AVANCE IVDr

- IVDr Data Browser

User Manual

Version 002

Innovation with Integrity

NMR

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1 Introduction

The Bruker In Vitro Diagnostics (IVDr) Data Browser is a convenient program to scan through NMR data. It simplifies selecting and sorting spectral data by gathering metadata from a locally existing repository of experimental NMR data. Additionally, the metadata of the NMR spectra can be augmented by metadata, e. g. concerning the origin of the measured sample.

Several tools to import and export data, to sort the data and to open data in TopSpin™ or AMIX™ are available.

Introduction

2 Getting Started

2.1 Searching for Spectral Data

After the initial start of the IVDr Data Browser the tables of the tool (i.e. **Main List** and **Work List**), which represent the main workbench, are empty. In order for data to show up here, select **Search for spectra…** and choose a directory to search in the local file system:

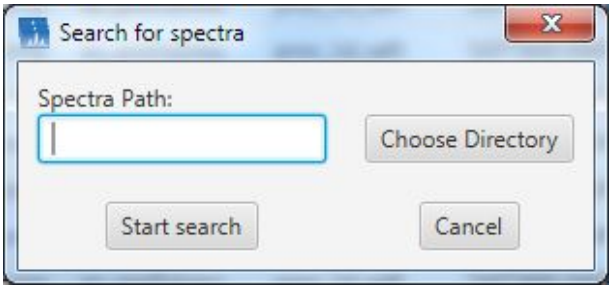

Figure 2.1: Searching for Spectral Data

Press **Start search** to begin the search, it may take several minutes depending on the folder selected and the computer performance.

2.2 Workbench Overview

The workbench consists of two tabs representing two tables with spectral data (see *Figure 2.2 [▶ 6]*).

- Main List
- Work List

The Main List contains the main spectra data. When a spectra search is performed, all of the metadata from the spectra found will be placed here. The Work List is a second table that can be used as a work area. Data from the Main List can be easily copied to the Work List, e.g. by selecting spectral data in the Main List and pressing the keys **Ctrl**+**C**. The menu item **Copy spectra to work list** is also available from the context menu of the Main List and from the main menu of the IVDr Data Browser.

As you will notice, certain functions are exclusively available for either the Main List or the Work List. For example, the **Search for spectra…** is only available for the Main List and the execution of TopSpin commands on spectra is only available from the Work List.

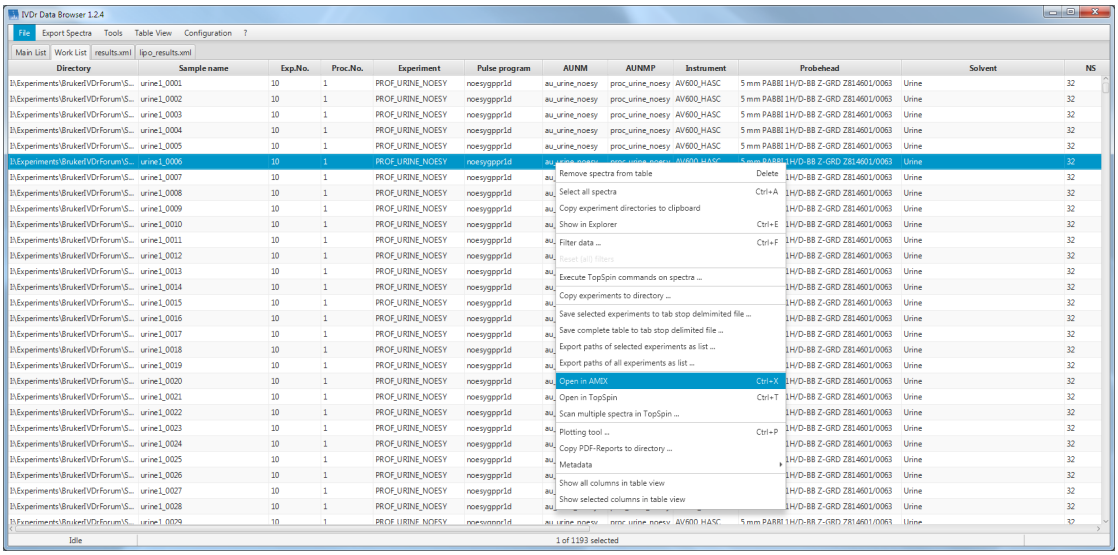

Figure 2.2: The IVDr Data Browser Workbench

2.3 Configuration

Before the functions from TopSpin or AMIX can be used, the IVDr Data Browser needs to be configured. To do this go to the configuration menu item and enter the correct path to TopSpin and AMIX (if available):

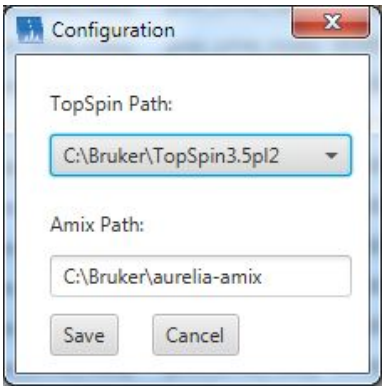

Figure 2.3: Configuration: Selecting the TopSpin and AMIX Path

3 Description of Menu Items and Functions

3.1 Miscellaneous Functions

Open and Save

The IVDr Data Browser saves the current data in the tables when the program is closed. After restarting the IVDr Data Browser, the data in the Main List and the Work List is reloaded.

To store the current data in the program to a file, select **Save** from the **File** menu item. Stored files have the ending ***.idb** and can be easily loaded by selecting **Open** from the same menu item.

Copy spectra to work list and remove spectra from table

When spectra are selected in the Main List, the list item **Copy spectra to work list** is available.

The item **Remove spectra from table** removes the selected spectra from the current tab.

Copy experiment directories to clipboard

This menu item copies the directories of the selected spectra to the clipboard. At the file system level the directories will be copied to the selected folder by clicking e.g. **Paste** from the context menu of the file browser.

Show in explorer

This menu item allows all the directories of the selected spectra to be opened at once. Use this function with care, because for each selected spectra a new window will be opened.

Filter Spectra and Reset (all) filter

The **Filter Spectra** menu item is available for the Main List and the Work List. It allows certain spectra to be filtered and selected in the foreground table. Through the use of filtering you can search for specific text in a selected column or all available columns.

Filters can also be combined and the complex filter queues can be saved to a file and reloaded from disk. The functions for removing a filter from the queue, loading and saving filters from or to disk are available via the context menu of the filter table:

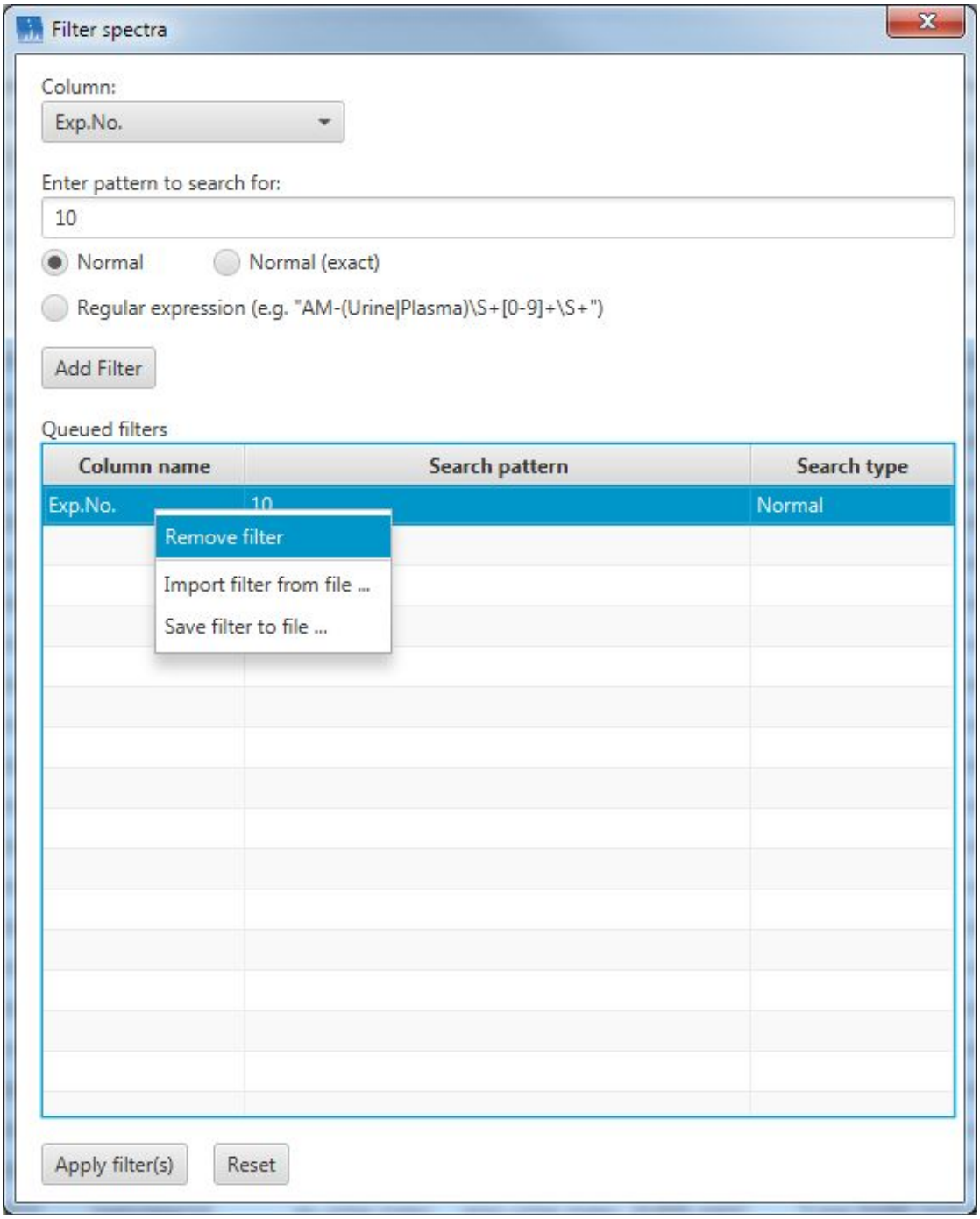

Figure 3.1: Filter Spectra

The menu item **Reset (all) filters** resets all the filters and shows the data of the complete table again. This menu item is only available if a filter was applied in advance.

3.2 Export Spectral Data

Execute TopsSpin commands on spectra

The menu item for the execution of TopSpin commands is only available for the Work List. A list of commands can be entered and is executed consecutively for each selected spectra in the Work List:

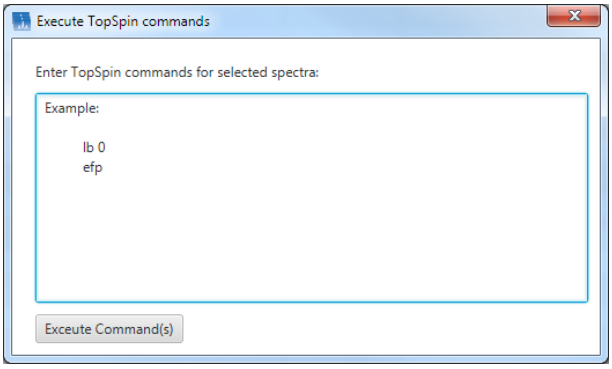

Figure 3.2: Execute TopSpin Commands on Spectra

This function is only available if the configuration for TopSpin was pre-assigned correctly.

Copy experiments to directory

The menu item **Copy experiments to directory …** copies the experiments folder of each selected spectra to a directory that has to be selected.

Export selected/all experiments to file

The menu items **Export selected experiments to file** and **Export all experiments to file** copy the complete data of the spectra that is observable in the table to a tab-delimited text file.

Export paths of selected/all experiments as list

The menu items **Export paths of selected experiments as list** and **Export paths of all experiments as list** copy the complete paths of the “1r” or “2rr” file of the spectra to a text file.

Open in AMIX

The menu item **Open in AMIX** opens the selected spectra of the table in AMIX. To use this function it is necessary to assign the path to AMIX in the IVDr Data Browser configuration.

Open in TopSpin

The menu item **Open in TopSpin** opens the selected spectra of the table in TopSpin. To use this function it is necessary to assign the path to TopSpin in the IVDr Data Browser configuration.

Scan multiple spectra in TopSpin

The menu item **Scan multiple spectra in TopSpin** opens the selected spectra of the table consecutively in TopSpin. A left limit and a right limit for the display of the spectra can be specified and also an interrupt that pauses the loading of the next spectra for a certain time (see figure below). If you interrupt the loading of spectra by pressing the **Pause** button, it is possible to jump forward or backward in the list of selected spectra. To use this function it is necessary to assign the path to TopSpin in the IVDr Data Browser configuration.

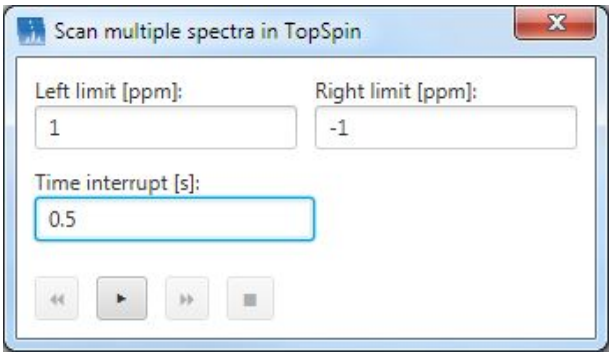

Figure 3.3: Scan Multiple Spectra in TopSpin

3.3 Miscellaneous Tools

3.3.1 Plotting Tool

The plotting tool provides several functions to plot data or metadata. In order to access the Plotting tool, entries in the foreground list have to be selected. The configuration of the popup window consists of 3 radio buttons to select the wanted diagram and 2 tables. The table on the left side is the selection table for columns and the table on the right side shows the selected columns. Columns can be added or removed via the corresponding buttons. Currently, the following diagrams are available:

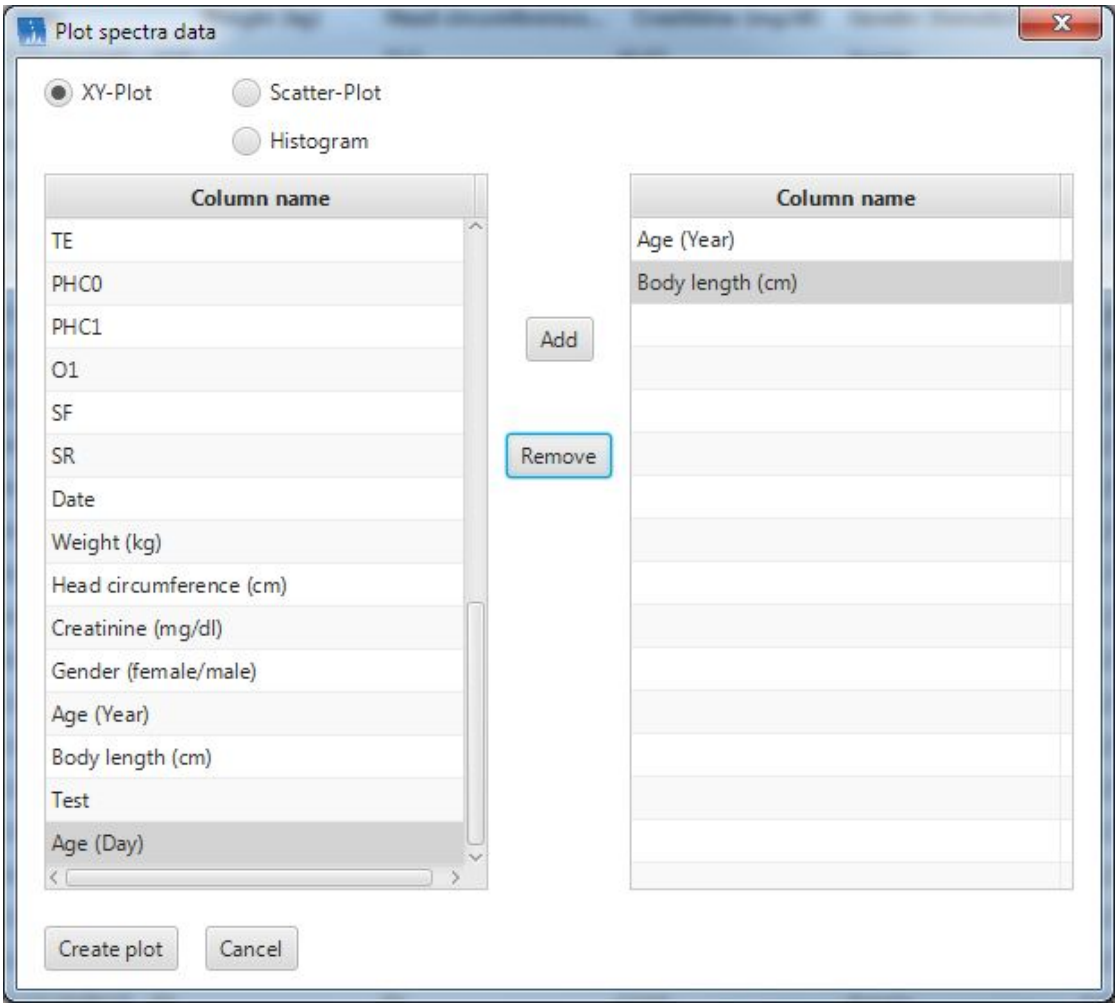

Figure 3.4: Plot Spectra Data

XY-Plot

The XY-Plot allows a simple representation of values on a XY-diagram with the value given on the y-axis and the number of the spectra in the selection on the x-axis. The XY-diagram allows for multiple x-axes, i.e. multiple columns with numerical values can be shown at once and compared. Zoom functionalities can be accessed by scrolling with the mouse wheel or rectangle selection with the left mouse button on the desired area. A double click resets the view. A click on a data point selects the entry in the foreground list.

Scatter-Plot

The scatter-plot allows obviously only two columns with numerical values. The first selected column is drawn to the x-axis and the second to the y-axis. Zooming features are the same as for the XY-Plot.

Histogram

The histogram allows only one selected column with numerical values. A small popup enables the configuration of the number of bins that have to be drawn. Zooming options are not available here, but a click on a bin selects the entries in the foreground list.

3.3.2 Copy PDF Reports to Directory

This function allows copying of all PDF-Files in the spectral path to a directory at once. The name of the PDF-Files has to be specified in the combo box and the folder where the files should be stored to has to be entered in text field or selected via a folder chooser (“Choose Directory”).

The names of the PDF-Files are collected automatically during the import of initial spectra data, invoked by “Search for spectra…”.

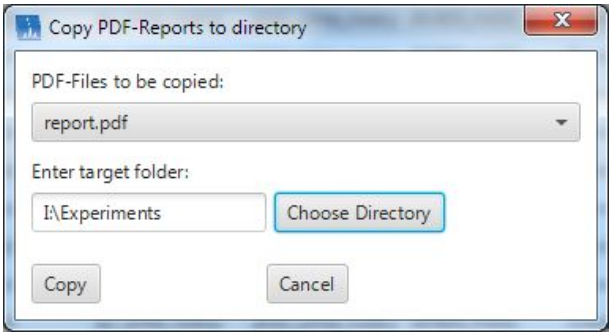

Figure 3.5: Copy PDF Reports to Directory

3.3.3 Metadata/XML

Besides the metadata that is gathered directly from the spectral data, it is possible to augment the data with additional data. For example, the data may contain information concerning the origin of the measured data. Most functions concerning metadata are only available for the Work List.

Import metadata from file

Metadata can be easily imported from a tab-delimited file. The sample name is used as an identifier and must be unique. The first row of the file must contain the identifiers of the given metadata. All consecutive rows contain the data.

Example file:

SampleName <Tab> Gender (male/female) <Tab> Weight (kg) <Tab> Body length (cm) ...
Urine_001 <Tab> male <Tab> 5.89 <Tab> 58.5 ...
Urine_002 <Tab> female <Tab> 4.53 <Tab> 51.5 ...
...

The importing of metadata is available for Main List and Work List.

Remove all metadata from table

The menu item **Remove all metadata from table** deletes all metadata that was previously added to the spectral data of the table in the foreground, i.e. Main List or Working List. The removing of metadata is also available for Main List and Work List.

Export metadata of selected spectra / all metadata to file

This menu item exports the metadata to a tab-delimited text-file. Besides the metadata the sample name is used as an identifier, thus the sample name should be unique. The identifiers for the columns are given in the first row of the file. See above for an example file output.

Import metadata/data from XML

The menu item and the successive popup-window for the import of metadata/data from XML allow for a serial import of data from XML-files. During the import of initial spectra data, invoked by **Search for spectra…**, also information on XML-files in the directories is gathered. Available XML-files can be selected as *Source XML-File* afterwards. On selecting a **Source XML-File** its data and available XML-items show up in the table below.

Fields and data that should be imported from the XML-file can be selected. If the selection pattern for this file should be used again in the future it is possible to store the selection pattern to a file and reload it via the context menu of the table.

Besides the selection of the data that should be imported, it has to be specified whether the new data is presented as *Metadata* in either the Main List or Working List depending on the tab in the foreground or if the data will be presented in a new tab (**New table**).

If **New table** is selected a new tab with the name of the **Source XML-file** will be created. The new tab has a reduced context menu that allows for only some operations that are available for Main List and Working List.

The checkbox for **Bruker results XML-file** is only available if a Bruker results file is selected (e.g. *lipo_results.xml*, *results.xml*, etc.). The importing of data works in a predefined way then and a selection of fields that should be imported is not necessary.

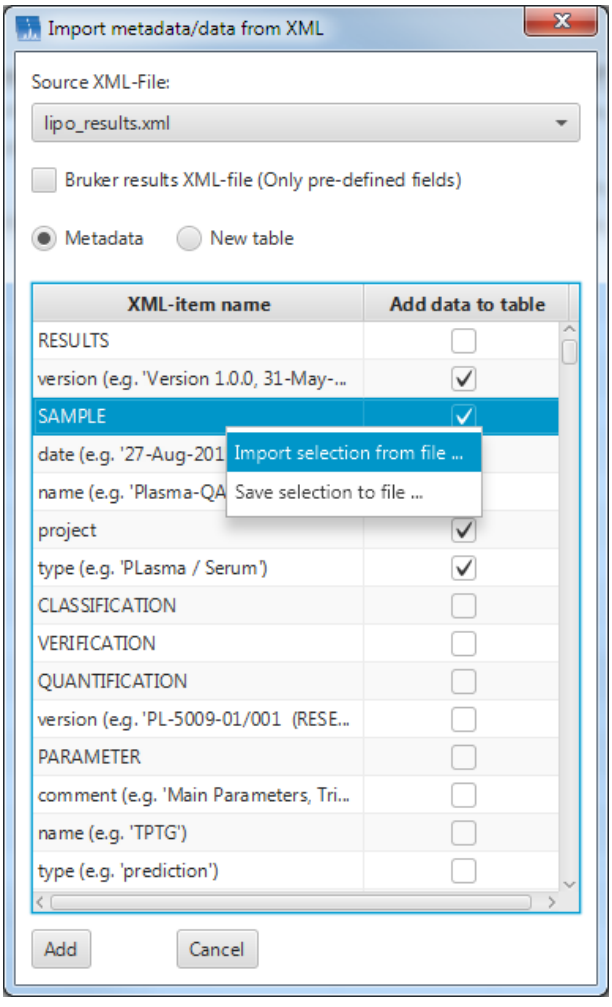

Figure 3.6: Import Metadata/Data from XML

Add metadata to XML

The **Add metadata to XML** augments existing XML-Files with the metadata or creates new XML-Files that contain the metadata of the spectrum. This function is only available if spectra in the Work List are selected.

Besides the name of the source XML-File, an export path has to be specified and if an XML-File with the metadata should be created, although the source XML-File is not found:

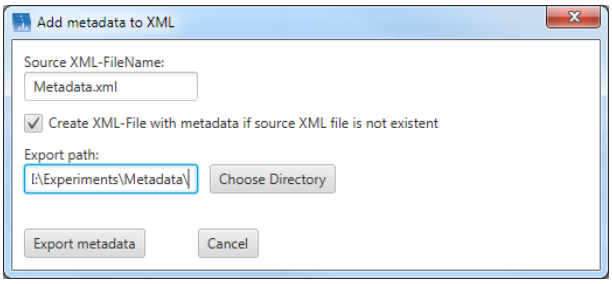

Figure 3.7: Add Metadata to XML

3.4 Customizing the Table View

Select columns in view

The **Select columns in view menu item** offers the opportunity to show or hide certain columns of the table in the foreground:

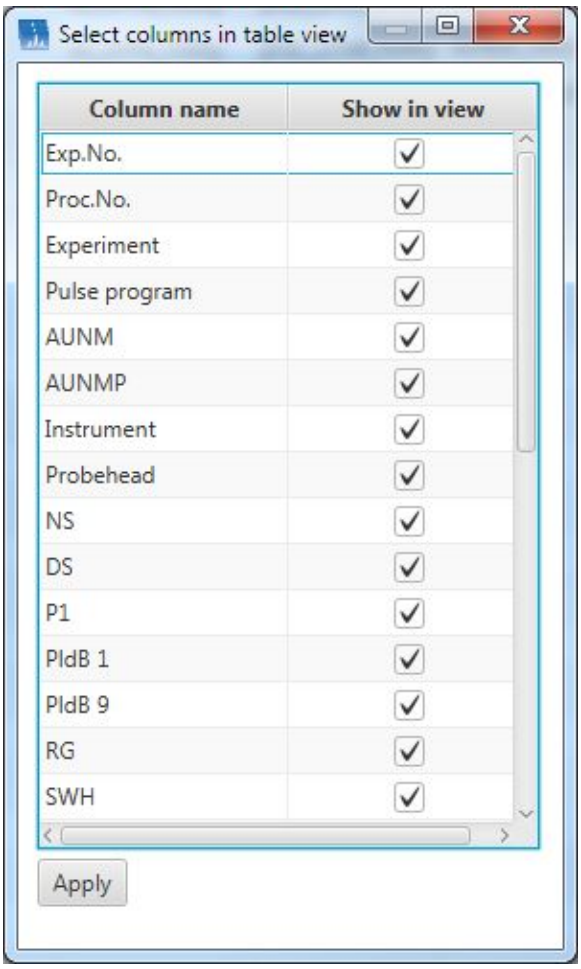

Figure 3.8: Select Columns in View

Show all/show selected columns in table view

These menu items toggle between the view of selected table columns and the view of all columns in the table in the foreground. The list of selected columns can either be modified via the menu item **Select columns in view** or by deleting columns from the table via the context menu of the column title. It is not possible to delete the columns “Directory” and “Sample name” from the view.

3.5 Persistence and Exiting of IVDr Data Browser

Whenever the IVDr Data Browser is closed, the current data in the table is written to a file and is reloaded when the IVDr Data Browser is restarted. Depending on the amount of data in the table and the performance of the computer, this may take a few seconds.

Description of Menu Items and Functions

4 Contact

Manufacturer

Bruker BioSpin GmbH
Silberstreifen 4
D-76287 Rheinstetten
Germany
http://www.bruker.com

WEEE DE43181702

NMR Hotlines

Contact our NMR service centers.

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

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

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

Phone: +49 721-5161-6155

E-mail: *nmr-support@bruker.com*

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