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 hmbc\_metab.nan

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NAN support at UGA

Network for Advanced NMR

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## ABSTRACT

This is a protocol for running the Bruker pulse program "hmbcetgpl3nd" 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.

OPEN  ACCESS



DOI:

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

Created: Feb 22, 2024

## BEFORE START INSTRUCTIONS

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PROTOCOL integer ID: 95619

Keywords: NAN, NMR, Metabolomics, HMBC

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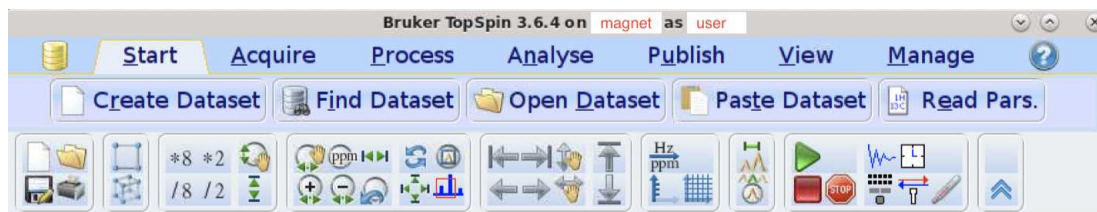
This protocol assumes:

- 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.

- **Directory:** Your directory.

Note

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

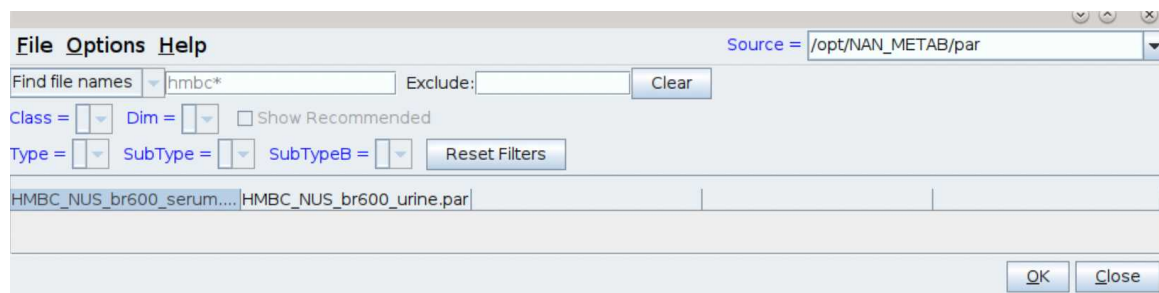
## Select

Click the button

## 1.4

protocols.io | <https://dx.doi.org/10.17504/protocols.io.4r3l22dm4l1y/v1>

Source = /opt/NAN\_METAB/par



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

For serum and plasma samples:

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

For urine samples:

- **HMBC\_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 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.



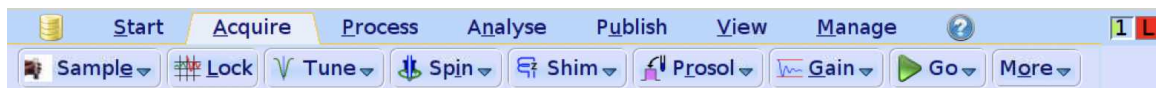
```
getprosol 1H [calibrated P1 value] [power level for P1]
```

(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**".