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 jres\_metab.nan

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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 "jresgpprqf".

## 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



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[dx.doi.org/10.17504/protocols.io.e6nvwd27wlmk/v1](https://dx.doi.org/10.17504/protocols.io.e6nvwd27wlmk/v1)

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

**Created:** Nov 27, 2023

## BEFORE START INSTRUCTIONS

**Last Modified:** Dec 20, 2023

This protocol assumes your sample is loaded, locked, tuned, and shimmed in the magnet.

**PROTOCOL integer ID:**  
91462

**Keywords:** NAN, NMR, metabolomics, JRES

### Funders

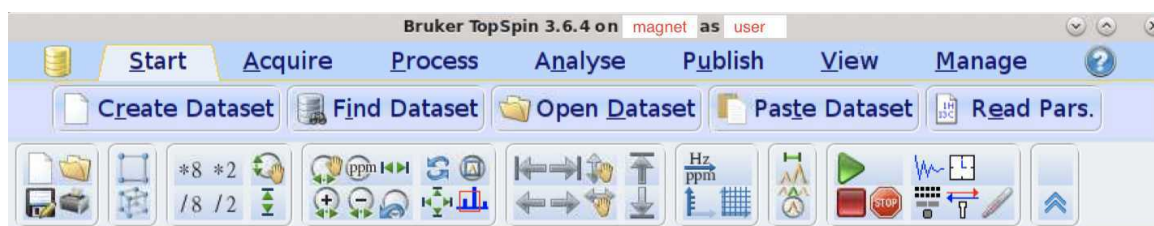
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## Create a new dataset

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 (do not use spaces)
  - **EXPNO:** Dataset number. Use a positive integer

**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/USER  
☐ Open in new window

**Parameters**

☐ Use current parameters  
☒ Read parameterset: JRES\_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**

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:

**JRES\_br600\_serum.par:** Parameter set optimized for serum and plasma samples.

**JRES\_br600\_urine.par:** Parameter set optimized for urine samples.

#### Note

Parameter set names in the list vary between spectrometers (e.g., JRES\_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.



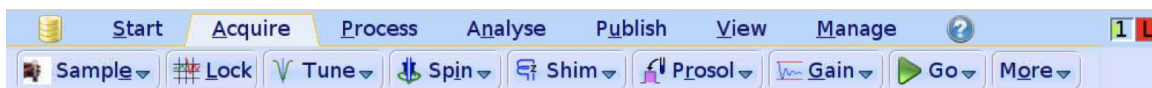
```
getprosol 1H [calibrated P1 value] [power level for P1]
```

(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

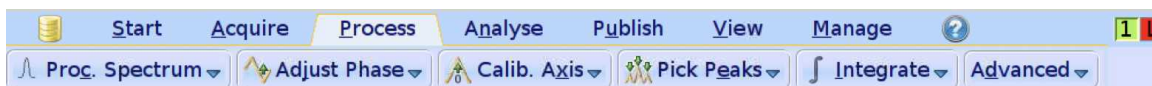
You can also use the **rga** command in the command line.

- 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**".