Apr 29, 2024

tocsy_metab.nan

Forked from tocsy.nan

DOI
dx.doi.org/10.17504/protocols.io.x54v92meml3e/v1

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NAN support at UGA
Network for Advanced NMR

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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://dx.doi.org/10.17504/protocols.io.x54v92meml3e/v1**

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

Disclaimer

Abstract

This is a protocol for running the Bruker pulse program "dipsi2gpphpr" 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

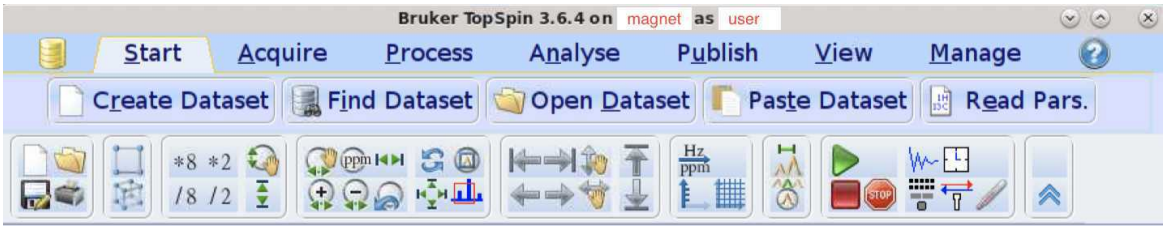
This protocol assumes:

- 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



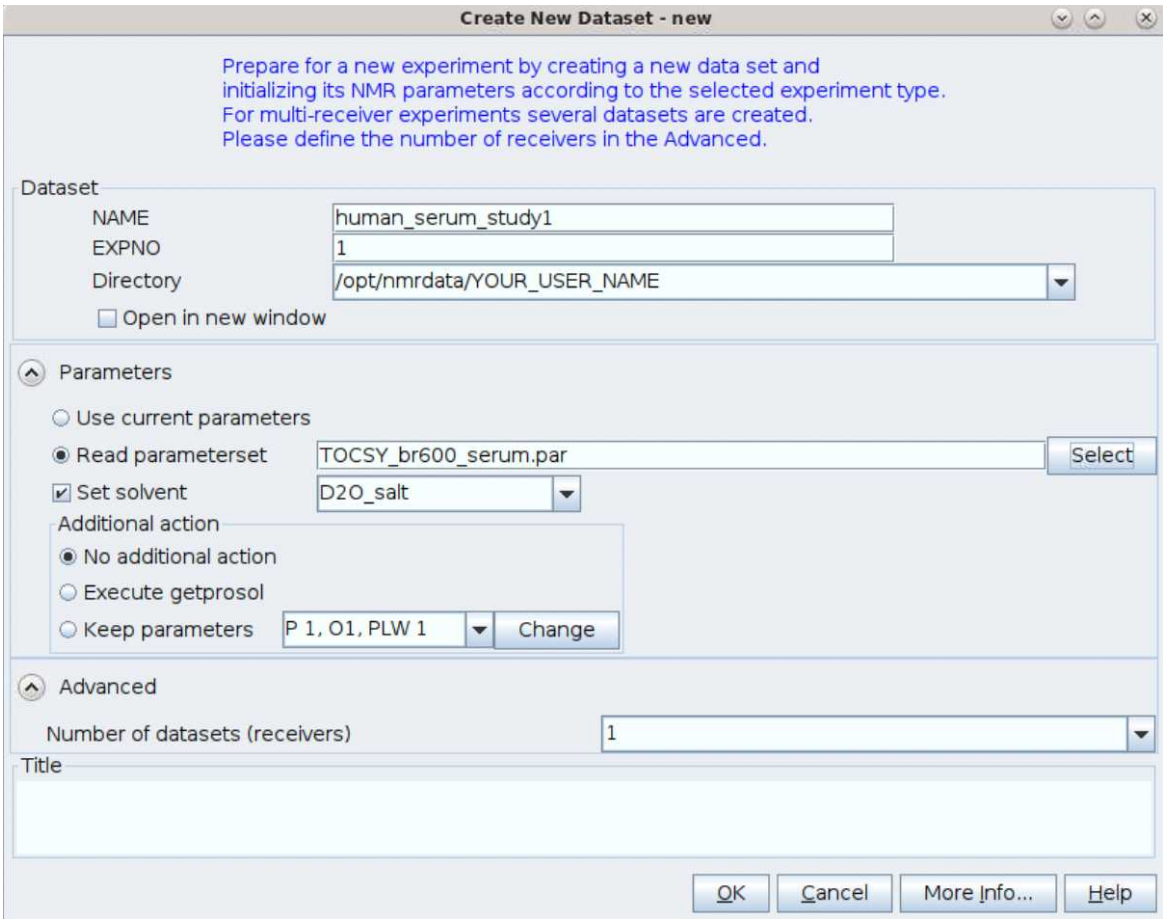
(This protocol uses TopSpin 3.6.4, and the interface may look different on other TopSpin versions.)

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.



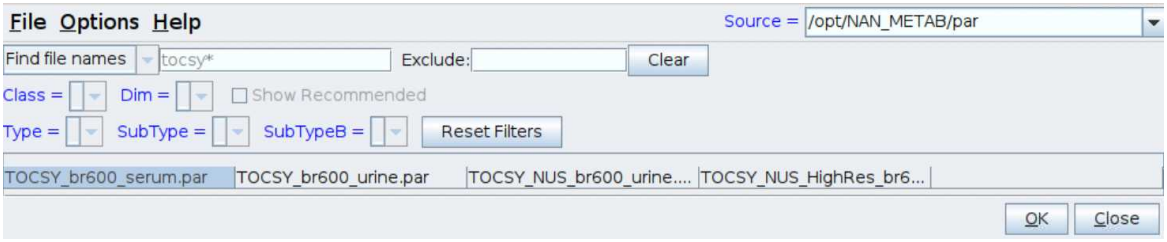
Note

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.

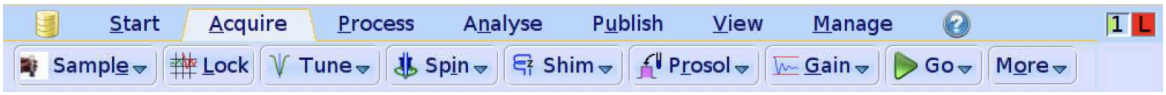
```
getprosol 1H [calibrated P1 value] [power level for P1]
```

(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**".