

Selective 1D experiments with IconNMR

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1. Contact BioNMR core staff Minli Xing (mlxing@umich.edu) to grant supervisor permission to your account on the 600 MHz NMR in Mary Sue Coleman Hall.
2. Login to your account, enter your sample information, in the **experiment drop down menu**, scroll down to the bottom and then select the selective 1D experiment you want to run. SELCOGP for selective 1D COSY, SELNOGPZS.2 for selective 1D NOESY, SELDIGPZS for selective 1D TOCSY and SELROGP for selective 1D ROESY.

N	UM_PROTON_1D	1H PROTON	
C	HMOCGP	sw opt.	HMOC with gradients (magn. mode)
C	HSQC	sw opt.	HSQC sens. improved with gradients (e/a TPPI)
C	HSQCEDETG	sw opt.	edited HSQC with gradients (e/a TPPI)
C	HMOCGPML	sw opt.	HMOC-TOCSY with gradients (magn. mode)
C	HMOCBI	sw opt.	HMOC using BIRD pulse (magn. mode)
C	HMOCBIPH	sw opt.	HMOC using BIRD pulse (States-TPPI)
C	HMOC	sw opt.	HMOC (magn. mode)
C	HMOCPH	sw opt.	HMOC (States-TPPI)
C	HMB	sw opt.	HMB with gradients
C	HMBCLPND	sw opt.	HMB with low pass J-filter (magn. mode)
C	HSQCETGPML	sw opt.	HSQC-TOCSY with gradients (e/a TPPI)
C	HSQCEDETGPSISP_ADIA	1H-13C	multiplicity edited HSQC with gradient selection BF1 >= 700 MHz
C	HSQCETGP	sw opt.	HSQC with gradients (e/a TPPI)
C	HSQC_TOCSY_ADIA	1H-13C	HSQC-TOCSY with gradient selection BF1 >= 700 MHz
C	HCCOSW	sw opt.	CH-correlation
C	HCCOLOCSW	sw opt.	COLOC
C	SELCOGP		selective COSY experiment w/gradients
C	SELNOGPZS.2		selective NOESY experiment w/gradients
C	SELDIGPZS		selective TOCSY experiment w/gradients
C	SELROGP		selective ROESY experiment w/gradients

3. Once you select the selective experiment, IconNMR will load two experiments for you, the first one is a 1D 1H experiment, the second one is your selective 1D experiment, you may modify parameters such as number of scans, and then click **submit** to run the experiments. A window will pop up and click **OK** to continue.

11	2	Available						
Available	/icondata	Aug16-2022-mlxing	20	CDCI3	chloroform-d	N PROTON	1H experiment	
Available	/icondata	Aug16-2022-mlxing	21	CDCI3	chloroform-d	C SELDIGPZS	selective TOCSY experimen	
F2	/icondata	Aug16-2022-mlxing	20					

Info

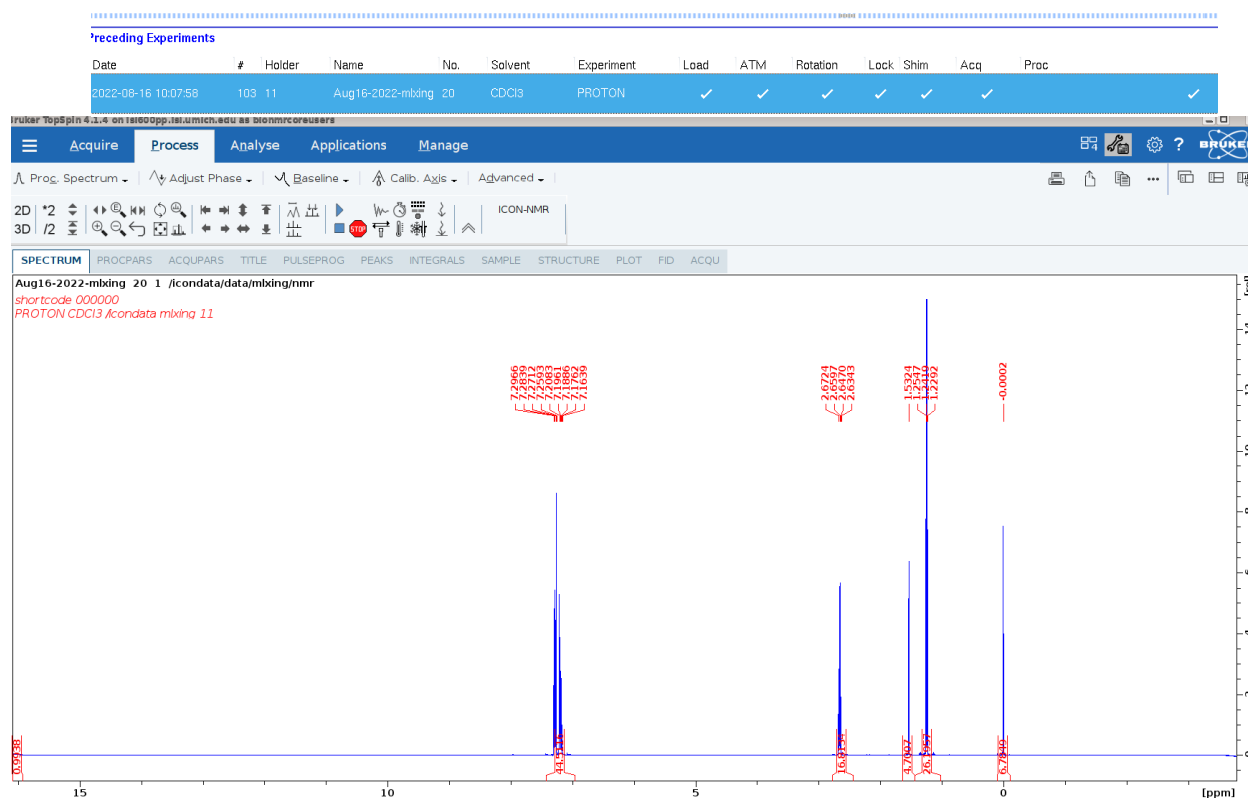
You have selected a selective experiment for submission where the corresponding region file entry has not been defined.

Please save a region file in the completed reference experiment first.

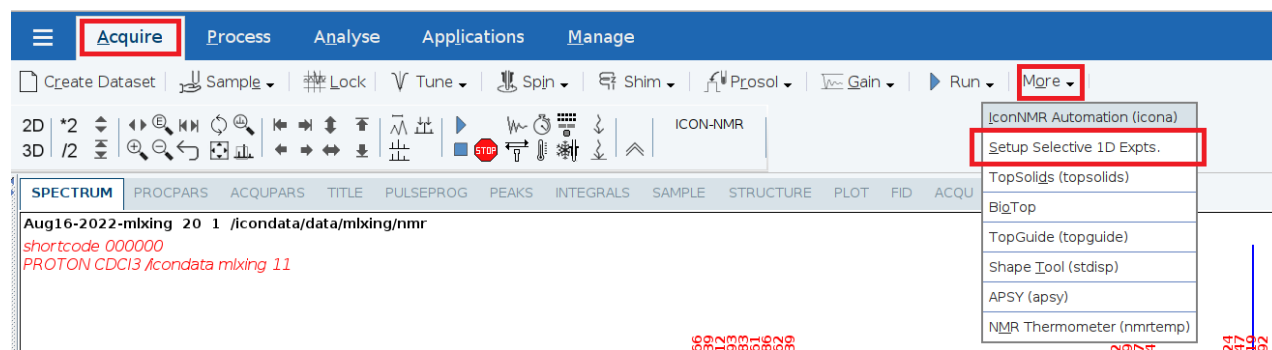
Click OK to go there automatically

OK Cancel

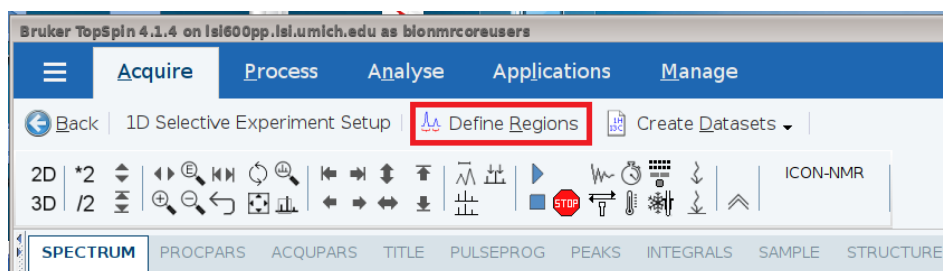
- The 1D 1H experiment will run first, once it is done, double click the 1D 1H experiment under the **Preceding Experiments** window, and topspin will automatically display your 1D 1H spectrum.



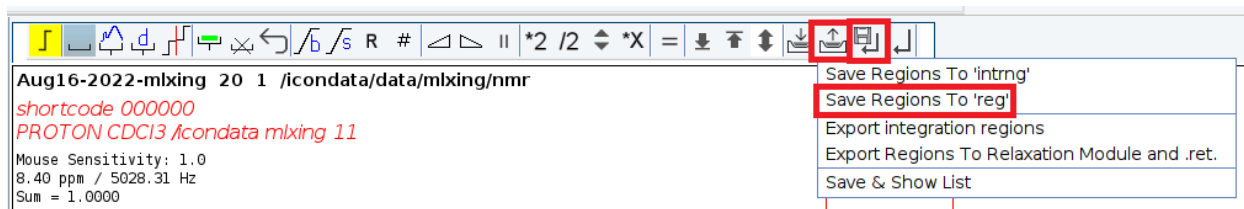
- Under the **Acquire** tab, click **More**, and select **Setup Selective 1D Expts.** in the drop down menu.



- A new menu will appear, click **Define Regions**.



- Click the **Save Regions To 'reg'** icon to save the regions you defined. Then click the **return, save regions** icon.



- Go back to IconNMR, if you defined more than one regions, add more selective 1D experiments so that the number of the selective 1D experiments matches the number of regions you defined. The F2 reference spectrum for all your selective experiments is the 1H experiment you just collected. Click on **submit** to submit all selective 1D experiments.

11 3 Available									
Finished	/icondata	Aug16-2022-mixing	20	CDC13	chloroform-d	N PROTON	1H experiment		
Available	/icondata	Aug16-2022-mixing	21	CDC13	chloroform-d	C SELDIGPZS	selective TOCSY experimen		
F2	/icondata	Aug16-2022-mixing	20						
Available	/icondata	Aug16-2022-mixing	22	CDC13	chloroform-d	C SELDIGPZS	selective TOCSY experimen		
F2	/icondata	Aug16-2022-mixing	20						