

Bruker **BioSpin**

• SAMPLEJET

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TRASHIELD

Firmware 5 User Manual

Version 002

think forward

NMR Spectroscopy

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This manual was written by

Reto Schmid

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Fällanden, Switzerland

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Introduction

What is a SampleJet?

The SAMPLEJET is a high capacity, high throughput sample robot system optimized for NMR applications. It is based on a modular concept.

The basic system takes care of common functionality of a sample handling robot and provides all parts to integrate the SAMPLEJET with standard AVANCE spectrometers. Although capable of stand-alone operation, the SAMPLEJET is connected to the console via a regular RS232 interface allowing standard control through IconNMR or the XwinNMR / TopSpin commands (B-ACS interface).

Figure 1.1. SAMPLEJET System



The SAMPLEJET is a push-button system, which runs under complete computer control enabling modern interfaces like Ethernet and a comprehensive communication link for service and diagnostics with Web based mechanisms. It's built-in electronics control and continuously monitor all operations needed for an entirely automatic sample handling.

The basic system provides all necessary parts (power supply, cables, etc.) to integrate a SAMPLEJET into a NMR laboratory.

The SAMPLEJET's capacity allows it to handle 5 racks of 96 samples (1 mm and 5 mm diameter) each and on the rotating tray 47 samples (5 mm diameter, max.

7^e length). The rotating tray system is designed for openshop operation with common spinners (the ones with yellow ring). The rack system works with a shuttle or a shuttle spinner.

SampleJet Benefits Overview

1.2

1.3

- SAMPLEJET can be mounted on magnets from 300MHz to 700MHz.
- Fast, high capacity sample changer.
- For high throughput and openshop applications.
- 480 sample tubes arranged in 5 racks in 96 well plate format for batch operation (1mm, 1.7mm, 3mm and 5mm tubes possible).
- 47 sample tubes in spinners for open shop sequential operation (3mm and 5mm tubes).
- Easy access for manual sample handling.
- Simple IconNMR control.
- Identify racks from IconNMR by reading their barcodes with a camera (option).
- Remote control (option) for changing openshop samples during measurement.
- Light and door switches kit (option) for safer, faster and more convenient work with the SAMLEJET.

SampleJet Overview

The SAMPLEJET is based on modules which are shown below.



Figure 1.2. SAMPLEJET front view with closed casing

It is mounted onto the magnet with the MAG MOUNTING. It accommodates the different heights of the BST shim upper part and magnet.



Figure 1.3. SAMPLEJET overview inside with partly removed casing

The SAMPLEJET will be placed on top of the MAG MOUNTING and tightened with 4 star screws.

Figure 1.4. SAMPLEJET CAROUSEL TYPE PMMA 5 RACKS



The CAROUSEL TYPE PMMA 5 RACKS can store up to 47 7" samples with standard BRUKER BIOSPIN spinners (the version with the yellow ring) and 5 racks with up to 96 samples. These racks are compatible to the BRUKER BIOSPIN modified Gilson Liquidhandler.

Figure 1.5. SAMPLEJET dimensions



Magnet, side view



Firmware Hints

What is New in Firmware 5

- Rack label handling supported (option) The firmware supports the new hardware SAMPLEJET GRIPPER ARM / 2 (Z108928) with the integrated camera. Barcode labels on the racks can be read to identify or search a specific rack.
- Cover light and door switches supported (option)
 Door Switches indicates, when probes in the storage may have changed. This leads to faster sample handling.
 The light inside the device, switched by the door switches, illuminates the stor-
 - The light inside the device, switched by the door switches, illuminates the storage and shows warnings and errors.
- One-click coordinate calibration for entire system There is now a "push button" calibration available with extended safety functionality for the complete SAMPLEJET. (The format of the calibration data changed, therefore the calibration has to be done again with the new firmware)
- Support of 1.7mm and 3mm sample tubes We introduced two new diameters of sample tubes with their accordant shuttle. The diameters 1mm, 1.7mm, 3mm and 5mm are now supported.
- Better web interface menu structure and account management The menu of the web interface has a new structure with new accounts and passwords for user and service.
- System configuration editable with web interface Every hardware part of the SAMPLEJET is listed in the "System Configuration" and recognized by the firmware. New hardware components can easily be updated through the web interface.
- New functionality on user settings page The "System Settings" has been split into "User Settings" and "System Settings". This leads to a safe and clear design which contains only the relevant values.
- Additional security checks. The firmware can now check if a sample tube is in a position of a rack before inserting a sample there. Empty spinner and shuttles in the openshop storage are now detected as well.
- General motion speedup The movement has been optimized in this firmware in order to accelerate sample changes.

Upgrading to Firmware 5

There are some important things to know when updating to Firmware 5. They are listed below.

- Since the firmware 5 uses a file called "User.xml, instead of the file "Sample-Jet.xml" all the user settings and the counters were transferred to this file. This is done only once when installing the firmware 5 when there is no "User.xml".
- The firmware 5 has a new concept of the calibrations. Calibrations from an older Firmware are not valid anymore. The device will refuse working unless all the calibrations are redone.



You have to do the calibration again after installing the firmware 5.

- If the software runs into a "Hardware Offline" (see <u>"Hardware Offline" on</u> <u>page 38</u>) after restarting the SAMPLEJET the "System Configuration" may be wrong or older hardware is not supported anymore. Contact BRUKER BIO-SPIN for assistance.
- To upgrade to new firmware read the instructions in .<u>"Loading new Firm-</u> ware" on page 50.
- After the installation you should check the "User Settings" for your original values and set the new options.

Safety

3.1

Warnings and Notes in this Manual

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



Potentially Hazardous Areas

3.2

The symbols below shown indicates a potentially hazardous area and strong LA-SER (ISO 3864;DIN 40008).

Warning hazardous area



The symbol is placed on the following areas of the SAMPLEJET:

1. On the front cover, just right of the door (side that is away from the magnet).

2. On the rear side left and right (side that is over the magnet). Warning: Keep cover closed unless manual action has to be done.

Warning LASER hazard



The symbol is placed on the following area of the SAMPLEJET:

1. On the "SAMPLEJET BST ADAPTER UNIVERSAL" on top of the magnet. Do not remove any parts until the SAMPLEJET is powered off.



If one of these symbols is missing, please contact BRUKER BIOSPIN for a replacement!

Disclaimer

- The unit should only be used for its intended purpose as described in this manual.
- Use of the unit for any purpose other than that for which it is intended is taken at the users own risk and invalidates any and all manufacturer warranties.
- Service or maintenance work on the unit must be carried out by qualified personnel.
- Only those persons trained in the operation of the SAMPLEJET should operate the unit.
- Read this manual before operating the unit. Pay particular attention to any safety related information.



BRUKER BIOSPIN is not responsible or liable for any injury or damage that occurs as a consequence of non-approved manipulations on the SAMPLEJET.

13 (87)

The red emergency button on top of the SAMPLEJET is used to disconnect the power supply of all the drives. This will immediately stop any movement of the carousel and the gripper. To turn off the power completely use the switch on the back side of the SAMPLEJET POWER SUPPLY.

Site Considerations

The SAMPLEJET should be setup in a standard laboratory environment. Maximum room temperature should not exceed the range from 17-25°C. For more information refer to the Avance spectrometer manual on site planning available from BRUKER BIOSPIN.

Before Mounting the SampleJet

- Make sure the magnet is firmly secured to its base in order to prevent the instrumentation from tipping over.
- Please check if this magnet needs a "sample changer foot" to extend the magnet base to get the desired stability. This is the case for some 300 and 400 MHz magnets. Contact BRUKER BIOSPIN if in doubt.

While Mounting the SampleJet

- Lifting the SAMPLEJET up to the magnet requires at least two people (ca. 40 kg). Do not try to do it on your own. You may get hurt.
- Beware of the strong magnetic field while working around the magnet. Keep all metal objects, such as tools, screws, or any metallic parts away from the magnet. Remove any mechanical watches or metallic objects while working around the magnet.
- Don't power on the SAMPLEJET during Installation.

During Operation

- Use only new sample tubes in the specified diameter range or otherwise the caps may fall off while the system is running.
- When the SAMPLEJET is running, avoid putting hands or objects in the path of the gripperarm or tray, as this may cause personal injury or damage to the equipment. Therefore it is recommended to keep the doors on the front and back side closed during normal operation.
- Be aware that the SAMPLEJET's horizontal and vertical axis, the tray or the gripper may start a movement unexpectedly.
- Glass tubes may contain hazardous substances. If a glass tube breaks, refer to the corresponding precautions and cleaning/disinfection instructions. Only trained personnel should be allowed to operate the SAMPLEJET. Staff training

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3.7

3.6

3.8

3.5

Emergency Stop

is the responsibility of the owner of the system, BRUKER BIOSPIN will not be responsible for damage resulting from improper training.

- The use of nitrogen as an operating resource instead of compressed air may lead to an oxygen deficiency in the laboratory, e.g. through a technical defect (burst in pneumatic hose). It is highly recommended that oxygen warning device(s) be installed in the laboratory.
- Always have the covers closed while working with the system.

Using the SampleJet

Introduction

In this chapter the handling of the SAMPLEJET for standard use is defined.

States of the SampleJet

Before doing any action on the SAMPLEJET it is important to know the general behavior of the device. It works as a state machine, that means it jumps from one defined state to an other. These are the simplified states:

- Booting
- Idle
- Busy, defined action
- Recovering
- Error, defined error
- · Shutting down
- Hardware offline

During operation the SAMPLEJET jumps from "idle" to "busy" state and back.





4.1

4.2

Accessing the SampleJet

In addition to the display in front of the SAMPLEJET, there is a built-in web server accessible. The web interface is used for service, the display for normal operation. Both of them depend on the firmware and can be different in any versions.

Access from the Display

4.3.1

The Display on the SAMPLEJET is equipped with a touchscreen. The menu is built as a tree shown in <u>"The menu tree of the display" on page 17</u>, all functions are guided.



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It is possible to protect the "service" menu by setting a code in the "User Settings" on the web interface. If no password is set you do not have to log in and out. The "Logout" button is disabled.

If the display is not accessed it shows the "System State" and is dimmed after a time-out of 3 minutes. The dimming options can be set trough the web interface in the menu "Basic Service" on the page "User Settings". Dimming of the display will increase the lifetime of the background light.



Hint: The background light of some of the displays is getting darker and darker with increasing operating hours. If it is unreadable contact BRUKER BIOSPIN.



Figure 4.3. The menu tree of the display

Access from the Web Interface



The web interface was built for service only. For normal operation use the display on the SAMPLEJET.

The SAMPLEJET is connected to a switch in the console with an ethernet connection. This switch connects all the NMR system internal devices in a closed network. This closed network is not connected to any other networks such as the company internal network. Do not connect the SAMPLEJET to an other network, because the fixed IP addresses may cause problems.

The only computer which can access the web interface is the spectrometer computer of the NMR system. One of the two installed ethernet cards belongs to the closed network of the spectrometer.

In this network BRUKER BIOSPIN defines fixed IP addresses, the same IP for the same device on every BRUKER BIOSPIN NMR system.

Every SAMPLEJET has the IP 149.236.99.55, which is defined in the hostfile of the spectrometer computer as "samplejet".



Figure 4.4. The SAMPLEJET web page



To access the SAMPLEJET just enter "samplejet "in a web browser window.

The dynamic web pages are created on the web server, the web browser will receive html pages only. Therefore no java extension is needed.



On the web pages, always use the mouse to press the buttons instead of hitting the "Enter" key.

The SAMPELJET shows different pages, depending on the user level. The "user" account should be used only by the NMR system administrator.

Login	Password	Rights
guest	default, when logged out	read only access
user	bruker	start simple action, change values
service		start service action

Table 4.1. Login table

If you log in as user, you can harm the system if you are not careful.



Figure 4.5. The menu tree of the web page

The SAMPLEJET can handle different sample diameters. The cap on top of each sample serves as an interface between the different samples and the gripper.

BRUKER BIOSPIN delivers factory assembled sample tubes and caps. There is a hole in the cap where sample liquid may be filled through. The Gilson liquid handler's needle fits through this hole. It can be closed once with a pellet.



If the cap does not hold with a sufficient force (6 Newton) on the sample, the sample could be lost during transportation in the SAMPLEJET.



The SAMPLEJET caps are consumables, they may be used only once. If caps are used over again, they might not sit tight enough on the tubes.

Depending on the operating mode of the SAMPLEJET, see <u>"Operating Modes of</u> <u>the SampleJet" on page 27</u>, different sample carriers are used. A Shuttle is a carrier which does not leave the shim system during operation. It just transports a sample up and down. Some of the shuttles clamp the sample for sample spinning.



Check if existing carriers can be used with the SAMPLEJET.

Tubes with Caps	Tube Attributes	Operating Mode	Caps Attributes	Carriers	Carrier Attributes
Z107374 (100 pcs.)	Diameter: 5 mm (+0.05 / -0.15) Length: 7"	Openshop	Violet Without hole	Z42516	Spinning Temperature: Max. 50°C
	Insertion depth: 15 to 21mm			H00177	Spinning (calibrated) Temperature: Max. 50°C
	Diameter: 3 mm (+0.05 / -0.15) Length: 7" Insertion depth: 15 to 21mm	Openshop	Green Without hole	Z45665	Spinning Temperature: Max. 50°C

Table 4.2.The attributes and usage of the carriers

Tubes with Caps	Tube Attributes	Operating Mode	Caps Attributes	Carriers	Carrier Attributes
Z107370 (96 pcs.)	Diameter: 5mm Length: 103.5mm Insertion depth: Configurable 15 to 21mm	5mm Rack	Violet With hole	Z105515	Shuttle Spinning Temperature: Max. 50°C
Z107377 (96 pcs.)	Diameter: 3mm Length: 103.5mm Insertion depth: Configurable 15 to 21mm	3mm Rack	Green With hole	Z105909	Shuttle Spinning Temperature: Max. 50°C
Z106407 (96 pcs.)	Diameter: 1.7mm Length: 100mm Insertion depth: Probe defined.	1.7mm Rack	Gray With hole Not remova- ble	Z106558	Shuttle No spinning Temperature: Max. 50°C
Black: Z73003 White: Z73004 (96 pcs.)	Diameter: 1mm Length: 100mm Insertion depth: Probe defined.	1mm Rack	White, Black With hole Not remova- ble	Z107648 (=Z105512)	Shuttle No Spinning Temperature: Max. 50°C

Table 4.2. The attributes and usage of the carriers

Caps	Description
Z106764 and Z106770.	For the sealed reference samples these special caps are used. The cap consists of two pieces, screwed together. This is not a consumable and can be used several times. Always order the two pieces together.
	Since these caps are higher than the standard caps and their position is not defined, check the height of the tube in the spinner. If it is to high the SAMPLEJET could break the sample tube while moving above it. The maximum allowed height is 60mm!

 Table 4.3.
 Special caps for sealed reference Samples

Part	Description		
Standard Caps	Only the SAMPLEJET caps have the right geometry to guarantee successful sam- ple transport with the SAMPLEJET.		
H00804	Ceramic carriers must not be used with the SAMPLEJET.		
Z5292	Older carriers without a yellow mark must not be used with the SAMPLEJET.		

Table 4.4.Parts not allowed to use with the SAMPLEJET

Using the SampleJet

Part	Description
Z70973	This is a 1mm carrier designed for the BACS samplechanger and must not be used with the SAMPLEJET.
Match System	Match spinner and samples must not be used with the SAMPLEJET.

Table 4.4.Parts not allowed to use with the SAMPLEJET

4.5

The SAMPLEJET has 3 basic operating modes.

- Manual mode
- Rack mode
- Openshop Mode

Changing the Mode

4.5.1

These modes are persistent and have to be changed only if the SAMPLEJET is used in an other way. To change between the modes, press "Change Operating Mode" on the main menu of the SAMPLEJET display. Then follow the instructions on the display. The list of available modes depends on the enabled operating modes in the system settings.

Figure 4.6. Changing the operation mode



Manual Mode

4.5.2

If you do not use the SAMPLEJET and work manually with the BSMS lift use this mode (the BSMS lift is used if the "Lift" button on the BSMS keyboard is pressed, "ej," or "ji" is entered in Topspin). All the sliders inside the SAMPLEJET BST ADAPTER UNIVERSAL are open and the gripper moves away from the BST.





Open the door on the back of the cover to insert and remove samples. The door stays open, if you slide it to the very top.

Figure 4.8. The door on the back



Openshop Mode

4.5.3

Figure 4.9. The openshop mode



If you use 7" tubes with standard spinners, then select this mode. To access a sample in the openshop storage use the "Change Sample" function in the "Main menu" of the SAMPLEJET display. This will rotate the choosen sample position to the door.

If the SAMPLEJET is equipped with a remote control accessing a sample is even easier. Read the chapter *<u>"Remote Control (Option)" on page 53</u>*.

The tray will rotate quickly if no Sample is in the magnet. If there is a sample in the Magnet, the tray will rotate very slowly to not disturb the NMR experiment.



Figure 4.10. Racks and openshop

Rack Mode

Figure 4.11. The rack mode



The rack mode uses the samples stored in the five racks in the carousel. Since these samples are not stored with a carrier, a shuttle is used.

To access a rack for inserting or removing it use the "Change Rack" function in the "Main menu" of the SAMPLEJET display. This will rotate the chosen rack position to the door.

The tray will rotate quickly if no Sample is in the magnet. If there is a sample in the Magnet, the tray will rotate very slow to not disturb the NMR experiment.

If the SAMPLEJET is equipped with a remote control accessing a rack is even easier. Read the chapter <u>"Remote Control (Option)" on page 53</u>.







Make sure that the racks stand flatly on the rotary tray, if you insert new racks.

Figure 4.13. How to insert a rack





In the "User Settings" of the SAMPLEJET a check for rack cover and positioning can be activated.

Sample Holder Numbers

In TopSpin, XwinNMR and IconNMR the samples are addressed by numbers.

Holder Numbers	Used for
1 - 47	For openshop holders
101 - 196	For Samples in the Rack 1
201 - 296	For Samples in the Rack 2
301 - 396	For Samples in the Rack 3
401 - 496	For Samples in the Rack 4
501 - 596	For Samples in the Rack 5

Table 4.5. The holder numbers



To set the sample position enumeration according to your needs, check <u>"User</u> <u>Settings of the SampleJet" on page 36</u>. The default starts with A1, B1 ... H1 and jumps to A2.



Figure 4.14. The enumeration of the rack

SampleJet Version 2.0

IconNMR will accept these sample numbers for the setup of orders. In TopSpin or XWinNMR the sx command can be used to change samples. "sx 25" will insert sample 25 into the magnet, which is an openshop sample and thus requires the SAMPLEJET to be in "openshop" mode. "sx 265" will transport the 65th sample of rack 2 into the magnet and therefore the SAMPLEJET has to be in a rack mode (for short tubes of a given diameter).

To eject a sample without putting a new one into the magnet use "sx ej".

There are gaps within the list. They should not be used, otherwise the SAMPLE-JET will return a "sample missing" message.

SampleJet together with IconNMR

- You can have an overview of the storage. In this overview the state of every sample is displayed with different colors.
- The expanded protocol for the communication between SAMPLEJET and IconNMR enables faster work and support for the SAMPLEJET VISION option.
- You can choose between working with tube positions or working with rack identifications (when using Bruker SampleTrack software).



BRUKER IconNMR software recognizes the SAMPLEJET from the version 4.2, included in TOPSPIN 2.1. From this IconNMR version on the SAMPLEJET is <u>not</u> defined as an BACS (see the "SAMPLEJET Installation Guide" for setting up Icon-NMR).



Figure 4.15. The SAMPLEJET storage overview in IconNMR



For detailed informations about the IconNMR please refer to the ICONNMR documentation.

User Settings of the SampleJet

There is a web page displaying the general user settings. The settings depend on the loaded firmware. To see them, do the following.

- 1. The system has to be in idle state.
- 2. Open a web browser and type "samplejet" or "http://149.236.99.55".
- 3. Log in to the web page as user (password: "bruker").
- 4. On the menu "Basic Service" click on "System Settings".

This page is not refreshed automatically. If you change a setting on the SAMPLE-JET display it will not show up on the page unless you click the "Refresh" button. After changing a setting the "Save" button has to be used to store the values.

System Parameters

 Sample order in the rack Some laboratories may have a certain habit how a rack is addressed. 8 different possibilities can be chosen (See also <u>"Sample Holder Numbers" on</u> <u>page 32</u>). If you use a IconNMR version supporting the SAMPLEJET (Icon-NMR 4.2 and up) this value will be overwritten with the settings from IconNMR.

- Sample insertion depth for samples in clampable shuttles The SAMPLEJET can measure the sample depth when clamping a sample tube with a shuttle. The depth is measured from the center of the magnet (= center of NMR coil) to the end of the glass. The default is set to 20mm and you can chose an offset from -5mm to +1mm.
- Touchscreen service code
 To protect critical functions on the SAMPLEJET display you can choose a
 code. This code is asked, when the functions are choosen from the display. If
 you enter a "0" no code will be asked.
- Backlight brightness when dimmed The lifetime of the backlight of the touch screen can be extended if it is dimmed when not used. You can choose the degree of dimming with this setting. The recommended value is 10%.
- Backlight brightness when not dimmed Depending on the ambient light in the lab the backlight of the touch screen can be adjusted.
- Door mode (only available if "Light and Door Switches" is installed) You can choose between two modes: In the "Normal" door mode the light flashes if a door is open and the device is working. This is a warning to prevent the user to grab a sample or rack when parts are moving.

In the "Service" door mode there is no warning when parts are moving.

Light mode (only available if "Light and Door Switches" is installed)
There are three different modes for the light behavior: In all modes the light
blinks slowly on an error and flashes on danger. You can switch the light on
and off or let the doors control the light automatically like the light in a fridge.

Options

Openshop: Free position check / Occupied position
 If a lot of different people are inserting and removing samples in the openshop
mode these safety options should be switched on. The SAMPLEJET will move to the openshop position and check if it is free before inserting the currently measured sample. If the position is occupied an error is displayed and the SAMPLEJET stops. If you do not want to stop the device choose the option of placing the sample to an other storage number if there is any free. The SAMPLEJET will check for both, tube and spinner.

If there are door sensors indicating the doors were not opened between inserting and removing a sample to the magnet, the check is not proceeded.

Rack: Insertion test

If an untrained person inserts a rack it may forget to remove the cover or checking if the rack stands flatly. If you switch on this option, the gripper will check the rack every time a new rack is accessed.

• Rack: Occupied position

If a the content of a rack changes during the NMR experiment of its tubes, a crash may be the result when returning this tube to the rack. With this option, the position in a rack is checked first before returning a sample to it. If there are door sensors indicating the doors were not opened between inserting and removing a sample to the magnet, the check is not proceeded. We recommend not to change the rack contents during NMR experiments.

Enabled Operating Modes

 Choose the modes to work with from the list. This will affect the available operating modes on the SAMPLEJET display when using the function "Change Operating Mode"

Error Recovery

The error recovery is used to set the SAMPLEJET in a well defined state. There are 4 occasions when an error handling is proceeded.

- After a power up
- After a restart of the application
- · If an error occurs during operation

To handle an error just click "Handle" on the SAMPLEJET display and follow the instructions.



If the SAMPLEJET application is restarted, an error recovery has to be started by pressing "Start" on the display.

4.9

Hardware Offline

The system goes into to the "Hardware Offline" state, if an error occurs during application startup. These errors cannot be handled with the "Error Recovery" sequence. There are 3 possible reasons for the "Hardware Offline" state.

If no hardware or firmware was changed:

1. There is a defective hardware.

If firmware was changed:

2. The new firmware does not support the old hardware.

If hardware was changed (and hardware is not defective):

3. The "System Configuration" has wrong values.



If you have a "Hardware Offline" contact your local BRUKER BIOSPIN representation. You cannot solve the problem on your own.



In the "Hardware Offline" state the web interface is operational for functions which do not access the SAMPLEJET hardware.

Emergency Stop

The red emergency button on top of the SAMPLEJET disconnects the power supply of all the drives. This will immediately stop any movement of the carousel and the gripper. The emergency button can also be used to restart the application.



If the emergency stop has been pressed, the application is restarted when the button is released. This will the lead to en error recovery in any case.

Important Things to Keep in Mind

4.12

- Never interrupt the "busy" state of the SAMPLEJET. Just wait until the operation is finished and the state is "idle" before sending commands to the SAM-PLEJET from the display or the web interface.
- Never apply any forces to the drives, axis and rotary tray of the SAMPLEJET. Applying forces may lead to a misadjusted calibration which may result in a crash and / or sample destruction.

Using the SampleJet

Vision (Option)

5.1

What is the Vision for?

The VISION option is a special GRIPPER ARM with a camera and a spot light integrated. The camera can read bar code labels on the racks and identify them to the BRUKER IconNMR software. This leads to the possibility to set up your Icon-NMR runs from the BRUKER SAMPLETRACK software to a specific rack.





Figure 5.2. A rack with a bar code label



Using the Vision

Since the SAMPLEJET needs more commands for communication with the Icon-NMR, older IconNMR versions cannot be used.



To enable the functionality of the SAMPLEJET GRIPPER ARM / 2 (Z108928) the device has to be listed on the "System Configuration". If it's listed, all of the coordinates and the camera need to be calibrated.

Bar Code Reading Behavior

5.2.1

For a SAMPLEJET equipped with the VISION option the SAMPLEJET LIGHT AND DOOR SWITCHES are recommended. The device can detect if a rack has been changed. Therefore all of the racks are read only as long as the doors are closed. If you open the door all racks are flagged as "ID not reliable" and every rack accessed has to be verified again. If the door stays open, the continuous verification of the racks slows down the working speed.



Always close the doors when using the VISION option to make faster work possible.

If a bar code could not be read the first time SAMPLEJET tries to read it again.



Stray light from outside the SAMPLEJET can disturb a reading. Closing the doors prevents from this problem.

Bruker specifies the bar codes for all automation devices in a separate manual.



Barcode Reading Problems

5.2.3

If the SAMPLEJET is not able to read a bar code it can have various reasons.

- The bar code does not match the specifications.
- The bar code label was not stuck on the right place or aslope.
- The camera is not properly calibrated.
- Light sources from outside the SAMPLEJET disturb the reading. Assure the cover is complete and the doors are closed.

To get an idea of the problem the last 10 unreadable codes are stored as a picture and can be downloaded. The pictures get lost if the SAMPLEJET is switched off.

Downloading unreadable bar codes

- 1. On the spectrometer control computer open a web browser and type in "samplejet" or "http://149.236.99.55".
- 2. Log in to the web page as user (password: "bruker").
- 3. In the "Basic Menu" choose "Download Images".
- 4. Unreadable codes will be shown as a images and can be downloaded.

Basic Service

Basic Service by Operator

There are some simple service operations the user may perform.

- Calibrating the device
- Changing the gripper
- Cleaning the SAMPLEJET
- · Storing the system data
- · Storing the log files
- · Loading new firmware

Calibrating the Device

The calibrating is described in chapter "Calibrating the SampleJet" on page 59.

Replacing the Gripper

If the SAMPLEJET should crash for any reason the gripper is the rated break point to prevent the system from serious damage. Once a gripper lost one or more of the four legs it has to be replaced. For this procedure the drives have to be switched off.

Switching off the drives

- 1. The system has to be in the idle state.
- 2. Press the red emergency button.
- 3. You can now move the gripper manually.

6.1

6.3

6.2

Removing the Broken Gripper.

4. Try to remove the gripper with your fingers. Pull the blue gripper down firmly while holding the gripper arm with the other hand. If it is not removable with your fingers then use a plier like on the picture shown.



The older design of the gripper could not be removed by hand. Use gripping pliers and take care of risks from the magnetic field!

Table 6.1.Replacing a gripper



Table 6.1.Replacing a gripper

Gripper new design	Gripper old design
Remove it with fingers	Remove it with a plier

Mounting a new gripper.

5. Insert the new gripper until a "click" sound can be heared



Take care of the right orientation of the gripper. Between the gripper and the black pen is no gap.



Figure 6.1. Inserting the gripper (new design)

Restarting the system.

Release the emergency button by turning it clock wise. The application will be restarted.

Cleaning the SampleJet

If a sample tube is broken you have to clean all the glass out of the SAMPLEJET. Otherwise the racks will not stand proper anymore on the rotary tray.



Stop the SAMPLEJET from doing any action before you start cleaning the device. Don't forget to stop the submitted jobs in IconNMR.

If proper cleaning is not possible through the front door, remove one of the side covers (--> Angled allen key 2.5).

If the gripper disturbs the cleaning it can be moved away. Choose the function "Change Rack" or "Change Sample" from the display.

6.4

Storing the System Data and the Log Files

In case of troubleshooting an unknown error, BRUKER BIOSPIN may ask you to send the log files and the system data. From these files BRUKER BIOSPIN can get additional debugging information.



These files do not contain any information about your company, samples or spectra. BRUKER BIOSPIN will not give any information to a third party.

System Data

6.5.1

6.5

In the system files, information about the software, the hardware and the user settings are stored. The files are textfiles, containing data in xml (Extensible Markup Language) structure. Three files are stored:

- BIS.xml Contains information about the SAMPLEJET hardware.
- Base.xml Contains default settings and software data and will be replaced with every firmware upload.
- User.xml Contains the user settings, the statistics and the calibration.

The files can be downloaded through the web interface.

- 1. Open a web browser and type in "samplejet" or "http://149.236.99.55".
- 2. Log in to the web page as user (password: "bruker").
- 3. On the menu "Basic Service" click on "Download System Data"
- 4. Follow the instructions shown on the webpage.

Log Files

6.5.2

The SAMPLEJET stores a lot of data in the log files. This is basically a list with an entry each time the SAMPLEJET starts an action. These textfiles may not make sense to users and service engineers. They are intended to be used by the development team.

If the "samplejet.log" file reaches the size of 5 megabytes it will be compressed and stored in a "samplejet_YYYYMMDD_hhmm.gz" file and a new log file will be written.

The "samplejet.log" is the log file with the most current entries.

BRUKER BIOSPIN

There is a simple way to download more than one file by creating a compressed package of files. This is described on the web page.

Downloading Logfiles

- 1. Open a web browser and type in "samplejet" or "http://149.236.99.55".
- 2. Log in to the web page as user (password: "bruker").
- 3. On the menu "Basic Service" click on "Download Logfiles"
- 4. Follow the instructions shown on the webpage.

Loading new Firmware

6.6

A SAMPLEJET firmware has the extension ".deb" and is an archive file. The filename contains some information about the software package.

To check the actually loaded firmware.

- 1. Open a web browser and type in "samplejet" or "http://149.236.99.55".
- 2. Log in to the web page as user (password: "bruker").
- 3. On the menu "Device Information" click on "Firmware"



Remove any samples from the magnet before loading a new firmware.

To load new firmware.

1. The system has to be in idle state

- 2. Open a web browser and type in "samplejet" or "http://149.236.99.55".
- 3. Log in to the web page as user (password: "bruker").
- 4. On the menu "Basic Service" click on "Upload Firmware"
- 5. Follow the instructions shown on the webpage. (The web site depends on the loaded firmware)

Remote Control (Option)

What is the Remote Control for?

The REMOTE CONTROL allows to change openshop samples without disturbing a running NMR measurement.

Further the exchange of a rack or an openshop sample is very easy. Only two buttons are used, the users do not have to know the menu on the display. This is useful if many users are placing racks and samples in the SAMPLEJET.

At least release 4 of the SAMPLEJET firmware is used to operate the REMOTE CONTROL.



It is not possible to harm the SAMPLEJET by uncontrolled pressing of the buttons on the REMOTE CONTROL.

Figure 7.1. The REMOTE CONTROL



How to Install the Remote Control

The installation of the REMOTE CONTROL is simple and can be easily done by the customer, if the REMOTE CONTROL is ordered after the installation of the SAMPLEJET.

- 1. The SAMPLEJET has to be in idle state.
- 2. Remove the cover on the right side. --> Angled allen key 2.5
- 3. Feed the plug trough the hole in the bottom of the frame.
- Connect the plug to the control box on top of the SAMPLEJET (position RES1) and fix the cable with lacing cord.
 --> Screw driver 2

There are several similar plugs! Use the "RES1" to connect the REMOTE CONTROL.



Figure 7.2. Where to connect the REMOTE CONTROL

5. Remount the cover on the right side. --> Angled allen key 2.5

6. If a SAMPLEJET STAIR 4 STEPS is used the REMOTE CONTROL can be mounted to the hand rail.

--> Angled allen key 2.5

If not, attach it to a ladder with the pads or place it on a table.

Figure 7.3. The pads

How to Use to Remote Control

7.3

Just press the + or - button to turn the rotary tray step wise to the left or the right. One step is half a rack or 5 samples.

If a sample is in the magnet the tray will move slower in order to not disturb a running measurement.



Figure 7.4. Using the REMOTE CONTROL

Table 7.1. The REMOTE CONTROL LEDs

LED "System locked"	LED's "Rotate Tray"	Meaning	
Off	Off	System locked by an other process.	
Off	On	The System is idle.	
On	On	The System is locked for the user of the REMOTE CONTROL, commands from the workstation are buffered.	
On	Blinking	The rotary tray is turning in the direction indicated by the LED.	
Blinking	On	REMOTE CONTROL is loosing the "locked" status.	
Blinking	Blinking	SAMPLEJET is in error state.	

If the "System locked" LED starts blinking, the SAMPLEJET will shortly accept commands from IconNMR and may start moving.



If the "System locked" LED is blinking you gain more time by pressing one of the buttons. In this case, the tray will not move if the button is only pressed shortly.



Pressing both buttons for more than 15 seconds will restart the application.



Figure 7.5. The standard sequence

Calibration

Calibrating the SampleJet

The first time after the SAMPLEJET is installed and powered up, the drives and the lift have to be calibrated. Every calibration is stored with its date.

The following calibrations have to be done in the given order. They are described on the next pages.

- 1. Coordinate Calibration Calibrates all the positions of the hardware
- 2. Lift Calibration Calibration of the lift for each shuttle or spinner type
- 3. Vision Calibration If the system is equipped with a camera, the camera needs a calibration



System is to calibrate when updating to firmware release 5 the first time.

8.1

Important Knowledge about the Calibration



Coordinate Calibration

8.3

8.2

You can calibrate the coordinates of the entire system or a specific part of it. The calibration routine can be started from the display or the web interface.

Calibrations

Calibrate Entire System

This routine will calibrate the sample storage, the BST and Extension if present. All calibrations will be saved with the date. It takes about 18 minutes to calibrate all.

- Calibrate Storage In about 13 minutes the sample storage is calibrated. Check if all the racks are inserted correctly before starting the calibration.
- Calibrate BST The SAMPLEJET will automatically find the calibration notch on the SAMPLE-JET BST ADAPTER UNIVERSAL and calibrate it in about 3 minutes.

Calibrate Extension.

SAMPLEJET will calibrate the parking and preheating positions. The calibration is only available if the hardware is listed in the "System Configuration",

Calibrate from display

- 1. The system has to be in idle state.
- 2. From "Main Menu" choose the "Advanced Menu."
- 3. In the "Advanced Menu" choose "Service".
- 4. If there is a service code set in the "System Settings" of the web interface, type in the number.
- 5. Click on "Calibration" and then "Coordinate Calibration".
- 6. Choose a calibration routine and follow the instructions on the display.

Calibrate from the web interface

- 1. The system has to be in idle state.
- On the spectrometer control computer open a web browser and type in "samplejet" or "http://149.236.99.55".
- 3. Log in to the web page as user (password: "bruker").
- 4. In the "Basic Menu" choose "Coordinate Calibration".
- 5. Choose a calibration routine and follow the instructions.

Lift Calibration

8.4

Given the fact that each type of shuttle or spinner has a different weight and a diameter tolerance, the SAMPLEJET needs to calibrate all of them. With some iterations the SAMPLEJET tries to find the fastest set up of the air flow without hitting the sample too hard on the bottom or on the top. Some carriers are calibrated with a sample tube, others without. The carriers for thicker tubes need the tubes to get the normal situation of weight and airflow.

The lift calibration routine can be started from the SAMPLEJET display only.



Only the "Enabled Operating Modes" in the "User Settings" (except the "Manual mode") are available for calibration.

Calibrate from display

- 1. The system has to be in idle state.
- 2. From "Main Menu" choose the "Advanced Menu."

- 3. In the "Advanced Menu" choose "Service"
- 4. If there is a service code set in the "System Settings" of the web interface type in the number.
- 5. Click on "Calibration" and then "Lift Calibration"
- 6. Choose a calibration routine and follow the instructions on the display.

Calibrate from the web interface

• The lift calibration is currently not available in the web interface.

Vision Calibration

8.5

Systems which are equipped with a camera require this calibration. The calibration is available when the appropriate gripper arm is listed in the "System Configuration". The calibration routine can be started from the display or the web interface. To start a vision calibration do the following.

Calibrate from display

- 1. The system has to be in idle state.
- 2. From "Main Menu" choose the "Advanced Menu."
- 3. In the "Advanced Menu" choose "Service".
- 4. If there is a service code set in the "System Settings" of the web interface type in the number.
- 5. Click on "Calibration" and then "Vision Calibration".
- 6. Follow the instructions on the display.

Calibrate from the web interface

- 1. The system has to be in idle state.
- On the spectrometer control computer open a web browser and type in "samplejet" or "http://149.236.99.55".
- 3. Log in to the web page as user (password: "bruker").
- 4. In the "Basic Menu" choose "Coordinate Calibration".
- 5. Follow the instructions.

Printout Section

9.1

What is this Chapter for?

The next pages contain drawings, forms and guidances for the daily work with the SAMPLEJET. Print or copy these pages and post it at a noticeable spot in your lab if required. Every topic is on one page.



Figure 9.1. A1,B1...H1 and Jump to A2



Figure 9.2. A1,A2...A12 and Jump to B1



Figure 9.3. H1,G1...A1 and Jump to H2



Figure 9.4. H1,H2...H12 and Jump to G1



Figure 9.5. A12,B12...H12 and Jump to A11



Figure 9.6. A12,A11...A1 and Jump to B12



Figure 9.7. H12,G12...A1 and Jump to H11



Figure 9.8. H12,H11...H1 and Jump to G12

Content of a Rack

Table 9.1. General information

Rack no.: (1) (2) (3) (4) (5)	Date:	Who:
Rack id.:		
Sample diameter: (1) (5)		

Table 9.2.Samples in the rack

No.	SAMPLE	No.	SAMPLE	No.	SAMPLE
1		33		65	
2		34		66	
3		35		67	
4		36		68	
5		37		69	
6		38		70	
7		39		71	
8		40		72	
9		41		73	
10		42		74	
11		43		75	
12		44		76	
13		45		77	
14		46		78	
15		47		79	
16		48		80	
17		49		81	
18		50		82	
19		51		83	
20		52		84	
21		53		85	
22		54		86	
23		55		87	
24		56		88	
25		57		89	
26		58		90	
27		59		91	
28		60		92	
29		61		93	
30		62		94	
31		63		95	
32		64		96	
Exchange a Rack Using the Display

1. Navigate to the main menu and press the "Change Rack" button.

2. Select the rack to exchange, it will move to the front.

Figure 9.9. Change rack Change Rack (1 of 3) X System State Main Menu x Select Rack Sample in magnet Change Sample Change Rack [2](3](4][5] 1 Change Operating Mode System State Advanced Menu System Idle System Idle System Idle

- 3. Open the front door and remove the old rack (if there is one).
- 4. Insert the new rack and close the front door. (The rack will fit only in one direction.)
- 5. Press "Done"



The SAMPLEJET may start moving after 60 seconds inactivity.





Exchange a Rack Using the Remote Control

- 1. Open the front door.
- 2. Press a button on the REMOTE CONTROL to rotate the rack to the front.
- Figure 9.11. The REMOTE CONTROL



- 3. Remove the old rack (if there is one).
- 4. Insert the new rack. (The rack will fit only in one direction.)
- 5. Close the front door.



The SAMPLEJET may start moving after 60 seconds inactivity.





Exchange a Sample Using the Display

9.6

- 1. Navigate to the main menu and press the "Change Sample" button.
- 2. Select the sample to exchange, it will move to the front.

Figure 9.13. Change sample



- 3. Open the front door.
- 4. Insert the new sample.
- 5. Close the front door.
- 6. Press "Done"



Exchange a Sample Using the Remote Control

- 1. Open the front door.
- 2. Press a button on the REMOTE CONTROL to rotate the sample to the front.
- Figure 9.14. The REMOTE CONTROL



- 3. Insert the sample
- 4. Close the front door.



Change the Operation Mode

1. Navigate to the main menu and press the "Change Operating Mode" button. *Figure 9.15. Change operating mode*



- 2. Select the desired mode.
- 3. Folow the instructions on the Display

BRUKER BIOSPIN Contact

Submit your inquiries about SAMPLEJET sales and service to your local BRUK-ER BIOSPIN representation. Use the following address to get further information.

Contact for Sales Information

For further technical assistance, please do not hesitate to contact us directly at:

BRUKER BIOSPIN AG SAMPLEJET Info Industriestrasse 26 CH-8117 Fällanden

Phone:[+41] 44 825 98 80

E-mail: samplejet-info@bruker.ch

Contact for Additional Technical Assistance

For further technical assistance, please do not hesitate to contact us directly at:

BRUKER BIOSPIN AG SAMPLEJET Service Industriestrasse 26 CH-8117 Fällanden

Phone:[+41] 44 825 98 90

E-mail: samplejet-service@bruker.ch

FTP: ftp://ftp.bruker.ch/pub/NMR/download/SampleJet/



10.1

10.2

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Bruker BioSpin Group

info@bruker-biospin.com www.bruker-biospin.com