Using the *Net12NMR* *ConsoleServer*

# Introduction

A NetNMR Server is a class of TCP/IP NMR data servers that respond to clients requesting NMR data. Custom NetNMR Servers have been developed for both Bruker and Agilent/Varian systems running on a variety of operating system. The role of the NetNMR Server is to provide listing services so that clients can browse the spectrometer for file and then, once the client has requested a specific file, the server then translates that NMR dataset to a common format and sends it to the client.

The *ConsoleServer* is a small, yet powerful type of personal NetNMR Server that can deliver both one- and two-dimensional data to a Net12NMR client (*Net12NMR*, *NetPlot* or *NetComPlot*). This data can be in either Bruker or Agilent (*nee* Varian) data format. While a NetNMR Server installed on NMR instruments is specifically designed to server data from only the specific vendor, the *ConsoleServer* can serve both Bruker and Agilent formatted data. Also, While the NMR instrument-based NetNMR Server runs as a service and is running constantly in the background, waiting for client connections, the *ConsoleServer* runs as a simple application and can be launched and shutdown whenever needed. It is intended to be a “personal” NetNMRServer, serving NMR files within the immediate domain of the local PC. That is, the data is on the PC or a share drive accessible from the PC.

While *Net12NMR* can open both Bruker and Agilent 1D data sets directly, *NetPlot* and *NetComPlot* cannot open any native data sets. To open and use new data, *NetPlot* and *NetComPlot* **must** connect to a NetNMR Server in order to open those datasets. Under most circumstances, clients will connect directly to a spectrometer with an installed NetNMR Server, but this is not always possible. Maybe the spectrometer doesn’t have an installed NetNMR Server, or maybe the spectrometer not connected to the network. In some cases NMR data is collected on a user’s share drive while the user is operating the instrument. Once the user logs off the instrument the user’s share drive will be disconnected and the NetNMR Server on the instrument will no longer have access to the user’s data. Finally, a remote collaborator may provide native NMR data that has to be evaluated. If there’s not an appropriate software package to do the evaluation, the *ConsoleServer* can be used to serve this data to a client application (one of the Net12NMR Application Suite programs).

# Requirements

*ConsoleServer* is written in Microsoft C# (C-Sharp) Visual Studio 2010 and so it has one requirement: The Microsoft .NET Framework version 4. Most modern PC systems will already have this installed. The presence of a “C:\Windows\Microsoft.NET\Framework\v4.0.<something>” directory indicates that the PC has a working version of the .NET Framework 4. If this directory is not present, using most any Web search engine can find the .Net Framework installer by searching for “Microsoft .NET Framework 4”. The current location of the Microsoft .NET Framework 4 installation program is:

<http://www.microsoft.com/en-us/download/details.aspx?id=17851>

# Installation and Configuration

*ConsoleServer* is installed as part of the Net12NMR Application Suite. If you can’t find it in the “GE Research” folder of the Windows Start button, the Application Suite must be reinstalled. Once launched, *ConsoleServer* runs in a simple “DOS box”-like console window. There are no graphical elements to ConsoleServer and there are no controls. To stop *ConsoleServer*, click the “X” in the upper right corner of the console frame. Once running, the *ConsoleServer* will report connection information from Net12NMR clients and the internal NetNMRServer commands those clients are executing. The only thing to configure is the “home” directory. The *ConsoleServer* home directory is where the Net12NMR client will open upon initial connection. The default value installed with *ConsoleServer* is your Documents folder. You must have authorized access to this directory, otherwise ConsoleServer will fail.

If the Bruker and/or Agilent files on your PC are in a different location, you can change the *ConsoleServer* “home” directory with the “Connection Manager” program found in the Net12NMR Application Suite. Launch this program and select “My Personal Server” in the drop-down list and then click the “Edit” button to bring up a dialog to change the home directory. Note: *ConsoleServer* does not support password authentication, so **do not set a password**!

Please note that once a valid Bruker or Agilent NMR dataset is found, that branch of the file system will not be searched for any additional directories or NMR data. (Don’t nest data inside other valid data.)

Once *ConsoleServer* is running, *Net12NMR*, *NetPlot* and *NetComPlot* will show a “My Personal Server” in the server list. Choosing that server, you should immediately be shown the contents of the configured “home” directory.

# Implementation Details (with special comments for Agilent data)

Both Bruker and Varian NMR datasets are complex, multiple file assemblages with sometimes deep layers of subdirectories. All the varieties of the NetNMR Servers understand these structures and make sure that the minimum subset of data is present before presenting those NMR datasets to the client:

1. Bruker files will begin with a directory with any name.
   1. There will be an integer-named <expno> subdirectory containing the untransformed FID data along with spectrum parameter and other files.
      1. “acqus” and “fid” files for 1D datasets.
      2. “acqus”, “acqus2” and “ser” files for 2D data.
   2. Processed data will be in a pdata\<procno> subdirectory. <procno> will also look like a positive integer.
      1. “procs”, “1r” and “1i” files are for 1D datasets.
      2. “procs”, “1rr” and “1ii” are for 2D data.
   3. Arrayed 1D data (like relaxation experiments, i.e., DOSY, T1, T2) will look just like 2D data and there will be additional files in the <expno> directory that contains a list of values for each of the arrayed data sets. The names of the additional files are highly variable and depend on the version of Bruker software that created them as well as the NMR parameter that was varied for the arrayed experiment.
   4. Additional optional files include:
      1. <expno>\format.temp is used to figure out which pulse program parameters were actually needed for the data collection.
      2. <expno>\sample\_info.prop will be used to fine a “sample” and “comment” for the data file. Additional variables searched for and used (at GEGR) are “user”, “workorder”, “project”, “submitted” and “dataclass”.
2. Agilent (Varian) files will begin with a directory name that will always have a “.fid” filename extension at the very end of the directory name.
   1. This \*.fid directory will contain a “procpar” and “fid” file that can be either a 1D or 2D FID dataset. Information in the procpar file and the fid file can be used to determine if the file is 1D or 2D, or an arrayed dataset.
   2. The \*.fid directory will contain a subdirectory called “datdir” containing “data” or “phasefile” that will contain the processed files. (Ordinarily, Agilent doesn’t ever save processed data. NetNMRServers for Agilent spectrometers come with an additional VNMRJ macro command, “svfs”, used to save the processed data along with the fid data.)
   3. Arrayed 1D data cannot be distinguished from 1D or 2D data without examining the procpar and the fid file. The list associated with the array is contained in the procpar file.
   4. There is only one optional file, \*.fid\text. The first line of the text file becomes the “sample” variable and the second line of this file becomes the “comment” variable. Subsequent lines become additional variable as in 1.d.ii.

Based on commands from the client, any NetNMR Server only shows files that a particular client can open and use. For example, 2D files are not presented to Net12NMR and untransformed file are not offered to NetComPlot. This is an outstanding and highly useful feature of any NetNMR Server, but it comes at a cost. The NetNMRServer must examine each suspected NMR dataset (and open files therein). Because of this, it is wise to not let a directory get “too full” of NMR data. You will know a directory too full when it takes a long time to expand and show it.

As explained earlier, Agilent’s VNMRJ software doesn’t ever store processed data. The only place processed data usually exists in in the “exp<n>” experiments. In order to save the processed data, you have to use the custom macro, “svfs”, supplied with the Agilent/Varian versions of the NetNMRServer software. This macro will fetch the “exp<n> processed data along with the FID data.

For 2D datasets, NetNMR Servers will only serve “simple” 2D processed files. Hypercomplex files are not supported. Also, here’s a tip to save some disk space on your Agilent spectrometer: Avoid using “svfs” on files where “Trace Axis: F2” is selected on the display panel. If you do, the resulting \*.fid/datdir/phasefile file will become twice as large as one where “TraceAxis:F1” (the default) is not changed. When you transpose the data by selecting “F2”, the transformed data is appended to the end of the ”phasefile” file. If you select “F2” before any processing and then process the data and save with “svfs”, the “phasefile” file will still be twice as large as it needs to be, but the first half of the “data” file will be filled with zeros! If you want to look at the data with the F2 as the trace axis, that’s okay, just set the trace back to F1 and reprocess the data.

Agilent/Varian uses a fixed frequency, variable field lock while Bruker uses a fixed field, variable frequency lock. This difference means that for Agilent data, nuclear chemical shift offsets are calculated from the lock frequency and the lock frequency depends on the lock solvent. All NetNMR Servers for Agilent/Varian spectrometers use the same calculating algorithm in order to calculate the nuclear window offset.

Basically, the fixed lock frequency is adjusted by the PPM offset of the lock solvent to in order to calculate the exact frequency of 2H deuteron with a zero PPM chemical shift. Zero PPM for any other nuclei is then calculated from a table of nuclear frequencies. The offset of any channel can then be calculated by comparing the actual channel frequency to the calculated zero PPM frequency.

NetNMR Servers do this, just like VNMRJ does, with two external files. NetNMR Servers on the spectrometer uses the exact same files as VNMRJ does. The *ConsoleServer* doesn’t have access to the spectrometer, so it has its own versions. The first file, Solvents.txt, lists solvent names with the PPM chemical shift of the locked resonance. The second file, nuctabref.txt lists the nuclei with their exact frequency of a zero ppm standard for that nucleus. While the file on the spectrometer scales these frequencies to a 100.000000 MHz proton frequency, *ConsoleServer* scales these nuclear values to a deuterium frequency of 1.000000 MHz.

Remember that if you add or modify a solvent to your Varian/Agilent spectrometer “solvents” file, you need to also or modify your *ConsoleServer* solvents.txt file. Likewise if you change the frequency of an entry in the nuctabref file on your Agilent or Varian spectrometer, you need to get out your calculator and also change the nuctabref.txt file. These two files are in the folder where you installed the Net12NMR software, usually C:\Program Files (x86)\Net12NMR Suite\Net12NMR.

Please note that *Net12NMR* can open 1D files from Bruker or Agilent that are accessible from a local or shared drive without the help of any NetNMRServer, and also uses Solvents.txt and nuctabref.txt to calculate offsets.