

PINMRF

Varian Inova NMR Spectrometers - How to Export VNMR Data to an ASCII File

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Overview

These notes cover the steps involved in exporting a Varian NMR dataset as an ASCII file that can be downloaded and imported into MS Excel or other plotting programs for better presentation of spectra. These notes are designed to be used in conjunction with the PINMRF Varian 1D Training and Secure File Transfer Guides.

Exporting Data Using writexy

1. After acquiring your NMR data, complete processing, ensuring proper phasing and chemical shift referencing. It is recommended that you save your data.
2. Type writexy in the command line. The 'group' window will indicate that a file called 'xytrace.1' has been saved. This file is saved in the experiment directory corresponding to the experiment number in which you acquired your data. If you acquired the NMR data in experiment 1, your ascii data will be located in /mnt/d2/*userid*/vnmrsys/exp1/xytrace.1, where *userid* is your NMR login.
3. Follow the Secure File Transfer instructions to download this file to your PC.
4. To open the file in Excel, open Excel first and choose File > Open from the menu. Make sure you are viewing 'all documents'. Choose the xytrace.1 file you downloaded and go through the import procedure for a delimited file.
5. Data should now be in a 2-column format, with frequency (in Hz) in the first column and arbitrary intensity in the second column. Frequency can be transformed to the ppm scale by inserting another column and dividing the frequency values by 1 part-per-million of the spectrometer frequency. E.g., if you acquired proton data at 300MHz, then divide the frequency by 300Hz. NOTE: to be strictly accurate the division should use the exact sfrq (spectrometer frequency) value for the nucleus as given in the spectrum's parameter listing.