

SampleCase standard, cooled & heated

User Manual Version 003

Innovation with Integrity

NMR

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1 About This Manual

This manual enables safe and efficient handling of the device.

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

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

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

1.1 Policy Statement

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

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

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

1.2 Symbols and Conventions

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

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

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



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

This is the consequence of not following the warning.

- 1. This is the safety condition.
- ► This is the safety instruction.



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

This is the consequence of not following the warning.

- 1. This is the safety condition.
- ► This is the safety instruction.



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

This is the consequence of not following the warning.

- 1. This is the safety condition.
- ► This is the safety instruction.

NOTICE

NOTICE indicates a property damage message.

This is the consequence of not following the notice.

- 1. This is a safety condition.
- ► This is a safety instruction.

SAFETY INSTRUCTIONS

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

This is the consequence of not following the safety instructions.

- 1. This is a safety condition.
- ► This is a safety instruction.



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

2 Introduction

2.1 Overview of Sample Case Options

The Sample Case[™] system is designed to easily transport the customers NMR tubes into the magnet and back. For this the NMR tube will be transported up and down with the lift gas and shifted horizontally by a pneumatic drive. This is all fully controlled from software and verified by optical sensors. Users have only to start the transport of a sample from the computer interface or at the hardware interface itself. Furthermore the user can observe the progress of the interaction indicated by the status LED on the SampleCase system.

The SampleCase system, often referred to as the device in this manual, can be ordered in three options all based on a carousel for the samples. This carousel provides holders for 24 carriers for samples. Beside the standard version with 24 holders in the carousel the SampleCase cooled and SampleCase heated option are available.

There are two system configurations with different linear axis lengths available. The short linear axis can be installed on most magnets, but for some magnets the long linear axis is mandatory. The SampleMail system with a standard transport tube can be mounted on most magnets.

Option	System	Sample Temperature Range	included
AH0171	SampleCase (24 position carousel)	• N/A	 1 SampleMail plus Z123384/Z133067
			 1 SampleCase Z122633
			Accessory
AH0172	SampleCase cooled	 Selectable 4°C up to 40°C Uniformity of +/-2 °C with setpoint @6°C 	 1 SampleMail plus Z123384/Z133067
			 1 SampleCase cooled Z143007
			• 1 BCUI
			Accessory
AH0178	SampleCase heated	 Selectable room temperature up to 125°C Uniformity of +/-5 °C with concept @125°C 	 1 SampleMail plus Z123384/Z133067
			 1 SampleCase heated Z155921
			Accessory

Table 2.1: Overview of SampleCase Options

2.2 Intended Use

The device has been designed and constructed solely for the intended use described above. Intended use also includes compliance with all specifications within this manual.

Any use which exceeds or differs from the intended use shall be considered improper use. No claims of any kind for damage will be entertained if such claims result from improper use.

2.3 Installation and Initial Commissioning



Installation, initial commissioning, retrofitting, repairs, adjustments or dismantling of the device must only be carried out by Bruker Service or personnel authorized by Bruker. Damage due to servicing that is not authorized by Bruker is not covered by your warranty.

2.4 Limitation of Liability

All specifications and instructions in this manual have been compiled taking account of applicable standards and regulations, the current state of technology and the experience and insights we have gained over the years.

The manufacturer accepts no liability for damage due to:

- Failure to observe this manual.
- Improper use.
- Deployment of untrained personnel.
- · Unauthorized modifications.
- Technical modifications.
- Use of unauthorized spare parts.

The actual scope of supply may differ from the explanations and depictions in this manual in the case of special designs, take-up of additional ordering options, or as a result of the latest technical modifications.

The undertakings agreed in the supply contract, as well as the manufacturer's Terms and Conditions and Terms of Delivery, and the legal regulations applicable at the time of the conclusion of the contract shall apply.

2.5 Warranty Terms

The warranty terms are included in the manufacturer's Terms and Conditions.

2.6 Customer Service

Our customer service division is available to provide technical information. See the chapter Contact for contact information.

In addition, our employees are always interested in acquiring new information and experience gained from practical application; such information and experience may help improve our products.

2.7 Product Safety and Electromagnetic Compatibility

The device complies with the standard

- IEC 61010-1 and with UL 61010-1 / CSA C22.2 No. 61010-1-04 Safety Requirements for Electrical Equipment.
- IEC 61326-1 for Electromagnetic Compatibility (EMC)

3 Safety

3.1 System Owner's Responsibility

System Owner

The term *system owner* refers to the person who operates the device for trade or commercial purposes, or who surrenders the device to a third party for use/application, and who bears the legal product liability for protecting the user, the personnel or third parties during the operation.

System Owner's Obligations

The device is used in the industrial sector, universities and research laboratories. The system owner of the device must therefore comply with statutory occupational safety requirements.

In addition to the safety instructions in this manual, the safety, accident prevention and environmental protection regulations governing the operating area of the device must be observed.

In this regard, the following requirements should be particularly observed:

- The system owner must obtain information about the applicable occupational safety regulations, and in the context of a risk assessment must determine any additional dangers resulting from the specific working conditions at the usage location of the device. The system owner must then implement this information in a set of operating instructions governing operation of the device.
- During the complete operating time of the device, the system owner must assess whether the operating instructions issued comply with the current status of regulations, and must update the operating instructions if necessary.
- The system owner must clearly lay down and specify responsibilities with respect to installation, operation, troubleshooting, maintenance and cleaning.
- The system owner must ensure that all personnel dealing with the device have read and understood this manual. In addition, the system owner must provide personnel with training and hazards information at regular intervals.
- The system owner must provide the personnel with the necessary protective equipment.
- The system owner must warrant that the device is operated by trained and authorized personnel as well as all other work, such as transportation, mounting, start-up, the installation, maintenance, cleaning, service, repair and shutdown, that is carried out on the device.
- All personnel who work with, or in the close proximity of the device, need to be informed of all safety issues and emergency procedures as outlined in this user manual.
- The system owner must document the information about all safety issues and emergency
 procedures in a laboratory SOP (Standard Operating Procedure). Routine briefings and
 briefings for new personnel must take place.
- The system owner must ensure that new personnel are supervised by experienced personnel. It is highly recommended to implement a company training program for new personnel on all aspects of product safety and operation.
- The system owner must ensure that personnel are regularly informed of the potential hazards within the laboratory. This is all personnel that work in the area, but in particular laboratory personnel and external personnel such as cleaning and service personnel.

- The system owner is responsible for taking measures to avoid inherent risks in the handling of dangerous substances, preventing industrial disease, and providing medical first aid in emergencies.
- The system owner is responsible for providing facilities according to the local regulations for the prevention of industrial accidents and generally accepted safety regulations according to the rules of occupational medicine.
- All substances needed for operating and cleaning the device samples, solvents, cleaning agents, gases, etc. have to be handled with care and disposed of appropriately. All hints and warnings on storage containers must be read and adhered to.
- The system owner must ensure that the work area is sufficiently illuminated to avoid reading errors and faulty operation.
- The system owner must ensure that the laboratory is equipped with an oxygen warning device, in case the device is operated with nitrogen.

Furthermore, the system owner is responsible for ensuring that the device is always in a technically faultless condition. Therefore, the following applies:

- The system owner must ensure that the maintenance intervals described in this manual are observed.
- The system owner must ensure that all (electrical, mechanical, etc.) safety devices are regularly checked to ensure full safety functionality and completeness.

3.2 Personnel Requirements



Only trained Bruker personnel are allowed to install, mount, retrofit, repair, adjust and dismantle the unit!



Risk to life for unauthorized personnel in the work area

Unauthorized personnel who do not meet the requirements described in this manual will not be familiar with the dangers in the work area. Therefore, unauthorized persons face the risk of serious injury or death.

3.2.1 Qualifications

This manual specifies the personnel qualifications required for the different areas of work, listed below:

Laboratory Personnel

Laboratory personnel are health care professionals, technicians, and assistants staffing a research or health care facility where specimens are grown, tested, or evaluated and the results of such measurements are recorded. Laboratory personnel are able to carry out assigned work and to recognize and prevent possible dangers self-reliant due to their professional training, knowledge and experience as well as profound knowledge of applicable regulations.

The workforce must only consist of persons who can be expected to carry out their work reliably. Persons with impaired reactions due to, for example, the consumption of drugs, alcohol, or medication are prohibited from carrying out work on the device.

When selecting personnel, the age-related and occupation-related regulations governing the usage location must be observed.

3.3 **Personal Protective Equipment**

Personal protective equipment is used to protect the personnel from dangers which could affect their safety or health while working.

Personnel must wear personal protective equipment while carrying out the different operations at and with the device.

This equipment will be defined by the head of the laboratory. Always comply with the instructions governing personal protective equipment posted in the work area.

3.4 **Position of the Emergency Stop Button**



Figure 3.1: Emergency stop button (1) of the SampleCase

The emergency stop button is placed on the left top of the SampleCase user interface.

Pressing the emergency stop button triggers an emergency stop. The emergency stop will not power off the system completely but will release the compressed gas in the SampleCase. All pneumatic driven actors on the system will stop immediately and the system indicates an *Error state*.

After the **Emergency Stop** button has been pressed, it has to be pulled in order to enable a restart. Releasing the emergency button will pressurize the system and reset the firmware. The system will go through the *Check state* first.

3.5 Location of the Safety Label



The laboratory supervisor is responsible for ensuring that all the warning labels are maintained in their proper place any time that the device is used.

The operating elements of the SampleCase are labeled with the biohazard symbol to warn the operator of the possible content of the substances in the carriers and samples. The operator himself must ensure that all the necessary safety precautions are taken for every NMR experiment in which biological or any other hazardous substances are used.

The device needs to be cleaned by the operator before maintenance work will be done by the Bruker service or before returning the equipment to Bruker for repair. In such a case the signed Equipment Clearance Format as part of the process Returning the Unit for Repair needs to be sent to the local Bruker office.

If a sample containing biohazard material is broken, due to user or machine error, there is a risk of injury due to contact with that material. The device itself generates no biological hazard.



Bruker is not responsible for the content or improper handling of the samples. The user themselves must ensure that all the necessary safety precautions are taken for every NMR experiment in which biologically hazardous substances are used. In the case of the unit becoming contaminated with biologically hazardous substances, the user is wholly responsible. Depending on the circumstances, this could lead to consequential damage to persons and machine components.

- Only trained operators are allowed to work on the device.
- Clean the device before maintenance work and/or returning to Bruker for repair.
- Prepare a list of materials which the device came into contact with.
- A signed confirmation of correctly carrying out cleaning/disinfection is required from the customer. Without this confirmation the parts delivered for repair will be rejected and returned to the customer.

In case of a contamination of the SampleCase the customer is responsible for the decontamination before Returning the Unit for Repair.



Risk to life due to chemical hazards. The device generates no direct chemical hazard.



The user must ensure that all the necessary safety precautions are taken for every NMR experiment in which substances are used that could represent a chemical and/or radioactive hazard or that are easily flammable. In the case of the unit becoming contaminated with the hazardous substances, the user themselves are wholly responsible. Depending on the circumstances, this could lead to consequential damage to persons and machine components.

In case of contamination of the device the customer is responsible for decontamination before Bruker employees access the system.

Risk of Injury due to Contact with Hot Surfaces

Contact with the hot surface of the carousel may result in burns.

- Do not touch parts of the heated carousel.
- Only exchange carriers with samples in the holder positions of the carousel when the temperature is below ≤ 35°C.
- Do not use damaged carousels.

3.6 Basic Dangers

The following section specifies residual risks which may result from using the device and have been established by means of a risk assessment.

In order to minimize health hazards and avoid dangerous situations, follow the safety instructions specified here as well as in the following chapters of this manual.

3.6.1 General Workplace Dangers

Danger to life from nonfunctional or insufficient safety devices!

If safety devices are not functioning or are disabled, there is a danger of serious injury or death.

- Check that all safety devices are fully functional and correctly installed before starting work.
- Never disable or bypass safety devices.
- Ensure that all safety devices are always accessible.

Danger of injury from tripping over dirt and scattered objects!

Dirt and scattered objects may cause people to slip or trip, resulting in personal injuries.

- ► Always keep the work area clean.
- Remove objects which are no longer required from the work area and particularly from the floor.
- Indicate unavoidable hazards using marking tape.



It is possible to fall from the ladder, when it is used to reach the devices on top of the magnet.

Wear appropriate non-slip footwear during work.

NOTICE

Risk of material damage due to a software error

Personnel should be alerted due to an unexpected malfunction.

NOTICE

Material damage hazard due to improper maintenance

Device deadlock may occur as a result of failures due to a lack of proper maintenance.

- ► Maintenance intervals must be properly followed.
- ▶ Use appropriate tools to avoid damaging parts or modules.
- ▶ Only trained personnel should carry out maintenance work.

3.6.2 Dangers from Electric Power

Danger of injury from electrical shock!

A life threatening shock may result when the housing is open during operation.

- Only qualified personnel should open the housing.
- Disconnect the device from the electrical power supply before opening the device. Use a voltmeter to verify that the device is not under power!
- ▶ Be sure that the power supply cannot be reconnected without notice.

3.6.3 Mechanical Dangers

A DANGER

Danger to life due to blocked or covered drop-off plate.

Therefore:

- ▶ Position the linear axis of the device such a way that it does not block the drop-off plate.
- Use the Velcro straps (included in the delivery) to fix the cables and hoses beside the drop-off plate.
- Apply the delivered drop-off plate sticker (see symbol on the side) in case it is missing on the drop–off plate.



Risk of injury due to moving parts

There are uncovered moving parts on the device. Users and non-users within proximity to the device must be aware of moving parts on the device and must keep clear when it is in use.



Accident hazard from movement of mechanical parts!

The fingers or hand may be pinched due to movement of mechanical parts.

▶ Shut off the device before accessing it.

Accident and material damage hazard from falling objects



Equipment my fall down during retrofitting or dismantling. This may result in personal injury or equipment damage.

- ▶ If necessary, assemble/disassemble the device in multiple parts.
- ▶ Use a platform with railings instead of a ladder to reach the assembly area.
- Avoid working over the head. When this cannot be avoided, wear a protective hard hat.

3.6.4 Dangers from Magnetic Fields

Risk to life due to high magnetic fields

A magnetic field of more than 0.5 mT (5 Gauss) is life-threatening for people with pacemakers or active metal implants. Exposure to more than 8 T can cause damage to health. Duration of exposure (8 h/day) above the limit of 200 mT can cause damage to health. Ferromagnetic tools in the magnetic field are significantly hazardous. Disks and electronic devices may be damaged.

- ▶ Mark the magnetic field of more than 0.5 mT (5 Gauss) before start up.
- Keep people with active medical implants or heart pacemakers away from the 0.5 mT (5 Gauss) area.
 - ▶ The permanent workplace of employees must be outside the 0.5 mT (5 Gauss) area.
- Do not stay or work at magnetic fields of more than 8 T.
- Prevent exposure of more than 200 mT for more than 8 h/day.
- ▶ Keep disks, credit cards and electronic devices away from the identified area.
- ▶ Do not use ferromagnetic tools or items within the identified area.
- Only use non-ferromagnetic transportation dewars or pressure cylinders for the cryogenic agents.
- Only use non-ferromagnetic ladders or steps.
- Remove magnetic items (jewelry, watches, pens etc.) before carrying out maintenance work.



The magnetic field of the device does not cause any personal injuries or property damage. For further information see the manual of the magnet used.

3.6.5 Dangers Due to High or Low Temperatures



Contact with the hot or cold surfaces of the carousel may result in serious burns.

- ▶ Do not touch carousel parts of cooled or heated carousels.
- Do not use damaged carousels.

A CAUTION

Accident hazard from hot or cold surfaces

When a sample holder is removed from the carousel, it might be hot or cold, which may result in serious burns.

- Ensure the personnel are aware of the risk.
- Ensure the personnel is trained how to operate the SampleCase cooled or heated and where to verify the temperature in the software interface before removing a sample holder.
- Do not touch carousel parts of cooled or heated carousels.
- ▶ Do not touch the lower part of a sample holder.

NOTICE

Risk of material damage due to an overflow of cryogens.

Material damage may result from the overflow of cryogens during the refill of the magnet.

- Be sure to use sufficient transfer line and Teflon evacuation hose for nitrogen and helium refills based on recommendations in the magnet manual. Connect those lines carefully in order to avoid spillage on the carousel.
- After refilling cryogens some parts of the magnet may be icy. Be sure to remove the ice to avoid its melting onto the device.

3.6.6 Danger from Chemical Substances

If a sample containing biohazard material is broken, due to user or machine error, there is a risk of injury due to contact with that material. The device itself generates no biological hazard.



Bruker is not responsible for the content or improper handling of the samples. The user themselves must ensure that all the necessary safety precautions are taken for every NMR experiment in which biologically hazardous substances are used. In the case of the unit becoming contaminated with biologically hazardous substances, the user is wholly responsible. Depending on the circumstances, this could lead to consequential damage to persons and machine components.

- Only trained operators are allowed to work on the device.
- Clean the device before maintenance work and/or returning to Bruker for repair.
- Prepare a list of materials which the device came into contact with.
- A signed confirmation of correctly carrying out cleaning/disinfection is required from the customer. Without this confirmation the parts delivered for repair will be rejected and returned to the customer.

Risk to life due to chemical hazards. The device generates no direct chemical hazard.



The user must ensure that all the necessary safety precautions are taken for every NMR experiment in which substances are used that could represent a chemical and/or radioactive hazard or that are easily flammable. In the case of the unit becoming contaminated with the hazardous substances, the user themselves are wholly responsible. Depending on the circumstances, this could lead to consequential damage to persons and machine components.

In case of contamination of the device the customer is responsible for decontamination before Bruker employees access the system.

Danger of injury from vapor formation!

During the work process, vapors may form which cause serious injury if inhaled.

▶ Only install the device in a well-ventilated room or ensure that an extractor is fitted.

Exposure and other health hazards to maintenance personnel.

The device must be cleaned if contaminated before performing any maintenance.

- Register all substances with which the device has come into contact.
- Sign a certification form verifying that the device has been properly cleaned if contaminated to protect maintenance personnel.
- Obviously contaminated, insufficiently cleaned units, as well as units without a signed cleaning certification will not be repaired and returned to the sender.

Danger of injury from glassware breakage.

Broken glassware may cause minor injuries or material damage, but may also result in a life threatening situation if hazardous substances are used.

- If glassware breaks, refer to the corresponding precautions and cleaning/disinfection instructions.
- ► Wear protective equipment.
- ▶ Perform all tasks with the glassware carefully.
- Before carrying out any maintenance work or cleaning of the device, remove the samples and use dummy samples if necessary.
- Strictly observe the correct sample adjustment, i.e. the maximum sample height.
- Always transport the glassware with a sample tube cap, if applicable.
- The laboratory supervisor is responsible for:
 - ⇒ Establishing and enforcing standard sample handling and cleaning procedures.
 - ⇒ Establishing and enforcing the use of protective clothing and equipment.
 - ⇒ Training laboratory personnel.
 - \Rightarrow Preparing an emergency plan.

NOTICE

Material damage hazard from material contact with NMR solvents!

Material damage may result when the device comes in contact with NMR solvents.

Follow instructions provided in the manual for correct handling of NMR sample holder, e.g. size.

3.7 Environmental Protection

NOTICE

Danger to the environment from incorrect handling of pollutants!

Incorrect handling of pollutants, particularly incorrect waste disposal, may cause serious damage to the environment.

- Always observe local environmental regulations regarding handling and disposal of pollutants.
- Take the appropriate actions immediately if pollutants escape accidentally into the environment. If in doubt, inform the responsible municipal authorities about the damage and ask about the appropriate actions to be taken.

The following pollutants are used:

Nitrogen gas

Nitrogen gas may cause suffocation at high concentrations. Disposal of the empty gas cylinders must be performed by a specialist disposal company.





3.8 Signage

The following symbols and information signs can be found in the work area. They refer to their immediate surroundings.



The identification and placement of warning labels are included in the manual. The laboratory supervisor is responsible for ensuring that all the warning labels are maintained in their proper place any time that the device is used.

Biohazard



Warning indicating a danger due to biohazard material. Infection, contamination, or other health endangerment as a result of contact with biological or chemical substances, e.g. from broken samples.

The SampleCase contains no biological hazard itself.

Danger Spot



Warning indicating a danger spot in work rooms. The warning label may be ordered using Bruker Part Number 67470.

4 Transport, Packaging and Storage

Installation, initial commissioning, retrofitting, repairs, adjustments or dismantling of the device must only be carried out by Bruker Service or personnel authorized by Bruker. Damage due to servicing that is not authorized by Bruker is not covered by your warranty.

4.1 Inspection at Delivery

Upon receipt, immediately inspect the delivery for completeness and transport damage.

Proceed as follows in the event of externally apparent transport damage:

- · Do not accept the delivery, or only accept it subject to reservation.
- Note the extent of the damage on the transport documentation or the shipper's delivery note.
- · Initiate complaint procedures.



Π

Issue a complaint in respect to each defect immediately following detection. Damage compensation claims can only be asserted within the applicable complaint deadlines.

4.2 Packaging

About Packaging

The individual packages are packaged in accordance with anticipated transport conditions. Only environmentally friendly materials have been used in the packaging.

The packaging is intended to protect the individual components from transport damage, corrosion and other damage prior to assembly. Therefore do not destroy the packaging and only remove it shortly before assembly.

Handling Packaging Materials

Keep the original container and packing assembly, at least as long the warranty is valid, in case the unit has to be returned to the factory. When the packaging material is no longer needed dispose of in accordance with the relevant applicable legal requirements and local regulations.

4.3 Storage

Storage of the Packages

Store the packages under the following conditions:

- Do not store outdoors.
- Store in dry and dust-free conditions.
- Do not expose to aggressive media.
- · Protect against direct sunlight.
- · Avoid mechanical shocks.
- Storage temperature: 15 to 35 °C.
- Relative humidity: max. 60%.
- If stored for longer than 3 months, regularly check the general condition of all parts and the packaging. If necessary, top-up or replace preservatives.



Under certain circumstances, storage instructions may be affixed to packages which expand the requirements specified here. Comply with these accordingly.

5 Design and Function

5.1 SampleCase

SampleCaseTM is the first NMR automation solution with capacity for 24 samples (*Figure 5.1* [\triangleright 25]) that provides easy, safe and convenient access to fully-fledged NMR automation at user height.



Figure 5.1: SampleCase carousel with 24 positions for samples

It is based on push-button operation for manual sample insertion and ejection directly at the instrument. The user-friendly system can be fitted to almost any Bruker NMR magnet from 300 - 900 MHz.



- 1. Transfer slider tube
- 2. Linear Axis
- 3. Mounting hardware
- 4. BST
- 5. SampleCase
- 6. Transport tube
- 7. SampleMail

Fully compatible with TopSpin[™] and IconNMR[™] software, it can be added to any modern NMR instrument equipped with AVANCE[™] II or AVANCE[™] III technology as shown in *SampleCase* [▶ 25], for further details see *Schematic Overviews & Requirements* [▶ 52].

 The SampleCase system is compatible with all Bruker room temperature and CryoProbes™.

- SampleCase also provides direct access to the BST and thus is compatible with MAS or CryoFit accessory.
- The sample carrier, e.g. spinner with sample transport is controlled by a specific pneumatic transfer within the SampleCase system which allows vibration-free acquisition without RF interference. Therefore, the compressed air or nitrogen pressure requirement is 5 bar and 100 Normliter/min. The status of the SampleCase system is indicated by a traffic light display (for further details please refer to *Operating States of the SampleCase* [> 29].
- The SampleCase system is compatible with all sample diameters from 1-10 mm and works with all sample tube length (including Shigemi tubes), for further information please refer to Sample Carrier and NMR Tubes [> 33].
- SampleCase is an automation accessory that not only offers safe and convenient sample access on routine NMR systems but is also an excellent choice for high field research instruments.

See also

Intended Use [▶ 8]

5.2 SampleCase Cooled

SampleCase cooled (SampleCase_cooled) takes the proven concept of safe and easy NMR Automation at user height to the next level. Providing a fridge-cold sample storage platform, it is possible to also submit temperature sensitive samples like Protein-, RNA- or Biofluid solutions for subsequent automation runs in smaller batches.

In the SampleCase cooled, the 24 holder cool all the carriers to a selectable temperature of 4 °C up to 40 °C. The uniformity is given for the setpoint with 279 K / 6 °C \pm 2 °C. All holders are on the same temperature level.



Figure 5.2: SampleCase cooled carousel

5.3 SampleCase Heated

SampleCase heated (*Figure 5.3 [* 27]) takes the proven concept of safe and easy NMR Automation at user height to the next level. Providing a heated sample storage platform is specially designed for work in polymer research.

In the SampleCase heated, the 24 holder individually heat the carriers to a selectable temperature between room temperature up to 398 K / 125 °C. When the temperature of a sample holder is above 313 K / 40 °C the related position LED will light up in red to indicate the warm state of the sample. For the exact temperature of the sample please refer to the user interface under TopSpin where the exact temperature measurement result is shown (*SampleCase Heated* [\triangleright 38]).

Thereby it is possible to keep polymers liquid and ready for measurement individually.



Figure 5.3: SampleCase heated carousel with 24 positions for samples to be individually heated

5.4 Retrofitting Capability

Retrofitting Capability

In the field the SampleCase cannot be modified or retrofitted to the cooled or heated option.

It is only possible to exchange the SampleCase (Z122633) with a SampleCase cooled (Z143007) or a SampleCase heated (Z155921). The subunit SampleMail (Z123384 / Z133067) can be re-used. Before an exchange of a SampleCase the Lab & System Requirements for the new type have to be checked.

6 Operation



SampleCase standard, cooled & heated

When SampleCase is used within the manual it applies to all three types, otherwise the type is explicitly mentioned.

The Sample Case standard, cooled & heated are designed to easily transport the NMR sample tubes from the carousel into the magnet bore and back. The NMR sample tube will be transported up and down with the lift gas in the Transport tube and shifted horizontally by the pneumatic drive along the linear axis on top of the magnet, fully controlled by software. At specific positions optical sensors verify the correct path of the sample.

The user only has to start the transport from the computer interface or at the carousel and can observe the progress via the status LEDs on the SampleCase itself.

The SampleCase can be operated stand alone at the user interface or remotely controlled with the Bruker TopSpin and IconNMR software (for details in relation to the three types of SampleCases please refer to the specific technical data: SampleCase: Lab & System Requirements [> 53], SampleCase Cooled: Lab & System Requirements [> 57] or SampleCase Heated: Lab & System Requirements [> 62]). There are no special functions for the SampleCase in IconNMR. But IconNMR needs to be configured correctly to 24 holders.

6.1 Operating States of the SampleCase

LED interfaces (1) at SampleMail and SampleCase highlight the operating state. The SampleCase has two separate lights to indicate its current state. One on the user interface of the carousel and the other on the SampleMail unit (see *Figure 6.1* [29])



Figure 6.1: LED interface (1) at SampleMail and SampleCase highlights the operating state.

The meaning of these LED states and state types are listed below. The user should know them in order to operate the system correctly and safely.

LED (blinking rhythm)	State Type	Meaning
	Stable	System is in a stable state with no actions pending
	Transient	System performs an action
	Urgent	System is in a time-critical state with actions pending

Table 6.1: Type of Sample Transporter States

LED	State	Meaning
Green	Idle	System is idle with no sample in magnet.
Blinking Yellow/ Green	Busy	System is busy transporting a sample or system received a command via TopSpin and is busy
Yellow	Measuring	System is Idle with a sample in magnet.
Blinking Yellow-	Warning	Check BSMS service web page for more information.
Fast blinking Yellow	Attention	System will start soon. Keep hands off.
Blinking Red	Checking	System is checking for errors.
Red	Error / Startup	System has detected an error or is starting up.

Table 6.2: Specific Sample Transport States

6.2 Operating Elements

The operating elements of the SampleCase are shown in the following Figure. There are two push buttons on the left side (1 & 3) which can only activate the described functions when the buttons are illuminated.



- 1. Rotate carousel clockwise blue push button (enabled)
- 2. Emergency stop button
- 3. Inject/Eject green push button (enabled)
- 4. State LED (green showing *idle* state)
- 5. Sample gate (open)
- 6. Sample over length latch
- The blue Rotate carousel button (1) will rotate the carousel one holder position when pressed once or will rotate the carousel continuously when held down. The design of the carousel allows only clockwise rotation. The carousel cannot be rotated when a carrier with an NMR sample tube (e.g. spinner, shuttle, solid or MAS) is in the magnet bore. In this case the rotation will be blocked because the jack which lifts the chosen holder with the NMR sample tube towards the transport gate under the transport tube will remain below the transport gate until the NMR sample tube comes back after the measurement.

 The green Inject/Eject push button (3) allows the operator to either inject the NMR sample tube below the Transport gate into the magnet bore or to eject the NMR sample out of the magnet bore and transfer it back to the place in the carousel. Ejecting an NMR sample tube out of the magnet bore will only work, when the spinning of the sample is switched off.



No power

When the two push buttons are not illuminated they are not active. Pushing a non-illuminated button has no effect.



- 1. Rotate carousel clockwise push button (disabled)
- 2. Emergency stop button
- 3. Inject/Eject push button (disabled)
- 4. State LED (yellow showing *measure* state)
- 5. Sample gate (closed)
- 6. Holder in Sample gate position

The operating elements of the SampleCase are labeled with the biohazard symbol to warn the operator of the possible content of the substances in the carriers and samples. The operator himself must ensure that all the necessary safety precautions are taken for every NMR experiment in which biological or any other hazardous substances are used.

The device needs to be cleaned by the operator before maintenance work will be done by the Bruker service or before returning the equipment to Bruker for repair. In such a case the signed Equipment Clearance Format as part of the process Returning the Unit for Repair needs to be sent to the local Bruker office.

If a sample containing biohazard material is broken, due to user or machine error, there is a risk of injury due to contact with that material. The device itself generates no biological hazard.



Bruker is not responsible for the content or improper handling of the samples. The user themselves must ensure that all the necessary safety precautions are taken for every NMR experiment in which biologically hazardous substances are used. In the case of the unit becoming contaminated with biologically hazardous substances, the user is wholly responsible. Depending on the circumstances, this could lead to consequential damage to persons and machine components.

- Only trained operators are allowed to work on the device.
- Clean the device before maintenance work and/or returning to Bruker for repair.
- Prepare a list of materials which the device came into contact with.
- A signed confirmation of correctly carrying out cleaning/disinfection is required from the customer. Without this confirmation the parts delivered for repair will be rejected and returned to the customer.

Risk to life due to chemical hazards. The device generates no direct chemical hazard.



The user must ensure that all the necessary safety precautions are taken for every NMR experiment in which substances are used that could represent a chemical and/or radioactive hazard or that are easily flammable. In the case of the unit becoming contaminated with the hazardous substances, the user themselves are wholly responsible. Depending on the circumstances, this could lead to consequential damage to persons and machine components.

In case of contamination of the device the customer is responsible for decontamination before Bruker employees access the system.

The carousel of the SampleCase is labeled with the symbol of hot surfaces to warn the operator that the content of the carriers and samples might be hot when the heating is on. Further details about the SampleCase heated interface is decribed in *SampleCase Heated* [> 37].

Risk of Injury due to Contact with Hot Surfaces

Contact with the hot surface of the carousel may result in burns.

- ▶ Do not touch parts of the heated carousel.
- Only exchange carriers with samples in the holder positions of the carousel when the temperature is below ≤ 35°C.
- ► Do not use damaged carousels.

6.3 Emergency Stop Button



Figure 6.2: Emergency stop button (1) of SampleCase

The emergency stop button (1) is on the left side of the SampleCase user interface as shown in the Figure above. Further details are explained under *Position of the Emergency Stop Button* [▶ 13].

6.4 Sample Carrier and NMR Tubes

NOTICE

Risk of material damage due to incorrect use of spinners and shuttles.

When setting up the experiments please make sure that the temperature specifications of both the NMR probe and the sample carriers (e.g. spinner/shuttle) are respected in order to avoid damage to the hardware.

- Consult the customer sample certificate to get information about the approved temperature range for your sample.
- Consult the Manual NMR Probes Variable Temperature Control for NMR Probes (Z33073, Chapter 3, Table 3.4.) to get the information about the approved temperature range of spinners and shuttles.



Spinner with yellow ring

The sample carrier can transport almost every Bruker Spinner and Shuttle except the older types with no yellow ring on the reflector foil.

Spinner SB PLA (PCTFE) 5+2,5 A (H00177A) with black marking inside
Spinner SB CERAMICS 5mm TYP:A (H00804A)
Spinner SB PLA (POM) 5+2,5 -A (Z42516A) with black marking inside

Table 6.3: Allowed spinner types with yellow rings

Further information about available samples can be found under *https://store.bruker-biospin.com/*.

Glass Tubes

NOTICE

Material damage due to broken glass tubes

The device is built to handle the NMR tubes carefully but glass tubes may break during the transport. Also while loading and removing tubes from the device the NMR tubes may break even without any force or impact.

Use general lab safety e.g. protective gloves, safety goggles when working with NMR tubes.

Sample Overlength Latch

The standard NMR reference sample tube of 5 mm has a total length of 184-187 mm (7 "). But there is an absolute sample length limitation of 97.5 mm (3.8 ") above the spinner which is the distance between the carousel holder, where the sample tube with spinner is placed, and the transport tube inlet. The sample overlength latch at the transport tube inlet will detect sample tubes with an overlength while the carousel is rotating which ends in an emergency stop.



Figure 6.3: Sample length limitation is given with 97.5 mm.

6.5 Manual Operation of the SampleCase





- The SampleCase carousel can be filled when the system is in the idle state shown by the green light on the user interface .
- Place the sample carrier in a free holder of the carousel.



• Press the blue button to rotate the carousel so that the sample carrier to measure next is below the Transport tube gate.



• When pressing the Inject/Eject button the sample carrier below the Transport tube gate will be lifted towards the Transport tube and transported to the magnet bore.



• When pressing the Inject/Eject button a second time the sample carrier will be removed from the magnet bore and transported to the SampleCase and placed in the holder below the Transport tube gate.

6.6 Remote Operation of the SampleCase with TopSpin

Risk of injury

When using the SampleCase in Remote Control with TopSpin, manual intervention can cause injuries.

- ► Check under TopSpin the status of the SampleCase.
- ▶ Don't intervene when the LEDs are blinking green.

The following commands of TopSpin[™] can be used to control the SampleCase.

TopSpin Command	Command Result
sx A	• The current sample carrier is removed from the magnet bore. The selected sample carrier A (1-24) is then inserted in the magnet bore.
sx ej	 The current sample carrier is removed (ejected) from the magnet bore and is placed back in the carousel.
ij (insert sample)	 Insert the current sample carrier of the holder under the transport gate into magnet.
ej (eject sample)	 Eject the sample carrier from the magnet bore and place it back in the carousel.
bsmsdisp	• Opens the graphical interface showing a button to switch on or off the lift. This will have the same effect as the ij and ej commands.
vtudisp	Opens the Temperature Control Suite which provides access to all temperature related parameters.

Table 6.4: TopSpin Commands for the SampleCase
6.7 Cooling and Heating Operation with TopSpin

6.7.1 SampleCase Cooled

• Start TopSpin and open the Temperature Control window from the Acquire – Sample menu or double click the Temperature Control window in the acquisition status bar.



• The status of the sample storage is shown with off, no cooling takes place.



- After pressing the ON button, the status of the sample storage is shown with on and the sample carrier in the 24 holder positions will be cooled.
- At any time the sample storage state can be deactivated by pressing the OFF button and the cooling will stop.

6.7.2 SampleCase Heated

NOTICE

Risk of material damage due to incorrect use of spinners and shuttles.

When setting up the experiments please make sure that the temperature specifications of both the NMR probe and the sample carriers (e.g. spinner/shuttle) are respected in order to avoid damage to the hardware.

- Consult the customer sample certificate to get information about the approved temperature range for your sample.
- Consult the Manual NMR Probes Variable Temperature Control for NMR Probes (Z33073, Chapter 3, Table 3.4.) to get the information about the approved temperature range of spinners and shuttles.

• Start TopSpin and check in the TopSpin GUI that TopSpin[™] Version >=3.5pl3 is installed.



 Then open the Temperature Control window from the Acquire - Sample menu or double-click the Temperature Control window in the acquisition status bar (or type on the command line vtudisp).



• Open the Sample storage view. At the beginning the system is OFF.

SampleCase	with High Temperature Heating	298.0 K (283 K398 K	Set			
Active	Name	Temperature	Active	Name	Temperature	
	Sample Position 1	299.0 K		Sample Position 13	299.0 K	
V	Sample Position 2	298.9 K	V	Sample Position 14	299.0 K	
	Sample Position 3	298.9 K		Sample Position 15	299.0 K	
V	Sample Position 4	298.7 K	×.	Sample Position 16	299.2 K	
	Sample Position 5	298.6 K		Sample Position 17	299.2 K	
V	Sample Position 6	298.7 K	V	Sample Position 18	299.1 K	
	Sample Position 7	298.7 K		Sample Position 19	299.1 K	
V	Sample Position 8	298.7 K	V	Sample Position 20	299.0 K	
	Sample Position 9	298.7 K		Sample Position 21	299.0 K	
V	Sample Position 10	298.7 K	V	Sample Position 22	299.1 K	
	Sample Position 11	298.8 K		Sample Position 23	299.0 K	
V	Sample Position 12	298.8 K	V	Sample Position 24	299.0 K	
		Activat	e all Deactivate	all		

 When selecting the Active button of a specific sample place as shown in the next step, the holder of the sample in the carousel will heat the sample to the specified temperature.

тетр	erature Monitoring	Record Correction Self 1	tune Configurat	Sample storage Log	
				💼 💽 🐨 Sample Storage State: 🛇 On	
	6	Dovice		mmon Target Temperature	
	SampleCase with H	igh Temperature Heating		24.9 °C (10 °C125 °C) 801	
Active	Name	Temperature	Active	Name Temperature	
	Sample Position 1	22.0 °C		nple Position 13 21.7 °C	
	Sample Position 2	22.1 °C		nple Position 14 21.7 °C	
	Sample Position 3	22.1 °C		npie Position 15 21.7 °C	
	Sample Position 4	22.1 °C		nple Position 16 21.7 19	
	Sample Position 6	25.1 °C		mple Position 17 21.8 °C	
	Sample Position 6	21.9 °C		npie Position 18 21.8 °C	
	Sample Position /	21.8 °C		nple Position 19 21.9 °C	
	Sample Position 8	21.7 °C		nplc Position 20 21.9 °C	
	Sample Position 9	21.8 °C		mptc Position 21 21.8 °C	
	Sample Position 10	21.8 °C		mple Position 22 21.8 °C	
	Sample Position 11	21.8 °C		nple Position 23 21.9 °C	
	Sample Position 12	21.7 °C		nptc Position 24 21.9 °C	
				Activate all Deactivate all	
TU: Or	Probe Temperat	ure: 26.0 °C Probe Regul	ation: Steady 🙄	e: Nistit 🔕 Recording: Off Probe: PA TXI 50052 H-C/N-D-05 XYZ	

- In the following screenshot an example of three selected holders, marked at the check boxes, is shown, while the others will not be actively heated.
- In set target temperature specify the temperature the samples should be heated-up to as shown for e.g. 370 K. The maximal temperature the sample can be heated-up to is given with 398 K / 125 °C.

SampleCase	with High Temperature Heating	350.0 K (283 K 398 K)	Set									
Active	Name	Temperature	Active	Name	Temperature							
	Sample Position 1	318.1 K		Sample Position 13	_							
	Sample Position 2	-		Sample Position 14	_							
	Sample Position 3	Set target temps	erature	Position 15	-							
V	Sample Position 4	Please enter the	common target temp	erature for e Position 16	_							
	Sample Position 5	"SampleCase wi	th High Temperature	Heating". e Position 17	-							
	Sample Position 6	Common target	temperature [K]: 🔢	e Position 18	_							
	Sample Position 7		OK	Cancel e Position 19	-							
	Sample Position 8			e Position 20	_							
	Sample Position 9	-		Sample Position 21	_							
	Sample Position 10	_		Sample Position 22	_							
	Sample Position 11	-		Sample Position 23	-							
	Sample Position 12	_		Sample Position 24	_							
		Activat	e all Deactivate	all		Activate all Deactivate all						

- When the target temperature has been reached, the SampleCase holder will keep the sample at this specified temperature until:
 - the specific sample holder is deactivated
 - or all sample holders are activated/deactivated
 - or the SampleCase heated is switched OFF.
- The temperature values will be displayed in red, as soon as the sample temperature is above 315 K / 40 °C. The position LED of the sample holder in the carousel is on as soon as the position holder is heating/active.

• Example view, in case all sample holders are heated, which can be started with the button Activate all.

Device Common Target Temperature						
SampleCase	with High Temperature Heating	398.0 K (283 K398 K)	Set			
Active	Name	Temperature	Active	Name	Temperature	
	Sample Position 1	381.1 K		Sample Position 13	357.6 K	
V	Sample Position 2	357.4 K	V	Sample Position 14	356.2 K	
	Sample Position 3	355.9 K		Sample Position 15	355.6 K	
V	Sample Position 4	382.6 K	V	Sample Position 16	352.9 K	
	Sample Position 5	382.9 K		Sample Position 17	355.7 K	
V	Sample Position 6	357.5 K	V	Sample Position 18	354.5 K	
	Sample Position 7	353.8 K		Sample Position 19	355.5 K	
V	Sample Position 8	353.8 K	V	Sample Position 20	354.7 K	
	Sample Position 9	357.1 K		Sample Position 21	352.2 K	
V	Sample Position 10	356.3 K	V	Sample Position 22	355.2 K	
	Sample Position 11	356.2 K		Sample Position 23	355.9 K	
V	Sample Position 12	355.0 K	V	Sample Position 24	354.9 K	
		Activat	e all Deactivate	all		

• Within the Configuration window of the Temperature Control Suite the general configuration of the Sample Storage State window can be set, for e.g. temperature in K or °C.

Temperature Montoring Record Connection Settune Configuration Sample storage Log General configuration Profile configuration Channel mapping Gas mode Use "External" for MAS probes with therpered bearing gas. (()) Use "External" for MAS probes with therpered bearing gas. (()) Use "External" for MAS probes with therpered bearing gas. (()) Use "External" for MAS probes with therpered bearing gas. (()) Use "External" for MAS probes with therpered bearing gas. (()) Use "External" for MAS probes with therpered bearing gas. (()) Use "External" for MAS probes with therpered bearing gas. (()) Use "External" for MAS probes with therpered bearing gas. (()) Use "External" for MAS probes with therpered bearing gas. () Use "External" for MAS probes with therpered bearing gas. () Use "External" for MAS probes with therpered bearing gas. () Use "External" for MAS probes with therpered bearing gas. () Use "External" for MAS probes with therpered bearing gas. () Use "External TopSpin withdow Use "External TopSpin withdow Use "External TopSpin withdow External TopSpin withdow External TopSpin withdow Use TopSpin withdow External TopSpin withdow Use TopSpin withdow External TopSpi	Temperature Control Suite			
General configuration Profile configuration Channel mapping Gas mode Temperature unit VTU retained settings (or generature unit, names, limits etc.) can be stored in a profile Channel mapping Casan de transmeterie (or generature unit, names, limits etc.) can be stored in a profile Use "External To AMAS probes with a stored in a profile Use "External To Sections" Use "External To Sections" Use "External To Sections" Sas four control: © resting To Officer (Target) Create new profile Create Load profile Load Sas four control: Standard © construction Delete profile Load Delete Delete Sas four control: Sas four control: Sas four control: Standard	Temperature Monitoring Re	cord Correction Self tune Configuration San	mple storage Log	
Internal TopSpin window Olisable NMR thermometer	General configuration Temperature unit.	Profe configuration VIU related service (a) temperature unit, names immis etc.) can be stored in a profile you can load a portle to apply the stored VIU settings to different hardware configurations or users. Create new profile Load profile Delete profile Delete	Channel mapping Set mapping between to-parameters (e.g. to2) or to-commands (e.g. to2est, to2get) and hardware channels. This determines which channel is used. Hardware channel Logical channel 2 <u>Jetter Set</u> Set	Gas mode Use "External for MAS probes with tempered bearing gas (folde: VTU gas supply is switched off) Gas fox control:
Channel configuration	Channel configuration			
1 Sensor: Standard Set 273 K. 353 K Set 186.0 % Set CPP BBO 50052 BB-H&F-D-05 Z Set NMR thermometer: Standard Set 573 K Set 186.0 % of 43.0 V) Set	1 CPP BBO 500S2 BB-H&F-D-	05 Z Set NMR thermometer: Standard	Set 273 K353 K Set 57	186.0 % 3 K Set (max. 186.0 % of 43.0 W) Set

6.8 **Operating SampleCase with MAS**

Depending on the application there may be situations where the SampleCase is not needed or cannot be used. A magnet with an SampleCase installed still offers access to insert carriers with sample by hand.

6.8.1 Deactivate the SampleCase to Allow Manual Operation for MAS Hardware

To bypass or work beside the SampleCase without interference, do the following steps:



• Disconnect the gas supply by closing the pneumatic valve (1) at the end of the linear axis.



- The pneumatic valve is closed when the switch is in this position.
- In case the Transfer slider tube stopped above the magnet bore and blocks the magnet bore, move the Transfer slider tube carefully by hand to the side. To do so, hold the Transfer slider tube near the linear axis to avoid tilting it away from the axis.

THER B	SampleTransporter Control	BRUK	R
Commands	JURER SURER	Story	E.P.
Lit	Eject Inject		lift off
Lift Service Loop	Loop ON Loop on all samples Lo	op OFF	Loop of
Reset Sample Transporter	Please verify that there is no carrier stuck in a position where it can be detected by the SampleTransporter is e.g. make sure that the CRP emergency lift is not active Reset	efore resetting ve.	2
THER (THER THER	Char	
Configuration	Bud Bud	ary	
Lift Mode	SampleTransporter: PLC on TTY1 of ELC	B 1) 🗘	
MAS Shuttle Mode enable	DREP CAREP	Char	
Set Refresh	Auto Refresh	ery-	~
Status	THER THER	C.L.	R
FSM State	en en	887	2
PLC State			
Sample Position	BER BER	-	sample do
PLC Firmware Version	BROWN BROWN	BRY	not availab
Hardware Type	u u		unknown
Handson Cards			1

• Within the BSMS service web go to the menu configuration and change the lift mode to the setting: Sample Transporter: PLC on TTY1 of ELCB 1

6.8.2 MAS Hardware Usage

The SampleCase will provide access for the MAS hardware, when the MAS adapter has the recommended shape with a recess as shown below on the left side.



Figure 6.4: MAS adapter

The MAS adapter has to be applied in the adapter ring (3) of the linear axis to the BST above the magnet bore. Therefore the adjusting ring (1) and the bayonet ring (2) have to be taken out.



- 1. Adjusting ring
- 2. Bayonet ring
- 3. Access hole to the magnet bore

The bayonet ring can be taken out after it has been loosened clockwise as shown in the figure below.



Figure 6.5: BST Mounting



6.8.3 Activate the SampleCase to Allow Automatic Operation Again

To activate the SampleCase after manual use, do the following steps:

- 1. Switch the lift mode to BSMS lift in the configuration.
- 2. Mount the bayonet ring and then the adjusting ring tightly.
- 3. Reconnect the gas supply





• Within the BSMS service web go to the menu configuration change the lift mode to *BSMS lift* in the configuration.

• Remount anticlockwise the bayonet ring (2) and then the adjusting ring (1) tightly in the adjusting ring (3) of the linear axis to the BST.

• Reconnect the gas supply by opening the pneumatic valve at the end of the linear axis.

7 Maintenance

7.1 Cleaning

NOTICE

Cleaning the device

Usage of cleaners like thinner or benzene may damage the surface of the unit.

► Use only water or neutral cleaning fluids.

7.1.1 **Preparation for Cleaning**

- 1. Stop the device from doing any actions.
- 2. Switch the pneumatic off
- 3. Disconnect all the power supplies of the SampleCase version.

7.1.2 Other Cleaning Operations

For all other cleaning operations contact Bruker Service for advice and support. It may be necessary to send in the device for a cleaning service.

No special precautions have been taken in the device to avoid contamination from leaking samples. Bruker accepts no responsibility for any damage which may occur when samples are containing biologically active, radioactive or other hazardous materials are used.

In case of an accident with toxic, radioactive, explosive, or biologically active substances, the device and associated equipment must be cleaned in such a way that no danger emanates from the device and associated equipment, especially for all uninformed personnel. If a device has to be cleaned of all remains of a substance for safety reasons, contact Bruker Service for advice and support.

Note that in serious cases it may be necessary for the owner to exchange the device with a new one, contact Bruker Service for details.

7.2 Preventive Maintenance

The SampleCase needs very few maintenance. The customer can do this on its own or ask the Bruker service for assistance. Proper service will increase the lifetime of the system and prevents form failures during operation. The following things need to be done after approximately 20.000 sample changes:

- Axis lubrication
- O-ring exchange



- 1. O-ring
- 2. Lubricant film on the linear axis

Accident hazard from falling from ladder!

It is possible to fall from a ladder when it is used to reach the device on some magnets.

- ▶ Do not use a ladder.
- ▶ Use an approved platform to reach the device on the magnet.
- ▶ Wear non-slip shoes.



A CAUTION

Accident hazard from movement of mechanical parts!

The fingers or hand may be pinched due to movement of mechanical parts.

Shut off the device before accessing it.

7.2.1 Exchange of the O-ring

The O-ring of the Transfer Slider tube will wear out if the system is in use or not, therefore exchange the O-ring twice a year. If the rubber rips are worn off the tube cannot be captured in the Transport slider. Spare O-rings are delivered with each SampleCase system.

7.2.2 Lubrication of the Linear Axis

The linear axis has some friction areas which need to be lubricated every half year otherwise they will wear out.





- Use only the silicone free grease that comes with the SampleCase system. If the grease (1803238) is missing please ask Bruker service for a replacement.
- Axis lubrication along the marked parts of the linear axis with silicone free grease.

8 Dismantling and Disposal

Installation, initial commissioning, retrofitting, repairs, adjustments or dismantling of the device must only be carried out by Bruker Service or personnel authorized by Bruker. Damage due to servicing that is not authorized by Bruker is not covered by your warranty.

8.1 Dismantling

Before starting dismantling:

- 1. Shut down the device and secure to prevent restarting.
- 2. Disconnect the power supply from the device; discharge stored residual energy.
- 3. Remove consumables, auxiliary materials and other processing materials and dispose of in accordance with the environmental regulations.
- 4. Clean assemblies and parts properly and dismantle in compliance with applicable local occupational safety and environmental protection regulations.

8.2 Disposal Europe

Environmental information for laboratory and industrial customers within the EU (European Union)



This laboratory product is developed and marketed for Business-to-Business (B2B), so does not fall under article 6 clause 3 of the German Act ElectroG. To meet the demands of the European Directive 2012/19/EU WEEE 2 (Waste of Electrical and Electronic Equipment) and the national Equipment Safety Act, electrical and electronic equipment that is marked with this symbol directly on or with the equipment and/or its packaging must not be disposed of together with unsorted municipal waste or at local municipal waste collecting points. The symbol indicates that the equipment should be disposed of separately from regular industrial/ domestic waste.

Correct disposal and recycling will help prevent potential negative consequences for the environment and risk to personal health. It is your responsibility to dispose of this equipment using only legally prescribed methods of disposal and at collection points defined by government or local authorities in your area.

The WEEE register number can be found on the product label of the equipment. If you need further information on the disposal of equipment or collection and recovery programs available, contact your local Bruker BioSpin sales representative. Local authorities or professional waste management companies may also provide information on specific waste disposal services available in your area.

Disposal - End of Life (EoL) information: the common procedure as defined in the sales contract with Bruker BioSpin

After the lifespan of an electrical and electronic product, Bruker BioSpin takes responsibility for final disassembly and correct disposal in accordance with the European directive 2012/19/ EU WEEE 2.

Bruker BioSpin offers to take back the equipment (only for deliveries after 23.03.2006) after termination of use at the customer site upon request by the customer. This request must be affirmed when the equipment is ordered from Bruker BioSpin. Additional costs for dismantling and transport service will apply!

Only 100% pre-decontaminated equipment can and will be accepted by Bruker BioSpin. A release document for decontamination can be inquired from your nearest Bruker BioSpin contact site, also to be used when repairs, going back to Bruker sites, are requested.

In compliance with WEEE II directive: 2012/19/EU

8.3 Disposal USA and Other Countries

Disposal of these materials may be regulated due to environmental considerations. For disposal or recycling information, please contact our local office or your local authorities, or in the U.S.A., contact the Electronics Industry Alliance web site at *www.eiae.org*.

9 Technical Data

9.1 **Overview of Sample Case Options**

The Sample Case[™] system is designed to easily transport the customers NMR tubes into the magnet and back. For this the NMR tube will be transported up and down with the lift gas and shifted horizontally by a pneumatic drive. This is all fully controlled from software and verified by optical sensors. Users have only to start the transport of a sample from the computer interface or at the hardware interface itself. Furthermore the user can observe the progress of the interaction indicated by the status LED on the SampleCase system.

The SampleCase system, often referred to as the device in this manual, can be ordered in three options all based on a carousel for the samples. This carousel provides holders for 24 carriers for samples. Beside the standard version with 24 holders in the carousel the SampleCase cooled and SampleCase heated option are available.

There are two system configurations with different linear axis lengths available. The short linear axis can be installed on most magnets, but for some magnets the long linear axis is mandatory. The SampleMail system with a standard transport tube can be mounted on most magnets.

Option	System	Sample Temperature Range	included
AH0171	SampleCase (24 position carousel)	• N/A	 1 SampleMail plus Z123384/Z133067
			 1 SampleCase Z122633
			Accessory
AH0172	SampleCase cooled	 Selectable 4°C up to 40°C 	 1 SampleMail plus Z123384/Z133067
		Uniformity of +/-2 °C with setpoint @6°C	 1 SampleCase cooled Z143007
			• 1 BCUI
			Accessory
AH0178	SampleCase heated	Selectable room temperature up to	 1 SampleMail plus Z123384/Z133067
		125°C Uniformity of +/-5 °C with setpoint @125°C	 1 SampleCase heated Z155921
			Accessory

Table 9.1: Overview of SampleCase Options

9.2 Schematic Overviews & Requirements

9.2.1 SampleCase



Figure 9.1: SampleCase System Overview

9.2.1.1 SampleCase Specifications

Shipping dimensions					
Package of Axis for SampleMail / SampleCase P/N Z133067 or Z123384	189 x 52 x 27 cm (L x W x H); 15 kg				
Package of Carousel for SampleCase P/N Z122633	75 x 75 x 65 cm (L x W x H); 35 kg				
Electrical specifications					
SampleMail (subunit)	24 VDC / 0.7 A (Use only the SampleCase adapter P/N: 1801324 supplied by Bruker)				
Pneumatic specifications					
Compressed air or Compressed nitrogen	Purity: ISO 8573-1:2010 [1:1:0 (0.005)] Pressure: 5 – 7 bar Volume flow: ≥ 100 l/ min at 1 bar (20°C, 1 bar)				

9.2.1.2 SampleCase: Lab & System Requirements

Electrical requirements					
SampleMail (su	bunit)	100 – 240 VAC / 50/60 Hz / 0.7 A			
Pneumatic rec	luirements				
Compressed ai	r Or Compressed	Purity: ISO 8573-1:2010 [1:1:0 (0.005)]			
nitrogen		Pressure: 5 – 7 bar Volume flow: ≥ 100 l/min at 1 bar (20°C, 1 bar)			
Temperature r	equirements				
Room temperat	ure	17°C – 25°C			
Temperature va variation not mo	ariation not more than 2 ore than 1°C per 24 h fe	2°C per 24 h for magnets ≤ 400 MHz Temperature or magnets > 500 MHz			
Hardware requirements					
ELCB		ECL 05.01 or more recent (ECL 05.00 and below on request, ECL 02.00 and below are not compatible)			
Either	SLCB	With PNK variant 3, 3s or 5			
	BSVT	SPB or SPB-E			
Software requ	irements				
TopSpin		2.0 or more recent			
ELCB firmware		elcb_firmware_150423.gz or more recent			

Software requirements					
SampleCase firmware		V6			
Either	SLCB firmware	090206 or more recent			
	BSVT firmware	all			

9.2.1.3 SampleCase Rating Plate



Figure 9.2: SampleCase rating plate

The rating plate is located at the flat bottom and includes the following information:

- Name of product
- Manufacturer



Figure 9.3: User interface of SampleCase with rating plate



Figure 9.4: SampleCase label

This label contains:

- PN: Part Number
- SN: Serial Number
- ECL: Engineering Change Level

The SampleMail (subunit) is marked with a separate label at the bottom of the unit:



Figure 9.5: Label at SampleMail (subunit)

This label contains the following information:

vorio proceuro
ienc pressure
$\Theta - \epsilon$
positive
polority
04/0000
n1/nnn2
1

Figure 9.6: SampleMail (subunit) label

- Name of product
- Manufacturer
- Voltage
- Current
- Gaspressure
- · Gasflow
- · Recommended power supply: Output, Safety Standards
- PN: Part Number
- SN: Serial Number
- ECL: Engineering Change Level

9.2.2 SampleCase Cooled



Figure 9.7: SampleCase cooled System Overview

9.2.2.1 SampleCase Cooled Specifications

Shipping specifications					
Package of Axis for SampleMail / SampleCase P/N Z133067 or Z123384	189 x 52 x 27 cm (L x W x H); 15 kg				
Package of Carousel for SampleCase cooled P/N Z143007	75 x 75 x 65 cm (L x W x H); 15 kg				
Package of BCU I and Transferline	80 x 60 x 64 cm (L x W x H); 45 kg				
Electrical specifications					
SampleMail (subunit)	24 VDC / 0.7 A (Use only the SampleCase adapter P/N: 1801324 supplied by Bruker)				
Carousel cooled	048 VDC / 1.4 A (use only the VTA or AUX-Channel of VPSB- board in console)				
Pneumatic specifications					
Compressed air Or Compressed nitrogen	Purity: ISO 8573-1:2010 [1:1:0 (0.005)] Pressure: 5 – 7 bar Volume flow: ≥ 100 I / min at 1 bar (20°C, 1 bar)				

9.2.2.2 SampleCase Cooled: Lab & System Requirements

Electrical requirements			
SampleMail (subunit)	100 – 240 VAC / 50/60 Hz / 0.7 A		
Carousel cooled	048 VDC / 1.4 A		
	(use only the VTA or AUX-Channel of VPSB- board in console)		
Pneumatic requirements			
Compressed air or compressed	Purity: ISO 8573-1:2010 [1:1:0 (0.005)]		
nitrogen	Pressure: 5 – 7 bar Volume flow: \geq 100 l/min at		
	1 bar (20°C, 1 bar)		
Transfer line connector	VT gas max 2bar; 25 l/min		
Flush gas connector	Flush gas max 2bar; 20 l/min		
Temperature requirements			
Room temperature	17°C – 25°C		
Temperature variation not more than 2° C per 24 h for magnets \leq 400 MHz Temperature variation not more than 1° C per 24 h for magnets > 500 MHz			

Hardware requirements			
ELCB	ECL 05.01 or more recent (ECL 05.00 and below on request, ECL 02.00 and below are not compatible)		
Spare heater output of VPSB/VPSB-DC/VPSB-DC-E			
BSVT	SPB or SPB-E		
Software requirements			
TopSpin	2.0 or more recent		
ELCB firmware	elcb_firmware_150423.gz or more recent		
SampleCase firmware	Samplecase_firmware_v6 or more recent		
	1 5 150010		

9.2.2.3 SampleCase Cooled Rating Plate



- 1. VT gas connector
- 2. Bruker rating plate
- 3. VTA connector
- 4. Flush gas connector

The rating plate is located at the power input and includes the following information:

- Name of product
- Manufacturer
- Voltage
- ElectroG Registration Number
- PN: Part Number



Figure 9.8: User interface of SampleCase cooled with rating plate

This plate contains:

- Year of Production
- PN: Part Number
- SN: Serial Number
- ECL: Engineering Change Level

The SampleMail (subunit) is marked with a separate label at the bottom of the unit:

Figure 9.9: Label at SampleMail (subunit)

This label contains the following information:

oumpien		
Voltage: Current:	24V- 0.7A	<u>)</u> s((
Gaspressure: Gasflow:	≥5bar;≤7bar ≥100 l/min at 1bar (atmos	pheric pressure)
Recommended p Output: Safety Standards:	eower supply: ≥25W (SET at 24V) UL60950-1,EN60950-1	O-C-
212 Z12	23384 / 00	0.01/ 00025

Figure 9.10: SampleMail (subunit) label

- · Name of product
- Manufacturer
- Voltage
- Current
- Gaspressure
- · Gasflow
- · Recommended power supply: Output, Safety Standards
- PN: Part Number
- SN: Serial Number
- ECL: Engineering Change Level

9.2.3 SampleCase Heated



Figure 9.11: SampleCase heated System Overview

9.2.3.1 SampleCase Heated Specifications

Shipping dimensions		
Package of Axis for SampleMail /	189 x 52 x 27 cm (L x W x H);	
SampleCase	15 kg	
P/N 2133067 OF 2123384		
Package of Carousel for	75 x 75 x 65 cm (L x W x H);	
SampleCase heated	41 kg	
P/N Z155921		
Electrical specifications		
SampleMail (subunit)	24 VDC / 0.7 A	
	(Use only the SampleCase adapter	
	P/N: 1801324 supplied by Bruker)	
Carousel heated	24 VDC / 6 A	
	(Use only the SampleCase AC/DC adapter	
	P/N: Z125236)	
Pneumatic specifications		
Compressed air Or Compressed	Purity: ISO 8573-1:2010 [1:1:0 (0.005)]	
nitrogen	Pressure: 5 – 7 bar Volume flow: ≥ 100 l/min at 1 bar (20°C, 1 bar)	

9.2.3.2 SampleCase Heated: Lab & System Requirements

Electrical requirements			
SampleMail (subunit)	100 – 240 VAC / 50/60 Hz / min 0.7 A		
Carousel heated	100 - 240 VAC / 50 - 60 Hz / 3.0 A ,		
	(Use only SampleCase AC/DC adapter, P/N: Z125236 supplied by Bruker))		
Pneumatic requirements			
Compressed air Or Compressed	Purity: ISO 8573-1:2010 [1:1:0 (0.005)]		
nitrogen	Pressure: 5 – 7 bar Volume flow: ≥ 100 l / min at 1 bar (20°C, 1 bar)		
Temperature requirements			
Room temperature	17°C – 25°C		
Temperature variation not more than 2°C per 24 h for magnets ≤ 400 MHz Temperature variation not more than 1°C per 24 h for magnets > 500 MHz			
Hardware requirements			
ELCB	ECL 05.01 or more recent (ECL 05.00 and below on request, ECL 02.00 and below are not compatible)		

Hardware requirements		
Spare AUX or heater output of VPSB/VPSB-DC/VPSB-DC-E		
BSVT	SPB or SPB-E	
Software requirements		
TopSpin	≥ 3.5pl3 or more recent	
ELCB firmware	elcb_firmware_160329.gz or more recent	
SampleCase firmware	samplecase_firmware_v6 or more recent	
SACA HEATER BOARD firmware	sacaheat_firmware_151216 or more recent	

9.2.3.3 SampleCase Heated Rating Plate



- 1. Power IN and VTA/AUX COM
- 2. Bruker rating plate

The rating plate is located at the power input and includes the following information:

- Name of product
- Manufacturer
- Voltage
- ElektroG Registration Number
- PN: Part Number



Figure 9.12: User interface of SampleCase heated with rating plate

• PN: Part Number

- SN: Serial Number
- ECL: Engineering Change Level

The SampleMail (subunit) is marked with a separate label at the bottom of the unit:



Figure 9.13: Label at SampleMail (subunit)

This label contains the following information:

Voltage:	241- 6	
Current:	0.7A	
Gaspressure:	≥5bar;≤7bar	
Gasflow:	≥100 l/min at 1bar (atmos	pheric pressure)
Recommended p	ower supply:	
Output:	≥25W (SET at 24V)	0-6-6
Safety Standards:	UL60950-1, EN60950-1	positive polarity
		polarity
	10001	0.041.00005

Figure 9.14: SampleMail (subunit) label

- Name of product
- Manufacturer
- Voltage
- Current
- Gaspressure
- · Gasflow
- · Recommended power supply: Output, Safety Standards
- PN: Part Number
- SN: Serial Number
- ECL: Engineering Change Level

9.3 **Operating Conditions**

Environment

Normal environmental conditions (CAN/CSA 61010112; IEC 610101:2010; ANSI/UL 610101).

- Indoor use only.
- Maximum operation altitude: 2000 m.
- Ideal operating temperatures: 22-25 °C. Minimum operating temperature: 18 °C Maximum operating temperature: 28 °C Humidity (non-condensing): 20-80 %
- Maximum operating temperature: 28 °C Humidity (non-condensing): 20-80 %
- Maximum relative humidity 80 % for temperatures up to 31 or decreasing linearly to
- 50 % relative humidity at 40 °C.
- MAINS supply voltage fluctuations up to ±10 % of the nominal voltage.
- TRANSIENT OVERVOLTAGES up to the levels of OVERVOLTAGE CATEGORY II.
- Pollution degree 2.
- Protection class IP20.

File LR1392

10 Certificate of Compliance

The SampleCase systems, namely Sample Case, Sample Case cooled and Sample Case heated, are checked by external inspectors to satisfy the safety requirements of the CAN/ CSA C22.2 No 61010-1-12 and UL 61010-1.



QPS Evaluation Services Inc Testing, Certification and Field Evaluation Body Accredited in Canada, the USA, and Internationally

	ICATE OF COMPLIANCE TYPE 3 CERTIFICATION SYSTEM)	
	Page 1 of 2	
Issued to	Bruker BioSpin AG	
Address	Industriestrasse 26, CH-8117 Fällanden, Switzerland	
Project Number	LR1392-1	
Product	Sample Transporter	
Model Number	 System AH0171 consists of SampleMail plus P/N Z123384, Z133067 with SampleCase Z122633 System AH0178 consist of SampleMail plus P/N Z123384, Z133067 with optional SampleCase heated Z155921 System AH0172 consist of SampleMail plus P/N Z123384, Z133087 with optional SampleCase cooled Z143007 	
Ratings	See page 2	
Applicable Standards	 CAN/CSA C22.2 NO 61010-1-12: Safety Requirements for Electrical Equipment for Measurement, Control, and Laboratory Use - Part 1: General Requirements - Third Edition; Update No. 1: July 2015 UL 61010-1 - UL Standard for Safety Electrical Equipment for Measurement, Control, and Laboratory Use; Part 1: General Requirements - Third Edition; Reprint with revisions through and including July 15, 2015 	
Factory & Manufacturing Location	Bruker BioSpin AG Industriestrasse 26, CH-8117 Fällanden, Switzerland	
Statement of Compliance: The product(s) identified in this Certificate and described in the Report covered under the above referenced project number have been investigated and found to be in compliance with the relevant requirements of the above referenced standard(s). As such, they are eligible to bear the QPS Certification Mark shown below, in accordance with the provisions of QPS's Service Agreement.		
Issued By: Steve Siu Stave Sim.		
Signature:	Date: June 10, 2016	

81 Keifield St., Units 7-9, Toronto, ON M9W 5A3 Tel: 416-241-8857; Fax: 416-241-0682 www.qps.ca

QSD 34

Rev 04



QPS Evaluation Services Inc Testing, Certification and Field Evaluation Body Accredited in Canada, the USA, and Internationally

CERTIFICATE OF COMPLIANCE (ISO TYPE 3 CERTIFICATION SYSTEM)	
Project Number: LR1392-1	Page 2 of 2
Ratings	
 System AH0171 consist of SampleMail plus P/N Z123384, Z133067 with SampleCase Z12 Input: 24Vdc, 0.7A 	2633
 System AH0178 consist of SampleMail plus P/N Z123384, Z133087 with optional Sam Z155921 Input 1: 24Vdc; 0.7A Input 2: 24Vdc; max. 6A for optional heating function 	npleCase heated
 System AH0172 consist of SampleMail plus P/N Z123384, Z133067 with optional Sar Z143007 Input 1: 24Vdc; 0.7A Input 2: 0-48Vdc, max. 1.4A for optional cooling function 	mpleCase cooled

81 Keifield St., Units 7-9, Toronto, ON M9W 5A3 Tel: 416-241-8857; Fax: 416-241-0682 www.qps.ca

QSD 34

Rev 04

File

11 Contact

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Samplemail-service@bruker.com

Samplecase-service@bruker.com

Please refer to the Model No., serial No. and Internal Order No. in all correspondence regarding the NMR system or components thereof. The Serial No. can be read in the BSMS setup web page.

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