## **Basic NMR Operation**

### Guide for the Bruker AV-III 600 MHz NMR Spectrometer TopSpin 3.X Instruction

Dr. Yun Qu

05/15/2024

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CDCI3-H

CUPS-PD

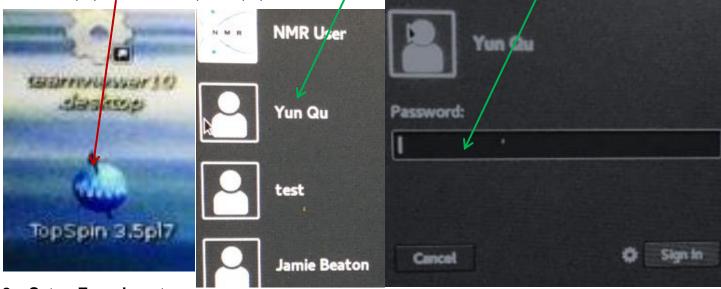
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## 1. Start TopSpin

Press any key to turn the screen back on. Click on your account and type in **password** in pop-up form to login. Click on TopSpin\_3.x icon to open TopSpin window



# 2. Setup Experiment

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Downloads

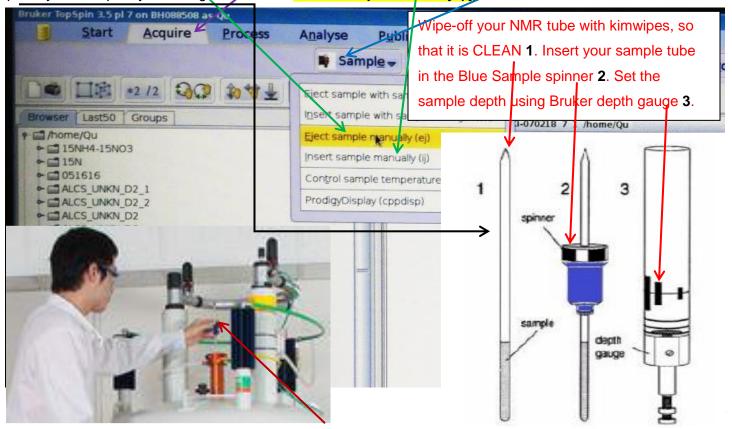
PSD-1-087-4

SD-1-087-5

(1). Create file, It can be done by Open an old dataset or Create Dataset. To Open an old dataset, in the Browser window to locate your data, right-click a dataset name, ruker TopSpin 3.5 pl 7 on BH088508 as Qu then select **Display** from the drop-down menu. Pro Start Acquire To Create Dataset, clicking on Start in the TopSpin menu bar, Create Dataset then click on Start Acquire Process Analyse Publish 200 \*2 Create Datase Browser Last50 Groups home/Qu \*2 /2 15NH4-15NO3 115N Last50 Groups Acquisition 051616 LCS UNKN D2 Spectrum . ALCS UNKN D2 1 LCS\_UNKN\_D3 COCL3 - 2 - zg 0 - CDCl3 BO-15N-HSQC INKN D2 2 ALCS BO-C13-CDCl3 ALCS UN Display DCI3-C13-QXI-091515 Display In New Window ► CALCS\_UN DCI3-H1-QXI-092016 DCI3-H1-QXI-102615 ► BBO-15 Display As 2D Projection UPS-PDF ► 📑 BBO-C1 Scroll to Active Dataset Jesktop CDCI3-C Fully Expand Selection Documents CDCI3-H

(2). Edit file, edc		8	6
type edc		Amplifier Control	Acquisition information
in the command line (at the bottom of TopSpin window)	For multi-receiver ex	periments several datasets are cr imber of receivers in the Options.	eated.
In the popup dialog box specify	NAME	QXI-070318	
on NAME	EXPNO	4	
EXPNO PROCNO	PROCNO	1	
select Use current parameters-	Use current paran	neters	
( or click on <b>Experiment</b>	O Experiment		Select
parameters from the drop-down menu).	Options		
type the dataset title in the <b>TITLE</b> box. Click on <b>OK</b> .			
(these can be done by typing <b>rpar</b> in the command line, then	CDCL3	111111111111111	MMMMMMM.
select experimental parameter			
set from the drop-down menu)			THURSDAY
3. Run Spectrum			More Info Help

(1). Exchange Sample Tube, click on Acquire in the TopSpin Menu bar, then click on select Eject sample manually (ej) from the drop-down menu, then take sealed CDCl<sub>3</sub> tube sample out and place your sample by following 1-3, click on Insert sample manually (ij).



A Solvent Descript A Solvent Descript Acetic acetic acid-d4 Acetone acetone-d6 C6D6 benzene-d6 CD2Cl2 dichlormethane-d2 CD3CN acetonitrile-d3 CD3CN_SPE LC-SPE Solvent (Acetonitrile) CD3OD_SPE LC-SPE Solvent (Methanol-d4) CDCl3 CN+D2O HPLC Solvent (Acetonitril/D2O) Tune Probe, click on V Tune c). Sample Spin, click on Spin (only spin the sample for 1D N	Acquire	Process	Analyse	Dublich	Solvents table	
Acetone acetone-d6 benzene-d6 cD2cl2 dichlormethane-d2 acetonitrile-d3 LC-SPE Solvent (Acetonitrile) Spectru 50/50, H CD3CN_SPE LC-SPE Solvent (Acetonitrile) CD3CN_SPE LC-SPE Solvent (Methanol-d4) CD3CN_SPE LC-SPE Solvent (Acetonitril/D2O) Tune Probe, click on V Tune c). Sample Spin, click on Spin (only spin the sample for 1D N	Sector Landstein	Liocos	Allaryse	Fuciisn	△ Solvent	Description
Acetone acetone-d6 C6D6 benzene-d6 CD2Cl2 dichlormethane-d2 CD3CN acetonitrile-d3 CD3CN_SPE LC-SPE Solvent (Acetonitrile) CD3OD_SPE LC-SPE Solvent (Methanol-d4) CD3OD_SPE LC-SPE Solvent (Methanol-d4)			Sampl	e- = = 100	Acetic	acetic acid-d4
Toups       CD2Cl2       dichlormethane-d2         2 Acquis       CD2Cl2       dichlormethane-d2         2 Spectru       Spectru       CD3CN_SPE         CD3OD_SPE       LC-SPE Solvent (Acetonitrile)         LC-SPE Solvent (Methanol-d4)         50/50, H       CD2Cl3         CD3OD_SPE       LC-SPE Solvent (Methanol-d4)         CDCl3       Chloroform-d         CH3CN+D20       HPLC Solvent (Acetonitril/D20)         Tune Probe, click on       V Tune         C). Sample Spin, click on       Spin         (only spin the sample for 1D N	and the second	and a second			Acetone	acetone-d6
Toups       CD2Cl2       dichlormethane-d2         CD3CN       acetonitrile-d3         CD3CN_SPE       LC-SPE Solvent (Acetonitrile)         CD3CN_SPE       LC-SPE Solvent (Methanol-d4)         CD3CN_SPE       Chloroform-d         CD3CN_SPE       Chloroform-d         CH3CN+D20       HPLC Solvent (Acetonitril/D20)         Tune Probe, click on V Tune C). Sample Spin, click on Spin (only spin the sample for 1D N	12 200	Ltop	(AAA	TH HA	C6D6	benzene-d6
2 Acquis       CD3CN_SPE       LC-SPE Solvent (Acetonitrile)         Spectrur       Spectrur       CD3CN_SPE       LC-SPE Solvent (Methanol-d4)         COCI3       Chloroform-d         FOUCH       CH3CN+B20       HPLC Solvent (Acetonitril/D20)         Tune Probe, click on V Tune C). Sample Spin, click on Spin (only spin the sample for 1D N			4. A. A. A.	Zu WV (	CD2Cl2	dichlormethane-d2
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CD30D_SPE       LC-SPE Solvent (Methanol-d4)         COCI3       Chloroform-d         CH3CN+D20       HPLC Solvent (Acetonitril/D20)         Tune Probe, click on V Tune C). Sample Spin, click on V Spin C (only spin the sample for 1D N				CD3CN SPF	LC-SPE Solvent (Acetonitrile)	
CH3CN+D20       HPLC Solvent (Acetonitril/D20)         Tune Probe, click on V Tune C). Sample Spin, click on Spin (only spin the sample for 1D N			-	spectrur	CD30D_SPE	LC-SPE Solvent (Methanol-d4)
Tune Probe, click on V Tune c). Sample Spin, click on U Spin (only spin the sample for 1D N				50/50, H	CDCI3 N	chloroform-d
Tune Probe, click on V Tune c). Sample Spin, click on U Spin (only spin the sample for 1D N					CH3CN+D20	
en click on <u>Gain</u> , <u>f).</u> Run Spectrum, to record spectrum, click on <u>Ga</u>	spin on mu	ltidimension	al NMR) <b>d)</b> .	. Shim, clicl	k on 🗟 Shim 🗸	to perform topshim e). click on Prosol

### 4. Data Processing

- (1). Open Dataset, Dataset can be opened by a) or b).
- a). Clicking on the Start in the TopSpin Menu bar, then click on Open Dataset, your dir/files will appear

<u>S</u> tart <u>A</u> cquire	<u>P</u> rocess A <u>n</u> alyse	P <u>u</u> blish <u>V</u> iew <u>M</u> anage
Create Dataset	d Dataset 🔄 Open <u>D</u> ataset	🖡 Paste Dataset 🔡 Read Pars.
Browser Last50 Groups	<b>U</b>	Display
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	<b>3-17-06-Qu</b>	
	Desktop     Jun19-2015-Qu	

select dir/file which you want to process, then click on **Open** 

J N	Jun22-2015-Qu	
Open = Displ Print = Print t	contains several EXPNO / PROCNO pairs,corresp ay the selected data set. he data set list. he data set list in a file.	onding to several raw/processed data files.
EXPNO / PRO	CNO dim pulseprog "title"	
2/1 3/1	1d2g30"1H sensitivity sample / in CDCI3"1d2gflqn"19F sensitivity sample / in C6D6"1d2gfhigqn.21d2gpg30"13C sensitivity sample / in C6D6"1d2gpg30	
Show din	n/pulseprog/title next time	Open Print Save Cancel

locate your data and right-click on a dataset name, and choose <b>Display</b> from the dram down many		
from the drop down menu (2). Process Spectrum,	-	
Click on the Process	2 ilay ilay In New Window	

then click on **Proc. Spectrum** there are a few options to choose from the drop-down menu

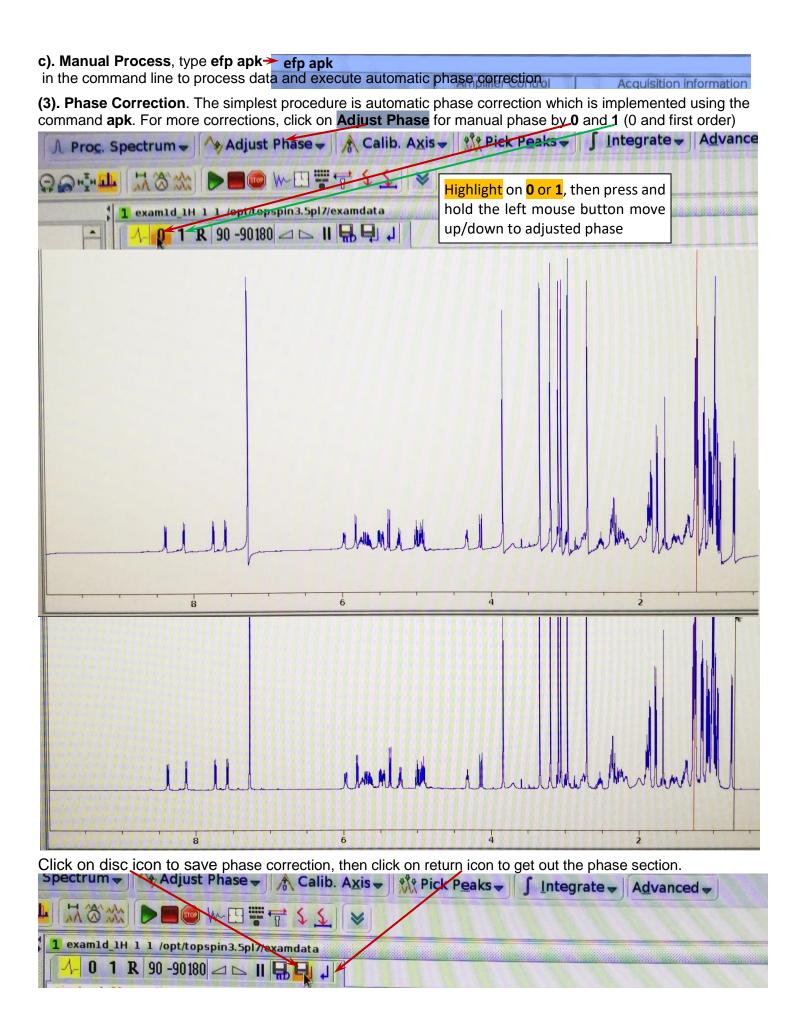
	<u>S</u> tart	<u>A</u> cquire	Process	Analys	e P <u>u</u> blish	<u>V</u> iew	<u>M</u> anage	0	
	Λ	Spectrum 🗲	Adjust P	hase 🗢	Å Calib. A <u>x</u> is <del>v</del>	M P	ick P <u>e</u> aks <del>▼</del>	∫ Integrate <del>→</del>	A <u>d</u> vanced <del>-</del>

a). Auto Process, for easy and quick, Select xaup to auto process spectrum with peak picking and integration.

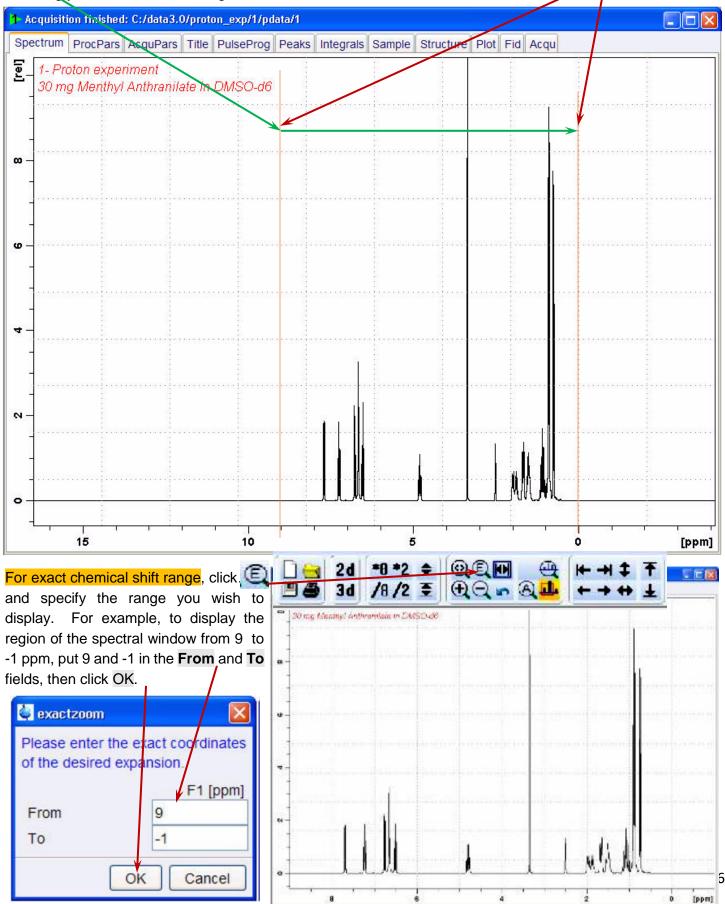
<b>V</b>	•	Configure Standard Processing (proc1d) Window Multiplication (wm)	TT S S S						
		Fourier Transform (ft) Eourier Transform Options (ftf)	Title PulseProg Peaks Integrals Sample Structure						
		Start Automation AU Program (xaup)							

b). Standard Process, Select proc 1d (2d, 3d), then fill in drop-down table to process spectrum

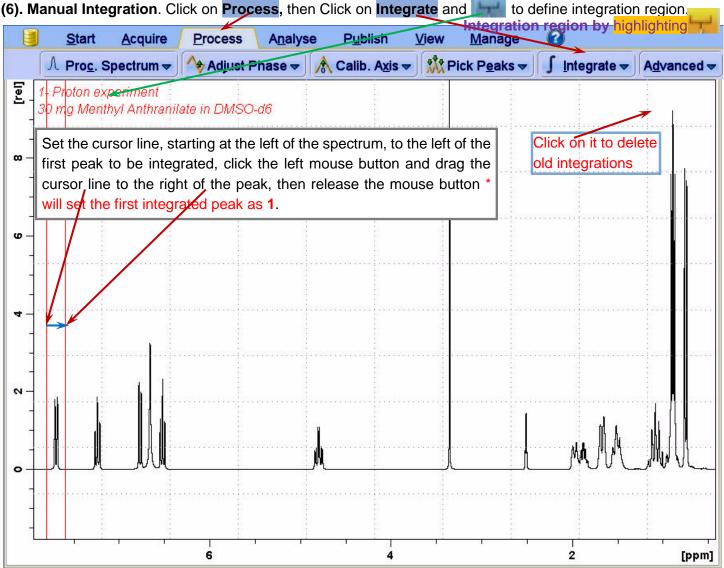
Start Acquire Proc	ess	Analys	e Pu	blish	View	Manage	. 0	
		TR	roc. Spec	ctrum 🚽	Adjus	st Phase		ib. A
12 +2 /2 20 20 10 10	1	00	Configure	Standard	Processing	(proc1d)	₩ 🖶 🖇	
Last50 Groups			Manufacture and American	A <u>u</u> ltiplicatio		Foria	• 1. *	-
procld							- d ×	ulseP
Press 'Execute' to process the cun Press 'Save' to just change the pro Changed options will be effective v one-click 'Proc. Spectrum' button.	cess	ing options.	•			*		
Exponential Multiply (em)		LB [Hz] =	10000	0.3				
Fourier Transform (ft)							1121	
Auto - Phasing (apk)							E.	
Set Spectrum Reference (sref)								
Auto - Baseline Correction (absn)		Include int	egration =	no				
Plot (autoplot)		LAYOUT =		+/1D_H	xwp		-	
							The second s	



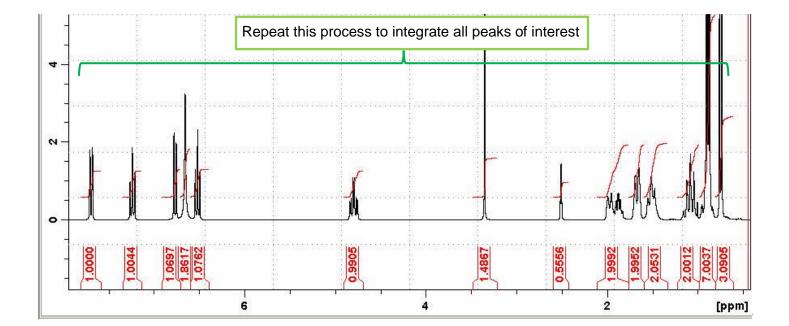
(4). Optimizing the Spectral Width. To display a specific region of your spectrum hold the left mouse button and drag your mouse over the region of interest.

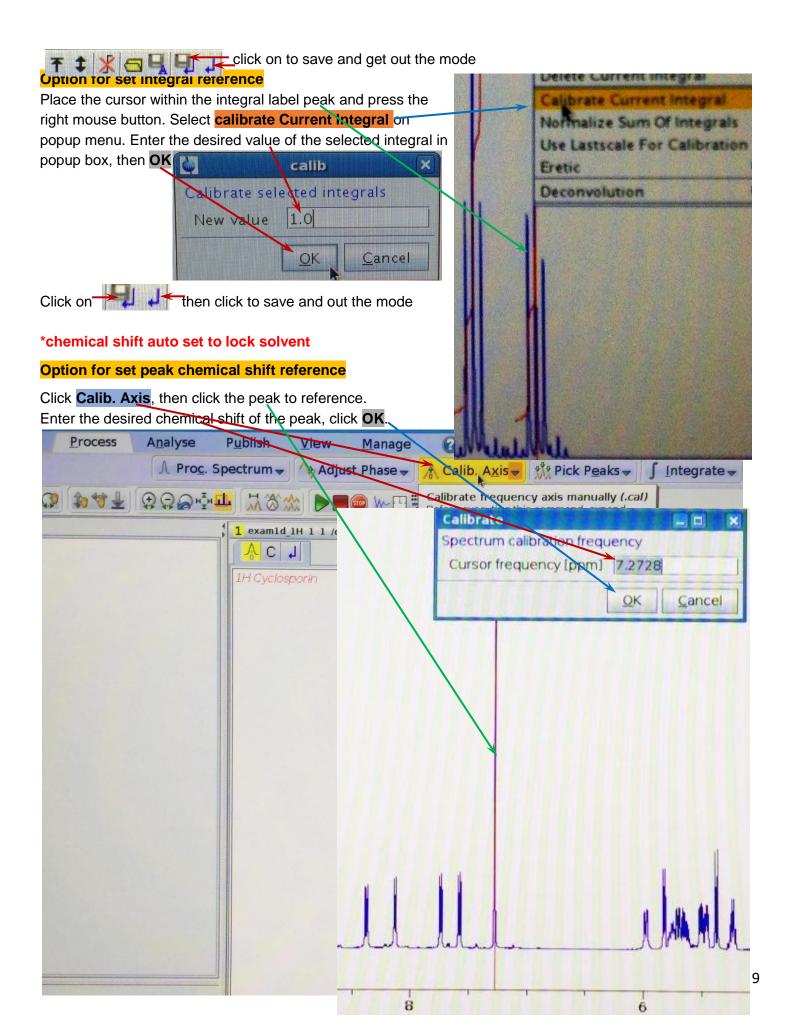




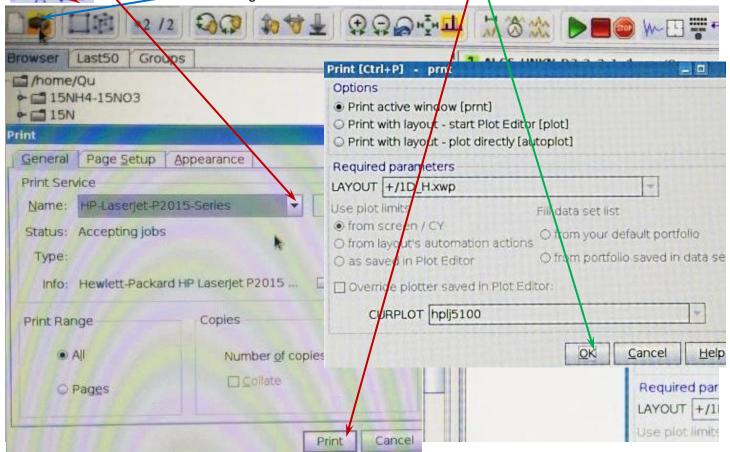








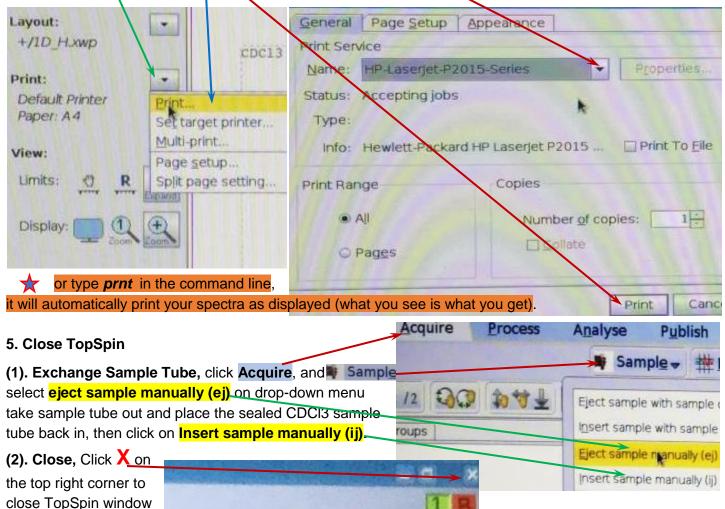
(7). Plotting a). Quick print, click on printer icon, then click ok on drop-down box, another Print box

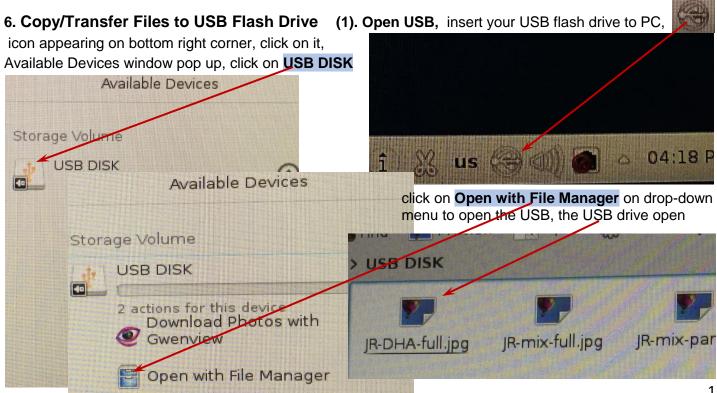


b). Plot Editor, click on Publish, then click on Plot Layout. Editing by a page at the left (active/select menu)

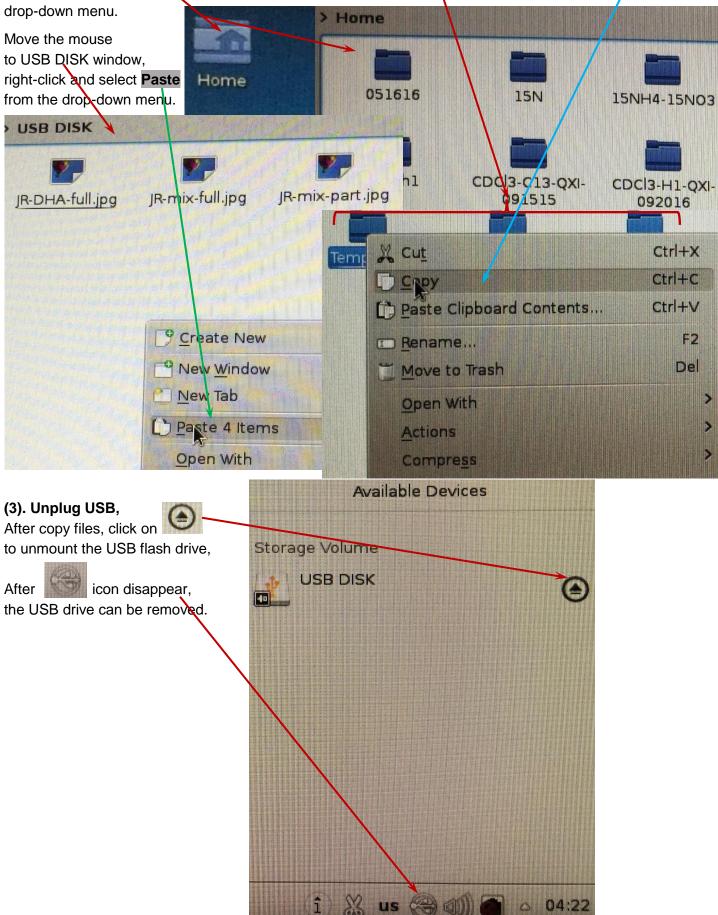
Analyse	Publish View Manage Copy Print - Plot Layout PDF - E-Mail Mobile -
ାହନ୍ଦ୍ର କ	Switch to plot layout editor         The spout currently set for this data set is used. The Limits buttons help to quickly choose axis limits:         ALCS_UNKN_D2_2_1_frame         Spectrum       PacPars         Acqui
	Layout: +/ID_Hxwp Print: Default Printer Paper: A4 View: Limits: R. R. Line Display: R. R. Line Click here to insert new ele Standard NMR MR MR MR MR MR MR

Print, click on ▼ and select Print... on drop-down list, click on ▼ to select HP-Laserjet-P2015-Series in Name on popup Print box, then click on Print





(2). Copy Files, click Home folder on desktop, then select the file/files, right-click and select Copy from the



# 7. Logout

1

Click on bottom left corner man, more icons appear on the bottom bar, place pointer on Log out on popup icons on the left column to logout your account. The screen shows as

, then select

Konsole TopSpin 3.5pl7 2 **Recently Used** orites Applications Computer Log out Lock Switch user NMR Super User Yun Qu Sleep NMR User Hibernate .... Pfizer Pha Restart ie Beaton Shut down Farrell N **VynnVisio** idorov L . **avorites** Applications .... CentOS 🛤