

BEST -NMR 215 Liquid Handler Installation and Users Manual

Version 211201

Order No. H9330

User's Guide

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1 Introduction

Safety precautions

- For safe and correct use of this instrument, it is recommended that both operating and service personnel follow the instructions contained in this guide when installing, cleaning and maintaining this instrument.
- Because the needle installed on the Z-drive may contain a dangerous substance, do not interfere in the work area of the instrument until the liquid handler has completed its procedures. If dangerous liquids are used, adequate protection such as proper ventilation, safety glasses, etc., should be used.
- Always switch the power to off when making adjustments to the liquid handler. The potential exists for bodily harm if you interfere with the work area of the instrument while it is running.

Description

The BEST 215 Liquid Handler is an XYZ robot that can automate any number of manual liquid handling procedures. The liquid handler's ability to pierce thick septa allows access to samples in clinical sample tubes without exposing the user to biological hazards. The built-in dilutor provides for the accurate and precise handling of liquids.



Unpacking

The 215 Liquid Handler is delivered with all major components already assembled except for auxiliary parts such as the Z-drive, probe, racks, tubing, etc. Keep the original container and packing assembly, at least as long the warranty is valid, in case the liquid handler has to be returned to the factory.

The 215 Liquid Handler and its components are shipped in several containers:

- One box contains the 819 Valve Actuator
- One box contains a set of vials and the capillary set, as well as the 10 m serial cable
- The biggest container holds the 215 Liquid Handler.
 - The container inside the 215 Liquid Handler box holds the auxiliary items, such as locator plate, tubing, probes, syringes, rinse inserts, Z-drive, and any other accessories like the rack code 211 you may have ordered with your system.

To remove the liquid handler from its container:

- 1. Cut the metal strapping.
- 2. Lift the outer box off and away from the liquid handler.
- 3. Lift the inner box off and away from the liquid handler.
- 4. Lift the unit off its base platform and place it on a lab bench or cart. Gilson recommends that two people lift the liquid handler off the base of the packing container. Do not lift or handle the 215 by the XY arm ! To lift the liquid handler:
 - a) Using the two cutouts for hand holds, place a hand at the base of the packing container.
 - b) Grip the liquid handler under the base plate.
 - c) Lift the unit up and out of the foam packing material. The side containing the electronics cabinet is the heavier side.

!! Do not attempt to lift the instrument from the XY-arm (the horizontal arm). Always lift the instrument from its base.

Standard Equipment

Once the liquid handler and the accessories containers have been unpacked, you should have the following:

Reference	Description
H9376	215 unit with dilutor
	Locator plate with one drain base (includes 4 mounting screws)
	Rinse drain package which includes : • 2-liter waste bottle • Cap with quick connect fitting • Rinse station with fittings • 5 feet of Tygon waste tubing with quick connect fitting
	125 mm Z-drive and control cable with retaining clip
	 Accessory package which includes : Fuse drawers, fuses, and power cords 10-pin terminal block 8-pin terminal block 9/64" ball driver for removal of armlock 8 tubing retaining clips Cable support rod with bracket and 2 Phillips-head attachment screws Level sensing cable Tubing support rod Dilutor valve and vent tubing
	 Inlet tubing package which includes: 1/4"-28 coupler PTFE inlet tubing (650 x 3 x 2 mm) with 20 µm stainless steel filter
H9303	BEST-NMR 215 Liquid Handler Manual 819 Valve Actuator with 7000 valve mounted Rack 211H
Accessories (H9437)	Based upon your configuration, you'll also receive additional accessories, such as the probe, dilutor syringe, transfer tubing, fittings, 211H bottles with caps and septa, racks, etc.

In Appendix A you will find a detailed list of spare parts and accessories.

Customer service

If you need assistance, please contact your Bruker representative. You can also contact the BEST-NMR group via its e-mail address: <bestnmr@bruker.de>. To help us serve you quickly and efficiently, please refer to the "**Before Calling us**" section 6 under "Repair and Return Policies" on page 81

Technical data

The following specifications are subject to change without notice.

The following information is subject to change without notice.

- Warning: Changes or modifications to the Liquid Handler not expressly approved by Bruker could void the user's authority to operate the Liquid Handler.
- **Note** : The Liquid Handler has been tested and found to comply with the limits for a Class A digital device, pursuant to Part 15 of the FCC commercial environment. The Liquid Handler generates, uses, and can radiate radio frequency energy and, if not installed and used in accordance with the instructions, may cause harmful interference to radio communications. Operation of the Liquid Handler in a residential area is likely to cause harmful interference; in which case, the user will be required to correct the interference at the user's own expense.

Shielded cables must be used with the Liquid Handler to ensure compliance with the Class A FCC limits.

manufacturing standards	Safety certification:
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- **CE** UL 1262
- • CSA C22.2 No. 151
- • EC 1010-1

EMC certification:

- • EN 50082-1
- • FCC Class A

EMI certification:

- • EN 50081-1
- **sampler type** XYZ robot with stationary rack design
- **pumping system** Integral high-precision single piston dilutor pump

dilutor syringe capacity 5000 µl,

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(100, 250, 500, 1000, 10000 or 25000 μl available from the local Gilson distributor)

front panel	8-cha	3-character display, Start and emergency Stop soft keys		
and precision Separate Se		Appendix C fo dure that Gils olumetric acc nums. Under	to Gilson Inc. USA) or details about the configuration and test on used to determine the limits below. uracy and precision listed are most circumstances, you can expect urpasses these specified limits.	
 Open bottle to open 50 µl A = 0 500 µl A = 0 	.25%, 0	CV = 0.38%		
 Sealed tube to ope 50 μl A = 2 500 μl A = 1 	.0%, C	V = 0.63%		
carryover	sensi		m-piercing probe (capacitive, level- ppendix C for information on the method carryover.	
liquid level sensing			uctive (currently 12.2001 not supported in ider development)	
needle rinse	outsic Optio	le of the need	ed rinse station for rinsing the inside and lle; selectable rinse volume and flow rate. level sensing, non-level sensing and	
probe positioning performance	Acc	uracy:	+/- 0.5 mm in X/Y dimensions +/- 1 mm in Z dimension	
	Rep	eatability:	+/- 0.25 mm in X/Y/Z dimensions	
arm speed			ec (> 18 in/sec) in X dimension ec (> 16 in/sec) in Y dimension	
vertical punch strength		4.9 kg (11.0	lb)	
horizontal motion strength		X: 5 kg (11.1 Y: 7 kg (15.6	,	

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rack capacity	Up to five code 200-series racks, up to seven code 20- or 30-series racks, or a combination of up to five racks of both types		
control	omputer control via RS-232 with Bruker-BEST-NMR Software		
electrical control	4 inputs (contact closure, TTL or open-collector), 4 relay outputs, and one switched +24 V DC, 1 A output		
power requirements	Frequency: 50/60 Hz Voltage: 100-120 V or 220-240 V; mains voltage fluctuations not to exceed ±10% of the nominal voltage Current rating: 2.0 A for 100-120 or 1.0 A for 220-240 V		
environmental condition Altitude: Temperature range Air pressure: Pollution degree: Humidity:	Up to 2000 m		
dimensions (w x d x h)	91.4 x 61 x 55.8 cm (36 x 24 x 22 in)*		
	Maximum height. Z-drive (vertical arm) height is adjustable to accommodate vessel heights between 1 and 150 mm (dependent on installed Z-drive).		
weight	39.9 kg (89 lb)		

2 Installation

Liquid handler setup



This section takes you through the steps for setting up your 215 Liquid Handler.

Locator plate installation

The locator plate serves two functions:

	rinse station base	
0		0
0		0
	holes to secure locator plate	ſ

1. Positions the racks and accessories that fit onto the bed of the liquid handler.

2. Contains liquid spills, such as those caused by overflowing vessels.

The locator plate and its four mounting screws are shipped in a separate box with the liquid handler's accessories. To install the locator plate onto the instrument bed : BEST- NMR Installation and Software Manual –Version 21.12.01

- 1. Make sure the locator plate's rinsing station base is at the rear of the instrument. (The locator plate will only install in this orientation.)
- Align the four corner holes of the locator plate with the four holes on the instrument bed and lower the plate onto the bed.
- Using a Phillips-head screwdriver, secure the locator plate using the four mounting screws.

Note: If you purchased the optional 6-position locator plate (Gilson Reference Number 25045513), the rinse station base is in the center rear of the locator plate.

Armlock removal

- The armlock on the liquid handler secures the Y-arm during shipment. You must remove the armlock prior to installing the Z-drive and operating the instrument. If the armlock is not removed, the liquid handler cannot move in the X direction. This results in an error state during operation.
- If you need to move the liquid handler, always re-install the armlock. This safeguards against mechanical damage.

To remove the armlock:

1. Remove the cardboard label in front of the armlock.



2. Using the 9/64" ball driver, loosen the tensioning screw that immobilizes the Y-arm.

3. Using the 9/64" ball driver, remove the two remaining screws that hold the armlock in place.

4. Remove the armlock and store it and the ball driver for future use.

Z-drive installation



Follow these steps to install the Z-drive:

1. Using a Phillips screwdriver, loosen the mounting screw on the Z-drive mounting bracket located on the Y-arm. Turn counterclockwise to loosen.

2. Partially pull out the bracket. Do not remove completely.

3. Place the Z-drive into the mounting bracket. You will need to insert one side of the Z-drive into place at a time.

4. Tighten the screw on the mounting bracket until the Z-drive is secure.

You'll adjust the Z-drive to its proper height after rack and rinse station installation. This adjustment is described on page 20.





Installing the Z-drive

Using the two Phillips-head screws, attach the cable support

Cable support rod

rod bracket in the holes located in the rear of the X-arm extrusion.

Plug the Z-drive control cable into the back topside of the control cabinet. The control cable should be tucked into the groove located in the top of the X-arm extrusion. The retaining clip that is already on the control cable should be snapped onto the top of the cable support rod. Refer to diagram at top of next page.

The control cable is correctly installed when the arm is extended to the extreme X and Y direction and the cable has enough slack.

Probe installation

There are different probes available for use on the 215 Liquid Handler. Depending upon your application, you have purchased the appropriate probe and probe holder/guide kit. BEST –NMR is already equipped with best suited probe for high throughput and septum piercing. When installing the probe, probe holder and probe guide, refer to the following procedures and diagram that shows where they are installed on the liquid handler.



Installing the probe guide

The probe guide is installed on the top of the Z-drive foot.

1. Place the probe guide into the opening in the top of the foot.

2. Use the two Phillips-head screws to secure the probe guide to the foot.

Installing the probe holder

To install the probe holder, screw it into the bottom of the isolation probe holder.

Installing the probe

Insert the probe into the top of the isolation probe holder and pull it through the holder until the tip of the probe is in the probe guide.

Installing the level sensing cable

(currently 12.2001 not supported under BEST, but under development)

- Plug the quick connector into the socket located on the Z-drive.
- Remove the screw from the right side of the isolation probe holder, install the ringtongue connector onto the screw, and re-attach the screw to the isolation probe holder.

Syringe installation

Your liquid handler has a built-in dilutor, and the piston operating rod will be shipped in the down position. If the rod is not in the down position, please refer to the instructions on changing a syringe in *Section 4*. Those instructions detail how to lower the rod.

The following procedure is important for correct syringe piston alignment. Improper alignment may cause premature piston seal failure.



7. Fully tighten the syringe to the valve.

1. Remove the valve and syringe from their packages.

2. Lubricate the piston with diluent in order to reduce piston seal friction during syringe installation.

3. Loosely screw the syringe into the valve. Do not fully tighten.

4. Loosely attach the valve to the dilutor with the supplied screws.

5. Pull down the piston so it comes into contact with the piston operating rod and firmly tighten the piston holding screw.

6. Fully tighten the valve screws to secure the valve.

Note: Remember the size of the syringe you are installing for later software configuration. (the standard size for BEST-NMR is 5000 μl) See Configuring the liquid handler in Section 3, page 29.

Plumbing connections

Inlet and sample loop installation

For the dilutor, you received inlet tubing and a sample loop. (For the detailed size and length of tubing refer to Appendix D)



1. Install the 1/4"-28 fitting of the 2 mm ID tubing (Gilson Reference Number 3645357) to the inlet side of the dilutor.

2. Place the filtered end of the assembly into the bottle containing your diluent or probe rinse solution.

Note: If you need to shorten your inlet tubing, remount the

filter, cut the tube with a proper cutter, fit it through the bottle cap and replace the filter

- 1. Snap three tubing retaining clips onto the tubing support rod. Equally space the clips.
- 2. Install the tubing support rod in its brackets on the control cabinet. Insert the front end of the rod into the hole before placing the back end of the rod in its cradle.
- Connect the sample loop (3000 x 1.0 mm ID 1/16"FEP tubing) between the port on the dilutor valve (see above) and port 6 of the 819 loop valve actuator (address ID29) using a long UNF 10/32 fitting. (Refer to diagram shown in Appendix D)
- 4. Gather any excess tubing into a coil to minimize the length of tubing and secure the coil using a twist tie. Position the excess tubing in a convenient location near the rear of the liquid handler.



Needle tubing installation

Snap three tubing retaining clips onto the Z-drive control cable. Equally space the clips.

1. Snap the tubing into the small grooves on the clips installed on the Z-drive control cable.

Note : You can thread the capillary through before mounting the fittings.

2. Connect one end of the needle tubing $(1300 \times 0.8 \ 1/16"$ FEP) to the loop valve port 1 using a short UNF 10/32 fitting. Finger-tighten. (Refer to diagram shown in Appendix D)

3. Connect the other end to the top of the isolation probe holder. Firmly tighten this fitting since it holds the probe in place.

Valve tubing installation

Use the precut capillaries and follow the scheme shown in Appendix E.



Rinse station and drain waste tubing installation

You'll clean the probe using the rinse station. To eliminate carryover of liquids, the rinsing procedure pumps excess diluent or probe washing solution through the probe and out into the rinse station. The small diameter of the rinse station inserts allows both the outside and the inside of the probe to be washed thoroughly.

There are three different types of rinse station inserts available from Gilson.

The rinse station insert for BEST-NMR is a deep pocket insert - This is a closed bottom rinse insert mainly used for non-level sensing applications. This type of insert allows for a deeper insertion of the probe into the rinse well resulting in a greater area of the outside of the probe to be rinsed. It may be necessary to vary the types and volumes of probe wash solutions to most efficiently eliminate carryover of particular compounds. Generally, the smaller the volume of probe wash solution used, the faster your automated liquid handling protocol.

Installing the rinse station

The base of one rinse station is shipped already secured to the rear of the locator plate.



rinse station

base

rinse station Before installing the rinse station, make sure the locator plate has been properly installed with the rinse station base to the rear.

Install the rinse station so that its tube fittings are pointing toward the rear of the liquid handler. That orientation is the one shipped from the factory.

To install the rinse station housing onto the base, follow these steps:

- 1. Align the triangle of the housing to the base.
- 2. Insert the housing into the base.

3. Press down and turn 60 degrees. The rinse station is secure when you feel the housing snap into place.



waste tubing

fittings

4. If you are satisfied with the standard orientation, follow steps 6, 7, and 8.

5. You may need to change the orientation if the current location of the waste tubing fittings will obstruct the installation of non-standard racks or other accessories.

6. Install the rinse station insert by pressing the insert down into the housing until it snaps into place. The top of the insert should be level with the rim of the housing.

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Note! It will be easier to push the insert into the rinse station by greasing the O-rings slightly with e.g. laboratory Silicon grease or a film of machine oil!

- 7. Connect the Tygon waste tubing to the rinse station housing by twisting the tubing onto the fittings on the rinse housing until secure. To be on the safe side you can also use the clamps in addition to secure the hose.
- 8. The Y-piece out of the capillary kit can be used to fit in directly behind the drain. The upper open end can then be used as an inlet for the waste capillaries coming from the 819 Valve Actuator.
- 9. Connect the other end of the Tygon waste tubing to the two-liter waste bottle. The waste bottle lid has a matching quick connect fitting that mates with the tubing's quick connect fitting.
- **Note!** Make sure the waste bottle is placed in a location that is lower than the instrument bed of the liquid handler and the that the waste hose will not build a knee, but will always descend.

Rack setup

The 215 Liquid Handler is equipped to locate code 200 racks. See *Appendix A* for a list of racks available for the liquid handler. For BEST – NMR all the 200 series racks are recommended.

Depending on the racks you're using, refer to the appropriate procedures below.

code 200-series racks

If all your racks are code 200-series, place them directly onto the locator plate:

- 1. Orient the rack so that the code number (e.g. 216) is facing forward.
- 2. Fit the rack on the locator plate so that the slots and holes on the underside of the rack align with the pins on the locator plate.
- **Note!** The Washing Rack (211, 304B or 306B) is always in the very left position on the 215 working bed. Its function is for cleaning and washing procedures and the software is expecting it in the first holder position. Using the closed injection port solution will give this position free for placing a sample rack.

Final Z-drive adjustment



Follow these steps to adjust the Z-drive to the proper height.

1. Move the arm to the **center** of its working field.

2. Loosen the mounting screw on the Z-drive mounting bracket until the Z-drive can slide up and down. Refer to diagram on page 13 for location of the mounting bracket, if necessary.

3. Slide Z-drive and adjust to proper height. The Z-drive should be set at a height of 125 mm. Use the supplied

cylindrical distance tube to adjust the proper height. Slide the mounting bracket to the front and place the distance tube directly underneath it. Turn the Z-drive into the mounting bracket and let it stand on the tube.

4. Tighten the screw on the mounting bracket until the Z-drive is secure.

Note! Be aware that with the bar code reader the delivered distance tube for 127 mm should be used to ensure the proper use of the 205B code racks.

Note! Changing the height will impact the entire system and has to be set in the hardware configuration in the BEST-NMR software to the proper value.

Electrical connections

Rear panel



- 1 Input/Output (I/O) ports
- 2 Gilson Serial Input/Output Channel (GSIOC) port
- 3 Keypad port
- 4 RS-232 port
- 5 Fuse drawer
- 6 Power switch
- 7 Power input socket
- 8 Unit ID selector
- 9 Baud rate/mode selector

Input/Output ports

You can use the input and output contacts found on the rear panel of the liquid handler to control peripheral devices.

Contact inputs

The input barrier strip of the liquid handler has 8 connections. All of the inputs are paired, and each pair include a GROUND reference.

The contact input pairs are labeled A, B, C, and D.

A contact is connected if it has a short across the input or is held low by a TTL output or other device.

• Never connect voltages higher than 5 V DC to an input. When using TTL signals, be sure to match GROUND connections.

Contact outputs

- The output barrier strip has 10 contacts.
- Pins 1 and 2 supply a +24 V DC output.
- Do not use this output unless the receiving device can accept 24 V power.
- Pins 3 through 10 are paired, isolated-relay contact closures and are labeled 1, 2, 3, and 4.

Items you'll need

To make connections, you'll need the following:

- 2-conductor cable (22 30 gauge for each wire)
- wire insulation stripper
- small-blade screwdriver

Making connections

To prepare and make connections with the 2-conductor cable:



1. Cut the cable into pieces of appropriate length.

2. Strip about 0.25 cm of insulation from each end of the cable.

3. Remove the barrier strip from the liquid handler.

4. Insert each wire into the appropriate slot on the barrier strip.

Note: When making connections, be sure to maintain the correct orientation of the barrier strip relative to the port.

Push the wire all the way in; then tighten its corresponding pin screw.

5. Re-connect the barrier strip to the liquid handler. The wires will be facing left and the pin screws will be facing you as you look at the rear of the instrument.

Push the barrier strip in as far as it will go. It is designed to fit snugly into its receptacle.

- 6. Connect the opposite ends of the wires to the other device(s). Be sure to match ground connections.
- 7. Label each cable to identify the purpose of the connection.

RS-232 port

The RS-232 port is used to transfer information between the liquid handler and a computer. For the location of the RS-232 port, refer to the diagram on page 21

Be sure your computer is turned off before making any connections.

To connect your computer to the liquid handler, you'll need an RS-232 cable. Obtain a cable with D-connectors that are appropriate for the liquid handler and your computer. The liquid handler requires a 25-pin male D-connector. Refer to the back panel of your computer or its documentation to determine which type of D-connector it requires. RS-232 cables are available from Gilson and your local computer store.

To connect the RS-232 cable attach the male end to the RS-232 port located on back panel of the 215 Liquid Handler. Tighten the retaining screws.

Attach the other end of the cable to the computer's RS-232 serial communications port. (Do not mistake it for the female 25-pin parallel printer port!) Again, tighten the retaining screws.

GSIOC port

Gilson systems feature a two-way communication interface between the computer and most Gilson modules. Communication occurs along the Gilson Serial Input/Output Channel (GSIOC).

The liquid handler can convert the RS-232 signal levels used by computers to the RS-422/485 signal levels required by the GSIOC and *vice versa*.

GSIOC cable

Use the GSIOC cable to link an additional Gilson GSIOC module to the liquid handler and control both devices via a program executed on the computer or Gilson Keypad Controller.



Insert the female connector, (refer to the above diagram), into the GSIOC port of the liquid handler. Tighten the retaining screws. (Gilson Part # 36078143)

GIOSC connection for **BEST** – **NMR**

GIOSC connection of 215 - 819 (ID 29)



GIOSC connection for BEST – NMR with solvent changing valve (Valvemate)

GIOSC connection of Valvemate - 215 - 819 (ID 29)



Connect the other female connector, located on the same end as the male connector, to the Gilson module. Tighten the retaining screws.

If you're connecting another Gilson module, use the male connector to join another GSIOC cable and make the necessary connection to the next Gilson module. The figure above shows you the connection of the BEST – NMR setup

Unit ID and baud rate/mode selection

Use the SW1 selector to choose a different unit ID and the SW2 to choose a different baud rate/mode. The standard setting for **SW2 is 6**. If necessary, refer to the diagram on page 21 for the location of these selectors.

Note! Switch off the system before changing any settings.

Unit ID

The unit ID identifies the liquid handler to the software packages that can issue GSIOC commands to the liquid handler.

At the factory, the 215 unit ID is set to **ID 22**. There is **no need** to change this number unless it is the same as that assigned to another Gilson device that's also connected along the GSIOC. The 819 with the injection port has to be set to **ID 29**

To change the unit ID:

- 1. Switch off the system
- 2. Gently insert a small flat blade screwdriver into the SW1 selector on the rear panel and turn it.
- 3. Align the white dot with one of the indicated numbers. The unit ID is 20 plus the selected number. This is valid for the 215 liquid handler and the 819-valve actuator. The ID for the Valvemate actuator is set via software. For details refer to appendix E. (in development)

Baud rate/mode

As a default, the baud rate/mode is set to 6, indicating that the liquid handler is set for a baud rate of 19200 and is a master device.

Ordinarily, this selection will not need to be altered.

To change the baud rate/mode, proceed as above:

Fuses

You may have received the liquid handler without any fuses installed. Depending on your local voltage mount the 110V or 230V fuse drawer.



Locate the accessory package containing the fuse drawer appropriate for your line voltage. Discard the other fuse drawer.

Locate the accessory package containing the 2.5 A "T" Slo-Blo fuse (5 x 20-mm size) fuses.

Install the fuse(s) into the fuse drawer. The fuse drawer for 100/120 V accepts one fuse. The fuse drawer for 220/240 V accepts two fuses.

Insert the fuse drawer into its receptacle in the liquid handler. See rear panel diagram on page 21.

Power cord connection

Locate the appropriate power cord for your line voltage. Discard the other power cord.

Use the power cord to connect the liquid handler to an AC power source.

The system is delivered with a set middle European and USA standard power cable.

Note! The power supply for the 606M Interface is only delivered in European standard.

3 System startup

The BEST-NMR 215 Liquid Handler is controlled via the supplied serial cable (Bruker # HZ10144/A)

Front panel

The front panel of the liquid handler contains a Start button, Stop button, LED display, and power indicator light.



Start button

The Start button can be used to home the XYZ-arm when the liquid handler is first powered up or when the motors for the XYZ-arm have been relaxed. When pressed, the yellow LED lights. Pressing the Start button will not resume the currently running program unless instructions were included in the program to do so.

Stop button

The Stop button is a large touch-sensitive pad that can be used to terminate a program and stop the liquid handler from responding to any more commands coming from the running program. This button also relaxes the motors for the XYZ-arm so that you can easily lift the probe and move the arm. When pressed, the yellow LED light is turned off.

In a situation where an emergency stop is required, pressing the Stop button immediately stops the liquid handler. The Stop button is so sensitive that if you just brush it with your hand it activates.

LED display

The 8-character LED display shows the current status of the liquid handler and any error codes as they are encountered. Your program can also contain instructions for showing 8-character messages on the display when the program is run. Refer to **Section 5, Maintainance**, 215 Liquid Handler Error Messages, for a list of current error codes and required actions.

Power indicator light

This indicator lights when you turn on power to the liquid handler using the power switch on the rear panel. Refer to the rear panel diagram on page 21 if necessary.

Start up

To start the liquid handler:

- 1. Make sure the liquid handler is connected to a power source.
- 2. Turn on the liquid handler and all other devices which are connected using the power switches located on the rear. (Refer to rear panel diagram on page 21 if necessary.) The power indicator light on the front panel becomes lit.
- 3. When power is turned on, the liquid handler beeps and displays the current version of its installed firmware. This message appears for about 1 second before the LED display returns to a blank state. (If starting the flow injection program refer to BEST software manual)
- 4. In order to determine what PROM version is installed in your liquid handler, you may need to turn the unit off then on again and watch the display for the version number to appear. (to guarantee correct functioning, the firmware should be at least 2.1 or higher
- 5. After the liquid handler powers up, press the Start button. This initiates the homing sequence that allows the liquid handler to determine its mechanical reference positions. The sequence takes approximately 1 minute to complete.
- 6. While the homing sequence progresses, the LED display shows Homing. When the sequence completes, it blanks.

Note! If the program being executed by the liquid handler doesn't include commands for homing the instrument, perform step 3 before starting the program. Just switch the power off and on again.

7. If necessary, use the utility and example programs supplied with the liquid handler, in order to home the instrument.

Configuring the liquid handler

The liquid handler comes from the factory with its configuration set by Gilson. Configuration information is stored in the non-volatile memory of the liquid handler. Prior to using the liquid handler for the first time, it is important to review and adjust the default configuration to make sure it is correct for your application.

The final configuration will be set with the BEST-NMR program. Please use the following instructions of the BEST software manual.

4 Operation of the BEST System

On install, the BEST system must be configured in the software according to the hardware such as racks and probes, that are required for a particular application. Once this is completed, this configuration should not change except when new racks or sample vials, probes or solvent changeovers are used.

As with Bruker's other auto-samplers, BEST is fully imbedded into the ICON-NMR automation routine. From the XWINNMR command line, the command <**bestadm**> starts the BEST administrator tool, from where the Hardware and Methods modules, the BEST-NMR Holder menu, the BEST optimization tool and Utilities can be chosen. The Gilson is connected to the NMR console through an RS-232 connection.

In ICON-NMR setup, a pictorial tray display can be used for ultra fast multiple sample definition. The status of each sample is visible in the tray display, and updated throughout the automated run.

The BEST administrator program

Typing <**BESTADM**> from the XWINNMR-Window starts the administrator program. From here you can select the following modules and routines :

🎀 BEST-NMR Administration Toolbox 📃 🗖 🗙					
Hardware	Holders	Solvents	Methods	Tests	Utilities
Next tool into separate window!					
For context help enter menu button with mouse pointer!					

Bestadm // Hardware:

BEST-NMR Hardware Setup **and** configuration;

...// Holders:

Selection of racks and needle z height adjustments;

...// Solvents:

Setting of solvents to the required positions

...// Method:

Selection of Methods and parameters affecting the sample transport;

...// Tests:

Start of the BEST-NMR optimization program, allowing manual choice of cleaning steps and run of individual samples or sample series outside of ICONNMR;

...// Utilities // Clean:

Removes older BEST-NMR versions (used after installation of new BEST-NMR versions).

The default operation mode of BESTADM is to close previous modules if new modules are selected. This can be changed by activating the "Next tool into separate window" button.

Configuration of the BEST-NMR System

The Hardware module is used to configure the Gilson autosampler. Specific types of hardware, lengths and diameters of capillaries, and communication ports are defined here. To start the routine, select **HARDWARE** from the BESTADM routine and enter the NMR-Superuser password.

The top of the window shows the BEST-NMR system graphically (see next Fig.). Each graphical component is a link to the dialog box in the routine that contains that parameter. By clicking on a different component with the left mouse button the cursor will jump to the corresponding dialog box on the appropriate page. The active item is highlighted in both graphic and text.

Three main pages are provided - *Autosampler Components*, *Needle Ports, Capillaries* and *Associated Hardware*. By clicking on the header it is possible to jump directly to the corresponding page.

In addition, there are two menu items at the top of the screen - *<File and View>*. File contains the usual commands for saving, opening, and deleting files. After configuring the system with the Hardware interface, the file can be stored. With the print option you can not only make a hardcopy of the Hardware setup, but also save the print out as a text file.

View has three viewing options - < *Graphic*>, < *Balloon*> and < *Description*>:

<Graphic>

→ shows the graphic of the BEST system;

<Balloon>

 \rightarrow shows a title of each component as it is highlighted and

<Description>

➔ provides a more detailed description of the highlighted component on the line just below the graphic.

Finally, there a four buttons across the bottom of the screen - *<OK*>, *<Apply*>, *<Rese*t>, and *<Cancel*>.

<0K>

→ accepts current changes and closes the window;

<Apply>

→ accepts current changes, but does not close the interface;

<*Rese*t>

→ restores previous information if a change was made, but not already saved;

<Cancel>

 \rightarrow closes the window without accepting any changes.

74 BEST-NMR Hardware Installation - Current Para File View _ 🗆 × Autosampler Components Robot Needle Ports, Capillaries Ŧ Robot Type: 215 Associated Hardware Needle Volume/µl: 111 Ŧ Z-Drive Height/mm: 125 Hood Switch Installed? no Dilutor Dilutor Type: 402 Ŧ Syringe Volume/µl: 5000 Ŧ Valvemate installed? no Number of ports: 0 *

Setting up the "Main Components of Autosampler" – Page

Robot

Robot Type: Needle Volume/µL:	Type of Gilson Autosampler in use, select < <i>215</i> > Volume of Needle in use. 111 µl needles are provided with the BEST system 215
Z-Drive Height/min	The standard height is 125 mm. Using a barcode reader and the Bruker 205B racks for well plates 127 mm must be adjusted.
	Dilutor Type

Dilutor Type:	Only Dilutor Type 402 is available;
Syringe Volume/µL:	5000 µl syringes are delivered as standard

Valvemate

Switch between installed *yes / no* Specify the Number of ports (usually 8) (for Valvemate users only)



Needle Ports

Setting up the "Needle Ports, Capillaries " - Page

Edit

1 Injection 🛓	
2 Recover 🛃	
3 Solvent 🛓	
4 Gas 👤	
ОК	

Port 1 is set to the injection position for standard BEST applications. The three other positions could be set optional for other actions. Using a "Bruker Close Injection Port" (Bruker # HZ06807) you can use the other positions either for recovering all measured sample to one destination, or to provide washing and cleaning solvent out of a larger bottle, or to provide inert gas for the gas gaps.

<u>NOTE</u>

The following values for the capillary lengths and diameters refer to the capillaries that are provided with the standard BEST-NMR set

Sample Loop	
Length/mm:	4000
Internal Diameter/mm:	1.00
Port Capillary	
Length/mm:	90
Internal Diameter/mm:	0.50
Inlet Capillary	
Length/mm:	3000 (Standard for a non-shielded 400 MHz NMR.)
Internal Diameter:	0.50

<u>NOTE</u>

To reduce sample cycle times, the shortest possible inlet and outlet capillaries should be used. UltraShield Magnets allow the placement of the Gilson closer to the Magnet (Recommended placement for the Gilson is outside the 5 Gauss line, see your Magnet Specifications for details).



Setting up the "Associated Hardware" - Page

Probe Head

Edit	With this button your are opening EDHEAD. The parameter of the current probe will be used for the following Probe Head
Installed Type:	parameter. fi (flow injection, BEST probe) or Ic (LC-NMR probe) The fi and Ic probes differ in their internal construction. Flow restrictions of 1ml/min to max. 2 ml/min apply to Ic probes.
Positioning Volume/µL	This depends on probehead type and cell volume. The volume can be initially determined with a syringe, but must be optimized. Measure the volume of a sample from inlet to outlet of the probe.
Temperature Unit For "Transfer Line and Probe installed" Switch between yes / no	

Barcode Scanner

Installed

-

Switch between yes / no

Connected to Specify the communication port

Communication port

Connected to: tty0n (where n = tty port designation)

Specifies communication port on the spectrometer (tty port = RS232 connection), or SGI Indy/O2 (com1/com2). See Appendix for details on how to configure the system if connected to the SGI. The default configuration is to the spectrometer.

When the appropriate information has been given, be sure to save the file. Then, click on <OK> to exit.

<u>NOTE</u>

The settings on this page are not stored, because e.g. the probe volume is not a Gilson specific parameter. Always the current set parameters will be used.
The BEST - Holders - Module

In this menu, the rack types currently in use are defined for each position. The active racks in your system can be pre-selected from a list of all supported racks.

<u>NOTE</u>

The racks have to be defined before moving on to the Solvent set up and the Test Tool.

76 BEST-NMR Holder N	lenu - Current Parameter Se	et 📃 🗆 🗙
File View		
Selection of facks, to t	l	uons.
Usable Racks	Usable Sa	ample Racks
Rack Ø	Usable Sample Racks:	Edit
Rack 1	Couble oumple racks.	
Rack 2		203 #tube:w6>
Rack 3		✓ 205 #wplt:1x2
Wellplate 3a		✓ 205H#wplt:1x:
Wellplate 3b Rack 4		206 #tube:w6>
NdLK 4		✓ 209 #tube:w6>
		✓ 209B#tube:w6>
		✓ 216 #tube:4x'
Сору		
]	Mark Unmark
		Selected Selected
ОК	Apply Res	All Items All Items
		ОК

Main Page

Gilson offers a wide variety of racks. This menu can be used to pre-select the racks used with the current system. Thus, only the pre-selected racks will be offered for selection inside the ICON-NMR BEST Holder Menu.

After highlighting the corresponding rack type, click on "*<MARK>* Selected" to choose that rack. To de-select a rack, click on "*<*UNMARK> Selected". In either case, All Items can be used to select or de-select all racks at once.

The top of the window shows a view of the racks in the Gilson 215 as seen from above. Each rack is a link to the dialog box in the routine that contains that rack information. By clicking on the different racks with the left mouse button the cursor will jump to the corresponding box. The active rack is highlighted in both graphic and text. Only those racks that have been pre-selected in the Hardware Module are offered for selection.

<View>

→ this button can be used to display the racks in a true pictorial form once the racks have been defined in the main window. Note that the racks must already be defined and the apply button clicked for this display to function. This display allows a sample position to be defined for use. Under the rack, an entry dialog box exists for giving the rack a label (not activated for well plates). This rack label will be carried over into the ICON-NMR status line in automation, but is not used here.

There are three buttons across the bottom of the screen - *<OK*>, *<Apply*>, and *<Cancel*>.

<OK> accepts current changes and closes the window;

< Apply> accepts current changes, but does not close the interface;

<*Cancel>* closes the window without accepting any changes.

Rack Pages 0 to 4



In contrast to the other racks positions1 to 4 this first rack position 0 can be equipped, either with the Gilson standard racks or with the so-called Wash Racks: 211, 304B or 306B.

If you have instead decided to use solvents for washing and cleaning from an optional "Bruker Closed Injection Port" #HZ06807, the first rack position could then be used for a sample rack.

Tube Type

Due to a variety of commercially available vial and well plates, (with different depth and inner volumes), it was necessary to provide the flexibility of adjusting the hardware to the required situation. In the most cases the standard vial values "#default" will fit. In the case of well plate racks, currently 1ml and 2ml are supported

In the case of well plate racks,	currently 1ml and 2ml are su	pported
TWH12DR #1mlx96	(96 Deep Well Plate 1ml	R = round vial)
TWH12DS #2mlx96	(96 Deep Well Plate 2ml	S = square vial)

Recover Holder

In this field you can define a recover destination which will be used in a Recover Method for samples out of the current rack position.

If no recover destination is defined, then the sample will be recovered back to the source vial, or if installed, to a recovery injection port (s. Hardware Setup)

Arrangement and Sequence Order

For each rack the sample numbering scheme the "Arrangement" and the Sequence Order can be chosen. The latter defines the sequence samples are taken from and put back into the rack. Notice the arrows indicate the vial or well plate numbering scheme, and how it progresses from one sample to the next.

Note! To avoid confusion, please use the same Arrangement and Sequence Order for vial racks and Wellplates. A different settings should only be used, if for example sample robots place the samples in a different order from the standard wellplate numbering scheme (A1 to H12).

The BEST - Solvents - Module

The BEST-NMR Solvent Menu is used to specify the actual solvents in your system. NMR-, Push- and Wash solvents can be defined individually and assigned to Valvemate- and Wash rack positions. **Users without a Valvemate have restricted choices in this windows.** System preparation steps and Intermediate Solvent and Solvent Switch cleaning procedures can be defined.



Is no Valvemate chosen in the Hardware Setup the picture will appear without the Valvemate symbol. Also the Valvemate parameter will be missing.

Usable Solvents

• NMR Sample Solvents

Use this table to select the actual NMR solvents. After highlighting the corresponding solvent, click on *ARK*> Selected to choose that solvent. To deselect a solvent, click on UNMARK Selected. In either case, all items can be used to select or deselect all solvents at once.

<u>Note</u>

The solvents in this table correspond to the XWINNMR solvent list. Use 'edsolv' from the XWINNMR command prompt for additions/changes, for example adding air or gas where appropriate.

• Push Solvents

Use this table to select the actual push solvents. These solvents are also used for solvent and intermediate solvent cleaning procedures. After highlighting the corresponding solvent, click on "<*MARK*> Selected" to choose that solvent. To deselect a solvent, click on "<UNMARK> Selected". In either case, All Items can be used to select or deselect all solvents at once. Use the <ADD> and <DELETE> button for changes. (*only for Users with a Valvemate*)

<u>Note</u>

In case of non deuterated solvents it is recommended to choose names which are clearly different from the deuterated names (e.g. DMSO-h6)

• Intermediate Solvents

Use this table to add/edit the solvent change combinations, where an intermediate step is necessary. Push solvent 1 refers to the current solvent, Push Solvent 2 to the target solvent. Example : Push Solvent 1 = DMSO, Push Solvent 2 = CDCl3, Intermediate Solvent = Acetone-h6. (*only for Users with a Valvemate*)

<u>Note</u>

Please use an intermediate solvent like Acetone-h6 for all changes between CDCI3 / water and vice versa (also DMSO contaminated with water).

• Wash Solvents

Use this table to select the actual wash solvents. These solvents are used for cleaning segments and the solvent in between air gaps After highlighting the corresponding solvent, click on "<*MARK*> Selected" to choose that solvent. To deselect a solvent, click on "<UNMARK> Selected". In either case, All Items can be used to select of deselect all solvents at once. Use the <ADD> and <DELETE> button for changes.

<u>Note</u>

In case of non deuterated solvents it is recommended to choose names which are clearly different from the deuterated names (e.g. DMSO-h6)

Provided Solvents

This function allows the assignment of solvents to Valvemate and/or wash rack positions.

Use the *<Valvemate>* button to assign up to 8 solvents for the corresponding positions. The button *<their volumes>* is not used in this version, so it can be left empty. *If a Valvemate is not installed, this part is greyed out.* Use the *<Wash Rack>* button to assign the wash liquids to wash rack positions. This assignment must be done also if a Valvemate is not installed. Again, the button *<their volumes>* is not used in this version.

System preparation

If set to "yes", this parameter allows the user to perform repetitive cycles instead of the push solvent cleaning procedure, The software stores the last solvent used by ICONNMR. By default, if it finds a different solvent at the next start of ICONNMR for the first sample, it executes a solvent cleaning procedure. By selecting to perform repetitive cycles, it will perform FLPR (flush and prepare) cycles with the old solvent. Please use this selection only if you do not change your current solvent between the last and next use of ICONNMR ! It should only be used if the system wasn't in use for some time and simple FLPR steps are necessary to clean it before an actual run with the same solvent ! (*For Valvemate Users only* !)

Intermediate Solvent Cleaning Procedure

Here the user chooses the PRIME and FLPR steps to be performed if an intermediate solvent is involved in the cleaning procedure. (*For Valvemate Users only*!)

- Number of dilutor syringe fillings
- This refers to initial PRIME procedures. This procedure fills the dilutor syringe and empties it using the needle. This step is useful to prime the dilutor liquid before a FLPR procedure is applied. A PRIME step uses only the sample loop and the needle capillary, while an FLPR step flushes the whole system including the probe.
- Drying with gas time (typically 40 to 120 s depending on dead volume and solvent) An FLPR step consists of a certain liquid volume (specified in the Methods module) and a drying gas period. Here the drying gas time can be set.
- Number of repetitive cycles (typically 2 to 4 depending on solvent) Number of FLPR steps to be executed if an intermediate solvent is included in a solvent change.
- Aspiration ml/min (typically 10 to 20 ml/min depending on solvent) Aspiration speed for the FLPR and PRIME solvent
- Dispense ml/min (typically 5 to 10 ml/min depending on back pressure and solvent) Dispense speed for the FLPR and PRIME solvent

Solvent Switch Cleaning Procedure

Here the user chooses PRIME and FLPR steps to be performed at a certain solvent changeover.

• Number of dilutor syringe fillings

This refers to initial PRIME procedures. This procedure fills the dilutor syringe and empties it using the needle. This step is useful to exchange the dilutor liquid before a FLPR procedure is applied. A PRIME step uses only the sample loop and the needle capillary, while an FLPR step flushes the whole system including the probe.

- Drying with gas time An FLPR step consists of a certain liquid volume (specified in the Methods module) and a drying gas period. Here the drying gas time can be set.
- Number of repetitive cycles Number of FLPR steps to be executed in a solvent change. FLPR steps will follow PRIME steps, if specified.
- Aspiration ml/min Aspiration speed for the FLPR and PRIME solvent
- Dispense ml/min Dispense speed for the FLPR and PRIME solvent

BEST Flow Injection Method Introduction

Before creating a BEST method, you have to know what you are expecting from your application.

In principle, there are two modes of sample treatment. One is called "**High Speed**" method (**HS**) and the other one "**High Quality**" method (**HQ**)

The **HS method** is focused on the fastest possible sample turnover. Using this mode the back mixing or carry over between two samples will be higher then in the HQ method. Even so, there are features in the software, which will reduce it to a certain minimum, without loosing too much time. It is clear that every cleaning action will need some time which will reduce the overall turnover.

In the **HQ method** the goal is to avoid any possible dilution and loss of the sample. Therefore no cleaning and separator liquid is used ahead of the sample. The sample will be transferred to the empty NMR probe through a cleaned and dried capillary. A more extensive washing, cleaning and drying action will also be carried out between the sample transfers to reduce the back mixing and carry over to almost zero. These actions will cost time.

The **recovering** of samples should generally be done in the HQ mode to achieve the best result

The time per cycle depends on solvent and sample. Lower viscosity solvents like Chloroform have to be treated in a different way to higher viscosity solvents like DMSO. Also the sample itself has a certain impact on the entire system. Low concentration samples behave differently to saturated samples. Typical values of transfer time for HS methods are 1 to 2.5 minutes per sample. For the HQ mode you can typically expect 3 to 5 minutes. If you are recovering the sample you must add 1 to 2 minutes to each cycle. These transfer times do not include the NMR measurement time.

Achieving high throughput and the lowest back mixing with minimal loss of sample will require a compromise. How to achieve the best method for your needs will be described in the following chapter.



BEST Method

7% BEST-NMR Method Setup -	Current Parameter Set
File View Comment: Default method	parameter set
Fundamental -	BEST Method
Parameters NMR Sample and	Emptying Procedure: Waste
Related Gaps Emptying	Quick Mode? yes
Wash and Dry System	Wash and Dry nothing
Further Cleaning Dilutor Speeds,	Additional WDS Period: 8
Temperatures	Additional WDS Solvents: Edit
	WDS Solvents on Stop: Edit
	Fundamental Solvents
	Sample solvent DMS0
	Push solvent DMS0
	Probe Head
	Type: 🚹

Fundamental Parameters

What do you want to do with the sample after the NMR measurement?

Emptng Procedure:

- a. None fastest turn over
- b. Waste lowest carry over slowest turn over
- c. Recover

If you choose "None" then the sample will be left in the probe after the NMR measurement and the next transfer action will replace it with the new sample. To achieve a cleaning effect you can set certain gas- and liquid gaps ahead of the sample plug. This will reduce the back mixing drastically.

Using the feature "Waste" the sample will be discarded. Either use gas to blow, or liquid to flush the probe, but a more efficient action is a combination of the two. The "Waste" action is most commonly used, even in the HS mode. Just using gas (ca. 30s to 60s depending on the solvent) will help dramatically to reduce the carry over.

If you want to get your sample back after the NMR measurement you must choose this option.

Your choices will enable and disable chapters in the Method Setup program. e.g. if you have clicked on "Recover" you will recognize that the next value "Quick Mode Y/N" will get inactive (it is grayed out) This will be done also on all the other pages to help you to set only the relevant parameter.

Do you want to save some additional seconds?

Quick ModeYeswill make the turn over faster – overlapping actionsNowill run one action after the other

If you have chosen to run your sample in Quick Mode, the system will prepare the next sample for transfer immediately after having delivered the previous one to the NMR. In doing this, we can save up to one minute of preparation.

Be aware that you can't use the "Quick Mode" together with a "Wash and Dry System" (WDS) action, as they will interfere each other.

During the evaluation phase of a method it is recommended not to run the methods in Quick Mode, as otherwise you might waste too much sample.

Do you want to save more time, allowing for higher back mixing?

Wash	Nothing	no wash actions, but blow out available	
	System	excessive washing and drying will be enabled	

The washing action will be done after each measurement. You can set the detailed values for this on the pages "Emptying", "Wash and Dry System" and "Further Cleaning"

Do you want to carry out additional washing action from time to time?

Additional WDS Period	0 - n You can insert a number between 0 and n
Additional WDS Solvents	you can create a solvent list for doing several WDS
	actions in a block

WDS means Wash and Dry the System. There is a separate page for all the required values for this action. The parameter "Additional WDS Period " will carry out this excessive washing procedure every "n" injections within a series. It has been shown that for several applications, especially for investigation of body fluids, it will make sense to have additional cleaning steps every 10th injection of sample to avoid bacterial growth.

Do you want to set your system to well known conditions after finishing a series of samples?

WDS on Stop You can create a solvent list for doing several WDS actions in a block at the end of a series of samples

An empty list means that there will be no WDS action carried out at the end of a series.

It is strongly recommended to use this feature. To be on the safe side, you should always keep the probe clean. If a sample remains in the probe and dries out, it may be impossible to remove. It will lead to background signals which can't be cleaned out.

Which solvents should be used for the sample and for the transfer?

Sample Solvent	(listing of usable sample solvents)
Push Solvent	(listing of usable push solvents)

The sample solvent will be used by the NMR program for setting the solvent related NMR parameters.

If the Valvemate is installed, the required push solvent is set here. If you choose a solvent in ICONNMR you will only have options on methods using this solvent. Applications using markedly different solvents for sample and pushing does not improve back mixing.

Deuterated sample solvent and protonated push solvent will safe some money, but will also need good suppression techniques to get a sufficient S/N. To minimize the protonated signal coming out of the push solvent, you can use small deuterated liquid gaps around the sample package.

? Which probe will be used ?

Probe Head Type	fi	will allow high aspiration and dispensing speed	
	lc	will slow down aspiration and dispensing speed	

The FI-probe is built for flow injection and allows an optimal speed for all aspiration and dispensing action due to its larger capillary IDs. s. The LC-probe is built for LC-NMR and has smaller inlet capillary IDs. This will lead to a limited speed for the transfer and washing actions and thus the turn over time will be much longer than with the dedicated FI-probe.

NMR Sample and related Gaps



Is the sample precipitating ?

Submersion Offset

0.0 – 99.9 mm

the needle will not go as deep with larger values

By setting the offset you can avoid the needle aspirating precipitated particles which might lie on the floor of the vial. The needle will start aspirating with the given distance to the basic Z-position of the chosen vial.

How much sample is available ?

Volume 0.0 – 999 µl

As described before, you will need a minimum of twice the active volume of your probe to get reasonable results. The more sample you can use the better for the reproducibility and minimal back mixing or carry over will be visible.

Is the sample placed correct in the probe ?

Corr. Pos. -999 – 999 μl

It might be necessary to adjust the position of your sample if you are need to use different solvents and speeds. This effect is especially visible if your sample volume is near the lower limit of factor 2 of the active volume.

Is the sample viscous ?

Getting Equil. Time	0 – 999 s
Inj. Equil. Time	0 – 999 s

These values are normally set between 0 and 3 seconds, depending on the viscosity of sample and solvents involved. Under certain circumstances they may be set higher. You must ensure that all movement has stopped before the needle starts its next action.

Leading / Trailing Gaps



do you want to create an HS or HQ method ?

Leading Gaps Solvent Volume Gas Volume	Solvent 0 - 999 μl 0 - 999 μl	(listing of provided washing solvents)	
	Add Copy Delete OK	will add a new line will copy the marked line will delete the last line will accept the settings	
The gas and liquid	gaps are set ahead	d of the sample beginning with a gas gap in the	

The gas and liquid gaps are set ahead of the sample beginning with a gas gap in the first line.

If you decide to create an HS method then you should set the solvent in the first line to a higher value. This solvent package will enter the probe first and can act as a cleaning segment.

Besides the wash liquids which could be provided out of a wash rack or an closed injection port it is also possible to set a part of the sample with a separator gap in front of it. This will reduce the diluting effect. You only have to ensure that enough sample will be available from the sample vial.

If you want to create a HQ method you delete all lines set. A gas gap (ca. 100 μ l) in front of the sample helps avoiding dilution with solvent rests in the capillary.

Trailing Gaps Solvent Volume Gas Volume	Solvent 0 - 999 μl 0 - 999 μl	(listing of provided washing solvents)
	Add Copy Delete OK	will add a new line will copy the marked line will delete the last line will accept the settings

The trailing gas and liquid gaps are set behind the sample beginning with the gas gap in the first line.

For both the HS and HQ method you should set at least two gap lines.

Besides the wash liquids from a wash rack or a closed injection port it is also possible to set a part of the sample with a separator gap in front of it. This will reduce the diluting effect further. You only have to ensure that enough sample will be available from the sample vial.

Is your sample viscous ?

Getting Equil. Time	0 – 999 s	
Use Gas from	Environment	
	Port requires closed injection port (# HZ06807)	

The equilibration values normally are set between 0 and 3 seconds, depending on the viscosity of sample and solvents involved. Under certain circumstances they may be set higher. You must ensure that all movement has stopped before the needle starts its next action If you have installed a closed injection port which is connected to an inert gas support (e.g. N_2) you can also set the inert gas gaps, which should improve the NMR performance, by improving the quality of the shimming on the sample.



How do you want to treat your sample after the measurement?

Sample Wasting

Blow Out Pulse Time	0 – 999 s how long should the gas/puls flow?		
	Blow	Out Intermissn. Time 0 – 999 s	how
		long should the Gas flow be	
		interrupted?	
Blow Out Pulse Counter	0 – 999	how often should the pulse be	
	repeated?		

A pulsing blow out has shown better efficiency than a constant flow of gas. In pauses, when the flow stops, liquid on the surface of the capillaries will have time to form a little drop. With the next blowing period this drop will be transported further out of the system. A gathering time from 4 to 6 seconds should sufficient for most cases. Adding pulse and intermission time and multiplying it with the counter value will lead to the entire time of this action.

Did you choose Recover as a fundamental parameter ?

Sample Recovering

Holder the reg		the re	ample will be recovered to its origin gion of the new target must be defined in the r menu	
Port			you also can gather all samples to one Vessel.	
		The port has to be defined in the hardware setup as a		
recover port.				
Leading Recover Offset 0 – 999 µl		99 µl	will place the sample saver in the needle	
Trailing Recover (Offset 0–9	99 µl	will dispense the set volume in addition to the	
			sample into the target	
Recover equil. Tin	ne 0–9	99 s	will wait before continuing.	

Generally it is recommended to recover the sample into a new vial. As we can not avoid a certain dilution we would also dilute the rest of the origin sample. To recover it into a new target it must be defined in the holder menu.

If you want to collect all samples into one vessel, you can use a closed inject port solution. The port position to be used for the recover action must be defined in the hardware setup. which. You can chose up to 3 ports. In the solvent menu you can assign the appropriate ports.

In the recover process the dilutor will aspirate the sample back into its needle. The gas valve will help this process in pushing the sample as long the aspiration is running. To minimize losses and to be on the safe side, it will in addition aspirate the value set under "Leading Recover Offset".

In the dispensing step the sample, the Leading Recover Offset and the Trailing Recover Offset value will all be pushed to the recover target.. This value shouldn't be larger then

the first gas gap which was set under "Trailing Gaps" the page before. Otherwise you will probably dilute your sample.

As the needle and its capillary are used for the recover process, Quick mode is disabled.

are you running a HQ method an do you want to minimize any dilution ?

Injection Port Emptying

Use Gas from	Environment Port	
Gas Volume	0 – 999 µl	reduces dilution in the HQ mode

If you want to use inert gas, you can use a closed inject port solution. The port position to be used for gas support must be defined in the hardware setup .

The path from the injector to the valve usually contains remaining push solvent as it can't be reached with the gas flow coming from the gas switch valve. However, this remaining liquid will dilute the following sample by a certain amount. Depending on the sample size 5% to 15% has been observed..

To empty the path you can set a gas volume which will be pushed into the injection port, so that the liquid will be pushed into the capillaries which will then be dried in the conventional way. To be on the safe side values around 250 μ l are recommended.

, , , , , , , , , , , , , , , , , , ,			
76 BEST-NMR Method Setup -	Current Parameter Set		
File View			
Comment Default method	parameter set		
Parameters for Wash and Dry			
Fundamental -	Wash and Dry System		
Parameters NMR Sample and	Use Gas from Environment		
Related Gaps	Leading Gas Volume/µl: 🕫 🔶		
Emptying Wash and Dry System	Wash solvent: H20		
Further Cleaning			
Dilutor Speeds,	Wash Solvent Volume/µl: 200		
Temperatures	Trailing Gas Volume/µl: 25		
	Gas Equil. Time/sec: 1		
	Solution Time/sec: 10		
	Push Solvent Volume/µl: 690		
	Dry w. Gas Pulse Time/sec: 10		
	Dry w. Gas Interm. Time/sec: 4		
	Dry with Gas Pulse Counter: 3		

Wash and Dry System

Do you need more extensive cleaning ?

Wash and Dry System

Use Gas from	Environment		
	Port		n optional closed injection port will be eeded
Leading Gas Volume	0 – 99		ill set a gas gap in front of the wash Divent plug
Wash Solvent	(listing of provided wash solvents)		
Wash Solvent Volume	0 – 999 µl		,
Trailing Gas Volume	0 – 999 μl will set a gas gap behind the wash Solvent plug		
Gas Equil. Time	0 – 999 s		-

In this special wash action, which can be carried out either after each injection or after a defined number of injections is be done.

Solution Time 0 – 999 s will wait the set time for the wash solvent to act in the NMR cell

The plug is stopped in the sample cell and you can adjust the cleaning reaction time with the parameter "Solution Time".

Push Solvent Volume 0 – 999 µl will push the wash solvent

Set the "Push Solvent Volume" such that the plug is definitely pushed through the probe and the outlet capillary, so that the drying action will not blow it back into the sample path.

On the "Fundamental Parameter" page you can also set a sequence of several wash solvent which will be carried out one after another. This is especially recommended if you use WDS on stop to clean your entire system after ending a whole series of sample.

Dry with Gas Pulse Time	0 – 999 s how long should the gas/puls flow?		
	Dry	with Gas Interm. Time	0 – 999 s
	-	how long should i	t the Gas flow
		be interrupted?	
Dry with Gas Puls Counter	0 – 999	how often should the pul	se be
		repeated?	

A pulsing gas blow out has shown better efficiency than a constant flow of gas. In pauses, when the flow stops, liquid on the surface of the capillaries will have time to form a little droplet. With the next blowing period this droplet will be efficiently pumped through the system. A gathering time from 4 to 6 seconds should sufficient for most cases. Adding pulse and intermission time and multiplying it with the counter value will lead to the entire time of this action.

Further Cleaning



Do you want to reduce the carry over ?

Wash Needle

Push Solvent Volume

0 – 999

will clean the needle after each run

Set the correct value for washing the needle. It is the main source of carry over of the previous sample. A volume of 250 μ l or more will be sufficient.

Is your system ready to start?

Flush and Prepare

Probe Flushing Volume	0 – 999
Dry with Gas Pulse Time	0 – 999
Dry with Gas Interm. Time	0 – 999

how long should the gas/puls flow? how long should it the Gas flow be interrupted?

s s Dry with Gas Puls Counter 0 – 999

how often should the pulse be repeated?

Flush and Prepare is only available in "Tests" in bestadm. You should use it to be sure that your system will be in a well known state before you starting your method after a period of inactivity.

The program is providing some standard HQ and HS methods which can be used as a base for the requested application.



Dilutor Speeds and Temperature

Do you use a dedicated FI-probe or will you work with a LC-probe ?

Dilutor Speeds

Aspiration Push Solv. 0 – 20 ml/min normally the highest value

The Push Solvent aspirates through a larger capillary ID so you can easily use the highest speed available for FI probes

Dispense to Rinse0 – 20 ml/minnormally the highest valueAs the dispensing is done directly into the waste you can easily use the highest speed
available

Aspiration for Cleaning0 – 20 ml/min5 to 10 ml/min recommendedThe sample is not involved so you can use a relatively high speed.

Dispense for Cleaning	0 – 20 ml/min	5 to 10 ml/min recommended
-----------------------	---------------	----------------------------

Because of the pressure resistance of the probe in the cleaning procedures you can use higher speeds but not as high as draining the solvent only.

Aspiration for Sample0 - 20 ml/min1 to 6 ml/min recommendedDispense for Sample0 - 20 ml/min1 to 6 ml/min recommendedHere the sample is involved and you should take care not to create a back pressurewhich will impact your transportation negatively.

Do you want to save time in getting the measurement temperature already during the transfer ?

The temperature controlled transfer line is an option and will make sense using DMSO and measurement temperatures over 300 °K. You can save minutes off each sample cycle using the preheating option.

Temperatures

Probe Temperature	0 – 373 °K	set probe temperature method depended
Transfer Line Temperature	0 – 373 °K	set transfer line temperature a few degrees higher then the probe temperature

Offset the transfer line temperature a few degrees above the probe temperature as there will be a loss from the TCTC through the capillaries to the NMR measurement cell. Depending on the temperature difference to the environmental temperature and depending on the flow rate the difference could be up to 15 degrees C. Also the probe design will have a certain impact.

FI-probes built before 1999 have very little insulation and will need a higher transfer line temperature.

FI-probes built later then October 2001 will need a lower temperature offset due to an active heated probe inlet line. The temperature offset for the transfer line could be set with such probes, even in using probe temperatures over 313 °K, only to 3 to 5 °K.

BEST – NMR Test Tool

This tool can be used to check a configuration and a BEST method under real conditions outside of ICONNMR.

WINDERST-NMR	Test Tool	<u>_ </u>	
Set_Parameter	rs	RESET	
VMPOS=	1	PRIME	
FLPR	WN	WDS	
Run	Continue	Break	
Barcode Scanner			
Start_Scanner Get_Barcodes			
Configure		Check	
Waiting for command.			



BEST Status Monitor

On opening the BEST-NMR Test Tool, the connected hardware will be checked for its status. If everything is connected and communicating correctly, the Status light will switch to GREEN. During communication and moving action of the 215, the RED light indicates the system is busy.

Further details about the current status are shown in the three lines of the Status Monitor If a time consuming action, like aspirating or dispensing, is running, the remaining time will be shown in the lowest bar.

BEST Test Tool

Set parameter

Before starting a run you have to transfer all necessary parameters to the robot. A choice of Hardware, Holder, Solvent and Method parameters are sent and can be tested.

To change one of the menus, you first have to click this button to enable them with your next run.

RESET

With "RESET" the whole Gilson will be initialized. Any current actions will be stopped and the hardware will be set to its initial values.

VMPOS

This button is only active if you have chosen the Valvemate in the "Hardware Setup" The Valvemate valve position will be always 1 after starting the Test Tool or doing an initialization.

! You have to set the right port for your testing, as it won't be set automatically!

In the ICONNMR automation it will be taken care of from the program. The ports at the Valvemate start with the port at "3:00 a clock" and are counted counter clockwise.

PRIME

This function will fill the syringe completely and dispense it to drain. It can be used to speed up the flushing of the capillaries and the dilutor, after the change of a dilutor solvent.

FLPR

With "FLush and PRepare" the entire system, including the flow path to the NMR probe It will use the solvent currently connected to the dilutor. The used values are set in "Method – Further Cleaning"

WN

"Wash Needle" will use the drain to clean the needle further on the outer side. The used values are set in "Method – Further Cleaning"

WDS

Having a Method loaded using the "Wash and Dry System" action, you will be able to run this action separately.

Run

Clicking "Run" without marking a sample or a sample array on the "Show Holder" Page the loaded method will be carried out on the first available sample position. If you marked a sample (or array) it will start on that position.

When the transfer is finished, the hardware will wait for you to hit the continue button. This will allow you to check and optimize the NMR parameters.

Continue

With "continue" it will finish this run in the set way, this means it will waste or recover it and then prepare the next sample for the transfer. If you want to check the behavior of a series then it is recommended to mark several samples. This is particularly useful if you want to prove the so called "Quick Mode" where a sample will be prepared during the NMR measurement.

Break

"Break" will stop a series, but will end it safely. "Recover" and Washing actions will be carried out. Also having chosen a "Quick Mode" the prepared sample will be transferred first to the NMR before ending it.

Barcode Scanner

This part of the tool will only be shown, if you have chosen "Barcode Scanner" in the "Hardware Setup"

Barcode will only make sense in combination with the Bruker LIMS software package "SampleTrack"

Start Scanner

With this function the scanner will be initialized and will look for possible barcode information and will set the found racks to the proper position in the holder menu

Get Barcodes

Here the barcodes will be read out of the information the "Holder" menu has given. In contrast to the previous action, the holder menu will be not overwritten if a different rack type has been found.

Configure

Is currently disabled.

Check

If a barcode reading problem occurs , you can check the function by pressing the "Check" button. A report file with the actual values will be created and can be printed out. This will help to locate the problem faster.



5 Maintenance

To obtain optimum performance and maximum life from the 215 Liquid Handler, it is important to keep the instrument well maintained.

This section contains some general guidelines that will help you to maintain your liquid handler.

Helpful hints

In order to keep your liquid handler at peak performance, Gilson Inc. recommends that you do the following:

- Change or clean the piston seals and tubing regularly in a monthly turn, to maintain maximum dilutor performance.
- Do not run the dilutor without fluid. Doing this causes excessive piston seal wear.
- If bubbles remain in the syringe after priming, clean the syringe with alcohol.
- Check periodically to ensure that all fittings are tight.
- Check that the syringe is tight in the dilutor valve fitting.
- Wipe up all spills immediately. DMSO will destroy the lacquer coating the metal parts of the 215
- Cold fluids may cause leakage; warm fluids to room temperature before running them through the system especially DMSO

Cleaning Cleaning the liquid handler

The liquid handler should be cleaned occasionally using a dry, clean cloth. Or, if necessary, use a cloth dipped in soapy water. If liquid is accidentally spilled on the liquid handler, wipe the instrument using a dry, clean cloth.

Cleaning the syringe

If your liquid handler is equipped with a dilutor, it may be necessary to clean the syringe. Cleaning the syringe is needed when some or all of the following occurs:

- Corrosive or hazardous liquids have been pumped
- Possible back flow of liquids into the waste tubing
- Leakage
- Aspiration of samples or reagents into the syringe

To clean the syringe, follow the procedures on the next page and use the diagram below as a reference.



Removing the syringe

1. Unscrew the syringe piston holding screw

2. Start the BESTADM Test Tool and press Lower Piston.

3. Disconnect the syringe piston from the piston-operating rod by unscrewing the piston holding screw on the underside of the rod when the prompt Install new syringe now appears.

4. Remove the two screws securing the valve to the dilutor and then remove the valve and syringe assembly.

5. Unscrew and remove the syringe from the valve.

Cleaning the syringe

Once the syringe has been removed, it can be cleaned:

- 1. Place the syringe in a beaker-containing methanol. Then aspirate and dispense several volumes of methanol through the syringe.
- 2. Place the syringe in a beaker containing distilled or deionized water. Then aspirate and dispense several volumes of water through the syringe.
- 3. Hold the syringe housing in one hand. Clean the syringe using a non-abrasive cloth dampened with alcohol. Remove the piston and clean the piston with a non-abrasive cloth dampened with alcohol.
- 4. Dry the syringe and piston using a clean, lint-free cloth.

Re-installing the syringe

When the syringe is clean, re-install it:

- 1. Lubricate the piston with diluent in order to reduce friction on the piston seals during re-installation.
- 2. Loosely screw the syringe into the valve. Do not fully tighten.
- 3. Loosely attach the valve with its screws to the dilutor.
- 4. Pull down the piston so it comes into contact with the piston operating rod and firmly tighten the piston holding screw.
- 5. Fully tighten the valve screws to secure the valve.
- 6. Fully tighten the syringe into the valve.
- 7. Press "Home Dilutor" to drive the piston rod to its upper position and tighten the screw.

Cleaning the fluid path

Depending upon your use of the liquid handler, it may be necessary to flush the entire fluid path. The following procedures use the PRIME command out of the BEST-NMR program. Start "bestadm" program in XWINNMR and open the test page. (Please refer to the BEST Software Manual how to set up BEST-NMR)

It's important to clean the fluid path if you won't be using the liquid handler for a while or if you're using a solution with a high salt concentration for a probe wash or as a diluent.

- 1. If necessary, place the dilutor's inlet tubing into a beaker containing distilled or deionized water. Check the beaker during the priming sequence to ensure it always has liquid in it.
- 2. press the PRIME button.
- 3. Inspect the dilutor for leaks.
- 4. Wipe up all spills on and around the dilutor immediately.

Cleaning methods

Depending on the samples or reagents that come into contact with the fluid path, you may need to vary your cleaning methods accordingly. Use the following cleaning protocols as references and make any changes to them as required for the samples and reagents being pumped for your application.

Proteins and peptides

Follow this procedure if the fluid path is in contact with proteins and peptides:

- 1. Place the dilutor's inlet tubing into a beaker containing a weak detergent solution.
- 2. Start PRIME and pump until the entire fluid path has come into contact with detergent.
- 3. After 30 minutes, remove the inlet tubing from the detergent solution and immerse it in a bottle containing distilled or deionized water.
- 4. Continue the priming sequence and pump the remaining detergent from the syringe and tubing into a waste container.
- 5. You might repeat the priming step several times to succeed.

Acidic and basic compounds

Follow this procedure if the fluid path is in contact with acidic and basic compounds:

- 1. Place the dilutor's inlet tubing into a beaker containing 0.1 N NaOH.
- Start PRIME and pump until the entire fluid path has come into contact with 0.1 N NaOH.
- 3. After 10 minutes, remove the inlet tubing from the 0.1 N NaOH and immerse it in a beaker containing distilled or deionized water.
- 4. Continue the priming sequence in PRIME Continue to prime until the fluid path has been flushed with water.

- 5. Place the dilutor's inlet tubing into a beaker containing 0.1 N HCl.
- 6. Press PRIME to continue the priming sequence. Continue to prime until the fluid path has been flushed with 0.1 N HCI.
- 7. After 10 minutes, remove the inlet tubing from the 0.1 N HCl and immerse it in a beaker containing distilled or deionized water.
- 8. Press PRIME to continue the priming sequence. Continue to prime until the fluid path has been flushed with water.
- 9. You might repeat the priming step several times to succeed.

Biological fluids

Follow this procedure if the fluid path is in contact with biological fluids such as blood products:

- 1. Make a solution of 10% bleach by adding one part of commercial bleach to nine parts of water.
- 2. Place the dilutor's inlet tubing into a beaker containing the bleach solution.
- 3. Start PRIME and pump until the entire fluid path has come into contact with bleach.
- 4. After 30 minutes, remove the inlet tubing from the bleach solution and immerse it in a beaker containing distilled or deionized water.
- 5. Press PRIME to continue the priming sequences and pump the remaining bleach solution from the syringe and tubing into a waste container.
- 6. Prime the fluid path a minimum of 10 cycles with distilled or deionized water.
- 7. You might repeat the priming step several times to succeed.

Cleaning the valve

Clean the dilutor's valve with a non-abrasive cloth after any of the following situations have occurred:

- Corrosive or hazardous liquids have been pumped
- Possible back flow of liquids into the waste tubing
- Leakage

Removing the valve

To clean the valve, first remove it from the dilutor:

- 1. Disconnect the inlet, transfer and vent tubing from the valve.
- 2. Disconnect the syringe from the valve and remove the valve from the dilutor as described on page 31.

Disassembling the valve

1. Hold the valve body firmly in one hand. Using a 17 mm open-ended wrench, turn the valve axle guide counterclockwise and separate the two halves.



2. Pull the valve axle away from the valve main body.

3. Separate the ceramic stator from the ceramic rotor.

4. Tap the valve axle guide against a solid level surface to remove the spring and PTFE end piece.

Note: Do not remove the ceramic stator from the valve main body.

Cleaning and re-installing

The disassembled parts of the valve can be cleaned using a non-abrasive cloth dampened with alcohol or by autoclaving.

- 1. Dry the components using a clean, lint-free cloth.
- 2. Re-assemble the valve parts by reversing the above procedure.
- 3. Re-install the syringe and valve by following the instructions on page 31.

Replacing parts

Replacing tubing

It is important to keep all tubing clean and free of crimps. Tubing that has become dirty, blocked or crimped can result in poor accuracy and precision, loss of air gap or the syringe stalling.

Removing the syringe

1. Use bestadm menu lower syringe

2. Select the MOUNT to lower the syringe piston. This causes the XYZ-arm to move to the rinse station and the dilutor's piston operating rod to descend as the dilutor aspirates from the reservoir. The dilutor will stop in the middle of its down stroke and the valve will switch to the outlet position.

Note: If the liquid handler is not homed when this option is selected, the unit will home before it moves to the rinse site.

- 3. Remove the screws attaching the valve to the dilutor and remove the valve and syringe.
- 4. Unscrew and remove the syringe from the valve.

Mounting new syringe

- 1. Loosely screw the replacement syringe into the valve. Do not fully tighten.
- 2. Loosely attach the valve to the dilutor with its screws.
- 3. Pull down the piston so it comes into contact with the piston operating rod and firmly tighten the piston holding screw.
- 4. Fully tighten the valve screws to secure the valve.
- 5. Fully tighten the syringe into the valve.
- 6. Press any key when finished. The liquid handler will move to the rinse site and the dilutor will re-initialize with the new syringe.
- **Note :** If you installed a new syringe of a different size to the one you replaced, you need to run "bestadm" "hardware" setup and change the syringe size.

Replacing the valve

To replace the dilutor's valve, follow the instructions below. If necessary, refer to the dilutor diagram on page 31.

- 1. Disconnect the inlet, transfer and vent tubing from the valve.
- 2. 2. Disconnect the syringe and the valve from the dilutor. Refer to the procedure for replacing the syringe
- 3. Re-install the syringe and the replacement valve. Refer to the procedure for mounting new syringe, above.
- 4. Re-connect the inlet, transfer and vent tubing to the newly installed valve.
- 5. Press the "Start" button at the 215 to home the hardware

Replacing the liquid handler probe

Refer to the appropriate instructions below depending on whether your replacing the probe with one of the same type or one of a different type.



4. Replace and tighten the 1/4"-28 fitting.

Installing same type To install a replacement probe of the same type that's currently

1. Remove the transfer tubing's 1/4"-28 fitting connected to the top of the isolation probe holder.

2. Grasp the current probe and push it up through the top of the isolation probe holder.

3. Install the new probe by pushing it through the top of the isolation probe holder. Make sure the tip of the probe sits inside the probe guide.

• Be aware that different types of probes will need also the corresponding Gilson Probe Holder/Guide Kits. Details are listed in the Gilson catalog.
Installing different type

To install a replacement probe of a different type to that currently installed, you'll need to obtain a probe kit. Each kit includes a probe guide, probe holder, and probe.

- 1. Remove the transfer tubing's 1/4"-28 fitting connected to the top of the isolation probe holder.
- 2. Grasp the current probe and push it up through the top of the isolation probe holder.
- 3. Remove the current probe guide from the opening in the top of the foot by unscrewing the two Phillips-head screws. Then place the new probe guide into the top of the foot and secure it using the screws.
- 4. Remove the current probe holder by unscrewing it from the bottom of the isolation probe holder. Then install the new probe holder by screwing it into the isolation probe holder.
- 5. Install the new probe by pushing it through the top of the isolation probe holder. Make sure the tip of the probe sits inside the probe guide.
- 6. Replace and tighten the 1/4"-28 fitting.

Replacing a fuse

A blown fuse may indicate another problem in the instrument. If the replacement fuses blow, don't try others. Contact your local representative. See **before calling us** in **Section 5**.

To change a fuse, follow these steps:

1. Disconnect the power cord from the power outlet and from the rear panel receptacle.



2. Locate the fuse drawer on the rear panel. See page 2-16 if necessary.

3. Insert a small screwdriver into the notch next to the fuse drawer.

4. Twist the screwdriver to open and remove the fuse drawer. The fuse drawer contains one 2.5 A "T" Slo-Blo fuse (5 x 20-mm size) for a 100/120-voltage selection. It contains two 2.5 A fuses for a 220/240 voltage selection.

5. Remove the old fuse(s) and insert the new fuse(s).



6. Insert the fuse drawer into its receptacle in the liquid handler.

Transporting the liquid handler

When moving the liquid handler to another location or when sending it back to the factory, do not use the Y-arm as a handle. Re-install the armlock (see *Section 2*) and always lift the liquid handler from the base.

6 Troubleshooting

Electrical

Unit completely dead

- Make sure power is turned on
- Check AC power cord connections.
- Try different AC outlet.
- Check fuse(s); replace if necessary.
- Check all valve actuator connections and make sure that the unit is plugged in.

Unit blows fuses

Contact the Bruker service department.

LED's flashing on front panel

Check that a valve is installed.

Input and Output functions Not operating

- Make sure terminal block connector is secure in input/output port.
- Check connections for proper pin assignments.
- Be sure pins from external devices are assigned correctly.
- Check polarity of input. Inputs should be a contact closure. If not, it must be TTL level (logic Ø activates).
- Output from valve actuator should be compatible with device to which it is interfaced. Outputs are contact closures.
- Confirm that source supplying input to valve actuator is working.

Error Massages at the 215 display

215 Liquid Handler Error Messages

A number of error messages may appear on the 215 front panel display either during system initialization or during a run. Refer to the following error message list to determine what action to take when an error message appears.

No.	Error Description	Possible solutions
10	Invalid Pump Type.	Run SET_215.EXE to correct problem.
		If this fails (and the SET_215 program appears to run correctly,) it most likely indicates a NV-RAM problem.
		The NV-RAM is socketed, and can be replaced. After NV-RAM replacement, the NV-RAM must be re-initialized and the alignment program, CORRECT.EXE must be run to assure best accuracy. It would be best to upgrade the PROM to the current rev level while replacing the NV-RAM.
		If this fails, there is likely a problem with the main electronics board. See 'Main board replacement' section.
11	Undefined syringe size.	Run SET_215.EXE to correct problem.
		If this fails, it most likely indicates a NV-RAM problem. See <i>possible solution</i> for Error 10 to handle suspected NV-RAM failures.
12	Pump not found.	This can be caused by an incorrect pump type. Check the pump type by running SET_215.EXE.
		This can also be caused by a loose cable. Turn off power to the unit, open the side panel, and check that the cables are properly and tightly connected. Removing and reseating the connectors on both ends (with power off) is recommended.
		If the cable connections are good, and the pump type is correct, the dilutor module itself may be malfunctioning. There are no field serviceable sub- assemblies in the dilutor module; the entire module should be replaced.
13	Syringe speed out of range.	Correct user program error.
14	Invalid syringe volume.	Correct user program error.
15	NV-RAM checksum is invalid.	The contents of the NV-RAM may be scrambled. This could be caused by a static discharge on the

16	X scale factor is invalid.	serial cable, power spike, or some other accident. First try to wipe the NV-RAM and reprogram by using CORRECT.EXE and SET_215.EXE. If this fails to restore proper operation, see the method for handling suspected NV-RAM failures under error 10. Rerun CORRECT.EXE. If this fails, try to wipe NV- RAM and rerun CORRECT.EXE. If this fails, then proceed with method for handling suspected NV- RAM failures in error 10.
17	Y scale factor is invalid.	See method for handling error 16.
18	Z scale factor is invalid.	See method for handling error 16.
20	X motor position error.	Cycle power to unit.
		If this does not clear the problem, or if the problem returns, it most likely indicates one of three problems:
		a) Binding in the X axis mechanics can be found by moving the Y-arm over its full range of travel, with the power off. (Note: Do not move the arm too quickly, or potentially damaging back-EMF may be generated in the stepper motors, blowing out the driver chips.) If a sticky or rough spot is found in the travel, see if there is a mechanical problem at that location that can be cleared (e.g. paint that can be scraped off of the bearing area). If the motion problem can't be resolved, contact Customer Service. The X-axis is hard to service in the field.
		 b) Belt tension could be a problem, although is it very rare with the belts used in the 215 (Kevlar fiber). Check that there is correct tension in the belts: use GSUTIL to move the arm to the midpoint of the X travel (buffered X command). Then, with the motor still powered, move the arm toward the pump end, and check that the sprocket moves, rather than having the belt jump the sprocket.
		c) A fault with the X axis position encoder could be the problem. If the encoder is the problem, check first that the cables are seated properly. With the power off, remove and re-connect the X axis encoder connector. If this fails to fix the encoder problem, replace the motor/encoder assembly.

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21	Y motor position error.	Cycle power to unit. See the method for handling error 20.
22	Z motor position error.	Cycle power to unit. See the method for handling error 20, except note that the Z-drive has no encoder, only a limit sensor. Also check that the Z- drive cable is secure, unplug and reconnect with the power off, making sure the connector snaps back into the socket with a click.
24	X target less than minimum X.	Correct user program error.
25	X target more than maximum X.	Correct user program error.
26	Y target less than minimum Y.	Correct user program error.
27	Y target more than maximum Y.	Correct user program error.
28	Z target less than minimum Z.	Correct user program error.
29	Z target more than maximum Z.	Correct user program error.
30	X encoder inactive.	Check that the cable is seated properly. With the power off, remove and re-connect the X axis encoder connector. If this fails to fix the encoder problem, replace the motor/encoder assembly.
31	Y encoder inactive.	See method for handling error 30.
32	Z position sensor inactive.	Check that the Z-drive cable is secure, unplug and reconnect with the power off, making sure the connector snaps back into the socket with a click. If failure continues, replace the Z-drive board assembly located in the Z-drive.
33	Safety contact activated.	Release contact, restart. If contact is not shorted, check the status of the safety contact configuration with the SET_215.EXE program.
34	X home phase is invalid.	Run SET_215.EXE to correct problem. If the home phase wanders too much during the home phase definition part of the program, (more than +/- 5 counts,) something is not right with the mechanics. Some possible problems are: slipping of the sprocket collar, or junk on the face of the X-car where it touches the left hand support (inside the enclosure.) Clean the face of the car and the side plate, or try to jiggle the Y arm side to side while the

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		motors are locked to determine the source of the problem.
35	Y home phase is invalid.	Run SET_215.EXE to correct problem. See method for handling error 34 if this fails.
36	X and Y home phases are invalid.	Run SET_215.EXE to correct problem. See method for error 34 if this fails.
39	Gilson m402 not initialized prior to use.	Correct user program error.
40	Gilson m402 invalid valve position.	This is caused by either the valve stem not turning properly, or the valve encoder not registering properly. Try operating without a valve. If that fails, you will probably need a new pump module. If it works check the valve assembly for smooth operation (follow procedure to clean the valve in Section 4 of the 215 <i>User's Guide</i>). If bad, replace valve.
41	Gilson m402 valve missing.	Contact the responsible Bruker Customer Service
42	Gilson m402 undefined valve command.	Contact the responsible Bruker Customer Service.
43	Gilson m402 valve communication error.	Contact the responsible Bruker Customer Service
44	Gilson m402 valve unit busy.	Contact the responsible Bruker Customer Service.
45	Gilson m402 plunger overload.	The piston may be operating at an excessively high speed, generating too much back-pressure. Try reducing the speed (flow rate) to see if this clears the problem. If this doesn't work, remove the fluid lines from the valve, and see if proper operation occurs. If it does, suspect blockage in the plumbing. If this does not work, try removing the piston and syringe, and see if it works. If it does, check for binding in the piston. If not, the 402 module must be replaced.
46	Gilson m402 syringe missing.	Replace 402 pump module.
47	Gilson m402 undefined syringe command.	Contact the responsible Bruker Customer Service
48	Gilson m402 syringe communication error.	Replace 402 pump module.
49	Gilson m402 valve unit busy.	Check for binding in the valve.

Repair and return policies

Before calling us

Bruker Service personnel will be able to serve you more efficiently if you have the following information:

- the serial number (located on the rear panel) of your valve actuator
- the installation procedure you used
- list of concise symptoms
- list of operating procedures and conditions you were using when the problem arose
- list of other devices connected to the valve actuator and a description of those connections

list of other electrical connections in the room

Warranty repair

Units covered under warranty will be repaired and returned to you at no charge. If you have any questions about applicability, please contact your authorized representative.

Non-warranty repair

For out-of-warranty repairs, contact your local Bruker representative. A Customer Service representative will discuss service options with you and can assist in making arrangements to return the instrument, if necessary.

Rebuilt exchange

For some units, rebuilt exchange components are available. Contact Bruker for details.

Application related Trouble Shooting

Problem :

Air bubbles in the syringe during the aspiration of solvent out of the main bottle (or Valvemate)

Possible reason :

- Empty bottle
- Leakage in the connection
- Clogged filter (clean or replace)
- DMSO at low Temperature
- Defective dilutor valve
- •
- Wrong position of Valvemate

Problem :

Two mixing phases in the syringe during the aspiration of solvent out of the Valvemate during the test procedure

Possible reason :

- Wrong Valvemate position
- Incomplete solvent change procedure

Problem :

Air bubbles in the needle capillary during the aspiration of wash solvent or sample Possible reason :

- Aspiration speed too high
- Clogged needle
- Wrong capillary ID

Problem :

Jerking movement in the needle capillary, during an aspiration step Possible reason :

• Older firmware (<2.30)

Problem :

Jerking movement in the needle capillary, when the needle is moving up after an aspiration step

Possible reason :

- Clogged needle
- Too short equilibrating time

Problem :

Liquid drops in the outlet capillary at the dilutor valve

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Possible reason :

- Overpressure due to high aspiration speed
- Overpressure due to wrong valve position
- Overpressure due to a clogged system

Problem :

Air bubbles and ruptured liquid segments during the transfer step Possible reason :

- Bad connections
- First injection with a new solvent
- Dispensing speed too high

Problem :

No gas gaps visible in the transfer action when sample is entering the NMR probe Possible reason :

- Aspiration speed too high
- Gas gaps too small
- LC- probe with a FI-Method
- Clogged outlet

Problem :

Solvent occurring on the top of the injection port during the transfer action Possible reason :

- Seal has to be exchanged
- Wrong needle
- Wrong seal
- Aspiration speed too high

Problem : Sample position is always different Possible reason :

- Leakage in system
- Not enough sample
- Gas gaps too small

Problem :

Sample movement is not smooth but jerking during the transfer Possible reason :

- Restriction in the pathway
- Over pressure due to a clogged needle
- Temperature too low (DMSO)

Problem :

Sample need several seconds to stop its movement after transfer action is finished Possible reason :

- overpressure in the outlet path
- Speed to high
- Gas gaps large
- Viscosity too high (DMSO)

Problem :

Sample keeps moving after transfer action is finished Possible reason :

- Leakage inside the 819 valve
- Recover Module valve defective

Problem :

Recovery is not working sufficiently anymore Possible reason :

- No gas flow at the Recover Module
- Recover Module valve defective
- No current to switch the Recover Module

Problem :

Needle is hitting between the vials Possible reason :

• Wrong rack code chosen

Problem :

Needle is hitting vial bottom Possible reason :

- Wrong rack code chosen
- Wrong Z-arm height (Bar Code)

Problem :

Needle makes a cracking noise in entering the injection port Possible reason :

- Wrong needle Guide/Holder
- Wrong position of closed injection port
- Wrong Z-arm height (Bar Code)

Appendix A

Replacement Parts and Accessories

Туре	Bruker #	Gilson #	Comment
Included parts			
Gilson Liquid Handler 215	69401	2510121G	generic
819 Valve Actuator	69407	251511G	generic
7000L Rheodyne Valve	84414	3303430	mounted
Injection Port	84421	2954640	
Septum Piercing Needle 1.5 mm	84536	27067376	2x
Probe Holder/Guide Kit f. Top Entry Needle	120446	253643	
Spare Seal 1.5 mm	84540	2954674	2x
Deep Pocket Rinse insert	84419	25245533	
Dilutor Syringe 5ml	69403	25025344	
Rack Code 211H	69409	2504611H	
Control Cable	HZ10144		
Capillary Set (Version November 2001)	H9336		
BEST Closed Injection Port	HZ06807		
4 x Rack Code 216 + 500 4ml Bottles	H9467**	2504616	Gilson Racks + vials
4 x Rack Code 209 + 500 2ml Bottles	H9466**	2504609	Gilson Racks + vials
4 x Rack Code 205H + 20 96 Well Plates	H9465**	2504605H	Gilson Racks + vials
BEST Installation Guide / Software Manual	H9330		
BEST-NMR Calibration Kit	H9643		
Wash Switch Valve	HZ10067		
Gas Switch Valve	HZ10068		
Upgrade Set for BEST under XWINNMR 3.1	H9770		

** Depending on the option of H9376

Additional Parts

Part	Bruker #	Gilson #
Description		
BEST Safety Hood	HZ07207	
BEST Temperature Controlled Transfer with 2.5 m	W1209598	
Capillary (complete)	Var.0	
BEST Temperature Controlled Transfer with 1.5 m Capillary (complete)	W1209598 Var.1	
BEST BVT3000 Controller (with two controlling circuits)	W1101266	
BEST Transfer Capillary 2.5 m	W1209791 Var.0	
BEST Transfer Capillary 1.5 m	W1209791 Var.1	
BEST Valvemate Solvent Changing System (equipped with 4 bottles)	H9619	331051G + 33035424
BEST Valvemate Capillary Set + 4 x Bottles 11	H9618	
BEST Gilson Barcode reader (compl.) (SampleTrack requested)	H9545	
BEST-NMR Calibration Kit (dyes for H_2O,CH_3OH , CHCN and CHCL ₃)	H9643	
BEST Fitting Set Gilson 215 (precut capillaries and fittings for Gilson 215)	H9436	
LC-NMR / BEST NMR Capillary Service Set	H9495	
Serial Cable 10m Gilson – NMR (direct control)	HZ10144	
Septum Piercing Needle 0.8mm ID 1.5mm – Top Entry - Vented	84536	27067376
Septum Piercing Needle 0.8mm ID 1.3mm – Top and Side Entry – Vented	84535	2507235
Probe Holder / Guide Kit 1.5mm	84537	253643
Probe Holder / Guide Kit 1.3mm	69404	253640
Injection Port Seal for 1.5mm Probe	84540	2954674
Injection Port Seal for 1.3mm Probe	84539	250510153
Cooling Rack controller 85x for up to five Cooling Racks	85309	2505850
Cooling Rack 843 for 2ml vials (13x35)	85306	2504853
Cooling Rack 842 for 96 Deep Well (Ritter / Riplate)	85307	2504854
Cooling Rack 526 for 1.8ml Cryo Vials - Gilson Rack Code	85557	MRACK526
Rack Heightener for Rack 200 series	85312	

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Part Description	Bruker #	Gilson #
Waste Bottle 2I + Cap with Connector	85183 85182 85289	23077310 23077314 23077332
Level Sensor Receiver (for up to 10 Sensors)	85310	Under development
Level Sensor positive (Waste Bottle)	(85311)	Under development
Level Sensor negative (Solvent Bottle)	(85311)	Under development
Rack 304B complete with bottles	H9697	
Rack 306B complete with bottles	H9698	
Bottle 150ml for Rack 30x	84756	
Bottle 500ml without Connector for Rack 30x	85757	
Bottle 500ml with connector for Rack 30x	84754	
Bottle Cap for Rack 30x	84758	
Bottle Septum for Rack 30x	84757	
Capillary Set for Rack 30x	H9696	
Vials 2ml 13x 35 for Rack 209 (100/pck) + Caps + Septum	36680 36724 36766	
Cryo Vials 1.8ml for Rack 526 (100/Pck) + Caps + Septum	85372	
96 Well Plate 1ml (Ritter - Riplate)	68964	
Mat for 96 Well Plates 1ml	n.a.	
96 Well Plate 2ml	68966	
Mat for 96 Well Plates 2ml	68965	
Vial 4ml 17x45 for Rack 216 (100/Pck) + Caps + Septum	68333 68337 68340	
Bottles Type Boston 125 ml for Rack 211 + Caps + Septum	84599 84600 84601	

Appendix B

Closed Injection Port

(Bruker Ord. # HZ06807)



Injection Port 0501.bmp 12.05.01 MHO

With every BEST System, in addition to the Gilson Injection port, a Bruker designed "Closed Injector Port" is included. The advantage of this device is minimal leakage of solvent and that the flow path to the NMR probe is always closed.

A further advantage of such a design will be that to provide inert gas for the gas gaps and solvent for heading and cleaning liquid gaps. In this case we are not limited to the bottle sizes fitting in a Gilson Rack. Now you can connect also 2 I or 5 I bottles. The new software version 3.1 will support this feature.

Customer experience shows that after approximately one year of use, the piston seal is worn and must be replaced.

The installation should be done always in the following steps.

- 1. Mount top through injector plate (always the far left hole)
- 2. Fix it with the screw (hand tight or use the wrench and large screw driver)
- 3. Check there is no play
- 4. Mount the lower part and tighten it with the wrench
- 5. Connect the capillary (be aware it is a different fitting (1/4" flangeless))

If you have to change the needle and/or the piston seal and you don't want to damage the needle seal, you might use a thin needle (< 0.8 mm OD) to push everything out through the top in leading the needle through the lower fitting hole.

Be aware that the tiny spring might be lost easily during this action.

In many cases you can continue your work by turning the seals upside down. However, it is better and safer to exchange them with new ones.

BEST Gas Switch Valve

(Bruker Ord. # H10067)

Description

For obtaining reproducible results in sample recovery using Syringe Mode this module is highly recommended .The gas switch valve can be mounted on the right hand side of the 215. You can use the same screws used for fixing the injection port plate.

It is recommended to adjust the gas pressure to < 2bar (<14 psi) The control of the module is possible with BRUK_XL version 990218 and higher. For installation with the Temperature Controlled Transfer Capillary, the back plate has to turned so that the mounting holes are placed under the module. In this position both parts, the recover module and the TCTC hose holder, can be secured with the two screws holding the injection port in place.



BEST Wash Switch Valve

(Bruker Ord. # H10068)

Description

To speed up the washing action and to improve the washing efficency a new device called the "Washing Switch Valve" was introduced. It should be mounted directly behind the dilutor pump 402.



The Wash Module will be mounted with its clamps to the metal rod on the upper right side of the 215.

With tightening of the clamps it will be fixed to its position.

The "Dilutor" capillary will be mounted to the right outlet to the 402 dilutor valve.

The "Needle" outlet will be connected to the 215 probe.

The "Wash" outlet should go to the 819 port 4.

The electrical connection will be I/O output 4 on the backside of the liquid handler.



The Gilson 215 Protecting Hood (Bruker Ord. No. HZ06623)

Safety precautions

- For safe and correct use of this hood, it is recommended that both operating and service personnel follow the instructions contained in this guide when performing installation, cleaning and maintenance.
- If dangerous liquids are used, adequate protection such as proper ventilation, safety glasses, etc., should be used.
- Always switch power off when making adjustments to the liquid handler. The potential exists for bodily harm if you interfere with the work area of the instrument while it is running.
- The hood is equipped with a safety power off door switch with green/yellow/red LED indicators to increase security The control of the LED is done via the Input/Output option from the 215
- Use the distance piece in the right front corner of the hood for correct placement of the 215. This will prevent the potential for interference of the Gilson Z-arm with the door.
- Avoid direct contact of organic solvents with the hood surface.

Unpacking

The fume hood is delivered with all major components already assembled except for auxiliary parts such as legs, security lights, fume hood adapter, etc.

To install the fume hood :

- 1. Open the box at the top and the front.
- 2. Lift the unit off the box and place it on a lab bench or cart. Due to its weight it is recommended that a minimum of two people lift the hood off the base of the packing container.
- 3. Leave enough space to dismount the hood from its wooden platform. It is possible to place the 215 through the open door and to do the installation inside. It is advisable and much easier to do the 215 installation and its respective connections without the cover in place.
- 4. You should place the hood on a table which is stable enough to hold ~120 kg (~250lbs)
- 5. If the legs are installed, the 4 leg mounts have to be installed first. Mount the legs and level the platform using the adjustable leg screws.
- 6. Finish the 215 installation before replacing the hood cover.
- 7. To get the stability and gas tightness of the hood, fix the hood to the wooden platform.
- 8. The serial cables can be fed through the outside via the center hole in the rear.
- 9. Plug all power cables inside before connecting the main power.

Technical data

The following information is subject to change without notice.

Material : Macralon Measures : (I x d x h) 130 x 81 x 71 cm open 191 cm Weight : 89 kg (including platform and legs)

• Warning: Modifications will void the safety feature of the hood

The Temperature Controlled Transfer Capillary

(Bruker Ord. No. W1209598 Var. x)

Two variations are available.

The basic version is equipped with a 2.5m hose and is recommended for the use with standard magnets >300MHz.

Variation 1 has a 1.5m hose and can be used also with Ultra Shielded magnets up to 600 MHz

The system is delivered with a BVT3000 BEST which has two control circuits. One is for the probe temperature, the other one for the TCTC. In addition there are 4 AUX temperature connections possible. E.g. to record the room temperature.

To secure the hose in place a holder plate mount to the Gilson is included. To prevent the hose from hanging and placing stress at connections, a clamp and stand at the magnet are included.

Appendix C

Customer Information Sheet

Company / Institute Customer Name (User) Department City code + City Street Country Telephone Fax e-mail Bruker Customer Number	
Order number Order Date Installation Date	System Information
 Autoinjector []Gilson 215 []Gilson 819 []Valvemate 	Hardware Serial Number 1) No. of Ports
 Software [] ICONNMR [] NMR Firmware [] Gilson 215 NMR Type / Field Probe Remarks	Version

Appendix D

Connection of the Capillaries



Nr.	Lenght	Dimension	Position	Fittings
1	500mm	Capillary FEP 1/16" x 1.0	Dilutor – Wash Switch	1⁄4" + 1⁄4"
2	4000mm	Capillary FEP 1/16" x 1.0	Wash Switch – Needle	1⁄4" + 1⁄4"
3	1500mm	Capillary FEP 1/16" x 1.0	Wash Switch - 819 Valve Port 4	¼" + UNF L
4	90mm	Capillary FEP 1/16" x 0.5	Inj. Port – 819 Valve Port 1	¼ + UNF L
5	3000mm	Capillary FEP 1/16" x 0.5	819 Valve Port 2 – Probe	UNF S +UNF L
6	3000mm	Capillary FEP 1/16" x 0.5	Probe – Gas Switch	UNFL+UNFS
7	1000mm	Capillary FEP 1/16" x 1.0	819 Valve Port 3 – Waste	UNF S + none
8	1000mm	Capillary FEP 1/16" x 1.0	819 Valve Port 6 – Waste	UNF L + none
9	300mm	Capillary FEP 1/16" x 0.5	Gas Switch – 819 Valve Port 5	None + UNFS

FEP	➔ Fluoro Po
1⁄4"	→ Fitting ¼"

UNF S

- lymer
- UNF L

- → Fitting ¼" 28 Thread for 1/6" Capillary Flangeless (Nut and Ferrule)
 → Fitting UNF 10/32 Nut short head for 1/6" Capillary
- → Fitting UNF 10/32 Nut long for 1/6" Capillary

WSV	➔ Wash Valve Module	(Bruker #H10067)
GSV	Gas Valve Switch	(Bruker #H10068)