

1. Upon arrival at the beamline, create a new data directory on the beamline computer named for the month and year of the run (.mmyyyy). In the following, we will use the February 2002 run as an example. After logging into the beamline computer, the default directory will be \$USER1:[B\_SCOTT]. First set the default to the data directory and create a new subdirectory.

```
$ SET DEF $DATA1:
$ CREATE/DIR [.022002]
```

Then, in XAS-Collect, set the default data directory to the newly created subdirectory.

```
$ XAS
```

In the XAS-Collect window, use Utilities | Directories and set the Data Directory: to \$DATA1:[B\_SCOTT.022002]

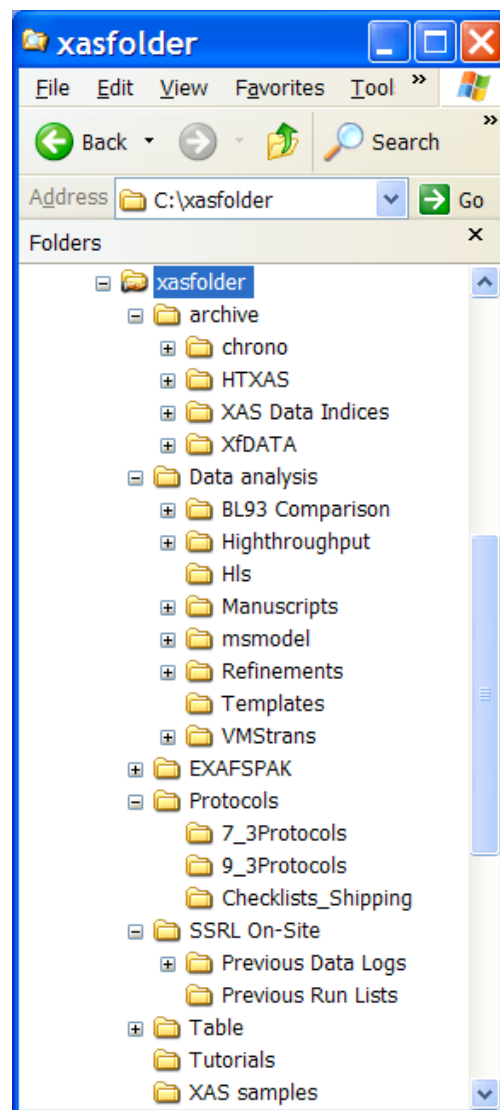
2. At the right is the overall directory structure of the XAS beamline laptop, starting in the directory c:\xasfolder. Create new folder\subfolders in the xasfolder\archive directory to hold the data log forms and data. There should be a new folder for each calendar year and a subfolder for each run, as follows

```
xasfolder\archive\chrono\2002\022002\raw73 (or \raw93)
xasfolder\archive\chrono\2002\022002\pre-run_log
xasfolder\archive\chrono\2002\022002\logforms
xasfolder\archive\chrono\2002\022002\aveandfrm
```

3. The preliminary sample list should be contained within the Excel file containing the comprehensive data index. This file is

```
xasfolder\archive\XAS Data
Indices\XAS_Data_Index_Proteins.xls
```

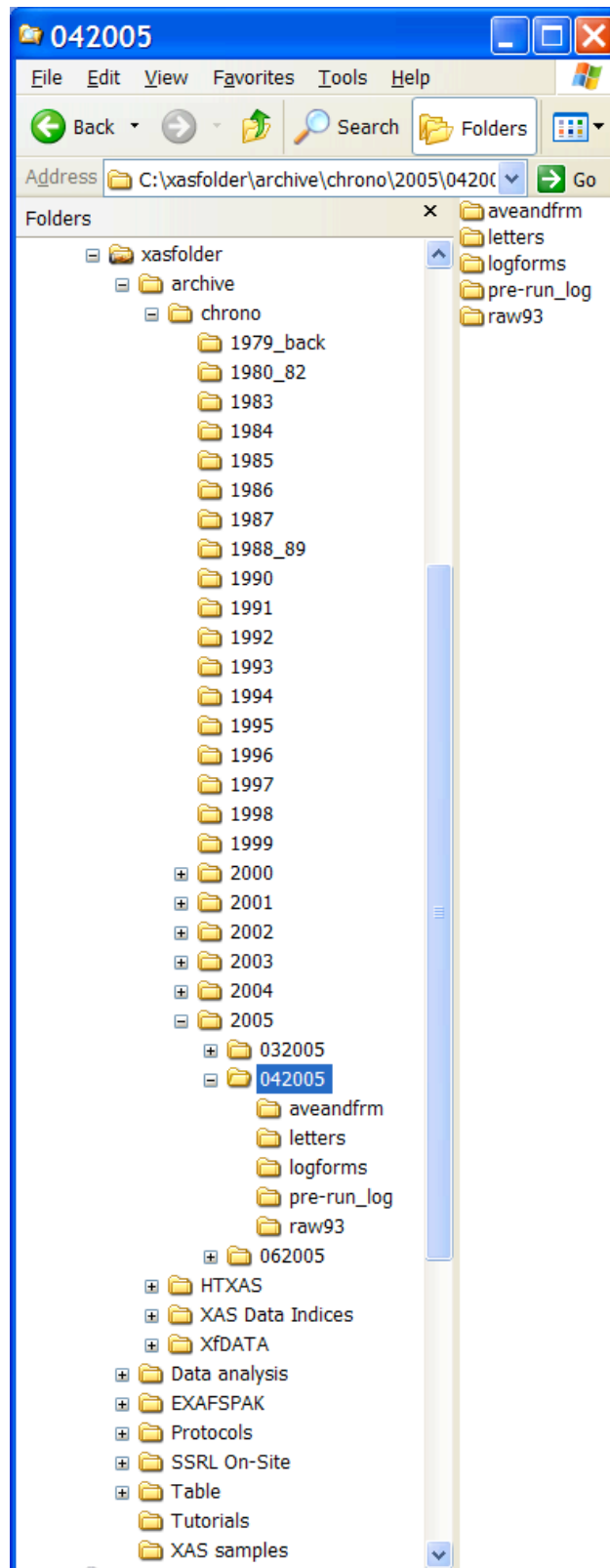
and the preliminary list will be on the runlist worksheet. This will become the comprehensive chronological list of samples examined. Download a data log form appropriate for the beamline from the Scott group website and place it in the \logforms subfolder. This can be used as a template for new data log forms. Place any partially filled data log forms from



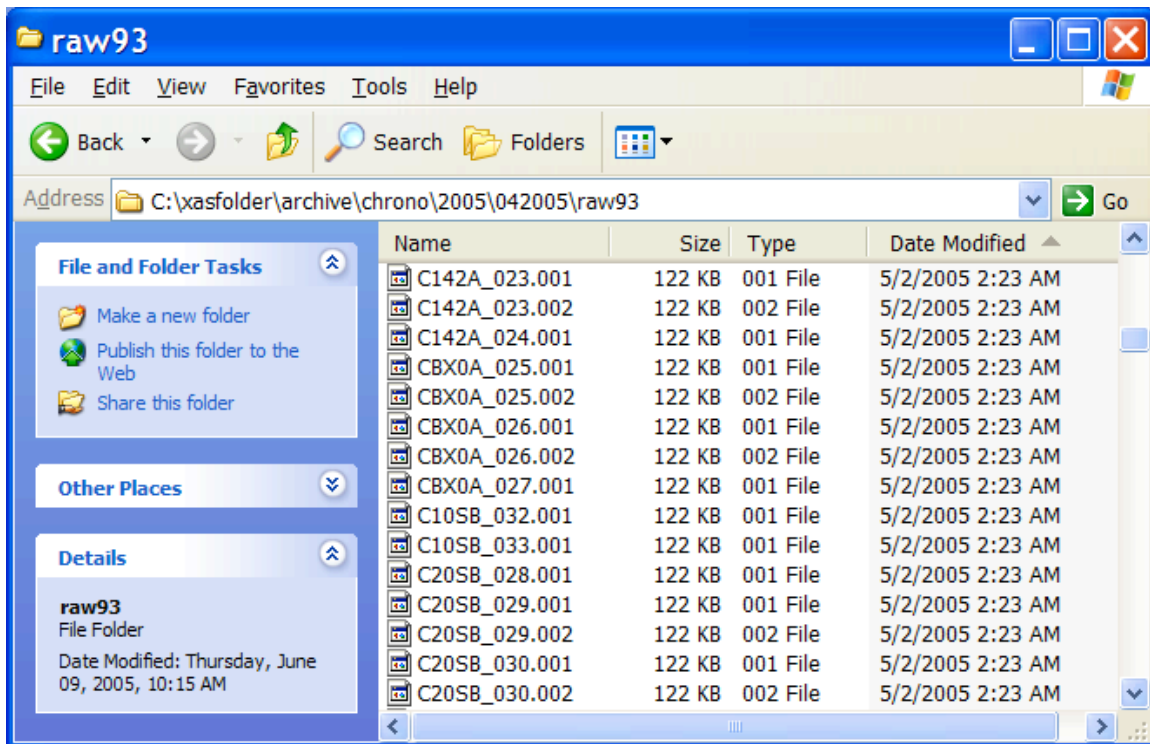
Revised 11 June 2005

collaborators in the \pre-run\_log subfolder and name them with the data filenames for those samples, when filenames are assigned.

- Every data file collected must be entered on an XAS Data Log Form appropriate for the beamline in use. BL73 forms have only a data reduction form below the data collection portion, whereas BL93 forms have a "cuvet map" in addition to the data reduction form.
- As soon as data collection for a sample is finished, enter the Date and BL in the XAS\_Data\_Index\_Proteins document (runlist worksheet). Then use binary ftp to transfer the raw data from the beamline computer data directory (above) to the \raw73 (for example) laptop subfolder. When it has been transferred, check the Data Transferred checkbox at the bottom of the data log form. (If more data are collected later on the same sample, use a *new* data log form; add a '\_B', etc., to the data log form filename.) Print a preliminary copy of each data log form after the checkbox has been checked (*before any data reduction*) and place it in the Master XAS Notebook binder.



6. ONLY the raw data files will be stored in the *raw\*\** folders:



7. When finished collecting data on a beamline, generate a list of the raw data on the beamline computer as follows

```
$ SET DEF $DATA1:[B_SCOTT.022002]  
$ DIR /DATE /OUT=[-]022002.LIS *.0*  
$ PRINT /QUEUE=120_BL7 [-]022002.LIS
```

Go through the printed data log forms, confirming that:

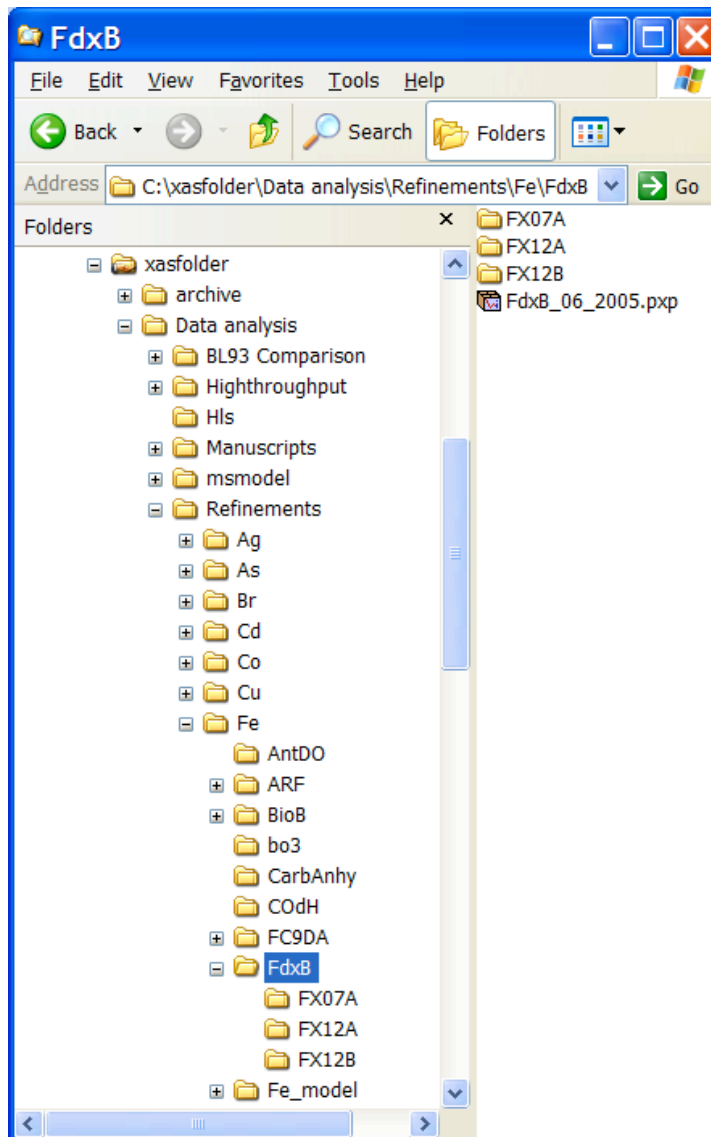
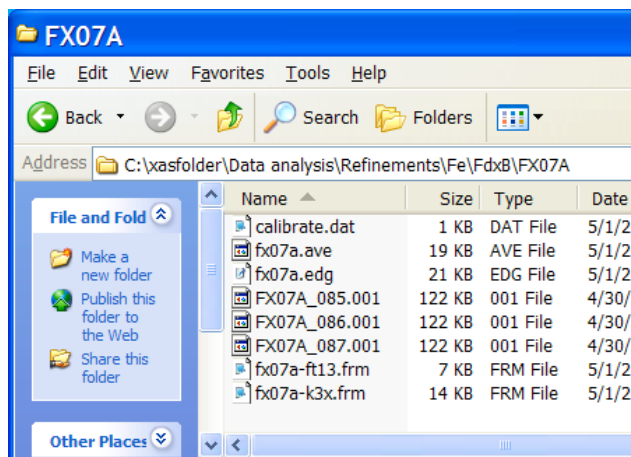
- (a) all data files on the printed beamline list are listed as sweeps on the log forms (print any missing log forms and add to log forms any missing sweeps)
- (b) all sweeps on log forms are data files in the directory (cross out or delete sweeps on log forms that don't have files on the beamline)

As you go through the printouts, remember that run numbers are used chronologically (missing run numbers should be a red flag).

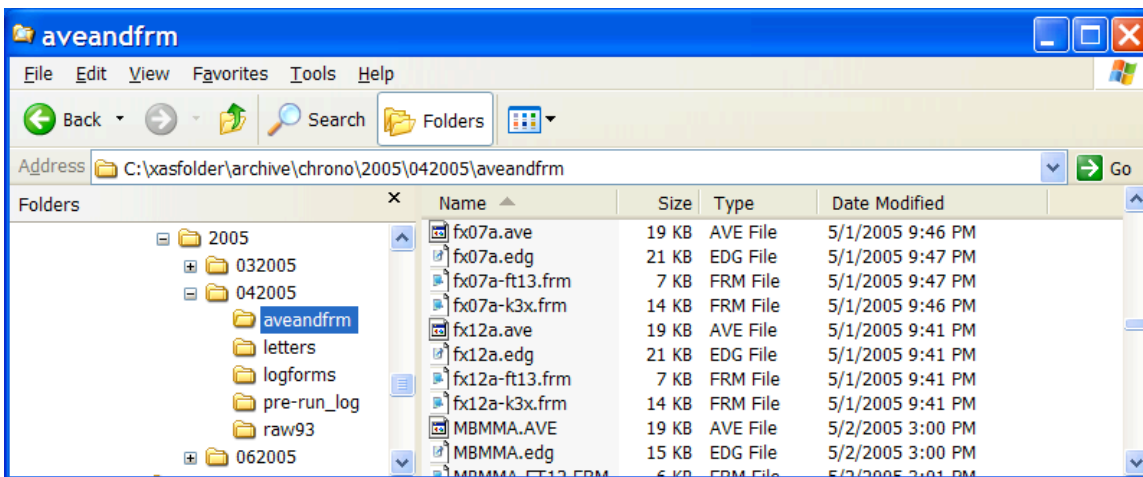
Then confirm that **ALL** data files in 022002.LIS have been copied by binary ftp to the laptop.

Revised 11 June 2005

- In preparation for on-site (preliminary) data reduction, an appropriate folder should be selected (or created) in the *\Refinements* subfolder of the *\Data analysis* subfolder of *\xasfolder*. For example, a workspace for Fe FdxB data should be created.
- The raw files should be **COPIED** into a new subfolder named for the sample filename (e.g., *\FX07A* below) where they will be reduced and appropriate FRM and EDG files will be created. For example, this folder should be within the ...*\Fe\FdxB* folder

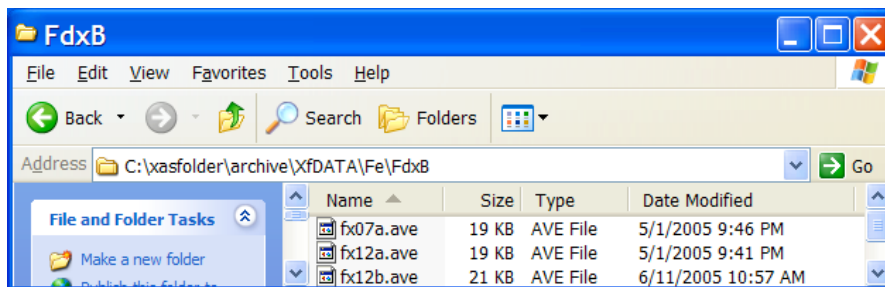


10. Once the data are reduced, the .AVE, .FRM, and .EDG files should be **COPIED** to the appropriate \aveandfrm folder in the *chrono* archive:



The final data reduction parameters should be recorded into the data log form for this particular sample (xasfolder\archive\chrono\2005\042005\logforms\FX07A in this example) and this completed data log form printed to replace the one from step 5. Complete the record in the runlist (see step 3) by entering Avg File and NB Page.

11. Then, the .AVE file should be placed in the appropriate XFDATA Archive folder.



At this point, the XAS\_Data\_Index\_Proteins.xls runlist worksheet should be updated to include the appropriate \xfdata\ folder for storage. Complete runlist records (that will be loaded into the running index on the by\_date worksheet) look like this:

Raw Files	Avg File	Protein	Derivative/Description	Source	Element	Date	T	NB	Page	\xfdata\	Cn	Cap	BL	Project
1552 FX12A	FX12A	FdxB	FdxB ISC-like at pH 12.3	Iwasaki	Fe	30-Apr-05	10	JES2-209		\Fe\FdxB	B	white	9-3	FdxB
1553 FX07A	FX07A	FdxB	FdxB ISC-like at pH 7.5 (as isolated).	Iwasaki	Fe	30-Apr-05	10	JES2-210		\Fe\FdxB	B	violet	9-3	FdxB
1554 FSH0A	FSH0A		FeSO4+Na2S at pH 12.3 without fractionation	Iwasaki	Fe	30-Apr-05	10	JES2-211		\Fe\ARF	C	red	9-3	ARF
1555 FSHCA	FSHCA		FeSO4+Na2S at pH 12.3 after centrifugation	Iwasaki	Fe	30-Apr-05	10	JES2-212		\Fe\ARF	B	green	9-3	ARF
1556 FSL1A	FSL1A		FeSO4+Na2S at pH 13.2	Iwasaki	Fe	30-Apr-05	10	JES2-213		\Fe\ARF	C	blue	9-3	ARF
1557 FSL0A	FSL0A		FeSO4+Na2S at pH12.3 jumped to pH9.6	Iwasaki	Fe	30-Apr-05	10	JES2-214		\Fe\ARF	C	Orange	9-3	ARF

*Once these steps have been completed for all data from a given run, burn a CD of the \archive, \Data analysis, and \SSRL On-Site folders.*

**Checklist to be completed for each data set**

- 4 Completed logging data collection in FILENAME.doc (in \logforms subfolder)
  - 5 Completion date entered in XAS\_Data\_Index\_Proteins.xls runlist worksheet
  - 5 Raw data ftp'd to \raw\*\* subfolder
  - 5 Data Transferred checkbox checked in data log form
  - 5 Data log form printed and placed in Master XAS Notebook
  - 9 Raw data files COPIED to appropriate \Refinements subfolder
  - 9 Data reduced in \Refinements subfolder
  - 10 .AVE and .FRM files COPIED to appropriate \aveandfrm subfolder
  - 10 Data reduction details recorded in FILENAME.doc (in \logforms subfolder)
  - 10 Avg File and NB Page entered in XAS\_Data\_Index\_Proteins.xls runlist worksheet
  - 11 .AVE file COPIED to appropriate \archive\XfDATA subfolder
  - 11 Directory entered in XAS\_Data\_Index\_Proteins.xls runlist worksheet
-