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 **hsqc-tocsy\_metab.nan**

 Forked from [hsqc-tocsy.nan](#)

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NAN support at UGA

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**protocols.io**

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

## 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

## BEFORE START INSTRUCTIONS

**Last Modified:** Nov 30, 2023

**PROTOCOL integer ID:**  
87729

### Funders

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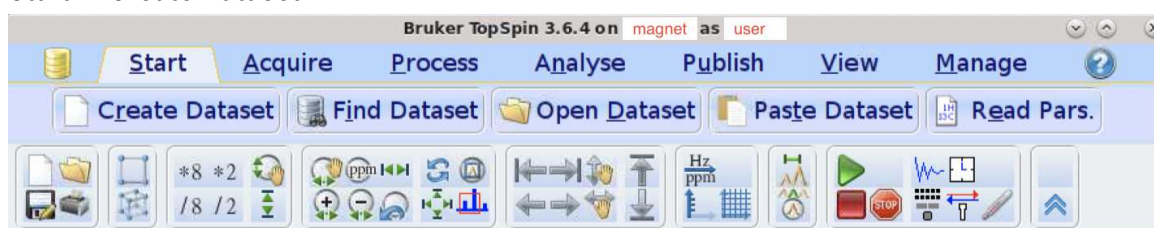
This protocol assumes:

- 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

**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: HSQC-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

**File Options Help** Source = /opt/NAN\_METAB/par

Find file names: hsqc-tocsy\* Exclude: **Clear**

Class = Dim = ☐ Show Recommended  
 Type = SubType = SubTypeB = **Reset Filters**

HSQC-TOCSY\_br600\_serum.par HSQC-TOCSY\_br600\_urine.par HSQC-TOCSY\_NUS\_br600\_ser... HSQC-TOCSY\_NUS\_br600\_uri...

**OK Close**

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]**

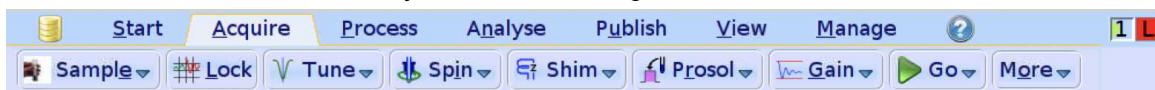
(e.g., getprosol 1H 10.01 -7.45)

#### 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".