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 projectpr1d_metab.nan

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Protocol status: Working

We use this protocol and it's working

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Abstract

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

This pulse program was originally proposed in:

Citation

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.

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

LINK

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.

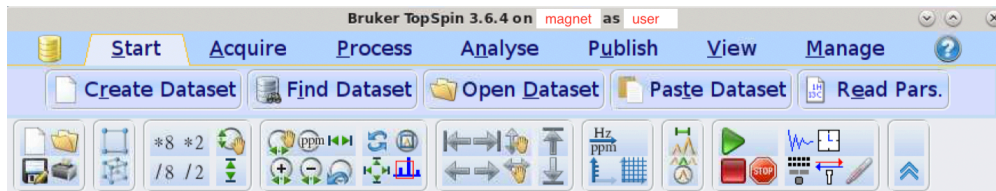
Before start

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.

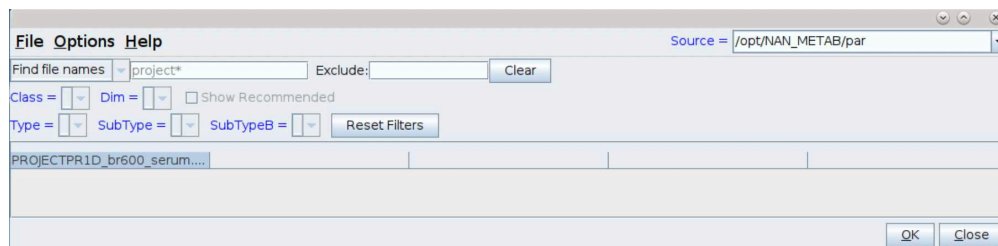


Note

Parameter set names in the list vary between spectrometers (e.g., PROJECTPR1D_br800_serum.par).

Click

OK



1.5 Click

OK

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)

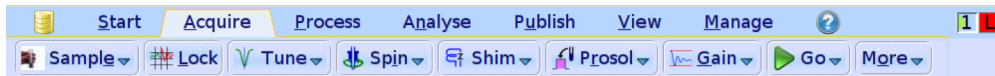




Note

[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".



Citations

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

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