

NMR Software Recommendations and Resources for the Department of Chemistry

Transfer via SSH/SCP, and NMR with VNMRJ, and MNova

GPU (personal cloud storage)

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Security on Personal Computers

First things first, no matter how complex or secure our computers are they can always be hacked. We are constantly battling between tighter security versus easy-of-use. A truly secure system is one that's inaccessible and therefore useless.

To this end we ask that users minimally make an effort to install the latest security patches for their laboratory and personal computers be they laptops, tablets, or mobile device. All it takes is a single compromised system for the entire facility to feel the effect.

The University of Alberta's computer network services provides excellent documentation and even **free security software** for faculty and students of the university. Please participate as much as time will allow. We appreciate it.

Primary UofA Computer Security Link

http://ist.ualberta.ca/ts/security

On the website linked above you will see extensive protection software both to prevent intrusion and to detect anything that may have already happened. It takes relatively little time to download and install, and can be set to automatically scan incoming information. Just as in life, please practice safe interactions.

Mac Security through Obscurity

It used to be that owning Apple products implied a certain level of protection. Due to the number of people using Macs, there wasn't the incentive to make MalWare for that population. However now due to the popularity of the iPhone, iPod, and iPads, along with an increase in the percent of people using Macintosh computers we can no longer expect immunity. Nefarious individuals will exploit vulnerabilities in browsers, the operating system, or communications (*i.e.* email). While Apple is a closed environment it is not invulnerable (*e.g.* Flash, Java, HeartBleed). With the use of BootCamp and virtual operating systems (see Chapters below), we can introduce all the problems and security holes of other operating systems on our Macs.

At the very least while Macs may not be susceptible to some forms of attack, we can certainly be carriers and pass along problems to others using different systems. In this regard please keep your OS updated (this can be set automatically) so that you don't indirectly compromise the NMR facility, *e.g.* by allowing someone to monitor your login and/or passwords.

Passwords

We all know what happens. An easy to remember password means little to no security (e.g. 'password' is the number one most used password in the world, followed closely by 'password1'). To combat this we make huge passwords that are impossible to remember. These get written on a Post-It note or taped to the monitor, or put in the top desk drawer. Yes, it's more common than you may think.

Please try your best to protect passwords and/or invest in a password manager that can generate and store passwords for you. If you're interested checkout programs such as "1Password" by AgileBits, available for iPhone, iPad, Mac, Windows, and Android or LastPass with a Yubikey for two-factor security.

http://www.yubico.com/. This is highly recommended and easy to use.

Transferring Files

BACKGROUND - WHAT DO I NEED?

Everyone wants a way to access data via computer communications, day or night, from anywhere in the world. Unfortunately there are tons of young adults continuously running software (*i.e.* script kiddies) looking for computers to takeover, and then use them to supply stolen programs, games, movies, music, *etc.* to others.

Most intruders don't care what your data is, what it's for, and will likely only damage it if they need additional space and your information is in the way.

However the hijacked host computer does have value to them as it can be used to run third party network attacks (*e.g.* overloading another computer's network, aka denial of service), host files for download, and basically become a real nuisance. These hijacked computers called "zombies" look for other machines to takeover and quickly take-up valuable network capacity. Once a zombie is discovered it has to be shut down, isolated from the network, wiped clean and rebuilt from scratch. The loss of functionality is bad enough, but the time wasted rebuilding machines can be hours to days.

Therefore we need a way for computers to trust communications, instructions, and access is from a reliable source and hence encryption is used. The NMR facility uses a well-established and highly reliable secure communication



called SSH (secure shell) and its corresponding file transfer method called SCP (secure copy). SSH allows one to communicate with another computer using password or SSHkeys access through a completely encrypted tunnel. All correspondence is encrypted so the login, password, and operations are safe and cannot be copied/used or modified by an outside party.

SSH and SCP are based on computer terminal command-line instructions. There is a vast amount of literature for interested users ranging from free/online to well

written books such as Barrett & Silverman's 'SSH The Secure Shell'.

This also comes into play for the university server (see GPU chapter below) and how to store data and login to your accounts from around the world.

SSH/SCP, DO I HAVE IT, AND HOW DO I USE IT?

SSH and SCP commonly require access to a command line usually via a terminal window (see right). Linux operating systems such as RedHat used on the NMR spectrometers have these capabilities built in as an inherent part of the system. Mac OSX is built upon a linux core (Darwin) and also has this capability though user access is atypical and may require selection of installation options but can also be added later depending on the version. For Windows, one will need to either access the windows command line prompt and/or install an X11 windowing



environment (*e.g.* Xming, Cygwin, *etc.*). Once a person has access to the command line the commands are simple:

Command Line Examples^{*}

List the contents of the current directory

-> ls –la

- -the '-la' are extra options added to specify "all" and "long" listings of information.
- -to see what extra options are available and what they do check the manual or "man" pages

Show manual or 'man' page for command

->man ls

Print Working Directory

'Prints' (to the screen) the present location of the user in the file structure, *e.g.* /home/john/data. The 'print' is a throw back to when computers output information to dot-matrix printers, *i.e.* before computer screens!

-> pwd

Change Directory

-to the directory named 'xxx', *e.g.* cd /home/john/data

-> cd xxx

-in order to go back up a directory use cd ..

^{*}we will use -> to indicate where and what a user types. The actual command to be typed is colored burgundy.

[†] Some machines will need the full name of the remote host, while others can use the short name.

Move File

->mv jon_file john_file

– great to correct a typo in the file name. Moves the name of the file, can also be used to move directories at the same time

e.g. mv jon_file /home/john/data/john_file

SSH Example

-> ssh –Y john@spectrometer.chem.ualberta.ca

-SSH would then form the connection, test the encryption and request the password for john, and if successful would provide direct control of the computer named 'spectrometer' as if john was sitting at the computer (see Remote Display section in the VNMRJ chapter below). The '-Y' sets the stage for remote display (more on that later).

SCP Example

->scp john@spectrometer.chem.ualberta:/home/john/data xxx/XXX /newhome/XXX

-this command forms a connection for john to 'spectrometer' and copies a file to the local computer that 'john' is sitting at. The colon tells the computer that the name is done and starts looking for a directory xxx and the file name XXX. Lastly as the file is being brought to the local computer, then put in the the "newhome" directory and called XXX. Any name can be used.

SCP Push Example

SCP can also be used to push files from the local computer to a remote computer

->scp xxx john@home-computer.ed.shaw.ca:/newlocation/.

-this command take the file xxx, and sends it to john's home-computer and keeps the same name using just the period '.' Instead of having to type the whole name again.

Setting up SSH and SCP Aliases

When faced with typing in the same command repeatedly, one can create a short-cut or 'alias'. For example instead of typing the full name of a remote system one could just type a few letters or the start of the computer's name.

Depending on what type of command line program (called a shell) you're using will determine how to set up the alias:

-> echo \$SHELL

The computer will respond with either /bin/csh, /bin/tcsh, or /bin/bash.

Bash Shell

For bash shell users you'll need to modify the .bashrc file in your home directory with the following entry (use the editor of your choice).

alias ibdw= 'ssh -Y john@ibdw.chem.ualberta.ca'

This will set the alias permanently in your account. Replace the 'john' with your login name, and the ibdw with the workstation assigned to your group.

Tcsh or csh

For csh or tcsh users you'll need to change the .cshrc file:

alias ibdw 'ssh -Y john@ibdw.chem.ualberta.ca'

You can build anything into your aliases. Feel free to explore and experiment. For ideas and resources, a simple Internet search will likely yield plenty of inspiration.

Wow command line is so old/hard, is there a Graphical Interface for SSH and SCP?

ileZilla

Features Screensh Download

ileZilla Serve

ommunity

nse acy P

Overview

Welcome to the homepa GNU General Public Lice

In addition, you will find do

Quick download links

Pick the client if you

New features:

O News

Yes, many! Doing a simple web **Z**FileZilla search will reveal a fantastic range of programs from professional purchase software (e.g. CyberDuck) to free utilities. A windows example would be "Putty" which is well described by ITS (see the chapter below). GPU We're recommending an excellent little free computer program called *FileZilla (The free ftp solution*). Ftp was the previous form of *f*ile *t*ransfer *p*rograms that did not use encryption for the login, password, or on the file being transmitted. It has been

replaced with sftp (secure-file transfer protocol).

Macintosh and Linux

FileZilla – filezilla-project.org

Opening a web browser and either searching for FileZilla or entering the address from above should get you immediately to the relevant site.

Click on the download button for client version (unless vou're the interested serving files in up to



Support is available through our forums, the wiki and the bug and feature request tracker

♦ 2014-06-22 - FileZilla Client 3.9.0-beta1 released



others...not common nor needed for NMR data). The file will download and should not take long.

On Macs you'll end up with a compressed file in .bz2 format. Double clicking the download will expand the compressed file, likely in your 'downloads' folder.

O O O I Downloads								
			Q					
FAVORITES	Name	Date Modified	Size	Kind	Date Added 🔻			
😻 Dropbox	🔁 FileZilla	Jun 1, 2014, 3:29 AM	18.8 MB	Application	Today, 11:18 AM			
frvan 🗇	FileZilla_3.8.1_macosx-x86.app.tar.bz2	Jun 1, 2014, 3:32 AM	6 MB	bzip2archive	Today, 8:55 AM			
	MestrelabLicServer-2.1.0-7177-2.dmg	Oct 11, 2011, 12:22 AM	30.4 MB	Disk Image	Jun 9, 2014, 10:09 AM			
All My Files	MestrelabLicServer-2.1.0-7177.dmg	Oct 11, 2011, 12:22 AM	30.4 MB	Disk Image	Jun 9, 2014, 10:04 AM			
Documents	indent.doc	Dec 13, 2013, 12:02 PM	134 KB	Microsument	May 22, 2014, 10:06 AM			
Library	EMR_2014.01-3.doc	Jan 10, 2014, 11:37 AM	564 KB	Microsument	May 16, 2014, 4:03 PM			
	EMR_2014.01-2.doc	Jan 10, 2014, 11:37 AM	564 KB	Microsument	May 16, 2014, 3:52 PM			
AirDrop	nvj-macosj6_9_0_0-b114.dmg	Apr 11, 2014, 10:33 AM	23.8 MB	Disk Image	Apr 11, 2014, 10:33 AM			
Applications	😼 5991–4097EN.pdf	Jan 26, 2014, 2:18 AM	896 KB	PDF Document	Mar 20, 2014, 10:09 AM			
Desktop	Lecture 15 Chem 681B2 February 10 2014.docx	Feb 9, 2014, 4:02 PM	569 KB	Microsument	Feb 10, 2014, 11:48 AM			
Desktop	Lecture 14 Chem 681B2 February 5 2014.docx	Feb 4, 2014, 11:02 AM	151 KB	Microsument	Feb 10, 2014, 11:47 AM			
Downloads	Lecture 13- Lung Surfactants v2.pptx	Feb 4, 2014, 11:17 AM	31 MB	Microstation	Feb 10, 2014, 11:47 AM			
Movies	Lecture 12 Chem 681B2 January 31 2014.docx	Jan 30, 2014, 7:31 PM	243 KB	Microsument	Feb 10, 2014, 11:47 AM			

lost:	Username:	Password:	Port:	Quickconnect	
local site: /			Remote site:		\$
	C Fil Th	eZilla 3.8.1 the free open source FTP solution	o FileZilla on	Z	
ilename ^ .DocumentRe .MobileBackups .PKInstallSan .Spotlight-V1 .Trashes	Filesize Filetype Director Director Director Director Director Director Director	scumentation <u>Basic usage instructions</u> <u>Configuring FileZilla and yor</u> <u>Further documentation</u> ttting help <u>Asking questions in the File</u> <u>Reporting bugs and feature</u> ou can always open this dialog	<mark>ur network</mark> Zilla forums requests 1 again through the	Last modified	Permissions Own
.fseventsd .vol Applications Groups	Director Director, Directory Directory	23/06/2014 14: 06/11/2012 09:	ĸ		
Library files and 34 directories.	Directory Fotal size: 8,448,284	13/05/2014 13: bytes	Not connected.		_
erver/Local file	Direction Ren	note file	Size Priority S	tatus	

"FileZilla" should then be moved (*e.g.* drag-and-drop) to your **Applications** directory along with all your other programs. Nothing else needs to be done for installation, it's ready to launch.

FileZilla for Linux

For Linux computers you'll need to either install the 'rpm' through your package manager (highly recommended), or download the file directly as seen on the right.

You'll need to make sure

the compressed file is opened, permissions set appropriately (*e.g.* chmod +x filezilla), and located in a directory acknowledged by the user's "path" (*i.e.* so the computer knows it's an executable program and where it is).

Compilation ready source code is also available for those so inclined or needing a customized version for their particular OS.

FileZilla for Windows

Instructions here should be very similar to the Mac. Download the Windows installer and follow the usual on-screen installation instructions.

So how do I use FileZilla's Graphic Interface?

Setting up FileZilla



For this example we'll be showing a mac, but it will be very similar for Windows and Linux installations.

⁽⁷⁾ Show Web Page Cancel Open Depending on your mac OS version it will likely ask you if it's OK to run the application since it's downloaded. You may need to enter your administrator password to allow the application to run. Once the application is active you'll see the opening window (see inset). Hitting "OK" will allow access to the underlying windows.

Under the opening credits you'll see the "Local Site:" information on the left, which is your computer and the default starting location is in the top most directory (call '/' in the Linux world). By default there is no connection to a remote computer (top and right side).

Connect to the Remote Host

To connect to the remote data storage you'll need three things:

1.) network name of the NMR computer, *e.g. ibdw.chem.ualberta.ca or ibdw*^{\dagger} default port should be fine but in case it asks use 22 (standard for SSH and SFTP).

2.) your login, *e.g. nmrlab*

3.) your password



In the example below we're using "ibdw" as the host computer. In order to equalize the workload, your laboratory will have been assigned a workstation for connections. Please check with the NMR group for

your assigned workstation and substitute your workstation name for ibdw as appropriate.

Once you've entered the information, the computer will attempt to form an encrypted tunnel to the Host computer you're connecting to.

If it is the first time that you are connecting to a particular host computer, FileZilla will ask you if that Host machine can be trusted and if you'd like to record the Host Key (see inset). This is OK and you can select the "Always trust" so you don't get asked



each time. You can find the trusted host-keys in your account usually in the .ssh directory. For Windows machines you'll have to locate where FileZilla stores the known hosts equivalent file for

your OS, if you want to modify or erase entries.

In the example you'll see that a local default directory (/User/ryan/Dropbox) has been selected where we always want to store our retrieved NMR data. On the right side we've selected the default 'nmrdata' directory where everyone's data resides. Please select on your local computer any directory you would like to use to store your NMR data. We recommend creating a desktop folder named



† Some machines will need the full name of the remote host, while others can use the short name. This depends on your network settings. Contact IST for assistance.

something like "NMR DATA" and copying all data from the server there. Please be aware that the connection is two-way so don't overwrite archive files. If you do let us know and we'll see what we can do to help resolve.

Now that we've entered the information, we want to use these settings as the defaults and automatically do this for us. When you quit FileZilla and re-launch it later we don't want to have to re-enter everything again.

By default your last 10 sessions will be saved in the Quick Connect pull down menu (downward facing triangle beside the Quickconnect button, top right) pull



down. Hitting the "Quickconnect" button should take you back to where you were. If you only connect to a single computer then this may work just fine.

To be safer, one can also enter the information in the Site Manger (see 'File' pull-down menu, and select Site-Manager) as seen above. This will allow you to enter your information and store it without worrying about the last 10 connections. You may also enter the default directories here so that FileZilla opens the connections and goes to the convenient directory of your choice. The absolute full path is required, and you may need to navigate



manually to that location the first time to determine the full path.

Each time FileZilla is started you will either have to use the QuickConnect or the Site-Manager to re-open the connection to the host computer downstairs.

How do I Move Files?

Once you've got the connection open moving files is simply a matter of clicking on the file or directory you want on the right, and dragging it across to the left to the local directory you want it copied to, e.g. a folder named "NMR Data" on your laptop.

So what can go wrong and how do I fix it?

The most common problem is a change to the SSH host-key for the computer you're connecting to. This happens after operating system updates, or network alterations. For linux and macintosh users, you need to go into your account

directory. find the .ssh sub-directory and either edit or remove the "known hosts" file (see inset). This error will not simply go away and you'll remove previous need to the known hosts entry. If you have trouble removing the entry, contact the NMR staff. For windows version the program should inform you of the key change



and you'll need to simply accept the new key.

The second most common problems are permissions. Either you don't have read permission from the source, or write permission for the destination. If the program responds about permissions errors come see the NMR staff and we'll try to help you out.

Other problems can arise if there is insufficient disk space available at the destination (less and less likely these days), or if the connection fails due to login/password errors. FileZilla should let you know if either of these is the case. If you come across a different problem check the extensive FileZilla help (see below).

FileZilla Instructions

https://wiki.filezilla-project.org/Using

For additional instructions, command line options, and other more advanced features there's a fair amount of information available in the FileZilla Wiki in addition to access to the discussion forums. Please let us know if you discover something you think might be useful for others and we'll include it in the program description.



VNMRJ – NMR Spectrometer Software

Agilent's VNMRJ 4 (left) and VNMRJ 3.2 (right) with Chemistry's 'EZ-NMR' interface by M. Miskolzie and A. Otter.

SOFTWARE

The University has a site license for Agilent's (formerly Varian Inc.) VNMRJ software. We are now making it easier for facility users to access the workstation version of the software. As of June 2014 we use VNMRJ version 3.2 on the spectrometers and also have the latest (v4.2) available for your use and trial.

There are native Windows (v3.2), Macintosh (v3.2, 4.0, & 4.2) and Linux versions (3.2 to 4.2) of VNMRJ. Agilent also provides a virtual operating system with VNMRJ installed in the virtual machine. The virtual device runs like any other program in a window on your computer. The virtual OS is RHEL 6, and this virtual device can be run on Windows, Macintosh or other flavors of linux. The advantage of the virtual device is they can stop making Windows/Macintosh/other versions and concentrate on a single virtual operating system. Emphasis is then placed on the program in that one environment.

REMOTE DISPLAY

One of the easiest ways to use VNMRJ is through the SSH connection described in the previous chapter to connect to one of our NMR data stations and display VNMRJ onto your laptop or local computer.

So what do I need for Remote Display?

Linux computers already come with all the software required built in. For Windows computers there is a detailed section on the NMR website under the FAQ section. For Macintosh computers X11 used to be an installation option, however now the XQuartz project (name of X11 on macs) is independent. To download the XQuartz installation package for your version of Mac OSX please visit:

http://xquartz.macosforge.org/landing/

At the time of writing there was one version of X11 (2.7.6) for Mac OSX 10.6 up to 10.9.

Once your X11 is installed, you can launch VNMRJ from the data station via the SSH connection and have it display on your screen. SSH is usually smart enough

to allow the incoming information though your firewall may have to be modified to all programs access to your screen.

You may find the following X11 setting in your X11 preferences advantageous (see inset).

To start VNMRJ, in the terminal SSH connection to the workstation simply type vnmrj to start the program. Once done exiting VNMRJ and closing the SSH connection will severe the link. Please don't forget to exit VNMRJ before closing the SSH tunnel or abandoned processes can build up on the remote workstation. You can leave the connection open with VNMRJ running for as long as you require for your work.

Cygwin - Remote VNMRJ Display for a Windows Computer





You'll need a program to display the X11 display information on your Windows computer. We recommend the free software Cygwin (https://www.cygwin.com) which is easy to use, download and allows similar functionality of Linux operating systems on a Windows platform.

Select the version of the program you'd like to download. We're recommending 64-bit versions both of your operating system and

the 3rd party software you'll be downloading.

For example you can click on the 'setup-x86_64.exe' (64-bit installation) link to download the setup program and save it to a known location. Start the setup program by double clicking on the application, and a new window should appear. The Cygwin welcome screen will indicate that the install process has begun. Click on Next to proceed, and the window will change to Choose A Download Source. At this point select Install from Internet and click on Next to continue. The installer will ask for install options, select the following or make changes as desired. Root Directory: C:\cygwin

Install For: All Users (RECOMMENDED)

Then click on Next.

The window will change to: Select Local Package Directory. The default location should suffice (where the setup.exe installer was downloaded). Click on Next again. The window should change to: Select Your Internet Connection. From here select Direct Connection or what is applicable to your computer setup. Again click the Next. The window should then change to: Choose A Download Site. Select a mirror site and again click on Next.

The setup will indicate what packages will be installed. In addition to the defaults select:

X11 (all)

search for and select: ssh - autossh, libssh2-devel, libssh2_1, openssh, and nedit. Then click on Next. The Setup.exe will now proceed with the install. The install is far from fast and has be known to take more than 1 hour to complete depending on the mirror site and your internet connection, so be patient and perhaps grab a coffee while you have the time. Once complete one can start the Cygwin Terminal. On the terminal command line enter:

touch .startxwinrc

to create a blank .startxwinrc profile. The default setup will inconsistently start an xterm if the profile is not established. We do not want to start an xterm but instead want to use the Cygwin Terminal. Please edit the .bashrc file (see SSH example section above) using previously described methods, or one can do this by opening a terminal window and issue the command:

nedit

to start the nedit text editor (you can also use NotePad) find the lines and either add/remove or comment them (# in front of the line means ignore the subsequent text as a comment) as applicable:

```
alias rm='rm -i' # the -i means ask before removing, copying or moving
alias cp='cp -i'
alias mv='mv -i'
#
# Dafault to human readable figures
alias df='df -h'
alias du='du -h'
#
alias ls='ls -p'
#
# remote access aliases
# replace xxx with your short-hand name for the computer e.g. ibdw
alias shortname='ssh -Y xxx@yyyy.chem.ualberta.ca'
```

where where xxx is your group's login name for the NMR spectrometers and data stations (*e.g.* gennmr) and yyyy.chem.ualberta.ca is the name of the computer the NMR staff will direct you to use. Once done, close the Cygwin terminal window and re-open or enter:

bash

on the terminal command line to re-initialize the shell. If desired create desktop shortcuts to the Xwin Server and Cygwin Terminal (both are in the Start Menu). To start a remote X session, first start the Xwin server and then open the Cygwin Terminal. On the terminal command line enter the shortname you established above to log in to the remote server. Your usual login name should have been defined in the alias above. Accept any rsa keys if asked, enter the system password and then start vnmrj by entering:

vnmrj

on the terminal command line. One can also use Xlaunch to set up a one button click application to start an application through ssh and remote X windows. When finished, exit VNMRJ, then type logout or exit on the command line in the Cygwin terminal window, and then close X-Win server by right clicking the X-Win icon in the Windows systray and select exit. When connecting to the NMR data stations only the last steps will need to be repeated.

Three Button Mice

VNMRJ and Linux computers make use of three button mice for processing and viewing NMR data. Similar to the Linux based NMR data stations pressing the scroll wheel of a mouse is the same a clicking on middle mouse button.

Three Button Mice on Mac

This gets a little bit trickier. Using control-Click or option-Click will usually suffice to emulate the right- and middle-Click, however sometimes this doesn't work (e.g. Apple's Magic TrackPad both stand-alone and laptops) and you may need a program like "Magic Prefs" in order to fully emulate the multiple button mouse. You can also purchase USB mice for Macintosh computers.

Remote Plotting Printing:

Note that the printer beside the NMR data station will perform all **REMOTE** plotting and printing tasks. This means that when remotely connected to the NMR data station using Cygwin all plot commands issued in VNMRJ will be sent to the printer attached to NMR data station. If you wish to plot your spectra in your lab please let the NMR staff know and we can configure the NMR data station to send all plots to your lab's network attached printer (see NMR news 2004-02).

VIRTUAL MACHINES

To run the virtual operating system on your computer you'll need something like Virtual Box, VMware, or Parallels. We're recommending Virtual Box as it's free, fast, and we have some experience with it. For Macintosh we also have experience with VMware Fusion which the

	요) [2년] [수 📷 Antus B www.virtualBox.org
	VirtualBox
	Welcome to VirtualBox.org!
About	VirtualBox is a powerful x86 and AMD64/Intel64 virtualization product for enterprise as well as home use. Not only is VirtualBox an extremely feature rich, high performance product for enterprise customers, it is also the only professional solution that is freely available as Open Source Software under the terms of the GNU General Nabil Liones (GPL) version 2. See "Nabul "VirtualBox" for an introduction.
Downloads Documentation	Presently, VirtualBox runs on Windows, Linux, Macintosh, and Solaris hosts and supports a large number of guest operating systems including but not limited to Windows (NT 40, 2000, XP, Server 2003), Vista, Windows 7, Windows 8), DOS/Windows 3.x, Linux (2.4, 2.6 and 3.x), Solaris and OpenSolaris, 05/2, and OpenBob.
End-user docs Technical docs	VirtualBox is being actively developed with frequent releases and has an ever growing list of features, supported guest operating systems and platforms it runs on. VirtualBox is a community effort backed by a dedicated company: everyone is encouraged to contribute while Oracle ensures the product always matter prefeasional quality criteria.
Community	Hot picks:
	the Julii Virtual machines for developer at Collect Ref Network thypethod Conservoir Virtual distribution Message Propriet site terminal and the Virtual machines of the Virtual Statement (Virtual Virtual Virtu
	Contact - Privacy policy - Terms of Use

university has available via their licensed software program. Contact Information Technology Services for pricing and pickup. The virtual environments can be a bit of a resource hog, and benefit greatly from a large amount of computer RAM, fast hard drives (*e.g.* SSD), and modern CPUs. However even with modest machinery the virtual devices are relatively easy to use and supply a standardized environment for researchers and the company's support services.

Pictured here is an example of a virtual device running RHEL v6 with VNMRJ 4.2-beta. The virtual device is running on a mac via VMware's Fusion6. The entire



virtual operating system is within a window just like another other computer The program. device acts like a separate computer and can be shutdown or put to sleep until needed.

DOWNLOAD LINKS

Virtual Device for VNMRJ

http://nmr.chem.ualberta.ca/downloads/centos_6.5_vj_3.2A.ova

Once the file is downloaded, Virtual Box on your computer will want to "import" the new file. This basically sets up everything for your particular machine. The conversion can take 4-5 minutes. When done and running, the default account is vnmr1 and there is no password. For those wanting to install other programs or options into the virtual space, the root password is @gilent1.

The virtual machine was updated to Centos 6.5, VNMRJ was patched to the most recent update, and Virtual Box guest additions were installed for you already (highly recommended if you create your own virtual box environment). Mark also installed FileZilla to be consistent with our spectrometers and workstations.

System Requirements for Virtual Machine

The virtual box will want 2 GB of RAM minimum which should available for most systems, if not the usage can be reduce to 1GB through Virtual Box's preferences menu options. Performance will take a hit. Feel free to adjust the settings to suit your needs and machine capabilities (e.g. use more or less CPU cores). A modern CPU (e.g. Intel core2duo or better) is recommended.

The virtual operating system is 64-bit, so a 64-bit or emulation compatible CPU is needed with a 64-bit operating system. Intel provides emulation in all chips for the past several years and both Windows and Mac have had that capability for some time.

VNMRJ for Mac

http://nmr.chem.ualberta.ca/downloads/vnmrj3.2_mac.zip -decompress disk image file and run the installer -pdf instruction manual included

VNMRJ for Windows

http://nmr.chem.ualberta.ca/downloads/vnmrj3.2_win.zip -decompress installer and run

VNMRJ MANUALS AND SUPPORT

The first place to check is the nmr.chem.ualberta.ca website for the UofA summary manual.

http://nmr.chem.ualberta.ca/AOVNMR_course/VNMRJ/content.html

One can also check the frequently asked questions section for common issues and solution.

http://nmr.chem.ualberta.ca/nmr_news.htm#FAQs

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NMR questions?try http://nmr.chem.ualberta.ca	
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Built in Manuals

The next best resource is inside VNMRJ itself. The program contains all the manuals in PDF and HTML format for the user. Under the "Help" menu (see above) you'll find menu options that will open the table of contents for the manuals (right). The manuals will be specific to the version of VNMRJ that is installed and may differ a bit from other versions. Each title is a separate manual and can be several hundred pages long. The "Safety", "Spectroscopy" and "Quick Start Guide" should be the place to begin. The other manuals can be left until later when specific needs arise.

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		Agilent VnmrJ 3.2 Manuals Table of Contents
	Safety	VmmJ 3.2 Installation and Administration Guide
	Automation	VnmrJ 3.2 Linux Installation Guide
	Spectroscopy	VnmrJ 3.2 Quick Start Guide
	BioPack	VnmrJ 3.2 Quick Submit Guide
	CPR	VnmrJ 3.2 Administration Quick Start Guide
	User Programming	VnmrJ 3.2 Experiment Guide
	DOSY	Good Laboratory Practices
	AutoTest	Amplifier Linearization
	3D Gradient Shimming	
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SpinSights

There is a large amount of information available on Agilent's website named SpinSights.

https://spinsights.chem.agilent.com/welcome

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HIMRI Imaging Centre Opening in Newcastle, Australia by John Rywin Solnajoths Blogs on Jun 2, 2014 "On Friday 14th March the Hunter Medical Research Institute, in association with Newcastle University and Hunter New England Health officially opened a new state-of-the-art magnetic resonance imaging more					ersity ling	Re: A question about 'bioref' and a comment on the weighting panels Thours ago in Discussion Forum Re: mrPipe trying to keep the complex number tay ago in MIRPipe					
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As a user of Agilent equipment here at the University of Alberta, you are all welcome to a free registration and access to the Agilent SpinSights site. After registering and receiving a password (takes about a day or so) you will be able to see various discussions forums, ask questions yourself, and access the Manuals (see above), notes, patches, and bug reports (often with solutions). Please make sure to read any regulations about posting before asking a forum question. Also the search window is very useful to make sure something hasn't been asked, and answered, before.

Mestrenova (MNova) from Mestralab Research

The University of Alberta has a 3 month (Summer 2014) trial license kindly provided by Metralab research. The Mnova software is relatively easy to use, powerful, and comes with all the expected bells and whistles of modern software. The program is available from their website (see inset) and automatically comes with a 30-day trial period.

We've been offered an extended license trial period of 3 months and comes with a license server. The server allows individuals to "check-out" a license and for the NMR group to edit who has licenses and for how long. Each time Mnova is

launched the program checks the license. If a network connection is not available it will continue to function for 3 months. At the end of that time a license will need to be purchased separately, or a network connection to the license server is required.

The license server will allow us to monitor usage and free up licenses for new users when people graduate and move to other institutions. To start we've been given 100 licenses. Let us know if you problems.

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SO HOW DO I GET THE MNOVA SOFTWARE?

This is the easiest part. Simply download the latest version from their website. Use the "Download and try it now" button.

http://mestrelab.com/software/

Should you have any problems with the installation there is a lot of information available on their website and if that fails give us a call and we can try to help. You will likely need administrator/root access.

WHERE DO I GET A LICENSE?

We have established an Mnova license server on the NMR website. Normally to use the server would require some configuring on the user's part to tell the program where to find the licenses, but to make things easier we have a configuration file that will do it all for you.

Direct your favorite browser to:

http://nmr.chem.ualberta.ca/downloads/mnova.zip

This should download a compressed file that contains all the preset configuration information regarding our license server. Please decompress the zip file.

When you start MNova, it will request information on what type of license you have. You will need to select the left option "Install" (see inset) because you'll have already downloaded the license configuration file. Once loaded, your copy of MNova will know how to 'check-out' an individual license and allow you to work. If you've already started a trial license and



want to switch to the 3-month license you'll need to find the license manager in the MNova software under the "Help" pull down menu. Use the manager to select the new license.

How do I use MNOVA?

Unlike VNMRJ there are no manuals or help files built into the software itself, but there is a great deal of information, documents and tutorials on their website.



GPU – University Server as Personal Cloud Storage

GPU (GENERAL PUBLIC UNIX) SERVER

The general public unix (GPU) server has been used on campus for decades. While a bit of an anachronism originally using command-line driven text based email (*e.g.* Pine), GPU now has new life. We can use the GPU server to remotely log into the university, and for cloud storage. GPU remains the central user and login system for the university (*i.e.* CCID).

Each student and faculty member is automatically given 24 Gb of storage space. Previously this capacity was much smaller and predominantly used for email and email attachments. Now it's like having a secure USB drive that you can open from anywhere in the world and don't have to remember to pack on trips.

Cloud storage provides disk space for files and content that can be accessed from multiple computer platforms, tablets, and mobile devices. You can use the programs in the previous chapters to put useful items such as presentations, images, or other types of digital data on the GPU server and then login into the server using your laptop or someone else's machine. You can then use FileZilla (or equivalent) to download the files to your current location. This is especially handy for working on documents at the University and then accessing them from home.

Instructions on how to use GPU

ITS (formerly AICT) has excellent details on how to use the server.

http://ist.ualberta.ca/selfhelp/howto/afs-howto/cls-login

The example uses the Windows program called "Putty". Putty is a Windows graphic interface to command line connections and access on remote computers. You can also use the instructions provided previously for other platforms.

GPU is also very secure with up-to-date encryption and intrusion detection. We therefore use GPU as a waypoint into departmental computers. Anyone with a University of Alberta CCID account is able to log into GPU, and from that computer then access computers behind the Chemistry department firewall. This is a two-step back-door into the department and quite handy. We don't have to worry about the trustworthiness of the connection; the screening is done at the GPU stage. That being said please be careful on borrowed machines such as public computers that your session is not logged.

General Link "How to's" from ITS – Terminals, VPNs, Google Aps, etc.

http://ist.ualberta.ca/selfhelp/howto

Of general interest are the FAQs provided by ITS in the link above.