI Biotyper applications

Before use, each disposable MALDI target plate must be checked using one of the following procedures.

A.9.1 New disposable MALDI target plates

- Remove the MALDI target plate from its packaging and inspect the upper surface for damage, such as deep scratches.
  - If no damage is apparent, the MALDI target plate can be used in IVD MALDI Biotyper applications.
  - If damage is apparent, contact Bruker.

A.9.2 Partially used disposable MALDI target plates

- Before each use, inspect the upper surface for damage, such as deep scratches.
  - If no damage is apparent, the MALDI target plate can be used in IVD MALDI Biotyper applications.
  - If damage is apparent, the remaining unused positions cannot be used and the MALDI target plate must be discarded.

A.10 General recommendations

Before starting

- Make sure that you have sufficient reagents (for example, dissolved matrix solution) and consumables (for example, pipette tips) at hand to be able to perform the sample preparation procedure without delay.
- Make sure that the MALDI target plate has been cleaned. If the MALDI target plate has not been cleaned, clean it using one of the procedures in section B.1.1.
- Check the surface of the MALDI target plate for severe scratches. If severe scratches are visible, check the suitability of the MALDI target plate using the procedure in section A.8.2.
- Make sure that the culture is suitable for IVD MALDI Biotyper testing. After incubation, culture plates can be stored for up to 12 hours at room temperature. If more than 12 hours have elapsed since the culture plate was removed from the incubator, subculture the microorganism before starting IVD MALDI Biotyper testing. Storing culture plates in a refrigerator will adversely affect the quality of spectra.

During preparation of MALDI target plates

CAUTION

- Smearing too little or too much biological material from an isolated colony onto the MALDI target plate may result in no final identification. The following figure shows examples of suitable and unsuitable amounts of Gram-negative bacteria. **Row B**: ideal amount of biological material (between 10^4 and 10^7 cells per sample position); **Row C**: small but nevertheless sufficient amount of biological material; **Row A**: too much biological material.

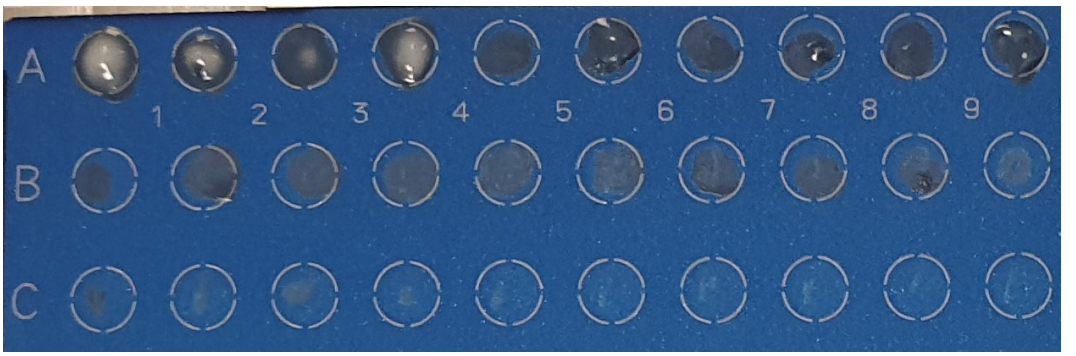

Figure A-1 Ideal (row B) and suboptimal (rows A and C) amounts of biological material on a MALDI target plate

- If IVD HCCA matrix solution is not added to samples within 30 minutes after they have dried, these positions cannot be tested.

After preparation of MALDI target plates

- Prepared MALDI target plates must be measured within 24 hours of preparation. If more than 24 hours have elapsed since preparation, the sample preparation procedure must be repeated on unused positions or on a new MALDI target plate. In case of reusable MALDI target plates, repeat the sample preparation procedure on a cleaned MALDI target plate.

A.10.1 Culturing samples

A.10.1.1 Culture media

The following isolation culture media have been tested for culturing samples to be identified using the IVD MALDI Biotyper:

- Columbia blood agar with 5% sheep blood
- Trypticase soy agar with 5% sheep blood
- Chocolate agar
- MacConkey agar
- Columbia CNA agar with 5% sheep blood
- Brucella agar with 5% horse blood
- CDC anaerobe agar with 5% sheep blood
- CDC anaerobe 5% sheep blood agar with phenylethyl alcohol
- CDC anaerobe laked sheep blood agar with kanamycin and vancomycin
- Bacteroides bile esculin agar with amikacin
- Clostridium difficile agar with 7% sheep blood
- Sabouraud-dextrose agar
- Brain-heart infusion agar
- Campylobacter agar with 5 antimicrobics and 10% sheep blood
- Bordet-Gengou (BG) agar with 15% sheep blood
- Buffered Charcoal Yeast Extract Agar (*Legionella* species)
- Buffered Charcoal Yeast Extract Selective Agar with polymyxin, anisomycin and vancomycin (*Nocardia* species)
- Modified Thayer-Martin Agar (*Neisseria* species)

A.10.1.2 Culturing bacteria

Generally, bacterial cultures should be incubated for 18–48 hours at 37°C ±2°C.

Species-specific culture conditions:

- *Bordetella*: Incubation on BG agar should not exceed 24 hours.
- *Campylobacter*: Incubation can be prolonged for up to 72 hours.
- *Streptococcus pneumoniae*: To prevent autolysis, incubation should not exceed 24 hours.
- *Neisseria*: Cultivation on Modified Thayer-Martin Agar (MTM) shall not be longer than 24 hours.
- *Nocardia*: Identification rate may decrease after incubation time >48h (+12h storage at room temperature).

After incubation, culture plates can be stored for up to 12 hours at room temperature. If more than 12 hours have elapsed since the culture plate was removed from the incubator, subculture the bacteria before starting IVD MALDI Biotyper testing.

A.10.1.3 Culturing yeasts

Yeast cultures should be incubated for 18–48 hours at 29°C ±2°C.

After incubation, culture plates can be stored for up to 12 hours at room temperature. If more than 12 hours have elapsed since the culture plate was removed from the incubator, subculture the yeasts before starting IVD MALDI Biotyper testing.

Appendix B — Sample preparation guide

This appendix contains the standard operating procedures for sample preparation in relation to the MBT Compass HT IVD workflow and may be printed for training purposes.

This appendix is part of the *MBT Compass HT IVD User Manual* and does not replace the *MBT Compass HT IVD User Manual*. The entire *MBT Compass HT IVD User Manual* must be read by every user.

B.1 Sample preparation

B.1.1 Reusable MALDI target plate cleaning procedures

Use either the trifluoroacetic acid or the guanidine hydrochloride procedure to clean reusable MALDI target plates. It is not necessary to perform both procedures sequentially.

(A) Trifluoroacetic acid procedure

1. Transfer the MALDI target plate into a suitable container (for example, a 100 mm diameter glass Petri dish) and cover the surface with 70% aqueous ethanol.
    - Alternatively, place the MALDI target plate on a stack of paper towels.
2. Incubate for five minutes at room temperature.
3. Remove the MALDI target plate and rinse it thoroughly under running tap water.
4. Using a paper towel, clean the MALDI target plate thoroughly with 70% aqueous ethanol.
5. Rinse the MALDI target plate with tap water and wipe it with a paper towel.
6. Transfer the MALDI target plate to a fume hood and using a pipette, deposit 100 (±10) µL 80% aqueous trifluoroacetic acid (prepared as described above) onto the MALDI target plate as a thin layer.
7. Thoroughly wipe all MALDI target plate positions with a paper towel. This step must be performed under a fume hood.
8. Rinse the MALDI target plate with HPLC-grade water and wipe it dry with a paper towel.
9. Air-dry the MALDI target plate for at least 15 minutes at room temperature.

   The MALDI target plate is ready for use. If the cleaned MALDI target plate will not be used immediately, store the cleaned MALDI target plate in the supplied container.

(B) Guanidine hydrochloride procedure

1. Transfer the MALDI target plate into a suitable container (for example, a 100 mm diameter glass Petri dish) and cover the surface with 70% aqueous ethanol.
    - Alternatively, place the MALDI target plate on a stack of paper towels.
2. Incubate for five minutes at room temperature.
3. Remove the MALDI target plate and rinse it thoroughly under running tap water.
4. Using a paper towel, clean the MALDI target plate thoroughly with 70% aqueous ethanol (prepared as described above).
5. Rinse the MALDI target plate with tap water and wipe it with a paper towel.
6. Cover the MALDI target plate with a layer of 4 M guanidine hydrochloride (prepared as described above) and incubate for 10 minutes at controlled room temperature.
7. Rinse the MALDI target plate with HPLC-grade water and wipe it dry with a paper towel.
8. Cover the MALDI target plate with a layer of 4 M guanidine hydrochloride and thoroughly wipe all MALDI target plate positions with a paper towel.
9. Rinse the MALDI target plate with HPLC-grade water and wipe it dry with a paper towel.
10. Repeat steps 8 and 9 twice.
11. Rinse the MALDI target plate with HPLC-grade water and wipe it dry with a paper towel.
12. Air-dry the MALDI target plate for at least 15 minutes at room temperature.

    The MALDI target plate is ready for use. If the cleaned MALDI target plate will not be used immediately, store the cleaned MALDI target plate in the supplied container.

B.2 Sample preparation procedures

B.2.1 Direct transfer sample preparation procedure

Required reagents

- Dissolved IVD Bacterial Test Standard (IVD BTS, # 8290190)[1]
- Dissolved IVD Matrix HCCA-portioned (IVD HCCA, # 8290200)[2]

►► Direct transfer sample preparation procedure

1. Deposit 1 µL of IVD BTS onto each of the assigned **BTS QC** positions and for each sample, smear an isolated colony as a thin film directly onto a sample position using a sample applicator.
2. Air-dry the spots at room temperature.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

3. Overlay each sample position and **BTS QC** position with 1 µL IVD HCCA matrix solution.

   Use a new sample applicator for each sample position to avoid cross-contamination.

   To minimize solvent evaporation, make sure that the screw cap tube containing matrix solution is tightly closed after use.

4. Air-dry the spots at room temperature.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

   Make sure that spots are well-separated from each other and that none of the spots has bled into a neighboring position.

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[1] *Preparation must be performed as described in the latest Instructions for Use IVD Bacterial Test Standard.*
[2] *Preparation must be performed as described in the latest Instructions for Use IVD Matrix HCCA-portioned.*

If bleeding occurs on a reusable MALDI target plate, the MALDI target plate must be cleaned carefully as described in section B.1.1 and the entire sample preparation must be repeated.

If bleeding occurs on a disposable MALDI target plate, the affected positions must be disregarded and sample preparation must be repeated on unused positions or a new disposable MALDI target plate must be used.

5. Load the MALDI target plate into the mass spectrometer.

CAUTION Before starting acquisition, double check that the target identifier of the target inserted into the IVD MALDI Biotyper instrument and the target identifier of the run are identical. Using a wrong target or run will cause wrong results and patient harm.

B.2.2 Extended direct transfer sample preparation procedure

If IVD MALDI Biotyper identification of the microorganism using the direct transfer sample preparation procedure does not result in a high-confidence identification with log (score) ≥2.0, testing can be repeated using the following extended direct transfer sample preparation procedure.

Alternatively, testing can be repeated using the extraction procedure in section B.2.3.

Required reagents

- Dissolved IVD Bacterial Test Standard (IVD BTS, # 8290190)[1]
- Dissolved IVD Matrix HCCA-portioned (IVD HCCA, # 8290200)[2]
- 70% formic acid
  - Transfer 300 µL of HPLC-grade water into a 1.5 mL Eppendorf tube. Carefully add 700 µL formic acid. Close the tube tightly and mix by inverting.

[1] *Preparation must be performed as described in the latest Instructions for Use IVD Bacterial Test Standard.*
[2] *Preparation must be performed as described in the latest Instructions for Use IVD Matrix HCCA-portioned.*

►► Extended direct transfer sample preparation procedure

1. Deposit 1 µL of IVD BTS onto each of the assigned **BTS QC** positions and for each sample, smear an isolated colony as a thin film directly onto a sample position using a sample applicator.
2. Air-dry the spots at room temperature.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

3. Overlay the sample position with 1 µL 70% formic acid.

   Note *Do not overlay BTS with formic acid!*

4. Air-dry the spots at room temperature.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

5. Overlay each sample position and **BTS QC** position with 1 µL IVD HCCA matrix solution.

   Use a new sample applicator for each sample position to avoid cross-contamination.

   To minimize solvent evaporation, make sure that the screw cap tube containing matrix solution is tightly closed after use.

6. Air-dry the spots at room temperature.

   Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

   Make sure that spots are well-separated from each other and that none of the spots has bled into a neighboring position.

If bleeding occurs on a reusable MALDI target plate, the MALDI target plate must be cleaned carefully as described in section B.1.1 and the entire sample preparation must be repeated.

If bleeding occurs on a disposable MALDI target plate, the affected positions must be disregarded and sample preparation must be repeated on unused positions or a new disposable MALDI target plate must be used.

7. Load the MALDI target plate into the mass spectrometer.

CAUTION Before starting acquisition, double check that the target identifier of the target inserted into the IVD MALDI Biotyper instrument and the target identifier of the run are identical. Using a wrong target or run will cause wrong results and patient harm.

B.2.3 Extraction sample preparation procedure

If a high- confidence identification with a log(score) ≥2.0 is not obtained for samples prepared using the direct transfer or extended direct transfer sample preparation procedure, testing can be repeated using the following extraction sample preparation procedure.

Required reagents

- Dissolved IVD Bacterial Test Standard (IVD BTS, 8290190)[1]
- Dissolved IVD Matrix HCCA-portioned (IVD HCCA, 8290200)[2]
- HPLC-grade water
- Absolute ethanol
- Acetonitrile
- 70% formic acid
  - Transfer 300 µL of HPLC-grade water into a 1.5 mL Eppendorf tube. Carefully add 700 µL formic acid. Close the tube tightly and mix by inverting.

[1] *Preparation must be performed as described in the latest Instructions for Use IVD Bacterial Test Standard.*
[2] *Preparation must be performed as described in the latest Instructions for Use IVD Matrix HCCA-portioned.*

►► Extraction sample preparation procedure

1. Transfer 300 µL of HPLC-grade water into an Eppendorf tube.
2. Using a 1 µL inoculation loop, transfer isolated colonies from the culture plate into the water and mix thoroughly until the material is completely in suspension.

   Alternatively, the recommended Eppendorf micropestle can be used to generate a homogenous suspension.

3. Add 900 µL pure ethanol and mix the suspension.
4. Spin down the microbial material in a bench-top centrifuge for two minutes at 13,000 –15,000 rpm.
5. Remove the supernatant using a pipette (avoiding contact with the microbial material).
6. Repeat step (4) and remove residual ethanol by pipetting (avoiding contact with the microbial material).
7. Air-dry the pellet for at least five minutes at room temperature.
8. Add 25 µL 70% aqueous formic acid and pipette the solution up and down until the pellet is resuspended.
9. Add 25 µL acetonitrile to the tube and mix by pipetting the solution up and down two or three times.
10. Centrifuge the tube for two minutes at 13,000 – 15,000 rpm.
11. Deposit 1 µL of the supernatant onto a vacant sample position of a MALDI target plate **and** deposit 1 µL of IVD BTS onto each of the assigned BTS QC positions. Use a new pipette tip for each sample position and each BTS QC position to avoid cross-contamination.

    Note *Sample extracts can be stored for up to 4 hours at room temperature before use. If more than 4 hours have elapsed since extraction, repeat the extraction procedure using fresh samples.*

12. Air-dry the MALDI target plate at room temperature.

    Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

13. Overlay each sample position and **BTS QC** position with 1 µL IVD HCCA matrix solution.

    Use a new pipette tip for each sample position to avoid cross-contamination.

    To minimize solvent evaporation, make sure that the screw cap tube containing matrix solution is tightly closed after use.

14. Air-dry the spots at room temperature.

    Note *As an alternative to drying at room temperature, you can accelerate the drying process at elevated temperature and under controlled conditions with the MBT FAST Shuttle IVD (# 1878263). For details, refer to the MBT FAST Shuttle IVD User Manual.*

    Make sure that spots are well-separated from each other and that none of the spots has bled into a neighboring position.

    If bleeding occurs on a reusable MALDI target plate, the MALDI target plate must be cleaned carefully as described in section B.1.1 and the entire sample preparation must be repeated.

    If bleeding occurs on a disposable MALDI target plate, the affected positions must be disregarded and sample preparation must be repeated on unused positions or a new disposable MALDI target plate must be used.

15. Load the MALDI target plate into the mass spectrometer.

CAUTION Before starting acquisition, double check that the target identifier of the target inserted into the IVD MALDI Biotyper instrument and the target identifier of the run are identical. Using a wrong target or run will cause wrong results and patient harm.

Appendix C — User management

MBT Compass HT IVD user management implements six user groups:

- The **Administrator** group is for users who perform specific administrative configurations (such as defining group/ user permissions).
- The **Laboratory Technician** group is for users who perform standard measurement tasks (such as defining and performing measurement using default settings).
- The **Laboratory Manager** group is for users who perform advanced measurement tasks (such as result export to a laboratory information management system).
- The **Data Administrator** group is for users who perform data administrative tasks (such as hiding, archiving, removing and restoring targets).
- The **Reviewer** group is for users who review the runs prepared and performed by other users.
- The **Approver** group is for users who approve the runs prepared and performed by other users.

C.1 Default mapping of MBT Compass HT IVD user roles to Windows groups

Table C-1 Default mapping of MBT Compass HT IVD user roles to Windows Groups

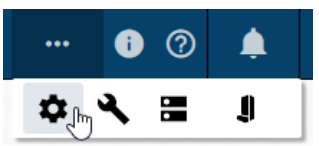
MBT Compass HT IVD user role	Windows user group
Administrator	BUILTIN\Administrators
Data Administrator	BUILTIN\Power Users
Laboratory Manager	BUILTIN\Power Users
Laboratory Technician	BUILTIN\Users
Reviewer	BUILTIN\Power Users
Approver	BUILTIN\Power Users

C.2 User group rights

User right	Lab Technician	Lab Manager	Data Admin	Admin	Service
Home view (options)					
Create a new run by providing/scanning a MALDI target identifier 	Yes	Yes	No	No	Yes
View the Statistics from Home view 	Yes	Yes	No	No	Yes
Import runs 	Yes	Yes	No	No	Yes
PREPARED TARGETS (list options)					
Open a prepared (unmeasured) run from Home view in Acquisition view 	Yes	Yes	No	No	Yes
Edit a run (preparation) that has not yet been measured 	Yes	Yes	No	No	Yes

User right	Lab Tech-nician	Lab Manager	Data Admin	Admin	Service
Hide prepared (unmeasured) runs from Home view 	Yes	Yes	No	No	Yes
Create a target layout of prepared (unmeasured) runs from Home view 	Yes	Yes	No	No	Yes
Show run info of prepared (unmeasured) runs from Home view 	Yes	Yes	No	No	Yes
Show run log of prepared (unmeasured) runs from Home view 	Yes	Yes	No	No	Yes
LATEST ID RUNS (list options)					
Open a completed (measured run) from Home view to view run results (this is the identical functionality like accessed via View Result Report) 	Yes	Yes	No	No	Yes

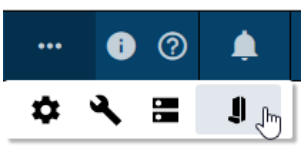
User right	Lab Tech-nician	Lab Manager	Data Admin	Admin	Service
Hide completed (measured) runs from Home view 	No	Yes	No	No	Yes
Show run info of completed (measured) runs from Home view 	Yes	Yes	No	No	Yes
Show run log of completed (measured) runs from Home view 	Yes	Yes	No	No	Yes
Run editor					
All controls	Yes	Yes	No	No	Yes
Acquisition view					
Start a measurement (acquisition) 	Yes	Yes	No	No	Yes
View a Result Report for the current identification run 	Yes	Yes	No	No	Yes

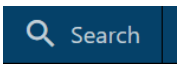
User right	Lab Tech-nician	Lab Manager	Data Admin	Admin	Service
Export all results marked as decided 	Yes	Yes	No	No	Yes
Reexport results (reset exported) – this enables results to be sent to the LIMS a second time 	No	Yes	No	No	Yes
Configuration settings					
Configure settings using **Show more > Configuration** 	No	Yes	No	Yes	Yes
Configure the Views Settings using **Show more > Configuration > Views**	No	Yes	No	No	Yes
Configure the Import Settings using **Show more > Configuration > Imports**	No	Yes	No	No	Yes
Configure the Export Settings using **Show more > Configuration > Exports**	No	Yes	No	No	Yes

User right	Lab Tech-nician	Lab Manager	Data Admin	Admin	Service
Configure the MSP abbreviations settings using **Show more > Configuration > MSP abbreviations**	No	Yes	No	No	Yes
Configure the Target types settings using **Show more > Configuration > Target types**	No	No	No	No	Yes
Configure the MSP Sources settings using **Show more > Configuration > MSP sources**	No	No	No	No	Yes
Configure the Sample types settings using **Show more > Configuration > Sample types**	No	Yes	No	No	Yes
Configure the Acquisition settings using **Show more > Configuration > Acquisition**	No	Yes (read only)	No	Yes (read – write)	Yes (read – write)
Configure the Remote identification settings using **Show more > Configuration > Remote identification**	No	No	No	Yes	Yes
Configure the Reporting settings using **Show more > Configuration > Reporting**	No	No	No	No	Yes

User right	Lab Tech-nician	Lab Manager	Data Admin	Admin	Service
Configure the Identification methods settings using **Show more > Configuration > Identification methods**	No	No	No	No	Yes
Configure the preprocessing methods settings using **Show more > Configuration > Preprocessing methods**	No	No	No	No	Yes
Configure the Quality check methods settings using **Show more > Configuration > Quality check methods**	No	No	No	No	Yes
Configure the Preparation protocols settings using **Show more > Configuration > Preparation protocols**	No	Yes	No	No	Yes
Configure the Authentication settings using **Show more > Configuration > Authentication**	No	No	No	Yes	Yes
Configure the Modules settings using **Show more > Configuration > Modules**	No	Yes	No	No	Yes
Configure the Signatures settings using **Show more > Configuration > Signatures**	No	No	No	Yes	Yes

User right	Lab Tech-nician	Lab Manager	Data Admin	Admin	Service
Configure the Global settings using **Show more > Configuration > Global**	No	Yes	No	Yes	Yes
Maintenance settings					
Maintain the Settings using **Show more > Maintenance** 	No	Yes	Yes	No	Yes
Maintain the E-Log book using **Show more > Maintenance > E- Log book**	No	No	Yes	No	Yes
Maintain the Consumables registration using **Show more > Maintenance > Consumables registration**	No	Yes	No	No	Yes
Maintain the Runs administration using **Show more > Maintenance > Runs administration**	No	No	Yes	No	Yes
Maintain the Troubleshooting using **Show more > Maintenance > Troubleshooting**	No	Yes	Yes	No	Yes

User right	Lab Tech-nician	Lab Manager	Data Admin	Admin	Service
Server connection					
Check Server Connection using **Show more > Server connection** 	Yes	Yes	Yes	Yes	Yes
Instrument connection					
Check Instrument Connection using **Show more > Instrument connection** 	Yes	Yes	Yes	No	Yes
Always hide flexControl using **Show more > Instrument connection**	Yes (read only)	Yes (read only)	Yes (read only)	No	Yes
Trigger Refresh status using **Show more > Instrument connection**	Yes	Yes	No	No	Yes
View Vacuum status details using **Show more > Instrument connection**	Yes	Yes	Yes	No	Yes
Trigger Source cleaning using **Show more > Instrument connection**	Yes	Yes	No	No	Yes

User right	Lab Tech-nician	Lab Manager	Data Admin	Admin	Service
Trigger Target in/out using **Show more > Instrument connection**	Yes	Yes	No	No	Yes
Ribbon bar (options)					
Search for ID results 	Yes	Yes	No	No	Yes
Access online help 	Yes	Yes	Yes	Yes	Yes
Access about box 	Yes	Yes	Yes	Yes	Yes

Appendix D — Sample report

See below for a typical report of an identification run without additional modules.

Bruker MALDI Biotyper IVD

Identification Results

BRUKER

Report Info:

Created by:	TEST-GV-Z2\expert
Creation Date/Time:	7/5/2021 10:19 AM
Tests coverage:	31 of 31 Tests selected for this report

Run Info:

Run Identifier:	210705-101623-IVD-101333332
Created by:	TEST-GV-Z2\expert
Run Creation Date/Time:	7/5/2021 10:16 AM
Run Result Review:	not yet reviewed
Run Result Approval:	not yet approved
Number of Tests:	31
Validation:	passed
Validation Position:	H12
Instrument Identifier:	TEST-GV-Z2-SIMU
Server Version:	5.2.200
BTS / Matrix Lot Numbers:	- / -

Report created at
7/5/2021 10:19 AM In Vitro Diagnostic Page 1 of 38

Figure D-1 Example of an identification result report

Index

A

Acquisition
- monitoring 39
- starting 37
- stopping 43

B

BTS QC position
- assigning 35

C

Calibration
- mass spectrometer 24

Cleaning MALDI target plates 80

I

Identification run
- adding positions 36
- changing position definitions 36
- creating 31
- reviewing status 36

Installation
- software 21

Intended purpose 9

L

License
- software 21

Limitations 15

M

MALDI target plates
- checking 85
- cleaning 80
- handling 79
- testing 83-84

Manufacturer 3

Mass spectrometer
- calibration 24

MBT Compass HT IVD
- performance evaluation 16
- starting 25
- troubleshooting 61
- workflow 14

Molecular fingerprint 13

P

Performance evaluation 16

R

Reagents and chemicals 77

Result report
- example 109
- generating 44

structure 44

Results

exporting 51

viewing 51

S

Sample position

assigning 35

Sample preparation

Direct transfer 93

Extended direct transfer 94

Reagents and chemicals 77

Samples

culturing 88

Scope of supply 19

Software

configuration 65

installing 21

licensing 21

maintenance 67

System

limitations 15

T

Troubleshooting 61

U

User group rights 100

W

Workflow

MBT Compass HT IVD 14