

A5 ICON NMR Short Acquisition Instructions

1. Launch **Topspin** from the desktop and log into your advisor's research account.
2. Select **Automation** on the new Icon NMR pop-up and then choose the account name for saving data (no password required).
3. In the center of Automation screen, right click on **Holder #1** and then select **Add**.
4. Type in the **Sample Name** and **Experiment #** (e.g. 10), select the **Solvent** and **NMR Experiment**. See the poster above the instrument for the experiment definitions. Parameters can be changed by clicking the blue/yellow icon.
5. Repeat step 4 to add any additional experiments for that sample. When done right click the top of the queue bar and select **submit**.
6. Click **Start** at the top left to begin automation (then click **Start** again in the new window).
7. After a few seconds click **OK** to begin the **sample eject**. Remove the std. sample.
8. Once you have loaded your sample into the magnet, click **OK** to begin **sample insert**.
9. All queued experiments for that sample will now run and be automatically saved.
10. When all experiment have been completed, Click **Stop** (Next to *Start*) and close **IconNMR**.
11. Type *ej* in the **Topspin command line** to eject your sample.
12. Replace your sample with the standard and type *ij* in the **Topspin command line** to insert it.
13. **Close Topspin** by clicking the **X** at the **TOP RIGHT**.
14. Launch **gFTP** from the desktop and in bookmarks select **FTP Server**. On the left side of the screen is the **A5 host PC** folders, on the right is the **ASDS Server** folders. Select the destination folder on the right and what you want to transfer from the left, and then click the right arrow in the center bar. **Close gFTP**.

PROTONRO	H detection with rotation
C13CPD	C detection with ¹ H decoupling and NOE enhancement (Typical Carbon)
C13IG	Quantitative C Detection
COSYGPSW	“routine” gradient COSY: H-H correlations; usually just 2 to 3 bond couplings
COSYGPDPF HSW	Gradient COSY: Minimizes strong singlets and solvent peaks via double-quantum filtering. Enables measurements of H-H coupling constants.
MLEVPHSW	TOCSY: H-H correlations based on couplings
HSQCEDETG PSISP	“routine” gradient multiplicity edited HSQC: H-C 1-bond correlations, -CH ₂ - inverted
HMBCETGPL 3ND	“routine” gradient HMBC: H-C n-bond correlations, 2 and 3-bond (usually), with 3-fold 1-bond filter
NOESYPHSW	2D-NOESY: H-H correlations based on proximity (also for exchange)
ROESYPHPR	2D-ROESY: H-H correlations based on proximity; for intermediate MW (1000-3000 MW)