


Apr 29, 2024

 tocsy\_metab.nan

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DOI

[dx.doi.org/10.17504/protocols.io.x54v92meml3e/v1](https://dx.doi.org/10.17504/protocols.io.x54v92meml3e/v1)




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**Protocol Citation:** NAN KB, John Glushka, Mario Uchimiya, Saraa Al Jawad, Christopher Esselman, Leandro I Ponce, Laura Morris, Arthur Edison 2024. tocsy\_metab.nan. [protocols.io](https://protocols.io) <https://dx.doi.org/10.17504/protocols.io.x54v92meml3e/v1>

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**Protocol status:** Working

**We use this protocol and it's working**

**Created:** April 08, 2024

**Last Modified:** April 29, 2024

**Protocol Integer ID:** 97922

**Keywords:** NAN, NMR, Metabolomics, TOCSY



**Funders Acknowledgement:**  
**National Science Foundation**  
**Grant ID: 194670**

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## Abstract

This is a protocol for running the Bruker pulse program "dipsi2gpghpr" for metabolomics samples.

## 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.

## Before start

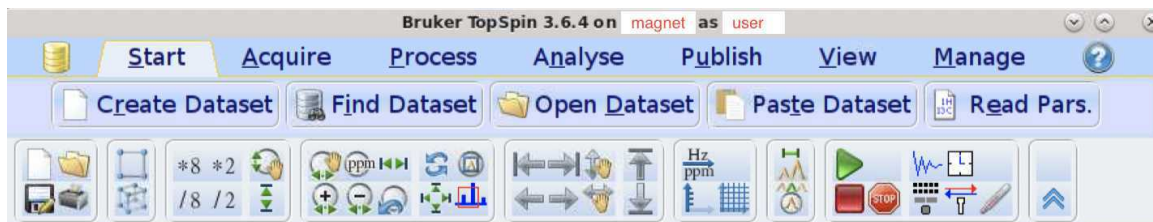
This protocol assumes:

- Your sample is loaded, locked, tuned, 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.



**Create New Dataset - new**

Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the Advanced.

**Dataset**

NAME: human\_serum\_study1  
EXPNO: 1  
Directory: /opt/nmrdata/YOUR\_USER\_NAME  
☐ Open in new window

**Parameters**

☐ Use current parameters  
☒ Read parameterset: TOCSY\_br600\_serum.par **Select**  
☒ Set solvent: D2O\_salt  
Additional action:  
☒ No additional action  
☐ Execute getprosol  
☐ Keep parameters: P 1, O1, PLW 1 **Change**

**Advanced**

Number of datasets (receivers): 1

Title:

**OK** **Cancel** **More Info...** **Help**

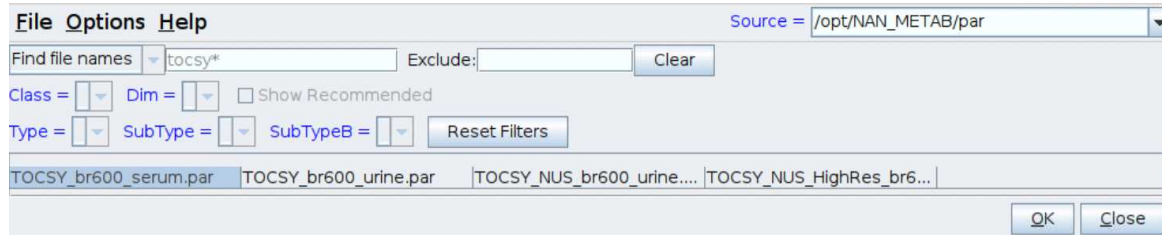
### Note

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:

- **TOCSY\_br600\_serum.par**: Parameter set optimized for serum samples.

For urine samples:

- **TOCSY\_br600\_urine.par**: Parameter set optimized for urine samples.
- **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., 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.

3

### STEP CASE

Use default parameters: 6 steps



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

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



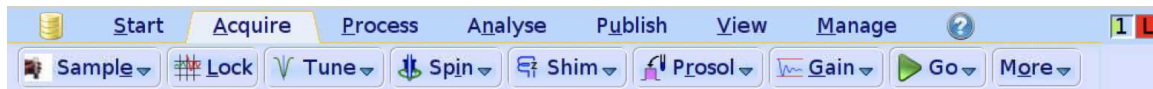
```
getprosol 1H [calibrated P1 value] [power level for P1]
```

(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.

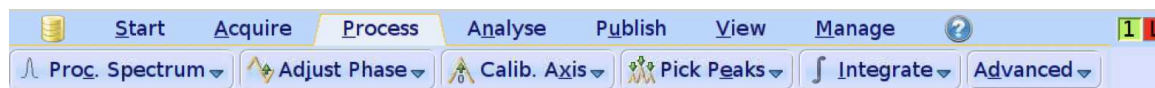
#### Note

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**".