Readme file for **bruk2igor**

bruk2igor is a win32 console program for batch conversion of Bruker 1r binary format frequency domain spectrum files into any one of three output formats: individual (0) .txt ascii text files (1) .dfp DFP compatible 1column format (2) .itx Igor-Pro text file. The files are placed in the fds subfolder of the main experiment folder.

If **bruk2igor** is entered with no command line argument, it looks for the file "list.txt" in the current working directory which contains a list of 1r filenames for files to be converted (for creation of this file, see below).

If the folder name is specified as the command line parameter, then bru2igor looks in that folder for the “list.txt” file.

Installation:

Copy the file bru2igor.exe into the directory where you keep all your console programs. For cygwin, this should be /usr/local/bin. For DOS, you would need to modify the PATH variable to include the directory containing bru2igor.exe, but this is not necessary in cygwin.

Execution:

(1) Create the "list.txt" file. The file "list.txt" contains a list of the binary "1r" files to be converted.

A convenient way to generate the list.txt file is to use the unix "find" command to search for 1r files in all subdirectories of the main experiment directory. The ">" operator sends the contents to a text file.

For example, to create a list of all "1r" files contained in the wag21d-rt experiment:

```
$ find wag21d-rt -name "1r" > wag21d-rt/list.txt
```

Note that the list.txt file was created inside the wag21d-rt experiment directory.

This generated the following list.txt contents:

```
wag21d-rt/2/pdata/1/1r
wag21d-rt/3/pdata/1/1r
wag21d-rt/4/pdata/1/1r
wag21d-rt/5/pdata/1/1r
```

Now that you have the list.txt file created, you can edit this file to remove entries that you do not wish to convert. You should remove all of the paropt (999) directories from the list.

(2) Running BRU2IGOR

At the system prompt enter

```
$ bru2igor expname
```

where expname is the name of the main experiment folder. For example:

```
$ bru2igor wag21d-rt
```

In this case bru2igor will use the wag21d-rt/list.txt.

```
program found 4 1r files listed in list.txt
series /2: sw=1.000e+005 npts=8192 -> 8192 points read
series /3: sw=1.000e+006 npts=8192 -> 8192 points read
series /4: sw=1.000e+006 npts=8192 -> 8192 points read
series /5: sw=1.000e+006 npts=8192 -> 8192 points read
```

The output of bru2igor can be sent to a text file for future reference by using the ">" operator, e.g.

```
$ bruk2igor wag21d-rt > wag21d-rt/out.txt
```

bru2igor will prompt for the output file format, where

0=create text file (.txt), 1st column is frequency, 2nd column is the real signal

1=DFP (.dfp), creates output as follows:
Line 1: # points in the spectrum
Line 2: dwell time, 1/sw
Line 3: name of the spectrum

2=IGOR A single Igor Pro text file (.itx) will be created containing all of the spectra in the list.txt file.

bru2igor will prompt for the data point interval

1=output every point
2=output every other point, etc…

(3) Output

bruk2igor creates a subdirectory named "fds" (frequency domain spectra) in the main experiment directory. For the example give above, this would be

wag21d-rt/fds

File extensions:

File extension ".txt" is used for output files in the 2-column text file (format 0 above). The first is the frequency, in Hz, the 2nd is the spectrum amplitude at that frequency.

The “.dfp” extension is used for DFP output files (format 1 above).

To combine .txt files into a single Igor Pro compatible file, use FDSTACK.