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 **hsqc\_metab.nan V.3**  
 Version 1 is forked from [hsqc.nan](#)

Saraa Al  
NAN KB<sup>1</sup>, John Glushka<sup>2</sup>, Mario Uchimiya<sup>2</sup>, Jawad<sup>2</sup>,  
Leandro I  
Christopher Esselman<sup>2</sup>, Ponce<sup>2</sup>, Laura Morris<sup>2</sup>,  
Arthur  
Edison<sup>2</sup>

<sup>1</sup>Network for Advanced NMR (NAN); <sup>2</sup>University of Georgia

Saraa Al Jawad: Protocol review;  
Christopher Esselman: Protocol review  
Leandro I Ponce: Protocol review



NAN support at UGA

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## ABSTRACT

This is a protocol for running the Bruker pulse program "hsqcetgpsisp2".

## 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.

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

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## BEFORE START INSTRUCTIONS

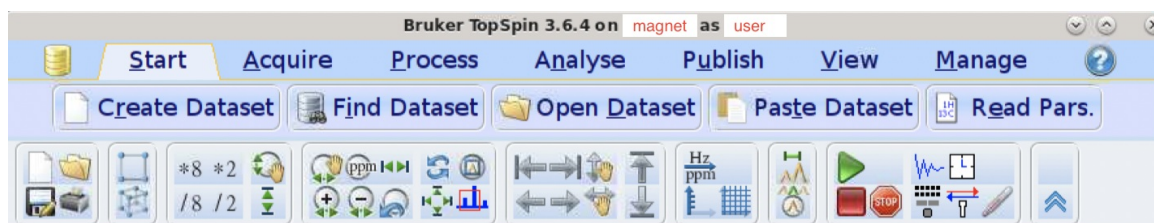
This protocol assumes:

- 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.

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/User

☐ Open in new window

**Parameters**

☐ Use current parameters

☒ Read parameterset: HSQC\_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

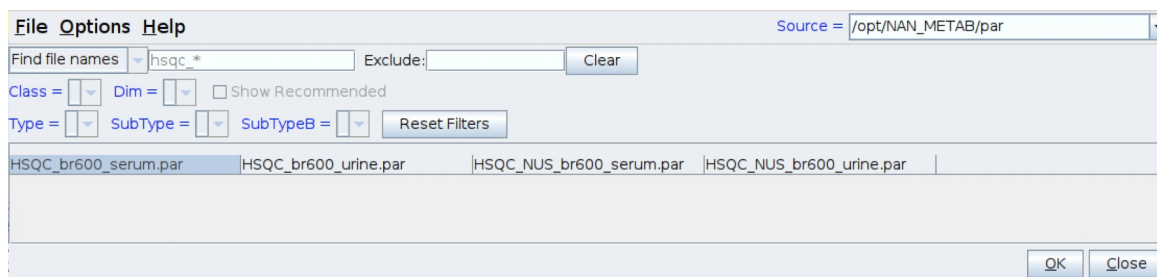
Your new dataset will be stored in **Directory/NAME/EXPNO**

### 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:

- **HSQC\_br600\_serum.par**: Parameter set using an acquisition mode "traditional planes"
- **HSQC\_NUS\_br600\_serum.par**: Parameter set using an acquisition mode "non-uniform sampling (NUS)". Higher resolution on the indirect dimension

For urine samples:

- **HSQC\_br600\_urine.par**: Parameter set using an acquisition mode "traditional planes"
- **HSQC\_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\_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

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".