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🌐 projectpr1d\_metab.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

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## ABSTRACT

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This is a protocol for running the Bruker pulse program "projectpr1d".

**PROTOCOL integer ID:** 92993

This pulse program was originally proposed in:

**Keywords:** NAN, NMR, metabolomics, projectpr1d

## CITATION

**Funders Acknowledgement:**  
National Science Foundation  
Grant ID: 194670

Le Guennec A, Tayyari F, Edison AS (2017). Alternatives to Nuclear Overhauser Enhancement Spectroscopy Presat and Carr-Purcell-Meiboom-Gill Presat for NMR-Based Metabolomics..

LINK

<https://doi.org/10.1021/acs.analchem.7b02354>

## GUIDELINES

This protocol intends to provide concise instructions to carry out the experiment. For more comprehensive information, see Bruker's documentation including "Basic NMR Experiments" by clicking ? → **Manuals (docs)** on the menu bar on TopSpin.

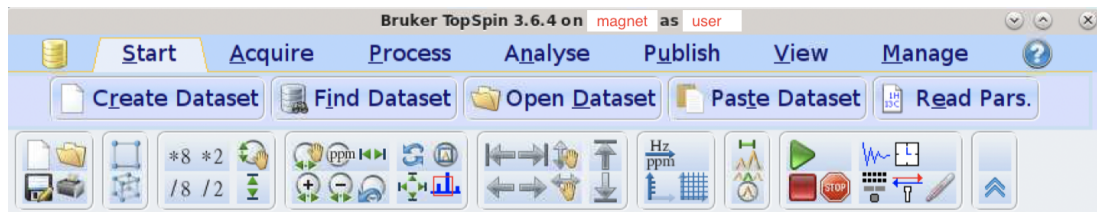
## BEFORE START INSTRUCTIONS

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

## 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: PROJECTPR1D\_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**

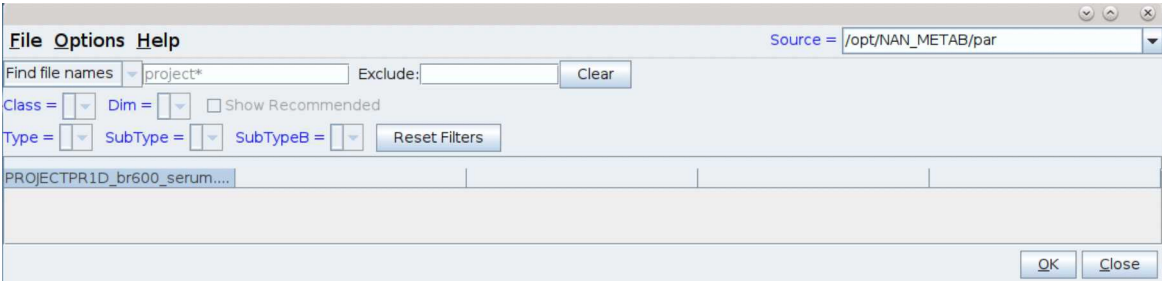
In the list, select the one you want to use:

**PROJECTPR1D\_br600\_serum.par**: Parameter set optimized for serum and plasma samples.

Note

Parameter set names in the list vary between spectrometers (e.g., PROJECTPR1D\_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.



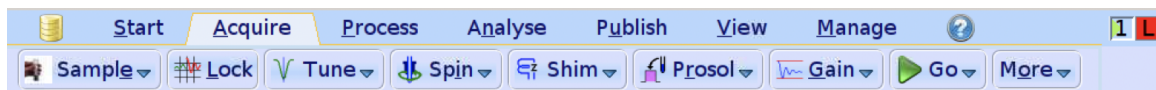
```
getprosol 1H [calibrated P1 value] [power level for P1]
```

(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 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 a step case "MODIFY PAR".