

Bruker BioSpin

• SAMPLEJET

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MPLEJ

BRUKER

TRASHIELD

Firmware 5 Installation Guide

Version 002

think forward

NMR Spectroscopy

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Contents

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







Safety

2.1

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

2.2

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.

Emergency Stop

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

2.4

2.7

2.8

2.5

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.

Mounting Instructions

3.1

Caution

Before mounting the SAMPLEJET, it is important to make sure that the magnet is

firmly anchored to its base in order to prevent the magnet from tipping over. Switch off the dampers of the magnet if existing.

Make sure that the shim system is firmly tightened, in order to prevent it from shifting.



All fixed screws have to be secured with LOCTITE. Otherwise the vibrations of the drives may loosen the screws!

But do not use LOCTITE on perspex and the whole cover.



Every SAMPLEJET is delivered with a TOOL KIT containing LOCTITE. Additional LOCTITE 243 Art. Nr. 45872 is available at BRUKER BIOSPIN.



Use the delivered screws for the shim systems which have the appropriate length and material.

Prevent screws and tools from falling into the BST by closing the top of it with the black protection lid.

The SAMPLEJET must be supplied by minimum 5.5 bar and maximum 7 bar. An airflow of 100l/min is needed to guarantee a proper behavior of the lift.

The SAMPLEJET POWER SUPPLY is running from 110 to 240 volts at a frequency of 50 to 60 hertz.

3.2

Required Tools and Consumables for the Installation

The SAMPLEJET comes with a TOOL KIT (Z107443) which contains all the special tools and consumables. An installation needs some additional standard tools which are listed below. All dimensions of the tools are metric system. Every time a tool is used it is marked in this manual by the "-->" sign.

Position	ΤοοΙ	Remark
1	Screwdriver 2	
2	Screwdriver 4	
3	Crosstip screwdriver 0	
4	Crosstip screwdriver 2	
5	Angled allen key 2.5	
6	Angled allen key 3	
7	Angled allen key 4	
8	Angled allen key 5	
9	Angled allen key 6	Only used with a samplechanger foot
10	Flat spanner 7	Comes with the TOOL KIT
11	Flat spanner 13	
12	Flat spanner 16	
13	Flat spanner 17	
14	Water level	Comes with the TOOL KIT
15	Cutter	
16	Metric Scale	
17	2 Ladders	

Table 3.1. Required tools

Table 3.2. Required consumables

Position	Consumable	Remark
1	Some medium size cable ties	
2	Loctite 243	Comes whit the TOOL KIT
3	Cleaning utilities	sometimes used
4	Rubbing alcohol	sometimes used

Installing the Samplechanger Foot

On some small and tall magnets (300 & 400 MHz), an additional samplechanger foot has to be used in order to get desired stability.

If your are not sure, if this additional samplechanger foot is required, please get in touch with the local BRUKER BIOSPIN dealer.



- 1. Switch on dampers if available.
- 2. Attach the samplechanger foot and secure the 4 screws with Loctite. --> Angled allen key 6
- 3. Check that the supporting leg does not touch the ground, to prevent picking up vibrations from the ground.
- 4. Switch off dampers and make sure the magnet is firmly anchored to its base

Installations on the Magnet	3.4
-----------------------------	-----

Determine which Parts to Use

The SAMPLEJET has always to be on the same height in relation to the BST shim upper part. Since the height of the BST shim upper part is different for every magnet, the height of the SAMPLEJET MAG MOUNTING has to be adjusted.

As shown in the picture, measure the length L between the top side of the flange and the lower side of the shim upper part.

3.3

3.4.1



Figure 3.2. Measure the height of the BST shimupperpart tube

Depending on the length L, select the appropriate parts in the table below.

Table 3.3.Matrix which parts to use

	SAMP ADJUSTAB	LEJET LE SLEEVE	SAMP THREAD	LEJET DED ROD	SAMPLEJET DISTANCE TUBE
length L [mm] [inch]					
	Z73988 length 64 mm (2 ¹ / ₂ ")	Z73990 length 94 mm (3 ^{11/} 16")	Z73989 length 60 mm (2 ^{3/} 8")	Z73991 length 90 mm (3 ¹ / ₂ ")	Z105622
0 - 45 0 - 1 ³ / ₄ "	x		x		x
45 - 110 1 ³ / ₄ " - 4 ³ / ₈ "		x		x	x
110 - 147 4 ³ / ₈ " - 5 ³ / ₄ "	x		x		
147 - 207 5 ³ / ₄ " - 8 ¹ / ₈ "		x		x	

Depending on the type of BST flange, different parts have to be used. Measure the height H and the diameter D to determine the proper mounting from the tables below.





Table 3.4. The SAMPLEJET PLASTIC WASHER

	SAMPLEJET PLASTIC WASHER		
height h [mm] [inch]			
<= 3 <= ¹ / ₈ "	Use the 2 plastic washers.		
> 3 < ¹ / ₈ "	Don't use the washers.		

Table 3.5. The SAMPLEJET SPREAD RING

	SAMPLEJET SPREAD RING	
diameter d [mm] [inch]		
85 3 ¹¹ / ₃₂ "	Use the spread ring.	
90 3 ¹ / ₂ "	Don't use the spread ring.	

- 1. Remove the two screws with rounded heads on top of the BST if present. --> Screwdriver 2
- Figure 3.4. The two screws with rounded heads



- 2. Make sure all the screws on top of the BST are not higher than the BST itself. --> Screwdriver 2 and 4
- 3. Place the protection lid on top of the BST.
- 4. Remove the connected air tubes and the spinning rate detection cable.
- Remove the existing air inlets, by screwing them out and replace them with the angled ones, which are shipped with the SAMPLEJET. Use the colored rings from the removed legris with the new legris by pressing them on it.
 --> Flat spanner 13 and 16





Adaptation for the SampleJet Mag Mounting

3.4.3



The BST flange must not be removed completely to install the SAMPLEJET MAG MOUNTING parts. Therefore the shim stack has not to be readjusted.

Skip the parts of the following list which are not necessary. To find out which parts to use check the chapter <u>"Determine which Parts to Use" on page 18</u>.

6. Attach the black SAMPLEJET SPREAD RING, regarding the proper gap orientation to the flange. This is important to a BST ring with gap's to exhaust the BST cooling air.



Figure 3.6. SAMPLEJET SPREAD RING

 Place the 2 special flattened SAMPLEJET PLASTIC WASHERS into the BST ring if needed. Align it so that it will fit into the countersink, the flat side on the outerside.







Mounting of the SampleJet Mag Mounting

3.4.4



Tighten the 6 screws described in point 8), 10) and 11) all together. Otherwise you will have problems introducing the screws in point 11).

8. Attach the SAMPLEJET TENSION RING. Make certain that the outer screws are aligned to the front of the magnet, ensuring access to it. **Slightly** tighten the SAMPLEJET TENSION RING with the delivered longer screws to the flange.

--> Angled allen key 4

Firmly tighten the three outer screws if it's not done already.
--> Angled allen key 4



 Tighten the 2 screws from the side slightly. Make sure that the resulting gaps on each side are symmetrical.
--> Angled allen key 3



Be informed of the fact that there will be a gap of about 1mm between the top flange of the magnet and the SAMPLEJET TENSION RING.

Figure 3.9. SAMPLEJET TENSION RING



11. Mount the SAMPLEJET THREDED ROD and the USC ADJUSTABLE SLEEVE on the SAMPLEJET TENSION RING definite by firmly tighten the 4 screws and the 4 screws from the *Figure 3.9.* above.

--> Angled allen keys 3,4,5

Figure 3.10. The complete thread





Skip this chapter if the SAMPLEJET DISTANCE TUBE is not necessary on this system. Check the result from <u>"Determine which Parts to Use" on page 18</u>. Figure 3.11. SAMPLEJET DISTANCE TUBE



- 12. Use the right-angled plug from the cable Z105098 to connect to the BST shimupperpart.
- Remove all of the 4 screws which are closing the air bypass on the bottom of the SAMPLEJET DISTANCE TUBE.
 --> Angled allen key 4
- Mount the SAMPLEJET DISTANCE TUBE with 2 screws on the BST shimupperpart. The BST lid switch goes into a bore in the bottom of the DISTANCE TUBE. Check if the tube stands flat on the BST.
 --> Angled allen key 2.5





15. Close the tube's opening with the protection lid. This is a precaution.

Adjusting the Height of the Thread

- 16. Place the SAMPLEJET BST ADAPTER UNIVERSAL together with its flange on top without screwing it.
- 17. Adjust the SAMPLEJET ADJUSTABLE SLEEVE until the height to the SAM-PLEJT BST ADAPTER UNIVERSAL measures approximate 160 mm ⁺/- 2 mm.

Hint: one full rotation is about 3 mm ($^{1}/_{8}$ ").



Given by the material of the SAMPLEJET ADJUSTABLE SLEEVE the adjusting may produce noise, smoke and smelliness.



18. Remove the BST UNIVERSAL ADAPTER.

Mount the SampleJet Mounting Universal

Adjust the position of the supporting feet to fit to the diameter of the given magnet. Use the outer most position possible. Depending on the magnet design you have to adjust the legs of the SAMPLEJET MAG MOUNTING.
--> Angled allen key 5



Figure 3.14. The legs of the SAMPLEJET MOUNTING UNIVERSAL

20. Mount the base plate to the positioning ring with 12 screws. --> Angled allen key 5

Figure 3.15. Mounting SAMPLEJET MOUNTING UNIVERSAL



- 21. Check the level of the magnet. A level can be found in the SAMPLEJET TOOL KIT.
- 22. Turn the two supporting feet until the base plate is leveled relative to the magnet.
- 23. Lock the nuts to fix the feet. --> Flat spanner 17

Installing the SampleJet BST Adapter Universal

3.4.8

24. Mount the SAMPELJET CONNECTION FLANGE to the BST or the SAMPLE-JET DISTANCE TUBE. If a SAMPLEJET DISTANCE TUBE is used, check if the flange stands flat on the BST and don't cover the BST lid switch <u>"Don't</u> <u>cover the BST lid switch" on page 24</u>. --> Angled allen key 2.5

Figure 3.16. SAMPLEJET CONNECTION FLANGE SMALL



25. If a SAMPLEJET DISTANCE TUBE is used, then the 4 air bypasses in the flange must be closed with the enclosed screws.

If the SAMPLEJET DISTANCE TUBE is not used, then open the bypasses on the flange by removing the 4 screws. In either case, the bypasses just above the BST are open.

Place the screws on unused positions on the SAMPELJET CONNECTION FLANGE.

--> Angled allen key 4

Figure 3.17. Bypass holes



26. Mount the SAMPLEJET BST ADAPTER UNIVERSAL onto the flange and line it up, so that it's long side is perpendicular to the line of the two helium towers of the magnet. The connectors on the BST ADAPTER UNIVERSAL have to be on the right side.



Top view of the SAMPLEJET BST ADAPTER UNIVERSAL

27. Check again the height of the BST UNIVERSAL ADAPTER.



Figure 3.18. Measuring height again

28. If no SAMPLEJET DISTANCE TUBE is used then use the right-angled connector from the cable Z105098 to connect to the BST ADAPTER. See <u>Figure</u> <u>3.19.</u>



Figure 3.19. SAMPLEJET BST ADAPTER UNIVERSAL cabling

Mount the SampleJet

3.5



For safety reasons, two stable ladders are recommended to stand on, while lifting the system up.

- 29. Remove the transport lock of the SAMPLEJET GRIPPER ARM and the SAM-PLEJET CAROUSEL.
- 30. Arrange the cables in order to prevent stepping over it while carrying the system.
- 31. For safety, two ladders are recommended in front of the magnet. Check that they are stable enough to carry the additional weight of the SAMPLEJET.



Figure 3.20. Lifting the SAMPLEJET onto the magnet

- 32. Lift the SAMPLEJET onto the SAMPLEJET MAG MOUNTING platform.
- 33. **Always** attach all 4 screws! (The original screws have a length shorter than 11mm, to prevent the screws from digging into the turntable.)

Figure 3.21. Fixing the SAMPLEJET on the platform



34. Move the SAMPLEJET towards the BST until the limit is reached. Fasten the 4 screws. The SAMPLEJET is now mechanically mounted.



Clean the area around the SAMPLEJET CAROUSEL. Swarf can damage the teeth of the SAMPLEJET CAROUSEL drive.





3.6

3.6.1

Connecting the SampleJet BST Adapter



2x2 black and blue hoses





39. Connect the air tubes to the BST. Insert a **Y** or **T** legris to the white air tube for lift function. Put the tubes to BST from underneath through the opening and connect them.



Connecting the SAMPLEJET to the Console

3.6.3

The necessary cables and hoses to connect the SAMPLEJET to the Console are part of the SAMPLEJET BASIC KIT.

- 40. Open the back cover of the Spectrometer Console.
- 41. Place the SAMPLEJET POWER SUPPLY between the BSMS and AQS rack and switch it off.
- 42. Use a free power cord to connect it to the main power.
- 43. Install the Ethernet Switch if no switch is already installed.
- 44. Lay out the long, black cable loom from the magnet to the console, so it is parallel to other cables going on top of the magnet. Use the side where the hoses and cables have the same length to direct to the magnet.
- 45. Insert the cable into the opening in front of the SAMPLEJET.



Figure 3.26. Inserting the cable into the SAMPLEJET

46. Connect the plugs into the corresponding connectors on the SAMPLEJET CONTROL BOX.



- 47. Use lacing cord to attach the cable loom to the magnet and in the SAMPLE-JET.
- 48. To allow further access to the BST, the frame of the SAMPLEJET can slide away from the magnet on the base plate. For this reason the cable should not be mounted too tight.





- 49. Insert the lacing cord cable into the console similar to the BSMS cable.
- 50. Connect the ETH_HOST plug into any port on the ethernet switch.

Figure 3.28. Ethernet switch



51. Place the SMAPLEJET POWER SUPPLY inside the console if there is some free space. The power switch on the back side should be accessible.

Do not obstacle neither the air circulation of the console nor the fan on top of the SAMPLEJET POWER SUPPLY.

52. Clamp the POWER connector into the plugs on SAMPLEJET POWER SUP-PLY and screw the grounding wire to the chassis as seen in *Figure 3.29.*

Figure 3.29. SAMPLEJET POWER SUPPLY in the console



- 53. Connect the TTY_SPECT cable to any free connector on the tty panel of the AQS rack. Default is tty08.
- 54. Connect the GAS_IN hose to the console using a **Y** or **T** legris. The SAMPLE-JET needs at least 5.5 bar, so it has to be connected before the pressure reduction unit in the console.
- 55. Close the back cover of the console.

Install the SampleJet Cover



Don't use LOCTITE for the cover.

- 56. Attach the side covers. --> Angled allen key 2.5
- 57. Put the top cover onto the 4 posts.
- Mount the front cover, but handle it with care. It is quite fragile. On some older system the screws can't be tightened to a dead stop.
 --> Angled allen key 4
- 59. Hook in the rear cover over the back of the SAMPLEJET by the center of the magnet.
Mounting Instructions

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 4.1. The REMOTE CONTROL



4.1

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 4.2. 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.



How to Use to Remote Control

4.3

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 4.4. Using the REMOTE CONTROL

Table 4.1. 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 4.5. 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.

5.1

Important Knowledge about the Calibration



Coordinate Calibration

5.3

5.2

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

5.4

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

5.5

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.

Initial Configurations

6.1

Introduction

This chapter will lead you through the configuration, fine adjustment procedures, pneumatic settings, and final setup of the SAMPLEJET. These adjustments should be made after the SAMPLEJET has been mounted in accordance with the mounting instructions.



Do not start the SAMPLEJET by any "SX" commands or IconNMR jobs unless the SAMPLEJET is calibrated correctly! This is described in <u>"Calibrating the SAMPLEJET" on page 51</u>

Power up the SAMPLEJET

- 1. Make sure the emergency button is released.
- 2. Switch on the 24 V power supply of the SampleJet, which is located in the Console.
- 3. Wait until the touch screen in front of the SampleJet is starting up. This may take up to 30 seconds.
- 4. Follow the startup procedure. Note: read the advice given on the display carefully.



If the power up sequence leads into the error state again and again, maybe some cabling/hoses are plugged in wrongly. Check the installation and try again.

Readjust the BSMS Lift

Except for the SAMPLEJET manual mode the SAMPLEJET controls the BST lift itself. After installing a SAMPLEJET, the BST lift (controlled by the BSMS) has to be set up again in the service mode of the BSMS. This lift mode is used if the SAMPLEJET is operated in manual mode.

- 5. Change the SAMPLEJET operation mode to "manual".
- 6. Switch on the BSMS lift.
- 7. Insert an long sample with the heaviest carrier the customer is using.
- 8. Adjust the BSMS lift to a value which brings the sample to the top.

Set up the Service Access with a Web Browser

A web server on the SAMPLEJET provides you with a simple way to manage the SAMPLEJET. With any common web browser on the spectrometer computer you get access to it.



You need an administrator or super user password to configure the hosts file. If you can not change the hosts file, the IP has to be used. In this case create a shot cut on the web browser to this IP and name the shortcut "SampleJet".

 Check if the hosts file contains an entry for the SampleJet. The SAMPLEJET uses the fixed IP address: 149.236.99.55. This IP address is only valid in the spectrometer network.

Table 6.1.Where the hosts file are located

Operating System	Path to the hosts file
Windows	C:\WINDOWS\system32\drivers\etc\hosts
Linux	/etc/hosts

6.3

Figure 6.1	. Hosts file		
🚺 hosts - Note	pad		
File Edit Form	at View Help		
127.0.0.1	localhost	localhost.localdomain	# Do not change this
# 149.236.99 149.236.99 149.236.99 149.236.99 150.205.48 149.236.99	1 ASP_ST2 99 spect av300 89 dru1 88 dru2 6 deliver 55 samplejet	# Second Et) av400 av500 av600 av700 # DRU entry # DRU entry # Address f	hernet Card av800 av900 # EthernetCar or delivering

10. Just type "samplejet" in any Web browser to get access to the service web if the hostfile is modified correctly.

The Main Window

6.3.1



The Login Window

6.3.2

		Br	uker Sam	pleJet			
Device Information System Configuration Statistics Date & Time Sample Database From	Current Login: Login as: Servi	Guest	Login	ningsen.	a freezen	angelen.	-9
Loglie Documentation	Login	100					
About Us Login							
	with the						
	antinda						
	angerst.	machen	© Bruker B	ioSpin AG (Switzerli	and)	aproxim.	anters
	State: System	idle (5mm-Rac	k)				Login:

Figure 6.3. Login web server window

For setting up the SAMPELET, use the user "Service". Log in to the web page as service (contact BRUKER BIOSPIN if you don't know the password). For more information about the users, read the user manual.

Check Firmware Version

6.3.3

6.4

The functionality of the SampleJet depends on the installed firmware version on the SampleJet. The installed version can be seen on the web page:

11. Open a web browser and type in "samplejet" or "http://149.236.99.55".

12. In "Device Information" see the "System Configuration".

Figure 6.4. Installed firmware version

		Bruke	r S	ampleJet			
		Display	y Syst	em Configuration			41
Device Information System Configuration Statistics Date & Time Sample Database Error	Software SampleJet Firmware Version 5b20070508			BE CORE	mp.GHR.	andr	
Logfie	1. C/22 C	Hardware		a			
Basic Service	Component	Production ID	ECL	Serial Number			
Advanced Service	Basic Kit	Z105514	0.0	1			
Documentation	Base Plate	Z104529	0.0	2			
About Us	Carousel Drive	Z73868	0.0	3. 8482			
	Carousel	Z105513	1.0	4			
Login	Axes System	Z104678	0.0	5			
	Gripper	Z73878	2.0	10			
	Control Unit	Z105243	1.0	11			
	Casing	Z105443	0.0	12			
	BST Adapter	Z105516	2.0	13			
	Preheating Unit	Z109174	0.0	14			
	Parking Unit	Z109175	0.0	15			
	Light + Door Switches	Z108935	0.0	16			
	all all	10 A.Y		ances			
			© Bru	ker BioSpin AG (Switze	rland)		
	State: System idle (5 Action:	imm-Rack)					Login: Service

Set up the System Settings

Currently there is only one setting you might have to change. This is the type of the shim system, it will affect the lift air.

- 13. Open a web browser and type in "samplejet" or "http://149.236.99.55".
- 14. Log in to the web page as service (contact BRUKER BIOSPIN if you do not know the password).
- 15. In the menu "Advanced Service" choose "System Settings".
- 16. Select the BST type installed at your system. The Z-number can be looked up from the label on the top of the BST.

6.5

The chapter describes the setup with a TopSpin 1.3 or 2.0 installed. With Xwin-NMR 3.5 do the setup analogical to the description.



- 17. Do "cf" in TopSpin or XwinNMR.
- 18. Enter the tty channel which the SampleJet is connected to.
- Figure 6.5. TopSpin TTY window

S-232/485 channels for external device	5 Ht 40			
BSMS Smart Magnet Control System	шуто •			
	tty02			
L C NMD Software Hyster				
VTI Variable Temperature Unit				
Cradient Temperature Unit (PCU 90)	цуор 🗸			
MAS Broumetic Centrel Unit				
RACS Prieumatic Control Onic	no v			
Baco Bruker Automatic Changer	ttyua 🗸			
Caro Controllor	no 🗸			
UPOLI List Rever Centrel Lisit	no 💌			
A Phose Medulater	no			
4 Priase Mouulator	no 💌			
Freeniphasis/Gradient Onic	nu			
ockswitch				
Lockswitch no 🖌 🗸				
.ockswitch no				

- 19. Tick the box "Should the sample changer control the lift."
- 20. Enter 0 in "Delay between SX and next command[s]."

Cf			
Additional configuration:			
Security configuration			
Enable peak power check (POWCHK):			
-Sample changer configuration			1
Should the sample changer control the lift:			
Delay between SV and next command [c]:			
Delay between 3x and next command [3].			
BACS options:	-		
Fast SampleRail mode:			
		Previous N	ext > Cancel

21. At the end of the "**cf**" you get a summary called "CONFIGURATION INFOR-MATION" of all the hardware installed. If the SAMPLEJET has been recognized by "**cf**" you can find it in this file.

Figure 6.7. CONFIGURATION INFORMATION after cf

```
BACS Sample Changer: device connected to 149.236.99.243:/dev/tty04
- Capacity: 596 holders
- Firmware: 970111
- use BACS air = yes
- BACS sx delay = 0 s
- Sample Rail fast changer mode = no
```

6.6

Table 6.2.Supported SX commands

Command	Remark
sx <holder number=""></holder>	Removes the previously inserted sample automatically. Inserts the choosen sample from the holder into the magnet
sx ej	Removes sample from the magnet and puts it back to its origin.

Set up IconNMR

The chapter describes the setup with a IconNMR version 4. With other versions do the setup analogical to the description.



IconNMR version 4.2 or later supports SAMPLEJET specific functions.

Depending on the version of IconNMR different Automation modes are available.

Table 6.3.Deciding the Automation Mode

IconNMR Version	Automation Mode	Description
< 4.2	"Standard BACS"	Working by relating on positions.
>= 4.2	"Sample Jet"	Working by relating on positions
	"Sample Track (Sample Jet)"	If a SampleTrack is installed you can work by relation on bar code ID's on the racks. (Only with the "VISION" option)

If the customer uses IconNMR for the first time the setup is slightly different than if IconNMR is already in use. If IconNMR is in use, continue with <u>"Setup IconNMR</u> if Already in Use" on page 56

Setup IconNMR for First-Time Use

6.6.1

- 22. Enter "IconNMR" in TopSpin.
- 23. In "Express Setup for First-Time Use" select the automation mode. See <u>"De-</u> <u>ciding the Automation Mode" on page 55</u>



24. In the menu "Automation Window" change the "Default Number of Sample Holders" to "596". See <u>"The number of sample holders" on page 58</u>

Setup IconNMR if Already in Use

6.7

- 25. Enter "IconNMR" in TopSpin.
- 26. Select "Configuration" in the IconNMR start window.
- Figure 6.9. IconNMR start window



27. Select the menu "Automation Configuration" (or "Master Switches") change "Default Automation Mode" to the desired automation mode. See <u>"Deciding</u> <u>the Automation Mode" on page 55</u>

The ICON MUD: Confirmation		
File		Help
	The Operation of States	Leb
User Settings	Start run at user login	
-User Manager	Default Automation Mode	Standard BACS -
-Additional Users	Eject last sample in queue	
Originator Items	Process Data Sets after Acquisition	Always
Automation Window	Generate Spectrum Print-Out file in data set for	In PDF Format
ToolBox Setup	possible dispatch to E-mail recipient.	
Automation Configuration Master Switches	Automatic Lock Program	
©-Shimming	Abort Acquisition on Shim Failure	
-Shimming Controls	Innore the TOPSPIN Prosol Parameters	
CON-NMR: Configuration		
-Au Eile		Help
Tel E User Settings	Run Control	
HLC User Manager	Default Automation Mode	Sample Jet
-Sar -Composite Experiment	s	
-WE Additional Users	Sample Sequence	$M \leq m \leq m \leq M$
ICON- E Automation		
-Master Switches	× Eject last sample in o	jueue
Automation Window	Start run at usen lor	
Solvent/Prohe	Processing Control	
Dependencies	Gononato a Shaothum Dr	ninteut
Tuning/Matching	ICON-NMR: Configuration	X - L
Temperature Handli	Eile	Help
-LC-NMR Options E	∃ User Settings F	un Control
-SampleTrack Option	User Manager	Default Automation Mode Sample Track (Sample Jet)
Veh Interface	Composite Experiments	
General Options	-Originator Items	Sample Sequence $\geq M \geq M \geq M \geq M$
ToolBox Setup E	3 Automation	X Fiert last samle in mene
Accounting	-Master Switches	× Never Rotate the Sample
	⊖ Lock/Shim Options	Start run at user login
	Solvent/Probe F	rocessing Control
	Dependencies	Generate a Spectrum Printout
	-Priority	Process Data Sets after Acquisition Always 👻
	- Temperature Handling	benerate Spectrum Print-Out file in data set for possible dispatch to E-mail recipient.
	-LC-NMR Options	Perform Structure Consistency Check
	-Fail Safe / Error Handling	ataSet Management
	L.Web Interface	Ignore the TopSpin Prosol Parameters
	General Options	Delete temporary datasets after experiment end
	ToolBox Setup	★ Hilow Uverwrite of existing Hoquisition Data EST Mode Settings
	The country is	Finable BEST-NMR
		SEST-N/R Automation Mode Standard (No Barcodes)
		Force Solvent Change after
		(Number of Hours - Day Time only)
		best Hoministration Tool

Figure 6.10. Selecting the automation device



28. In the menu "Automation Window" change the "Default Number of Sample Holders" to "596"

Acceptance Test

This chapter describes the tests which are done at the customer site at the end of the installation. The test shows the customer the proper function of the SAMPLE-JET.

Error Preventing Routines

The software has some special routines to avoid errors. Those routines can handle minor problems by repeating an action several times until it works. This should prevent the system from stopping, but they should rarely occur in a newly installed system. If you see one of the following actions, repeat the calibration procedure.

- Glass sensor does not find a sample tube. The gripper moves to different positions away from the center of the magnet when inserting or removing an open shop sample. The system tries to see the glass tube. Often an aslope mounted sample cap is the reason for this behaviour.
- Problems with lowering the sample to the probehead. If a sample hangs in the SAMPLEJET BST ADAPTER UNIVERSAL the software tries to free it by switching on and off the lift several times. If this will still not help the software opens and closes the gate slider in a fast interval to shake the sample a little bit.
- Problems with ejecting a sample. The Software switches on and off the lift to eject the sample.



The error preventing routines must not permanently occur during acceptance test.

Test Procedure

7.3

Each mode the customer works with has to be demonstrated to the customer. During this demonstration no error must occur. If there is an error try to solve the problem and repeat the test.

7.2

7.1

Rack Mode

Use "SX" command from Topspin or XwinNMR to insert the defined samples from the racks. It is possible to use one rack in all positions.

- Rack 1: Sample position A1.
- Rack 2: Sample position A12.
- Rack 3: Sample position H1.
- Rack 4: Sample position H12.
- Rack 5: Sample position D6.

Figure 7.1. The used rack positions



Use the user setting for the rack numbering of the customer to do the test. To see them do the following procedure.

- 1. The system has to be in idle state
- 2. 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. On the menu "Basic Service" click on "User Settings".
- 5. Lock at the setting "Sample order in the racks".

Table 7.1.	The	position	numbers
------------	-----	----------	---------

Setting	Rack 1	Rack 2	Rack 3	Rack 4	Rack 5
Start with A1,B1H1 and jump to A2	101	289	308	496	544
Start with A1,A2A12 and jump to B1	101	212	385	496	542
Start with H1,G1A1 and jump to H2	108	296	301	485	545

Table 7.1. The position numbers

Setting	Rack 1	Rack 2	Rack 3	Rack 4	Rack 5
Start with H1,H2H12 and jump to G1	185	296	301	412	554
Start with A12,B12H12 and jump to A11	189	201	396	408	552
Start with A12,A11A1 and jump to B12	112	201	396	485	543
Start with H12,G12A12 and jump to H11	196	208	389	401	553
Start with H12,H11H1 and jump to G12	196	258	312	401	555

If there is any problem, the storage calibration has to be repeated.

Open Shop Mode

7.3.2

7.3.3

Use "SX" command from Topspin or XwinNMR to insert the defined samples from the openshop. It is possible to use one sample for both positions.

- Openshop: Sample position 12.
- Openshop: Sample position 35.

Settings of IconNMR

If the customer uses IconNMR, you have to set up a job and let it run.

• Any sample position higher than 120.

Vision Option	7.3.4

If the System is equipped with a VISION option, try the bar code reading by processing some experiments from SampleTrack.

Remote Control Option	7.3.5

Try to rotate the storage in both directions.

Light and Door Switches Option	7.3.6
--------------------------------	-------

Both switches, front and back door, have to be tested. If you open a door, the light should turn on.

User Training

Introduction

After the installation of the SAMPLEJET the customer has to learn some basic knowledge about the SAMPLEJET. All these important things and the often used procedures are listed below.



Procedures to be done by the customer are all described in the SAMPLEJET "User Manual". In this chapter you will find only references to the "User Manual".

Basic Operations

The user has to be informed about the basic operations:

- How to start the web interface and log in.
- How to access the menu on the display on the SAMPLEJET.
- How to handle an error.
- The function of the emergency button (it just switches the drives off, the power is still on!).
- The "busy", "idle" and "error" state of the SAMPLEJET.
- · How to change between the modes "manual", "openshop" and "rack"
- Knowing the function of the shuttles, special spinners and the tube caps.
- How to insert racks and openshop samples.
- How to run the SAMPLEJET from XwinNMR, TOPSPIN and IconNMR.

BRUKER BIOSPIN

Don't do...

The following points are important.

- Never interrupt a "busy" state.
- Never apply any forces to the drives.

8.3



8.1

Basic Service

These basics can be done by the customer.

- Calibrating the device.
- Replacing a gripper.
- Cleaning the SAMPLEJET.
- Storing the system data and the log files.
- Loading new Firmware.

After Sales Service

8.5

Inform the customer about how to get help and information.

- 1. Contact information of the local BRUKER BIOSPIN representative.
- 2. If this will not solve the problem refer to the "Contact" chapter in every SAM-PLEJET manual.

BRUKER BIOSPIN Contact

General Questions

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/

9.2

9.3

BRUKER BIOSPIN Contact

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5 Calibration

6

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