

Bruker BioSpin

PrepGilsonST

Preparation Gilson with SampleTrack
User Guide - Version 004

NMR

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P/N: Z31695 DWG-Nr.: 1402004

Contents

	Contents	3
1	Introduction	7
1.1	Introduction	7
1.2	Warnings and Notes	
1.2	Note on SPE Tube Transfer and 1 mm Applications	
1.3	Contact for Additional Technical Assistance	
2	Menus	9
2.1	The Main Menu	9
2.2	File Menu Commands	
	Application Settings	
	Open Current Session	
	Open Old Session	
	Save As	
	Save Current Protocol (log) Files	
	Open Print Dialog	
	Compare Procedures Dialog Box	
	Configuration Save/Load	
	Exit	13
2.3	Edit Settings Menu	. 14
	For Applications with SampleTrack (Profiler, Samp	le-
	Track)	14
	For Applications without SampleTrack (Easy, SPE	TT)
		15
2.4	Preparation Menu Commands	16
	Start Preparation Automation	17
	For Applications without SampleTrack (Easy, SPE	TT)
		17
	For Applications with SampleTrack (Profiler and Sa	am-
	pleTrack)	
	Start Verify Test Loop for All Orders	18
	For Applications without SampleTrack (Easy, SPE	
		18
	For Applications with SampleTrack (Profiler and Sa	am-
	pleTrack)	
	Preparation Pause	18
	Continue	
	End After Current Order	19
	Abort Current Order	
2.5	Service Tools Menu Commands	
	Initialize Gilson	20
	Initialize Pump	20

	Initialize + Home Gilson	
	Read Barcodes	
	Create New Orders Dialog Box	
	Create Orders SPE Tube Transfer	
	Load Orders and Verify	
	Prepare Orders	
	Copy Orders Back From\in\save\	
	Modify Procedure	
	Delete Map: Source/Destination Matrix	
	Connect Gilson	
	Delete all Orders and Protocols in ST folders	
	Test	
	Check Positions in Tray	
2.6	Clean Procedures Menu Commands	
	Clean Needle	
	Prime Dilutor	
	Prime Inject Port	
	Set ValveMate Default Solvent Position	
0.7	Modify Clean Procedures	
2.7	View Menu Commands	
	Toolbar	
	Status Bar	
	Modify Procedure	
	Configuration	
	Tray View	
	View Main Protocol FileView Current Protocol File	
	Error History Procedure Step View	
2.8	Help Menu Commands	
2.0	Help Topics	
	Help 1MM Application	
	About	
	About	
3	Start Selections	35
3.1	Defining Procedure Type	35
3.2	Default Procedure Selection	
4	Configuration	27
-	Configuration	
4.1	Open Configuration View	
4.2	Base Configuration	
4.3	Gilson Liquid Handler 215 Configuration	
	Default Files Configuration	
	Execution Mode Configuration	
4.4	Dilutor Configuration	
4.5	Working Area Configuration	
	For Applications with SampleTrack (Profiler, Sa	
	Track)	
	For Applications without SampleTrack (Easy, S	
		44

	Tray File Configuration	
	Adding Rack Tubes to a Zone	
	Remove Racks from the Tray	
	Solvents in Tray Configuration	
	Reagent in Tray Configuration	
	Barcode Zone Configuration	
	Defining Barcode Defined Racks	
	Checking Barcode Rack Information	
	Ports in Tray Configuration	
4.6	Z-Tower Configuration	
4.7	Solvent Names Configuration	
4.8	Valve & Carillan Configuration	
4.9	Valves & Capillary Configuration	
4.10	Gilson Cover & LED Configuration	55
5	The Rack Editor	57
5.1	Opening the Rack Editor	57
5.2	Rack Selection	
	Carrier Selection	59
5.3	Creating a New Rack	60
	Deleting a Rack	61
5.4	Bruker or Custom Racks	62
	Bruker Racks:	62
	Custom Racks:	
5.5	Modifying Racks	62
5.6	Service Tools	64
6	Preparation Data Files	65
6.1	Data Directory Structures	65
0.1	Main Folder	
	Configuration Files Directory	
	Preparation Procedure Files Directory	
	Temporary Settings Files	
	Temporary Protocol Files	
6.2	Viewing Preparation Procedure Data Files	
6.3	Protocol Files	
7	Order Files	69
7.1	Directory Structure of Order Files	
7.1	Main Directory	
	Input Order Files Directory	
	Output Order Files Directory	
	Order Protocol Files Directory	
7.2	Viewing Order Files	
8	Solvents	79
8.1	Defining Solvents for Preparation Defining External NMR Solvents	
8.2		

Contents

9	Edit Procedures	75
9.1	Modifying TASK Procedures	75
9.2	TASK Procedures	
	Common TASK dialog box Elements	75
9.3	Types of TASK Procedures	76
	Task Procedure Wash	76
	Task Procedure Clean	77
	Automatic Cleaning	77
	Task Procedure Add	78
	Task Procedure Dispense	79
	Task Procedure Mix	80
	Task Procedure 1MM Samples	80
9.4	Modifying the Procedure Dialog Box	81
10	Test/Service Tips	83
10.1	Service Information	83
A	How To	85
A.1	Introduction	85
A.2	Define Application Type	
A.3	Create Orders	
A.4	Modify Task Procedures	
A.5	Insert Racks	
	Inserting a New Rack	
A.6	Insert Racks with Barcode Simulation	
A.7	Adding Zones and Tubes to a Zone	
	Adding a Zone Manually	
	Adding Tubes to a Zone Manually	
	Removing Tubes from a Zone Manually	
	Adding Zones and Tubes Automatically	
A.8	Define Sort Orders	
	Figures	95
	Tables	97

Introduction

Introduction 1.1

Preparation Gilson + SampleTrack (PrepGilsonST) is a sample preparation program which controls a Gilson "215" or "235" instrument with additional "8xx" valves and "ValveMate".

Predefined preparation step procedures can be modified by the user and will be executed.

Depending on the application type, a barcode reader identification can be used and orders can be defined by the "SampleTrack" program.

The type of destination racks can be specified and used to define destination positions automatically.

When SampleTrack is not used, the user can create orders when defining source samples, procedures, and push solvents.



Note: Throughout this manual Preparation Gilson + SampleTrack will simply be referred to as ${\bf PrepGilsonST}$.

Warnings and Notes

1.2

There are two types of information notices used in this manual. These notices highlight important information or warn the user of a potentially dangerous situation. The following notices will have the same level of importance throughout this manual.



Note: Indicates important information or helpful hints



WARNING: Indicates the possibility of severe personal injury, loss of life or equipment damage if the instructions are not followed.

Note on SPE Tube Transfer and 1 mm Applications

1.2.1

For information on the "SPE-TT System" refer to the manual SPE-TT system Installation and Users Manual for Solid Phase Extraction Tube Transfer Systems available from Bruker.

For additional help on 1 mm applications, refer to the online help included with the PrepGilsonST program.

Contact for Additional Technical Assistance

1.3

For further technical assistance on the PrepGilsonST, please do not hesitate to contact your nearest BRUKER dealer or contact us directly at:

BRUKER BioSpin GMBH am Silberstreifen D-76287 Rheinstetten Germany

Phone: + 49 721 5161 0 FAX: + 49 721 5171 01

E-mail: martin-beck@bruker-biospin.de

Internet: www.bruker.de

Menus 2

The Main Menu 2.1

The main menu consists of:

"File Menu Commands"

"Edit Settings Menu"

"Preparation Menu Commands"

"Service Tools Menu Commands"

"Clean Procedures Menu Commands"

"View Menu Commands"

"Help Menu Commands"

File Menu Commands

2.2

The File menu offers the following commands:

Table 2.1. The File Menu Commands

Application Settings	Open Current Session	Opens the current session file curr_session.pgi.
	Open Old Session	Opens an old session file *.pgi
	SaveAs	Saves the current session file under a different file name.
Save Current Protocol (log) Files		Saves the current protocol files.
Open Print Dialog		Opens the print dialog box allowing selection of print options for the current order protocol.
Compare Procedures Dialog		Opens a dialog box allowing the comparision of procedures.
Configuration save/load		Used to backup and reload coniguration files *.cfg and *.735.
Exit		Exits the PrepGilsonST program.

Open Current Session

Use this command to reload the current session (settings) file (**curr_session.pgi**) after checking an old session file.

The current session file is loaded automatically when the program is opened and the application type is selected (see <u>"Default Procedure Selection" on page 35</u>).

The name of the current session file is visible in the caption of the main window. The content of the current session file can be viewed in the Edit Settings dialog box (see <u>"Edit Settings Menu"</u>).

Shortcut Keys: CTRL+O

Open Old Session

Use this command to open an old session file (*.pgi) in the PrepGilsonST program.

This is used only to view the old session file contents in the <u>"Edit Settings Menu"</u>. Several menus will be disabled and the contents cannot be changed and saved. After opening an old session the program should be closed and reopened for automatic preparation.

The name of the current session file of the selected application will remain visible in the caption of the main window.

Save ... As

Use this command to save the active session as a file with another name (only used for checking the settings at later time!).

PrepGilsonST displays the Save As dialog box so you can name the file.

Save Current Protocol (... log) Files

2.2.2

Saves the current protocol files. During this procedure a copy of the current protocol files are produced as follows:

log_current.log saved to ...\G215Data\Exec\saved_log_current.log

log_exec.log saved to ...\G215Data\Exec\saved_log_exec.log

A copy of the session file is also made:

curr_session.pgi saved to ...\G215Data\Exec\saved_curr_session.pgi

Open Print Dialog

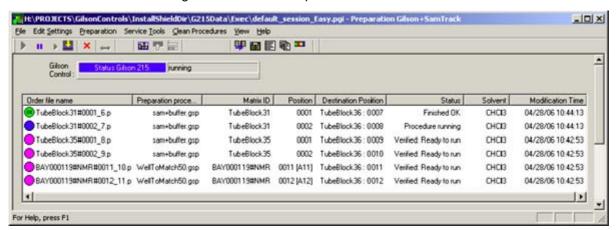
2.2.3

Selecting this menu option will open the **Print Order List** dialog box where all information for the automatically generated print list can be selected:

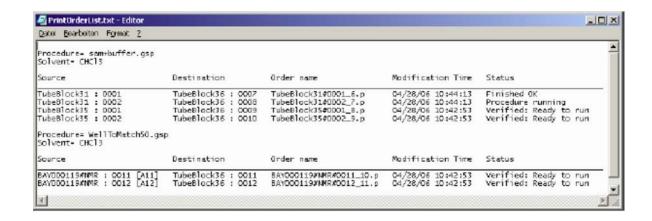


Figure 2.1. Print Order List Dialog Box

For each header combination of procedure files and solvents, one separate list will be generated. For example for the order list...



...the following print list will be generated, saved in the PrintOrderList.txt file and then be displayed in the Notepad program.



The Print List will be saved in the default print file:

[Order Folder]\bstsdata\gilson\out\protocol\PrintOrderList.txt (when running with SampleTrack)

[Order Folder]\bstsdata\gilson\out_no_ST\protocol\PrintOrderList.txt (when running without SampleTrack)

Compare Procedures Dialog Box

2.2.4

With the Checkbox "Compare folders" disabled, two single procedures can be compared.

With the Checkbox "Compare folders" enabled, all procedures of the selected folder can be compared.

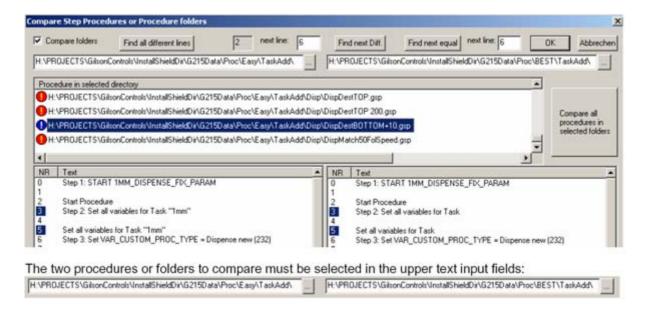


Figure 2.2. Compare Step Procedures Dialog Box

When comparing all procedures in two folders the color in the Procedure List shows the procedure status:

- Green: No differences between the procedure in first and second folder.
- **Blue**: Differences detected between the procedure in first and second folder.
- Red: The procedure in the first folder does not exist in the second folder.

In the two procedure text boxes for the first (left) and the second folder (right) different lines of the selected procedure are displayed "blue" (in the column "NR"), e.g. line 3 and 5 in the example.

Configuration Save/Load

2.2.5

Backups and reloads the configuration files *.cfg and *.735 of the current application in the working folder [Install Folder Data]\G215Data\Config\.

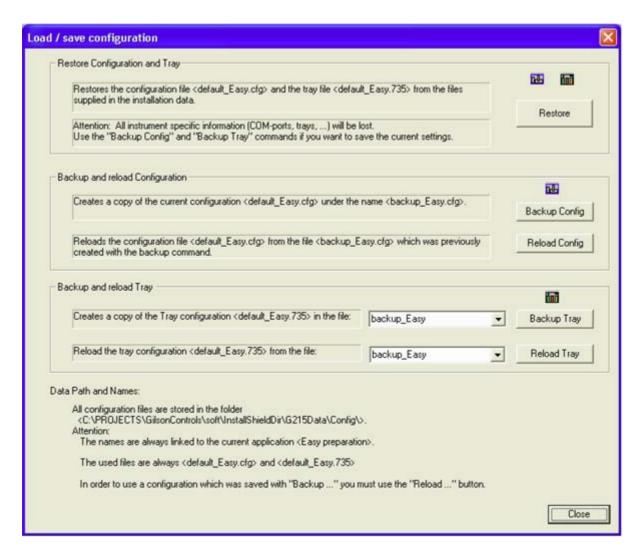


Figure 2.3. The Load/Save Configuration Dialog Box

Default config files for each Application are written at Installation time into the Install folder: [Install Folder Data]\G215Data\Config\Restore\

When starting an Application the program is checking if config files are existing in the working folder: [Install Folder Data]\G215Data\Config\

If there are no files found, a copy of the default files from the Install folder ...\Restore\ will be moved automatically into the working folder.

Note: For applications with SampleTrack (Profiler, SampleTrack) the tray configuration is grayed (only automatically changeable using the barcode reader).

Exit 2.2.6

Exits the PrepGilsonST session. You can also use the **Close** command on the application control menu. The program will prompt you to save documents with any unsaved changes if applicable.

Shortcuts: Double-click the applications control menu button, or click on the close button, or prest ALT + F4.

Edit Settings Menu

2.3

For Applications with SampleTrack (Profiler, SampleTrack)

The **Edit Settings** menu opens the Edit Settings dialog box from SampleTrack where the following preparation modes can be defined:

- Web service server URL.
- Procedure export folder.
- SampleTrack order folder.

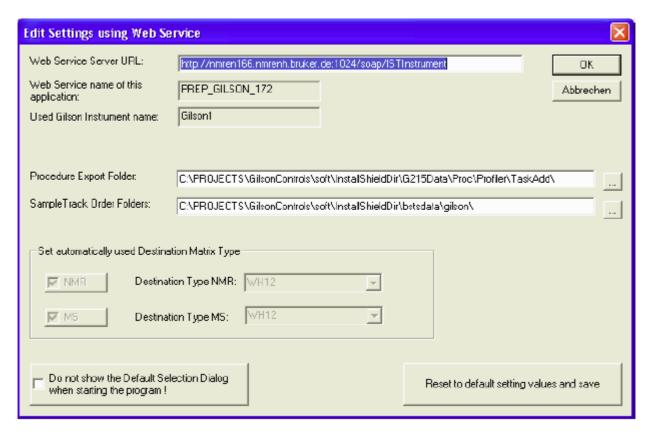


Figure 2.4. The Edit Settings Using Web Service Dialog Box

Reset to default settings values and save:

Restores all setting values to the default values delivered with the installation in the file "...\G215Data\Exec\Restore\default_session_xxxx.pgi" ("xxxx" depends on the selected application type).

For Applications without SampleTrack (Easy, SPETT)

The **Edit Settings** menu opens the Edit Settings dialog box where the following preparation modes can be defined.

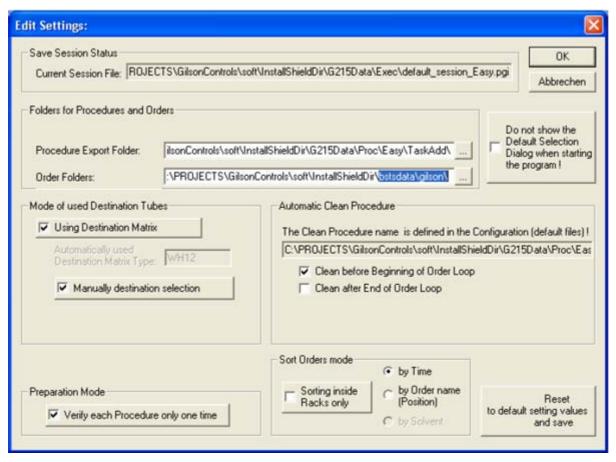


Figure 2.5. The Edit Settings Dialog Box

Table 2.2. Description of the Edit Settings Fields

Folders for Procedures and Orders	Order Folders	Orders and protocols are stored in the path of the edit box Order Folders + \in_no_ST\
Mode of Used Destination Tubes	Using Destination Matrix	If checked, the field Destination Matrix Type is used to find an empty destination matrix of this type for orders loaded in the currently inserted source racks.

Table 2.2. Description of the Edit Settings Fields

Manually Destination Selection

If checked source tubes and destination tubes can be defined in the Create Orders dialog box (see

"Create Orders" on page 85).

If this is not checked only source tubes can be defined in the Create Orders dialog box and destination racks shown in the Automatically used Destination Matrix Type field will be used auto-

matically.

Preparation Mode Verify Each Proce-

dure Only One Time

Procedures with the same name will be checked

only one time before execution.

Automatic Clean Proce-

dure

The Clean Procedure name is defined in the "Configuration" section (see also "Clean Proce-

dures Menu Commands").

Select the appropriate options to run this procedure before the beginning of the order procedure

loop OR/AND after the last order.

Sort Orders mode

Sort Orders Inside

Rack By

Orders can be sorted inside racks by Creation

time (default), Position, or Solvent.

Reset Default Values

The reset default values button restores all setting values to the default values delivered with the

installation in the file:

"...\G215Data\Exec\Restore\default_session_xx xx.pgi

("xxxx" depends on the selected application type).

Preparation Menu Commands

2.4

The **Preparation** menu offers the following commands:

Table 2.3. The Preparation Menu Commands

D	Start Preparation Automation	Start Automation = Init + Read Barcodes + Read Orders + Verify + Preparation
2	Start Verify Test All Orders Test Loop	Starts the verify test loop for Profiler applications.

Table 2.3. The Preparation Menu Commands

п	Pause after current movement	Stops after the current movement and waits. Select the menu Continue to continue the preparation.
•	Continue	Continues the preparation after Pause .
	End after current order	Stops after the current order and finish order loop.
×	Abort current order	Aborts the current order and finish order loop.

Start Preparation Automation

2.4.1

For Applications without SampleTrack (Easy, SPETT)

When the automation is started using one of the shortcuts listed below, a new preparation loop for all available orders will be started:

- Initialize Gilson
- Read Barcodes if the barcode reader is selected in the configuration.
- Deletes all old orders.
- Load orders
- Verify orders
- Run default Clean procedure if selected in the settings dialog box.
- Run **Preparation** procedures loop (for all available orders).
- Run default Clean procedure if selected in the settings dialog box.

For Applications with SampleTrack (Profiler and SampleTrack)

A new preparation loop will be started:

- One order will be loaded via the web service server, verified and executed before the next order will be requested.
- All urgent order will be delivered from the SampleTrack web service server first.

Select the menu <u>"Preparation Pause"</u> or the Toolbar to stop the preparation.

Select the menu <u>"End After Current Order"</u> or the Toolbar to stop after current order and to finish the order loop.

Select the menu <u>"Abort Current Order"</u> or the Toolbar to abort the preparation immediately.

Shortcuts: Toolbar: or Keys: CTRL+A

If the user wants to check all available orders when starting the program this menu could be used.

For Applications without SampleTrack (Easy, SPETT)

A new verification test loop for all orders will be started:

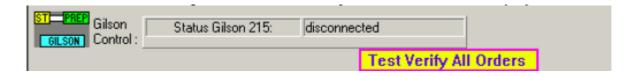
- Initialize Gilson.
- Read Barcodes if the barcode reader is selected in the configuration.
- Deletes all old orders.
- Create orders in the Create New Orders dialog box.
- Load orders.
- Verify orders.

For Applications with SampleTrack (Profiler and SampleTrack)

A new verification test loop for all orders will be started:

- A test loop will be started.
- All available orders will be loaded from the Web Services server.
- All available orders will be verifyed.
- All available orders will be removed from the order list and the status will be resetted via Web Services.

When the Test is running, the text "Test Verify All Orders" will be displayed:



Preparation Pause 2.4.3

Preparation pause: Stops after current movement and waits for the menu <u>"Continue"</u>. Select the menu <u>"Continue"</u> or the Toolbar button to continue the preparation.

Continue 2.4.4

Select this menu to continue the preparation after Pause.

Shortcuts: Toolbar

End After Current Order

2.4.5

Stops after the currently running order and finishes the order loop.

Shortcuts: Toolbar

Abort Current Order

2.4.6

The currently running order will be stopped immediately with an error status and if the order loop was running it will be stopped. A **Home Seek** will be performed automatically.

Shortcuts: Toolbar X

Service Tools Menu Commands

2.5

The **Service Tools** menu offers the following commands:

Table 2.4. The Preparation Menu Commands

	Initialize Gilson	Intializes the Gilson instrument.
	Initialize Pump	Initializes the Gilson instrument and the dilutor pump.
	Initialize + Home	Initializes the Gilson instrument and performs a home seek.
	Read Barcodes	Runs the Read Barcodes task.
	Create New Orders Dialog	Creates new orders dialog box.
	Load New Orders and Verify	Loads orders from order directory and verifies orders.
	Prepare all Orders	Prepares the orders.
₹	Modify Procedure	Shows or hides a Procedure View in the main window in order to modify task procedures at a high edit level for customers.
	Connect Gilson	Connects the Gilson after changing the configuration.
	Delete Map: Source-Destination Matrix	Delete Map: Source destination matrix
	Change Syringe	For service personnel only! Used to change the syringe.
	Delete all Orders and Protocols in ST Folders	Reloads the configuration file.
	Test: Check Positions in Tray	Special dialog box used to check all XYZ positions in the tray (racks, ports, etc.).

Initialize Gilson 2.5.1

Note: Menu enabled only for applications without SampleTrack (Easy, SPETT).

Runs the Initialize Gilson task:

- 1. Write procedure List file of all useable procedures in SampleTrack.
- 2. Write solvent List file of all defined solvents for SampleTrack.
- 3. Start to write a new Current protocol file.
- 4. Reset Errors.
- 5. Set Gilson Z Tower clamp height variable.
- 6. Set Gilson liquid level detection threshold variable.
- 7. Initialize barcode reader (if installed).
- 8. Checking Z axis.
- 9. Checking XY axis.
- 10. Checking Dilutor pump (not homing!)

Initialize Pump 2.5.2

Runs the Initialize Pump task:

- Writes a procedure list file of all usable procedures in SampleTrack.
- 2. Writes a solvent list file of all defined solvents for SampleTrack.
- 3. Starts to write a new current protocol file.
- 4. Resets errors.
- 5. Sets the Gilson Z-tower clamp height variable.
- 6. Sets the Gilson liquid level detection threshold variable.
- 7. Initializes the barcode reader (if installed).
- 8. Checks the Z-axis.
- 9. Checks the XY-axis.
- 10. Checks the dilutor pump at the rinse station.

Initialize + Home Gilson

2.5.3

Note: Menu enabled only for applications without SampleTrack (Easy, SPETT).

Runs the Initialize + Home Gilson task.

- 1. Write procedure list file of all useable procedures for order creation.
- 2. Write solvent list file of all defined solvents for order creation.
- 3. Start to write a new current protocol file.
- 4. Reset Errors.

- 5. Set Gilson Z-tower clamp height variable.
- 6. Set Gilson liquid level detection threshold variable.
- 7. Initialize barcode reader (if installed).
- 8. Homing Z axis.
- 9. Homing XY axis.
- 10. Homing dilutor pump at rinse station.

Read Barcodes 2.5.4

Note: Menu enabled only for applications without SampleTrack (Easy, SPETT).

 Called automatically when starting automation loop with the start toolbar button.

Runs the Read Barcodes task.

- 1. Reads both **ID** and **TYPE** barcodes at all defined barcode racks (displayed with red frames in the barcode view of the tray configuration).
- 2. Deletes old barcode defined racks in the tray configuration if they are removed from the Gilson.
- 3. Creates new barcode defined racks and zones (with the name of the Rack ID barcode) in the tray configuration if the barcodes are found.

All sites in the tray can be defined as barcode defined sites: See also <u>"Barcode Zone Configuration" on page 48</u>.

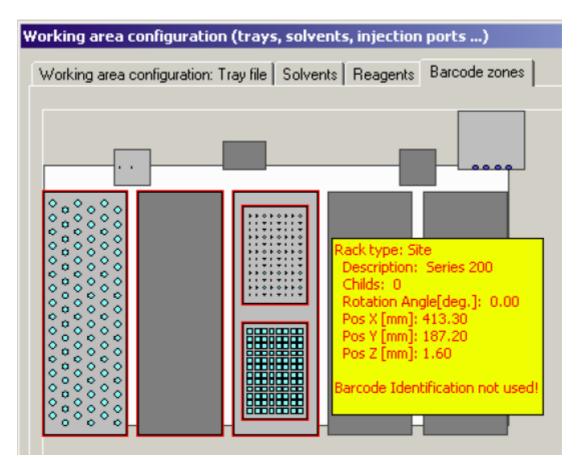


Figure 2.6. Working Area Configuration: Barcode Zones

Create New Orders Dialog Box

2.5.5

Note: Menu enabled only for applications without SampleTrack (Easy, SPETT).

 Called automatically when starting the automation loop with the start toolbar button.

Orders can be created in this dialog box without SampleTrack.

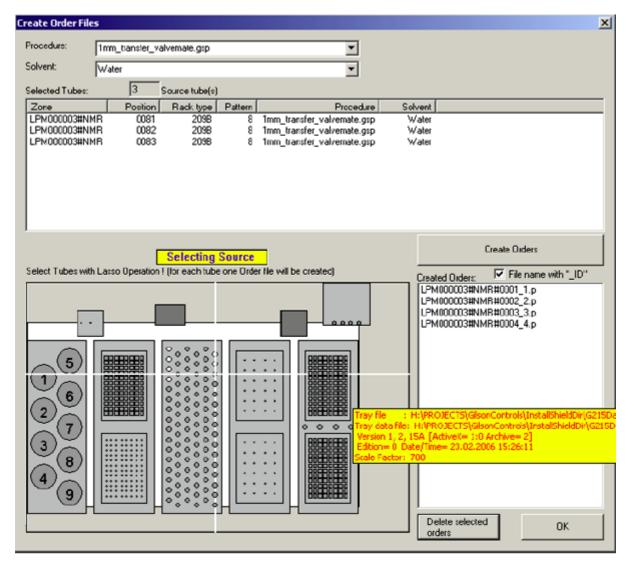


Figure 2.7. The Create Order Files Dialog Box

When checking **File name with '_ID'** an additional number will be added to the order name, so multiple orders for the same source position are possible.

Create Orders SPE Tube Transfer

The solvent selection is grayed. The Delete Created Orders is enabled.

Load Orders and Verify

2.5.6

Note: Menu enabled only for applications without SampleTrack (Easy, SPETT).

Runs the Load Orders and Verify task (without **Automation after Initialize** and **Read Barcodes**).

 Called automatically when starting automation loop with the start toolbar button.

For applications with SampleTrack (Profiler, SampleTrack):

- Only called automatically when starting automation loop with the start toolbar button.
- One order will be loaded via WEB SERVICE Server, verified and executed before the next order will be requested.
- All Urgent orders will be delivered from the SampleTrack Web Service Server first.

Prepare Orders

2.5.7

Note: Menu enabled only for applications without SampleTrack (Easy, SPETT).

Runs the procedures preparation loop (for all available orders without **Automation after Initialize**, **Read Barcodes**, and **Load Orders and Verify**).

Called automatically when starting automation loop with the start toolbar button.

Copy Orders Back From...\in\save\

2.5.8

Copies orders from the directory ...\in\save into the directory ... \in\

Used for tests or if racks with the same Barcode ID and the same samples are used again.

Not used for "1 mm Sample preparation" or "SPE Tube Transfer" applications.

Modify Procedure

2.5.9

See "Edit Procedures" on page 75.

Delete Map: Source/Destination Matrix

2.5.10

Deletes all relations between the source Matrix ID Racks and Destination Matrix ID Racks.

Not used for 1mm Sample Preparation or for SPE tube transfer applications!

Only relevant with option "Preparation Mode: Using Destination Matrix" in the <u>"Edit Settings Menu"</u> dialog box!

After reading the Rack ID barcodes during the "Loading and Verifying Orders" procedure, all orders will be checked if they need a new Destination Rack of the Destination Rack Type, as defined in the field "**Destination Matrix Type**" of the <u>"Edit Settings Menu"</u> dialog box.

If there is no Destination Rack defined for the current Source Rack in the Source/ Destination Map, and an empty Destination Rack is found in the tray, then the current Source Rack of the Order and the empty Destination Rack will be written as "connected" into the **Source/Destination Map**.

The Source/Destination Map will then be saved.

After restarting the program, or for new Source Rack orders in the Source/Destination Map, the Destination Rack will be the same.

If a Barcode ID is used more than one time (not recommended!):

- The customer must clear the Destination Rack and fill the Source Rack.
- If only the Source or the Destination ID has changed, this menu has to be used to delete all relations between Source Matrix ID Racks and Destination Matrix ID Racks.

Connect Gilson 2.5.11

NOTE: Not for BEST or Profiler applications!

This menu could be used to connect the Gilson liquid handler, if the Gilson is disconnected after an Error when starting this program.

Typically the Gilson will be connected automatically when starting this program. If another configuration is used when starting the program with different values in the Gilson "non volatile memory" (e.g. Z-tower clamp height or syringe size) the Gilson reports an error and will be disconnected. In this case the user could close this program and restart again or use this command for correct connection to the Gilson.

Delete all Orders and Protocols in ST folders

2.5.12

Typically all executed orders and protocols will be saved in the appropriate file folders. This menu can be used to delete all orders and protocols in the appropriate file folders. The folder names are different depending on whether the current application is using SampleTrack or not (see "Directory Structure of Order Files" on page 69).

Test 2.5.13

Check Positions in Tray

Special dialog box used to check all XYZ positions in the tray (racks, ports, etc.).

Clean Procedures Menu Commands

2.6

The **Clean Procedures** menu offers the following commands, which enable you to arrange multiple views of multiple documents in the application window:

Table 2.5. The Clean Procedures Menu Commands

Clean Needle	The clean needle menu command starts the clean needle procedure.
Prime Dilutor - Purge System	Runs the Prime Dilutor procedure.

User Guide Version 004 BRUKER BIOSPIN 25 (99)

Table 2.5. The Clean Procedures Menu Commands

Prime Inject Port	Runs the Prime Inject Port procedure.
Set ValveMate default solvent position	Moves ValveMate to the default solvent position (defined in the Dilutor configuration).
Modify Clean Procedure	Opens the Clean TASK procedure edit dialog box.

The procedures **Clean Needle**, **Prime Dilutor** and **Prime Inject Port** are defined in the default file configuration.

When the Default File Configuration is called from the clean procedures menu, the Gilson Liquid Handler 215 configuration is displayed in the configuration view.

Clean Needle 2.6.1

The clean needle menu command starts the clean needle procedure. The procedure is defined in the Gilson Liquid Handler 215 section of the configuration.

Prime Dilutor 2.6.2

Runs the **Prime Dilutor** procedure.

The procedure is defined in the Gilson Liquid Handler 215 section of the configuration.

Prime Inject Port 2.6.3

Runs the Prime Inject Port procedure.

The procedure name is defined in the Gilson Liquid Handler 215 section of the configuration.

Set ValveMate Default Solvent Position

2.6.4

Moves ValveMate to the default solvent position (defined in <u>"Dilutor Configuration" on page 42</u>).

Modify Clean Procedures

2.6.5

Opens the Clean TASK procedure edit dialog box (see <u>"Task Procedure Clean"</u> on page 77).

The View menu offers the following commands:

Table 2.6. The View Menu Commands

	Toolbar	Shows or hides the toolbar.
	Status Bar	Shows or hides the status bar.
	Barcode List	Shows or hides the barcode list of connected source and destination barcode racks.
₹	Modify Procedure	Shows or hides a Procedure View in the main window to modify Task procedures at a high edit level for customers.
7-U-	Configuration	Shows or hides the configuration dialog box.
100	Tray	Shows or hides the tray dialog box.
	Main Protocol File	Shows or hides the main protocol in the protocol dialog box.
电	Current Protocol File	Shows or hides the current protocol in the protocol dialog box.
	Procedure Steps	Shows or hides the current master step procedure dialog box.
	Solvent Consumption Information	For applications without SampleTrack only. This command is used to show a message box with the required solvent amounts for all orders after the verification.
	Error History	Shows the error history dialog box with all the errors which have occurred after starting the program. In each line of the list one error will be displayed. When clicking on an error line all details of the error will be displayed in the information field.

Toolbar 2.7.1

Use this command to display and hide the Toolbar, which includes buttons for some of the most common commands in PrepGilsonST, such as **File Open**. A check mark appears next to the menu item when the Toolbar is displayed.

The Toolbar

The Toolbar is displayed across the top of the application window, below the menu bar. The Toolbar provides quick mouse access to many tools used in PrepGilsonST.

To hide or display the Toolbar, choose Toolbar from the View menu (ALT, V, T).

Table 2.7. Menus with Toolbar Buttons

D	Start Preparation Automation	Start Automation = Init + Read Barcodes + Read Orders + Verify + Preparation.
п	Pause after current movement	Preparation Pause: Stop after current movement and wait. Select the Menu Continue to continue the preparation.

Table 2.7. Menus with Toolbar Buttons

Þ	Continue	Continue the preparation after a pause.
	End After Current Order	End after current order and finish order loop.
×	Abort Current Order	Abort current order and finish order loop.
+	Move Arm to Other Side	Moves the Gilson arm into a different position if the barcode reader did not allow the rack exchange.
₽.	Configuration	Shows or hides the Configuration View to see configuration details or to perform modifications if the instrument is not running.
₹	Modify Procedure	Shows or hides a Procedure View in the main window to modify task procedures at a high edit level for customers.
	Start Verify Test All Orders	Starts the verify test loop.
	Barcode List	Shows or hides the barcode list of connected source and destination barcode racks.
	Tray View	Shows or hides the tray dialog box.
	View Main Log File	Shows or hides the main protocol in the protocol dialog box.
	Log File	Shows or hides the current protocol in the protocol dialog box view.
	Procedure Steps	Shows or hides the current master step procedure dialog box.

Status Bar 2.7.2

Use this command to display or hide the **Status Bar**, which describes the action to be executed by the selected menu item or depressed Toolbar button, and the keyboard latch state. A checkmark appears next to the menu item when the status bar is displayed.

The status bar is displayed at the bottom of the PrepGilsonST window. To display or hide the status bar, use the Status Bar command in the View menu.



Figure 2.8. The Status Bar

The left area of the status bar describes actions of menu items as you use the arrow keys to navigate through menus. This area similarly shows messages that de-

scribe the actions of Toolbar buttons as you depress them, before releasing them. If after viewing the description of the Toolbar button command you wish not to execute the command, then release the mouse button while the pointer is off the Toolbar button.

The right areas of the status bar indicate which of the following keys are latched down:

<u>Indicator</u>	<u>Description</u>
CAP	The Caps Lock key is latched down.
NUM	The Num Lock key is latched down.
SCRL	The Scroll Lock key is latched down.

Modify Procedure 2.7.3

Shows or hides a Procedure View in the main window, which is used to modify Task procedures at a high edit level for customers.

See "Modifying the Procedure Dialog Box" on page 81.

Configuration 2.7.4

Shows or hides the configuration view in order to see configuration details or to perform modifications if the instrument is not running (see <u>"Open Configuration View" on page 37</u>).

Shortcuts: Toolbar 114

Tray View 2.7.5

Shows or hides the tray dialog box. By moving the cursor over **Containers** (dark gray), **Racks** (light gray) or **Tubes** (colors defined) different information for the object under the cursor will be displayed in a yellow pop-up window:

User Guide Version 004 BRUKER BIOSPIN 29 (99)



Figure 2.9. The Tray View Dialog Box

Different view modes can be selected by checking the "Status" or "Barcode" check boxes in the View Mode block.

- When **Status** is checked the status information for each tube will be shown.
- When Barcode is checked the barcode defined racks will be highlighted within a red frame.

Shortcuts: Toolbar

View Main Protocol File 2.7.6

Shows or hides the main protocol file with all the important information after the program is started.



Figure 2.10. Main Protocol File

This view can also be used to display other information:

- 1. Input order files from SampleTrack.
- 2. Output result order files to SampleTrack.

View Current Protocol File

2.7.7

2.7.8

Shows or hides the cuurent protocol file with all the important information from the selected/current order.

This view can also be used to display other information:

- Input order files from SampleTrack.
- 2. Output result order files to SampleTrack.

Shortcuts: Toolbar



Error History

This command is used to show a dialog box with all errors after starting the program:

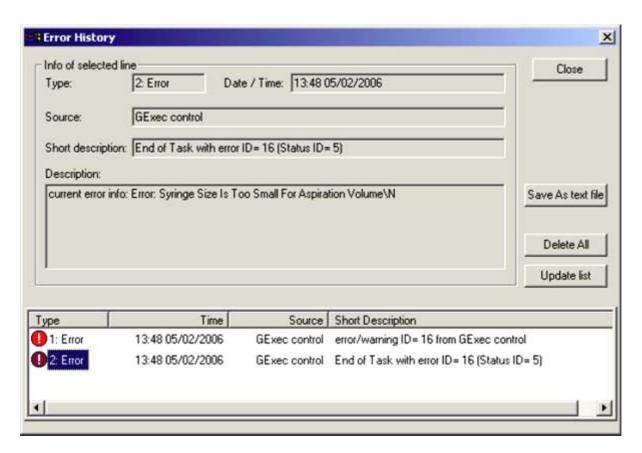


Figure 2.11. The Error History View

In each line of the list one error will be displayed (old errors on the top of the list based on the time stamp).

When clicking on one error line all details of the error will be displayed in the information fields.

Procedure Step View

2.7.9

Shows the **Procedure Step** View:

- Move the mouse cursor over one step, or click on the step icon to see details of one step!
- Shows the currently loaded or running main procedure in the upper part of the window.
- If there is a sub-procedure running, it is shown in the lower part of the window.

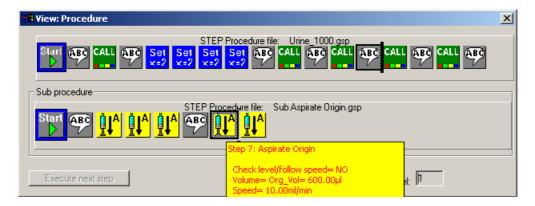


Figure 2.12. Procedure Step View

Note:

- It is not possible to display the procedure as a text file, but only as a protocol text file after execution.
- For service personal only: Procedures that are not running can be displayed in the Procedure Editor program.

Shortcuts: Toolbar

Help Menu Commands

2.8

The **Help Menu** offers various options which provide assistance with this application:

Table 2.8. The Preparation Menu Commands

Help Topics	Offers you an index of topics on which you can get help.
Help 1MM Application	Open the help file for 1 mm applications.
About	Displays the version number of this application

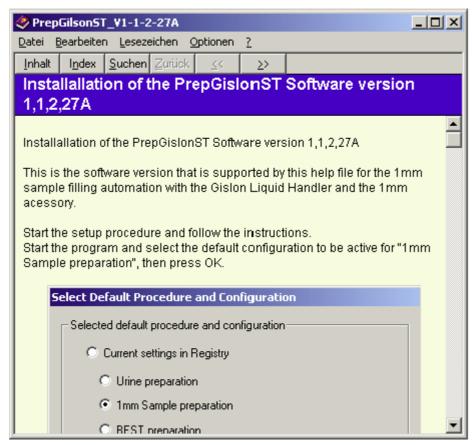
Help Topics 2.8.1

Use this command to display the opening help window. From this window, you can jump to step-by-step instructions on using PrepGilsonST and various other types of reference information.

Once you open the help window you can click the **Contents** button whenever you want to return to the opening screen.

User Guide Version 004 BRUKER BIOSPIN 33 (99)

Use this command to display the online help file for 1MM applications.



About 2.8.3

Use this command to display the copyright notice and version number of your copy of PrepGilsonST.

When starting the program the first time after installation the <u>"Default Procedure Selection"</u> dialog box appears enabling you to define the type of procedure and configuration settings in the registry.

Five types of procedures can be selected:

- Easy Preparation
- 1mm Sample Preparation
- SPE Tube Transfer
- Profiler Preparation
- SampleTrack Preparation

After performing an initialization using the menu "Service tools" -> "Initialize Pump", all procedures in the Export directory (defined in the "Edit Settings Menu" dialog box) will be exported to enable a selection of these procedures in the selection box of SampleTrack or in the BEST program.

Default Procedure Selection

3.2

When starting this program after installation, the following box appears which allows you to define the application type (to perform different settings in the Registry), or to modify the path inside all the procedures:

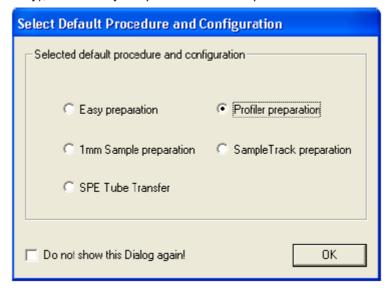


Figure 3.1. The Select Default Procedure and Configuration dialog box

The following files will be set in the registry (in HKEY_LOCAL_MACHINE->SOFT-WARE->Bruker BioSpin->):

1. Easy Preparation: ->Gilson Control->ApplicType=7

->Gilson Control->GExecCtrl->Config file= \Config\default_Easy.cfg

->Gilson Control->EditProcedure->Procedure= \Proc\Easy\default_Easy.gsp

2. 1mm Sample Preparation: ->Gilson Control->ApplicType= 2

->Gilson Control->GExecCtrl->Config file= \Config\default_1mm.cfg

->Gilson Control->EditProcedure->Procedure= \Proc\1mm\default_1mm.gsp

3. SPE Tube Transfer: ->Gilson Control->ApplicType= 5

->Gilson Control->GExecCtrl->Config file= \Config\default_SPETT.cfg

->Gilson Control->EditProcedure->Procedure= \Proc\SPETT\default_SPETT.gsp

4. Profiler Preparation: ->Gilson Control->ApplicType= 6

->Gilson Control->GExecCtrl->Config file= \Config\default_Profiler.cfg

->Gilson Control->EditProcedure->Procedure= \Proc\Profiler\default Profiler.gsp

5. SampleTrack preparation: ->Gilson Control->ApplicType= 8

->Gilson Control->GExecCtrl->Config file= \Config\default_SampleTrack.cfg\

->Gilson Control->EditProcedure->Procedure= \Proc\SampleTrack\default_SampleTrack.gsp\

The following "Current session" default files will be copied into the file \exec\curr_session.pgi:

Easy Preparation: default_session_Easy.pgi
 1 mm Sample preparation: default_session_1mm.pgi
 SPE Tube Transfer: default_session_SPETT.pgi
 Profiler Preparation: default_session_Profiler.pgi

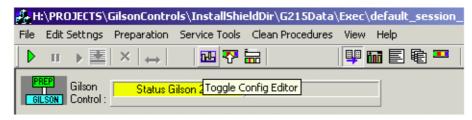
5. SampleTrack Preparation: default_session_SampleTrack.pgi

If it is desired that this box does not appear the next time the program is started, please select:

- The check box "Do not show this dialog box again!" in this dialog box, or,
- The check box "Do not show the Default Selection dialog box when starting the program!" in the <u>"Edit Settings Menu"</u> dialog box.

4.1

To open the configuration view, start the program:



 $\begin{tabular}{ll} \textbf{Then press the $\textbf{Configuration View}$ button from the toolbar.} \end{tabular}$

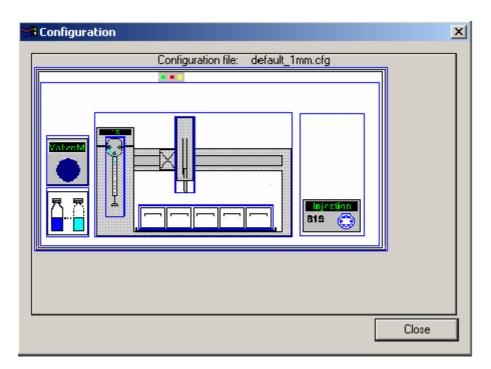


Figure 4.1. The Configuration View dialog box

Each of the different configuration sections are displayed inside a blue frame.

Configuration

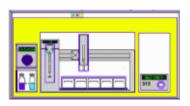
By moving the mouse cursor around inside the blue frames, various configuration tool tips will be displayed:

By clicking inside the blue frames (here shown as yellow areas) special dialog boxes will open shown various configurations.

"Base Configuration"

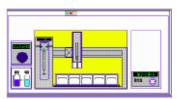
Defines the installed components of the

configuration.



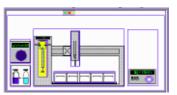
"Gilson Liquid Handler 215 Configuration"

Defines default files and Gilson instrument type specific configuration.



"Dilutor Configuration"

Defines the usable solvent list, the dilutor syringes and the default solvent.

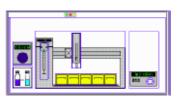


"Working Area Configu-

ration"

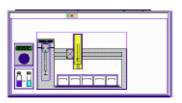
Defines the working area:

- "Tray File Configuration"
- "Solvents in Tray Configuration"
- "Reagent in Tray Configuration"
- "Barcode Zone Configuration"



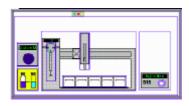
"Z-Tower Configuration"

Defines the needle adjustment.



"Solvent Names Configuration"

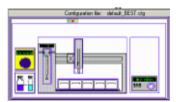
Defines the solvent names.



BRUKER BIOSPIN 38 (99) **User Guide Version 004**

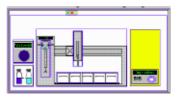
<u>"ValveMate Configuration"</u>

Defines the Valvemate solvents.



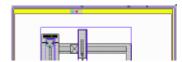
"Valves & Capillary Configuration"

Defines the valves and capillary configuration.



"Gilson Cover & LED Configuration"

Defines the reaction after opening the cover.



Base Configuration

4.2

In the base configuration dialog box the following items can be defined:

- The liquid handler type, either '215' or '235'.
- The basic GSIOC ID.
- The serial ports (RS232) used (for the Gilson, barcode reader, and SPE tube transfer).
- Other additional installation options used.

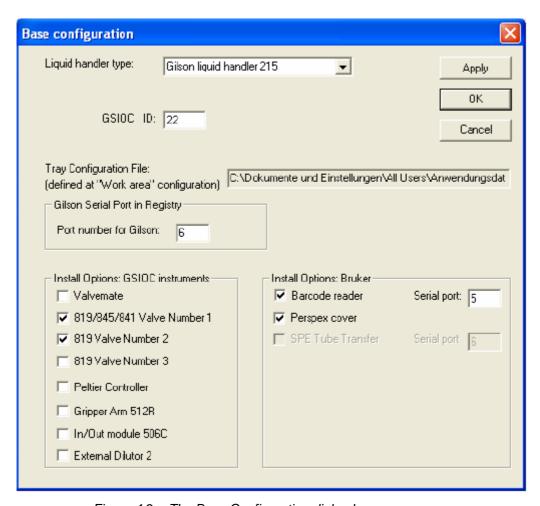


Figure 4.2. The Base Configuration dialog box

Gilson Liquid Handler 215 Configuration

4.3

The Gilson Liquid Handler 215 configuration defines default files and the Gilson execution mode configuration.

Default Files Configuration

4.3.1

In the Default Files configuration, the following Gilson liquid handler 215 files can be configured:

- A default path for all procedures can be defined (application specific).
- When clicking on a line in the list, a default file for the selected type can be defined in a dialog box.

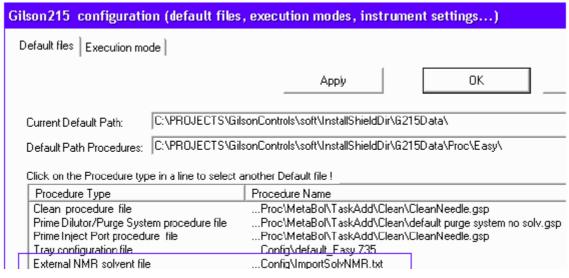


Figure 4.3. The Gilson Default Files Configuration Dialog Box

Execution Mode Configuration

4.3.2

In the Execution Mode configuration, the following Gilson liquid handler 215 information can be configured:

- When the program is running, protocol files can be written.
- Different wash procedures can be defined for various ValveMate solvent changes.
- The Solvent Configuration button can be used to define solvent names in the <u>"Dilutor Configuration"</u>.
- The Edit Solvent Positions at ValveMate button can be used to define solvent positions in the <u>"ValveMate Configuration"</u>.

User Guide Version 004 BRUKER BIOSPIN 41 (99)

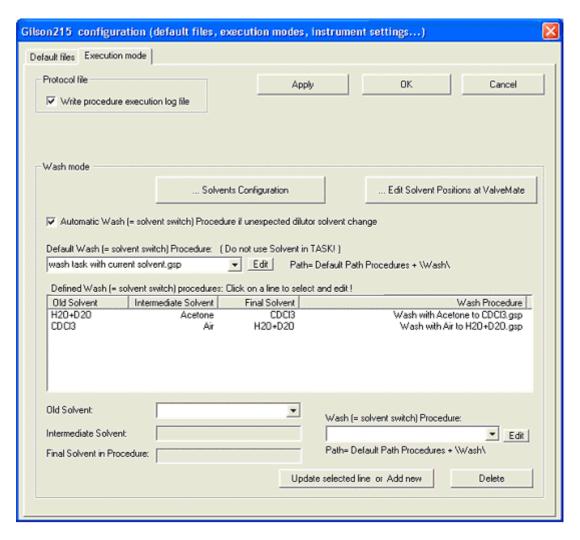


Figure 4.4. Gilson 215 Execution Mode Configuration

Dilutor Configuration

4.4

The Dilutor Configuration dialog box can be used to define:

- The dilutor type (currently only "Type 402" is supported):
- The number of syringes that can be used (currently only one syringe is supported);
- The size and the maximum speed of the syringe;
- A reduced maximum speed of the syringe.

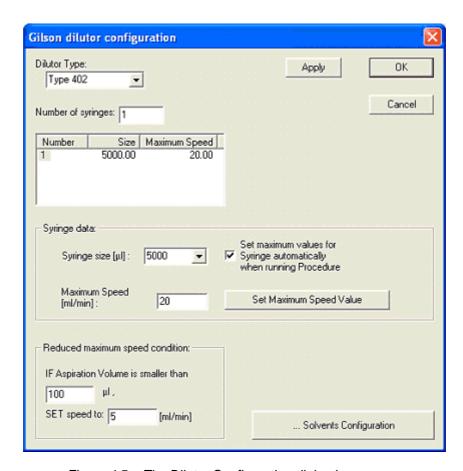


Figure 4.5. The Dilutor Configuration dialog box

The **Solvents Configuration** button can be used to define solvent names in the <u>"Solvent Names Configuration"</u> dialog box and provides a link to define solvent positions in the (<u>"Tray File Configuration"</u>) dialog box.

Working Area Configuration

4.5

The **Working Area Configuration** allows configuration of the working area. The areas that can be configured depend on the applications that will be used. The working area for applications using SampleTrack are slightly different then those used without SampleTrack.

For Applications with SampleTrack (Profiler, SampleTrack)

Four configuration dialog boxess are available for applications with SampleTrack:

- "Tray File Configuration"
- "Solvents in Tray Configuration"
- "Reagent in Tray Configuration"
- "Ports in Tray Configuration"

For Applications without SampleTrack (Easy, SPETT)

Four configuration dialog boxes are available for applications without Sample-Track:

- "Tray File Configuration"
- "Solvents in Tray Configuration"
- "Reagent in Tray Configuration"
- "Barcode Zone Configuration"

Each application uses a different predefined default tray configuration file (*.735):

Application Easy: default_Easy.735
Application 1MM: default_1mm.735
Application SPETT: default_SPETT.735
Application Profiler: default_Profiler.735
Application SampleTrack: default_SampleTrack.735

The current default path can be checked in the Gilson Liquid Handler 215 configuration.

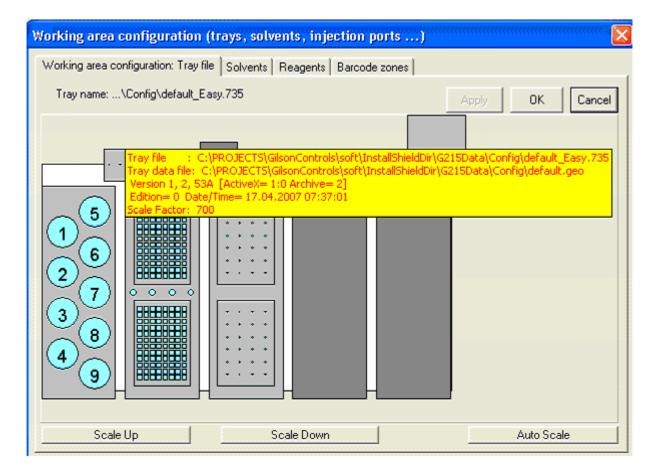
The solvent and reagent information and the tray file name can be saved in the *.cfg file (path written in the tool tip on the configuration name) and the tray information in the tray file *.735 when the **Apply** and **OK** buttons are pressed.

Tray File Configuration

4.5.1

For applications with SampleTrack (Profiler, SampleTrack):

- Modification of racks and zones in the tray area are not allowed.
- All rack insert and remove operations are done automatically with the barcode reader.



For applications without SampleTrack (Easy, SPETT):

Figure 4.6. The Tray Configuration dialog box for Applications without Sample-Track

Press the **Apply** or **OK** button to save the tray configuration to the *.735 file.

Adding Rack Tubes to a Zone

Only tubes assigned to a zone can be used in other configuration dialog boxes or in procedure steps.

- 1. Insert rack with a zone and tubes for one rack.
- A very fast way to define a tube when inserting a new rack manually.
- A new zone is defined after inserting the rack and all tubes of the rack will be added to the zone.
- See <u>"Insert Racks with Barcode Simulation" on page 88.</u>
- 2. Inserting rack tubes with a zone for more than one rack or for a part of one rack.
- The very flexible tube definition will be performed manually in three steps:
 - Insert a rack into a carrier (shown as a dark gray area, other names "container" or "site".

User Guide Version 004 BRUKER BIOSPIN 45 (99)

Configuration

- Add a new zone (see "Adding Zones and Tubes to a Zone" on page 90).
- Add tubes to a zone (see <u>"Adding Zones and Tubes to a Zone" on page 90</u>).
- 3. Insert racks with a zone and tube using the barcode reader.
- When a barcode reader is installed, tube definition will be done automatically when reading the barcodes of barcode defined racks (see <u>"Barcode Zone</u> <u>Configuration" on page 48</u>).

New customer racks could be created and modified using the context menu Rack Editor of the tray control (see "The Rack Editor" on page 57).

Remove Racks from the Tray

4.5.2

- Open the Tray Configuration in the Configuration View.
- Double-click on the gray rack area (not on a tube) or use the context menu "Remove selected rack".
- Confirm the delete operation in the popup message with "Yes".

Solvent can be defined at all positions in the tray configuration. The position must be a member of a zone (see <u>"Adding Zones and Tubes to a Zone" on page 90</u>).

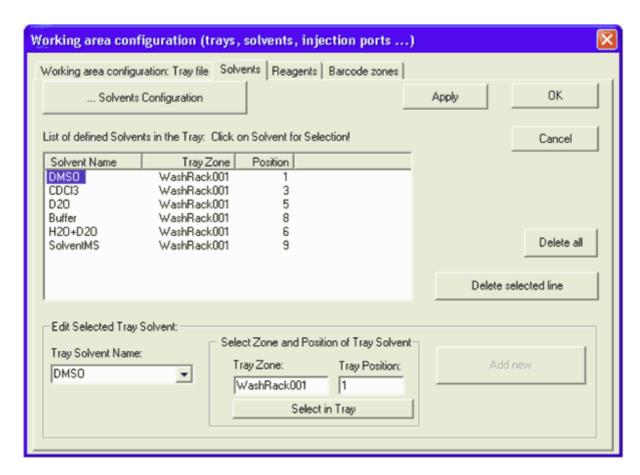


Figure 4.7. The Solvent Configuration dialog box

The **Solvents Configuration** button can be used to define solvent names in the **"Solvent Names Configuration"**.

Reagent in Tray Configuration

4.5.4

Reagents can be defined at all positions in the tray configuration. The position must be a member of a zone (see <u>"Adding Zones and Tubes to a Zone" on page 90</u>).

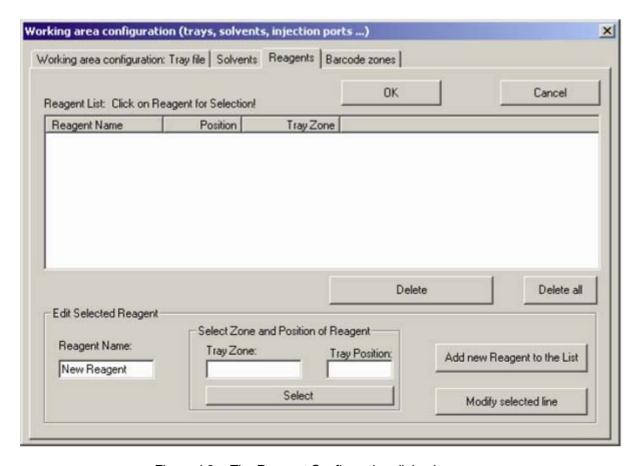


Figure 4.8. The Reagent Configuration dialog box

Reagents can be used in TASK procedures with the type "ADD".

Barcode Zone Configuration

4.5.5

The barcode configuration dialog box can only be used if a barcode reader is installed.

Containers (carriers for racks) can be defined as "barcode defined racks", whereas an automatic barcode reading can be performed here when starting the preparation program.

Defining Barcode Defined Racks

• "Double click" on the rack area, or on a dark gray container area, to define it as a "barcode defined rack" (or to undo this definition).

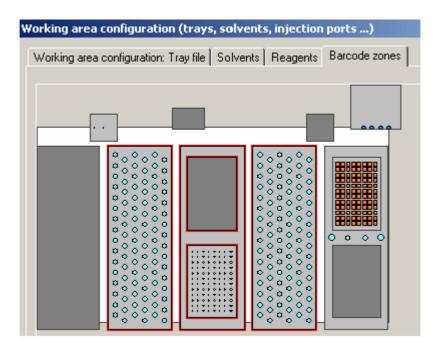


Figure 4.9. The Barcode Zones Configuration dialog box

Checking Barcode Rack Information

Open the Tray View and select the "Barcode" view mode to see all "barcode defined racks":

- A red frame will be displayed if the rack is a "barcode defined rack"
- See Tool tips for details on rack information

When starting the preparation with "Autostart", two barcodes from each "barcode defined rack" are read automatically:

If a valid Type Barcode and Barcode ID are read when executing the program, any older rack will automatically be removed and the new rack inserted.

See also: "Insert Racks with Barcode Simulation" on page 88.

User Guide Version 004 BRUKER BIOSPIN 49 (99)

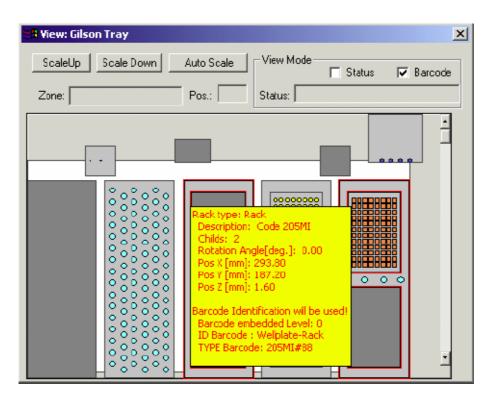


Figure 4.10. Example of a Gilson Tray Configuration

(The example shows a tray configuration file (*.735) with only two "barcode defined racks")

Ports in Tray Configuration

4.5.6

This configuration dialog box is for use only with applications used **with** Sample-Track (Profiler, SampleTrack)!

Ports with predefined names can be defined in predefined zones (one position only) in the tray configuration. Automatically defined ports include **Injection** and **InjectionMS**.

The **Switch NMR and MS Port** button can be used to switch the right/left position of the valves 819 in the tray.

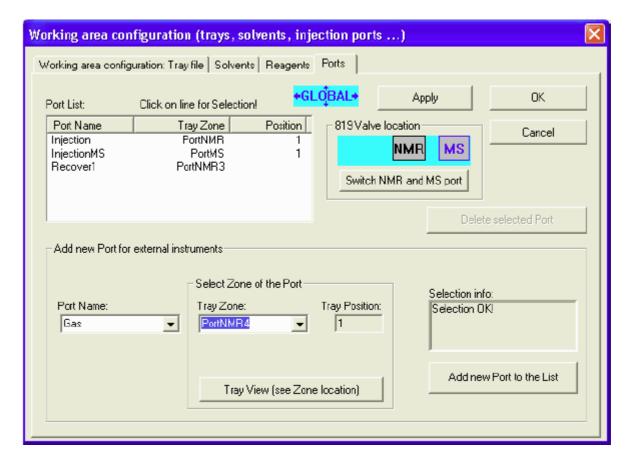


Figure 4.11. Example of a Ports in Tray Configuration

Z-Tower Configuration

4.6

The Z-Tower configuration dialog box allows the following settings to be changed:

- The Z-Tower size can be defined to 125 mm or 175 mm.
- The Z-Tower calibration clamp height can be defined (use the value written on the adjustment tube!).
- The barcode reader mounting position can be defined (old position: X = -49).

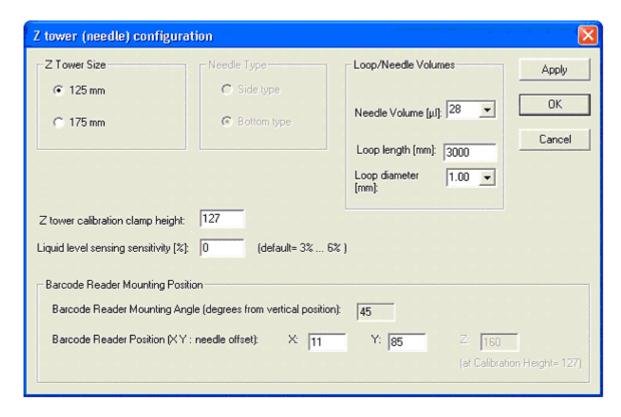


Figure 4.12. The Z-Tower Configuration dialog box

Note: Liquid level sensing is not used!

Solvent Names Configuration

4.7

The Solvent Names Configuration dialog box is used to define the names of the solvents used in experiments.

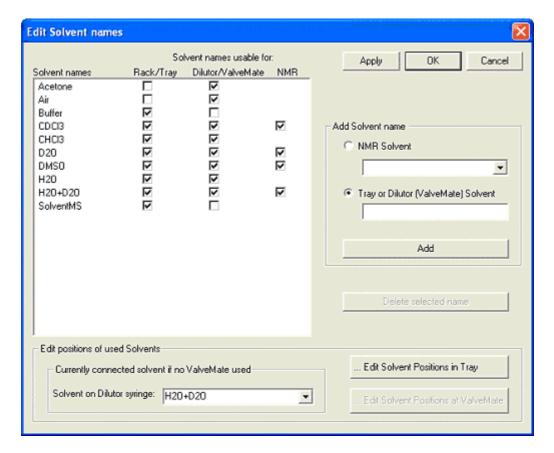


Figure 4.13. The Edit Solvent Names Dialog Box

To insert a solvent name select the name from the NMR Solvent list or enter a tray or dilutor solvent. Press **Add** to add the solvent to the list.

ValveMate Configuration

4.8

In the ValveMate configuration dialog box, solvents can be assigned to the Valve-Mate positions.

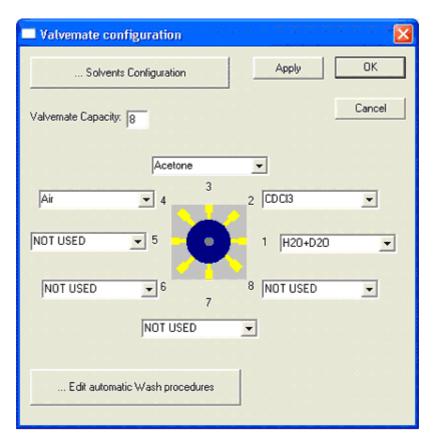


Figure 4.14. The ValveMate Configuration dialog box

The **Solvents Configuration** button can be used to define solvent names in the <u>"Solvent Names Configuration"</u> dialog box.

The **Edit Automatic Wash Procedures** button can be used to define wash procedures in the <u>"Execution Mode Configuration"</u>.

Valves & Capillary Configuration

4.9

In the Valves & Capilllary Configuration dialog box:

- Properties of "Gilson 819" valves can be defined: name, GSIOC ID, default position.
- Properties of additional Bruker valves can be defined: name, Gilson output connector, default position.

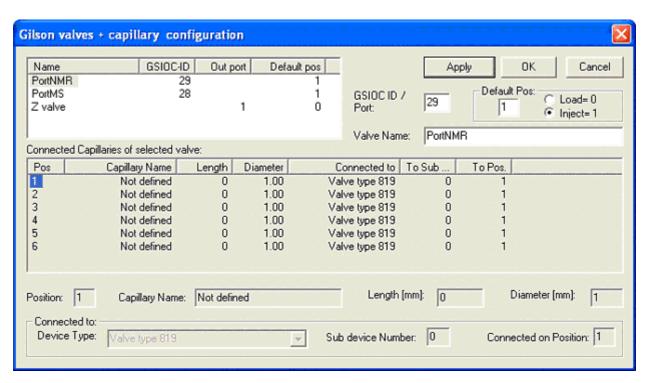


Figure 4.15. The Valves & Capillary Configuration Dialog Box

Gilson Cover & LED Configuration

4.10

The Gilson Cover & LED Configuration dialog box is used to define the reaction after the cover is opened. Specifically:

- The input port of the "cover open switch".
- The output ports of the Gilson status LED's.
- The reaction when opening the cover (stop and wait until closed).
- The reaction when closing the cover (reading all barcodes again).

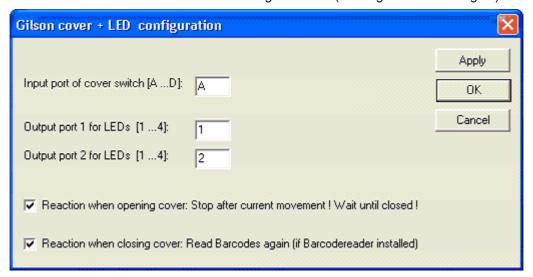


Figure 4.16. The Cover Configuration Window

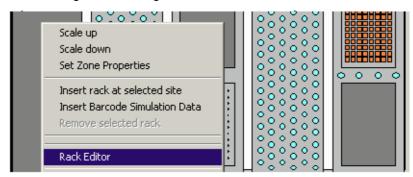
User Guide Version 004 BRUKER BIOSPIN 55 (99)

Configuration

Opening the Rack Editor

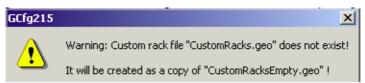
5.1

To open the Rack Editor select "Rack Editor" from the Tray Control in the Tray Configuration dialog box.

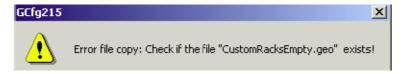


The file "CustomRacks.geo" is used for customer defined racks. By a new installation it is not overwritten if it already exists. If it does not exist, it will be created as a copy of the empty rack file "CustomRacksEmpty.geo" (delivered with the setup file).

Warning shown when the file "CustomRacks.geo" does not exist when opening the Tray Configuration dialog box:



Warning shown when the file "CustomRacks.geo" can not be created:



Error shown if both custom rack files do not exist when opening the "Rack Editor" dialog box:



Rack Editor without a carrier (other names: container or site) selected:



See also:

- 1. "Rack Selection"
- 2. "Creating a New Rack"
- 3. "Bruker or Custom Racks"
- 4. "Modifying Racks"

Rack Selection 5.2

When you click on a rack (that is placed in a carrier) it will show a light blue frame around the selected carrier, and the rack information will be displayed in the Rack Editor.

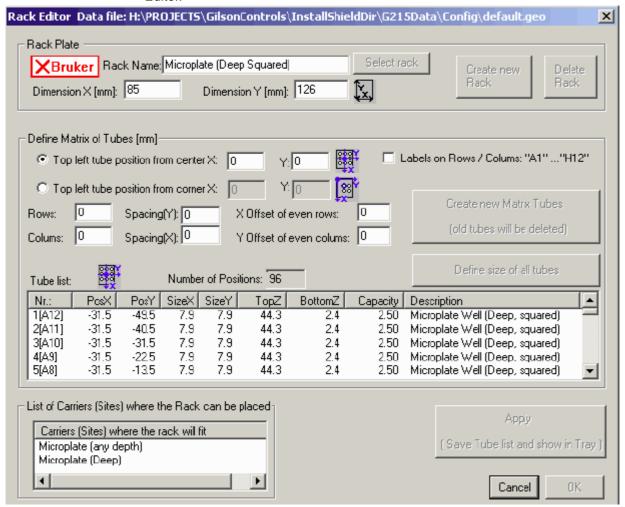


Figure 5.1. Rack Editor with Rack Selected

Old Gilson defined racks do not have values for rows or columns. Only tube values in the tube list can be displayed!

Carrier Selection 5.2.1

When you click on a dark gray carrier area, it will show a light blue frame around the selected carrier and the **Select rack** button will be enabled:

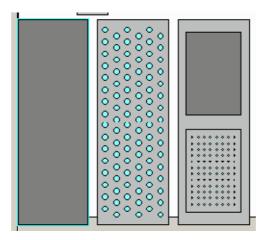


Figure 5.2. Selecting a Carrier

Using the **Select rack** button, a rack can be selected from a list of all racks that can be used for the selected carrier.

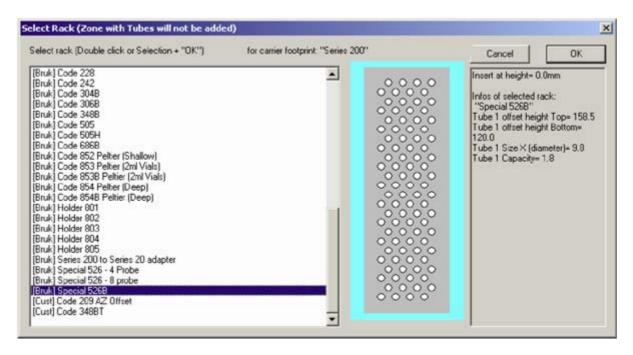


Figure 5.3. Selecting a Rack

"[Bruk]" racks in the selection list are delivered from Bruker with the installation and cannot be modified.

"[Cust]" racks in the selection list (at the end) are customer racks and can be modified.

Creating a New Rack

5.3

After opening the Rack Editor the button "Create new Rack" is disabled:





Existing rack values can be used by clicking on an existing rack in the tray view! Use existing rack values to add the new rack to the carrier list of an existing rack!

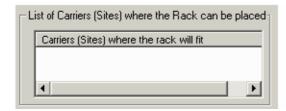
After manually changing the "Rack Name" edit field to a new rack name (not an existing Bruker rack name or custom rack name!) the button "Create new Rack" will be enabled.

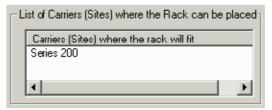


Define the total size of the new rack in the fields "**Dimensions x**" and "...y" (the values of an existing rack can be used by clicking on the rack in the tray view before changing the name).

Define the **Carrier** (list), where the new rack can be placed by clicking on an existing rack in the tray view (otherwise the new rack can only be displayed in the current selected carrier after typing the rack name manually)

List with no carriers defined (left) - List with carriers defined (right):

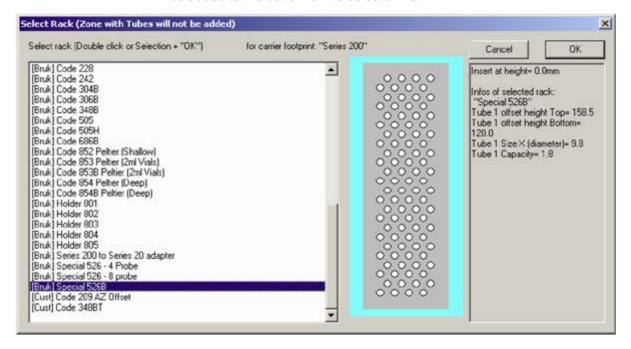






The Create New Rack button will create the new rack as a "Custom" rack:

When the button is pressed and a carrier is defined for the new rack, the new rack will be added to the bottom of the selection list:



"[Bruk]" racks in the selection list are delivered from Bruker with the installation and cannot be modified.

"[Cust]" racks in the selection list (at the end) are customer racks and can be modified.

Deleting a Rack 5.3.1

A custom rack can be deleted using the **Delete Rack** button. Bruker racks cannot be deleted.

Bruker or Custom Racks

5.4

Racks can be defined as Bruker racks or Custom racks.

Bruker Racks:

Bruker is shown in the upper left corner of the Rack Editor:



- Rack data is delivered from Bruker with the installation and cannot be modified
- Rack data is defined only in the file "default.geo"
- Racks are displayed in the selection list with the prefix: "[Bruk]"

Custom Racks:

• Custom is shown in the upper left corner of the Rack Editor:



- Rack data is defined by the customer and can be modified and deleted.
- Rack data is defined in the file "default.geo" and in the file "CustomRacks.geo".
- Racks are displayed in the selection list with the prefix: "[Cust]".

Modifying Racks

5.5

First select an existing rack in the Rack Editor (see <u>"Rack Selection" on page</u> <u>58</u>).

Note: Only custom racks can be modified!

The Rack Editor can be used to define a Tube Matrix in a rack.

Old Gilson defined racks do not have values for rows or columns. Only tube values in the tube list can be displayed!

The total rack size can be defined in the edit fields "Dimension X" and "Dimension Y":



The position of the top left tube of the matrix can be defined relative to the center of the rack or relative to the top left corner of the rack.



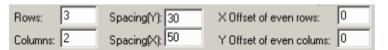
The values of the opposite mode are calculated automatically using the total rack size in the fields "Dimension X" and "Dimension Y".

The number of rows and columns can be defined in the edit fields "Rows" and "Columns".

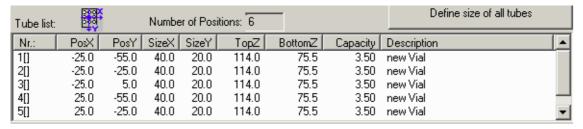
The space between two rows can be defined in the edit field "Spacing (Y)".

The space between two columns can be defined in the edit field "Spacing (X)".

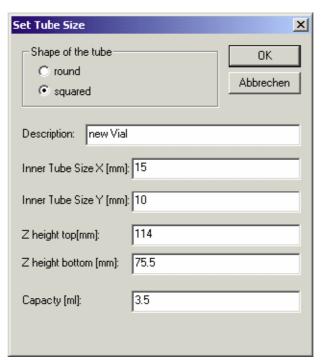
An additional offset of even rows/columns can be defined in the edit fields "X Offset of even rows" and "Y Offset of even columns".



The **Create New Matrix Tubes** button will create all matrix tubes and display them in the tube list:



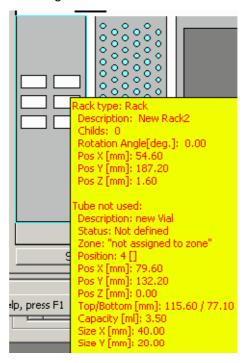
The **Define size of all tubes** button is used to open the "Set Tube Size" dialog box where the matrix tube size can be defined:



The mode **Labels on Rows / Columns:** "A1"..."H12"should be only selected if there is no offset defined for even rows or columns!

User Guide Version 004 BRUKER BIOSPIN 63 (99)

Pressing the **Apply** button saves the modified rack data in the files "default.geo" and "CustomRacks.geo" files and displays the data in the selected carrier highlighted with the light blue frame:



The yellow pop-up window displays all the tube values for easy verification!

Service Tools 5.6



The Service Tools are for trained Bruker Service Personnel Only!

Preparation Data Files

Data Directory Structures

6.1

```
Structure:
```

[Install Folder Data]\G215Data\

\Config\

\Config\Restore\

\Proc\

\Easy\

1mm

\SPETT\

\Profiler\

\SampleTrack\

\Test\

for release test files

\ProcTest\

\Easy\

\Profiler\

\Exec\

\Exec\Restore\

Obsolete folders:

\Custom\

\BEST\

Main Folder 6.1.1

[Install Folder Data]\G215Data\ (defined when installing the program)

Configuration Files Directory

6.1.2

[Install Folder Data]\G215Data\Config\

Preparation Data Files

- 1. All data in the current configuration (file extension: *.cfg), including the tray file name, e.g. Current_Config_data.cfg.
- 2. Data in the current tray (file extension: *.735), including the tray geometry database file name, e.g.: Current_Tray_Config.735.
- 3. Data of tray geometry database (file extension: *.geo). This file is used when inserting racks (e.g. after barcode reading). e.g.: GRack_data_all.geo.

Preparation Procedure Files Directory

6.1.3

[Install Folder Data]\G215Data\Prep\

Common procedure files used for initial control settings (file extension: *.gsp or *.gfp).

Temporary Settings Files

6.1.4

[Install Folder Data]\G215Data\Exec\

- Saved Session file after an error or Menu <u>"Save Current Protocol (... log)</u> <u>Files"</u>.
- 2. Current preparation status file (file extension: *.sts currently not used).

[Install Folder Data]\G215Data\Exec\Restore\

All default setting files (file extension: *.pgi) to restore to installation values.

Temporary Protocol Files

6.1.5

[Install Folder Data]\G215Data\Exec\

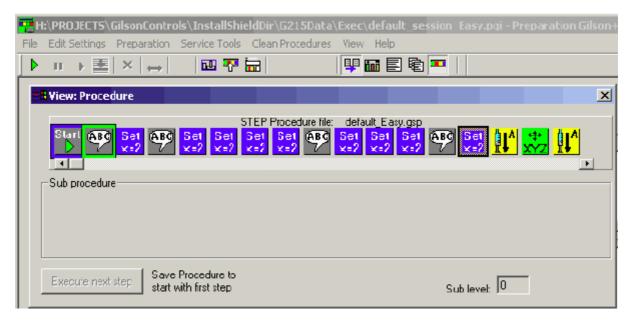
- 1. Current main protocol file of the current session (**log_exec.log**).
- 2. Current protocol file of the running procedure (log_current.log).
- Saved protocol files (saved_log_exec.log and saved_log_current.log) after an
 error occurs or after saving the file with the menu <u>"Save Current Protocol (... log) Files"</u>.

After completion of the SampleTrack order procedure the current protocol file, [Install Folder Data]\G215Data\Exec\log_current.log, will be renamed (to the order name) and saved in the SampleTrack order files directory:

[Order Folder]\bstsdata\gilson\out...\protocol\

See also: <u>"View Current Protocol File" on page 31</u>) and the <u>"Directory Structure of Order Files" on page 69</u>.

Press the Step View button in the Toolbar to display the currently loaded/running master step procedure.



The menu selection Compare Procedures can be used to check/compare any procedure. All steps are displayed in a text file similar to the current protocol file.

To find the file directory see the "Data Directory Structures" on page 65.

Protocol Files 6.3

Current Preparation Protocol File Directory: (see also: <u>"View Current Protocol File" on page 31</u>).

[Install Folder Data]\G215Data\Exec\

Two protocol files are written automatically:

- 1. Current main procedure protocol file: log_exec.log
- 2. Current protocol file of running procedure: log_current.log

After an error or when selecting menu option <u>"Save Current Protocol (... log)</u> <u>Files"</u> a copy of the current protocol files will be performed:

log_current.log to ...\G215Data\Exec\saved_log_current.log log_exec.log to ...\G215Data\Exec\saved_log_exec.log

After completion of the order procedure the current protocol file, [Install Folder Data]\G215Data\Exec\log_current.log, will be renamed (to the order name) and saved in the order files directory:

C:\bstsdata\gilson\out...\protocol\

Preparation Data Files

(See the "Data Directory Structures" on page 65)

Directory of saved protocol files after execution of orders:

[Order Folder]\bstsdata\gilson\out\protocol\ - (when running with SampleTrack)

[Order Folder]\bstsdata\gilson\out_no_ST\protocol\ - (when running without SampleTrack -

e.g. BAY000100 NMR 31.log

(See the "Directory Structure of Order Files" on page 69).

Order Files

Directory Structure of Order Files

7.1

Note: To allow access to old order information, old files will not be automatically deleted!

The user should delete all old orders in the subdirectories listed below by using:

The menu option "Service Tools" + the button:

Delete all orders and protocols in ST folders

Note: "order files" in the JCAMP format will be used when working **without** SampleTrack

Note: "order files" in the JCAMP format will be used when working **with** Sample-Track using the old file system (1 mm applications)!

Note: "order files" in the XML format will be used when working **with** SampleTrack via a **SOAP** server (Profiler and SampleTrack applications)!

Directory Structure for Order Files:

[Order Folder]\bstsdata\gilson\

\in\

\in\exec\

\in\save\

\in\error\

\out\

\out\save\

\out\error\

\out\protocol\

 \ln_{no_ST}

\out_no_ST\

Main Directory 7.1.1

[Order Folder]\bstsdata\gilson\ (defined by SampleTrack)

7.1.2

[Order Folder]\bstsdata\gilson\in\ (when running with SampleTrack).

[Order Folder]\bstsdata\gilson\in_no_ST\ (when running without Sample-Track).

Contains all order files (file extension: *.p) to carry out.

After pressing OK, the files will be moved into the directory \in...\exec\.

After verifying an error the files will be moved into the directory \in...\error\.

After execution of the order, the files will be moved into the directory \in...\save\.

Output Order Files Directory

7.1.3

This results after execution.

[Order Folder]\bstsdata\gilson\out\ (when running with SampleTrack).

[Order Folder]\bstsdata\gilson\out_no_ST\ (when running without Sample-Track).

Contains all order files with results after execution (file extension: *.r).

After result handling by the SampleTrack Communicator, the files will be moved into the directory **\out\save** if status OK, or into the directory **\out\error** if an error occurs.

Order Protocol Files Directory

7.1.4

Results after running the order procedure.

[Order Folder]\bstsdata\gilson\out\protocol\ (when running with SampleTrack).

[Order Folder]\bstsdata\gilson\out_no_ST\protocol\ (when running without SampleTrack).

After completion of the SampleTrack Order procedure, the current protocol file [Install Folder Data]\G215Data\Exec\log_current.log will be renamed (to the order name) and saved in the SampleTrack order files directory:

[Order Folder]\bstsdata\gilson\out...\protocol\

(See also "Data Directory Structures" on page 65).

7.2

To see the JCAMP SampleTrack order files:

- 1. Right-click on the order in the order list and select **Show input order file** to display the order information.
- 2. Right-click on the order in the order list and select **Show output report file** to see the report information.

To see the protocol files: Double-click on the order in the order list!

To find the file directory refer to <u>"Directory Structure of Order Files" on page 69</u>.

Order Files

Solvents

Defining Solvents for Preparation

8.1

To edit the solvents names used for preparation, open the <u>"Solvent Names Configuration"</u>, whereas:

- All defined external NMR solvents can be used.
- Additional solvents can only be defined for the preparation.

To define the solvent positions in the Gilson tray area for preparation, open the configuration dialog box (see <u>"Solvents in Tray Configuration" on page 47</u>) and click on the place where you want to use the solvent:

To define the solvent positions at the Gilson ValveMate open the <u>"ValveMate Configuration"</u>.

Defining External NMR Solvents

8.2

The external NMR solvents are used inside the <u>"Solvent Names Configuration"</u>, which is a dialog box used to define the preparation solvents used.

For **Profiler applications** the external NMR solvents are delivered by the Web Services server directly.

For other applications:

- The external NMR solvents are defined inside a text file (e.g. solvents.txt).
- The name of this text file can be defined in the configuration dialog box (see
 "Default Files Configuration" on page 40) or by clicking on the Gilson liquid
 handler 215 (default files, ...) to open the configuration Gilson 215 dialog box.

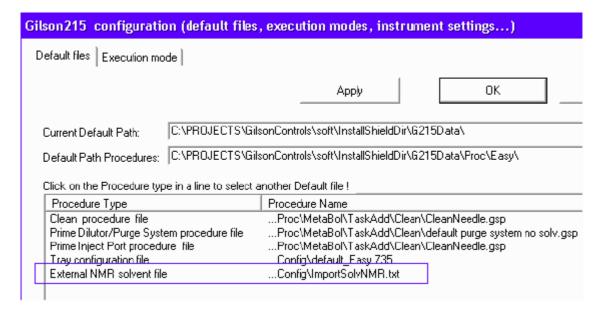


Figure 8.1. External NMR Solvent Configuration

In the property sheet **Default Files**, the default file name and directory of the type External NMR solvent file can be changed to define the ambient solvent file used.

To view or edit the configuration see "Open Configuration View" on page 37.

Edit Procedures

Modifying TASK Procedures

9.1

If the source TASK procedure is selected in the registry, then you must:

- 1. Modify the procedure in the menu "Service tools" -> "Modify Procedure" or using the Toolbar button. Select another TASK procedure if there is no correct TASK procedure in the Registry entry.
- 2. Export the procedures and display them in the SampleTrack selection box using the menu "Service tools" -> "Initialize Pump"

TASK Procedures 9.2

TASK procedures are special procedures with a customer dialog box for each different type, used to easily change procedure parameters.

Common TASK dialog box Elements

9.2.1

In the top of the dialog box the name of the procedure and the **Custom** (green) or **Bruker** (red) type is shown:



(see "Bruker or Custom Racks" on page 62)

With the '...' button another TASK procedure of the same type can be loaded.

TASK procedures can be saved using the 'Save As' button (for all procedures) or using the 'Save' button (for CUSTOM procedures only). Names of existing Bruker procedures can not be used!

The 'Cancel' button can be used to close the dialog box without saving modifications.

9.3

- 1. Common TASK procedures:
 - "Task Procedure Wash"
 - "Task Procedure Clean"
 - "Task Procedure Add"
 - "Task Procedure Dispense"
 - "Task Procedure Mix"
- 2. Application specific TASK procedures:
 - "Task Procedure 1MM Samples"

Task Procedure Wash 9.3.1

Wash tasks are only used to perform an automatic wash procedure for a different ValveMate solvent if this option is selected in the execution mode configuration (see <u>"Execution Mode Configuration" on page 41</u>).

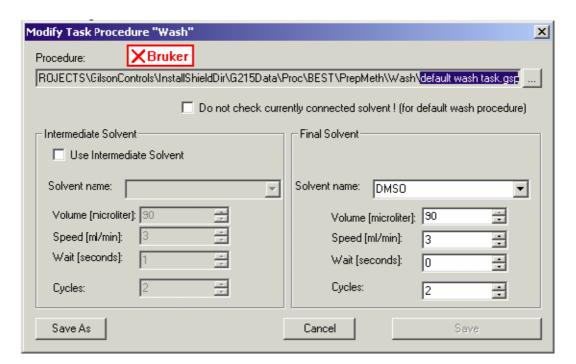


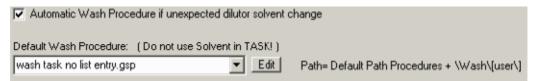
Figure 9.1. Editor Dialog Box of a Wash TASK

Optionally an intermediate solvent can be used.

If the Wash TASK will be used as the default wash procedure in the configuration, the following check box must be selected:

✓ Do not check currently connected solvent! (for default wash procedure)

The default wash procedure can be selected in the configuration dialog box:



Task Procedure Clean

9.3.2

Clean tasks can be defined as sub-procedures in each line of an **Add Task!**

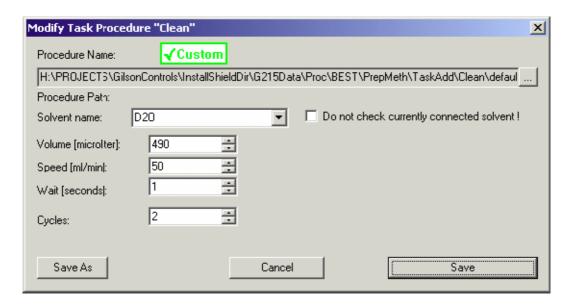


Figure 9.2. The Modify Task Procedure Clean dialog box

Clean tasks can be started using the menu without adding a task.

To edit or to run clean procedures: see <u>"Clean Procedures Menu Commands"</u> on page 25.

Automatic Cleaning

The clean procedure name is defined in the default files configuration (see <u>"Clean Procedures Menu Commands" on page 25</u>).

Select the appropriate options in the Settings dialog box (see <u>"Edit Settings Menu" on page 14</u>) to run this procedure. Automatic cleaning can be performed before the beginning of the order procedure loop, and/or after the last order.



This feature works only when starting with AutoStart button (shown at left)!

Task Procedure Add 9.3.3

An **Add** task is a flexible procedure that is designed to be modified by the user. All lines in the Add Task procedure list are executed from the top of the list to the bottom.

In the Add Task the user can modify a selected line (after selecting a line by clicking in the left column of the list) or add additional lines or delete lines.

In each line of an Add Task other tasks of the type can be defined and modified with the **Edit** button:

- Task Dispense
- Task Mix
- Task Clean

At execution time they will be performed after the execution of the line. In each line of an Add Task modifications must be updated in the list with the button!

The procedure list will be saved with the buttons Save As or Save.

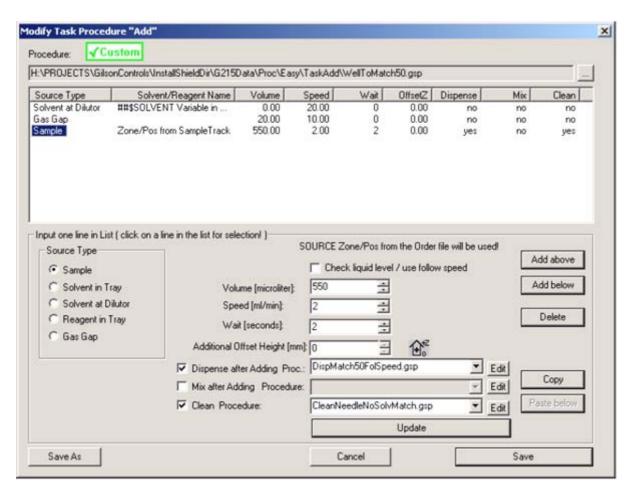


Figure 9.3. Modify Task Procedure ADD

Dispense tasks can be defined as sub-procedures in each line of an Add Task.

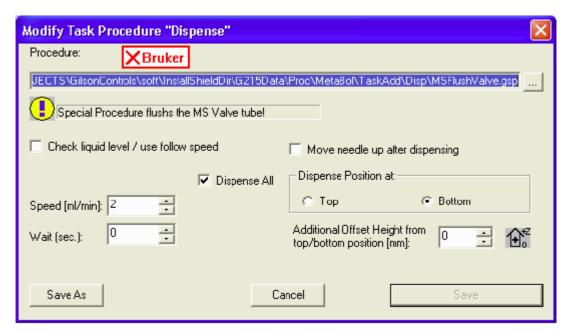


Figure 9.4. Modify Task Procedure Dispense

Task Procedure Mix 9.3.5

Mix tasks can be defined as sub-procedures in each line of an Add Task, but only after a Dispense Task in the list.

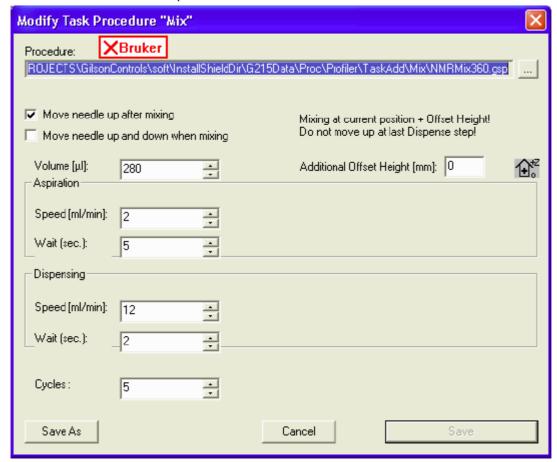


Figure 9.5. Modify Task Procedure Mix

Task Procedure 1MM Samples

9.3.6

Note: It is recommended that you use the <u>"Task Procedure Add"</u> in most circumstances!

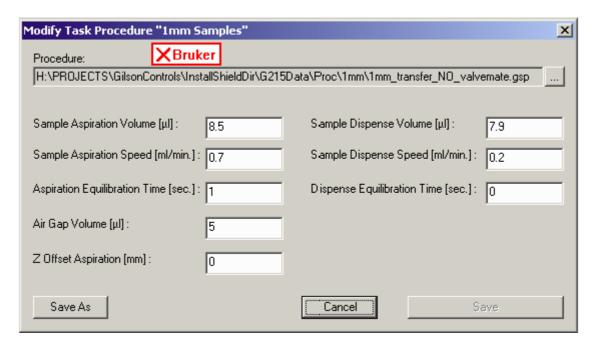


Figure 9.6. Modifiy 1mm Samples Task

Modifying the Procedure Dialog Box

9.4

This dialog box is called from the Modify Procedure option in the View menu (see "View Menu Commands" on page 27). When selected this option shows or hides a Procedure View in the main window, which is used to modify Task procedures at a high edit level for customers.

The last selected TASK procedure is written in the registry (entry: ProcedureLast-Task)

Modification:

 "Custom" procedures have a green "Custom" identification at the top of the dialog box and can be modified:



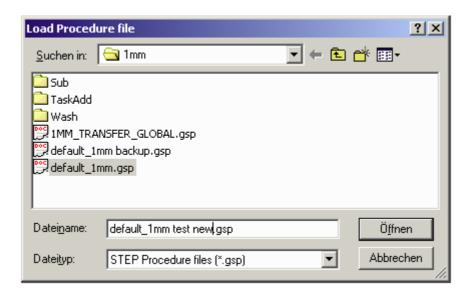
 "Bruker" procedures are delivered from Bruker with the installation, have a red "Bruker" identification and can NOT be modified.



User Guide Version 004 BRUKER BIOSPIN 81 (99)

With the button on the right, which is found on the right side of the current procedure, another TASK procedure of the same type can be selected:





If there was a TASK procedure of a different type selected the following message box appears:



All procedures can be saved as a file with another name with the button:



But only "Custom"- procedures can be saved in the current file with the button:



For "Bruker" procedures the following button is not active:



If the current procedure in the Registry is not a TASK procedure the following message box appears:



Test/Service Tips

10

Service Information 10.1

1. Default Speed Z Axis

• Can be defined in the registry:

Software > Bruker Biospin > Gilson Control > GExecCtrl > Z Speed

• Values 1...5 (default= 4)

Test/Service Tips

How To...



Introduction A.1

The following tasks are discussed in the appendix:

"Define Application Type"

"Create Orders"

"Modify Task Procedures"

"Insert Racks"

"Insert Racks with Barcode Simulation"

"Adding Zones and Tubes to a Zone"

"Define Sort Orders"

Define Application Type

A.2

When starting the program the first time after installation the default procedure selection dialog box appears, allowing you to define the type of procedure and config settings in the registry.

Types of applications: (5 different types of applications can be selected)

- Easy Preparation (working only without SampleTrack)
- 1mm Sample Preparation
- SPE Tube Transfer (working only without SampleTrack)
- Profiler Preparation (working only without SampleTrack)
- SampleTrack Preparation (working only without SampleTrack)

After performing an initialization using menu "Service tools" -> Initialize Pump, all procedures in the export directory (defined in the <u>"Edit Settings Menu"</u>) will be exported to enable a selection of these procedures in the Create Orders dialog box (without SampleTrack) or in the selection box of SampleTrack.

Create Orders A.3

The Create Orders dialog box is used to create test order files if SampleTrack is not selected in the Edit Setting dialog box (see <u>"Edit Settings Menu" on page 14</u>).



The Toolbar button shown to the left is used to open the Create Test Order Files dialog box. If SampleTrack is selected in the Edit Settings dialog box, then the button will be shadowed and unavailable.

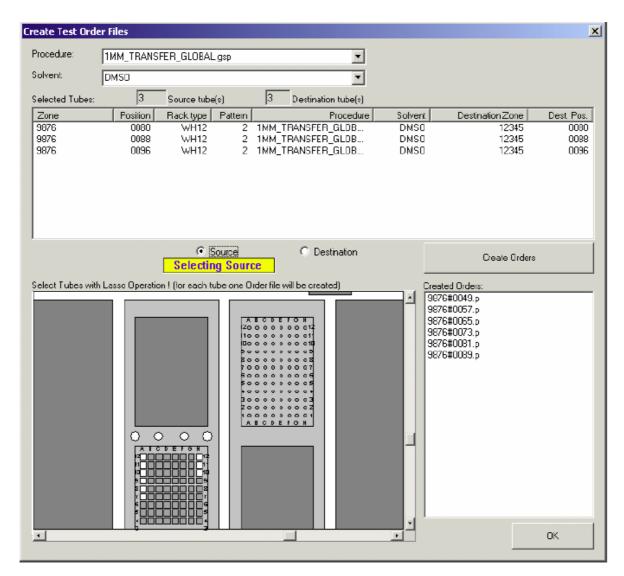


Figure A.1. Create Test Order Files

Variants for different settings:

"Insert Racks with Barcode Simulation"

Modify Task Procedures

A.4

To modify a task procedure:

Open the modification dialog box with the menu "Service tools" -> Modify Procedure (see <u>"Modifying the Procedure Dialog Box" on page 81</u>) or Toolbar button.

If the procedure export path is not correct, (e.g. another application was running) a message box will appear:



In this case select another TASK procedure in the current application folder.

2. Export procedures with the menu "Service tools" -> Initialize Pump (see <u>"Ini-tialize Pump" on page 20</u>).

Exported procedures will be displayed it in the selection box of SampleTrack or in the "Create Orders Dialog Box" (without SampleTrack).

Insert Racks A.5

For applications with SampleTrack (Profiler, SampleTrack):

- Modifications of racks and zones in the ray area are not allowed!
- All rack insert and remove operations will be done automatically with the barcode reader!

In this step only the rack will be inserted. A zone will not be created and tubes will not be added to a zone! Use this method to define a zone for more than one rack or for a part of one rack.

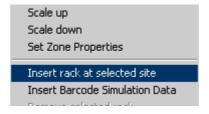
To insert racks with a new zone and to add rack tubes to a zone see <u>"Insert Racks with Barcode Simulation" on page 88</u>.

Inserting a New Rack

A.5.1

Open the tray configuration in the configuration view.

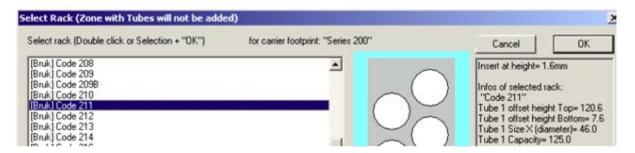
With the mouse right-click on an empty (gray) container area (= site), which will open the following context menu:



Select "Insert rack at selected site".

User Guide Version 004 BRUKER BIOSPIN 87 (99)

This will open the Select Rack dialog box where you can select a rack (you can also double-click on "Create Order Dialog" with your mouse):



"[Bruk]" racks in the selection list are delivered from Bruker with the installation and cannot be modified.

"[Cust]" racks in the selection list (at the end) are customer racks and can be modified.

All tubes from the inserted rack are **not** assigned to a zone (with the color "white"). Only tubes assigned to a zone can be used in other configuration dialog boxes or in procedure steps.

Insert Racks with Barcode Simulation

A.6

Barcode racks could be simulated manually without a barcode reader when defining the barcodes in a special input dialog box:

There are two ways to open the Tray Configuration:

1. Using the Configuration View

Open the **Tray Configuration** in the Configuration View.

2. Using the edit mode in the "Create Order" dialog box.

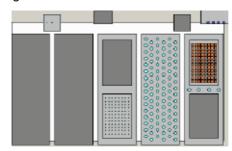
Use this only if no barcode reader is installed (defined in the base configuration):



Selecting the checkbox "Edit Mode" will change the mode of the tray control:



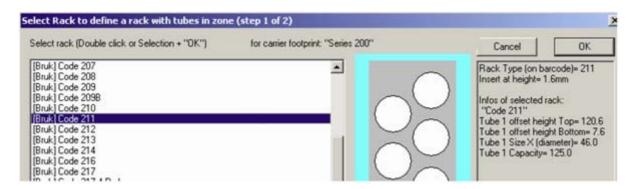
Tray Configuration:



Step 1: Insert a barcode rack

With the mouse double-click on an empty (dark gray) container area or right-click on an empty (gray) container area, and select "Insert Barcode Simulation Data" from the context menu.

In either case this will open the Select Rack dialog box where you can select a rack:

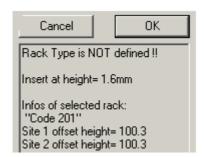


"[Bruk]" racks in the selection list are delivered from Bruker with the installation and cannot be modified.

"[Cust]" racks in the selection list (at the end) are customer racks and can be modified.

Selection Error:

• The following selection error occurs when no barcode type label is defined for the selected rack (e.g. "Code 202"):



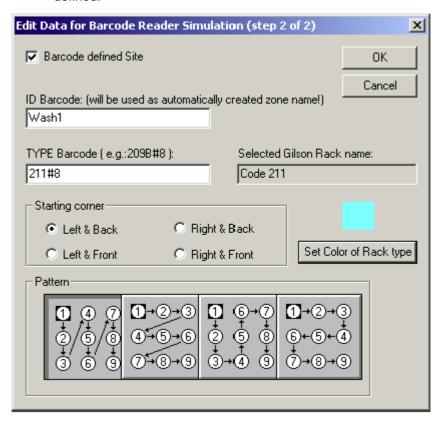


Please contact Bruker or use another rack type if this error occurs!

User Guide Version 004 BRUKER BIOSPIN 89 (99)

Step 2: Insert zone and add tubes to zone

After selecting the Rack Type, the tube numbering order and the rack ID must be defined:



To insert wellplates into a container rack, first insert the container rack (e.g. "205" or "205MI"), then the wellplates (e.g. "WH12" or "WH12@1MM").

The automatically assigned zone can be checked in the tool tip information of the new tubes.

When using a barcode reader to detect barcode racks automatically, refer to "Barcode Zone Configuration" on page 48 for information on the configuration!

Adding Zones and Tubes to a Zone

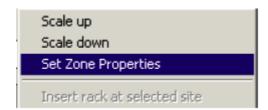
A.7

Open the Tray Configuration in the Configuration View.

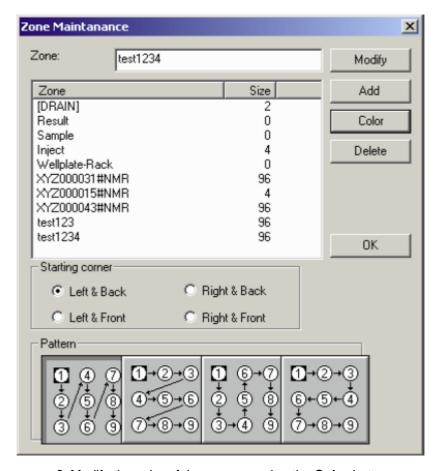
Note: Only tubes assigned to a zone can be used in other configuration dialog boxes or in procedure steps.

When using <u>"Insert Racks"</u>, all tubes are not assigned to a zone (displayed with the color white).

• Open the context menu **Set Zone Properties** from the tray control menu:



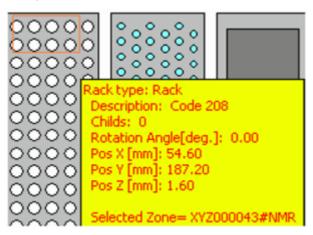
 In the Zone Maintenace dialog box select a zone from the zone list, or write a new zone name in the edit field, and press the Add button.



- Modify the color of the zone pressing the **Color** button.
- Modify the numbering order of the tubes that will be added to the zone in the section Starting Corner and Pattern.
- Press the **OK** button to temporarily save the new zone definitions in the tray configuration diaglog.

User Guide Version 004 BRUKER BIOSPIN 91 (99)

- Select a defined zone in the Zone Maintenance dialog box list, or click on a tube already assigned to this zone (the selected zone will be displayed in the zone edit dialog box).
- Use a "Lasso" mouse operation (the Lasso frame will have the color of the selected zone) to add all tube in the lasso frame to the selected zone (only white-colored tubes that are not yet assigned to a zone can be added to the selected zone).



Removing Tubes from a Zone Manually

A.7.3

Tubes can not be removed individually from a zone, the whole rack with the tube must be removed (see <u>"Deleting a Rack" on page 61</u>).

Adding Zones and Tubes Automatically

A.7.4

A barcode reader must be installed for this procedure.

Two barcodes will be read on each rack automatically:

- 1. Type Barcode
- 2. ID Barcode

During this procedure:

- A new rack of the type **Type Barcode** will be automatically inserted.
- A new zone with the name **ID Barcode** will be automatically created.
- All tubes for the rack will be automatically assigned to the new zone with the name "ID Barcode" (see <u>"Barcode Zone Configuration" on page 48</u>).

Define Sort Orders A.8

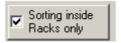
Only for applications without SampleTrack!

Sorting orders defines which order will be at the top of the order list and prepared first.

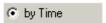
Select the sorting mode in the Edit Setting dialog box



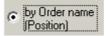
All orders for all currently inserted racks can be sorted, or all orders inside one rack can be executed together:



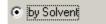
Orders can be prepared according to there creation time (first created order will be prepared first) - check **by Time**:



The sorting by Order name (Position) sorts the preparation in ascending order:



Sorting by Solvent sorts the preparation in ascending order (when ValveMate is installed), but all orders with the currently connected solvent will be prepared first.



User Guide Version 004 BRUKER BIOSPIN 93 (99)

Figures

1 Introd	uction	7
2 Menus	;	9
Figure 2.1.	Print Order List Dialog Box	11
Figure 2.2.	Compare Step Procedures Dialog Box	12
Figure 2.3.	The Load/Save Configuration Dialog Box	13
Figure 2.4.	The Edit Settings Using Web Service Dialog Box	14
Figure 2.5.	The Edit Settings Dialog Box	
Figure 2.6.	Working Area Configuration: Barcode Zones	
Figure 2.7.	The Create Order Files Dialog Box	23
Figure 2.8.	The Status Bar	
Figure 2.9.	The Tray View Dialog Box	
-	Main Protocol File	
•	The Error History View	
Figure 2.12.	Procedure Step View	33
3 Start S	Selections	35
Figure 3.1.	The Select Default Procedure and Configuration dialog box	.35
4 Config	uration	37
Figure 4.1.	The Configuration View dialog box	37
Figure 4.2.	The Base Configuration dialog box	
Figure 4.3.	The Gilson Default Files Configuration Dialog Box	41
Figure 4.4.	Gilson 215 Execution Mode Configuration	42
Figure 4.5.	The Dilutor Configuration dialog box	
Figure 4.6.	The Tray Configuration dialog box for Applications without S	
	pleTrack	
Figure 4.7.	The Solvent Configuration dialog box	
Figure 4.8.	The Reagent Configuration dialog box	
Figure 4.9.	The Barcode Zones Configuration dialog box	
-	Example of a Gilson Tray Configuration Example of a Ports in Tray Configuration	
	The Z-Tower Configuration dialog box	
•	The Edit Solvent Names Dialog Box	
•	The ValveMate Configuration dialog box	
	The Valves & Capillary Configuration Dialog Box	
-	The Cover Configuration Window	
5 The Ra	ack Editor	57
Figure 5.1.	Rack Editor with Rack Selected	58
Figure 5.2.		
•	Soloeting a Pack	EC

User Guide Version 004 BRUKER BIOSPIN 95 (99)

6	Preparation Data Files		65
7	Order	Files	69
8	Solve	nts	73
Fig	ure 8.1.	External NMR Solvent Configuration	. 74
9	Edit P	rocedures	75
Fig	ure 9.1.	Editor Dialog Box of a Wash TASK	. 76
Fig	ure 9.2.	The Modify Task Procedure Clean dialog box	. 77
Fig	ure 9.3.	Modify Task Procedure ADD	. 78
		Modify Task Procedure Dispense	
Fig	ure 9.5.	Modify Task Procedure Mix	
Fig	ure 9.6.	Modifiy 1mm Samples Task	. 81
10	Test/S	ervice Tips	83
A	How T	·o	85
Fig	ure A.1.	Create Test Order Files	86

Tables

1	Introduc	etion	7
2	Menus		9
Tab	le 2.1.	The File Menu Commands	9
Tab	le 2.2.	Description of the Edit Settings Fields	15
Tab	le 2.3.	The Preparation Menu Commands	
Tab	le 2.4.	The Preparation Menu Commands	
Tab	le 2.5.	The Clean Procedures Menu Commands	25
Tab	le 2.6.	The View Menu Commands	27
Tab	le 2.7.	Menus with Toolbar Buttons	27
Tab	le 2.8.	The Preparation Menu Commands	33
3	Start Se	lections	35
4	Configu	ration	37
5	The Rac	k Editor	57
6	Prepara	tion Data Files	65
7	Order Fi	iles	69
8	Solvents	S	73
9	Edit Pro	cedures	75
10	0 Test/Service Tips		
A	How To.	••	85

User Guide Version 004 BRUKER BIOSPIN 97 (99)

Tables

Notes:

User Guide Version 004 BRUKER BIOSPIN 99 (99)

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