

Importing Varian 2D data into XEasy

[cg fry and c cairo: 9 Feb 99]

I. Make directory for XEasy data

```
cd /starbase/cairo
mkdir xeasy
cd xeasy
mkdir data
```

II. Transform a 2D set in VNMR

XEasy will only import data which has been transformed already. You must go into VNMR, transform and phase your spectrum. When finished, simply exit *without* transforming a slice. NOTE: This will leave a large file in your account, you should remember to return to vnmr and remove this data, the easiest method being transformation of the first slice (*i.e.*: wft(1), exit)

III. Move Data to XEasy

```
cd /starbase/cairo/xeasy/data
cp -r /starbase/cairo/vnmrsys/exp1 .
```

IV. Convert Data

```
var2x
Enter the location of your data >      ./exp1
Enter name of file for output >      spectrum1
Enter scaling factor >      2
Enter parameter for spec freq>      <CR>
Do you agree with these parameters?>      y
Macro will take a few moments to complete the transformation.
Creates files named: spectrum1.3D.16
and                  spectrum1.par
```

V. Execute XEasy

```
xeasy
Load spectrum with ns, or right click for a menu.
Your converted file should be in the ../xeasy/data directory
Load the file with the .16 extension
```

VI. Furthur Reading:

The workstations have a copy of the HTML Manual in:

/zhadum/xeasy/xeasy/html_manual/index.html

Also see:

<http://www.mol.biol.ethz.ch/software/xeasy>
for updates and current information.

XEasy Installation Notes:

I Install GZip/GunZip

```
login as vnmr1
cd /vnmr/bin
extract bin gzip.tar.Z /vnmr
rehash
Usage: gzip -h    for help
gunzip filename
```

II Retrieve XEasy files from server

```
ftp ftp.mol.biol.ethz.ch
name: anonymous
password: email@chem.wisc.edu
cd pub/software/xeasy_spscan
lcd /zhadum/xeasy
bin
get xeasy.tar.gz.crypt
get xeasy.sun5a.gz.crypt
bye
```

III Decrypt and extract files

```
cd /zhadum/xeasy
crypt rwg3sv7 < xeasy.sun5a.gz.crypt > xeasy.sun5a.gz
crypt rwg3sv7 < xeasy.tar.gz.crypt > xeasy.tar.gz
gunzip xeasy.tar.gz
gunzip xeasy.sun5a.gz
tar xvf xeasy.tar
tar xvf xeasy.sun5a
```

IV Install XEasy

```
cd /zhadum/xeasy/xeasy
./configure sun new
cd /zhadum/xeasy
chmod 777 xeasy.sun5a
execute as: ./xeasy.sun5a
```

V Modifications to (to each user's) .cshrc files

```
#Xeasy additions
#Tell XEasy where your data is located
setenv XEASY_GROUP /starbase/cairo/vnmrsys
#Tell XEasy where the library file is (for biopolymers)
setenv XEASY_LIB /zhadum/xeasy/xeasy/src.new/ecepp.lib
#Add aliases for executables, -l forces xeasy to retain last spec in memory
alias xeasy '/zhadum/xeasy/./xeasy.sun5a -l'
alias var2x '/zhadum/xeasy/xeasy/external/varian_xeasy/./varian_xeasy2d'
```