NOV 30, 2023

OPEN ACCESS

DOI:
dx.doi.org/10.17504/protocols.io.8epv5x2rng1b/v1

Protocol Citation: NAN KB, John Glushka, Mario Uchimiya, Saraa Al Jawad, Christopher Esselman, Leandro I Ponce, Laura Morris, Arthur Edison 2023. hsqc-tocsy_metab.nan. **protocols.io** https://dx.doi.org/10.17504/protocols.io.8epv5x2rng1b/v1

Protocol status: Working
We use this protocol and it's working

hsqc-tocsy_metab.nan

Forked from hsqc-tocsy.nan

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NAN support at UGA

DISCLAIMER

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ABSTRACT

This is a protocol for running the Bruker pulse program "hsqcdietgpsisp.2".

GUIDELINES

This protocol intends to provide concise instructions to carry out the experiment. For more comprehensive information, see Bruker's documentation "Basic NMR Experiments" by clicking ? → Manuals (docs) on the menu bar on TopSpin. See also "Pulse Program Catalogue. 1D/2D" for the details about the pulse program used in this protocol.

Created: Sep 13, 2023

Last Modified: Nov 30, 2023

PROTOCOL integer ID: 87729

Funders Acknowledgement:
National Science Foundation
Grant ID: 194670

BEFORE START INSTRUCTIONS

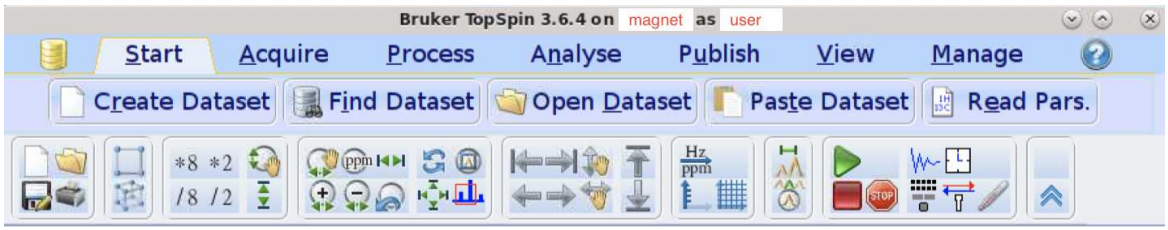
This protocol assumes:

- Your sample is loaded, locked, tuned for both proton and carbon channels, and shimmed in the magnet
- The calibrated 90° pulse value for proton (i.e., P1) for the sample has been collected

Create a new dataset

1

1.1 On the menu bar on TopSpin, click on
Start → Create Dataset



(This protocol uses TopSpin 3.6.4, and the interface may look different on other TopSpin versions.)

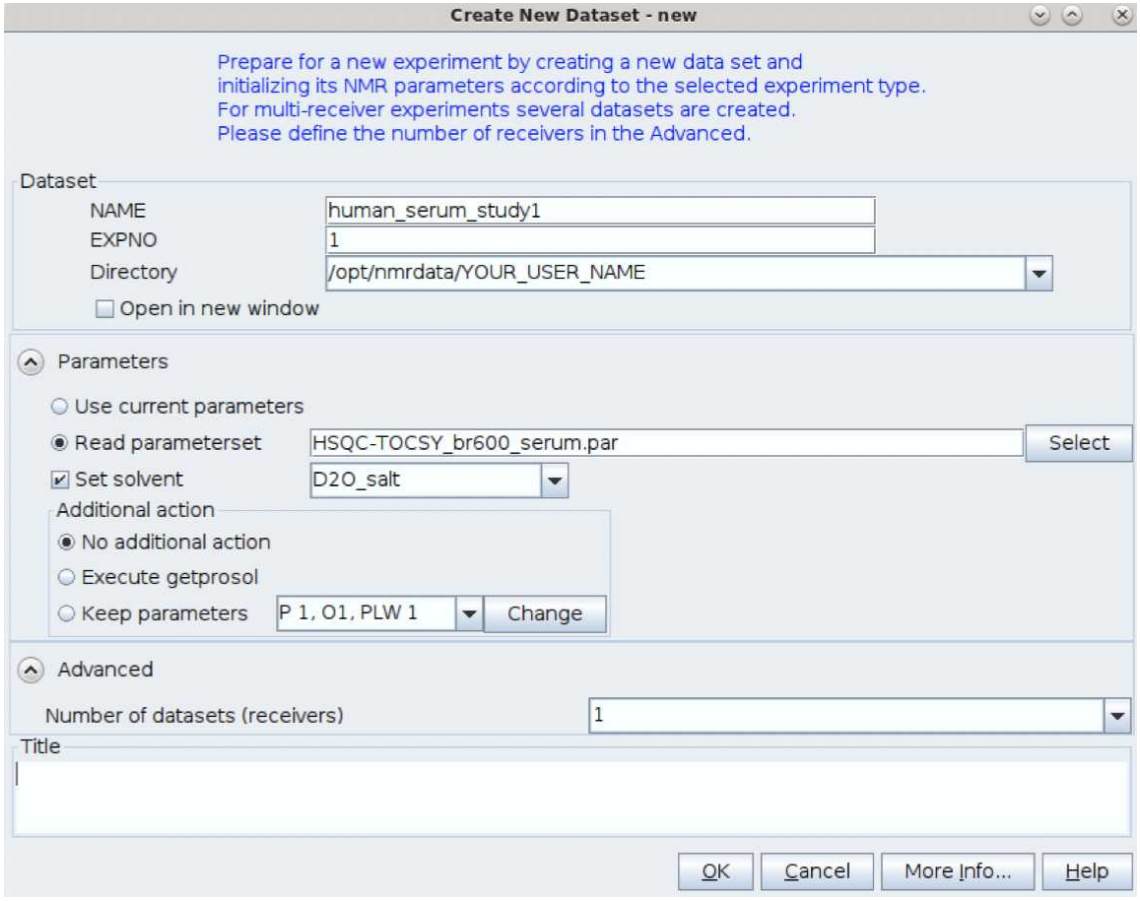
> **Note**
>
> You can also use the **new** command in the command line to do this step.

1.2 Enter

- **NAME**: Name of a set of datasets (e.g., human_serum_study1). Use a single string
- **EXPNO**: Dataset number. Use a positive integer

Select

- **Directory**: Your directory



Note

Your new dataset will be stored in **Directory/NAME/EXPNO**.

1.3 Select
Read parameterset

Click the button
Select

1.4 A new window opens. On the right top bar, select
Source = /opt/NAN_METAB/par

In the list, select the one you want to use:

For serum and plasma samples:

- **HSQC-TOCSY_br600_serum.par**: Parameter set using an acquisition mode "traditional planes"
- **HSQC-TOCSY_NUS_br600_serum.par**: Parameter set using an acquisition mode "non-uniform sampling (NUS)". Higher resolution on the indirect dimension
-

For urine samples:

- **HSQC-TOCSY_br600_urine.par**: Parameter set using an acquisition mode "traditional planes"
- **HSQC-TOCSY_NUS_br600_urine.par**: Parameter set using an acquisition mode "non-uniform sampling (NUS)". Higher resolution on the indirect dimension

Note

Parameter set names in the list vary between spectrometers
(e.g., HSQC-TOCSY_br800_serum.par).

Click
OK

1.5 Click
OK

Acquire a spectrum

2 Go to the "**USE DEFAULT**" tab below to proceed with the default optimized parameters.

STEP CASE

Use default parameters

6 steps

This step case uses the default optimized parameters to acquire a spectrum.

3

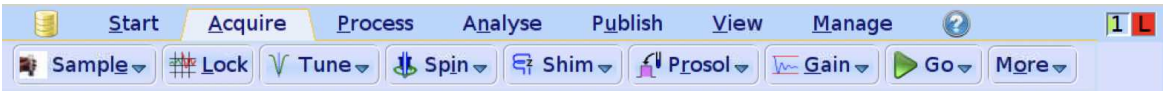
3.1 Load the calibrated P1 using the following command in the command line.

```
getprosol 1H [calibrated P1 value] [power level for P1]
```

(e.g., getprosol 1H 10.01 -7.45)

> Note
>
> **[power level for P1]** varies between spectrometers. Never use a wrong **[power level for P1]**.

3.2 Click on
Acquire → Gain
in the menu bar to automatically set the receiver gain.



> Note
>
> You can also use the **rga** command in the command line.

3.3 Click
Go
in the menu bar to acquire a spectrum.

> Note
>
> You can also use the **zg** command in the command line.

3.4 After the run, click on
Process → Proc. Spectrum
in the menu bar to execute an automated processing macro.

3.5 If you want to modify parameters to improve your spectrum, go to step #2 and move to the step case "MODIFY PAR".