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noesypr1d_metab.nan V.3

Version 1 is forked from noesypr1d.nan

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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.

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

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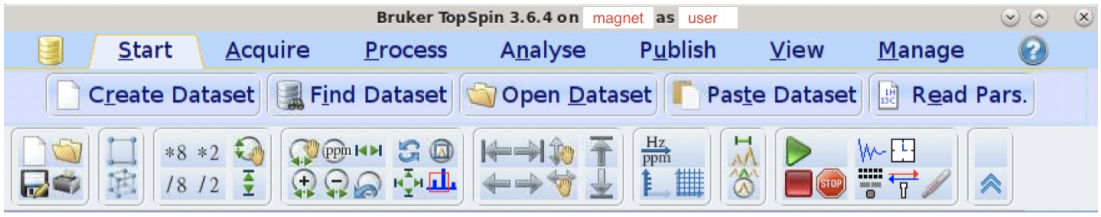
BEFORE START INSTRUCTIONS

This protocol assumes your sample is loaded, locked, tuned, 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.)

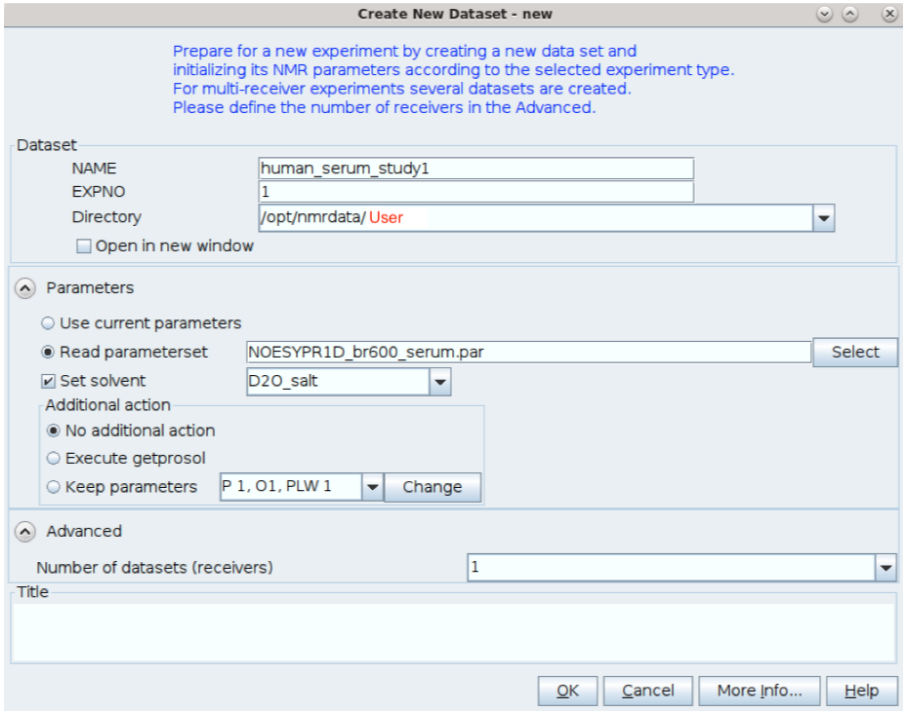
Note

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.



Note

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

1.3 Select
Read parameterset

Click the button
Select

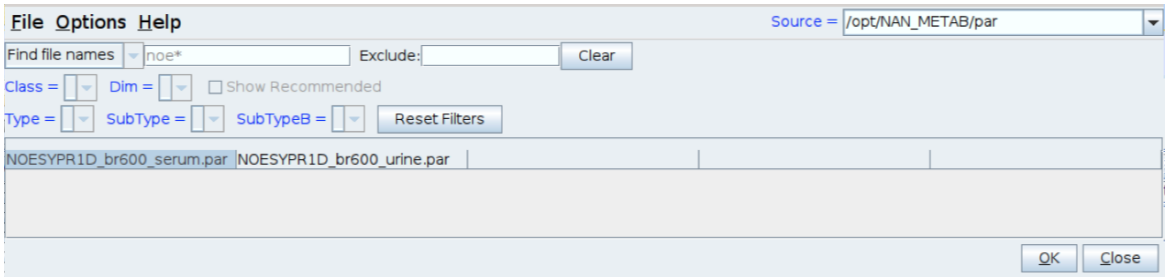
1.4 A new window opens. On the right top bar, select
Source = /opt/NAN_METAB/par

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 CASE

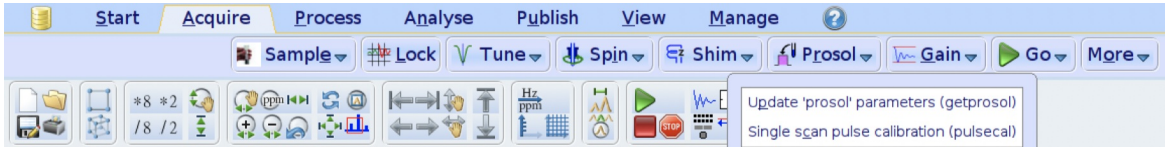
Use default parameters:

7 steps

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

3

3.1 Click on
Acquire → Prosol → Single scan pulse calibration (pulsecal)
to calibrate the 90° proton pulse (i.e., P1).



A new window will appear to show the calibrated P1.

Note

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

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".