

# VnmrJ JS300-NMR User Guide

The JS300 NMR is NOT Fully Automated as of 8/1/2014.

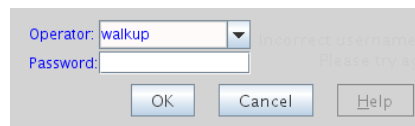
You MUST check LOCK and SHIM status – just as you did before the upgrade - or your results will be poor.

## Scheduling and Accounting

Note the reservation sheet provided by the door. JS300 usage is on a first-come, first-served, open-access, walkup basis. Logging is done electronically, recording number of samples, experiments / protocols used, log time and acquisition time. The reservation sheet is for your convenience only.

## CIF Lab NMR General Login info

NMR:	JS300	Inova 400	Robot 400
Username:	(your eName)	(your eName)	(your eName)
Default Password:	nmr4CSU	nmr4CSU	nmr4CSU



## Sample Preparation

**DO NOT EVER USE BROKEN, CHIPPED, DISTORTED, ETCHED NMR TUBES!** These tubes are fragile, break more often in the NMR, will damage the probe and **YOU AND YOUR ADVISOR** will be held responsible for mishaps.

Use a deuterated solvent whenever possible. You need about 0.650 ml total solvent volume or 3.5 cm in the NMR tube. The NMR is sensitive and good proton can be obtained on 5mg. You will have poor lineshape / shim results if you try to use to short a column of solvent (less than 3cm).

## Check and Gauge Sample:

- Before putting your sample tube in the spinner, clean the tube and insert it into the glass gauge. If the tube is warped, it will not insert fully into the gauge, and must not be used, or else it will damage the probe.
- If the tube is ok, place the spinner into the metal depth gauge, and insert the tube into the spinner. Center the sample volume around the dotted lines on the gauge.
- Using a Kimwipe with a drop of ethanol, carefully wipe the sample tube and spinner. Be sure you are inserting a sample with a deuterated solvent (unless you have cleared otherwise with staff).

## Login to the Instrument

The JS300 is already in “New Study Submit” Mode for convenience. Press Cancel to leave this mode if you like.

## Sample Insertion

**Caution: The magnet produces a very powerful magnetic field. It cannot be turned off and on. Observe all posted precautions when approaching the magnet. Do not approach the magnet if you have a pacemaker, other medical implant, or any metal objects in your body. Remove from your pocket and put in a safe place any magnetic media, such as computer disks, or magnetic strip ID cards or credit cards. Some watches may also be damaged. Do not bring any ferromagnetic objects near the magnet. If in doubt, please ask any of the CIF staff. Read the accompanying Magnetic Resonance (MR) Safety documents. The 5 Gauss limit involves the ENTIRE JS-300 NMR Lab.**

- **Important: The eject air must be ON before you insert the sample!**
- Press the <Eject> button to turn on the eject airflow.
- Wait for the eject air to come on (it can be heard and felt rushing out the top tube of the NMR), and then insert the spinner with the sample into the NMR.
- Press the <Insert> button to turn off the airflow. The sample will descend into the magnet, you will hear it settle.
- The JS300 **only** should begin to SPIN the sample after it settles. Other CIF NMRs do NOT spin the sample.

Recall Default Shims from the <Shim> Panel

Check the LOCK

SHIM “Z1C” and “Z2C” (see attached spectra that display the effects of shimming)

## Study Queue

- Each NMR sample is a “Study” and will require a “Sample Name” and at least one Experiment or Protocol.
- The JS300 is already in New Study Submit mode for convenience. You may begin adding experiments from the list OR you may click <Cancel> to exit submit mode.

### For each sample that you have:

- Click on one or more desired protocols from those available, (e.g. Proton, Carbon and/or protocols on other tabs).
- If you select the wrong protocol, simply drag it from the study queue into the trash.
- Enter sample information: Sample Name is **required**, select appropriate solvent, check your email, etc..

### You may modify the experimental protocol

- right click and select from the popup, or double click on the protocol.
- Change parameters you wish from the panels below the “white board” display area.
- Save – or Quit without saving – to return the parameters to the Study.

### Submit Study Queue

- LOCKED and SHIMMED the sample yet ?
- Click Submit and wait for acquisition to complete.

*{check the QUICK SUBMIT Panel Mode – Another option to consider for Speed}*

### Retrieve your sample

- When your sample is completed
- Click Eject to eject sample
- Remove sample from magnet, return spinner to tray.
- Click Logout button on *Enter sample info panel*.

### Data

- Your data will automatically be saved
- A PDF survey spectrum will be emailed to you for each experiment.
- You will also receive data (FID) email for each Protocol or Experiment.
- If there has been an error, you will receive an error email.

Please be considerate to your colleagues and avoid doing data processing at the console when lab is busy.

### Data Retrieval

You will need to use an ftp program that uses SSH2/SFTP security and be Chemistry Department internet domain (but stay tuned, we are working on a data server that will be generally available to authenticated users inside the CSU domain. The original, non-encrypted FTP will NOT work.

NMR	IP Address	Username	Password
JS300	129.82.76.80	js300	nmr4CSU
I400	129.82.76.87	i400	nmr4CSU
400MR	129.82.76.82	400mr	nmr4CSU

Your data will be found in `/home/_data/walkup/your-operator-name/`

## Menthol – With and Without Quick Shim

