NMR Sample Manager for TopSpin: Quick Reference

Documentation: nmr-samples.github.io/topspin   **Web app:** nmr-samples.github.io/online

Record what's in the magnet alongside your experiment data. All fields are optional – annotate as much or as little as you need. Sample metadata is stored as JSON files in your data directories. No data leaves your computer.

Getting Started

Type `samples` in TopSpin to open the Sample Manager. The window shows a timeline of your experiments, a sample list, and a searchable catalogue.

Commands

Use these instead of the standard TopSpin commands. They perform the same physical operations and additionally capture sample metadata.

Command	Replaces	What it does
`ija`	`ij`	Injects sample (lift air off), then opens annotation form
`eja`	`ej`	Ejects sample (lift air on), closes annotation with timestamp
`sxa 15`	`sx 15`	SampleJet: exchanges sample then opens annotation form
`sxa ej`	`sx ej`	SampleJet: ejects and returns to storage, closes annotation

What You Can Record

Everything is optional. Fill in what's relevant for you.

Section	Fields
People	Users, research groups
Sample	Label, components (names, concentrations, isotopic labelling)
Buffer	pH, solvent, chemical shift reference, buffer components
NMR Tube	Diameter, tube type (regular, Shigemi, solid-state rotor, …), sample volume
Lab Reference	Sample ID, lab book entry
Notes	Free-form text

Key Features

Retrospective annotation: Right-click experiments in the timeline to create an annotation at any time.

Duplicate: select a sample and click Duplicate to copy it as a template (ideal for titration series).

Catalogue: search across all your data directories for samples by user, buffer, components, or any text.

Timeline: see everything you've run within a directory. Double-click to open an experiment in TopSpin.

One active sample: creating a new sample automatically marks the previous one as ejected.

Feedback Is Welcome!

Please send any feedback and comments to c.waudby@ucl.ac.uk.
Alternatively, raise an issue at https://www.github.com/nmr-samples/topspin/.