





SEP 13, 2023

 noesypr1d_metab.nan

 Forked from [noesypr1d.nan](#)

Saraa Al

NAN KB¹, John Glushka², Mario Uchimiya², Jawad²,

Leandro I

Christopher Esselman², Ponce²,

Laura Morris²,

Arthur

Edison²

¹Network for Advanced NMR (NAN); ²University of Georgia

Saraa Al Jawad: Protocol review;

Christopher Esselman: Protocol review

Leandro I Ponce: Protocol review

OPEN  ACCESS



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 "noesypr1d".

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.

Created: Aug 31, 2023

BEFORE START INSTRUCTIONS

Last Modified: Sep 13, 2023

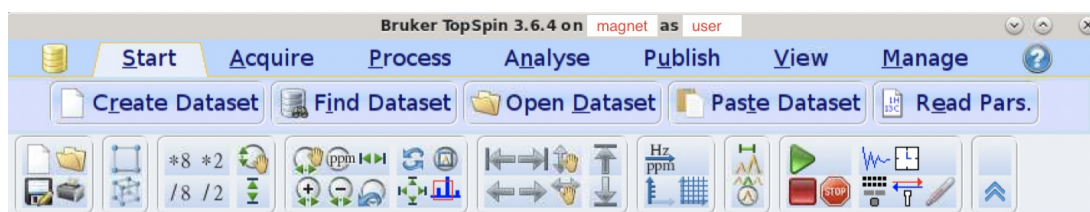
This protocol assumes your sample is loaded, locked, tuned, and shimmed in the magnet.

PROTOCOL integer ID:
87222

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/User

☐ Open in new window

Parameters

☐ Use current parameters

☒ Read parameterset: NOESYPR1D_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:

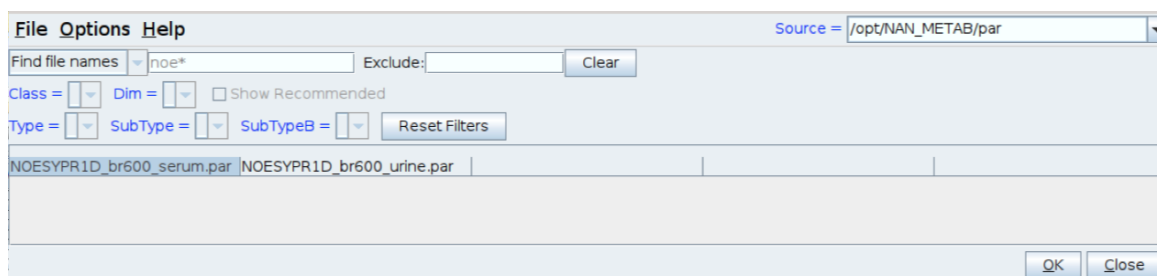
NOESYPR1D_br600_serum.par: Parameter set optimized for serum and plasma samples.

NOESYPR1D_br600_urine.par: Parameter set optimized for urine samples.

Note

Parameter set names in the list vary between spectrometers (e.g., NOESYPR1D_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 2 includes a Step case.

USE DEFAULT
MODIFY PAR

step case

USE DEFAULT

This step case uses the default optimized parameters to acquire a spectrum.

- 3
 - 3.1 Calibrate the 90° proton pulse (i.e., P1) using the following command in the command line.

```
pulsecal
```

A new window will appear to show the calibrated P1.

- 3.2 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

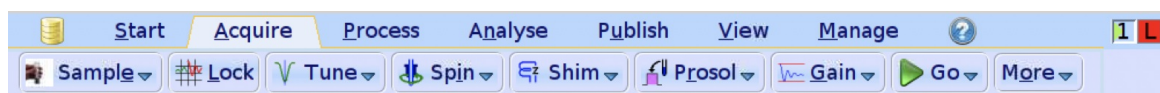
[power level for P1] varies between spectrometers. Never use a wrong **[power level for P1]**

3.3

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.

3.4

Click

Go

in the menu bar to acquire a spectrum.

Note

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


3.5

Click on

Process → Proc. Spectrum

in the menu bar to execute an automated processing macro.



3.6 If you want to modify parameters to improve your spectrum,  [go to step #2](#) and move to a step case "MODIFY PAR".