minispec

Automation Software

User Manual

Version 006

Innovation with Integrity

AIC

This manual was written by

Bruker BioSpin AIC

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1 About This Manual

This manual enables safe and efficient handling of the device.

This manual is an integral part of the device, and must be kept in close proximity to the device where it is permanently accessible to personnel. In addition, instructions concerning labor protection laws, operator regulations tools and supplies must be available and adhered to.

Before starting any work, personnel must read the manual thoroughly and understand its contents. Compliance with all specified safety and operating instructions, as well as local work safety regulations, are vital to ensure safe operation.

The figures shown in this manual are designed to be general and informative and may not represent the specific Bruker model, component or software/firmware version you are working with. Options and accessories may or may not be illustrated in each figure.

1.1 Policy Statement

It is Bruker's policy to improve products as new techniques and components become available. Bruker reserves the right to change specifications at any time.

Every effort has been made to avoid errors in text and Figure presentation in this publication. In order to produce useful and appropriate documentation, we welcome your comments on this publication. Field Service Engineers are advised to check regularly with Bruker for updated information.

Bruker is committed to providing customers with inventive, high-quality, environmentally-sound products and services.

1.2 Symbols and Conventions

Safety instructions in this manual and labels of devices are marked with symbols. .

The safety instructions are introduced using indicative words which express the extent of the hazard.

In order to avoid accidents, personal injury or damage to property, always observe safety instructions and proceed with care.

⚠ DANGER

DANGER indicates a hazardous situation which, if not avoided, will result in death or serious injury.

This is the consequence of not following the warning.

1. This is the safety condition.

▶ This is the safety instruction.

⚠ WARNING

WARNING indicates a hazardous situation, which, if not avoided, could result in death or serious injury.

This is the consequence of not following the warning.

1. This is the safety condition.

▶ This is the safety instruction.

⚠ CAUTION

CAUTION indicates a hazardous situation, which, if not avoided, may result in minor or moderate injury or severe material or property damage.

This is the consequence of not following the warning.

1. This is the safety condition.

▶ This is the safety instruction.

NOTICE

NOTICE indicates a property damage message.

This is the consequence of not following the notice.

1. This is a safety condition.

▶ This is a safety instruction.

SAFETY INSTRUCTIONS

SAFETY INSTRUCTIONS are used for control flow and shutdowns in the event of an error or emergency.

This is the consequence of not following the safety instructions.

1. This is a safety condition.

▶ This is a safety instruction.

This symbol highlights useful tips and recommendations as well as information designed to ensure efficient and smooth operation.

1.3 Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All what you can enter"	Arial bold	Type or enter **fromjdx zg**
Button, Tab, Pane and Menu Names "All what you can click"	Arial bold, initial letters capitalized	Use the **Export To File** button. Click **OK**. Click **Processing**…
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names **Data Path Variables** **Table Column Names** **Field Names (within Dialog Windows)**	Arial Italics	*$tshome/exp/stan/nmr/lists* *expno, procno,*
Parameters	Arial in Capital Letters	VCLIST

Program Code
Pulse and AU Program Names
Macros
Functions
Arguments
Variables
	Courier	`go=2`
		`au_zgte`
		`edmac`
		`CalcExpTime()`
		`XAU(prog, arg)`
		`disk2, user2`

AU Macro	Courier in Capital Letters	`REX` `PNO`

Table 1.1: Font and Format Conventions

About This Manual

2 Introduction

The minispec Sample Automation software is a feature-packed, easy-to-use solution that provides significant flexibility, usability and the performance required to maximize your lab efficiency by automating your Time Domain Nuclear Magnetic Resonance (TD-NMR) minispec applications.

With the minispec automation software you can process computerized measurements with your minispec. The software controls the processing of the sample tubes, the measurement using the minispec, and supports other devices, like a robot, tempering blocks, etc.

minispec Automation manages the methods for the measurement and all sample data with their results.

Additionally, an interface between the minispec Automation and LIMS is available. This interface is bidirectional, which means that the interface imports the sample orders from the LIMS and exports the results back to the LIMS.

The sample data are archived and can be selected easily using search tools. The search results can be exported to other applications via the Windows clipboard.

Introduction

3 Installation

For detailed instructions on how to install the software please refer to the Installation Manual.

The program is installed locally on a PC using the setup program. The program files and the user-specific files are copied to the directory specified during the installation process.

When the software is started for the first time, the user-specific files are saved in the system folder “..\minispec-Automation". This system folder can be found in the following directory:

Windows 7:

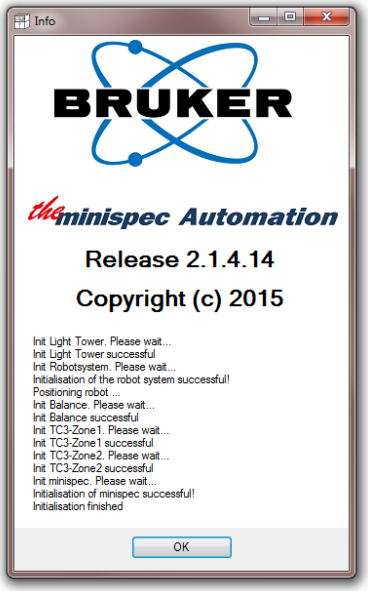
c:\ProgramData\

In operating systems with a different language, the directories are named based on the language selected.

4 Starting the Software

To start the software go to the Start menu and click on **Start** - **Programs** and then **minispec Automation**.

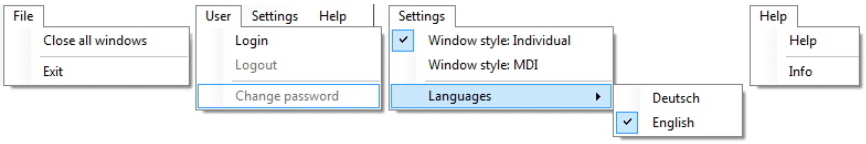
When the program starts, the main window will be displayed. If available, other devices such as a robot, tempering blocks and minispec are initialized.



If a robotic system detects a tube at startup in the gripper or in the minispec, the system will attempt to place it in the 'emergency position'. This is the last position of the storage area of the TC6-block. Make sure that this position is not occupied.

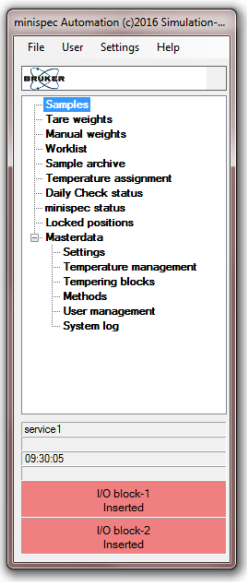
5 Setting up the System

General settings for the software can be set using the menu bar:



The software functions are accessible from the toolbar on the left side of the main window.

The toolbar displays the enabled features, for example, when you use a robot system for the measurement, the toolbar displays additional functions for the configuration and control of the robot.



5.1 Setting the Language

To change the language:

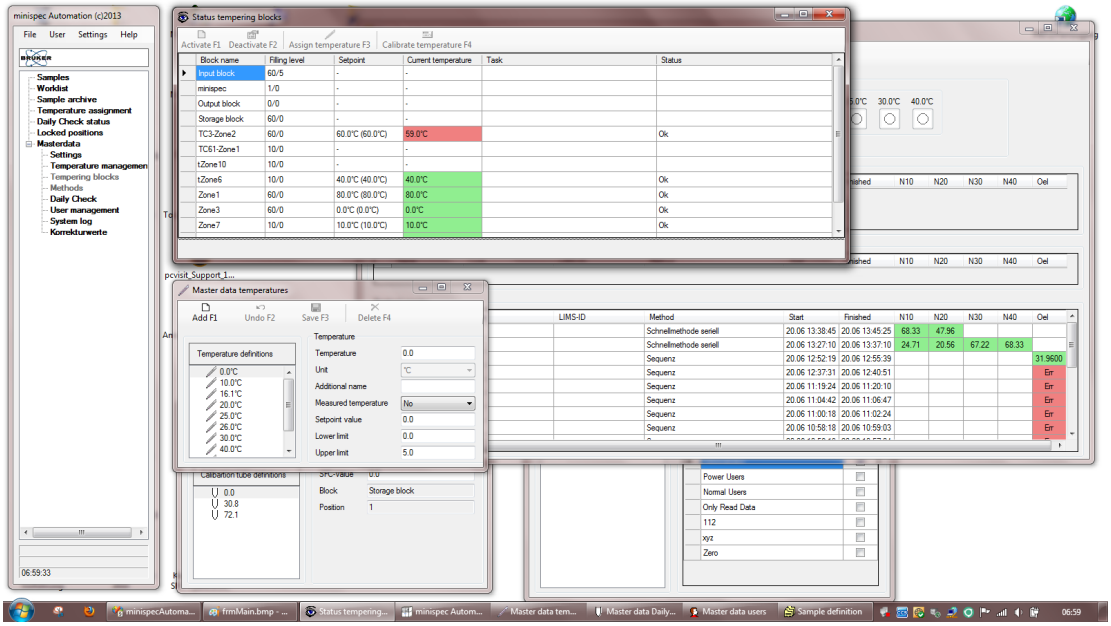
- Click on the main window menu item **Settings** and select the menu item **Languages**.
- Select the desired language from the list that is displayed.

The settings for the new language are immediately applied and the text in the windows is displayed in the selected language without restarting the software. Some language-specific properties are displayed only after reopening the corresponding window.

5.2 Setting the Window Style

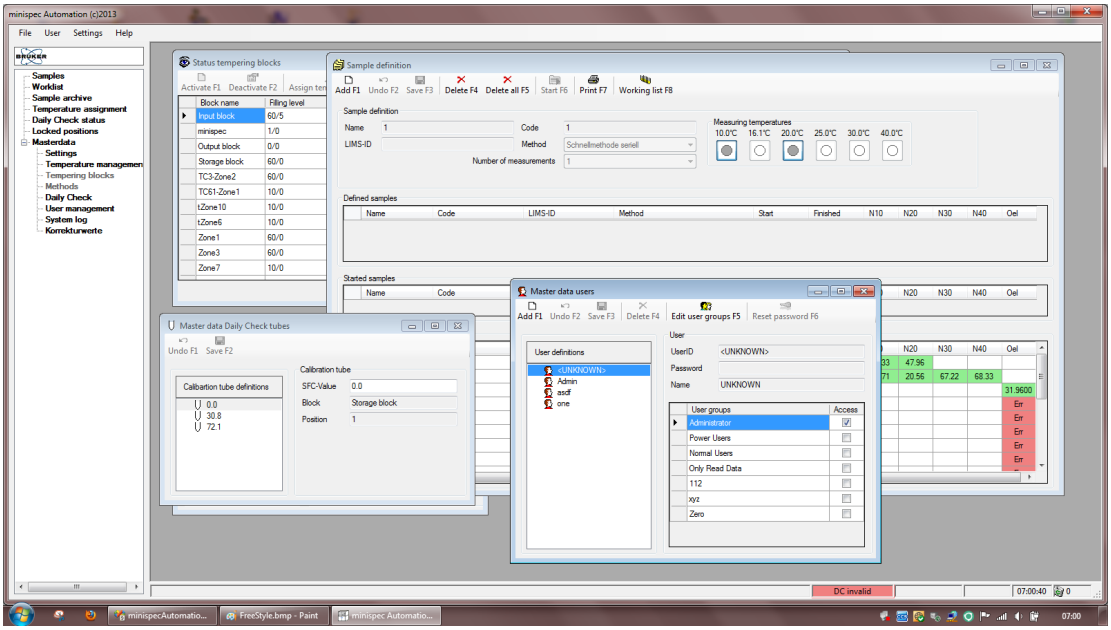
minispec Automation can be displayed using different window styles.

5.2.1 Free Floating Windows



This window style is especially suited for dual monitor operation because the windows can be displayed on two separate monitors. To work with the different windows, you must first focus on a window by clicking on the window with the mouse.

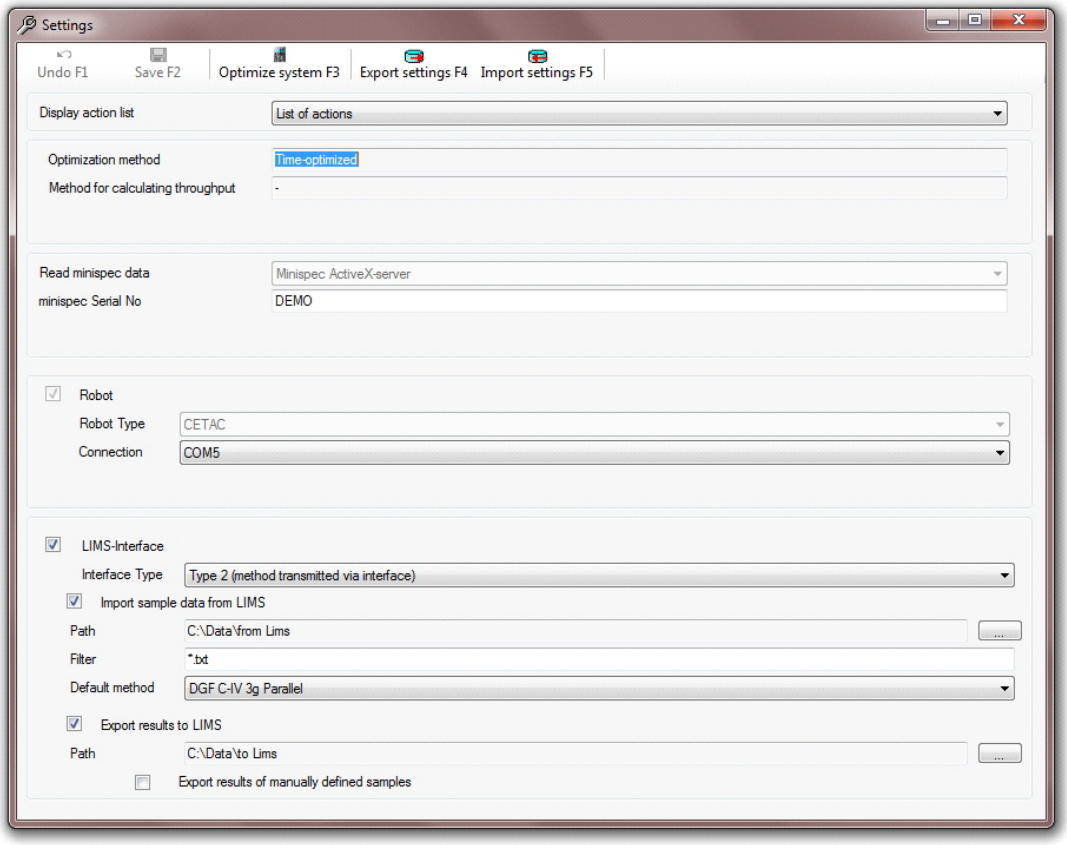
5.2.2 MDI Windows



This window style (MDI = Multi document interface) displays all of the dialogs in a main window. The focus is set automatically to the window with which you want to work.

5.3 Communication with the minispec

To set the parameters for communication with the minispec select **Master data** / **Settings** from the main toolbar. If *Settings* is not displayed, expand the master data menu by selecting the entry **Master Data**.



Before the automation software can control the minispec, the serial number of the minispec must be entered in the corresponding field. It is advisable to first establish communication by means of the minispec software, and then configure the automation software.

After you have completed the settings, save the changes by pressing the **Save** button or by pressing the **F2** key.

After saving, a message is display stating that the changes will only take effort after restarting the software.

To discard the changes, click on the **Undo** button or press the **F1** key.

5.4 Robotic Communication

To set the parameters for communication with the robot, select the menu item **Master Data** / **Settings** from the main toolbar. If this entry is not displayed, expand the master data menu by selecting the entry **Master Data**.

Before the automation software can control the robot, the COM port with which the robot is connected to the PC must be specified.

After you have completed the settings, save the changes by pressing the **Save** button or the **F2** key.

After saving, a message is displayed stating that the changes will only take effect after restarting the software.

To discard the changes, click on the **Undo** button or press the **F1** key.

5.5 Tempering Block Communication

To set the parameters for communication with the tempering blocks, select the menu item **Master Data** / **Settings** from the main toolbar. If this entry is not displayed, expand the master data menu by selecting the entry **Master Data**.

Before the automation software can control the temper blocks, the COM port with which the tempering blocks are connected to the PC must be specified.

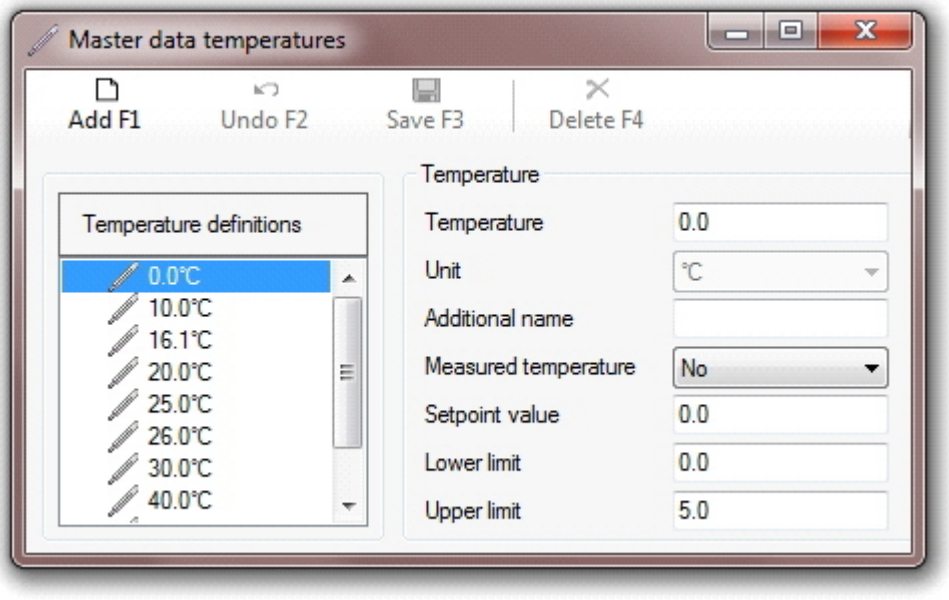
After you have completed the settings, save the changes by pressing the **Save** button or the **F2** key.

After saving, a message is displayed stating that the changes will only take effect after restarting the software.

To discard the changes, click on the **Undo** button or press the **F1** key.

5.6 Defining Temperatures

To define temperature ranges select **Master data** / **Temperature Management** from the main toolbar. If **Temperature Management** is not displayed, expand the master data menu by selecting the entry **Master Data**.



In this dialog, all temperatures are displayed which are managed by the system.

For each temperature the following details are required:

- Temperature

  Definition of the temperature with one decimal place.
- Unit

  The temperature unit is preset to °C and cannot be changed.
- Additional name

  For each temperature, an additional description can be assigned.
- Measured temperature

  This option specifies whether the temperature is displayed in the window for sample management or in the sample reports. In general this option is activated for each measurement temperature.
- Set point value

  Definition of the set point for the temperature control of the tempering blocks. The set point corresponds to the defined temperature.
- Lower limit

  Specification of the lower limit for the defined temperature. When the temperature of the assigned tempering block is lower than the defined value, an alarm message will be displayed.
- Upper limit

  Specification of the upper limit for the defined temperature. When the temperature of the assigned tempering block is higher than the defined value, an alarm message will be displayed.

Each temperature must have a unique assignment. This assignment is derived from the two items 'Temperature' and 'Additional name'.

This definition allows, for example, **0°C Crystallization** (0°C is the temperature, 'Crystallization' is the additional name) and **0°C Measuring Temperature** (0°C is the temperature, 'Measuring Temperature' is the additional name) to be defined as different temperatures.

To change an existing temperature definition, select the desired temperature on the left side and make the changes.

After completing the changes click on the **Save** button or press the **F3** key to save your changes. The changes are effective immediately.

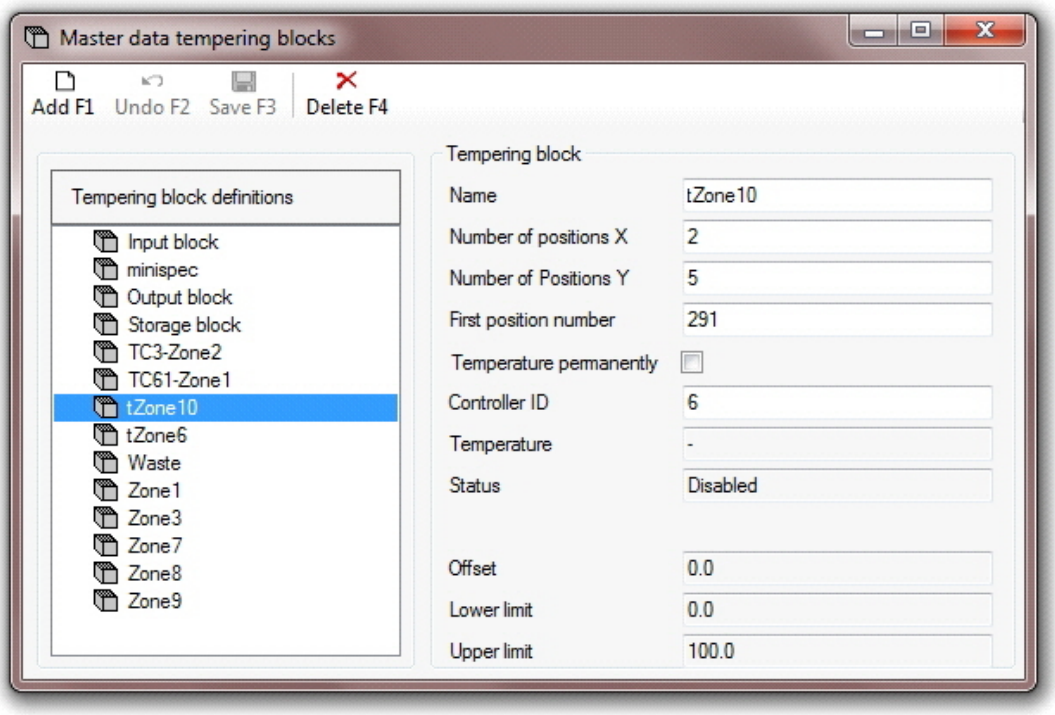
To discard the changes, click on the **Undo** button or press the **F2** key.

To define a new temperature, click on the **Add** button or enter the **F1**key, input the definitions and save as described above.

If you change an existing temperature, the data of all thermostating blocks and method steps assigned to this temperature must also be adapted! Delete any temperatures that are no longer required and do not overwrite any existing temperature.

5.7 Defining Tempering Blocks

To define tempering blocks select **Master data** / **Tempering blocks** from the main toolbar. If **Tempering blocks** is not displayed, expand the master data menu by selecting the entry **Master Data**.



In this dialog, all tempering blocks are displayed which are managed by the system.

For each tempering block the following details are required:

- Name

  Definition of a unique name for the block. For system-relevant blocks the names are fixed and cannot be changed.
- Number of X positions

  Maximum number of tubes that can fit on the X-axis in the specified block.
- Number of Y positions

  Maximum number of tubes that can fit on the Y-axis in the specified block.
- First position number

  Specification of the first position number of the robot controller for this block.
- Temperature permanently

  This setting specifies whether the standard user can change the temperature of the block or if the temperature is permanently assigned in the system.
- X-Co, Y-Co

  Here the coordinates for the block coordinates are defined (currently not used).
- ControllerID

  Internal ID of the temperature controller for the defined block.
- Temperature

  The temperature which is assigned to the block.

Changes are made in the dialog **Temperature assignment** (see *Temperature Assignment [▶ 22]*).

- Status

  Actual status of the block (enabled / disabled).
- Offset

  Offset of the temperature calibration.
- Lower Limit

  Lower limit of the block temperature.
- Upper Limit

  Upper limit of the block temperature.
- Label Design

  Here the different numbering sequence of the blocks are defined:

  Type 1: Input block/Output block

  Type 2: TC3-Blocks

  Type 3: TC6-Blocks

  Type 4: TC6-Storageline

  Type 5: Reserved

To change an existing block definition, select the desired block on the left side and make the changes.

Most of the settings can be changed only if the block is disabled (see chapter *Temperature Assignment [▶ 22]*).

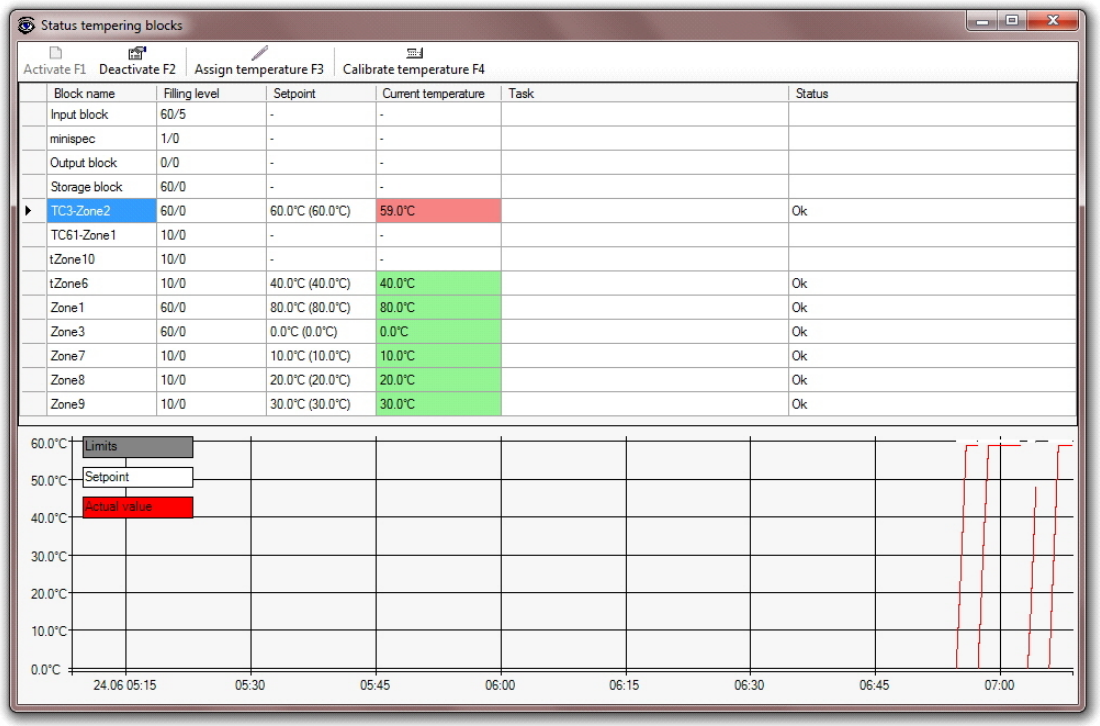
After completing the changes click on the **Save** button or press the **F3** key to save your changes. The changes are effective immediately.

To discard the changes, click on the **Undo** button or press the **F2** key.

To define a new block, click on the **Add** button or enter the **F1** key, input the definitions and save as described above.

5.8 Temperature Assignment

Once the master data for temperatures and tempering blocks are defined, the assignment between temperatures and the blocks can be performed.



The actual temperature for each block and the temperature graph are displayed only if communication between the temperature controller and the minispec Automation is set up.

In the graph the last two hours of the temperature profile are displayed. You can select different display areas by right-clicking on the area to be displayed.

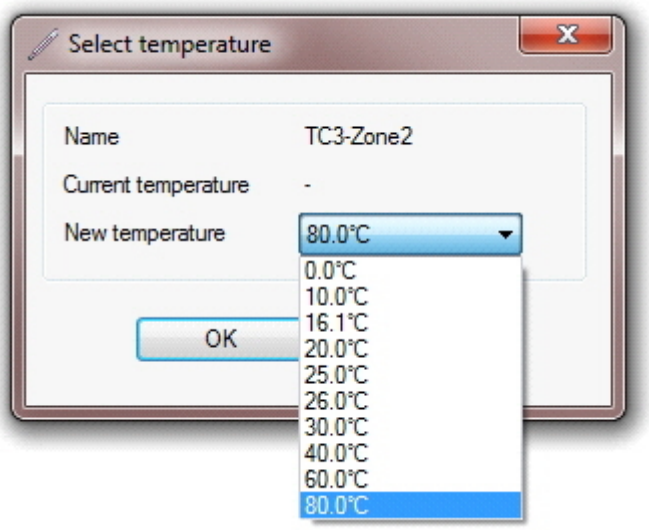
The limit range of the temperature is shown in gray, the set point temperature in white, and the actual temperature in red.

Use the mouse to enlarge a region of the temperature graph. To do this, move the mouse to the start point of the desired region, then press the left mouse button and move the mouse to the end point of the desired region. After releasing the mouse button, the selected region is enlarged. To undo the enlargement, press the right mouse button on the temperature graph.

Each tempering block can be enabled or disabled. When a block is disabled, no temperature is assigned and the block is not used by the system. It is therefore possible to define replacement blocks which can be switched on as required. When a block is enabled, a temperature is assigned and this block is used by the system.

To enable a disabled block, first select the block in the table and then click on the **Activate** button or press the **F1** key.

A dialog to select the temperature opens.



After selecting the temperature, click on the **OK** button to implement the new temperature.

The status display will show that the corresponding block is enabled.

TC3-Zone2	60/0	80.0°C (80.0°C)	-	Activate block	Wait for the end of timestep

In the first step the system waits until the actual robot step is executed.

TC3-Zone2	60/0	80.0°C (80.0°C)	35.9°C		Wait for reaching the new temperature

The block is then connected to the system and the system waits until the set point temperature of the block is reached.

If the temperature of an enabled block is changed, the following changes in the status are executed:

TC3-Zone2	60/0	80.0°C (80.0°C)	80.0°C	Change block temperature to 20.0°C	Wait for the end of timestep

In the first step the system waits until the actual robot step is executed.

TC3-Zone2	60/0	80.0°C (80.0°C)	80.0°C	Change block temperature to 20.0°C	Wait for emptying of the block

The next step is to determine whether the block is still needed by the system to process the registered sample tubes.

TC3-Zone2	60/0	20.0°C (20.0°C)	80.0°C	Change block temperature to 20.0°C	Wait for reaching the new temperature

The block is then heated or cooled to the new set point temperature. After reaching the temperature the block can be used by the system.

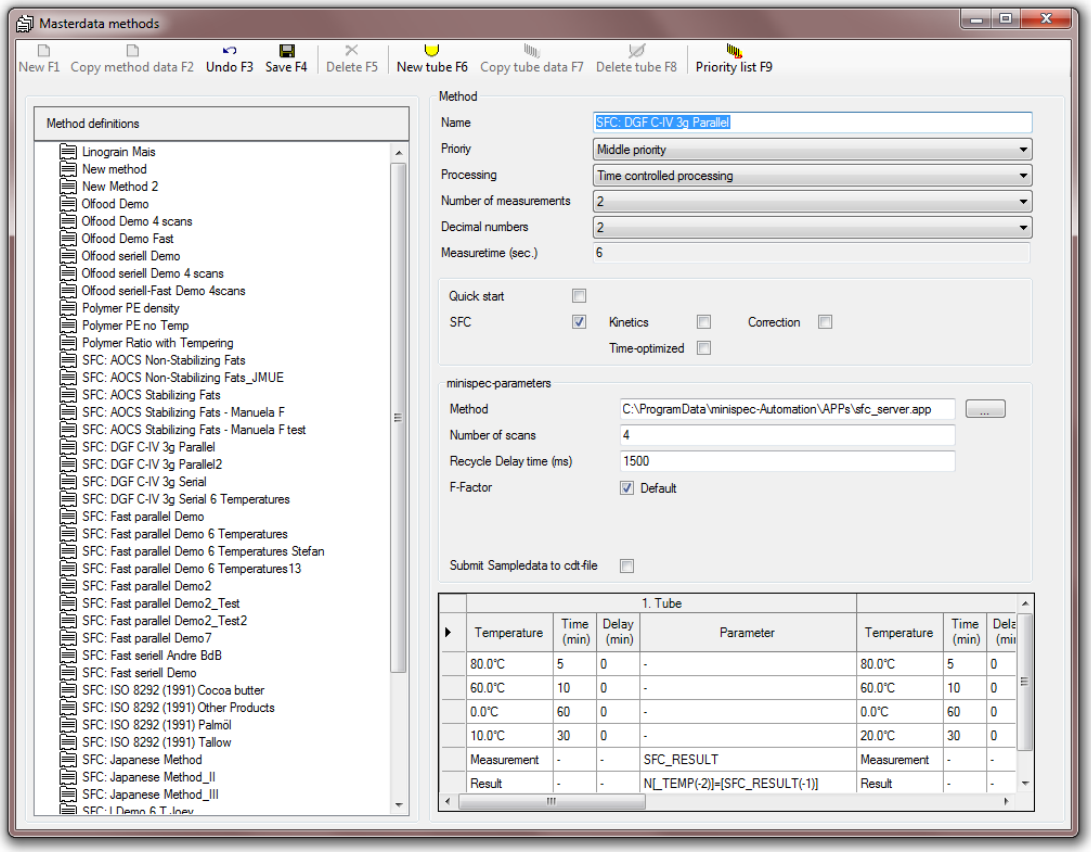
Disabling of a block is analogous to the change in the temperature of a block. The difference is that the block is turned off.

5.9 Definition of Methods

To define a method, select **Master data** | **Methods** from the main toobar. If **Methods** is not displayed, expand the master data menu by selecting the entry **Master Data**.

The methods implemented with the installation are read-only. After copying the methods can be edited as a new method.

Note the special features of the 21 CFR Part 11 option in the chapter *CFR 21 Part 11 [▶ 53]*.



In this dialog, all methods are displayed which are managed by the system.

For each method, the following information is required:

- Name

  Definition of a unique name for the method.

- Priority

  Here the priority of the method is given. If multiple samples with methods of different priorities are started simultaneously, the samples are processed in accordance with the priority order.

- Processing

  You can select between time controlled or sequential processing. In the time controlled processing the residence times of the tubes in each tempering block are accurately maintained. In the sequential processing the method steps are executed one after the other.

- Number of measurements

  Default setting for the number of measurements. This setting can be changed during sample registration.

- Number of decimals

  Here you can specify how many decimal places the final result has. The intermediate values are displayed with one decimal place more.

  The number of decimals used is that which is specified in the result column.

- SFC (not valid for non-SFC installations)

  If the SFC flag is set for a method, than this flag must also be set in the minispec software. In this case the Daily Check is performed with three tubes. When the SFC flag is not set, the minispec applications must be calibrated before use.

- Time optimized

  With this option, a method can be processed with optimized timing of the sample tubes. This means the residence time in each tempering block is maintained accurately. Normally the system is throughput optimized. For a detailed description of this option, see *System Optimization [▶ 61]*.

- Quick start

  With this option, a method can be started although there are no time windows for robot actions available. When used with the G-Var application, this method will make sure that cooled samples (at 5°C) are immediately transferred to a cooling bath after they have been introduced. For a detailed description of this option, see *System Optimization [▶ 61]*.

- Kinetics (not valid for non-SFC installations)

  With this option, a method can be defined as a kinetic method.

- Correction (not valid for non-SFC installations)

  With this option, quick SFC-methods can be defined. The measurement values will be corrected by the defined correction values (see *Master Data: Correction Values [▶ 29]*).

- Number of Scans

  Number of scans is a minispec parameter. This setting is available only if the SFC flag is set.

- Recycle Delay Time

  Recycle delay time is a minispec parameter. This setting is available only if the SFC flag is set.

- F-Factor (not valid for non-SFC installations)

  By default, the SFC value is determined by the F factor of the minispec. For every method, the F-Factor can be changed to a fixed value or to an offset of the minispec-factor.

At least one tube must be specified for a processing cycle (methods steps).

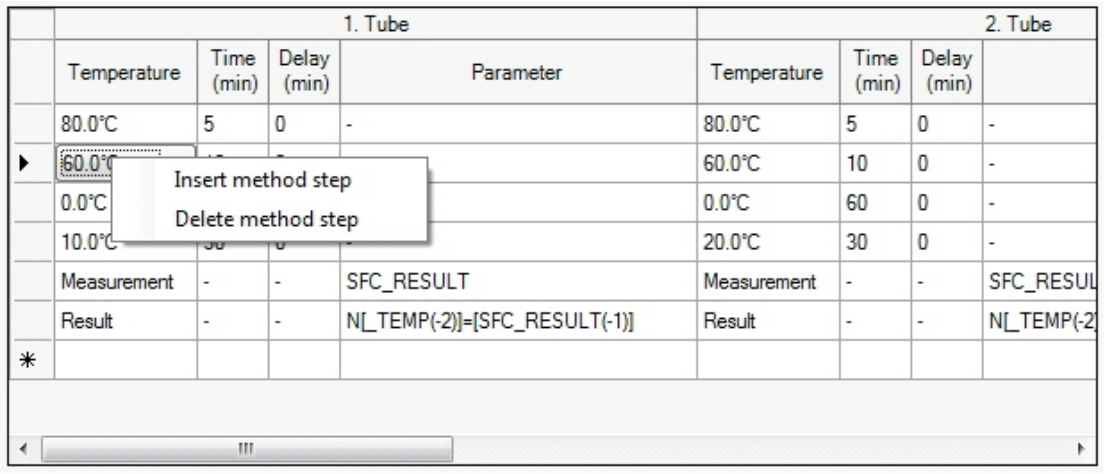
5.9.1 Changing a Method

To change a method, select the desired method from the left side of the window, and make the changes.

When entering the method steps, note the following instructions:

- For each step, temperature, residence time and the maximum time deviation can be defined (for sequential processing the time specifications are omitted). Should there be a measurement at the end of the tempering steps, enter the value **Measurement** in the field 'Temperature'. In this case the time values are deleted.
- If a weighing should be performed, enter the value **Weighing** in the field 'Temperature'.
- If you want to define a serial method, enter additional tempering and measurement steps.
- If you want to define a parallel method, enter the data for the next tube. Click on the **New Tube** button or press the **F6** key to define another tube.

- To define a new tube, it is possible to make a copy of an already defined tube. Select the tube data to copy by clicking on the header line of the tube, then click the **Copy tube data** button or press the **F7** key.
- To delete a tube definition, click on the header line of the tube, then click on the **Delete tube** button or press the **F8** key.



To insert or delete a method step, click with the right mouse button on the corresponding position in the sequence of steps and select the desired function.

At the end of a measurement a result line must be defined. In the result line the calculation of the result is performed.

After changing the method, save the data by clicking on the **Save** button or pressing the **F4** key. The changes are effective immediately.

To discard the changes, click on the **Undo** button or press the **F3** key.

5.9.2 Creating a New Method

To define a new method:

- Click on the **New** button or press the **F1**key.
- Enter the method data.
- Save the method by clicking on the **Save** button or pressing the **F4** key.

Methods can be changed at any time. Internally, a version management is used. This means that samples which are already started continue processing according to the old method version. Samples which are started after changing the method are processed according to the new method version.

With the function **Copy method data** or **F7** a defined method can be copied to a new method, which can be further processed.

5.10 Principles of Method Creation

minispec-Automation supports different minispec applications.

For *Solid Fat Content (SFC)* parallel and serial methods, as well as crystallization, kinetics are supported.

For the *G-Var applications*, we currently distinguish between: water droplets (g-var_mq_nf_wds.app), water droplets/fitting including free water function (g-var_mq_nf_wds_fw.app) and oil droplets (g-var_mq_nf_ods.app).

If the method steps can be executed sequentially, select the **sequential processing** workflow. If residence times in tempering blocks are needed, select the **time controlled** workflow.

For each method, at least one tube has to be defined with the method steps for tempering and measurement. Any number of tempering and measurement steps can be defined for each tube.

For each measurement step the parameter for the minispec application must be defined. If several parameters are required, the parameters can be separated with commas in the same line.

If a sample weight is to be sent to the minispec application, it must be entered in the parameter list using the form:

```
WEIGHT<12.345
```

Where:

- The character '<' indicates, that a value is transmitted to the minispec application.
- On the left of that character is the minispec parameter that contains the value.
- After the '<' character is the associated value. The value can be a number, but also a parameter value, e.g.: a result of a weighing could be:

  ```
  WEIGHT<[GROSS(-2)].
  ```

- The square brackets indicate that the parameter value is to be calculated. 'GROSS' is the name of the parameter. The value (-2) indicates, that the value was defined 2 rows above the current row.

For the calculation of results a result row is required. In this case the parameter is the name of the result. The calculation is specified in the form:

```
Result name=Calculation
```

The decimals can also be defined in curved brackets.

For a detailed description of this information, please refer to the *Examples of Methods [▶ 69]*. In general the methods are created at the delivery. Later the methods can be modified and extended only by trained users.

The software automatically searches for regularities in the measuring cycles. This function works with both parallel and serial methods.

If regularities are found (i.e. the same steps for each measuring temperature), then additional measuring temperatures can be selected or deselected during sample registration. In this case the temperatures in the method definition are targets that can be changed.

When no regularities are found, the measuring cycles are carried out exactly as defined in the method.

A special feature of the automation software is SFC measurements for crystallization kinetics. For kinetics measurements, a new tube is created for measurement time, e.g. 1 min., 2 min., 3 min., 5 min., 10 min., 15 min., etc. In order to show a crystallization curve, the data (temperature and time) are extracted from the variable:

```
name - = Result.
```

To do this, the variable name must comply with the following conventions:

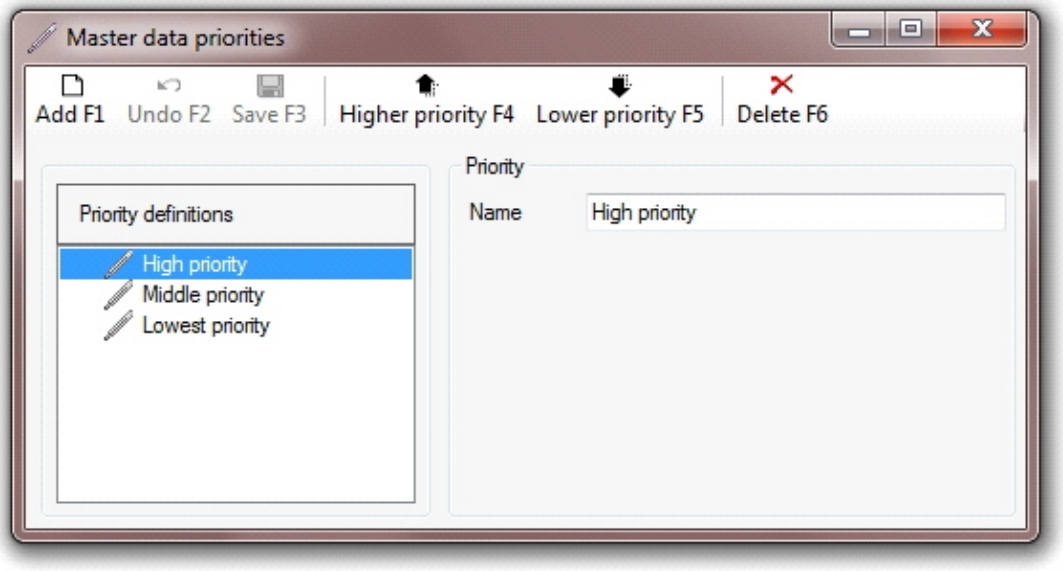
- T10_01min for 10°C, 1 minute
- T20_10min for 20°C, 10 minutes
- T40_60min for 40°C, 60 minutes

An example of the definition of a kinetic method is shown in the Parameter field in the next figure:

	1. Tube				2. Tube			
	Temperature	Time (min)	Delay (min)	Parameter	Temperature	Time (min)	Delay (min)	Parameter
	80.0°C	1	0	-	80.0°C	1	0	-
	10.0°C	1	0	-	10.0°C	2	0	-
	Measurement	-	-	SFC_RESULT	Measurement	-	-	SFC_RESULT
	Result	-	-	T10_01min=[SFC_RESULT(-1)]	Result	-	-	T10_02min=[SFC_RESULT(-1)]
*								

5.11 How to Edit the Priority List

The dialog to edit the priority list is called from the methods dialog. To open this dialog, click on the **Priority list** button or press the **F9** key.



In the left table, the available priorities are displayed in descending order.

To edit an existing priority, select the desired priority on the left and change the name on the right.

After changing the priority, save the data by clicking on the **Save** button or pressing the **F3** key. The changes are effective immediately. To discard the changes, click on the **Undo** button or press the **F2** key.

To define a new priority:

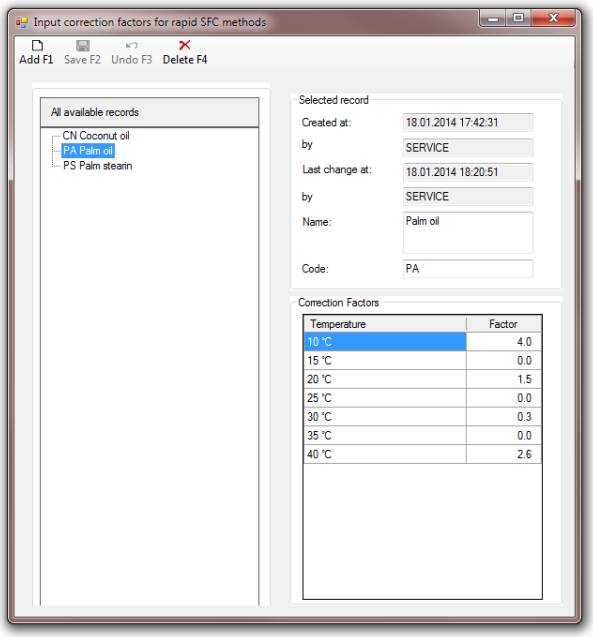
- Click on the **New** button or press the **F1** key.
- Enter the priority name.
- Save the priority as described above.

To change the priority order, select the entry to modify, than click on the **Higher priority** button or **Lower priority** to change the order.

To delete a defined priority, click on the **Delete** button or press the **F6** key.

5.12 Master Data: Correction Values

To edit the calibration data select **Master data** / **Correction Factors** from the main toolbar. If **Correction Factors** is not displayed, expand the master data menu by selecting the entry **Master Data**.



The correction values are needed for all SFC rapid methods. One possible rapid method is, for example:

- Cooling of the SFC tubes in liquid nitrogen.
- Then immediate placement in the tempering blocks for measuring temperatures.
- Measuring after 20 minutes.

The advantage of a rapid method is that the results are available after about 25 minutes. The disadvantage is that the measured values are as a rule, too low, but reproducible. Using the correction factors, the measured values can be corrected so that they correspond to those measured by the standard method.

For this purpose a table must be created with the correction values for each product (see table above). The correction values are obtained from measurements of the SFC values using the standard method or with a rapid method. To obtain accurate values, the measurements are performed several times, and then averaged. The average values of the rapid method are then subtracted from the values of the standard method for each temperature. The resulting difference is the correction value and is placed in the table. The values are usually positive, but in rare cases can also be negative. The correction value is always added to the measured value when using the rapid method.

To utilize the correction values, the options **Correction** and **Quick Start** must be selected when setting up the method. When these options are selected the SFC tubes are moved immediately from the input block into the blocks for the respective measurement temperatures.

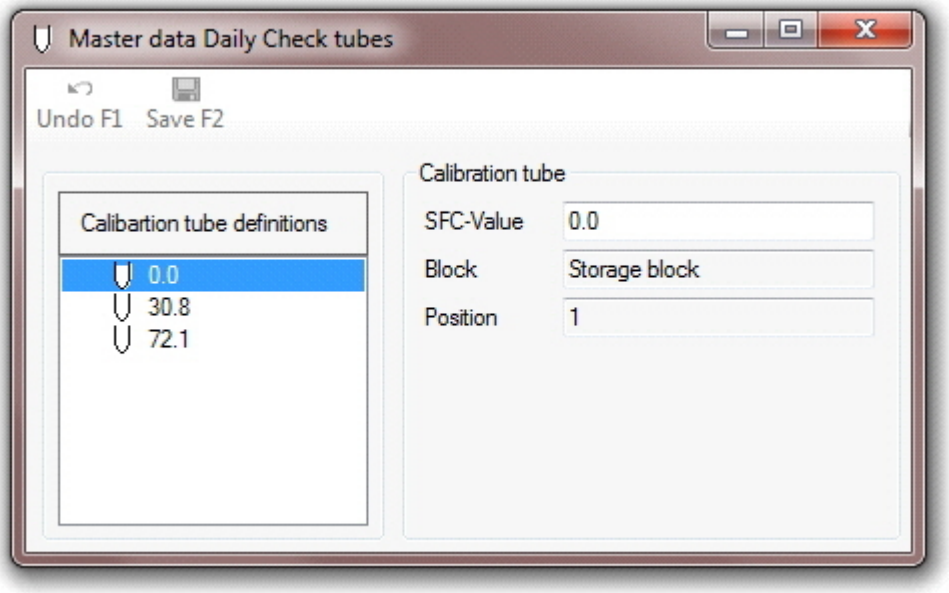
To ensure that the appropriate correction values are assigned to the right product, a unique code is used. When entering a new sample, the code of the product must be the same as the product in the table (see figure above).

5.13 Definition of the Tubes for Daily Check

To edit the calibration data select **Master data** / **DailyCheck** from the main toolbar. If **Daily Check** is not displayed, like for non-SFC installations, expand the master data menu by selecting the entry **Master Data**.

For the G-Var installations, the daily check sample is provided and its default position is 1 in the storage block.

For the SFC installation, three calibration tubes are shown in this dialog, which are needed for the calibration of the minispec.



For each tube the following information is required:

- SFC-Value

  Specified value of the calibration tube. The value is on the tubes supplied by Bruker.
- Block

  The block where the calibration tube will be permanently kept.
- Position

  The position number in the block defined above.

To change the data of one of the tubes, select the desired tube from the calibration tube definitions, and make the changes desired.

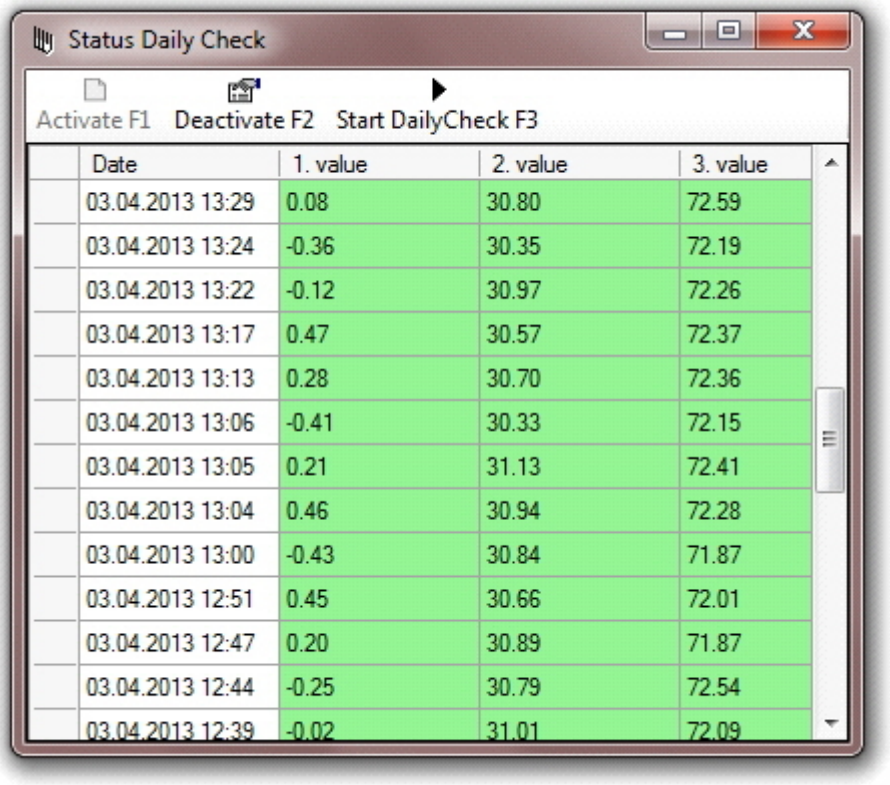
After changing the tube data, save the data by clicking on the **Save** button or pressing the **F2** key. The changes are effective immediately.

To discard the changes, click on the **Undo** button or press the **F1** key.

The positions of the calibration tubes in the system are permanently assigned. When no robot is available, the calibration tubes are not managed by the system. In this case the calibration tubes should be stored on the minispec tray.

5.14 Daily Check

To get an overview of the calibration status, select **Status Daily Check** from the main toolbar.



Date	1. value	2. value	3. value
03.04.2013 13:29	0.08	30.80	72.59
03.04.2013 13:24	-0.36	30.35	72.19
03.04.2013 13:22	-0.12	30.97	72.26
03.04.2013 13:17	0.47	30.57	72.37
03.04.2013 13:13	0.28	30.70	72.36
03.04.2013 13:06	-0.41	30.33	72.15
03.04.2013 13:05	0.21	31.13	72.41
03.04.2013 13:04	0.46	30.94	72.28
03.04.2013 13:00	-0.43	30.84	71.87
03.04.2013 12:51	0.45	30.66	72.01
03.04.2013 12:47	0.20	30.89	71.87
03.04.2013 12:44	-0.25	30.79	72.54
03.04.2013 12:39	-0.02	31.01	72.09

Click on the **Activate** button or press the **F1** key to activate the Daily Check. When activated, the minispec is automatically calibrated every 23.5 hours. If the last calibration was done prior to the last 23.5 hours, the calibration will start immediately. To deactivate the automatic calibration, click on the **Deactivate** button or press the **F2** key.

To start a Daily Check manually outside of the predefined period, click on the **Start Daily Check** button or press the **F3** key. In this case the software will look for free time slots to start the Daily Check. This may take longer if the system has to process a lot of sample tubes. For future reference, the Daily Check is recorded in the work list.

If the Daily Check is automatically processed, the future time slots are always reserved. If you stop and restart the system, and there are no time slots available, the Daily Check is performed first and then the sample tubes are processed.

In the table above is an example of Daily Checks that were performed in the past. The displayed SFC values were determined when the Daily Check is executed.

When the Daily Check is cancelled, the system will stop and a corresponding message will be displayed. In this case the automatic Daily Check will also be disabled.

6 System Layout

When a robot system is used, 3 different systems layouts can be used depending on the application.

Important: For the insertion or removal of tubes from the system, one of the above system layouts must be selected!

6.1 System with Waste Container

In this system configuration, the two transfer blocks are managed as input blocks.

When the Sample Start dialog is opened, both input blocks are automatically suspended for the robot handling (the status on the status bar changes from red to green).

When the robot is performing an action in the input blocks, the software waits until the end of the robot action.

When the Samples Start dialog is closed, the input blocks are released back for robot handling.

6.2 System with Input and Output Block

In this system configuration one of the transfer blocks is used as sample input, the other one as sample output.

When the Sample Start dialog is opened, both input blocks are automatically suspended for the robot handling (the status on the status bar changes from red to green).

When the robot is performing an action in the input blocks, the software waits until the end of the robot action.

When the Samples Start dialog is closed, the input blocks are released back for robot handling.

To remove the finished samples from the output block, the removal must be logged into the system:

- Click on the output block in the status line.
- The status will change from red to green.
- The respective positions can now be released in the Locked Positions dialog. Alternatively, all the items can be released simultaneously.

Important: After removing the tubes, the output block for the robot must be released again. Click on the output block on the status line again, this will change the status from green to red.

6.3 System with Combined Input/Output Block

In this system configuration, both transfer blocks are managed as input and output blocks. When a tube is started, the position is immediately reserved for when the tube is returned.

When the Sample Start dialog is opened, both Input/Output blocks are automatically suspended for robot actions (the status on the status bar changes from red to green).

When the robot is performing an action in the input blocks, the software waits until the end of the robot action.

When the Samples Start dialog is closed, the input blocks are released back for robot handling.

To remove the finished samples from the blocks, the removal must be logged into the system:

- Click on a block on the status bar.
- The status will change from red to green.
- The respective positions can now be released in the Locked Positions dialog. Alternatively, all the items can be released simultaneously.

Important: After removing the tubes the two blocks must be released for the robot. Click on the status bar again, this will change the status from green to red.

7 Calibrating for Oil Droplet Sizes/ Water Droplet Sizes

Prior to using the minispec Sample Automation software, the minispec mq20 system has to be calibrated for droplet size analysis (o/w or w/o emulsions) like margarine or mayonnaise samples. For the new G-Var method Bruker delivers the application pre-calibrated so that only a fine adjustment of the calibration is needed on the customer side.

Two software packages are delivered with the equipment:

- The minispec Sample Automation GUI software (mA).
- The Bruker minispec control software (minispec.exe).

The new G-Var method needs only one calibration for any copy of the G-Var server application file.

Use one of the applications like *g-var_mq_nf_wds.app* to do a fine adjustment of the factory pre-calibration. Parameters are to be adjusted according to the corresponding G-Var Droplet Size manual (P/N E1400013). During the calibration process, manual sample handling is expected.

Select the parameters properly for all the methods (refer to the G-Var Droplets Manual for details). Bruker has already provided the server application files with the correct parameters (by supplying *.cdt files in a sub-directory **NFxxxx** where **xxxx** needs to be adapted to the corresponding instrument serial number), however please double check. The server applications (plus the corresponding calibration files) for automated operation must be located in:

C:\ProgramData\minispec-Automation\APPs

Only when all files (*.app and *.cdt files in the sub-directories) are available, can the required calibration data for the corresponding method be found by the software.

Once the calibration is ready, unknown samples can be measured either via the minispec Sample Automation software.

The calibration procedure has fixed values for the most of the parameters, with only a few of them being accessible to the user, as the configuration table is used only in the measurements.

Calibrating for Oil Droplet Sizes/Water Droplet Sizes

After clicking on **Calibrate**, a window will pop up, displaying all parameters that the user can change. The calibration is divided into 3 steps, which the user can decide to do or not, as long as they have executed the whole calibration procedure at least once. The options available are:

- **Water Droplets or Oil Droplets**: The standard temperature for the calibration is 5 °C for water droplets, or 20 °C for oil droplets.
- **Calibrate the Steady Gradient**: Calibrates the steady gradient in order to guarantee a defined magnetic field homogeneity of 0.5 ms. Sample required: CuS04 solution.
- **Calibrate the Gradient Amplitude**: Calibrates the gradient strength [T/m]. Sample required: CuS04 solution.
- **Calibrate the Balance**: Calibrates the pulse gradient balance for pre-defined values of gradient strength. Sample required: Bruker G-Var Balance Calibration sample or a customer sample that fulfills the requirements stated above.
- **Calibration at Standard Temperature**: Upon entering the administrator password, the user can perform the calibration at non-standard temperatures.
- **Balance Deviation Adjustment**: Upon entering the administrator password, the user can define the balance deviation limit.

Click on **OK** and follow the instructions given by the application.

During the balance calibration, the application will check the goodness of the balance fitting. When the minimum criterion is not reached, the application will recommend repeating this calibration step.

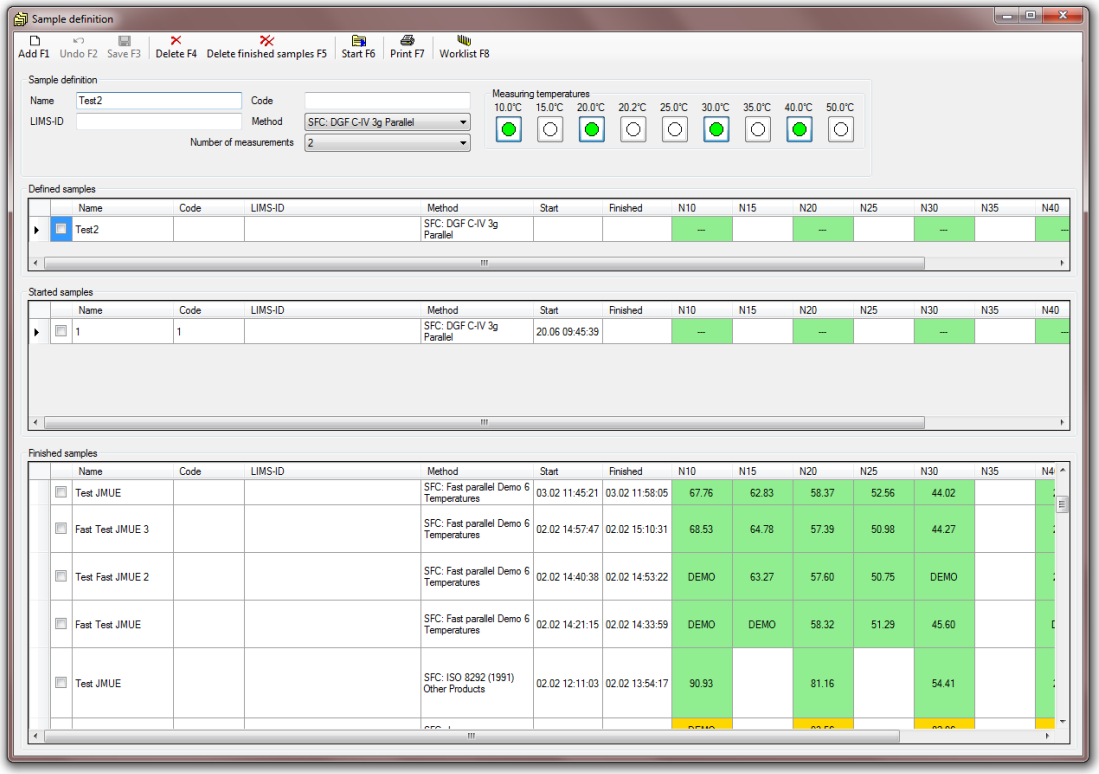
The same calibration can be used either for water droplet measurements or oil droplet measurements. Moreover duplications of the application can use the same calibration file as long as they are created in the same folder where the original application was.

It is recommended to update the calibration every month or whenever the instrument was turned off for long periods.

Once the calibration is done, close the minispec application and open the minispec Automation to perform the measurements in an automated way.

8 Sample Management

To define a sample in Sample Management, select **Samples** from the main toolbar to open the Sample Definition dialog.



The Sample Definition dialog lists all of the current samples which are defined.

For each sample the following information is required:

- Name

  Name of the sample.
- Code

  Code of the sample.
- LIMS-ID

  Unique LIMS-ID, used to export the results automatically to the LIMS.
- Method

  Selection of the method for the actual sample.
- Number of measurements

  Number of complete tempering and measurement cycles.
- Number of samples

  The number of samples which are created if sample data is saved. The sample name is supplemented by a counter, which runs from 1 to the number of samples.
- Measuring temperatures

  If a method was selected, the temperatures for the measurement can be selected or deselected in this area. (see *Principles of Method Creation [▷ 27]*)

The sample data are presented in three groups.

- On the top of the table, all samples which are defined, but not yet started are displayed.
- In the middle all samples which are started, but not yet finished are displayed.
- At the bottom the finished samples are shown. The time period for this display can be defined.

To select multiple samples simultaneously in a group, click in the corresponding checkboxes in front of the sample. To select all samples of a group, click in the header row of the corresponding column.

To show the status of the measurement five colors are used:

- Green:

  The measurement was performed with no errors.
- Yellow:

  During the measurement a time deviation was detected. The delay of the tube is greater than the maximum delay defined in the method. The yellow status is only used in systems with robot automation.

  If the move deviates by more than the predefined maximum delay, then the corresponding measured value is also highlighted in yellow.
- Light orange:

  The measurement was carried out during a temperature deviation, which was outside the predefined temperature limits.
- Orange:

  During the measurement there was a time difference and a temperature deviation that were outside the predefined limits.
- Red:

  The measurement could not be performed.

  If the sample order or the tube was deleted, the robot gripper can not detect the tube, or the intended position for the tube is blocked, the measurement of the tube is aborted and the field for the value is marked in red.

8.1 Define and Edit Samples

To define a new sample:

- Click on the **Add** button or press the **F1** key.
- Enter the sample data.
- Save the changes by clicking on the **Save** button or press the **F3** key.

To cancel the new input click on the **Undo** button or press the **F2** key.

With SFC measurements, the temperature selection display is visible; with non-SFC measurements it is not visible.

The sample name, sample code and the LIMS ID do not need to be unique. Each defined sample is displayed in one line. If you define multiple samples with the same sample name, multiple rows are created using the same sample name. The sample is then selected by selecting the row.

The data for samples that have not started can be changed at any time. To change the data:

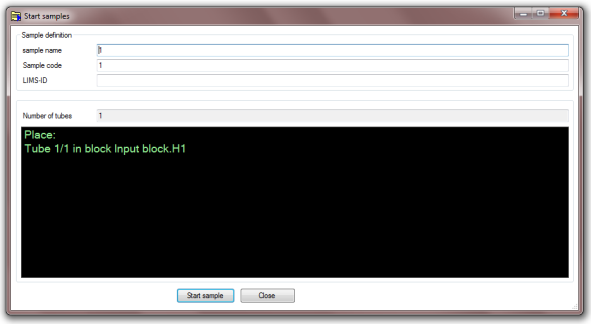
- Select the corresponding sample by clicking on the row in the table.
- Change the data as required.
- Save the changes by clicking on the **Save** button or press the **F2** key.

To cancel the changes click on the **Undo** button or press the **F2** key.

8.2 Start Samples

For systems without robotic automation you can distinguish between a normal **Start** and a **Quick Start**. With Quick Start, the sample is started immediately. With the normal start, the samples are first collected in a batch and only processed every 30 or 60 minutes (collection function).

To start processing a sample, click on the **Start** button, or press the **F6** key.



A dialog opens which shows exactly where to put the tubes of one sample (block and position).

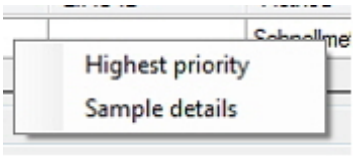
To start another sample:

- Enter the sample data (name, code, LIMS ID) in the dialog.
- Follow the instructions provided.
- Click on the **Start sample** button.

When a robot system is used, the samples are released for processing when the dialog is closed. As long as the dialog remains open, the system will wait before starting additional samples.

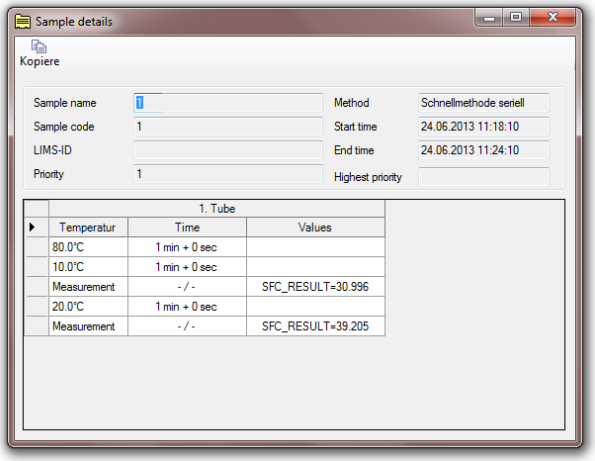
All samples are processed according to the starting sequence and the priority of the method.

To change the priority of the sample processing, right click on the sample row and select the option **Highest priority**.



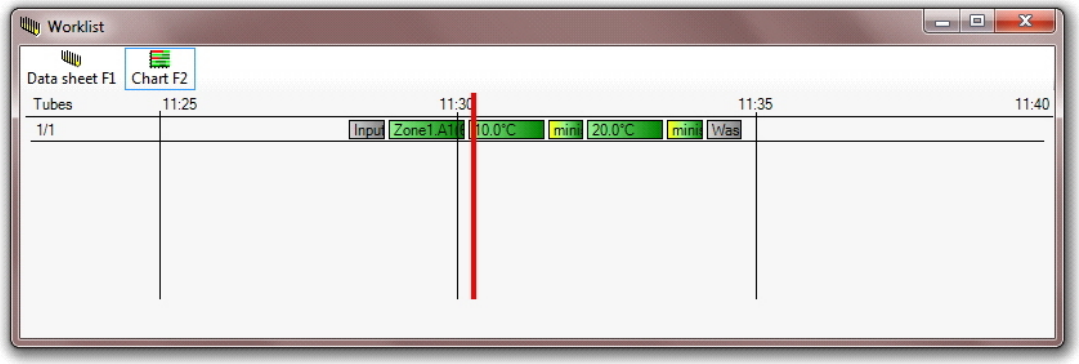
This option is available for a sample as long as there are no defined end times for the sample tubes.

To view details of a sample measurement, right click on the sample row and select the option **Sample details**. The Sample Details dialog opens:



For each tempering step, the target and actual times, as well as the measurements are displayed. For temperature or time deviations the corresponding color codes are used.

Click on the **Work list** button or press the **F8** key to open the work list:



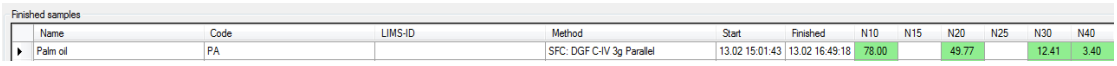
All tubes processed in the system are displayed, including all the tempering and measurement actions that need to be executed. To display the work list as a table, clicking on the **Data sheet** button.

The work list can also be accessed via the main toolbar by selecting **Work list**.

8.3 Performing Sample Measurements

For systems with a robot, the individual sample measurement steps are performed automatically.

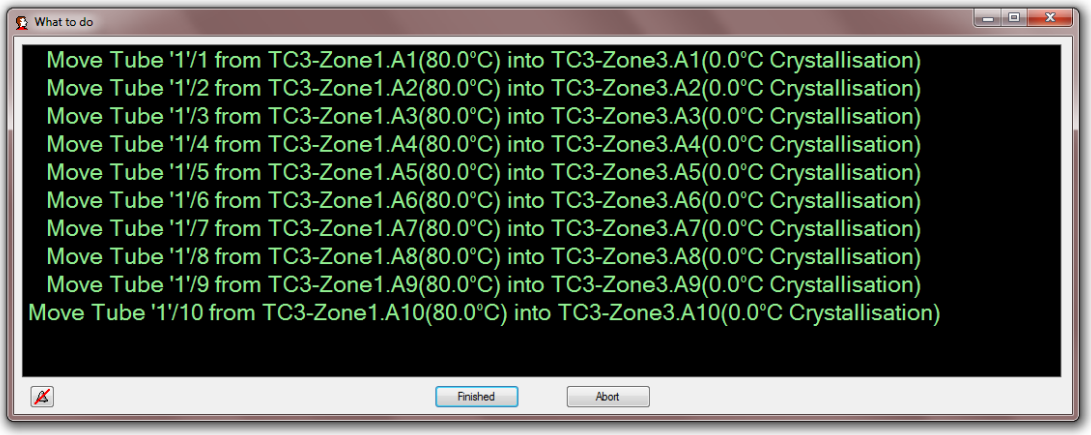
The measured values are immediately displayed in the sample list.


Finished samples

	Name	Code	LIMS-ID	Method	Start	Finished	N10	N15	N20	N25	N30	N40
▸	Palm oil	PA		SFC: DGF C-IV 3g Parallel	13.02 15:01:43	13.02 16:49:18	78.00		49.77		12.41	3.40

For systems without robotic automation, a countdown window is displayed showing when the next individual action will begin.

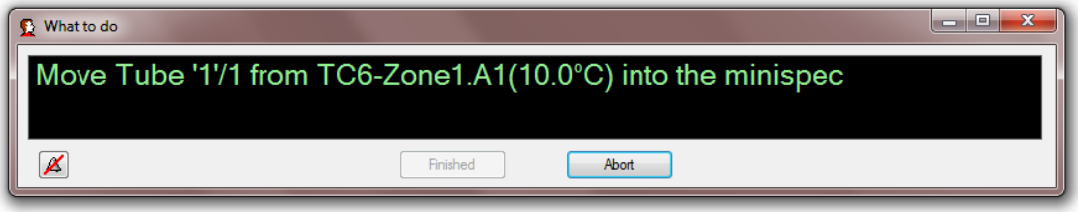
If movements are to be executed, a window appears in which the movements are displayed. In addition, an alarm is used, so that the user is informed of the movement. This can be switched off via the button with the crossed-out bell icon.



The display of the movement actions can be changed using **Master Data** / **Settings**. Here you can select whether to display a list of all the actions, or show the actions step by step.

For experienced users, the list view is recommended because the action list must only be confirmed once using the **FINISHED** button. For inexperienced users, we recommend the single-step display because each movement action is displayed showing the user exactly what to do.

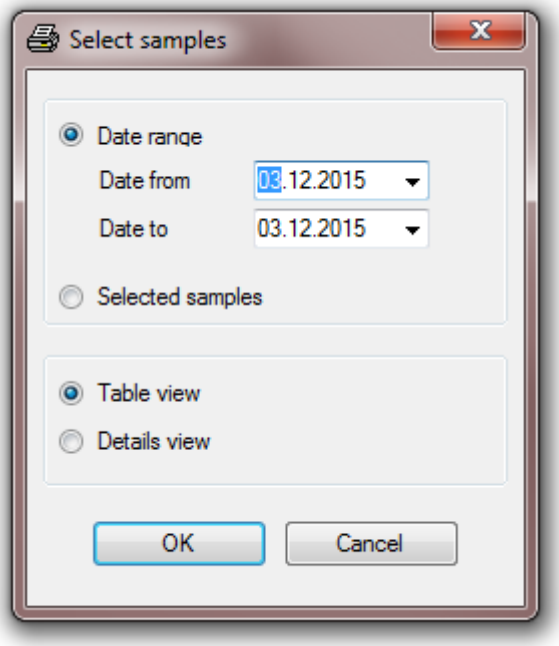
If a tube can no longer be used (for example, because it is broken or leaking), the **ABORT** button needs to be pressed to abort the measurement of this tube. When this happens while using the list view, all actions are redisplayed, step by step, so that the appropriate action can be cancelled.



If the next action is a sample measurement, the action is shown as a single step. After the tube is placed in the minispec, the result is automatically transferred and the next action is displayed. In case of failure the **ABORT** button can be pressed again.

8.4 Print Sample Data

To print finished samples, press the **Print** button or the **F7** key. A dialog to select the data to be printed is displayed:



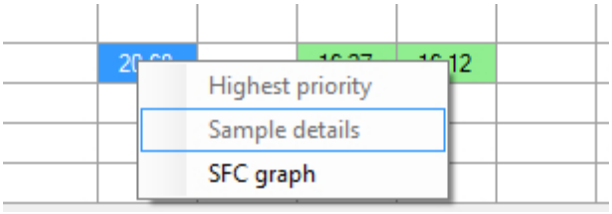
Depending on the currently selected sample(s), the selected sample or all selected samples in a defined time range can be printed. The print out can be selected in table form or with details of the sample data.

8.5 Empty Tube Container

For systems with a robot the used sample tubes are disposed of in a tube container. The tube container should be emptied at regular intervals.

8.6 Displaying the SFC Graph

To display the measured SFC graph, right click on the line with the desired sample in the table of the finished samples. In the menu that opens, click on the menu item **SFC graph**.



A new window with the SFC graph opens (see figure below). In addition, the melting point and the dropping point are estimated from the measured SFC values.

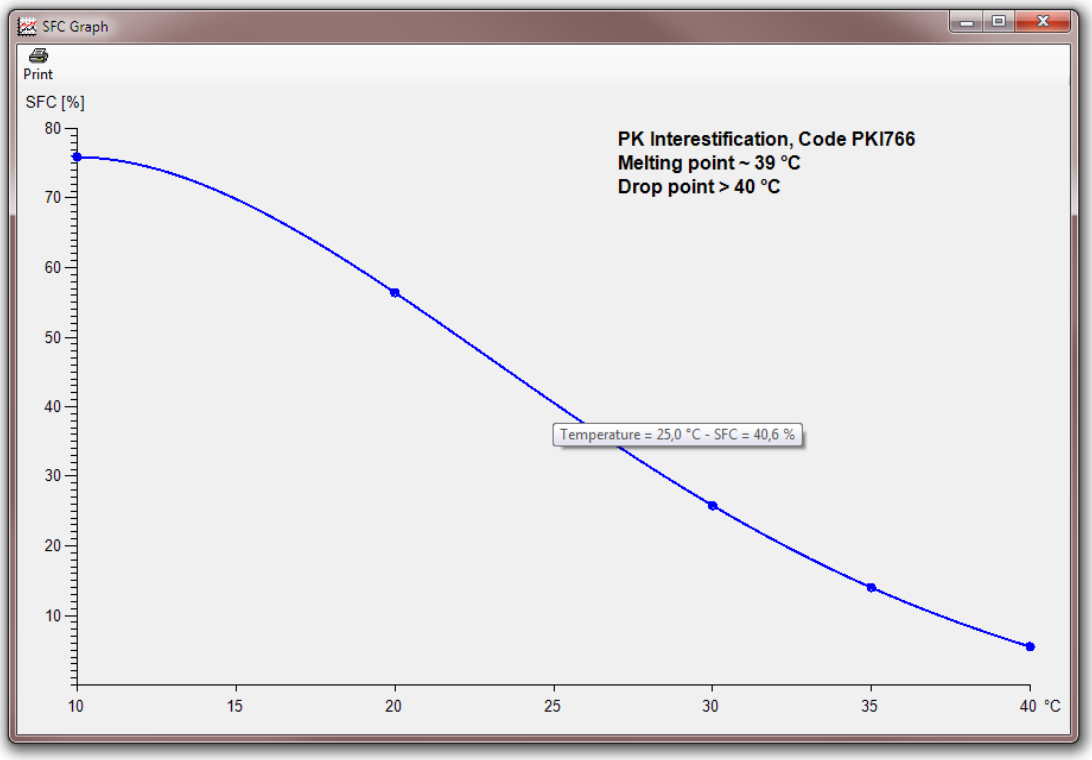
This estimate is based on the fact that the melting point temperature is between 5% and 6% of the SFC value and the dropping point temperature is between 2% and 3% of the SFC value. To estimate the melting point, the software uses the value 5.5%, and for the dropping point 2.5%. Because this procedure is based on experience, the estimated values are not very accurate.

If the highest temperature SFC value measured, for example 40°C, exceeds 6%, the melting and dropping points are indicated as: melting point/dropping point > 40°C.

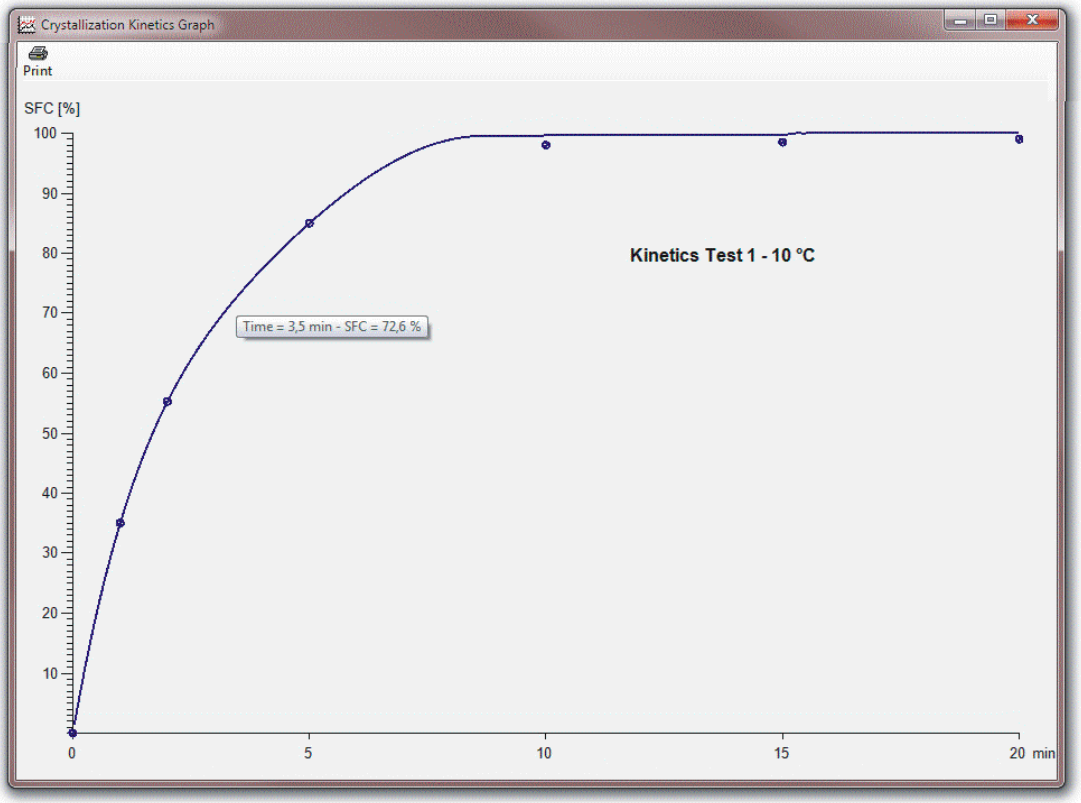
The display can be enlarged or reduced as required by dragging the mouse to the edges of the window.

When you click the mouse on a point on the curve, the temperature and the corresponding SFC value are displayed for that point. This way you can subsequently calculate the SFC values for arbitrary temperatures. These values are interpolated, and only can be calculated within the measured temperature range. Please note that the accuracy of the interpolated values is lower than the measured values.

To print the graph, click on the **Print** symbol.



If the sample is a kinetic method, the graph is shown in a different form (see figure below). This requires that the correct convention is used for the variables (column headings), otherwise the error message **Not enough data points** will be displayed. Again, the intermediate values are displayed by clicking on the curve at the corresponding location.



9 The Weighing Module

For systems with an integrated scale the measurement sequence is carried out according to the following scheme:

- The tare weight of the empty tube is determined by weighing the tube.
- The weighted tubes are assigned to a sample during sample input.

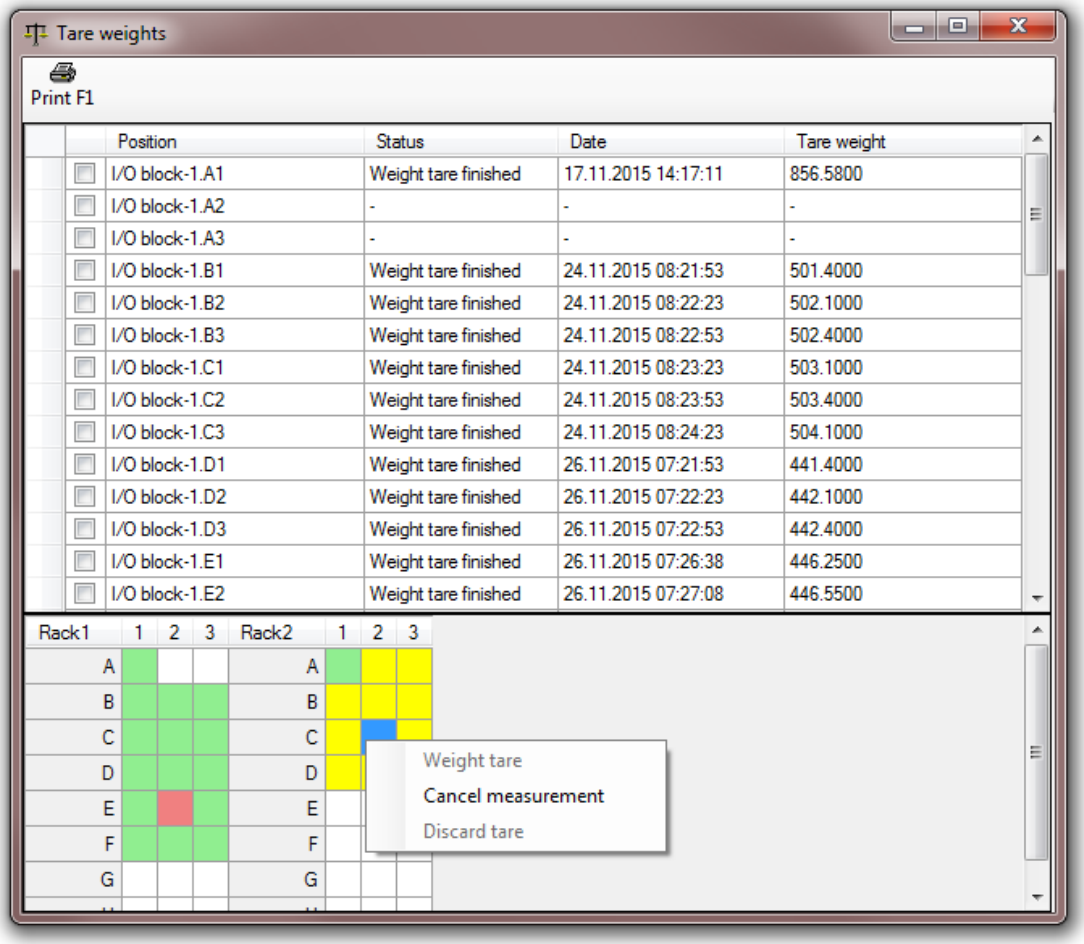
In this case the user specifies the position for the tube.

There are two methods for handling the weighted tubes, which are set at initial installation:

- Tare weight assignment of the weighted tubes based on positions.
- Tare weight assignment of the weighted tubes based on unique tube numbers.

9.1 Tare Weight Assignment Based on Positions

To determine the tare select **Tare Weights** from the left side of the toolbar. The dialog below will open:



In the figure above, the measured tare weights are shown for each position of the input blocks. In the area below all positions of the input blocks are highlighted in color:

- **White**

  The position is free.

- **Yellow**

  The position was selected to determine the tare weight of the tube.

- **Green**

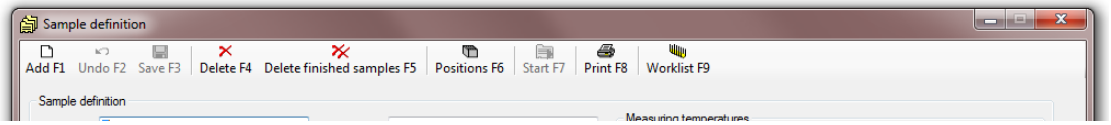
  The tare weight of the tube was determined for the selected position.

- **Red**

  There is a sample tube in the selected position or the position is locked.

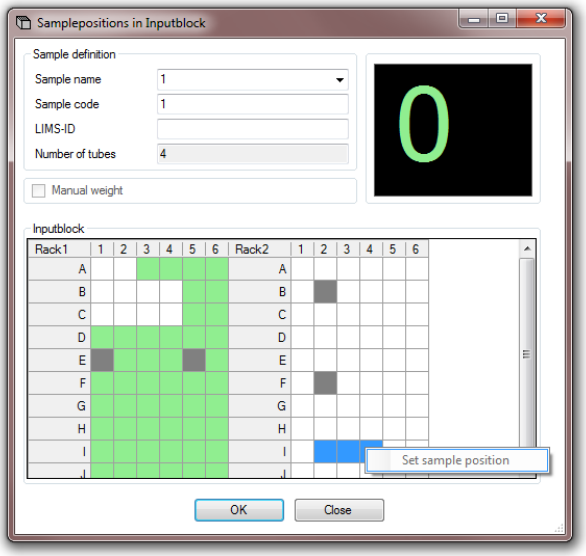
To start the determination of tare weight, select free positions for the weighted tubes by double clicking with the mouse. Alternatively, you can select multiple positions and start the weighing using the right mouse button.

Using the right mouse button will also cancel the measurements or discard the weights.



If tare weights were determined, these can now be assigned to a sample.

To assign positions to samples, select the appropriate sample in the sample window and select the function **Positions**.



At the top of the sample data window the number of current positions to allocate is displayed.

At the bottom of the sample data window the input blocks are displayed. The color highlighting corresponds to the **Tare Weights** window, whereas selected items are grayed out.

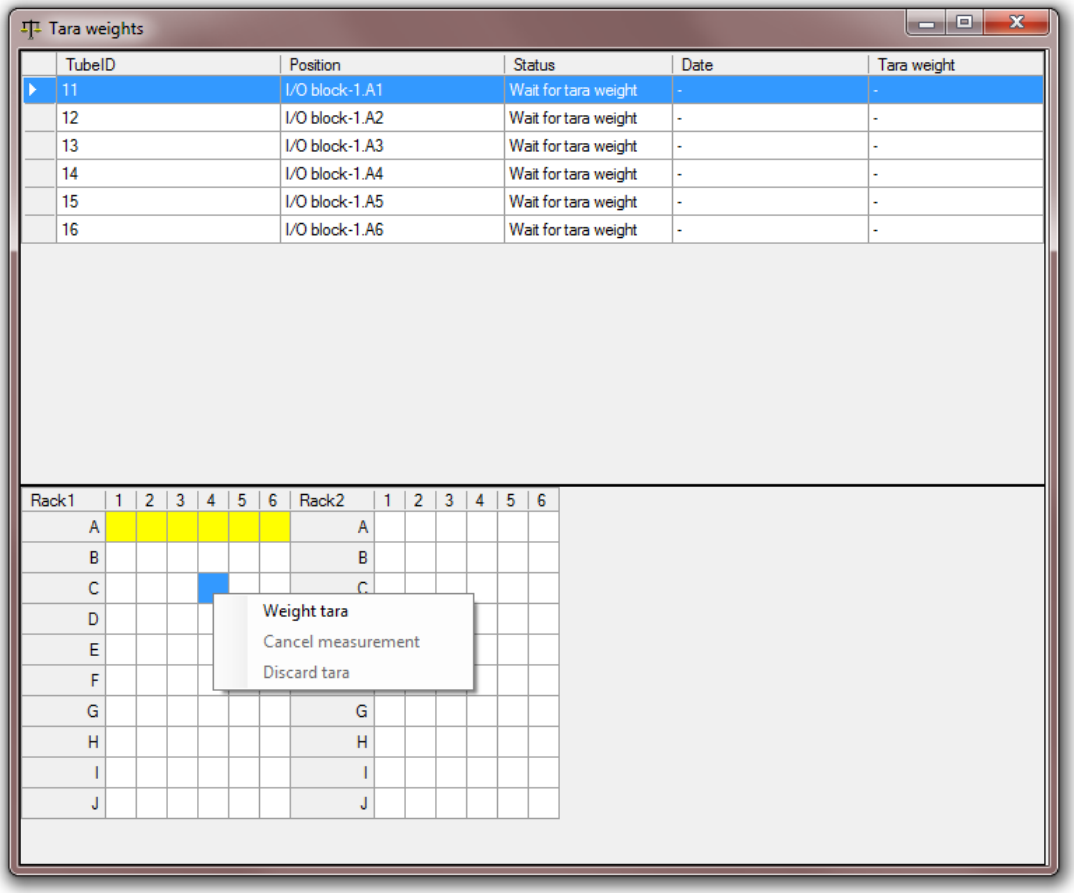
If weight determination is required for the sample, only positions with a finished tare weight (highlighted green) can be selected. If no weight determination is defined in the method, free positions can also be selected.

To select positions, double click on the corresponding position, or select one or more positions, and allocate the position using the right mouse button.

After allocation of the position the sample can be started.

9.2 Tare Weight Assignment Based on Unique Tube Numbers

To determine the tare select **Tare Weights** from the left side of the toolbar. The following dialog will open:



In the table above the last measured tare weight and the position are displayed for each tube. If there is already a new measurement of tare weight in work, this will be displayed accordingly.

In the area below all positions of the input blocks are highlighted in color.

- White

  The position is free.

- Yellow

  The position was selected to determine the tare weight of the tube.

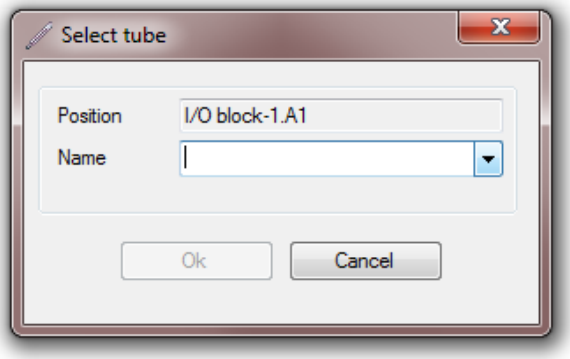
- Red

  There is a sample tube in the selected position or the position is locked.

To start the determination of tare weight, free positions can be selected by double clicking with the mouse. Alternatively you can select multiple positions and start the weighing using the right mouse button.

A list of the selected tare weights can be created using the print function.

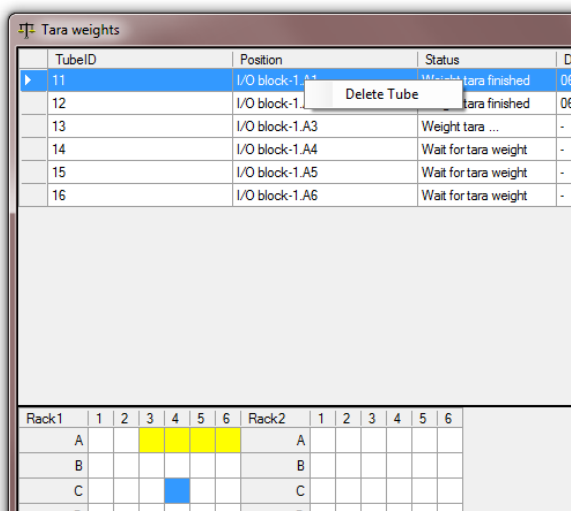
A window for selecting the tube to be measured is displayed for each selected position:



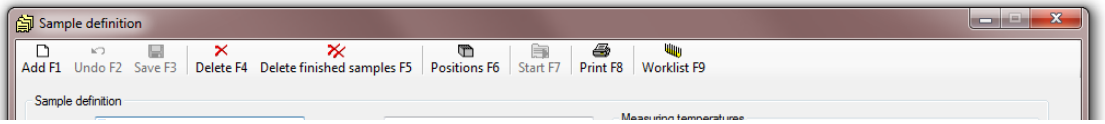
Here an already defined tube can be selected or a new tube can be entered.

Measurements can be canceled using the right mouse button,.

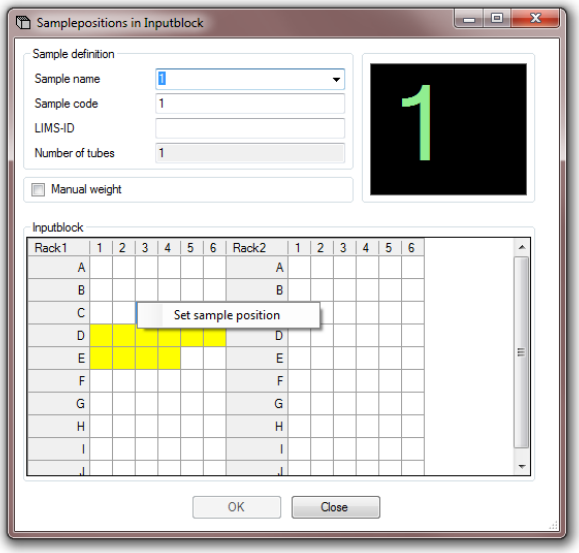
To delete a tube, select a tube in the table and delete using the right mouse button:



If tare weights were determined, these can now be assigned to a sample.



To assign positions to samples, select the appropriate sample in the sample window and select the function **Positions**.



At the top of the dialog window the number of current positions to allocate is displayed.

At the bottom of the sample data window the input blocks are displayed. The color highlighting corresponds to the **Tare Weights** window, whereas selected items are grayed out.

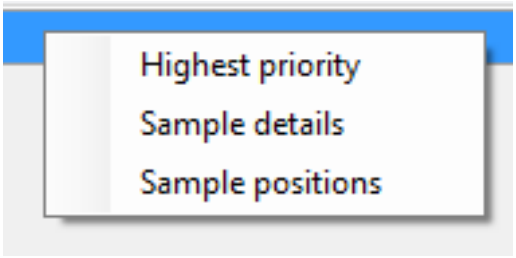
If a weight measurement is required for the sample, only free positions (white) can be selected. If no weight determination is defined in the method, free positions can also be selected.

To select positions, double click on the corresponding position, or select one or more positions, and allocate the position using the right mouse button. For each position a dialog opens allowing the desired tube to be selected.

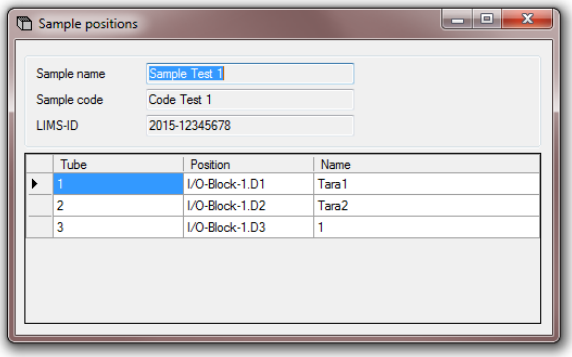
After allocation of the position the sample can be started.

9.3 Displaying Sample Tube Positions

To display the position assigned to a sample, right click on the appropriate sample and select **Sample positions** in the menu:



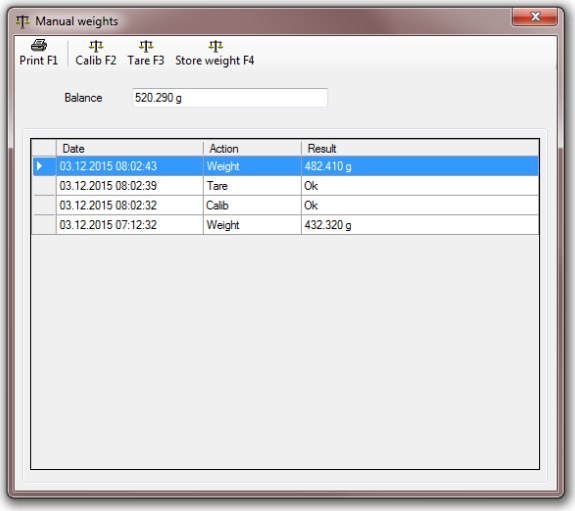
A dialog opens with the sample tubes and the assigned positions. If the option **Unique tube names** is selected, the corresponding names are also shown in the dialog:



9.4 Manual Weighing Operations

To select manual weighing operations click on **Manual Weighing** on the left toolbar.

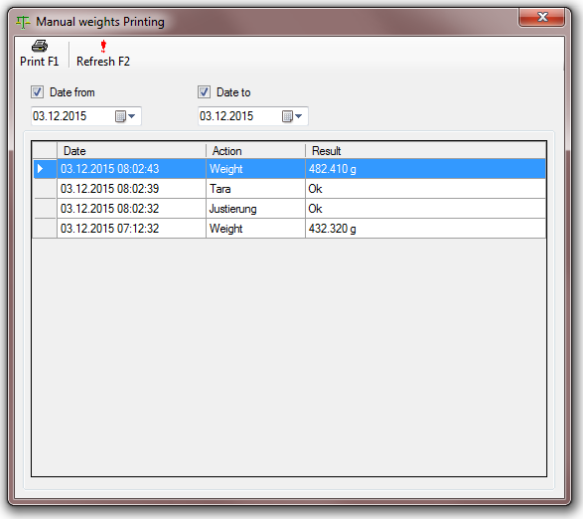
This function can only be executed if currently no automation tasks are at work. As long as the dialog is open, no automation tasks can be performed or started.



The following weighing operations can be performed manually:

- Calibration: The balance performs the adjustment automatically.
- Tare weight: The balance is tared.
- Save weight: The actual measured weight of the balance is saved.

To print the data select the **Print** function.



In the print dialog the data can be filtered by changing the time period.

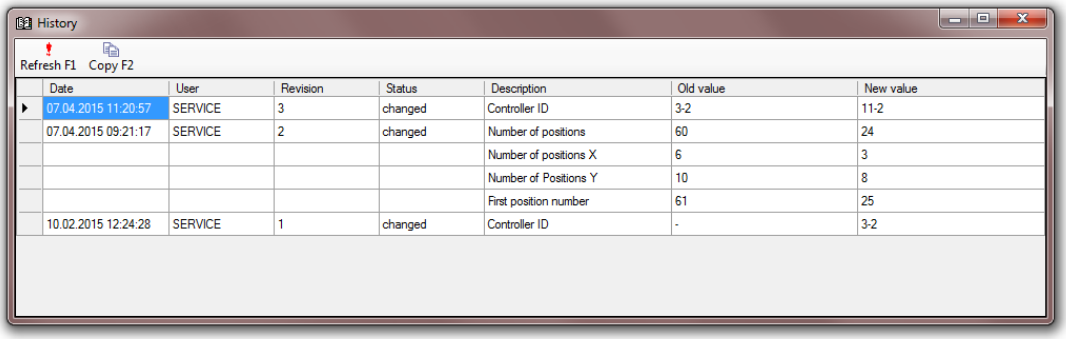
The print data is selected by highlighting the table rows (Windows conform with the Shift/ Control option). Click the **Print** button to start the output.

10 CFR 21 Part 11

With the 21 CFR part 11 option the regulations for this standard can be fulfilled. Any changes in the data are documented and defined password definitions are respected. With this regulation the transfer of the minispec methods to the minispec application has also changed.

10.1 History of Changes

For each record, a history is created, to display the history, press the **History** button:



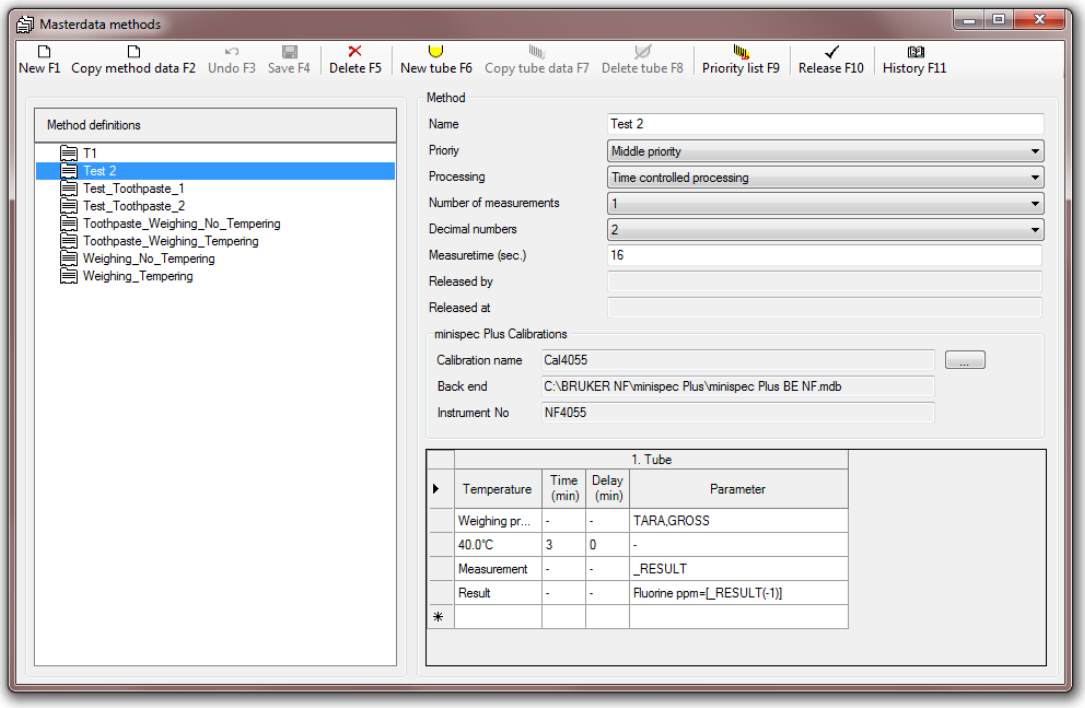
For each record the following changes are shown:

- Who made the change.
- What changed.
- When the change was made.

In each case, the old and the new values are documented.

10.2 Methods

In the method management a calibration of a minispec Plus application must be selected. To do this, a calibration is created in the minispec Plus application and then exported.



The complete settings for the calibration are taken from the export of the minispec Plus application. Note that the calibration is carried out with the same minispec which is used for the actual measurements.

Input a time in seconds in the **Measure time** field which is slightly higher than the actual measurement time. This time value is then reserved for the measuring step. If this value is set too low, subsequent actions in the system are carried out with a time lag. If the value is too high, then there will be unnecessary delays. When adjusting the time, use an increment of 15 seconds.

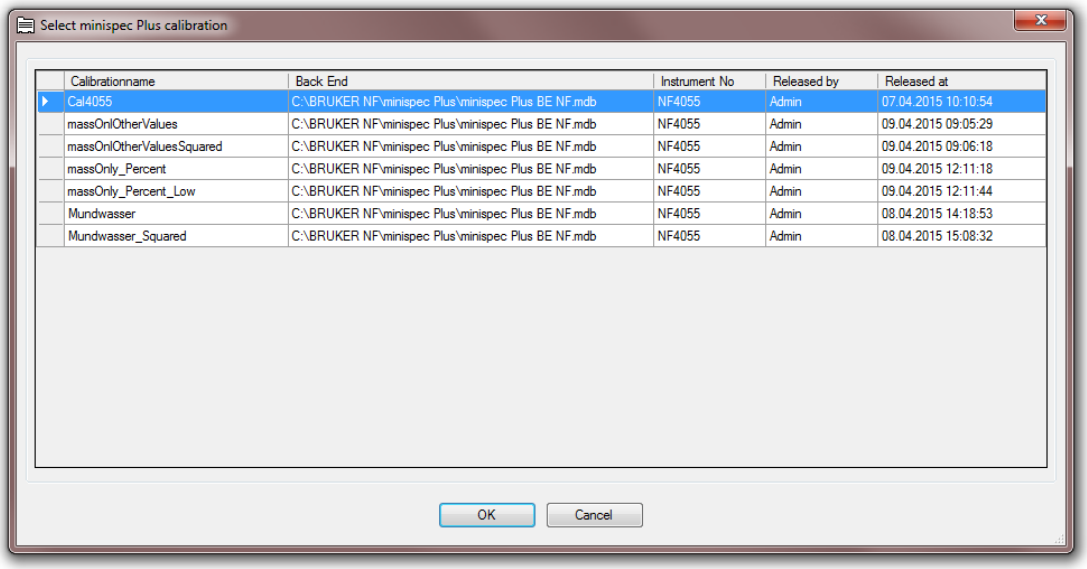
Before using a method enable the method by pressing the **Release** button. After releasing, no changes to the method are possible.

If a released method has to be changed, the first action is to duplicate the method data using the function **Copy method data**. The method data can then be changed and saved under a different name.

For each measuring step, the following additional parameters are available:

- Slope, Intercept: Calculation parameters from the minispec Plus calibration.
- Result1, Result2, Result3: Raw data of the minispec measurement.
- Result: Result of the measurement according to the minispec Plus calibration.

To select the minispec Plus calibration click on the button next to the name of the calibration. A dialog appears with the calibrations provided from minispec Plus:



Click on the desired calibration and press **OK** to select the calibration.

10.3 User Management

New users must create a password during the first login. Each password must be at least 9 characters long. Passwords expire after 90 days.

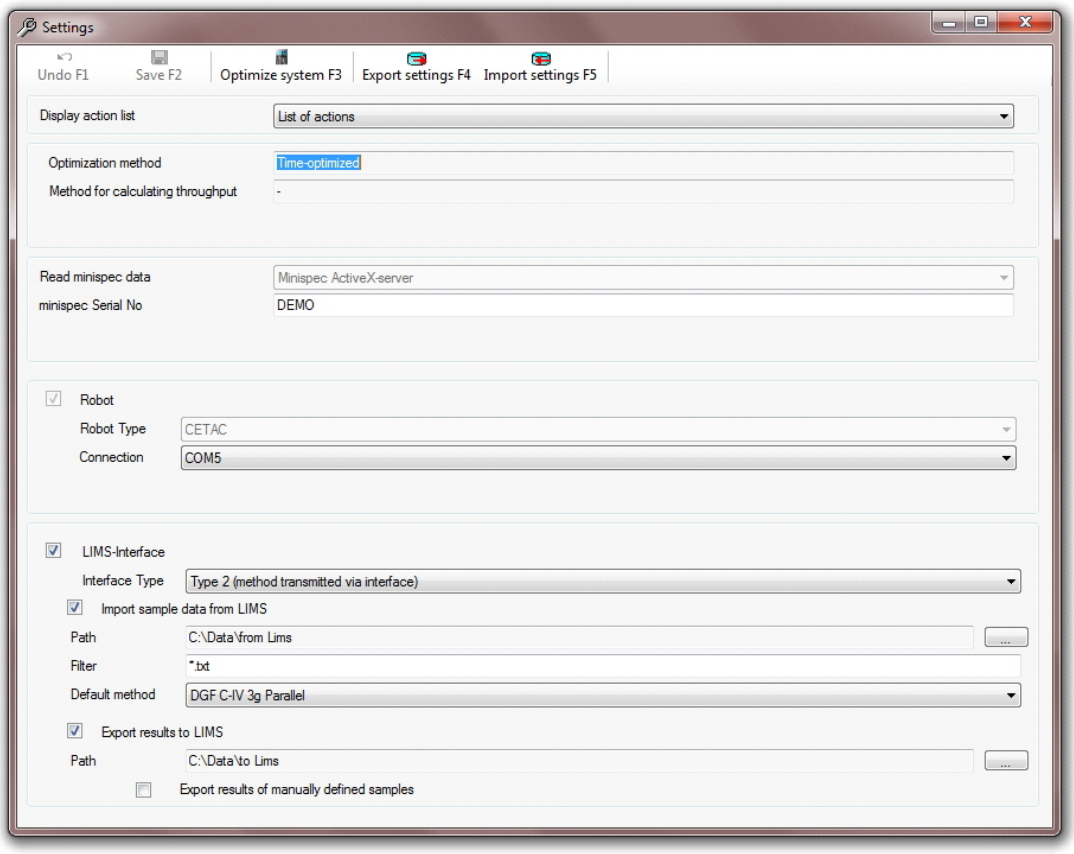
When the password is entered 3 times incorrectly, the account is locked. A reset of the locked account can only be done by the administrator.

CFR 21 Part 11

11 LIMS Interface

A bidirectional LIMS interface is integrated in the software. Sample registrations from the LIMS are imported automatically into the minispec automation software, and results are automatically exported back to the LIMS.

To set the parameters for the LIMS interface select **Master data** / **Settings** from the main toolbar. If the **Settings** dialog is not displayed, expand the master data menu by selecting **Master Data**.



Select **LIMS-Interface** to enable the interface.

11.1 Importing Sample Definitions

To import sample definitions from the LIMS, activate the option **Import sample data from LIMS**.

Path is the directory where the sample data is stored by the LIMS. By specifying a **Filter** such as '*.txt', only the data files corresponding to the filter are imported. The option **Default method** is used to define a method which is used if no method information is imported with the import file, or the imported method is not available.

11.2 Exporting Sample Results

To export the sample results automatically to the LIMS, activate the option **Export results to LIMS**.

Path is the directory where the sample data for the LIMS are stored by the minispec automation software. By default, data is only sent to the LIMS if the sample registration was carried out via the LIMS. If you also want to export the results of manually defined samples, select the option **Export results of manually defined samples**.

11.3 File Format Types

The minispec automation software supports two different file formats, which are described in the following sections.

11.3.1 Type 1 (Standard Method)

The methods for processing the sample tubes are not imported with the sample data. The minispec automation software uses the standard method, but the method can be changed by the user before starting the procedure.

The data import takes place via ASCII files, whereas the name of the file must correspond to the filter, for example **INPUT*.TXT** or ***.***, where * is a wildcard for any string.

Example:

```
[Automation]
031001022-001
Testsample 1
20°C
30°C
40°C
```

Format for the text file:

- The first line must always contain the string **[Automation]**.
- The second line specifies the unique LIMS ID.
- In the third line the sample name is defined.
- If an SFC method was selected, the temperatures for the measurement must be defined in the lines that follow.
- In the lines after this the temperatures for measuring are defined.
  - Each line should contain only one temperature, followed by **°C**.

After a sample is measured, the minispec automation software generates an ASCII file used to export the results to the LIMS.

Example:

```
Automation Output]
031001022-001
Testsample 1
N20:41.21
N30:1.22
N40:-100
```

The name of the file must follow the format **OUTPUT<yymmddhhmmss><counter>.TXT**, whereas **<yymmddhhmmss>** is for year, month, day, hour, minute and **<counter>** is for a serial number.

Format for the text file:

- The first line must always contain the string **[Automation Output]**.
- The second line specifies the unique LIMS ID.
- In the third line the sample name is defined.
- In the next lines the temperatures for measuring are listed, followed by the results being specified:
  - Each line begins with the result-parameter, followed by a colon and the result.
  - The result -100 means that no value could be measured by the minispec.

11.3.2 Type 2 (Method Forwarded)

For each sample the method is transferred from the LIMS. The minispec automation software uses the transferred method to process the sample tubes. If the transferred method is not available, the standard method is used, but the method can be changed by the user before starting the procedure.

The data import takes place via ASCII files.

The name of the file must correspond to the filter, for example **INPUT*.TXT** or ***.*,** where * is a wildcard for any string.

Example:

```
[minispec-Automation]
031001022-001
Testsample 1
DGF C-IV 3g
N20
N30
N40
```

Format for text files:

- The first line must always contain the string **[minispec-Automation]**.
- The second line specifies the unique LIMS ID.
- In the third line the sample name is defined.
- In the fourth line the method is defined.
- If an SFC method was selected, the temperatures for the measurement must be defined in the lines that follow.
- In the lines after this the temperatures for measuring are defined:
  - Each line should contain only one temperature.
  - The line should begin with **'N'**, followed by the temperature.

After a sample is measured, the minispec-automation software generates an ASCII file used to export the results to the LIMS.

Example:

```
[minispec-Automation Output]
031001022-001
Testsample 1
DGF C-IV 3g
N20=41.21
N30=1.22
N40=-100
```

The name of the file must follow the format **OUTPUT<yymmddhhmmss><counter>.TXT**, whereas **<yymmddhhmmss>** is for year, month, day, hour, minute and **<counter>** is for a serial number.

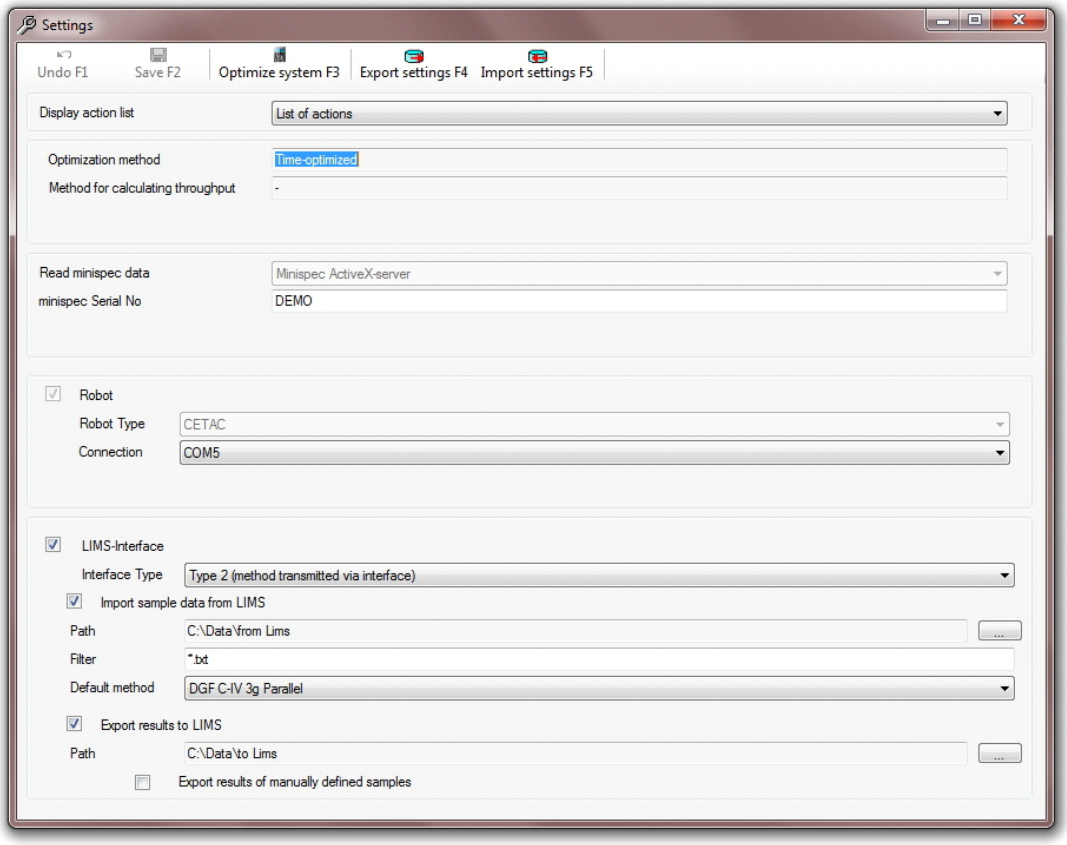
Format for the text file:

- The first line contains always the string **[minispec-Automation Output]**.
- The second line specifies the unique LIMS ID.
- In the third line the sample name is defined.
- In the next lines the results are specified:
  - Each line begins with the result parameter, followed by the equal sign and the result.
  - The result -100 means that no value could be measured by the minispec.

12 System Optimization

When a robot is available, there are two different optimization methods available, which are described in the following sections.

To set the parameters for the optimization, select **Master data** / **Settings from the main toolbar**. If the **Settings** dialog is not displayed, expand the master data menu by double clicking on **Master Data**.



12.1 Throughput Optimization

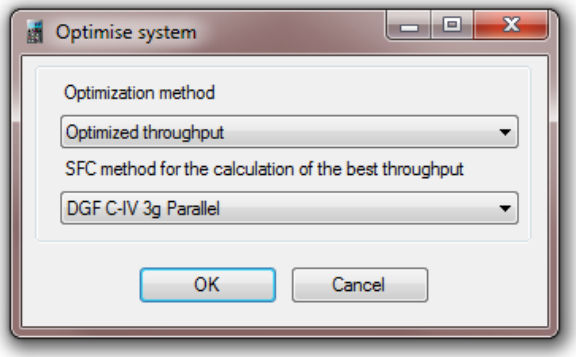
With this method the system is optimized for the highest possible throughput for a selected method.

With this option, the system ensures that new samples can be started at any time. In this case, the system reserves time slots for each execution step of the selected method.

This setting is recommended if you process a large number of samples tubes and mostly use the same method (or methods with the same number of actions from one tempering block to another).

Through the reservation of time slots for each step, the measurement times shift to a reproducible fixed length. This time shift is dependent on the selected method and the speed of the robot system, but is usually less than 1 minute.

To set the optimization parameters, click on the **Optimize system** button or press the **F3** key.



Select the optimization method and the method you want to optimize.

To save the selected parameters click on **OK**.

To discard the settings click on **Cancel**.

12.2 Time Optimization

With time optimization the system is set to the highest level of precision for all time controlled actions.

When this option is used, sample tubes are started as soon as possible, depending on available time slots for tempering blocks and the minispec. This allows you to place a lot of sample tubes in the system, but the processing of the tubes only starts when time slots are available.

This setting is recommended when the maximum possible throughput is not needed and the samples are coming at irregular intervals.

12.3 Selecting the Right Optimization

In general, the following guidelines are recommended when deciding on which optimization method to use.

If you mostly use standard methods, or methods with the same number of actions from one tempering block to another, use the throughput optimization. Samples with different methods reduce the throughput. The disadvantage of this optimization is the time shift (max. 1 minute).

Example:

- Selected method DGF C-IV 3g (4 tempering steps).
- Robot with high speed.

Step No.	Temperature	Method time	Execution time
1	80 °C	5 min.	5 min. 30 sec.
2	60 °C	10 min.	10 min. 45 sec.
3	0 °C	60 min.	61 min. 30 sec.
4	Meas. Temp.	30 min.	30 min. 0 sec.

When the time shift in the standard method can be tolerated, you can still select the option **Time optimization** for other methods. In this case the other methods will have no time shift, which will allow you to achieve a high sample throughput, but this will reduce the number of time slots. This method is recommended for the execution of methods for crystallization kinetics.

Note: If you use many different methods at the same time, it's better to use the option internal **Time optimized**, rather than the **time optimization** option.

If you are constantly using different methods, or if you require a high time accuracy tempering, use the **time optimization** option. With this option the processing time for all the tubes for one sample will depend on the available time slots. In some cases it may be required to put the tubes from the input block into the first tempering block as quickly as possible (e.g., external cooling of the sample in liquid nitrogen). In such a case the Quick Start option must be used. The Quick Start uses the next available time slot to start processing the sample tubes and all other actions are shifted one time slot (max. 1 minute).

Note: With throughput optimized systems, the Quick Start option results in throughput loss because reserved time slots are used for the samples. When using the Quick Start option, the timing accuracy for other samples also cannot be ensured.

13 User Management

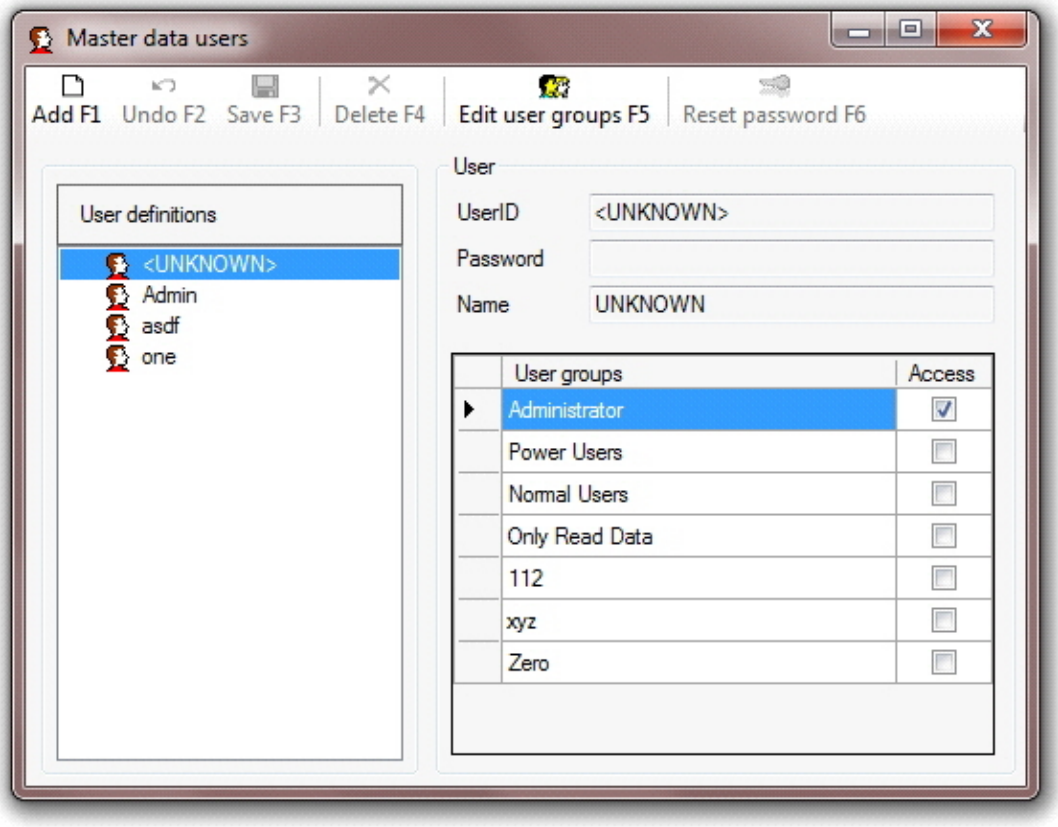
The minispec automation software contains extensive user management for access control.

The access control is based on the following principles:

- Each function within a dialog can be separately enabled for a user. Only those functions that have been enabled can be used by the user. One of the functions available is the write access required for the saving data. The user can only process the data in the selected dialog if the right access is enabled.
- Individual functions used to process the data for a dialog are grouped into user roles. Some user roles are predefined in the software, such as Edit, Delete, Start, etc.
- These user roles are assigned to user groups. Each user group can contain one or more user roles.
- Each user is then assigned to one or more user groups.

13.1 Master Data: Users

To edit the user data select **Master data** / **User management** from the main toolbar. If the **User management** dialog is not displayed, expand the master data menu by double clicking on **Master Data**.



The Master Data users dialog shows all users which are actually managed by the system.

For each user the following information is required:

- UserID

  Unique user identification (may be the same as in Windows).
- Password

  The password should be set by the user. By default the UserID is set as the password.
- Name

  The name of the user.
- User groups

  List of possible user groups for the user.

To modify an existing user, select the desired user from the left table and then make the changes.

After completing the changes click on the **Save** button or press the **F3** key to save your changes. The changes are effective immediately.

To discard the changes, click on the **Undo** button or press the **F2** key.

To define a new user, click on the **Add** button or enter the **F1**key, input the user definitions and save as described above.

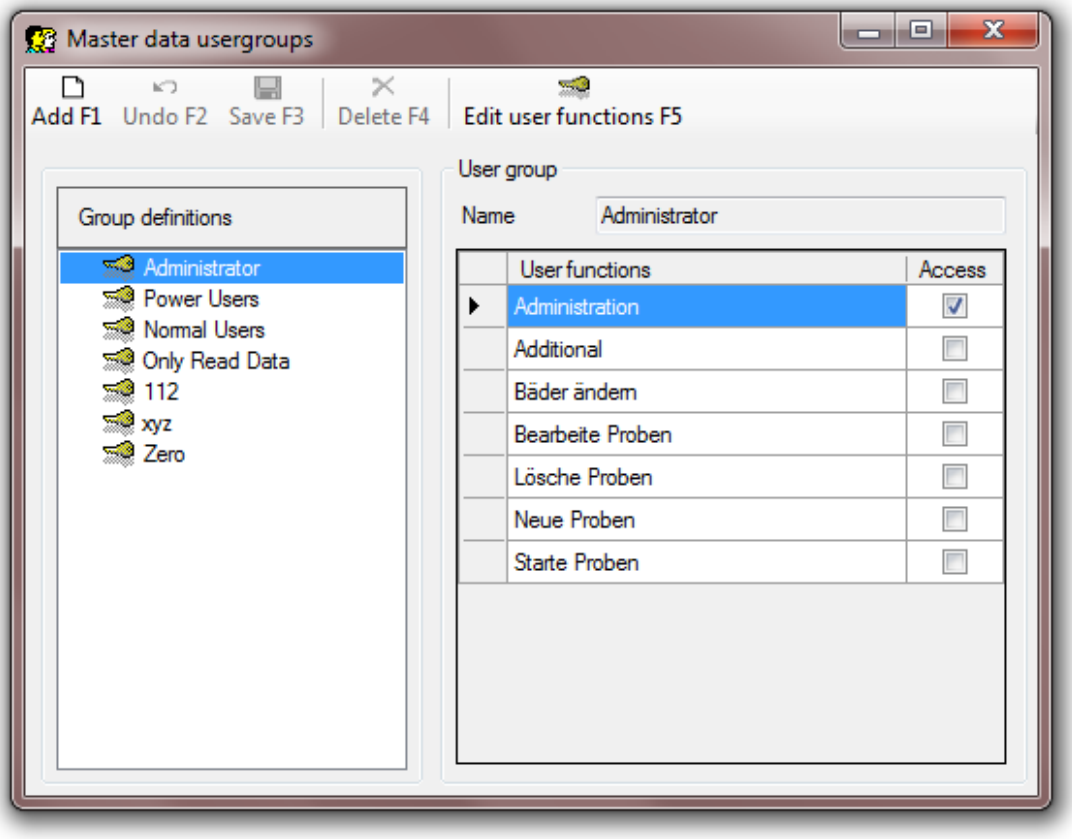
To delete a user, select the desired user from the left table and then click on the **Delete** button or press the **F4** key.

The system is delivered with a default user *UNKNOWN*, which has administrator rights. This user is automatically loaded if no other user is logged into the system.

For information on how to modify user groups refer to *Master Data: User Groups [▶ 67]*.

13.2 Master Data: User Groups

The User Groups dialog shows all user groups which are actually managed by the system.



For each user group, the following information is required:

- Name

  Name of the user group.
- User functions

  Selection of the functions for each user group.

To modify an existing user group, select the desired user group from the left table and then make the changes.

After completing the changes click on the **Save** button or press the **F3** key to save your changes.

To discard the changes, click on the **Undo** button or press the **F2** key.

To define a new user group, click on the **Add** button or press the **F1** key, input the user group definitions and save as described above.

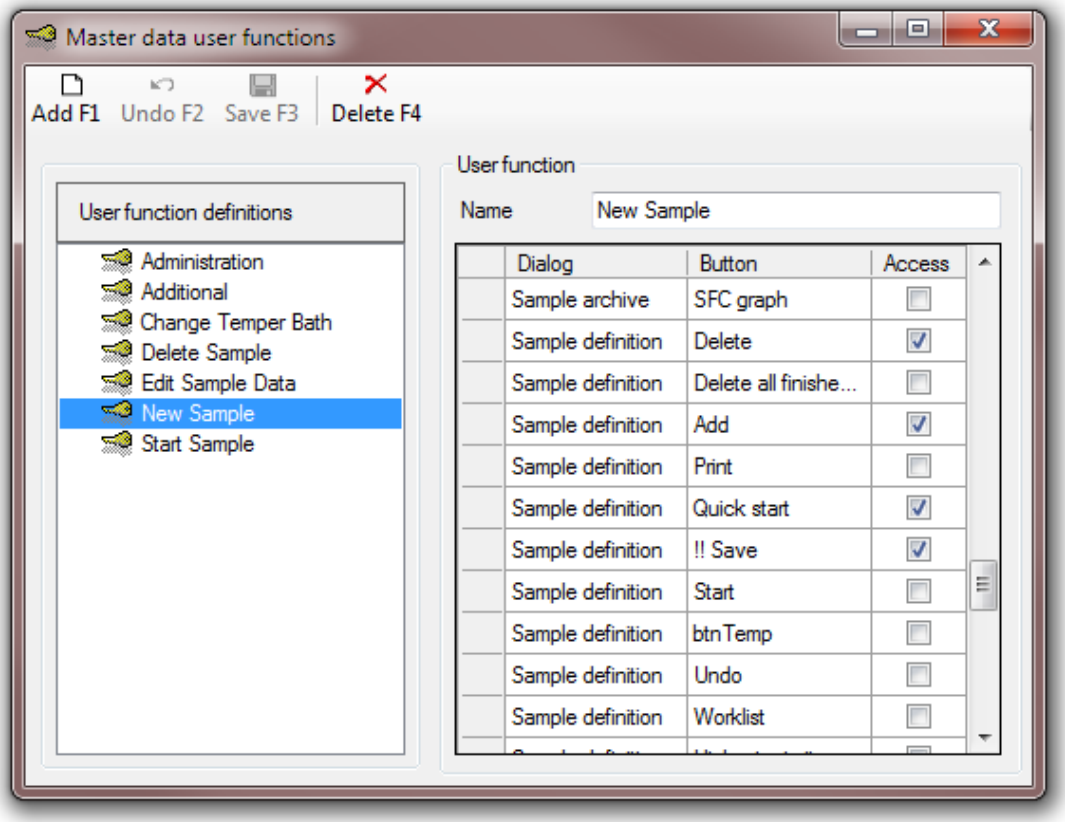
To delete a user, select the desired user from the left table and click on the **Delete** button or press the **F4** key.

There is a special user group **Adminstrator**. This group automatically receives all the rights for the complete system.

For information on how to edit user functions refer to *Master Data: User Functions [▶ 68]*.

13.3 Master Data: User Functions

The User Functions dialog lists all of the user functions which are managed by the system.



For each user function the following information is required:

- Name

  Name of the user function.

- Selection of functions

  The functions for each dialog are defined in the table. A function that requires write access (e.g. **Save**) is marked with two exclamation marks before the name.

To modify an existing function, select the desired function from the left table and make the changes.

After completing the changes click on the **Save** button or press the **F3** key to save your changes.

To discard the changes, click on the **Undo** button or press the **F2** key.

To define a new user function, click on the **Add** button or enter the **F1** key, input the function definitions, and save as described above.

To delete a function, select the desired function from the left table and click on the **Delete** button or press the **F4** key.

There is a special user function **ADMINISTRATION**. This function automatically receives all the rights for the complete system.

14 Examples of Methods

14.1 Example 1

Line	Temperature	Time	Delay	Parameter
1	80°C	5	0	
2	60°C	10	0	
3	0°C	60	0	
4	10°C	30	0	
5	Measurement	-	-	SFC-RESULT
6	Result	-	-	N[_Temp(-2)]=[SFC-RESULT(-1)] {2}

In line 5 the result value of the measurement is saved in the minispec-application under the parameter SFC-RESULT.

In line 6, the final result is calculated:

- N[_temp(-2)] means that the name of the result variable begins with 'N', followed by the formula in brackets. In the example _temp(-2) indicates that the temperature value is two rows above (-2). In the example the temperature value is 10 (line 4).
- The result is a formula (indicated by brackets), containing the parameter SFC-Result. The parameter (-1) indicates that SFC-Result is defined up one line.
- The {2} indicates that the result is shown with two decimals independent of the defined decimals in the method.

14.2 Example 2

Line	Temperature	Parameter
1	Weighing	GROSS
2	20°C	
3	Measurement	WEIGHT<[GROSS(-2)],EAA
4	Result	OIL=[EAA(-1)]

In the first line a weighing parameter is defined. If no scale is available, the parameter value for the weighing result is always requested when starting the sample, regardless in which line of the method the weighing parameter is defined.

In the next line, a temperature for storing the sample is defined.

In line 3 is the measurement, whereas:

WEIGHT<[GROSS(-2)] means the parameter WEIGHT in the minispec application uses the parameter GROSS defined two lines above (-2).

The value of the measurement is saved in the parameter EAA of the minispec application.

In the line 4 the result is defined as a formula:

OIL=[EAA(-1)] means that the name of the result is OIL and is obtained from the measured parameter EAA, which is defined one line above (-1).

14.3 Example 3

Line	Temperature	Parameter
1	Weighing	TARA
2	20°C	
3	Weighing	GROSS
4	Measurement	WEIGHT<GROSS(-1)-TARA(-3)],EAA
5	Result	OIL=[EAA(-1)]

In this example two weighing's, TARA and GROSS, are carried out. If no scale is available, both parameter values for the weighing result are requested when starting the sample, regardless in which line of the method the weighing is defined.

In the next line, a temperature for storing the sample is defined.

The next line is the measurement, whereas:

WEIGHT<GROSS(-1)-TARA(-3)] means the parameter WEIGHT in the minispec application is using the two parameters GROSS, defined one line above (-1) and TARA, defined three lines above (-3), to calculate the net weight.

The value of the net weight is saved in the parameter EAA of the minispec application.

In line 5 the result is defined as a formula:

OIL=[EAA(-1)] means that the name of the result is OIL and is obtained from the measured parameter EAA, which is defined one line above (-1).

15 Software Bugs

The software was developed with great care, nevertheless it is still possible that an error may occur.

When a software error occurs, a message is displayed on the screen and the error is documented in a corresponding log file.

The user must now decide whether to continue working despite the error. Depending on the error, other errors may also occur. In worst case, an error may lead to glass breakage in the system.

If it is not clear why the error occurred, we recommend that the software be stopped and restarted.

If the actual sample workflow cannot be read, the sample data will be deleted when the software reboots.

The error log where the error is documented is named **Error.log** and is placed in the folder for user files (see *Installation [▶ 11]*). Typically this is in the folder:

```
c:\programdata\minispec-Automation\error.log
```

To obtain technical support, send the **Error.log** file to *minispec.SLS@bruker.com*.

Be sure to include a brief description of what was being done when the error occurred. With this information Bruker service will typically be able to understand how this error could be caused.

It may also be necessary that the Bruker service will ask for additional information. Typically in this case the complete folder “minispec-Automation” located in the directory below should be e-mailed to the Bruker service team at *minispec.SLS@bruker.com*:

```
c:\programdata\minispec-Automation
```

Software Bugs

16 Contact

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Bruker BioSpin Hotlines

Contact our Bruker BioSpin service centers.

Bruker BioSpin provides dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

Please select the service center or hotline you wish to contact from our list available at:

https://www.bruker.com/service/information-communication/helpdesk.html

Contact

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