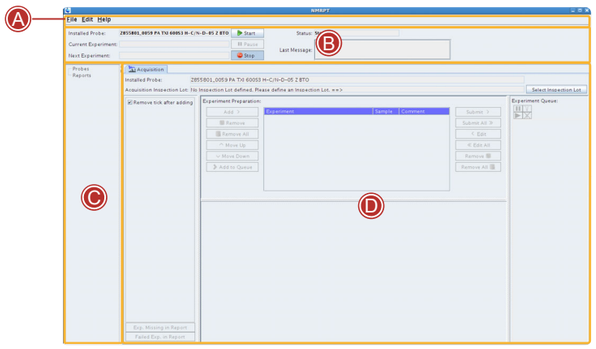
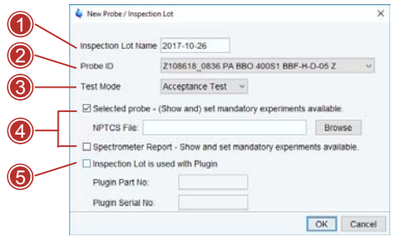
1 Starting-Up NMR Product Test Software

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:
Ⓐ Menu Bar, Ⓑ Acquisition Bar, Ⓒ Navigation Panel and Ⓓ Workspace.



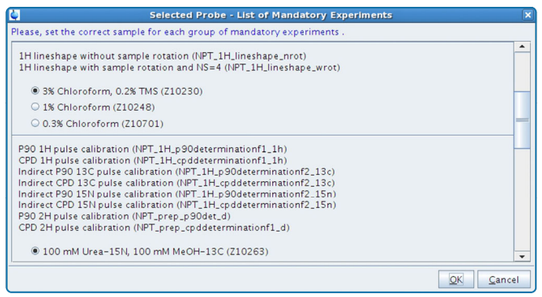
The usage of a **sample changer** is set in “Edit > Configuration” dialogue selected from Menu Bar. A **new product test** is started by choosing “File > New > Probe / Inspection Lot” from Menu Bar. In New Probe / Inspection Lot dialog window name the ① Inspection Lot, select the ② Probe ID and the ③ Test Mode for your product test. Two further options provide ④ **Standard Inspection Lot Configuration**: First one **automatically sets all mandatory experiments** available for the probe type specified and the second one adds an additional set of experiments mandatory for a spectrometer report.

To include a plugin as a subject to a product test activate ⑤ plugin option and enter part and serial number of the plugin.



Important The Test Mode selected during setup defines the resulting Report Type. A report consists of a test protocol and a spectra PDF.

The subsequent dialogue opens up if “Selected probe – (Show and) set mandatory experiments available” was selected. This dialog window offers the opportunity to choose between standard samples if mandatory experiments can be executed using multiple samples. For each experiment subsection provided, a sample needs to be selected.



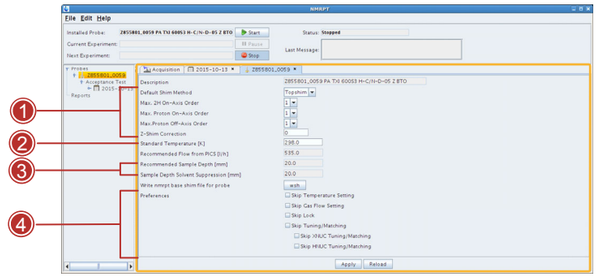
Detailed Options

Acquisition Panel: As a **space-saving option** detach the Ⓑ Acquisition Panel from NMRPT main window in “Edit > Configuration” dialog.

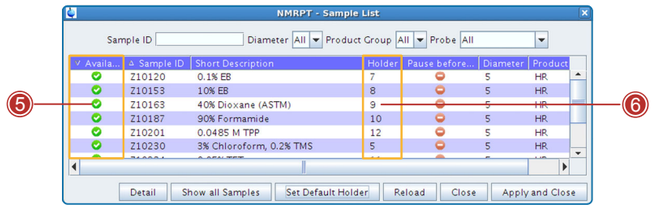
2 Inspection Lot and Probe Setup

Inspection Lot tab opens up in workspace area after a new Inspection Lot was created. This tab offers options to set the individual availability of experiments and corresponding samples or to set experiment specification values manually. If complete Standard Inspection Lot Configuration options were selected in New Inspection Lot dialog, there is no need to modify the given options except for experiment specifications (see Detailed Options below).

Open **Probe Setup** tab from Ⓒ Navigation Panel to set probe-specific parameters such as ① **shim options**, ② **standard temperature**, ③ **sample depth** and ④ **global experiment preferences**. These allow to set default acquisition parameters for all future experiments set up for this probe. The Maximum Order shim settings are applied according to the TopShim ordmax parameter. Tooltips provide further information about the specific settings in this tab.



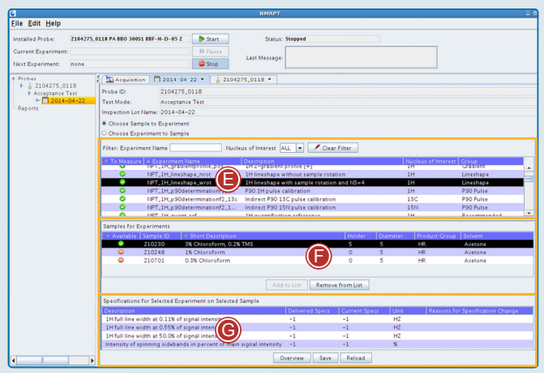
Open “Edit > Sample List” dialogue to define ⑥ **holder positions** for the samples either by choosing Set Default Holder button or entering numbers manually inside the table. Holder position 0 means **manual sample change** (deselect usage of sample changer from configuration to activate manual mode). You may also change sample`s ⑤ availability status.



Important Please, ensure approximate pulse settings using edprosol command in TopSpin before measurement. Check for all holder positions to be set correctly.

Detailed Options

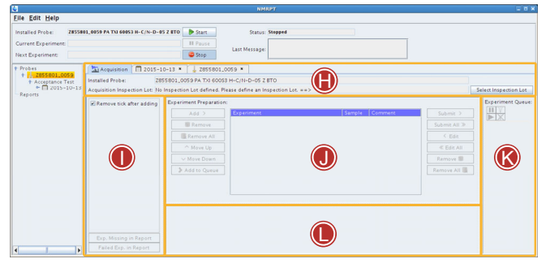
Inspection Lot: The Ⓔ upper table shows the experiments or samples depending on the option set above the table. If you select one entry, the Ⓕ second table shows the corresponding samples or experiments. A selected combination of experiment and sample is set available for the current Inspection Lot by choosing Add to List button. To **specify the experiment values** of a certain experiment, select the experiment and sample combination already set available and edit the “Current Specs” provided in Ⓖ third table. All changes need to be saved!



General Configuration: “Edit > Configuration” dialogue offers additional settings concerning the **usage of a sample changer**, a **time span, in which to ignore samples with option Pause before Change,** and a **waiting time for temperature equilibrium after sample change**.

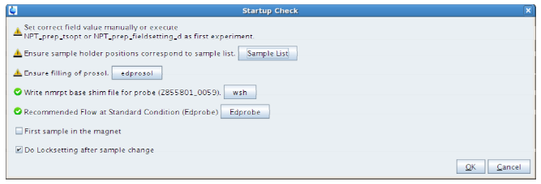
3 Acquisition

The **Acquisition** tab in Ⓓ workspace is a global tab and only available for installed probe. The tab is subdivided into five areas: An Ⓗ Information Bar, a Ⓘ Library Panel, the Ⓙ Experiment Preparation Panel with Ⓛ Detail Configurations and the Ⓚ Experiment Queue.



First you need to **select an Inspection Lot** in Information Bar to set experiments for. Choose a sample with all its experiments at once from Library Panel or open a subtree of experiments by sample and mark selected experiments to use. Enqueue selected experiments using **Add to Queue** button. Start execution of all experiments as shown in Experiment Queue by using the **Start** button in Acquisition Bar.

In **startup check window** you must confirm that all preparation steps are finished correctly.



Monitoring of your acquisition is provided in Ⓑ Acquisition Bar: Current experiment, next experiment enqueued, acquisition status and messages are displayed. The **Pause** button allows you to pause before subsequent acquisition. **Restarting** proceeds the same run with the next experiment enqueued. The sample will only be changed if required by the experiment. To terminate immediately the current experiment use the **Stop** button. **Restarting** proceeds with a sample change due to security purpose and the next experiment enqueued. The terminated experiment will not be re-executed. Failed experiments or experiments missing in report can be accessed by two buttons at the bottom of Library Panel.

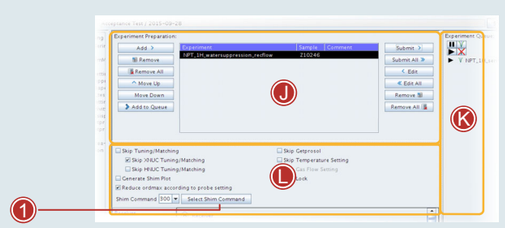
Detailed Options

Experiment Preparation Panel: Use Add button (instead of Add to Queue) to list selected experiments in **Experiment Preparation** Panel before enqueuing. This panel allows to **change the order** or **delete certain experiments** by using the corresponding buttons to the left. Submit or Submit All button move the experiments from Experiment Preparation Panel to Experiment Queue. To **edit an already enqueued experiment** select it and use Edit button to shift it back to Experiment Preparation Panel. Edit All gives the opportunity to reedit and reorder all experiments in queue. To **delete experiments from Experiment Queue** use Remove or Remove All button.

Important It is not possible to apply any changes to the experiment currently running!

Detail Configurations: To **set specific parameters for experiments** select the experiment from table in Experiment Preparation Panel. The parameters of the selected experiment are shown in Detail Configuration Panel below. A list of Shim Commands can be accessed by Select ① Shim Command button.

Experiment Queue: To pause before an experiment but after a possible sample change or to skip atma, select all affected experiments listed in queue. Toggle the corresponding icons in front using the buttons at the top of the list.



4 Results

In **Results** tab the results of all experiments executed for a specific Inspection Lot are listed. Open this tab by selecting the related icon from Ⓒ Navigation Panel tree.

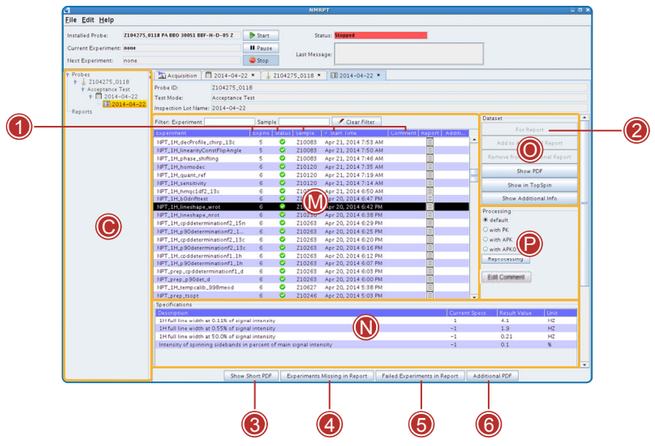
In Ⓜ **result list** alongside ① row categories Start Time, Expno and Sample a **Status icon** is given to show if an experiment was successfully finished. A green check means no errors occurred and all specifications were achieved. A yellow exclamation mark indicates that specifications were not achieved. A red error icon is shown if errors occurred during acquisition or processing. Ⓝ **Experiment values** are shown below experiment table if an experiment is selected. As a default a report icon is shown behind the latest run of each experiment without error to show which results will be **used for product test report**. To change the selection of **experiments used for report**, mark another equivalent experiment run in the list and use ② For Report button to select.

The Ⓞ Button Panel provides access to experiment information and report settings. Retrieve information about the currently selected experiment by Additional Info button. Show PDF previews the individual **experiment`s PDF** file. Furthermore directly **access experiment data in TopSpin**.

Lists of experiments failed or not measured though mandatory according to the Inspection Lot are accessed by ⑤ **Failed Experiments in Report** and ④ **Experiments Missing in Report**.

Preview a short version of the Report PDF using ③ Show Short PDF button. The preview collates an overview of the experiments in the subsequent report.

To add **additional PDF content** (e.g. external TopSpin measurements or additional data) load those PDF files by using dialogue provided by ⑥ Additional PDF button.

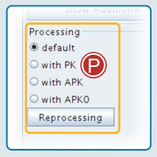


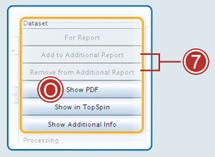
Detailed Options

Reprocessing: In Results tab multiple Ⓟ Phase Correction Options to **reprocess experiment data** are offered.

Important Please consider that reprocessing of data may change the experiment status due to recalculation of results in comparison to the specified values. Changing **Current Specs** (see Ⓒ 2. Inspection Lot and Probe Setup, Detailed Options) also causes a reprocessing of the measurement data.

Additional Report: Manage **supplementary experiments** from Inspection Lot (e.g. measured under different conditions) as part of the report using ⑦ Add to / Remove from Additional Report buttons in Ⓞ Button Panel. They will also be marked by a report icon in column Additional Report. The Additional Report option will create a separate report section covering those additional measurements.

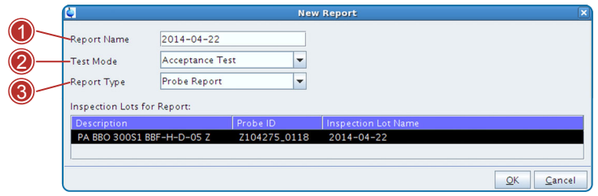




Copy Inspection Lot: To create a new Inspection Lot based on the specifications of an existing one use “Edit > **Copy Inspection Lot**” from Menu Bar. This will copy the corresponding Inspection Lot to a new name including existing specifications. No experiment results will be copied to the new Inspection Lot.

5 Report

A **new report** is created using “File > New > Report” from Ⓐ Menu Bar. In the subsequent dialogue window ① name the report and select ② Test Mode and ③ Report Type. Select from all available Inspection Lots listed below filtered by the above settings. The Report Type option Spectrometer Report allows multiple Inspection Lots to be selected for one report.

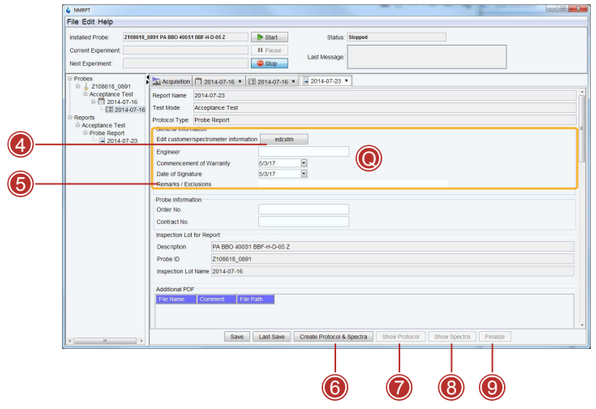


The Report tab opens in Workspace Area. All Ⓠ **General Information** fields including customer/system information (accessible via ④ edcstm button) are to be filled properly. Special **remarks** about the product test, **special conditions**, **agreements** etc. are to be provided in ⑤ Remarks field. Save all data.

To **create a product test report** consisting of a test protocol and a spectra PDF use ⑥ Create Protocol & Spectra button in Report tab. ⑦ Show Protocol button allows you to **open the** ⑧ **current protocol** once a protocol has been created. The assorted **spectra PDF** is accessible via Show Spectra button.

To get a **valid document** for your product test you must **finalize the report**. If the compilation of measurements from Inspection Lot and additional PDF-documents meets your requirements create the final document using ⑨ Finalize button.

Important For a finalized report all corresponding data will be locked, the Inspection Lot cannot be used anymore and no additional experiments or changes can be performed within this Inspection Lot – the product test is finished.



Detailed Options

Rename Inspection Lot or Report: To **rename** either an Inspection Lot or a report use “Edit > Rename” dialogue from Menu Bar.

Delete Probe, Inspection Lot or Report: To **delete** either a probe, an Inspection Lot or a report use “File > Delete” Menu Bar dialogue.

Important Deletion of a report reopens data and Inspection Lot for the creation of another report. Deletion of a probe / Inspection Lot also deletes all corresponding NMR measurement data.

NMRPT Help Files: All NMRPT Help Files are accessible from Menu Bar. Please choose “Help” and select the appropriate help option. The latest version of NMRPT Short Guide is also available from help menu.

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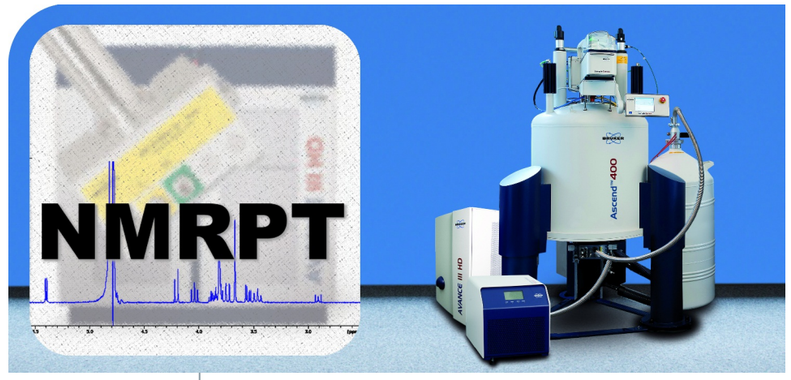

NMR Product Test

Internal NMRPT Short Guide

NMRPT Automation Software for Product Test purposes providing acceptance reports
– including protocol and spectra.

Spectrometer Report

- Final Test Protocol
- Acceptance Protocol
- Field Service Protocol

Probe Report

- Final Test Protocol
- Acceptance Protocol
- Field Service Protocol

Accessories Report

- Final Test Protocol
- Acceptance Protocol
- Field Service Protocol