

# NMRPT

- BRUKER User Manual for  
NMR Product Test Software

Version 020





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<b>1</b>	<b>Introduction .....</b>	<b>7</b>
<b>2</b>	<b>Conventions .....</b>	<b>9</b>
<b>3</b>	<b>Overview .....</b>	<b>13</b>
<b>4</b>	<b>Practical Advices .....</b>	<b>29</b>
<b>5</b>	<b>GUI-Description.....</b>	<b>39</b>
<b>6</b>	<b>Contact.....</b>	<b>99</b>
	<b>Appendix .....</b>	<b>101</b>

<b>1</b>	<b>Introduction .....</b>	<b>7</b>
1.1	Purpose.....	7
1.2	Area of Application.....	7
1.3	Warning / Notice Signs .....	7
1.4	Requirements.....	7
1.5	Referenced Documents .....	8
<b>2</b>	<b>Conventions .....</b>	<b>9</b>
2.1	Abbreviations .....	9
2.2	Terms and Definitions .....	9
<b>3</b>	<b>Overview .....</b>	<b>13</b>
3.1	About <i>NMRPT</i> .....	13
3.2	Test Modes .....	14
3.3	Report Types .....	14
3.4	<i>NMRPT</i> Documents .....	15
3.4.1	Test Report .....	15
3.4.1.1	Protocol.....	16
3.4.1.2	Spectra PDF .....	16
3.4.2	Single Spectrum PDF .....	17
3.4.3	Short PDF .....	18
3.5	Workflow .....	19
<b>4</b>	<b>Practical Advices .....</b>	<b>29</b>
4.1	Sample Change Modes .....	29
4.2	Gas Flow Control .....	29
4.3	Temperature Control.....	30
4.3.1	Selftune.....	30
4.4	<i>NMRPT</i> Shim Handling.....	31
4.5	Locksetting.....	32
4.6	Converted Parameter Sets .....	33
4.7	Additional Information .....	33
4.8	How to Debug .....	34
4.9	Troubleshooting .....	35
4.10	How to Report a Bug .....	38
<b>5</b>	<b>GUI-Description.....</b>	<b>39</b>
5.1	Menu Bar .....	39
5.1.1	File .....	39
5.1.1.1	New > Probe / Inspection Lot .....	40

5.1.1.2	New > Report.....	42
5.1.1.3	NMRSAVE .....	43
5.1.1.4	Close.....	44
5.1.2	Edit.....	44
5.1.2.1	Copy Inspection Lot.....	45
5.1.2.2	Rename > Inspection Lot.....	45
5.1.2.3	Rename > Plugin .....	46
5.1.2.4	Rename > Report .....	47
5.1.2.5	Delete > Probe.....	48
5.1.2.6	Delete > Inspection Lot.....	49
5.1.2.7	Delete > Report .....	49
5.1.2.8	Shim Command .....	50
5.1.2.9	Sample List.....	52
5.1.2.10	Remove Converted Parameters .....	55
5.1.2.11	Configuration .....	56
5.1.3	Help .....	58
5.1.3.1	NMR Product Test Graphical User Interface Manual.....	58
5.1.3.2	NMR Product Test Experiment Manual .....	58
5.1.3.3	NMR Product Test Short Guide.....	58
5.1.3.4	About .....	58
5.2	Acquisition Bar.....	60
5.3	Navigation.....	63
5.3.1	Navigation: Probes .....	64
5.3.2	Navigation: Reports .....	64
5.3.3	Navigation Context Menus .....	65
5.4	Workspace.....	69
5.4.1	Inspection Lot Tab .....	70
5.4.2	Probe Setup Tab.....	72
5.4.3	Acquisition Tab .....	74
5.4.4	Results Tab.....	80
5.4.5	Report Tab.....	85
5.4.5.1	Report Tab for Acceptance Test.....	86
5.4.5.2	Report Tab for Final Test.....	91
5.4.5.3	Report Tab for Field Service Test.....	94
<b>6</b>	<b>Contact.....</b>	<b>99</b>
	<b>Appendix .....</b>	<b>101</b>
A.1	Figures .....	101
A.2	Tables .....	106
A.3	Index .....	107





# 1 Introduction

## 1.1 Purpose

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This reference manual describes the functionalities of *NMR Product Test (NMRPT)* software. *NMRPT* software is used for the standardized installation, the Acceptance, the NMR Final and Service Test of *Bruker AVANCE III*-series (and newer) instruments, and components. *NMRPT* provides standard Test Reports including spectra for documentation and signature.

For a short introduction to *NMRPT* see ZHUB0001 in [1.5 Referenced Documents](#). For information about the test procedure and included experiments see ZUEP0102 in [1.5 Referenced Documents](#). Both documents are also available from *NMRPT* [Help menu](#).

## 1.2 Area of Application

---

This manual is written for all Bruker employees engaged in final testing, service and installation of NMR products using the *NMRPT* software. In addition to the installation procedure, a list of technical demonstrations (see Customer Acceptance [Protocol](#) of the installation) is outlined in the test documents in order to provide an effective introduction to the NMR system.

## 1.3 Warning / Notice Signs

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Provides important information for the user.

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## 1.4 Requirements

---

- |           |   |
|-----------|---|
| Software: | The <i>NMRPT</i> software is included in <i>TopSpin 3.5</i> (and newer)                 |
| Hardware: | <i>AVANCE III</i> (and newer)<br><i>FOURIER</i> is not supported                        |
| Samples:  | Bruker standard samples<br>(see ZUEP0102 for information about samples and experiments) |

## 1.5 Referenced Documents

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ZHUB0001	Internal <i>NMRPT</i> Short Guide (see <i>NMRPT</i> <a href="#">Help menu</a> )
ZUEP0102	Bruker Test Procedures for <i>Avance</i> NMR Systems (see <i>NMRPT</i> <a href="#">Help menu</a> )
H9469SA3	<i>TopSpin</i> User Manual
H9776SA3	Processing Commands and References
n.a.	<i>TopShim</i> Automatic Shimming Users Manual
Z33073	Variable Temperature Control for NMR Probes User Manual

## 2 Conventions

### 2.1 Abbreviations

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GUI	Graphical User Interface
NMRPT	NMR Product Test
NMRSAVE	Call of <code>nmr_save</code> including <i>NMRPT</i> data
PICS	Probe Identification and Control System
probe ID	Probe Identification (unique, consists of the part number and the serial number of an NMR probe)
sample ID	Sample Identification (unique)

### 2.2 Terms and Definitions

---

Additional PDF (of Inspection Lot)	<i>NMRPT</i> allows additional PDF files to be included to the Additional Report of an Inspection Lot (e.g. additional experiments acquired outside <i>NMRPT</i> ).
Additional PDF (of report)	<i>NMRPT</i> allows additional PDF files to be included to a report (e.g. additional experiments acquired outside <i>NMRPT</i> ).
Additional Report	The Additional Report is an optional part of the <i>NMRPT</i> spectra PDF of each Inspection Lot. Additional measurements of <i>NMRPT</i> experiments (e.g. acquired under different conditions) can be added to the test document as Additional Report.
base shim file	A basic shim file for a probe, read in at the beginning of most Shim Commands. The shim file is named by the Probe ID. The base shim file is updated in <code>NPT_prep_tsopt</code> experiment.
converted parameters	The datasets included with <i>NMRPT</i> are automatically adjusted and optimized to the current hardware.
Current Specs	Specifications that can be set or changed in <i>NMRPT</i> . If Delivered Specs are available, Current Specs are set to the same values as a default. See <i>Specs</i> for further information.
Customer Sample	Each <i>NMRPT</i> test has to be done using standard samples. For comparison of results, a Customer Sample of the same composition can be used. It is created using laboratory chemicals available on site.
Delivered Specs	Specifications that are delivered with an external Inspection Lot.

Experiment Queue	Sequence of experiments in measurement order to be executed.
finalized report	A finalized report is the final document of a Final Test, Acceptance Test or Field Service Test for signature. Finalized means no further changes to the Inspection Lot, its experiments and results or documents can be done.
Inspection Lot	The Inspection Lot defines the test procedure for an NMR probe. It is created from Inspection Lot tab. The Inspection Lot consists of all experiments for a test combined with the required Bruker NMR standard samples. The experiment specifications are also included in the Inspection Lot.
irregular experiment	Depending on the experiment, it is set to irregular if measured under non-standard conditions (e.g. L23 options, temperature settings, flow settings). See documentation of experiments in ZUEP0102 for further information. Experiments are also set to irregular if status parameters of the data set are changed. Irregular experiments can not be used for report, but can be included in Additional Report.
Library	The set of experiments available in currently selected Inspection Lot.
Nucleus of Interest	The nucleus in focus of the experiment. The main result of the experiment is determined for this nucleus.
Pairing	A combination of an <i>NMRPT</i> experiment and a Bruker NMR standard sample defined in the Inspection Lot.
permitted characters	Permitted characters in <i>NMRPT</i> GUI text fields are the letters a-z(A-Z), the digits 0-9, '-' and '_'. No white space and no further special characters are permitted.
protocol	The <i>NMRPT</i> test protocol is part of the <i>NMRPT</i> report. It includes the signature page. Further content depends on the Test Mode and the Report Type of the report.
Queue	see <i>Experiment Queue</i> .
report	The <i>NMRPT</i> report is the document of an Acceptance, Field Service or Final Test. It consists of a test protocol and a spectra PDF. An Additional PDF can be included.
Recommended Flow	The Recommended Flow is the gas flow for temperature control, defined in the PICS of a probe.
Report Type	<i>NMRPT</i> knows three different Report Types: Spectrometer Report, Probe Report and Accessories Report. The Report Type affects how many Inspection Lots can be included to the report.
Shim Command	<i>NMRPT</i> Shim Commands are shim sequences represented by Shim Command numbers. All commands included in a sequence have to be executable from <i>TopSpin</i> command line. User Shim Commands can be created.

Short PDF	The Short PDF collates all single spectrum PDF files set to be used for report.
single spectrum PDF	A single spectrum PDF file is available from Results tab for each run of an experiment successfully acquired and processed.
Specs/Specifications	Specifications are target values to be proved by <i>NMRPT</i> results. Depending on the experiment also specifications for the definition of acquisition parameters exist. A Specs value of -1 means determination of results, but no comparing evaluation of results against specifications. Only positive values can be set as Specs.
spectra PDF	The <i>NMRPT</i> spectra PDF is part of the <i>NMRPT</i> report. It includes all single spectrum PDF files of experiment runs set to be used for report.
Test Mode	<i>NMRPT</i> knows three different Test Modes: Final Test, Acceptance Test and Field Service Test. The Test Mode defines the kind of resulting report and affects the set of mandatory experiments for an Inspection Lot.
Workspace	Area in the <i>NMRPT</i> GUI hosting tabs of different functionality.



## 3 Overview

### 3.1 About *NMRPT*

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*NMRPT* software provides a standardized Final Test, Acceptance Test and Field Service Test procedure of spectrometers and probes.

A set of standardized experiments is provided by *NMRPT* as described in ZUEP0102 accessible from *NMRPT* [Help menu](#) (see [1.5 Referenced Documents](#)). But the user can select only from the subset feasible to the current hardware (combination of probe, console, and routing). The datasets included with the *NMRPT* are automatically adjusted and optimized to the current hardware. If user interaction is necessary, the software will guide the user (e.g. through the parameter optimization).

A PDF file documents the results and spectra for each measurement successfully evaluated. *NMRPT* collates the results and spectra of all acquired experiments (one measurement per experiment) in a report. This report is the test document for the acceptance, a final test or a service of a spectrometer, parts of a spectrometer, a probe, or accessories.

#### Receiver Gain (RG)

The value for RG is predefined in each experiment. It is adjusted during setup. The usual standard values are  $RG_{min}$  or  $RG_{max}$ . In first case, *NMRPT* executes RGA to set the optimum value. In second case, *NMRPT* adopts the value. For a user controlled RG, the RG is set in the [Preparation panel](#) of *NMRPT* Acquisition page.  $RG_{min}$  and  $RG_{max}$  are derived from *TopSpin* configuration information (after execution of *cf*, see *TopSpin* manual). In *NMRPT* the maximum value of  $RG_{max}$  is limited to 203. If the  $RG_{max}$  value of the *TopSpin* configuration is lower, this value will be used.

#### Carrier Frequencies (O1 and O2)

The carrier frequency offset can be changed in all experiments where *NMRPT* does not optimize these settings. It is not recommended to change this except for the water suppression and MAS experiments when using specific options of L23 (see ZUEP0102, chapter [1.5 Referenced Documents](#) or *NMRPT* [Help menu](#)).

#### Loopcounter Parameter L23

The loopcounter L23 is used to apply special conditions in *NMRPT* experiments. The values allowed for each experiment are provided in the experiment description in ZUEP0102 (see chapter [1.5 Referenced Documents](#) or *NMRPT* [Help menu](#)). For some experiments (e.g. L23=27 in watersuppression experiment) changing the L23 value results in a non-standard experiment without a regular experiment output.

#### Gradient Strength (GPZx)

The used gradient strength (given in %) of all experiments (see ZUEP0102, chapter [1.5 Referenced Documents](#) or *NMRPT* [Help menu](#)) is related to a maximum gradient current of the probe. If the maximum current of a gradient amplifier differs from the one of the probe, the gradient strength is recalculated accordingly.

## 3.2 Test Modes

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The *NMRPT* software knows 3 different Test Modes:

- Final Test
- Acceptance Test
- Field Service Test

The Test Mode has to be selected at the beginning of a new NMR product test while [creating the Inspection Lot](#). Every Test Mode has its own test protocol. For example the Acceptance Test includes a Customer Training Checklist, the acceptance agreement and the signature line for customer's signature.

## 3.3 Report Types

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The *NMRPT* software knows three different Report Types:

- Spectrometer Report
- Probe Report
- Accessories Report

A report consists of a [test protocol](#) and a [spectra PDF](#). A Spectrometer Report consists of one or more probe tests. To cover a complex spectrometer type, it can be necessary to test with more than one single probe. So the Spectrometer Report includes the sum of all necessary probe tests and the specific spectrometer NMR tests.

Therefore 9 different test protocols exist as a combination of Test Mode and Report Type:

- Final Test Protocol, NMR Spectrometer
- Acceptance Protocol, NMR Spectrometer
- Field Service Protocol, NMR Spectrometer
- Final Test Protocol, NMR Probe
- Acceptance Protocol, NMR Probe
- Field Service Protocol, NMR Probe
- Final Test Protocol, Accessories
- Acceptance Protocol, Accessories
- Field Service Protocol, Accessories



## 3.4 NMRPT Documents

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The main document of *NMRPT* is the test report for signature. Beside this test report and its components, there are single spectra PDF files and a Short PDF providing information about the test results of an [Inspection Lot](#).

### 3.4.1 Test Report

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The *NMRPT* test report consists of a test protocol and a spectra PDF. As an optional part an Additional Report can be included to the spectra PDF. Optional additional PDF files (e.g. additional experiments from outside *NMRPT*) can also be included to the report.

Three different Report Types are provided (see [3.3 Report Types](#) and [5.4.5 Report Tab](#)):

- **Spectrometer Report**  
To cover a complex spectrometer type, it can be necessary to test with more than one single probe. So the Spectrometer Report can be based on multiple Inspection Lots. Therefore the report includes the sum of all necessary probe tests and the specific spectrometer NMR tests.
- **Probe Report**  
A Probe Report covers the test of a single probe. It is based on one Inspection Lot covering all probe tests necessary for the probe type.
- **Accessories Report**  
An Accessories Report covers all tests specific for the tested accessories. Therefore it can be based on multiple Inspection Lots, but can also be created without any Inspection Lot (e.g. if no NMR tests are applicable to an accessory).

In combination with the available Test Modes – Final Test, Acceptance Test and Field Service Test (see [3.2 Test Modes](#)) – 9 different test protocols are provided by *NMRPT*.

A test report is created from Report tab (see [5.4.5 Report Tab](#)). Each report is marked as preliminary while under review. To remove the label “preliminary” and to get the valid documents for signature, a report needs to be [finalized](#).

## 3.4.1.1 Protocol

The *NMRPT* test protocol consists of a signature page and a summary of all included Inspection Lots covering the test results of all experiments set to be **used for report**. In case of an Acceptance Protocol an Installation Checklist is included. The Service Protocol of a spectrometer includes a Service Checklist.

Acceptance Protocol		NMR Spectrometer	
<b>Customer Information</b>			
Customer Name	A. Muster	Operator Name	B. Kundenoperator
Company	Mustercompany AG	Address	WSW 502.1308
Postal Code / City / Country	4051 Basel, Schweiz	Phone Contact Customer	+41 (0)1234567
Fax	+41 (0)1234567	E-Mail	a.muster@mustercompany.com
<b>Bruker Information</b>			
Office	Bruker, Faelanden	Engineer	M. Brukerengineer
Central Hotline Phone	+49 (0)721 5161 6155	Central Hotline E-Mail	support@bruker-biospin.com
<b>Spectrometer Information</b>			
Order No.	10014051	Contract No.	123456789
System	AVIII 500	Coil	BZH 002 30 40E
Dewar	D123 45-6789	Location	3.123
TopSpin Version	3.5.b.27 pl 0 (of October 5 2014) - Build 1784		
<b>Acceptance</b>			
1) I confirm that below-mentioned tests were performed during installation and meet the published or contractually agreed specifications.			
2) In accordance with the terms of sale, the period of warranty will end (see exclusions) on Jan 15, 2014.			
3) I accept that installation is complete (see exclusions) as per sales agreement and I authorize payment of the outstanding balance due for this system.			
Place:	4051 Basel, Schweiz	Place:	4051 Basel, Schweiz
Date:	Oct 14, 2014	Date:	Oct 14, 2014
Customer Representative Signature		Bruker Representative Signature	
A. Muster		N. Brukerengineer	
ZPPT0008		Bruker Biospin AG	
Index: 00		BBD	
		Report Name: CA2Test	

Figure 3-1: Signature page of Acceptance Protocol NMR Spectrometer

The signature page meets the requirements of each combination of Test Mode and Report Type. It provides information about tested hardware and the signing parties. In case of all Acceptance protocols also the wording of acceptance is included on signature page.

## 3.4.1.2 Spectra PDF

The spectra PDF includes all single spectrum PDF files of experiment runs set to be **used for report**. These spectra and the optional Additional Reports (including optional Additional PDFs of each Inspection Lot) are grouped to chapters by the Inspection Lot. Probe and spectrometer related information, information about the PICS, ATMA data and required samples are also included to the Inspection Lot chapter. Additional PDFs of the report are appended to the end of the Spectra PDF.

A Probe Report covers one Inspection Lot chapter. In case of an Accessories Report the spectra PDF may collate multiple Inspection Lot chapters. The spectra PDF of a Spectrometer Report may also cover multiple Inspection Lot chapters and includes configuration information and IP config information about the spectrometer.

### Additional Report (optional)

The Additional Report is an optional part of *NMRPT* spectra PDF of each Inspection Lot. Additional measurement runs (e.g. acquired under different conditions) of *NMRPT* experiments can be [added to the test document](#) as Additional Report.

### Additional PDFs of Inspection Lot (optional)

Additional PDF files can be included to the Additional Report of each Inspection Lot (e.g. additional experiments acquired outside *NMRPT*) from Results tab. See chapter [5.4.4 Results Tab](#) for further information.

### Additional PDFs of Report (optional)

Additional PDF files can also be appended to the spectra PDF of each report on Report tab. See chapter [5.4.5 Report Tab](#) for further information.

## 3.4.2 Single Spectrum PDF

A single spectrum PDF file is available from [Results Tab](#) for each run of an experiment successfully acquired and processed (indicated by a green status icon or yellow exclamation mark – see chapter [5.4.4 Results Tab](#)).

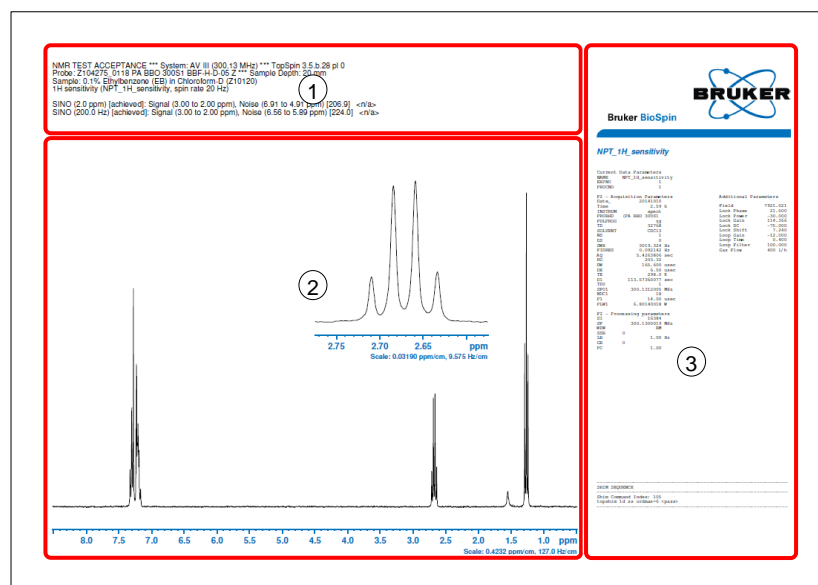


Figure 3-2: Single spectrum PDF

The single spectra PDF shows the resulting spectrum (Figure 3-2 (2)). Depending on the experiment also an expansion, multiple spectra or plots are provided. The title of the single spectrum PDF (Figure 3-2 (1)) provides the results of the acquired experiment including the comparison to [specification values](#) if available (see chapter [5.4.1 Inspection Lot Tab](#)). The title also includes information about the used NMR system, the *TopSpin* version, the probe and the sample the experiment was acquired on. Further information e.g. about the sample depth or rotation status may also be provided. Right of the spectrum (Figure 3-2 (3)) acquisition, processing and additional parameters are shown and information about the applied shim sequence is provided.

The single spectrum PDF is the result page of an experiment run as collated by the [short PDF](#) or the [spectra PDF](#) of a [report](#) if the respective run is included.

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**i** Further information about experiments, parameters and resulting spectra is provided in ZUEP0102 accessible via *NMRPT* [Help menu](#) (see chapter [1.5 Referenced Documents](#)).

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### 3.4.3 Short PDF

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The Short PDF provides a shortened preview of the current spectra PDF for this Inspection Lot: It collates all single spectrum PDF files set to be [used for report](#) but includes no further information about the probe and no [Additional Report](#) or [Additional PDF](#) files. The Short PDF is accessible from [Results tab](#).

### 3.5 Workflow

This basic *NMRPT* workflow shows the procedure from setup over measurement to the creation of a finalized report. All additional options and optional settings beside this basic workflow can be found in chapter 5 [GUI-Description](#).

An Acceptance Test of a probe is used as an example. The probe is assumed to be installed and configured in *TopSpin* via *edprobe* and all customer and spectrometer information to be provided via *edcstm*. The *TopSpin* prosol tables are assumed to be prefilled with approximate pulse values. The standard samples are assumed to be available. A sample changer is not required (see chapter 4.1 [Sample Change Modes](#)), but if available, the sample changer is recommended to be ready for use.



The commands *edprobe*, *edcstm* and the prosol functionality are part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter 1.5 [Referenced Documents](#)).

1. Enter *nmrpt* to *TopSpin* command line to start *NMRPT*. The *NMRPT* main window is divided into four main areas:

- (1) [Menu Bar](#)
- (2) [Acquisition Bar](#)
- (3) [Workspace](#)
- (4) [Navigation](#)

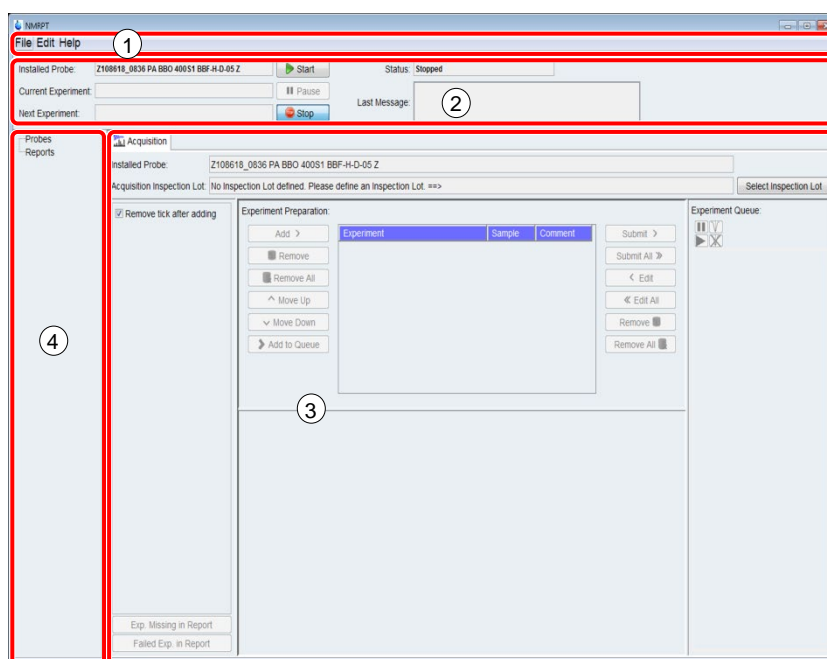


Figure 3-3: *NMRPT* main window at first start.

- On the **File** menu shown in Figure 3-4 (1), point to **New**, and then click **Probe / Inspection Lot** (2). The New Probe / Inspection Lot dialog opens up.

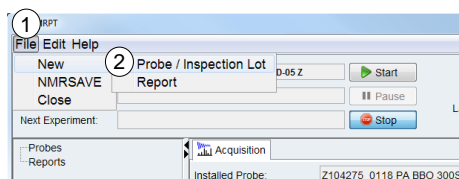


Figure 3-4: Create new Inspection Lot for probe

- Enter an **Inspection Lot Name** (Figure 3-5 (1)) and select the **Probe ID** from the list (Figure 3-5 (2)). Keep the default settings of further options. Click **OK** to apply and continue.

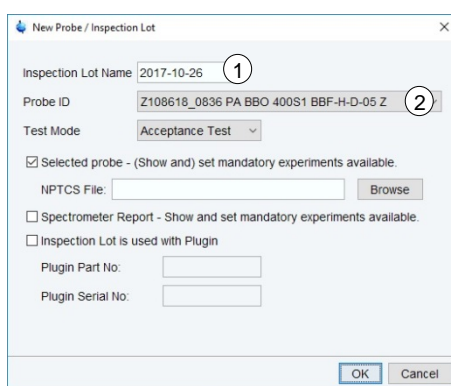


Figure 3-5: Basic settings for a new Inspection Lot

- Select a sample for each experiment or a group of experiments as shown in Figure 3-6. Click **OK** to apply and continue.

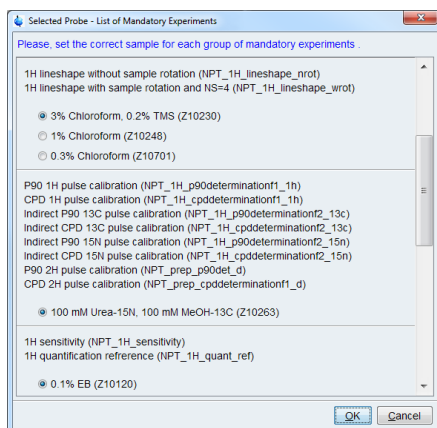


Figure 3-6: Sample selection for experiments

5. The **Inspection Lot** tab opens in **NMRPT Workspace**. Click on table entries to select a combination of experiment (Figure 3-7 (1)) and sample (Figure 3-7 (2)). The corresponding experiment specifications are listed in a third table shown in Figure 3-7 (3).

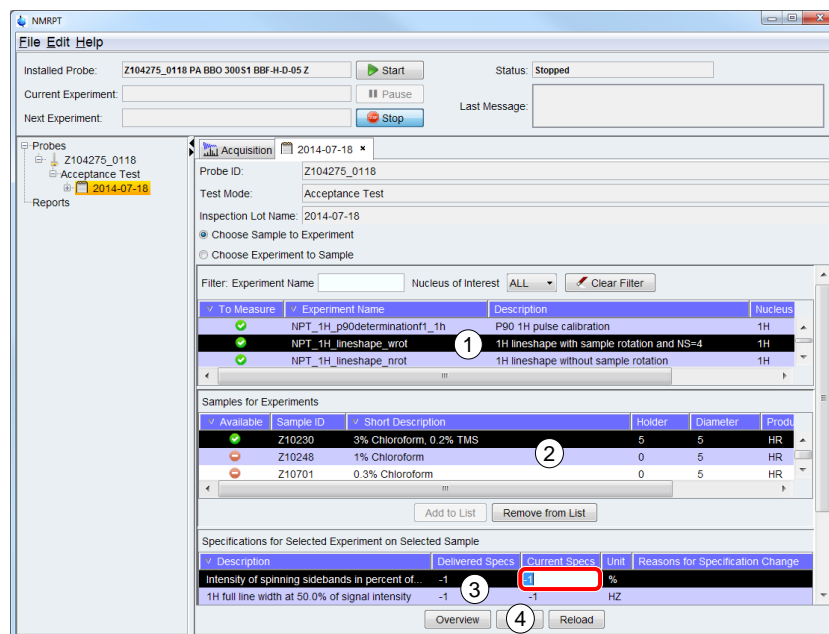


Figure 3-7: Set experiment specifications on Inspection Lot tab

6. Click into **Current Specs** cell of an experiment specification item in table (3) shown in Figure 3-7. Enter the new value to be applied.
7. Repeat step 5 and 6 for all experiments to be specified.
8. When finished, click **Save** (Figure 3-7 (4)) to apply all changes.
9. In Menu Bar, select **Edit** menu shown in Figure 3-8 (1) and click **Sample List** (2). The Sample List dialog opens up.

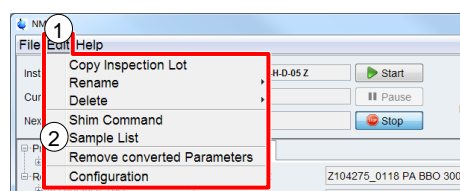


Figure 3-8: Open Sample List

**i** Step 9 and 10 can be skipped if no sample changer is used. These steps are only relevant to set appropriate default sample changer positions.

- In Sample List dialog (Figure 3-9) click **Set Default Holder** (3) and place each sample in the sample changer position shown in **Holder** column (1). Click **Apply and Close** (2) when finished.

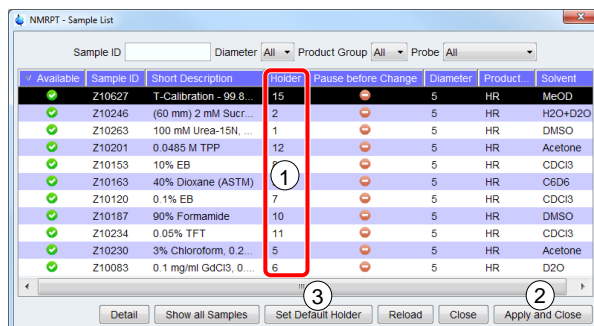



Figure 3-9: Set Default Holder in Sample List

- Click the  **Acquisition** tab (Figure 3-10 (1)) in *NMRPT Workspace* to switch to the **Acquisition** tab.

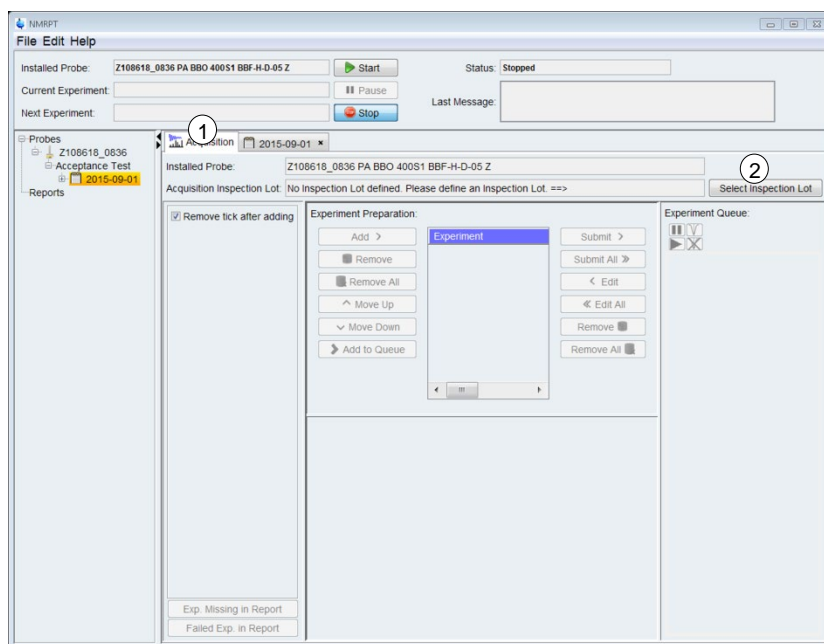


Figure 3-10: Select Inspection Lot on Acquisition tab

- On the **Acquisition** tab (Figure 3-10) click **Select Inspection Lot** (2).
- Choose Inspection Lot to measure** from the list in the dialog window shown in Figure 3-11. Click **OK** to apply the selection. Click **Cancel** to abort selecting an Inspection Lot for acquisition.

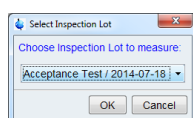


Figure 3-11: Select Inspection Lot from list



14. Click the **Recommended Experiment Sequence** check box (Figure 3-12 (1)) in the **Library**. The recommended set of experiments in recommended measurement order is selected.

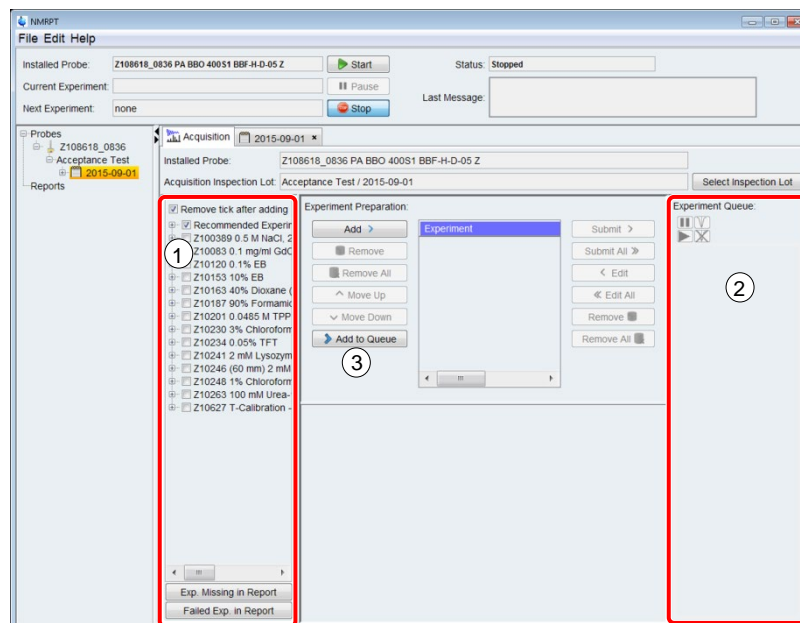


Figure 3-12: Enqueue Recommended Experiment Sequence

15. Click **Add to Queue** (Figure 3-12 (3)) located in **Experiment Preparation** panel to enqueue experiments for measurement. The experiments are then listed into the **Experiment Queue** (Figure 3-12 (2)).

16. Click **Start** (Figure 3-13 (1)) located in the **Acquisition Bar** to start the sequence of experiments as listed in Experiment Queue (Figure 3-13 (2)).

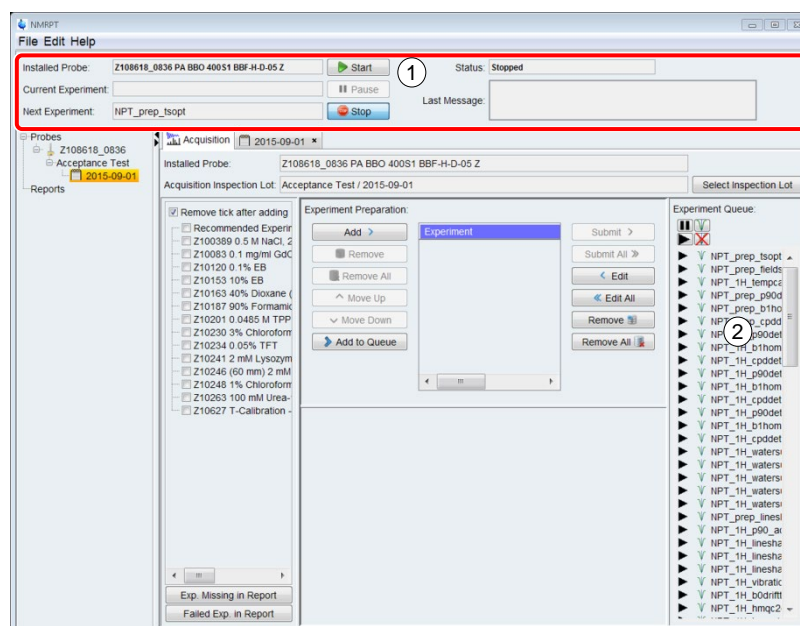


Figure 3-13: Start of Experiment Queue

- In the Startup Check dialog (Figure 3-14) click **wsh** (1). A base shim file is written.

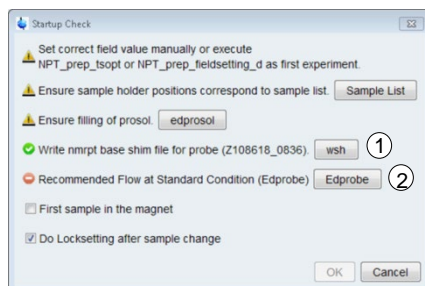




Figure 3-14: Startup Check dialog

**i** The write shim command **wsh** is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter 1.5 Referenced Documents).

- If a red error symbol  appears next to **Recommended Flow at Standard Condition (Edprobe)** in Startup Check dialog (Figure 3-14): Click **Edprobe** (Figure 3-14 (2)) to set Recommended Flow in *TopSpin* edprobe dialog.

**i** The **edprobe** command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter 1.5 Referenced Documents).

- In Startup Check dialog (Figure 3-14) click **OK** to start the measurements.
- Open  **Results** tab from **Navigation** (Figure 3-15 (1)): The Results tab is a sub-item of the Inspection Lot. Expand the Inspection Lot item and click the Results item to open. While the Queue is acquired, the results will appear one after another.

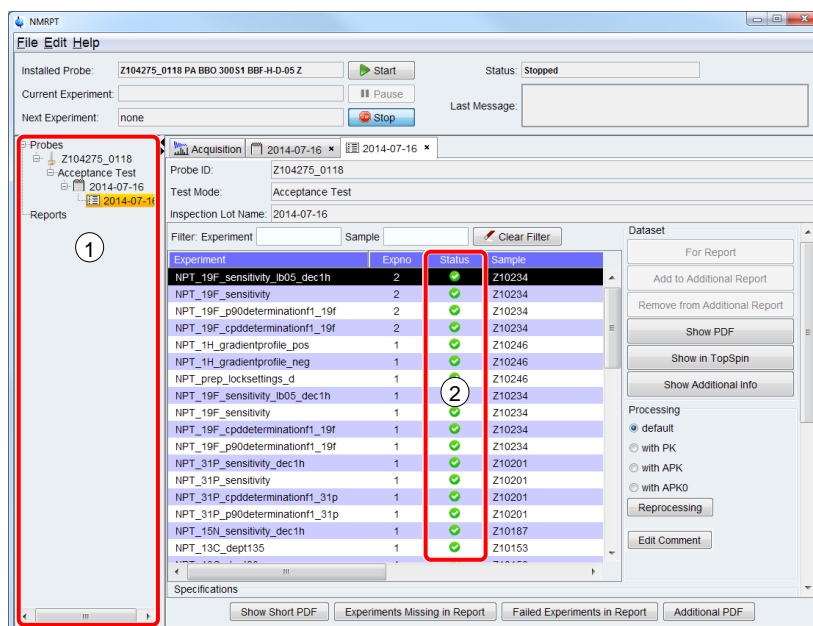



Figure 3-15: Check of experiments on Results tab

21. Check if all experiments were successful. Success is indicated by a green icon  in **Status** column (Figure 3-15 (2)).
22. Working with non-successful experiments: To re-execute, go back to step 14 but select the individual experiments instead of the Recommended Experiment Sequence. To change specifications, edit as described in steps 5 and 6. See chapter 5 [GUI-Description](#) for additional options.
23. On the **File** menu shown in Figure 3-16 (1), point to **New**, and then click **Report** (2). The New Report dialog opens.

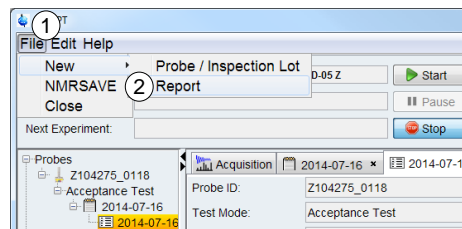


Figure 3-16: Create new Report for probe

24. Enter a **Report Name** (Figure 3-17 (1)) and select the Inspection Lot from the list (Figure 3-17 (2)). Keep the default settings of further options. Click **OK** to apply and continue. The **Report** tab (Figure 3-18) opens in [NMRPT Workspace](#).

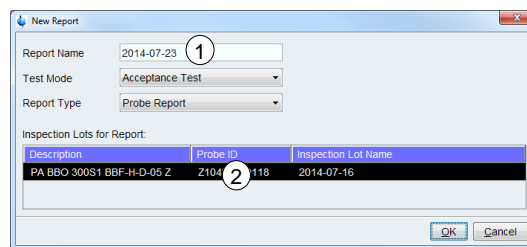


Figure 3-17: New Report dialog

## i

### Information for Report Creation

Enter all available information on Report tab. This information is used to create and fill the final document for signature. Empty information may result in an invalid document.

Figure 3-18: Preparation of NMRPT report on Report tab

25. Click **edcstm** (Figure 3-18 (1)) under **General Information** to open *TopSpin* Edcstm dialog. Enter all mandatory information.

**i**

The `edcstm` command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter 1.5 Referenced Documents).

26. Under **General Information** (Figure 3-18) enter **Engineer** and **Duration of Warranty in months**.
27. Under **Probe Information** (Figure 3-18) enter **Order No.** and **Contract No.**
28. Scroll down to find **Installation, Training, Acceptance and Warranty** and **Optional Components** check lists. Select statuses for the list entries.
29. Click **Save** (Figure 3-18 (6)) to apply all changes.
30. Click **Create Protocol & Spectra** (Figure 3-18 (5)) to create a preliminary report.
31. Check the report documents. Click **Show Protocol** (Figure 3-18 (4)) to access protocol PDF. To access spectra PDF click **Show Spectra** (Figure 3-18 (3)).
32. Click **Finalize** (Figure 3-18 (2)) to create the valid report.

33. In Finalize dialog (Figure 3-19) click **Yes** to accept, that the Inspection Lot used for the finalized report can not be used for another report.

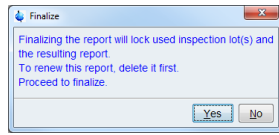


Figure 3-19: Finalize report message

34. Access the finalized report as described in step 31.



---

For basic information about *NMRPT* also see the *NMRPT* Short Guide accessible via *NMRPT* [Help menu](#) (ZHUB0001, chapter [1.5 Referenced Documents](#)).

---



## 4 Practical Advices

### 4.1 Sample Change Modes

*NMRPT* can be used with a sample changer but also handle manual sample change.

If a sample changer is detected, the option to use the sample changer (see [5.1.2.11 Configuration](#)) is set automatically as a default but can be deselected. If deselected, all samples are automatically configured to be changed manually.

It is also possible to change specific samples manually. Set manual change option for individual samples in Sample List (see [5.1.2.9 Sample List](#)).

If no sample changer is detected by *NMRPT*, the usage of a sample changer is automatically deselected. All samples are automatically configured to be changed manually.

In manual changing mode, *NMRPT* pauses the Queue and after an acoustic signal dialogs are provided to guide the user through sample change procedure.

**i**

Holder position 0 means manual sample change. If the Use Sample Changer option is deselected in [NMRPT Configuration](#), all holder positions are set to 0.

If the Use Sample Changer option is selected, samples set to be changed manually are not included to the [Recommended Experiment Sequence](#). For LC, HRMAS and MAS often there is no appropriate sample changer available. Therefore especially in these cases it may be useful to deselect usage of a sample changer to include all experiments to Recommended Experiment Sequence.

### 4.2 Gas Flow Control

As a default *NMRPT* handles setting the gas flow for temperature control in each experiment. The desired flow value is set at the beginning of each experiment. The [Recommended Flow](#), a value provided by the PICS of a probe, is applied for all experiments except for watersuppression experiments. These watersuppression experiments are named by the individual flow value applied.

Select **Skip Gas Flow Setting** (Figure 4-1 (5)) on [Probe Setup tab](#) to skip setting the gas flow by *NMRPT* for all experiments of all Inspection Lots of this probe as a default.

To skip setting the gas flow by *NMRPT* for a single experiment, Select **Skip Gas Flow Setting** in [Experiment Preparation](#) panel on [Acquisition tab](#).

If the temperature unit is set to external mode (e.g. operating some MAS and HRMAS probes), Skip Gas Flow Settings are disabled and automatically applied.

**i**

Watersuppression experiments are set to [irregular](#) if setting the gas flow is skipped.

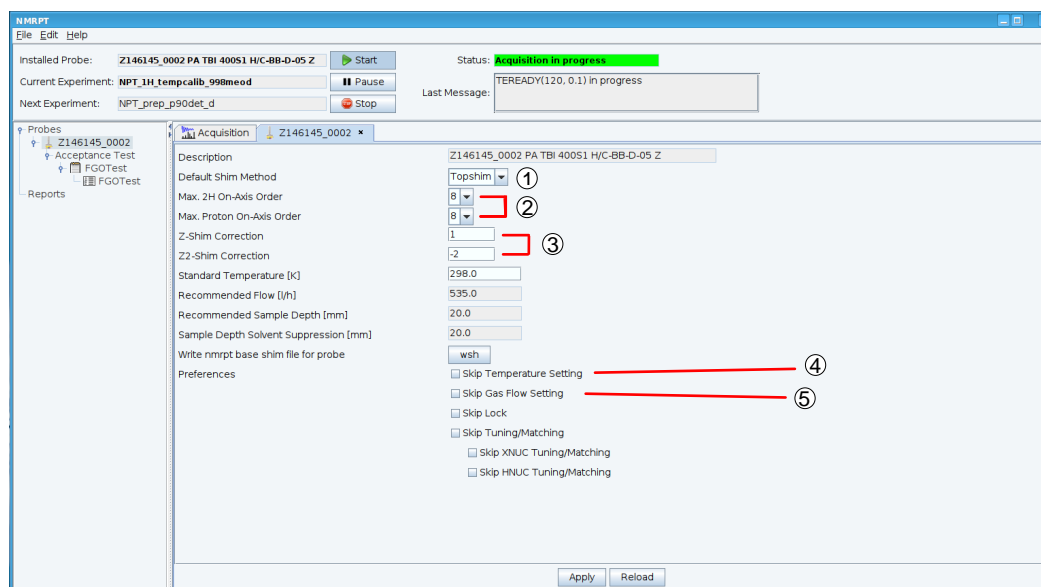


Figure 4-1: Probe Setup tab – Flow, Temperature and Shim options

## 4.3 Temperature Control

By default, the target temperature for temperature control is handled by *NMRPT*. The desired temperature is set at the beginning of each experiment. The Standard Temperature, as set on [Probe Setup tab](#), is applied for all experiments.

Select **Skip Temperature Setting** (Figure 4-1 (4)) on Probe Setup tab to skip setting the temperature by *NMRPT* for all experiments of all Inspection Lots of this probe as a default.

To skip setting the temperature by *NMRPT* for a single experiment, Select **Skip Temperature Setting** in [Experiment Preparation](#) panel on [Acquisition tab](#).



Watersuppression experiments are set to [irregular](#) if setting the temperature is skipped.

### 4.3.1 Selftune

#### BSVT temperature unit installed

If option [Skip Temperature Setting](#) is not applied, *NMRPT* handles selftune process automatically. *NMRPT* reads the selftune settings for the current probe and target flow before acquisition of each experiment. If no selftune settings are available for this flow, *NMRPT* initializes a selftune and the creation of the corresponding selftune settings.



The selftune settings are named by the [Probe ID](#) and the [relevant gas flow](#) (or “external” in case of external mode for gas flow) appended with underscore, e.g. Z104275\_0118\_400.

All available selftune settings are listed in *Temperature Control Suite* window, accessible via `vtudisp` command from *TopSpin* command line. To re-execute a selftune for a specific gas flow, delete the corresponding selftune settings from this list.



The *Temperature Control Suite* is a software interface available if a Bruker Smart Variable Temperature unit is installed. See Z33073 (chapter [1.5 Referenced Documents](#)) for further information.

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## 4.4 NMRPT Shim Handling

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[NMRPT Shim Commands](#) encompass sequences of combined *TopSpin* and *TopShim* commands. The *NMRPT* Shim Commands are indicated by shim numbers.

### Default Shim Method

In *NMRPT* Probe Setup Tab (see [5.4.2 Probe Setup Tab](#)) select the **Default Shim Method** (Figure 4-1 (1)) for this probe. The selection is applied to all Inspection Lots of the probe.



The selected Default Shim Method affects the default Shim Commands of all experiments included to all Inspection Lots of the probe. The default Shim Command is the preselected [Shim Command](#) provided in [Experiment Preparation](#) panel on [Acquisition tab](#).

---

### Reduce Ordmax Options

The `ordmax` parameter of *TopShim* defines an upper limit for the order of shim functions used by *TopShim*. In *NMRPT* [Probe Setup tab](#) multiple options (Figure 4-1 (2)) are provided to reduce the maximum shim orders according to this `ordmax` parameter.

These *NMRPT* maximum shim order options are applied to the *NMRPT* Shim Commands and therefore the complete sequence encompassed. Available options are:

- Max. 2H On-Axis Order
- Max. Proton On-Axis Order
- Max. Proton Off-Axis-Order

As a default, these settings are applied to all experiments. To skip these settings, deselect Reduce Ordmax according to probe setting in [Experiment Preparation](#) of a single experiment.

### Z-Shim Correction (not MAS, SOL probes)

*NMRPT* [Probe Setup Tab](#) provides a Z- and Z2-Shim Correction (Figure 4-1 (3)) to be set for a probe. The correction is applied at the end of the shim process during water

suppression experiments. If *NMRPT* Shim Command 999 (skip shimming) is selected for an experiment, Z- and Z2-Shim Correction is not applied.

## 4.5 Locksetting

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For HR and HRMAS probes *NMRPT* provides the opportunity of an automatic and solvent-dependent optimization of lock parameters.

The locksetting experiment optimizes the lock parameters according to the LOOPADJ macro. As a basis of computation the standard parameters of the corresponding solvent from EDSOLV are used. The results are written to the Edlock tables. In case of the solvents Acetone and Benzene-D6 stronger coupling conditions (according to a lock gain of 83.9 dB) are applied.

Select [Do Locksetting after sample change](#) option in [Startup Check dialog](#) (see chapter [5.2 Acquisition Bar](#)) to execute a 2H locksetting experiment after each sample change. This experiment is acquired automatically in background before the first experiment of this sample is executed.

To do 19F locksettings, acquire the corresponding locksetting experiment from Queue.

The locksetting experiments are named NPT\_prep\_locksettings and the lock nucleus appended with underscore.



The LOOPADJ macro, the Edlock and the Edsolv tables are part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

---

## 4.6 Converted Parameter Sets

The datasets included with *NMRPT* are automatically adjusted to the current hardware and spectrometer routing when an experiment is added from [Library](#) to [Experiment Preparation panel](#) or [Experiment Queue](#). *NMRPT* keeps converted experiment parameters while open and a probe stays defined as current via `edprobe` in *TopSpin*. Converted parameters can be deleted manually (see [5.1.2.10 Remove Converted Parameters](#)) to enforce parameters to be converted again, e.g. if manual re-routing is necessary.

**i**

The definition of the spectrometer routing is part of *TopSpin*. It can be accessed via `edaspt` command from *TopSpin* command line. The `edprobe` command is also part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

## 4.7 Additional Information

[Additional Information](#) for each run of an experiment is accessible from Results tab (see [5.4.4 Results Tab](#)). The Show Additional Info dialog provides detailed status and log messages of the run. Show Expert Messages option provides more detailed expert information.

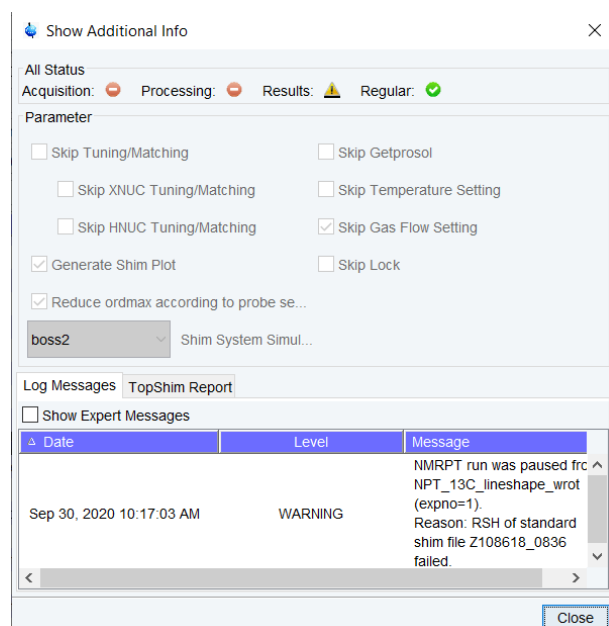


Figure 4-2: Show Additional Info dialog (see Additional Information in 5.4.4 Results Tab)

Besides the log messages one can find the information included in the TopShim report file via clicking on the TopShim Report field next to the Log Messages field.

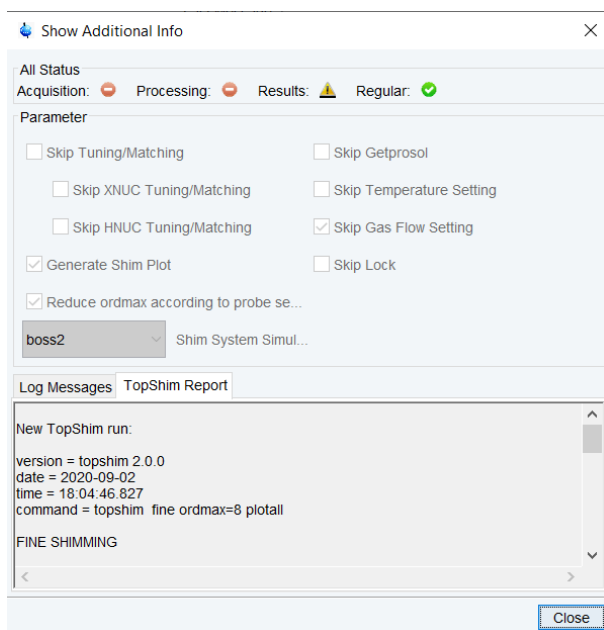


Figure 4-3: Show Additional Info dialog with TopShim report (see Additional Information in 5.4.4 Results Tab)

## 4.8 How to Debug

Information for debugging purposes concerning *NMRPT* can be found in several places, specific for the problems which occurred:

- The [Additional Information](#) dialog of each experiment, accessible from Results tab, provides detailed status and text messages of the experiments including Expert Messages for debugging purposes.
- Use [Show in TopSpin](#) button on [Results tab](#) to access the spectrum, the data set, acquisition and processing parameters, the routing etc. of an *NMRPT* experiment run to debug experiment related problems.
- *TopSpin* history file includes experiment related log entries of *NMRPT*.
- *TopSpin* Java history file provides GUI related log information about *NMRPT*.

**i**

*TopSpin* history file and Java history file are both available combined in *TopSpin* history and protocol dialog. Use `hist` command from *TopSpin* command line to open this dialog. The `hist` command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

## 4.9 Troubleshooting

### Configuration, Sample List, Shim Command

Indication	Solution
Configuration dialog: Usage of Sample Changer not selected, number of holder positions not set	Check if the sample changer is correctly installed and configured in <i>TopSpin</i> . If so, select <a href="#">usage of sample changer</a> in <i>NMRPT</i> and set number of holder positions manually.
Sample List dialog: Availability of sample can not be changed	The availability of <a href="#">Customer Samples</a> can not be changed. <a href="#">Delete a Customer Sample</a> to remove it from the list of available samples.
Shim Command dialog: Edit Command button is disabled	Default Shim Commands can not be edited. Select a Shim Command Number between 800 and 824 to <a href="#">create a custom</a> Shim Command.

Table 4-1: Troubleshooting – Configuration, Sample List, Shim Command

### Inspection Lot

Indication	Solution
Probe not listed to create a new Inspection Lot for	The probe needs to be installed to <i>TopSpin</i> via <i>edprobe</i> at least once. See <i>TopSpin</i> manuals (chapter <a href="#">1.5 Referenced Documents</a> ) for information about how to install a probe via <i>edprobe</i> .
Empty List of Mandatory Experiments while creating a new Inspection Lot	An empty List of Mandatory Experiments indicates missing or inappropriate probe information. Continue the creation of the Inspection Lot to see if experiments are available on Inspection Lot tab.
Experiments / samples missing in Inspection Lot tab	Use <i>TopSpin edprobe</i> functionality (chapter <a href="#">1.5 Referenced Documents</a> ) to check all probe properties (e.g. probe type, diameter, nuclei, peak powers etc.). Correct probe properties are required to get an appropriate set of experiments for Inspection Lot. To fix incorrect PICS, please contact NMR support (see <a href="#">6 Contact</a> )
Inspection Lot can not be changed	The Inspection Lot is included to a <a href="#">finalized report</a> can not be changed. Corresponding buttons are disabled. <a href="#">Delete</a> the finalized report first and then edit the Inspection Lot.

Table 4-2: Troubleshooting – Inspection Lot

## Acquisition

Indication	Solution
Wrong probe shown as Installed Probe	The probe to be used needs to be the current probe according to <i>TopSpin</i> <code>edprobe</code> . See <i>TopSpin</i> manuals (chapter 1.5 Referenced Documents) for information about <code>edprobe</code> .
Inspection Lot can not be selected for acquisition	The Inspection Lot is included to a <a href="#">finalized report</a> . Therefor the Inspection Lot is locked and can not be changed, e.g. by acquisition of new data. <a href="#">Delete</a> the finalized report to make the Inspection Lot available again.
Empty Library of experiments	Check if the desired <a href="#">Inspection Lot is selected</a> for Acquisition. Ensure that the required pairings of experiments and samples for this Inspection Lot are <a href="#">set to be measured</a> . Check if the required samples are set available in <a href="#">Sample List</a> .
Non-Routable Experiments are listed in Library	Depending on the hardware not all required nuclei for experiments of the Inspection Lot may be routable at the same time. Change current routing or check for errors via <code>edasp</code> and <code>edasp probe</code> . See <i>TopSpin</i> manuals (chapter 1.5 Referenced Documents) for information about <code>edasp</code> .
Unexpected experiment settings in Experiment Preparation or Queue	Check default settings for the current probe on <a href="#">Probe Setup tab</a> . Also check settings for sample change modes in <a href="#">Sample List</a> and NMR
Queue is paused but Pause button was not used	Check if <a href="#">Pause before Acquisition</a> was selected for the upcoming experiment in <a href="#">Experiment Queue</a> . Check if <a href="#">Pause before Sample Change</a> was selected for the upcoming sample in <a href="#">Sample List</a> . In both cases, press <a href="#">Start</a> to continue. Check if Experiment Queue was paused due to failed experiments. If general steps of experiments fail (like RSH of standard shim file), the Queue is paused to avoid a series of failed experiments.
Experiments in Queue are skipped	Check if <i>NMRPT</i> was <a href="#">configured</a> to skip experiments on samples with option <a href="#">Pause before Change</a> in a certain time span. The experiments will remain enqueued while others are executed. Deselect this option to acquire all experiments in Queue order.
A message about missing pulse or power values occurs	Check if generic prosol tables for the current probe are filled correctly. For experiments including a manual interaction part demanding to check parameters: Set and check all required values including the ones listed in the message. See <i>TopSpin</i> manuals (chapter 1.5 Referenced Documents) for information about prosol.
Experiment is aborted due to missing Specs	A few experiments need certain specification values for acquisition. The abort dialog message provides further information. <a href="#">Set these Specs</a> on Inspection Lot tab.

Table 4-3: Troubleshooting – Acquisition

## Results

Indication	Solution
Experiment run is marked successful but can not be selected for report	The experiment run was set <a href="#">irregular</a> due to non-standard conditions of the experiment (e.g. some L23 options). Select the experiment run <a href="#">for Additional Report</a> to include it to the test report. See ZUEP0102 (chapter <a href="#">1.5 Referenced Documents</a> ) for further information about standard and irregular conditions.

Table 4-4: Troubleshooting – Results

## Report

Indication	Solution
Inspection Lot not available for creation of new report	Select the correct Test Mode in <a href="#">New Report dialog</a> . Only Inspection Lots of the selected Test Mode are listed and can be included to a report. Inspection Lots can only be included to one report. To make an Inspection Lot available again, <a href="#">delete</a> the existing report.
Selection of multiple Inspection Lots for creation of a report is not possible	Select the correct Report Type in <a href="#">New Report dialog</a> . For Spectrometer and Accessories Reports multiple Inspection Lots can be selected for report. In case of a Probe Report only one Inspection Lot can be selected.
Information on first page of report or checklist incomplete	Check if all details on Report tab are filled with appropriate data. Click edcstm button on Report tab to check if all details of customer/spectrometer information are filled.
Report can not be finalized	Use <a href="#">Experiments Missing in Report</a> button on <a href="#">Results tabs</a> of all included Inspection Lots to check if all experiments included to the Inspection Lots have been acquired. To force finalization, <a href="#">remove</a> the experiments from Inspection Lot. Check if all details on Report tab are filled with appropriate data. Click edcstm button on Report tab to check customer/spectrometer information.

Table 4-5: Troubleshooting – Report

## 4.10 How to Report a Bug

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If you have questions or problems concerning *NMRPT*, please, contact your local Key User. Further support is provided by the NMR Support (see chapter 6 [Contact](#)).

When you identify a major bug in *NMRPT*, please, report it to Bruker NMR/MRI Software Knowledge Base:

[http://www.bruker.com/nc/bkb\\_access.html](http://www.bruker.com/nc/bkb_access.html)

All *NMRPT* specific bug reports can be found under the category combination of “TOPSPIN” (**Program** list) and “product test” (**Component** list). Please, ensure that the bug was not reported yet. Assign a new bug report to the category combination of “TOPSPIN” and “product test” (select from **Component** list), too.

When reporting a bug, always have an **NMRSAVE** backup of the reported state ready at hand. Select **NMRSAVE** from *NMRPT* file menu to create this backup of installation specific files including all *NMRPT* data and *NMRPT* measurement results.



## 5 GUI-Description

This *NMRPT* GUI Description is a reference manual with detailed descriptions of all functionalities, options and settings in *NMRPT*, their application, effects and results.

To start *NMR Product Test* software (*NMRPT*) use `nmrpt` command in *TopSpin* command line. The *NMRPT* software opens up in a separate window divided into four main areas:

- (1) Menu Bar
- (2) Acquisition Bar
- (3) Workspace
- (4) Navigation

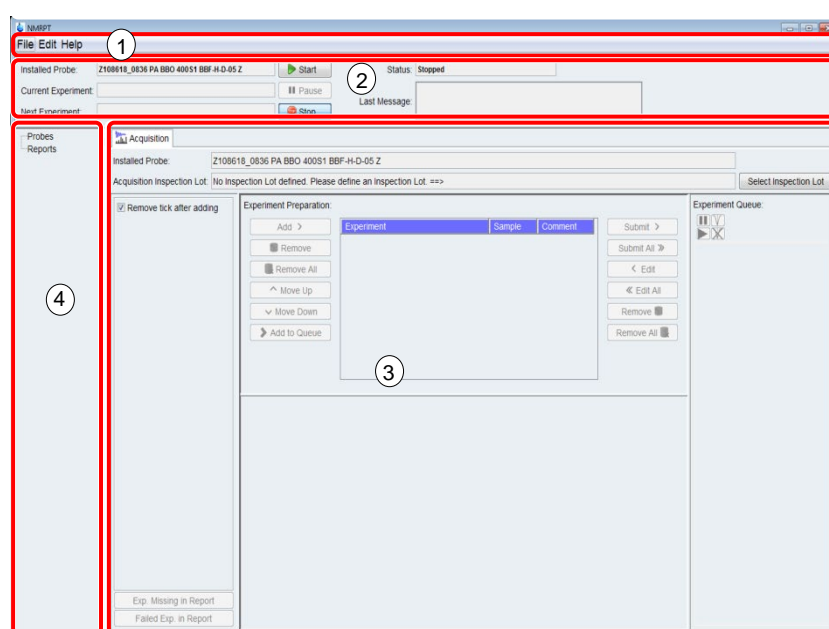


Figure 5-1: NMRPT main window with main areas

### 5.1 Menu Bar

#### 5.1.1 File

File menu shown in Figure 5-2 (1) provides

- the creation of new Inspection Lots (3)
- the creation of new reports (2)
- NMRSAVE option (including all *NMRPT* data) (5)
- the option to close *NMRPT* (4)



#### 5.1.1.1 New > Probe / Inspection Lot

On the **File** menu shown in Figure 5-2 (1), point to **New** (6), and then click **Probe / Inspection Lot** (3). The New Probe / Inspection Lot dialog (Figure 5-3) opens up.



### New Probe / Inspection Lot Dialog (Figure 5-3)

- (1) **Inspection Lot Name**  
Enter an individual name for the new Inspection Lot (see chapter 2.2, [permitted characters](#)). The current date is suggested as a default.
- (2) **Probe ID**  
From the list select the probe the new Inspection Lot is created for. The list contains all probes registered to *TopSpin* via *edprobe*. The probe does not need to be currently installed to create the Inspection Lot. The characteristics of the probe affect the sets of available and [mandatory experiments](#) (4).

The `edprobe` command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter 1.5 Referenced Documents).

- (3) **Test Mode**  
Select the **Test Mode** from the list. The Test Mode defines the kind of resulting report and affects the set of **mandatory experiments** (4) for the Inspection Lot.
- (4) **Selected Probe – Show and set mandatory experiments available**  
Select this checkbox to set combinations of mandatory experiments and samples available for this Inspection Lot. The selected **Probe ID** (2) and **Test Mode** (3) affect the set of mandatory experiments. This option opens a subsequent dialog (shown in Figure 5-4) during the creation of the Inspection Lot.

## (5) NPTCS File

This file contains the customer specification.

It can be downloaded from <http://nmr-product-test.bruker.com> for probes produced after August 2016. When a file has been loaded earlier on, the input field is disabled and shows the text "From existing File".

For newer probes, connected direct with BFB, the file is provided by the probe. In this case the input field is disabled and shows the text "From Probe".

## (6) Spectrometer Report – Show and set mandatory experiments available

If a Spectrometer Test is done, select this check box to add a set of spectrometer specific experiments to the Inspection Lot. These experiments usually have to be included in only one of the Spectrometer Report related Inspection Lots. An additional dialog (shown in Figure 5-5) opens during the creation of the Inspection Lot.

## (7) Inspection Lot is used with Plugin

If the probe is equipped with a plugin, select this check box. **Plugin Part No** (8) and **Plugin Serial No** (9) need to be entered. This option modifies the sets of recommended respectively [mandatory experiments](#) for a plugin test.

## (8) Plugin Part No

If (7) is selected, enter the part number of the plugin. The input is disabled if (7) is deselected.

## (9) Plugin Serial No

If (7) is selected, enter the serial number of the plugin. The input is disabled if (7) is deselected.

(10) Click **OK** to apply all settings and continue the creation of the Inspection Lot. Depending on the selected options (see (4) and (6)) additional dialogs as shown in Figure 5-4 and Figure 5-5 open subsequently.

(11) Click **Cancel** to abort the creation of the Inspection Lot.

## Selected Probe – List of Mandatory Experiments Dialog (Figure 5-4)

If [Selected Probe – Show and set mandatory experiments available](#) (Figure 5-3 (4)) was selected and no NPTCS file is provided in New Probe / Inspection Lot dialog, this dialog opens.

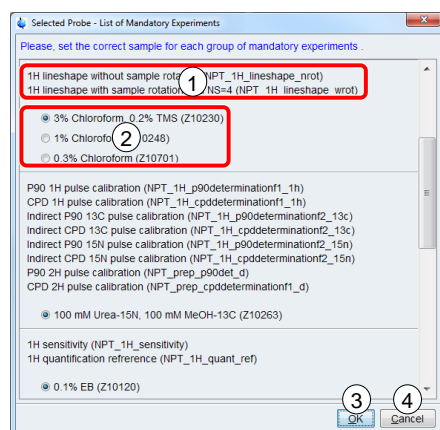


Figure 5-4: List of Mandatory Experiments

(1),(2) Select a sample (2) for each group of experiments (1). Use scroll bar to access all entries.

- (3) Click **OK** (3) to apply and continue the creation of the Inspection Lot. Depending on the selected option for a spectrometer test (Figure 5-3 (5)) a subsequent dialog opens.
- (4) Click **Cancel** (4) to skip setting the mandatory experiments available. The creation of the Inspection Lot is not aborted. Depending on the selected option for a spectrometer test (Figure 5-3 (5)) a subsequent dialog opens.

## List of mandatory Spectrometer Report Experiments (Figure 5-5)

If [Spectrometer Report – Show and set mandatory experiments available](#) (Figure 5-3 (5)) was selected in New Probe / Inspection Lot dialog, this dialog opens up.

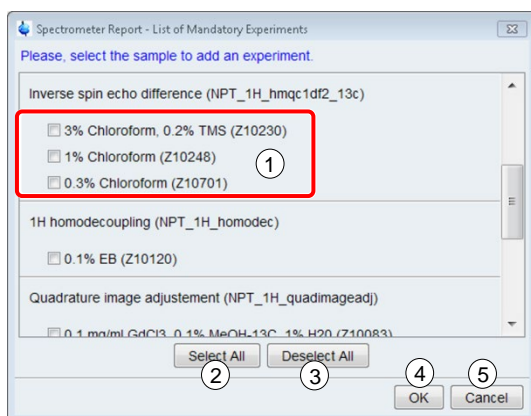


Figure 5-5: List of mandatory Spectrometer Report Experiments

- (1) Select a sample (1) for each experiment to set combinations of experiments and samples available for this Inspection Lot. Use scroll bar to access all entries.
- (2) Click **Select All** (2) to select all experiments from list.
- (3) Click **Deselect All** (3) to deselect all experiments.
- (4) Click **OK** (4) to apply and continue the creation of the Inspection Lot.
- (5) Click **Cancel** (5) to skip setting spectrometer experiments available. The creation of the Inspection Lot is not aborted.

Finally the new Inspection Lot opens as a tab in the [Workspace](#) of *NMRPT* main window. In this tab, further adjustments can be made (see 5.4.1 Inspection Lot Tab).

### 5.1.1.2 New > Report

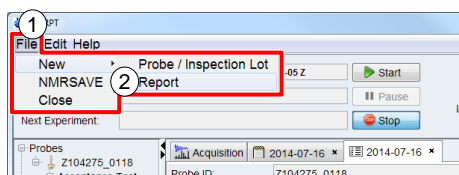


Figure 5-6: File menu, New Report

To create a new report, on the **File** menu shown in Figure 5-6 (1), point to **New**, and then click **Report** (2). The New Report dialog (Figure 5-7) opens up.

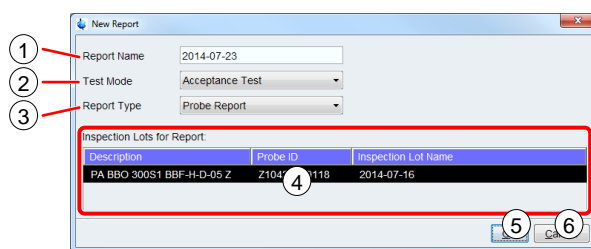


Figure 5-7: New Report dialog

## New Report Dialog (Figure 5-7)

- (1) **Report Name**  
Enter an individual name for the new report (see chapter 2.2, [permitted characters](#)). The current date is suggested as a default.
- (2) **Test Mode**  
Select the [Test Mode](#) from the list. The selected Test Mode affects the list of available Inspection Lots for Report (4) listed below. Only Inspection Lots of the selected Test Mode are available.
- (3) **Report Type**  
Select the [Report Type](#) from the list. The selected Report Type affects the number of selectable Inspection Lots in the list below (4).
- (4) **Inspection Lots for Report**  
Select the Inspection Lot respectively multiple Inspection Lots from the list to be included in the report. The list shows all Inspection Lots available in the selected [Test Mode](#).
  - In case of a Probe Report one Inspection Lot can be selected.
  - In case of a Spectrometer Report multiple Inspection Lots can be selected.
  - In case of an Accessories Report from zero to multiple Inspection Lots can be selected.

To select multiple Inspection Lots, press and hold CTRL, and then click each item.
- (5) Click **OK** to apply and continue the creation of the report.
- (6) Click **Cancel** to abort the creation of the Inspection Lot.

### 5.1.1.3 NMRSAVE

NMRSAVE saves installation specific files in a backup TAR-file as done by *TopSpin* au program `nmr_save`, but includes all *NMRPT* data and *NMRPT* measurement results.

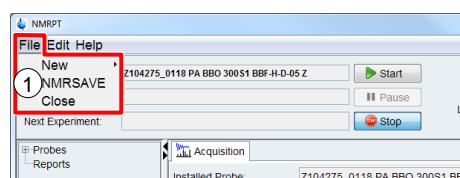


Figure 5-8: NMRSAVE

On the **File** menu shown in Figure 5-8, point to **New**, and then click **NMRSAVE** (1). The resulting file is located in `<tshome>/nmr_backup` folder.

**i** The `nmr_save` command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

## 5.1.1.4 Close

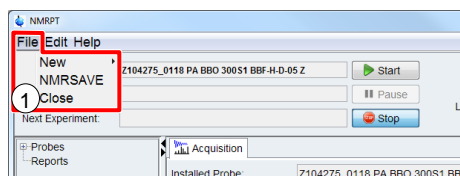


Figure 5-9: Close *NMRPT*

Click **Close** (Figure 5-9 (1)) to exit *NMRPT*. Closing is prohibited if acquisition of the Experiment Queue is active or paused. To stop current Acquisition Queue use [Stop button](#) in [Acquisition Bar](#).

## 5.1.2 Edit

Edit Menu (1) shown in Figure 5-10 provides functionalities to

- copy an [Inspection Lot](#) (2)
- rename an [Inspection Lot](#) (3)
- delete an [Inspection Lot](#) (4)
- rename a report (3)
- delete a report (4)
- rename a plugin (3)
- delete a probe (4)
- show and edit the Shim Command list (5)
- show and edit the Sample List (6)
- remove converted experiment parameters from *NMRPT* (7)
- set *NMRPT* wide configurations (8)

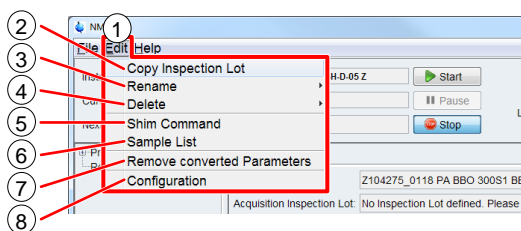


Figure 5-10: Edit menu

## 5.1.2.1 Copy Inspection Lot

On the **Edit** menu shown in Figure 5-10 (1), click **Copy Inspection Lot** (2) to copy an Inspection Lot including its experiment specifications to a new one.

The new Inspection Lot can be assigned to a different **Test Mode**. This way, e.g. specifications of an Acceptance Test can be applied to a Service Test. No experiment results will be copied.

### Copy Inspection Lot Dialogs

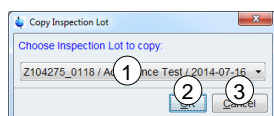


Figure 5-11: Copy Inspection Lot – source

- (1) Select an existing Inspection Lot to copy from the list (Figure 5-11 (1)).
- (2) Click **OK** (Figure 5-11 (2)) to continue copy process. The subsequent dialog shown in Figure 5-12 opens.
- (3) Click **Cancel** (Figure 5-11 (3)) to abort copying an Inspection Lot.

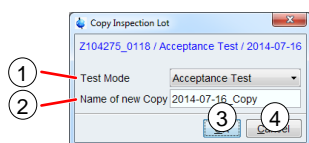


Figure 5-12: Copy Inspection Lot – target

- (1) **Test Mode**  
Select the **Test Mode** (Figure 5-12 (1)) for the copy.
- (2) **Name of new Copy**  
Enter an individual **Name of new Copy** (Figure 5-12 (2)) (see chapter 2.2, **permitted characters**). The old name labeled as Copy is suggested as a default (see Figure 5-12).
- (3) Click **OK** (Figure 5-12 (3)) to finish the copy process. The new Inspection Lot opens in the **Workspace** of **NMRPT main window**.
- (4) Click **Cancel** (Figure 5-12 (4)) to abort copying the Inspection Lot.

## 5.1.2.2 Rename > Inspection Lot

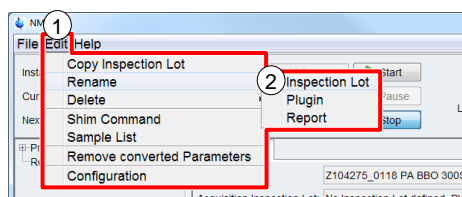


Figure 5-13: Rename Inspection Lot in menu

To rename an Inspection Lot, on the **Edit** menu shown in Figure 5-13 (1), point to **Rename**, and click **Inspection Lot** (2).

## Rename Inspection Lot Dialogs

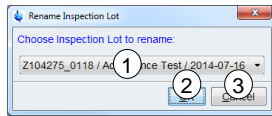


Figure 5-14: Rename Inspection Lot – choose Inspection Lot

- (1) Select the Inspection Lot to rename from the list (Figure 5-14 (1)) of available Inspection Lots.
- (2) Click **OK** (Figure 5-14 (2)) to continue to rename the Inspection Lot. The subsequent dialog shown in Figure 5-15 opens.
- (3) Click **Cancel** (Figure 5-14 (3)) to abort renaming an Inspection Lot.

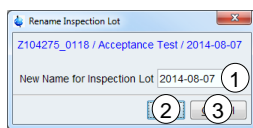


Figure 5-15: Rename Inspection Lot – rename

- (1) **New Name for Inspection Lot**  
Enter an individual **New Name for Inspection Lot** (Figure 5-15 (1)) ([permitted characters](#), see chapter 2.2). The old name is suggested as a default (see Figure 5-15).
- (2) Click **OK** (Figure 5-15 (2)) to finish renaming the Inspection Lot.
- (3) Click **Cancel** (Figure 5-15 (3)) to abort renaming the Inspection Lot.

### 5.1.2.3 Rename > Plugin

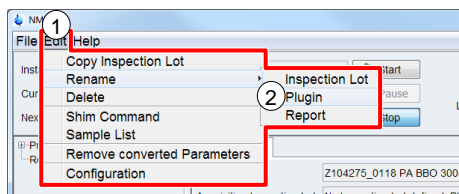


Figure 5-16: Rename Plugin in menu

To rename a plugin, on the **Edit** menu shown in Figure 5-16 (1), point to **Rename**, and click **Plugin** (2).

## Rename Plugin Dialogs

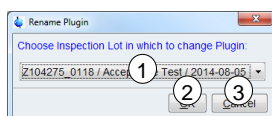


Figure 5-17: Rename Plugin – choose Inspection Lot

- (1) Select the Inspection Lot including the plugin to rename from the list (Figure 5-17 (1)) of available Inspection Lots with plugins.



- (2) Click **OK** (Figure 5-17 (2)) to continue to rename the plugin. The subsequent dialog shown in Figure 5-18 opens.
- (3) Click **Cancel** (Figure 5-17 (3)) to abort renaming a plugin.

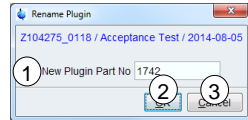


Figure 5-18: Rename Plugin – rename Part No

- (1) **New Plugin Part No**  
Enter the **New Plugin Part No** (Figure 5-18 (1)) (see chapter 2.2, [permitted characters](#)). The old Part No is suggested as a default.
- (2) Click **OK** (Figure 5-18 (2)) to continue to rename the plugin. The subsequent dialog shown in Figure 5-19 opens.
- (3) Click **Cancel** (Figure 5-18 (3)) to abort renaming a plugin.

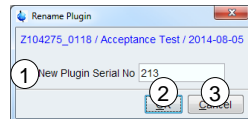


Figure 5-19: Rename Plugin – rename Serial No

- (1) **New Plugin Serial No**  
Enter the **New Plugin Serial No** (Figure 5-19 (1)) (see chapter 2.2, [permitted characters](#)). The old Serial No is suggested as a default.
- (2) Click **OK** (Figure 5-19 (2)) to finish renaming the plugin.
- (3) Click **Cancel** (Figure 5-19 (3)) to abort renaming a plugin.

## 5.1.2.4 Rename > Report

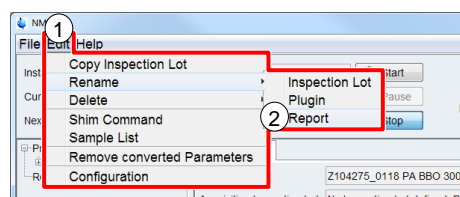


Figure 5-20: Rename Report in menu

To rename a report, on the **Edit** menu shown in Figure 5-20 (1), point to **Rename**, and click **Report** (2).

### Rename Report Dialogs

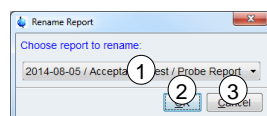


Figure 5-21: Rename Report – choose report

- (1) Select the report to rename from the list (Figure 5-21 (1)).

- (2) Click **OK** (Figure 5-21 (2)) to continue to rename the report. The subsequent dialog shown in Figure 5-22 opens.
- (3) Click **Cancel** (Figure 5-21 (3)) to abort renaming a report.

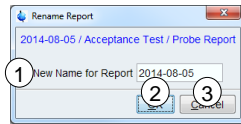


Figure 5-22: Rename Report – rename

- (1) **New name for Report**  
Enter the **New Name for Report** (Figure 5-22 (1)). (see chapter 2.2, [permitted characters](#)). The old name is suggested as a default.
- (2) Click **OK** (Figure 5-22 (2)) to finish renaming the report.
- (3) Click **Cancel** (Figure 5-22 (3)) to abort renaming a report.

## 5.1.2.5 Delete > Probe

If a probe is deleted from *NMRPT*, all Inspection Lots, results and measurement data of this probe are deleted. Deletion of a probe is not possible if reports are based on at least one Inspection Lot of the probe. These reports need to be [deleted](#) first.

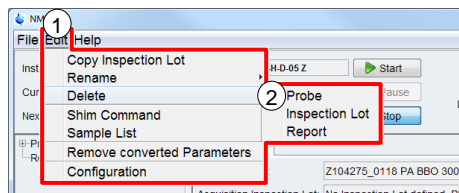


Figure 5-23: Delete Probe in menu

To delete a probe from *NMRPT*, on the **Edit** menu shown in Figure 5-23 (1), point to **Delete**, and click **Probe** (2).

### Delete Probe Dialog (Figure 5-24)

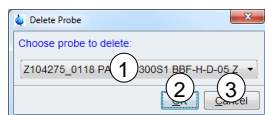


Figure 5-24: Delete Probe – choose probe

- (1) In the dialog (Figure 5-24) select the probe (1) to delete.
- (2) Click **OK** (2) to continue to delete the probe.
- (3) Click **Cancel** (3) to abort deleting a probe.



## Deleting a probe from *NMRPT*:

All Inspection Lots, results, and measurement data of this probe are deleted!  
Deletion of a probe is disabled if Inspection Lots of the probe are used in reports.

### 5.1.2.6 Delete > Inspection Lot

If an Inspection Lot is deleted, all measurement data and results of this Inspection Lot are deleted. Deletion of an Inspection Lot is not possible if a report based on the Inspection Lot exists. The report needs to be **deleted** first.

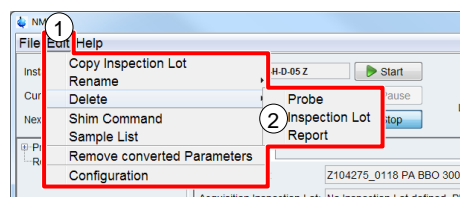


Figure 5-25: Delete Inspection Lot in menu

To delete an Inspection Lot from *NMRPT*, on the **Edit** menu shown in Figure 5-25 (1), point to **Delete**, and click **Inspection Lot** (2).

### Delete Inspection Lot Dialog (Figure 5-26)

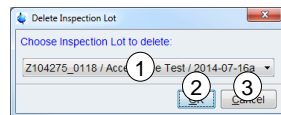


Figure 5-26: Delete Inspection Lot – choose Inspection Lot

- (1) In the dialog (Figure 5-26) select the Inspection Lot (1) to delete.
- (2) Click **OK** (2) to continue to delete the Inspection Lot.
- (3) Click **Cancel** (3) to abort deleting an Inspection Lot.



## Deleting an Inspection Lot from *NMRPT*:

Attention! All results and NMR measurement data of this Inspection Lot are deleted!  
Deletion of an Inspection Lot is disabled if it is used for a report.

### 5.1.2.7 Delete > Report

- If a report is deleted, the corresponding Inspection Lot can be deleted.
- If the deleted report was of **finalized** state, the corresponding Inspection Lot and its results are unlocked: The Inspection Lot can be changed.
- Deleting all reports of one probe allows deleting the probe from *NMRPT*.
- Deleting a report does not delete any Inspection Lot or measurement data.

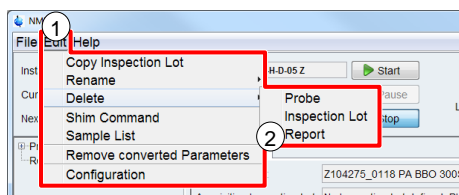


Figure 5-27: Delete Inspection Lot in menu

To delete a report from *NMRPT*, on the **Edit** menu shown in Figure 5-27 (1), point to **Delete**, and click **Report** (2).

## Delete Report Dialog (Figure 5-28)

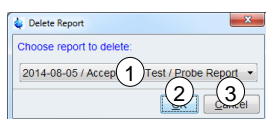


Figure 5-28: Delete Report – choose report

- (1) In the dialog (Figure 5-28) select the report (1) to delete.
- (2) Click **OK** (2) to continue to delete the report.
- (3) Click **Cancel** (3) to abort deleting a report.

## i

### Deleting a report from *NMRPT*:

The corresponding Inspection Lot is available again and can be changed or deleted. Deleting all reports of one probe allows deleting the probe from *NMRPT*.

## 5.1.2.8 Shim Command

The *NMRPT* Shim Command list (Figure 5-30) shows the shim sequences connected to each *NMRPT* Shim Command Number. Entries with Shim Command numbers 800 to 824 are editable and can be filled with user defined shim sequences.

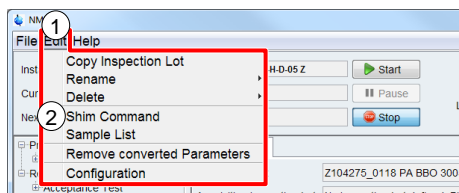


Figure 5-29: Shim Command list in menu

On the **Edit** menu shown in Figure 5-29 (1), click **Shim Command** (2) to open Shim Command list dialog.

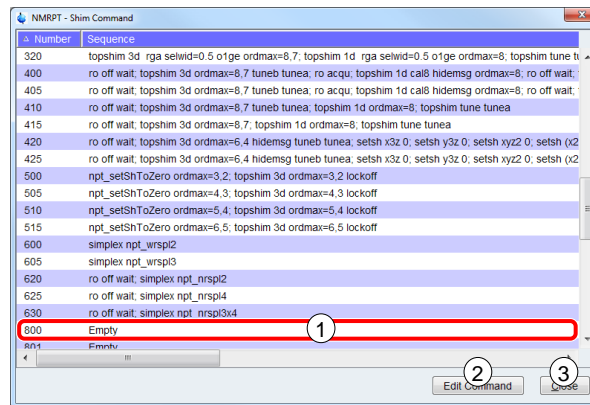


Figure 5-30: Shim Command list

## Shim Command Dialog (Figure 5-30)

- (1) In Shim Command list the shim sequences connected to each *NMRPT* Shim Command Number (1) are shown.
- (2) **Edit Command**  
Select a Shim Command list item (1) and click **Edit Command** (2) to edit the sequence of this Shim Command number. The **Edit Command** dialog (Figure 5-31 ) opens. The **Edit Command** button is disabled for default Shim Command numbers other than 800 to 824.
- (3) Click **Close** (3) to close Shim Command dialog.

## Edit Command Dialog (Figure 4-32)

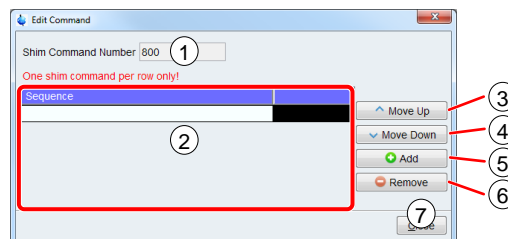


Figure 5-31: Edit Shim Command dialog

- (1) **Shim Command Number**  
The **Shim Command Number** (1) which is currently edited is shown above the Sequence list (2).
- (2) **Sequence**  
The Shim Commands are listed one per row in the **Sequence** list (2) in the order of execution. Click an item in Sequence column to edit.
- (3) **Move Up**  
Select an item in **Sequence** list (2) and click **Move Up** (3) to move the item up in the Sequence list.
- (4) **Move Down**  
Select an item in **Sequence** list (2) and click **Move Down** (4) to move the item down in the Sequence list.

- (5) **Add**  
Click **Add** (5) to add a new item to the Sequence list.
- (6) **Remove**  
Select an item in **Sequence** list (2) and click **Remove** (6) to remove the item from the Sequence list.
- (7) Click **Close** (7) to close Edit Command dialog.

**i**

**NMRPT** Shim Command Number **999** means **skip shimming**.

All shim commands added to a sequence of a Shim Command Number are to be executable via *TopSpin* command line. Further information about shim commands is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

## 5.1.2.9 Sample List

In *NMRPT* Sample List all samples required by experiments included in available Inspection Lots are listed.

- Detail information about the samples is provided.
- The sample changer holder positions are set.
- The availability of the samples can be changed.
- Customer Samples can be created (as a copy of the standard samples).

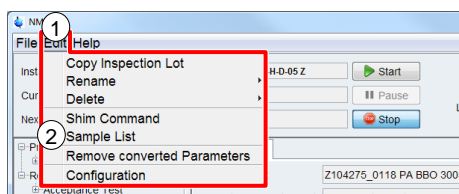


Figure 5-32: Sample List in menu

On the **Edit** menu shown in Figure 5-32 (1), click **Sample List** (2) to open Sample List dialog.

### Sample List Dialog (Figure 5-33)

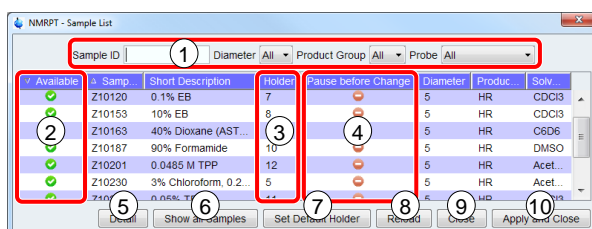




Figure 5-33: Sample List

- (1) The filter bar (1) allows to list only samples matching the selected criteria in the sample list below. Available criteria are: **Sample ID**, **Diameter**, **Product Group** and **Probe**.
- (2) Click the status icon of a listed sample in **Available** column (2) to change its availability. A green icon  means available, a red icon  means not available.

---

**i** Setting a sample unavailable removes all dependent experiments from [Library](#) on [Acquisition tab](#). Experiments already enqueued are also affected and will be lost from Queue. The affected experiments remain part of the Inspection Lot and will become executable again when the sample is set to status available.



---

- (3) Click the holder position of a sample in **Holder** column (3) to edit the holder position. Holder position 0 means manual change of the sample. To set default holder positions see (7).

---

**i** Holder position 0 means manual sample change. If the Use Sample Changer option is deselected in [NMRPT Configuration](#), all holder positions are set to 0. If the Use Sample Changer option is selected, samples set to be changed manually are not included to the [Recommended Experiment Sequence](#). For LC, HRMAS and MAS often there is no appropriate sample changer available. Therefore especially in these cases it may be useful to deselect usage of a sample changer to include all experiments to Recommended Experiment Sequence.

---

- (4) Click the status icon (4) in **Pause before Change** column to pause the Acquisition Queue before changing to this sample. A green icon  means pause, a red icon  means no pause before sample change.
- (5) **Detail**  
Click **Detail** (5) to open Sample Detail information dialog (see below and Figure 5-34).
- (6) **Show all Samples**  
Click **Show all Samples** (6) to open Show all Samples dialog (see below and Figure 5-35). In this dialog Customer Samples can be created.
- (7) **Set Default Holder**  
Click **Set Default Holder** (7) to assign default holder positions to the most frequently used standard samples currently listed in Sample List. This option requires those samples to be placed in these holder positions. This button is disabled if the [use of a Sample Changer](#) is deselected.
- (8) **Reload**  
Click **Reload** (8) to revert all changes not applied yet.
- (9) Click **Close** (9) to close Sample List dialog without applying recent modifications.
- (10) **Apply and Close**  
Click **Apply and Close** (10) to save all recent modifications and close Sample List.

## Sample Detail Dialog (Figure 5-34)

In Sample List dialog (Figure 5-33) select a sample and click **Detail** (Figure 5-33 (5)) to open Sample Detail dialog.

Figure 5-34: Sample Detail information

Details about the selected sample are shown: Sample ID, Short Description, Solvent, Physical Condition, Sample Type, TopSpin Description, Temperature Max. [C], Temperature Min. [C], Diameter and Batch Number.

- (1) Enter an optional **Batch Number** (1) to add it to detail information of the sample.
- (2) Click **Close** (2) to apply changes and close Sample Detail dialog.

## Show all Samples Dialog (Figure 5-35)

In Sample List dialog (Figure 5-33) click Show all Samples (Figure 5-33 (6)) to open Show all Samples dialog.

Figure 5-35: Show all Samples

In **Show all Samples** dialog all samples known by *NMRPT* are listed. The details provided for each sample can not be edited and are for information only.

- (1) The filter bar (1) allows to list only samples matching the selected criteria in the sample list below. Available criteria are: **Sample ID**, **Diameter**, **Product Group** and **Probe**.
- (2) The status icons in **Used** column (2) show if a sample was used in *NMRPT* before (independent of its current availability status (Figure 5-33 (2))). A green icon 🟢 means used, a red icon 🔴 means not used.



## (3) Copy selected sample to Customer Sample

If a standard sample is not available and an equivalent sample based on common laboratory chemicals has to be used: Select the standard sample and click **Copy selected sample to Customer Sample**.

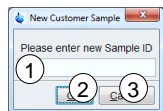


Figure 5-36: New Customer Sample dialog

In the subsequent dialog (Figure 5-36) enter a new **Sample ID** (Figure 5-36 (1)) (see chapter 2.2, [permitted characters](#)) and click **OK** (Figure 5-36 (2)) save the sample and to close the dialog. Click **Cancel** (Figure 5-36 (3)) to abort copying a standard sample to a new Customer Sample.

I

The creation of a Customer Sample needs to be applied to the [Sample List](#) by Apply and Close button (Figure 5-33 (10)). The same experiments assigned to the original standard sample are assigned to the Customer Sample and the [Pairings](#) can be added to an Inspection Lot on [Inspection Lot](#) tab.

## (4) Delete Customer Sample

To delete a Customer Sample, select the Customer Sample and click **Delete Customer Sample** (4). This option is disabled, if the sample is part of an Inspection Lot.

I

A Customer Sample that is part of an Inspection Lot can not be deleted. The sample-experiment Pairings have to be removed from Inspection Lots first. The deletion of a Customer Sample needs to be applied to the [Sample List](#) by Apply and Close button (Figure 5-33 (10)).

(5) Click **OK** (5) to apply all changes of Customer Samples and to close Show all Samples dialog.

(6) Click **Cancel** (6) to discard all changes of Customer Samples and to close Show all Samples dialog.

### 5.1.2.10 Remove Converted Parameters

*NMRPT* keeps [converted experiment parameters](#) as long as the probe is defined as current via `edprobe` in *TopSpin*. To delete converted parameters manually use Remove Converted Parameters entry in File menu.

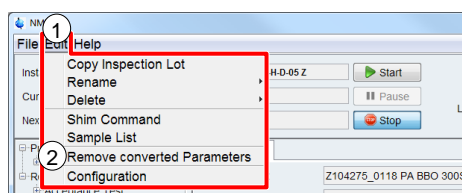


Figure 5-37: Remove Converted Parameters in menu

On the **Edit** menu shown in Figure 5-37 (1), click **Remove Converted Parameters** (2) to open Remove converted Parameters dialog.

**I** The `edprobe` command is part of TopSpin. Further information is provided in the TopSpin manuals (see chapter [1.5 Referenced Documents](#)).

## Remove converted Parameters Dialog (Figure 5-38)

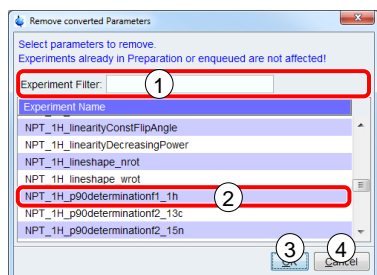


Figure 5-38: Remove Converted Parameters

- (1) Enter part of an experiment name to the filter bar (1) to list only experiments containing this pattern.
- (2) Select an experiment (2) for which to delete the converted parameters. To select multiple experiments, press and hold down CTRL, and then click each item.
- (3) Click **OK** (3) to continue to remove the selected converted parameters.
- (4) Click **Cancel** (4) to abort removing converted parameters.

## 5.1.2.11 Configuration

In *NMRPT* Configuration window global settings are located to configure general options for sample change behavior and the location of the Acquisition Bar.

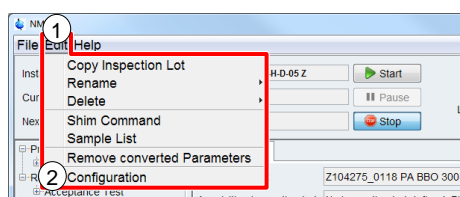


Figure 5-39: Configuration in menu

On the **Edit** menu shown in Figure 5-39 (1), click **Configuration** (2) to open *NMRPT* Configuration dialog.

## Configuration Dialog (Figure 5-40)

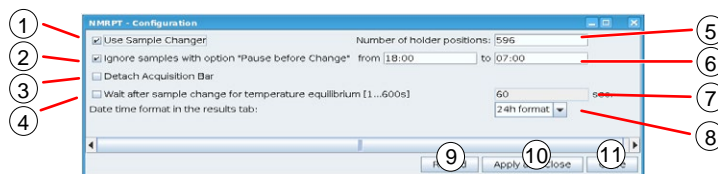


Figure 5-40: Configuration dialog

- (1) **Use Sample Changer**  
Select the usage of a Sample Changer (1). As a default the option is selected if a Sample Changer is detected. If no Sample Changer is recognized, the Use Sample Changer option is automatically deselected.
- (2) **Ignore samples with option "Pause before Change"**  
Select this option to set a time span (see (6)) in which to skip experiments on samples with option "Pause before Change". The experiments will remain enqueued.
- (3) **Detach Acquisition Bar**  
Select this option to detach *NMRPT* Acquisition Bar from *NMRPT* main window as a space-saving option especially for small screens.
- (4) **Wait after sample change for temperature equilibrium [1...600s]**  
Select this option to wait for temperature equilibrium in the sample after insert into the magnet and before starting the experiment. The waiting time is provided in seconds (see (7)).
- (5) **Number of holder positions**  
The Number of holder positions (5) of a sample changer is automatically set if available. Enter the number of holders to set it manually. This box is disabled if (1) is deselected.
- (6) Enter a time span (6) for **Ignore samples with option "Pause before Change"** (see(2)). This box is disabled if (2) is deselected.
- (7) Enter a number between 1 s and the maximum of 600 s for **Wait after sample change for temperature equilibrium** option (see (4)). This box is disabled if (4) is deselected.
- (8) **Change time format**  
Click the **dropdown menu** (8) to change the time format of the results table in the results tab.
- (9) **Reload**  
Click **Reload** (8) to revert all changes not applied yet.
- (10) **Apply and Close**  
Click **Apply and Close** (9) to save all recent modifications and close Configuration dialog.
- (11) Click **Close** (10) to close Configuration dialog without applying recent modifications.

## 5.1.3 Help

In Help menu section access to the *NMRPT* manuals is located. Further information about the *NMRPT* software version is provided.

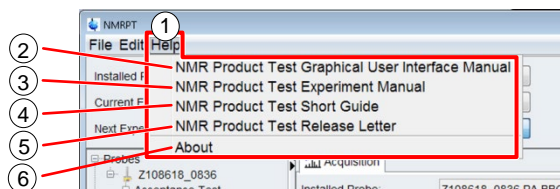


Figure 5-41: Help menu

### 5.1.3.2 NMR Product Test Graphical User Interface Manual

On the **Help** menu shown in Figure 5-41 (1), click **NMR Product Test Graphical User Interface Manual** (2) to access this document (ZHUB0002). The Graphical User Interface Manual provides detailed information about the *NMRPT* user interface.

### 5.1.3.3 NMR Product Test Experiment Manual

On the **Help** menu shown in Figure 5-41 (1), click **NMR Product Test Experiment Manual** (3) to access the Bruker Test Procedures for *Avance* NMR Systems (see chapter [1.5 Referenced Documents](#), ZUEP0102). The Product Test Experiment Manual provides detailed information about the *NMRPT* set of experiments, including example parameters, available options and sample plots.

### 5.1.3.4 NMR Product Test Short Guide

On the **Help** menu shown in Figure 5-41 (1), click **NMR Product Test Short Guide** (4) to access the *NMRPT* Short Guide. The Short Guide provides basic information and a basic standard workflow in *NMRPT*.

### 5.1.3.5 NMR Product Test Release Letter

On the **Help** menu shown in Figure 5-41 (1), click **NMR Product Test Release Letter** (5) to access the *NMRPT* Release Letter. The Release Letter provides changes in the *NMRPT* software since last software release.

### 5.1.3.6 About

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On the **Help** menu shown in Figure 5-41 (1), click **About** (6) to access information about the current *NMRPT* version and the *TopSpin* version in which *NMRPT* is integrated (see Figure 5-42).

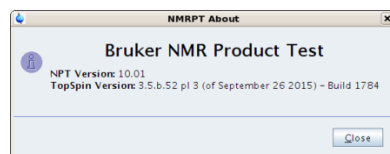


Figure 5-42: *NMRPT* About information

## 5.2 Acquisition Bar

The control to operate an assembled [Experiment Queue](#) and essential information about this queue are provided in Acquisition Bar.



Figure 5-43: Acquisition Bar

### (1) Installed Probe

Installed Probe information (Figure 5-43 (1)) shows the description of the currently installed probe as provided by `edprobe` in *TopSpin*.



The `edprobe` command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

### (2) Current Experiment

The **Current Experiment** information (Figure 5-43 (2)) shows the name of the experiment which is currently in progress. This experiment is not listed in Experiment Queue anymore. Click the information field to open the experiment in *TopSpin* window.

### (3) Next Experiment

**Next Experiment** information (Figure 5-43 (3)) shows the name of the upcoming experiment. This experiment is also listed at the top of the Experiment Queue.

### (4) Start

Click **Start** (Figure 5-43 (4)) to start the queue of experiments as listed in Experiment Queue. If the acquisition of the queue is interrupted either by [Stop](#) or [Pause](#) button, click **Start** to continue with the next experiment enqueued (including sample change if required).

The Startup Check window (Figure 5-47) appears if a queue is started for the first time or restarted after [Stop](#) (Figure 5-43 (6)) was applied.

### (5) Pause

Click **Pause** (Figure 5-43 (5)) to complete the current experiment and interrupt the queue afterwards. If the upcoming experiment requires to change the sample, the queue is interrupted before sample change. The upcoming experiment stays enqueued.

### (6) Stop

Click **Stop** (Figure 5-43 (6)) to stop immediately, independent of the current status (7). If acquisition was running **Stop** aborts the current experiment. The acquisition of the experiment is not completed, no evaluable data will be available. The experiment is not automatically re-enqueued. The spectrometer may remain in an undefined state.



A running queue (all status except for Stopped) blocks several commands, e.g. closing *NMRPT* and multiple *TopSpin* commands.

## (7) Status

The **Status** information (Figure 5-43 (7)) provides the current status of *NMRPT* respectively the status of the current experiment queue. Possible status indicators are listed in Table 5-1.

Message	Explanation
Waiting	green, static – Queue active: <a href="#">Experiment Queue</a> empty, <i>NMRPT</i> waiting for the next experiment to be enqueued.
Acquisition in progress	green, flashing – Queue active: Current experiment of <a href="#">Queue</a> in progress. The message provides further information about the current process.
Processing in progress	
Locksetting in progress	
Cooldown in progress	
Inserting correct sample	
Waiting for temp. equilibrium	
Paused	orange, static – Queue paused: <a href="#">Experiment Queue</a> manually <a href="#">paused</a> . Click <a href="#">Start button</a> to continue Experiment Queue with upcoming experiment, including sample change if required.
Pause before acquisition	orange, flashing – Queue paused: <a href="#">Experiment Queue</a> paused automatically by <i>NMRPT</i> option <a href="#">Pause before Acquisition</a> or <a href="#">Pause before Change</a> . Click <a href="#">Start button</a> to continue.
Pause before sample change	
Stopped	Red, static – Queue stopped: <a href="#">Experiment Queue</a> was stopped immediately, independent of the current status (7). If an experiment was currently executed it was aborted and dropped from queue. Spectrometer might be in an undefined state. Start handles remaining experiments like a new queue.

Table 5-1: Status indicators in NMRPT Acquisition Bar

## (8) Last Message

**Last Message** information (Figure 5-43 (8)) shows individual messages from experiments. Each message is shown until the next message appears.

## Probe dependent options

### Skip Cooldown (CryoProbe and Prodigy only)

Status: **Stopped** ☒ Skip Cooldown

Last Message:

Figure 5-44: Skip Cooldown

The Skip Cooldown option can be used in case that the connection to the cooling unit is broken or a special debugging is necessary.

## MAS Off Timer (CMP, HRMAS and MAS Probe only)

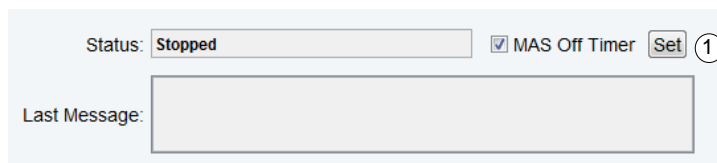


Figure 5-45: MAS Off Timer

The MAS off timer automatically stops the MAS spinning when no experiment is running.

- (1) **Set timer** is used to define the time (in minutes) between last experiment and switching MAS spinning off. Default time after NMRPT start is 5 minutes.

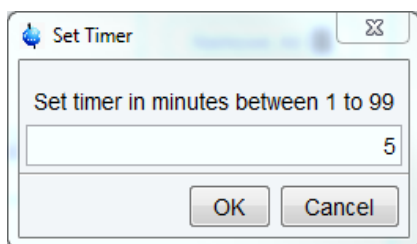


Figure 5-46: Set Timer dialog

## Startup Check Dialog (Figure 5-47)

The Startup Check dialog shows information about the status of mandatory preparation steps and settings. It includes reminders and provides access to most of these settings. A green checkmark ✓ indicates a successful check of an option. A yellow exclamation mark ⚠ marks a reminder not checked automatically. A red error sign ✖ indicates a mandatory preparation step or setting not met yet.

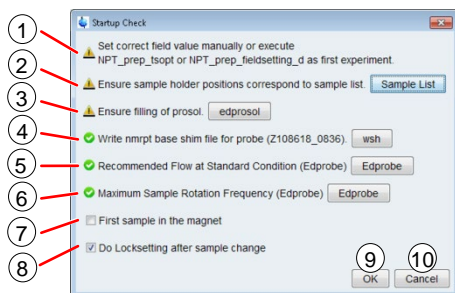


Figure 5-47: Startup Check dialog

- (1) **Set correct field value manually / Set correct field value manually or execute NPT\_prep\_tsopt or NPT\_prep\_fieldsetting\_d as first experiment**  
This message reminds to set the correct field value manually. If the experiment NPT\_prep\_tsopt is available for the current Inspection Lot it can be enqueued to set the field automatically.
- (2) **Ensure sample holder positions correspond to sample list**  
(visible if sample changer is set to be used)  
Click **Sample List** (2) to check if all sample holder positions in [Sample List](#) correspond to the real holder positions in the sample changer. Holder position 0 means manual change of the sample.
- (3) **Ensure filling of prosol**  
Click **edprosol** (3) to check if all needed 90 degree pulses for the actual probe are filled in prosol.



- (4) **Write nmrpt base shim file for probe**  
Click **wsh** (4) to write a [base shim file](#) for current probe.
- (5) **Recommended Flow at Standard Condition (Edprobe)**  
(visible if gas flow is controlled by BSVT)  
Click **Edprobe** (5) to set Recommended Flow in *TopSpin* edprobe dialog.
- (6) **Maximum Sample Rotation Frequency (Edprobe)**  
(visible for MAS / HRMAS probes)  
Click **Edprobe** (6) to set Maximum Rotation Frequency in *TopSpin* edprobe dialog.  
This setting is only available for MAS / HRMAS probes.



The write shim command `wsh` and the `edprobe` command are part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

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- (-) **Ensure correct gas flow and temperature settings**  
(visible if no BSVT is available)  
Ensure correct temperature and gas flow are applied before starting the Queue.
- (7) **First sample in the magnet** (manual sample change)  
Select this option (7) to skip sample change process if the correct sample for the next experiment is already inside the magnet.  
**Current Holder Position** (sample changer)  
Shows the current holder position at magnet bore. A negative number indicates an unknown state.
- (8) **Do Locksetting after sample change**  
(visible if lock is available)  
Select this option (8) to execute automatic locksettings after each sample change.  
This option is missing if no lock is available.
- (9) Click **OK** to confirm all mandatory preparation steps and settings listed in Startup Check dialog and to start the queue by acquisition of the first experiment.
- (10) Click **Cancel** to abort starting the queue.



The OK button (9) of Startup Check dialog is disabled if mandatory preparation steps or settings are not met.

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## 5.3 Navigation

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The Navigation panel on the left in *NMRPT* window is structured into the main sections **Probes** (Figure 5-48 (1)) and **Reports** (Figure 5-48 (2)). Both sections are divided into individual subnavigations. Expand either Probes or Reports navigation item to access the corresponding subnavigation. Context menus for the Navigation entries provide short access to operations also provided in [Edit menu](#).

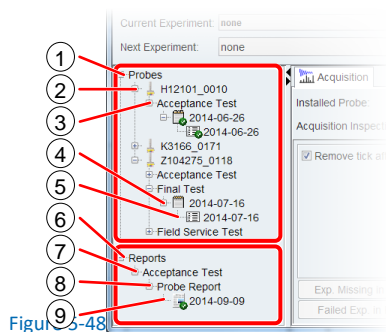







Figure 5-48

## 5.3.1 Navigation: Probes

- (2) **Probe**  Click a Probe item (Figure 5-48 (2)) to open the corresponding [Probe Setup Tab](#) in [Workspace](#). Each probe item is named by its Probe ID, a unique identifier composed of part and serial number of the probe.
- (3) **Test Mode** Expand a Probe item (2) to access the subordinated Test Mode navigation items (Figure 5-48 (3)). These items provide grouping of the Inspection Lots of a probe according to their [Test Mode](#) (Final Test, Acceptance Test, Field Service Test).
- (4) **Inspection Lot**  Expand a Test Mode item (3) to access the subordinated Inspection Lot items (Figure 5-48 (4)). Click an Inspection Lot item open the corresponding [Inspection Lot Tab](#) in [Workspace](#). Inspection Lot navigation items are listed by their name.
- (5) **Results**  Expand an Inspection Lot item (4) to access its Result item. Click the Result item (Figure 5-48 (5)) to open the corresponding [Results Tab](#) in [Workspace](#). Result navigation items are listed by the Inspection Lot name.
- Finalized Entries**  Navigation items for Inspection Lots and Results show a green checkmark when finalized. Inspections Lots are finalized if the results are used by a [finalized report](#).

## 5.3.2 Navigation: Reports

- (7) **Test Mode** The Test Mode navigation items (Figure 5-48 (7)) provide grouping of the [Report Types](#) in each [Test Mode](#) (Final Test, Acceptance Test, Field Service Test).
- (8) **Report Type** Expand a Test Mode item (7) to access the subordinated Report Type navigation items (Figure 5-48 (8)). These items provide grouping of the reports.
- (9) **Report**  Expand a Report Type item (8) to access the subordinated Report items (Figure 5-48 (9)). Click a Report item to open the corresponding [Report Tab](#) in [Workspace](#). Report navigation items are listed by their name.

## Finalized Entries

Navigation entries for reports show a green checkmark when **finalized**.

### 5.3.3 Navigation Context Menus

#### Probe Context Menu (Figure 5-49)

Right-click the probe item to edit in Navigation panel. The context menu for this probe opens up.

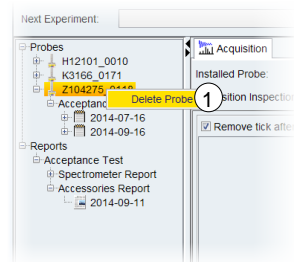


Figure 5-49: Navigation context menu – probe

#### (1) Delete Probe

Click **Delete Probe** (1) in probe context menu to delete the selected probe. A subsequent confirmation dialog opens up (Figure 5-50).

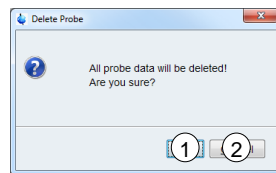


Figure 5-50: Navigation context menu – Delete Probe confirmation dialog

Click **OK** (Figure 5-50 (1)) to confirm and continue the deletion of the probe. Click **Cancel** (Figure 5-50 (2)) to abort and keep the probe in *NMRPT*.

If a probe is deleted from *NMRPT*, all Inspection Lots, results and measurement data of this probe are deleted. Deletion of a probe is not possible if reports are based on at least one Inspection Lot of the probe. These reports need to be **deleted** first.

#### Inspection Lot Context Menu (Figure 5-51)

Right-click the Inspection Lot item to edit in Navigation panel. The context menu for this Inspection Lot opens up.

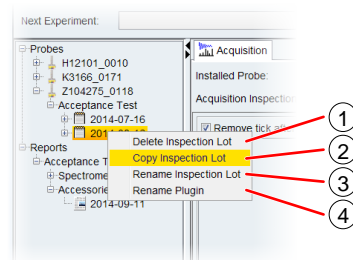


Figure 5-51: Navigation context menu – Inspection Lot

## (1) Delete Inspection Lot

Click **Delete Inspection Lot** (1) in Inspection Lot context menu to delete the selected Inspection Lot. A subsequent confirmation dialog opens up (Figure 5-52).

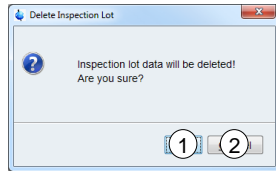


Figure 5-52: Navigation context menu – Delete Inspection Lot confirmation dialog

Click **OK** (Figure 5-52 (1)) to confirm and continue the deletion of the Inspection Lot. Click **Cancel** (Figure 5-52 (2)) to abort and keep the Inspection Lot.

If an Inspection Lot is deleted from *NMRPT*, all results and measurement data of this Inspection Lot are deleted. Deletion of an Inspection Lot is not possible if a report based on the Inspection Lot exists. The report needs to be **deleted** first.

## (2) Copy Inspection Lot

In Inspection Lot context menu click **Copy Inspection Lot** (2) to copy an Inspection Lot including its experiment specifications to a new one. The new Inspection Lot can be assigned to a different **Test Mode**. This way, e.g. specifications of an Acceptance Test can be applied to a Service Test. No experiment data and results will be copied. A subsequent dialog (Figure 5-53) opens up.

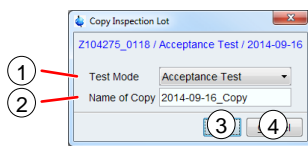


Figure 5-53: Navigation context menu – Copy Inspection Lot dialog

Select the **Test Mode** (Figure 5-53 (1)) for the copy. Enter an individual **Name of Copy** (Figure 5-53 (2)) (see chapter 2.2, **permitted characters**). The source name supplemented with “\_Copy” is suggested as a default (see Figure 5-53). Click **OK** (Figure 5-53 (3)) to confirm and finish the copy process. Click **Cancel** (Figure 5-53 (4)) to abort copying the Inspection Lot.

## (3) Rename Inspection Lot

Click **Rename Inspection Lot** (3) in Inspection Lot context menu to rename the selected Inspection Lot. A subsequent dialog (Figure 5-54) opens up.

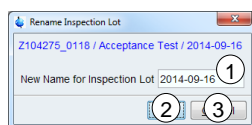


Figure 5-54: Navigation context menu – Rename Inspection Lot dialog

Enter an individual **New Name for Inspection Lot** (Figure 5-54 (1)) (see chapter 2.2, **permitted characters**). The old name is suggested as a default (see Figure 5-54). Click **OK** (Figure 5-54 (2)) to finish renaming the Inspection Lot. Click **Cancel** (Figure 5-54 (3)) to abort renaming the Inspection Lot.

## (4) Rename Plugin (Inspection Lots including plugins only)

In Inspection Lot context menu click **Rename Plugin** (4) to correct the part or serial number of the plugin connected with the selected Inspection Lot. Subsequent dialogs (Figure 5-55) open up.

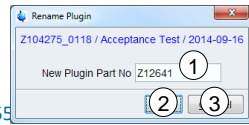


Figure 5-55: Rename Plugin dialog, New Plugin Part No

Enter the **New Plugin Part No** (Figure 5-55 (1)) (see chapter 2.2, [permitted characters](#)). The old Part No is suggested as a default. Click **OK** (Figure 5-55 (2)) to continue to rename the plugin. The subsequent dialog shown in Figure 5-56 opens. Click **Cancel** (Figure 5-55 (3)) to abort renaming a plugin.

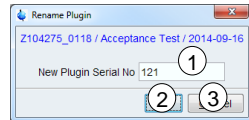


Figure 5-56: Navigation context menu – Rename Plugin dialog, New Plugin Serial No

Enter the **New Plugin Serial No** (Figure 5-56 (1)) (see chapter 2.2, [permitted characters](#)). The old Serial No is suggested as a default. Click **OK** (Figure 5-56 (2)) to confirm and finish renaming the plugin. Click **Cancel** (Figure 5-56 (3)) to abort renaming the plugin.

The Rename Plugin menu item is only available for Inspection Lots including plugins.

## Report Context Menu (Figure 5-57)

Right-click the report item to edit in Navigation panel. The context menu for this report opens up.

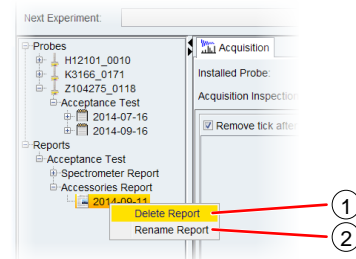


Figure 5-57: Navigation context menu – report

### (1) Delete Report

Click **Delete Report** (1) in report context menu to delete the selected report. A subsequent confirmation dialog opens up (Figure 5-58).

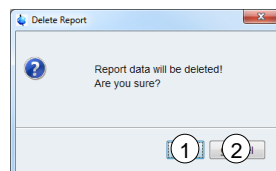


Figure 5-58: Navigation context menu – Delete Report confirmation dialog

Click **OK** (Figure 5-58 (1)) to confirm and continue the deletion of the report. Click **Cancel** (Figure 5-58 (2)) to abort the deletion of the report. Deleting a report makes the corresponding Inspection Lot available again. It can be changed or deleted. Deleting all reports of one probe allows deleting the probe from *NMRPT*.

### (2) **Rename Report**

Click **Rename Report** (2) in report context menu to rename the selected report. A subsequent dialog (Figure 5-59) opens up.



Figure 5-59: Navigation context menu – Rename Report dialog

Enter an individual **New Name for Report** (Figure 5-59 (1)) (see chapter 2.2, [permitted characters](#)). The old name is suggested as a default (see Figure 5-59). Click **OK** (Figure 5-59 (2)) to finish renaming the report. Click **Cancel** (Figure 5-59 (3)) to abort renaming the report.

## 5.4 Workspace

In Workspace area of *NMRPT* main window (Figure 5-60) multiple tabs for different functionalities can be accessed:

- Acquisition tab
- Probe Setup tab
- Inspection Lot tab
- Results tab
- Report tab

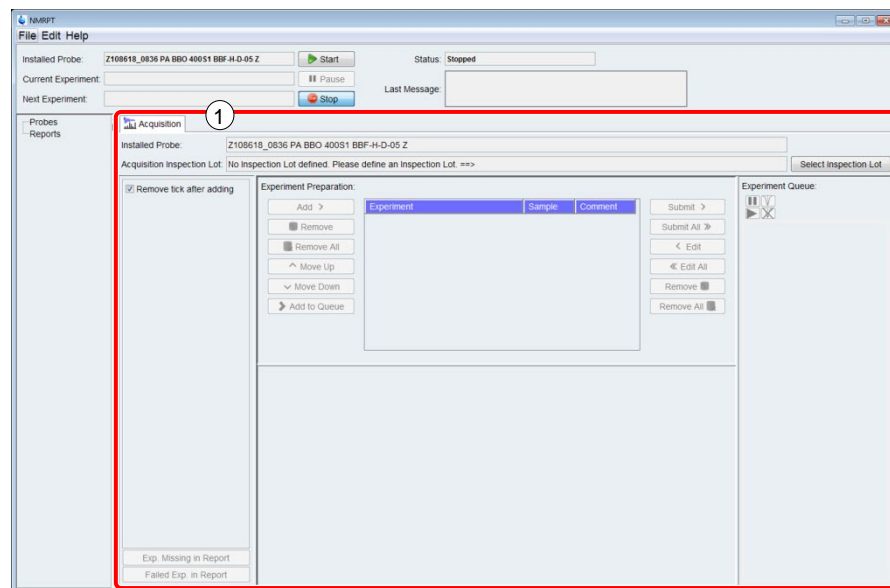


Figure 5-60: Workspace area

Click the corresponding item in [Navigation](#) panel to open a tab.

To close a tab, click the **x** symbol (Figure 5-60 (1)) on the right of its title.

Change the order of open tabs by drag and drop: Click and hold the title of a tab and move it to its new position.

**i** The Acquisition tab is unique and only available for the Inspection Lot currently selected (see [5.4.3 Acquisition Tab](#)). It can not be closed.

## 5.4.1 Inspection Lot Tab

On Inspection Lot tab (Figure 5-61), the content of the Inspection Lot is prepared. **Pairings** of experiments and samples are included to the Inspection Lot and their specification values are set. The Inspection Lot tab consists of three tables:

- (1) Experiments
- (2) Samples
- (3) Specifications

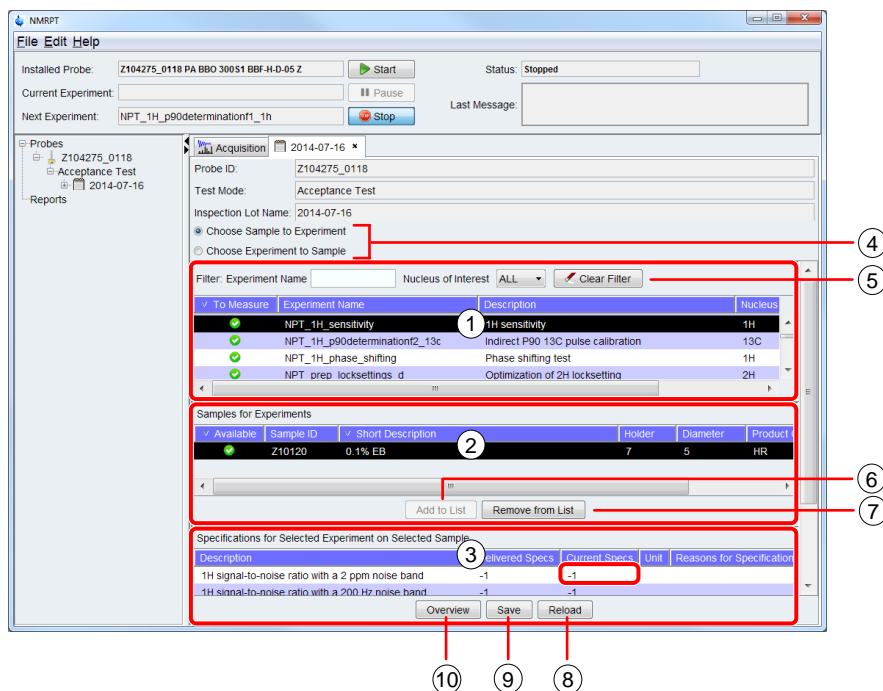


Figure 5-61: Inspection Lot tab – overview

- (1) Select an experiment from the experiment table (Figure 5-61 (1)) to show the respective samples in table (2) (Figure 5-61). The experiment table contains all experiments suitable for the probe of the Inspection Lot.
- (2) Select a sample for the selected experiment from the sample table (Figure 5-61 (2)) to show the respective specification values in table (3) (Figure 5-61). Click **Add to List** (Figure 5-61 (6)) to add the Pairing of experiment and sample to the Inspection Lot.
- (3) Click a cell in **Current Specs** column of the specification table (Figure 5-61 (3)) and enter a specification value. In case of changed Specs, enter **Reasons for Specification Change** to the corresponding cell. Click **Save** (Figure 5-61 (9)) to apply the changes.

**i**

A **Specs** value of -1 means determination of results, but no comparing evaluation of results against specifications. It is mandatory to enter a comment if Delivered Specs are available and Current Specs are changed. The results in spectra PDF are marked accordingly. Only positive values can be set as Specs.



- (4) Select **Choose Experiment to Sample** to swap the order of experiment table (Figure 5-61 (1)) and sample table (Figure 5-61 (2)). Selecting a sample in first table shows all experiments available for this sample in second table. **Select Choose Sample to Experiment** to switch back to default order.
- (5) **Filter Bar**  
Enter an **Experiment Name** or select a **Nucleus of Interest** to filter the experiment table content. Click **Clear Filter** to reset filter conditions and to show the unfiltered experiment table.

**i** The Nucleus of Interest is the nucleus in focus of the experiment. The main result of the experiment is determined for this nucleus .

- (6) **Add to List**  
Click **Add to List** (Figure 5-61 (6)) to add the selected Pairing of experiment and sample to the list of experiments to be executed, collated in this Inspection Lot.
- (7) **Remove from List**  
Click **Remove from List** (Figure 5-61 (7)) to remove the selected Pairing of experiment and sample from the list of experiments to be executed, collated in this Inspection Lot.

**i** Experiments removed from an Inspection Lot are also removed from the Results tab if already executed. The measurement data is not deleted. The results will be shown again in Results tab if the experiments are again added to the Inspection Lot.

- (8) **Reload**  
Click **Reload** (Figure 5-61 (8)) to revert all changes not applied yet.
- (9) **Save**  
Click **Save** (Figure 5-61 (9)) to apply all changes. Changed specifications are also applied to experiments of the Inspection Lot already acquired. The experiments are reprocessed and evaluated against the new specification value. Therefore the [status](#) of the results might change. Experiments removed from the Inspection Lot are also removed from the [Results tab](#). The measurement data is not deleted.
- (10) **Overview**  
Click **Overview** (Figure 5-61 (9)) to open Overview dialog (Figure 5-62).

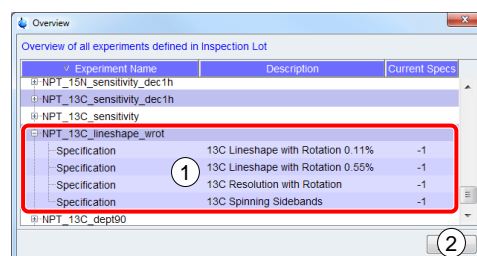


Figure 5-62: Inspection Lot tab – Overview dialog

In Overview dialog (Figure 5-62) the experiments currently selected for the Inspection Lot are listed. Expand an experiment item (1) to see its specification values. Click **Close** (Figure 5-62 (2)) to close the dialog.

## 5.4.2 Probe Setup Tab

The Probe Setup tab (Figure 5-63) offers global settings for a specific probe. These settings are applied as defaults for all future experiments of Inspection Lots for this probe.

- i** The default settings in Probe Setup tab can be changed for each experiment individually in [Preparation](#) panel of the [Acquisition](#) tab.

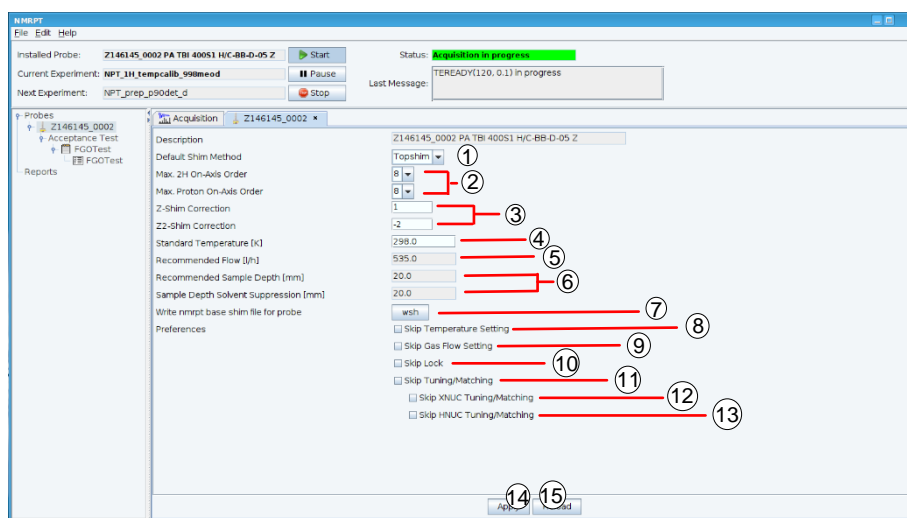


Figure 5-63: Probe Setup tab – overview

- (1) **Default Shim Method**  
Select the Shim Method from the list (Figure 5-63 (1)) to be set as default for the probe. If None is selected as a default, *NMRPT Shim Command Number* 999 ([skip shimming](#)) is set as a default for experiments.
- (2) **Maximum Shim Order (not HRMAS, MAS, CMP probes)**  
Select a **Max. 2H On-Axis Order** and a **Max. Proton On-Axis Order** from the corresponding lists (Figure 5-63 (2)). These maximum orders are applied according to the TopShim `ordmax` parameter.
- (3) **Z-Shim Correction (not MAS, SOL probes)**  
Enter a value for **Z- or Z2-Shim Correction** (Figure 5-63 (3)) to be applied for this probe. The correction is applied at the end of the shimming process during water suppression experiments. If *NMRPT Shim Command* 999 ([skip shimming](#)) is selected for an experiment, Z-Shim Correction is not applied.
- (4) **Standard Temperature [K]**  
Enter a **Standard Temperature** (Figure 5-63 (4)) in Kelvin to be applied if Temperature und Flow settings (Figure 5-63 (8)) are active.
- (5) **Recommended Flow from PICS [l/h]**  
This information shows the PICS value for Recommended Flow (Figure 5-63 (5)) in litre per hour to be applied if Temperature und Flow settings (Figure 5-63 (8)) are selected.
- (6) **Sample Depth [mm] (Figure 5-63 (6)) (HR probes only)**  
**Recomanded Sample Depth** below magnetic centre in millimeters for all standard samples.

**Sample Depth Solvent Suppression** in millimeters for best solvent suppression results.

This information shows the PICS values for Sample Depth.

- (7) **Write nmrpt base shim file for probe**  
Click **wsh** (Figure 5-63 (7)) to write a [base shim file](#).
- (8) **Skip Temperature Setting**  
Select this option (Figure 5-63 (8)) to skip setting the [Standard Temperature](#) of the probe to temperature control unit.
- (9) **Skip Gas Flow Setting**  
Select this option (Figure 5-63 (9)) to skip [setting the gas flow](#) for temperature control by *NMRPT*. Experiments that require a defined flow will become [irregular](#). This option is disabled if temperature control unit is set to external mode.
- (10) **Skip Lock (probes with 2H only)**  
Select **Skip Lock** option (Figure 5-63 (10)) to measure the experiment unlocked or to lock manually. This option is missing if no lock is available.
- (11) **Skip Tuning/Matching**  
Select this option (Figure 5-63 (11)) to skip tuning and matching of all nuclei used in an experiment. If selected, **Skip XNUC Tuning/Matching** (Figure 5-63 (12)) and **Skip HNUC Tuning/Matching** (Figure 5-63 (13)) are disabled.
- (12) **Skip XNUC Tuning/Matching**  
Select this option (Figure 5-63 (12)) to skip tuning and matching of all X nuclei used in an experiment. This option is disabled if **Skip Tuning/Matching** (Figure 5-63 (11)) is selected.
- (13) **Skip HNUC Tuning/Matching**  
Select this option (Figure 5-63 (13)) to skip tuning and matching of the H nucleus if used in an experiment. This option is disabled if **Skip Tuning/Matching** (Figure 5-63 (11)) is selected.
- (14) **Apply**  
Click **Apply** (Figure 5-63 (14)) to apply all settings as defaults for future experiments set up for this probe.
- (15) **Reload**  
Click **Reload** (Figure 5-63 (15)) to revert all changes not applied yet.

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[NMRPT Shim Commands](#) encompass sequences of combined *TopSpin* and *TopShim* commands. Maximum Shim Order is applied to these *NMRPT* Shimcommands and therefore the complete sequence included. More Information about *NMRPT* Shim Commands is provided in chapter [4.4 NMRPT Shim Handling](#). General information about shimming in *TopSpin* and the write shim command **wsh** are provided in the *TopSpin* and *TopShim* manuals (see chapter [1.5 Referenced Documents](#)).

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## 5.4.3 Acquisition Tab

The Acquisition tab (Figure 5-64) is divided into three main areas:

- (1) Library
- (2) Experiment Preparation
- (3) Experiment Queue

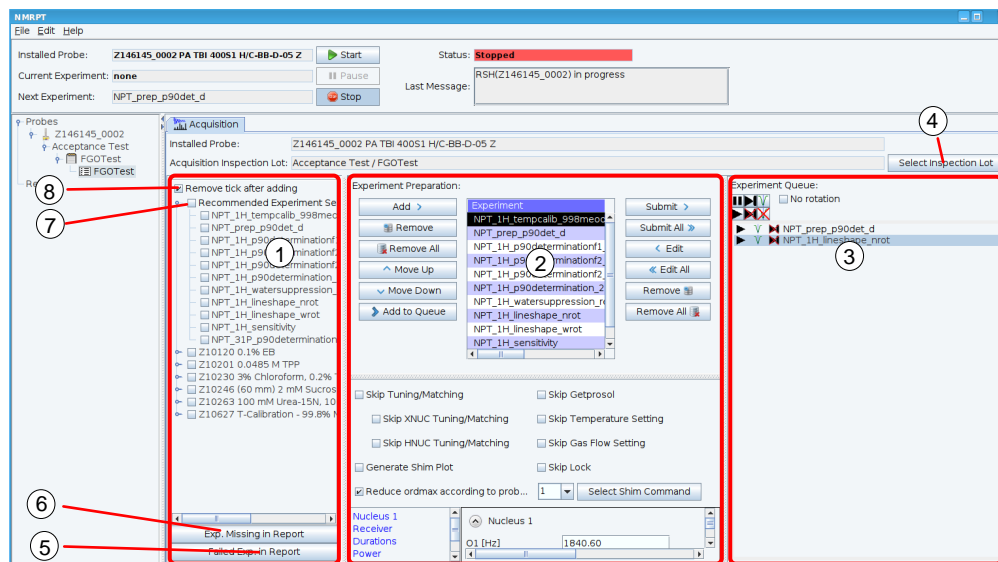


Figure 5-64: Acquisition tab – overview

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Experiments in Acquisition tab can also be moved from Experiment Preparation to Experiment Queue and back – or inside these lists, using drag and drop. Click and hold an experiment item and move it to the new position.

### Select Inspection Lot (Figure 5-64 (4))

On the **Acquisition** tab (Figure 5-64) click **Select Inspection Lot** (4). The Select Inspection Lot dialog opens.

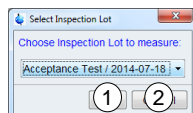


Figure 5-65: Acquisition tab – Select Inspection Lot dialog

Select the **Inspection Lot** to measure from the list in the dialog window shown in Figure 5-65. Click **OK** (Figure 5-65 (1)) to apply the selection. Click **Cancel** (Figure 5-65 (2)) to abort selecting an Inspection Lot for acquisition.

## Library (Figure 5-64 (1))

In the Library all experiments of the current [Inspection Lot](#) are listed grouped by the samples of the [Pairing](#). Expand a sample entry to access the corresponding experiments. Click the check box in front of an experiment to select experiments individually.

### (7) Recommended Experiment Sequence

Select **Recommended Experiment Sequence** (7) from [Library](#) to select all experiments from Library in recommended measurement order. The Recommended Experiment Sequence contains all experiments listed below, grouped by sample.

### (8) Remove tick after adding

Select **Remove tick after adding** (8) to automatically deselect experiments in Library when added to the [Experiment Preparation](#) or [Experiment Queue](#).

### (6) Exp. Missing in Report

Click **Exp. Missing in Report** (6) to show a list of experiments (Figure 5-66) of the Inspection Lot not measured yet. Only experiments for current routing and samples currently available are listed.

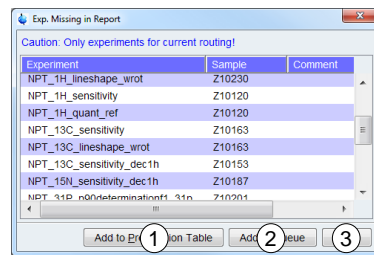


Figure 5-66: Acquisition tab – Exp. Missing in Report dialog

Select experiments from the list (Figure 5-66) and click **Add to Preparation Table** (Figure 5-66 (1)) to move the experiments to the table for [Experiment Preparation](#). Click **Add to Queue** (Figure 5-66 (2)) to add the experiments directly to the [Experiment Queue](#). Click **Close** (Figure 5-66 (3)) to close the dialog.

### (5) Exp. Failed in Report

Click **Exp. Failed in Report** (5) to show a list of experiment runs set to be used for report (Figure 5-67) that do not meet specifications. Only experiments for current routing and samples currently available are listed.

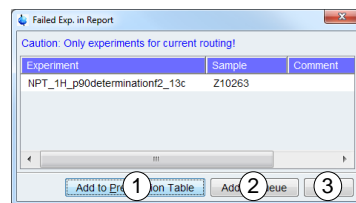


Figure 5-67: Acquisition tab – Failed Exp. in Report

Select experiments from the list (Figure 5-67) and click **Add to Preparation Table** (Figure 5-67 (1)) to move the experiments to the table for [Experiment Preparation](#). Click **Add to Queue** (Figure 5-67 (2)) to add the experiments directly to the [Experiment Queue](#). Click **Close** (Figure 5-67 (3)) to close the dialog.

## Experiment Preparation – Workflow (Figure 5-68)

The Experiment Preparation panel provides individual settings for experiments. Therefore select an experiment in the table for Experiment Preparation (7) and modify the settings below (24).

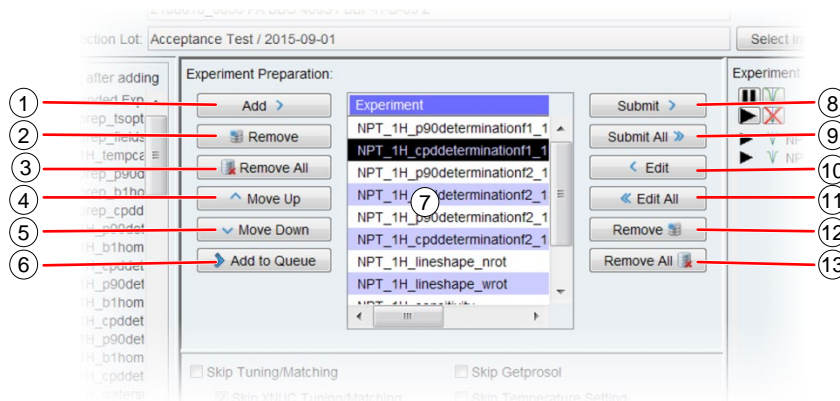


Figure 5-68: Acquisition tab – detail: Experiment Preparation (Figure 5-64 (2)), workflow

- (1) **Add**  
Select experiments in [Library](#) (Figure 5-64 (1)) and click **Add** (1) to move these experiments to Experiment Preparation table (7).
- (2) **Remove**  
Select experiments in Experiment Preparation table (7) and click **Remove** (2) to remove these experiments from Experiment Preparation table (7).
- (3) **Remove All**  
Click **Remove All** (3) to remove all experiments from Experiment Preparation table (7).
- (4) **Move Up**  
Select an experiment in Experiment Preparation table (7) and click **Move Up** (4) to move the experiment up in the table. A higher position in the table means an earlier acquisition in the [Experiment Queue](#) (Figure 5-64 (3)).
- (5) **Move Down**  
Select an experiment in Experiment Preparation table (7) and click **Move Down** (5) to move the experiment down in the table. A lower position in the table means a later acquisition in the Experiment Queue (Figure 5-64 (3)).
- (6) **Add to Queue**  
Click **Add to Queue** (6) to add selected experiments from [Library](#) (Figure 5-64 (1)) directly to the [Experiment Queue](#) (Figure 5-64 (3)). This skips the Experiment Preparation step. The measurement order is based on the **Recommended Experiment Sequence** (Figure 5-64 (8)).
- (8) **Submit**  
Select experiments in Experiment Preparation table (7) and click **Submit** (8) to move the experiments to Experiment Queue (Figure 5-64 (3)).
- (9) **Submit All**  
Click **Submit All** (9) to move all experiments in Preparation table (7) to Experiment Queue (Figure 5-64 (3)).

- (10) **Edit**  
Select the experiments to edit in Experiment Queue (Figure 5-64 (3)). Click **Edit** (10) to move the experiments to [Experiment Preparation](#) table (7) to change settings or measurement order.
- (11) **Edit All**  
Click **Edit All** (11) to move all experiments from Experiment Queue (Figure 5-64 (3)) to Experiment Preparation table (7) to change settings or measurement order.
- (12) **Remove**  
Select the experiments to be removed in Experiment Queue (Figure 5-64 (3)). Click **Remove** (12) to remove the experiments from the Queue.
- (13) **Remove All**  
Click **Remove All** (13) to remove all experiments from Experiment Queue (Figure 5-64 (3)).

## Experiment Preparation – Detail Settings (Figure 5-69)

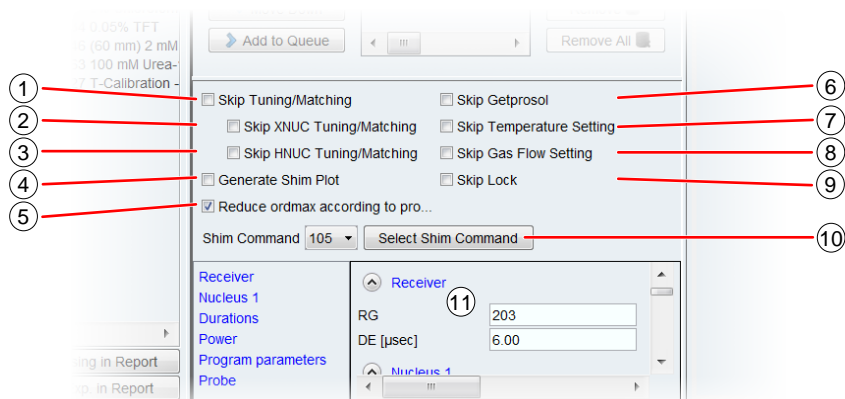


Figure 5-69: Acquisition tab – detail: Experiment Preparation (Figure 4 47 (2)), detail settings

- (1) **Skip Tuning/Matching**  
Select this option (1) to skip tuning and matching of all nuclei used in the experiment. If selected, **Skip XNUC Tuning/Matching** (2) and **Skip HNUC Tuning/Matching** (3) are disabled.
- (2) **Skip XNUC Tuning/Matching**  
Select **Skip XNUC Tuning/Matching** (2) to skip tuning and matching of all X nuclei used in the experiment. This option is disabled if **Skip Tuning/Matching** (1) is selected.
- (3) **Skip HNUC Tuning/Matching**  
Select **Skip HNUC Tuning/Matching** (3) to skip tuning and matching of the H nucleus if used in the experiment. This option is disabled if **Skip Tuning/Matching** (1) is selected.
- (4) **Generate Shim Plot**  
Select **Generate Shim Plot** (4) to add a shim plot to the results of the experiments.
- (5) **Reduce ordmax according to probe setting (not HRMAS, MAS, CMP probes)**  
Select **Reduce ordmax according to probe setting** (5) to apply the settings for maximum shim order which were set for the probe in [Probe Setup](#) tab.

## (6) Skip Getprosol

Select **Skip Getprosol** (6) to skip setting pulses applying the *TopSpin* `getprosol` command for the experiment.

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If Skip Getprosol is selected, pulse determination experiments also skip writing the determined pulses to the prosol tables (`setprosol`).

The `getprosol` and `setprosol` commands are part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

## (7) Skip Temperature Setting

Select **Skip Temperature Setting** (7) to skip setting the [Standard Temperature](#) of the probe, as defined on [Probe Setup tab](#), to temperature control unit.

## (8) Skip Gas Flow Setting

Select this option (8) to skip [setting the gas flow](#) for temperature control by *NMRPT*. Experiments that require a defined flow will become [irregular](#). This option is disabled if temperature control unit is set to external mode.

## (9) Skip Lock

Select **Skip Lock** (9) to measure the experiment unlocked or to lock manually. This option is missing if no lock is available.

## (10) Shim Command / Select Shim Command

Select a [Shim Command](#) number from the list (10) to select a shim sequence to be applied for the experiment. Click **Select Shim Command** (10) to open Select Shim Command dialog (Figure 5-70).

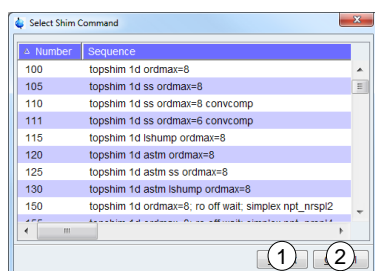


Figure 5-70: Acquisition tab – Select Shim Command dialog

Select a Shim Command from the list and click **Select** (1) to apply the Shim Command to the experiment. Click **Cancel** (2) to abort changing the Shim Command.

## (11) TopSpin Experiment Parameters

Edit specific TopSpin experiment parameters



## Experiment Queue (Figure 5-71)

The **Experiment Queue** (Figure 5-64 (3)) shows the sequence of experiments in measurement order. The experiment listed in first line will be executed next. To change the order of the sequence, see [Experiment Preparation](#).

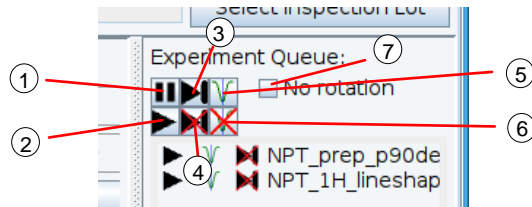




Figure 5-71: Acquisition tab – detail: Experiment Queue (Figure 5-64 (3))


### (1) **Pause before Acquisition**

Select experiments in Experiment Queue (Figure 5-64 (3)) and click  to pause the queue before the acquisition of the selected experiments. If a sample change is required, the Experiment Queue is paused after sample change (unlike the sample specific [Pause before Change](#) option available from [Sample List](#)).


### (2) **Run Experiment without Pause before Acquisition**

Select experiments in Experiment Queue (Figure 5-64 (3)) and click  to pause the queue before the acquisition of the selected experiments.


### (3) **Skip Experiment**

Select experiments in Experiment Queue (Figure 5-64 (3)) and click  to skip these experiments when doing the acquisition.


### (4) **Execute Experiment**

Select experiments in Experiment Queue (Figure 5-64 (3)) and click  to mark these experiments for acquisition.

### (5) **Execute Tuning/Matching**

Select experiments in Experiment Queue (Figure 5-64 (3)) and click  to execute Tuning/Matching during acquisition of the selected experiments.

### (6) **Skip Tuning/Matching**

Select experiments in Experiment Queue (Figure 5-64 (3)) and click  to skip execution of Tuning/Matching during acquisition of the selected experiments.

### (7) **No Rotation**

The rotation will be turned off for all experiments in the Experiment Queue (Figure 5-64 (3)) when this checkbox is marked.

## 5.4.4 Results Tab

The Results tab provides an overview of all experiments executed and their results. It offers access to additional information about each run of an experiment and allows selecting the run for report. It also offers access to the measurement data in TopSpin and provides options for reprocessing of a selected run. The Results tab (Figure 5-72) consists of three main areas:

- (1) Results table
- (2) Dataset options
- (3) Processing options

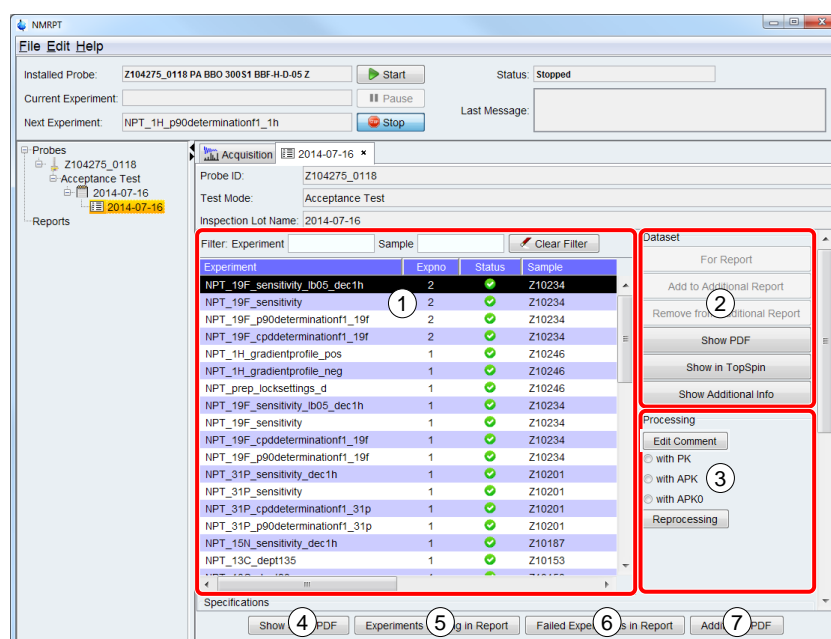


Figure 5-72: Results tab – overview

The button panel of Results tab provides access to information about the current state and content of the Inspection Lot:

- (4) Click **Short PDF** (Figure 5-72 (4)) to access the [Short PDF](#) of this Inspection Lot.
- (5) **Experiments Missing in Report**  
Click **Experiments Missing in Report** (Figure 5-72 (5)) to show a list of experiments of the Inspection Lot not measured yet (Figure 5-73). Only experiments for samples currently available are listed.

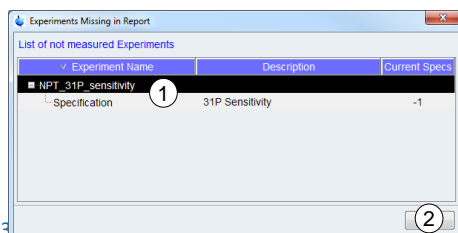


Figure 5-73

Expand experiment items from the **List of not measured Experiments** (Figure 5-73) to show the Current Specs of the experiments. Click **Close** (Figure 5-73 (2)) to close the dialog.

## (6) Failed Experiments in Report

Click **Failed Experiments in Report** (Figure 5-72 (6)) to show a list of experiment runs set to be used for report (Figure 5-67) that do not meet specifications. Only experiments for samples currently available are listed.

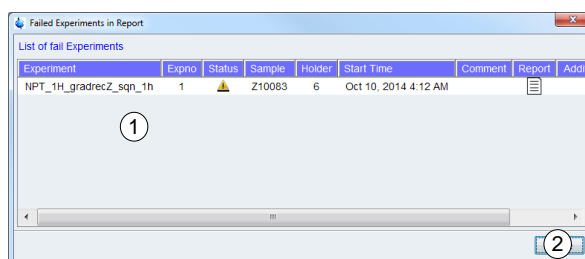


Figure 5-74: Results tab – Failed Experiments in Report dialog

The **List of failed Experiments** (Figure 5-74 (1)) contains all non-successful experiment runs set to be used for report. Non-successful experiments are either experiments with status error (red status icon) or experiments that do not meet the specifications (yellow exclamation mark). Further information about each of these experiment runs is provided. Click **Close** (Figure 5-74 (2)) to close the dialog.

## (7) Additional PDF (of Inspection Lot)

Click **Additional PDF** to include [additional PDF files](#) (e.g. external measurements acquired outside *NMRPT*) to the Additional Report of the Inspection Lot.

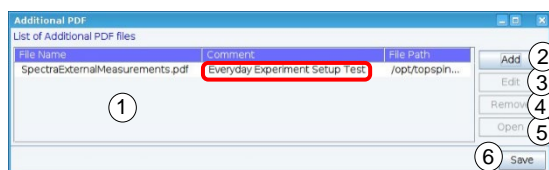


Figure 5-75: Results tab – Additional PDF dialog

In the subsequent Additional PDF dialog the PDF files to be included are shown in **List of Additional PDF files** (Figure 5-75 (1)). Click **Add** (Figure 5-75 (2)) to open a file browser and to select a PDF file from hard disk. The file is added to the list. Click the **Comment** cell of a file entry in the list to enter a comment if required. Select a file list entry and click **Edit** (Figure 5-75 (3)) to edit an Additional PDF entry. Select a file list entry and click **Remove** (Figure 5-75 (4)) to remove an Additional PDF file. Select a file list entry and click **Open** (Figure 5-75 (5)) to open an Additional PDF file with a PDF viewer. Click **Save** (Figure 5-75 (6)) to apply all changes and close Additional PDF dialog.

Results Table (Figure 5-76)

Test Mode: Acceptance Test  
Inspection Lot Name: 2014-07-16  
Filter: Experiment Sample Clear Filter

Experiment	Expno	Status	Sample	Holder	Start Time	Comment	Report	Additional
NPT_19F_sensitivity_lb05_dec1h	2	✔	Z10234	11	Jul 17, 20...			
NPT_19F_sensitivity	2	✔	Z10234	11	Jul 17, 20...			
NPT_19F_p90determinationf1_19f	2	✔	Z10234	11	Jul 17, 20...			
NPT_19F_cpddeterminationf1_19f	2	✔	Z10234	11	Jul 17, 20...			
NPT_1H_gradientprofile_pos	1	✔	Z10246	2	Jul 16, 20...			
NPT_1H_gradientprofile_neg	1	✔	Z10246	2	Jul 16, 20...			
NPT_prep_locksettings_d	1	ⓘ	Z10246	2	Jul 16, 20...			
NPT_19F_sensitivity_lb05_dec1h	1	✔	Z10234	11	Jul 16, 20...			
NPT_19F_sensitivity	1	✔	Z10234	11	Jul 16, 20...			
NPT_19F_cpddeterminationf1_19f	1	✔	Z10234	11	Jul 16, 20...			
NPT_19F_p90determinationf1_19f	1	✔	Z10234	11	Jul 16, 20...			
NPT_31P_sensitivity_dec1h	1	✔	Z10201	12	Jul 16, 20...			
NPT_31P_sensitivity	1	✔	Z10201	12	Jul 16, 20...			
NPT_31P_cpddeterminationf1_31p	1	✔	Z10201	12	Jul 16, 20...			
NPT_31P_p90determinationf1_31p	1	✔	Z10201	12	Jul 16, 20...			
NPT_15N_sensitivity_dec1h	1	✔	Z10187	10	Jul 16, 20...			
NPT_13C_dept135	1	✔	Z10153	8	Jul 16, 20...			

Description	Current Specs	Result Value	Unit
19F signal-t...	-1	365.5	
19F full line ...	-1	0.74	Hz

Show Short PDF Experiments Missing in Report Failed Experiments in Report Additional P

Figure 5-76: Results tab – detail: results table (Figure 5-72 (1))

- (1) A green icon ✔ in the **Status** column (1) means no errors occurred and all specifications were achieved. A yellow exclamation mark ⚠ indicates that specifications were not achieved. A red error icon ❌ is shown if errors occurred during acquisition or processing.

**i** More information about each run of an experiment and its status is provided as [Additional Info](#) (see (6))

- (2) A report icon 📄 in **Report** column (2) indicates which run of an experiment is used for [report](#). As a default, the last run of each experiment is used if no error (see (1)) occurred.
- (3) A report icon 📄 in **Additional Report** column (2) indicates which run of an experiment is selected to be used for [Additional Report](#).
- (4) Select an experiment in results table to see the corresponding specifications and results in **Specifications** table (4). Results not reaching specifications are printed in red.

## Dataset Options (Figure 5-77)

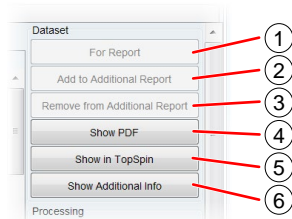




Figure 5-77: Results tab – detail: Dataset options (Figure 5-72 (2))

### (1) For Report

Select a run of an experiment in results table (Figure 5-72 (1)) and click **For Report** (1) to select the run to be used for [report](#). A report icon  in the **Report** column of the run indicates the run is used for report. If errors occurred during measurement or processing, this option may be disabled.

### (2) Add to Additional Report

Select a run of an experiment in results table (Figure 5-72 (1)) and click **Add to Additional Report** (2) to add the run of the experiment to the [Additional Report](#). A report icon  in the **Additional Report** column of the run indicates the run is used for report. If errors occurred during measurement or processing, this option may be disabled.

### (3) Remove from Additional Report

Select a run of an experiment in results table (Figure 5-72 (1)) and click **Remove from Additional Report** (3) to remove the run of the experiment from the Additional Report. This option is only available for runs added to the Additional Report.



[Irregular](#) experiments can not be part of a report but can be added as [Additional Report](#).

### (4) Show PDF

Select a run of an experiment in results table (Figure 5-72 (1)) and click **Show PDF** (4) to access the single spectrum PDF of this run. If errors occurred during measurement or processing, this option may be disabled.

### (5) Show in TopSpin

Select a run of an experiment in results table (Figure 5-72 (1)) and click **Show in TopSpin** (5) to access the measurement data of this run in *TopSpin* window.

### (6) Show Additional Info

Select a run of an experiment in results table (Figure 5-72 (1)) and click **Show Additional Info** (6) to open Additional Information dialog (Figure 5-78).

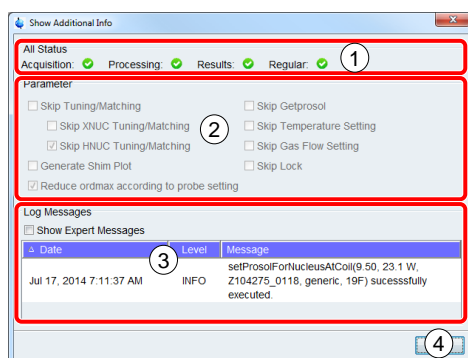


Figure 5-78: Results tab – Show Additional Info dialog

The **Show Additional Info** dialog (Figure 5-78) provides detailed information about **All Status** (Figure 5-78 (1)) of the run. Separate icons indicate if **Acquisition** and **Processing** occurred without errors and if the **Results** match the specifications. A fourth icon indicates if the experiment was executed under **Regular** conditions.

An overview about the applied *NMRPT* control **Parameters** (Figure 5-78 (2)) is provided for information.

**Log Messages** (Figure 5-78 (3)) are listed to provide detailed information about the specific run. Click **Show Expert Messages** to access more detailed expert information.

Click **Close** (Figure 5-78 (4)) to close Show Additional Info dialog.

## Processing Options (Figure 5-79)

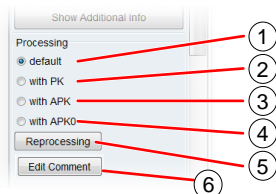


Figure 5-79: Results tab – detail: Processing options

- (1) Select a run of an experiment in results table (Figure 5-72 (1)), select **default** (1) and click **Reprocessing** (5) to reprocess the run of the experiment applying the default phase correction option for this experiment. (see Experiment Documentation, [1.5 Referenced Documents](#))
- (2) Select a run of an experiment in results table (Figure 5-72 (1)), select **with PK** (2) and click **Reprocessing** (5) to reprocess the run of the experiment applying TopSpin PK command.
- (3) Select a run of an experiment in results table (Figure 5-72 (1)), select **with APK** (3) and click **Reprocessing** (5) to reprocess the run of the experiment applying TopSpin APK command.
- (4) Select a run of an experiment in results table (Figure 5-72 (1)), select **with APK0** (4) and click **Reprocessing** (5) to reprocess the run of the experiment applying TopSpin APK0 command.
- (5) **Reprocessing**  
Click **Reprocessing** (5) to start reprocessing the selected experiment applying selected processing option.

## (6) Edit Comment

Click Edit Comment (6) to edit the comment of selected experiment. Reprocessing will be executed afterwards.



The phase correction commands PK, APK and APK0 are part of *TopSpin*. Further information is provided in the TopSpin manuals (see chapter [1.5 Referenced Documents](#)).

## 5.4.5 Report Tab

The *NMRPT* report, consisting of a spectra PDF and the test protocol for signature, is created from Report tab. In Report tab all information for a test report is summarized. Therefore the content of the tab (Figure 5-80 (1)) depends on the [Test Mode](#) and the [Report Type](#). The button panel (Figure 5-80 (2)) is the same for all modes and types (see individual report tab chapters for detailed information).



### Information for Report Creation

Enter all available information on Report tab. This information is used to create and fill the final document for signature. Empty information may result in an invalid document.

The screenshot shows the NMRPT Report tab interface. The left sidebar contains a tree view with the following structure:

- Probes
  - B0945\_0020
  - F12345\_0001
  - H6565\_1
  - Z104450\_0004
- Reports
  - Final Test
  - Acceptance Test
  - Accessories Report
  - Probe Report
  - Spectrometer Report

The main content area is titled 'Report Name: 2020-08-03' and contains the following fields:

- Test Mode: Acceptance Test
- Protocol Type: Probe Report
- General Information
  - Edit customer/spectrometer information: edit
  - Engineer: [text field]
  - Date of Signature: 8/5/20
  - Language: English
  - Remarks / Exclusions: [text field]
- Probe Information
  - Order No: [text field]
  - Contract No: [text field]
- Inspection Lot for Report
  - Description: TXD
  - Probe ID: F12345\_0001
  - Inspection Lot Name: 2020-08-03
- Additional PDF
  - File Name: [text field]
  - Comment: [text field]
  - File Path: [text field]

The bottom button panel includes the following buttons:

- Save
- Last Save
- Create Protocol & Spectra
- View Spectra
- Print

Figure 5-80: Report tab – overview

## 5.4.5.1 Report Tab for Acceptance Test

The Acceptance Test Report tab is divided into different sections. Some sections differ depending on the subject to the acceptance. As an example the Acceptance Report tab of a probe is shown in Figure 5-81.

### Acceptance Test Report Tab – General Sections (Figure 5-81)

Figure 5-81: Report tab – Acceptance Test Probe

#### (1) General Information

In General Information section (Figure 5-81 (1)) click **edcstm** to open the Customer / System Setup dialog of *TopSpin*. In this dialog enter at least all information marked as required. Save all changes before closing the dialog.

In **Engineer** text field of the Report tab (Figure 5-81), enter the name of the engineer responsible for the Acceptance Test. Select the **Date of Signature** from the dropdown calendar. Remarks can also be added to the report filling the **Remarks / Exclusions** text field.

**i**

The **edcstm** command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter [1.5 Referenced Documents](#)).

#### (2) Probe Information (Probe Report only)

Enter the **Order No.** and **Contract No.** of the tested probe in the text fields of Probe Information section (Figure 5-81 (2)).



## (2) Accessory Information (Accessories Report only)

Figure 5-82: Report tab – Acceptance Test Accessories, Accessory Information

Enter the **Order No.** (Figure 5-82 (1)) and **Contract No.** (Figure 5-82 (2)) of the tested accessories in the text fields of Accessory Information section (Figure 5-82). Click **Add** (Figure 5-82 (3)) to add a new line to the table of accessories that are subject to this report. Enter the part (**P/N**) and serial (**S/N**) numbers of the tested accessories into the corresponding cells. Select a line in the table and click **Remove** (Figure 5-82 (4)) to delete this item.

## (3) Inspection Lot for Report

In case of a Probe Report, the **Inspection Lot Name**, the **Probe ID** and the **Description** are shown in Inspection Lot for Report section (Figure 5-81 (3)) for information.

Figure 5-83: Report tab – Acceptance Test Spectrometer/Accessories, Inspection Lot for Report

In case of Spectrometer and Accessories Reports multiple Inspection Lots can be included to a report. The Inspection Lots are listed in a table (Figure 5-83) providing the **Description**, the **Probe ID** and the **Inspection Lot Name** in columns. Select an Inspection Lot in the table and click **Remove and Save** (Figure 5-83(2)) to remove an Inspection Lot from the report. Click **Add and Save** (Figure 5-83(1)) to add further Inspection Lots. The Add Inspection Lot dialog (Figure 5-84) opens.

Figure 5-84: Report tab – Acceptance Test Spectrometer/Accessories, Add Inspection Lot dialog

Select the Inspection Lot to add from the list in the dialog and click OK (Figure 5-84 (1)) to apply the selection. Click Cancel (Figure 5-84 (1)) to abort adding an Inspection Lot to the report.



Only in case of an Accessories Report a report without any Inspection Lot can be created.

## (4) Additional PDF (of report)

**Additional PDF** documents can be included in the report. These documents are listed in **Additional PDF** section (Figure 5-81 (4)) of Report tab. Click **Add** to open a document browser to select files from hard disk. To add a comment to a file, enter the text into the cell in Comment column of the PDF list item. Select an Additional PDF list item and click **Edit** to edit the PDF entry. Select an Additional PDF list item and click **Remove** to remove the PDF from report. Select an Additional PDF list item and click **Open** to open the PDF with a PDF viewer.

## Acceptance Test Report Tab – Checklist Sections (Figure 5-85)

Scroll down to find multiple checklist sections on Acceptance Test Report tab. Select the status for each item out of three different options: **Pass**, **Fail** and **n/a** (not applicable).

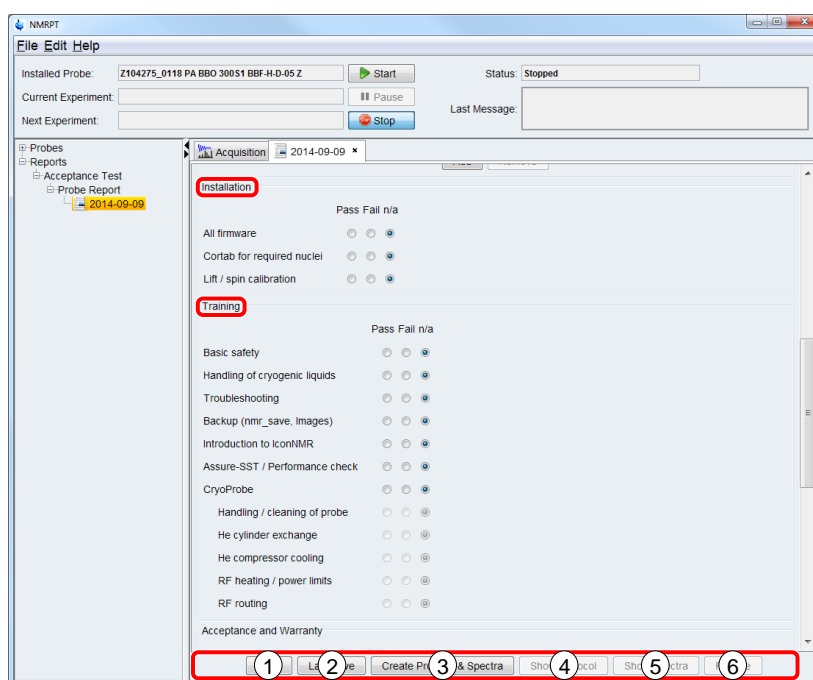


Figure 5-85: Report tab – Acceptance Test Probe, checklist sections

### • Installation

In Installation Checklist information about completed installation steps and aspects is collected for documentation. In all cases of Acceptance Reports the following items are available:

- All connections and grounding
- All Firmware
- Cortab for required nuclei
- Lift / spin calibration

For a Spectrometer Report additional items are:

- Software licenses
- He / N<sub>2</sub> log files activated
- MICS installed

- **Training**

In Training Checklist information about the customer training is collected. In all cases of Acceptance Reports the following items are available:

- Basic safety
- Handling of cryogenic liquids
- Troubleshooting
- Backups (nmr\_save, images)
- Introduction to IconNMR
- Assure-SST / Performance check

If a **CryoProbe** is subject to a Probe or Spectrometer Report additional items are:

- Handling / cleaning of probe
- He cylinder exchange
- He compressor cooling, RF heating / power limits
- RF routing

In case of a Spectrometer Report further items are:

- Magnet safety and refilling
- Hardware overview
- Console on/off operation
- Basic operation

- **Acceptance and Warranty**

This checklist collates all information concerning acceptance and warranty to be provided to the customer:

- Explanation of warranty
- Customer support hotlines

In case of a Spectrometer Report further item is:

- Spectrometer documentation

- **Optional Components (Probe and Spectrometer Report only)**

In Optional Components Checklist information about optional components being subject to the report is collected. Despite a list of suggested components five custom fields are provided. Enter further optional components to these custom fields.

- Sample changer
- MAS controller
- High power equipment
- LC-NMR
- Liquid Handler SamplePro Tube
- Micro-Imaging
- Diffusion
- CryoProbe, Cryoplatfrom
- BNL / BSNL
- Additional cooling/heating units (like BCU1 / BCU2)
- LT-MAS (Low Temperature MAS equipment)

- Gyrotron magnet and DNP console
- five custom fields

### Acceptance Test Report Tab – Button Panel (Figure 5-85 )

- (1) **Save**  
Click **Save** (1) to apply all changes to the current report.
- (2) **Last Save**  
Click **Last Save** (2) to revert all changes in Report Tab not applied yet.
- (3) **Create Protocol & Spectra**  
Click **Create Protocol & Spectra** (3) to create the spectra PDF and the protocol PDF of the report. All results set to be [used for report](#) and [for Additional Report](#) are included. Both parts of the report are marked as preliminary until it is [finalized](#).
- (4) **Show Protocol**  
Click **Show Protocol** (4) to open protocol PDF file. The protocol PDF is marked as preliminary until it is [finalized](#). This button is disabled if no protocol PDF was created yet.
- (5) **Show Spectra**  
Click **Show Spectra** (5) to open spectra PDF file. The spectra PDF is marked as preliminary until it is [finalized](#). This button is disabled if no spectra PDF was created yet.
- (6) **Finalize (non-finalized reports only)**  
Click Finalize (6) to create the final report for signature. The finalized spectra and protocol PDF files can not be recreated. Finalizing a report finalizes the Inspection Lots and results the report is based on.
- (6) **Export (finalized reports only)**  
Click Export (6) to open a file browser to export the finalized report to hard disk.

### i

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Finalized means, no further changes to the report, the included Inspection Lots, their experiments and results can be done. In the [Navigation panel](#), the corresponding icons are signed with a green checkmark. To make an Inspection Lot available again, the finalized report has to be deleted first.

---

## 5.4.5.2 Report Tab for Final Test

The Final Test Report tab is divided into different sections. Some sections differ depending on the subject to the Final Test. As an example the Final Test Report tab of a probe is shown in Figure 5-86.

Figure 5-86: Report tab – Final Test Probe

### Final Test Report Tab – General Sections (Figure 5-86)

#### (1) General Information

In General Information section (Figure 5-86 (1)) click **edcstm** to open the Customer / System Setup dialog of *TopSpin*. In this dialog enter at least all information marked as required. Save all changes before closing the dialog.

In **Engineer** field of the Report tab (Figure 5-86) enter the name of the engineer responsible for the Final Test. Enter the name of the **Supervisor** in the corresponding text field. Also enter the **Approval Postal Code**, **Approval City** and **Approval Country** in the corresponding text fields. Select the **Date of Signature** from the dropdown calendar. Remarks can be added to the report filling the **Remarks / Exclusions** text field.



The **edcstm** command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter 1.5 Referenced Documents).

#### (2) Probe Information (Probe Report only)

Enter the **Order No.** of the tested probe in the text field of Probe Information section (Figure 5-86 (2)).

## (2) Accessory Information (Accessories Report only)

Figure 5-87: Report tab – Final Test Accessories, Accessory Information

Enter the **Order No.** (Figure 5-87 (1)) and **Contract No.** (Figure 5-87 (2)) of the tested accessories in the text fields of Accessory Information section (Figure 5-87). Click **Add** (Figure 5-87 (3)) to add a new line to the table of accessories that are subject to this report. Enter the part (**P/N**) and serial (**S/N**) numbers of the tested accessories into the corresponding cells. Select a line in the table and click **Remove** (Figure 5-87 (4)) to delete this item.

## (3) Inspection Lot for Report

In case of a Probe Report, the **Inspection Lot Name**, the **Probe ID** and the **Description** are shown in Inspection Lot for Report section (Figure 5-86 (3)) for information.

Figure 5-88: Report tab – Final Test Spectrometer/Accessories, Inspection Lot for Report

In case of Spectrometer and Accessories Reports multiple Inspection Lots can be included to a report. The Inspection Lots are listed in a table (Figure 5-88) providing the **Description**, the **Probe ID** and the **Inspection Lot Name** in columns. Select an Inspection Lot in the table and click **Remove and Save** (Figure 5-89 (2)) to remove the Inspection Lot from the report. Click **Add and Save** (Figure 5-89 (1)) to add further Inspection Lots. The Add Inspection Lot dialog (Figure 5-89) opens up.

Figure 5-89: Report tab – Final Test Spectrometer/Accessories, Add Inspection Lot dialog

Select the Inspection Lot to add from the list in the dialog and click OK (Figure 5-89 (1)) to apply the selection. Click Cancel (Figure 5-89 (2)) to abort adding an Inspection Lot to the report.



Only in case of an Accessory Test a report without any Inspection Lot can be created.

(4) **Additional PDF (of report)**

[Additional PDF](#) documents can be included in the report. These documents are listed in **Additional PDF** section (Figure 5-86 (4)) of Report tab. Click **Add** to open a document browser to select files from the hard disk. To add a comment to a file, enter the text into the cell in Comment column of the PDF list item. Select an Additional PDF list item and click **Remove** to remove the PDF from report.

**Final Test Report Tab – Button Panel (Figure 5-86)**

(5) **Save**

Click **Save** (5) to apply all changes to the current report.

(6) **Last Save**

Click **Last Save** (6) to revert all changes in Report tab not applied yet.

(7) **Create Protocol & Spectra**

Click **Create Protocol & Spectra** (7) to create the spectra PDF and the protocol PDF of the report. All results set to be [used for report](#) and [for Additional Report](#) are included. Both parts of the report are marked as preliminary until it is [finalized](#).

(8) **Show Protocol**

Click **Show Protocol** (8) to open protocol PDF file. The protocol PDF is marked as preliminary until it is [finalized](#). This button is disabled if no protocol PDF was created yet.

(9) **Show Spectra**

Click **Show Spectra** (9) to open spectra PDF file. The spectra PDF is marked as preliminary until it is [finalized](#). This button is disabled if no spectra PDF was created yet.

(10) **Finalize (non-finalized reports only)**

Click Finalize (10) to create the final report for signature. The finalized spectra and protocol PDF files can not be recreated. Finalizing a report finalizes the Inspection Lots and results the report is based on.

(10) **Export (finalized reports only)**

Click Export (6) to open a file browser to export the finalized report to hard disk.



Finalized means, no further changes to the report, the included Inspection Lots, their experiments and results can be done. In the [Navigation panel](#), the corresponding icons are signed with a green checkmark. To make an Inspection Lot available again, the finalized report has to be deleted first.

---

## 5.4.5.3 Report Tab for Field Service Test

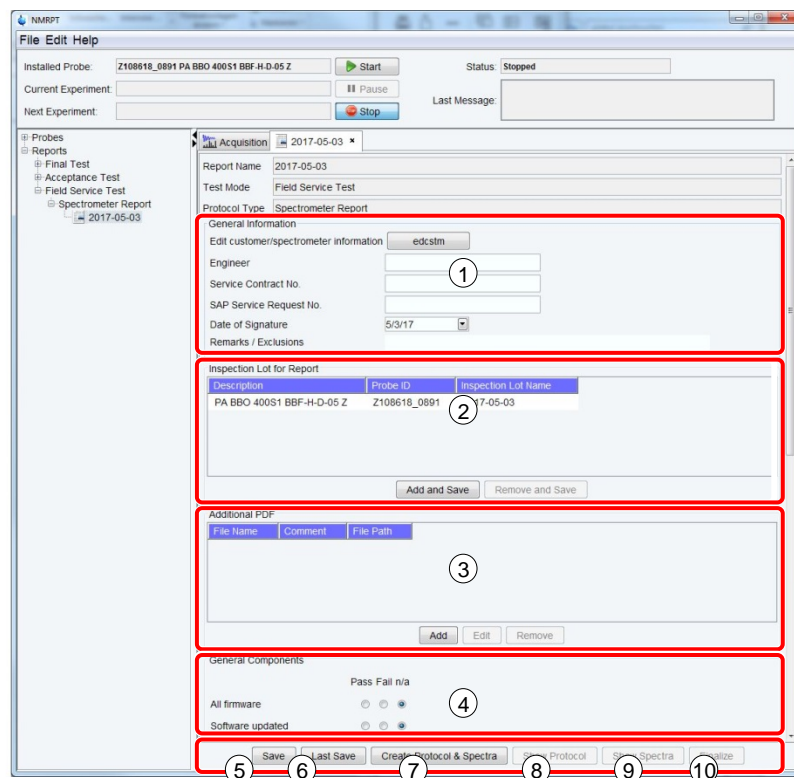


Figure 5-90: Report tab – Field Service Test Spectrometer

### Field Service Test Report Tab – General Sections (Figure 5-90)

#### (1) General Information

In General Information section (Figure 5-90 (1)) click **edcstm** to open the Customer / System Setup dialog of *TopSpin*. In this dialog enter at least all information marked as required. Save all changes before closing the dialog.

In **Engineer** field of the Report tab (Figure 5-90) enter the name of the engineer responsible for the Field Service Test. Enter the **Service Contract No.** and the **SAP Service Request No.** in the corresponding text fields. Select the **Date of Signature** from the dropdown calendar. Remarks can be added to the report filling the **Remarks / Exclusions** text field.



The **edcstm** command is part of *TopSpin*. Further information is provided in the *TopSpin* manuals (see chapter 1.5 Referenced Documents).



## (-) Probe Information (Probe Report only)

Figure 5-91: Report tab – Field Service Test Probe, Probe Information

Enter the **Order No.** of the tested probe in the text field of Probe Information section (Figure 5-91 (1)).

## (-) Accessory Information (Accessories Report only)

Figure 5-92: Report tab – Field Service Test Accessories, Accessory Information

Enter the **Order No.** (Figure 5-92 (1)) and **Contract No.** (Figure 5-92 (2)) of the tested accessories in the text fields of Accessory Information section (Figure 5-92). Click **Add** (Figure 5-92 (3)) to add a new line to the table of accessories that are subject to this report. Enter the part (**P/N**) and serial (**S/N**) numbers of the tested accessories into the corresponding cells. Select a line in the table and click **Remove** (Figure 5-92 (4)) to delete this item.

## (2) Inspection Lot for Report

In case of Spectrometer and Accessories Reports multiple Inspection Lots can be included to a report. The Inspection Lots are listed in a table (Figure 5-90 (2)) providing the **Description**, the **Probe ID** and the **Inspection Lot Name** in columns. To remove an Inspection Lot from the report, select an Inspection Lot in the table and click **Remove** and **Save** button in Inspection Lot for Report section (Figure 5-90 (2)). Click **Add and Save** button in Inspection Lot for Report section (Figure 5-90 (2)) to add further Inspection Lots. The Add Inspection Lot dialog (Figure 5-93) opens.

Figure 5-93: Report tab – Final Test Spectrometer/Accessories, Add Inspection Lot dialog

Select the Inspection Lot to add from the list in the dialog and click OK (Figure 5-93 (1)) to apply the selection. Click Cancel (Figure 5-93 (2)) to abort adding an Inspection Lot to the report.

In case of a Probe Report, the **Inspection Lot Name** (Figure 5-94 (3)), the **Probe ID** (Figure 5-94 (2)) and the **Description** (Figure 5-94 (1)) are shown in Inspection Lot for Report section for information.

Figure 5-94: Report tab – Final Test Spectrometer/Accessories, Inspection Lot for Report

**i** Only in case of an Accessory Test a report without any Inspection Lot can be created.

### (3) Additional PDF (of report)

**Additional PDF** documents can be included in the report. These documents are listed in **Additional PDF** section (Figure 5-90 (3)) of Report tab. Click **Add** to open a document browser to select files from hard disk. To add a comment to a file, enter the text into the cell in Comment column of the PDF list item. Select an Additional PDF list item and click **Remove** to remove the PDF from report.

### Field Service Test Report Tab – Checklist Sections (Figure 5-90 (4))

Scroll down on Field Service Test Report tab to find multiple checklist sections. Select the status for each item out of three different options: **Pass**, **Fail** and not applicable (**n/a**).

- **General Components (Spectrometer Report only)**

In General Components Checklist information about general aspects of a Field Service Test is collected for documentation:

- All firmware
- Software updated
- Cortab
- Lift / spin calibration
- He / N2 log files
- MICS
- BSMS
- AQS chassis
- Shim system turbine cleaned
- Door filter(s) replaced

- **Optional Components (Probe and Spectrometer Report only)**

In Optional Components Checklist information about optional components being subject to the report is collected. Despite a list of suggested components five custom fields are provided. Enter further optional components to these custom fields.

- Sample changer
- MAS controller
- High power equipment
- LC-NMR
- BEST
- Liquid handler
- Micro-Imaging
- Diffusion, Cryoplatfrom
- Additional cooling/heating unit
- five custom fields

## Field Service Test Report Tab – Button Panel (Figure 5-90)

- (5) **Save**  
Click **Save** (5) to apply all changes to the current report.
- (6) **Last Save**  
Click **Last Save** (6) to revert all changes in Report tab not applied yet.
- (7) **Create Protocol & Spectra**  
Click **Create Protocol & Spectra** (7) to create the spectra PDF and the protocol PDF of the report. All results set to be [used for report](#) and [for Additional Report](#) are included. Both parts of the report are marked as preliminary until it is [finalized](#).
- (8) **Show Protocol**  
Click **Show Protocol** (8) to open protocol PDF file. The protocol PDF is marked as preliminary until it is [finalized](#). This button is disabled if no protocol PDF was created yet.
- (9) **Show Spectra**  
Click **Show Spectra** (9) to open spectra PDF file. The spectra PDF is marked as preliminary until it is [finalized](#). This button is disabled if no spectra PDF was created yet.
- (10) **Finalize (non-finalized reports only)**  
Click Finalize (10) to create the final report for signature. The finalized spectra and protocol PDF files can not be recreated. Finalizing a report finalizes the Inspection Lots and results the report is based on.
- (10) **Export (finalized reports only)**  
Click Export (10) to open a file browser to export the finalized report to hard disk.

### i

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Finalized means, no further changes to the report, the included Inspection Lots, their experiments and results can be done. In the [Navigation panel](#), the corresponding icons are signed with a green checkmark. To make an Inspection Lot available again, the finalized report has to be deleted first.

---



## 6 Contact

We provide service support as follows:

The Bruker Service Stations or the Bruker Representatives will take care of virtually all aspects of Service world-wide.

- Telephone support from Bruker Main Offices and remote diagnosis (NMR-check) is provided during working hours every working day, local holidays are observed.
- Our laboratories to diagnose Covered Equipment malfunction(s).
- Our replacement parts as required on an exchange (refurbished) or new part basis.
- On site service will be provided by us during normal working hours and during our standard working week (Monday through Friday), excluding our observed holidays.
- When a Bruker Service Engineer is sent to customer site, the customer will provide our personnel an unrestricted access to the Covered Equipment to perform service. If the Bruker Service Engineer is unable to gain access at a time previously agreed upon, wasted time or waiting time service will be charged additionally at our standard service rates.

The customer will get a list of important e-mail addresses, telephone- and fax-numbers.

Manufacturer:

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Silberstreifen 4  
76287 Rheinstetten, Germany  
Germany  
Phone: +49 721-5161-0  
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Service Hotline:  
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Bruker Switzerland AG  
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8117 Fällanden  
Switzerland

Service Hotline:  
Phone: +41 44 825 9898  
E-mail: [Service.BBIO.CH@bruker.com](mailto:Service.BBIO.CH@bruker.com)

Bruker BioSpin S.A.S  
34, rue de l'industrie  
67166 Wissembourg, France

Service Hotline:  
Phone: +33 3 88 06 60 00  
Email: [support-rmn@bruker.com](mailto:support-rmn@bruker.com)

Please refer to the Model No., Serial No. and Internal Order No. in all correspondence regarding the NMR system or components thereof.



# Appendix

- Figures
- Tables
- Index

## A.1 Figures

Figure 3-1: Signature page of Acceptance Protocol NMR Spectrometer .....	16
Figure 3-2: Single spectrum PDF .....	17
Figure 3-3: <i>NMRPT</i> main window at first start. ....	19
Figure 3-4: Create new Inspection Lot for probe .....	20
Figure 3-5: Basic settings for a new Inspection Lot .....	20
Figure 3-6: Sample selection for experiments .....	20
Figure 3-7: Set experiment specifications on Inspection Lot tab .....	21
Figure 3-8: Open Sample List .....	21
Figure 3-9: Set Default Holder in Sample List .....	22
Figure 3-10: Select Inspection Lot on Acquisition tab .....	22
Figure 3-11: Select Inspection Lot from list .....	22
Figure 3-12: Enqueue Recommended Experiment Sequence .....	23
Figure 3-13: Start of Experiment Queue .....	23
Figure 3-14: Startup Check dialog .....	24
Figure 3-15: Check of experiments on Results tab .....	24
Figure 3-16: Create new Report for probe .....	25
Figure 3-17: New Report dialog .....	25
Figure 3-18: Preparation of <i>NMRPT</i> report on Report tab .....	26
Figure 3-19: Finalize report message .....	27
Figure 4-1: Probe Setup tab – Flow, Temperature and Shim options .....	30
Figure 4-2: Show Additional Info dialog (see Additional Information in 5.4.4 Results Tab .....	33
Figure 4-3: Show Additional Info dialog with TopShim report (see Additional Information in 5.4.4 Results Tab) .....	34

Figure 5-1: NMRPT main window with main areas.....	39
Figure 5-2: File menu .....	40
Figure 5-3: New Probe / Inspection Lot dialog.....	40
Figure 5-4: List of Mandatory Experiments .....	41
Figure 5-5: List of mandatory Spectrometer Report Experiments .....	42
Figure 5-6: File menu, New Report.....	42
Figure 5-7: New Report dialog .....	43
Figure 5-8: NMRSAVE .....	43
Figure 5-9: Close <i>NMRPT</i> .....	44
Figure 5-10: Edit menu.....	44
Figure 5-11: Copy Inspection Lot – source .....	45
Figure 5-12: Copy Inspection Lot – target.....	45
Figure 5-13: Rename Inspection Lot in menu.....	45
Figure 5-14: Rename Inspection Lot – choose Inspection Lot .....	46
Figure 5-15: Rename Inspection Lot – rename .....	46
Figure 5-16: Rename Plugin in menu .....	46
Figure 5-17: Rename Plugin – choose Inspection Lot.....	46
Figure 5-18: Rename Plugin – rename Part No.....	47
Figure 5-19: Rename Plugin – rename Serial No.....	47
Figure 5-20: Rename Report in menu .....	47
Figure 5-21: Rename Report – choose report .....	47
Figure 5-22: Rename Report – rename .....	48
Figure 5-23: Delete Probe in menu.....	48
Figure 5-24: Delete Probe – choose probe.....	48
Figure 5-25: Delete Inspection Lot in menu .....	49
Figure 5-26: Delete Inspection Lot – choose Inspection Lot.....	49
Figure 5-27: Delete Inspection Lot in menu .....	50
Figure 5-28: Delete Report – choose report .....	50
Figure 5-29: Shim Command list in menu.....	50
Figure 5-30: Shim Command list.....	51
Figure 5-31: Edit Shim Command dialog.....	51
Figure 5-32: Sample List in menu .....	52



Figure 5-33: Sample List.....	52
Figure 5-34: Sample Detail information .....	54
Figure 5-35: Show all Samples .....	54
Figure 5-36: New Customer Sample dialog.....	55
Figure 5-37: Remove Converted Parameters in menu.....	55
Figure 5-38: Remove Converted Parameters.....	56
Figure 5-39: Configuration in menu .....	56
Figure 5-40: Configuration dialog .....	57
Figure 5-41: Help menu .....	58
Figure 5-42: <i>NMRPT</i> About information .....	59
Figure 5-43: Acquisition Bar.....	60
Figure 5-44: Skip Cooldown.....	61
Figure 5-45: MAS Off Timer.....	62
Figure 5-46: Set Timer dialog .....	62
Figure 5-47: Startup Check dialog .....	62
Figure 5-48: Navigation.....	64
Figure 5-49: Navigation context menu – probe.....	65
Figure 5-50: Navigation context menu – Delete Probe confirmation dialog .....	65
Figure 5-51: Navigation context menu – Inspection Lot .....	65
Figure 5-52: Navigation context menu – Delete Inspection Lot confirmation dialog .....	66
Figure 5-53: Navigation context menu – Copy Inspection Lot dialog .....	66
Figure 5-54: Navigation context menu – Rename Inspection Lot dialog.....	66
Figure 5-55: Navigation context menu – Rename Plugin dialog, New Plugin Part No.....	67
Figure 5-56: Navigation context menu – Rename Plugin dialog, New Plugin Serial No ...	67
Figure 5-57: Navigation context menu – report .....	67
Figure 5-58: Navigation context menu – Delete Report confirmation dialog .....	67
Figure 5-59: Navigation context menu – Rename Report dialog.....	68
Figure 5-60: Workspace area .....	69
Figure 5-61: Inspection Lot tab – overview .....	70
Figure 5-62: Inspection Lot tab – Overview dialog .....	71
Figure 5-63: Probe Setup tab – overview .....	72
Figure 5-64: Acquisition tab – overview.....	74

Figure 5-65: Acquisition tab – Select Inspection Lot dialog .....	74
Figure 5-66: Acquisition tab – Exp. Missing in Report dialog .....	75
Figure 5-67: Acquisition tab – Failed Exp. in Report .....	75
Figure 5-68: Acquisition tab – detail: Experiment Preparation (Figure 5-64 (2)), workflow .....	76
Figure 5-69: Acquisition tab – detail: Experiment Preparation (Figure 4 47 (2)), detail settings .....	77
Figure 5-70: Acquisition tab – Select Shim Command dialog.....	78
Figure 5-71: Acquisition tab – detail: Experiment Queue (Figure 5-64 (3)) .....	79
Figure 5-72: Results tab – overview .....	80
Figure 5-73: Results tab – Experiments Missing in Report dialog .....	81
Figure 5-74: Results tab – Failed Experiments in Report dialog .....	81
Figure 5-75: Results tab – Additional PDF dialog .....	81
Figure 5-76: Results tab – detail: results table (Figure 5-72 (1)) .....	82
Figure 5-77: Results tab – detail: Dataset options (Figure 5-72 (2)).....	83
Figure 5-78: Results tab – Show Additinal Info dialog .....	84
Figure 5-79: Results tab – detail: Processing options .....	84
Figure 5-80: Report tab – overview.....	85
Figure 5-81: Report tab – Acceptance Test Probe .....	86
Figure 5-82: Report tab – Acceptance Test Accessories, Accessory Information.....	87
Figure 5-83: Report tab – Acceptance Test Spectrometer/Accessories, Inspection Lot for Report.....	87
Figure 5-84: Report tab – Acceptance Test Spectrometer/Accessories, Add Inspection Lot dialog .....	87
Figure 5-85: Report tab – Acceptance Test Probe, checklist sections .....	88
Figure 5-86: Report tab – Final Test Probe .....	91
Figure 5-87: Report tab – Final Test Accessories, Accessory Information.....	92
Figure 5-88: Report tab – Final Test Spectrometer/Accessories, Inspection Lot for Report .....	92
Figure 5-89: Report tab – Final Test Spectrometer/Accessories, Add Inspection Lot dialog .....	92
Figure 5-90: Report tab – Field Service Test Spectrometer .....	94
Figure 5-91: Report tab – Field Service Test Probe, Probe Information .....	95
Figure 5-92: Report tab – Field Service Test Accessories, Accessory Information.....	95

Figure 5-93: Report tab – Final Test Spectrometer/Accessories, Add Inspection Lot dialog .....	95
Figure 5-94: Report tab – Final Test Spectrometer/Accessories, Inspection Lot for Report.....	96

A.2 Tables

---

Table 4-1: Troubleshooting – Configuration, Sample List, Shim Command.....	35
Table 4-2: Troubleshooting – Inspection Lot.....	35
Table 4-3: Troubleshooting – Acquisition.....	36
Table 4-4: Troubleshooting – Results .....	37
Table 4-5: Troubleshooting – Report .....	37
Table 5-1: Status indicators in NMRPT Acquisition Bar .....	61

## A.3 Index

---

### A

abbreviations 9  
 Acceptance Test 14  
   acceptance 86  
   checklist 88  
   remarks 86  
   report 86  
 accessories  
   report 15  
   report without Inspection Lot 43  
 acquisition  
   Acquisition Bar 60  
   Acquisition tab 22  
   pause 60, 79  
   select Inspection Lot 22, 74  
   start 23, 60  
   status 61  
   stop 60  
 Acquisition Bar 60  
   detach 57  
 Acquisition tab 74  
 Additional Information 33, 83  
   log messages 84  
 Additional PDF  
   of Inspection Lot 9, 17, 81  
   of report 9, 17, 88, 93, 96  
 Additional Report 9, 17  
   Additional PDF of Inspection Lot 9, 17  
   Additional PDF of report 17  
   remove results 83  
   results included 82  
   select results 83  
 approval 91

### B

base shim file 9, 21, 24  
 bug  
   how to debug 34  
   how to report 38

### C

carrier frequency offset 13  
 checklist  
   Acceptance and Warranty 89  
   Acceptance Test Report 88  
   Field Service Test Report 96  
   General Components 96  
   Installation 88  
   Optional Components 89, 96

Training 89  
 close  
   NMRPT 44  
 configuration  
   NMRPT 56  
   probe 72  
 converted parameters 9, 33  
   remove 55  
 copy  
   Inspection Lot 45, 66  
 create  
   Inspection Lot 20, 40  
   protocol 26, 90, 93, 97  
   report 25, 26, 42, 90, 93, 97  
   spectra PDF 26, 90, 93, 97  
 current experiment 60  
 Current Specs 9  
 Customer Sample 9, 55

### D

debugging  
   Additional Information 84  
   experiment log messages 84  
   how to debug 34  
   how to report a bug 38  
   troubleshooting 35  
 default shim method 31  
 definitions 9  
 delete  
   Inspection Lot 49, 66  
   probe 48, 65  
   report 49, 67  
 Delivered Specs 10

### E

edit  
   Inspection Lot 44, 45, 49, 70  
   plugin 46  
   probe 48  
   report 44, 47, 49  
   Sample List 52  
   Shim Command 50  
 Edit menu 44  
 exclusions 86, 91, 94  
 Experiment Preparation 76  
   add experiment 76  
   add to queue 76  
   change experiment acquisition order 76  
   edit enqueued experiments 77  
   remove all experiments 76  
   remove experiment 76  
 Experiment Queue 10, 79

- pause 60
- start 60
- status 61
- stop 60

## experiments

- add to Experiment Preparation 76
- add to queue 76
- change acquisition order 76
- current experiment 60
- edit enqueued experiments 77
- edit specifications 70
- failed in report 75, 81
- generate shim plot 77
- irregular 29, 30
- Library 75
- mandatory experiments 40
  - probe 41
  - spectrometer 41, 42
- missing in report 75, 80
- next experiment 60
- Pairing 10
- recommended experiments
  - spectrometer 41, 42
- recommended sequence 23, 75
- re-execute 25
- remove all from Experiment Preparation 76
- remove from Experiment Preparation 76
- remove from Inspection Lot 70
- reprocessing 84
- select for Inspection Lot 70
- set specifications 70

export finalized report 90, 93, 97

---

## F

- failed experiments in report 75, 81
- Field Service Test 14
  - checklist 96
  - report 94
- File menu 39
  - close NMRPT 44
  - new
    - Inspection Lot 40
    - report 42
  - NMRSAVE 43
- Final Test 14
  - report 91
- finalize report 26, 90, 93, 97
- finalized 10, 90, 93, 97

---

## G

- gas flow
  - external mode 29
  - gas flow control 29
  - recommended flow from PICS 73
  - skip gas flow 78
  - skip gas flow setting 73
- getprosol

- skip getprosol 78

gradient strength 13

GUI 9

---

## H

- help 58
- holder position
  - default 21, 53
  - number 57
  - set 53
- how to report a bug 38

---

## I

Inspection Lot 10

- Additional PDF 81
- copy 45, 66
- create 20, 40
- delete 49, 66
- edit 44, 70
- edit specifications 70
- Inspection Lot tab 21
- remove experiments 70
- rename 45, 66
- select
  - for acquisition 22, 74
  - for report 43, 87, 92, 95
  - multiple for report 43
- select experiments 70
- set specifications 70
- with plugin 41

Inspection Lot tab 70

installed probe 60

irregular experiments 10, 29, 30

---

## L

L23 13

Library 10, 75

- experiments missing in report 75
- failed experiments in report 75

lock

- do locksetting after sample change 32, 63
- locksetting 32
- skip 73, 78

locksetting 32

log messages 84

loopcounter parameter L23 13

---

## M

- main window 19, 39
- mandatory experiments 40
  - probe 41

select samples 20, 41  
 spectrometer 41, 42  
**MAS Off Timer** 62  
**Menu Bar** 39  
 missing experiments in report 75, 80

---

## N

**navigation** 63  
   context menu 65  
**new**  
   Inspection Lot 40  
   report 42  
**NMRPT**  
   about 13, 59  
   configuration 56  
   GUI 9  
   help 58  
   log messages 84  
   main window 19, 39  
   requirements 7  
   status 61  
**NMRSAVE** 9, 43  
**Nucleus of Interest** 10

---

## O

**offset** 13

---

## P

**Pairing** 10  
**parameters**  
   converted parameters 33  
   remove converted parameters 55  
**pause**  
   before acquisition 79  
   before sample change 53  
   button 60  
   Experiment Queue 53, 60, 79  
**permitted characters** 10  
**PICS** 9  
**plugin**  
   Inspection Lot 41  
   rename 46, 66  
**probe**  
   delete 48, 65  
   report 15  
**Probe ID** 9  
**Probe Setup tab** 72  
**protocol** 10, 16  
   create 26, 90, 93, 97  
   show 26, 90, 93, 97  
   signature page 16

---

## Q

**Queue** see Experiment Queue

---

## R

**reciever gain** 13  
**recommended**  
   experiment sequence 23, 75  
   flow from PICS 10, 73  
   spectrometer experiments 41, 42  
**reduce ordmax** 31, 72, 77  
**remarks** 86, 91, 94  
**remove**  
   converted parameters 55  
   results from Additional Report 83  
**rename**  
   Inspection Lot 45, 66  
   plugin 46, 66  
   report 47, 68  
**report** 10, 14, 85  
   Acceptance Test 86  
   Accessories Report 15, 43, 87, 92, 96  
   Additional PDF 88, 93, 96  
   create 25, 42  
   delete 49, 67  
   edit 44  
   export 90, 93, 97  
   Field Service Test 94  
   Final Test 91  
   finalize 26, 90, 93, 97  
   Probe Report 15  
   rename 47, 68  
   results included 82  
   select Inspection Lot 43, 87, 92, 95  
   select multiple Inspection Lots 43  
   select results 83  
   Spectrometer Report 14, 15, 43  
   without Inspection Lot 43, 87, 92, 96  
**Report tab** 85  
**Report Type** 10, 14  
**reprocessing**  
   APK 84  
   APK0 84  
   default 84  
   PK 84  
**requirements** 7  
**results**  
   detailed status 84  
   experiments missing in report 80  
   failed experiments in report 81  
   for Additional Report 82  
   for report 82  
   of experiment run 82  
   processing options 84  
   Results tab 24  
   show in TopSpin 83  
   status 82  
**Results tab** 80

routing 33, 36

---

## S

### sample changer

- change modes 29
- default holder positions 21, 53
- number of holder positions 57
- options 57
- set holder positions 53
- usage 57

### Sample ID 9

### Sample List 22

- edit 52
- holder position 21, 53

### samples 7

- availability 53
- change modes 29
- Customer Sample 55
- default holder positions 21, 53
- details 53, 54
- mandatory experiments 20, 41
- manual sample change 29
- Pairing 10
- required samples 7
- sample depth 73
- Sample List 22, 52
- set holder positions 53
- show all 53, 54
- standard samples 7

### select

- Inspection Lot for acquisition 22, 74
- Inspection Lot for report 43, 87, 92, 95
- results for Additional Report 83
- results for report 83
- Shim Command 78

### selftune 30

- BSVT 30

### service hotlines 99

### shim

- default shim method 31, 72
- maximum shim order 31, 72, 77
- NMRPT shim handling 31
- reduce ordmax 31, 72, 77
- Shim Command 11
  - edit 50
  - number 50
  - select 78
- Shim Command List 50
- shim plot 77
- wsh 21, 24
- Z-shim corrections 31, 72

### shim method

- default 31, 72

### Short PDF 11, 18, 80

### show

- Additional Info 83
- protocol 26, 90, 93, 97
- results in TopSpin 83
- results of experiment run 82

Short PDF 80

single spectrum PDF 83

spectra PDF 26, 90, 93, 97

### signature page 16

### single spectrum PDF 11, 17

show PDF 83

### skip

- gas flow setting 73, 78
- getprosol 78
- lock 73, 78
- temperature setting 73, 78
- tuning/matching 73, 77, 79
  - HNUC 73, 77
  - XNUC 73, 77

### Skip Cooldown 61

### specifications 11

- Current Specs 9, 21, 70
- Delivered Specs 10
- edit 70
- set 70

### Specs see specifications

### spectra PDF 11, 16

- create 26, 90, 93, 97
- show 26, 90, 93, 97

### spectrometer

- experiments 41, 42
- multiple Inspection Lots for report 43
- report 14, 15

### standard temperature 72

### start

- acquisition 23, 60
- button 60
- NMRPT 39

### Start button 23

### Startup Check dialog 24, 62

### status 61

- results 82, 84

### stop

- button 60
- Experiment Queue 60

### support 99

---

## T

### tab

- Acquisition tab 22, 74
- Inspection Lot tab 21, 70
- Probe Setup tab 72
- Report tab 85
- Results tab 24, 80

### temperature

- external mode 29
- gas flow 29
- selftune BSVT 30
- skip temperature setting 73, 78
- standard temperature 72
- temperature control 30

### terms 9

### Test Mode 11, 14



TopSpin Experiment Parameters 78  
troubleshooting 35  
tuning/matching  
    skip 73, 77, 79  
    skip HNUC 73, 77  
    skip XNUC 73, 77

    checklist 89  
    commencement 86  
    duration 86  
    remarks 86  
workflow 19  
Workspace 11, 69  
wsh 21, 24

---

## W

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