

# **AVANCE IVDr**

IVDr Data Browser
 User Manual
 Version 001

Innovation with Integrity

NMR

#### Copyright © by Bruker Corporation

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form, or by any means without the prior consent of the publisher. Product names used are trademarks or registered trademarks of their respective holders.

This manual was written by

Applied, Industrial & Clinical MR Market Division

© September 21, 2016 Bruker Corporation

Document Number: 10000057225

P/N: H161805

# **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  $TopSpin^{TM}$  or  $AMIX^{TM}$  are available.

# **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:

Search for spectra	×
Spectra Path:	Choose Directory
Ctud unurk	
Start search	Cancel

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* [ b 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.

File Exp	ort Spectra Metadata Table View	Configuration	?														
Main List																	
	Directory Samp s\BrukerIVDrForum\S., urine1 0013	ple name	Exp.No.	Proc.No.	Experiment PROF URINE NOESY	Pulse program	AUNM au urine noesy	AUNMP proc urine noesy	Instrument	Probehead 5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	NS 32	DS	P1 13.11	PIdB 1	PIdB 9 45.6479257	RG	
	s\BrukerIVDrForum\S., urine1 0014		10		PROF_URINE_NOESY	noesygpprld		proc_urine_noesy		5 mm PAB8 1H/D-88 Z-GRD 2814601/0053		4	12.87		45.8084107		-
-	opv spectra to work list	Ctrl+C	10	1	PROF URINE NOESY	noesygpprld	au_urine_noesy au_urine_noesy	proc_urine_noesy		5 mm PA8811H/D-88 Z-GRD Z814601/0063		4	13.35		45,4838516		-
	emove spectra from table	Delete	10	1	PROF URINE NOESY	noesygpprid	au urine noesy	proclutine_noesy	-	5 mm PA88I 1H/D-88 Z-GRD 2814601/0063		4	12.58	-12.000018	46.0063662		
	elect all spectra	Ctrl+A	10	1	PROF URINE NOESY	noesygpprid	au urine noesy	proclutine noesy		5 mm PA88I 1H/D-88 Z-GRD 2814601/0063		4	13.47		45.4126276		
		Ctri+A	10	1	PROF URINE NOESY	noesygpprid	au_urine_noesy	proc urine noesy	-	5 mm PARRI 1H/D-BR 7-GRD 7814601/0063		4	12.85	-12.000018	45.8219179.		
voerime	opy experiment directories to clipboard		10	1	PROF URINE NOESY	noesygpprid	au_urine_noesy	procurine noesy		5 mm PA88I 1H/D-88 Z-GRD Z814601/0063		4	13.24	-12.000018	45.5622211		
voerime	how in Explorer	Ctrl+E	10	1	PROF URINE NOESY	noesygpprid	au urine noesy	procurine noesy	-	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063		4	11.68	-12.000018	46.6511237		
xperime	ilter spectra	Ctrl+F	10	1	PROF URINE NOESY	noesygpprid	au_urine_noesy	procurine noesy		5 mm PARRI 1H/D-RR 7-GRD 7814601/0063		4	11.87	-12.000018.	46.5109669		
xperime	leset (all) filters		10	1	PROF_URINE_NOESY	noesygpprid	au_urine_noesy	proc_urine_noesy		5 mm PA88I 1H/D-88 Z-GRD Z814601/0063		4	13.01		45.7144359		
	opy experiments to directory		10	1	PROF_URINE_NOESY	noesygpprid	au_urine_noesy	proc_urine_noesy			32	4	13.51		45.3868759		
	xport selected experiments to file		10	1	PROF URINE NOESY	noesygpprid	au urine noesy	proc urine noesy		5 mm PA88I 1H/D-88 Z-GRD Z814501/0063		4	12.77		45.8761640		
	xport all experiments to file		10	1	PROF URINE NOESY	noesygpprid	au urine noesy	proc urine noesy			32	4	12.55		46.0271070		
	xport paths of selected experiments as lis	t.,	10	1	PROF URINE NOESY	noesygpprid	au_urine_noesy	proc urine noesy	-		32	4	13.65	-12.000018.	45.2973287		
	xport paths of all experiments as list		10	1	PROF URINE NOESY	noesygpprid	au urine noesy	proc urine noesy		5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	12.36	-12.000018	46.1596108	86.63	
	Open in AMIX	Ctrl+X	10	1	PROF URINE NOESY	noesygpprid	au_urine_noesy	proc urine noesy	-		32	4	11.99	-12.000018	46.4235954		
	Dpen in TopSpin	Ctrl+T	10	1	PROF URINE NOESY	noesygpprid	au_urine_noesy	proc urine noesy	-	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	13.74	-12.000018	45.2402462	86.63	
	can multiple spectra in TopSpin	Contra	10	1	PROF URINE NOESY	noesygppr1d	au urine noesy	proc urine noesy	AV600 HASC	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	11.88	-12.000018	46.5036507	86.63	
voerime		Ctrl+I	10	1	PROF URINE NOESY	noesygppr1d	au_urine_noesy	proc urine noesy	AV600 HASC	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	13,47	-12.000018	45.4126276	86.63	
operime	mport metadata from file	Ctrl+I	10	1	PROF_URINE_NOESY	noesygpprld	au_urine_noesy	proc_urine_noesy	AV600 HASC	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	13.87	-12.000018	45.1584513	86.63	
xperime	how all columns in table view		10	1	PROF_URINE_NOESY	noesygpprld	au urine noesy	proc urine noesy		5 mm PA88I 1H/D-88 Z-GRD Z814501/0053	32	4	12.29	-12.000018	46.2089417	86.63	
xperime	how selected columns in table view		10	1	PROF URINE NOESY	noesygppr1d	au urine noesy	proc urine noesy	AV600 HASC	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	11.94	-12.000018	46.4598957	86.63	
xperiment	s\BrukerIVDrForum\S urine1 0035		10	1	PROF URINE NOESY	noesyapprid	au urine noesy	proc_urine_noesy	AV600 HASC	5 mm PA8811H/D-88 Z-GRD Z814601/0063	32	4	13.23	-12.000018	45.5687867	86.63	
Experiment	s\BrukerIVDrForum\S urine1_0036		10	1	PROF_URINE_NOESY	noesygppr1d	au_urine_noesy	proc_urine_noesy		5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	13.91	-12.000018	45.1334386	86.63	
Experiment	s\BrukerIVDrForum\S urine1_0037		10	1	PROF_URINE_NOESY	noesygpprid	au_urine_noesy	proc_urine_noesy	AV600_HASC	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	12.4	-12.000018	46.1315462	86.63	
xperiment	s\BrukerIVDrForum\S urine1_0038		10	1	PROF_URINE_NOESY	noesygpprid	au_urine_noesy	proc_urine_noesy	AV600_HASC	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	12.57	-12.000018	46.0132752	86.63	
xperiment	s\BrukerIVDrForum\S urine1_0039		10	1	PROF_URINE_NOESY	noesygppr1d	au_urine_noesy	proc_urine_noesy	AV600_HASC	5 mm PAB8I 1H/D-BB Z-GRD Z814601/0063	32	4	11.81	-12.000018	46.5549808	86.63	
xperiment	s\BrukerIVDrForum\S urine1_0040		10	1	PROF_URINE_NOESY	noesygppr1d	au_urine_noesy	proc_urine_noesy	AV600_HASC	5 mm PA88I 1H/D-88 Z-GRD Z814601/0063	32	4	11.79	-12.000018	46.5697052	86.63	
xperiment	s\BrukerIVDrForum\S urine1_0041		10	1	PROF_URINE_NOESY	noesygppr1d	au_urine_noesy	proc_urine_noesy	AV600_HASC	5 mm PAB8I 1H/D-88 Z-GRD Z814601/0063	32	4	11.79	-12.000018	46.5697052	86.63	
xperiment	s\BrukerIVDrForum\S urine1_0042		10	1	PROF_URINE_NOESY	noesygpprld	au urine noesy	proc_urine_noesy	AV600_HASC	5 mm PAB8I 1H/D-88 Z-GRD Z814501/0053	32	4	12.09	-12.000018	46.3514557	86.63	

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):

Configuration	
TopSpin Path:	
C:\Bruker\TopSpin3.5pl2 -	1
Amix Path:	
C:\Bruker\aurelia-amix	
Save Cancel	

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:

Filter spectra			×
Column:			
Exp.No.	•		
Enter pattern to sea	rch for:		
10			
Normal	Normal (exact)		
Regular express	ion (e.g. "AM-(Urine	e Plasma)\S+[0-9]+\S+")	
Add Filter			
0			
Queued filters Column name		Search pattern	Search type
Exp.No.	10		Normal
Remo	ve filter		
Impor	t filter from file		
Save f	ilter to file		
Apply filter(s)	Reset		

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:

 Execute TopSpin commands	Γ
Enter TopSpin commands for selected spectra:	
Example:	
Ib 0	
efp	
Exceute Command(s)	

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.

🚡 Scan multiple spectra in T	opSpin 💌
Left limit [ppm]:	Right limit [ppm]:
1	-1
Time interrupt [s]:	_
0.5	
₩ ► > =	

Figure 3.3: Scan Multiple Spectra in TopSpin

#### 3.3 Metadata

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 sample for example.

#### 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. The other functions concerning metadata are only available for the 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.

#### 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.

When using this function, you have to enter the name of the source XML file and specify the export path. When the source XML file does not exist, then you should check **Create XML-File with metadata if source XML-File is not existent** to create the file with metadata:

Add metadata to XML	
Source XML-FileName: Metadata.xml	
Create XML-File with metadata if source XML file is not existent	
Export path:           I\Experiments\Metadata\         Choose Directory	
Export metadata Cancel	

Figure 3.4: 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:

Column name	Show in view
Exp.No.	V
Proc.No.	$\checkmark$
Experiment	$\checkmark$
Pulse program	
AUNM	$\checkmark$
AUNMP	$\checkmark$
Instrument	$\checkmark$
Probehead	$\checkmark$
NS	$\checkmark$
DS	$\checkmark$
P1	$\checkmark$
PIdB 1	$\checkmark$
PIdB 9	$\checkmark$
RG	$\checkmark$
SWH	
<	>

Figure 3.5: 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.

# 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

### H161805\_1\_001

### **Bruker Corporation**

info@bruker.com www.bruker.com