






One-Minute NMR Quick Start Guide

August 11, 2010

The One-Minute NMR system from Protasis Corporation connects NMR spectrometers to the LEAP/CTC liquid handler with custom solvent conditioning and pumping systems using the MRM CapNMR probe for detection. The system is a high-throughput open-access Web-based control application running on the MS-Windows platform and is accessible through the web from many platforms.



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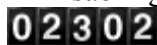
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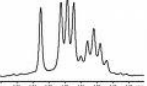
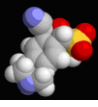







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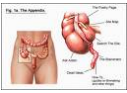
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Understanding One-Minute NMR

Overall System Design

The system uses TCP connections for communication to the spectrometer, RS232 connections to the CTC/LEAP liquid handler and HTSL pump, and fluidic connections between the HTSL, LEAP, and CapNMR probe.

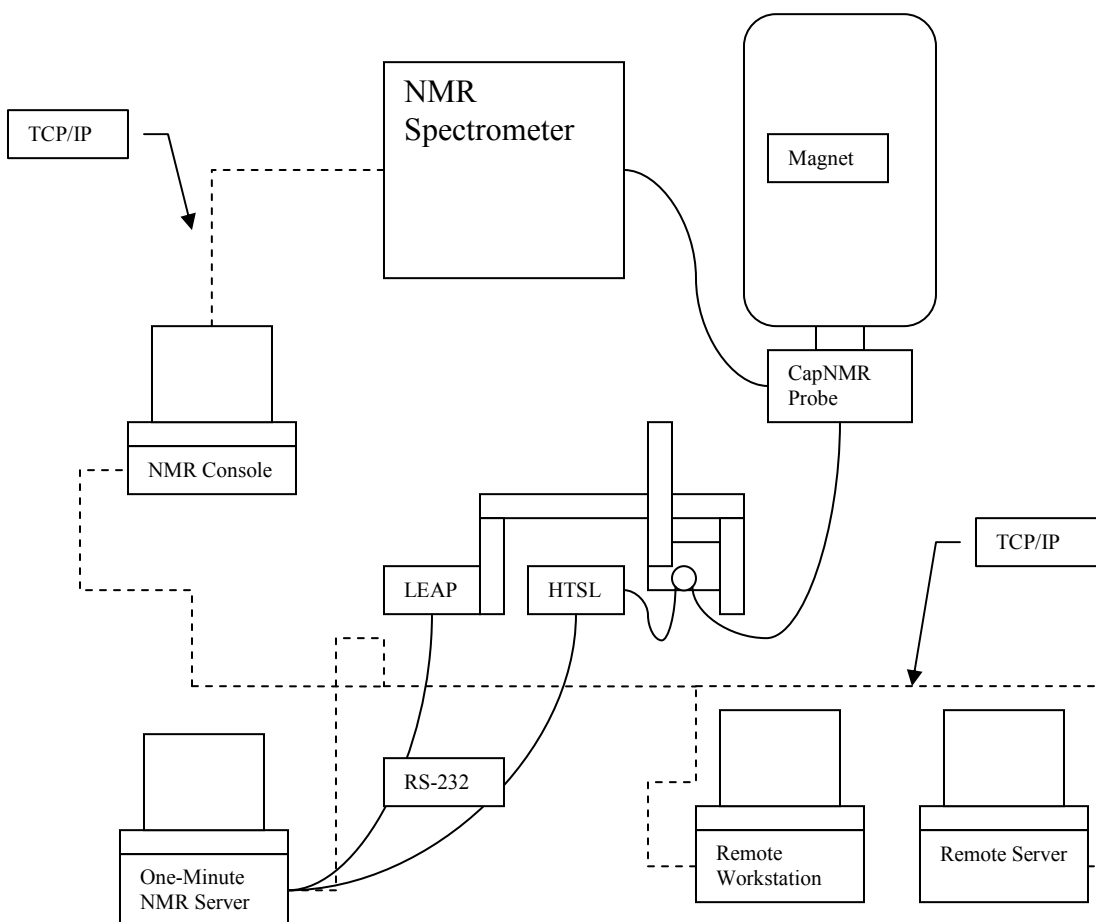


Figure – One-Minute NMR schematic

Software Architecture

The One-Minute NMR software consists of four pieces:

1. The **Web Application** is the primary user interface. It communicates with a database and the RunProcess.
2. The **RunProcess** communicates with the HTSL pump and CTC/LEAP liquid handler through RS232 Connections and to the NMR spectrometer computer using a TCP socket connection or direct file interface.

3. The TCL **Listener** listens for commands sent to the NMR spectrometer console computer from the RunProcess.
4. The Listener invokes **NMR Scripts** in the Magical or AU scripting languages to control the NMR.

Installation

The One-Minute NMR Software comes pre-installed on a PC. For Windows-based spectrometers it is possible to install the One-Minute NMR software on the NMR console computer. Detailed installation information is available in the [One-Minute NMR Installation Guide](#).



Starting One-Minute NMR

1. Turn on the LEAP and HTSL(s)

Turn the switch to ON. Make sure the RS232 cables are still connected. Wait until the lights stop blinking on the HTSL before running samples.

2. Start The Listener

Varian

Open a new UNIX shell window.

Change the current directory to /vnmr/tcl, type `cd /vnmr/tcl [ENTER]`

Start the listener: type `listener.tcl [ENTER]`

You should see a message indicating that it is OK.

Use Of Foreground VNMR or VNMRJ

If The Brain parameter `NMR.Varian.Foreground` is set to True all VNMR commands are sent using “send2Vnmr \$vnmruser/.talk autorun...”. The `$vnmruser/.talk` argument can be set as the brain parameter

`NMR.Varian.TalkFile`, its default is `$vnmruser/.talk`. **Before foreground VNMR can be used the *listenon* macro must be typed on the VNMR command line.**

Listenon creates the `$vnmruser/.talk` file.

Bruker.Windows

Start the Bruker listener: From the XWIN-NMR command line type `wait4cmd [ENTER]`.

Bruker.Linux

Open a new Linux shell window.

Change the current directory to your installation location, typically `/home/mrm` type `cd /home/mrm [ENTER]`

Start the listener: type `./listener.tcl [ENTER]`

You should see a message indicating that it is OK.

2. Start the RunProcess

The RunProcess must be started on the PC that is connected to the LEAP and HTSL (CONTROLLER). The One-Minute NMR software is in a folder on the desktop named *One-Minute NMR*. Open this folder and double-click on *Start-First RunProcess*.

The RunProcess will perform a system check and report any errors in its main window. The liquid handler will re-home to indicate it is connected. If the RunProcess appears to hang it is probably having trouble communicating with the NMR computer. It will report an error after a timeout period. One-Minute NMR Versions 1.1.3 and above report *Ready* in the status bar and *System Check Complete* in the main window. Errors are reported in the main window.

The Listener on UNIX systems will report “Connected” when the RunProcess is started.

All errors must be cleared before the system can be operated.

3. Open the Web Page

The One-Minute NMR Web site is located on the computer that is connected to the LEAP and HTSL (CONTROLLER). This computer is configured to have the One-Minute NMR web page come up as the default in MS Internet Explorer.

The link will be:

<http://localhost/OneMinuteNMR/main.aspx?RunEnable=true>

If you do not want the CONTROLLER computer to be able to start runs, you should use the following link:

<http://localhost/OneMinuteNMR/main.aspx>

On Remote Computers you need to know the machine name, DNS name, or IP address of the CONTROLLER. This is set up during on-site installation. The computer name is useful for MS Windows-based networks, while the DNS name or IP address is used for UNIX-based networks. The computer name can be discovered or changed by from *Start Menu/Control Panel/System* on the *Computer Name* tab. The DNS name can be obtained from your system administrator. The IP address can be obtained by typing *ipconfig* on the command line. Remote connection links will look like this:

<http://ComputerNameOrDNS/OneMinuteNMR/main.aspx>

or

<http://10.0.0.10/OneMinuteNMR/main.aspx>

or

<http://ComputerNameOrDNS/OneMinuteNMR/main.aspx?RunEnable=true>

if you want to run the system from the remote computer. This is especially handy for the NMR console computer.



One-Minute NMR Operation

The main user interface for the program is the One-Minute NMR Web site. The Web site consists of five pages. The main page is divided into four numbered sections.

Main Page

The Main Page is used for all system operation and is accessible to all users and non-users. Features of this page may be inactivated depending on whom, if anyone, is logged in.

1. Log In

Select your Account from the list. This list will have been set up by your system administrator.

Select your Username from the list. It will have been set up by your system administrator.

Enter your password. Hit **[ENTER]** or click the **Log In** button.

Plate	Location	Inj.	Status	Name	Scans	Submit Time	Start Time	End Time	Account	User	SMILES	Title	Ret.To	Results
Edit Delete	MT1-Fmt	A10	1	finished_A10	16	12/27/2007 1:06:16 PM	2/22/2008 4:35:04 PM	2/22/2008 4:37:02 PM	Protasis	Bob Albrecht		Self	c:\ACD\VerificationTestData_A10\autoqc.fid	
Edit Delete	MT1-Fmt	A11	1	finished_A11	16	12/27/2007 1:06:16 PM	2/22/2008 4:48:55 PM	2/22/2008 4:50:53 PM	Protasis	Bob Albrecht		Self	c:\ACD\VerificationTestData_A11\autoqc.fid	

Figure – The Main Web Page

2. Sample Information and Experiment(s)

The defaults can be accepted for all fields here, but it is best to choose a sample name and enter a title for your sample.

Name: This, along with the extension (after the _) is used to form the name of the file that your NMR data are stored in. The data are stored in your NMR data directory as set up by your system administrator.

Title: This title is stored along with your NMR data. It will appear on printouts and can be as long as you wish.

Number of Injections: The number of injections for each sample.

Solvent: Choose the solvent you want to use. On Varian systems if you choose an experiment with the default as the first word in the name, the solvent is used to set up an experiment.

SMILES formula: Informational. The SMILES for the molecule you are running.

NMR Experiments: Choose one or more experiments from the list. The list will have been set up by the system administrator.

Parameters for: Allows you to change the run parameters for the selected experiments. Select an experiment from the drop-down box and enter the **Number Of Scans**, **Spectral Width**, and **Spectrum Center**. The parameters for individual experiments can be hidden from walkup users by setting The Brain variable *System.ShowExperimentSettings* to False. Settings for individual experiments must still be entered in the Available Experiments section of The Brain, but this requirement can be eliminated by commenting-out lines in the *autorun* script running on the spectrometer.

Extra Parameters is a list of parameters associated with this experiment that is used by the NMR automation script *autorun*.

On Bruker systems you can choose which **Experiment number** to use for corresponding experiments and whether to use a particular experiment or make an experiment number from the Vial plus some value.

On Varian systems you can choose which background **Experiment number** is used to run your samples.
















Run order of the experiments can be changed by clicking the [+] and [-] buttons. The order of the experiment will change in the list box above.

3. Sample Location

The location of your samples on the CTC/LEAP liquid handler can be selected with a few simple mouse clicks.

The Tray that your samples are located in is selected from the drop-down tray selector. A picture of the tray will appear for visual confirmation. The pictures will have been configured for your system during on-site installation. When a tray is selected the format of the samples on the tray appears to the right. The configuration of the trays is determined by the settings on the CTC/LEAP liquid handler.

Graphic Symbols represent the state of samples on the tray.

 no sample	 selected ¹	 pending	 waiting
 priority waiting	 night waiting	 loading	 running
 error	 finished	 not yours ²	 confirmed ³
 rejected ³	 ambiguous ³	 quality control	

¹ all samples can be selected

² samples that are not yours have a darker color

³ results of automated structure confirmation

Sample Selection

Select individual samples with the mouse, multiple samples by holding down the shift key and clicking with the mouse. Depending on your user settings you may not be able to select other users' samples. The *Select All* button allows all samples, or all samples of a specific type to be selected. This is convenient when removing multiple plates or vials from the system. Clicking Cancel will stop Select All. The System.ShowSelectAll Brain setting enables and disables the Select All button.

Returning Samples is controlled by the *Return To:* Selector

Self returns the sample to the original well.

Waste returns the sample to the waste port

TrayNN, *MT-XXX*, or *StkNN* returns the sample to another tray or plate at the same index as the sample in its tray.

Importing

The import template will be set up by your administrator. Click the *Import...* button, select the .CSV or .ZIP file you want to import, click *Import File Now* to import the file, or *Cancel Import* to abort.

Removing Samples

Cancel any pending samples. The state changes to no sample.

Remove selected samples. The state changes to no sample.

4. Submitting Samples

Sample Submission is controlled by buttons.

Run pending samples to be run. The state changes to waiting.

Priority submit pending samples. The state changes to priority waiting.

Night submit pending samples. The state changes to night waiting.

Pause and Resume

Pause Automation stops the liquid handler and pumps but does not stop the NMR.

Automation is also paused when errors occur.

Resume Automation Automaiton re-starts the liquid handler and pumps.

Run Order Rules

Night samples will not start during the day, but have the highest priority at night.

Priority samples run ahead of waiting samples.

For samples with the same waiting state, samples submitted first are run first. For samples with the same submit time trays/plates are run in alphabetical order. Samples on a tray or plate are run in the natural order of the plate or tray. Samples that are run from the same vial using multiple injections are ordered by injection number. The order that samples are run on the plate can be controlled with the supplied SQL scripts RowOrder.sql (default) and ColumnOrder.sql that are found in the c:\protasis\SQL directory.

Samples Grid

The grid at the bottom of the main page shows one of many possible views of samples and each experiment that is scheduled for that sample. The current view of the grid can be changed using the selections in the query bar on the top. You can edit or delete samples and experiments in the grid. You may not be able to edit or delete samples that do not belong to you depending on your user settings. When you edit samples you must click Update for the changes to be accepted.



Data Storage Locations

The location of NMR data storage is important for planning and installation and to located data after runs are complete. The exact location depends on the brand of NMR system you are using and the operating system, and can be changed by modifying the autorun script for your system. The default (unmodified) file locations are described here.

Varian

The *userpath* where Varian data are stored is defined by the user's NMR Data Path on the People page. The name of the FID directory is specified by the *name* and *extension* fields on the login page. For samples with a single experiment the data are stored in ***userpath/name_extension.FID***. For example:
/vnmr/data/johnsmith/sample1234_A1.FID, where /vnmr/data/johnsmith is the NMR Data Path, sample1234 is Name, and A1 is the extension, set as the Location.

For multiple experiment samples data are stored in ***userpath/name_extension/experiment.FID***. For example
/vnmr/data/johnsmith/sample1234_A1/COSY.FID, where /vnmr/data/johnsmith is the NMR Data Path, sample1234 is Name, A1 is the extension, set as the Location, and COSY is the name of the NMR experiment.

Bruker.Linux

The *disk* where user data are stored comes from either the **NMR.Disk** Brain parameter, or the user's NMR Data Path as specified in the People section. The *disk* can be located on another computer for networked systems, for example //dataserver/. A user's **NMR Data Path** will override the **NMR.Disk** Brain setting. The **NMR User Name** in the People section specifies the *userdata* directory. The dataset name is created from the *name* field on the login screen plus the *extension*. The *experiment* number is associated

with the One-Minute NMR experiment, and can be a fixed number or a vial index plus some value. Data are stored in *disk/data/userdata/nmr/name_extension/experiment*.

Bruker.Windows

The *disk* where user data are stored comes from either the **NMR.Disk** Brain parameter, or the user's NMR Data Path as specified in the People section. The *disk* can be located on mapped drive for networked locations. A user's **NMR Data Path** will override the **NMR.Disk** Brain setting. The **NMR User Name** in the People section specifies the *userdata* directory. The dataset name is created from the *name* field on the login screen plus the *extension*. The *experiment* number is associated with the One-Minute NMR experiment, and can be a fixed number or a vial index plus some value. Data are stored in *disk\data\userdata\nmr\name_extension\experiment*.

Alternative Data Locations

There is often a need to store NMR in an alternative location. This can be controlled with the autorun macro on Varian and Bruker systems. For structure confirmation purposes the alternate location must be reported back to One-Minute NMR using the *omnmr_filelocator* script.

Development Credits

Click the link at the bottom of the main page to find out who contributed to One-Minute NMR.

System Administration

There are two system administration pages; People and The Brain. People is for setting up users, accounts, and passwords. The Brain is for controlling the operation of the system.



People

The People page is available by clicking the people icon in the login section of the Main Page. Only users with the Edit User Accounts permission can access the People page.

Name	e-mail	NMR User
-> Another User		Name of this user on the NMR system
-> Bob Albrecht	b.albrecht@protasis.com	
-> Service	info@protasis.com	
< >		

Username:
 Accounts: Novartis
 Protasis
 Service
 Add Account +
 Password:
 Confirm Password:
 E-Mail:
 NMR Data Path:
 NMR Experiment Path:
 NMR User Name: Name of this user on the NMR system
 NMR Password:
 Confirm NMR Password:
 Permissions
 Edit User Accounts:
 Select Other Users' Samples:
 Change Automation Settings:
 Add User Clear Update Delete
 Home

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Figure – People Page

The People page is divided into two sections; the left side has a grid with the list of users. The right side has information specific to the selected user or a new user.

User Grid (left)

Select users by clicking on the -> at the left of the user grid. The user's information will appear on the right.

User Form (right)

Username: is the name that will appear in the drop-down box during login.

Accounts: are the list of accounts that this user belongs to. Users can have multiple accounts selected with shift-click or ctrl-click.

Add Account: is used to add accounts to the system. Enter an account name and click [+].

Password: the optional password for the user.

Confirm Password: enter the password again.

E-mail: the address of the user for error and completion alerts.

NMR Data Path: the location where the user's data are stored. One-Minute NMR will attempt to make create this directory when the user's data is updated.

NMR Experiment Path: Not used yet

NMR User Name: The username on the NMR system for this user. This may be the same for all users.

NMR Password: Optional password for NMR user.

Confirm NMR Password: Enter again.

Permissions

Edit User Accounts: Check if this user has access to People page.

Select Other Users' Samples: Check if this user can select samples of another.

Change Automation Settings: Check if this user can access the Brain page.

Buttons

Clear the information for a user.

Update the information for a user.

Delete the currently selected user.

Home go back to the main page.

Add User to add a new user.

Service User

The first user in the system is Service. The password for this user is “protasis”. The Service user has all permissions and can be used to add other users. Please **do not delete the Service user or change its password**. You may need to have a service representative access the system using this account.

Adding Users

Click *Clear*.

Fill in the fields on the User Form. Be sure to select one or more accounts.

Click *Add User*.

Updating Users

Click -> next to the user you want to update in the users grid.

Change the fields on the User Form.

Click *Update*



The Brain

The brain is used to control automation settings and solvent lists, available experiments and import settings. Only people with Change Automation Settings permission can access The Brain. The selector at the top of the page controls what information is being viewed.

General Settings

The general settings is a list with values and descriptions. The **Setting** is used internally by the software. The **Value** is the value used by the system and the **Description** is a detailed English description of the setting. Most of the settings are self-explanatory. A few of them require more treatment here.

	Setting	Value	Description
Edit	Communication.CTC.COM	COM1	The serial port for communication with the CTC/LEAP liquid handler
Edit	Communication.Email.AlertRecipients	Bob Albrecht	Comma separated list of One-Minute NMR user names to send alerts to.
Edit	Communication.Email.FromAccount	b.albrecht@protasis.com	Account used to send mail to users. Identified in the FROM of messages.
Edit	Communication.Email.FromName	One-Minute NMR 1	The name of the One-Minute NMR system that is sending e-mail messages.
Edit	Communication.Email.Host	protasis.com	The SMTP server for sending e-mail messages to users.
Edit	Communication.Email.LinkToMe	http://localhost/OneMinuteNMR/main.aspx?RunEnable=True	Link to this One-Minute NMR system added to the bottom emails.
Edit	Communication.Email.Password	methods	Password for e-mail account that sends mail when authentication is required.
Edit	Communication.Email.SendAlerts	True	True if warnings and errors should be sent by e-mail.
Edit	Communication.Email.SendFinishedNotice	True	Set to True if One-Minute NMR sends messages about finished batches.
Edit	Communication.Email.SendPasswords	False	Set to True to e-mail passwords to users.
Edit	Communication.Email.Username	albrecht	The username when authentication is needed for sending e-mail.
Edit	Communication.HTSL.COM	COM4	The serial port for communicating with the HTSL
Edit	Communication.NMRIP	10.0.0.101	IP address or DNS of the NMR system
Edit	Database.RemovedSampleExpiration	24	The number of months after which removed samples are automatically purged
Edit	Database.Version	8	The version of the database schema used for automatic updates
Edit	Load.CleanInjector1.cycles	1	Number of clean cycles
Edit	Load.CleanInjector1.delay	0	Fill delay in seconds
Edit	Load.CleanInjector1.ejectSpeed	5	Eject speed in microliters per second
Edit	Load.CleanInjector1.fillSpeed	5	Fill speed in microliters per second

Figure – The Brain

Click **Edit** to edit a setting. **Warning:** Changing the name of the setting may cause the system to malfunction.

Sample Load Cycle

The sample load cycle uses the following settings in this order:

1. *Macro.Load.BeforeClean*
2. *Load.CleanSyringe.pre1*
3. *Load.CleanSyringe.pre2*
4. *Macro.Load.BeforeGetSample*
5. *Load.GetSolvent*
6. *Load.GetSample*
7. *Load.InjectSample*
8. *SampleReturn.CleanSyringe.pre1*
9. *SampleReturn.CleanSyringe.pre2*
10. *SampleReturn.EjectSpeed*
11. *Macro.Load.AfterInject*
12. *Load.CleanSyringe.post1*
13. *Load.CleanSyringe.post2*
14. *Load.CleanInjector1*
15. *Load.CleanInjector2*
16. *Load.ReverseRinse*

Communication.CTC.COM is the RS232 port for the LEAP liquid handler. If you are using a USB to Serial cable the COM port will sometimes change when the cable is unplugged and plugged back in. If the COM port is left blank the CTC will be simulated.

Database.Version is managed internally and should not be changed.

Load.CleanInjector1.station, *Load.CleanInjector2.station*,
Load.CleanSyringe.post1.station, *Load.CleanSyringe.post2.station*,
Load.CleanSyringe.pre1.station, *Load.CleanSyringe.pre2.station*
SampleReturn.CleanSyringe.pre1.station, *SampleReturn.CleanSyringe.pre2.station*
and, *Load.GetSolvent.location* need to be set to the LEAP/CTC Wash Station to be used.
If the value for these settings is blank the step will be skipped, which is sometimes
necessary to increase sample throughput or limit solvent use.

The *NMR.ErrorLevel* and *NMR.ScriptStatus* settings are used to handle NMR errors on
Varian systems. *NMR.ScriptStatus* should be set to *nmrstatus* if you want to handle
NMR errors (a good idea), or *showstat* if you do not want to handle NMR errors. Set
NMR.ErrorLevel to *Warning*, *Soft Error*, or *Hard Error* depending on what errors you
want to stop the system on. See the installation guide for more information.

Note: CTC/LEAP Quirk with Syringe Clean Volume

For The Brain syringe clean volume *Load.CleanSyringe.*.volPercent* to take effect the
Wash station CleanVolume on the CTC must be set to 0%.



Setting Up E-Mail Alerts and Reports

*Communication.Email.** is used to set up e-mail alerts, finished notices, and password
reminders, it is optional but this will make the system much more friendly.

A Test Email Account on Protasis.com

A Protasis.com e-mail account can be used for testing e-mail settings in One-Minute
NMR. To set up the test e-mail client use Database/Run Script... menu in the RunProcess
and choose c:\protasis\ProtasisEmail.sql. **CAUTION:** You should not use the Protasis
account to send proprietary information to One-Minute NMR users. Protasis Corporation
is not responsible for confidential information sent through the protasis.com server.

Setting	Description
Communication.Email.AlertRecipients	Comma separated list of One-Minute NMR user names to send alerts to. For example: Bob Albrecht,Tim Peck,Dean Olson
Communication.Email.FromAccount	Account used to send mail to users. Identified in the FROM of messages. This is the actual account used To Whom It May Concern: send the e-mail. Multiple One-Minute NMR systems can share the same e-mail account. You can use a personal account or set an account up especially for One-Minute NMR.
Communication.Email.FromName	The name of the One-Minute NMR system that is sending e-mail messages. This can be used to identify the system that is sending the e-mail. For example: OneMinuteNMR1
Communication.Email.Host	The SMTP server for sending e-mail messages to users. Use your company's e-mail server.

Communication.Email.LinkToMe	Link to this One-Minute NMR system added to the bottom emails. Enter the address of the One-Minute NMR server. For example, if the One-Minute NMR server's address is 192.168.0.1 enter http://192.168.0.1/OneMinuteNMR/main.aspx
Communication.Email.Password	Password for e-mail account that sends mail when authentication is required.
Communication.Email.SendAlerts	True if warnings and errors should be sent by e-mail.
Communication.Email.SendFinishedNotice	Set to True if One-Minute NMR sends messages about finished batches.
Communication.Email.SendPasswords	Set to True to e-mail passwords to users.
Communication.Email.Username	The username when authentication is needed for sending e-mail.

Table – E-Mail Settings

One-Minute NMR is an E-mail Client.

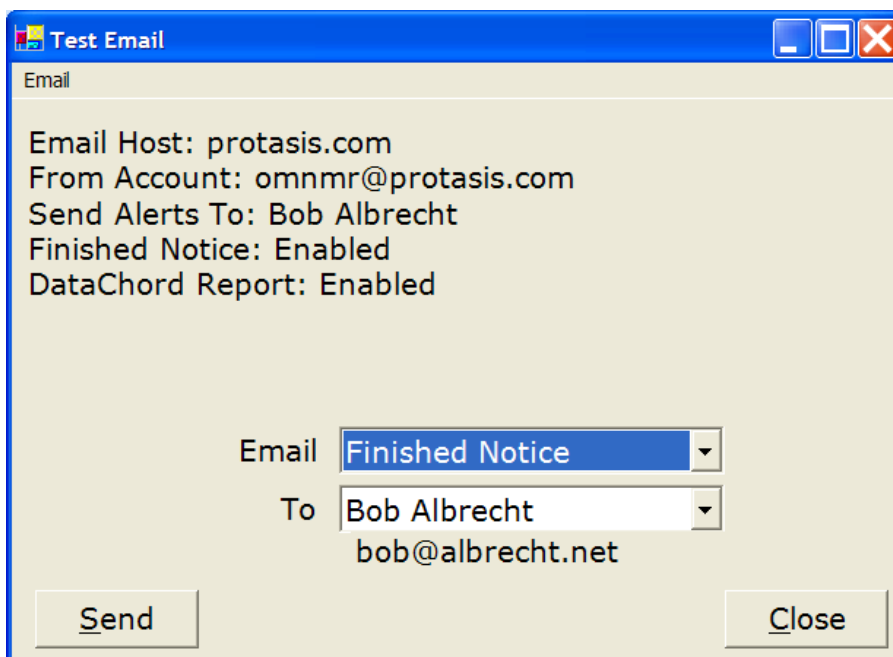
It can connect with your e-mail server (like Exchange Server), or any e-mail server on the Internet (say Hotmail) to send reports and alerts to users of the system. You can use a personal e-mail account or create a new e-mail account for the One-Minute NMR system. Unless you feel like sharing your company's private information with the world, you will not want to use a public e-mail server like Hotmail.

E-mail is buffered so that e-mail server outages or network disruptions do not prevent alerts and reports from being sent to their recipients. To force the e-mail queue to empty when e-mail service is restored use the menu File/Test Email in the RunProcess then the /Email/Empty Queue menu. The queue will disappear when the RunProcess is terminated.

The following e-mails are sent by One-Minute NMR: 1) Alerts when errors occur on the system. 2) Password reminders for users who have forgotten their password. 3) Notices that a user's samples are finished and need to be removed from the system. 4) HTML-formatted e-mail containing structure confirmation reports and links to the ACD Web Librarian.

Testing Email

The File/Test Email menu in the run process allows testing of the current configuration and modes of e-mail transmission.



The Mail drop-down selects between Alert, Finished Notice, and Full Report. The To drop-down allows to pick the One-Minute NMR user to send a Finished Notice or Full Report to. Users are configured in the People section of the One-Minute NMR web page. Alert recipients are configured in The Brain under General Settings / Communications.Email.AlertRecipients.

Disabling E-mail

The preferred way to disable e-mail communications is to set The Brain settings Communications.Email.SendAlerts, Communications.Email.SendPassword, and Communications.Email.SendFinishNotice to False. If Communication.Email.FromAddress is blank e-mail communication will also be disabled.

02302 Injection Counters

The *Counters* section of The Brain is used to hold user-defined counters for the system. Each time a sample is loaded all of the counters are incremented by one. Counters can be reset by changing the value directly. The counters are useful for keeping track of wear items such as syringe wear, injector valve rotor wear, injection port wear, and pump maintenance intervals.

Counter Alerts

As an alternative to manually checking various counters periodically in The Brain, e-mail alerts can be configured for each critical counter. The level of counters is checked when the RunProcess is started and when a Startup Sequence is initiated. An alert is sent for each counter that exceeds its limit. If the Alert flag is set to True an e-mail is sent. If Alert is not set to True the alert is sent to the One-Minute NMR log file.

Counter Alert Setup

To set up a counter alert two additional brain settings need to be associated with each counter. The *Counters.MyCounter.Limit* must specify the limit for the counter. The *Counters.MyCounter.Alert* must be set to True if e-mail alerts are desired.

For example, if the syringe needs to be changed after every 1000 injections, you would set up the following counter:

```
Counters.SyringeChange = 0
Counters.SyringeChange.Alert = True
Counters.SyringeChange.Limit = 1000
```



Automatic Instrument Pause

In order to force more careful inspection of the instrument when samples are submitted for the first time, there is now an optional parameter *System.AutomaticIdlePause=*True that automatically pauses automation when the system is inactive.



Probe Cleaning

For biological samples and samples or a matrix that has an affinity for the silica flow cell of the CapNMR probe it may be necessary to do an automatic cleaning of the probe after a certain number of samples. Probe cleaning is also a part of the Startup and Shutdown sequences.

If the Sample Return feature is engaged Probe Clean will use the current solvent to return the sample in the probe before proceeding with Probe Clean. This takes extra time but eliminates the possibility of dissimilar solvents in the returned sample.

Three Brain parameters control when and if a probe cleaning is performed.

<i>ProbeClean.Enabled</i>	True to activate Probe cleaning.
<i>ProbeClean.Frequency</i>	How often to clean the probe. 0=never, 1=every, n=every nth
<i>ProbeClean.Countdown</i>	Countdown for probe cleaning. When counter reaches zero, cleaning is done.

Probe Cleaning consists of ordered steps in The Brain, some of which are optional. The table below is color coded to show operations that are grouped.

Before Clean Macro	
<i>Macro.Load.BeforeClean</i>	Macro before the first syringe cleaning.
Syringe Cleaning	
<i>Load.CleanSyringe.pre1.*</i>	First syringe clean.
<i>Load.CleanSyringe.pre2.*</i>	Second syringe clean
If there is a first cleaning solution:	

Get Solvent	
<i>Load.GetSolvent.*</i>	Pick up push solvent before sample.
Get First Cleaning Solution	
<i>ProbeClean.Tray</i>	Vial tray for wash solution.
<i>ProbeClean.Index</i>	Vial index for wash solution.
<i>Load.GetSample.*</i>	Pick up was solution as a sample.
Inject First Cleaning Solution	
<i>Load.InjectSample.*</i>	Inject as a sample.
If a Sample Needs Returning:	
Pre-Return Clean Syringe	
<i>SampleReturn.CleanSyringe.*</i>	Clean syringe before returning sample.
Cleaning Solution To Probe and Wait	
<i>Pumps, Delivery Rate and Volume</i>	Cleaning solution is delivered as a sample.
<i>ProbeClean.Duration</i>	Seconds to leave solution in probe.
Expel Returned Sample From Syringe	
If there is a second probe clean vial	
Syringe Cleaning	
<i>Load.CleanSyringe.pre1.*</i>	First syringe clean.
<i>Load.CleanSyringe.pre2.*</i>	Second Syringe clean.
Get Solvent	
<i>Load.GetSolvent.*</i>	Pick up push solvent before sample.
Get Second Cleaning Solution	
<i>ProbeClean.Tray2</i>	Vial tray for second wash solution.
<i>ProbeClean.Index2</i>	Vial index for second wash solution.
<i>Load.GetSample.*</i>	Pick up cleaning solution as a sample.
Inject Second Cleaning Solution	
<i>Load.InjectSample.*</i>	Inject cleaning solution as a sample.
Cleaning Solution To Probe and Wait	
<i>Pumps, Delivery Rate and Volume</i>	Deliver cleaning solution as a sample.
<i>ProbeClean.Duration2</i>	Seconds to leave solutions in probe.
Clean Syringe	
<i>Load.CleanSyringe.post1.*</i>	Final syringe clean 1
<i>Load.CleanSyringe.post1.*</i>	Final syringe clean 2
Clean Injector	
<i>Load.CleanInjector1.*</i>	Injector clean 1
<i>Load.CleanInjector2.*</i>	Injector clean 2
Reverse Rinse	
<i>Load.ReverseRinse.*</i>	Reverse rinse
Solvent Flush	
<i>ProbeClean.SolventFlush1.*</i>	Solvent flush 1
<i>ProbeClean.SolventFlush2.*</i>	Solvent flush 2



Available Solvents and Pumps

This is the list of solvents that are available on the main page. It also defines which HTSL pumps are associated with solvents and defines the arrangement of multiple pumps.

Single Solvent

For single solvent you need only to define one solvent and one pump. The **Solvent** field must match (case sensitive) one of the solvents used on your NMR system. The **Pump** field in the solvents table must contain the name of the one pump, listed in the **Pumps Table**, you are using. This is typically HTSL1. All other fields in the Solvents table can be left blank when there is only one solvent.

The **Pumps Table** must define the one pump that is used. The **Master** field must be left blank and **Port** should be set to 1. The **COM** field is the port used to control the HTSL.

Multiple Solvents

When there are multiple solvents each solvent needs to have a pump assigned to it. One of the HTSL pumps needs to have a second valve for solvent switching; this is a Type C HTSL, or *Master* pump.

Solvent	Pump	Sparge	Wash	Vol. Full (mL)	Vol. Remaining (mL)	Polar (Yes/No)
Acetone	HTSL2	1	Wash2	0	0	yes
D2O	HTSL1	1	Wash1	0	0	yes

Name	Master	Port	COM	Delivery Rate	Fill Rate	Volume
HTSL1	HTSL1	1	COM9	30	30	25
HTSL2	HTSL1	2	COM10	30	29	35

Table – Typical two-solvent setup. Solvents and Pumps tables.

Each *Solvent* needs to match (case sensitive) one of the solvents used on your NMR system. The *Pump* field references the pump in the *Pumps Table* that is used for this solvent. *Sparge* is reserved for future use and should be set to 1. With multiple solvents it is necessary to use a separate wash station for each solvent to avoid shimming problems with dissimilar solvent. The Wash field references the CTC Liquid Handler wash station that is used for this solvent. One Pump needs to be defined for each solvent. One of the pumps, the one with a second solvent switching valve, is the Master pump. Each pump, including the *Master* needs to reference the Master pump. The *Port* field must be set to the 6-way valve port on the solvent switching valve of the master that the pump is connected to. The *COM* field defines the RS232 port that communicates with the pump. The *Polar* field is important and used in solvent switching. When the system switches from one solvent to another it checks to see that the solvent is *Polar* or not. If a switch is being made from polar to non-polar or non-polar to polar, a universal solvent, defined by the *Brain Setting SolventSelect.UniversalSolvents* is used to flush the system. Good universal solvents are Acetone and DMSO.

Solvent Volumes

The Vol. Full (mL) and Vol. Remaining (mL) are reserved for future use.

Pump Rates/Volumes

The Delivery Rate and Fill Rate need to be set to the fastest values that can be used for a particular solvent. These will be configured when the system is installed, but can be adjusted if the pressure is too high, or if the maximum pressure is less than 1800PSI. The Volume is the pump volume that is delivered to move one sample into the flow cell. However, the delivery volume can differ depending on the flow rate so if the flow rate is changed, the volume must be re-calibrated experimentally using repeated NMR scans.

Solvent Selection

One-Minute NMR is capable of switching between multiple solvents automatically. Besides the Solvent and Pump tables there are several Brain parameters that control solvent selection.

Setting	Value	Description
SolventSelect.BunchNightSamples	True	Run night samples with the same solvent together.
SolventSelect.BunchSamples	False	Runs samples with the same solvent together.
SolventSelect.CurrentSolvent	Acetone	The current solvent used by the system. For detecting changes.
SolventSelect.ExchangeVolume	200	Volume (uL) to push when changing solvents.
SolventSelect.FlushCycles	3	OBSOLETE
SolventSelect.FlushFillSpeed	25	Flush fill speed in microliters per minute.
SolventSelect.PrioritySwitch	False	Priority samples can force a solvent switch.
SolventSelect.UniversalSolvents	Acetone,DMSO	List of universal solvents. Typical universal solvents are Acetone and DMSO.
SolventSelect.ValveWastePort		The port to eject waste solvent to. Default probe port.

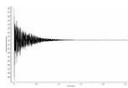
Table – Solvent Selection Brain Parameters

Solvent Change

To allow for efficient transition between solvents the Solvent Change table was implemented with a set of two volumes and two flow rates for each solvent change. The first flow rate is often slower because mixtures of solvents can have higher viscosities than pure solvents. If a Solvent Change entry is available for the transition between two solvents the *SolventSelect* settings are overridden.

From Solvent	To Solvent	Flow Rate1	Volume1	Flow Rate2	Volume2
D2O	DMSO	30	80	45	20
DMSO	D2O	25	30	80	70

Table – Solvent Change



Available Experiments

This is the list of experiments that are available to users. Experiments are attached to the default user, a particular user, and every sample that is entered. The *default* user has the parameters for the experiments before they are modified by specific users. To select the experiments available for the default user, or a particular user, select from the drop-down list. The experiments attached to individual samples cannot be changed after the sample has been created, except by editing values in the samples grid on the main page.

There are a number of parameters for experiments, some of which are not available for all NMR systems.

Exp. Name is the name of the experiment as it appears on the Main Page. If the first word of the experiment name is “default” on Varian systems, a setup is done using the name of

the solvent and Nucleus. Otherwise an experiment (AU or Magical script) must exist with this name on the NMR spectrometer.

Nucleus is the nucleus to use for the experiment. This nucleus name must exist on the NMR system.

Exp.# is the experiment number to use when running this experiment. On Varian systems you cannot be logged into this experiment.

Exp.# Fill (Bruker) is a code for filling experiment numbers, either *Use* or *=Vial+*. This is useful where each sample can have multiple experiment numbers.

Proc.# (Bruker) is the process number to use for processing. Usually 1.

Proc.# (Bruker) Fill *Use* or *=Vial+*

Num. Scans is the default number of scans to do using this experiment. This can be changed during sample submission.

Spectral Width is the default width of the spectrum in ppm.

Spectrum Center is the center of the spectrum in ppm.

ProcessFile is the AU or Magical macro used to process data.

Parameters are a set of optional parameters that are sent to autorun. A modified autorun must be used to implement the parameters.

Life Cycle of Experiments

1. The experiments for the "default" user are created.
2. When a user logs in any experiments that are in the default list are copied to the user's list. Any experiments that are not in the default list are removed. This means that everyone always has the same experiments as the default user.
3. A user can change the parameters for their experiments. Usually this is just the number of scans or run order.
4. When a sample is queued, the experiments that were selected are copied to the sample. Because there is a copy of each experiment for a sample the parameters can be changed by the user for other experiments without changing the ones that are already queued.
5. When a sample is removed and deleted from the system its list of experiments is deleted.

Copying Experiments to All Users

Because experiments and their settings are specific to each user it may be difficult to manage experiments for all users at the same time. To accommodate global changes to experiments edit the experiment list for the default user, then click the **Copy default Experiments To All Users** button to copy the entire default experiment list and the settings for each experiment to every user.

Setting up Experiments with a Custom Parameter Set

OneMinuteNMR creates and runs experiments on the NMR console computer using au or magical scripts. The autorun script, which is defined by the Brain parameter **NMR.ScriptTemplate**, imports the experiment setup parameters for creating the experiment while the full list of acquisition parameters are called in from a location on the console computer.

The experiment has to be pre-defined in two locations 1) on the OneMinuteNMR computer in the brain under 'Available Experiments' and 2) on the console computer with the full acquisition parameter set.

Settings Category: Available Experiments

		Exp. Name	Nucleus	Exp. #
Delete	Edit	Custom_expt_from_Bob	H1	1
Delete	Edit	OMNMR_s2pul	H1	1

NMR Experiments To Run:

Custom_expt_from_Bob
OMNMR_s2pul

In the OneMinuteNMR computer, go into the brain and select 'available experiments' from the first drop-down menu. Click on new and edit the name 'New experiment' to match the parameter set (OMNMR_s2pul). This experiment will then be an

available selection on the main OneMinuteNMR webpage.

Varian Setup:

- 1) Begin by saving the acquisition parameters (i.e. svp('OMNMR_s2pul') to a specific location (i.e. /export/home/userdirectory /vnmrsys/parlib).
- 2) Varian requires that an executable macro be written to call in the parameters. This macro only needs to consist of one line that reads in the saved parameter set (i.e. rtp('/export/home/userdirectory/vnmrsys/parlib/OMNMR_s2pul').
- 3) In order to test this pathway, type the experiment name (i.e. OMNMR_s2pul) into the VNMR command line. That should load the experiment parameters properly.

Bruker Setup:

- 1) Save the desired acquisition parameters (i.e. wpar OMNMR_s2pul)
- 2) In order to test this pathway, load the experiment parameters using the Bruker command line (i.e. rpar OMNMR_s2pul).



Autorun

The autorun script, which is defined by the Brain parameter *NMR.ScriptTemplate*, imports the experiment setup parameters for creating the experiment while the full list of acquisition parameters are called in from a location on the console computer. The autorun setup script (shown in the listener) is as detailed below.

```
autorun('user','solvent','probe','datasetname','experiment',nt,d1,sw,tof,'path','text','nucleus','proc','locktable','shimfile', OMNMRUser, email, sampleID, CustomFields...)
```

Arguments to autorun on Varian systems

1. NMRUserName

2. Solvent
3. ProbeFile
4. DataSet (FID)
5. ExperimentName
6. NumberOfScans
7. PulseDelay
8. SweepWidth
9. SpectrumCenter
10. DataPath
11. Title
12. Nucleus
13. ProcessFile
14. LockTable
15. ShimFile
16. OMNMR.username
17. UserEmail
18. SampleID
19. Plate (Optional when NMR.SendPlateID=True)
- 20+. Extra Parameters (NMR.UseExtraParamters=True)
- 20+. CustomFields, in the order that they appear on the web page.

Arguments to autorun on Bruker systems

1. Autorun response file. Defined by NMR.ResponseFile.
2. NMR.TemperatureEquilibrationTime
3. Title
4. Experiment Number
5. NMR Data Path for user or NMR.Disk
6. NMR User Name
7. Solvent
8. Nucleus
9. Shim File
10. Experiment Name
11. Number of scans
12. Sweep Width
13. Spectrum Center
14. Data file name
15. Processing script
16. One-Minute NMR User Name
17. User e-mail
18. Plate (Optional when NMR.SendPlateID=True)
19. Extra Parameters (NMR.UseExtraParamters=True)
- 19+. Custom Fields in the order they appear on the web page.

Named Parameters Files

The parameters to autorun, and some extra parameters, are optionally sent to a file of your choice on the NMR computer. The parameter file is created when you specify the name of the file in the NMR.NamedParameterFile in The Brain. The file name is relative to the directory on the UNIX or Linux system where autorun is located for Bruker and Varian systems on UNIX or Linux, or relative to the One-Minute NMR computer for Bruker systems. On Varian systems the lookup macro can be used to lookup individual parameters, on Bruker systems an AU script can read the file.

Each parameter has a name, a tab character, and an associated value followed by an end-of-line sequence. The names are guaranteed not to contain any white space, but the values may contain string of information.

An advantage of the parameter file is that custom parameters are named and appear just as they would on the main web page, except with the trailing colon removed and spaces converted to an under-bar character. If the label of a custom field differs from the declared name of the field the custom field is listed twice in the file.

Here is an example of the contents of a parameter file:

```
Parameter      Values
timestamp      10/3/2008 11:44:02 AM
Samples.Username Bob Albrecht
Samples.Account Protasis
Samples.CustomFields notebook1`page2`Dec `11` `08
Samples.InjectionNum 1
Samples.Location G5
Samples.ReturnTo
Samples.RunStartTime 10/3/2008 11:42:40 AM
Samples.RunVolume 0
Samples.SampleID sampleID_77
Samples.SMILES
Samples.Solvent D2O
Samples.Status running
Samples.SubmitTime 9/29/2008 11:10:11 PM
Samples.Title This is the title
Samples.TrayPlate MT1-Rear
Samples.uniqueID 4333
Samples.VialIndex 77
User.Username Bob Albrecht
User.email b.albrecht@protasis.com
User.NMRdataPath c:\ACD\VerificationTestData
User.NMRexperimentPath
User.NMRusername boba1
NMRExperiment.ExperimentName autoqc
NMRExperiment.ExperimentNumber 1
```

```

NMRExperiment.ExperimentNumberFill Use
NMRExperiment.ProcessNumber 1
NMRExperiment.ProcessNumberFill Use
NMRExperiment.NumberOfScans 1
NMRExperiment.SweepWidth 10
NMRExperiment.SpectrumCenter 0
NMRExperiment.RunOrder 12
NMRExperiment.Nucleus PROTON
NMRExperiment.ProcessFile autoprocqc
NMRExperiment.ProcessLink
NMRExperiment.Extra
CustomField.Notebook notebook1
CustomField.Page page2
CustomField.Collection_DateDec -11- 08
BrukerNMR.DataPathc:\ACD\VerificationTestData
BrukerNMR.DataFile sampleID_77
NMR.ShimFile D2Omrn
Status.RemainingSamplesForUser 0
Status.RemainingSamplesForUserOnTray 0

```



Import Conversion

This is a table that defines the layout of .CSV or .SDF files that can be imported from external sources.

Importing CSV Files

The first row of the .CSV file defines the column names and all subsequent rows specify sample data. The job of the import template is to tell One-Minute NMR which Samples Table field is used to store named fields in a CSV file.

In the following example CSV file:

```

Notebook-Page,Index,UserID,experiment,Solvent,Well,Title
01851042-003-001D01,1,crjone,scout1d&wet1d,DMSO,A1,01851042-003-001D01

```

The imported fields are: Notebook-Page, Index, UserID, experiment, Solvent, Well, and Title

An import template needs to define the location of a sample on a plate, and can supply any other information about the sample. The following import conversion table is given as an example.

Import ID	Imported Field	Samples Table Field
------------------	-----------------------	----------------------------

default	Solvent	Solvent
default	Well	Location
default	experiment	Experiments
default	Title	SampleID

Contact Technical Support for help creating an import template.

Importing ZIP Files

You can import ZIP files that contain multiple CSV files optionally combined with molecule files. The importer will scan the directory tree of the ZIP archive and attempt to import each file with a .CSV extension.

The procedure for preparing a ZIP file for import is as follows:

1. Create a directory for your archive. Use a name that represents the plate or tray of samples that you are importing.
2. Copy the .CSV file sample list into the directory.
3. If the .CSV file references Molecule files, copy them into the directory.
4. ZIP the entire directory. The easiest way is to right-click the directory in Windows Explorer and select ZIP to directory name option.

Importing User Lists

If an import template does not specify the VialIndex or Location user-only information can be imported. This is useful for importing lists of users. The user 'template' must be present as a template for new user creation.

Importing Structure Data Files (SDF)

SDF files contain lists of associated sample information including molecule data. One-Minute NMR automatically recognizes SDF files by the ".sdf" (not case-sensitive) file extension.

SDF files are imported using the current import template to translate associated sample information into the sample. Any associated data in the imported file can be mapped to one of the Import Fields described for CSV files.

For example, an associated data field named Unique ID in an SDF file looks like this:

```
> <Unique_ID>
XCA3464366
```

An entry in the Import Conversion table can be made to use Unique ID as the file name:

Imported Field	Samples Table Field
UniqueID	FileName

Custom Fields with SDF

Multiple associated data fields can be combined into a list of One-Minute NMR custom fields using a comma-separated list and the Custom Combo Samples Table Field.

Imported Field	Samples Table Field
Molecular Weight, Notebook Entry, Notebook Page, Notebook Number	Custom Combo

The custom fields are stored in the sample queue and are transmitted to the NMR computer and displayed on the web page. Imported custom fields must appear in the same order as defined custom fields in The Brain.

Importing Molecules with SDF

Molecules can be imported automatically and attached to samples in the queue. Molecule data is then transmitted to the NMR computer and placed in the directory associated with each sample's data. The name of the file is the same as the imported FileName for the sample with a .mol extension.

Enabling Molecule Import in The Brain

Enabling molecule import from SDF files and the main web page also enables transmission of molecules to the NMR computer. The *Import Molecule...* button will be active on the main web page to enable manual molecule imports. After molecules have been successfully imported the structures can be visualized using ctrl-click on the sample wells. See the Structure Confirmation section for more information.

The following Brain settings are used.

1. If *NMR.UseMoleculeData* is set to True, or
2. Automated structure confirmation is enabled (*Confirmation.License* is set) and *Confirmation.MoleculeAutomatic* is set to False.

Note: See the section on Automated Structure Confirmation.

Import Conversion Fields

Each entry in the Import Conversion table correlates a field in a .CSV or .SDF file to one of the One-Minute NMR Samples Table Fields listed below.

Samples Table Field	Length	Description
FileName	80	The name of the sample. Used on the NMR system as the name of the directory where results are stored. If multiple experiments are run on the same sample results are stored in the SampleID/Experiment directory.
InjectionNum	Integer	The number of iterative injections for the sample.
TrayPlate	20	The CTC/LEAP tray name where the sample is located. Typically tray01 – tray08, but can be anything defined on the Leap.
Location	20	The well address for the sample. A1 – H12 for 96 well plates. If VialIndex is not specified Location is

VialIndex	Integer	used to compute VialIndex. The 1-based index of the vial on the tray. 1-96 for a 96 well plate.
Username	40	The name of the user the sample belongs to. When importing, if the username is not an existing user, and there is a user named "template", template will be copied for the new user.
Account	40	The account name of the user.
SMILES	4096	Molecular formula for the proposed structure. Used by automated structure confirmation.
SampleID	4096	The title text for the sample. For historical reasons this field is named SampleID. It may be changed to Title in the future.
Solvent	20	The name of the solvent. This must be one of the configured solvents on the system.
ReturnTo	16	The location where the sample is returned to. This can be either "Self", "Waste", or the name of a liquid handler tray.
Experiments	N/A	A list of one or more experiments for the sample. Multiple experiments are separated by an ampersand (&). Experiments must be configured in One-Minute NMR and on the NMR system.
Scans	N/A	& separated list of the number of scans for each experiment in the Experiments list.
Email	N/A	The e-mail address of the User. If this is a new user the new e-mail address is assigned when the template user is copied and saved with the new user name.
Molecule	N/A	The file name of a molecule file* to be used for structure confirmation.
CustomFields	4096	The values of a list of custom fields. Each value is separated by a backwards single quote ('). The values must match the defined custom fields in the CustomField section of The Brain.
NMRDataPath	4096	If this is a new user this is their data path on the NMR system.
Password	40	If this is a new user this is their One-Minute NMR password. It is ignored for existing users.
Custom Combo	N/A	Multiple fields can be combined from SDF files. A comma separated list of associated sample data fields is combined as a list of CustomFields. CustomFields and Custom Combo will override each other in an import template.

Table - Import Fields and Extension

* See Allowed Molecule Files below

Note: Information that is not specified in the import file is taken instead from the sample information section (2.) of the main web page, and from the default values for the experiment in the case of the spectral window and number of scans.

Please contact Technical Support for help in building an import template.



Startup Sequence

The startup sequence is used to prepare the system for automated use. A probe clean, 2 syringe cleans, 2 injector cleans, and 2 solvent flushes (in that order) can be programmed. The probe clean may include syringe cleans, injector cleans, or return of sample. Each of the system preparation steps is optional and separate from normal operation.

Manual Start

The Startup Sequence can be started manually using the Run / Startup Sequence menu item in the RunProcess.

Automatic Start

The startup sequence is triggered automatically after a period of inactivity. The RunProcess looks at the date / time of the last sample and last time startup sequence ran to start automatically. Checks are made when samples are submitted, when automation resumes, and after retries from errors.

The system decides to do an automatic startup sequence when the following criteria are met:

- A. A sample is being queued to run and,
- B. The system is not paused, loading a sample, or running and,
- C. The *Startup.Enabled* Brain setting is True and,
- D. The elapsed time since the last sample's run end time exceeds the *Startup.Timeout* Brain parameter and,
- E. The elapsed time since the last startup sequence defined by *Startup.TimeOf* exceeds the *Startup.Timeout* period.

<i>.Enabled</i>	Turns on or off the automatic instrument startup sequence.
<i>.TimeOf</i>	The date/time the startup sequence last ran. Used to determine if the startup sequence needs to start again.
<i>.Timeout</i>	Minutes of down time needed before startup sequence is used again.

The Sequence

a. Probe Cleaning

A special probe clean for the startup sequence can be used or you can use the standard probe clean.

.Enabled	Turns on or off the startup probe clean.
.Duration	Seconds to leave solution in probe. (blank to use ProbeClean.Duration)
.Duration2	Seconds to leave solution in probe. (blank to use ProbeClean.Duration2) for second probe cleaning.
.Index	Vial index for cleaning solution. (blank to use ProbeClean.Index)
.Index2	Vial index for second cleaning solution. (blank to use ProbeClean.Index2).
.Tray	Vial tray for probe cleaning solution. (blank to use ProbeClean.Tray)
.Tray2	Vial tray for second probe cleaning solution. (blank to use ProbeClean.Tray2)
.SolventFlush1.Solvent	Name of solvent used for first probe flush (blank disables)
.SolventFlush1.Volume	Microliters of solvent for first solvent flush.
.SolventFlush1.Flow	Flow rate for first solvent flush.
.SolventFlush2.Solvent	Name of solvent used for second probe flush (blank disables)
.SolventFlush2.Volume	Microliters of solvent for second solvent flush.
.SolventFlush2.Flow	Flow rate for second solvent flush.

b. Syringe Cleaning

The syringe cleans should be tuned to properly prime the syringe for normal automation. The first syringe clean is **Startup.CleanSyringe.1** and the second is **Startup.CleanSyringe.2**. If **Startup.CleanSyringe.X.Station** is blank that syringe clean step is skipped. If **.Station** is set to **Solvent** the current solvent is used for the cleaning.

c. Injector Cleaning

The two injector cleans should be tuned to properly prime the injector before normal operation. The injector cleans are defined by **Startup.CleanInjector1** and **Startup.CleanInjector2**. If **Startup.CleanInjectorX.Station** is blank the step is skipped. If **.Station** is set to **Solvent** the current solvent is used.

d. Solvent Flush

Two solvent flush steps defined by **Startup.SolventFlush1** and **Startup.SolventFlush2** are available. They should be tuned to prime the flow path through the probe to eliminate bubbles and prepare the system for normal operation.

.Flow	Flow rate for first solvent flush (microliters/min)
.Solvent	Name of solvent used for first probe flush (blank disables)
.Volume	Microliters of solvent for first solvent flush.



Shutdown Sequence

The shutdown sequence is used to prepare the system for a period of inactivity by expelling remaining sample and leaving a suitable solvent in the system. A probe clean, 2 syringe cleans, 2 injector cleans, and 2 solvent flushes (in that order) can be programmed. The probe clean may include syringe cleans, injector cleans, or return of sample. Each of the system shutdown steps is optional and separate from normal operation.

Manual Start

The shutdown sequence can be started manually using the Run / Shutdown Sequence menu item in the RunProcess.

Automatic Start

The shutdown sequence is triggered automatically after a period of inactivity. The RunProcess looks at the date / time of the last sample and last time Shutdown sequence ran to start automatically. Checks are made using a timer when the system is idle.

The system decides to do an automatic shutdown sequence when the following criteria are met:

- A. The system is not paused, loading, or running a sample and,
- B. The *Shutdown.Enabled* Brain setting is True and,
- C. The elapsed time since the last run is greater than the *Shutdown.Timeout* Brain parameter and,
- D. The elapsed time since the last shutdown sequence is greater than the *Shutdown.Timeout* Brain parameter and,
- E. The elapsed time since the last shutdown sequence is greater than the elapsed time since the last sample run.

<i>.Enabled</i>	Turns on or off the automatic instrument shutdown sequence.
<i>.TimeOf</i>	The date/time the shutdown sequence last ran. Used to determine if the Shutdown sequence needs to start again.
<i>.Timeout</i>	Minutes of down time needed before shutdown sequence is used.

The Sequence

a. Probe Cleaning

A special probe clean for the shutdown sequence can be used or you can use the standard probe clean.

<i>.Enabled</i>	Turns on or off the Shutdown probe clean.
<i>.Duration</i>	Seconds to leave solution in probe. (blank to use ProbeClean.Duration)
<i>.Index</i>	Vial index for wash solution. (blank to use ProbeClean.Index)
<i>.Tray</i>	Vial tray for wash solution. (blank to use ProbeClean.Tray)

b. Syringe Cleaning

The syringe cleans should be tuned to prepare the system for inactivity. The first syringe clean is *Shutdown.CleanSyringe.1* and the second is *Shutdown.CleanSyringe.2*. If *Shutdown.CleanSyringe.X.Station* is blank that syringe clean step is skipped. If *.Station* is set to *Solvent* the current solvent is used for the cleaning.

c. Injector Cleaning

The two injector cleans should be tuned to properly prepare the injector for down time. The injector cleans are defined by *Shutdown.CleanInjector1* and *Shutdown.CleanInjector2*. If *Shutdown.CleanInjectorX.Station* is blank the step is skipped. If *.Station* is set to *Solvent* the current solvent is used.

d. Solvent Flush

Two solvent flush steps defined by *Shutdown.SolventFlush1* and *Shutdown.SolventFlush2* are available. They should prepare the flow path to be idle by using the stable and non-reactive solvent such as D2O.

<i>.Flow</i>	Flow rate for first solvent flush (microliters/min)
<i>.Solvent</i>	Name of solvent used for first probe flush (blank disables)
<i>.Volume</i>	Microliters of solvent for first solvent flush.

e. Syringe Parking

The syringe is optionally parked in the wash station current solvent. This prevents the needle from drying out for more volatile solvents such as chloroform.

<i>.ParkSyringe</i>	True if the needle should be parked in the wash station at the end of the shutdown sequence. The current solvent is defined by <i>SolventSelect.CurrentSolvent</i> .
---------------------	--



Using Sample Vial Barcodes

Vial barcodes are used to reduce or eliminate the information that is entered during sample submission and to reduce the number of potential errors. Several optional features work together to enable walkup sample submission where clients can place a vial in a holder with no data entry and minimal maintenance by facility managers.

CTC Liquid Handler Barcode Reader

Barcode reader Laser scanner for barcode labels on 2ml/10ml/20ml vials including electrical connection cable (needs firmware >2.2). This option is installed and configured by your CTC or Protasis service technician. The barcode reader picks up each vial using a magnet and a magnetic vial cap then scans the barcode with the laser scanner.

If Sample Information Lookup (see below) is not configured the value from the barcode reader is placed in the SampleID / FileName field for the sample. If a sample name was provided during data entry it is overwritten.

If no sample vial is found there are three different behaviors that can be configured in the software:

- 1) Generate an error and pause the automation queue.
- 2) Wait and retry the sample location until a vial is placed in the designated position.
- 3) Skip missing samples and move to the next position in the queue.

Sample Information Lookup

The barcode can be used to lookup all of the information for a sample including file name, title, and experiments. When a barcode is obtained from the scanner on the liquid handler it is stored in a temporary location and passed to an optional program that returns information about the sample.

The program that returns detailed information about the sample is referenced by The Brain setting GetBarcode.SampleLookup. It is a Windows-based console program that takes the barcode as an argument, and returns the information to the console. Each line of output from the SampleLookup program is scanned for pre-defined tags. The information after each tag is then used to populate fields associated with the current sample.

The currently supported return values from the Sample Information Lookup program are:

Sample Lookup Tag	Description
FileName:	The name of the NMR data file / FID directory for the sample and the primary identifier in the software.
Location:	The well location for the sample. If the location does not match the current vial position a message is sent to the log file, but no error is generated.
Solvent:	The solvent for the sample. This must be one of the currently configured Available Solvents.
Experiments:	One or more experiments to run for this sample. Experiments must be in the currently configured Available Experiments list. Multiple Experiments are separated by the ampersand (&) symbol.

In the example below, SampleLookup.exe is run by the One-Minute NMR RunProcess using the barcode of 1234. The results are sent to the console.

SampleLookup.exe 1234*FileName:MySampleName**Solvent:DMSO**Experiments:PROTON&COSY***Automatic Queue Regeneration**

Automatic sample queue regeneration was created to keep an automated walkup systems running without intervention from facility managers. Each time a sample finishes running its entry in the sample queue is automatically removed and another sample is submitted in its place at the end of the queue. The liquid handler will move through each position in the sample queue and collect data for the samples it finds.

With automatic queue regeneration, wait for missing samples, and sample information lookup enabled the liquid handler will wait for vials to be placed on the liquid handler, read barcodes of new vials, lookup their sample information, acquire NMR data, and add another sample at the end of the queue.

Barcode Brain Settings**GetBarcode.Enabled**

True enables reading barcodes from CTC liquid handler. The barcode reader must be configured on the CTC or an error will result.

GetBarcode.RegenerateSampleQueue

Regenerates samples in the queue to run forever on barcoded samples.

GetBarcode.SampleLookup

Program to lookup sample information for barcode.

GetBarcode.SkipMissingSamples

True to abort missing samples, log error, and continue sample queue.

GetBarcode.WaitForMissingSamples

Number of seconds to wait for missing samples to arrive.

GetBarcode.WaitForMissingSamplePeriod

Number of seconds to wait for missing samples to arrive.

**Lock Monitoring**

Lock monitoring is used to prevent samples from crystallizing in the NMR probe. A special process monitors the lock signal during long experiments. If the lock signal drops

below a pre-specified percentage of the original signal a Probe Clean is optionally performed. You may choose to continue to the next sample or stop and generate an error.

Note: Currently lock monitoring only works with Varian spectrometers.

Setting	Value	Description
LockMonitor.AveragingPeriod	1	Minutes of averaging for lock signal monitoring.
LockMonitor.ContinueNext	False	True continues to next sample. False pauses instrument.
LockMonitor.Enabled	True	Enables Lock Monitoring and corrective action.
LockMonitor.LimitPercent	10	Percentage drop before returning or flushing sample.
LockMonitor.ReportOnly	False	True to only report when the lock level drops.



Custom Fields

The *CustomField* section allows you to create custom fields that are passed to your NMR spectrometer as additional command line arguments to the Autorun macro. On Varian systems custom fields start at argument number 19. On Bruker systems custom fields start at argument number 18, Custom Fields can be entered in section 2. of the sample login page and can be imported in a CSV file.

Note: An example set of custom fields can be imported into the database by selecting the Database / Run Script... menu item in the RunProcess and selecting the c:\protasis\SQL\CustomFields.sql script. They can then be accessed and modified in The Brain Custom Fields section.

2.

Name: Vial ▾

Notebook:

Page:

Collection Date: Jan ▾ - 9 ▾ - 08 ▾

Title:

Figure – Custom fields on login screen.

Each custom field is declared in the General Settings/CustomField category/filter section of The Brain. To make new custom fields click *New Setting* and add the declaration, format, and label for the new field.

Settings Category: General Settings		Settings Filter: CustomField		
		Setting	Value	Description
Edit	Delete	CustomField.1NotebookEntry.Declare	Custom1	Internal ID for custom field.
Edit	Delete	CustomField.1NotebookEntry.Format	50px-50px-50px	Format of field. Fields are specified by width. Valid separators are - / _ ; + .
Edit	Delete	CustomField.1NotebookEntry.Label	Notebook Entry:	Label for custom field.
Edit	Delete	CustomField.Custom2.Declare		
Edit	Delete	CustomField.Custom2.Format	100%	
Edit	Delete	CustomField.Custom2.Label	User weight:	
Edit	Delete	CustomField.Custom3.Declare		
Edit	Delete	CustomField.Custom3.Format	60px/30px/30px	Collection Date (yyyy/mm/dd)
Edit	Delete	CustomField.Custom3.Label		

Figure – CustomField in The Brain

Each custom field is described with 3 or 4 Brain parameters.

<u>Brain Parameter</u>	<u>Purpose</u>
CustomField. <i>FIELDNAME</i> .Declare	Declaration of unique custom field.
CustomField. <i>FIELDNAME</i> .Format	The layout of the custom field on the page.
CustomField. <i>FIELDNAME</i> .Label	Label that appears to the left of the field.
CustomField. <i>FIELDNAME</i> .Choices	Choices for drop-down lists.

The declaration follows the pattern CustomField.*FIELDNAME*.Declare where *FIELDNAME* is the name of the new field. For example: CustomField.NotebookEntry.Declare creates a new field named NotebookEntry. The name of the field is not seen by the user. Custom fields are sorted alphabetically by their name when they are displayed. The sort order can be forced by beginning the field name with a number; for example: CustomField.1NotebookEntry.Declare.

The format of a custom field determines how many parts it has, the separator between parts, and the width of each part. Formats are defined by creating a new setting CustomField.*FIELDNAME*.Format. For example: CustomField.NotebookEntry.Format = 55px-55px-55px will create 3-part field where each part is 55px (pixels) wide and the fields are separated by a dash. Width values are specified in px and percent; e.g. 55px or 30%.

The label of a custom field specifies the visual label on the data entry page. Labels are specified by creating a new setting CustomField.*FIELDNAME*.Label. For example CustomField.NotebookEntry.Label = Notebook Entry:. The label is for visual display only.

Drop-down lists are created using CustomField.*FIELDNAME*.Choices. Each selectable item in the list is separated by a comma. For example: Yes,No,Maybe. The item in the list is selected by default. If no default choice is desired include a comma at the beginning to indicate a blank item. Spaces are automatically removed from the beginning and end of each item. It is useful to add spaces between items to allow the grid to word-wrap. Multi-part fields use multiple lists of items separated by the ‘|’ character. If there are no items in the list of choices for a field a text box is used. For example: *True, False||Large, Medium, Small* define the choices for a three-part custom field. The first item has two choices, True and False, the second field has no choices and a text entry field is used, and the third item has three choices Large, Medium, and Small.

Custom fields are passed as the last arguments to the autorun macros for your system. Each part of a custom field is passed as a separate argument. They are sent in the order that they appear on the sample login screen. In the figure above 7 additional arguments are passed to autorun, the first three are the parts of the Notebook Entry, the fourth is the User Weight, and the last three are the Collection Date.

Custom fields are stored in the CustomFields column of the Samples table. The values of the fields are positional so if you change the name and alphabetical order of the fields they and can be mixed up. It is not a good idea to change CustomFields when there are existing samples in the queue because it could negatively affect existing samples.

Custom fields are displayed in the Tool Tip for samples.

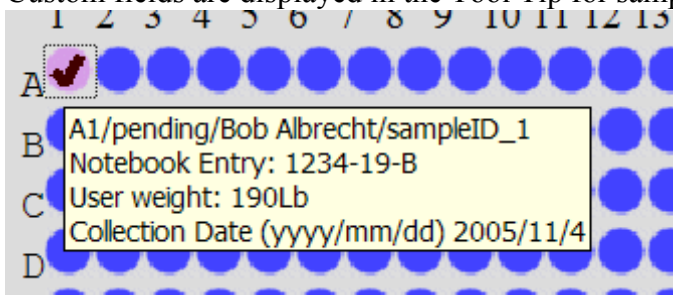


Figure – Custom Field Tool Tip

One-Minute NMR Macros

Macros provide a means to communicate to the NMR computer, CTC liquid handler, or HTSL pump. They are defined as file names in the Macros section of The Brain. The macro files must be located in the c:\protasis\macros directory but can have any name.

Each line of the macro must be preceded with one of three tokens to indicate the target device. *NMR*: indicates the NMR console computer, *CTC*: indicates the CTC liquid handler, and *HTSL*: indicates the HTSL pump.

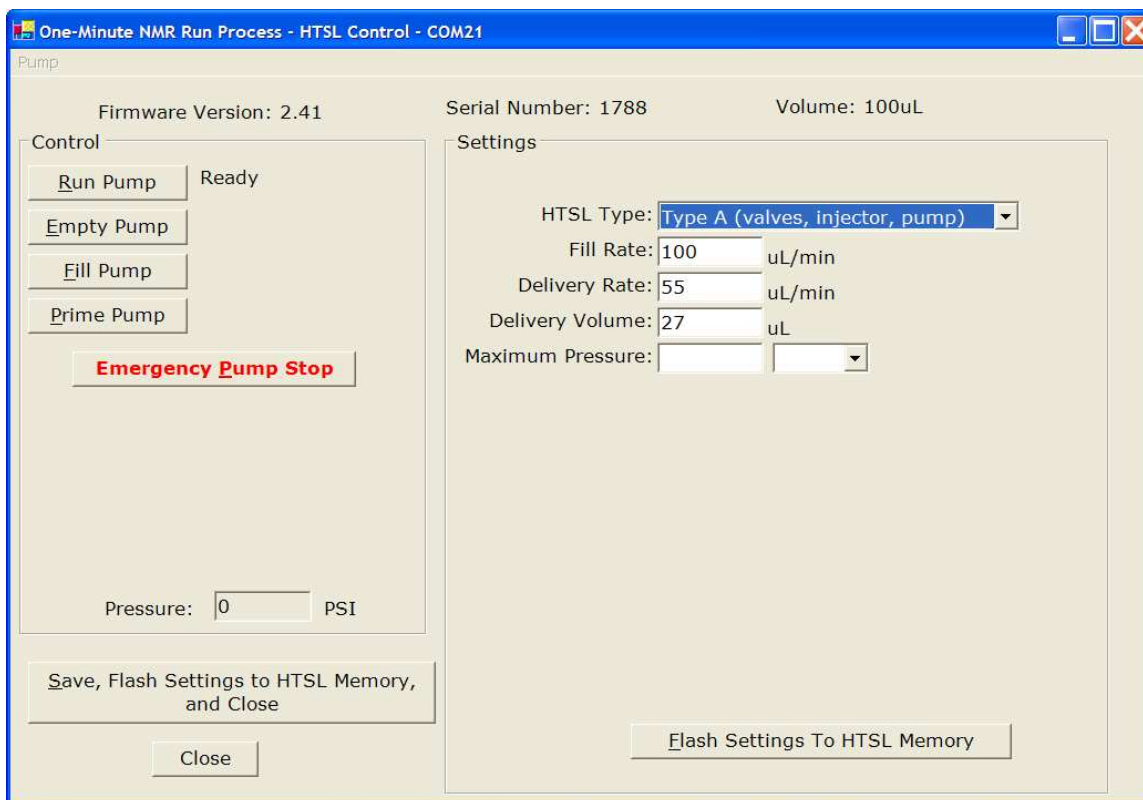
NMR commands are sent directly to the NMR console computer as UNIX commands. They can be commands sent to the NMR or they can be standard UNIX script commands. The symbol *\$sample* is replaced with the current sample ID (FID file name) in the for NMR commands.

CTC commands are sent to the CTC liquid handler and must follow the CTC liquid handler command set (available from CTC). The symbols *\$tray* and *\$index* are replaced in CTC commands to indicate the tray and index of the current sample.

HTSL commands provide a means to run the HTSL pump to push one sample volume to the probe. HTSL:RUN is the only possible command.

HTSL (Pump) Control

Direct control of the HTSL pumps is achieved through the HTSL menu in the RunProcess and the stand-alone HTSL control program. There are different configurations of the HTSL control program depending on the HTSL Type and its firmware version. Some of the features of HTSL control are hidden behind menu items because they are typically used by service personnel.



Do not change the HTSL Type unless instructed by Protasis technical support.

The Run, Empty, Fill, and Prime Pump buttons are used to control the flow of solvent. If the pump exceeds the maximum pressure it will stop without harming it.

The Fill and Delivery rates, the Delivery Volume and the Maximum Pressure are stored in the pump immediately after changing them, but are not stored permanently until settings are flashed to HTSL memory.

The Save, Flash Settings to HTSL Memory, and Close button saves all settings and closes the window.

Solvent Conditioner Brain Settings

The Solvent Conditioner Brain settings enable and disable control of the solvent conditioner and control what components are tested automatically and how often they are tested.

Setting	Value	Description
SolventConditioner.BottleA.Enabled	True	True to enable Bottle A.
SolventConditioner.BottleB.Enabled	False	True to enable Bottle B.
SolventConditioner.BottleC.Enabled	True	True to enable Bottle C.
SolventConditioner.BottleTestInterval	24	Number of hours between bottle tests.
SolventConditioner.Enabled	True	True to enable solvent conditioner control.
SolventConditioner.HistoryExpiration	4000	Hours until Solvent Conditioner history expires.
SolventConditioner.LastBottleTest	5/30/2008 2:10:19 AM	Date/time of last bottle test.
SolventConditioner.LastPressureCheck	5/30/2008 2:10:18 AM	Date/time of last bottle test.
SolventConditioner.LastPurge	5/30/2008 2:10:18 AM	Date / time of last purge.
SolventConditioner.PressureCheckInterval	8	Number of hours between manifold pressure checks.
SolventConditioner.PurgeInterval	72	Number of hours between manifold purge operations.
Communications.SolventConditioner.COM	COM6	COM port for Solvent conditioner.

Solvent Conditioner History

Test Component	Time	Manifold Pressure (psi)	Initial Pressure (psi)	Final Pressure (psi)	Test Duration (sec)	Pressure Drop Rate (psi/min)
Manifold	5/30/2008 2:00:18 AM	0.0	0.0	0.0	3	0.0
Solvent A	5/30/2008 2:00:18 AM	0.0	0.0	0.0	30	0.0
Solvent C	5/30/2008 2:00:18 AM	0.0	0.0	0.0	30	0.0
Solvent C	5/30/2008 2:12:54 AM	0.0	0.0	0.0	30	0.0
Solvent A	5/30/2008 2:12:54 AM	0.0	0.0	0.0	30	0.0
Manifold	5/30/2008 2:12:54 AM	0.0	0.0	0.0	3	0.0

The Solvent Conditioner History stores test results is available from the *Solvent Conditioner* link in the middle of the main web page. The time range can be selected along with a Filter of the individual items that are tested. Items on the solvent conditioner history automatically expire according to the *SolventConditioner.HistoryExpiration* Brain setting.

A set of Solvent Conditioner tests can be scheduled immediately as a background process by selecting the *Solvents / Start Bottle Test* menu item. The test results will appear in the history.

Database Backup and Restore

The One-Minute NMR software stores all of its data in a single SQL Server database supported by the Microsoft Data Engine (MSDE) server. Because the free MSDE server package does not include any client tools for database management, One-Minute NMR provides a simple utility for backup and restoration of the database. The contents of the database are stored to a file that can later be restored. This can be useful for saving alternative instrument configurations, or for saving your current configuration in case of a hard drive failure.

NOTE for SQL Server Client Owners: Scheduled automated backups of the database can be set up using the Microsoft SQL Server client software.

Backup

Select the Database / Backup Database... menu item in the RunProcess. You will be prompted for the file to back the database up to. If the backup file exists it will be removed before the backup starts.

Note: Files can't be backed-up to a network drive due to a quirk in MSDE.

Hint1: Back up your database after making changes to the Brain or People so that your changes will not be lost.

Hint2: Store your backup file on a network drive to prevent loss in case of a computer failure.

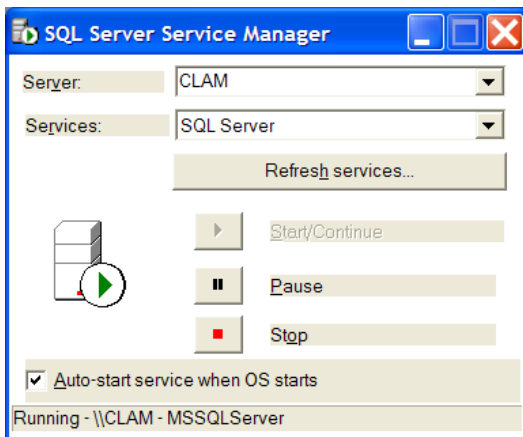
Restore

Caution: A database restore will erase any changes you have made since your last database backup.

Before a database restore starts you must exit the RunProcess and stop any web access. This can be accomplished immediately after computer boot,

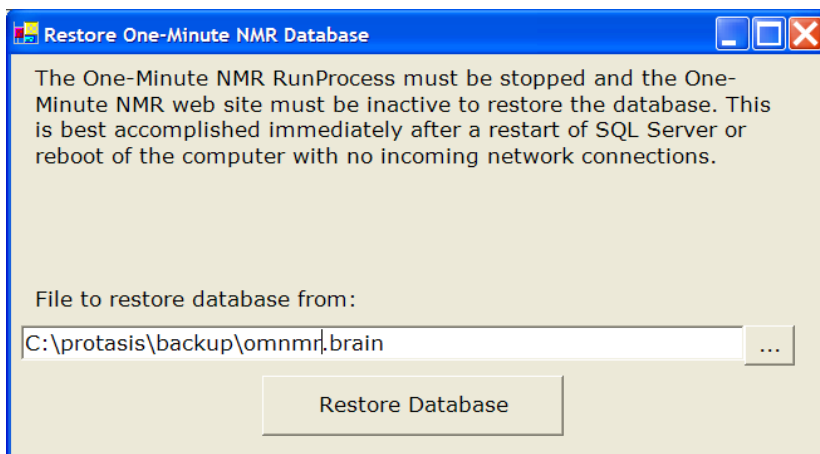
The One-Minute NMR web site can be paused with: Start Menu / Control Panel / Administrative Tools / Internet Information Services. Select the DefaultWebSite then click Pause Item in the tool bar.

The SQL Server engine can be stopped and re-started by right-clicking on the MSSQLServer icon in the task bar and selecting SQL Server Service Manager or the Stop menu item.



MSSQL Server Service Manager

When all One-Minute NMR database activity has stopped open the RestoreDatabase application in the One-Minute NMR desktop folder. The name of your last backup will automatically be displayed in the text box. You can select a different backup with [...].



RestoreDatabase program

Click Restore Database to start database restoration. The process may take several minutes.



Location of Experiments sent back to One-Minute NMR

It is possible to have One-Minute NMR retain the location of the results that were obtained from your NMR experiments. This feature is turned on when the System.ResultColumnEnabled is set to True. The locations of the NMR FID directories are displayed in the Results column on the sample table and in the tool tips for each sample when the experiments are completed.

Because some NMR implementations archive or database NMR data files a script named omnmr_filelocator is run on the NMR system to query the location of the data file based on the information entered for each sample and experiment. The omnmr_filelocator script must be present, but if it does not return the location of the FID the default FID location will be constructed from the inputs for that experiment.

File Locator

By using a programmatic interface on the NMR console computer the file locator gives you complete flexibility over the location of the files produced by your system.

One-Minute NMR calls the script that you implement called *omnmr_filelocator* on the NMR console computer to obtain the locations for the FID directory associated with your

sample. **You implement omnmr_filelocator** to tell One-Minute NMR where your files are located.

On Varian Linux or SUN systems the `omnmr_filelocator` is placed in the same directory as the `listener.tcl` script, usually `/home/mrm` or `/vnmr/mrm`. On Bruker Linux systems the location of the file locator is specified by the *NMR.Bruker.Windows.FileLocator* Brain Parameter. This allows the a program or batch file with any name to be used for the file locator.

The command line syntax of *omnmr_filelocator* is:

```
omnmr_filelocator "OMNMRUSER" "NRUSER" "SAMPLE" "EXPERIMENT"
"PLATEID" "CUSTOM1" "CUSTOM2" "CUSTOM3" ...
```

WHERE:

OMNMRUSER is the name of the One-Minute NMR user for the current sample.

NRUSER is the name of the NMR user for the current sample.

SAMPLE is the name of the sample. OMNMR uses this name to create the `.FID` directory for the sample, or to make a sub-directory for multi-experiment samples.

EXPERIMENT is the name of the experiment (macro) that is being run for the current sample.

CUSTOM1 is the name of the first custom field.

OUTPUT:

The output of the script goes to the standard output.

FID: **FIDDIR**

WHERE:

FIDDIR is the full path and file name to the phase file for this sample. The path is relative to the One-Minute NMR computer so must contain the correct machine name or mapped drive designation.

FIDDIR can be omitted if it is in the standard location used by One-Minute NMR.

Example *omnmr_filelocator*

The following example was written in C Shell script for a UNIX system. It will need to be modified to work with your system.

```
#!/bin/csh -f
set user=$argv[1]:q
set nmruser=$argv[2]:q
```

```
set sample=$argv[3]:q
set experiment=$argv[4]:q

echo "MOL:X:\molfiles\"$sample".mol"
echo "PHASE:X:\data\"$sample\"$experiment".FID\phasefile
echo "FID:X:\data\"$sample\"$experiment".FID"
```

In the above example if One-Minute NMR requested the location of the files by calling *omnmr_filelocator* with the following command line arguments:

```
omnmr_filelocator "Bob Albrecht" "nmrbob" "ABC123" "HSQC"
```

the response from this example program would be:

```
MOL:X:\molfiles\ABC123.mol
PHASE:X:\data\ABC123\HSQC.FID\phasefile
FID:X:\data\ABC123\HSQC.FID
```



Pressure History

One-Minute NMR systems configured with pumps that have a pressure transducer will record their pressure history in a database table. The pressure history is useful for tracking trends in pressure to predict necessary probe clean and filter change maintenance. Pressure history is accessed by clicking on the [Pressure](#) link in the middle of the main web page next to the pressure reading. Only systems that have a pressure transducer installed will have this link. Pressure transducers can be added to existing HTSL pumps by Protasis.

Pressure and flow rate X10 are displayed graphically at the top of the page. Pressure readings are only stored when the pump is delivering so that the pressure history for each sample can be viewed.

The pressure history time frame controls the graphical display of the pressure history and the tabular display below. The ***From*** and ***To*** values control the beginning and ending times of the pressure window. The ***Select*** control chooses a pre-set time from the last 15 minutes to the last 30 days.

The tabular display shows the ***Date*** and ***Time*** of the pressure reading, the ***Pressure*** in PSI, the ***Flow*** rate in microliters per minute, the name of the HTSL ***Pump*** that the pressure reading was taken from, and the ***Name*** of the sample that was running when the pressure reading was taken. Samples that have been purged from the system cannot show their Name. Pressure readings are sorted by date and time.

HTSL.PressureHistoryEnabled is set to True to enable the pressure history feature.

HTSL.PressureHistoryExpiration sets the number of hours that the pressure history is maintained in the database.



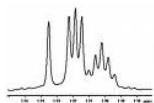
Controlling the Direction of the Liquid Handler

By default samples are selected from trays on the liquid handler in row order. That is they are taken from the back left of the tray in horizontal rows until the row is finished, then the next row is sampled.

Control of the direction that the liquid handler takes samples is done through two SQL queries built into the One-Minute NMR database. The queries are called RunQueue and NightQueue. Each of them returns the unique ID of the next sample to run and the order that samples are sorted in controls the direction of sampling.

One-Minute NMR provides two SQL scripts to control the direction of sampling globally. The scripts are c:\protasis\SQL\RowOrder.sql (the default) and c:\protasis\ColumnOrder.sql. You can run one of these scripts using the Database/Run Script... menu in the RunProcess. Once this change is made it applies to all samples until another script is run.

Contact technical support for assistance if you need the liquid handler to sample in a different order.



QC Check Samples

The integrity of the entire NMR system can be automatically checked using pre-defined quality control check samples for each solvent. Special QC samples are designated on the One-Minute NMR system. QC samples can be run on demand or periodically. When the software detects a QC sample, the signal to noise, line shape, and number of peaks in a selected region are compared to limits stored in The Brain.

Setting-up QC Samples


QC Samples contain a known concentration of a known compound in a specific solvent. Trays and plates of sealed QC Samples can be purchased from Protasis Corporation. User created QC samples must use the same compound and solvent as the Protasis / MRM QC samples or use specialized processing macros. Tightly-sealed vials must be used for QC samples to prevent evaporation and contamination from moisture in the air.

Brain Settings

The brain settings for QC samples are located under the Settings Category: *General Settings*, Settings Filter: *QC*.

Setting	Value	Description
QC.BrukerWindows.omnmr_qc	c:\protasis\omnmr_qc.bat	Analysis program to run for Bruker.Windows to get QC results.
QC.Countdown	0	Counter for QC samples. The countdown starts at QC.Frequency and when the counter is down to zero a QC sample is run.
QC.Enabled	False	True enables automatic running of QC samples. QC samples can still be run manually by selecting the QC experiment and running it as a sample.
QC.ExperimentName	autoQC	The name of the experiment to run for QC samples, typically <i>autoQC</i> .
QC.Frequency	10	How often to run a check sample automatically. A value of zero is never. A value of one is every other sample. A value of 10 is every 10 th sample.
QC.LineShapeLimit	1.5	The maximum line shape deformation. One is a perfectly symmetrical line, values greater than one are more asymmetric.
QC.LineShapeLimit.Solvent	1.5	The maximum line shape deformation for a specific solvent. The solvents DMSO and D2O are pre-defined, but additional solvents need to be added here. If this value is not specified for a solvent the limit defined by QC.LineShapeLimit will be used.
QC.MaximumNumberOfSignals	2	The maximum number of signals in the region tested for S/N.
QC.SignalToNoiseLimit	10	The minimum signal to noise value for the QC Sample.
QC.SignalToNoiseLimit.Solvent	3	The minimum signal to noise value for a specific solvent. If this value is not defined for a solvent then QC.SignalToNoiseLimit is used.
QC.SignalToNoiseLowerPPM	2	Lower ppm limit for signal to noise and number of signals calculation.
QC.SignalToNoiseUpperPPM	12	Upper ppm limit for signal to noise and number of signals calculation.

Designating Automatic QC Samples

In order to run QC samples automatically the *QC.Enabled* Brain setting must be True. Place the plate, vial tray, or partial vial tray of QC Samples on the liquid handler. On the One-Minute NMR web page select the tray where the samples are located. Click the QC icon  on the web page to designate the samples as QC samples. One-Minute NMR will automatically assign the QC experiment to this set of samples.

Running QC Samples Manually

One-Minute NMR recognizes any sample that uses the single QC experiment as defined by QC.ExperimentName as its NMR experiment. To run a QC experiment select the QC experiment from the list and run a sample as you normally would.

When QC Samples Run

There is one mode of success and several modes of failure for QC Samples. A QC check passes if a QC sample is available when it is needed, and all of test criteria pass. If no QC samples are available when the *QC.Countdown* reaches zero, or if any of the QC criteria are not met, then the run is stopped and an error message is issued. The error messages will indicate the each of the criteria that are out of range or the fact that no QC samples are available.

QC Samples for VNMRJ

This document describes how to install and use the autoQC macros to perform automated system integrity tests. The macros assume a single sample per solvent will be used to measure both S/N and Lineshape (FWHM). The raw fid data from the SIT will be saved, along with the calculated S/N and FWHM. The numbers will also be appended to a log file with a timestamp.

Installation

1. Copy the following Varian macros to the 'maclib' directory where the other OMNMR macros reside (such as 'autorun'). The macros and what they do are described as follows:

Macro	Description
autoQC_init	Initialize variables, provide instructions on next step.
autoQC_setls	Set the window parameters for Lineshape processing
autoQC_setsnr	Set the window parameters and integral resets for S/N processing
autoQC_save	Save the autoQC parameters and NMR acquisition parameters
autoQC_setup	Setup autoQC experiment
autoQC_proc	Process and save data from autoQC experiment
autoQC_createglobal	Utility function that sets up necessary global parameters
autosnr_getsolvent	Utility function that returns solvent name in lower case
autosnr_proc	Subroutine to process S/N data
autols_proc	Subroutine to process LS data

2. Go through the macros and edit the paths marked "EDITME". The UNIX tool 'grep' can be handy for this.

Setting up the QC experiment

1. Inject the sample you are going to use. In order to get a good QC baseline, use

- the automatic sample loading as you would during normal testing.
2. In VNMR, set up the basic 1D experiment to be used. Be sure the 'solvent' parameter matches the name in OMNMR ('DMSO', 'DMSO-d6' and 'CD3(SO)CD3' are all different, but the solvent name is case-insensitive, so 'DMSO' and 'dmsO' are the same).
 3. Take a test acquisition, and display the data, be sure to 'setref'
 4. Run the 'autoQC' macros:
 - a. Type 'autoQC_init'
 - b. Set the display to the peak that will be used for the LS measurement, then type 'autoQC_setls'
 - c. Set the integral resets to cover all the peaks, set the display to the peak and noise region to be used for the S/N measurement, then type 'autoQC_setsnr'
 - d. Type 'autoQC_save'. This will prompt you to confirm the settings and provide a sample name.
 5. Setup the 'autoQC' experiment in OMNMR.
 - a. The experiment name is 'autoQC_setup'
 - b. The processing macro is 'autoQC_proc'
 - c. The spectrum window and spectrum center must match those used in setting up the experiment on VNMR. If these do not match the integral resets will not be correct.

Using autoQC

To run autoQC, put the test sample on the LEAP and run the 'autoQC_setup' experiment on it. The results will be stored in the file 'qc.log' on the OMNMR home directory on the spectrometer. The data will also be reported back to the OMNMR software.

QC Samples for Bruker Systems

The system consists of some macros, scripts, and parameter files that report the signal-to-noise ratio, asymmetry for a single peak, and the number of peaks in a selected region. One-Minute NMR then analyzes the results and compares them to acceptable values to decide to continue.

System Components

AU Macros

autoqc

Runs as a processing macro for QC samples. It is a shell that runs processing, peak picking, signal-to-noise calculations, asymmetry calculations and writes the results to a file for later use

qcproc

Processing macro for autoqc. The default processing sequence is efp, apk, abs.

asym

Calculates peak asymmetry for a single peak in the plot region at 10% of the peak height.

Parameter Table

autoqc.table

A table of parameters used to analyze the QC sample in each solvent.

Scripts

qmmnr_qc.bat

Windows batch file that returns the results of the QC sample calculations to One-Minute NMR.

omnmr_qc

Linux script that returns the results of the QC sample calculations to One-Minute NMR

Operational Details

Setting up the AutoQC Experiment

The experiment used for QC calculations must be specified in the Available Experiments list of the brain and the process file for the QC experiment must be the autoqc AU macro.

QC Brain Settings

Under General Settings in the One-Minute NMR Brain the QC.ExperimentName parameter must be set to the name of the QC experiment set up in the Available Experiments list. Other parameters for the QC experiment must also be set up including the signal-to-noise, lineshape, and maximum number of signals for each solvent, and a default that applies to unknown solvents.

Parameter Table

The parameter table autoqc.table is located in the XWIN or Topspin prog directory (e.g. /bruker/XWIN-NMR/prog) and is accessed by the autoqc macro on the Bruker computer. It contains one line for each solvent. It is expected that the QC sample properties or the parameters required to correctly process the QC sample in a solvent will vary.

The first line of the autoqc.table has column headings for the table. Each of the parameters is described below.

```
solvent asym_start, asym_end, pp_start, pp_end, sigf1, sigf2, noisf1,
noisf2, mi, maxi, pc, cy
```

The following lines in autoqc.table have the name of the solvent followed by the parameters for that solvent.

```
DMSO      1.1      1.4      1.5      3.5      1.1      1.4      3.3
4.5      2.2      .34      12      2
```

solvent

The name of the solvent that this set of parameters is for.

asym_start, asym_end

The ppm range for the peak used in asymmetry calculations that correspond to the plot region parameters F1P and F2P.

pp_start, pp_end

The ppm range for peak picking for the purpose of counting peaks in the spectrum that correspond to the plot region parameters F1P and F2P.

sigf1, sigf2

The NMR field range for the signal in signal to noise calculations corresponding to SIGF1 and SIGF2 parameters.

noisef1, noisef2

The NMR field range for the noise in signal to noise calculations corresponding to the NOISEF1 and NOISEF2 parameters.

mi

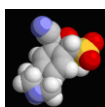
Minimum intensity for peak picking corresponding to the MI parameter.

maxi

Maximum relative intensity for peak picking corresponding to the MAXI parameter.

Scripts

The omnmr_qc Linux script of the omnmr_qc.bat batch file must display the contents of the file generated by autoqc. The autoqc file will be located in the XWIN or Topspin prog directory and have the name autoqc.txt. The omnmr_qc scripts are easy to edit with a text editor.

**Automated Structure Confirmation**

One-Minute NMR provides an interface for automated structure confirmation using the ACD Automation Server 9 software. Structures are confirmed using your molecular structure files and one or two NMR runs. The first NMR run must be a 1D Proton experiment, and the second an HSQC experiment. After the 1D proton experiment the ACD software is used to check if the HSQC experiment is necessary by deciding if the confirmation level is above the cutoff. After runs are complete confirmation results are visible on the One-Minute NMR web site and are sent in an HTML formatted e-mail.

Operator Interface


The operator interface includes the extra step of importing molecules for each sample and the display of confirmation results on the web site and in an HTML formatted e-mail. These features are only available after the proper licensing and setup procedures have been followed.

Importing Molecules

The native Molecule file format is MDL MOL file format. Molecule files in other formats are converted when they are imported into MDL MOL format. The list of acceptable file formats is below. Files are stored in the One-Minute NMR database as Binary Large Objects (BLOBs) in the One-Minute NMR sample queue. The files are copied to the NMR console computer immediately before experiments for each sample are started.

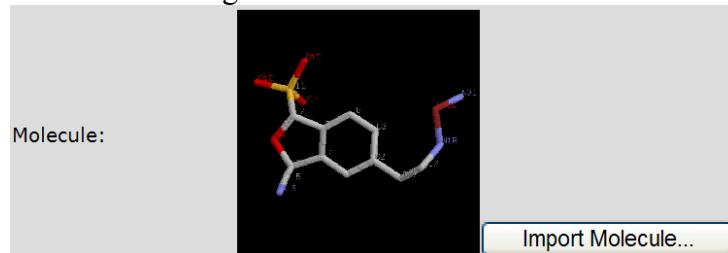
Single Molecules

When single, or small numbers, or samples are run the **Import Molecule...** button is used to import your molecule file. The allowed molecule file formats and proper file extensions are listed below.

1. Click the  button under (2) on the main web page.
2. Enter the full file path to the molecule in the text box or click **Browse...** to select the file.

Molecule:

3. Click Upload to send the file to One-Minute NMR or Cancel to cancel the operation. When the import is successful One-Minute NMR will display a ball and stick drawing of the molecule.



4. This molecule will be used when you select a plate/well or tray/vial under (3) on the main web page.
5. With this mode of operation you will have to repeat these steps for each sample that has a different molecular structure. For multiple samples use Sample Lists.

Sample Lists with Molecules

When importing multiple samples or multiple vial trays of samples that include molecule files it is best to import .CSV file sample lists and molecule files. Details of the Import Conversion template are given above.

If you use SMILES strings for your molecular structures the molecules can be embedded in the .CSV file, otherwise molecule files need to be referenced by the .CSV file in the **Molecule** field. When molecular structures are referenced by the .CSV file the .CSV file and all of the referenced molecules must be included in a single .ZIP archive so that One-Minute NMR can access both the sample list and all of the molecules in a single operation.

SAMPLE	EXPERIMENT	MOL	VIAL
td_1	H11D&HSQC	td_1.mol	1
td_2	H11D&HSQC	td_2.mol	2
td_3	H11D&HSQC	td_3.mol	3
td_4	H11D&HSQC	td_4.mol	4
td_5	H11D&HSQC	td_5.mol	5
td_6	H11D&HSQC	td_6.mol	6
td_7	H11D&HSQC	td_7.mol	7
td_8	H11D&HSQC	td_8.mol	8
td_9	H11D&HSQC	td_9.mol	9

Table - Example .CSV File with Referenced Molecules

Note that the EXPERIMENT column contains H11D&HSQC. One-Minute NMR will first run the experiment (macro) named H11D and start a structure confirmation immediately after this experiment is complete. If the confirmation level is not above the cutoff the experiment HSQC is performed. When the results of the HSQC experiment are available One-Minute processing is re-done on the H11D experiment and done for the first time on the HSQC experiment.

Import ID	Imported Field	Samples Table Field
default	EXPERIMENT	Experiments
default	MOL	Molecule
default	SAMPLE	FileName
default	VIAL	VialIndex

Table - Example Import Conversion Template from *The Brain*

Experiments

There are specific requirements for experiments used with automated structure confirmation. The best confirmation results are generated from a 1D proton NMR and an HSQC experiment.

One-Minute NMR requires that the name of the experiment (macro) for the 1D proton have the letters “1D” in the name. This is how One-Minute NMR distinguishes between 1D and 2D experiments. There are no specific requirements for the name of the HSQC experiment (macro), but HSQC is a good identifier.

When there are good positive results from the 1D proton experiment that are above the cutoff level, the sample is considered to be confirmed and the HSQC experiment is skipped.

Experiments that contain the word “scout” are skipped by the structure confirmation interface because they are assumed to be scouting runs for solvent suppression experiments.

Web Page Display of Results

After each sample is complete the results are displayed on the One-Minute NMR web page. You can access the results

Confirmation Symbols

Structure confirmation results are displayed graphically on the One-Minute NMR web page using three different shaped symbols. The **confirmed symbol** ▲ is used to indicate that the average of the ACD Verification Product for all experiments is above the acceptance level specified in the One-Minute NMR brain. The **rejected symbol** ▼ indicates that the Verification Product is below the rejection level specified in the brain. The **ambiguous symbol** ✕ indicates that the Verification Product is between the rejection level and the acceptance level specified in the brain. By default the acceptance and rejection level are the same so ambiguous samples will not be displayed.

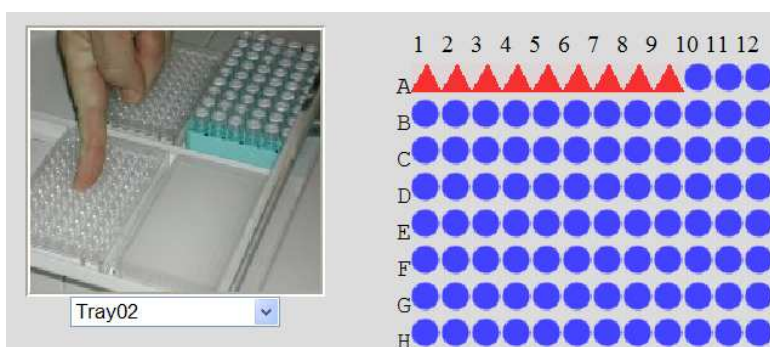


Figure - Structure confirmation results on the One-Minute NMR Web Page

Instant Tool Tips

Tool tips, accessed by holding the mouse pointer over a sample well location, are used to instantly display the structure confirmation results for samples displayed on the One-Minute NMR web page. This gives you a way to quickly view the verification product for each sample without using the ACD Web Librarian or Links To Data.

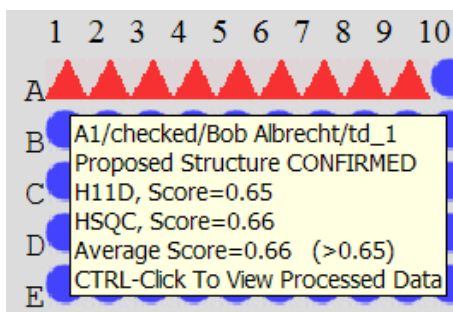


Figure - Confirmation Results Instant Tool Tip

Links to Data

CTRL-Click on a sample with structure confirmation information will display the molecule for the sample and the structure confirmation results with links to the processed NMR data through the ACD Web Librarian.

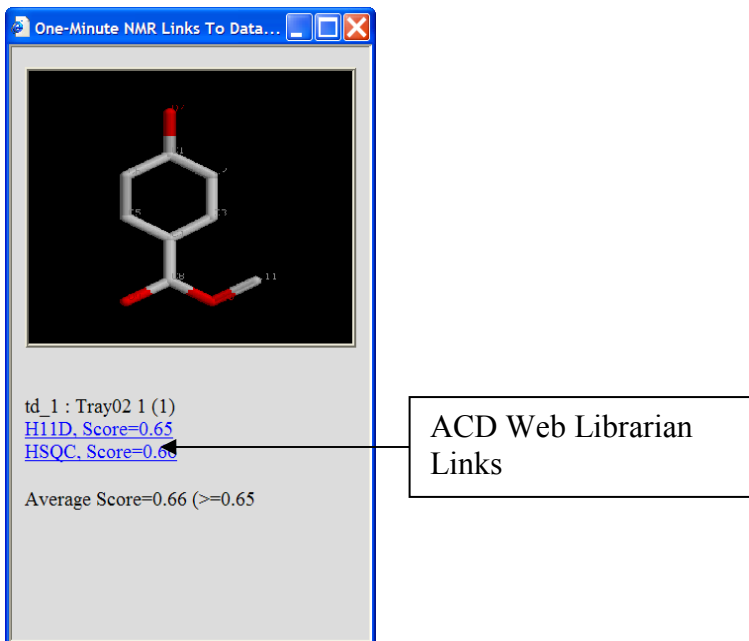


Figure - "Links To Data" popup

HTML E-Mail

If One-Minute NMR is configured to send e-mail to users, and if e-mail addresses are specified in One-Minute NMR, an HTML formatted e-mail is sent with all of the structure confirmation results and direct links to the ACD web librarian. The e-mail is sent only when all samples are finished complete for a particular user in order to summarize the results on a single page. You can log into One-Minute NMR and get results before all of your samples are complete.

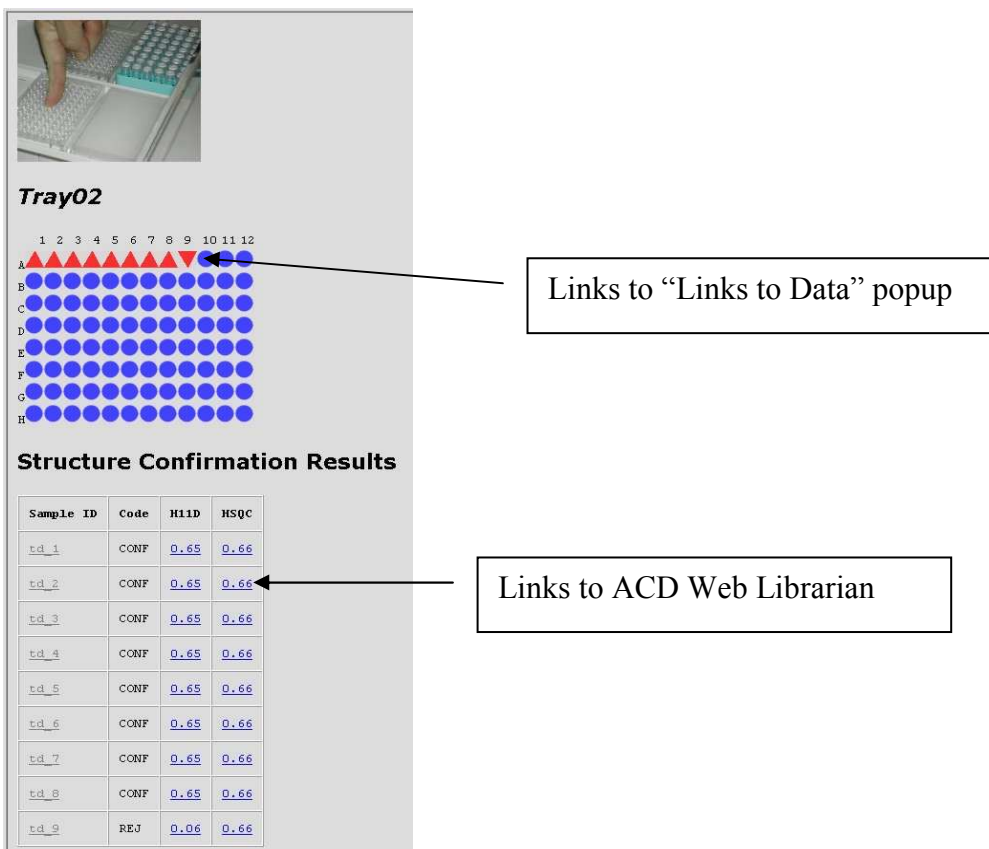


Figure - HTML E-Mail results

ACD Web Librarian

The ACD Web Librarian is the easiest way to access complete results for your samples. By clicking on the links in the HTML E-Mail or the Links To Data window you are taken directly to the ACD Web Librarian displaying the results for your sample.

qm1gp	Ghemical QM
hin	HyperChem HIN
jout	Jaguar Output
bin	OpenEye Binary
mmd, mmod, out, dat	MacroModel
car	MSI Biosym/Insight II CAR
sdf, sd	MDL Isis SDF
mdl, mol	MDL Molfile
mopert	MOPAC Cartesian
mopout	MOPAC Output
mmads	MMADS
mpqc	MPQC
bgf	MSI BGF
nwo	NWChem Output
pdb, ent	PDB
qcout	Q-Chem Output
res	ShelX
smi	SMILES
mol2	Sybyl Mol2
unixyz	UniChem XYZ
vmol	ViewMol
xyz	XYZ

Table - Supported molecule types and extensions

Structure Confirmation Setup

The structure confirmation interface is a linkage between ACD Automation Server and Protasis One-Minute NMR. The connections between the software are simple to manage but require attention to detail to work correctly.

ACD Software Installation

Use the ACD/Labs installation program to install Automation Server 9 and Web Librarian. The Oracle-based version of ACD software must be used due to concurrency issues with the flat-file based version of the ACD software.

Disabling ACD Service Manager (SM.EXE)

Due to a software conflict the ACD Service Manager must be disabled. Check the Windows Task Manager to see that SM.EXE is not running. If it is, kill the task. Disable the server manager from ***Start Menu/Control Panel/Administrative Tools/Services***. Right click on ***ACD/Labs Server Manager***, select ***Properties***, from the ***Startup Type*** select ***Disabled***.

Licensing

The One-Minute NMR interface to the ACD structure confirmation software is an optional feature and requires that a license key be set in the **Confirmation.License** brain setting. The correct license key for your specific system is available from your Protasis sales representative.

Confirmation Brain Settings


The settings for structure confirmation are stored in the Confirmation section of the One-Minute NMR Brain.

Setting	Value	Description
Confirmation.1DH1.AcceptanceLevel	.85	Acceptance level to stop after 1D proton acceptance.
Confirmation.AcceptanceLevel	.65	Level at which a structure is considered confirmed.
Confirmation.ACD.1DScript	C:\protasis\ACD\1DMRM_ACDv10_rev3.0.cpp	ACD Script template for 1D data.
Confirmation.ACD.2DScript	C:\protasis\ACD\2DMRM_ACDv10_rev3.2.cpp	ACD Script template for 2D data.
Confirmation.ACD.Database	C:\AS_MRM\DATA	ACD Database location.
Confirmation.ACD.DataRoot	P:	Root of data path. Users NMR Data Path is appended to find results.
Confirmation.ACD.Hostname	10.0.0.100	Name of server or IP address for links to ACD Web Librarian
Confirmation.ACD.LogResults	True	Logs the results from the ACD confirmation software to protasis.log.
Confirmation.ACD.Path	C:\AS_MRM\ESPFiles	The path to structure confirmation files for ACD.
Confirmation.ACD.Program	C:\ACDSRV10\SMROBOT.SRV\smrobot.exe	The name of the program to run for ACD confirmations.
Confirmation.ACD.XMLConfig	C:\protasis\ACD\Config_MRM_signal.xml	ACD Script template for 2D data.
Confirmation.Interface	ACD	Current interface for structure confirmation.
Confirmation.License	Call Protasis Sales	License for structure confirmation module.
Confirmation.PhaseFile	phasefile	The name for phase files stored in FID directory (e.g. SampleID.FID/phasefile).
Confirmation.ProcessDelay	90	Number of seconds to delay for processing to complete.
Confirmation.RejectionLevel	.65	Level at which structure is rejected.
Confirmation.MoleculeAutomatic	True	Set to True finds molecules with omnmr_filelocator.
Confirmation.ShowMoleculeUpload	True	Set to True to allow Mol file entry.
Confirmation.ShowSmiles	False	Set to True to allow SMILES string entry.
Confirmation.ContaminantSolvents		Comma-separated list of contaminant solvents.
Confirmation.SuppressedSolvents		Comma-separated list of suppressed solvents for all samples.

Table - Confirmation Section of *The Brain*


Decision Levels

The structure confirmation interface has three decision levels that control how experiments are performed and results are displayed.

Confirmation.AcceptanceLevel is used to display the graphic results of the confirmation. Samples that have an average ACD Verification Product equal to or higher than the Acceptance Level are displayed with the **confirmed symbol**  and the results are labeled with the word CONFIRMED. The AcceptanceLevel can be changed after

experiments are completed to change the display of samples in the One-Minute NMR web page, but e-mails sent with embedded graphics are not affected.

Confirmation.1DH1.AcceptanceLevel is used to decide when a 1D proton experiment has good enough results to not require a subsequent HSQC experiment. Immediately after the first 1D proton experiment One-Minute NMR calls on ACD software to do a structure confirmation based on that experiment. If the ACD Verification Product for the 1D proton experiment exceeds this level no further experiments are performed.

Confirmation.RejectionLevel is used to display the results of the confirmation graphically. Samples that have an average ACD Verification Product less than or equal to this level are displayed with the **rejected symbol**  and the results are labeled with the word REJECTED. The RejectionLevel can be changed after experiments are completed to change the display of samples in the One-Minute NMR web page, but e-mails sent with embedded graphics are not affected.

When the average ACD Verification Product **falls between** the **Confirmation.RejectionLevel** and the **Confirmation.AcceptanceLevel** the results are displayed with the **ambiguous symbol**  and results are labeled with the word AMBIGUOUS.

Software Interface Parameters

Confirmation.ACD.DataRoot is the network location of the NMR data files relative to the Protasis Discovery Tower or One-Minute NMR computer; how One-Minute NMR finds your data. The path is usually a network drive, possibly referencing a SAMBA share, set up in Windows to the data storage location on the NMR console computer.

The **Confirmation.ACD.1DScript** and **Confirmation.ACD.2DScript** define the locations of the script templates. The ACD Software is controlled by two custom script templates provided by ACD Labs. During the structure confirmation process One-Minute NMR replaces parameters in these scripts and starts the ACD software.

Confirmation.ACD.Database is used to define the directory where the ACD database is stored. This can be stored on any computer, but very fast access to the specified drive is required for to avoid slowdown of the sample queue.

Confirmation.ACD.Hostname is the network address or DNS name of the computer that serves the ACD Web Librarian. The hostname is included in links to the ACD Web Librarian that are sent by e-mail or displayed in the **Links To Data** popup. This can be a Protasis Discovery Tower or Protasis supplied computer used for One-Minute NMR, or another system on a network that hosts ACD Web Librarian.

Confirmation.ACD.LogResults is set to True if you want to log results from ACD confirmations to the C:\Protasis\Protasis.log file. Set this parameter to False if you do not need this information.

Confirmation.ACD.Path is the path to the directory used by the ACD software for temporary data processing.

Confirmation.ACD.Program is the complete file and path to the program used to do the ACD Structure Verification.

Confirmation.ACD.XMLConfig is the complete path and file name to the XML configuration file used by the ACD software.

Confirmation.Interface identifies the type of confirmation interface, currently ACD is the only valid value.

Confirmation.License the license key for the structure confirmation interface. Contact Protasis Sales.

Confirmation.PhaseFile specifies the name that is used for the phase file. One-Minute NMR expects that the phase file will be located in the .FID directory for the experiment.

Confirmation.ProcessDelay is the delay in seconds from the end of the last experiment to the time e-mail results are sent. This delay is necessary because processing of 2D experiments is done in parallel with other processes. If the results of the last sample in e-mailed results are not completely processed, extend this time.

Confirmation.MoleculeAutomatic is set to True when you want the omnmr_filelocator to tell the confirmation sub-system where the molecule files for a sample are located without having to upload them to One-Minute NMR.

Confirmation.ShowMoleculeUpload is set to True if the molecule upload section is visible on the main One-Minute NMR web page. This will allow users to upload structures to One-Minute NMR.

Confirmation.ShowSmiles is set to True if the SMILES entry field is to be made available on the One-Minute NMR main web page.

Confirmation.ContaminantSolvents comma-separated list of contaminant solvents that is passed to the ACD scripts.

Confirmation.SuppresseSolvents comma-separated list of suppressed solvents that is passed to the ACD scripts.

Confirmation.DatabaseOnly is set to True if the databasing-only scripts are used.

Requirements for Experiments (macros)

Experiments are macros that control the NMR system. There are specific requirements for experiments when using the ACD Structure confirmation interface:

1. Experiments that have the word “scout” in the name are skipped and not used in structure confirmation. They are assumed to be scouting runs for solvent suppression.
2. The first experiment after any scouting runs, must be a 1D proton experiment.
3. The 1D proton experiment must contain the substring “1D” in the name. Processing is different for 1D experiments.
4. A 2D HSQC experiment must follow the 1D proton experiment. The experiment can have any name.
5. Extra experiments that you do not want to take part in the structure verification process can be labeled by including the word “extra” in the experiment name.

Importing

The easiest way to get sample and molecule information to One-Minute NMR is through imported sample lists. If you use correct import features very little interaction will be required with the Web interface. Here are some suggestions for importing:

1. Specify all of the experiments you want to perform in the Experiments field. For example: “Scout1D&Wet1D&WetHSQC”.
2. Use MDL MOL files for molecules unless it is difficult to obtain them. This is the native format for One-Minute NMR and using them prevents the need to translate files.
3. Always include the FileName field is necessary, but you should also add the SampleID (title text) to better identify the sample.
4. New users can be imported automatically by specifying them in the Username field. Their e-mail address should be included so that results reach the right person. Be sure to set up a user named “template” so that the parameters for the new user can be set up automatically.
5. Multiple vial trays or plates can be imported simultaneously, but you must specify the TrayPlate for each sample that is not going to the currently selected tray.
6. The only way to import lists of samples (CSV files) that reference molecule files is to put them together in a directory, make a ZIP archive of the whole directory, import the ZIP archive.

File Locator

By using a programmatic interface on the NMR console computer the file locator gives you complete flexibility over the location of the files that One-Minute NMR and the ACD software uses for structure confirmation. With the file locator you can keep your files in any location on your network without having to copy them for structure confirmation.

One-Minute NMR calls the script that you implement called *omnmr_filelocator* on the NMR console computer to obtain the locations for the MDL MOL file associated with your sample, the phase file, and the FID directory. **You implement omnmr_filelocator** to tell One-Minute NMR where your files are located.

The command line syntax of *omnmr_filelocator* is:

**omnmr_filelocator "OMNMRUSER" "NRUSER" "SAMPLE" "EXPERIMENT"
"CUSTOM1" "CUSTOM2" "CUSTOM3" ...**

WHERE:

OMNMRUSER is the name of the One-Minute NMR user for the current sample.

NRUSER is the name of the NMR user for the current sample.

SAMPLE is the name of the sample. OMNMR uses this name to create the .FID directory for the sample, or to make a sub-directory for multi-experiment samples.

EXPERIMENT is the name of the experiment (macro) that is being run for the current sample.

CUSTOM1 is the name of the first custom field.

OUTPUT:

The output of the script goes to the standard output.

MOL: **MOLFILE**

PHASE: **PHASEFILE**

FID: **FIDDIR**

WHERE:

MOLFILE is the full path and file name to the MDL MOL file for this sample. The path is relative to the One-Minute NMR computer so must contain the correct machine name or mapped drive designation.

PHASEFILE is the full path and file name to the phase file for this sample. The path is relative to the One-Minute NMR computer so must contain the correct machine name or mapped drive designation. Note: This is not used by ACD Version 10 scripts and higher.

FIDDIR is the full path and file name to the FID directory for this sample. The path is relative to the One-Minute NMR computer so must contain the correct machine name or mapped drive designation.

MOLFILE, **PHASEFILE**, and **FIDDIR** can be omitted if they are in the standard location used by One-Minute NMR.

Example *omnmr_filelocator*

The following example was written in C Shell script for a UNIX system. It will need to be modified to work with your system.

```
#!/bin/csh -f
set user=$argv[1]:q
```

```

set nmruser=$argv[2]:q
set sample=$argv[3]:q
set experiment=$argv[4]:q

echo "MOL:X:\molfiles\"$sample".mol"
echo "PHASE:X:\data\"$sample\"$experiment".FID\phasefile
echo "FID:X:\data\"$sample\"$experiment".FID"

```

In the above example if One-Minute NMR requested the location of the files by calling *omnmr_filelocator* with the following command line arguments:

```
omnmr_filelocator "Bob Albrecht" "nmrbob" "ABC123" "HSQC"
```

the response from this example program would be:

```

MOL:X:\molfiles\ABC123.mol
PHASE:X:\data\ABC123\HSQC.FID\phasefile
FID:X:\data\ABC123\HSQC.FID

```

E-Mail Configuration

Proper configuration of the *Communication.Email* section, which is **described in The Brain** section of the documentation is necessary to obtain e-mail reports of completed sample sets.

Each user that receives e-mail notifications must have their e-mail address configured. The e-mail address of users can be set in the People section of One-Minute NMR and/or can be imported as a part of a sample list. See the **Import Conversion** section of the documentation.

DataChord Integration

One-Minute NMR will optionally attach a file that is used by One-Moon Scientific DataChord to start automatic processing and to reference results produced by the One-Minute NMR system. The attached file has the .dcs1 extension which is registered by the DataChord client to automatically start the program. When the attachment is double-clicked DataChord opens and loads the data referenced in the attachment. The feature is turned on by The Brain setting *Communication.Email.DataChordReport=True* combined with *System.ResultColumnEnabled*.

Internet Explorer and Web Librarian

Because the ACD Web Librarian uses ActiveX controls with Java to provide its functionality, it is necessary to use Microsoft Internet Explorer to connect with the links to data provided by the One-Minute NMR structure confirmation system.

ActiveX controls and plugins must be enabled in Internet Explorer for Web Librarian to work. The Tools/Internet Options.../Security tab in Internet Explorer has options to enable ActiveX and scripting.

Enabling Popups For This Web Site

Popups should be enabled to allow the “Links To Data” popup to work on the One-Minute NMR web site. Popups should be enabled for the Google or Yahoo toolbar and controlled through Internet Explorer options. For Google click the Options button, select the Browsing tab, and un-select Popup Blocker. From Internet Explorer select the Tools/Popup Blocker/Popup Blocker Settings... For the One-Minute NMR computer itself add *localhost* to Address of website to allow and click Add. For remote computers add the IP address or the machine name of the One-Minute NMR computer.

Firewall Configuration

On the One-Minute NMR Instrument server port 8100 needs to be opened in the Windows firewall for ACD Web Librarian. Open Start Menu/Control Panel/Windows Firewall/Exceptions..., click Add Port, type in WEBLIB for the name and 8100 for the port. Click OK to make the change.

Enabling Web Librarian

The ACD Web Librarian Service must be enabled in Start Menu/Control Panel/Administrative Tools/Services/ACD Web Librarian Service. The startup type should be Automatic.

Web Librarian Settings

1. From the Web Librarian server, go to the installation directory C:\ACDSRV9\WEBLIB.SRV\CONF\ and open the file ACCESS.CONF
2. There is a section called “access groups” in the file. Here you should put all the IP addresses of the computers that are to access Web Librarian. In your case, you would probably want to add the IP of the Protasis computer as well as your office PCs:

```
[access_groups]
acd_protasis      = 10.37.8.26 <your computer> 127.0.0.1
all               = 0.0.0.0/0.0.0.0
```

where *<your computer>* is the IP address of your computer. Notice, the IPs are separated by spaces. If your PC is using DHCP, then you can use an IP range instead:

e.g.

```
[access_groups]
acd_protasis      = 10.37.8.26 10.37.8. 127.0.0.1
all               = 0.0.0.0/0.0.0.0
```

3. In the “Web Librarian” section of the ACCESS.CONF file, make sure that the “acd_protasis” access group is added. Notice that all the other unnecessary access methods are commented out using “#”.

```
[WebLibrarian]
none              = acd_protasis
#emulate         = mitya
#ldap (195.209.47.4) = somebody
#oracle (bugdb.world:WL_ROLE) = surnin
```

```
#oracle (lims.acd)           = somebody
#domain (ACD_NT:WL)         = acd_bakuleva
#domain (BUILDB:LIMS)      = acd_lims
#webapp (http://www2.acdlabs.com/ilab/ session_id;user_id;access_group)
= valt acd_toronto
#extapp (authprog.exe)     = acd_all
deny                       = all
```

4. Save the ACCESS.CONF file.
5. Using the Service Control Panel, restart the Web Librarian Service.
6. Open a new browser and try accessing.

Disabling ACD/Labs Server Manager

The ACD/Labs Server Manager is incompatible with the One-Minute NMR structure confirmation software which uses ACD/Labs Automation Server and must be disabled. Open Start Menu/Control Panel/Administrative Tools/Services. Locate ACD/Labs Server Manager. Right-Click and select Properties. Change the Startup Type to disabled. Click the Stop button. Click OK. Close the Services Window.

Leap Liquid Handler

Password Protection

Go to Menu, F3, Setup-Access. There are three setting that can be changed from the default 0. Once you input a number or letter in the individual field that number or letter needs to be input before access to the function will be allowed.



Alternative Login

It is easy to develop alternative login pages for One-Minute NMR that verifies users against an LDAP server or other user directory. An example web page written in C# for ASP.NET is provided with source code One-Minute NMR. The login information is delivered to One-Minute NMR in a temporary browser cookie.

Using the alternative login procedure it is possible to:

- 1) Log-in existing users
- 2) Automatically specify new users with a name, password, e-mail, and private data directory.
- 3) Return to the alternative login screen automatically on logout.
- 4) More easily maintain an open access environment.
- 5) Maintain users and passwords in a central directory and remove the need to maintain a separate user list for One-Minute NMR.


Setting-Up Alternative Login

Login Web Page

Your login web page should check the authenticity of the username and password. If the e-mail address and data directory for the user are available that information should also be passed to One-Minute NMR.

Creating a template user

To allow automatic creation of new users by the alternative login procedure you will need

to create a new user in the One-Minute NMR People  page named “template”. You should specify the user account, NMR data directory, and e-mail for the template user. These values will be used as defaults for when they are not specified by login cookie. The template user and its fields are also used for importing sample and user lists when new users to the system are imported.

Creating the login cookie

The One-Minute NMR login information is communicated in a single HTTP cookie named *protasis.com.OneMinuteNMRAuthentication*. The value string for the cookie contains a set of name/value pairs that represent the information needed for login.

The names of the fields used by One-Minute NMR

Name	Value
<i>adminUsername</i>	The name of a One-Minute NMR user that has “can edit user accounts” rights. This is required.
<i>adminPassword</i>	The password of the administrative user.
<i>account</i>	The One-Minute NMR account for the user. This field can be omitted and the first listed account for the user, or template user, will be used by default.
<i>username</i>	The name of the One-Minute NMR user to log in. If this user does not exist and the template user exists, then a new user with this name is created.
<i>Email</i>	The e-mail address of the existing user. If the e-mail address is specified for an existing user it will be updated to this value. If this is a new user the e-mail address will be used for this new user.
<i>datadir</i>	The private data path for the user. If this is a new user the value will be used for the NMR Data Path for the user. If this is an existing user the NMR Data Path will be modified.
<i>failpage</i>	If this value is specified and login fails the web page is redirected to this address. If this value is not specified the login page is displayed after the failure. Login can fail because there is no template user or because the administrative user does not exist or does not have administrative rights.
<i>LogoutRedirect</i>	In some circumstances, secure web sites for instance, the referrer is obscured. Use this element to specify the page to direct to on logout.

The Login Cookie should expire within 1 minute of when it is created to reduce the possibility of security problems. The expiration time for the login cookie should be only slightly longer than is needed for the server to process the submit of the web page.

C# Method for making cookies

```
private void make_OMNMR_cookie(string adminUsername, string
adminPassword, string account, string username, string password, string
email, string datadir, string failpage)
{
    HttpCookie cookie = new
    HttpCookie("protasis.com.OneMinuteNMRAuthentication");

    StringBuilder cookieInfo = new StringBuilder();

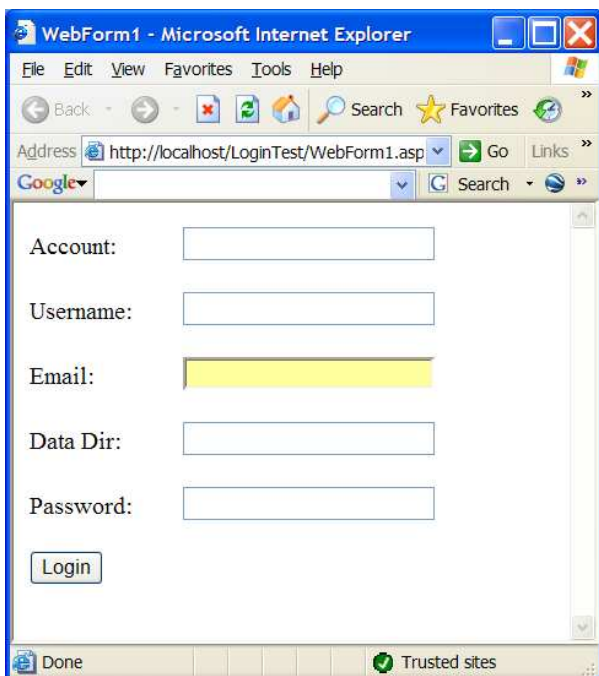
    cookie.Values.Add("adminUsername", adminUsername);
    cookie.Values.Add("adminPassword", adminPassword);
    cookie.Values.Add("account", account);
    cookie.Values.Add("username", username);
    cookie.Values.Add("password", password);
    cookie.Values.Add("email", email);
    cookie.Values.Add("datadir", datadir);
    cookie.Values.Add("failpage", failpage);
    //Set the cookie to expire in 1 minute
    TimeSpan tsMinute = new TimeSpan(0, 0, 1, 0);
    cookie.Expires = DateTime.Now + tsMinute;
    //Add the cookie
    Response.Cookies.Add(cookie);
}
```

A typical alternative login implementation might request the Username and Password from the *username*, verify that the *password* is correct, look up the *email* address, create the *datadir* using a standard template for data directories (e.g. /data/username), and internally specify the *adminUsername*, *adminPassword*, *account*, and *failpage*.

Preventing Normal Login

To increase security normal login should be prevented. If it is not it may be possible for users to log in using a direct connection to the web site. Normal login is prevented by setting The Brain setting `System.AlternativeLoginOnly=True`.

The Example Login Page



The LoginTest example program.

The source for the example web site written for Microsoft Visual Studio ASP.NET in C# is located in the c:\protasis\LoginTest directory. This example was used to test the alternative login screen feature for One-Minute NMR.



Automated Setup

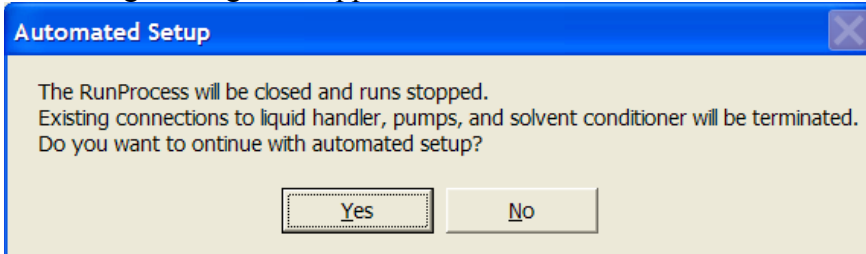
Automated setup is used to configure the serial communications ports for HTSL pumps, the CTC liquid handler, and the solvent conditioners. The initial solvent volumes are calculated based on the length of 100 micron tubing to the NMR probe, the type of solvent, and if sample return is used.

If you have an existing One-Minute NMR configuration you should do perform a Database Backup before running Automated Setup.

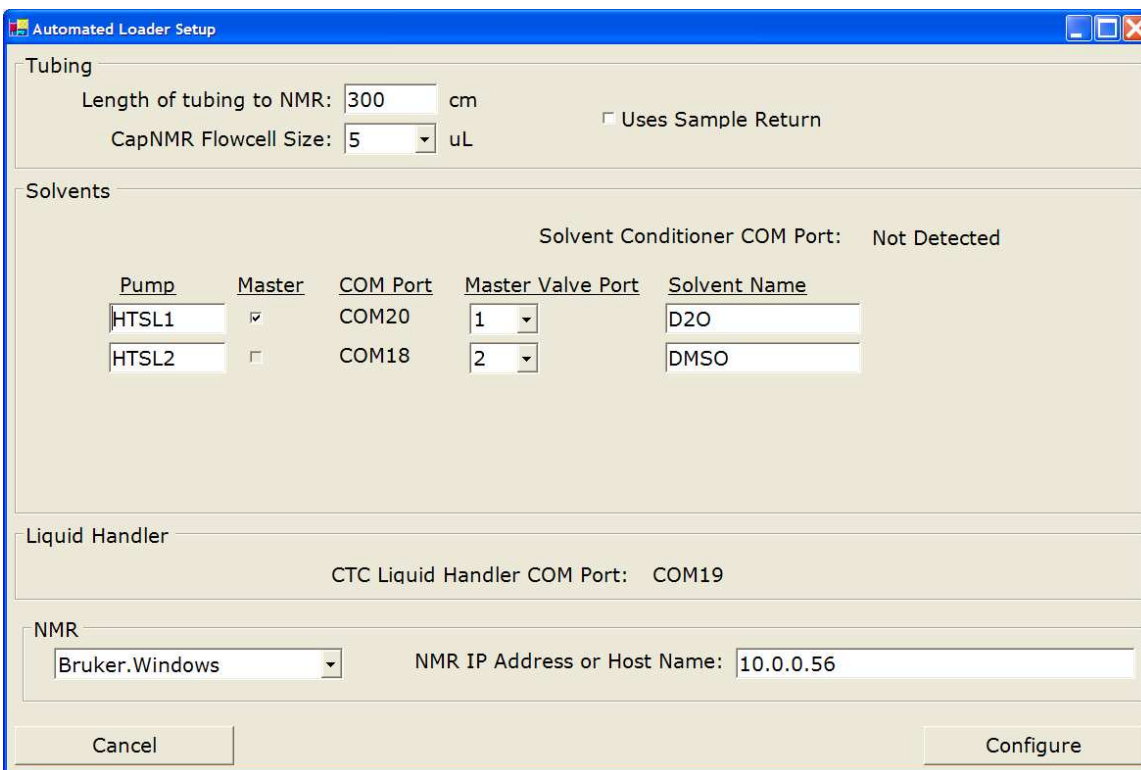
The Brain data that are configured by Automated Setup are defined in the Settings Category: General, Pumps, Available Solvents, and Solvent Change, and in Communications and NMR sections of the General category.

The Automated Setup window should be used for initial system configuration, or if changes have been made to the serial connections or additional devices have been added. To access Automated Setup open the One-Minute NMR RunProcess and select the *Run/Automated Setup* menu item. Automated setup is disabled when the system is running.

A warning message will appear.



Choose *Yes* to continue with Automated Setup. Some time, up to a few minutes, will pass as the serial ports on the instrument controller computer are scanned. You may hear the CTC liquid handler beep a few times. This is normal.



The length of tubing from the CTC injector to the NMR probe should be measured and entered in the first field. Choose between 5 and 10 microliter flow cells. The serial port for the solvent conditioner and CTC liquid handler are detected automatically.

Pump configuration can be changed, but the initial configuration will work in most cases. If you are using different solvents than the ones indicated enter the names of the solvents here.

The type of NMR system you will be connecting to and the IP address or host name of the NMR system is entered at the bottom of the window. The NMR system is not configured automatically by Automated Setup.

To accept the changes you have made in Automated Setup, click the Configure button. The RunProcess will be automatically closed. HTSL flow rates and volumes settings will be changed automatically when the system re-starts.



Automated Delivery Volume Experiments

The Automated Delivery Volume calculation allows the delivery volume to be measured for each selected solvent. It is accessed through the Run / Delivery Volume Experiment menu item in the Run Process.

Run Delivery Volume Experiment

A series of experiments are set up to measure find the delivery volume by detecting the maximum signal-to-noise for a series of runs. The HTSL.Setup variables are initialized and a set of experiments is defined for the selected Tray and Vial location.

Account: ENC
 Username: Bob Albrecht
 Password: *****

Delivery Volume Range

Initial Volume: 26 uL
 Final Volume: 50 uL
 Volume Increment: 1 uL

Tray: MT1-Frnt
 Vial: 1
 Experiment: autoqc
 Solvent: D2O

Experiment will have 25 injections from vial 1 using tray MT1-Frnt. The experiment autoqc will be used in the solvent D2O. The delivery volume with the maximum S/N will be saved automatically for your pump.

The Run Delivery Volume Experiment dialog sets up a series of experiments at different delivery volumes. If a QC sample, and the QC experiment (*autoqc*) are used the Signal / Noise (S/N) is measured at each delivery volume in the series and the volume with the best S/N is written into the pump (HTSL) run volume automatically. If the QC experiment is not used the NMR spectra from the series of experiments must be visually inspected for the best S/N.

Start by entering your Account, Username, and Password. Enter the desired delivery volume range and increment. The starting values for the range can be calculated using the volume of the injection loop plus the volume of the tubing, plus the volume of the NMR flow cell. Select the tray and vial for the experiment. A single 2mL vial can be used, or a range of vial or plate wells can be used (e.g. 1-25). If you are using the QC sample solution select *autoqc* as the Experiment for automatic S / N calculation and pump setup.

The Setup as Pending sets up the series of experiments and requires that you go to the One-Minute NMR Web site to actually start the instrument. The Run As Priority button sets up the series of experiments and starts them immediately.



Accounting Information Web Site

The One-Minute NMR Accounting web page is an optional web site that can be used by administrators to keep track of the use of the system. The web site uses the start and end times for each sample along with the user and account information.

Username	Hours	Amount
Bob Albrecht	65.64	\$6,564.33
Protasis Service	0.13	\$12.56
TOTAL	65.77	\$6,576.89

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Installation

The installer for the accounting website is located on the One-Minute NMR installer under the One-Minute NMR/Accounting Website directory. To install double-click setup.exe.

Web Link

The link for the accounting application on the local machine is: <http://localhost/OMNMRAccounting/Index.aspx> to access the accounting application from a remote computer, replace “localhost” with the network address or name of the One-Minute NMR computer.

Web Page

The One-Minute NMR Accounting web page displays two calendars. By default the previous whole month is displayed. The starting and ending date can be selected by clicking on the calendars. Information can be tabulated by users or users and accounts. Clicking on the *Show Accounts* box displays the account information. The hourly billing rate can be entered and the total bill summed for customers and accounts.

Data Expiration

The data used by the accounting website is derived from current and removed samples in the One-Minute NMR database. The length of time the data are available is in The Brain setting *Database.RemovedSampleExpiration* = N months.



Dual-Flow Cell Operation

The Dual-flowcell CapNMR Probe is supported by One-Minute NMR. The CTC liquid handler is configured with two injectors. Two pumps push solvent through the two independent flow paths. NMR Experiments can be run synchronized on two flow cells or individually. When two flow paths are synchronized the same set of experiments can be run for two samples at the same time.

MultiFlowcell settings filter in The Brain

Dual flow cell operation is configured using Settings Category: General Settings, Settings Filter: MultiFlowcell section of The Brain.

MultiFlowcell.Enabled turns on/off the multi-flowcell feature.

MultiFlowcell.Injectors lists the injectors, in order, for the system.

MultiFlowcell.NamedParameterFiles lists the base names of the named parameter files used for each flow path. The name of the NMR experiment is appended to this name.

MultiFlowcell.Solvents lists the solvents, in order, that correspond to each injector. Samples are directed to each flow cell based on the solvents that are assigned the flow path.

MultiFlowcell.Synchronized determines the behavior of the NMR experiments. In synchronized mode a sample is loaded into the first flow path, named parameter files are written for each experiment, but the NMR experiments are not run. When the second sample is loaded into flow path 2 the combined experiments are started.

Configuration for Synchronized Mode

Two flow paths are configured to run in synchronized mode with one pump dedicated to each. No solvent switching valve is required because each flow path uses its own solvent. Either HTSL or Citation based pumps can be used. Each pump is configured without a

Setting	Value	Description
MultiFlowcell.Enabled	False	Enables multi-flowcell mode.
MultiFlowcell.Injectors	LC Vlv1,LC Vlv1	List of injectors for flowpaths.
MultiFlowcell.NamedParameterFiles	npf1,npf2	List of named parameter files for flowpaths.
MultiFlowcell.Solvents	DMSO,DMSO2	List of solvents for flowpaths.
MultiFlowcell.Synchronized	True	All flowcells are synchronized. Experiments start on last flowcell.

Master switching valve.

Name	Tech	SubSys	Master	Port	COM	Delivery Rate	Fill Rate	Volume
HTSL1	CITN	pump1		1	COM27	60	60	60
HTSL2	CITN	pump2		1	COM27	60	60	30

Citation pump configuration for synchronized mode.

Solvent	Pump	Sparge	Wash	Vol. Full (mL)	Vol. Remaining (mL)	Polar (Yes/No)
DMSO	HTSL1	1	Wash2	0	0	yes
DMSO2	HTSL2	1	Wash1	0	0	no

Solvent configuration for synchronized mode.

When the system is configured for synchronized mode samples must be submitted with alternating solvent designations. This forces the system to pick samples up in pairs and load them into separate injectors. Submitted samples are ordered in a sequence that is independent of the vial number or well location. Odd samples in the sequence (1,3,5...) must be assigned to the first solvent listed in *MultiFlowcell.Solvents*. Even samples (2,4,6...) must be assigned to the second solvent in *MultiFlowcell.Solvents*.

When pairs of samples are submitted each experiment for each sample in a pair is given a One-Minute NMR named parameter file. The parameter files are assigned according to *MultiFlowcell.NamedParameterFiles* setting and are given an extension of the name of the NMR experiment. The odd samples in the sequence do not trigger an NMR run to start and all of the named parameter files for their experiments are written immediately after the sample is positioned in the flowcell. The Even samples in the sequence run their assigned experiments on the NMR and have all of their named parameter files written before a set of experiments start.

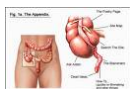
Specialized processing must be performed for synchronized samples. Contact Protasis/MRM for assistance.



Technical Support

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Marlboro, MA 01752

Tel: 508-481-4163
e-mail: b.albrecht@protasis.com



Appendix A

Alphabetical listing of One-Minute NMR General Settings

Setting	Value	Description
Communication.CTC.COM	COM7	Communication port for CTC Liquid Handler

Communication.Email.AlertRecipients	Bob Albrecht	Comma separated list of One-Minute NMR user names to send alerts to.
Communication.Email.DataChordReport	True	Adds a DataChord sample list to e-mail reports.
Communication.Email.FromAccount	omnmr@yourdomain.com	Account that e-mail is sent from.
Communication.Email.FromName	One-Minute NMR	The name of the One-Minute NMR system that is sending e-mail messages.
Communication.Email.Host	protasis.com	E-mail host
Communication.Email.LinkToMe	http://localhost/protasis/main.aspx?RunEnable=True	Link to this One-Minute NMR system added to the bottom emails.
Communication.Email.Password		Password for e-mail account that sends mail when authentication is required.
Communication.Email.SendAlerts	True	True if warnings and errors should be sent by e-mail.
Communication.Email.SendFinishedNotice	True	Set to True if One-Minute NMR sends messages about finished batches.
Communication.Email.SendPasswords	True	Set to True to e-mail passwords to users.
Communication.Email.Username	omnmr	The username when authentication is needed for sending e-mail.
Communication.Email.WebSite	localhost/OneMinuteNMR	Link to One-Minute NMR Web Site
Communication.NMRIP	albrechtsoft	IP address or DNS of the NMR system
Communication.SolventConditioner.COM	COM17	COM port for the solvent conditioner. Blank for stub mode.
Confirmation.1DH1.AcceptanceLevel	.70	Acceptance level to stop after 1D proton acceptance.
Confirmation.AcceptanceLevel	.35	Level at which a structure is considered confirmed.
Confirmation.ACD.1DScript	c:\protasis\ACD\mrm-db.script.base_rev1.0.c pp	ACD Script template for 1D data.
Confirmation.ACD.2DScript	c:\protasis\ACD\mrm-db.script.base_rev1.0.c pp	ACD Script template for 2D data.
Confirmation.ACD.Database	C:\protasis\ACD	ACD Database location.
Confirmation.ACD.DataRoot	P:	Root of data path. Users NMR Data Path is appended to find results.
Confirmation.ACD.Hostname	localhost	Name of server or IP address for links to ACD Web Librarian.
Confirmation.ACD.LogResults	True	Logs the results from the ACD confirmation software to protasis.log.
Confirmation.ACD.Path	C:\protasis\ACD\Data	The path to structure confirmation files for ACD.
Confirmation.ACD.Program	C:\ACDSRV11\SMROBOT.SRV\smrobot.exe	The name of the program to run for ACD confirmations.
Confirmation.ACD.XMLConfig	C:\protasis\ACD\Config_MRM_signal.xml	ACD Script template for 2D data.
Confirmation.ContaminantSolvents		Comma-separated list of contaminant solvents.
Confirmation.DatabaseOnly	False	True when only databasing is done..
Confirmation.Debug	True	
Confirmation.Interface	ACD	Current interface for structure confirmation.
Confirmation.License	OFF-98KK75YZ-SQ19UQ-88VBS2XX-88Y1933SD4	License for structure confirmation module.
Confirmation.MoleculeAutomatic	False	Set to True finds molecules with omnmr_filelocator.
Confirmation.New Setting		

Confirmation.NMRProcessDelay1D	0	1D Acquisition processing delay in seconds.
Confirmation.NMRProcessDelay2D	0	2D acquisition processing delay in seconds.
Confirmation.PhaseFile	phasefile	The name for phase files stored in FID directory (e.g. SampleID.FID/phasefile).
Confirmation.ProcessDelay	90	Number of seconds to delay for processing to complete.
Confirmation.RejectionLevel	.35	Level at which structure is rejected.
Confirmation.ShowMoleculeUpload	True	Set to True to allow Mol file entry.
Confirmation.ShowSmiles	True	Set to True to allow SMILES string entry.
Confirmation.SuppressedSolvents		Comma-separated list of suppressed solvents for all samples.
Counters.InjectorReplacement	3442	Number of samples since injector was replaced.
Counters.InjectorReplacement.Alert	True	
Counters.InjectorReplacement.Limit	6000	
Counters.ValveRotor	326	
Counters.ValveRotor.Alert	True	
Counters.ValveRotor.Limit	2500	
CustomField.HideName	False	Hides name field so custom fields can be used instead.
CustomFields.Disabled	False	Disables custom fields.
Database.BackupLocation	C:\protasis\backup\omnmr.brain	Location for backup database files.
Database.CurrentImportTemplate	AmgenSDF	Import template to use.
Database.PendingSampleExpiration	None	The number of minutes before the system automatically removes pending samples.
Database.RemovedSampleExpiration	24	
Database.Version	39	The version of the database schema used for automatic updates
GetBarcode.Enabled	True	True enables reading barcodes from CTC liquid handler.
GetBarcode.RegenerateSampleQueue	True	Regenerates samples in the queue to run forever on barcoded samples.
GetBarcode.SampleLookup	C:\Documents and Settings\Bob Albrecht\My Documents\Visual Studio Projects\TestSampleLookup\bin\Debug\TestSampleLookup.exe	Program to lookup sample information for barcode.
GetBarcode.SkipMissingSamples	False	True to abort missing samples, log error, and continue sample queue.
GetBarcode.WaitForMissingSamplePeriod	20	Number of seconds to wait for missing samples to arrive.
GetBarcode.WaitForMissingSamples	True	True for the CTC to retry missing sample positions and not generate an error.
HTSL.AutoRecoverValveMotorSlip	True	Set True to automatically recover on motor slippage.
HTSL.InitializeOnStartup	True	Set True to initialize HTSL on startup.
HTSL.LogCommands	True	Log all HTSL commands.
HTSL.Pressure	2614	Current HTSL Pressure reading.
HTSL.PressureEnabled	true	True if the pressure transducer is enabled.
HTSL.PressureHistoryEnabled	True	Set to True to turn on pressure history log to PressureHistory table.
HTSL.PressureHistoryExpiration	2000	Number of hours the pressure history is kept.
HTSL.PressurePercent	100	Percentage of maximum pressure.
HTSL.PressureUnit	PSI	Units for HTSL pressure. PSI or MPa.
HTSL.PressureUpdateInterval	3	Interval, in seconds to update pressure reading.

HTSL.Setup.BestDeliveryVolume	0	The delivery volume with the best S/N.
HTSL.Setup.BestSN	20	The best S/N for push volume experiments.
HTSL.Setup.DeliveryVolumeIncrement	1	delivery volume increment.
HTSL.Setup.Enabled	true	True if push volume experiment is enabled.
HTSL.Setup.EndingDeliveryVolume	30	Ending delivery volume for a multi delivery volume experiment.
HTSL.Setup.StartingDeliveryVolume	25	The starting delivery volume for a multi delivery volume experiment.
Load.CleanInjector1.cycles	1	Number of clean cycles
Load.CleanInjector1.delay	0	Fill delay in seconds
Load.CleanInjector1.ejectSpeed	25	Eject speed in microliters per second
Load.CleanInjector1.fillSpeed	25	Syringe fill speed in microliters per second
Load.CleanInjector1.rinseTime	1	Time to open rinse valve in seconds
Load.CleanInjector1.station	Solvent	Wash station to use for cleaning the injector
Load.CleanInjector1.volPercent	50	Percent of syringe to use for cleaning injector
Load.CleanInjector2.cycles	1	Number of clean cycles
Load.CleanInjector2.delay	0	Fill delay in seconds
Load.CleanInjector2.ejectSpeed	5	Eject speed in microliters per second
Load.CleanInjector2.fillSpeed	5	Syringe fill speed in microliters per second
Load.CleanInjector2.rinseTime	1	Time to open rinse valve in seconds
Load.CleanInjector2.station	Solvent	Wash station to use for cleaning the injector
Load.CleanInjector2.volPercent	30	Percent of syringe to use for cleaning injector
Load.CleanSyringe.post1.cycles	1	Number of cleaning cycles, first post-injection cleaning
Load.CleanSyringe.post1.delay	0	Pullup delay in seconds,first post-injection cleaning
Load.CleanSyringe.post1.ejectSpeed	5	Eject speed in microliters per second, first post-injection cleaning
Load.CleanSyringe.post1.fillSpeed	5	Fill speed in microliters per second, first post-injection cleaning
Load.CleanSyringe.post1.rinseTime	1	Time to open rinse valve in seconds
Load.CleanSyringe.post1.station		Wash station where the syringe is cleaned, first post-injection cleaning
Load.CleanSyringe.post1.volPercent	100	Percent of syringe to clean, first post-injection cleaning
Load.CleanSyringe.post2.cycles	1	Number of cleaning cycles, second post-injection cleaning
Load.CleanSyringe.post2.delay	0	Pullup delay in seconds,second post-injection cleaning
Load.CleanSyringe.post2.ejectSpeed	5	Eject speed in microliters per second, second post-injection cleaning
Load.CleanSyringe.post2.fillSpeed	5	Fill speed in microliters per second, second post-injection cleaning
Load.CleanSyringe.post2.rinseTime	1	Time to open rinse valve in seconds
Load.CleanSyringe.post2.station		Wash station where the syringe is cleaned, second post-injection cleaning
Load.CleanSyringe.post2.volPercent	100	Percent of syringe to clean, second post-injection cleaning
Load.CleanSyringe.pre1.cycles	2	Number of cleaning cycles, first pre-injection cleaning
Load.CleanSyringe.pre1.delay	0	Pullup delay in seconds,first pre-injection cleaning
Load.CleanSyringe.pre1.ejectSpeed	25	Eject speed in microliters per second, first pre-injection cleaning
Load.CleanSyringe.pre1.fillSpeed	25	Fill speed in microliters per second, first pre-injection cleaning
Load.CleanSyringe.pre1.rinseTime	1	Time to open rinse valve in seconds

Load.CleanSyringe.pre1.station	Solvent	Wash station where the syringe is cleaned, first pre-injection cleaning
Load.CleanSyringe.pre1.volPercent	50	Percent of syringe to clean, first pre-injection cleaning
Load.CleanSyringe.pre2.cycles	1	Number of cleaning cycles, second pre-injection cleaning
Load.CleanSyringe.pre2.delay	0	Pullup delay in seconds,second pre-injection cleaning
Load.CleanSyringe.pre2.ejectSpeed	5	Eject speed in microliters per second, second pre-injection cleaning
Load.CleanSyringe.pre2.fillSpeed	5	Fill speed in microliters per second, second pre-injection cleaning
Load.CleanSyringe.pre2.rinseTime	1	Time to open rinse valve in seconds
Load.CleanSyringe.pre2.station		Wash station where the syringe is cleaned, second pre-injection cleaning
Load.CleanSyringe.pre2.volPercent	100	Percent of syringe to clean, second pre-injection cleaning
Load.GetSample.delay	1	Fill delay in seconds
Load.GetSample.fillStrokes	0	Number of fillVolume strokes of sample to rinse the syringe with
Load.GetSample.fillVolume	0	Microliters of sample for each rinse of syringe
Load.GetSample.InjectAfterRun	False	True to prevent loop load before previous run finished.
Load.GetSample.InjectAfterRun.ParkSyringe	False	True parks syringe in current wash station while waiting.
Load.GetSample.rate	2	Fill rate in microliters per second
Load.GetSample.SkipMissingSamples	False	True to abort missing samples, log error, and continue sample queue.
Load.GetSample.volume	10	Sample volume in microliters
Load.GetSample.WaitForMissingSamplePeriod	120	Number of seconds to wait for missing samples to arrive.
Load.GetSample.WaitForMissingSamples	False	True for the CTC to retry missing sample positions and not generate an error.
Load.GetSolvent.delay	1	Fill delay in seconds
Load.GetSolvent.location		Location for picking up push solvent
Load.GetSolvent.rinseTime	0	Time in seconds to activate wash station, or default (0).
Load.GetSolvent.speed	2	Push solvent fill speed in microliters per second
Load.GetSolvent.volume	0	Push solvent volume in microliters
Load.Injector.valve	CTC	Injector valve. CTC for Injector valve,or HTSL
Load.InjectSample.delay	1	Eject delay in seconds
Load.InjectSample.injector	LC Vlv1	Name of injector
Load.InjectSample.rate	5	Eject speed in microliters per second
Load.InjectSample.volume	0	Volume to inject if different from GetSample.volume + GetSolvent.volume
Load.LogObjects	False	
Load.ReverseRinse.delay	2	Delay in seconds after reverse rinse
Load.ReverseRinse.ejectSpeed	2	Microliters per second for eject
Load.ReverseRinse.fillSpeed	1	Microliters per second for reverse rinse
Load.ReverseRinse.volume	1	Number of microliters for reverse rinse
Load.ReverseRinse.waste		Waste port to use for reverse rinse
LockMonitor.AveragingPeriod	5	Minutes of averaging for lock signal monitoring.
LockMonitor.ContinueNext	False	True continues to next sample. False pauses instrument.
LockMonitor.Debug	False	Turns on messages to the log file.
LockMonitor.Enabled	False	Enables Lock Monitoring and corrective action.
LockMonitor.LimitPercent	50	Percentage drop before returning or flushing

		sample.
LockMonitor.ReportOnly	True	True to only report when the lock level drops.
Macro.AfterRun		Macro after run.
Macro.Load.AfterInject	HOME.txt	Macro after inject.
Macro.Load.BeforeClean		Macro before the first syringe cleaning.
Macro.Load.BeforeGetSample		Macro after syringe cleaning, before getting sample.
MultiFlowcell.AutomaticSolventPick	True	Enables automatic assignment of solvents and flow paths.
MultiFlowcell.Enabled	False	Enables multi-flowcell mode.
MultiFlowcell.Injectors	LC Vlv1,LC Vlv2	List of injectors for flowpaths.
MultiFlowcell.NamedParameterFiles	npf1,npf2	List of named parameter files for flowpaths.
MultiFlowcell.Solvents	DMSO1,DMSO2	List of solvents for flowpaths.
MultiFlowcell.Synchronized	True	All flowcells are synchronized. Experiments start on last flowcell.
NightSample.Begin	18:20	The 24-hour time after which night samples can start
NightSample.End	6:00	The 24-hour time after which night samples cannot start
NMR.AllowManualStop	True	Allows manual stopping of runs with wexpDoneCheck on Varian systems.
NMR.Bruker.CleanupMacro		Executed on startup to delete debug file.
NMR.Bruker.Windows.FileLocator	C:\bruker\omnmr_filelocator.bat	Called to locate files based in sample information.
NMR.CommandFile	C:\bruker\XWIN-NMR\prog\xwin_cmd.txt	File for sending commands to the NMR
NMR.Disk		The disk where NMR data are stored
NMR.DriveShareName	//10.0.0.56	
NMR.ErrorLevel	Soft Error	Varian error level. Warning, Soft Error, or Hard Error (acqstat[1]=14,13,15)
NMR.Interface	Bruker.Windows	The NMR Interface to use.(Varian,Bruker.Windows,Bruker.Linux,JEOL.Windows)
NMR.JEOL.AutocompleteFile	P:\Protasis Loader\JEOLInterface\autocomplete.ec500.jeol.comcom	Autocomplete file for monitoring status.
NMR.JEOL.AutomationTemplate	P:\Protasis Loader\JEOLInterface\macros\omnmr.atm.auto2	File where automation template is written.
NMR.JEOL.AutomationTemplateMaster	C:\Protasis Documents\Protasis Loader\JEOL Interface\AutomationTemplateMaster.txt	
NMR.JEOL.MacroDir	P:\Protasis Loader\JEOLInterface\macros	Directory where .atm macro files are placed.
NMR.JEOL.MacroTemplate	C:\Protasis Documents\Protasis Loader\JEOL Interface\MacroTemplate.txt	Template for JEOL macro file.
NMR.LockTable	autolock	Table for initial lock settings on Varian, blank turns off autolocking.
NMR.LogVNMRResults	True	The name or the NMR instrument for One-Minute NMR.

NMR.Name	600 MHz	The name or the NMR instrument for One-Minute NMR.
NMR.NamedParameterFile	params.txt	Name of the named parameters file.
NMR.NetworkRetries	1	Maximum Number or Retries for listener communications.
NMR.NetworkTimeout	30	Timeout period in seconds for listener communications.
NMR.PostStartDelay	0	Varian. Seconds delay before Vnmr commands change showstat status.
NMR.PreStartDelay	1	Delay before starting experiments to account for processing.
NMR.ProbeFile	capnmr	Probe file to use for Varian spectrometers.
NMR.PulseDelay	1	Number of seconds of delay after each pulse
NMR.ResponseFile	C:\bruker\XWIN-NMR\prog\cmd_respons e.txt	File for getting status back from the NMR
NMR.ScriptStatus	nmrstatus	The command sent for monitoring status on the Varian system. (showstat)
NMR.ScriptTemplate	autorun	Basic script used to run all samples.
NMR.SendPlateID	True	Sends the Plate ID as the last argument to autorun before custom fields.
NMR.ShimFile	D2Omrm	File for shimming the probe.
NMR.ShimFileExtension	mrm	Varian extension to add to solvent for shim file e.g. d2omrm
NMR.TemperatureEquilibrationTime	0	Time in seconds to wait after sample is loaded before lock
NMR.UseExtraParameters	True	True sends extra parameters to autorun.
NMR.UseMoleculeData	True	True to use molecule data when structure confirmation is turned off.
NMR.Varian.Foreground	False	If set to true use send2Vnmr.
NMR.Varian.InstrumentRestartDelay	120	Idle time in seconds before attempting instrument restart.
NMR.Varian.InstrumentRestartTime	240	Time in seconds it takes restart instrument.
NMR.Varian.Simulator	True	
NMR.Varian.TalkFile	\$vnmruser/.talk	Name of VNMR talk file for use with send2Vnmr
NMR.Varian.wexpDoneCheck	True	Checks that experiments are done using wexp.
ProbeClean.Countdown	5	Countdown for probe cleaning.
ProbeClean.Duration	5	Seconds to leave solution in probe.
ProbeClean.Duration2	5	Seconds to leave solution 2 in probe.
ProbeClean.Enabled	False	True to activate Probe cleaning.
ProbeClean.Frequency	6	How often to clean the probe. 0=never, 1=every, n=every nth
ProbeClean.Index	25	Vial index for wash solution.
ProbeClean.Index2	26	Vial index for second wash solution.
ProbeClean.OldSolvent	DMSO1	The solvent switched from for probe cleans.
ProbeClean.Solvent	DMSO1	The solvent to switch to for probe cleans.
ProbeClean.SolventFlush1.Flow	100	Flow rate for first solvent flush.
ProbeClean.SolventFlush1.Solvent	DMSO2	Name of solvent used for second probe flush (blank disables)
ProbeClean.SolventFlush1.Volume	10	Microliters of solvent for first solvent flush.
ProbeClean.SolventFlush2.Flow	100	Flow rate for second solvent flush (microliters/min)
ProbeClean.SolventFlush2.Solvent	DMSO1	Name of solvent used for second probe flush (blank disables)
ProbeClean.SolventFlush2.Volume	10	Microliters of solvent for second solvent flush.
ProbeClean.Tray	MT1-Frnt	Vial tray for wash solution.
ProbeClean.Tray2	MT1-Frnt	Vial tray for second wash solution.

QC.BrukerWindows.omnmr_qc	c:\protasis\omnmr_qc.bat	Program to run for Bruker.Windows to get QC results.
QC.Countdown	3	Counter for QC samples.
QC.Enabled	False	True enables QC samples.
QC.ExperimentName	autoqc	The name of the experiment to run for QC samples.
QC.Frequency	4	How often to run a check sample.
QC.LineShapeLimit	1.5	The maximum line shape deformation.
QC.LineShapeLimit.DMSO1	1.5	The maximum line shape deformation.
QC.LineShapeLimit.DMSO2	1.5	The maximum line shape deformation.
QC.MaximumNumberOfSignals	3	The maximum number of signals in the region tested for S/N.
QC.SignalToNoiseLimit	10	The minimum signal to noise value.
QC.SignalToNoiseLimit.DMSO1	10	The minimum signal to noise value.
QC.SignalToNoiseLimit.DMSO2	10	The minimum signal to noise value.
QC.SignalToNoiseLowerPPM	2	Lower ppm limit for signal to noise calculation.
QC.SignalToNoiseUpperPPM	12	Upper ppm limit for signal to noise calculation.
SampleReturn.CleanSyringe.pre1.cycles	1	Number of cleaning cycles, first pre-return cleaning
SampleReturn.CleanSyringe.pre1.delay	0	Pullup delay in seconds, first pre-return cleaning
SampleReturn.CleanSyringe.pre1.ejectSpeed	25	Eject speed in microliters per second, first pre-return cleaning
SampleReturn.CleanSyringe.pre1.fillSpeed	25	Fill speed in microliters per second, first pre-return cleaning
SampleReturn.CleanSyringe.pre1.rinseTime	1	Time to open rinse valve in seconds
SampleReturn.CleanSyringe.pre1.station	Solvent	Wash station where the syringe is cleaned, first pre-return cleaning
SampleReturn.CleanSyringe.pre1.volPercent	100	Percent of syringe to clean, first before sample return.
SampleReturn.CleanSyringe.pre2.cycles	1	Number of cleaning cycles, second pre-return cleaning
SampleReturn.CleanSyringe.pre2.delay	0	Pullup delay in seconds, second pre-return cleaning
SampleReturn.CleanSyringe.pre2.ejectSpeed	5	Eject speed in microliters per second, second pre-return cleaning
SampleReturn.CleanSyringe.pre2.fillSpeed	5	Fill speed in microliters per second, second pre-return cleaning
SampleReturn.CleanSyringe.pre2.rinseTime	1	Time to open rinse valve in seconds
SampleReturn.CleanSyringe.pre2.station	Wash2	Wash station where the syringe is cleaned, second first pre-return cleaning
SampleReturn.CleanSyringe.pre2.volPercent	100	Percent of syringe to clean, second before sample return.
SampleReturn.EjectSpeed	25	Syringe eject speed in microliters/second.
SampleReturn.Enabled	False	Set to True if sample return is enabled and plumbed.
SampleReturn.LoadedSample	6977	The ID of the last loaded sample so it can be returned.
SampleReturn.Penetration	4000	Micrometers of needle penetration for sample return.
Setting.MonitorPressure	True	Allows pressure monitoring in Citation direct control.
Settings.AllowDelete	True	True if deletes are allowed. (DANGEROUS)
Settings.LastAccount	Protasis	Remembers and recalls the last Account used.
Settings.LastSampleExtension	Vial	Remembers and recalls the last setting for vial extension.

Shutdown.CleanInjector1.cycles	1	Number of clean cycles
Shutdown.CleanInjector1.delay	0	Fill delay in seconds
Shutdown.CleanInjector1.ejectSpeed	25	Eject speed in microliters per second
Shutdown.CleanInjector1.fillSpeed	25	Syringe fill speed in microliters per second
Shutdown.CleanInjector1.rinseTime	1	Time to open rinse valve in seconds
Shutdown.CleanInjector1.station		Wash station to use for cleaning the injector
Shutdown.CleanInjector1.volPercent	100	Percent of syringe to use for cleaning injector
Shutdown.CleanInjector2.cycles	1	Number of clean cycles
Shutdown.CleanInjector2.delay	0	Fill delay in seconds
Shutdown.CleanInjector2.ejectSpeed	25	Eject speed in microliters per second
Shutdown.CleanInjector2.fillSpeed	25	Syringe fill speed in microliters per second
Shutdown.CleanInjector2.rinseTime	1	Time to open rinse valve in seconds
Shutdown.CleanInjector2.station		Wash station to use for cleaning the injector
Shutdown.CleanSyringe.1.cycles	1	Number of cleaning cycles, first syringe cleaning
Shutdown.CleanSyringe.1.delay	1	Pullup delay in seconds,first cleaning
Shutdown.CleanSyringe.1.ejectSpeed	25	Eject speed in microliters per second, first cleaning
Shutdown.CleanSyringe.1.fillSpeed	25	Fill speed in microliters per second, first cleaning
Shutdown.CleanSyringe.1.rinseTime	1	Time to open rinse valve in seconds, first cleaning
Shutdown.CleanSyringe.1.station		Wash station syringe is cleaned at, first cleaning (Solvent,Wash1,Wash2)
Shutdown.CleanSyringe.1.volPercent	100	Percent of syringe to clean, first cleaning
Shutdown.CleanSyringe.2.cycles	1	Number of cleaning cycles, first syringe cleaning
Shutdown.CleanSyringe.2.delay	1	Pullup delay in seconds,first cleaning
Shutdown.CleanSyringe.2.ejectSpeed	25	Eject speed in microliters per second, first cleaning
Shutdown.CleanSyringe.2.fillSpeed	25	Fill speed in microliters per second, first cleaning
Shutdown.CleanSyringe.2.rinseTime	1	Time to open rinse valve in seconds, first cleaning
Shutdown.CleanSyringe.2.station		Wash station syringe is cleaned at, first cleaning (Solvent,Wash1,Wash2)
Shutdown.CleanSyringe.2.volPercent	100	Percent of syringe to clean, first cleaning
Shutdown.Enabled	False	Turns shutdown procedure on and off
Shutdown.ParkSyringe	True	Parks the syringe in the wash station.
Shutdown.ProbeClean.Duration	60	Seconds to leave solution in probe. (blank to use ProbeClean.Duration)
Shutdown.ProbeClean.Duration2	5	Seconds to leave solution 2 in probe.
Shutdown.ProbeClean.Enabled	False	Turns on or off the startup probe clean.
Shutdown.ProbeClean.Index		Vial index for wash solution. (blank to use ProbeClean.Index)
Shutdown.ProbeClean.Index2		Vial index for second wash solution.
Shutdown.ProbeClean.Solvent	Solvent	The solvent to switch to for probe cleans.
Shutdown.ProbeClean.Tray		Vial tray for wash solution. (blank to use ProbeClean.Tray)
Shutdown.ProbeClean.Tray2		Vial tray for second wash solution.
Shutdown.SolventFlush1.Flow	40	Flow rate for first solvent flush.
Shutdown.SolventFlush1.Solvent		Name of solvent used for first probe flush (blank disables)
Shutdown.SolventFlush1.Volume	75	Microliters of solvent for first solvent flush.
Shutdown.SolventFlush2.Flow	40	Flow rate for second solvent flush.
Shutdown.SolventFlush2.Solvent		Name of solvent used for first probe flush (blank disables)
Shutdown.SolventFlush2.Volume	25	Microliters of solvent for first solvent flush.
Shutdown.TimeOf	1/27/2010 12:06:03 PM	The date/time the shutdown sequence last ran.

Shutdown.Timeout	1	Minutes of down time needed before shutdown sequence is used.
SolventConditioner.BottleA.Enabled	True	True to enable Bottle A.
SolventConditioner.BottleB.Enabled	True	True to enable Bottle B.
SolventConditioner.BottleC.Enabled	True	True to enable Bottle C.
SolventConditioner.BottleTestInterval	24	Number of hours between bottle tests.
SolventConditioner.Enabled	False	True to enable solvent conditioner control.
SolventConditioner.HistoryExpiration	4000	Hours until Solvent Conditioner history expires.
SolventConditioner.LastBottleTest	4/30/2010 11:14:46 AM	Date/time of last bottle test.
SolventConditioner.LastPressureCheck	4/30/2010 12:03:49 PM	Date/time of last bottle test.
SolventConditioner.LastPurge	4/30/2010 12:08:20 PM	Date / time of last purge.
SolventConditioner.PressureCheckInterval	8	Number of hours between manifold pressure checks.
SolventConditioner.PressureHistoryFile	c:\protasis\sypressure.hist	History file for the Solvent Conditioner Control window.
SolventConditioner.PurgeInterval	72	Number of hours between manifold purge operations.
SolventSelect.BunchNightSamples	True	Run night samples with the same solvent together.
SolventSelect.BunchSamples	False	Runs samples with the same solvent together.
SolventSelect.CurrentSolvent	DMSO1	The current solvent used by the system. For detecting changes.
SolventSelect.ExchangeVolume	20	Volume (uL) to push when changing solvents.
SolventSelect.PrioritySwitch	False	Priority samples can force a solvent switch.
SolventSelect.UniversalSolvents	Acetone,DMSO	List of universal solvents.
Startup.CleanInjector1.cycles	1	Number of clean cycles
Startup.CleanInjector1.delay	0	Fill delay in seconds
Startup.CleanInjector1.ejectSpeed	25	Eject speed in microliters per second
Startup.CleanInjector1.fillSpeed	25	Syringe fill speed in microliters per second
Startup.CleanInjector1.rinseTime	1	Time to open rinse valve in seconds
Startup.CleanInjector1.station	Wash3	Wash station to use for cleaning the injector
Startup.CleanInjector1.volPercent	100	Percent of syringe to use for cleaning injector
Startup.CleanInjector2.cycles	1	Number of clean cycles
Startup.CleanInjector2.delay	0	Fill delay in seconds
Startup.CleanInjector2.ejectSpeed	25	Eject speed in microliters per second
Startup.CleanInjector2.fillSpeed	25	Syringe fill speed in microliters per second
Startup.CleanInjector2.rinseTime	1	Time to open rinse valve in seconds
Startup.CleanInjector2.station	Wash4	Wash station to use for cleaning the injector
Startup.CleanInjector2.volPercent	100	Percent of syringe to use for cleaning injector
Startup.CleanSyringe.1.cycles	1	Number of cleaning cycles, first syringe cleaning
Startup.CleanSyringe.1.delay	1	Pullup delay in seconds,first cleaning
Startup.CleanSyringe.1.ejectSpeed	25	Eject speed in microliters per second, first cleaning
Startup.CleanSyringe.1.fillSpeed	25	Fill speed in microliters per second, first cleaning
Startup.CleanSyringe.1.rinseTime	0	Time to open rinse valve in seconds, first cleaning
Startup.CleanSyringe.1.station	Wash1	Solvent Wash station syringe is cleaned at, first cleaning (Solvent,Wash1,Wash2)
Startup.CleanSyringe.1.volPercent	100	Percent of syringe to clean, first cleaning
Startup.CleanSyringe.2.cycles	1	Number of cleaning cycles, second syringe cleaning
Startup.CleanSyringe.2.delay	1	Pullup delay in seconds, second cleaning
Startup.CleanSyringe.2.ejectSpeed	25	Eject speed in microliters per second, second

		cleaning
Startup.CleanSyringe.2.fillSpeed	25	Fill speed in microliters per second, second cleaning
Startup.CleanSyringe.2.rinseTime	1	Time to open rinse valve in seconds, second cleaning
Startup.CleanSyringe.2.station	Wash2	Wash station syringe is cleaned at, second cleaning (Solvent,Wash1,Wash2)
Startup.CleanSyringe.2.volPercent	100	Percent of syringe to clean, second cleaning
Startup.Enabled	False	Turns on or off the instrument startup sequence.
Startup.ProbeClean.Duration	60	Seconds to leave solution in probe. (blank to use ProbeClean.Duration)
Startup.ProbeClean.Duration2	5	Seconds to leave solution 2 in probe.
Startup.ProbeClean.Enabled	False	Turns on or off the startup probe clean.
Startup.ProbeClean.Index	95	Vial index for wash solution. (blank to use ProbeClean.Index)
Startup.ProbeClean.Index2		Vial index for second wash solution.
Startup.ProbeClean.Solvent	Solvent	The solvent to switch to for probe cleans.
Startup.ProbeClean.Tray	MT1-Frnt	Vial tray for wash solution. (blank to use ProbeClean.Tray)
Startup.ProbeClean.Tray2		Vial tray for second wash solution.
Startup.SolventFlush1.Flow	40	Flow rate for first solvent flush (microliters/min)
Startup.SolventFlush1.Solvent	D2O	Name of solvent used for first probe flush (blank disables)
Startup.SolventFlush1.Volume	120	Microliters of solvent for first solvent flush.
Startup.SolventFlush2.Flow	40	Flow rate for second solvent flush (microliters/min)
Startup.SolventFlush2.Solvent	D2O	Name of solvent used for first probe flush (blank disables)
Startup.SolventFlush2.Volume	10	Microliters of solvent for second solvent flush.
Startup.TimeOf	9/13/2007 6:55:07 PM	The date/time the startup sequence last ran.
Startup.Timeout	120	Minutes of down time needed before startup sequence is used.
System.AlternativeLoginOnly	False	(DANGER) Turns off normal login and requires cookie login.
System.AutomaticIdlePause	False	Forces the instrument to pause after the last sample is run.
System.ClearLogOnStartup	False	Deletes c:\protasis\protasis.log on startup of the run process.
System.EnableNumberOfInjections	True	True enables the number of injections field.
System.LiteConfiguration	False	Enables / Disables OMNMR Lite.
System.LoadResumeStatus		Sample ID and current load step for resumed sample.
System.LogoutTime	30	Minutes of inactivity before web page logout. Blank disables.
System.MessageDebug	True	
System.NMRResumeStatus		Sample ID and current step for NMR resume.
System.Paused	false	Set to True when the system is paused
System.ResultColumnEnabled	True	Set to true to turn the Results column on in the grid.
System.SampleCounter	3346	Counts the number of samples that have run.
System.ShowExperimentSettings	True	Enables / Disables the NMR experiment settings.
System.ShowSelectAll	True	Shows the Select All button.
System.Status	>Sample Acquisition Done >NMR Run Complete >Cleaning Syringe >Go Home >Done Loading >Loading Sample:	Current system status message.

	SLTEST1 >Finished Load Sequence >Go Home	
System.SuppressOverwriteWarning	False	Suppress main web page overwrite warning.