Chemistry 2312 Honors Organic Chemistry Laboratory September 7, 2022 T. R. Hoye

Instructions for NMR data retrieval from the NMR lab server

FTP via, e.g., WinSCP (for Windows) or Transmit, CyberDuck, or Filezilla (for Mac) (a link to a WinSCP download can be found at <u>https://cse.umn.edu/chem/nmr-resources</u>) (Transmit, CyberDuck, and Filezilla can be downloaded from their sites (find via Google)

All applications are FREE to download

SFTP data connection information:

Server: <u>echo.chem.umn.edu</u> Login: zzzhon

Password: Rabi1944 Port: 22

As an alternative to using an FTP application:

For Mac Users

Initial Path, once connected to the server under "Go" and "Go To Folder" (command/opt+g), type "zzzhon"

For Windows Users

Select the icon "open directory/bookmark" (ctrl+o) and type "zzzhon" after the slash in the path

Search "/zzzhon" in the **Remote site** once you've accessed the server. Your data will be in the folder named "nc400" (a new 400 MHz spectrometer added in Sept 2020). FTP/copy/drag the *entire folder* of your sample name to your computer desktop (store in a folder there; include your name or initials in that folder name if you are using a desktop computer in 491a).

Open the folder with the **MNova** application. One convenient way is to drag-and-drop the entire folder into an already opened window in MNova.

FYI, you can later save any MNova main window as a PDF for insertion into your lab reports by "export to PDF" (as a single page).

Instructions for installing the MNova application on your laptop

reproduced on the following pages from the .txt files that are also on the 2312 website.

Those file names are:

Installation Instructions for Mnova - Mac - 2022.txt

Installation Instructions for Mnova - Windows - 2022.txt

for Macintosh [from "Installation Instructions for Mnova - Mac - 2022.txt"]

Notes:

- An account with administrator privileges is required to install this software.
- Before attempting to install Mnova, be sure you have an active internet connection.
- To download the Mnova license files you need to be logged in to your U of MN Gmail account.
- For the software to see the U of M's License Server, it needs to have a U of M IP address.
- If you are on campus, be sure to use the "eduroam" wireless connection to see the license server.
- If you are off campus you'll need to use VPN software to see the license server.
- (if needed, you can download the U of MN VPN software here: http://www.oit.umn.edu/vpn/)

Procedure:

-----step 1: download the software and license files-----

- download the latest Mnova software from http://mestrelab.com/download/mnova
- download the license file(s) for MestReNova Mnova registration
- NMR
- <u>https://drive.google.com/file/d/1Nd9zaStcp-HT0Q9hk9W5bxcQTuqevIzV</u>
- only download these two license files if you need to use qNMR or RM plug-ins
- <u>qNMR</u>
- https://drive.google.com/file/d/1_Iz1R59yzd-5Nd7PXYUtv3K96lRaUXDv
- Reaction Monitoring
- https://drive.google.com/file/d/1QuZ9AXNzR9FwBl4OXBy3xAQFFHWVSVWx

-----step 2: install software and license files-----

- Open MestReNova-XX.XXX.XXX.AMg on your desktop and copy MestReNova to the Applications folder.
- Copy the Manual to a folder of your choosing.
- Open MestReNova from the Applications folder.
- "MestReNova" is an application downloaded from the Internet. Are you sure you want to open it?
- Select "Open" (enter your admin username and password, if needed)
- You may see this message:
- "Mnova has detected that wrong permissions were set to the 'cache' folder. Mnova needs to be able to write to that folder in order to run. Do you want to allow Mnova to try fix it? You'll have to provide a user password with administrative privileges."
- Select "Yes" and (enter your admin username and password, if asked)
- The "Registration Wizard" window will appear.
- Choose, "Install" under the "If you already have your license file(s) press the button to install it (them)."
- Navigate to a license file and "Open". An example would be: Macintosh HD/Users/<
 Users/<
 Users/<
 NMR v1.12.lic
- This window with the following will appear when successful: "The following license files were successfully installed: Mnova: [University of Minnesota Campus NMR v1.12.lic] It is necessary to restart MNova for the changes to take effect"
- Repeat these two steps to install any additional license files.
- To make the license files active, close and re-open the MNova software.

-----step 3: verify the license files are active-----

• From the menu options, go to "File", "Help", "License Manager" or "Help", "License Manager..." and look for green or blue (happy) check marks.

Enjoy the software!

for PC [from "Installation Instructions for Mnova - Windows - 2022.txt"]

Notes:

- An account with administrator privileges is required to install this software.
- Before attempting to install Mnova, be sure you have an active internet connection.
- To download the Mnova license files you need to be logged in to your U of MN Gmail account.
- For the software to see the U of M's License Server, it needs to have a U of M IP address.
- If you are on campus, be sure to use the "eduroam" wireless connection to see the license server.
- If you are off campus you'll need to use VPN software to see the license server.
- (if needed, you can download the U of MN VPN software here: http://www.oit.umn.edu/vpn/)

Procedure:

-----step 1: download the software and license files-----

- download the latest Mnova software from http://mestrelab.com/download/mnova
- download the license file(s) for MestReNova Mnova registration
- NMR
- https://drive.google.com/file/d/1Nd9zaStcp-HT0Q9hk9W5bxcQTuqevIzV
- only download these two license files if you need to use qNMR or RM plug-ins
- <u>qNMR</u>
- https://drive.google.com/file/d/1_Iz1R59yzd-5Nd7PXYUtv3K96lRaUXDv
- Reaction Monitoring
- https://drive.google.com/file/d/1QuZ9AXNzR9FwBl4OXBy3xAQFFHWVSVWx

-----step 2: install software and license files-----

- Install MestReNova and accept all default options.
- If you previously installed the client software, it is recommended you update to the latest version.
- From the menu options, go to "Help", "Check For Updates" or "File", "Help", "Check For Updates"
- Open the MestReNova software.
- A "Registration Wizard" window will appear.
- You can manually open the "Registration Wizard" window by clicking on "Help", "Get\Install Licenses..." or "File", "Help", "Request Licenses"
- Click <Install> to continue.
- A "Select a License File" window will appear. Path to a license file and click < Open>.
- A "License File Installation" window should appear stating the file was successfully installed.
- Repeat these two steps to install all desired license files.
- To make the license active: Close and re-open the MNova software.

-----step 3: verify the license files are active-----

• From the menu options, go to "File", "Help", "License Manager" or "Help", "License Manager..." and look for green or blue (happy) check marks.

Enjoy the software.