Maximizing NMR Productivity by Using Batch Submissions with the VnmrJ 3.1A Software

Technical Overview

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The utility of NMR systems is often measured by such things as console specifications, performance numbers, and probe geometries. While these are important system attributes, there are many subjective measures of system performance that are equally important to overall system utility. For example, there are instances when simultaneous submission of multiple samples to the NMR spectrometer queue is required to meet a laboratory's needs. The ease and flexibility with which such tasks can be accomplished has a significant impact on the productivity and utility of the overall NMR operation. The VnmrJ 3.1 software provides all the tools necessary to easily and efficiently support the workflows NMR users need, including batch submission of samples to be run in an unattended fashion. This technical overview describes three VnmrJ 3.1 tools that simplify and accelerate the batch submission workflow.

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On-the-fly Batch Submission Using the Tray Display

The simplest batch submission example is a user's need to analyze several related samples, such as a series of column fractions or aliquots from a series of parallel synthetic chemistry reactions. In this situation the VnmrJ 3.1 user interface provides a quick and intuitive method for batch submission. After populating the Study Queue with the desired experiments and filling in the required sample information, the user need only select multiple tray locations prior to clicking **Submit**. The system automatically adds an index number to the sample directories it creates, generating a list of directories rather than overwriting a previous data set (i.e., MySample_01, MySample_02, MySample_03, etc.).

To submit sample locations sequentially, the location in the tray display that corresponds to the first sample to be run is selected, and then the **Shift** key is held down while selecting the last location in the series. All intervening locations are automatically highlighted, and the system submits them all to acquisition in ascending order (See Figure 1).

Sample locations can be selected at random by simply holding the **Control** key down while clicking on various locations in the tray display. Each location is highlighted as it is selected, and the system submits them all to acquisition in the order in which they were selected (Figure 2).

One of the best ways to exploit the power of batch submission is to combine multiple sample submissions with a customized NMR method, called a Study Clone. For example, a user might have 60 samples of neat apple juice from a metabolomics investigation, and NMR data is needed on each sample. Submitting these samples using the standard protocols would provide useful data by optimizing the frequency offsets and solvent suppression parameters for every sample, but a more homogenous dataset would be returned if each sample was collected using identical experimental conditions. Accomplishing this result is straightforward using the VnmrJ 3.1 software. Sample 1 is submitted, and the system is allowed to optimize parameters for the desired experiments on this sample. Once the data set for Sample 1 is complete, two mouse clicks convert those results into a Study Clone (see the VnmrJ 3 Automation User Guide, Chapter 3, Pub. No. 91001987), which can then be used to submit samples #2 through #60 to acquisition with parameters identical to those determined for Sample 1.

Quick and easy setup of batch submissions

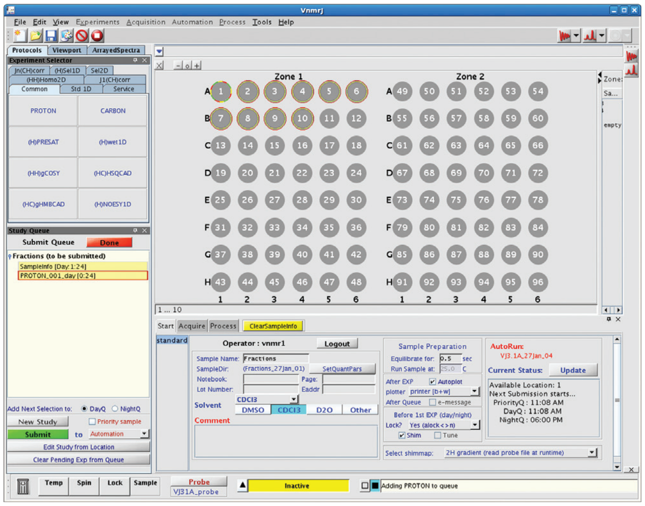


Figure 1. Tray display showing multiple, sequential locations selected for submission.

Samples can be assigned to random locations

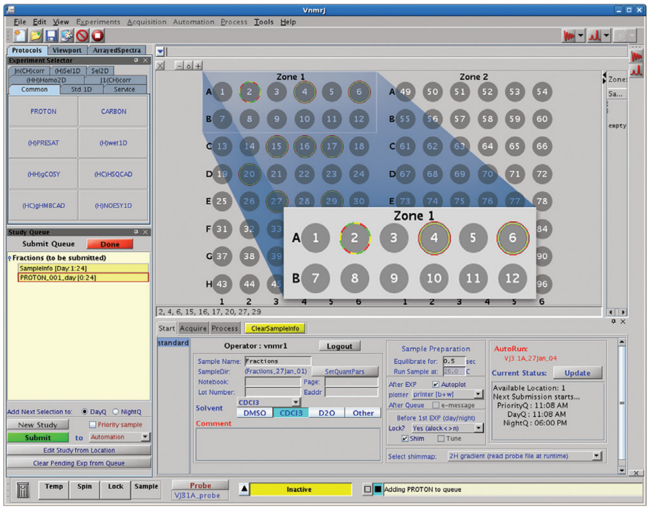


Figure 2. Tray display showing multiple, random locations selected for submission.

Batch Submission Using a Spreadsheet

When a research investigation involves a significant number of NMR samples, such as a metabolomics study or a sample library verification project, the scale of the project requires a completely automated method for transferring sample information and experimental parameters to the spectrometer. The VnmrJ 3.1 software offers a simple and flexible tool that imports sample information from a comma separated values spreadsheet (CSV), allowing single-point automated sample submission for as many samples as the user desires.

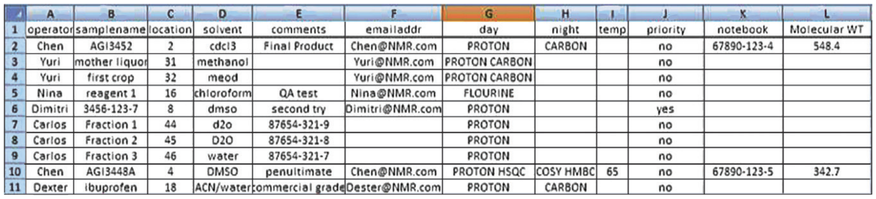
The utility that interprets the spreadsheets is very flexible and can accept a wide variety of inputs. If information that is not related to the NMR study is present in a spreadsheet, that information is ignored when submitted to the NMR. Thus any existing spreadsheet containing the desired sample information can be used so long as the first row in the spreadsheet contains the variable names to be populated in VnmrJ (Figure 3).

Investigators often want to collect data on a large number of samples using identical acquisition parameters for all the samples, but with a unique sample name for each. The workflow to accomplish this task would simply be:

1. Using the standard interface tools, set up a new Study in the Study Queue with the experiment list and instrument parameters as desired.
2. Submit to acquisition a one-column spreadsheet containing only the list of sample names.

The system then automatically creates the automation queue by integrating the requested experiments with the sample names supplied in the spreadsheet.

Spreadsheets automate large sample set submissions



	A	B	C	D	E	F	G	H	I	J	K	L
1	operator	samplename	location	solvent	comments	emailaddr	day	night	temp	priority	notebook	Molecular WT
2	Chen	AGI3452	2	cdcl3	Final Product	Chen@NMR.com	PROTON	CARBON		no	67890-123-4	548.4
3	Yuri	mother liquor	31	methanol		Yuri@NMR.com	PROTON CARBON			no		
4	Yuri	first crop	32	meod		Yuri@NMR.com	PROTON CARBON			no		
5	Nina	reagent 1	16	chloroform	QA test	Nina@NMR.com	FLOURINE			no		
6	Dimitri	3456-123-7	8	dmso	second try	Dimitri@NMR.com	PROTON			yes		
7	Carlos	Fraction 1	44	d2o	87654-321-9		PROTON			no		
8	Carlos	Fraction 2	45	D2O	87654-321-8		PROTON			no		
9	Carlos	Fraction 3	46	water	87654-321-7		PROTON			no		
10	Chen	AGI3448A	4	DMSO	penultimate	Chen@NMR.com	PROTON HSQC	COSY HMBC	65	no	67890-123-5	342.7
11	Dexter	ibuprofen	18	ACN/water	commercial grade	Dester@NMR.com	PROTON	CARBON		no		

Figure 3. An example of a spreadsheet that might be used for batch submissions. Note that this utility allows control of a wide variety of parameters and can flexibly interpret various header fields.

While this example exploits the simplest spreadsheet possible, the system is capable of handling as much detailed information as desired for each sample. For instance, a spreadsheet submission could specify not just different sample names, but also different solvents, sample temperatures, e-mail addresses, comments, an individualized list of experiments to be acquired (separated into Day and Night Queues, as desired), and variables to control the path for saving and archiving the final data, all for each sample (Figure 3).

Sometimes the user might not have control over the header information in a spreadsheet, such as spreadsheets created by a corporate LIMS system, or spreadsheets supplied by an outside vendor or customer. The VnmrJ 3.1 software provides the capability to use a simple text file as a synonym list to translate headers from the input template into VnmrJ 3.1 parameter values. For instance, the term "Investigator" supplied by the spreadsheet could be interpreted as "Researcher" and "Sample ID" could be converted to "samplename," all automatically, and all locally customizable with a simple, human-readable synonym table (Figure 4).

A spreadsheet batch submission can handle anything from a simple proton spectrum to the most complex study clone in any manner or combination. Batch submissions do not prevent the use of other NMR submission tools, as all submissions are treated identically by the queuing mechanism. This allows batch and manual walk-up operations to be carried out on a single NMR system in any order and in any combination

Spreadsheet submissions can be initiated using several methods. Most commonly, the csv file is simply submitted to automation using the command line. Alternatively, the submission can be scheduled at a specified time and date using the atcmd utility.

Example of a Synonyms File

```
PARAM_sample#        location
PARAM_sample         location
PARAM_location#      location
PARAM_loc            location
PARAM_traylocation   location

SOLV_meoh            cd3od
SOLV_meod            cd3od
SOLV_methanol-d4     cd3od
SOLV_methanol        cd3od
SOLV_50:50acn/water  d2o
SOLV_1nnaoh          d2o

EXP_H1               PROTON
EXP_1H               PROTON
EXP_Proton           PROTON
```

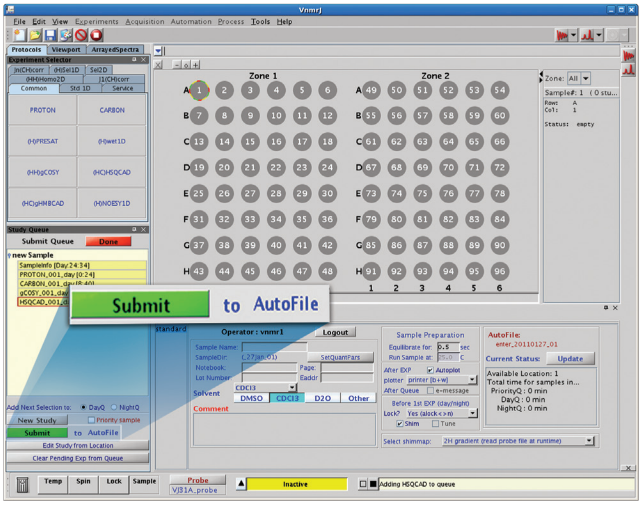
Figure 4. A section of the /vnmr/adm/walkupadm/csv2cpQ_synonyms file. The first column holds the list of synonyms, grouped by parameter type. These entries represent the various ways that a user might express parameters such as sample location, solvent, experiment type, user name, sample ID, etc. The second column is the VnmrJ3.1 parameter or value that will be used as the aliased value for the term in the first column. This file can be edited by the System Administrator to reflect the local needs of a specific installation.

Off-line Batch Submission

There are occasions when the ability to submit samples to a queue for acquisition at a later time or another place can prove valuable. For example, an undergraduate organic chemistry laboratory may have a spectrometer that is physically remote from the teaching laboratory itself. In this situation, the VnmrJ 3.1 software provides a useful tool that allows an automation queue to be constructed off-line at a remote workstation, and then transferred at a later time to the spectrometer for submission to acquisition. Once completed, the data can be emailed to the students automatically, stored on a server, or even uploaded to an outside service such as Google Groups where students can access their results.

The workflow students would use to build the off-line batch file is identical to that used to operate the spectrometer itself, eliminating the need for user training with two different interfaces (Figure 5). Moreover, in such a teaching environment, the off-line workstation can be used as a tool to train the students to operate the spectrometer interface without the need to tie up the spectrometer itself.

Off-line Batch Submissions are ideal for academic and industrial applications



SampleInfo [Day:24:34]
PROTON_001_day [0:24]
CARBON_001_day [8:40]
gCOSY_001_day
HSQCAD_001_d

Sample#: 1 (0 stu...
Row: A
Col: 1
Status: empty

standard
Operator : vnmr1
Sample Name:
SampleDir: (_27jan_01)
Notebook:
Page:
Lot Number:
Eaddr
Solvent: CDCl3

Equilibrate for: 0.5 sec
Run Sample at: 25.0 C
After EXP ☑ Autoplot
plotter printer (b+w)
After Queue ☐ e-message
Before 1st EXP (day/night)
Lock? Yes (alock<>n)
☑ Shim ☐ Tune
Select shimmap: 2H gradient (read probe file at runtime)

AutoFile:
enter_20110127_01
Current Status:
Available Location: 1
Total time for samples in...
PriorityQ : 0 min
DayQ : 0 min
NightQ : 0 min

VJ31A_probe
Inactive
Adding HSQCAD to queue

Figure 5. Tray display showing the off-line interface for batch sample submission, using the Submit to Autofile function.

Conclusions

Batch submissions provide a powerful workflow for many applications. The VnmrJ 3.1 software provides multiple ways to easily enter batch submissions to meet the varied needs of NMR users. For quick, on-the-fly submissions, the interface supports the selection of multiple sample locations, either sequentially or randomly, for submitting samples directly to the automation queue. A unique spreadsheet utility enables easy, automated submission of large batches of samples for extensive studies such as metabolomics. This tool can be used to satisfy a broad range of submission needs, from addition of individual sample information to an existing queue to controlling nearly any aspect of a complex sample set. Finally, the ability to create an automation queue for later submission to the spectrometer opens up a whole range of possible uses in many academic and industrial settings. In all of these cases the standard algorithm that automatically stores the data can be used to write the completed studies to any available network location and/or email the results electronically. The ease and flexibility with which batch submission can be accomplished using the VnmrJ 3.1 software have a significant impact on the productivity and utility of the overall NMR operation.

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