TopSpin

- IconNMR Automation Guide

User Manual

Version 001

Innovation with Integrity

NMR

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1 About

1.1 This Manual

This manual is intended to be a reference guide for IconNMR related operations within the TopSpin software. It describes the complete IconNMR functionality, both interactive and automated based on TopSpin3.5.

The figures shown in this manual are designed to be general and informative and may not represent the specific Bruker model, component or software/firmware version you are working with. Options and accessories may or may not be illustrated in each figure.

For older version of TopSpin, please refer to the manual supplied at the time.

1.2 Policy Statement

It is the policy of Bruker to improve products as new techniques and components become available. Bruker reserves the right to change specifications at any time.

Every effort has been made to avoid errors in text and figure presentation in this publication. In order to produce useful and appropriate documentation, we welcome your comments on this publication. Support engineers are advised to regularly check with Bruker for updated information.

Bruker is committed to providing customers with inventive, high quality products and services that are environmentally sound.

1.3 Symbols and Conventions

Safety instructions in this manual are marked with symbols. The safety instructions are introduced using indicative words which express the extent of the hazard.

In order to avoid accidents, personal injury or damage to property, always observe safety instructions and proceed with care.

DANGER

This combination of symbol and signal word indicates an immediately hazardous situation which could result in death or serious injury unless avoided.

⚠ WARNING

This combination of symbol and signal word indicates a potentially hazardous situation which could result in death or serious injury unless avoided.

⚠ CAUTION

This combination of symbol and signal word indicates a possibly hazardous situation which could result in minor or slight injury unless avoided.

SAFETY INSTRUCTIONS

This combination of color and signal words are used for control flow and shutdowns in the event of an error or emergency.

NOTICE

This combination of color and signal word indicates a possibly hazardous situation which could result in damage to property or the environment unless avoided.

This symbol highlights useful tips and recommendations as well as information designed to ensure efficient and smooth operation.

2 Introduction

2.1 What is IconNMR

Welcome to IconNMR, a comprehensive user interface, tailor made for all your NMR laboratory management and control needs. IconNMR was designed to make the execution of routine NMR experiments easy and straightforward by providing a state of the art icon based user interface. The steps necessary to acquire, process, and plot a spectrum are reduced to inserting a new sample, defining the data file name, the solvent, and the experiment. No other knowledge about the instrument, the parameters, or the software is necessary. Although running on top and under the control of the computer's Linux/ Windows operating system and Bruker's Topspin program, providing the acquisition and processing functions, IconNMR shields the user entirely from both. Accessing Topspin commands is only possible if permission has been granted by the laboratory manager. As such, IconNMR is particularly suited for open access spectrometers with a large number of users.

2.2 Blueprint for setting up IconNMR

IMPORTANT! Before you start to configure IconNMR answer the following questions. To use Assure or SampleTrack you will need extra licenses to use those features.

How many users will have access to the spectrometer?

Are there different groups of users (e.g. teachers vs. students)?

How many different groups of users are needed?

Are group members allowed to see each other's results?

Are the users familiar with NMR in general and the TopSpin software?

How many samples will be run on a daily basis?

Is there a need to run samples during day and night including weekends?

Is there a need for running priority samples?

Are there any needs for security / passwords?

Are there any needs to upload the data for archiving to a central computer?

Is there a need for running samples at high or low temperatures?

Is there a need to modify standard Bruker experiments?

Is there a need to run IconNMR remotely?

Do you intend using e-mail to send NMR data?

In what format would you like to send the data by e-mail (PDF, JDX or ZIP)?

Is there a need to print out spectra?

What spectrometer type do you have (AV or Fourier)?

Do you have a sample changer and if yes, what type is it?

Do you use Topshim or Gradshim?

Is the probe equipped with automatic tuning (ATMA)?

Is there a need to use the IconNMR accounting feature?

Do you use SampleTrack to submit samples?

Do you use Assure to run samples?

Do you use LC-NMR to run samples?

Introduction

3 IconNMR configuration

3.1 Adding a new user

There are two types of users which can use IconNMR. Users which have a workstation log in and the so called additional users with the permission to use IconNMR but have no log in on the workstation.

3.2 Adding new users to the operating system

To add new users to the Window or the LINUX operating system, follow the instructions documented respectively for each software.

To activate new users in IconNMR, follow the steps in **3.4 Activate new users in IconNMR**.

3.3 Adding a new additional user to run IconNMR

Additional Users are Spectrometer Users who do not have a System user account on the workstation managing the spectrometer. They may, however, still perform experiments and the experiment information FID's etc. will be stored using the NMR effective users ID and permission as defined. Additional Users is an extra feature available only in IconNMR. These users must not be defined for normal operation.

All Additional Users may have their own password and may initialize or reset it once they have logged into the IconNMR system.

1. Type **Icon** inside the TopSpin command line and hit Enter.

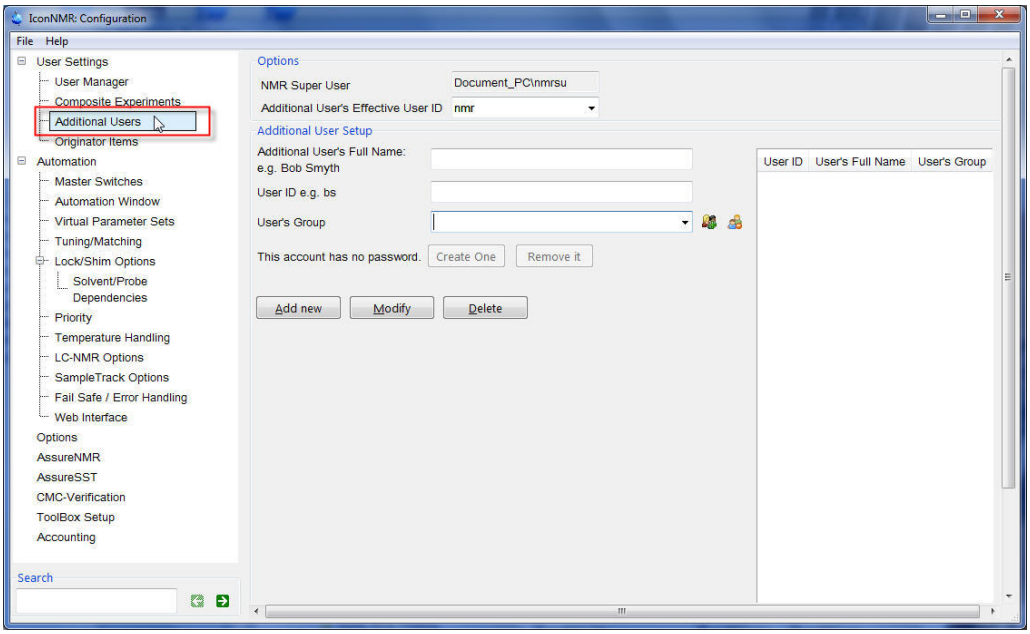
2. Select **Configuration**.

3. Enter the NMR Administrator password.

4. Hit Enter.

Alternatively, which involves more steps you can open the IconNMR Configuration window by selecting the **Acquire** tab in the Workflow tab bar and select **IconNMR Automation** from the **More** button in the Workflow button bar. Selecting the User and entering password will open the Icon Automation window. Select **Configuration** in the **Options** menu and enter the Administrator password.

5. Select **Additional Users** from the menu selection to the left of the IconNMR Configuration window.



6. Enter the Additional user's Full name (e.g. **Scientist_1**).

7. Enter the User ID (e.g. **sc1**).

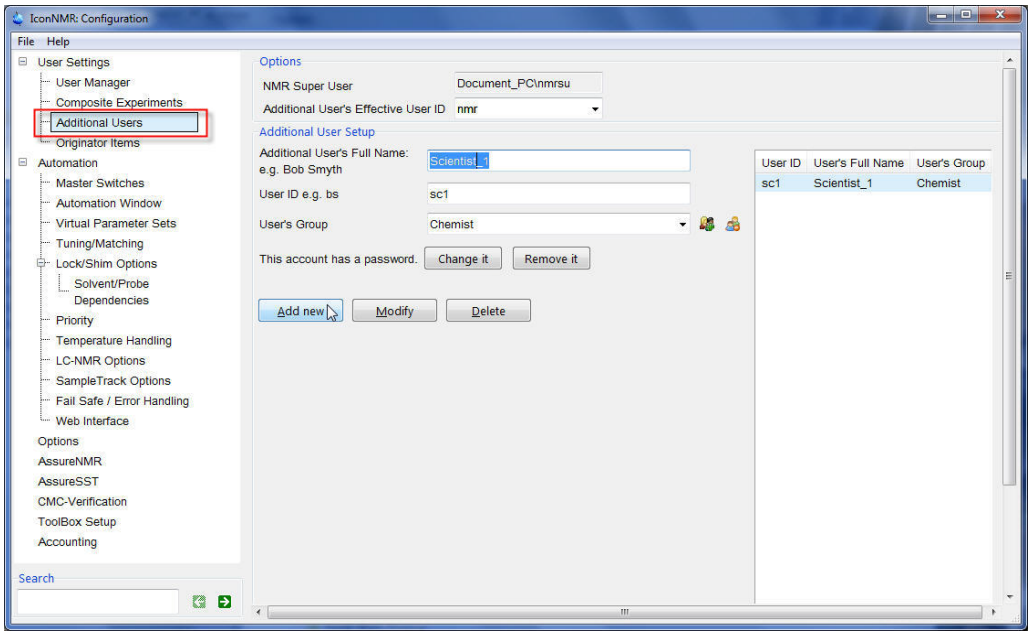
8. Enter a User's Group name (e.g. **Chemist**).

Grouping users together making handling multiple users simpler.

9. Select a **Additional User's Effective USER ID** (e.g. **nmr**).

Experiments and the experiment information FID's etc. are stored using the NMR effective user's ID and permissions as defined. This can be any user which has a System login.

10. Click on the **Add new** button.



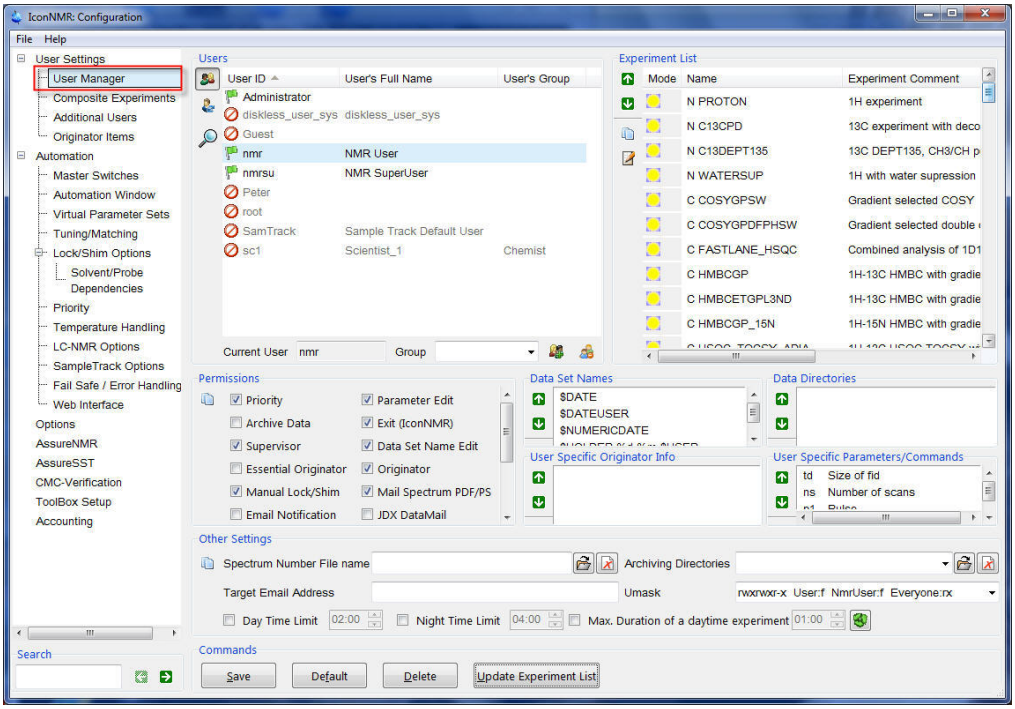
11. To add a password, click on the **Create One** button.

12. Enter a password and hit Enter.

13. Re-enter the password and hit Enter.
14. Click on **File** in the main menu bar.
15. Select **Save**.

3.4 Activating new users in IconNMR

1. Select **User Manager** from the menu selection to the left of the IconNMR Configuration window.

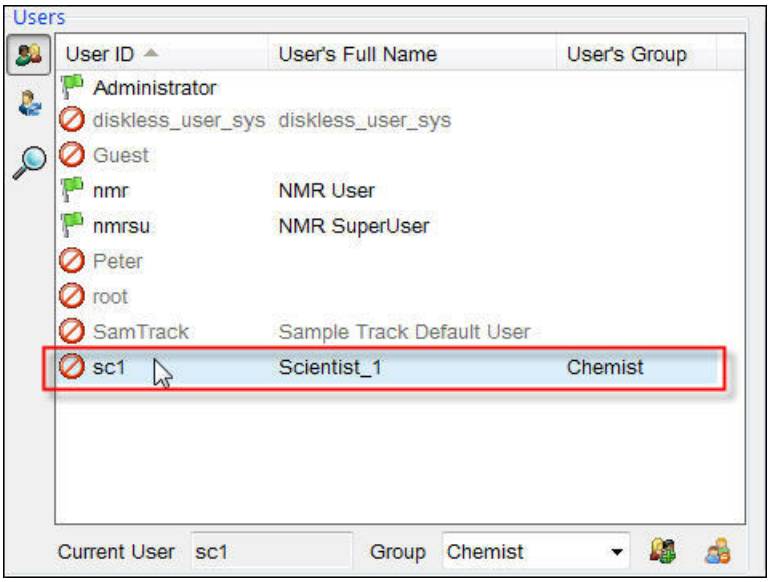


All settings in the User Manager window are user specific.

3.4.1 Users

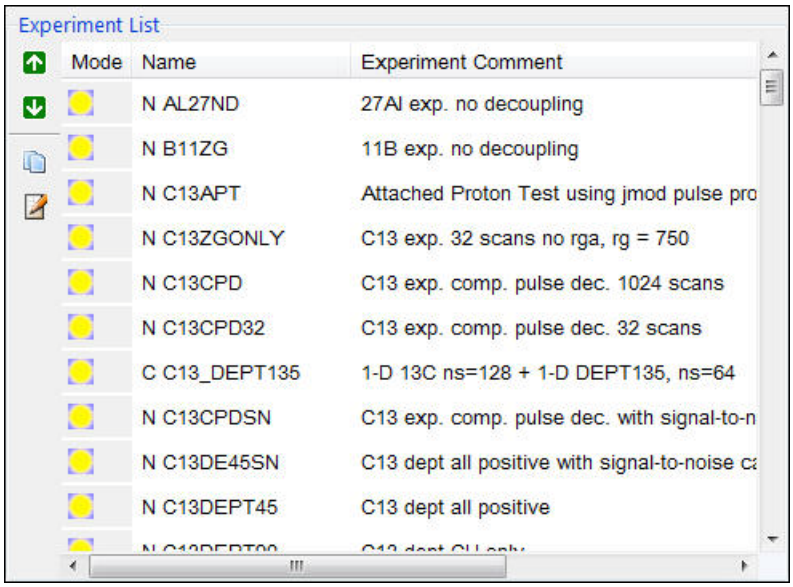
As default the users which can log in to IconNMR are highlighted and display a green flag in the user ID box. New users appear in gray letters and display a red circle.

1. Select the new user (e.g. **sc1**).



3.4.2 Experiment List

When IconNMR is started for the first time, a list of default experiments are loaded automatically. The picture below shows only a section of the experiments. This list can be individually tailored for any users which have an IconNMR login.



3.4.2.1 Mode

Click on the icon, the mode can be changed.to a sun icon which stands for **anytime** or a moon icon for **night time** operation only. To make use of this feature, the Priority and Night/Day switch over has to be enabled and the switch over time has to be set (see **3.13 Priority** in this chapter). Each user can be setup to have their own customized day and night time experiments. This way the users may run experiments only at a specific time.

3.4.2.2 Name

The letter **N** in front the experiment name stands for Normal which denotes a single or stand-alone experiment. The parameters for such an experiment are stored in the <TOPSPIN-home>/exp/stan/nmr/par/ directory under the same name.

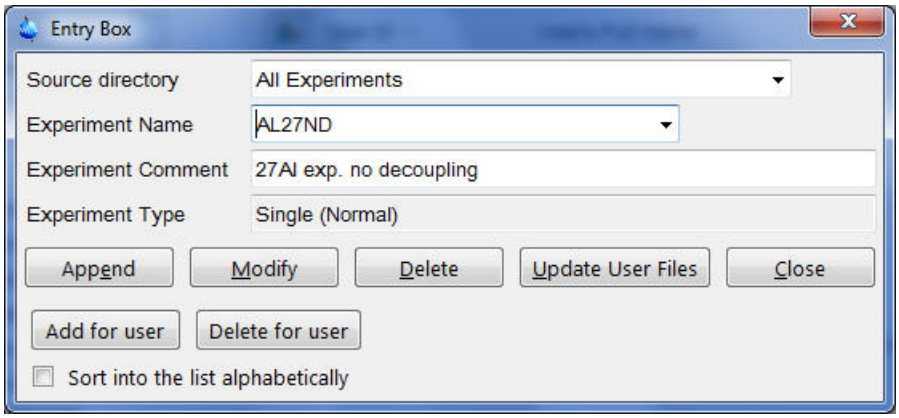
The letter **C** in front of the experiment name stands for Composite experiment and represents a series of two or more experiments combined under one name.

To add to a new user defined **N**- or **C**-experiments and the corresponding parameter sets (**see Chapter 6. Adding new experiments**).

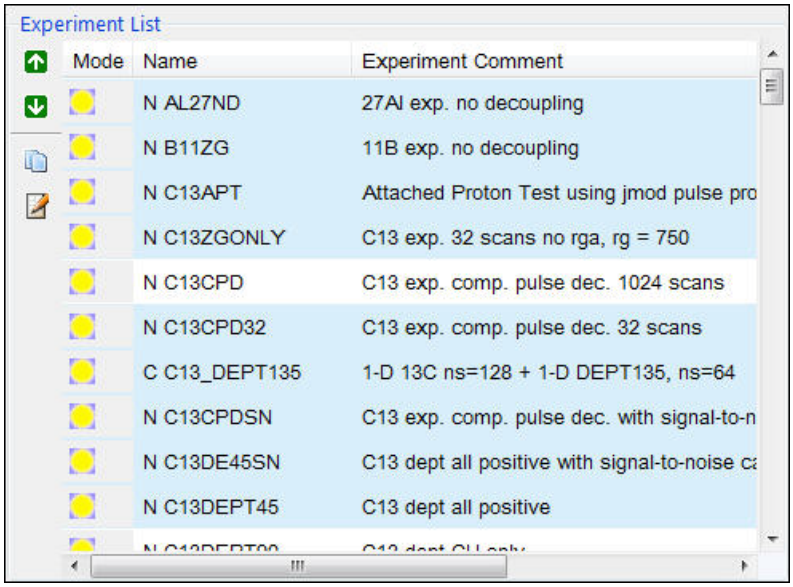
To customize the experiment list by deleting unwanted experiments, follow the steps below:

1. Click on the first to be deleted experiment.

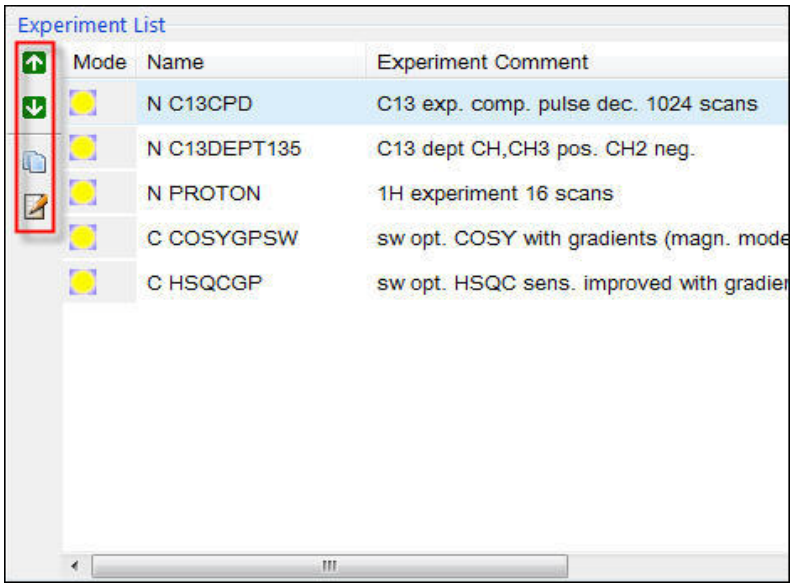
An Entry Box is displayed to manage the experiment list (see below).



2. In the Experiment List window, use the **Ctrl** or **Shift** key to select multiple experiments which you like to delete.



3. Click on the **Delete** button inside the Entry box.
4. Click on the **Close** button inside the Entry box.
5. Click on the **Save** button in the Commands section.



6. If desired, use the **up** or **down arrow** buttons on the left side of the Experiment List window to arrange the order the entries.

7. If desired, use the **Copy** button on the left side of the Experiment List window to copy the selected entry or entries to another users.

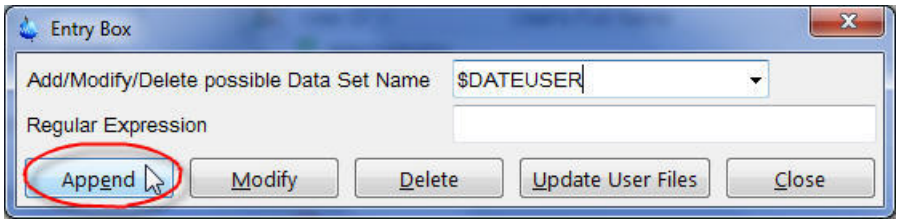
8. If desired, use the **Edit** button on the left side of the Experiment List window to edit the selected entry.

3.4.3 Data Set Names

Predefined data set names can be assigned to the different users. The name(s) can then be chosen from a list during the setup of the experiments in Routine Spectroscopy and Automation. See the IconNMR Reference Manual, **5.2.1.6 The Data Set Names box** for more details.

1. Click inside the **Data Set Name** window.

An Entry Box is displayed to manage the DataSet Name (see below).



2. Type Name in the Data Set Name window, or click on the down arrow and select one of the names provided by Bruker (e.g.**$DATEUSER**).

Input of data set names may be supervised via regular expressions. To use this option, refer to the IconNMR Reference Manual, **5.2.3 The Originator Items Editor**.

3. Click on the **Append** button inside the Entry box.

4. Click on the **Close** button inside the Entry box.

5. Click on the **Save** button in the Commands section.

6. If desired, changes and modifications can be done using the icons to the left of the Data Set Names window (see **3.4.2.2 Name**, steps **6** through **8** in this chapter).

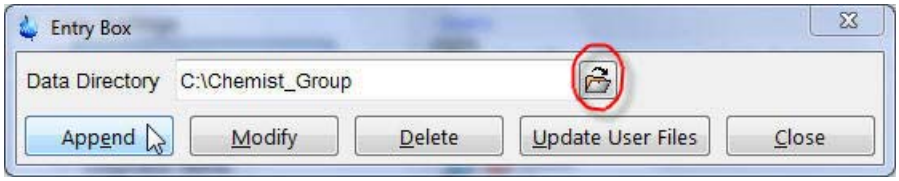
3.4.4 Data Directories

Predefined disk partition(s) for data storage can be assigned to the users. The partition(s) name(s) can be chosen from a list during the experiment set up within the Automation and Routine Spectroscopy. If the **Data Directories** window shows no assigned partitions and is empty, then the data are stored as default in the TopSpin home directory.

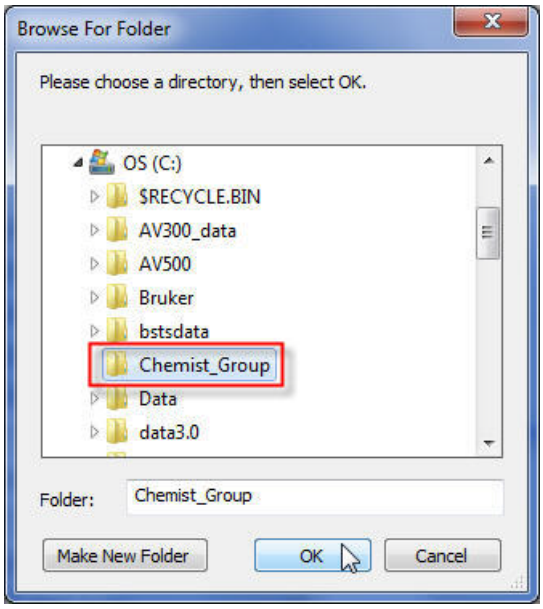
A default data path: **/data/<user name>/nmr** is added automatically to the disk partition name.
If desired, use the options in the configuration **Master Switches** window: **Data set management** to eliminate data, nmr or user from the data set path.

1. Click inside the Partition Names window.

An Entry Box is displayed to manage the Data Directories (see below).



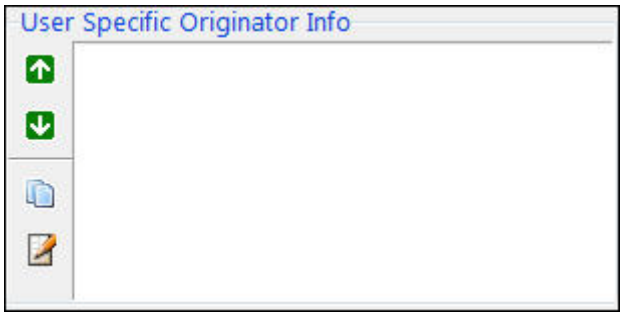
2. Click on Folder icon next to Data directory inside the Entry Box.



3. Select the directory name (**e.g. C:\Chemist Group**).
4. Click on the **OK** button inside the Browse For Folder window.
5. Click on the **Append** button inside the Entry Box.
6. Click on the **Close** button inside the Entry Box.
7. Click on the **Save** button in the Commands section.
8. If desired, changes and modifications can be made using the icons to the left of the

Data Set Names window (see **3.4.2.2 Name**, steps **6** through **8** in this chapter).

3.4.5 User Specific Originator Info



By default this box is empty. Information, such as Instrument name, Company, Department, etc. can be assigned to different users as predefined entries. The users can also enter the information during the experiment set up within the Automation or Routine Spectroscopy. To make use of this option, follow instructions in **chapter 7**, section **7.2**, **How to assign User Specific Originator Information**.

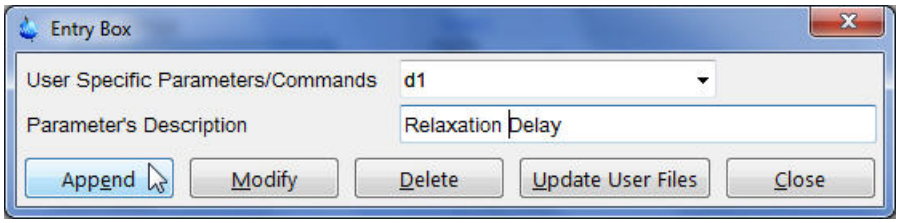
3.4.6 User Specific Parameters/Commands

Within a laboratory environment, users maybe allowed to change parameters or some TopSpin commands specified by the system manager. To take advantage of this option during the experiment set up with in Automation or Routine Spectroscopy, the **Parameter Edit** permission in the Permissions window has to be disabled. If enabled the users will have access to all parameters and in addition the User Specific Parameters/Commands.

1. Click inside the **User Specific/Commands** window.

An Entry Box window is displayed to manage the User specific Parameters/ Commands. (see below).

2. Click on the down arrow next to the User Specific Parameters/Commands field and select the parameter (e.g. **d1**).



The text **Delay** is automatically entered in to the Parameter Description field. If desired this text can be edited (e.g. **Relaxation Delay**).

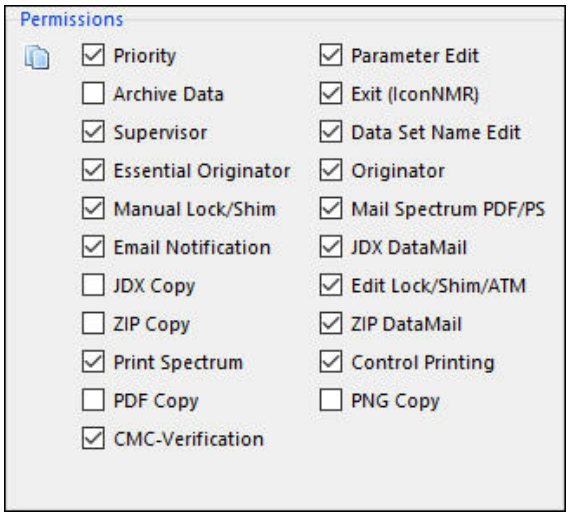
3. Click on the **Append** button inside the Entry box.

4. Click on the **Close** button inside the Entry box.

5. Click on the **Save** button in the Commands section.

6. If desired, changes and modifications can be made using the icons to the left of the Data Set Names window (see **3.4.2.2 Name**, steps **6** through **8** in this chapter).

3.4.7 Permissions



When the User Manager is started for the first time, default permissions are set. To change any permissions, click on any permission names. No check mark means no permission and a check mark means permission is granted. The permission settings can be copied to other users by clicking on the **Copy** icon to the left of the Permissions window. Below are the descriptions of the permission boxes.

3.4.7.1 Priority

A user may declare a sample or experiment to have a priority status. This option should only be used for automation with a random access sample changer. The Six-Pack and Nmr-Case changers may only operate in a sequential manner and Priority will be disabled automatically if such sample changers are in use. See **3.13 Priority** in this chapter to define how the priority switch is to be handled.

3.4.7.2 Archiving Data

This option applies for both the Automation and Routine Spectroscopy. If permission is granted, the user's data (after processing has been completed) is copied into a directory whose path is specified in the Archiving Directory box, see **3.4.9 Archiving Directory**.

3.4.7.3 Supervisor

This option applies for both the Automation and Routine Spectroscopy. If permission is granted, the user can minimize the IconNMR windows to access other programs on the desktop of the operating system. The user also has full control of all Topspin features.

3.4.7.4 Essential Originator

This option applies for both the Automation and Routine Spectroscopy. To use this feature, both the Originator and Essential Originator permissions have to be enabled. The user must then fill in the originator value in to the title field of the Automation set up window. The experiment cannot be submitted unless the originator information is entered.

3.4.7.5 Manual Lock/Shim

This option applies for both the Automation and Routine Spectroscopy. If enabled, the user is granted permission to activate the Manual Lock/Shim/ATMM feature in the Run menu in the Routine Spectroscopy or Automation set up window (see **7.3 How to use the Manual Lock/Shim/ATMM options**).

3.4.7.6 E-mail Notification

This option applies for both the Automation and Routine Spectroscopy. Permission can be granted to different users to be notified through E-mail when an experiment or sample is finished. This feature requires an E-mail address (see the section **Other Settings** in **3.4.8 Target E-mail Address**) or the E-mail address can be entered as a Originator value during the Automation set up (see **3.6 Originator Items**). It also requires an SMT mail server address and other options can be set (see the section **3.18.6 Mail** in the **Options** window).

3.4.7.7 JDX Copy

If enabled, IconNMR generate a copy of the data set in JCAMP-DX format and stores the data with an unique name in a directory as specified by the fields shown in **3.18.9 JDX Copy Mode**, in the **Options** window. This feature is in addition to all the other Archiving/Data Mail modes.

3.4.7.8 Zip Copy

If enabled, IconNMR generate a copy of the data set in JCAMP-DX format as a ZIP file and stores the data with an unique name in a directory as specified by the fields shown in **3.18.10 ZIP Copy Mode**, in the **Options** window. This feature is in addition to all the other Archiving/Data Mail modes.

3.4.7.9 Print Spectrum

If enabled, sets the check button controlling printing in Automation to on or off. This will then be the default setting for the user and determines whether a printout is to be made or not.

3.4.7.10 PDF Copy

If enabled, IconNMR generate a copy of the data set in PDF format and store the data with an unique name in a directory as specified by the fields shown in **3.18.7 PDF Copy Mode**, in the **Options** window. This feature is in addition to all the other Archiving/Data Mail modes.

3.4.7.11 Parameter Edit

This option applies for both the Automation and Routine Spectroscopy. If enabled, the user then can change any parameters during the set up of an experiment (acquisition, processing and plotting) and also have access to the User Specific Parameters/ Command.
If disabled, only the User Specific Parameters/Commands are accessible.

3.4.7.12 Exit (IconNMR)

This option applies for both the Automation and Routine Spectroscopy. If enabled the user is granted permission to exit IconNMR and open other software applications.
If disabled, the NMR Superuser password is required to exit IconNMR.

3.4.7.13 Data Set Name Edit

This option applies for both the Automation and Routine Spectroscopy. If enabled, the user can type a data set name during the set up of an experiment or choose one from the predefined names.
If disabled, only the predefined data set names are accessible and the user can only choose a data set name from the list created in the Data Set Names box (see **3.4.3 Data Set Names**).

3.4.7.14 Originator

This option applies for both the Automation and Routine Spectroscopy. If enabled, the Originator information and the associated User Specific Information (see **3.4.5 User Specific Originator Info**) is displayed in the file name set up box for Routine Spectroscopy and in the title window for Automation.

3.4.7.15 Mail Spectrum PS/PDF

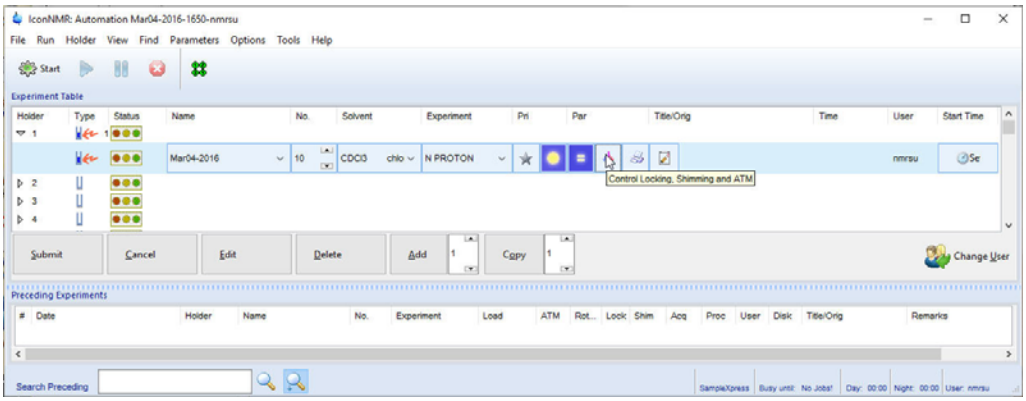
This option applies for both the Automation and Routine Spectroscopy. If enabled the user receives a general plot file as either a **PS** or **PDF** format. This feature requires the same set up as for the E-Mail Notification and in addition choose the format (see in **3.7.2.3 Generate Spectrum Print-Out file in data set for possible dispatch to E-mail recipient**, in the **Master Switches** window).

3.4.7.16 JDX Data Mail

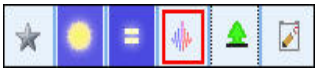
This option applies for both the Automation and Routine Spectroscopy. If enabled the user receives the data as a **JCAMP** format file. This feature requires the same set up as for the E-Mail Notification and in addition choose the format, (see in **3.18.9 JDX Copy Mode**, in the **Options** window).

3.4.7.17 Edit Lock/Shim/ATM

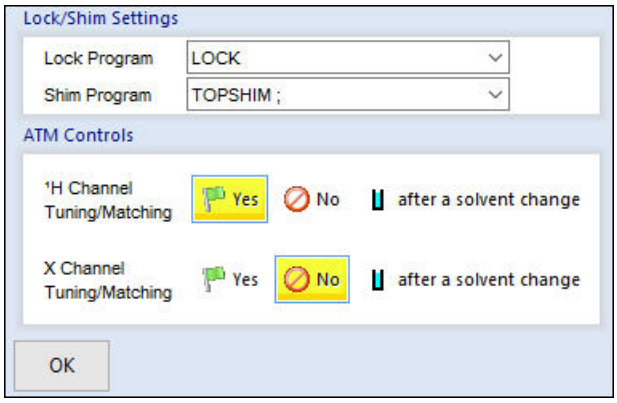
This option applies only for the Automation only. If enabled, permission is granted to users to use the “Automatic Lock Program, Automatic Shim Program and ATM Control” options in the Automation set up window in figure below, the cursor is pointing to the Control icon.



Below is a close up of the control icons.



Click on the icon and a pull down menu appears.

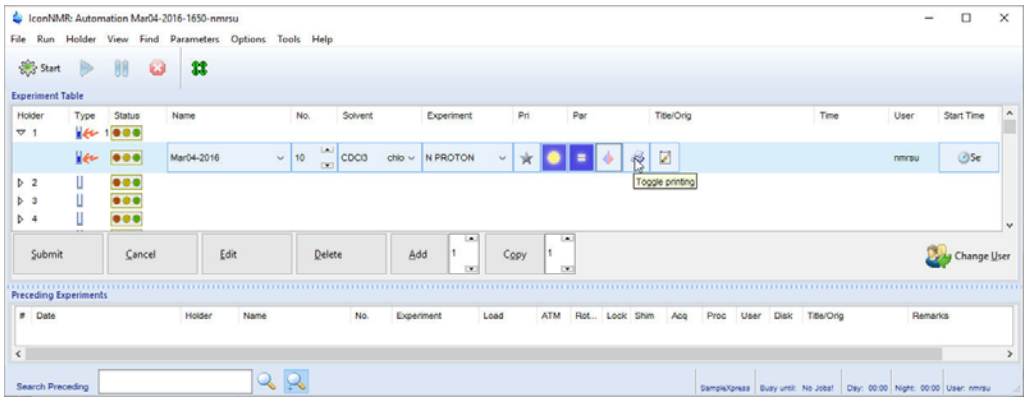


3.4.7.18 Zip Data Mail

This option applies for both the Automation and Routine Spectroscopy. If enabled the user receives the data as a **ZIP** file. This feature requires the same set up as for the E-Mail Notification and in addition choose the format, (see in **3.18.10 ZIP Copy Mode**, in the **Options** window).

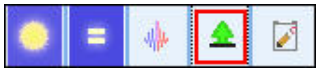
3.4.7.19 Control Printing

If enabled, the option for printing or not printing a spectrum can be set in the Automation set up window before submitting a sample.

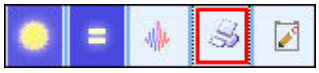


Below is a close up of the control icons.

No Printing



Printing to the default printer



3.4.7.20 PNG Copy

If enabled, IconNMR generate a copy of the data set in PNG format and store the data with an unique name in a directory as specified by the fields shown in **3.18.8 PNG Copy Mode**, in the **Options** window. This feature is in addition to all the other Archiving/Data Mail modes.

3.4.8 Other Settings

3.4.8.1 Spectrum Number File name

This entry which is located in the **Other Settings** section, provides an additional method of prescribing data file names. The contents of this entry field will be considered as a path name of a text file set up by the laboratory manager. The file name must start with letters and ending with a number. The data set name will automatically increment on setting up the next sample. To create this file, follow the steps below:

3.4.8.2 For LINUX, follow the steps below to create the text file:

1. Open a shell window

2. Choose a directory where the text file should reside (e.g. /usr/adm)

3. Type **cd /usr/adm**

4. Use an editor to create a text file which contains the data set file name which must start with letters and end with a number (e.g. **sample000**).

5. Store the file (e.g. **data set name**).

6. Start IconNMR.

7. Open the IconNMR Configuration window.

8. Select one or multiple users using the Ctrl or Shift key.

9. Click on the folder icon next to the **Spectrum Number Filename** box and select **/usr/adm/data set name**

10. Click on the **Save** button inside the IconNMR Configuration window (Commands section).

3.4.8.3 For Windows, follow the steps below:

1. Open the Note Pad application

2. Type a data set filename which must start with letters and end with a number (e.g. **sample000**)

3. Click on Save As

4. Select a directory (e.g. **C:\Temp**)

5. Choose a file name (e.g. **datasetname.txt**)

6. Start IconNMR

7. Open User Manger

8. Select one or multiple users using the Ctrl or Shift key

9. Click on the **folder** icon next to the **Spectrum Number Filename box** and select **C:\Temp\datasetname.txt**

10. Click on the **Save** button inside the IconNMR Configuration window (Commands section).

3.4.8.4 Target E-mail Address

This option is used to send Notification of completed experiments, Data or a PS/PDF file to be attached to an E-mail. A valid E-mail address have to be entered in to the Target E-mail Address window (e.g. **scientist2@company.com**). If an E-mail address is entered as a value for the Originator item **Data Mail/Notify to** in the title window, then it will

overwrite this **Target E-mail Address**.

3.4.8.5 Archiving Directories

This entry allow the above items to be defined on a per user basis, even for so-called NMR users who do not have a direct login on the workstation. The archiving directory could be used for example, to define an NFS mounted file system which is to be used to store a copy of any experiments data after processing.The workstation manager is responsible for the setup of such an archiving directory.

All data sets generated by the programs have audit trail files which catalog what has been done on the data set.

The archive function never overwrites data set directories which already exist on the target drive. If the Data Set directory with the particular expno already exists, IconNMR will add a prefix _<Number> to the Data Set Name and try to do the copy again. It will keep incrementing the <Number> prefix until a free directory is found.

3.4.8.6 Umask

The Umask entry stems from the Unix world and has some influence over the data permissions on Windows workstations. In that case, the order of the rw (read, write flags in as follows. (rw-rw-rw-). The first rw refers to the currently logged in User, the second refers to the group NmrUser, and the last refer to Everyone. It should be noted that the ownership of the data cannot be given to another Windows user. Ownership on Windows® systems can only ever be taken.

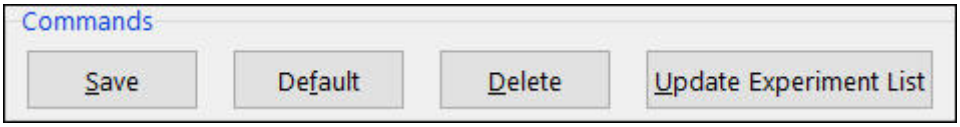
Important: This is for all Windows operating systems only. The group name:
NmrUser must be added to all Window users, using IconNMR to assure the correct data permission.

3.4.8.7 Experiment Time Limits

The maximum permissible total experiment duration may be entered for users to prevent any one user commanding too much time on the instrument. The times entered are granted to each user per each calendar day. Using the entry Max. Daytime. Experiment

Duration' specifies how long any individual experiment can take be before it is declared too time consuming to run in 'Day Time'. To make use of this option, follow instructions in **chapter 7**, section **7.1, How to set Day and Night Time limits for users**.

3.4.9 Commands



3.4.9.1 Save

The Save button saves the current settings on disk, in the file:
TOPSPINHOME/conf/instr/<instrument-name>/inmrusers/<userid>

You may save everything you have set up so far for several users at once. Hold down the <ctrl> key and mark all desired users in the User Names box by clicking on them. Or keep the <shift> key depressed while clicking on a user. This will automatically mark all users from the currently selected one to this position. Then click on the Save button.

3.4.9.2 Default

The Default button initializes all boxes with the default information stored in the file: TOPSPINHOME/exp/stan/nmr/lists/sam_users_exam.inmr.

3.4.9.3 Delete

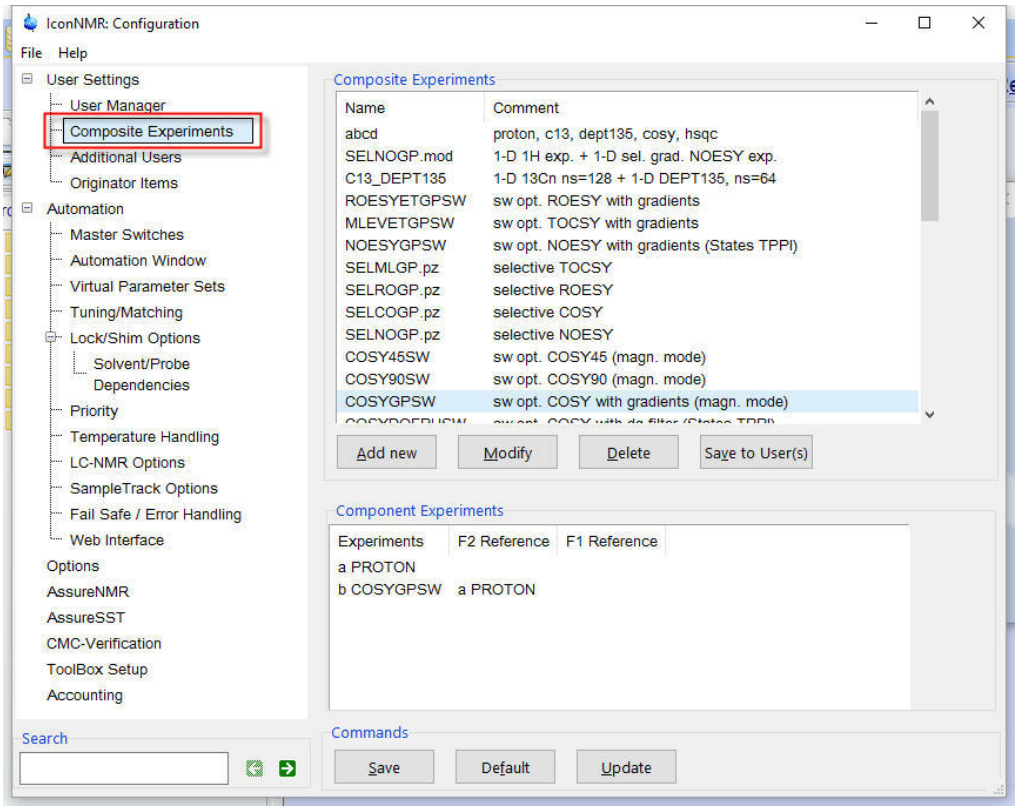
Use the Delete button to remove users from IconNMR. Mark the users you wish to delete and click on the delete button. Their user file will be deleted.

3.4.9.4 Update Experiment List

Loads experiments from the current IconNMR version into the Experiment list. Delete all current experiment entries.

3.5 Composite Experiments

1. Click on **Composite Experiments** on the left side of the IconNMR Configuration window.



A composite experiment is a series of two or more experiments combined under one name. To add a new composite experiment to the existing list, follow the instructions in **Chapter 6**, **Adding new experiments**, section **6.7**.

Composite experiments may not include other composite experiments.

3.5.1 Add new-, Modify-, Delete-, Save to buttons

3.5.1.1 Add new

Add a new composite experiment to the Composite Experiment list.

3.5.1.2 Modify

Modify a existing composite experiment listed in the Composite Experiment list.

3.5.1.3 Delete

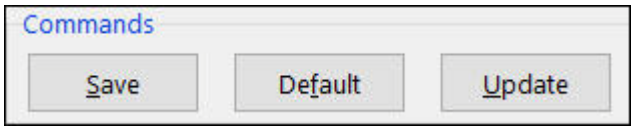
Delete a composite experiment from the Composite Experiment list.

The same experiment has to be also deleted from the Experiment list in the User Manager window.

3.5.1.4 Save to

Save a new or existing composite experiment to one or multiple users adding to the Experiment list bypassing the User manager.

3.5.2 Commands



3.5.2.1 Save

Saves the current Composite Experiment list to the disc into the directory: TOPSPINHOME/conf/instr/<instrument-name>/inmrusers/.pool_txt. This command is also accessible via the file menu.

3.5.2.2 Default

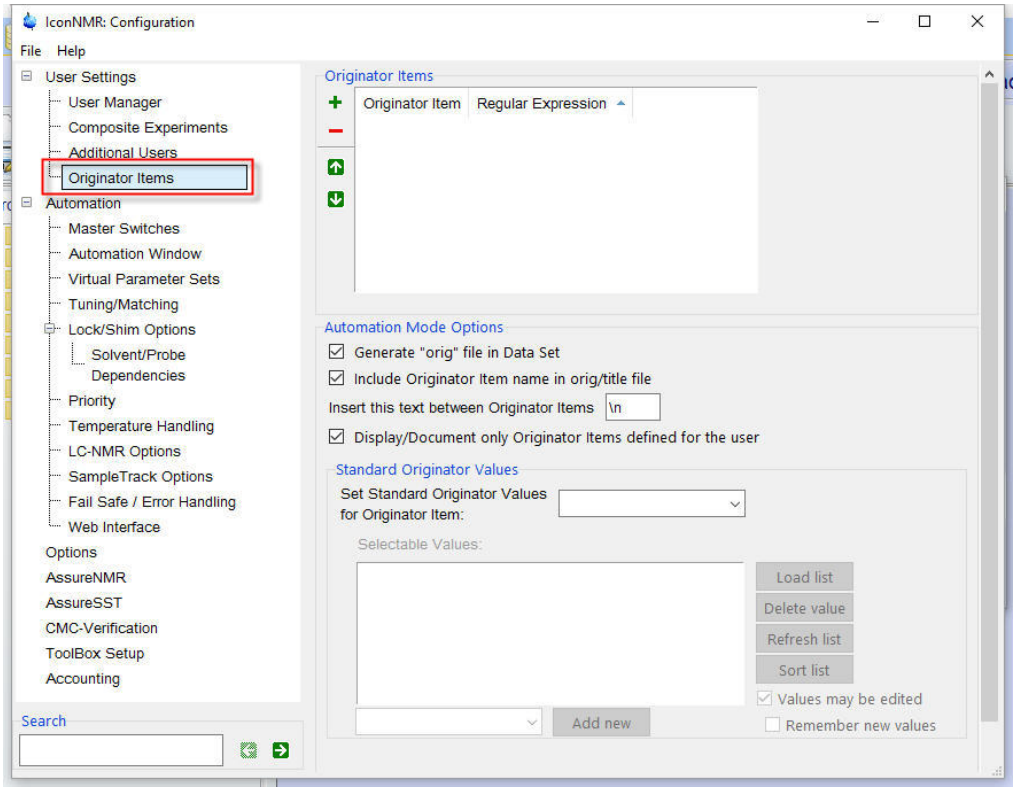
Loads the default composite experiments into the Composite Experiment list from the disc in the directory:
TOPSPINHOME/exp/stan/nmr/lists/def_comp_exps.inmr.
It will discard all present composite experiments.

3.5.2.3 Update

Extends the current list with new composites from this version of IconNmr.

3.6 Originator Items

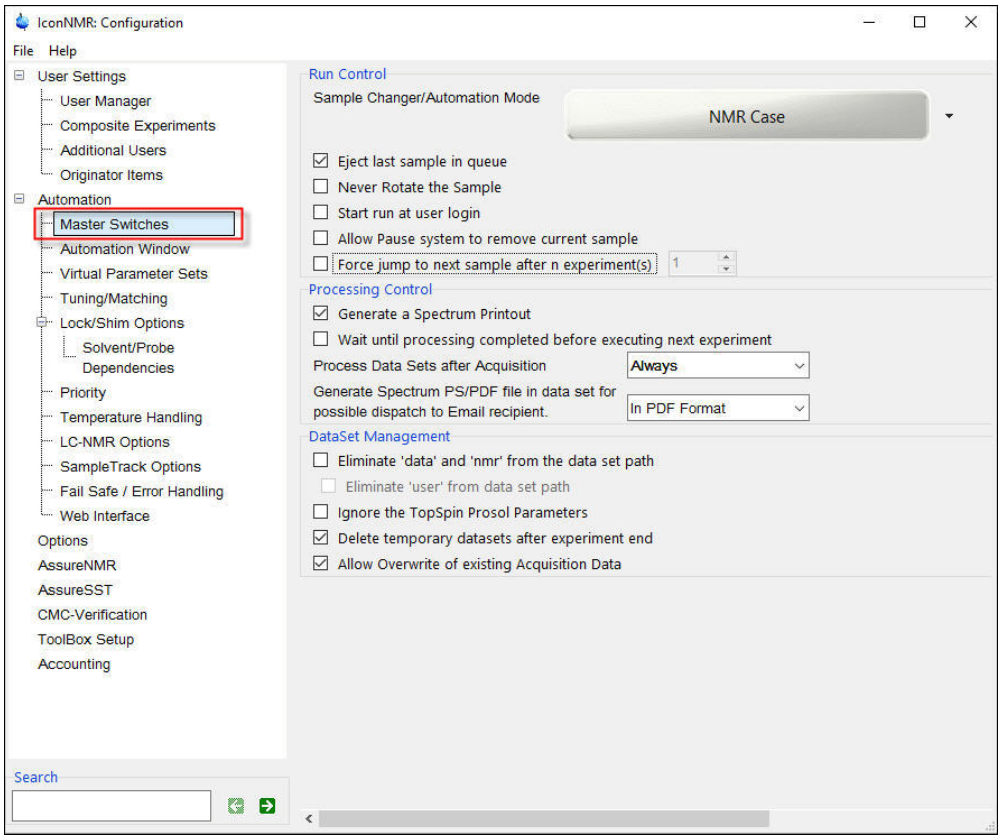
1. From the configuration item window select **Originator Items**.



To use this option and to add the Originator items and values to users, follow the instructions in **chapter 7**, section **7.2 How to assign User Specific Originator Information**.

3.7 Master Switches

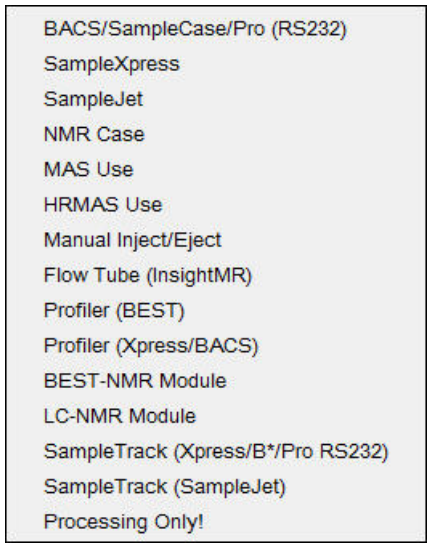
1. Click on **Master Switches**



3.7.1 Run Control

3.7.1.1 Default Automation Mode

This option applies only for Automation and not for Routine Spectroscopy. By clicking on the gray box a list of different automation modes or “drivers” appears.



The selection of the default mode is primary designed for starting the run at the users login option.

3.7.1.2 Eject last sample in a queue

This option applies only for Automation and not for Routine Spectroscopy. If enabled, the last sample will eject after all experiments are completed and if there are no new samples submitted to the run. Some automation modes do this regardless of the setting e.g. MAS, HRMAS.

3.7.1.3 Never Rotate the Sample

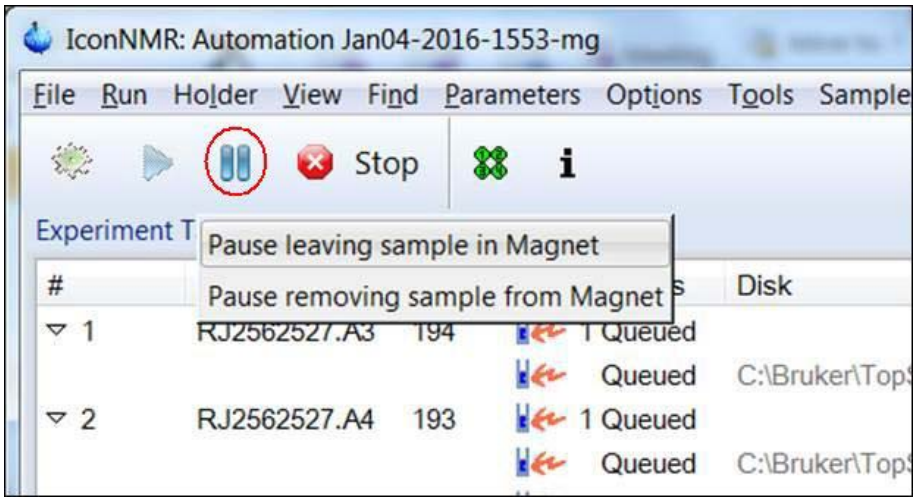
If enabled, all sample are run non spinning. This option applies for both the Automation and Routine Spectroscopy and should be used whenever sample spinning is not desired (e.g. BBI-, TXI- probes).

3.7.1.4 Start run at users login

This option applies only for Automation and not for Routine Spectroscopy. If enabled, the run will start when the user logs into IconNMR Automation. The current default automation mode selected in **3.7.1.1 Default Automation Mode** will be used.

3.7.1.5 Allow Pause system to remove current sample

If enabled, a popup window appears when hitting the pause button in the Automation window. It inquires as to whether the sample should be removed after the experiment is completed or leaving the sample in the magnet (see picture below).



3.7.1.6 Force jump to next sample after every experiment

Instead of Icon running all experiments on a sample before proceeding to the next one, use this flag to force Icon to only execute one experiment on a sample and then jump to the next sample.

3.7.2 Processing Control

3.7.2.1 Generate Spectrum Print-Out

If enabled, it will suppress the printing normally associated with the execution of the processing AU program. Processing will proceed as normal but no paper printout will be generated.

3.7.2.2 Wait until processing completed before executing next experiment

If enabled, it halts the run from continuing with the next experiment/sample until the processing of the current experiment/sample is finished. This may be useful if processing of the acquired experiment is part of an analysis.

3.7.2.3 Process Data Sets after Acquisition

This option applies only for Automation and not for Routine Spectroscopy. By clicking on the gray box, a list of choices appear.

Always

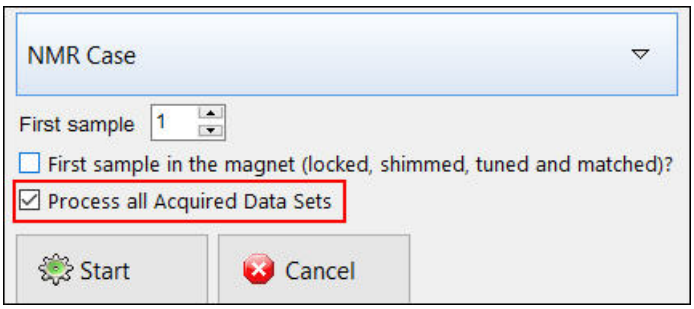
all experiments are processed.

Never

no processing done on any of the experiments.

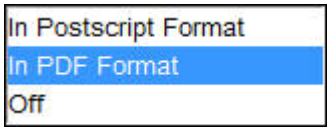
Ask on Startup

in the Initialize Run Window a check box will give the option to process the data after acquisition.



3.7.2.4 Generate Spectrum Print-Out file in data set for possible dispatch to E-mail recipient

Use of this feature creates a PS or PDF file in the pdata procno directory of the data set. IconNMR will send it to the currently defined user E-mail address. After sending the file, it will be deleted from the data set directory.



3.7.3 DataSet Management

3.7.3.1 Eliminate ‘data’ and ‘nmr’ from the data set path

Use this feature to change the way IconNMR creates data paths for your data. With this button unchecked (default) ICON continues to create data sets in the old style: /data/<User>/nmr/<Data Set Name>/<Expno>/pdata/<Procno> Activate the feature and ICON will remove the data and nmr parts of the path. This feature requires that IconNMR be restarted, no change will occur before that. This feature requires TopSpin Version 3 or

better.

3.7.3.2 Eliminate ‘user’ from data set path

Use this in conjunction with the above feature to also remove the user directory. The same rules apply as in the data and nmr case.

3.7.3.3 Ignore the TOPSPIN Prosol Parameters

If enabled, IconNMR does not execute a pulse sort and therefore ignores the prosol parameters. This option is primarily used for non standard pulse programs and instrument configurations.

3.7.3.4 Delete temporary datasets after experiment completion

When an experiment is submitted, IconNMR creates a temporary data set in the directory /<TOPSPINHOME>/prog/curdir/changer/inmrchanger. This data set contains all information to run the experiment including any changes in experimental parameters. The main purpose of using this option is to save disk space.

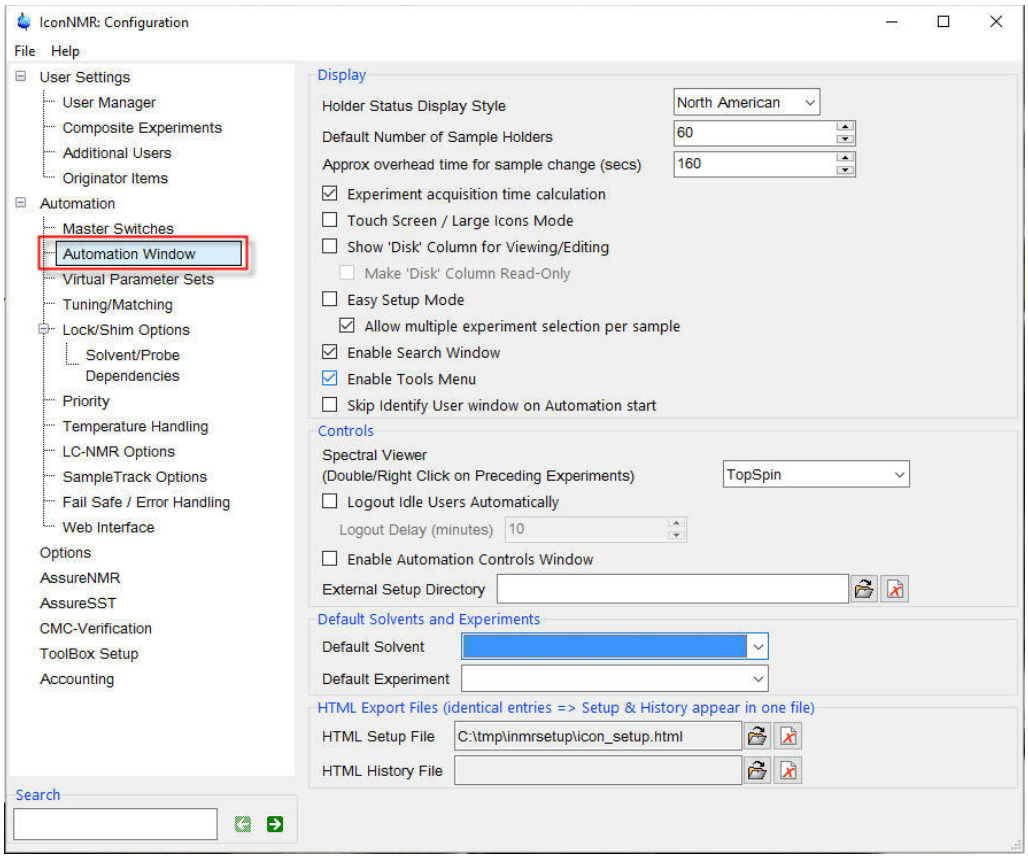
- **!!!WARNING!!!: IT IS NOT RECOMMENDED TO USE THIS OPTION WHEN THE SET UP FILE HAS TO BE SAVED FOR REPEATED USE SINCE ANY PARAMETER CHANGES WOULD BE LOST.**

3.7.3.5 Allow Overwrite of existing Acquisition Data

If enabled, IconNMR will overwrite a existing dataset. If this option is not checked, the experiment is skipped and the remarks column in the history window will indicate that the data already exist.

3.8 Automation window

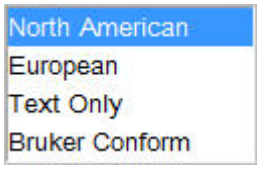
1. Click on **Automation window**.



3.8.1 Display

3.8.1.1 Holder Status Display Style

This options applies for Automation only and not for Routine Spectroscopy. One of four display modes can be selected:



North American traffic light style

no lights = experiment may be set up

yellow = sample submitted, waiting to run

green = experiment in progress

red = experiment done, sample measured

lights black = experiment aborted or failed

European traffic light style

green = experiment may be set up

red & yellow = sample submitted, waiting to run

red = experiment in progress

yellow = experiment done, sample measured

lights black = experiment aborted or failed

Text only

Available = experiment may be set up

Queued = sample submitted, waiting to run

Running = experiment in progress

Finished = experiment done, sample measured

Failed = experiment aborted or failed

Bruker Conform

Conformity between Bruker's various Automation software programs

3.8.1.2 Default Number of Sample Holders

This option applies for Automation only and not for Routine Spectroscopy. A number of sample holders can be chosen for various sample changers or manual sample change operation. The default number of sample holders are set during the **Sample changer configuration** as part of **cf**.

3.8.1.3 Approx overhead time for sample change (secs)

This option applies for Automation only and not for Routine Spectroscopy. The time entered in Seconds defines how long a sample change takes and it is used in calculating the **Expt Time** and **Busy until Times** displayed in the Automation set up window.

3.8.1.4 Experiment acquisition time calculation

This option applies for Automation only and not for Routine Spectroscopy. If enabled, the acquisition time is calculated on submitting an experiment or when parameters of an experiments are changed. The picture below shows the time calculation displayed on the bottom of the Automation window.

3.8.1.5 Touch Screen / Large Icons Mode

When enabled, the icons in the Automation set up screen are enlarged. This option is primarily used for touch screen operation.

3.8.1.6 Show 'Disk' Column for Viewing/Editing

When enabled the disk column is shown and can be edited in the Automation set up window. Disabling will remove the disk column.

3.8.1.7 Make 'Disk' Column Read-Only

Enabling this option together with the previous one will show the Disk column in the Automation set up window but can not be edited.

3.8.1.8 Easy Setup Mode

When enabled, a simplified entry window is used to set up samples in Automation. For more detailed information, see **7.4 How to use the Easy Setup Mode**.

3.8.1.9 Enable Search Window

When enabled, users can search through Icon's records of previous experiments in the Automation set up window (see picture below).

3.8.1.10 Enable Tools Window

When enabled, users will have access to the features shown in the Tool Menu of the Automation window (see **5.3 Tool Menu**).

3.8.1.11 Skip Identify User window on Automation start

Use this to have the automation window appear immediately with IconNMR Automation logged in as the current <system> user.

3.8.2 Controls

3.8.2.1 Spectral viewer

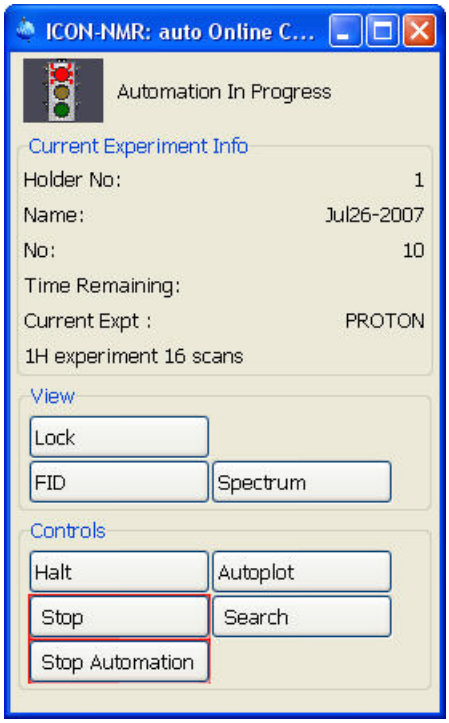
This option selects to view the spectrum in either the TopSpin or the Amix-viewer program. To apply, double click in the history window on the completed experiment in the Automation set up display.

3.8.2.2 Logout Idle Users automatically

This option applies for both the Automation and Routine Spectroscopy. It is designed for users who are required to log themselves out after all of their experiments have been submitted. If enabled, user's are automatically logged out after the specified idle time in Minutes.

3.8.2.3 Enable Automation controls Window

This option applies for Automation only and not for Routine Spectroscopy. If enabled The Automation Controls window as shown here appears during a run when an acquisition is in progress.



3.8.2.4 External Setup Directory

In this option a external set up directory can be entered. This is especially useful if a pool directory is to be used where multiple IconNMR programs scan the same directory looking for a external setup file based on for example a BEST-NMR well plate barcode.

3.8.3 Default Solvent and Experiment

3.8.3.1 Default Solvent

In cases where the same solvent is repeatedly used, a default solvent can be selected in this option. This selection is then entered automatically in the respective fields during the automation set up of a sample.

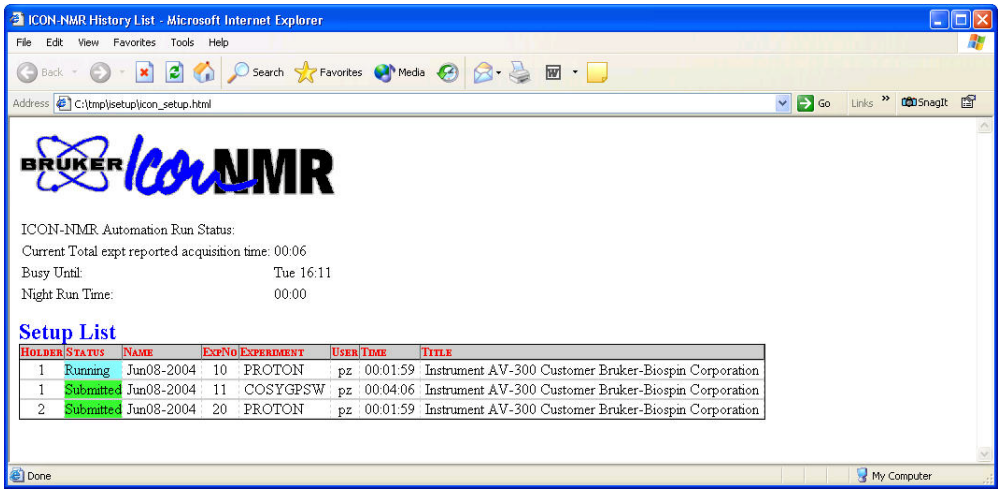
3.8.3.2 Default Experiment

In cases where the same experiment is repeatedly used, a default experiment can be selected in this option. This selection is then entered automatically in the respective fields during the automation set up of a sample.

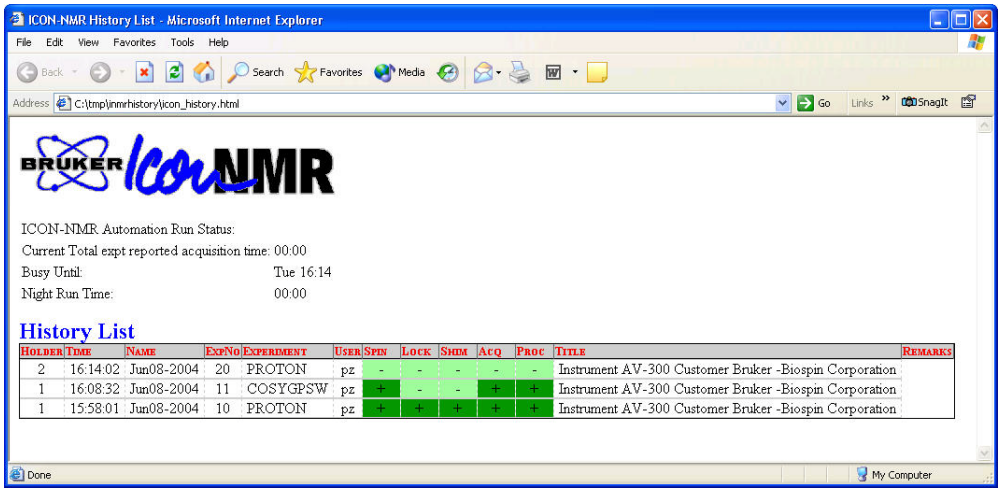
3.8.4 HTML Export Files

A directory path can be chosen to store the IconNMR setup and history files which are created during an automation run. This files are in HTML format and can be viewed through an Internet browser as shown below. (e.g. c:/tmp/inmrsetup and c:/tmp/inmrhistory). Identical entries results in that the Setup and History appear in one file.

3.8.4.1 IconNMR Setup file

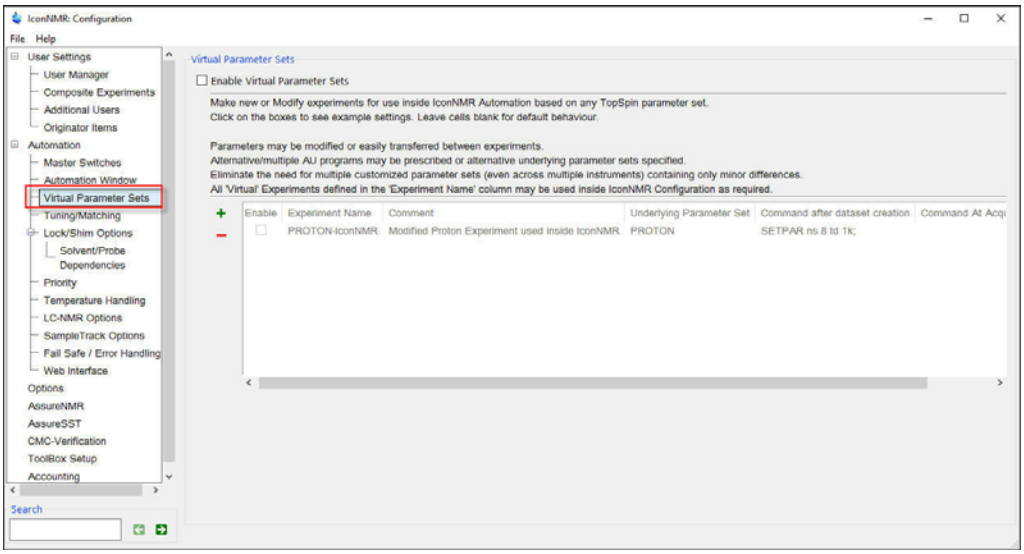


3.8.4.2 IconNMR History file



3.9 Virtual Parameter Sets

1. Click on **Virtual Parameter Sets**.



Make new/Tweak experiments for use inside IconNMR Automation based on any TopSpin parameter set.

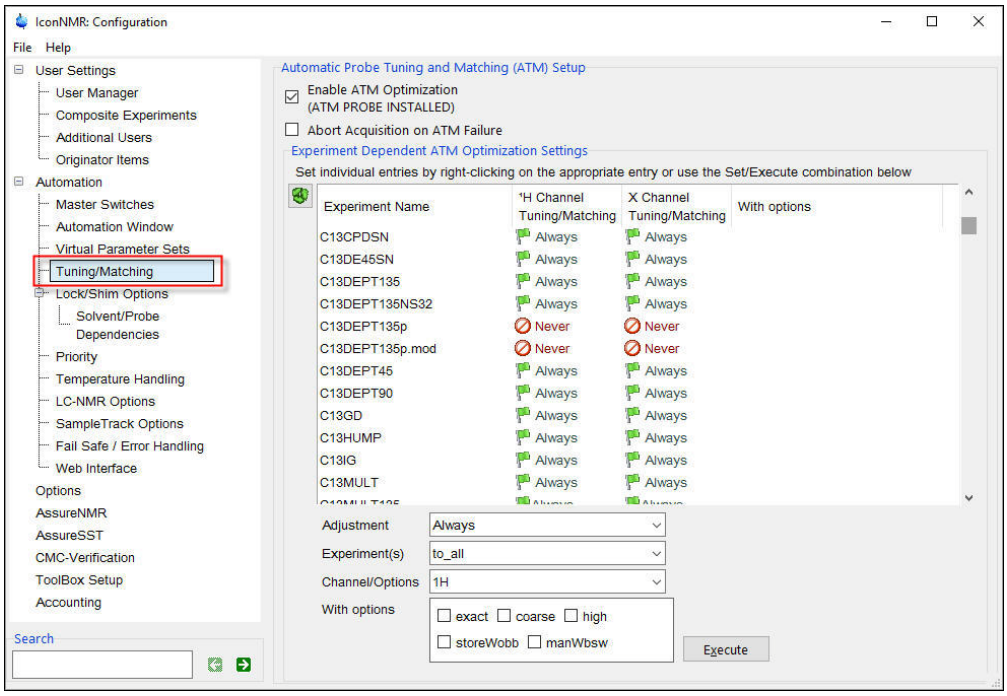
Parameters may be modified or even inherited by other experiments. Alternative/ multiple Acquisition AU programs/commands may be prescribed or alternative underlying parameter sets selected.

Eliminate the need for multiple customized parameter sets (even across multiple instruments), with only minor differences.

To use this option follow the example in **chapter 6**, **Adding new experiments**, section **6.9**.
For more in-depth information, consult the Reference Manual, page 111, **5.6 Virtual Parameter Sets.**

3.10 Tune / Matching

1. Click on **Tune / Matching**



3.10.1 Automatic Probe Tuning and Matching (ATM) Setup

Most of the high resolution probes with some exceptions are equipped with automatic tuning and matching capabilities (ATM). The TopSpin command atma tunes and matches the probe automatically according to the NUC settings in the current data set. To make use of this feature, follow the steps below.

3.10.1.1 Enable ATM Optimization (ATM PROBE INSTALLED)

1. Click inside the square next to enable ATM Optimization.

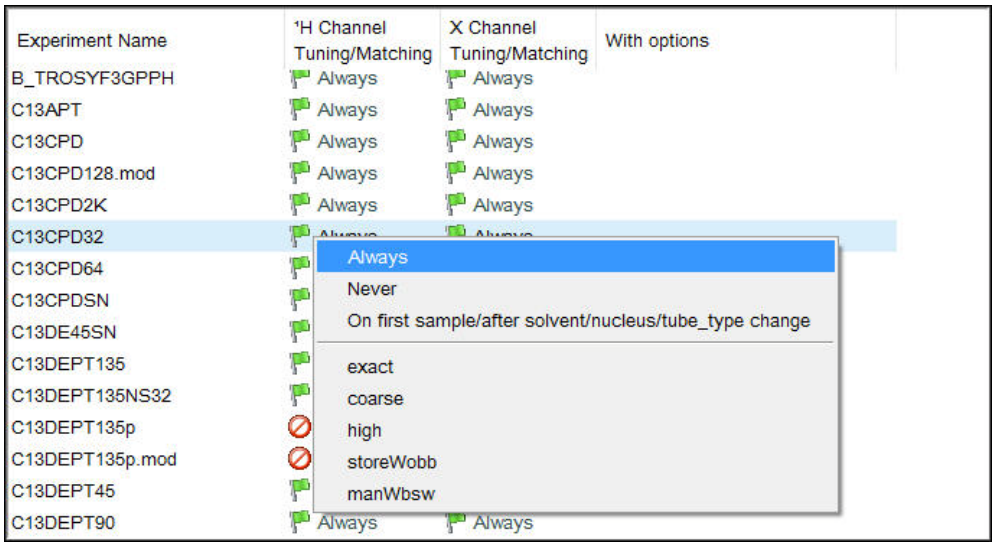
3.10.1.2 Abort Acquisition on ATM Failure

Using this option will stop the acquisition if the ATM fails to optimize.

3.10.2 Experiment Dependent ATM Optimization Settings

Single experiment

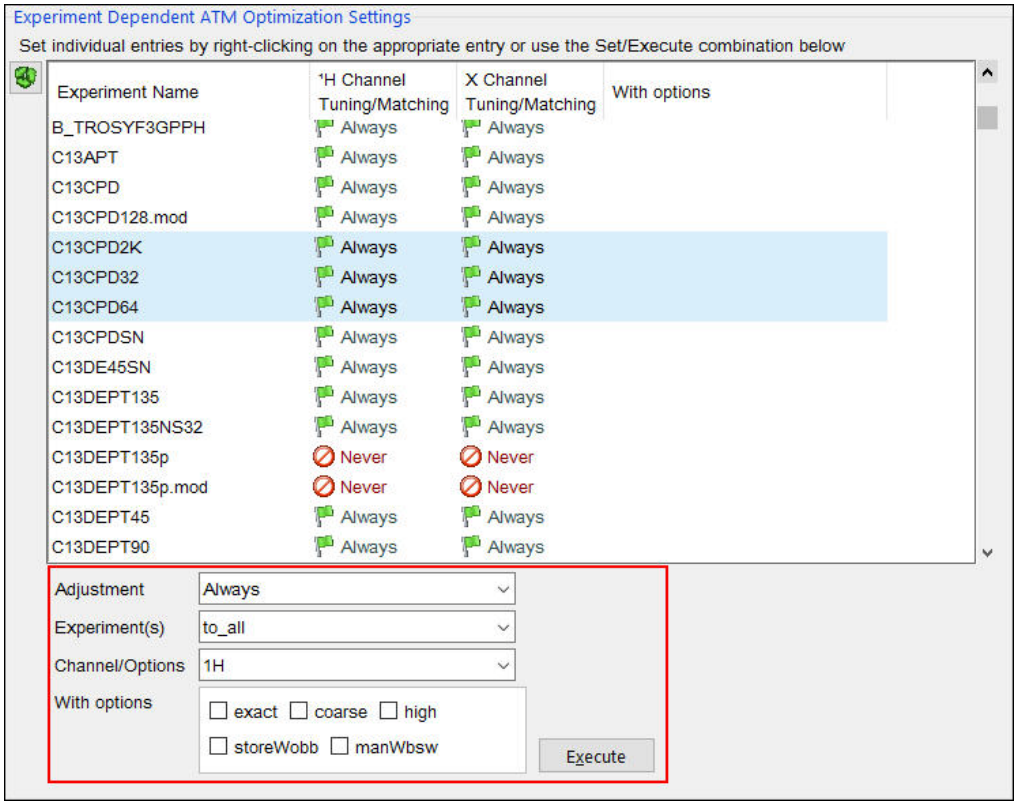
1. Click the right mouse button when the cursor is over a channel setting (1H or X).



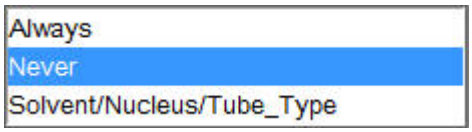
2. Select the setting from the pop up menu by clicking on it.

Multiple experiments

1. Use the ‘Ctrl’ or ‘Shift’ key to select multiple experiments.



2. Click on the down arrow next to **Adjustment**.



3. Select the setting from the pop up menu by clicking on it
4. Click on the down arrow next to **Experiment(s)**.

5. Select **'to selected'** from the pop up menu by clicking on it.
6. Click on the down arrow next to **Channel/Options**.

7. Select the setting from the pop up menu by clicking on it.
8. In the With options select any of the options listed below:

exact

This option will do the tuning and matching more precise, but takes time.

Coarse

This option will do the tuning and matching faster but may not be optimized.

high

store Wobb

This is a ATM option to save the Wobble curve after an **atma** command.

man Wbsw

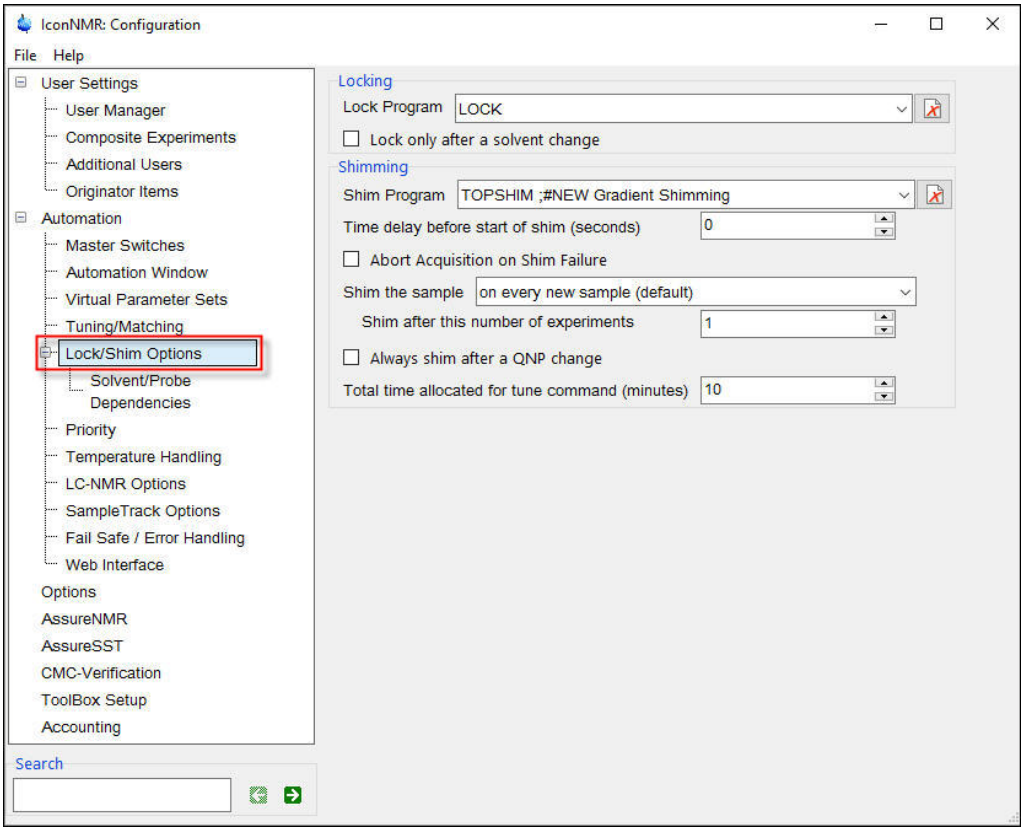
This option is for manual Tune and Matching.

8. Click on the **Execute** button to store the selected settings.

3.11 Locking/Shimming Options

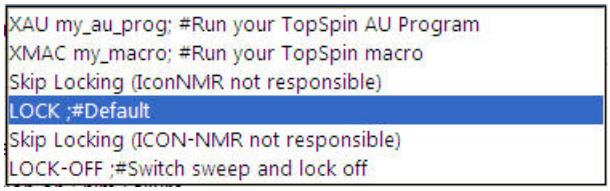
1. Click on **"Locking/Shimming Options"**

3.11.1 Locking



3.11.1.1 Lock Program

This option applies for both the Automation and Routine Spectroscopy. The locking procedure in IconNMR is controlled through this selection. If the Edit Lock/Shim/ATM permission is enabled (see 4.4.12 Permissions) the user can change the Lock Program in the IconNMR setup window.



Lock

The automatic lock is activated on every new sample.

Skip Locking (IconNMR not responsible

This option is primarily in throughput operation, used for samples with the same solvent.

LOCK-OFF;#Switch sweep and lock off

This option is primarily used for samples with none deuterated solvents.

Use the button to remove an item from the list box.

3.11.1.2 Lock only after a solvent change

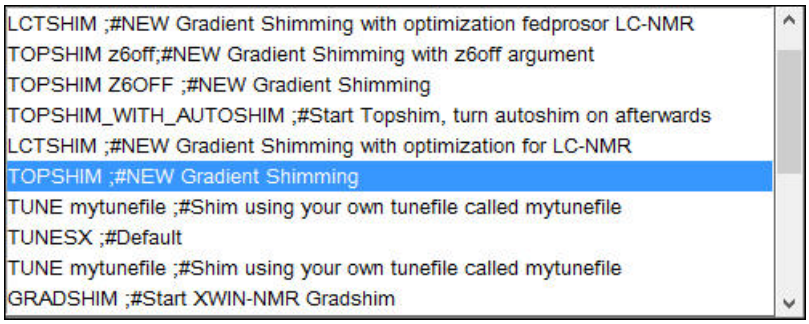
This option applies only in Automation and the use of a sample changer. It is primarily for use with BEST NMR accessory and samples in a queue with the same deuterated solvent.

Consult the IconNMR reference manual for more lock options.

3.11.2 Shimming

3.11.2.1 Shim Program

This option applies for both the Automation and Routine Spectroscopy. The shim routine can be selected by clicking on the down arrow button.



Use this to decide which type of shimming you'll be using. IconNMR provides 3 default options:

TUNESX

Computer shimming using the tune file created in edprosol. This file is probehead and solvent dependent. The probe head, all solvent tune file is stored in the directory: [TOPSPIN home]/conf/instr/spect/prosol/[probe ID]. The probe head, solvent tune file is stored in the directory: [TOPSPIN home]/conf/instr/spect/prosol/[solvent.probe ID]

GRADSHIM

Shimming using the Gradient shimming method defined in the TOPSPIN gradient shimming interface (gradshim). The iteration control file for gradient shimming is defined in the setup/automation menu.

TOPSHIM

Shimming using the TOPSHIM gradient shimming. TOPSHIM will select 1H gradient shimming when H2O+D2O as a solvent is selected. On all other Deuterium solvents, 2H gradient shimming is performed.

TOPSHIM_WITH_AUTOSHIM <args>

Standard gradient shimming followed by an autoshim on command. Arguments are passed to the topshim routine.

TUNE mytunefile

Computer shimming using a personal tune file created with edtune. This file is not probe-head or solvent dependent. It is stored in the directory: [TOPSPIN home]/exp/stan/nmr/lists/group.

Skip Shimming

Use this setting when shimming is not required, or where the shim control is handled externally, (e.g. by the Acquisition AU program see the AUNM parameter).

Use the button to remove an item from the list box.

3.11.2.2 Time delay before start of shim (seconds)

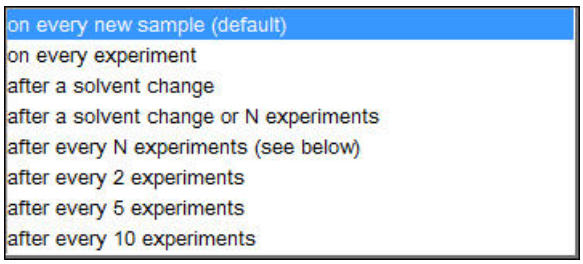
A time delay can be entered in seconds to start shimming the sample.

3.11.2.3 Abort Acquisition on Shim Failure

If enabled, the run on the current sample is discontinued after a shim failure.

3.11.2.4 Shim the Sample

This option applies only for the Automation. Different settings can be selected by clicking on the arrow.



On every new sample

This is a Default option and it will shim on every new sample using the shim program selected.

On every experiment

This Default option will shim on every new experiment on the inserted sample using the shim program selected.

After a solvent change

This option will only shim when a new solvent is detected. Grouping samples with the same solvent is useful to take advantage of this feature.

After a solvent change or N experiments

This option works like the one above, except it also skips the shimming on every experiments selected on the inserted sample.

After every N experiments

This option is useful if some of the experiments have a long acquisition time before the next experiment is started. Also some experiments have the spinning turned on or of (e.g 1D and 2D experiments). Set the number of experiments in **Shim after this number of experiments**. The next three options work the same way except they have a fixed number of experiments.

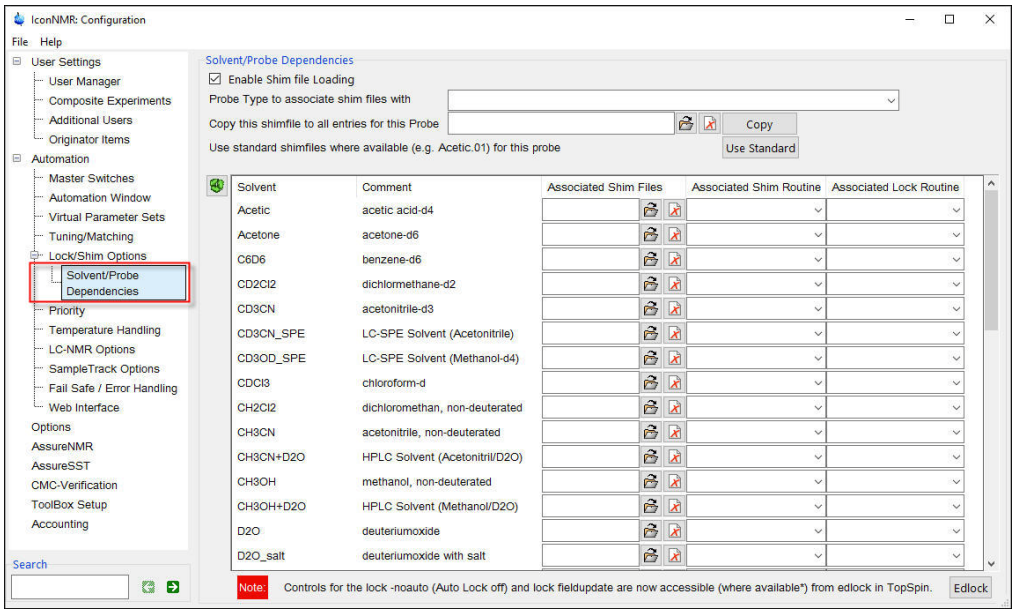
3.11.2.5 Always shim after a QNP change

If enabled, this option applies when the nucleus is changed on a QNP (quad nucleus) probe).

3.11.2.6 Total time allocated for tune command (minutes)

This option applies for both the Automation and Routine Spectroscopy. The setting is only active for the Automatic Shim Program **TUNESX**, **TUNE mytunefile**.

3.12 Solvent\Probe Dependencies



3.12.1 Solvent\Probe Dependencies

3.12.1.1 Enable shim file loading

If enabled, IconNMR will load a standard shim file in Routine Spectroscopy and Automation modes. The shim files are loaded automatically each time a new sample has been inserted into the magnet, before the system reaches the lock stage. That way it is always ensured that the system is in a well defined state for each new operator/sample. The shim files will be linked to the solvent and the probe being used. This window consists of a list of file entries (one for each solvent). The file entries apply to the probe which is shown in the Current Probe Type box.

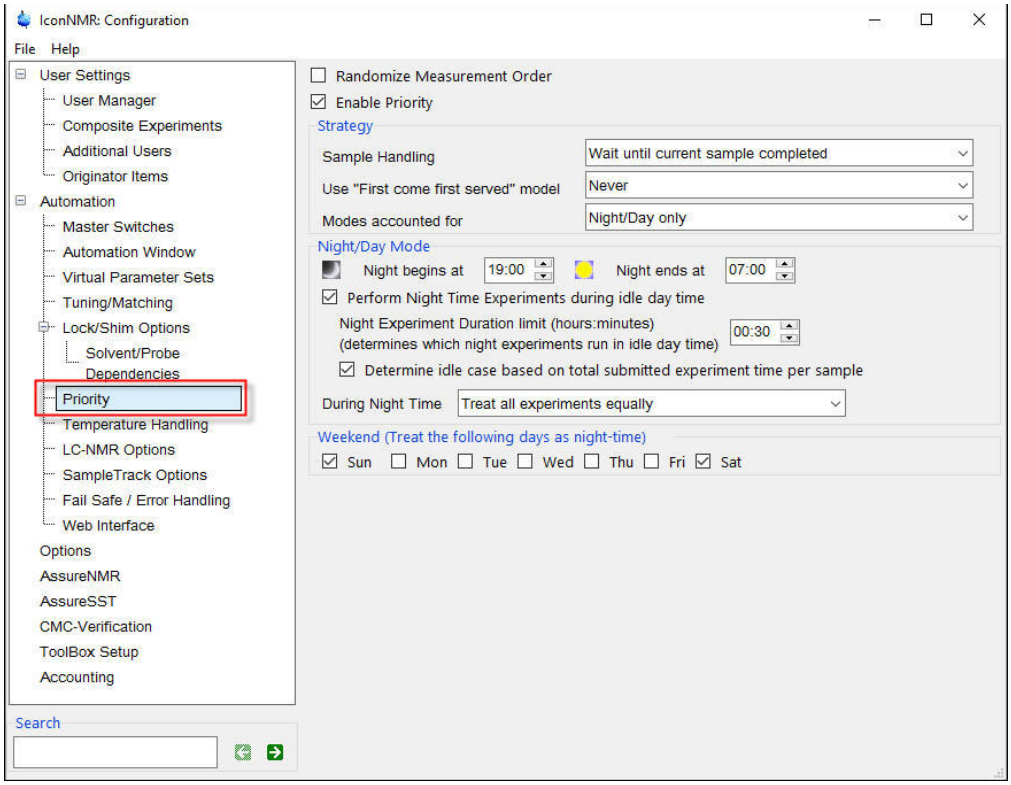
A shim file, shim routine and a lock routine can be chosen for each solvent. If the shim and lock routine entry box is empty, then the default lock and shim options are used (see 3.9 Lock/Shimming options).

For further information consult the IconNMR reference manual,

3.13 Priority

Users may decide to prioritize certain experiments. Such experiments will then be run before non prioritized experiments. The priority will be based on the time of their submission. Such experiments will either be run after the current experiment is completed or when all experiments scheduled on the current holder have been completed.

1. Click on **Priority**



3.13.0.2 Randomize Measurement Order

If enabled, this option chooses samples at random from all the submitted samples. In BEST-NMR this will be handled on a per well plate/rack fashion. If priority is assigned to a sample, it will over ride the randomize measurement.

3.13.0.3 Enable Priority

If enabled the priority in the order of running the samples can be granted. It is also possible to assign a day and night time option for various experiments.

3.13.1 Strategy

3.13.1.1 Priority Sample Handling

1. Click on the arrow next to the **Priority Sample Handling** window to select the choice of priority

Wait until current sample completed

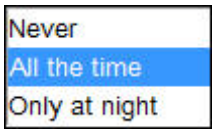
The priority sample is measured after all experiments on the current sample have been completed.

Do Priority Sample immediately

The priority sample is measured after the current experiment on the current sample is completed.

3.13.1.2 Use “First come first served Model”

1. Click on the arrow next to the **First come first served** window.



Never

The sample changer advances to the next highest sample holder, ignoring the time the sample was submitted.

All the time

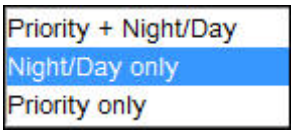
IconNMR recognizes the time when the sample was submitted and therefore measures the sample in the order of submission.

Only at night

This option is the same as the previous one, but only during night time operation.

3.13.1.3 Modes accounted for

1. Click on the arrow next to the **Modes accounted for** window.



Priority + Night/Day

The user has full control to use the priority sample handling and Night/Day time option.

Night/Day only

The user has control over Night/Day option only

Priority only

The user can only use the priority sample handling

3.13.2 Night/Day Mode

The values for begin and end the night time are entered as Military time.

3.13.2.1 Perform Night time experiments during idle day time

If enabled the assigned night time experiments will run during idle day time operation

3.13.2.2 Night Experiment Duration for Idle Limit

This option can be used to allow assigned night time experiments to run during idle day time on a experiment time limit. This will limit the very long term experiments to be run during night time only and the shorter assigned night time experiments to be run during idle day time hours.

3.13.2.3 Determine idle case based on total submitted exp. time per sample

When enabled the idle time is calculated according to the total time of all experiments submitted on a sample.

3.13.2.4 During Night Time

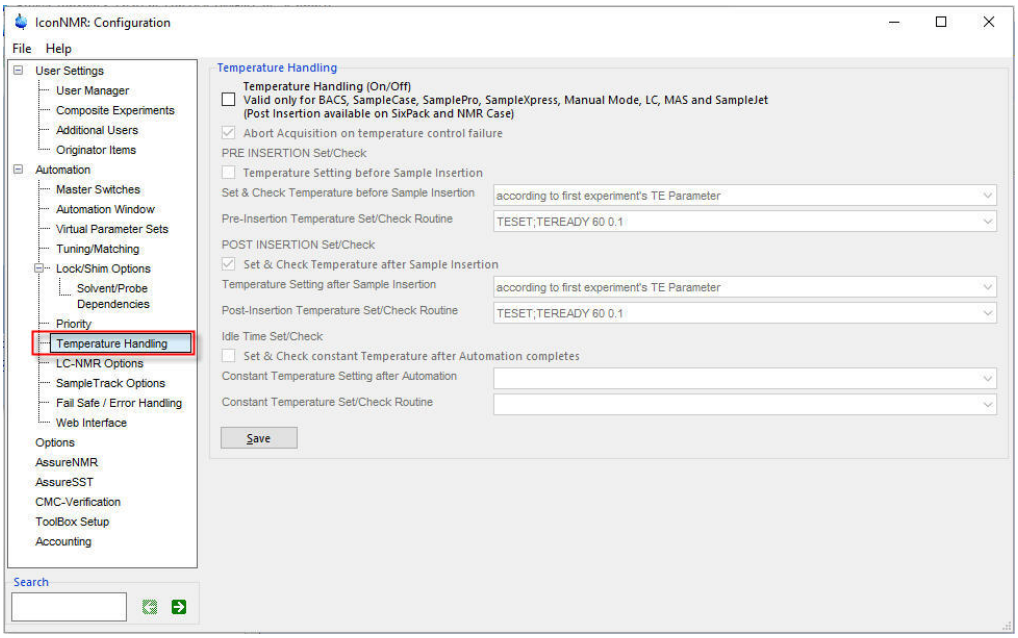
1. Click on the arrow next to the **During Night Time** window.

3.13.3 Weekend (Treat the following days as night-time)

Choose which days of the week should be treated as night time operation.

3.14 Temperature Handling

1. Click on Temperature Handling



3.14.1 Temperature Handling

3.14.1.1 Temperature Handling (ON/OFF)

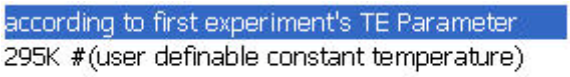
This Option is used to set and check the temperature before and after the sample is inserted. The pre-insertion is valid only for Standard BACS, Manual Mode, LC, MAS and Sample Track Automation Systems. Post Insertion is available on SixPack and NMR Case. Define TE as a user specific parameter.

3.14.2 PRE INSERTION Set/Check

3.14.2.1 Temperature Setting before Sample Insertion

This option is primarily used if samples have to be run at different temperatures. This would set the probe to a specific temperature, before the sample is inserted. If all samples in a sample changer run are to be run at the same temperature setting, then this option is not used and only POST INSERTION should be enabled.

3.14.2.2 Set & Check Temperature before Sample Insertion



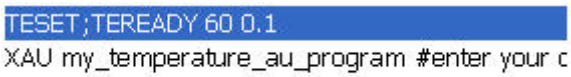
according to experiment's TE Parameter

If selected, the temperature value is been taken from the TE parameter

295K # (user definable constant fixed temperature)

if selected, this value can be changed to the desired temperature.

3.14.2.3 Pre-Insertion Temperature Set/Check Routine



TESET; TEREADY 60 0.1

If selected, TESET sets the temperature while TEREADY takes two arguments: The first argument defines an equilibrium time which is inserted after the temperature unit reports that the temperature, with reference to the tolerance, has been reached. The second parameter determines to what degree of accuracy the program should require temperature conformance to the desired value. Where multiple experiments are run on a single sample, the temperature will be updated according to the Post insertion routine. If the temperature is to be changed between experiments, in cases where the required temperature does not change the Temperature Set/Check routine will automatically be skipped.

For VT experiments in Automation it's a good idea to define TE as a user specific parameter. That way you can access the TE value quickly from the experiment definition line.

XAU my_temperature_au_program'

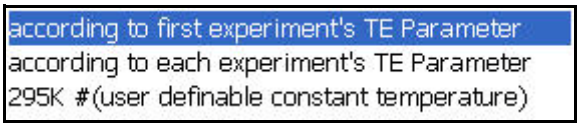
If selected, a user defined AU program can be used. The name has to be" my_temperature_au_program"

3.14.3 POST INSERTION Set/Check

3.14.3.1 Set & Check Temperature after Sample Insertion

This option is primary used to make sure the sample has reached the desired temperature after the sample has been inserted in to the magnet. If all samples have to be run at the same temperature, then only this option should be enabled.

3.14.3.2 Temperature Setting after Sample Insertion



according to first experiment's TE Parameter

If selected, the temperature value is been taken from the TE parameter of the first experiment.

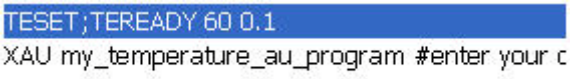
according to each experiment's TE parameter

If selected the temperature value is been taken from the TE parameter of each experiment.

295K # (user definable constant fixed temperature)

If selected, this value can be changed to the desired temperature.

3.14.3.3 Post Insertion Temperature Set/Check Routine



TESET; TEREADY 60 0.1

If selected, TESET sets the temperature while TEREADY takes two arguments: The first argument defines an equilibrium time which is inserted after the temperature unit reports that the temperature, with reference to the tolerance, has been reached. The second parameter determines to what degree of accuracy the program should require temperature conformance to the desired value. Where multiple experiments are run on a single sample, the temperature will be updated according to the Post insertion routine. If the temperature is to be changed between experiments, in cases where the required temperature does not change the Temperature Set/Check routine will automatically be skipped.

For VT experiments in Automation it's a good idea to define TE as a user specific parameter. That way you can access the TE value quickly from the experiment definition line.

XAU my_temperature_au_program

If selected, a user defined AU program can be used. The name has to be”my_temperature_au_program”

3.14.3.4 Idle Time Set/Check

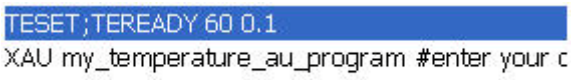
If no other experiments are in the queue and the sample is either removed out or stays in the magnet the temperature maybe reduced. The temperature can be changed by enabling the **Set & Check constant Temperature after Automation completes**, This option should not be used if running multiple experiments with delay between the measurements on a sample for Kinetics/Inside NMR

3.14.3.5 Constant Temperature Setting after Automation

295K # (user definable constant fixed temperature)

If selected, this value can be changed to the desired temperature.

3.14.3.6 Constant Temperature Set/Check Routine



TESET; TEREADY 60 0.1

If selected, TESET sets the temperature while TEREADY takes two arguments: The first argument defines an equilibrium time which is inserted after the temperature unit reports that the temperature, with reference to the tolerance, has been reached. The second parameter determines to what degree of accuracy the program should require temperature conformance to the desired value. Where multiple experiments are run on a single sample, the temperature will be updated according to the Post insertion routine. If the temperature is to be changed between experiments, in cases where the required temperature does not change the Temperature Set/Check routine will automatically be skipped.

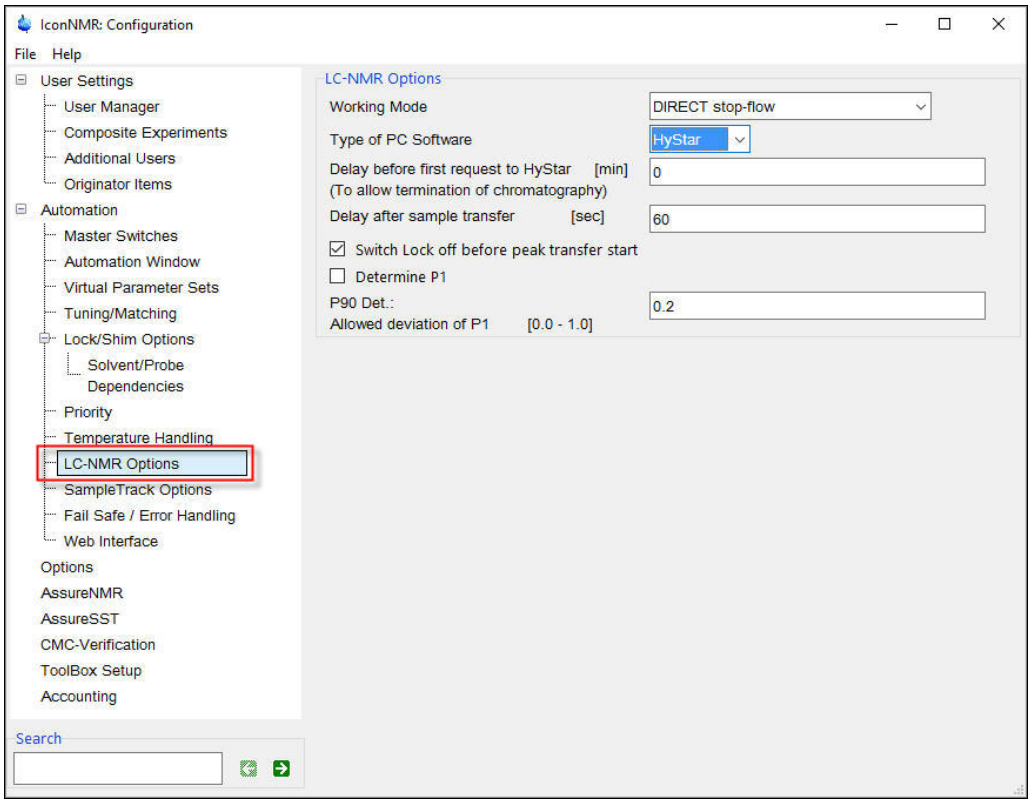
For VT experiments in Automation it’s a good idea to define TE as a user specific parameter. That way you can access the TE value quickly from the experiment definition line.

XAU my_temperature_au_program

If selected, a user defined AU program can be used. The name has to be”my_temperature_au_program”.

3.15 LC-NMR Options

1. Click on **LC-NMR Options**

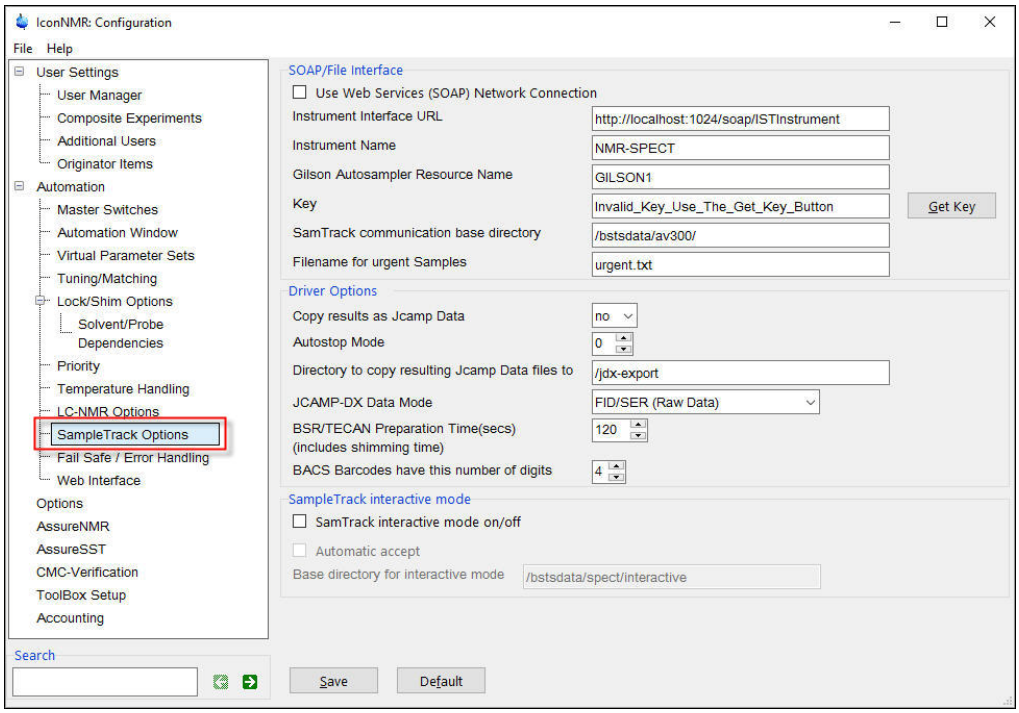


Routines in IconNMR are able to perform all tasks for the acquisition of LC-NMR spectra in full automation without user interaction. This includes preparation like tuning and matching, shimming and lock and pulse determination as well as the complex actions for multiple solvent suppression and signal-to-noise controlled acquisition.

To Use this option, refer to the **LCNMR** manual. The **HYSTAR LCNMR** software is required.

3.16 Sample Track options

1. Click on **Sample Track Options**

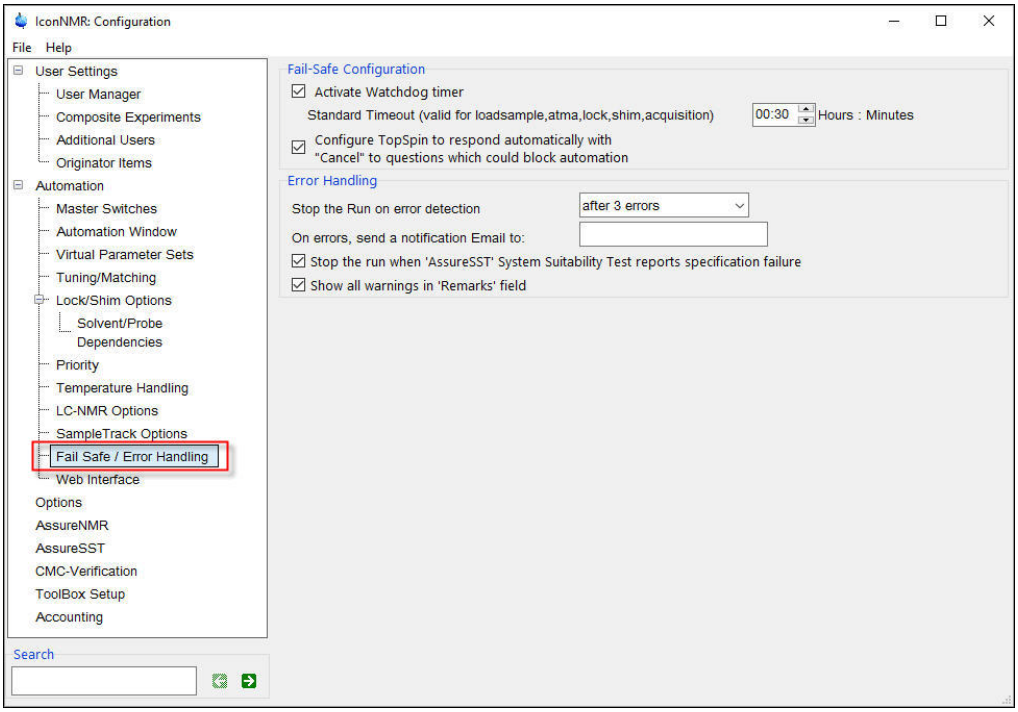


SampleTRACK is a Laboratory Management System with a standardized interface for BRUKER spectrometers. It is a software package that provides the link between the analytical laboratory, the synthesis laboratory and the information processing department. More importantly, it is the software tool for the laboratory network that coordinates all automation steps in analytical measurements.

To use this option refer to the **Sample Track** manual.

3.17 Fail Safe / Error Handling

1. Click on **Fail Save / Error Handling**



3.17.1 Fail Save Configuration

3.17.1.1 Activate Watchdog timer

When enabled a timer is started whenever a spectrometer operation is started on the instrument. If the operation has not responded after this time, IconNMR will assume the operation will not complete and the run will be terminated and restarted. Measurement will pick up where it had left off, so for example, if the acquisition was the problem, then only the acquisition will be restarted.

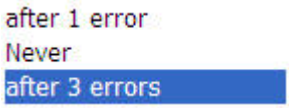
The acquisition time is taken into consideration and the experiment will only be terminated if the acquisition time plus the Standard Time out time has expired.

3.17.1.2 Configure TopSpin to respond automatically with “cancel” to questions which could block automation

When enabled the auto response such as clicking on the **Cancel** button.

3.17.2 Error Handling

3.17.2.1 Stop the on error detection



This feature available only in Automation mode allows for even more Instrument supervision. If one of the systems being used in Automation fails completely, for example the lock, then the complete Automation Run may be stopped automatically. Optionally you may choose to allow the run to continue (Never),

3.17.2.2 On errors. send a notification E-mail to

A E-mail address can be typed in to the window next to it and the error message is been sent to that address. Multiple addresses may be separated by a semicolons.

3.17.2.3 Stop the run when ‘AssureSST’ System Suitability Test reports specification failure

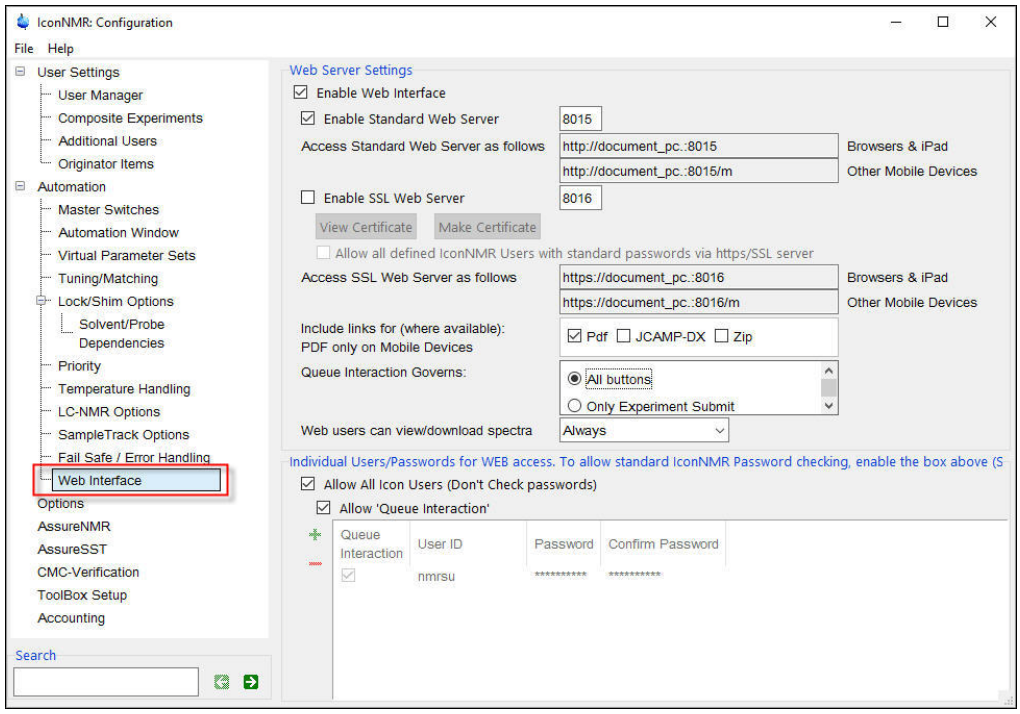
This option applies only on running AssureSST.

3.17.2.4 Show all warnings in ‘Remarks’ field

When enabled, all warnings are displayed in the Preceding Experiments history field in the Remark section of the Automation set up window.

3.18 WEB Interface

1. Click on **WEB Interface**



This option gives the users to access IconNMR through a Web interface and to submit samples using any desktop-, laptop- or pocket -computers connected to the Net. IconNMR Automation has to be running on the computer connected to the spectrometer to access the Web interface.

3.18.1 Web Server Settings

3.18.1.1 Enable Web Interface

When enabled a user may log in to the IconNMR automation using a Web server using the settings below.

3.18.1.2 Enable Standard Web Server

When enabled, choose a Port Number or use the default one

3.18.1.3 Access Standard Web server as follows

This is the address used in your internet browser. In some cases you may have to use the network address. Consult with your IT department for the correct address.

In cases where a secure Web connection is to be used, choose the ‘Enable SSL Web Interface’ as an option. SSL connections to the ICON Web server are encrypted for security and cannot be easily decoded. Contact your IT department for assistance or refer to the IconNMR Reference manual.

3.18.1.4 Include links for (where available): PDF only on Mobile Devices

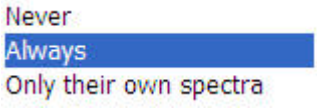
Click these items to include up to 3 links in the desktop mode Web Interface. The PDF link opens the installed viewer for pdf files, JCamp-DX and Zip options will allow for downloading the respective data file if the user has such automatically generated files.

3.18.1.5 Queue Interaction Governs

This setting may be used to allow all buttons except Submit. This may be useful where the sample position is remotely reserved at the spectrometer, the Final Submit always takes place when the sample arrives at the instrument.

3.18.1.6 Web users can view/download spectra

This option allows users to view the processed data in PDF format by double clicking on the data set name in the history section of the Web interface set up window.



Never

The users will not be able to view their spectra as a PDF file.

Always

All users can view theirs and others spectra as a PDF file.

Only their own spectra

All users can only view their own spectra as a PDF file.

3.18.2 Individual Users/Password for WEB access

3.18.2.1 Allow All Icon Users (Don’t check password)

If enabled all IconNMR users can submit samples through the Web interface. No

passwords are being checked.

If not enabled individual users can be selected for login to use the IconNMR Web interface and their Password is being checked.

3.18.2.2 Allow Queue Interaction

When enabled, the users have the options to Add, Submit and Cancel experiments through the WEB Interface and the buttons are visible in the WEB Interface window.

If disabled, the Add, Submit and Cancel button will not be shown in the WEB Interface window and the users will have ‘View Only’ permission.

3.18.3 Using the Iconweb

1. Close the **Configuration** window.

2. Select **Automation**.

Using the Web to access IconNMR, the Automation set up window has to be open.

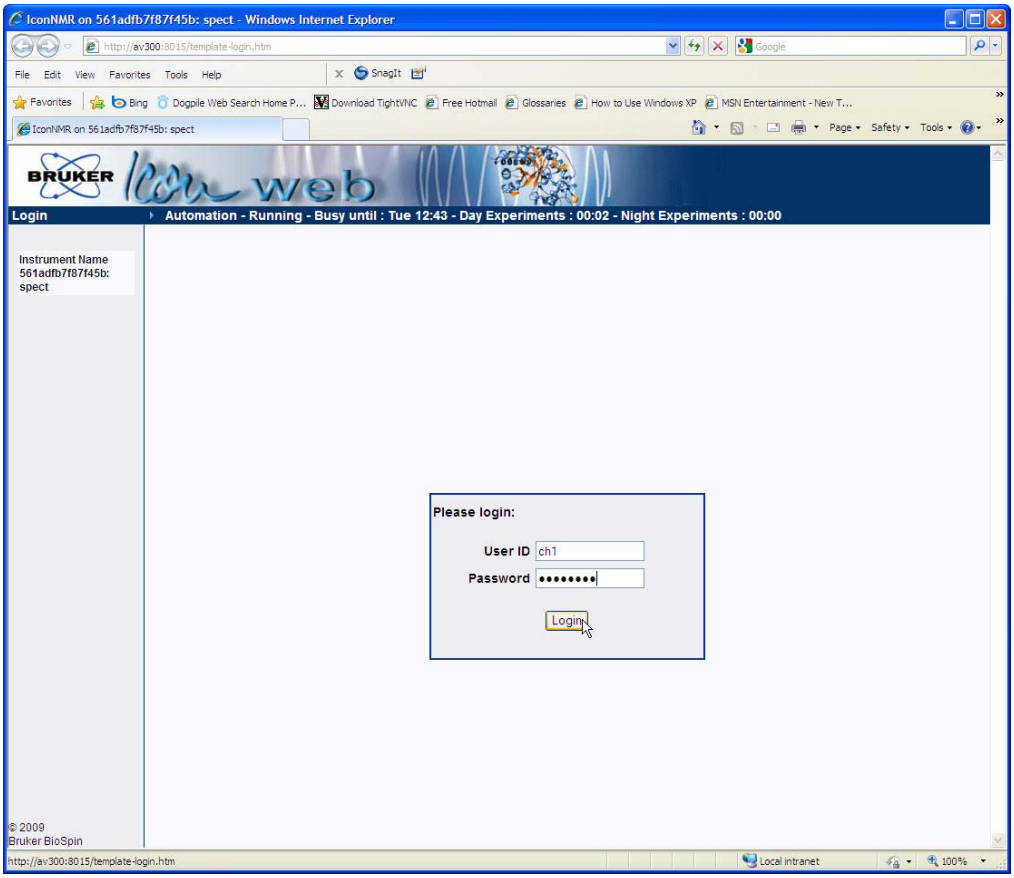
3. Using a Desktop, Laptop, Pocket PC or an I phone, open up the Internet Web browser.

4. Type the following line in to the Address window.

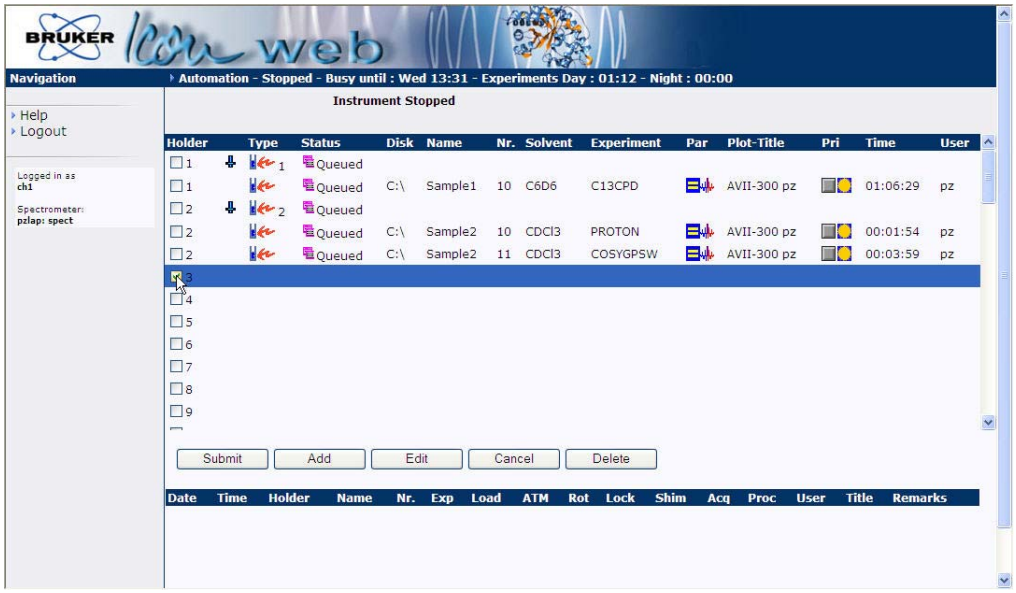
http://<computer name>:8015/icon

Where <computer name> is the full name of the computer or the IP address on the network and 8015 is the socket number for the server.

5. Press the **Enter** key.



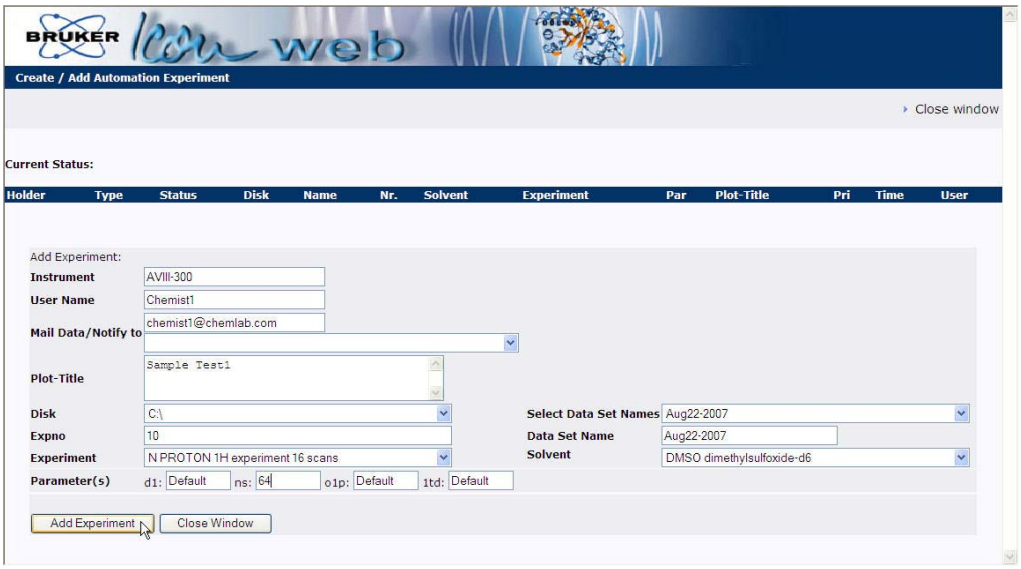
5. Enter **User Name** and **Password** and press the **Login** button.



If the user which started IconNMR Automation is the same user to start the Web interface e.g. nmrsu, then this user is allowed to Start, Hold or Stop the Run and the commands are visible in the Navigation section. No other users will have this possibility.

6. Click on the first Holder.

7. Click on the **Add** button.



8. Select the Experiment, Solvent, Parameters and Title

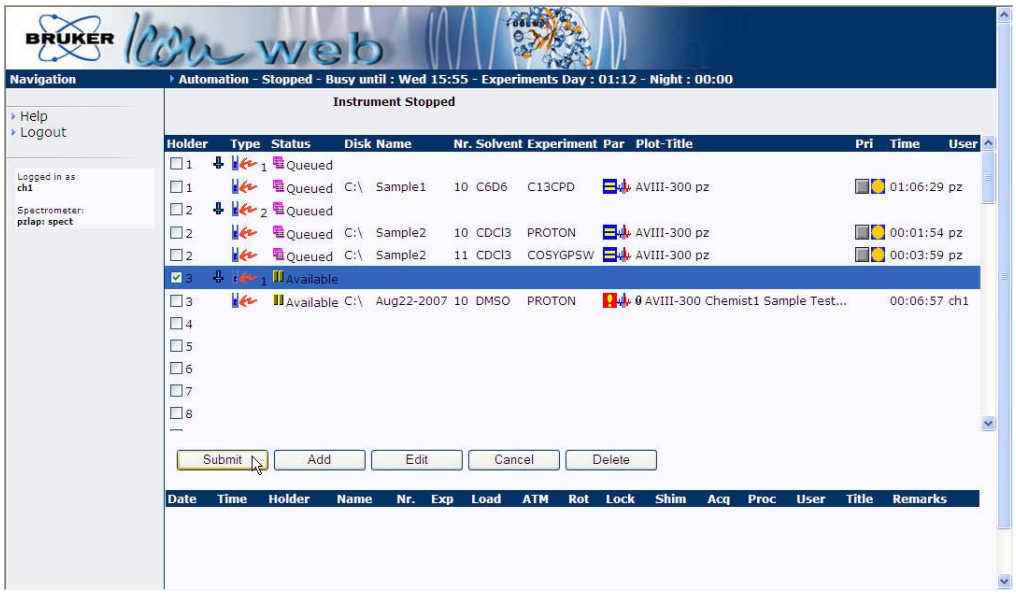
The List of Experiments, Parameters and User Permissions are set in the User Manager.

9. Click on the **Add Experiment** button.

10. If desired additional experiments can be added.

11. Click on the **Close Window** button.

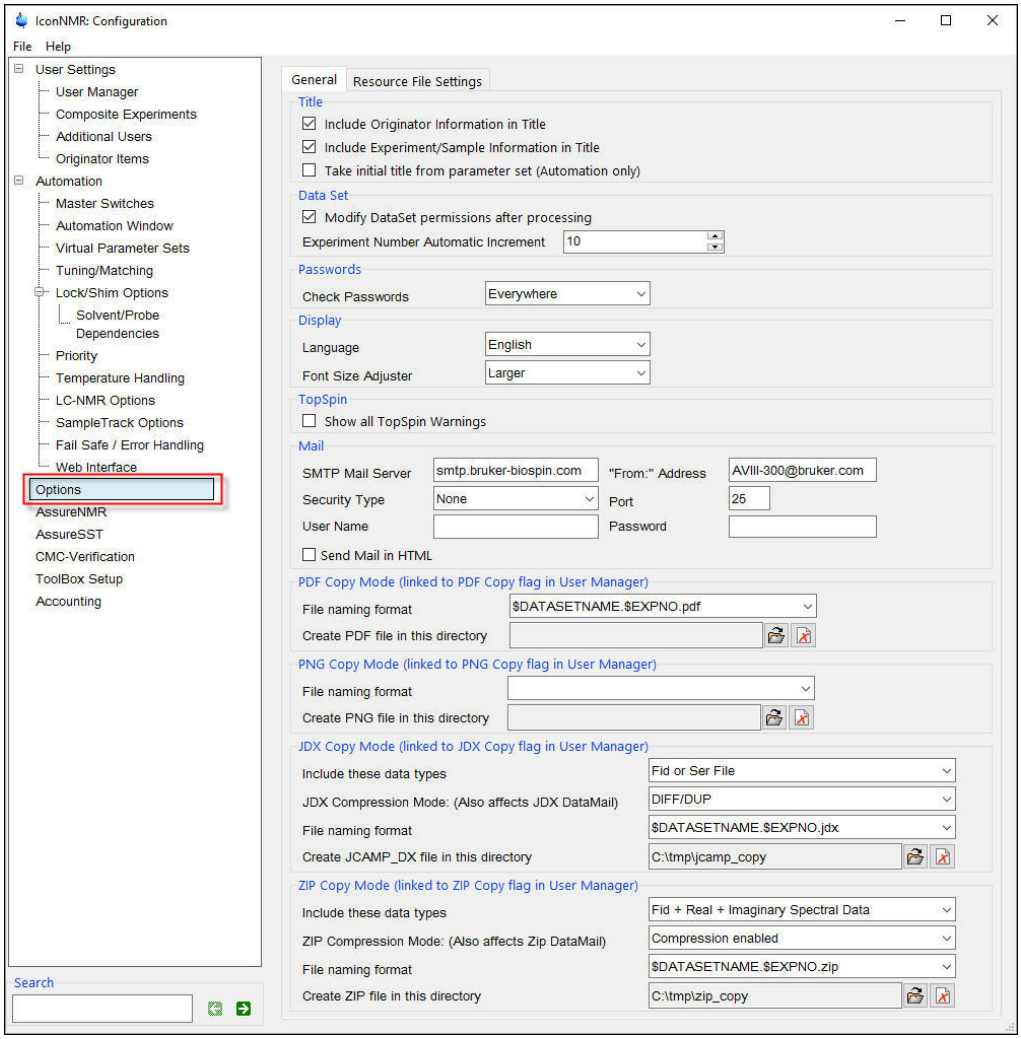
12. Click on the holder with the new created experiment. For multiple holders use the shift key.



13. Click on the **Submit** button.
14. Click on **Logout** at the upper left of the Icon Web window.

3.19 Options (General)

1. Click on **Options**



3.19.1 Title

3.19.1.1 Include Originator Information in Title

When enabled, the Originator information is being added to the title and will appear in the spectrum plot.

3.19.1.2 Include Experiment/Sample Information in Title

When enabled, the experiment name, solvent, disk drive, user and processing number

are added to the title and will appears in the spectrum plot.

3.19.1.3 Take initial title from parameter set (Automation only)

When enabled, always have the title initially taken from the parameter set.

3.19.2 Data Set

3.19.2.1 Modify DataSet permissions after processing

IconNMR acquires a data set having the permission and ownership according to the current logged on Workstation user. After processing has completed however, the permissions and ownership will be changed according to the user who submitted the experiment and the Umask setting in the User Manager.

3.19.2.2 Experiment Number Automatic Increment

The increment of the experiment number during a setup can be changed. As default, the experiment number starts with 10 and increments by one for each additional experiment. If the same data set name is used on different samples during the set up, the experiment number increments by 10 to the nearest multiple of 10.

3.19.3 Password

3.19.3.1 Check Password

Use this option to reduce the password checking. Click on the gray box, a list of password checking possibilities appear.

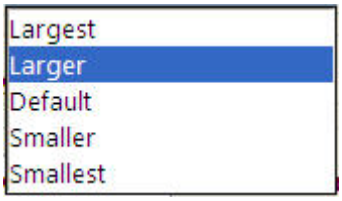
3.19.4 Display

3.19.4.1 Language

In this option English, German Japanese language can be selected to display the text in IconNMR.

3.19.4.2 Font Size Adjuster

This option makes a limited adjustment to the font size used in all IconNMR programs. Changes will be made after a restart of the program. By clicking on the gray box, a list Fonts possibilities appear.



3.19.5 TopSpin

3.19.5.1 Show all TopSpin warnings

When enabled, all TopSpin warnings such as the “seen” type are displayed. If disabled the information will still be reported in the TopSpin history file.

3.19.6 Mail

3.19.6.1 SMT Mail Server

Enter the name of your company/institution mail server in to the window provided. IconNMR will contact the server and attempt to use it for the transmission of all mail. If unsuccessful TopSpin error will be generated and visible in the TopSpin history file.

3.19.6.2 “From:” Address

Enter a legal E-Mail address.

3.19.6.3 Security Type

For a titer security, choose TLS/SSL when encryption is to be used.

3.19.6.4 Port

This information is available from your IT department.

3.19.6.5 User Name

As required by the SMTP server. If this and the password field is left blank then no Authentication will be used.

3.19.6.6 Password

As required by the SMTP server. If this and the User Name field is left blank then no Authentication will be used

3.19.6.7 Send Mail in HTML

Use this to send Mails in HTML format instead of plain text. A default Bruker logo and separator image is embedded in the mail. IconNMR will try and use image files in the Home Directory of the user starting TopSpin to allow for flexibility on this point. The files it looks for are:

IconNMR-Mail-Logo.png and

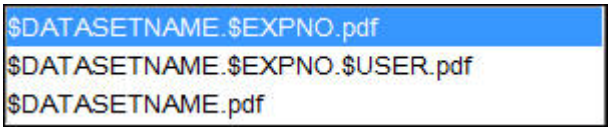
IconNMR-Mail-Separator.png respectively.

Start IconNMR with the argument ‘info’ from TopSpin to find out what the correct home directory is.

3.19.7 PDF Copy Mode (linked to PDF Copy flag in User manager)

3.19.7.1 File naming format

A filename can be set for the PDF file. Click on the pull down menu to choose from some examples.



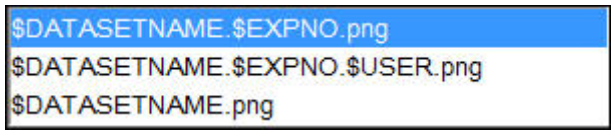
3.19.7.2 Create PDF file in this directory

Click on the Browse icon to select a directory where the PDF file will be stored. To clear the field, click on the X- icon.
This mode applies, when the PDF Copy permission in the User Manager menu is enabled.

3.19.8 PNG Copy Mode (linked to PNG Copy flag in User manager)

3.19.8.1 File naming format

A filename can be set for the PNG file. Click on the pull down menu to choose from some examples.



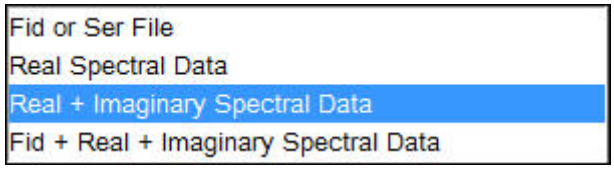
3.19.8.2 Create PNG file in this directory

Click on the Browse icon to select a directory where the PNG file will be stored. To clear the field, click on the X- icon.
This mode applies, when the PNG Copy permission in the User Manager menu is enabled.

3.19.9 JDX Copy Mode (linked to JDX Copy flag in User manager)

3.19.9.1 Include these data types

There are 4 choices to select from, when clicking on the window next to it This mode applies when the JDX Copy permission in the User Manager menu is enabled.

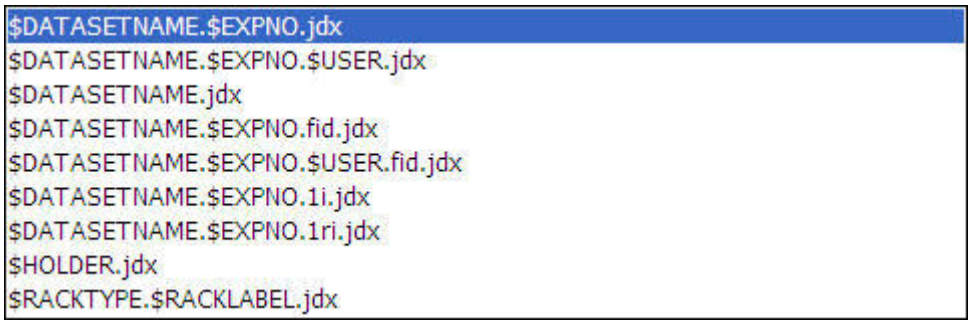


3.19.9.2 JDX Compression Mode (Also affects DataMail)

Defines the compression mode to be used. Clicking on the arrow for a list of settings.

3.19.9.3 File naming format

There are several Joyce's to select from, when clicking on the arrow next to the window. This mode applies, when the JDX Copy permission in the User Manager menu is enabled.



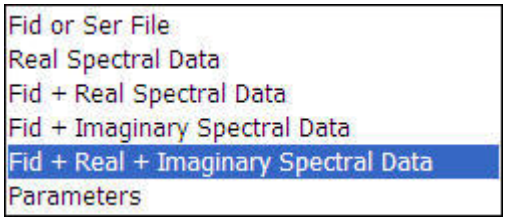
3.19.9.4 Create JCAMP_DX file in this directory

Click on the Browse icon to select a directory where the JCANMP_DX file will be stored. To clear the field, click on the X- icon.
This mode applies, when the JDX Copy permission in the User Manager menu is enabled.

3.19.10 ZIP Copy Mode (linked to ZIP Copy flag in User Manager)

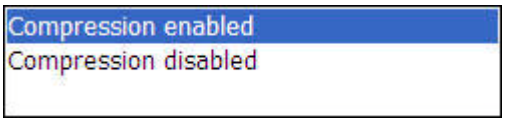
3.19.10.1 Include these data types

There are 6 choices to select from, when clicking on the window next to it This mode applies when the ZIP Copy permission in the User Manager menu is enabled.



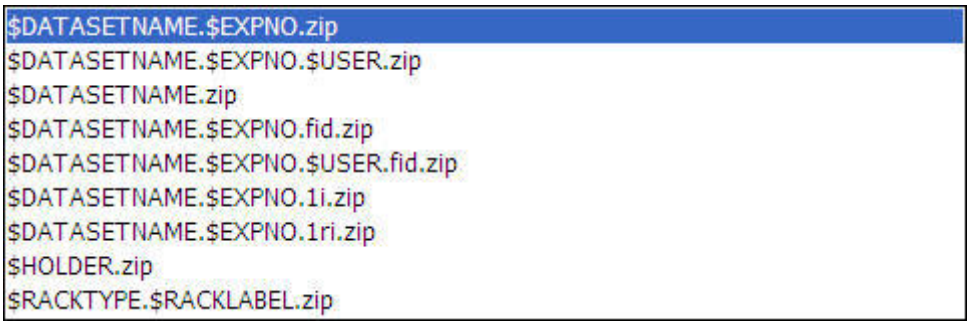
3.19.10.2 ZIP Compression Mode: (Also effects ZIP DataMail)

Defines the compression mode to be used. Clicking on the arrow for a list of settings.



3.19.10.3 File naming format

There are several Joyce's to select from, when clicking on the arrow next to the window. This mode applies, when the ZIP Copy permission in the User Manager menu is enabled.



3.19.10.4 Create ZIP file in this directory

Click on the Browse icon to select a directory where the ZIP file will be stored. To clear the field, click on the X- icon.
This mode applies, when the ZIP Copy permission in the User Manager menu is enabled.

3.20 Options (Resource File Settings)

Hidden Options from _iconnmrrc.txt are now fully accessible from this Options Resource File Settings menu. All settings below are for Automation only and does not apply for Routine Spectroscopy.

3.20.1 Automation

3.20.1.1 Prevent multiple users from submitting experiments for the same sample

This corresponds to the variable:
PREVENT_SAMPLE_EXPERIMENTS_FROM_MULTIPLE_USERS

3.20.1.2 Do not allow another user's experiment to be copied

This corresponds to the variable:
STOP_COPY_ON_DIFFERENT_USERS

3.20.1.3 Experiment numbers commence at

This corresponds to the variable:
EXPNO_START_VALUE

3.20.1.4 Increment Experiment numbers by this value on the same sample

This corresponds to the variable:
EXPNO_ADD_INCREMENT

3.20.1.5 Enforce 'User Manager' IconNMR 'Exit' permission for Automation window

This corresponds to the variable:
EXIT_PERMISSION_CHECK_FROM_AUTOMATION_WINDOW

3.20.1.6 Only allow users with 'Supervisor' permission to start the run

This corresponds to the variable:
ALLOW_ONLY_SUPERVISOR_RUN_START

3.20.1.7 Permit users without 'Supervisor' permission to use standard parameter editor

like eda, edp, ased etc.

This corresponds to the variable:
ALLOW_EDIT_PARAMETERS_WHEN_NOT_SPERVISOR

3.20.1.8 Optional help menu name and the corresponding http site

e.g. “My Help Menu” “http://www.bruker.com
This corresponds to the variable:
LOCAL_AUTOMATION_HELP

3.20.1.9 Include E-mail Address from Originator items in title

This corresponds to the variable:
SAVE_EMAILADDR_TO_TITLE

3.20.1.10 Keep Easy Setup originator item setting after submit

This corresponds to the variable:
KEEP_EASY_ORIGS_AFTER_SUBMIT

3.20.1.11 “Start Time” setting only available for Users with Supervisor permission

This corresponds to the variable:
STARTTIME_ONLY_FOR_SUPERVISOR

3.20.1.12 Easy Setup Mode ‘Help’ Text

This corresponds to the variable:
KIOSK_HELP

3.20.2 Domain

3.20.2.1 Use Domain Users

This corresponds to the variable:
DOMAIN_USERS

3.20.2.2 Domain Controller

This corresponds to the variable:
DOMAINCONTROLLER

3.20.2.3 Show saved domain accounts without actually questioning the domain controller

This corresponds to the variable:
SHOW_SAVED_DOMAIN_USERS

3.20.3 Driver

3.20.3.1 For jdx conversion use this routine

This corresponds to the variable:
TOJDX_PROGRAM

3.20.3.2 Standard Time-out (min.)

This corresponds to the variable:
STANDARD_TIMEOUT

3.20.3.3 ZG Time-out (min.)

This corresponds to the variable:
ZG_TIMEOUT

3.20.3.4 Quick Time-out (min.)

This corresponds to the variable:
QUICK TIMEOUT

3.20.3.5 Create the “last” style log file

../prog/logfile/inmrlog.txt

This corresponds to the variable:
LAST_STYLE_ACCOUNTING

3.20.3.6 Append this additional text (with variables) to ‘Status in Sample Information in title’ text

This corresponds to the variable:
ADDITIONAL_STATUS_VARIABLES

3.20.3.7 Before IconNMR changes the sample try to reduce the gas flow

This corresponds to the variable:
REDUCE_GASFLOW_AT_SAMPLE_CHANGE

3.20.4 Miscellaneous

3.20.4.1 Guide Site

This corresponds to the variable:
GUIDE_SITE

3.20.4.2 Mark Sample Positions starting at position

This corresponds to the variable:
MARK_NIGHT_HOLDERS_FROM

3.20.4.3 Allow IcoNMR to change file permissions on configuration files/data sets

This corresponds to the variable:
CHANGE_FILE_PERMISSIONS

3.20.4.4 Open new data sets in TopSpin in a new window

This corresponds to the variable:
TOPSPIN_MULTIPLE_DATA_WINDOWS

3.20.4.5 Always issue shimcntl command

This corresponds to the variable:
DO_SHIMCNTL

3.20.4.6 Allow TopSpin's browser to update itself, keeping track of the data sets which are chosen for viewing in IconNMR's preceding experiment list

This corresponds to the variable:
TOPSPIN_SCOLLTOCURDATA

3.20.4.7 Check for the least one valid BEST-NMR method per sample

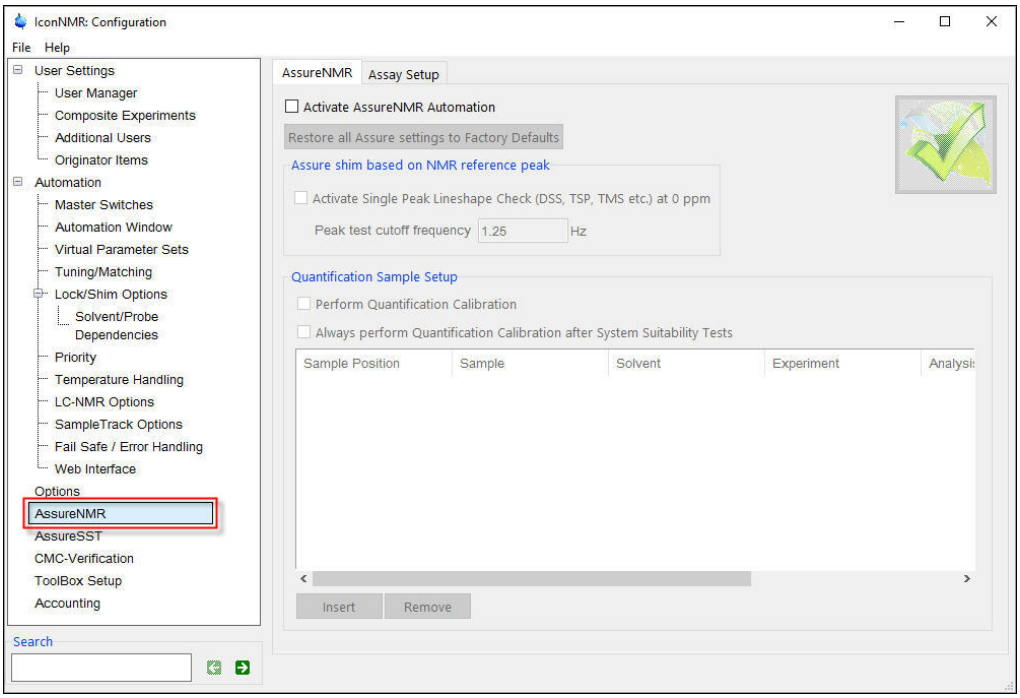
This corresponds to the variable:
CHECK_FOR1VALIDMETHOD

3.20.4.8 Copy Inmracct.full here on Automation close

This corresponds to the variable:
INMRACCT_COPY_DIR

3.21 AssureNMR

1. Click on **AssureNMR**.

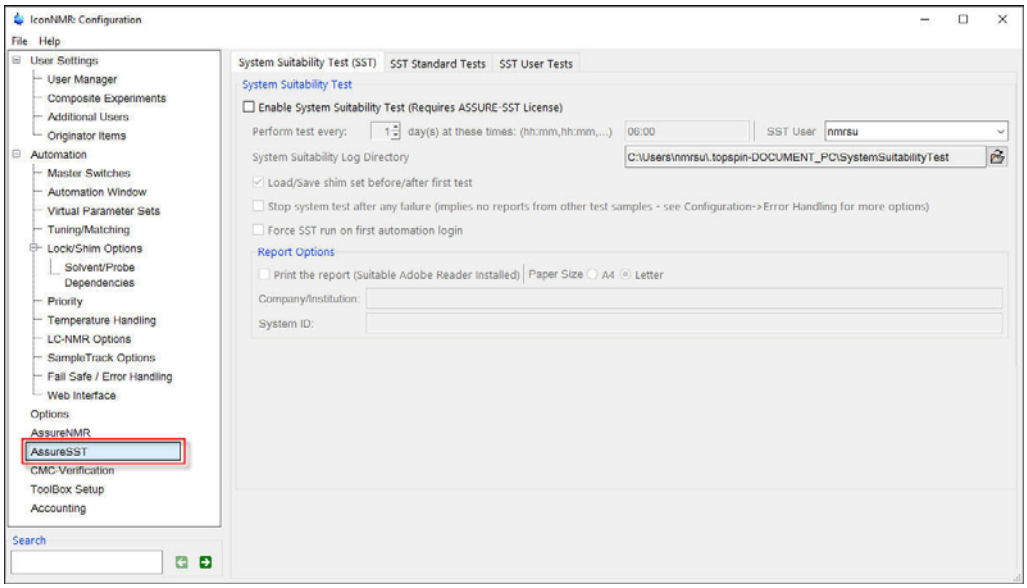


AssureNMR is the suite of tools for analyzing spectra. AssureNMR automation simplifies data acquisition and analysis using parameter sets and analysis methods customized for the material of interest, from purified raw materials to natural products to biofluids.

For detailed information how to use AssureNMR consult the **AssureNMR, Software and System Suitability Test, User Manual**.

3.22 AssureSST

1. Click on **AssureSST**.

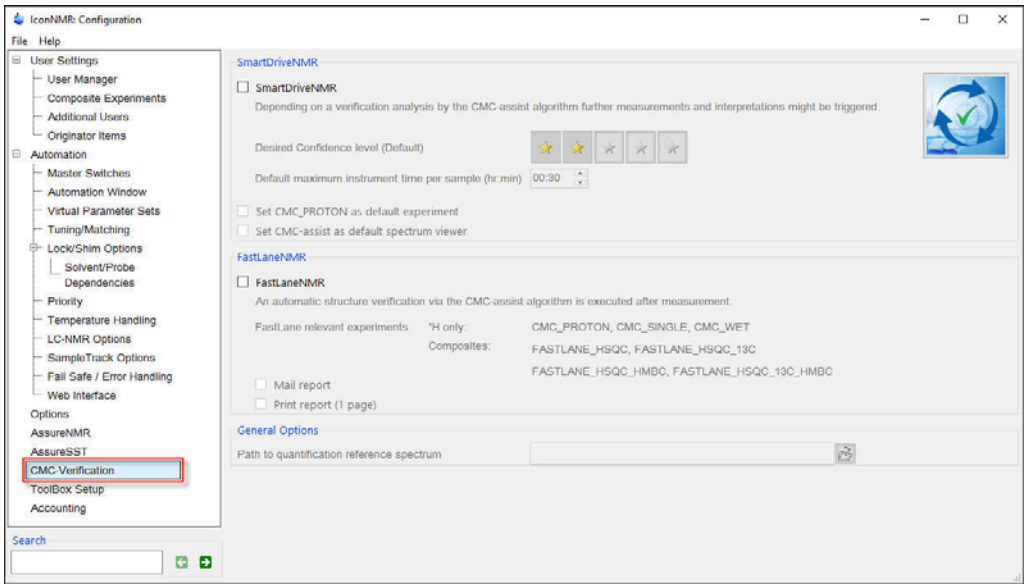


AssureNMR has two modules: AssureSST (System Suitability Test) and AssureNMR. The SST module is designed to monitor and maintain instrument performance. SST runs a set of user-selected tests, compares the results to user-defined specifications, and generates a dated summary report.

For detailed information how to use AssureNMR consult the **AssureNMR, Software and System Suitability Test, User Manual**.

3.23 CMC-Verification

1. Click on **CMC-Verification**.



SmartDriveNMR

Depending on a verification analysis by the CMC-assist algorithm, further measurements and interpretations may be triggered. Get the most out of your instrument by allowing it to decide what to measure. The ideal combination of NMR experiments for the verification task is identified and carried out. It is decided on the-fly if further experiments can improve significantly the verification confidence while complying with the user's demands concerning allocatable spectrometer time and confidence.
The relevant inputs are intuitive and NMR independent - only relating to the structure verification task Desired verification confidence, Maximum measurement time, Molecular structure and Solvent.

For more information consult your CMC documentation.

Fast Lane NMR- a member of the CMCTM Product family -now provides the user with additional post processing information for 1D 1H spectra. Fast Lane NMR delivers meaningful integration regions, multiplet interpretation, consistency evaluation, signal assignments, and quantification results. Fast Lane NMR can be activated via a check box within Iconnmr's Master Switches. To benefit fully from Fast Lane NMR the user needs to:

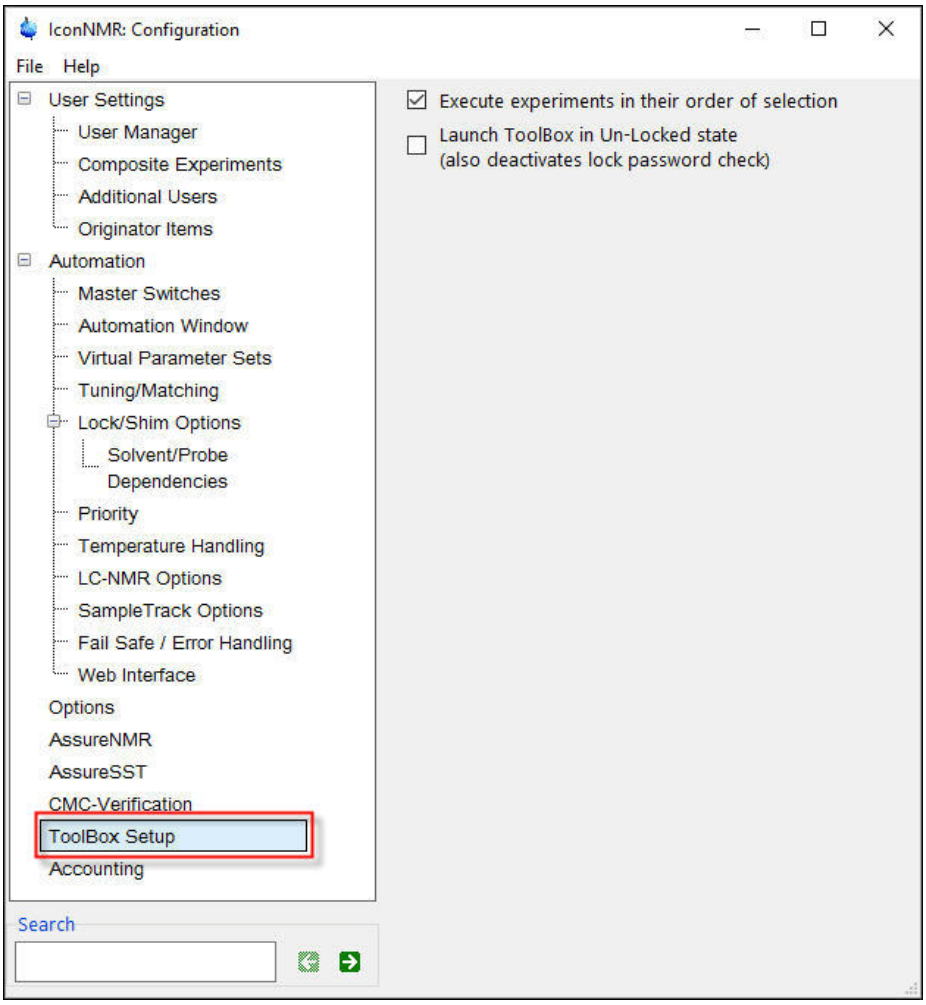
- Set a reference spectrum for quantification via the ERETIC dialog within Topspin's integration mode and indicate this spectrum within Iconnmr's Master Switches.
- Select the Experiment "CMCQ_PROTON" within Iconnmr's Automation.
- Add the .mol file to the dataset within Iconnmr's Automation either via drawing or browsing.

It seamlessly works with the **CMC-assist** - a newly designed Graphical User Interface which enables the user to view and edit the Fast Lane NMR results in avery convenient way. Please note that Fast Lane NMR requires the same license as CMC-assist.

For further information please contact cmc_service@bruker.ch or nmr-support@bruker.com.

3.24 ToolBox Setup

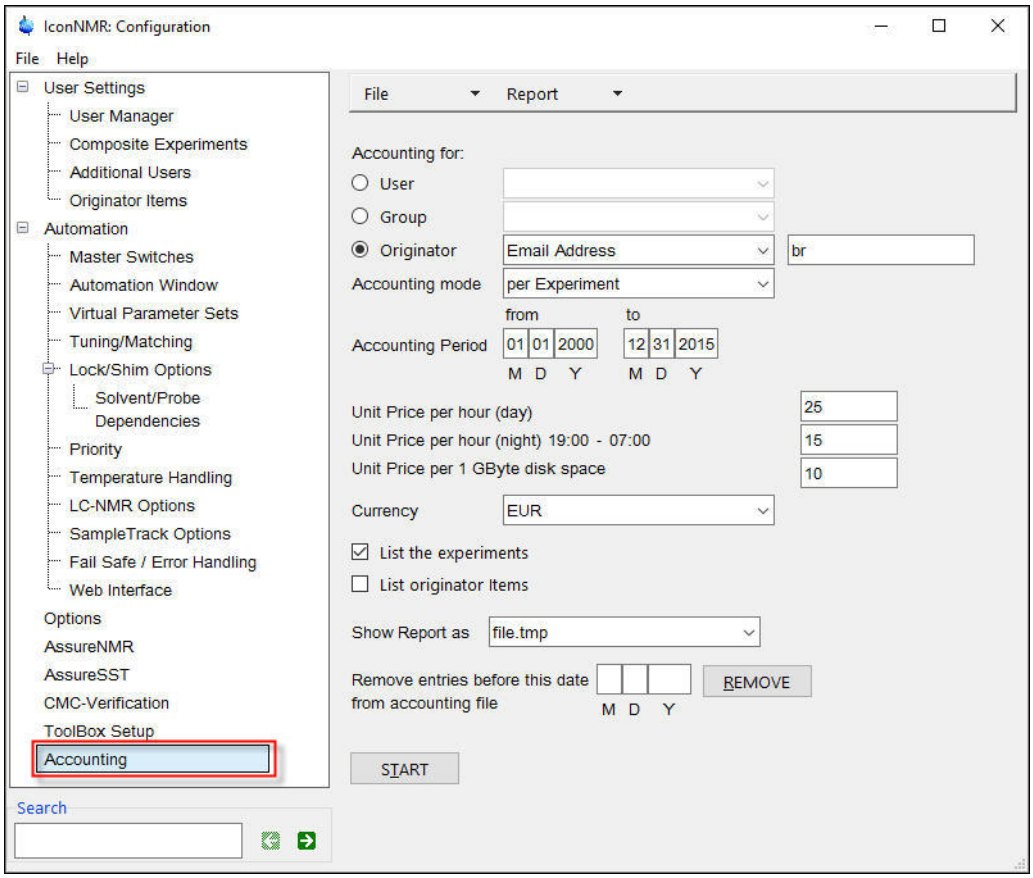
1. Click on **ToolBox Setup**



The IconNMR Toolbox is a user-configurative graphical interface providing a experiment oriented template setup which interfaces seamless with IconNMR's Automation front-end. See the IconNMR Reference manual for more information.The operators can quickly grasp a complex system whereby the details of how it all works are neatly tidied up and where necessary concealed. This is indeed possible without having to adapt standard Bruker AU macros or parameter sets.

3.25 IconNMR Accounting

1. Click on **Accounting**



The Accounting Manager gathers the information required to calculate prices for spectrometer usage from an accounting file. Each time an experiment is executed under control of IconNMR, the standard accounting file:

TOPSPINHOME/conf/instr/<instrument name>/inmrusers/Inmracct.brief

is updated.

At start up time the accounting program collects and sorts all user information stored in this file. Depending on its size (which can grow significantly during e.g. a month's period), you will have to wait some time until the dialog box similar to the one shown in Figure 4.124 appears.

3.25.0.9 The File menu

The following commands are available:

Open accounting file

By default, Inmracct.brief is the standard file responsible for all accounting information. However, the accounting information search can also be performed on other files with the extension.brief. The open command will display all files of this type stored in the

directory TOPSPINHOME/conf/instr/<instrument name>/ inmrusers/. Select the one you wish to use for accounting. Its name will be displayed in the header bar of the dialog box. After you have chosen a new file the accounting information is collected and sorted.

Save parameters

Saves the accounting file.

3.25.0.10 The Report menu

The following commands are available:

Display on screen

Re-display the report generated via the Start button.

Print

Print the report generated via the Start button on the current printer.

Save as

Store the report generated via the Start button in the specified file. If the file name does not begin with a "/"character, the report will be stored in the login user's home directory.

3.25.1 The Accounting for

In this box, you enter the users or the department etc. for which you want to generate an accounting report. The accounting mode is also selectable.

3.25.1.1 User

Enabling the User button will instruct the accounting software to generate a report for the user which you may select from a list. Click on the down arrow button to the right of the User button to display the list. This list is determined at startup time from the standard accounting file, or from the file you have chosen via the Open command in the File menu. The special list entry All will compile a report for all users present in the list.

3.25.1.2 Group

The Group button is similar to the previous User item, however, accounting is performed for the specified group. The special list entry All will compile a report for all groups present in the list.

3.25.1.3 Originator

Enabling the Originator button provides the most flexible accounting method in the per Experiment mode. Click on the down arrow button to get the list of originator items displayed that you have set up with the Originator Template Editor, and select one of them (e.g. Department). Enter the suitable accounting criterion into the field to the right

of it (e.g. a department identifier).

Example 1:

Assume you have selected the accounting type Department. The item Department is member of the list because you have defined it as originator item with the Originator Template Editor. Assume further that in your organization departments are identified by numbers. In order to generate the accounting report for the department 8009, enter this number as the accounting criterion. As a result you will get the total sum of spectrometer usage for all users belonging to this department.

Example 2:

Assume you have selected the accounting type E-mail Address. The item E-mail Address is member of the list because you have defined it as originator item with the Originator Template Editor. Assume further your E-mail addresses have the general form user@organisation.country. In order to generate the accounting report for all users belonging to organization, enter the text @organization as the accounting criterion. Accounting would then be performed for all users of organization, also for different country extensions. This example indicates that the accounting program applies a slightly different identification method to alphanumeric text as compared to plain numbers: In the first case substring matching is employed, while numbers must be matched exactly.

3.25.1.4 Accounting Mode

Setting the per Experiment mode will instruct the accounting software to account the time between the start and end of an experiment. Setting the mode per Login will instruct the accounting software to compute the accounting information based on the time between Login and Logout.

3.25.1.5 The Accounting Period and Unit Prices

Fill in the date of the first and last day of the accounting period (the sequence is month, day, year). If you want to charge night time rates specify the start and end time. Otherwise set the time of night start and end to 0, in this case the accounting program requires less calculation time. Then fill in unit prices that you intend to charge to the spectrometer users: A unit price per hour of spectrometer usage and a unit price per megabyte disk storage consumed during the accounting period. The total is calculated according to number of hours of spectrometer usage (day) * unit price per hour (day) + number of hours of spectrometer usage (night) * unit price per hour (night) + number of Megabytes consumed * unit price per Mbyte If you don’t want to charge for the disk space, set the unit price per MByte to 0. You can also enter a currency. The program will append it to all prices printed in the report, but will not perform any calculations with it. You can select the currency from a list. If you don’t find that of your country, you may add it to the file C:/prog/<version>/curdir/<user>/.currency Next time you enter the accounting software, your own currency will be included in the list. You may also delete unwanted items from this file.

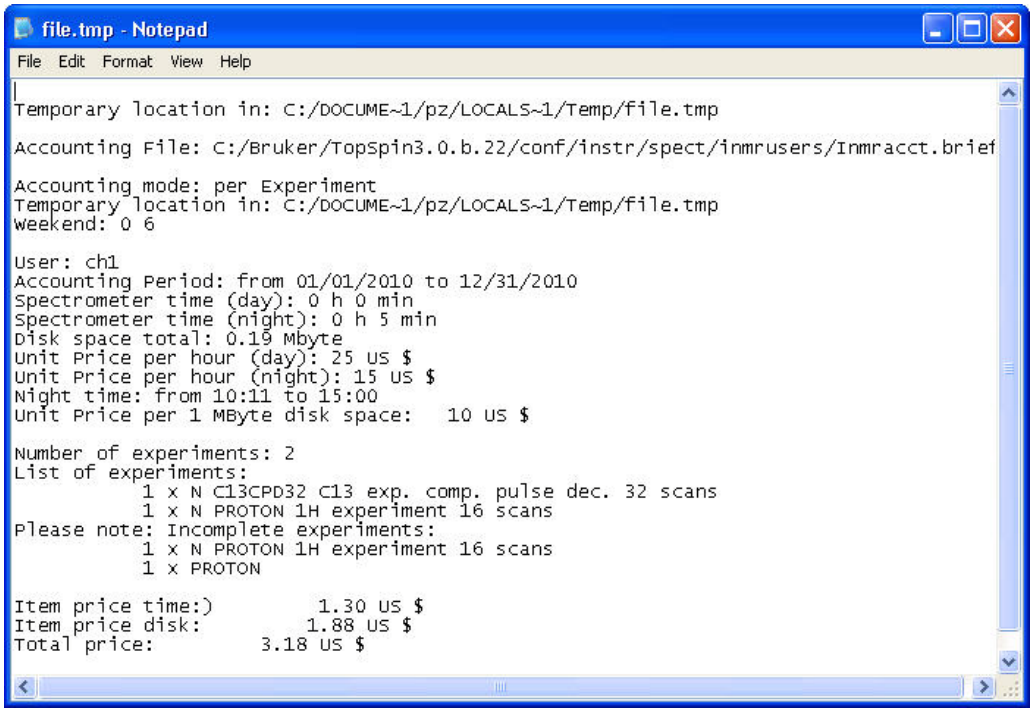
3.25.1.6 List the experiments

When enabled, the report lists how many time experiments have been run and also will

include the incomplete experiments.

3.25.1.7 The Start button

The program will start accounting according to the parameters you have defined during the previous steps, and display the report. Figure 4.124 shows a typical report including the performed experiments. The number close to each experiment name indicates the number of times this type of experiment was executed during the accounting period. The report also lists incomplete experiments which have been started but were interrupted either by the operator or because of an error situation. Failed experiments are not included in the price calculation.



4 Routine Spectroscopy

4.1 Starting the Routine Spectroscopy window

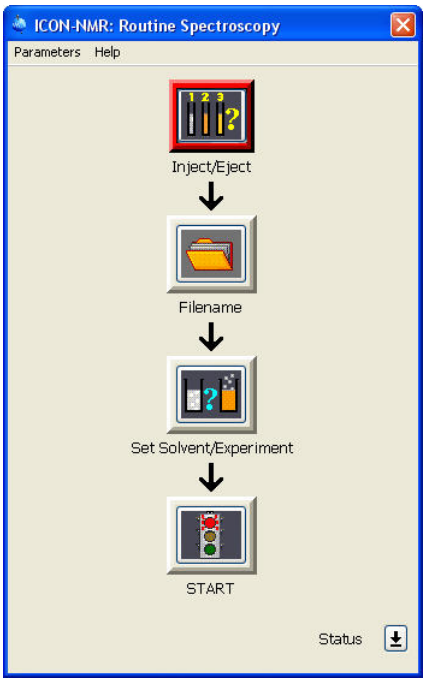
Routine Spectroscopy is designed to help users perform NMR experiments by following a step by step menu.

1. Type **Icon** inside the TopSpin command line and hit Enter.

2. Select **Routine Spectroscopy**.

Alternatively, you can also type **IconNMR** on the TopSpin command line.

3. Enter the User password.
4. Hit Enter.



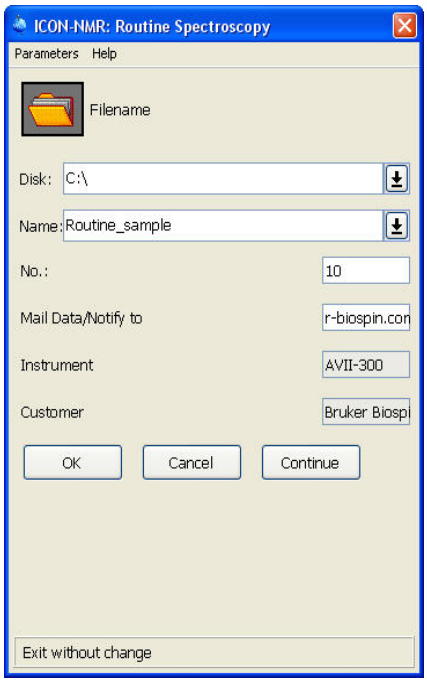
5. Click on the **Inject/Eject** button.

6. Click on the **Insert New Sample** button.

The sample lift air is turning on and the Insert Sample window appears.

7. Insert the sample on the top of the magnet.

8. Click on the **OK** button inside the Inject/Eject window.



9. Type a file name into the Name window or select one of the predefined file names, by clicking on the down arrow button.

The user may be requested to select a Disk Unit or to fill in the originator information. If the experiment number, e.g. 10, of the current data set name already exists, a Data Set Report window appears which gives the option to overwrite the existing data set or to increment the experiment number to the next available one.

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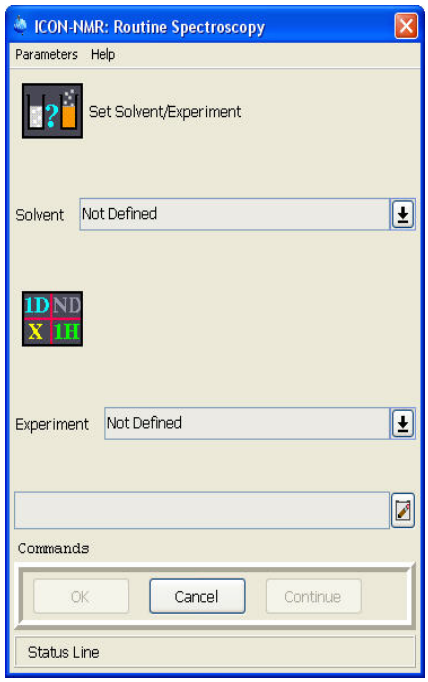
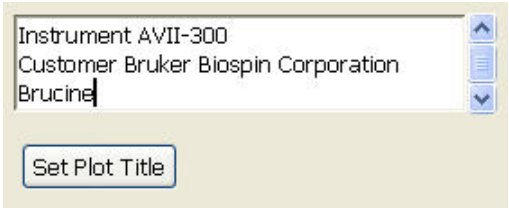
10. Click on the **Continue** button inside the IconNMR: Routine Spectroscopy window.

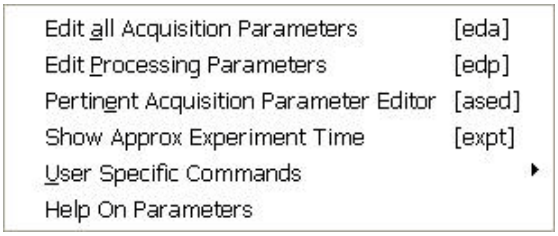


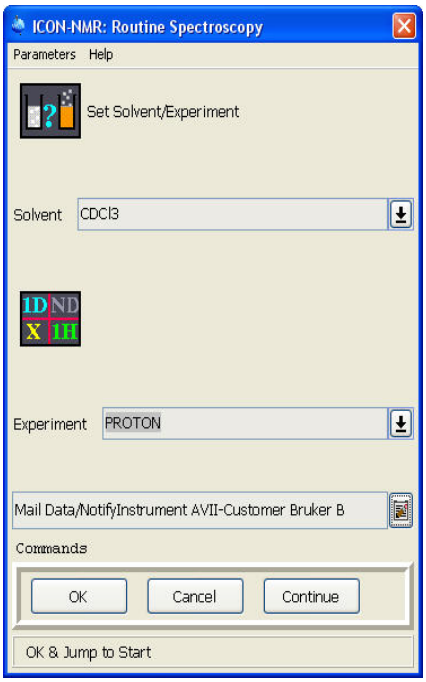
11. Click on the arrow next to the Solvent window.
12. Select the solvent e.g.**CDCl3** by clicking on it.
13. Click on the arrow next to the Experiment window.
14. Select the experiment e.g. **PROTON** by clicking on it.
15. Click on the note pad icon next to the title window.



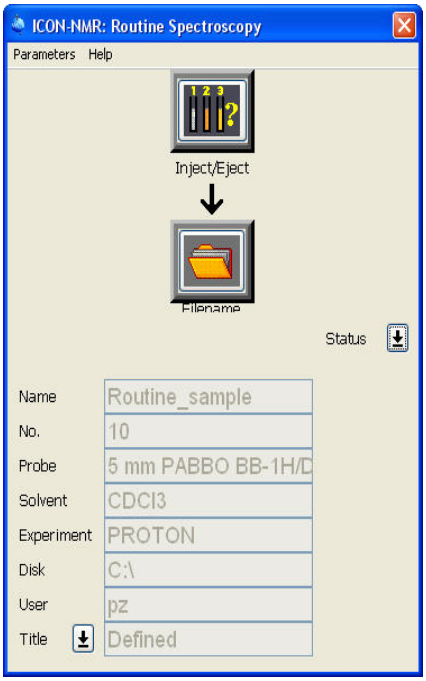
16. Enter a title and click on the Set Plot Title inside the title window.

At this time it is possible to change parameters by clicking on **Parameters**. Depending on the user's permission, the access to all parameters may be granted or only for user specific parameters (see the figure below).

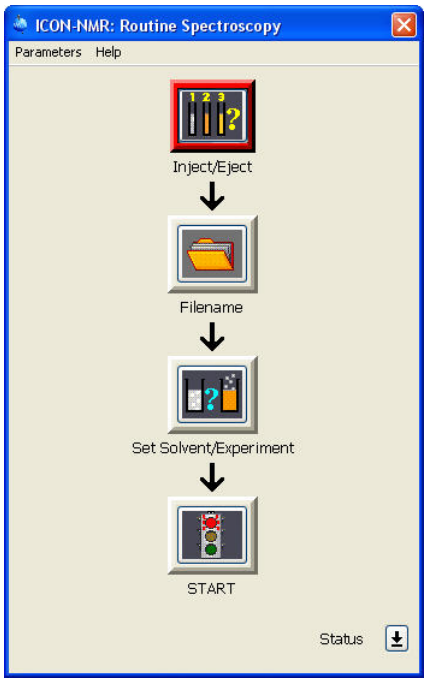




17. Click on the **Continue** button inside IconNMR: Routine Spectroscopy window.
18. Click on the **Status** button to check the information status of the current sample.

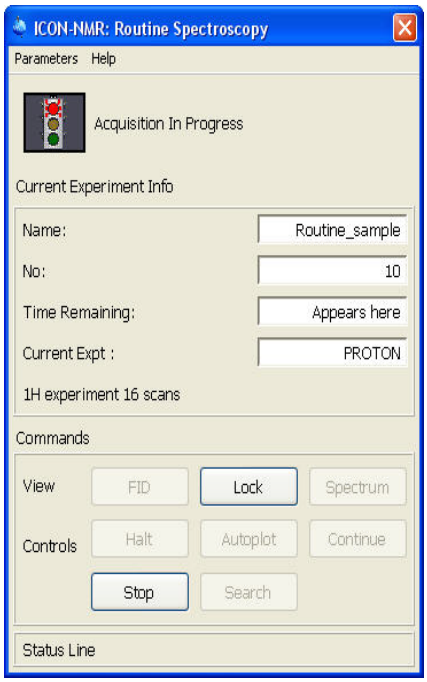


19. Click on the **Status** button to return to the Routine Spectroscopy flow chart.



20. Click on **Start** button.

At this point an Online Control window and the acquisition status icons appear on the screen.



Online Control function keys:

FID

display the acquisition window (active after the acquisition has started)

Lock

view the lock window

Spectrum

view the spectrum

Halt

stop the acquisition after the next scan is completed then start the processing

Autoplot

plot data or additional expansions

Continue

to exit back to the ICON-NMR/Routine window

Stop

stop all processes and do not continue

Search

open the Portfolio Editor

21. Click on the Continue button inside the Online Control function window after all processing status icons stop flashing.

22. Choose one of the options:

EXIT

Exit without change.

Eject + Terminate

Ejects the sample and logs out the user.

Insert New Sample

A window to change the sample will appear and a new file name, solvent and experiment can be selected. The current user stays logged in.

Use Same / Continue

The sample stays in the magnet, (locked and shimmed) and a new experiment can be selected.

Same with Lock/Shim

Use the same sample, repeating Lock and Shim.

23. Click on the **Exit** button inside IconNMR: Routine Spectroscopy window.

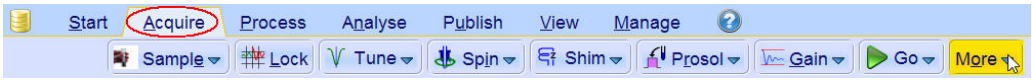
27. Click on **File** and select **Exit**.

5 Automation

5.1 Starting the Automation Setup window

Automation is designed to run experiments using a variety of sample changers and can also be used in manual sample change operation allowing greater flexibility than the Routine Spectroscopy (Chapter. 4).

1. In the TopSpin Menu bar click on the **Acquire** tab.

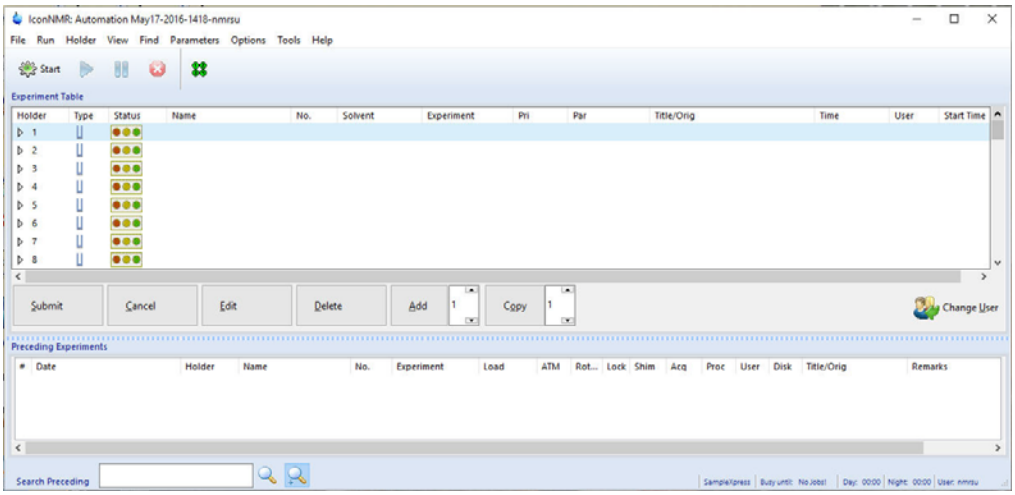


2. Click on the down arrow inside the **More** button.

3. Select **IconNMR Automation**

Alternatively, you can also type **icona** on the TopSpin command line.

4. Enter the User password.
5. Hit Enter.



5.1.1 Sample preparation

The following setup examples are simple exercises to demonstrate the different acquisition methods in IconNMR using 4 samples.

5.1.1.1 Samples

30 mg Cholesterylacetate in 0.6 ml CDCl3

30 mg Carvone in 0.6 ml Acetone-d6

30 mg Strychnine in 0.6 ml CDCl3

0.1% Ethylbenzene in CDCl3 (Standard Sample)

5.2 Experiment Setup

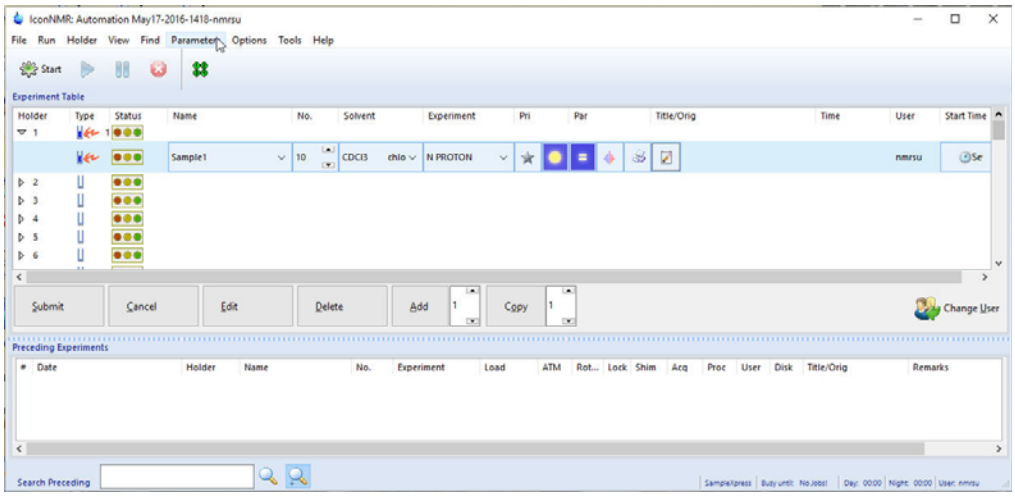
5.2.1 Set up of one single experiment

1. Double click on **Holder 1**
2. Click inside the Name window and change the name to **Sample1**

The experiment number automatically increments to the next available number if a data set already exists with that name and experiment number.

3. Click on the down arrow next to the Solvent window and select **CDCl3**.

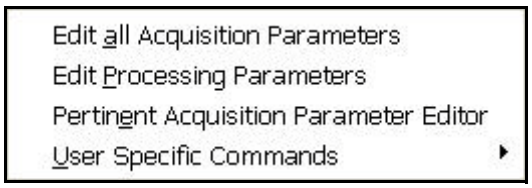
4. Click on the down arrow next to the Experiment window and select **PROTON**.



Depending on the user's permissions, parameters of the experiment can be changed using the following options.

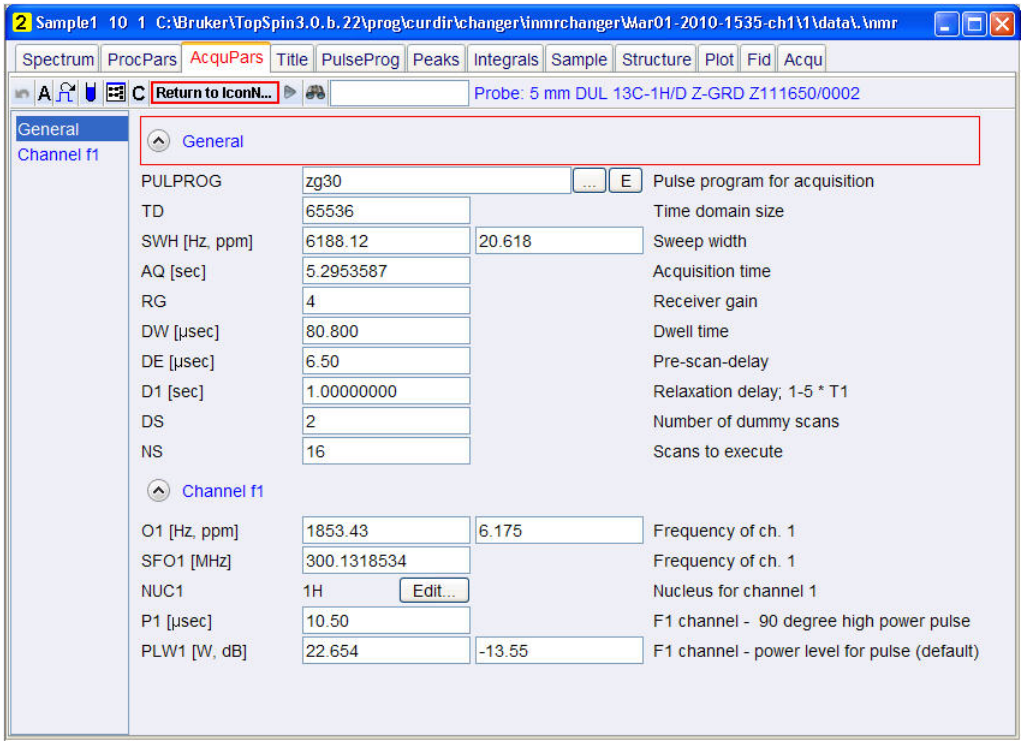
5.2.1.1 Change all parameters

5. In the IconNMR menu bar, click on **Parameters** and choose any of the options shown in the figure below.



6. Select e.g. **Edit all Acquisition Parameters**.

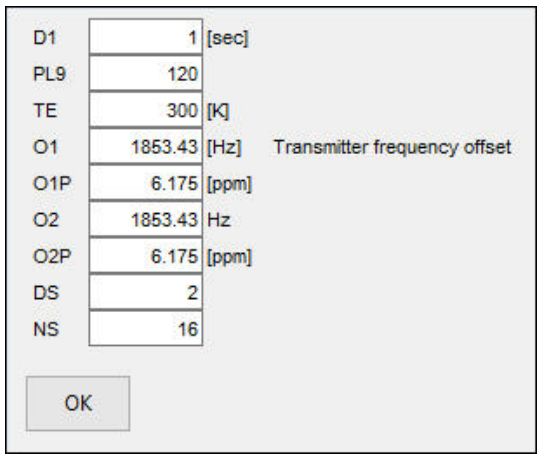
7. Change any of the parameters in the TopSpin AcquPars window shown in the figure below.



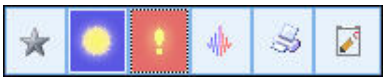
8. Click on the **Return to IconNMR** button to return to the Automation set up window.

5.2.1.2 Edit User specific parameters

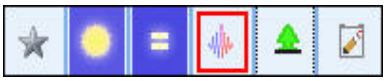
9. Click on the **Edit specific parameters** button.



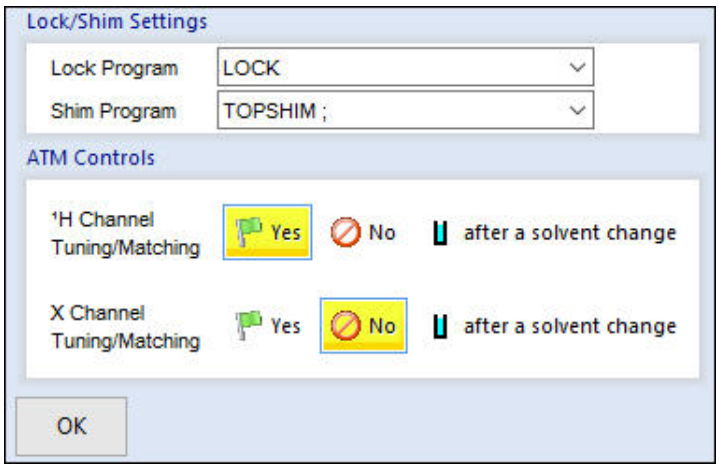
Any of the displayed parameters can be changed. If done so, the icon of the Edit specific parameters button will change as illustrated in the picture below.



5.2.1.3 Control Locking Shimming and ATM

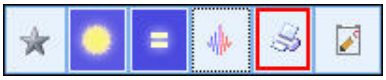


10. Click on the Control Locking, Schimming and ATM button to change any options in the figure below.



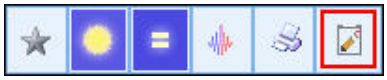
11. Click on the **OK** button inside the Lock.Schim Settings window, when done

5.2.1.4 Toggle Printing

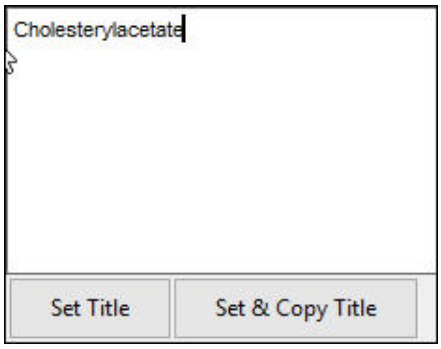


12. Select the **printer** icon for printing the spectrum or select the **green tree** icon for no print.

5.2.1.5 Setting the Title



13. Click on the Set a title button.
14. Type a title e.g. **Cholesterylacetate**



15. Click on the **Set Title** button inside the Title window.
16. Click on the first line of **Holder 1**

17. Click on the Submit button.

The user may be requested to fill in the originator information before the sample can be submitted. Proceed to paragraph **5.4 Sample run** to start the automation in this chapter.

5.2.2 Set up of two single experiments

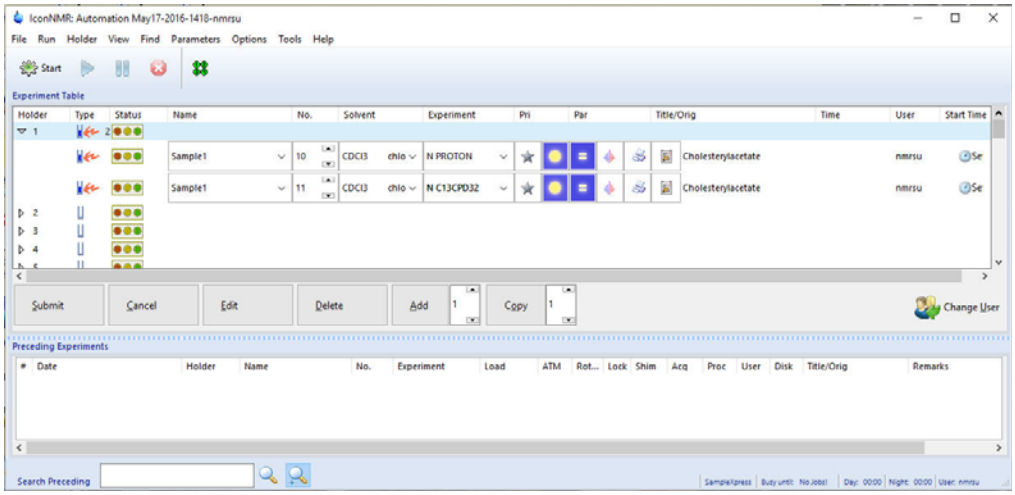
1. Follow steps **1** through **17** in paragraph **5.2.1 Setup of one single experiment**.

2. Click on the **Add** button.

To add one experiment, regardless if it is a single or composite one, a “1” should be displayed in the window next to the Add button. A new line opens up containing the same information for the Disk, Name, Solvent and Orig/Title. The Exp No is incrementing by 1.

3. Click on the small button to the right of the Experiment window and select **C13CPD32**.

4. Click on Holder 1



5. Click on the **Submit** button.

The Status traffic lights of the two experiments change to yellow to indicate the holder is ready to run and the experiment time of each experiment is calculated. Proceed to Paragraph 5.4 Sample run to start the automation.

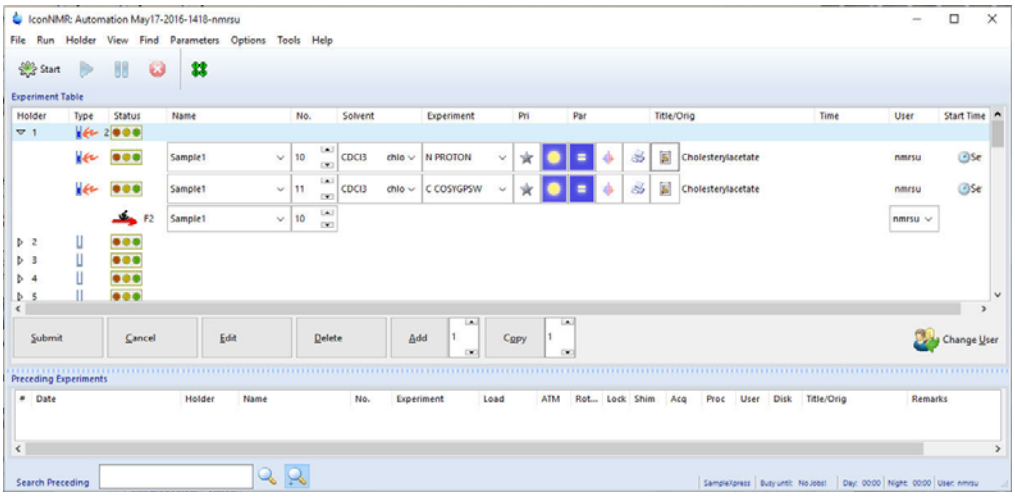
5.2.3 Set up of a composite experiment

1. Double click on **Holder 1**.

2. Click inside the Name window and change the name to **Sample1**.

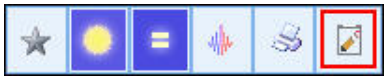
The experiment number automatically increments to the next available number if a data set already exists with that name and experiment number.

3. Click on the down arrow next to the Solvent window and select **CDCl3**.
4. Click on the down arrow next to the Experiment window and select **COSYGPSW**



A letter C will be displayed to mark the COSYGPSW to be composite experiment. A composite experiment contains two or more single experiments. In this case, the COSYGPSW is a 2D Homonuclear Correlation experiment which needs a PROTON experiment to optimize the parameters. The PROTON experiment is automatically entered into the present holder.

5. Select and highlight the PROTON experiment.



6. Click on the **Set a title** button.
7. Type a title e.g. **Cholesterylacetate**
8. Click on the **Set & Copy Title** button inside the Title window.
9. Click on the first line of Holder 1.

10. Click on the **Submit** button.

The user may be requested to select a Disk Unit or to fill in the originator information before the sample can be submitted.
The Status traffic lights of the two experiments are changing to yellow to indicate the experiments are in the queue and the experiment time of each experiment is calculated.
Proceed to 5.4 Sample run to start the automation.

5.2.4 Set up of two composite experiments

1. Follow steps 1 through 9 in 5.2.3 Setup of a composite experiment.

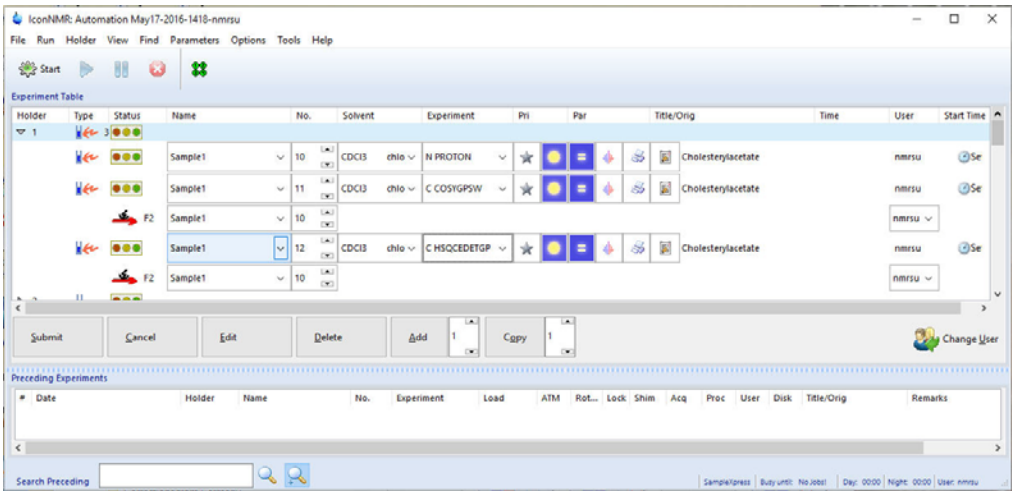
2. Click on the **Add** button.

To add one experiment, regardless if it is a single or composite experiment, a “1” should be displayed in the window next to the Add button. A new line opens up which contains the same information for the Disk, Name, Solvent and Orig/Title. The Exp No is incrementing by 1.

3. Click on the small button to the right of the Experiment window and select **HSQCEDETGP**.

HSQCEDETGP is a composite experiment like COSYGPSW and is marked with the letter C. It is a 2D Hetero inverse correlation experiment which needs a Proton 1D-preparation experiments to optimize the 2D parameters in F2. Since the PROTON experiment already exists, it will use this experiment to optimize the 2D parameters.

4. Click on the first line of Holder 1.

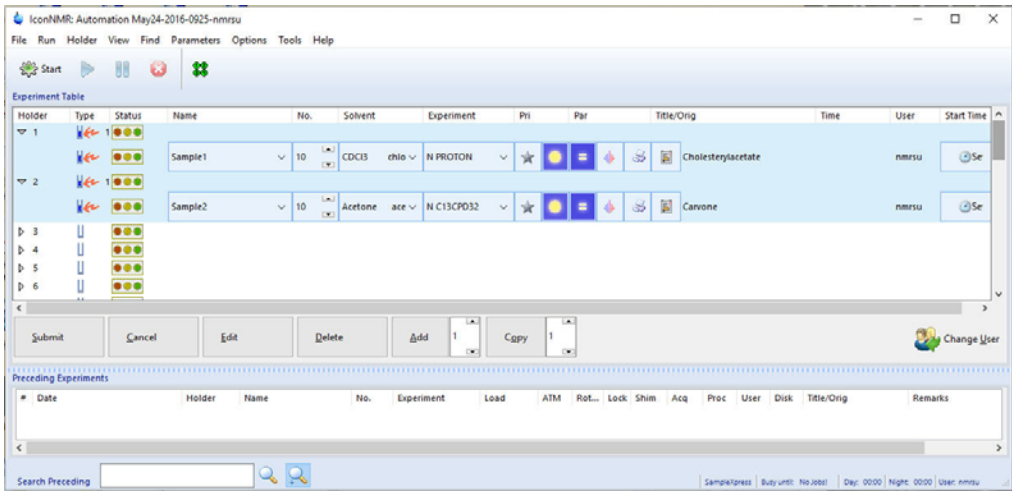


5. Click on the **Submit** button.

The Status traffic lights of the four experiments change to yellow to indicate the holder is ready to run and the experiment time of each experiment is calculated. To start the Automation Run, proceed to Paragraph 5.4 Sample run to start the Automation.

5.2.5 Set up of two or more holders with different solvents and experiments

1. Follow steps 1 through 17 in 5.2.1 Setup of one single experiment.
2. Double click on Holder 2.
3. Click inside the Name window and change the name to **Sample2**
4. Click on the down arrow to the right of the solvent window and select **Acetone**.
5. Click on the down arrow to the right of the Experiment window and select **C13CPD32**.
6. Click on the **Set a title** button.
7. Type a title e.g. **Carvone**.
8. Click on the **Set Title** button inside the Title window.
9. Click on the first line of Holder 1.
10. Hold down the **Shift** key and click on the last experiment line of Holder 2.

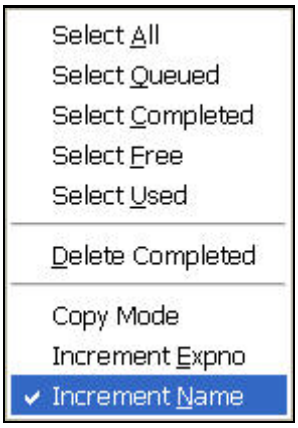


11. Click on the **Submit** button.

The Status traffic lights change to yellow to indicate the holders are ready to run and the experiment time is calculated. Proceed to Paragraph 5.4 Sample run to start the automation.

5.2.6 Set up of two or more holders with the same solvents and experiments

1. In the menu bar click on **Holder** and select **Increment Name.**



2. Follow steps **1** through **17** of **5.2.1 Setup of one single experiment**.

3. Click on the first line of Holder 1.

4. Increment the number next to the **Copy** button to **2**.

5. Click on the **Copy** button.

To copy the setup from one holder into another holder click on the **Copy** button. The number displayed in the window next to the Copy button is to how many holders it will copy. For this example use **2**. The next two holders will have the same setup as the previous one except that the Name **Sample1** increments to **Sample2** and **Sample3**.

---

6. Click on the experiment line in Holder 2.

7. Click on the **Edit** button.

8 Click on the **Set a title** button.

9. Type a title e.g. **Ethylbenzene**.

10. Click on the **Set Title** button inside the Title window.

In addition to the title all other entries can be edited in the new holder by clicking on **Edit**. DO NOT CHANGE the Exp No, unless you are sure the new Exp No does not already exist.

---

11. Click on the experiment line in Holder 3.

12. Click on the **Edit** button.

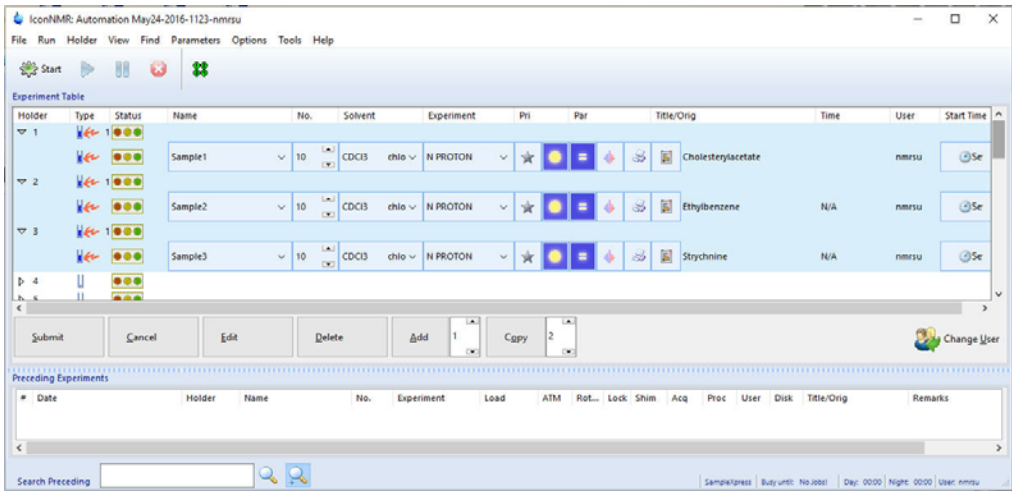
13. Click on the **Set a title** button.

14. Type a title e.g. **Strychnine**.

15. Click on the **Set Title** button inside the Title window.

16. Click on the first line of Holder 1.

17. Hold down the **Shift** key and click on the last experiment line of Holder 3.



18. Click on the **Submit** button.

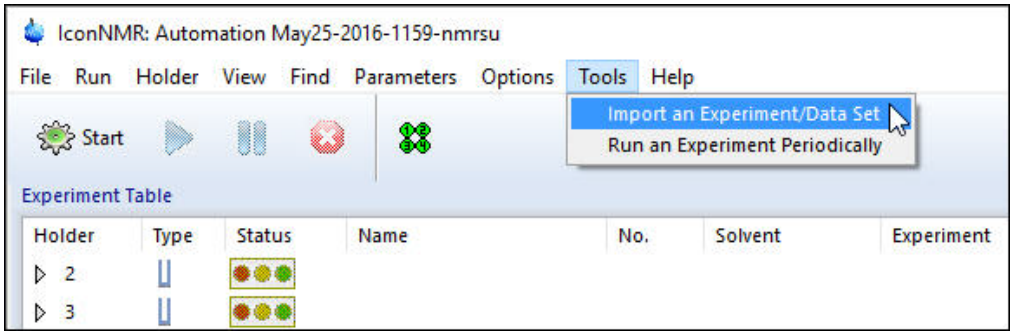
The Status traffic lights on both holders change to yellow to indicate the holder's ready to run and the experiment time for each experiment is calculated. Proceed to paragraph 5.4 Sample run to start the automation.

5.3 Tool Menu

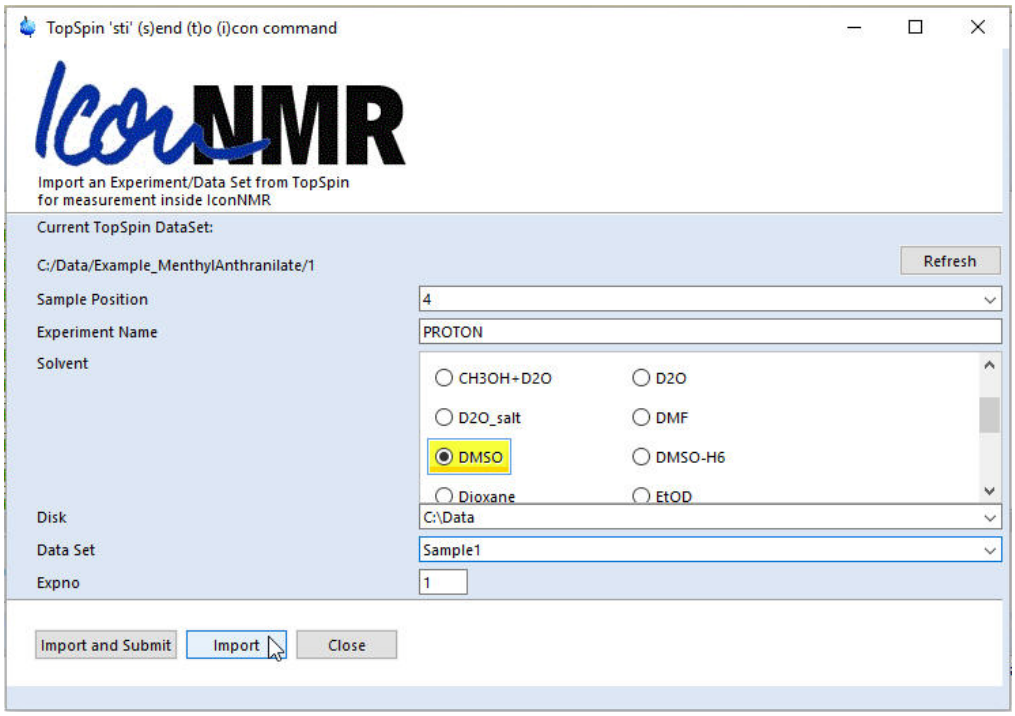
5.3.1 Import an Experiment/Dataset

Use this tool to import the current data set on display in TopSpin in to the Automation set up window, choosing any Holder. After the data set has been imported it may be modified, copied, iterated or prioritized as any standard IconNMR experiment.

1. Open a data set in TopSpin e.g. **Menthyl Antranilate in DMSO-d6**.
2. Start IconNMR and open the Automation set up window.
3. Click on **Tool** in the main menu bar.

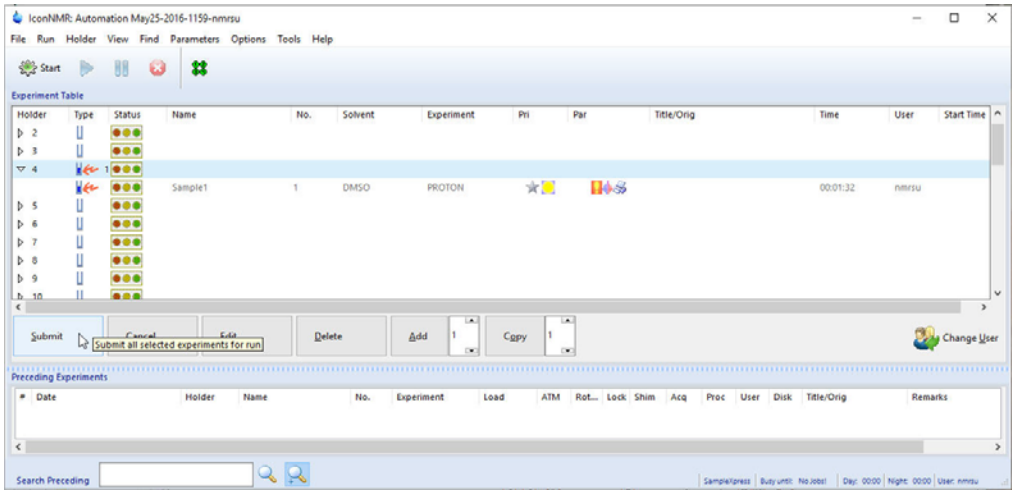


4. Select **Import an Experiment/Data Set**.
5. Click on the down arrow next to **Use Holder Position**
6. Select Holder e.g. **4**.
7. Change the Data Set name to e.g. **Sample1**.



8. Click on the **Import** button inside the TopSpin ‘sti’ window.

Using the Import button will add the Data set to the IconNMR Automation window and then can be submitted at a later time. The Import and Submit button will add and submit the Data set automatically.



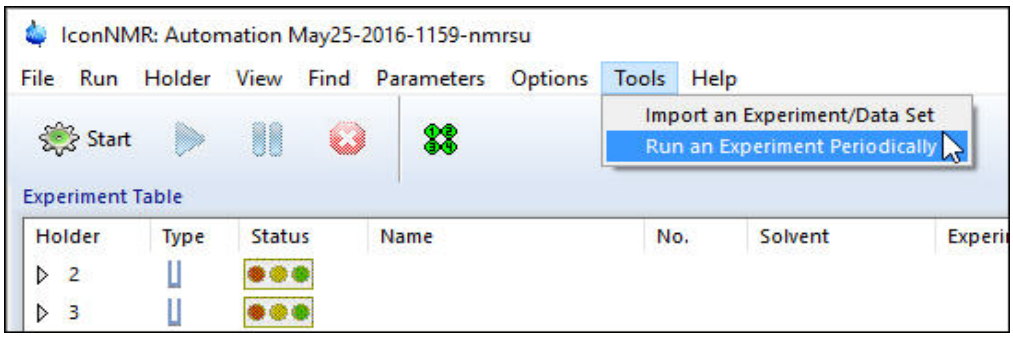
9. Click on the **Close** button inside the TopSpin ‘sti’ window.

10. Start the run by following the instructions in 5.4 Sample run

5.3.2 Run an Experiment Periodically

Use this tool to repeat any experiment automatically any number of times on a particular sample with a specific time delay between experiments. Up to 10 such periodic measurements may run simultaneously.

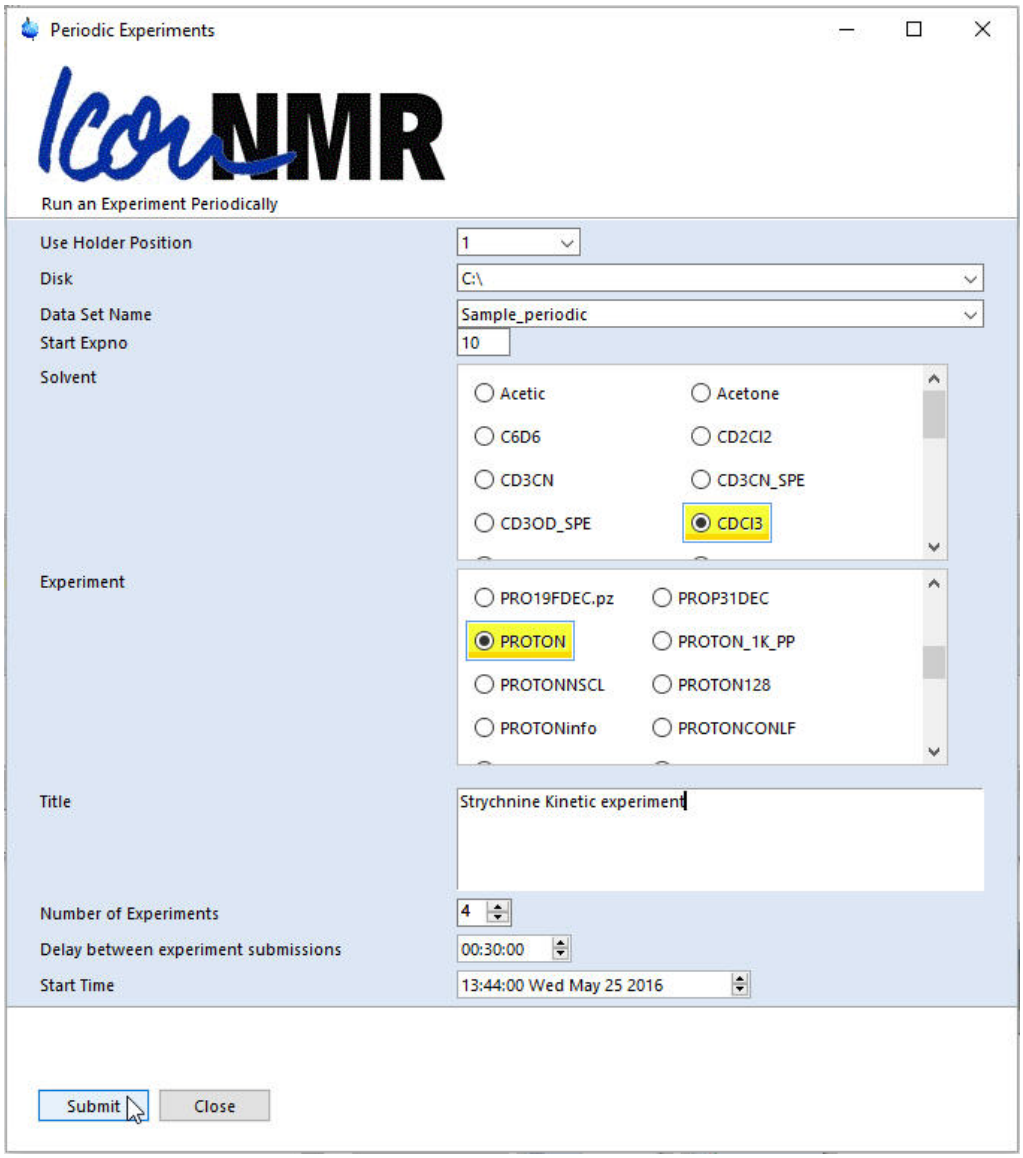
1. Start IconNMR and open the Automation set up window
2. Start the run by following the instructions in 5.4 Sample run.
3. Click on **Tool** in the main menu bar.
4. Select **Run an Experiment Periodically**.



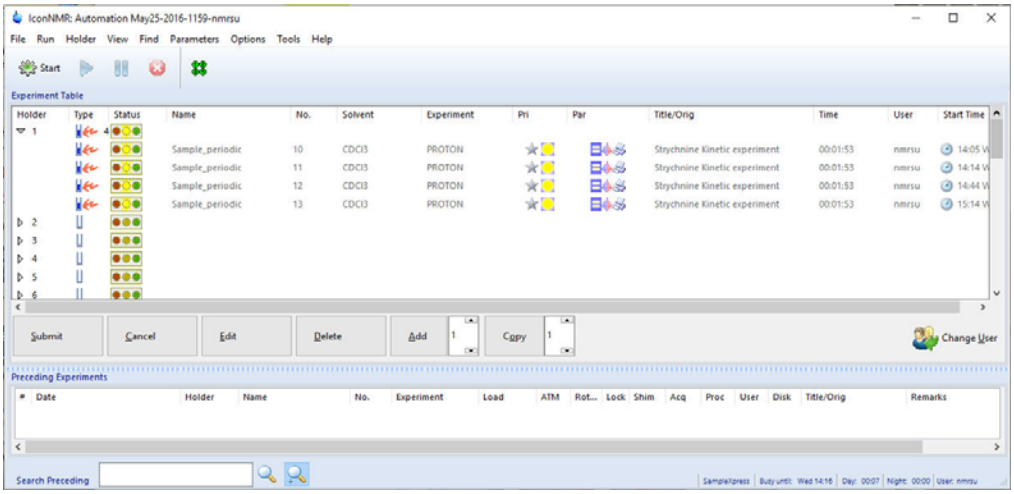
5. Click on the down arrow next to **Use Holder Position**.
6. Select Holder e.g. **1**.
7. Click on the down arrow next to **Disk**.
8. Select the disk e.g. **C:**.

9 Click on the down arrow next to **Data Set Name**.

10. Select a data set name or type a name e.g. **Sample_periodic**.
11. Select a solvent e.g. **CDCl3**.
12. Select the Experiment e.g. **PROTON**.
13. Enter a **Title** e.g. **Strychnine Kinetics experiment**.
14. Enter the Number of experiments e.g. **4.**
15. Enter the value for the Delay between experiments submissions e. g. **30** Min.
16. Enter a Start Time.



17. Click on the **Submit** button inside the Periodic Experiment window.



The experiments are automatically submitted and the Priority flag is set. The first experiments starts at the entered Start Time.

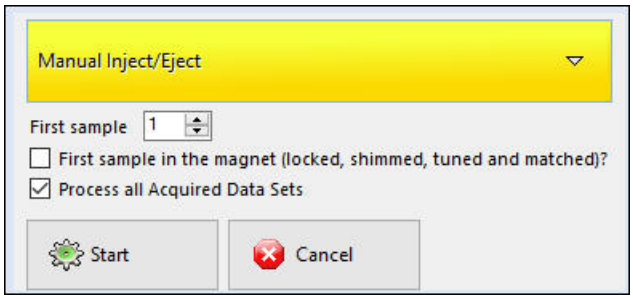
5.4 Sample run

5.4.1 Manual Inject/Eject

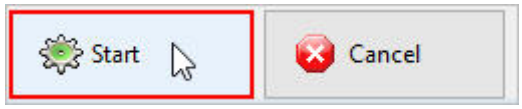
1. Click on the **Start** button.

The Initialize Run window appears. The default Automation mode displayed is what has been set in the ICON-NMR configuration.

2. Click on Automation mode button and select **Manual Inject/Eject**.
3. Select or type **1** for **First sample**.



IconNMR gives you the option to lock and shim the sample prior to running the automation or, if you have stopped or halted the previous automation run, to continue on the sample already in the magnet. For that purpose click on the small button next to **First sample in the magnet (locked and shimmed)?** and a check mark will appear. The system will skip the inject/eject, locking and shimming for that sample. In addition the user can choose to process all acquired data sets or do it later. This option can be set in the Icon configuration, Master Switches under the Process control section when Ask on Startup is selected.



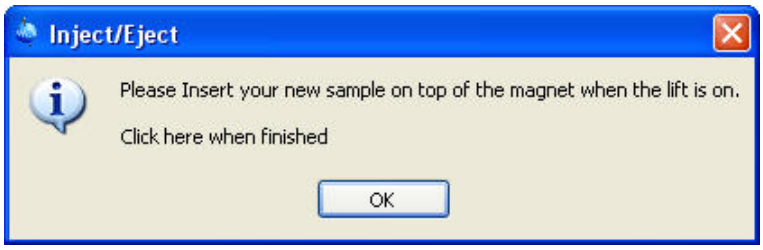
4. Click on the **Start** button

At this point the acquisition status icons and message window to change the sample appear.

5. Click on the **OK** button inside the Inject/Eject window.

The sample lift air will turn on and the Inject/Eject window appears.

6. Insert sample.



7. Click on the **OK** button inside the Inject/Eject window.

At this point the Automation begins locking, shimming, adjusting the receiver gain, acquisition and processing. A history box on the bottom of the “Automation Manager” window shows the detailed information of what tasks have been completed or failed for experiment(s) that have been setup to run on the sample. Double click on a completed entry, displays the data in the Topspin window.

5.4.2 NMR case

If the NMR Case is not installed on top of magnet, check if there is no sample in the magnet and then install the changer.

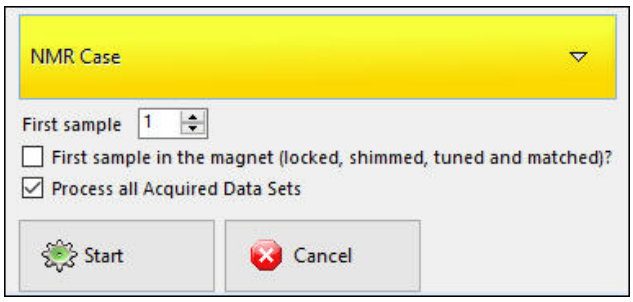
1. Turn the switch on the sixpack/case controller box to OFF position.
2. Turn on the sample lift and remove the sample and leave the lift air on.
   - **!!!WARNING!!!: Be absolutely sure that no sample is in the magnet and the sample holder is empty before proceeding to the next step.**
3. Install the NMR Case on to the top of the magnet.
4. With the sample lift air still on, move the sample holder to the start position (set the small hole over the shim stack).
5. Turn off the sample lift.
6. Load the samples into the sample holders.
7. Turn the switch on the sixpack/case controller box to ON position.

The sample in Holder 1 must be submitted before proceeding to the next step.

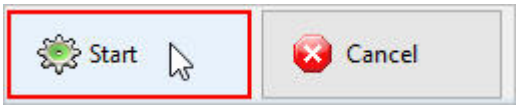
8. Click on Start button.

The Initialize Run window appears. The default Automation mode displayed is what has been set in the IconNMR configuration.

9. Click on Automation mode button and select **NMR Case**.
10. Select or type **1** for **First sample**.



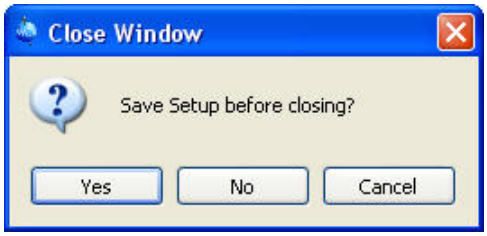
IconNMR gives you the option to lock and shim the sample prior to running the automation or, if you have stopped or halted the previous automation run, to continue on the sample already in the magnet. For that purpose click on the small button next to **First sample in the magnet (locked and shimmed)?** and a check mark will appear. The system will skip the inject/eject, locking and shimming for that sample. In addition the user can choose to process all acquired data sets or do it later. This option can be set in the Icon configuration set up.



11. Click on the **Start** button.

At this point the “IconNMR / Auto Online Controls” window and the “acquisition status icons” appears. The Automation begins changing the sample, locking, shimming, adjusting the receiver gain, acquisition and processing. A history box on the bottom of the “Automation Manager” window shows the detailed information of what tasks have been completed or failed for experiment(s) that have been setup to run on the samples. Double click on a completed entry, displays the data in the Topspin window.

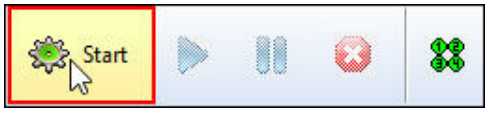
12. Wait until the last sample has finished running and has been ejected.
13. Turn the switch on the case controller box to OFF.
14. Remove all samples from the sample holders.
15. Click on **‘File’** and select **‘Close’** in the Automation set up window.



16. Click on the Yes button to save the Setup.

5.4.3 Standard BACS, Sample Case, Pro (RS232)

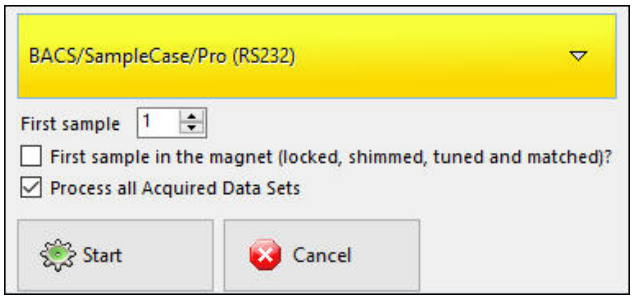
1. Insert the samples into the holders.
2. Press RESET on the front of the sample changer.



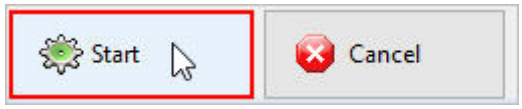
3. Click on the **Start** button,

The Initialize Run window appears. The default Automation mode displayed is what has been set in the Icon-NMR configuration.

4. Click on Automation mode button and select **BACS/SampleCase/Pro (RS232)**.
5. Select or type **1** for **First sample**.



IconNMR gives you the option to lock and shim the sample prior to running the automation or, if you have stopped or halted the previous automation run, to continue on the sample already in the magnet. For that purpose click on the small button next to **First sample in the magnet (locked and shimmed)?** and a check mark will appear. The system will skip the inject/eject, locking and shimming for that sample. In addition the user can choose to process all acquired data sets or do it later. This option can be set in the Icon configuration set up.



6. Click on the **Start** button.

At this point the “IconNMR / Auto Online Controls” window and the “acquisition status icons” appears. The Automation begins changing the sample, locking, shimming, adjusting the receiver gain, acquisition and processing. A history box on the bottom of the “Automation Manager” window shows the detailed information of what tasks have been completed or failed for experiment(s) that have been setup to run on the samples. Double click on a completed entry, displays the data in the Topspin window.

6 Adding new experiments

6.1 Introduction

- **!!!IMPORTANT!!!: Before creating a new experiment for automation, make a layout of how the new experiment should work and how you would like to present the result. Check the parameter library first to see if the new experiment already exists. If not, check in the pulse program library for an existing pulse program and in the au program library for the acquisition and processing programs to satisfy the plans for the new experiment. If you have to create a new pulse program or have to write an au program, be sure to follow to the nomenclature of file names, pulse widths and delay numbering that Bruker has defined. Any deviation may result in a malfunction of the new experiment. Always test out the new experiment before you add it to IconNMR.**

The parameter sets of any new user defined experiments are stored in the **<TopSpin home>\exp\stan\nmr\par\user** directory and can be copied to other Bruker instruments. With the use of the paracon program the parameters can the be converted to the frequency of the instrument. To avoid converting the parameter sets, you can create a **virtual parameter set** in IconNMR. To illustrate this feature, follow paragraph **6.9 1D Carbon and 1D DEPT135 composite exp.** in this chapter.

6.2 Single 1D Proton exp. with peak labels in print out

This example requires to make changes of some acquisition and processing parameters. There are no changes to the pulse sequence of the acquisition and processing AU-programs.

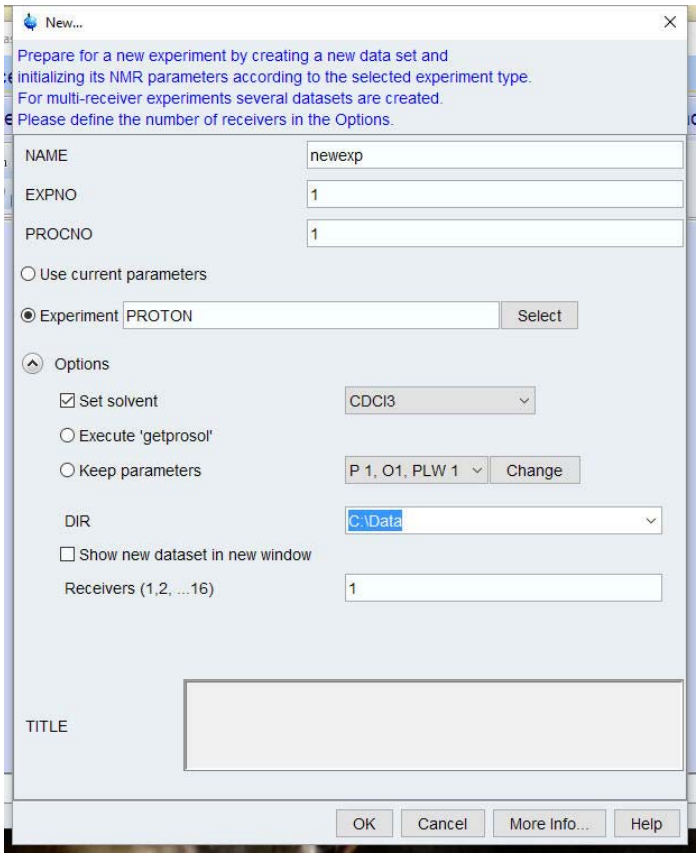
6.2.1 Layout of the new experiment

- Experiment: Proton, **128** scans, printing **11ppm** with **peak picking** and **integration**
- Starting parameter file: **PROTON**
- New parameter file: **PRO128PP**

6.2.2 Creating the parameter file

In this case the new experiment PRO128PP does not exist in the parameter set library. To create the new experiment, the existing PROTON parameter file can be used as a template, since the acquisition and processing parameters are similar.

1. Type **edc** and enter the following parameters:



2. Click on the **OK** button inside the New window.

3. Click on the **AcquPars** tab and in the section Experiment, change the following parameter:

   NS = **128**

4. Click on the **ProcPar** tab and in the sections Peak picking / plotting and Automation change the following parameters:

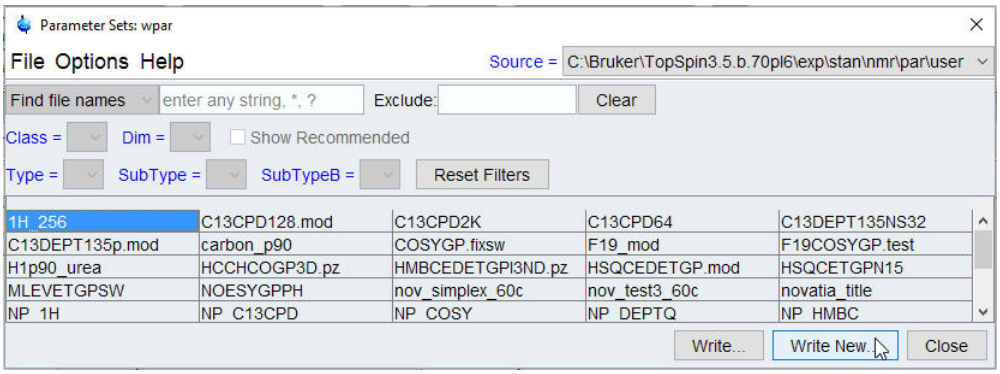
   F1P (ppm) = **10**

   F2P (ppm) = **-1**

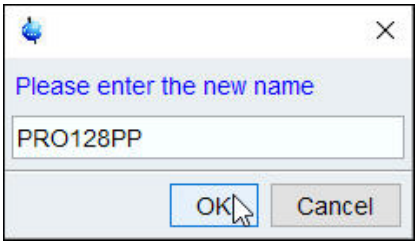
   LAYOUT = **+/1D_H+pp.xwp**

5. Type **wpar**

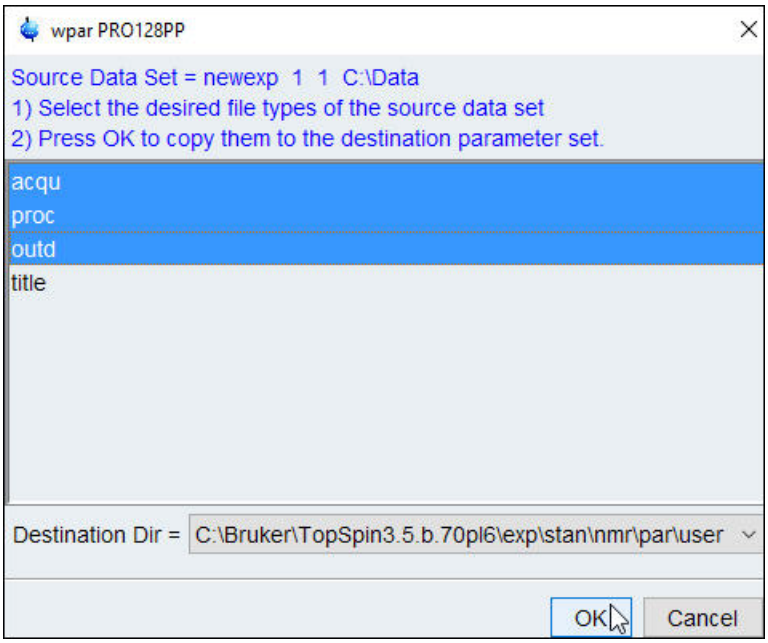
6. Select the user parameter source directory.



7. Click on the **Write New** button inside the Parameter Sets: wpar window.
8. Enter **PRO128PP**



9. Click on the **OK** button inside the new name window.
10. Select the **acqu**, **pro** and **outd** parameters.



11. Click on the **OK** button inside the wpar window.
12. Click on **Close** button inside the Parameter Sets: wpar window.

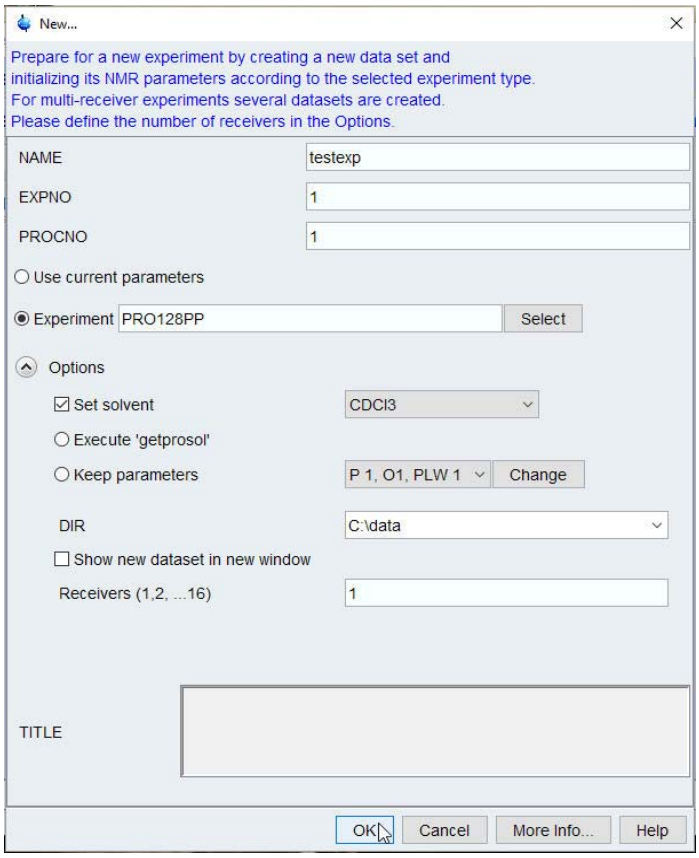
6.2.3 Testing the experiment

6.2.3.1 Sample

0.1% Ethylbenzene in CDCl3 or any other sample

6.2.3.2 Running the experiment

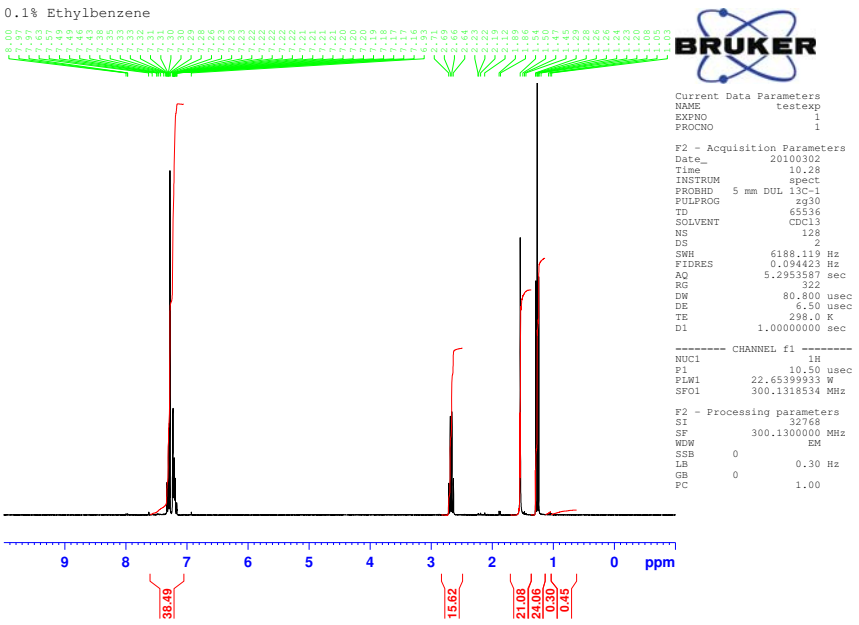
1. Type **edc** and enter the following parameters:



2. Click on the **OK** button inside the New window.
3. Type **lock** and select **CDCl3**.
4. Tune the probe.
5. Shim for best homogeneity.
6. Type **getprosol**

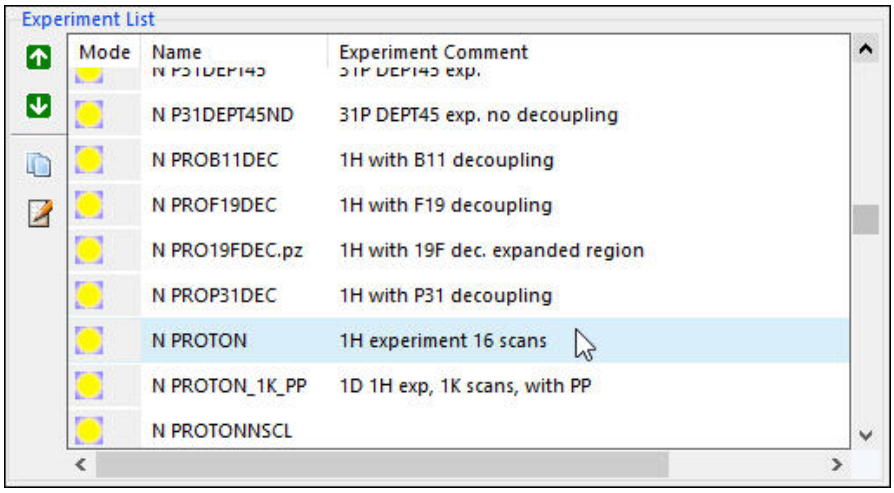
7. Type **xaua**
8. Type **xaup**

xaua is executing the acquisition AU-program ‘au_zg’ as a AUNM entry in the Automation section of the AcquPars and xaup executes the processing AU-program ‘proc_1d’ as a AUNMP entry in the Automation section of the ProcPars. If you want to make changes to the parameters, repeat steps 7 and 8 for testing, then store the parameter file PRO128PP with the wpar command.



6.2.4 Adding the new experiment to ICON-NMR

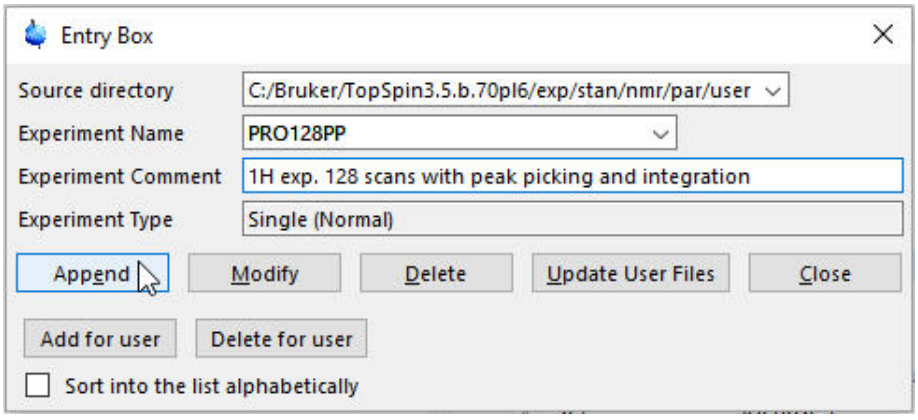
1. Start IconNMR **Configuration**.
2. Select **User Manager**.
3. Select a **user name**.
4. Click on any experiment listed inside the **Experiment list box**.



If there are already some N-Proton experiment listed in the Experiment list box, then you may consider clicking on one of the Proton experiment to append the new experiment to the list.

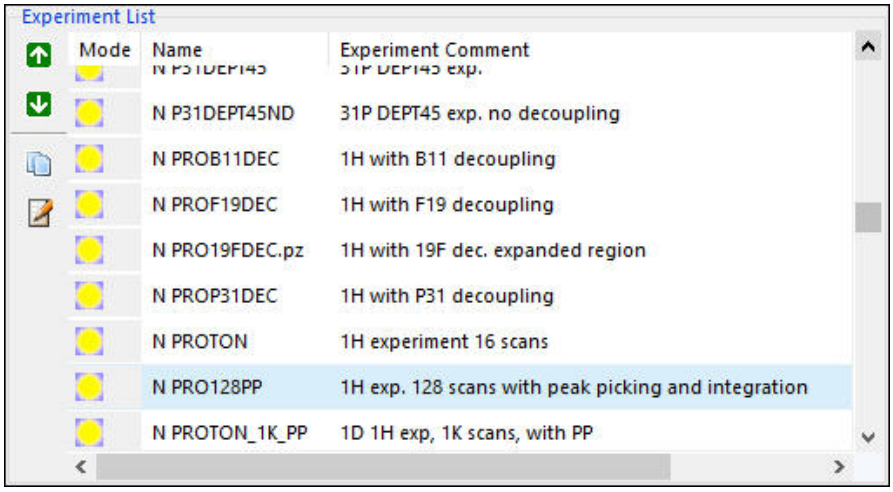
5. Click on the down arrow next to Source directory.
6. Select **<TopSpin-Home>/exp/stan/nmr/par/user**.
7. Click on the down arrow next to Experiment Name.
8. Select **PRO128PP**.
9. Click on the Experiment Comment Text window and enter the following text:

   1H exp. 128 scans with peak picking and integration



The Experiment Type is a Single (Normal) experiment and will be marked with an N inside the Experiment list box.

10. Click on the **Append** button inside the Entry Box.
11. Click on the **Close** button inside the Entry Box.



12. Click on **File** and select **Save**.
13. Click on **File** and select **Close**.

Test the new added experiment for proper operation using the IconNMR Automation.

6.3 NOTES:

6.4 Single 2D COSY exp. with a predefined sweep width

This example requires to make changes to the acquisition AU-program and parameters. There are no changes to the pulse sequence of the processing AU-programs or parameters.

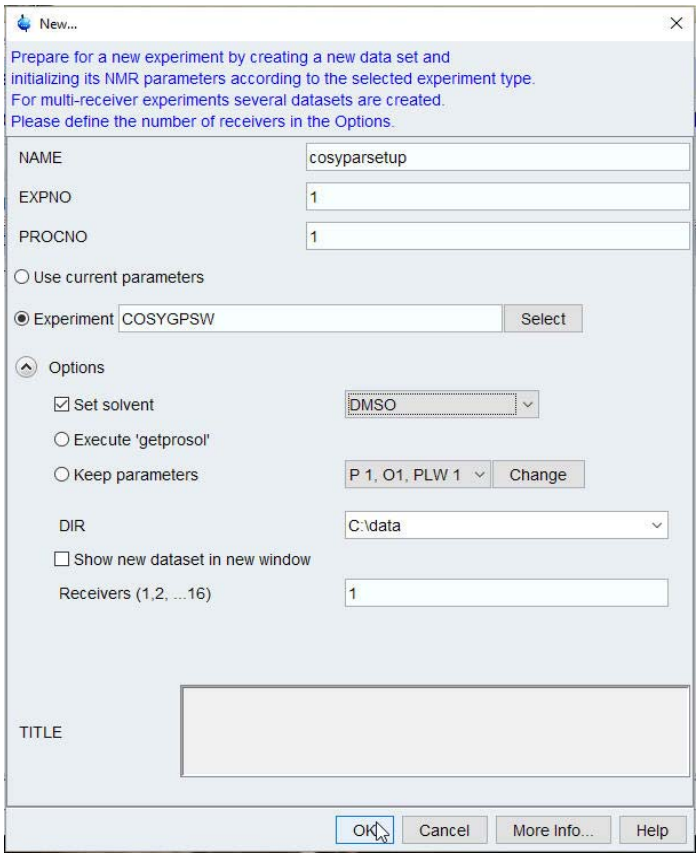
The COSY type experiments in Automation are composite experiments. A 1D Proton experiment is obtained first and the acquisition AU-program ‘au_getlcosy’ is used to optimize the sweep width. This example will guide you through the set up of creating a 2D gradient COSY experiment using a fixed predefined sweep width. This experiment can be run as a stand alone experiment or as a composite experiment together with a 1D Proton experiment to get the better resolution external projections.

6.4.1 Layout of the new experiment

- Experiment: **gradient COSY**, using a fixed SW from (**9** ppm - **0** ppm)
- Starting parameter file: **COSYGPSW**
- New parameter file: **COSYGP.fixsw**

6.4.2 Creating the COSY parameter set

1. Type **edc**
2. Change the following parameters:



3. Click on the **OK** button inside the New window.

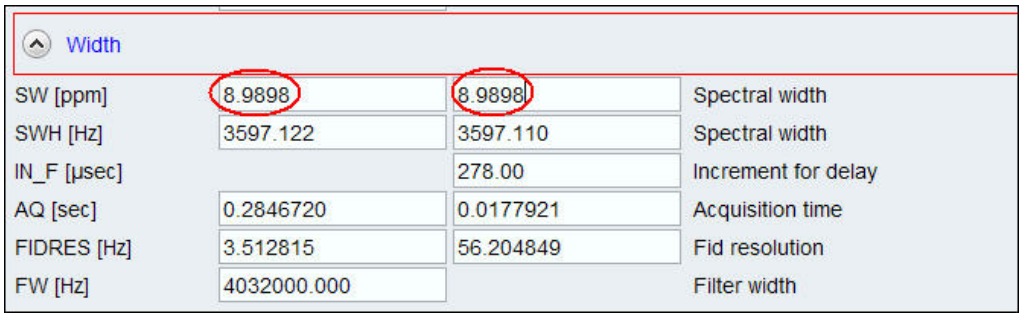
Some parameters have to be changed before the experiment is added to IconNMR. In addition to the parameter change below, any other parameters such as **ns**, **td**, **d1** etc. can be administered at this point.

---

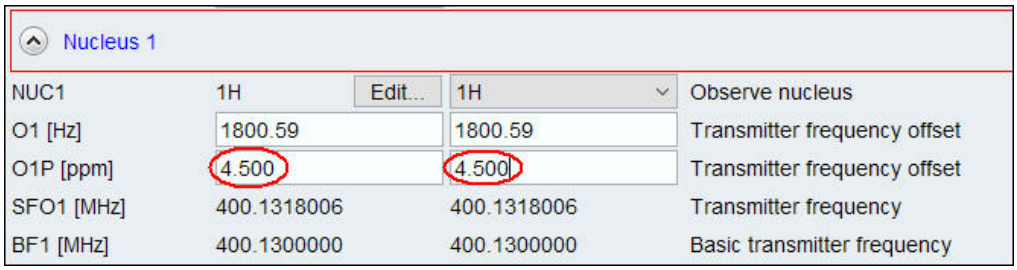
4. Select the **AcquPars** tab.
5. Display all parameters.
6. Change the following parameters:

   SW [F2] = **9**

   SW [F1] = same exact value as SW (F2)

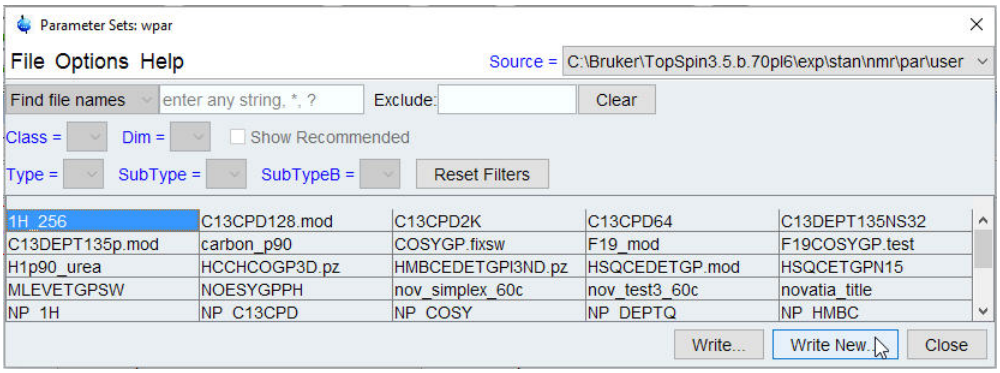


O1 [ppm] = **4.5**



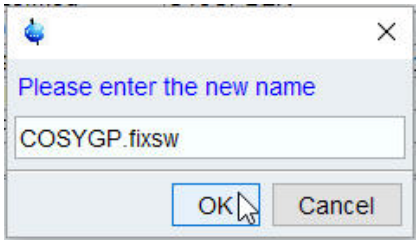
AUNM = **au_zgcosy**

7. Type **wpar**
8. Select the user parameter source directory.

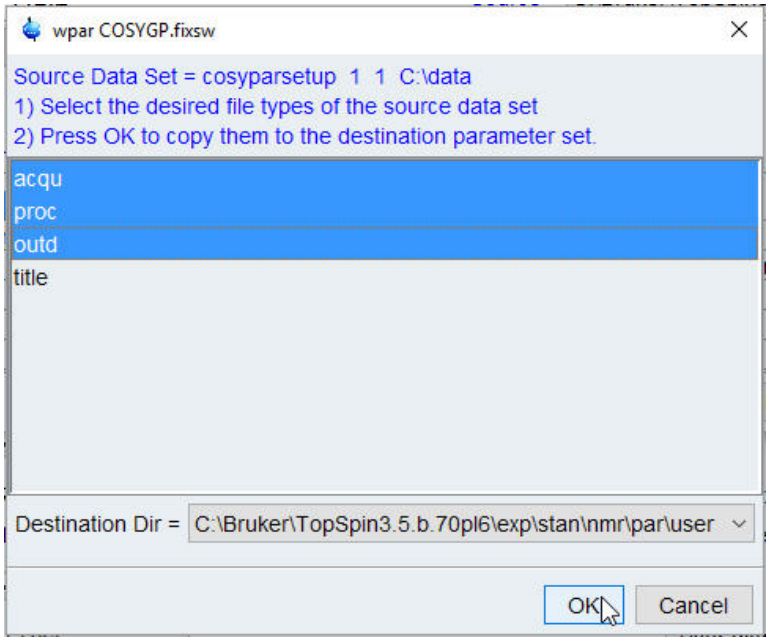


9. Click on the **Write New** button inside the Parameter Sets: wpar window.

10. Enter **PCOSYGP.fixsw**



10. Click on the **OK** button inside the new name window.
11. Select the **acqu**, **pro** and **outd** parameters.



12. Click on the **OK** button inside the wpar window.
13. Click on **Close** button inside the Parameter Sets: wpar window.

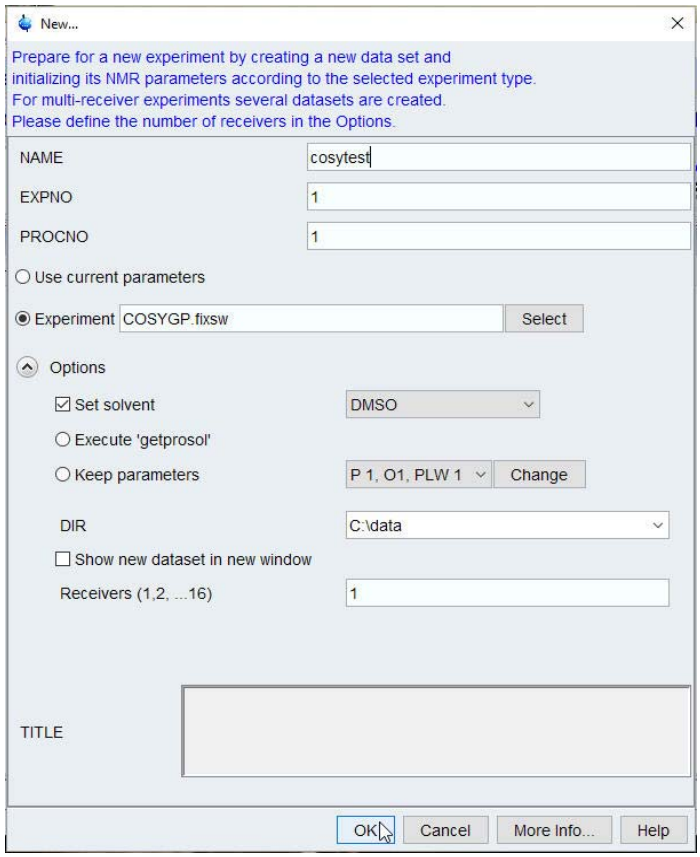
6.4.3 Testing the experiment

6.4.3.1 Sample

50 mM Gramicidin in DMSO-d6 or any other sample

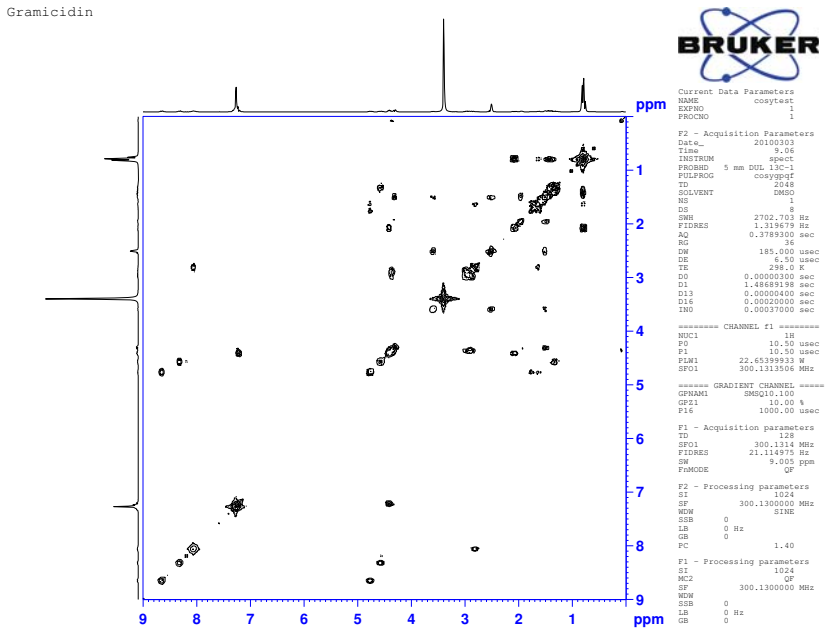
6.4.3.2 Running the experiment

1. Type **edc** and enter the following parameters:



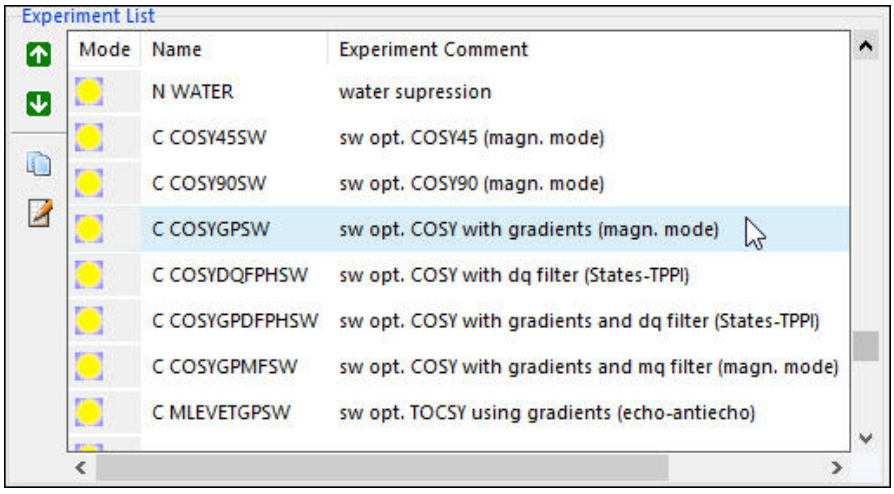
2. Click on the **OK** button inside the New window.
3. Type **lock** and select **DMSO.**
4. Tune the probe.
5. Turn off the spinner.
6. Shim for best homogeneity.
7. Type **getprosol**
8. Type **xaua**
9. Type **xaup**

xaua is executing the acquisition AU-program au_zgcosy as a AUNM entry in the Automation section of the AcquPars and xaup executes the processing AU-program proc_2dsym as a AUNMP entry in the Automation section of the ProcPars. The internal F1 and F2 projections are automatically added to the spectrum. If you want to make changes to the parameters, repeat steps 8 and 9 for testing, then store the parameter file COSYGP.fixsw with the wpar command.



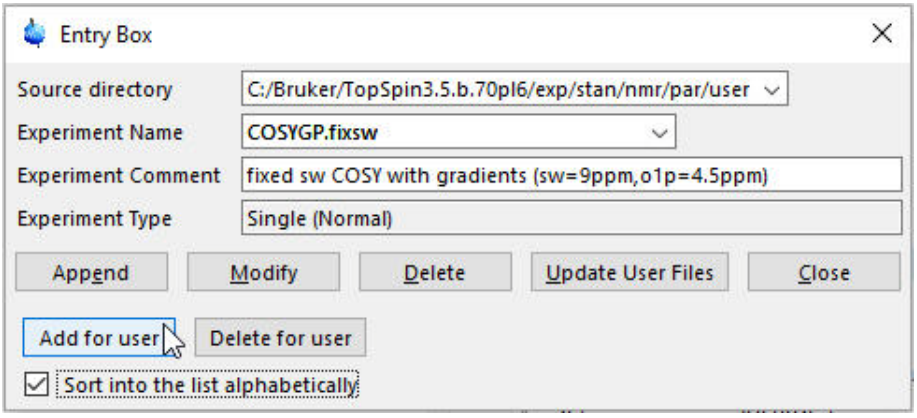
6.4.4 Adding the experiment COSYGP.fixsw to ICON-NMR

1. Start IconNMR **Configuration**.
2. Select **User Manager**.
3. Select a **user name**.
4. Click on any experiment listed inside the **Experiment list box**.

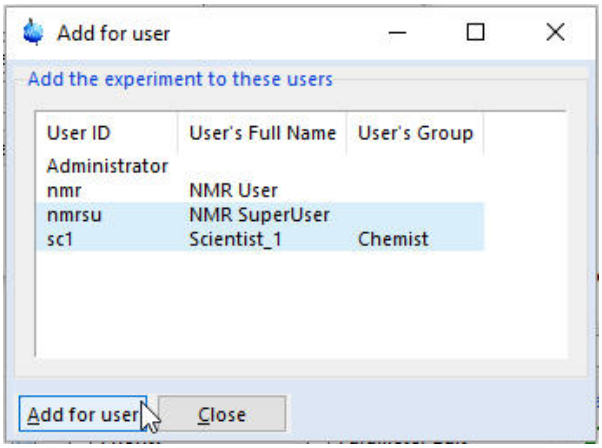


5. Click on the down arrow next to Source directory.
6. Select **<TopSpin-Home>/exp/stan/nmr/par/user**

7. Click on the down arrow next to Experiment Name.
8. Select **COSYGP.fixsw**.
9. Click on the Experiment Comment Text window and enter the following text:
   fixed sw COSY with gradients (sw=9 ppm, o1p=4.5 ppm)
10. Enable **Sort in to list alphabetically**.



11. Click on the **Add for user button** inside the Entry Box.



12. Select the users which will have this experiment added to the list.
13. Click on the **Add for user** inside the Add for user window.
14. Click on the **Close** button inside the Add for user window.
15. Click on **File** and select **Save**.
16. Click on **File** and select **Close**.

Test the new added experiment for proper operation using the IconNMR Automation.

6.5 NOTES:

6.6 1D Proton, 2D COSY and 2D HSQC Composite exp.

This example will guide you through the set up of creating a composite experiment consisting of a 1D Proton experiment followed by a 2D COSY and a 2D HSQC experiment. There are no changes made to the AU-programs, acqusition and processing parameters.

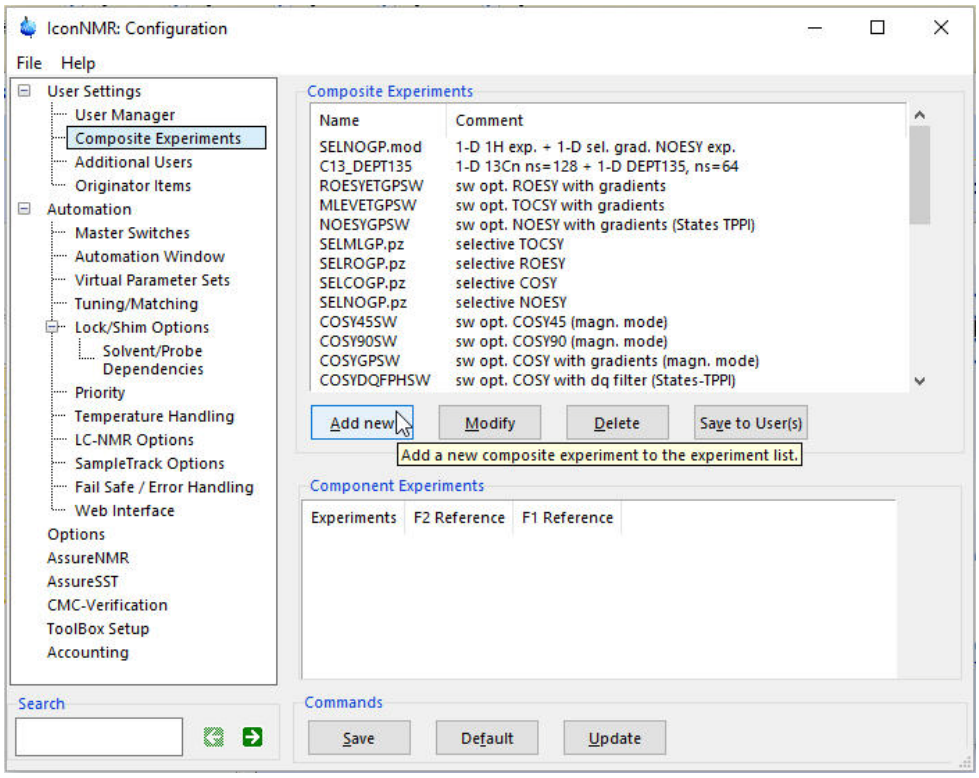
Before creating a new Composite experiment, make a layout of how the new experiment should work and how you would like to present the result. Check the parameter library first to see if the experiments of interest for the composite already exist. If any parameters have to be changed then store the parameter set using a different name or use an extension. The example below uses the default parameters stored in the Bruker parameter set library.

6.6.1 Layout of the new composite experiment

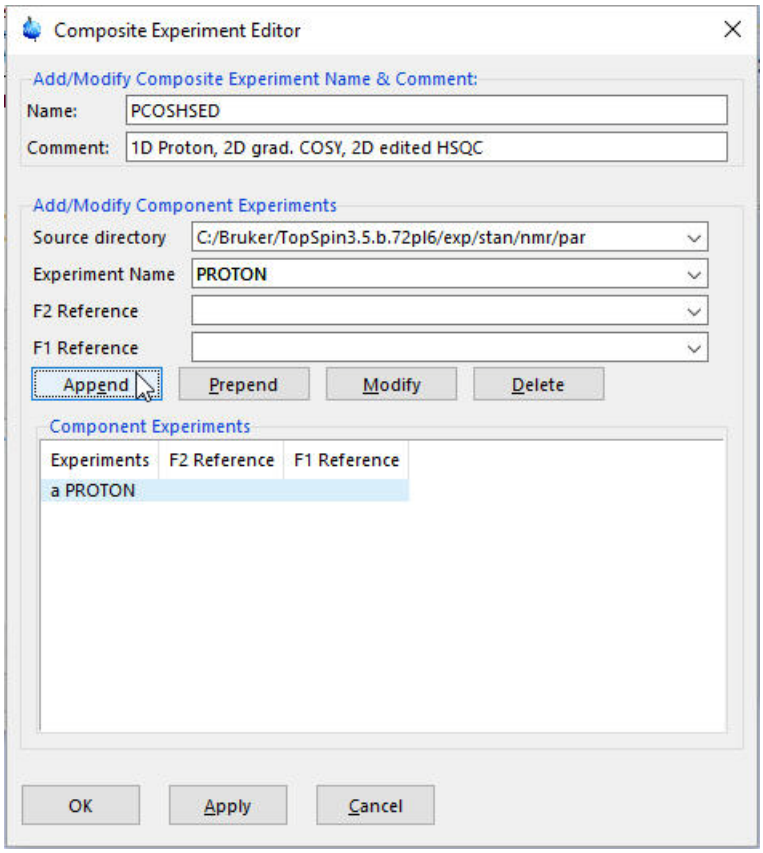
- Experiments:**1D-Proton** followed by a **2D COSY** and a **2D edited HSQC**
- Starting parameter files: **PROTON**, **COSYGPSW and HSQCEDETGP**
- Name of composite experiment: **PCOSHSED**

6.6.2 Creating the new composite experiment

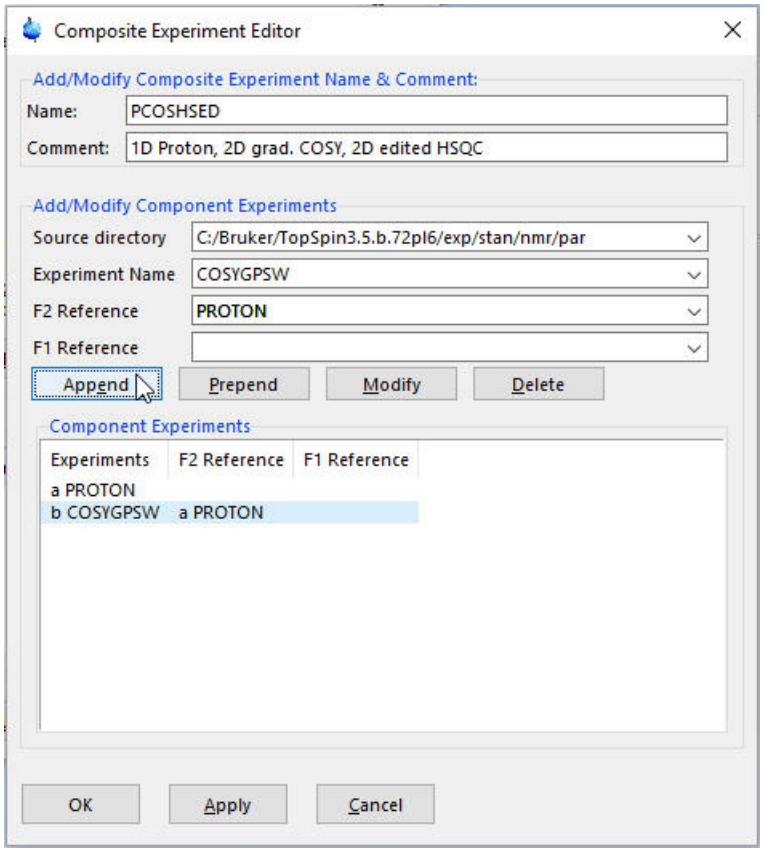
1. Start IconNMR **Configuration**.
2. Select **Composite Experiments**.



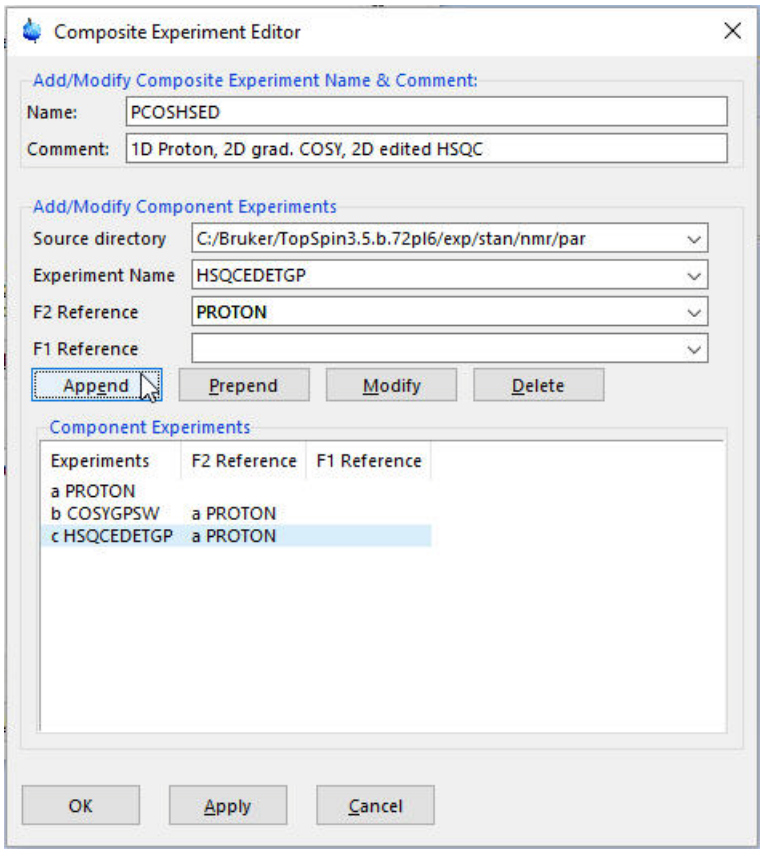
3. Click on the **Add new** button inside the Composite Experiment window.
4. Type **PCOSHSED** in to the Name field.
5. Type **1D Proton, 2D grad. COSY, 2D edited HSQC** in to the Comment field.
6. Click on the **down arrow** next to Source directory.
7. Select **<TopSpin-Home>/exp/stan/nmr/par** directory.
8. Click on the **down arrow** next to the Experiment Name window.
9. Select **PROTON** from the pop up window.
10. Click on the **Append** button inside the Composite Experiment Editor window.



11. Click on the **down arrow** next to the Experiment Name window.
12. Select **COSYGPSW** from the pop up window.
13. Click on the arrow next to the **F2 Reference** window.
14. Select **PROTON**.
15. Click on the **Append** button inside the Composite Experiment Editor window.



16. Click on the **down arrow** next to the Experiment Name window.
17. Select **HSQCEDETGP** from the pop up window.
18. Click on the **down arrow** next to the F2 Reference window.
19. Select **PROTON**.
20. Click on the **Append** button inside the Composite Experiment Editor window.

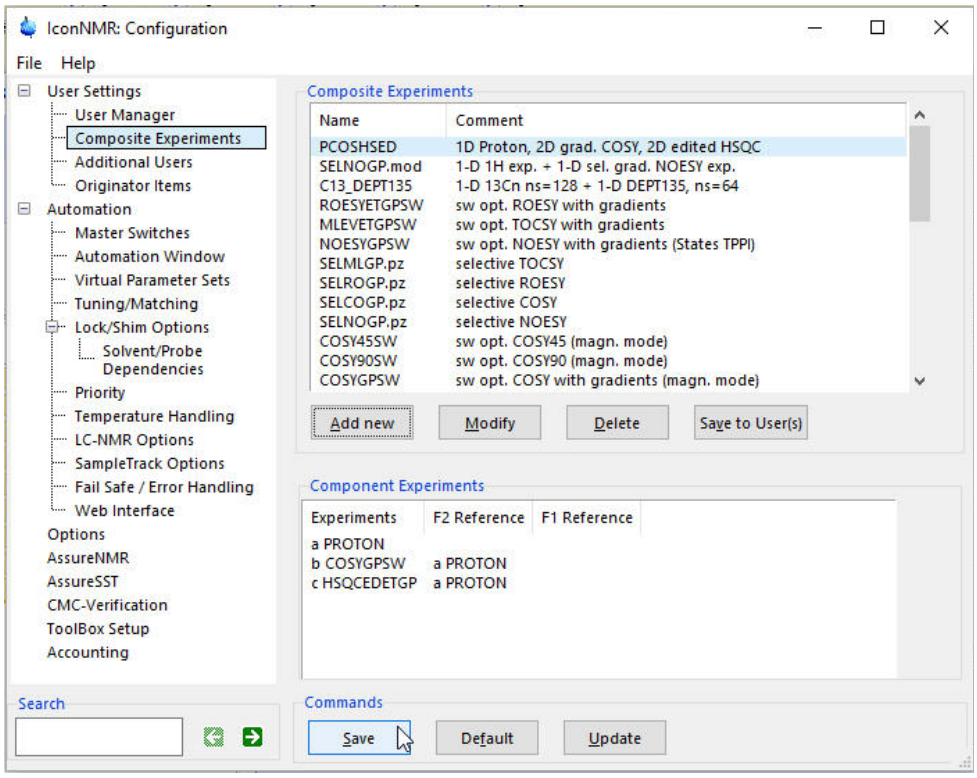


21. Click on the OK button inside the Composite Experiment Editor window.

The new composite experiment has now been added to the Composite Experiment List in the Composite Experiment Manager. To add this experiment to the user experiment list, stay in the ‘Composite Experiments’ window and follow the next steps.

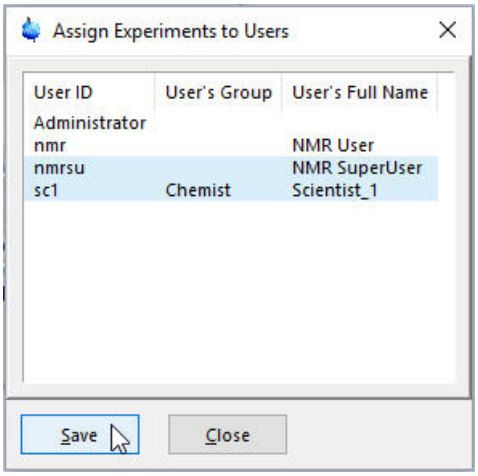
6.6.3 Adding the new composite experiment to the user experiment list

1. Click on the new experiment **PCOSHSED**.



2. Click on the **Save** button inside the Composite Experiment window.
3. Click on the **Save to User(s)** button inside the Composite Experiment window.

To select multiple users, hold down the Shift or Control key when selecting them.



4. Click on the **Save** button inside the Assign Experiments to Users window.
5. Click on the **Close** button inside the Assign Experiments to Users window.

6.Click on **File** and select **Save**.

7. Click on **File** and select **Close**.

If the probe is equipped with ATM, you may want to turn off the automatic tuning for 1H of the COSYGPSW and 13C for the HSQCEDETGP experiment. (Tuning/Matching option in ICONNMR configuration) The 1H tuning is performed on the first experiment which is PROTON and the 13C tuning is executed on HSQCEDETGP experiment.

6.7 NOTES:

6.8 1D Carbon and 1D DEPT135 Composite exp.

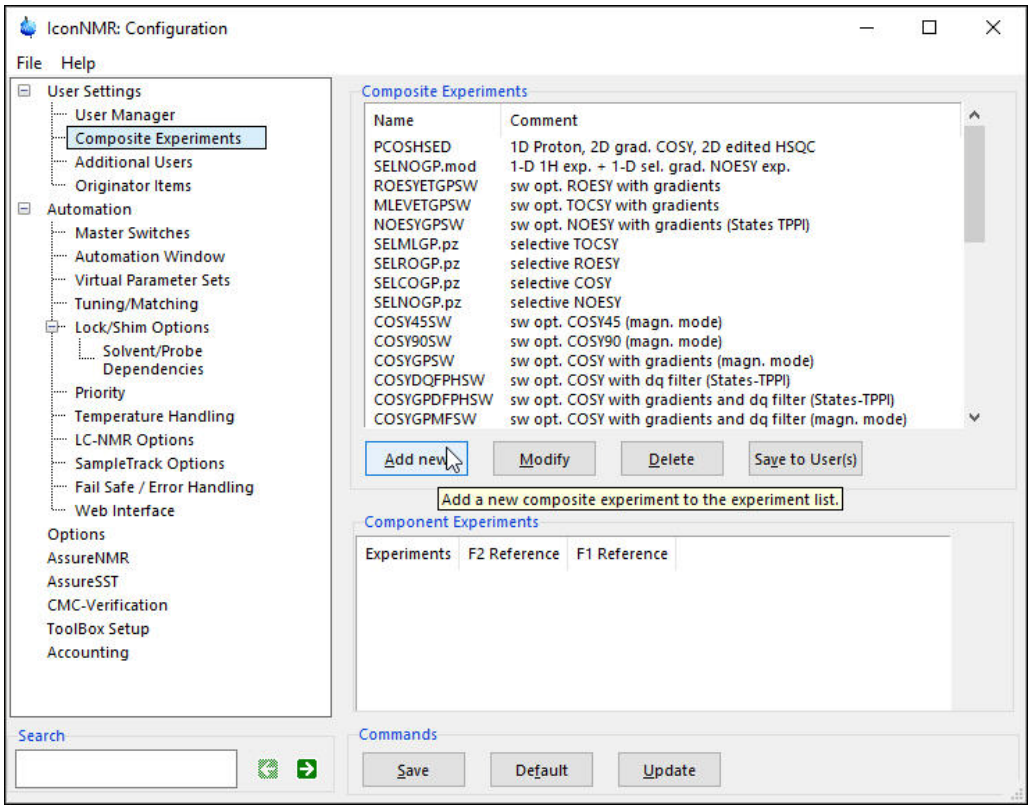
This example will guide you through the set up of creating a composite experiment consisting of a 1D C13CPD experiment followed by a 1D DEPT135 experiment. The parameters rg, sw, o1 and the phase values are transferred from the completed C13CPD experiment in to the C13DEPT135 experiment. The example below uses the default parameters stored in the Bruker parameter set library. The number of scans are then changed in creating the virtual parameter set.

6.8.1 Layout of the new composite experiment

- Experiments:**1D Carbon** followed by a **1D Carbon DEPT-135**
- Starting parameter files: **C13CPD** and **C13DEPT135p**
- Name of the composite experiment: **C13CPD_DEPT135**

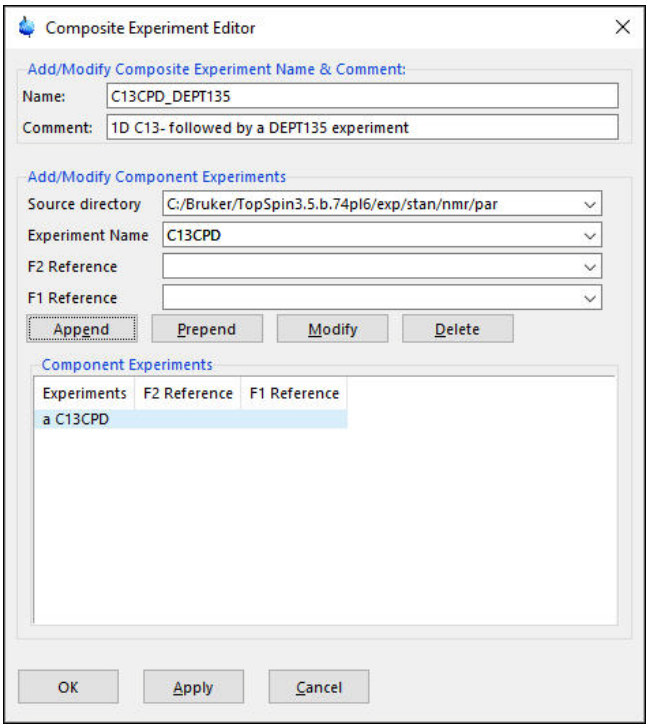
6.8.2 Creating the composite experiment in IconNMR

1. Start IconNMR **Configuration**
2. Select **Composite Experiments**

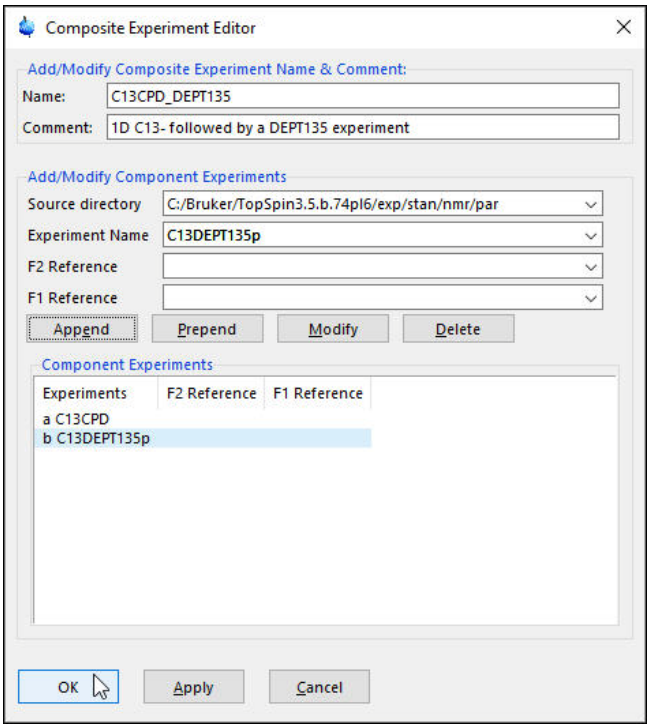


3. Click on the **Add new** button inside the Composite Experiment window.
4. Type **C13CPD_DEPT135** in to the Name field.

5. Type **1D C13- followed by a DEPT135 experiment** in to the Comment field.
6. Click on the **down arrow** next to Source directory.
7. Select **<TopSpin-Home>/exp/stan/nmr/par** directory.
8. Click on the **down arrow** next to the Experiment Name window.
9. Select **C13CPD** from the pop up window.
10. Click on the **Append** button inside the Composite Experiment Editor window.



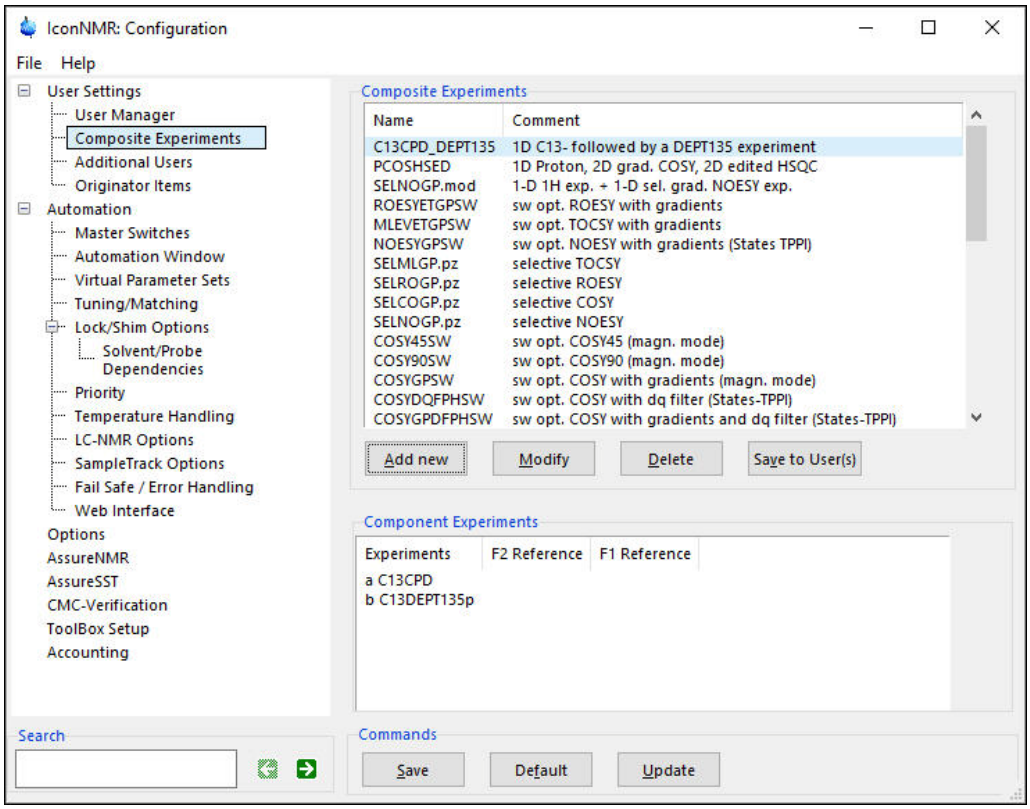
11. Click on the **down arrow** next to the Experiment Name window.
12. Select **C13DEPT135p** from the pop up window.
13. Click on the **Append** button inside the Composite Experiment Editor window.



14. Click on the OK button inside the Composite Experiment Editor window.

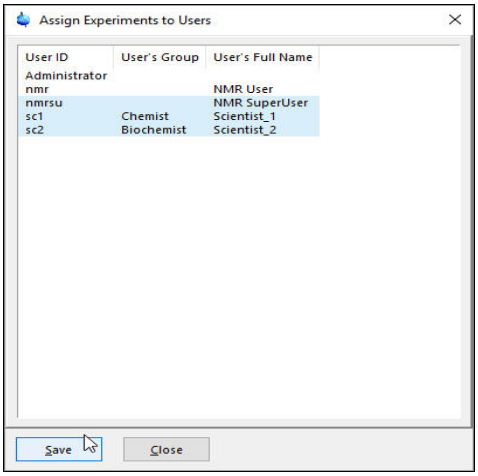
6.8.3 Adding the new composite experiment to the user experiment list

1. Click on the new experiment **C13CPD_DEPT135**.



2. Click on the **Save** button inside the Composite Experiment window.
3. Click on the **Save to User(s)** button inside the Composite Experiment window.

To select multiple users, hold down the Shift or Control key when selecting them.



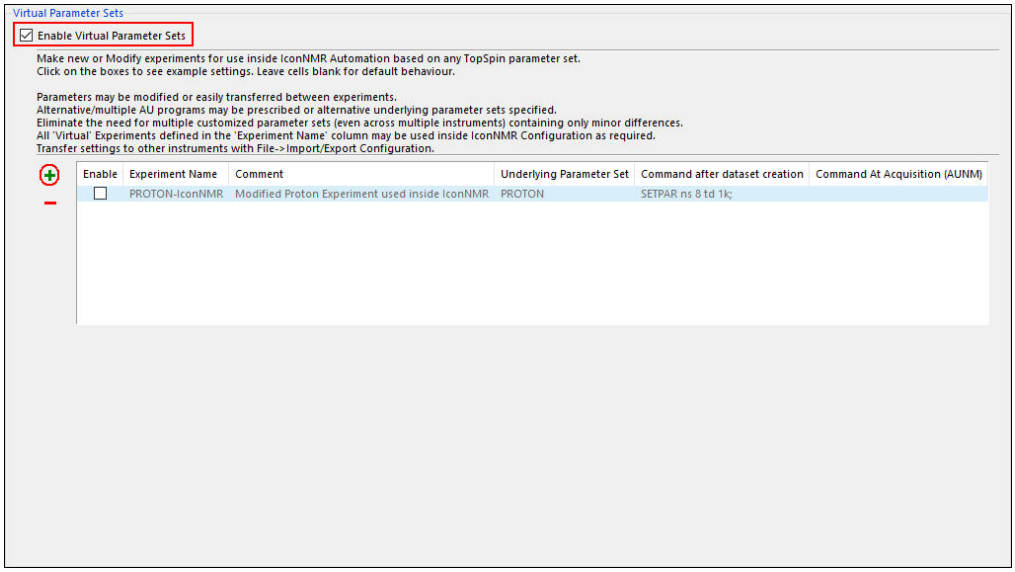
4. Click on the **Save** button inside the Assign Experiments to Users window.

5. Click on the **Close** button inside the Assign Experiments to Users window.

If the probe is equipped with ATM, you may want to turn off the automatic tuning for the C13DEPT135p.mod experiment. (Tuning/Matching option in IconNMR configuration). The tuning is performed on the first experiment which is C13CPD and does not have to be executed on the second experiment.

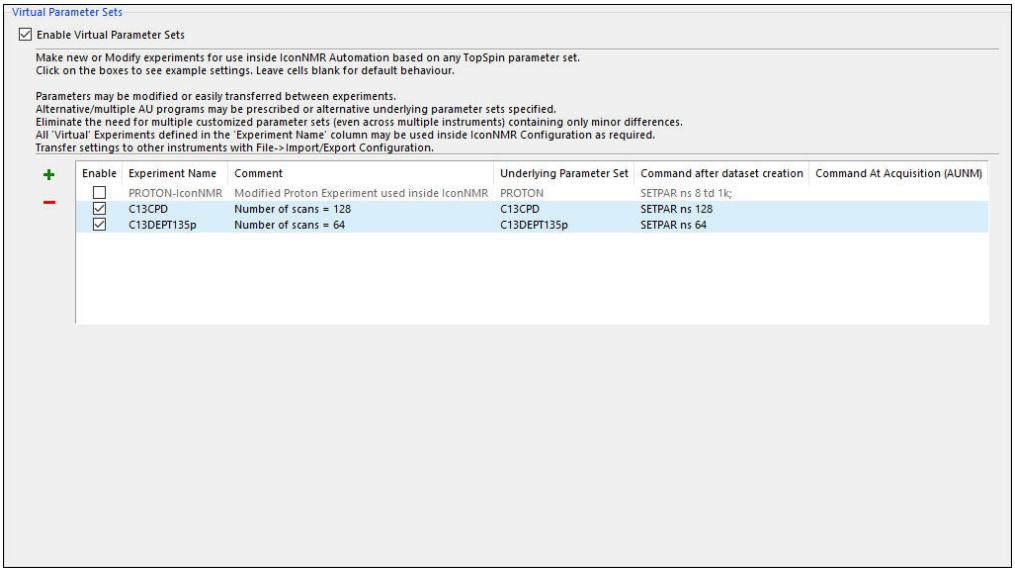
6.8.4 Setup the Virtual Parameter Set

1. Select **Virtual Parameter Sets**.
2. Enable **Virtual Parameter Sets**.



3. Click on the green "**+**" sign.
4. Click on the **down arrow** for the **Experiment Name**.
5. Select **C13CPD** from the pull down window.
6. Type e.g. **Number of scans = 128** in to the **Comment** section.
7. Click on the **down arrow** for the **Underlying Parameter Set**.
8. Select **C13CPD** from the pull down window.
9. Type e.g. **SETPAR ns 128** in to the **Command after dataset creation** section.
10. Leave the **Command At Acquisition (AUNM)** blank.
11. Click on the green "**+**" sign.
12. Click on the **down arrow** for the **Experiment Name**.
13. Select **C13DEPT135p** from the pull down window.
14. Type e.g. **Number of scans = 64** in to the **Comment** section.

15. Click on the **down arrow** for the **Underlying Parameter Set**.
16. Select **C13DEPT135p** from the pull down window.
17. Type e.g. **SETPAR ns 64** in to the **Command after dataset creation** section.
18. Leave the **Command At Acquisition (AUNM)** blank.



19.Click on **File** and select **Save**.

20. Click on **File** and select **Close**.

6.8.5 Testing the C13_DEPT135 experiment in IconNMR

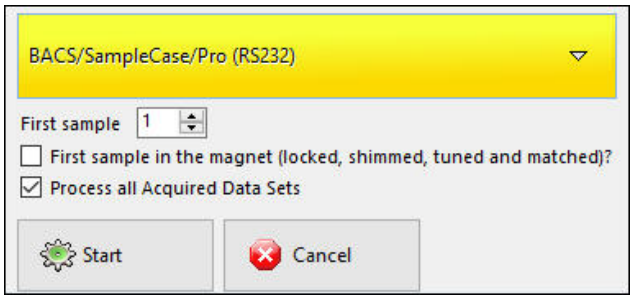
6.8.5.1 Sample:

100 mg Cholesterylacetate in CDCl3

6.8.5.2 Running the experiment

1. Log in to IconNMR Automation.

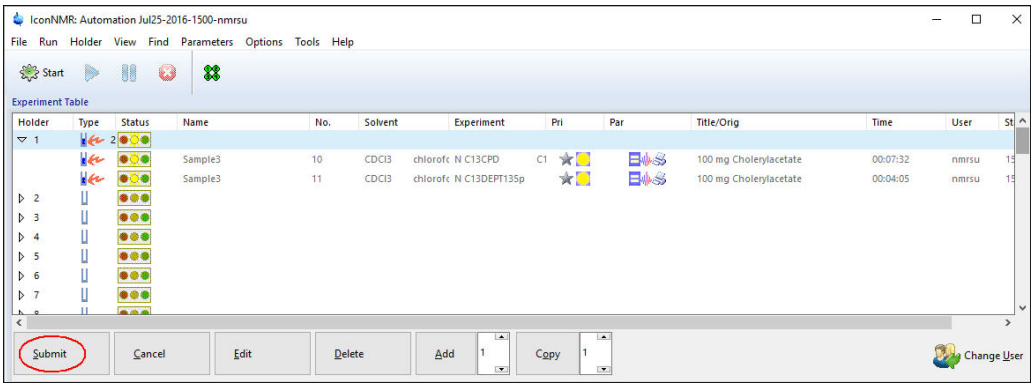
2 Click on the **Start** button to initialize the run.



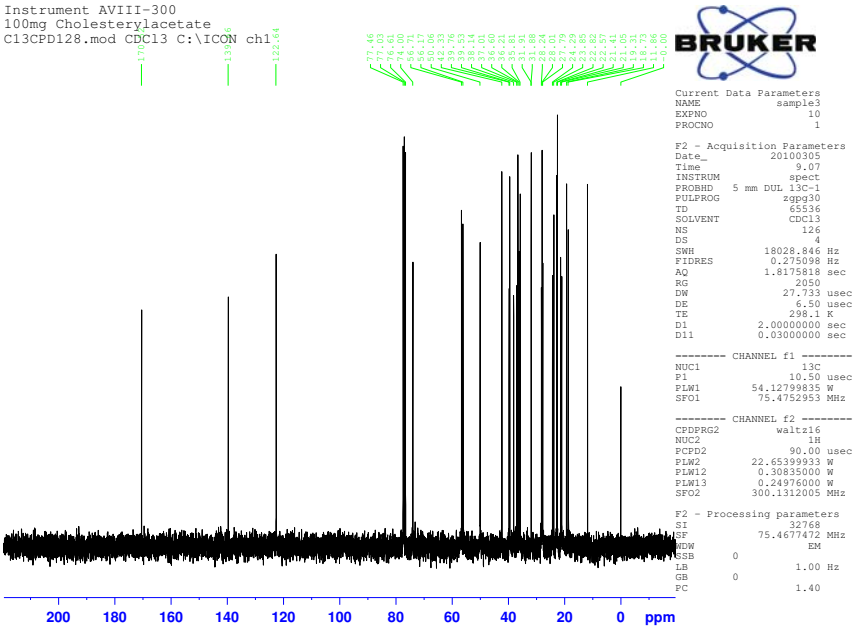
3. Select the appropriate Automation Mode.
4. Click on the **Start** button.
5. Double click on **Holder 1**
6. Click inside the Name window and choose a name e.g. **Sample3**
7. Click on the arrow next to the Solvent window and select the solvent (e.g. **CDCl3**).
8. Click on the arrow next to the Experiment window and select **C13CPD_DEPT135**.

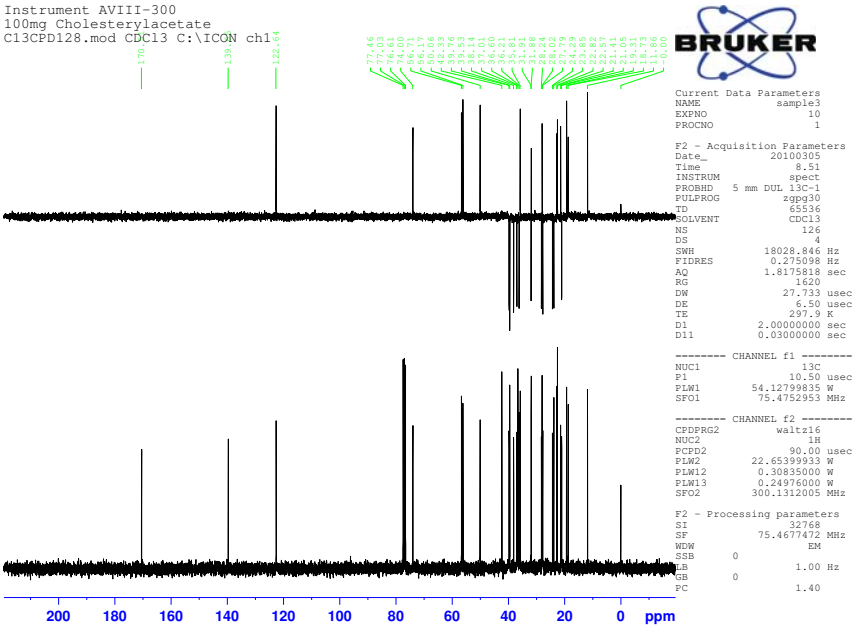
The two experiments C13CPD and C13DEPT135p appear in the experiment windows.

9. Click on the Title icon button and change the title e.g. **100 mg Cholesterylacetate**
10. Click on the **Set & Copy Title** button.
11. Click on the first line of **Holder 1**
12. Click on the **Submit** button.



This experiment produces two plots, a 13C spectrum only and a second plot with both the DEPT and 13C spectra.


Instrument AVIII-300
100mg Cholesterylacetate
C13CPD128.mod CDCl3 C:\ICON ch1
BRUKER
Current Data Parameters
NAME sample3
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100305
Time 9.07
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 126
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 2050
DW 27.733 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 10.50 usec
PLW1 54.12799835 W
SFO1 75.4752953 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 22.65399933 W
PLW12 0.30835000 W
PLW13 0.24976000 W
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677472 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm


Instrument AVIII-300
100mg Cholesterylacetate
C13CPD128.mod CDCl3 C:\ICON ch1
BRUKER
Current Data Parameters
NAME sample3
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100305
Time 8.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 126
DS 4
SWH 18028.846 Hz
FIDRES 0.275098 Hz
AQ 1.8175818 sec
RG 1620
DW 27.733 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 10.50 usec
PLW1 54.12799835 W
SFO1 75.4752953 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 22.65399933 W
PLW12 0.30835000 W
PLW13 0.24976000 W
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677472 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

6.9 NOTES:

Adding new experiments

7 Examples of user specific settings

7.1 How to set Day and Night Time limits for users

7.1.1 Introduction

This option is limiting the instrument time for a user. The day and night time limit can be set separately and the time entered are granted to each user per calendar day. In addition the maximum duration of a daytime experiment can also be set.

7.1.2 Configuring IconNMR

1. Open the **IconNMR configuration** window or type in the TopSpin command line **iconc**.

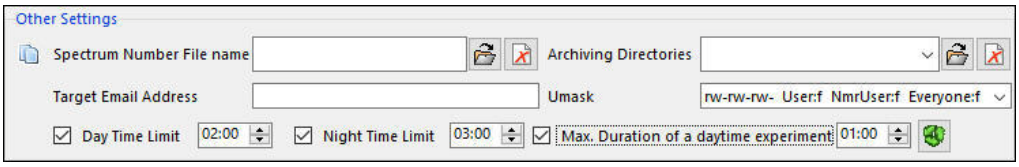
2. Under **User Settings**, select **User Manage**.

3. Under **Other Settings Option** enable the following options:

   Day Time Limit = **2 hour**

   Night Time Limit = **3 hours**

   Max. Duration of a daytime experiment = **1 hour**



4. Click on **File** and select **Save** or click on the **Save** button on the bottom of the User Manager window.

5. Select the **Priority** window.

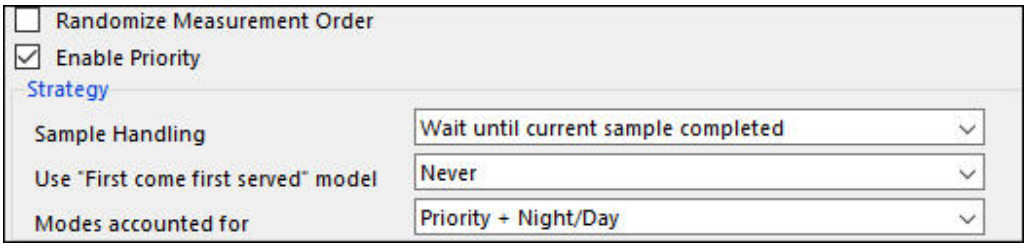
6. Enable **Priority**.

7. Under **Strategy** select the following options:

   Priority Sample Handling: **Wait until current sample completed**

   Use “First come first served” model: **Never**

   Modes accounted for: **Priority + Night/Day**



8. Under **Night/Day Mode** set the following options:

   Night begins at = e.g. **19:00**

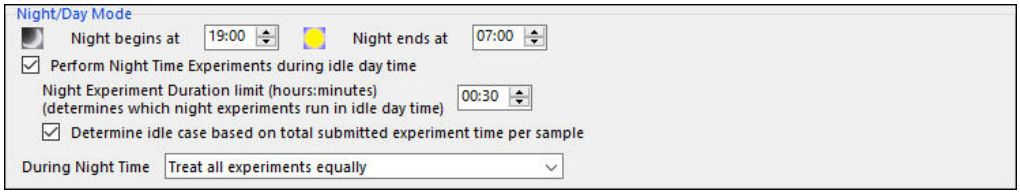
   Day begins at = e.g. **07:00**

   Enable **Perform Night Time Experiments during idle daytime**

   Night Experiment Duration = e.g. **00:30**

   Enable **Determine idle case based on total submitted experiment time for sample**

   During Night Time select: **Treat all experiments equally**



9. Under **Weekend (Treat the following days as night-time)** set the following options:

   Enable **Sun** (Sunday)

   Enable **Sat** (Saturday)

10. Click on **File** and select **Save**.

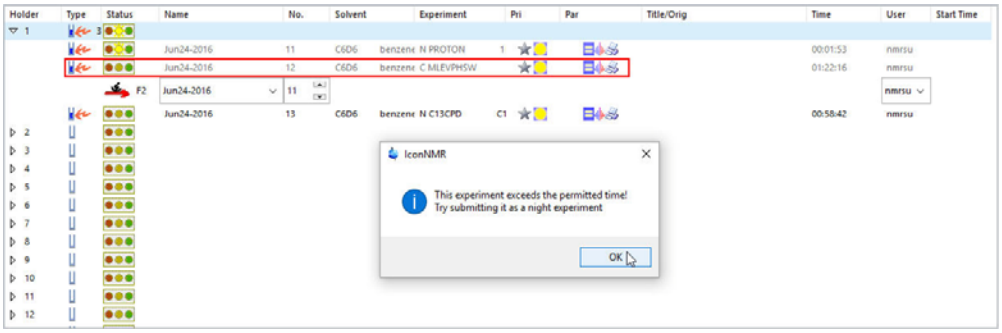
11. Click on **File** and select **Close**.

7.1.2.1 Starting the Automation

It is a good laboratory practice that the Automation is started by the NMR Administrator such as nmrsu or a neutral user which password is not known by other users. This assures that the Automation run can't be stopped or started by other users.

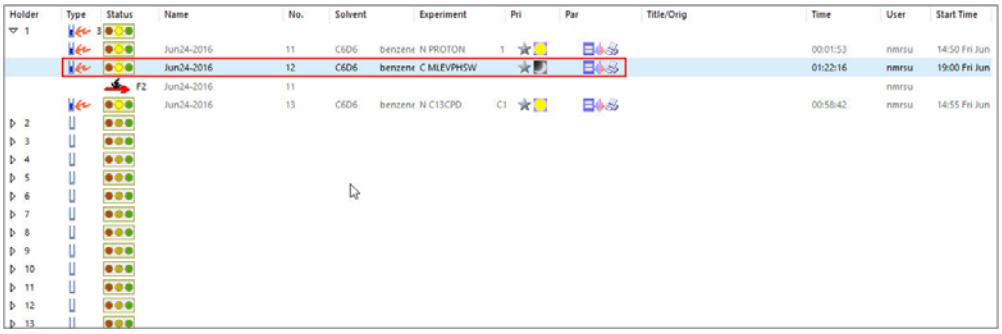
1. To start the Automation, follow the instructions in **5.4.3 Standard BACS, Sample Case, Pro (232)** steps **1** through **6**.

2. Double click on the Holder #1 and fill in all the required fields.

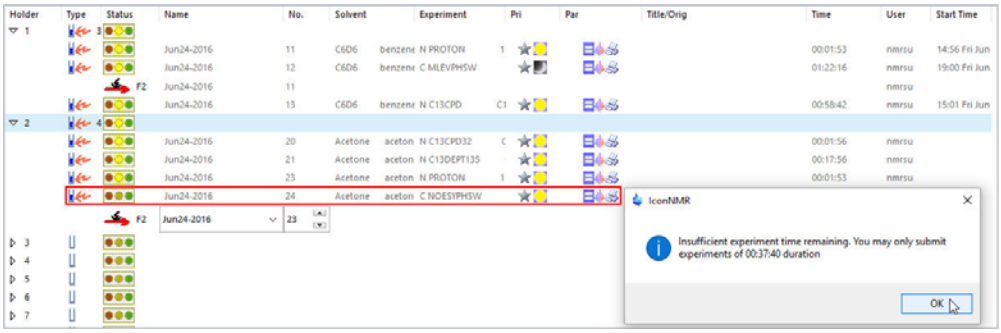


In this example the experiments are as follows: Proton, MLEVPHSW and C13CPD. The default time for the MLEVPHSW experiment is 1 hour and 22 minutes. Time wise this exceeds the maximum duration time of more than 1 hour and therefore this experiment has to be submitted as a night time experiment.

3. Click on the **OK** button inside the IconNMR pup up window.
4. Click on the **MLEVPHSW** experiment line.
5. Click on the **Edit** button.
6. Change the **MLEVPHSW** experiment to a night time experiment.
7. Click on the **Submit** button.

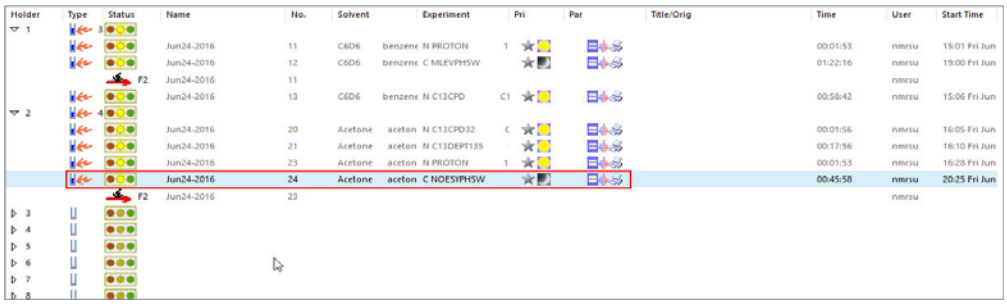


8. Double click on the Holder #2 and fill in all the required fields.



In this example the experiments are as follows: C13CPD32 C13DEPT135, PROTON and NOESYPHSW. The NOESYPHSW experiment exceeds the Day Time limit of 1 hour. This requires that this experiment has to be run at night time. Another experiment could be set up for daytime operation, but the experiment time has to be 39 Minutes or less.

9. Click on the **OK** button inside the IconNMR pup up window.
10. Click on the **NOESYPHSW** experiment line.
11. Click on the **Edit** button.
12. Change the **NOESYPHSW** experiment to a night time experiment.
13. Click on the **Submit** button.



This user has still night experiment time left of 39 Minutes.

14. Log out.

7.2 How to assign User Specific Originator Information

7.2.1 Introduction

This section will guide you through the set up how to assign different user specific Originator items and its informations for multiple users. For practical reasons for the example below, only two users, Scientist_1 and Scientist_2 are used. Four Originator items are chosen: **Instrument**, **Mail Data/Notify to**, **Research project** and **Department**.

7.2.2 Configuring the Originator Items

1. Open the **IconNMR configuration** window or type in the TopSpin command line **iconc**.

2. Under **User Settings**, select **Originator Items**.

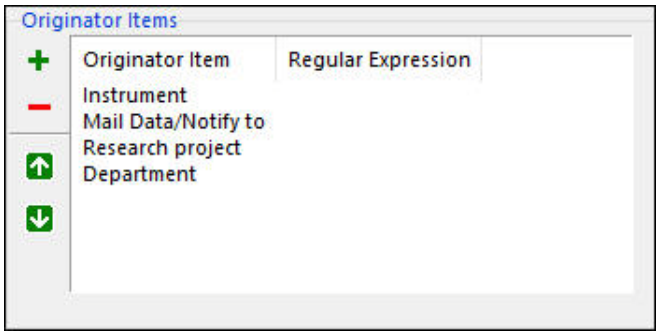
3. Select or create the following Originator Items:

   Instrument

   Mail Data/Notify to

   Research project

   Department

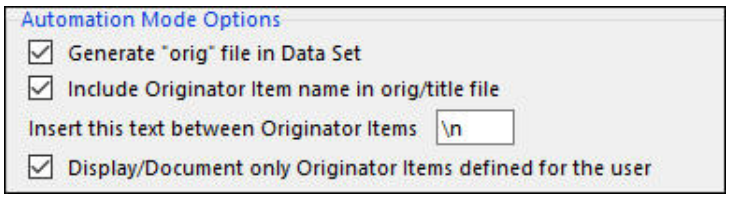


4. Under **Automation Mode Options** enable the following options:

   Generate "orig" file in Data set

   Include Originator Item name in orig/title file

   Display/Document only Originator Items defined for user



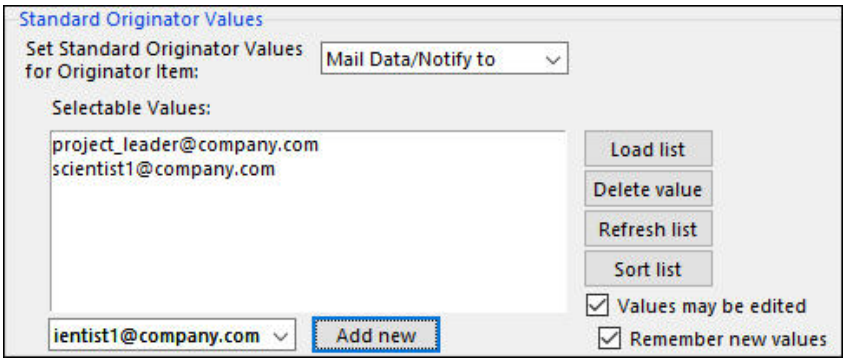
5. Under **Standard Originator Values** click on the down arrow of the **Set Standard Originator Values for Originator Items** window and select: **Mail/Notify to**.

6. For the **Selectable Values** enter a list of e-mail addresses:

7. Disable the following options:

   Values may be edited

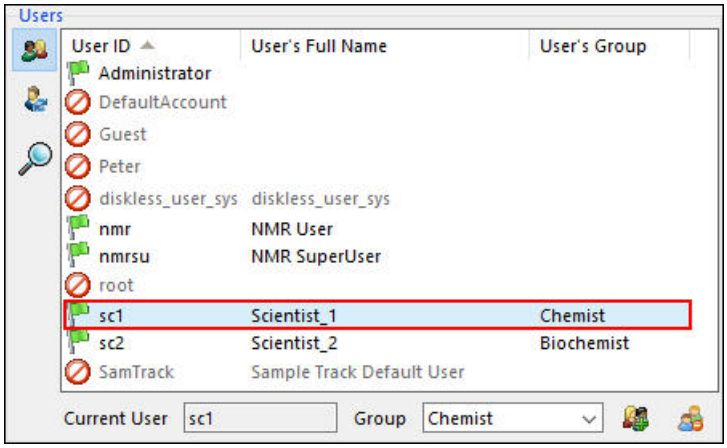
   Remember new values



8. Click on **File** and select **Save**.

9. Select the **User manager** window.

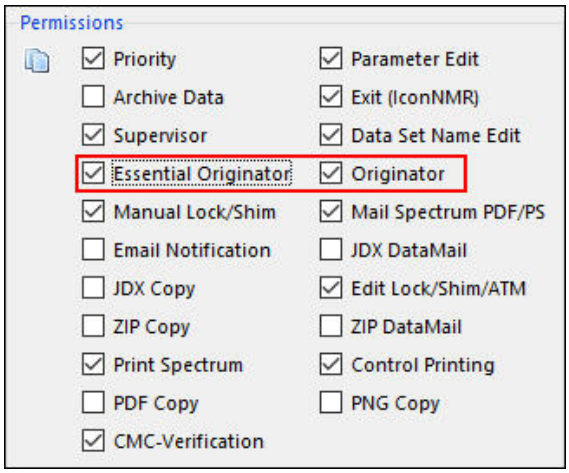
10. Select user **Scientist_1** inside the Users window.



11. Under **Permissions** enable the following options:

   Essential Originator

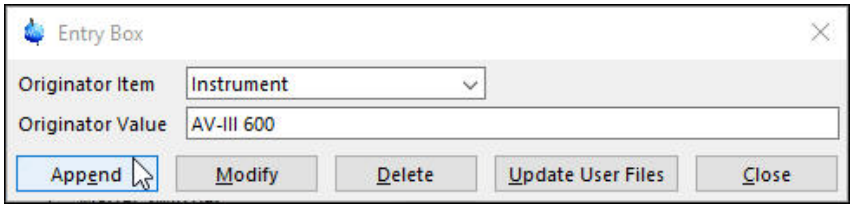
   Originator



12. Click inside the **User Specific Originator Info** window.
13. Select the following **Originator Item** inside the Entry box:

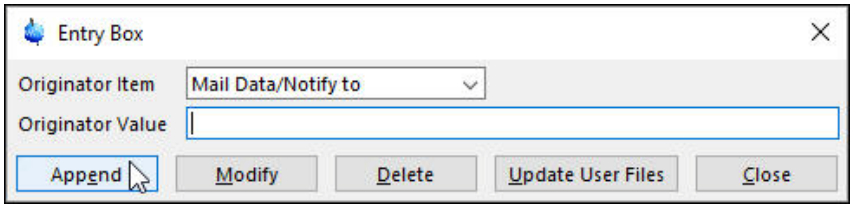
    Instrument name
14. Enter the following **Originator Value**:

    AV-III 600

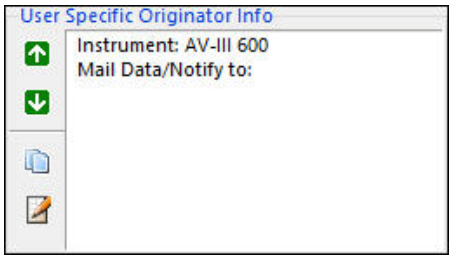


15. Click on the **Append** button inside the Entry Box.
16. Select the following **Originator Item** inside the Entry box:

    Mail/Data Notify to
17. Keep the **Originator Value** empty.

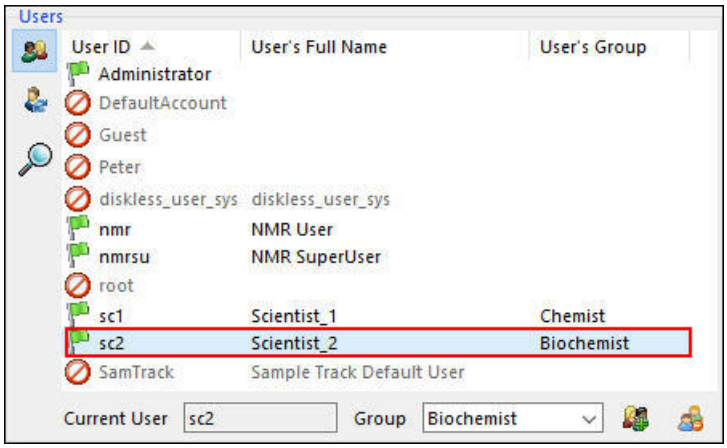


18. Click on the **Append** button inside the Entry Box.
19. Click on the **Close** button inside the Entry Box.



20. Click on **File** and select **Save** or click on the **Save** button on the bottom of the User Manager window.

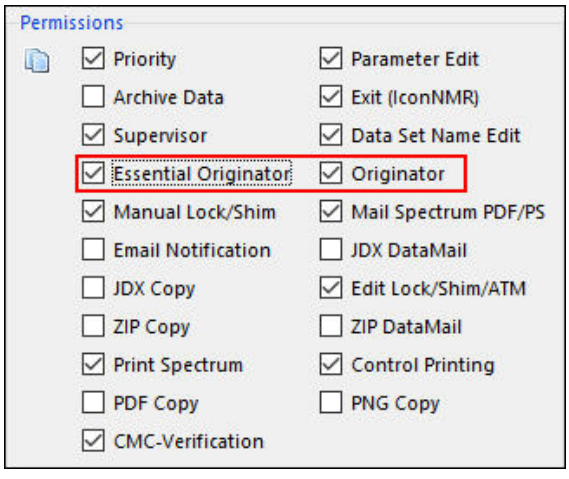
21. Select user **Scientist_2**.



22. Under **Permissions** enable the following options:

Essential Originator

Originator



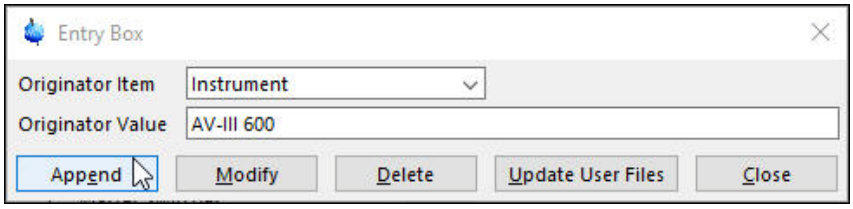
23. Click inside the **User Specific Originator Info** window.

24. Select the following **Originator Item** inside the Entry box:

Instrument name

25. Enter the following **Originator Value**:

    AV-II 600

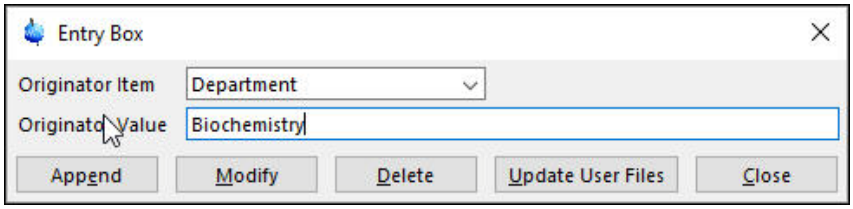


26. Click on the **Append** button inside the Entry Box.
27. Select the following **Originator Item** inside the Entry box:

    Department

28. Enter the following **Originator Value**:

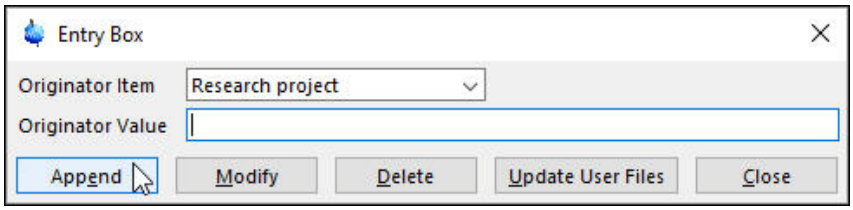
    Biochemistry



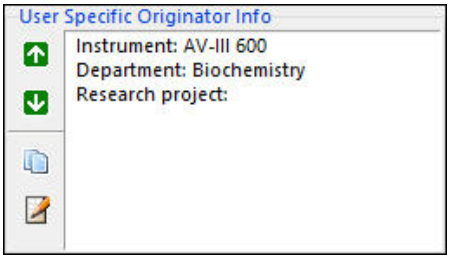
29. Click on the **Append** button inside the Entry Box.
30. Select the following **Originator Item** inside the Entry box:

    Research project

31. Keep the **Originator Value** empty.



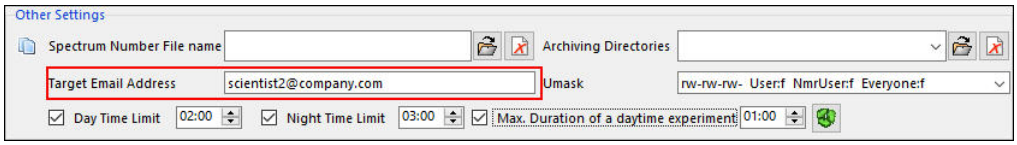
32. Click on the **Append** button inside the Entry Box.
33. Click on the **Close** button inside the Entry Box.



34. Under **Other Settings**' in the **Target E-mail Address** window enter the user's E-mail

address:

scientist2@company.com



35. Click on **File** and select **Save** or click on the **Save** button on the bottom of the User Manager window.

36. Click on **File** and select **Close**.

Depending on the need of the users, there are four E-mail Permissions to choose from (see **3.4.7 Permissions** in this Chapter). One, two, tree or all four Permissions can be enabled: **E-mail Notification**, **Mail Spectrum PDF/PS**, **JDX Data Mail** and **ZIP Data Mail**.

7.2.3 Starting the Automation

It is a good laboratory practice that the Automation is started by the NMR Administrator such as nmrsu or a neutral user which password is not known by other users. This assures that the Automation run can't be stopped or started by other users.

1. To start the Automation, follow the instructions in **5.4.3 Standard BACS, Sample Case, Pro (232)** steps **1** through **6**.

2. Click on the **Change User** button to log out temporarily.

3. Log in as **Scientist_1**.

4. Double click on the Holder #1 and enter all required fields.

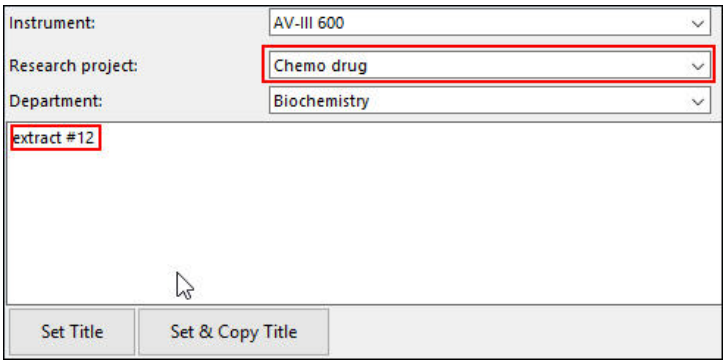
5. Click on the **Title** button to open up the title window.

6. Type a Title name: e.g. **Sample from Lot #653**.

7. Click on the down arrow of the **Mail/Notify to** window.

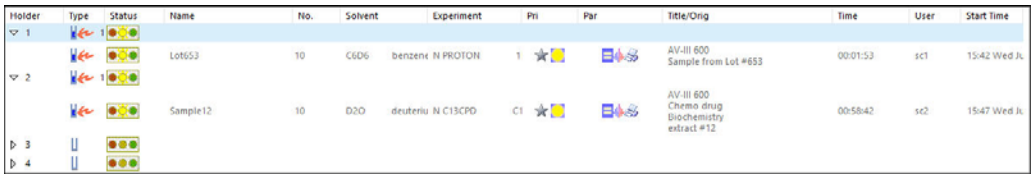
8.Select **scientist1@company.com** for the E-Mail address.

9. Click on the **Set & Copy Title** button to store the contents of the title window to other experiments.
10. Click on the **Submit** button to submit the experiment to the queue.
11. Click on the **Change User** button to log out temporarily.
12. Log in as **Scientist_2**.
13. Double click on the Holder #2 and enter all required fields.
14. Click on the **Title** button to open up the title window.
15. Type a Title name: e.g. **extract #12**.
16. Type the name of the **Research project** e.g. **Chemo drug**.



The user **Scientist_2** is required to enter the name of the **Research project** otherwise he will not be able to submit the experiment.

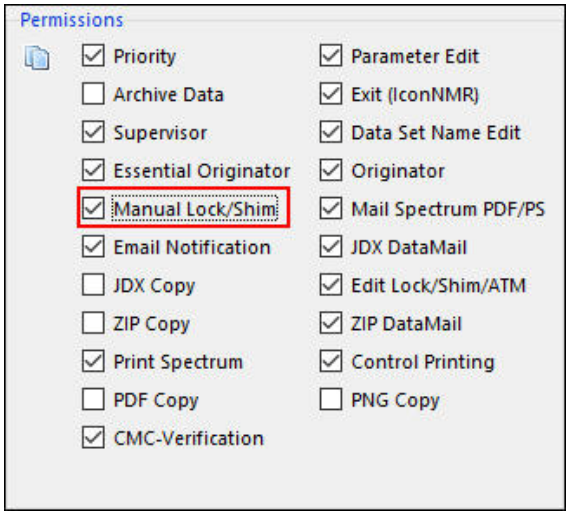
17. Click on the **Set & Copy Title** button to store the contents of the title window to other experiments.
18. Click on the **Submit** button to submit the experiment to the queue.



19. Click on the **Change User** button to log out temporarily.

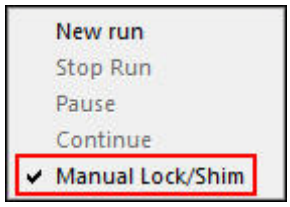
7.3 How to use the Manual Lock/Shim/ATMM options

1. Enable the Manual Lock/shim permission in the IconNMR Configuration, User Manager window.



7.3.1 Starting the Automation

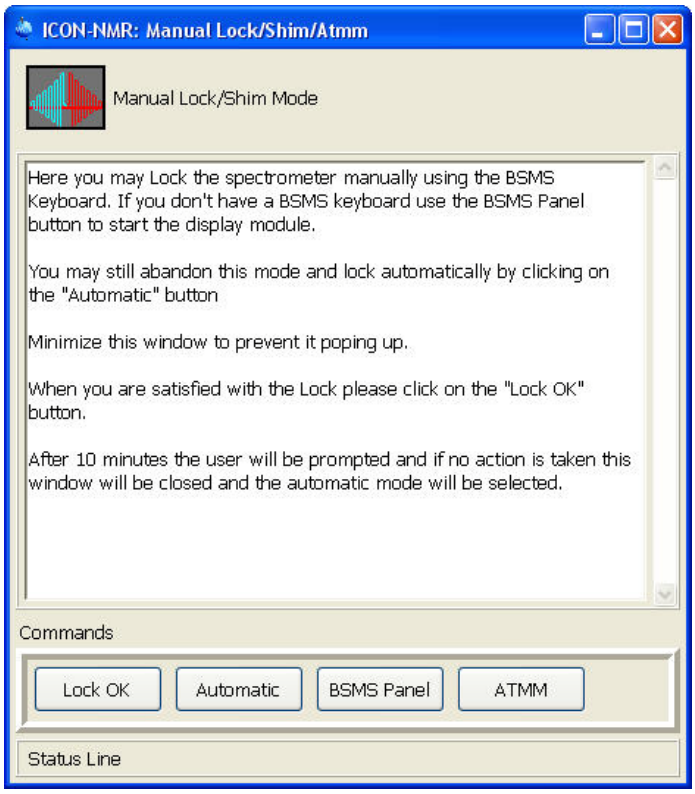
1. Type **icona** in the TopSpin command line to open the **IconNMR Automation** window.
2. Click on **Run** in the main menu of the Automation window.



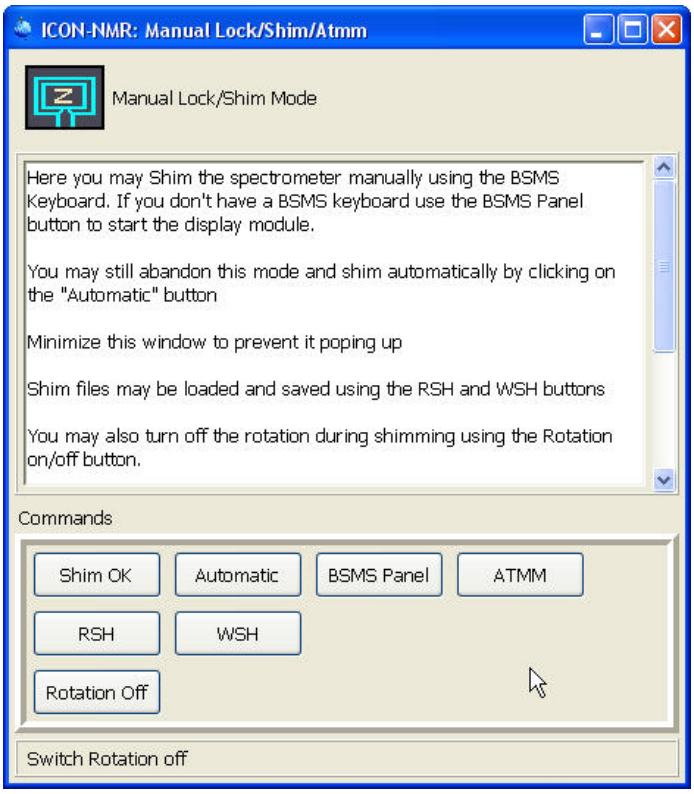
The Manual Lock/Shim option is check marked. The user then can choose between manual or automatic locking shimming and probe tuning.

3. Setup and submit a sample.
4. Click on the **Start** icon to initialize a run.

The IconNMR: Manual Lock/Shim/ATMM information box appears.



5. Click on the **Lock OK** button a second window appears with the Shim options.
6. Click on the **Shim OK** button, IconNMR continues with the acquisition.


ICON-NMR: Manual Lock/Shim/Atmm
Manual Lock/Shim Mode
Here you may Shim the spectrometer manually using the BSMS Keyboard. If you don't have a BSMS keyboard use the BSMS Panel button to start the display module.
You may still abandon this mode and shim automatically by clicking on the "Automatic" button
Minimize this window to prevent it poping up
Shim files may be loaded and saved using the RSH and WSH buttons
You may also turn off the rotation during shimming using the Rotation on/off button.
Commands
Shim OK
Automatic
BSMS Panel
ATMM
RSH
WSH
Rotation Off
Switch Rotation off

7.4 How to use the Easy Setup Mode

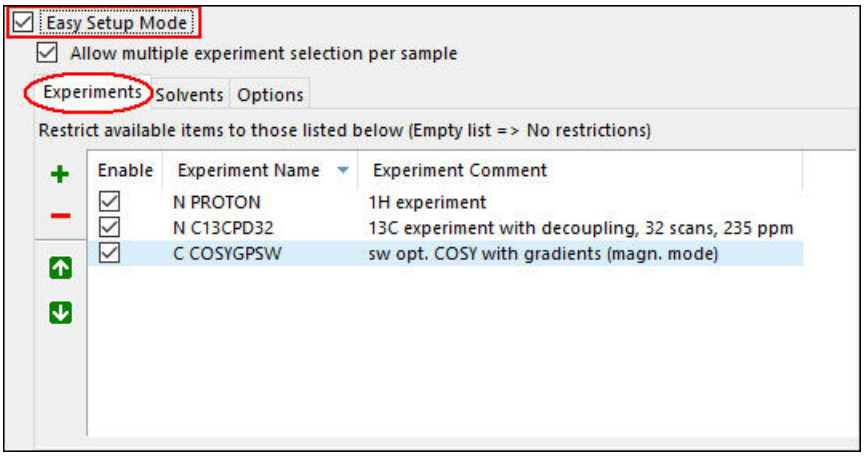
This section will guide you through the set up how to enable and use the Easy Setup Mode.

7.4.1 Setting up the Easy Setup Mode

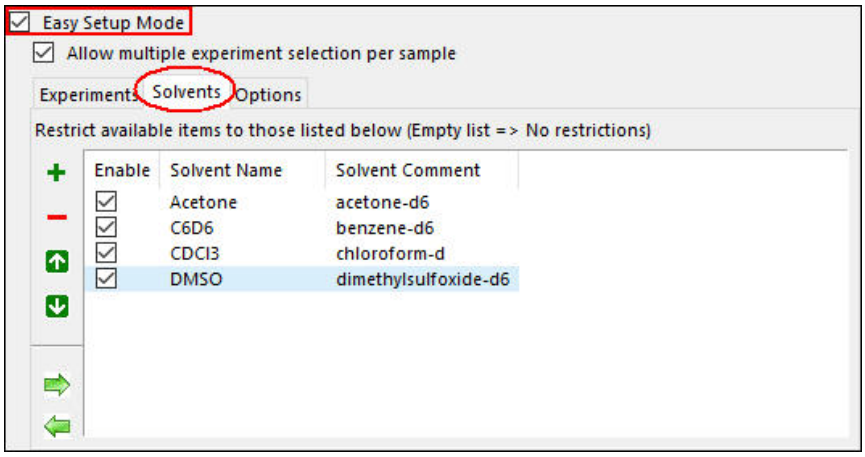
1. Open the **IconNMR configuration** window or type in the TopSpin command line **iconc**.
2. Under **Automation**, select **Automation Window**.
3. Enable **Easy Setup Mode** in the Display section.
4. Enable Allow multiple experiment selection per sample.

For practical reasons in the example below, 4 solvents and 3 experiments have been assigned to restrict allowing the user to access the list of all experiments and solvents.

5. Click on the **Experiment** tab.
6. Add 3 experiments e.g. **Proton**, **C13CPD32**, **COSYGPSW**.
7. Enable all 3 experiments.



8. Click on the **Solvent** tab.
9. Add 4 solvents e.g. **acetone-d6**, **benzene-d6**, **chloroform-d**, **dimethylsulfoxide-d6**.
10. Enable al 4 solvents.

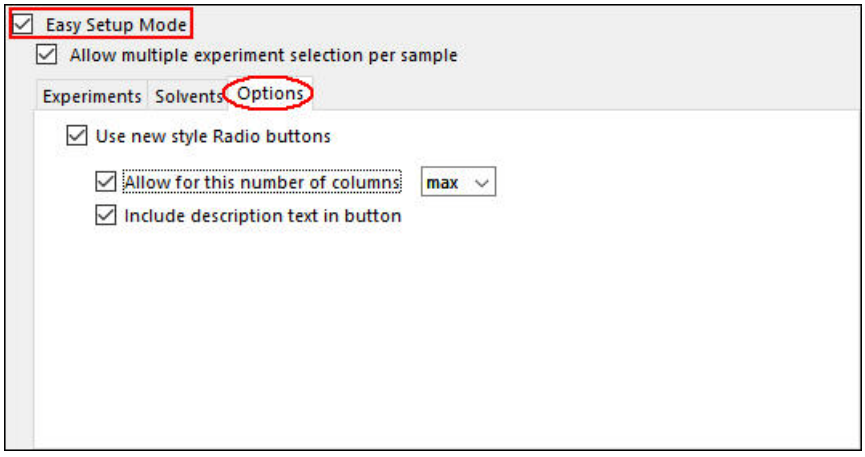


11. Click on the **Options** tab.
12. Enable the following options:

    Use new style Radio buttons

    Allow for this number of columns and select **max**

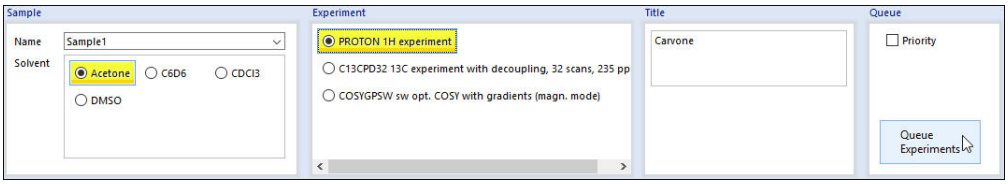
    Include description text in button



13. Click on **File** and select **Save**.
14. Click on **File** and select **Close**.

7.4.2 Using the Easy Setup Mode

1. To start the Automation, follow the instructions in **5.4.3 Standard BACS, Sample Case, Pro (232)** steps **1** through **6**.
2. Click on the **Change User** button to log out temporarily.
3. Log in as **Scientist_1**.

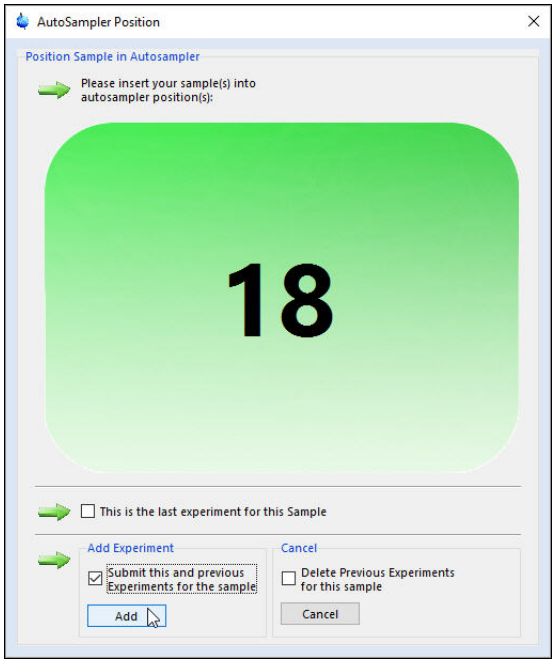


The data set name and experiment number is automatically entered using either the Spectrum Number Filename or the predefined Data Set Names option in the User manager configuration window. The only information the user has to input is the solvent, experiment and the title information.

4. Select the solvent e.g. **Acetone**.
5. Select the experiment e.g. **PROTON**.
6. Enter a name in to the Title block e.g. **Carvone**.

If there are many solvents and experiments listed, you can click inside the solvent or experiment window. Then jump through the radio buttons to select the solvent or experiment you want by hitting the first letter of the name.

7. Click on the **Queue Experiment** button.



The AutoSampler Position window appears. At this point insert the sample in to the displayed position of the sample changer e.g. 18.

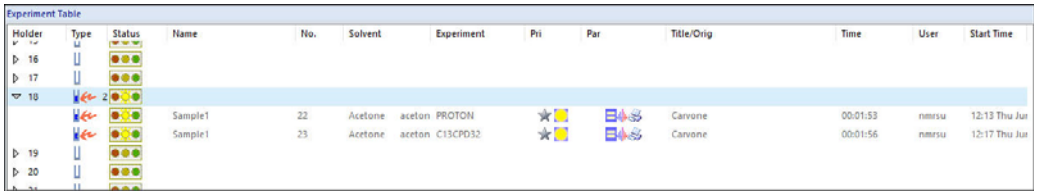
8. Enable in the Add Experiment section **Submit this and previous Experiments for the sample**.

9. Click on the **Add** button inside the AutoSampler Position window.

10. Select the experiment e.g. **C13CPD32**.

11. Click on the **Queue Experiment** button.

12. Click on the **Add** button inside the AutoSampler Position window.



Both experiments are submitted in to the queue at the sample position 18.

Examples of user specific settings

8 Experiment list

8.1 Default experiment list

N AL27ND - 27Al exp. no decoupling
N B11ZG - 11B exp. no decoupling
N C13APT - Attached Proton Test using jmod pulse program
N C13CPD - C13 exp. comp. pulse dec. 1024 scans
N C13CPD32 - C13 exp. comp. pulse dec. 32 scans
N C13CPDSN - C13 exp. comp. pulse dec. with signal-to-noise calc.
N C13DE45SN - C13 DEPT all positive with signal-to-noise calc.
N C13DEPT45 - C13 DEPT all positive
N C13DEPT90 - C13 DEPT CH-only
N C13DEPT135 - C13 DEPT CH,CH3 pos. CH2 neg.
N C13DEPT135p - dept135 with phase of previous C13
N C13GD - C13 exp. gated decoupling
N C13IG - C13 exp. inverse gated decoupling
N C13MULT - 13C automatic multiplicity determination
N C13OFF - C13 exp. off resonance
N C13PPTI - C13 exp. with peak picking in title
N C13HUMP - 13C hump (lineshape) test
N C13RESOL - 13C resolution (half width) test
N C13SENS - 13C sensitivity (SINO) test
N CD111ZG - 111Cd exp. no decoupling
N CD113ZG - 113Cd exp. no decoupling
N CL35ZG - 35Cl exp. no decoupling
N CL37ZG - 37Cl exp. no decoupling
N F19 - 19F exp. no decoupling
N F19CPD - 19F exp. comp. pulse decoupling
N GA71ZG - 71Ga exp. no decoupling
N HG199CPD - 199Hg exp. comp. pulse decoupling
N HMQC1D - 1D version of the HMQC
N MULTIPRESAT - 1H, multiple presaturation
N LC1D12 - 1H, double presaturation
N LC1DCWPS - 1H, multiple presaturation

N LC1DWTDC - 1H, mult. WET suppr., 13C decoupling
N LCML12 - TOCSY double presaturation
N LCMLCWPS - TOCSY TPPI, mult. presat., 13C decoupling
N MLEVDCPHWT - TOCSY TPPI, WET suppr., 13C decoupling
N COSYCWPHPS - COSY TPPI, multiple presat.
N COSYDCPHWT - COSY TPPI, WET suppr., 13C decoupling
N HSQCETGPSIWT - HSQC e/a TPPE, WET suppr. 1 solvent
N N15 - 15N exp. no decoupling
N N15IG - 15N exp. inverse gated
N N15INEPT - 15N exp. inept
N NA23ZG - 23Na exp. no decoupling
N NOEDIFF - 1H noe difference
N O17ZG - 17O exp. no decoupling
N P31 - 31P exp. no decoupling
N P31CPD - 31P exp. comp. pulse decoupling
N PROB11DEC - 1H with B11 decoupling
N PROF19DEC - 1H with F19 decoupling
N PROP31DEC - 1H with P31 decoupling
N PROTON - 1H experiment 16 scans
N PROTON128 - 1H experiment 128 scans
N PROTONinfo - 1H experiment with info table
N PROTONCONLF - 1H exp. with conditional low field plot
N PROTONEXP - 1H experiment + expansions
N PROTONLF - 1H experiment + low field plot
N PROTONLFEXP - 1H experiment + low field plot + expansions
N PROTONNR - 1H exp. non spinning
N PROTONNREXP - 1H exp. non spinning + expansions
N PROTONNRLF - 1H exp. non spinning + low field plot
N PRONRLFEXP - 1H exp. non spinning + low field plot + expansions
N PROHOMODEC - 1H homo decoupling experiment
N PROTONT1 - 1H T1 Relaxation measurement
N PROHUMP - 1H hump (lineshape) test
N PRORESOL - 1H resolution (half width) test
N PROSENS - 1H sensitivity (SINO) test
N PT195ZG - 195Pt exp. no decoupling
N RH103ZG - 103Rh exp. no decoupling

N SE77ZG - 77Se exp. no decoupling
N SELCO1H - 1D COSY using sel. excitation w/a shaped pulse
N SELMLZF1H - 1D homo. using MLEV17 and sel. exc. w/a shaped pulse
N SELNO1H - 1D NOESY using sel. exc. w/a shaped pulse
N SELRO1H - 1D ROESY using sel. exc. w/a shaped pulse
N SELZG1H - 1D sequence using sel. exc. w/a shaped pulse
N SI29IG - 29Si exp. inverse gated decoupling
N SN119IG - 119Sn exp. inverse gated decoupling
N WATERSUP - 1H water supression test
N WATER - water supression
C COSY45SW - sw opt. COSY45 (magn. mode)
C COSY90SW - sw opt. COSY90 (magn. mode)
C COSYGPSW - sw opt. COSY with gradients (magn. mode)
C COSYDQFPHSW - sw opt. COSY with dq filter (States-TPPI)
C COSYGPDFPHSW - sw opt. COSY with gradients and dq filter (States-TPPI)
C COSYGPMFSW - sw opt. COSY with gradients and mq filter (magn. mode)
C MLEVPHSW - sw opt. TOCSY (States-TPPI)
C NOESYPHSW - sw opt. NOESY (States-TPPI)
C ROESYPHSW - sw opt. ROESY (States-TPPI)
C HMQCGP - sw opt. HMQC with gradients (magn. mode)
C HMBCGP - sw opt. HMBC with gradients, low pass J-filter, no decoupling
C HSQCGP - sw opt. HSQC sens. improved with gradients (e/a TPPI)
C HSQCEDETGP - sw opt. edited HSQC with gradients (e/a TPPI)
C HMQCGPML - sw opt. HMQC-TOCSY with gradients (magn. mode)
C HMQCBI - sw opt. HMQC using BIRD pulse (magn. mode)
C HMQCBIPH - sw opt. HMQC using BIRD pulse (States-TPPI)
C HMQC - sw opt. HMQC (magn. mode)
C HMQCPH - sw opt. HMQC (States-TPPI)
C HMBCGPND - sw opt. HMBC with gradients
C HMBCLPND - sw opt. HMBC with low pass J-filter (magn. mode)
C HSQCETGPML - sw opt. HSQC-TOCSY with gradients (e/a TPPI)
C HSQCETGP - sw opt. HSQC with gradients (e/a TPPI)
C HCCOSW - sw opt. CH-correlation
C HCCOLOCSW - sw opt. COLOC
C SELCOGP - selective COSY experiment w/gradients
C SELNOGP - selective NOESY experiment w/gradients

C SELMLGP - selective TOCSY experiment w/gradients

C SELROGP - selective ROESY experiment w/gradients

9 Contact

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NMR Hotlines

Contact our NMR service centers.

Bruker BioSpin NMR provide dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

Please select the NMR service center or hotline you wish to contact from our list available at:
http://www.bruker.com/service/information-communication/helpdesk.html

9.4 Glossary

NMR

Nuclear Magnetic Resonance

Glossary

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