1. INTRODUCTION

1.1. Capabilities of the Inova 600

A summary of the capabilities of the Inova 600 in comparison to the Bruker 400 and Bruker 600 are presented here. For a full discussion, please see the "NMR Spectrometer Capabilities and Specifications" notes.

Table 1. Capabilities of the Bruker 400, Bruker 600 and Inova 600

Spectrometer	^{1}H	^{13}C	^{19}F	^{31}P	Other nuclei	Variable Temperature
Bruker 600	Yes	Yes	Yes	Yes	Yes	Upon request
Inova 600	Yes	Yes[a]	Yes[a]	Yes	Yes[a]	-100 °C to +130 °C[b]
Bruker 400	Yes	Yes	Yes	Yes	Yes	No

[a]Requires manual probe tuning.
[b]Chiller is used until -30 °C. Below -30 °C, liquid nitrogen must be used.

1.2. Specific Inova Policies

1) NMR time must be reserved regardless of the time or day using the FACES website.
2) Under no circumstances are users allowed to book time using another user's FACES account.
3) NMR reservations can be deleted up to a maximum of 1 hour before your reservation's start time.
4) For standard experiments, no more than two hours of time can be booked on weekdays between 9:00 am – 6:00 pm. However, a maximum of 3 hours is permitted for variable-temperature experiments and for samples requiring numerous experiments in which the user must remain at the spectrometer at all times (eg. for titrations, kinetics studies, etc.).
5) Overnight experiments (i.e. standard experiments longer than 2 hours) beginning on weekdays must start after 6:00 pm. Overnight experiments ending on a weekday must be completed by 9:00 am.
6) Odd nuclei or variable-temperature experiments and probe tuning are not to be performed until training has been received from NMR facility staff.

BASIC OPERATION OF THE INOVA 600

2. INITIAL STEPS

2.1. Logging into VnmrJ

1) At the VnmrJ welcome screen, select your group's name from the drop-down list.
2) Enter your group's password and then hit the enter key.

2.2. Inserting your Sample and Selecting your Solvent

1) Verify that the temperature is 25 ºC. If not, set the temperature to 25 ºC and wait for the temperature to regulate before proceeding.
2) Click on the **Start** panel and then select the **Standard** page.
3) Press Eject . You should hear air flowing and the $CDCl_3$ sample should eject.

CAUTION: The eject air MUST ALWAYS be initiated in order to insert a sample, regardless of whether a sample is in the magnet or not.

4) Remove the $CDCl_3$ sample from the magnet's upper barrel and insert your sample in its place.
5) Place the $CDCl_3$ sample into the metal NMR sample holder on the spectrometer's computer table.
6) Back at the computer, press Insert . The eject air will slowly dissipate and your sample will smoothly drop into place.
7) Select your solvent from the solvent drop-down list.

2.3. Locking and Shimming your Sample

1) Click Find z0 to find the lock (^2H) frequency and get your solvent on resonance.

IMPORTANT
Make sure you observe the following 3 things after the FindZ0 routine has finished:

1. *In the message window, you should see "Z0 set to XX", where X is a number between ± 32768.*
2. *The status window at the bottom of the screen should read "Idle".*
3. *In the blue banner at the top of the window, it should read your experiment name (eg. PROTON).*

2) Click Gradient Shim to automatically shim your sample.

IMPORTANT
Make sure you observe the following 3 things after the Gradient Shim routine has finished:

1. *In the message window, you should see "Gradient autoshimming on Z done, X iterations".*
2. *The status window at the bottom of the screen should read "Idle".*
3. *In the blue banner at the top of the window, it should read your experiment name (eg. PROTON).*

2.4. The Next Step

NMR experiments can be performed manually, in which each experiment is started by the user (see Section 3) or in a sample queue, where the experiments are queued and are run automatically (see Section 4).

3. PERFORMING NMR EXPERIMENTS MANUALLY

3.1. Selecting your Experiment

1) Select the desired experiment from the **Experiment Panel** located on the left-hand side of the screen.

3.2. Filling out the Sample Information

1) Go to the **Start** panel, **Standard** page.
2) Fill out the information needed to save your data. Do not use any special characters (eg. !, *, (,), etc.)
   a) Complete the "User Name:" section.
   b) Complete the "Sample Name:" section.
   c) ***(Optional)*** Enter any information in the "Comments" section. This section is free-form and can contain any information you want.

NOTE
Your data will automatically save on after completion on the server in the following directory:
/home/nmr-data/Group/UserName/SpectrometerName/SampleName_Date/

3.3. Modifying Select Parameters and Starting your Experiment

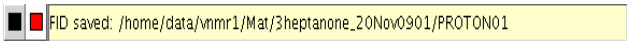
1) Go to the **Acquire** panel, **Default** page.
2) The acquisition parameters that can be modified depend on the chosen experiment, but generally at least two of the following choices are available:
   a) Spectral width: Determines the chemical shift range of the spectrum.
   b) Number of scans: The more scans, the longer the experiment takes, but the better the signal-to-noise of your spectrum.

NOTE
The signal-to-noise of an NMR spectrum does not increase linearly with the number of scans, but increases proportional to the square-root of the number of scans. Thus, to double the signal-to-noise of your spectrum, you must acquire 4 times the number of scans.

3) ***(Optional)*** Click Show time to see how long your experiment will take. The time will be displayed in the Information Panel.

4) Click Acquire to start your experiment
5) As the experiment proceeds, the time remaining and the number of scans/transients completed (CT) are displayed in the Spectrometer Status Window at the bottom of the screen.

6) Your spectrum will automatically save and be displayed when the experiment is finished. The message, "FID saved: …" should appear in the Information Panel.



IMPORTANT
If you do not see the "FID saved..." message, then the NMR experiment did NOT save and the data will be lost. Do the following to save the spectrum:

1. *Go to the Start → Standard page and click on "Clear Sample Info".*
3. *Select your name from the user drop-down list.*
4. *Enter your sample name.*
5. *Go to the Acquire panel.*
6. *Click on "Save Spectrum" button.*

3.4. Monitoring and Stopping your Experiment *(Optional)*

If you would like, you may see your spectrum before the experiment is completed.

1) Go to the **Process** panel.
2) When you see the message, "exp#: BS # completed" (it doesn't matter which number it is) in the Information Panel, click on Auto process. Your spectrum will be displayed.

3) In the top right-hand corner, click on  to display the full spectrum.
4) If you are happy with your spectrum and do not wish to complete all the scans, click "Stop & Save".

3.5. Performing Additional Experiments

Scenario 1

If you have additional 1D experiments to perform on the *same* sample, go back to the start of this section (section 3) for each additional experiment you wish to perform.

Scenario 2

If you have additional experiments to perform on a *different* sample, do the following:

- Go to the **Start** panel, **Standard** page
- Click on Clear Sample Info.
- Go to section 2.2.

Scenario 3

If you have no more experiments you wish to perform, move onto section 5.

BASIC OPERATION OF THE INOVA 600

4. PERFORMING NMR EXPERIMENTS USING THE STUDY QUEUE

4.1. Preparing your Sample

1) Click on New study on the left-hand panel of VnmrJ.
2) Go to the **Start** panel, **Standard** page.
3) Fill out the information needed to save your data. Do not use any special characters (eg. !, *, (,), etc.)
   a) Complete the "User Name:" section.
   b) Complete the "Sample Name:" section.
4) ***(Optional)*** Enter any information in the "Comments" section. This section is free-form and can contain any information you want.
5) If you would like the spectra to print automatically after completion by selecting or deselecting the Autoplot box.

4.2. Selecting and Customizing your Experiments

1) Select your experiments from the Experiment Panel on the top-left of the screen by clicking on the experiments in the order that you wish them to be performed.
2) ***(Optional)*** Customize your experimental parameters.
   a) Double-click on the experiment in the list of chosen experiments on the bottom left-hand side of the screen (not the Experiment Panel). This reads in the experiment.
   b) Go to the **Acquire** panel, **Default** page and modify any parameters that you wish.
   c) If desired, click Show time. The experiment time will be updated and displayed in the experiment list.
   d) Then click on Save to save the modified parameters and return to the previous screen.
   e) Repeat steps a – d for any additional experiments that you would like to customize.
3) ***(Optional)*** Delete unwanted experiments by selecting the experiment from the Experiment List and dragging it into  on the bottom left corner of the screen. The total sample time will be updated.
4) Click on Submit.
5) When prompted, go to the **Acquire** panel and click on Acquire to start the queue. Your data will automatically save when each experiment finishes.
6) If you decide that you do not want to perform the sample queue, click on Cancel.

5. FINAL STEPS

1) Eject your sample and insert the standard $CDCl_3$ sample:
   a) Click on the **Start** panel, then select the **Standard** page.
   b) Press Eject . You should hear air flowing and your sample should eject.
   c) Remove your sample from the magnet and insert the standard $CDCl_3$ sample in its place.

d) Press Insert . The eject air will slowly dissipate and your sample will smoothly drop into place.

2) Click Logout.