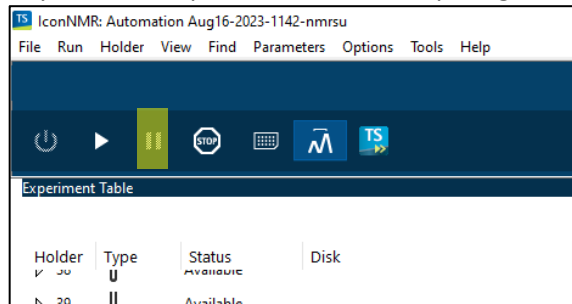


## Selective 1D Experiments in ICONNMR: 1D NOESY, 1D TOCSY

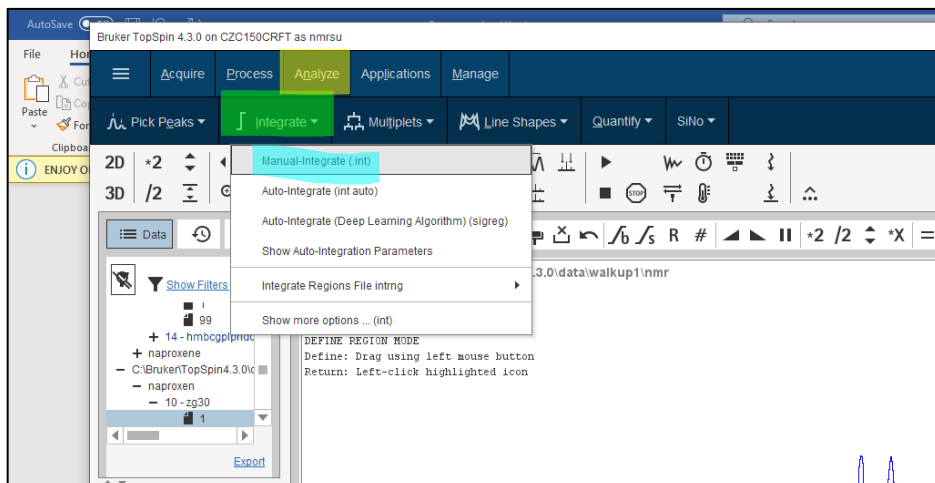
- Setup and submit a routine 1H NMR experiment in ICONNMR.
- **After the sample is in the magnet** and collecting data, hit **Pause** button. This way the autosampler won't eject your sample while you complete the setup of your 1D NOE experiment. Allow your 1D 1H spectrum to finish acquiring.



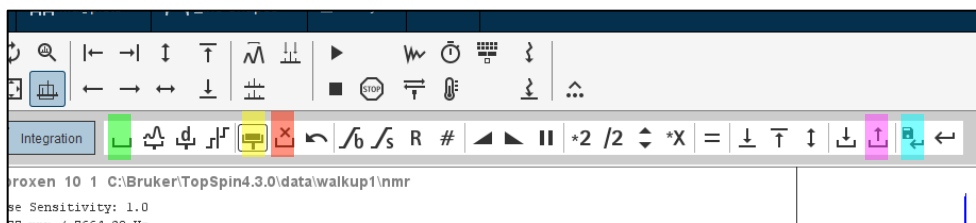
- Double click on your experiment in the **history list** to load 1D 1H spectrum. You will be automatically taken to the Topspin window. You should see your 1H NMR processed and loaded.

Date	Holder	Name	No.	Solvent	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig	Remarks
2023-08-18 09:53:37	41	naproxen	10	DMSO	PROTON	✓	✓	✓	✓	✓	✓	✓	walkup1	C:\Bruker\TopSpin4.3\data\walkup1	ref. reference peak not found default calibration done.	
2023-08-16 22:52:01	49	naproxen-NQ	14	DMSO	HMBCGP	✓	✓	✓	✓	✓	✓	✓	walkup1	C:\Bruker\TopSpin4.3\data\walkup1		

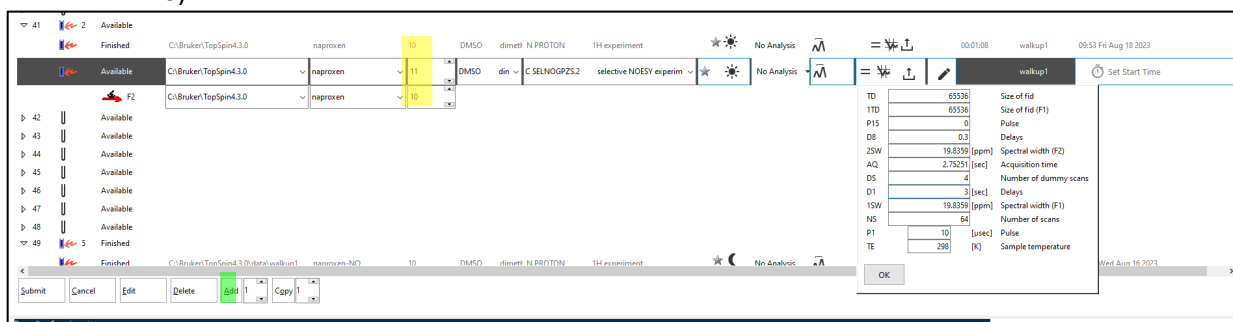
- In Topspin Select **Analyze** -> **Integrate** and select **Manual-integrate**



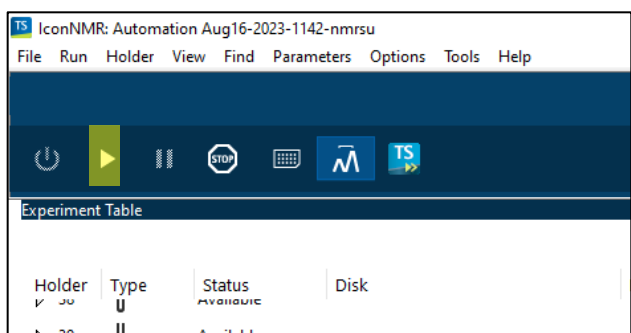
- Click the **select/deselect all regions button** and then click the **delete selected regions button** to delete all integrals.
- Zoom in to the peak of interest that you will irradiate.



- Click the **integration button** to highlight it and then drag over the peak of interest then click **save/export integration regions** and select “**save regions to reg**” then **return/save regions button**.
- Return to the Iconmr window.
- Highlight your experiment and click the **Add** button and select the SELNOGPZS.2 for 1D NOESY (or SDELDIGPZS for 1D TOCSY). Make sure the **F2 reference** spectrum for your selective experiment is the 1H experiment you just collected (typically experiment number 10).



- Click the = button to edit parameters for either NOESY or TOCSY:
  - NOESY: D1=3, D8 (NOESY mixing time) 0.3 – 0.5 sec
  - TOCSY: D9 = 0.03 (for 2-3 bonds) or 0.08 sec (long range- full spin system)
- Highlight experiment and hit **submit** button to queue your experiment and then click the **play** button to start the acquisition.



END!