DIFFRAC.SUITE

- User Manual

DIFFRAC.MEASUREMENT SUITE
FILE EXCHANGE

Original Instructions

Innovation with Integrity

XRD

We have checked the contents of this manual for agreement with the hardware and software described. Since deviations cannot be precluded entirely, we cannot guarantee full agreement. However, the data in this manual are reviewed regularly and any necessary corrections are included in subsequent editions. Suggestions for improvement are welcome.

All configurations and specifications are subject to change without notice.

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FILE EXCHANGE User Manual

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1 Introducing FILE EXCHANGE

1.1 What is FILE EXCHANGE

FILE EXCHANGE is a software designed for easy data conversion and management between different formats. The list of formats includes both the Bruker internal ones and the most recognized data formats from public domain software. FILE EXCHANGE is designed similarly to widely used (Windows) Total Commander file manager, however, does not replicate all the features of mentioned software and emphasizes the most important and typical operations with Bruker experimental data.

Main features of FILE EXCHANGE

- Easy-to-use operations with data files
- Intuitively clear Graphical User Interface similar to widely used file managers Norton Commander, Total Commander, Windows Commander, etc
- Filters to display/hide different file formats
- Connection to all network drives and Bruker Database
- Script interface for automated data conversion
- Basic file operations included (copy, delete, view, etc)

1.2 FILE EXCHANGE Installation

FILE EXCHANGE operation requires the Microsoft .NET Framework 3.5 installation, which is performed automatically during the installation of legal FILE EXCHANGE CD or Bruker measurement software CD. After successful installation, the FILE EXCHANGE program link is placed into Bruker AXS Programs group.

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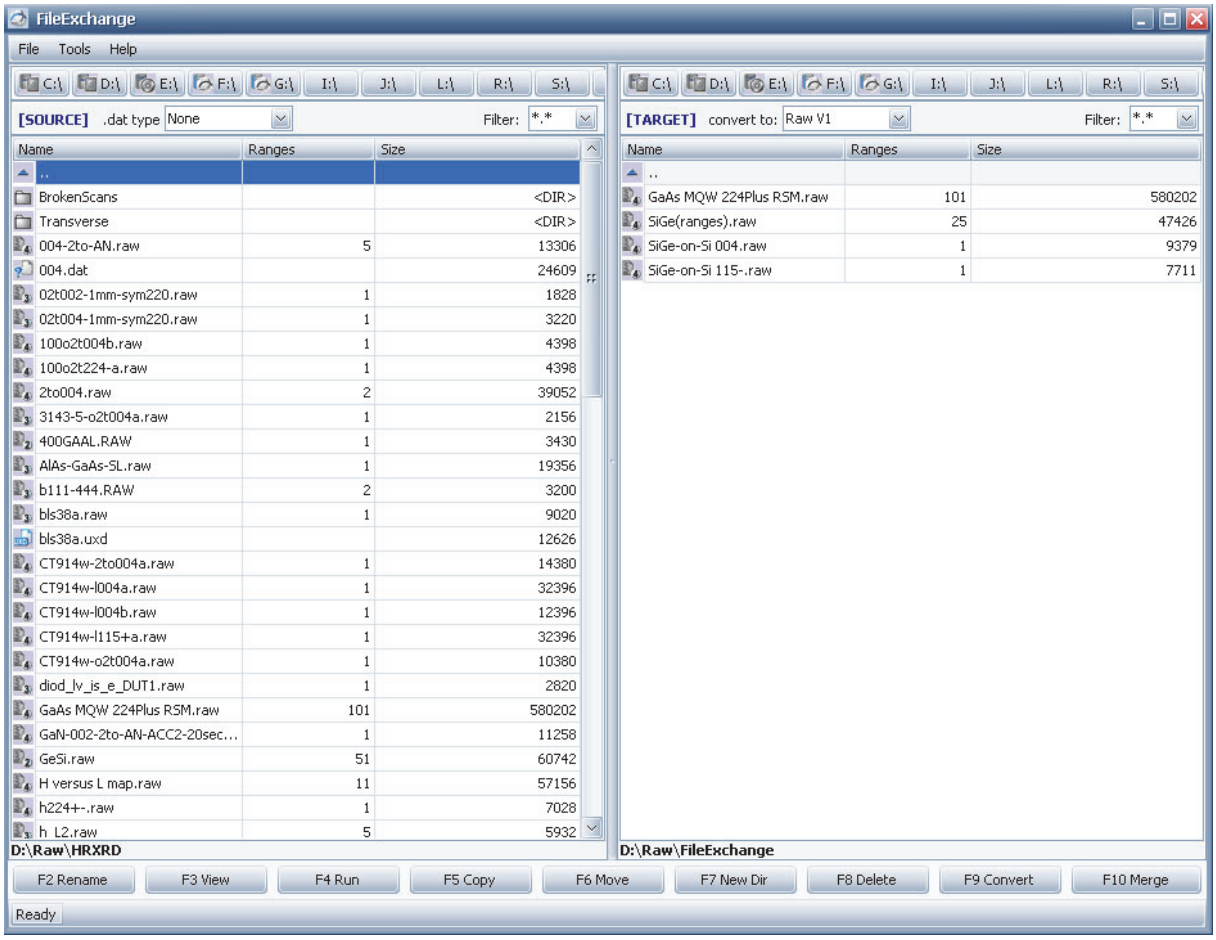
2 Data Conversion

2.1 Graphical User Interface

FILE EXCHANGE Graphical User Interface is designed similarly to standard file manager interface as two panels containing the list of files and directories (folders) with supplemental information on list objects.



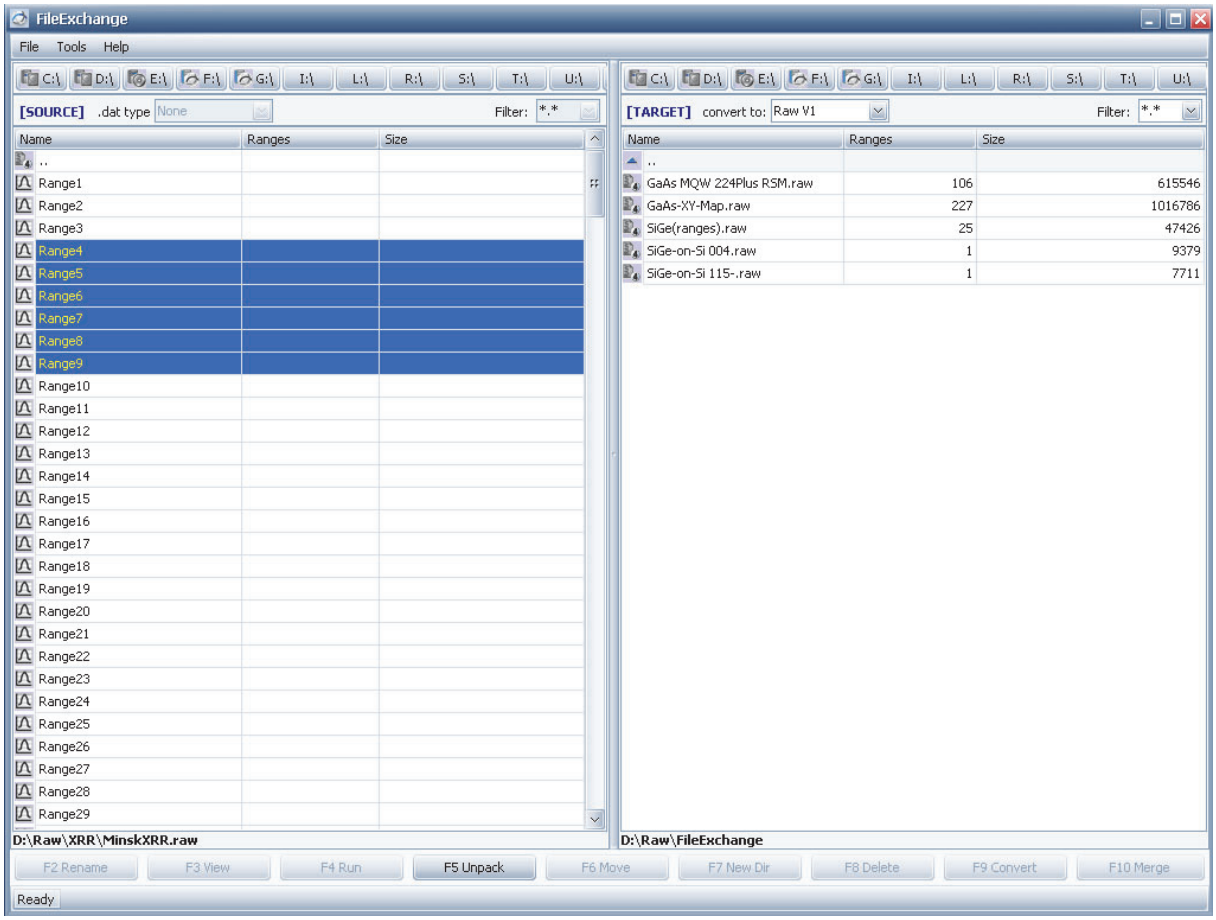
Both panels display the structure of logical drives including directories and files. The available drives list is shown in toolbars of each panel and includes all local and network drives and direct access to Bruker Database if available.

The left and right panels are not equivalent in operations. The left ***SOURCE*** panel is designed for selection of files for conversion, whereas right ***TARGET*** panel is assigned for the selection of the location and the format of the converted files. Both panels support common file operations like copy, delete, move, rename, view by external viewer. The filters in both panels allow to display only the files with selected extension and to hide other file types.

Each panel displays the file ***Names***, the number of single measured ***Ranges*** in Bruker raw files, and the ***Size*** of the files. Below the panels, the functional buttons ***Rename, View, Run, Copy, Move, New Directory, Delete, Convert,*** and ***Merge*** are located. Each button is associated with functional hot key, which is displayed on the button. The status bar shows the current status of the program.

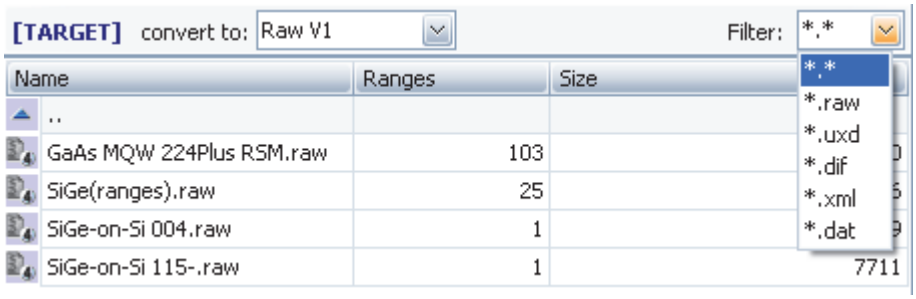
FILE EXCHANGE also has system menus File, Tools, and Help, which provide the access to the options and on-line help of the program. The splitter dividing both panels is movable, thus user may change as the size of the main window as well the sizes of each panel.

The raw files containing multiple ranges can be expanded as directories by left mouse button double-click or Enter key. In this case FILE EXCHANGE displays the list of the separate ranges named ***Range*** and enumerated from one to maximal number.



The data files format is automatically recognized by FILE EXCHANGE and displayed with a specific icon. The recognized formats are listed in the Section File Formats.

The ***Filters*** in both Source and Target panels help to display/hide desired file types:



2.2 File Operations

FILE EXCHANGE supports the following file operations, which are allowed in both (***Source*** and ***Target***) or ***Source*** only panels:

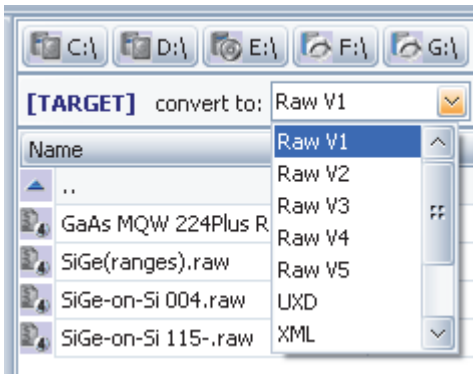
Command (Function key)	Description	Applicability
Rename (F2)	rename files	Source & Target
View (F3)	open file in external viewer specified in Options	Source & Target
Run (F4)	open file in Windows application, associated with file extension	Source & Target
Copy or Unpack (F5)	copy file(s) in opposite panel, or unpacks the range(s) from multirange file into file(s)	Source & Target, Source
Move (F6)	move file(s) to opposite panel	Source & Target
New Directory (F7)	create new directory	Source & Target
Delete (F8)	delete file(s)	Source & Target
Convert (F9)	convert file(s) from Source panel to Target one by creating new file(s)	Source
Merge or Append (F10)	merge two or more files selected in source panel into one created in Target panel, if header information is conformal; append file(s) from Source panel to expanded multi-range file in Target panel	Source

Attention!

FILE EXCHANGE supports multiple selection of files using Space bar or Insert key for batch operations when applicable.

2.2.1 Conversion

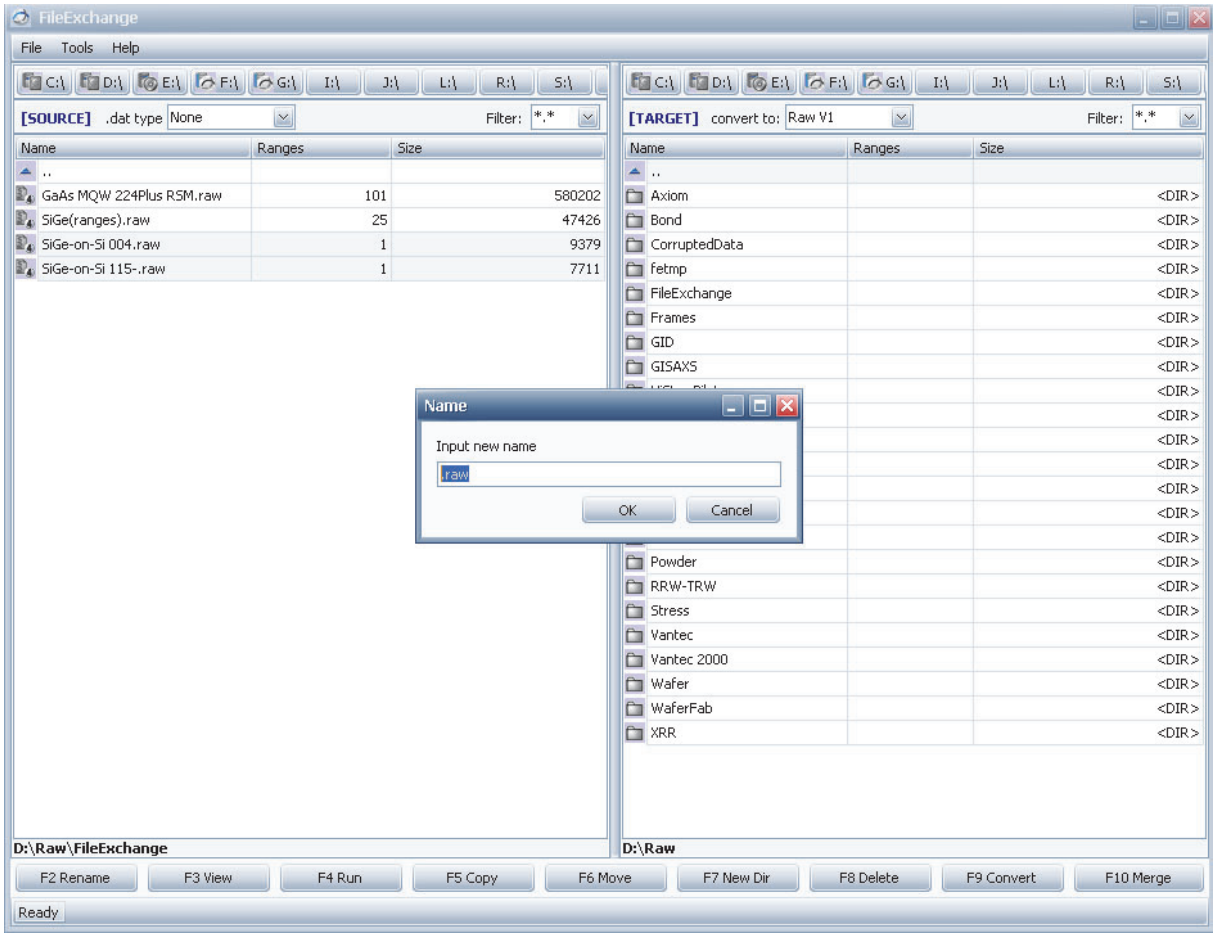
The conversion of data files from Source panel in Target panel is performed by selecting the file(s) in left panel, choosing the result file(s) format in the ***Convert to*** combobox of Target panel and pressing button Convert or key F9.



The list of available resulting formats is displayed in combobox. The multirange Bruker raw source files are converted in multirange target file, correspondingly. If the target ASCII file format is selected (UXD, XML, etc), then the ranges are stored in resulting file successively.

2.2.2 Merging

FILE EXCHANGE allows merging several Bruker raw files into single raw file by selecting in Source panel several files and using key ***F10 Merge***. The software firstly checks the compatibility of header information on the fields checked in ***Options*** in ***Merge/Append Matching*** list. The fields are Scan Type, Scan Start, Scan Stop, Step Size, Time per Step, X, Y, Z, Chi, Phi, Theta, Wavelength, Units, and Bragg reflection. If all the fields are compatible, FILE EXCHANGE prompts the new file name to be created in the selected in Target panel directory.



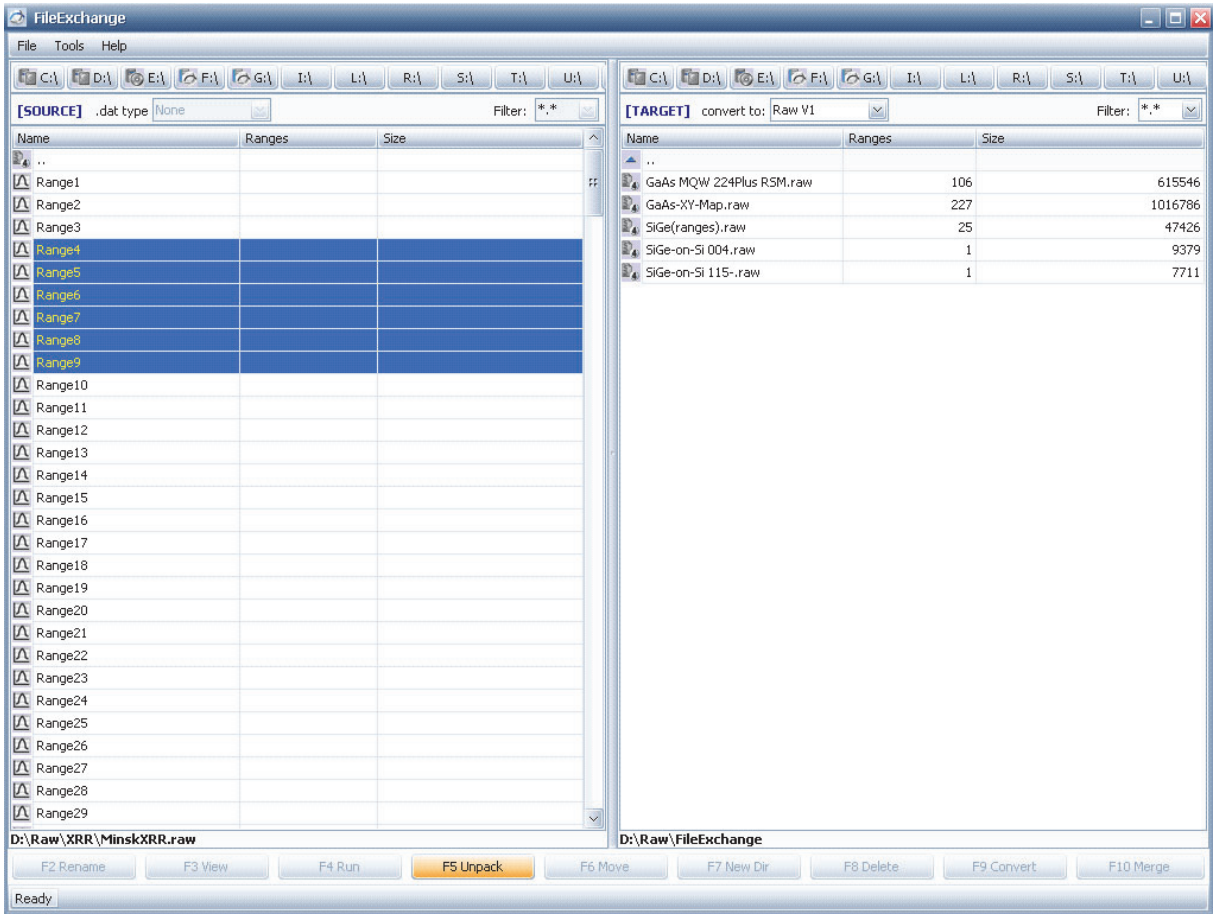
A new created raw file has always Bruker file format version 4.

Attention!

FILE EXCHANGE supports only merging of Bruker format raw files.

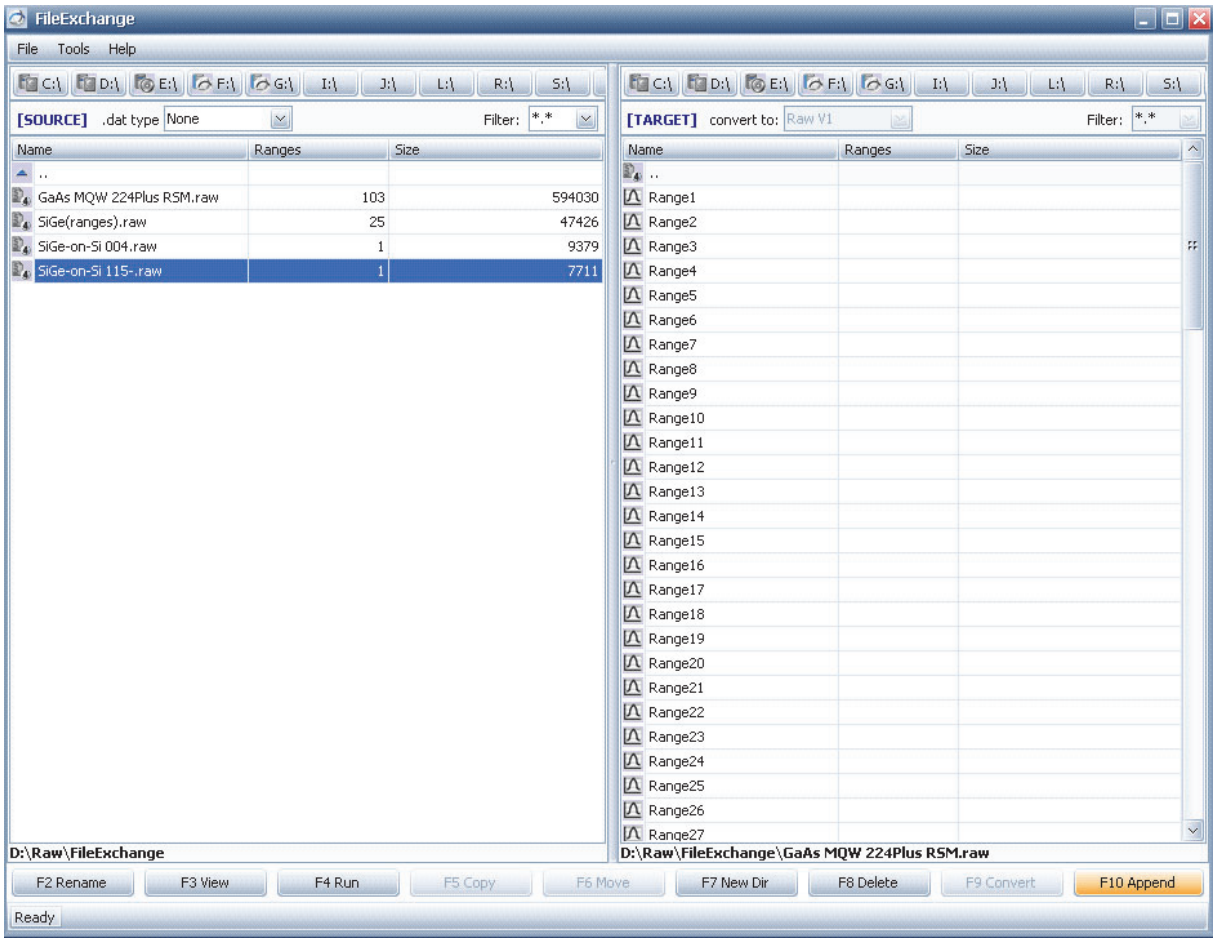
2.2.3 Unpacking

When expanding a multi-range Bruker raw file, FILE EXCHANGE makes possible to Unpack selected ranges in separate raw files in Target panel. The header of initial raw file is transferred unchanged into new raw files. In this situation, the functional button F5 takes Unpack functionality:



2.2.4 Appending

The operation Append is similar to opertation Merge with the difference that FILE EXCHANGE appends the selected in Source panel file to the expanded in Target panel multi-range file. The check of the file headers compatibility is performed on the basis of the selected fields in ***Options*** in ***Merge/Append Matching*** list.



Attention!

FILE EXCHANGE supports only appending in Bruker format raw files.

2.3 File Formats

FILE EXCHANGE operates with all internal formats of Bruker data taken with 0- or 1-dimensional detectors. The public domain software formats are also partly supported. The full list of data formats with comments is given below.

Format versions and types are displayed on the icons left to the file name.

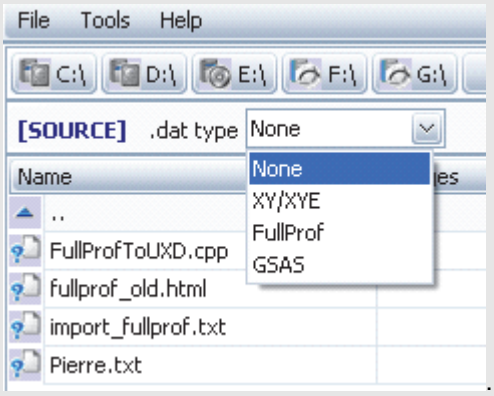
RAW V1..5	Bruker raw data formats; single range / multi-ranges; direct and reverse conversions;
DIF V1..3	Bruker raw data formats; conversion to ASCII only
UXD	Bruker Diffrac exchange format
XML	format for VÅNTEC-1 stand-alone mode
2 theta/counts	coupled scan

XY, ***XYE***	2 columns: angles, intensity; 3 columns: angles, intensity, intensity error; supported conversion from XYE into other formats, no conversion into XYE
VCT	Bruker variable counting time
FullPROF	FullProf public software for powder diffraction
GSAS	GSAS public software for powder diffraction
RRW/TRW	Bruker raw data formats for texture
PART11 RAW	Bruker raw data collected under CFR 21 Part 11 regulations

The external FullProf and GSAS formats are read by FILE EXCHANGE in short header length, i.e. only limited information is taken from these formats.

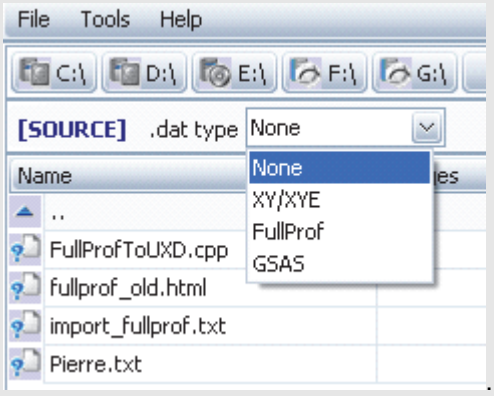
Attention!

To help FILE EXCHANGE in distinguishing general ASCII formats FullProf, GSAS, and XY/XYE, the ****.dat type*** combobox makes a selection of the intended source data format:



Attention!

To help FILE EXCHANGE in distinguishing general ASCII formats FullProf, GSAS, and XY/XYE, the ****.dat type*** combobox makes a selection of the intended source data format:



2.4 Automated Data Conversion

FILE EXCHANGE supports automated file conversion in three ways: (i) running FILE EXCHANGE application in command line mode, (ii) using FILE EXCHANGE function available in ***script*** interface, and (iii) in implementing the C# functions via the provided Dll.

The command line mode uses syntax:

```
FileExchange source [version] target
```

where `source` means source filename, `version` is a version of Bruker raw data format, and `target` is a target filename.

For example, the command `FileExchange C:\si004.raw v4 C:\si004_v4.raw` will convert raw file si004.raw located in root C:\ directory into si004_v4.raw file version 4 and place it in the same directory.

The list of C# conversion functions accessible in script interface or via inclusion of the Dll is given below. Their functionality is self-explanatory from the names:

```
Exchange.ConvertV1toV2(string inputFile, string outputFile)
Exchange.ConvertV1toV3(string inputFile, string outputFile)
Exchange.ConvertV1toV4(string inputFile, string outputFile)
Exchange.ConvertV1toUXD(string inputFile, string outputFile)
Exchange.ConvertV1toXML(string inputFile, string outputFile)
Exchange.ConvertV1toXY(string inputFile, string outputFile)
Exchange.ConvertV1toXYE(string inputFile, string outputFile)
Exchange.ConvertV1toFullProf(string inputFile, string outputFile)
Exchange.ConvertV1toGSAS(string inputFile, string outputFile)
Exchange.ConvertV2toV4(string inputFile, string outputFile)
Exchange.ConvertV2toV1(string inputFile, string outputFile)
Exchange.ConvertV2toV3(string inputFile, string outputFile)
Exchange.ConvertV2toUXD(string inputFile, string outputFile)
Exchange.ConvertV2toXML(string inputFile, string outputFile)
Exchange.ConvertV2toXY(string inputFile, string outputFile)
Exchange.ConvertV2toXYE(string inputFile, string outputFile)
Exchange.ConvertV2toFullProf(string inputFile, string outputFile)
Exchange.ConvertV2toGSAS(string inputFile, string outputFile)
Exchange.ConvertV3toV1(string inputFile, string outputFile)
Exchange.ConvertV3toV2(string inputFile, string outputFile)
Exchange.ConvertV3toV4(string inputFile, string outputFile)
Exchange.ConvertV3toUXD(string inputFile, string outputFile)
Exchange.ConvertV3toXML(string inputFile, string outputFile)
Exchange.ConvertV3toXY(string inputFile, string outputFile)
Exchange.ConvertV3toXYE(string inputFile, string outputFile)
Exchange.ConvertV3toFullProf(string inputFile, string outputFile)
Exchange.ConvertV3toGSAS(string inputFile, string outputFile)
Exchange.ConvertV4toV1(string inputFile, string outputFile)
```

```
Exchange.ConvertV4toV2(string inputFile, string outputFile)
Exchange.ConvertV4toV3(string inputFile, string outputFile)
Exchange.ConvertV4toV4Text(string inputFile, string outputFile)
Exchange.ConvertV4toXML(string inputFile, string outputFile)
Exchange.ConvertV4toUXD(string inputFile, string outputFile)
Exchange.ConvertV4toXY(string inputFile, string outputFile)
Exchange.ConvertV4toXYE(string inputFile, string outputFile)
Exchange.ConvertV4toFullProf(string inputFile, string outputFile)
Exchange.ConvertV4toGSAS(string inputFile, string outputFile)
Exchange.ConvertUXDtoV1(string inputFile, string outputFile)
Exchange.ConvertUXDtoV2(string inputFile, string outputFile)
Exchange.ConvertUXDtoV3(string inputFile, string outputFile)
Exchange.ConvertUXDtoV4(string inputFile, string outputFile)
Exchange.ConvertUXDtoXML(string inputFile, string outputFile)
Exchange.ConvertUXDtoFullProf(string inputFile, string outputFile)
Exchange.ConvertXYEtoV4(string inputFile, string outputFile)
Exchange.ConvertXMLtoV4(string inputFile, string outputFile)
Exchange.ConvertFPtoV1(string inputFile, string outputFile)
Exchange.ConvertFPtoV2(string inputFile, string outputFile)
Exchange.ConvertFPtoV3(string inputFile, string outputFile)
Exchange.ConvertFPtoV4(string inputFile, string outputFile)
Exchange.ConvertFPtoUXD(string inputFile, string outputFile)
Exchange.ConvertFPtoXML(string inputFile, string outputFile)
Exchange.ConvertFPtoXY(string inputFile, string outputFile)
Exchange.ConvertFPtoXYE(string inputFile, string outputFile)
Exchange.ConvertRWtoV1(string inputFile, string outputFile)
Exchange.ConvertRWtoV2(string inputFile, string outputFile)
Exchange.ConvertRWtoV3(string inputFile, string outputFile)
Exchange.ConvertRWtoV4(string inputFile, string outputFile)
Exchange.ConvertRWtoUXD(string inputFile, string outputFile)
Exchange.ConvertRWtoXML(string inputFile, string outputFile)
Exchange.ConvertRWtoXY(string inputFile, string outputFile)
Exchange.ConvertRWtoXYE(string inputFile, string outputFile)
Exchange.ConvertRWtoFullProf(string inputFile, string outputFile)
Exchange.ConvertGSAStoV1(string inputFile, string outputFile)
Exchange.ConvertGSAStoV2(string inputFile, string outputFile)
Exchange.ConvertGSAStoV3(string inputFile, string outputFile)
Exchange.ConvertGSAStoV4(string inputFile, string outputFile)
Exchange.ConvertGSAStoUXD(string inputFile, string outputFile)
Exchange.ConvertGSAStoXML(string inputFile, string outputFile)
Exchange.ConvertGSAStoXY(string inputFile, string outputFile)
Exchange.ConvertGSAStoXYE(string inputFile, string outputFile)
```

```
Exchange.ConvertV4toV5(string inputFile, string outputFile)
Exchange.ConvertV5toV4(string inputFile, string outputFile)
```

To access the options for UXD conversion (see chapter 2.6) there are three different properties:

```
Exchange.UXDMode
```

0 - Intensity
1 - Intensity in CpS
2 - Angle + Intensity
3 - Angle + Intensity in CpS

```
Exchange.UXDPeakMode
```

0 - dValue + Intensity
1 - Angle + Intensity
2 - dValue + Intensity in %
3 - Angle + Intensity in %

```
Exchange.ItemsPerLine
```

The typical call of these function from the C# script can be done as:

```
using System;
using BrukerAXS.FileExchange;

class FEScript
{
      public void Execute()
      {
        Exchange.ConvertV1toV4(@"D:\FileV1.raw", @"D:\FileV4.raw");

      }
}
```

The script is launched by a command line

```
FileExchange D:\Temp\FEScript.cs
```

A similar program can be build when referencing to the Dll that can be found in the program files directory:

```
C:\Program Files\Bruker AXS\DIFFRAC.FileExchange\
BrukerAXS.FileExchange.dll
```

Or for 64 bit systems:

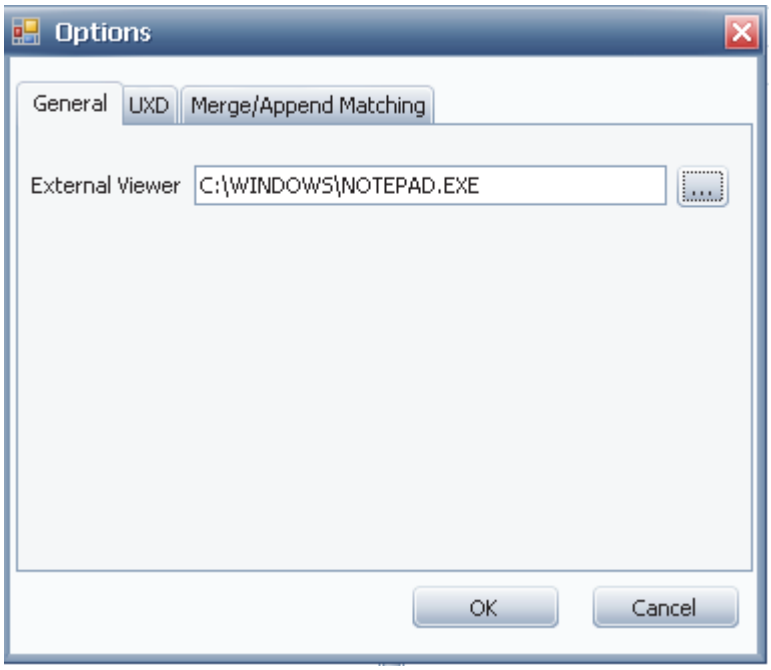
```
C:\Program Files (x86)\Bruker AXS\DIFFRAC.FileExchange\
BrukerAXS.FileExchange.dll
```

2.5 Bruker Database Access

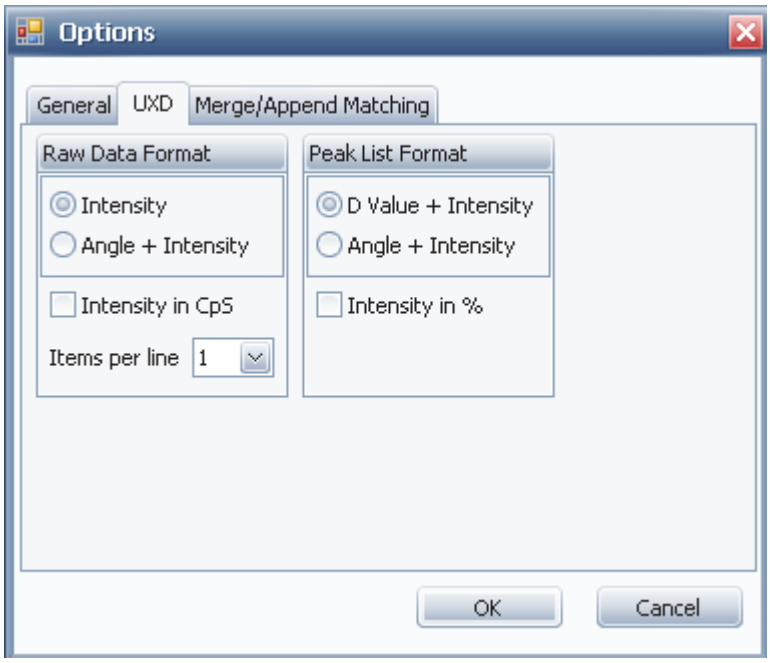
The recent Bruker V5 raw data format allows the storage of measured data as in files as well directly in Bruker Database. FILE EXCHANGE permits to connect directly to database for extracting and conversion of measured data in different formats. The connection with database is performed automatically after start of FILE EXCHANGE, if the database is installed and registered on computer.

2.6 Options

The FILE EXCHANGE ***Options*** are accessible via system ***Tools*** menu:

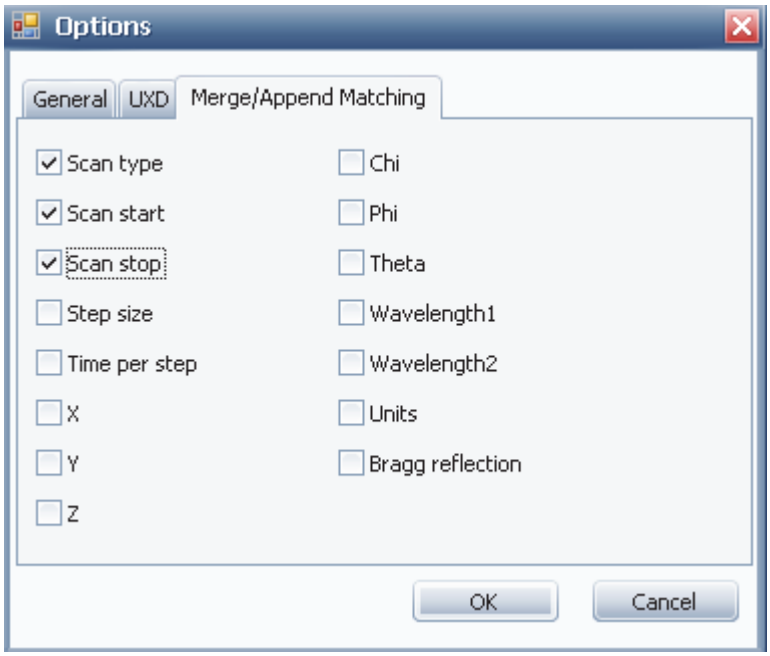


The ***General*** tab prompts user to select external viewer, which will be used when functional button F3 View is pressed. The ***UXD*** tab specifies the conversion from raw file format to UXD format, namely the data and peak list formats. The raw data can be converted as one column ***Intensity*** or two columns ***Angles and Intensity***. The latter can be stored in ***Counts*** or in ***Counts per seconds***. ***Items per line*** defines the number of data stored in a single line.



Peak list format defines the peaks as ***d-value*** and ***Intensity*** or ***Angles and Intensity***. The latter can be also stored in ***percentage*** from maximal peak.

The Merge/Append Matching tab determines the header fields to be compared for valid data merging or appending. The selected fields will be compared in the selected in the Source/Target panels files, and the files will be only merged/appended if the checked fileds are equal for all files.

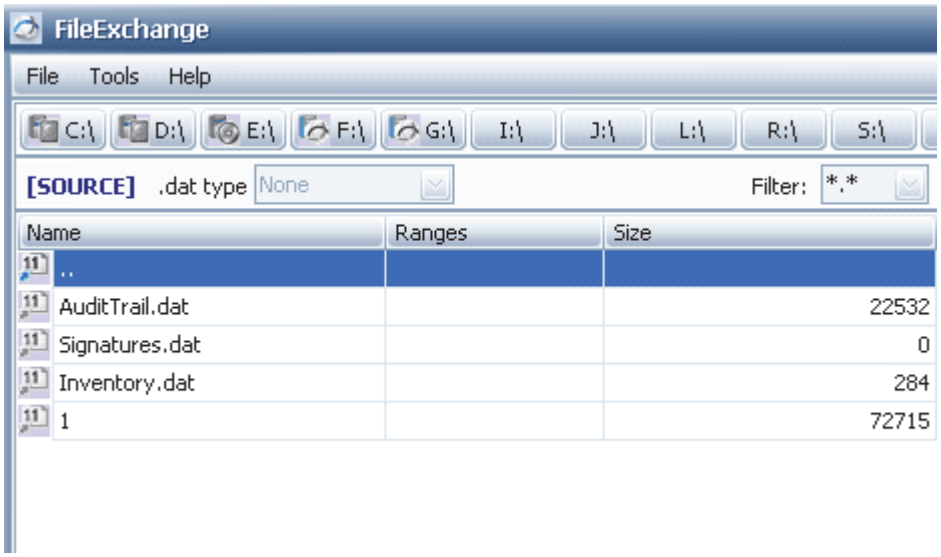


The meaning of the parameters is the following:

Scan Type	type of measured scan
Scan Start	scan start position
Scan Stop	scan stop position
Step Size	scan step value
Time per Step	measurement time per step
X	X-drive position
Y	Y-drive position
Z	Z-drive position
Chi	χ-drive position
Phi	ϕ-drive position
Theta	θ-drive position
Wavelength1	principal X-ray wavelength
Wavelength2	secondary x-ray wavelength
Units	scan units, e.g. degrees, arsecs, etc
Bragg Reflection	measured Bragg reflection

2.7 CFR 21 Part 11

FILE EXCHANGE displays the content of measured CFR 21 part 11 files by expanding this file type into directory. The Audit Trail, Signatures and Inventory data can be extracted along with the data themselves. The Part 11 files have special icon with mark 11 to distinguish them from regular Bruker raw files.



Attention!

CFR 21 part 11 files content is not allowed to be changed, merged or appended.

3 Glossary

1. ***RAW*** is Bruker experimental data format
2. ***FullProf*** is data format of public powder diffraction software http://www.ill.eu/sites/fullprof/
3. ***DIF*** is Bruker powder diffraction data format including peak positions
4. ***GSAS*** is data format of public software http://www.ncnr.nist.gov/xtal/software/gsas.html
5. ***CRF 21 Part 11*** is FDA guidance for industry http://www.21cfrpart11.com/
6. ***VCT*** is variable count time format
7. ***RRW/TRW*** are transmission and reflection texture Bruker data formats
8. ***UXD*** is a Bruker ASCII data format

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