

InsightMR

- User Manual

Version 003



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1 About This Manual

This manual enables safe and efficient handling of the device.

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

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

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

1.1 Policy Statement

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

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

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

1.2 Symbols and Conventions

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

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

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

DANGER



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

This is the consequence of not following the warning.

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

WARNING



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

This is the consequence of not following the warning.

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

CAUTION



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

This is the consequence of not following the warning.

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

NOTICE

NOTICE indicates a property damage message.

This is the consequence of not following the notice.

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

SAFETY INSTRUCTIONS

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

This is the consequence of not following the safety instructions.

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



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

2 Introduction

Designed for the analysis of chemical processes by NMR, InsightMR is the ideal solution for both industrial and academic scientists studying or optimizing reactions. InsightMR's two components, a flow unit and dedicated software, enable online monitoring of chemical reactions in real-time under real process conditions.

2.1 Concept

The flow unit enables online monitoring of chemical reaction in real-time under real conditions. This is achieved by fast and continuous transfer of reactions mixtures from a reaction vessel into a glass flow tube, located in the NMR probe, with temperature control from the flow interface to the probe. Designed to work with 5 mm probes, the flow unit is a versatile proposition to flow chemistry by NMR.

The dedicated InsightMR software is a platform designed for the analysis of chemical processes by NMR. Integrated acquisition control and data processing features enable on-the-fly acquisition parameter adjustment based on real-time kinetic data.

2.2 Intended Use

The InsightMR glass flow tube is an insert for standard 5 mm NMR probes. It allows the transfer of liquid from an external container through a transfer line into the NMR detection area and back. Once the liquid is in the detection area, NMR data can be acquired either under static or continuously flowing conditions. A schematic of the intended setup is shown in the figure [Figure 4.2 \[▶ 16\]](#).

Typically the InsightMR flow unit is used to continuously circulate the liquid from a reaction vessel through the NMR probe. By this procedure the changing composition of the liquid in the vessel, i.e. the progress of the reaction, can be continuously monitored. The low volumes of the system ensure that after a short time the composition in the NMR glass flow tube corresponds to the composition in the reactor.

The InsightMR modular design allows the user to maintain the system easily. In the case of contamination from compounds that cannot be removed with simple flushing, the glass flow tube can be removed and cleaned or replaced. The glass flow tube, and various other components are highlighted in the figure [Figure 4.1 \[▶ 15\]](#).

The system can be used for other purposes where a flow with changing composition should be monitored. However the usage as an HPLC-NMR system is not recommended since it is designed to allow fast transfer with high flow rates, which would cause peak broadening in an HPLC chromatogram.

2.3 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.

2.4 Copyright

All rights reserved. This manual is protected by copyright and intended solely for internal use by customers.

This manual must not be made available to third parties, duplicated in any manner or form – whether in whole or in part – and the content must not be used and/or communicated, except for internal purposes, without the written consent of the manufacturer.

Product names used are trademarks™ or registered trademarks® of their respective holders.

Violation of the copyright will result in legal action for damages. We reserve the right to assert further claims.

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.

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

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

Laboratory Personnel

Laboratory personnel are professionals, technicians, and assistants staffing a research facility where specimens are grown, tested, or evaluated and the results of such measures 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.

3.2.1 Unauthorized Persons

 **WARNING**



Risk to life for unauthorized personnel due to hazards in the danger and working zone!

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

- ▶ Unauthorized persons must be kept away from the danger and working zone.
- ▶ If in doubt, address the persons in question and ask them to leave the danger and working zone.
- ▶ Cease work while unauthorized persons are in the danger and working zone.

3.2.2 Instruction

Personnel must receive regular instruction from the owner. The instruction must be documented to facilitate improved verification.

Date	Name	Type of Instruction	Instruction Provided By	Signature

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 General Workplace Dangers

Please refer to the figure [Figure 4.1 \[▶ 15\]](#) for the location of parts mentioned in this section.

CAUTION

Risk of contamination from toxic liquids or vapors during operation.

Contamination may occur from sample liquid leaking into the laboratory environment.

- ▶ Clean any chemical leakages or spills immediately following all appropriate safety precautions for safe chemical handling and laboratory cleaning procedures.
- ▶ Wear proper personal protective equipment. Examples include but are not limited to gloves, goggles, lab coat, etc.
- ▶ The volume of sample liquid in the reactor must not exceed 2.5 liters.
- ▶ Utilize a fume hood over the reactor, fluid pump, and the sample and temperature control connectors to the reaction transfer line.
- ▶ Place a container that can hold up to 10 liters of liquid, and is appropriately rated for chemical spills, below the probe.
- ▶ Only reactions with moderately hazardous products should be carried out. The cleaning of accidental spillage of sample liquid must be possible using standard safety equipment (goggles, lab coat, gloves, etc.).



CAUTION

Risk of injury from broken glass during glass flow tube replacement.

Incorrect handling of the glass flow tube during installation may result in broken glass and possible injury.

- ▶ Wear proper personal protective equipment. Examples include, but are not limited to, gloves, goggles, lab coat, etc.
- ▶ Always use the flow tube protector to exchange the glass flow tube (see [Mounting the Glass Flow Tube \[▶ 50\]](#)).

CAUTION

Risk of contamination from toxic liquids or vapors during service and installation.

Insufficient cleaning/flushing of the flow unit prior to storage may result in a risk of contamination from toxic liquids or vapors during service and installation.

- ▶ Wear proper personal protective equipment. Examples include, but are not limited to, gloves, goggles, lab coat, etc.
- ▶ Clean and flush the sample line after usage with a suitable solvent that is compatible with the solubility of all components used in the experiment.
- ▶ Seal the inlet and outlet of the sample line and temperature control lines while the system is outside the magnet and prior to storage.
- ▶ Use an inert, non-toxic temperature control liquid like glycol.



NOTICE**Material damage to the NMR probe from sample liquid after a glass flow tube breakage.**

Sample liquid leaking into the NMR probe as a result of breakage of the glass flow tube may result in material damage to the NMR probe.

- ▶ Do not apply pressure above 10 bar to the flow unit assembly.
- ▶ Before introducing the flow unit assembly in the magnet, check for leakages in the unit at the flow rate and temperature values that will be later used during the experiment.
- ▶ Handle the flow unit assembly with care when inserting it into the magnet.
- ▶ Use a sample delivery pump with a maximum operating pressure below the specified pressure limit of the flow unit assembly or set the pressure limit of the pump not to exceed the specified pressure limit.
- ▶ The maximum allowed flow rate for the flow unit and reaction sample line is 5 mL/min = 0.3 L/h.

NOTICE**Material damage to the NMR probe from sample liquid leaking from flow unit.**

Sample liquid leaking into the NMR probe as a result of flow unit leakage may result in material damage to the NMR probe.

- ▶ Do not apply pressure above 10 bar to the flow unit assembly.
- ▶ Before introducing the flow tube assembly in the magnet, check for leakages in the unit at the flow rate and temperature values that will be later used during the experiment.
- ▶ Exchange the glass flow tube sealing O-rings regularly. If using solvents that are known to be destructive to polymers (Kalrez) exchange the O-rings after each use.
- ▶ Do not exceed the maximum flow rate for the flow unit and reaction sample line of 5 mL/min = 0.3 L/h.

NOTICE**Material damage to the magnet from sample liquid after a glass flow tube breakage or from flow unit leakage.**

Sample liquid leaking into the bore of the magnet as a result of a glass flow tube breakage or from flow unit leakage may cause material damage to the magnet.

- ▶ The volume of sample liquid in the reactor should not exceed 2.5 liters.
- ▶ Exchange the glass flow tube sealing O-rings regularly. If using solvents that are known to be destructive to polymers (Kalrez) exchange the O-rings after each use.
- ▶ Do not exceed the maximum flow rate for the glass flow tube and sample line of 5 mL/min = 0.3 L/h.

NOTICE**Material damage to the NMR probe or magnet from temperature control liquid.**

Leakage of temperature control liquid from reaction control connectors into the NMR probe or magnet may result in material damage.

- ▶ Use a temperature control unit with a maximum operating pressure set to ≤ 0.5 bar.
- ▶ Do not apply pressure greater than 1 bar to the reaction temperature line.
- ▶ Before introducing the flow unit assembly in the magnet, check for leakages in the unit at the flow rate and temperature values that will be later used during the experiment.
- ▶ Use an inert, non-toxic temperature control liquid like glycol.
- ▶ The volume of the temperature control liquid must not exceed 5 liters.

 **CAUTION****Risk of contamination from toxic liquids or vapors after a glass flow tube breakage or from flow unit leakage.**

Contamination from toxic liquids or vapors may result after a glass flow tube breakage or from leakage of sealing O-rings or connectors.



- ▶ Wear proper personal protective equipment. Examples include but are not limited to gloves, goggles, lab coat, etc.
- ▶ For test purposes, use only non-toxic harmless compounds, for example sucrose in $\text{H}_2\text{O}/\text{D}_2\text{O}$.
- ▶ Clean and decontaminate the entire flow unit assembly prior to service tasks and confirm the decontamination.

NOTICE**Material damage to the reactor due to movement of the flow unit assembly.**

Movement of the flow unit assembly during insertion/removal of the flow unit and InsightMR transfer line into or from the magnet may cause damage to the reactor. Accidental movement of the reaction transfer line by persons accessing the system may also cause material damage.

- ▶ Secure the end of the InsightMR transfer line close to the reactor to prevent movement (e.g. push/pull or rotation).
- ▶ Prevent access to the space between the reactor and magnet where the InsightMR transfer line is installed.

4 Design and Function

4.1 Description

InsightMR hardware consists of an insulated transfer line with an NMR glass flow tube on one end and a flow interface with an isolation valve on the other end:

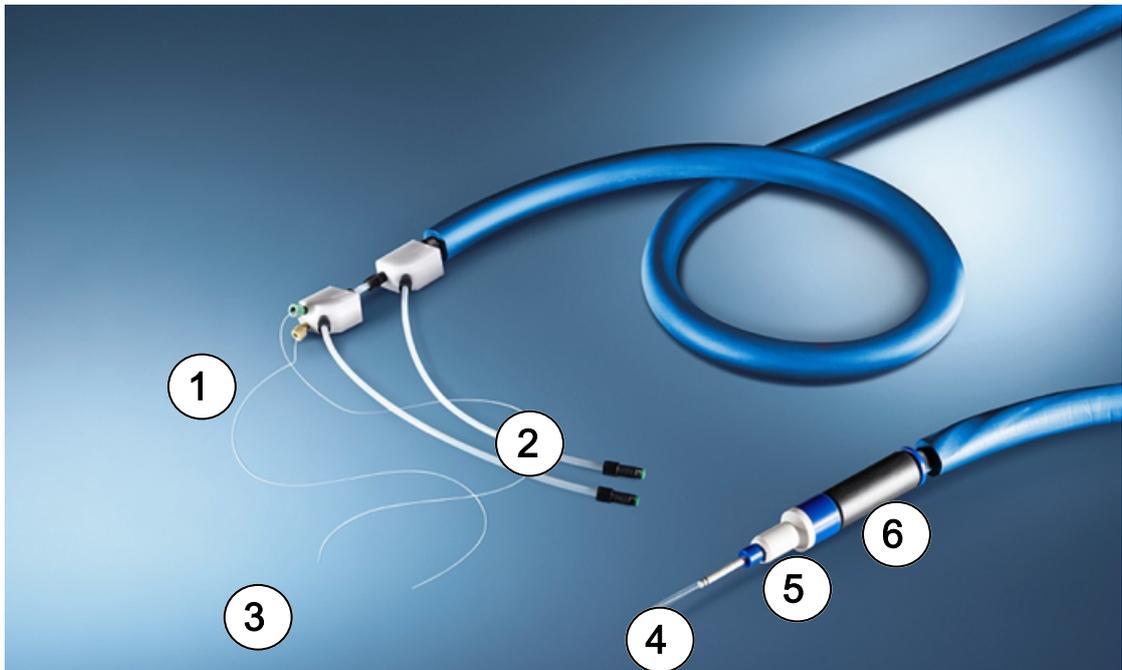


Figure 4.1: InsightMR Flow Tube Assembly and the Transfer Line

1	Sample Lines	4	Glass Flow Tube
2	Temperature Control Lines	5	Tube Holder
3	The Transfer Line. Consists of the temperature control lines, sample lines and insulation. Available in standard lengths of 4 and 7 meter, or in custom lengths of 5, 6 and 9 meters.	6	Holder Body

In addition, a sample line holder (shown in the following figure, on top of the magnet), a spare parts kit and documentation are provided. Refer to [Connecting the Transfer Line Holder \[▶ 24\]](#) for instructions on how to install it.

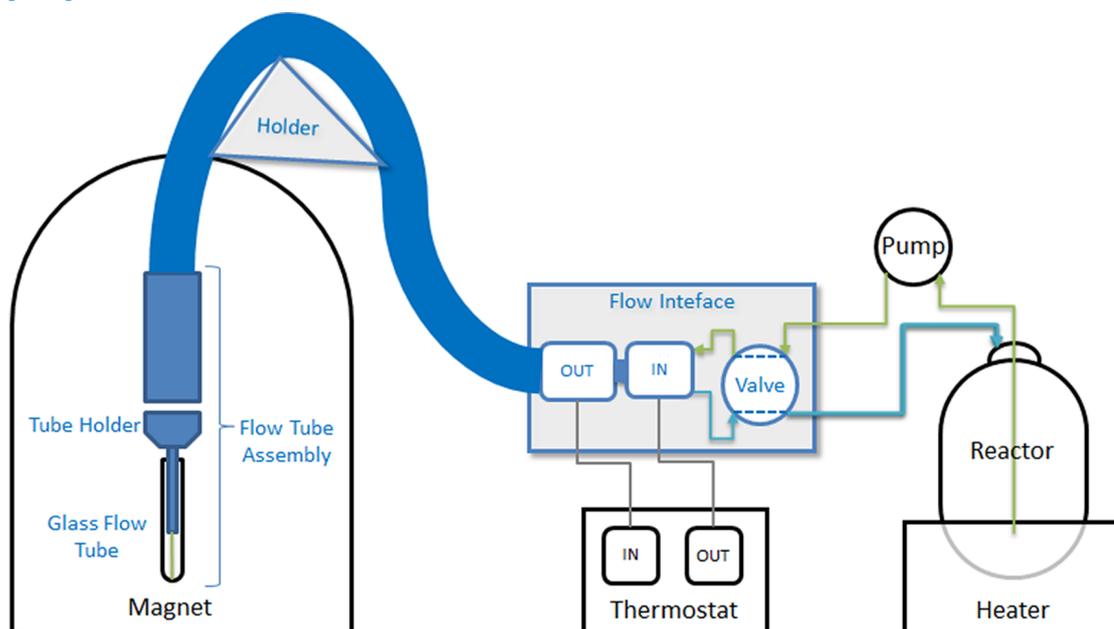


Figure 4.2: Recommended Laboratory Setup

The glass flow tube with flow tube protector and flow interface are shown in the figure [Figure 4.3 \[▶ 17\]](#).

The 5 mm NMR glass flow tube together with the tube holder, which has the shape of a spinner, is compatible with any standard Bruker 5 mm NMR probe with insertion depth of 20 mm. The InsightMR glass flow tube volume corresponds approximately to the active volume of a standard 5 mm tube.

The transfer line is composed of 2 sample lines, sample in and sample return, and 2 concentric temperature control lines surrounding the sample lines. Thermostatic liquid is flushed through the temperature control lines to maintain the temperature during the sample transfer to the NMR and back. Insulating foam around the transfer line prevent temperature loss, condensation and injury through high temperatures.

The recommended laboratory set up is shown in the figure [Figure 4.2 \[▶ 16\]](#). The pump and the thermostat can be purchased together with InsightMR, as options. They are not included as default.

The reaction mixture is pumped from the vessel, through the pump, the valve (flow interface) and the sample lines, to the NMR and back. Tubing and standard HPLC fittings are provided to connect the vessel to the pump, the pump to the valve and the valve back to the reactor.

The temperature control line inlets and outlets are fixed to the flow interface, which can be secured to a laboratory stand.

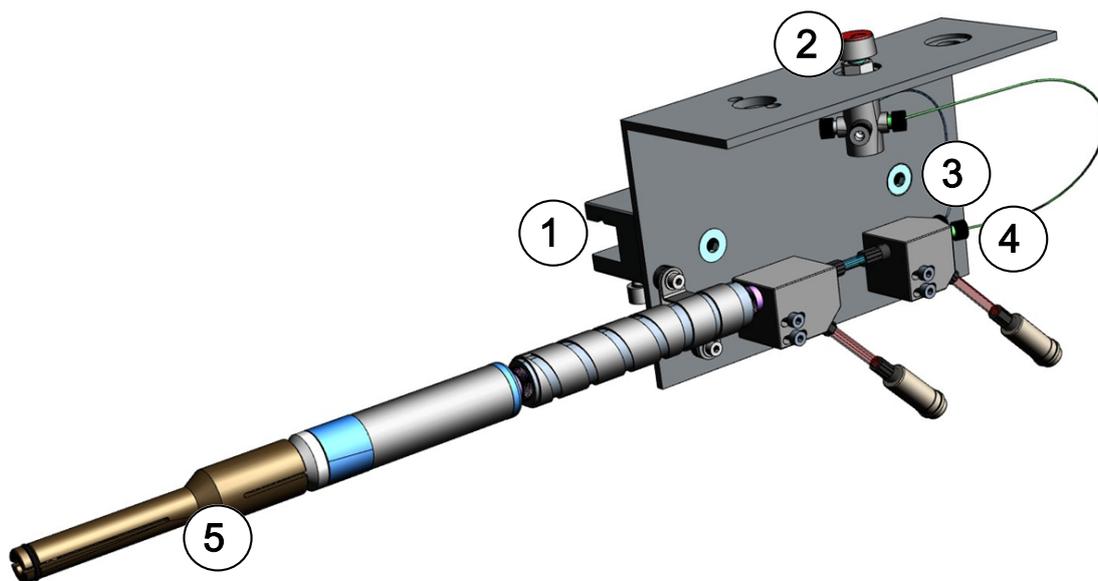


Figure 4.3: InsightMR Flow Tube Assembly, Flow Tube Protector and Flow Interface

1	Flow Interface	4	Sample Valve Outlet
2	Flow Control Valve	5	Flow Tube Protector
3	Sample Valve Inlet		

4.2 Software

InsightMR includes the flow unit and dedicated software. Use of this software is highly recommended. The software integrates acquisition control and data processing features, enabling on-the-fly acquisition parameter adjustment based on real-time kinetic data.

Please refer to the section [Software Installation \[27\]](#) for instructions on the software installation.

Upon installation and launch, a quick start guide is available under **Help - QuickStart**.

NOTICE

Material damage to flow unit due to incorrect automation mode

Failure to set the **Sample Changer/Automation** mode to Flow Tube (InsightMR) may result in flow tube breakage.

- ▶ Set the **Sample Changer/Automation** to Flow Tube (InsightMR) in IconNMR configuration **Automation/Master Switches**.

5 Transport, Packaging and Storage



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.

5.1 Symbols on the Packaging

The following symbols are affixed to the packaging material. Always observe the symbols during transport and handling.

Top		The arrow tips on the sign mark the top of the package. They must always point upwards; otherwise the content may be damaged.
Fragile		Marks packages with fragile or sensitive contents. Handle the package with care; do not allow the package to fall and do not allow it to be impacted.
Protect Against Moisture		Protect packages against moisture and keep dry.
Attach Here		Lifting gear (lifting chain, lifting strap) must only be attached to points bearing this symbol.
Center of Gravity		Marks the center of gravity of packages. Note the location of the center of gravity when lifting and transporting.
Weight, Attached Load		Indicates the weight of packages. Handle the marked package in accordance with its weight.
Permitted Stacking Load		Indicates packages which are partially stackable. Do not exceed the maximum load-bearing capacity specified on the symbol in order to avoid damaging or destroying the content.

<p>Do not Damage Air-tight Packaging</p>		<p>The packaging is air-tight. Damage to the barrier layer may render the contents unusable.</p> <p>Do not pierce.</p> <p>Do not use sharp objects to open.</p>
<p>Component Sensitive to Electrostatic Discharge</p>		<p>The packaging contains components which are sensitive to an electrostatic discharge.</p> <p>Only allow packaging to be opened by trained personnel.</p> <p>Establish potential equalization before opening.</p>
<p>Protect from Heat</p>		<p>Protect packages against heat and direct sunlight.</p>
<p>Protect from Radioactive Sources</p>		<p>Protect packages against radioactive sources.</p>

Table 5.1: Symbols on the Packaging

5.2 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.



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

5.3 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.

5.4 Storage

The following instructions should be followed when the flow unit will be stored for a longer period:

- Before storage, the flow unit should first be thoroughly cleaned – this is described in [Removing the Flow Unit for Storage in the Transport Box \[▶ 41\]](#).
- Close the inlet and outlet of the sample line to protect the system against dust and dirt.
- Leave the glass flow tube connected to tube holder. Protect it against damage.
- Coil up the transfer line ($\varnothing > 50$ cm) and place the system into the transport box.

To store the flow unit temporarily when not in use, follow the instructions in the section [Removing the Flow Unit for Storage in the Transport Box \[▶ 41\]](#)

6 Flow Unit Installation

Before installing the InsightMR flow unit:

- Familiarize yourself with all the safety measures in [General Workplace Dangers \[12\]](#).
- Take the appropriate safety measures (risk assessment, PPE, fume cupboard etc.) for monitoring reactions and processes.
- Familiarize yourself with safety measures when working with magnetic fields (refer to the AVANCE Systems General Safety Considerations User Manual, available on the BASH DVD or from Bruker).
- Place a collection vessel (rated for chemical waste according to local EH&S standards) below the NMR probe with sufficient volume to contain the thermostat liquid and the reaction mixture, in the unlikely case of a leak.

6.1 Choose the Position of the Reactor

The transfer line has a standard length of 4 or 7 meters. Depending on the magnet type 1 or 2 meters of transfer line are required inside the magnet.

- Identify the place where the vessel can be placed and reached by the remaining length of the transfer line.
- Fix the flow interface by connecting it to a laboratory stand.



Figure 6.1: Typical Laboratory Setup for Monitoring Chemical Reaction

The example shown in the figure above is equipped with a 4 meter transfer line.

6.2 Connecting the Transfer Line Holder

Attach the transfer line holder to the Bruker Sample Transport (BST).

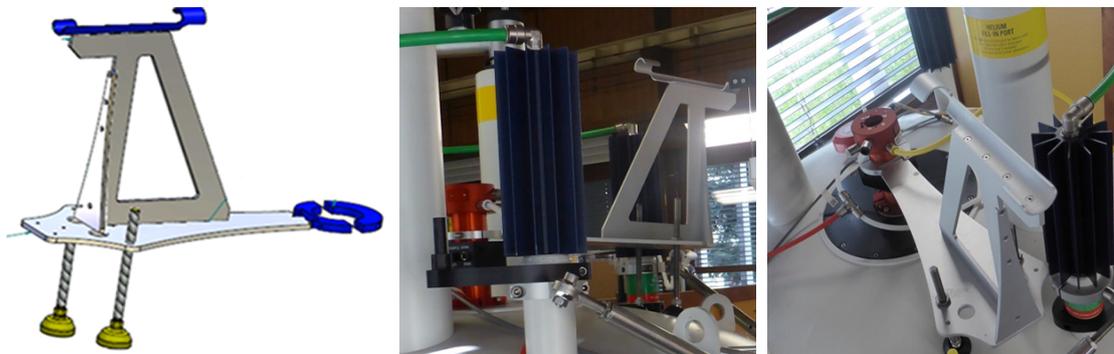


Figure 6.2: The Transfer Line Holder

Note that this is not for the SampleJet.

6.3 Testing the Flow Unit Prior to Inserting it into the Magnet



Figure 6.3: The InsightMR Flow Unit. From left to right: the pump, the reactor, the flow tube assembly secured with a clamp stand and the thermostat.

Note that the pump shown in the picture is not the InsightMR pump that can be purchased optionally with the system.

- Place the flow unit on a table and temporarily secure it against any movement.

- Inspect the glass flow tube for damage, contamination and leaks. The glass flow tube must not show any cracks or damage. No solid particles must be visible in the glass flow tube. No liquid must be visible behind the sealing O-rings. If necessary, clean or replace the glass flow tube and O-rings.

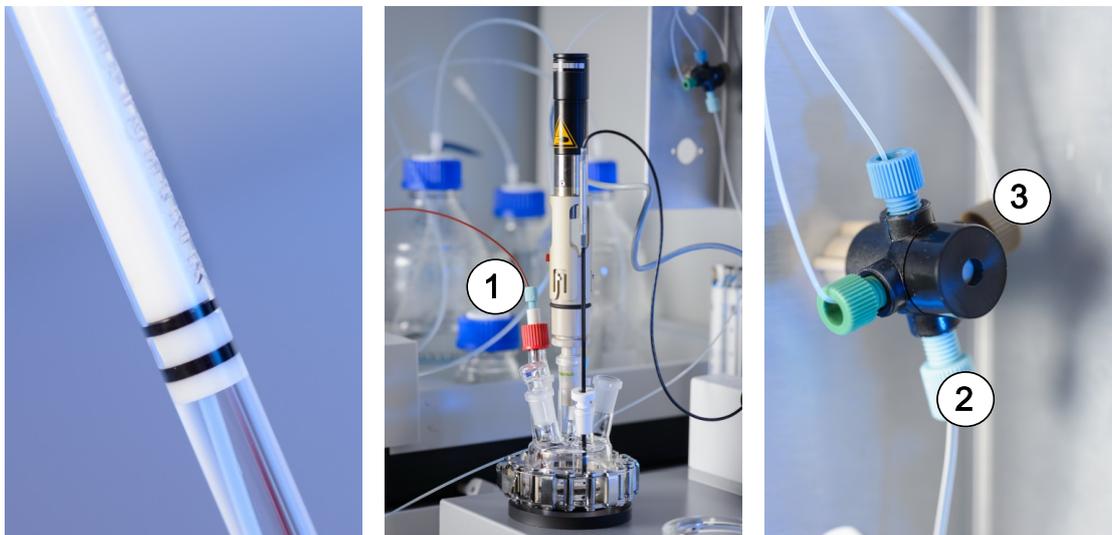


Figure 6.4: From Left to Right, Glass Flow Tube O-Rings, Vessel Connections, and Flow Interface Valve

- Connect the vessel to the pump [1].
 - Connect the pump outlet to the flow interface valve inlet [2, adjacent to the green connector] and the valve outlet [3, adjacent to the blue connector] back to the vessel or to the waste.
- Note that there are two valve positions: i) through the flow tube and ii) bypass it.
- Flush the flow unit with the reaction solvent at the maximum planned flow rate for 30 minutes and check for leaks, paying specific attention to all O-rings and seals.
 - Stop the flow.

6.4 Temperature Control (optional)

- Connect the inlet and outlet of the temperature control lines to the back of the thermostat.



Figure 6.5: Temperature Control Connections

- Set the thermostat to the target temperature; start it and wait for the desired temperature to be reached.
- Verify that the temperature control liquid returns to the chiller.
- Check for leakages at the upper part of the sample tube holder, all O-rings and seals.
- Check that no liquid appears at the outlet of the transfer lines (for both sample and temperature control lines).
- Check that the temperature control liquid does not leak into the sample line.

6.5 Software Installation

InsightMR software compatibility

InsightMR requires TopSpin 3.5.pl2 or higher.

Insight software download (includes TopSpin and InsightMR)

<https://www.bruker.com/service/support-upgrades/software-downloads/nmr.html>

InsightMR software can be installed from the TopSpin DVD (TopSpin 3.5.pl5 and above for windows and 3.5.pl6 and above for Linux). It can also be downloaded from the web page as an ISO image of the TopSpin DVD or as a separate executable file. The downloadable file (> 700 Mb) is a compressed self-extracting executable that contains TopSpin, IconNMR, InsightMR, Diskless and FlexIm.

InsightMR license request (hostID needed)

https://www.bruker.com/nmr_license_requests.html

InsightMR does not require an extra license when operated connected to a Bruker spectrometer (new from February 2017). The spectrometer needs to have a valid TopSpin 3 or above license.

Off-line analysis is supported by Dynamics Center, which does not require an extra license either.

If the user operates in conditions different from above, please contact your local Bruker representative. Three months demo licenses can also be requested through the [license request page](#). Once the software is installed the host-ID is visible under the **Help | About** tab.

InsightMR software installation

InsightMR must be installed together with the TopSpin's and IconNMR's versions included in the executable, ISO image or DVD. If a previous version of TopSpin exists it is recommended to do a parallel installation (i.e. set up a different directory name for the new TopSpin installation). After the new installation **expinstall** (command line) is required. The user should check that the topspin installation has been successful and topspin is fully functional before launching insightMR. Detailed instructions on the installation procedure are below.

The following instructions should be followed to install InsightMR software:

- If TopSpin is currently installed, launch TopSpin and at the command prompt type **nmr_save** to save the current configuration of the system.

Some installation and user files may be overwritten during a TopSpin installation/update. These files are easily restored if an **nmr_save** is performed in advance.

- Shut down all TopSpin and related programs.
- Start the installation by either:
 - **Windows:** After downloading the installer ReactionMonitoring<version>.zip, double-click and execute.
 - **Linux:** Download and install ./ReactionMonitoring<version>.sh

The <version> stands for the current program version, e.g. 1.0.7.

Note that one must have admin (Windows) or super user (Linux) rights to install the file.

- The TopSpin Setup tool will appear. Click **Next**.

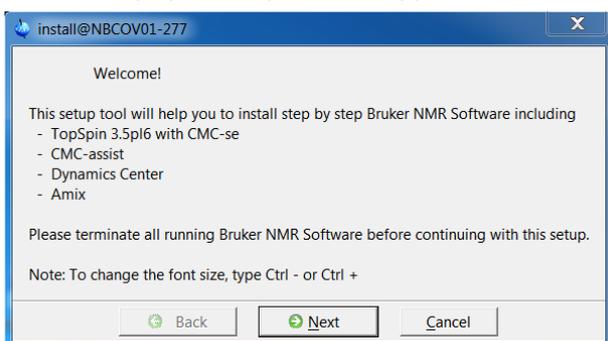


Figure 6.6: The TopSpin Setup Tool

- A new dialog box with **Install Bruker NMR Software** and **Install GPL licensed Cygwin 1.7.4 Software** checked will appear. Click **Next**.

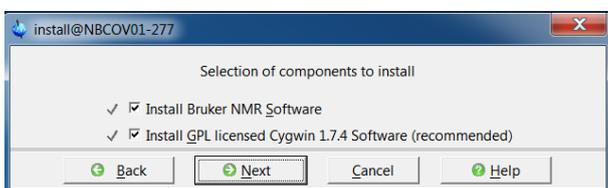


Figure 6.7: Selection of Components to Install

- The TopSpin release letter will appear and a dialog box to acknowledge you have read the letter. Click **Next** once you have read the letter.

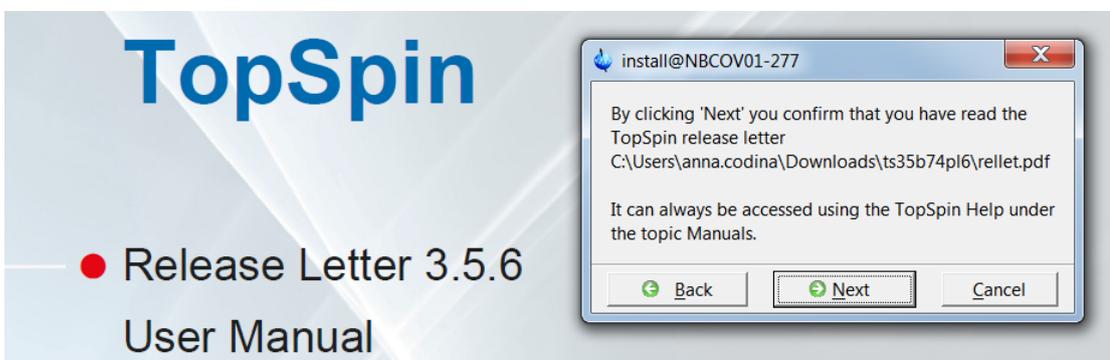


Figure 6.8: TopSpin Release Letter Confirmation

- Select the directory where you want to install the new TopSpin (as below). In cases where TopSpin is already installed, we highly recommend to do a parallel installation to ensure the compatibility of TopSpin, IconNMR and InsightMR (they must all come from the same source: same executable, ISO image or DVD). This means you should define a new TopSpin directory. Do NOT install on top of an existing TopSpin directory. Use **Browse** to see the different existing directories in case of any doubts.

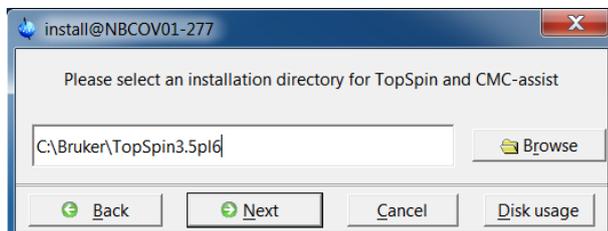


Figure 6.9: Select an Installation Directory

- Click **Yes** in the next warning message.

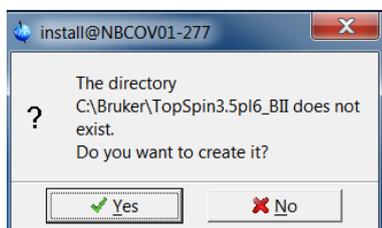


Figure 6.10: Warning Message when the Installation Directory does not Exist

- Choose **Customized** setup type.

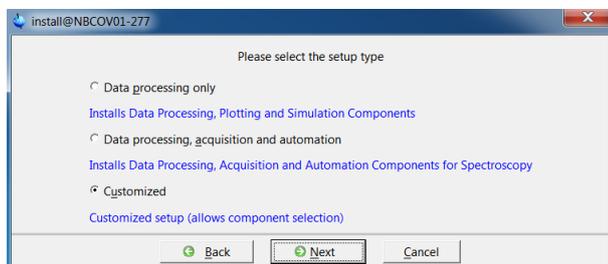


Figure 6.11: Select Setup Type

- Click on **More information** to see the current installed versions vs. the new ones for the different software parts. Select at least **TopSpin**, **IconNMR** and **InsightMR**. Also select **Diskless** if you are installing on the spectrometer a version with newer firmware. Also select **FLEXIm** in case there is no FLEXIm already installed. The rest of the programs are optional.

It is highly recommendable to install Dynamics Center either on the spectrometer or on a processing station or personal computer to use as off-line kinetics analysis tool. The Kinetics module of Dynamics Center contains the analysis tools also in InsightMR but it is not linked to acquisition.

When installing from a ReactionMonitoring ----.exe, the default installation setup type selects the adequate software parts required for InsightMR.

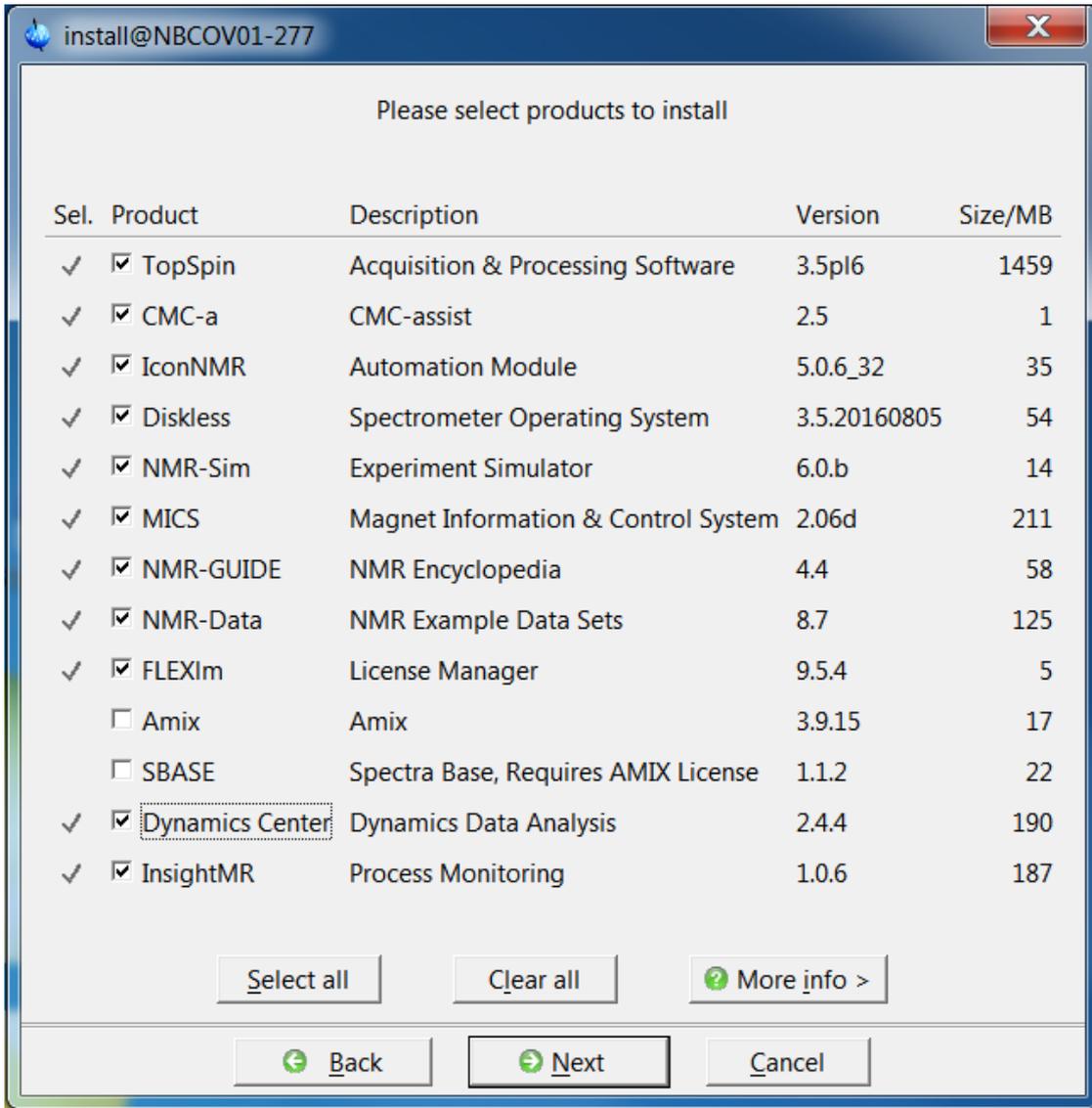


Figure 6.12: Select Products to Install

- Select the NMR Super User. It could be one of the domain users or traditionally **nmrsu**.

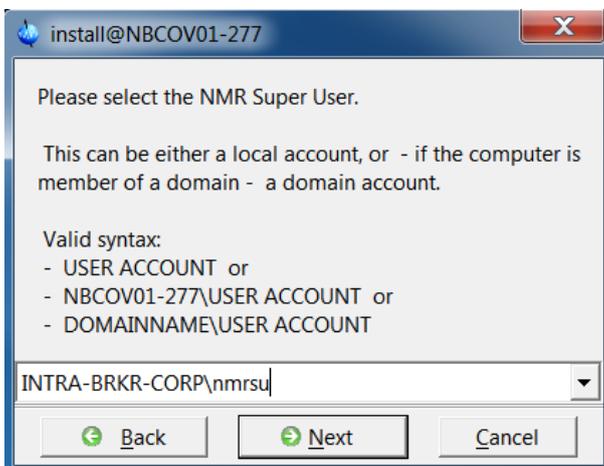


Figure 6.13: Select the NMR Super User

- Enter the password of the domain user that is going to be also NMR administrator. Or choose a password for the NMR administrator.

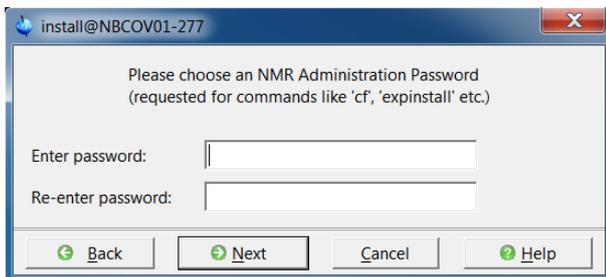


Figure 6.14: Select an NMR Administration Password

- Acknowledge that you are in agreement with the programs to be installed displayed in the next message window by clicking **Next**. The installation will start.
- If the installation has been successful you will see two messages similar to those below with all steps in green. If it is a windows installation, you should have at least two new icons in your desktop: TopSpin and InsightMR.

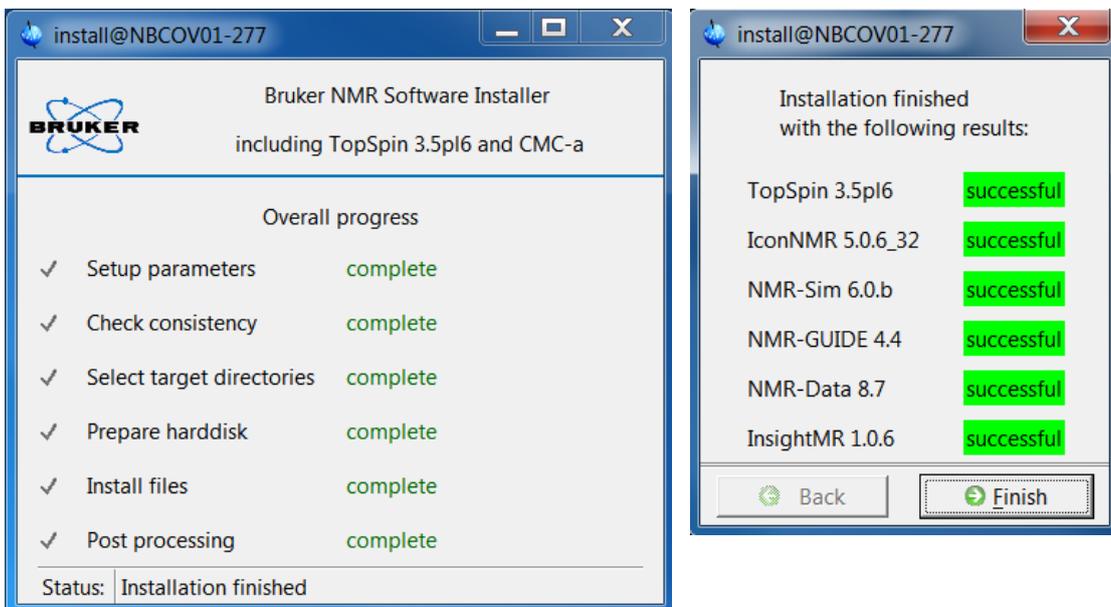


Figure 6.15: Installation Finished

- When you click **Finish**, the InsightMR release letter will appear.



Figure 6.16: InsightMR Release Letter

Refer to the TopSpin Installation Manual, Chapter 2, if more detailed instruction is needed.

6.6 Software Configuration

6.6.1 TopSpin Configuration

- Launch the newly installed TopSpin.
- Select **Expinstall (datastation)** in the dialog that appears.
- Click on **Next** until the Expinstall is finished.

Refer to the TopSpin installation manual (Chapter 4, page 44 onwards) for details on configuring TopSpin.

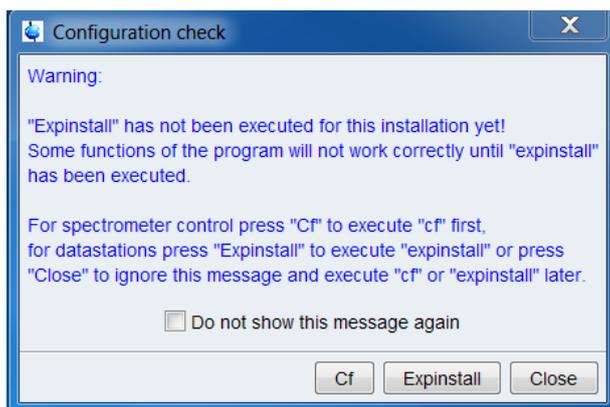


Figure 6.17: Configuration Check

Once Expinstall is complete, configure IconNMR as described in the next section.

6.6.2 InsightMR Flow Mode Configuration

If not launched already, launch InsightMR by clicking on the desktop Icon. If the operating system is Linux, there may not be a desktop icon and you may have to launch the program by going to the folder applications/Bruker software/InsightMR.



Figure 6.18: InsightMR Icon

This will launch TopSpin, InsightMR and IconNMR.

- Start Icon configuration by clicking on **configuration** in the icon below or typing **iconc** at the TopSpin command prompt.

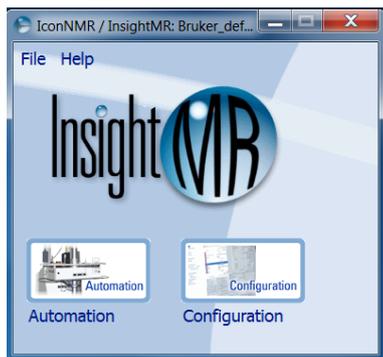


Figure 6.19: Starting the Icon Configuration

In TS3.5.pl6 and beyond, switch off the domain users if you are not going to use them since they slow down the program. Uncheck anything under Domain (**Options | Resource File Settings**).

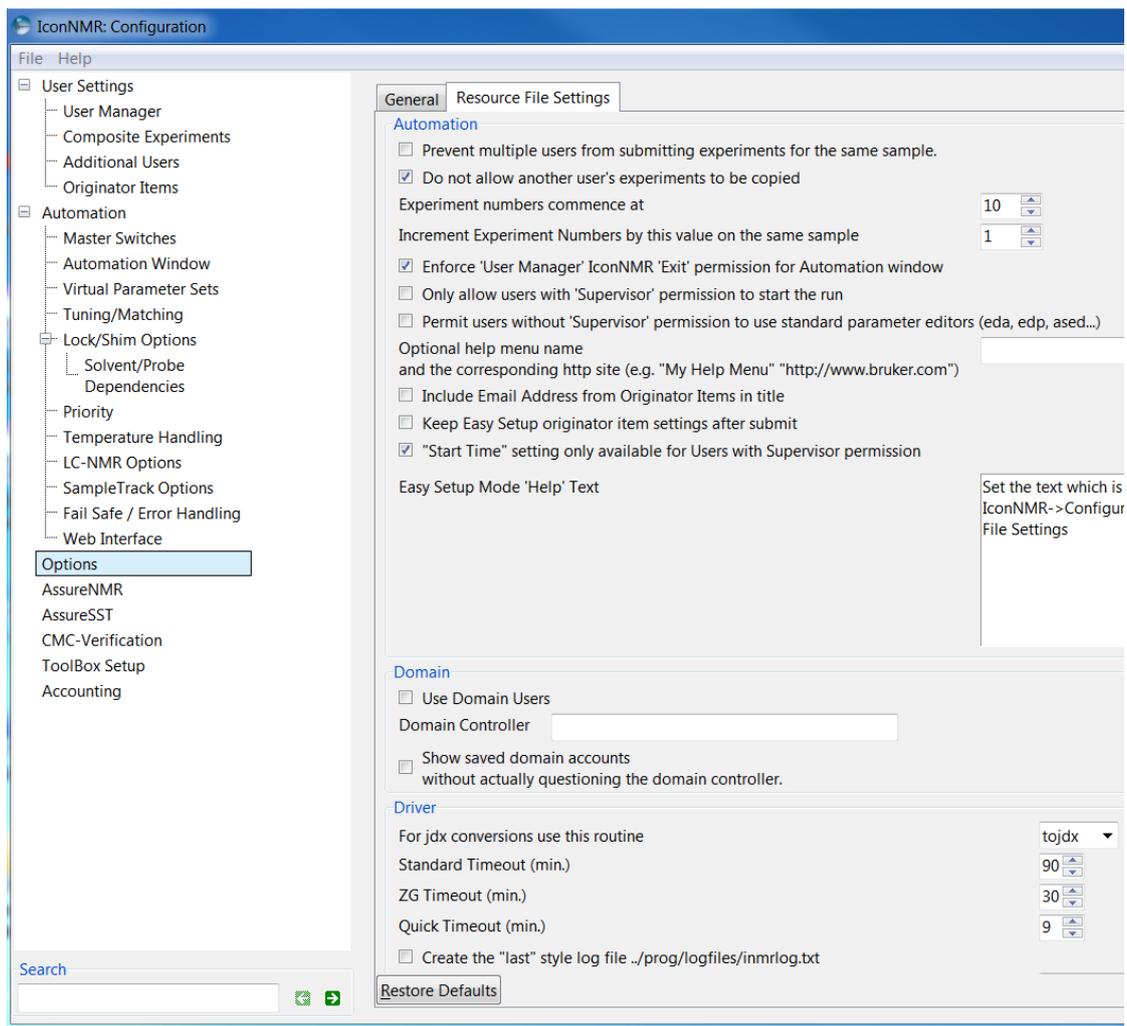


Figure 6.20: IconNMR Configuration - Resource File Settings

- IconNMR settings are important for InsightMR to work correctly. The user can either decide to restore default settings or check that all IconNMR settings are adequate for the use of InsightMR.
- To restore defaults, click on **File/Restore Defaults/Flow Tube (InsightMR)**.

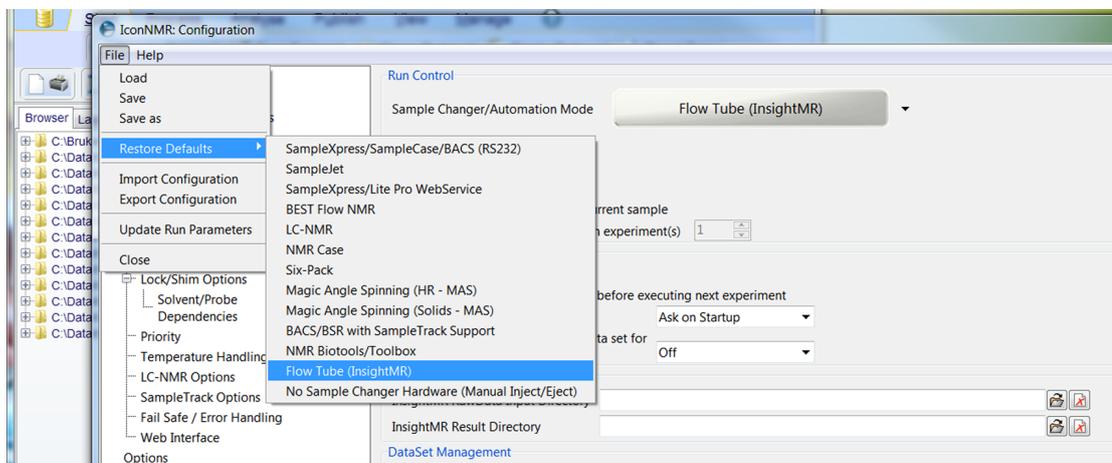


Figure 6.21: Restoring the Default Settings

6.6.2.1 Recommended Settings

This section lists the recommended settings to work with InsightMR software and flow unit.

Automation / Master Switches

The **Eject last sample in queue** should be unchecked.

The **Never rotate the sample** should be checked.

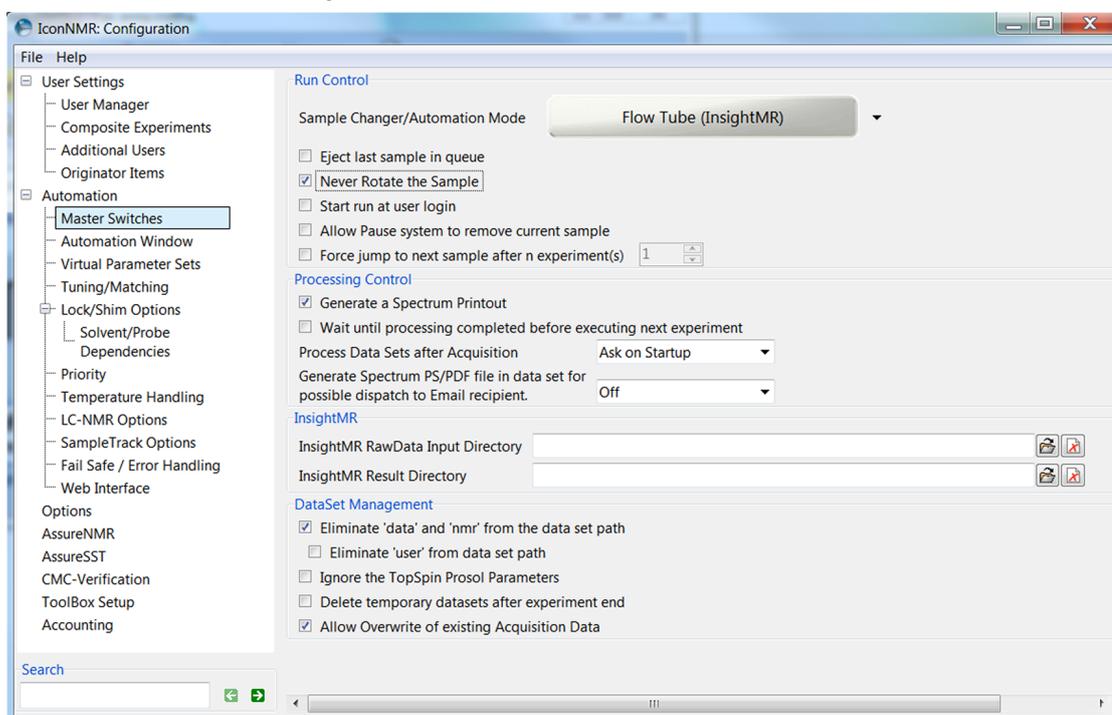


Figure 6.22: Configuring the Master Switches

Automation / Automation Window

The **Easy Setup Mode** should be checked.

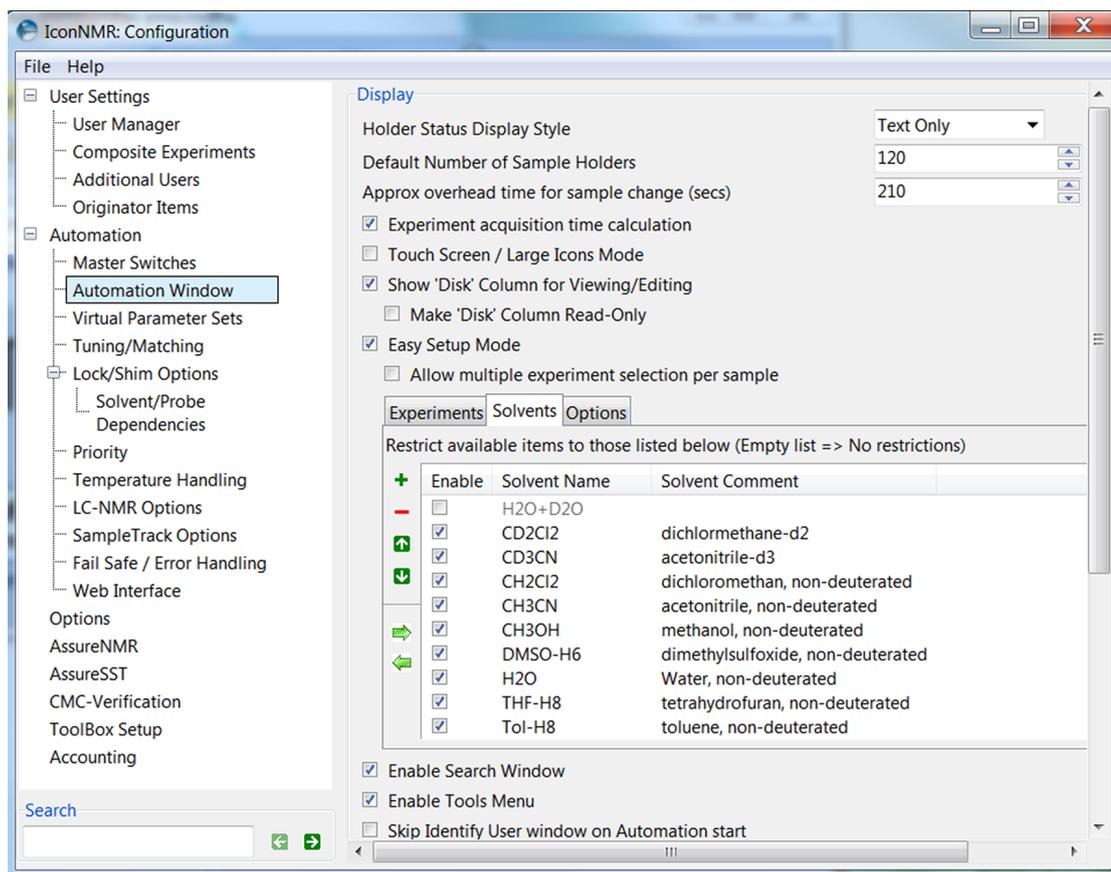


Figure 6.23: Configuring the Automation Window

Automation/Solvent/Probe Dependencies

Non deuterated solvents must have **XAU Ictshim flow** and **LOCK-OFF** as **Associated Shim** and **Lock Routine** respectively.

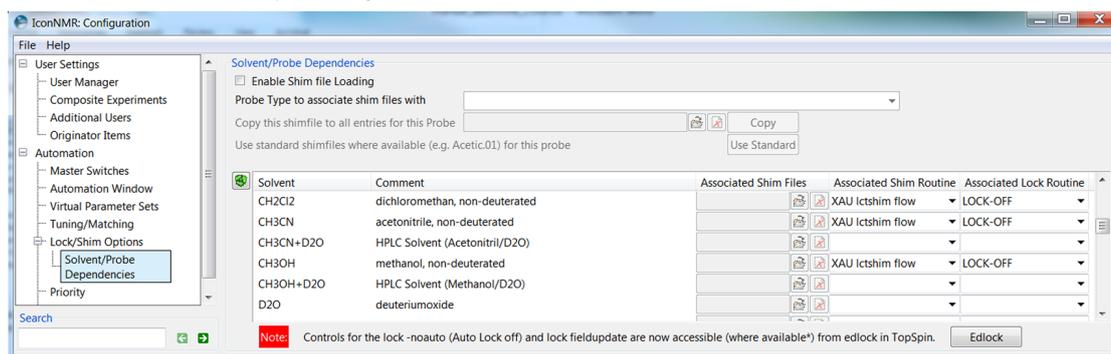


Figure 6.24: Selecting the Solvent and Probe Dependencies

Automation/Tuning/Matching

Set up the kinetic parameters so that the instrument only tunes and match after a solvent change.

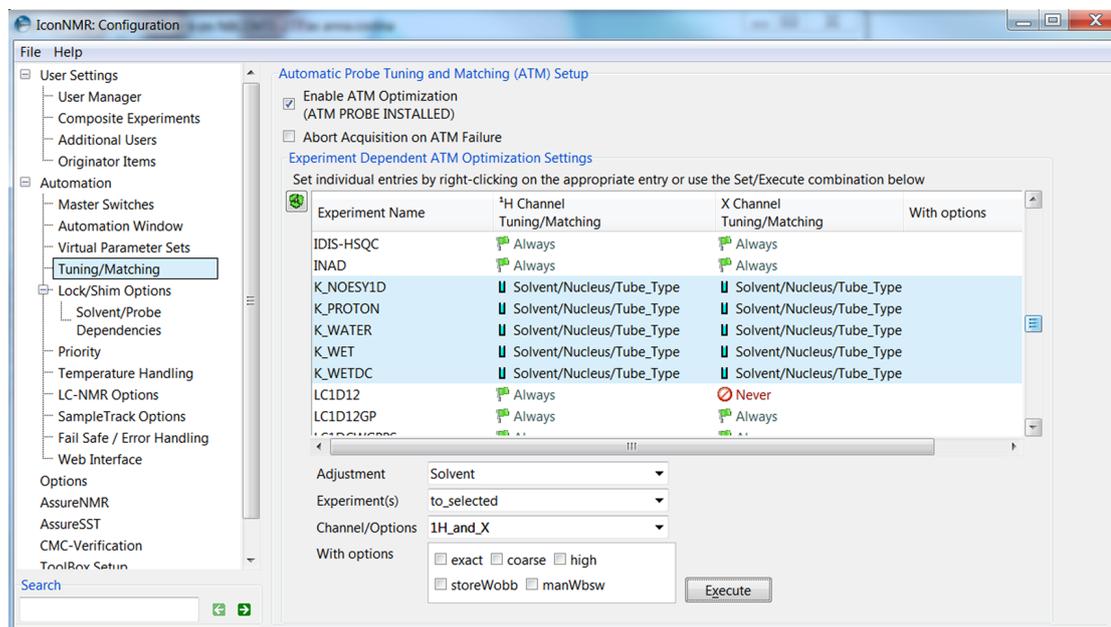


Figure 6.25: Selecting the Tuning and Matching Options

Settings for Solvents

Should protonated solvents (such as CH₂Cl₂, CH₃CN, DMSO-H₆) be missing from the Solvent tab in IconNMR shown below, follow the next steps.

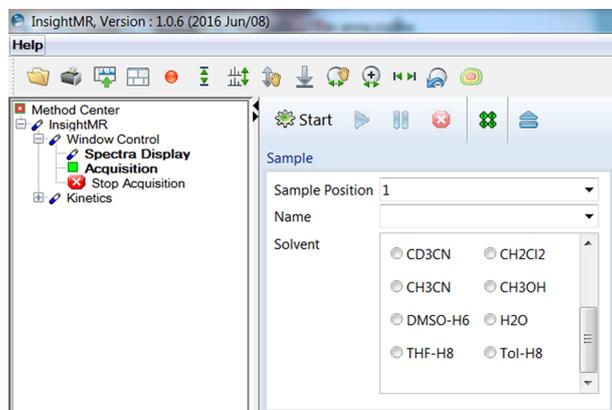


Figure 6.26: InsightMR Acquisition Window Expansion Showing the New Protonated Solvents

- Type **Edsolv** in the TopSpin command line to check whether those solvents are present in the solvent table.

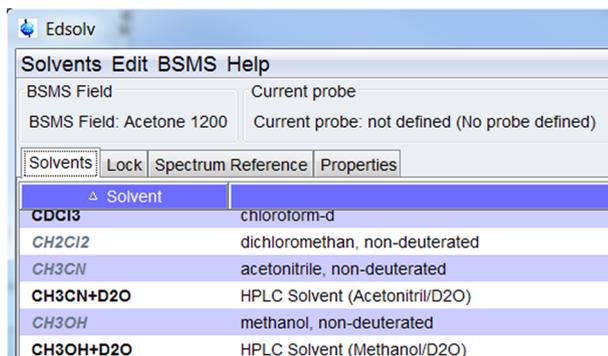


Figure 6.27: Edsolv in TopSpin

- If they are also missing from the solvent table, click on **Solvents**, select **Import Solvents** and import the new solvent file: C:/Bruker/TopSpinHOME/exp/stan/nmr/lists/solvents.xml.
- One could also select the **Restore Default Solvents** option, but this would DELETE any solvent previously defined by the user.
- Add the protonated solvents in the **Solvents** tab in IconNMR configuration **Automation / Automation Window** by clicking on the + sign and then selecting (check the box) the new added solvent.

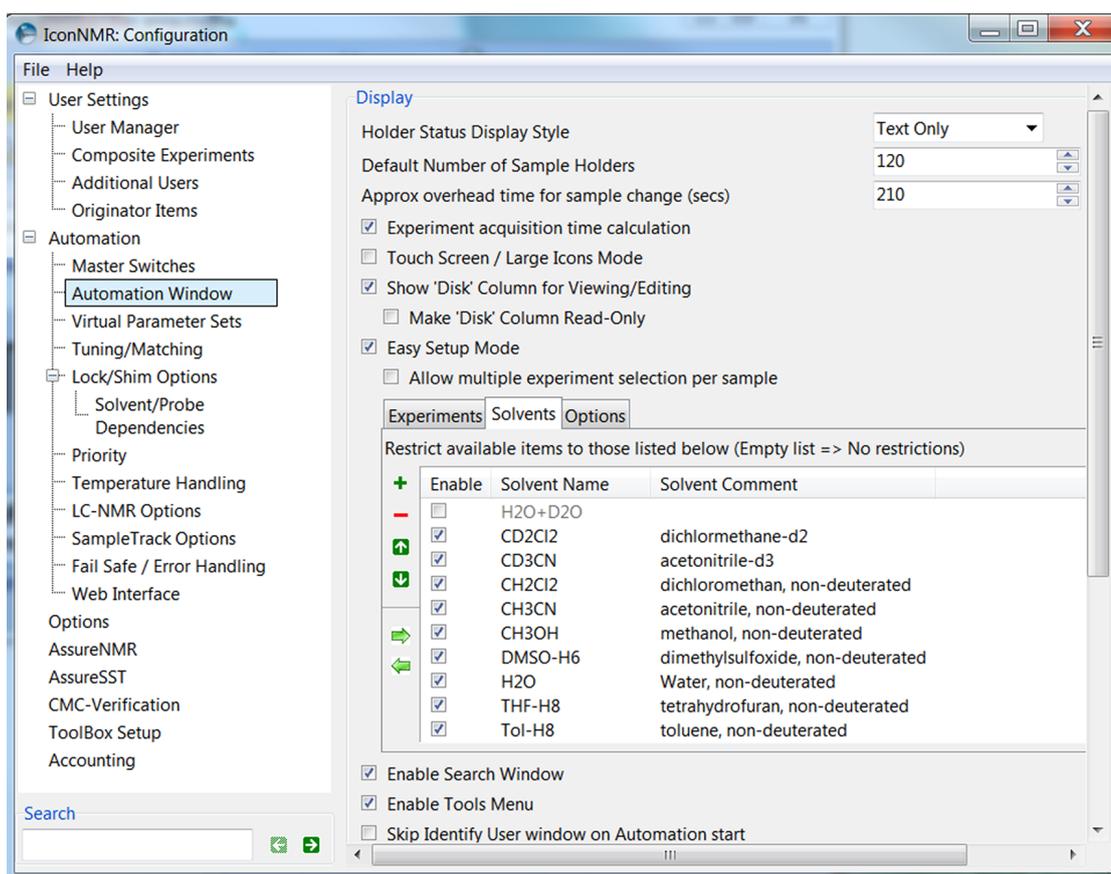


Figure 6.28: Solvents in the IconNMR Configuration

6.6.3 Adding a New Protonated Solvent

- Refer to the Edlock Guide (under the help button (?) / **Manuals** in TopSpin) to add the new solvent and its properties in the edlock table.
- Ensure the new solvent will also be shown in IconNMR.
- Non deuterated solvents must have **XAU lctshim flow** and **LOCK-OFF** as **Associated Shim and Lock Routine** respectively, as shown in the previous section.

7 Operation

Before using the flow unit, familiarize yourself with all the safety measures in [General Workplace Dangers \[12\]](#).

Before inserting and using the glass flow tube:

- Ensure there is no sample in the magnet.
- Ensure the NMR probe is at the desired temperature before inserting the glass flow tube.
- Inspect the flow unit looking for condensation, especially around the glass flow tube, tube holder and holder body. Wipe any observed condensation.

7.1 Inserting and Using the Flow Unit

- Carefully insert the flow unit assembly into the magnet and push it completely down. To ensure proper insertion, lift it 1 cm upwards and push it back down. You should feel a *solid* resistance.



Figure 7.1: Inserting the Flow Unit Assembly into the Magnet

- Fix the insulated transfer line to the top of the magnet using the transfer line holder or Velcro tape.

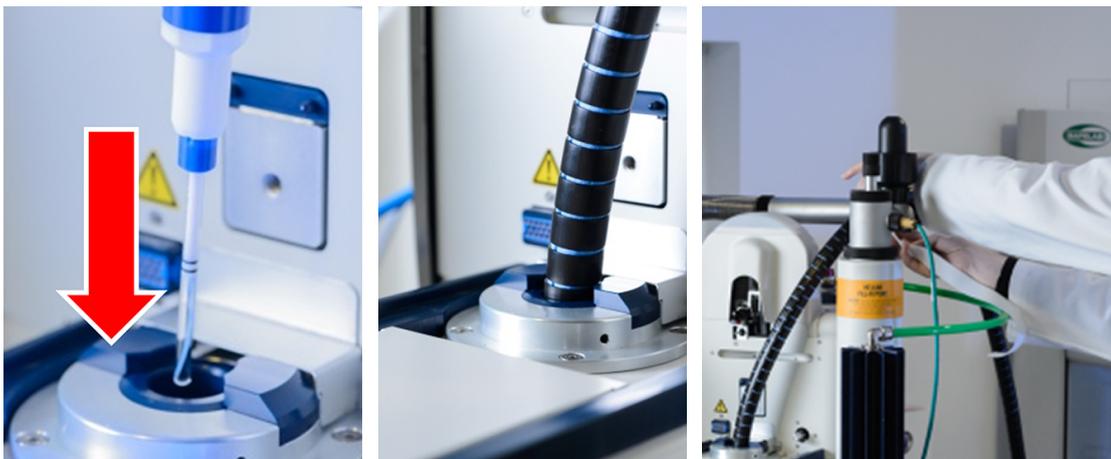


Figure 7.2: Mounting the Insulated Transfer Line

- Switch the pump on.
- Check that the solvent returns to the vessel and that the total volume remains stable.
- Check that the liquid level in the thermostat remains stable.
- Start the process to monitor (e.g. by adding the last reagent to the reaction mixture).

7.2 Acquiring NMR Data Using InsightMR Software

Upon installation of InsightMR, launch the program by clicking on the InsightMR desktop icon.



InsightMR 1.0

Refer to the InsightMR quick start guide under **Help - QuickStart** for instructions on how to use the software. Under **Help** there are also manuals for IconNMR and Dynamics Center, the foundation platforms of InsightMR.

Additional information, a video and an educational webinar can be found at our webpage: <https://www.bruker.com/insightmr>

NOTICE

Material damage to flow unit due to incorrect automation mode

Failure to set the **Sample Changer/Automation** mode to Flow Tube (InsightMR) may result in flow tube breakage.

- ▶ Set the **Sample Changer/Automation** to Flow Tube (InsightMR) in IconNMR configuration **Automation/Master Switches**.

7.3 Removing the Flow Unit for Storage in the Transport Box

To remove the flow unit for storage in the transport box when not being used:

- Rinse the sample line first with the reaction solvent, to avoid any compounds crashing out of solution, and then with any suitable cleaning/rinsing solution or solvent.
- When the InsightMR sample lines are blocked and do not allow flushing, replace the sample lines.
- Switch the chiller off.
- Disconnect the sample/solvent supply; connect a syringe to the outlet and empty the flow path by pushing air.
- Remove the flow tube assembly from the magnet.
- Place the flow unit on a table and temporarily secure it against any movement.
- Disconnect the inlet of the temperature control line from the chiller and empty the liquid through the outlet into the chiller. Flush with compressed air to speed the process up.
- Visually inspect the glass flow tube for damage, contamination and leaks. The glass flow tube must not show any cracks or damage and no solid particles should be visible. There should be no liquid behind the sealing O-rings. If necessary clean or replace the glass flow tube and/or the sealing O-rings.

7.4 Returning the Spectrometer to Normal Operation

To return the spectrometer to normal (non-flow) operation:

- Set the temperature of the NMR probe to the desired working temperature.
- Remove the holder from the BST (not for SampleJet).
- Remove the safety container that was placed underneath the magnet.
- Define the sample changer in the IconNMR configuration.
- Optional: Press the **Unhook** button shown below to disconnect IconNMR from InsightMR software, enabling the spectrometer to return to the standard data acquisition mode.



Figure 7.3: The Unhook Button

8 Flow Tube Assembly - Insertion Checklist

8.1 Prepare the NMR System

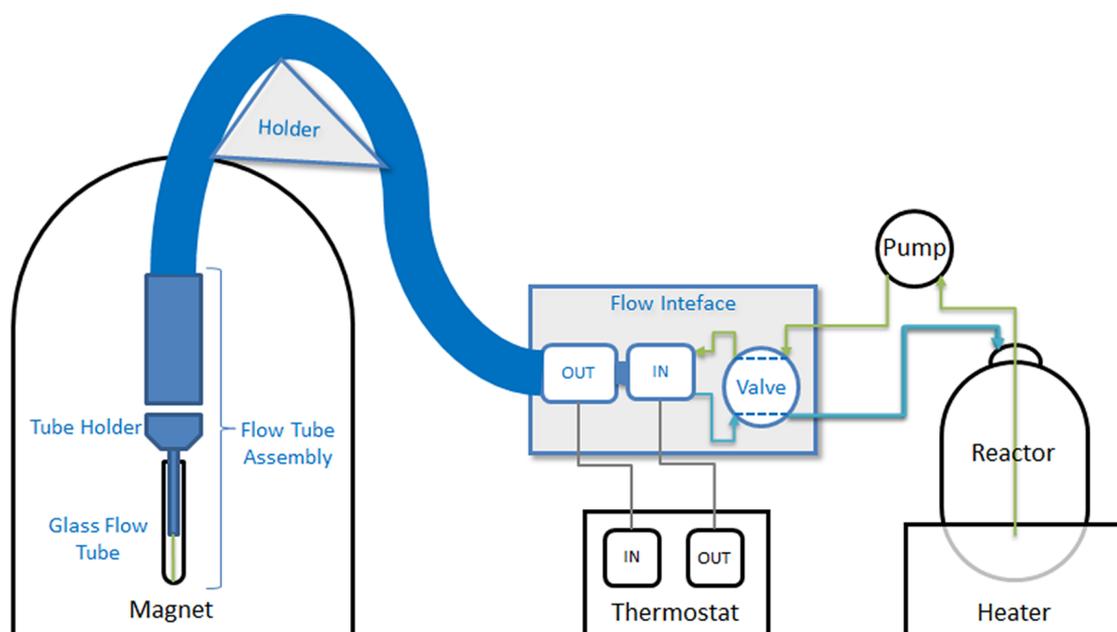


Figure 8.1: InsightMR Flow Unit Laboratory Setup

1. Launch InsightMR software.
2. Insert a standard 5 mm sample with deuterated solvent.
3. Run a K_PROTON experiment (optionally run a BESTPROFILE from TopSpin).
4. Remove the sample from the magnet.
5. Deactivate the sample changer if there is any.
6. Set the 'Sample Changer/Automation Mode' to 'Flow Tube (InsightMR)' in the IconNMR configuration.
7. Set the desired spectrometer temperature and leave the gas flow at least at 270 l/h in TopSpin.
8. Set the desired temperature parameters in InsightMR, IconNMR configuration.
9. Attach the transfer line holder to the Bruker Sample Transport (note the transfer line holder cannot be used with a SampleJet).

8.2 Prepare the Flow Tube Assembly

1. Secure the InsightMR flow unit (flow tube assembly, transfer lines and flow interface) against movements, with laboratory stands for example, ideally in a fume cupboard.
2. Inspect the flow unit, looking for damages, contamination and leaks. Clean or replace the glass flow tube and/or the sealing O-rings, if necessary.
 - The glass flow tube must not show any cracks or damages.
 - No solid particles must be visible in the glass flow tube.
 - No liquid must be visible behind the sealing O-rings.

8.3 Connect the Temperature Control Equipment (Optional)

1. Connect the thermostat to the in/outlet of the temperature control line.
2. Set the thermostat to the target temperature; start it and wait for the desired temperature to be reached.
3. Ensure that at the set temperature the sample or reaction mixture is in solution.
4. Ensure that the set temperature is in the recommended range for the probe and the flow unit.
5. Verify that the thermostatic liquid returns to the thermostat. Ensure that the liquid level remains stable.
6. Check for leakages at the upper part of the tube holder.
7. Check that no liquid appears at the outlet of the transfer line (both sample lines and temperature control lines). Ensure that the thermostatic liquid does not leak into the sample line.

8.4 Connect the Sample Supply (Reactor or Equivalent)

1. Connect the sample supply (reactor or equivalent) to the pump and the pump to the inlet of the flow interface.
2. Connect the flow interface valve output back to the sample supply or to waste.
3. Set the pump to the highest planned flow rate.
4. Add solvent to the sample supply (reactor); start the pump and check the flow rate at the outlet.
5. Check for leakages along the flow tube assembly paying close attention to all O-rings and seals in the glass flow tube.
6. Check that there are no bubbles in the glass flow tube.
7. Test the desired experimental conditions (temperature, pressure, reaction mixture) outside the magnet first.

8.5 Insert the Flow Tube Assembly

1. Temporarily switch the sample flow off.
2. Inspect the flow tube assembly and the transfer line. Remove any condensation from the outside of the glass flow tube, the tube holder and the holder body.
3. Hold the flow tube assembly; insert it in the magnet and carefully push it down until the glass flow tube seats on the probe. To ensure proper insertion, lift it 1 cm up and push it back down. You must feel a “solid” resistance.
4. Optionally acquire a BESTPROFILE and compare the result to that obtained from a standard 5 mm sample.
5. Switch the sample flow on.
6. Fix the transfer line to the holder on top of the magnet or use ‘Velcro’ tape to secure it.
7. Block the path where the transfer line is installed to ensure that the transfer line is not a tripping hazard.

8.6 The System is Ready to be Used

Refer to the InsightMR software quick guide (provided or under InsightMR help menu) for a quick start.

9 Flow Tube Assembly - Removal Checklist

9.1 Prepare the Flow Tube Assembly

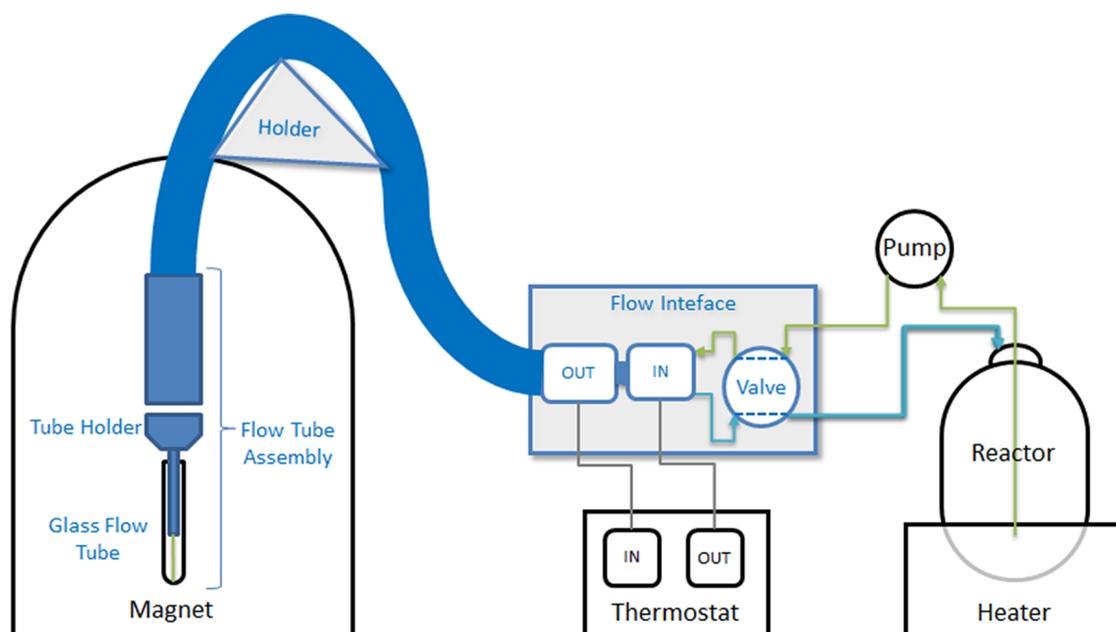


Figure 9.1: InsightMR Flow Unit Laboratory Setup

1. Stop the sample flow.
2. Rinse the sample line with a suitable solvent and switch the flow off.
3. Set the thermostat to ambient temperature; wait until the temperature is reached and switch the thermostat off.

9.2 Remove the Flow Tube Assembly

1. Remove the flow tube assembly from the magnet.
2. Secure the flow tube assembly and transfer lines to a clamp stand, ideally in the fume cupboard.
3. Disconnect the sample supply; connect a syringe to the outlet of the sample line and empty the flow path by flushing the lines with air.
4. Disconnect the inlet of the temperature control line from the thermostat and empty the liquid through the outlet into the thermostat.
5. Visually inspect the flow tube assembly looking for damages, contamination and leaks. Clean or replace the glass flow tube sealing's O-rings if necessary.
 - The glass flow tube must not show any cracks or damages.
 - No solid particles should be visible in the glass flow tube.
 - No liquid should be visible behind the sealing O-rings.

9.3 Storage

1. Close the inlet of the sample line to protect it against dust and dirt.
2. Leave the glass flow tube connected to the tube holder and insert it into the flow tube protector to protect it against damage.
3. Coil up the transfer line and place the system into the original transport box.

9.4 Prepare the NMR System

1. Activate the sample changer.
2. Set the temperature of the NMR probe and the gas flow back to normal values.
3. Remove the transfer line holder from the Bruker Sample Transport (note the transfer line holder cannot be used with a SampleJet).
4. Define the sample changer in InsightMR/IconNMR configuration.
5. Select the desired user in InsightMR/IconNMR part.
6. Optional: press the **Unhook** button to disconnect IconNMR from InsightMR software.



9.5 The system is ready for normal usage

10 InsightMR Glass Flow Tube Exchange Instructions

10.1 Removing the Glass Flow Tube

Note: Use lint free gloves to keep the glass flow tube clean.

Important: Be aware that the glass flow tube is made out of thin walled glass and is very fragile! Take all required precautions to avoid breakages and injuries. Avoid scratches or dirt on the surface or inside the glass flow tube.

Follow these instructions to safely remove the glass flow tube from the tube holder:

- Turn the twist cap 90°.



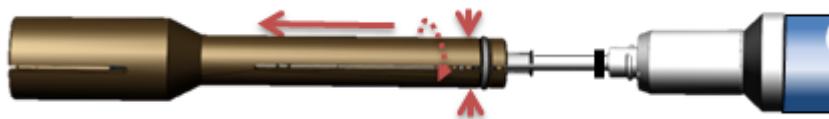
- Pull it off the glass flow tube together with the O-ring 5x1.



- Use the flow tube protector to pull the glass flow tube off the tube holder. Slide it with the O-ring in front, close to the glass flow tube.



- Squeeze the flow tube protector gently at the front: turn it a bit and pull the glass flow tube straight off. Avoid bending the rod of the tube holder, as the tube may break.



- Inspect the two O-rings 5x1 looking for damage. Replace them if it is required.

10.2 Mounting the Glass Flow Tube

Note: Use lint free gloves to keep the glass flow tube clean.

Important: Be aware that the glass flow tube is made out of thin walled glass and is very fragile! Avoid scratches or dirt on the surface or inside the glass flow tube!

Follow these instructions to safely mount the glass flow tube on the tube holder:

- Insert an O-ring 5x1 over the tube holder rod. Insert another O-ring 5x1 over the glass flow tube.



- Insert the glass flow tube in the flow tube protector. Squeeze it gently until you feel some friction and push the glass flow tube with a slight turn over the two O-rings of the tube holder rod. Push the tube with the tool to the far end. Avoid bending the rod of the tube holder, as the tube may break. Release the pressure on the flow tube protector and remove it from the glass flow tube.



- Push the twist cap to the far end of the tube. At this moment the markers on the twist cap and the tube holder must be in the opposite direction (180°).



- Lock the twist cap by turning it 90°.



Note: Now the position of the markers on the twist cap and the tube holder must match (0°). Only then will the glass flow tube be locked securely.

- Mount the tube protector so that it protects the glass flow tube.



11 Dismantling and Disposal

Following the end of its operational life, the device must be dismantled and disposed of in accordance with the environmental regulations.



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.

11.1 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.

11.2 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**

11.3 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.

12 Technical Data

NMR System Requirements

- 5 mm probe.
- 300-950 MHz magnet.
- AVIII console if InsightMR software is to be used (compatible with TopSpin 3.5pl2 and above).

Data Acquisition and Analysis

It is highly recommended that InsightMR software (refer to the InsightMR release letter) is used for data acquisition and analysis.

Recommended Temperature Range

The range in which temperature loss was measured is -5 °C to +60 °C. Temperature loss using a thermostat type like the Julabo FE25-HE at -5 °C is < 4 °C and at +60 °C is < 2 °C (remark: the loss is very dependent on the flow-power a thermostat can create, therefore these numbers are based on the thermostat type we recommend).

The unit can be used at a wider range of temperatures according to the recommended working temperatures of the wet materials, probe, pump and chiller.

Recommended Pressure

The recommended pressure is < 10 bar.

Wetted Materials for the Sample and Temperature Control Lines

Wetted materials for the sample lines are glass, PTFE (Teflon®) and FFKM (Kalrez®).

Wetted materials for the temperature control lines are PTFE (Teflon®), PEEK, POM (Delrin®).

Note: The temperature control line's wet material only come in contact with the thermostat liquid.

13 Contact

Manufacturer

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<http://www.bruker.com>

WEEE DE43181702

NMR Hotlines

Contact our NMR service centers.

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

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

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

Phone: +49 721-5161-6155

E-mail: nmr-support@bruker.com

Applications Support

E-mail: InsightMR@bruker.com

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