Jan 19, 2024

projectpr1d_metab.nan

DOI
https://dx.doi.org/10.17504/protocols.io.ewov1qkzkgr2/v1

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OPEN ACCESS

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Protocol Citation: NAN KB, John Glushka, Mario Uchimiya, Christopher Esselman, Saraa Al Jawad, Leandro Ponce, Laura Morris, Arthur Edison 2024. projectpr1d_metab.nan. **protocols.io** https://dx.doi.org/10.17504/protocols.io.ewov1qkzkgr2/v1

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

Created: January 05, 2024

Last Modified: January 19, 2024

Protocol Integer ID: 92993

Keywords: NAN, NMR, metabolomics, projectpr1d, bruker pulse program, projectpr1d, pulse program, protocol, bruker

Funders Acknowledgements:
National Science Foundation
Grant ID: 194670

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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.

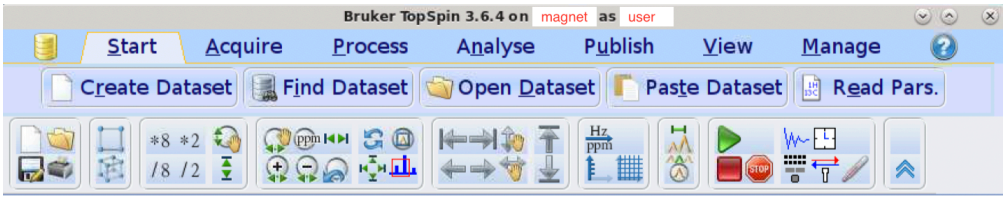
Before start

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



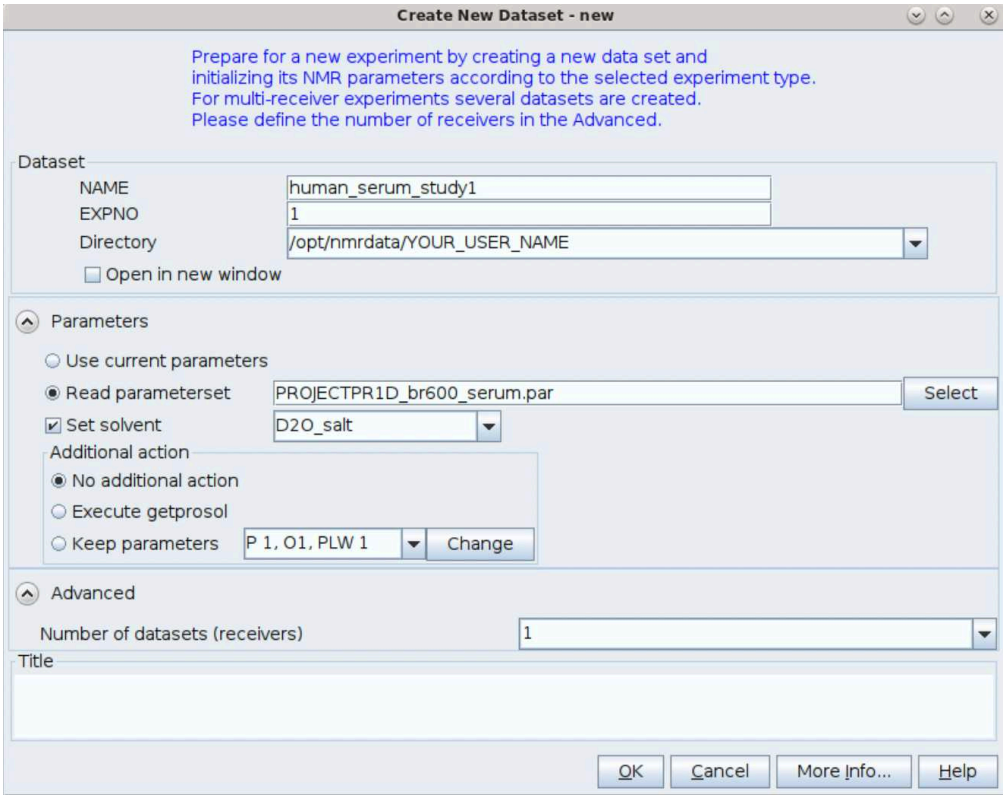
(This protocol uses TopSpin 3.6.4, and the interface may look different on other TopSpin versions.)

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.



Note

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

1.3 Select
Read parameterset

Click the button
Select

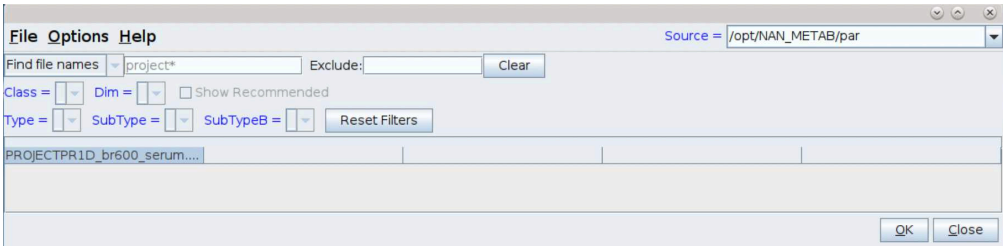
1.4 A new window opens. On the right top bar, select
Source = /opt/NAN_METAB/par

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