Transfer and Installation of NUTS 1D Software, v. 20080731

Availability

The Chemistry Department has a site license for NUTS 1D (full version). The program is available to all Chemistry Department members and CIC NMR Facility users on a no-cost basis for use on their PCs at work and/or at home. Student, staff and faculty members should delete any copies upon leaving the University.

The facility has three licenses for the NUTS 2D Pro software. These copies are installed on all computers in room 2224, and are not available for distribution.

Obtaining Copies of NUTS 1D

All the needed NUTS files are available on the facility's NMR ftp server, apollo.chem.wisc.edu. The username and password needed to access this server outside the facility are posted at room 2224. Go to \\ac300\DataArchives \NUTS transfer station on the server to obtain all the needed files. Required files include:

- i) the license file for NUTS 1D, license.nmr,
- ii) a file, **sam.dll**, which is required to read the license file,
- iii) a text file, nuts.ini, which sets defaults upon starting the program, and
- iv) the zipped nuts95.exe.

The license + sam.dll files will enable the full features of the 1D version of the software; see the instructions below. The **nuts.ini** file will configure the program similarly to the PCs within the facility. The most recent version of the NUTS 1D program for PC or Mac can be downloaded from the Acorn NMR website at http://www.acornnmr.com/customers.htm. Make certain you download the version for registered users, and not the shareware/demonstration version on the Acorn website.

NUTS 2D cannot be run except at the PCs within the facility.

Installation Instructions for Win98/WinNT/Win2000/WinXP PCs

- 1. Place the downloaded copy of NUTS (win_nuts.exe, for version 20080731) into any directory.
- 2. A password is required to run the self-extracting executable file, **win_nuts.exe**. Specify the directory into which NUTS should be installed. (This will not create an icon or an entry from the Start button.)
- 3. Follow the prompts for installing NUTS. Note in particular the path for the NUTS installation (the default is C:\NUTS).
- 4. Copy the **nuts.ini**, **sam.dll** and **license.nmr** files from the Transfer station folder into the NUTS installation directory (e.g., C:\NUTS).
 - Note: these files must be copied into the NUTS directory after installing NUTS.
- 5. Edit the **nuts.ini** file as needed; the parameters DATADIR and IMPORTDIR <u>must be</u> changed to correctly specify data locations for your PC. Mac users see CALCTYPE.

Note: the parameter INSERT_PRINTER_FUDGE = 1.0084 has been checked for our HP Laserjet printers to give accurate plotting of insets with fixed Hz/cm scaling. Other printers and/or the Mac version may need a different fudge factor to give accurate inset plot expansions; users should verify the correct factor for their own use.

- 6. Do not give the **license.nmr** file or the passwords to non-facility users, or use them after you leave UW Chemistry. To do so is a violation of our site license agreement.
- 7. Users should bring questions, suggestions, and bug reports about NUTS to Facility personnel, rather than directly to Acorn NMR. The site license provides support primarily through one contact person, who is currently Charlie Fry for our Facility.

Accessing NMR Data Within the Chemistry Department

Data on ftp:\\apollo.chem.wisc.edu can be accessed using any ftp program. The user willl need to download the required data on your local computer. Internet Explorer provides ftp functionality; simply type in the apollo address. FireFTP, an add-on, works well within Firefox. We have use many other programs, including WS_FTP and FireZilla, that all work fine.