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hmbc_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 "hmbcetgpl3nd" for metabolomics samples.

Guidelines

This protocol intends to provide concise instructions to carry out the experiment. For more comprehensive information, see Bruker's documentation "Basic NMR Experiments" by clicking ? → **Manuals (docs)** on the menu bar on TopSpin. See also "Pulse Program Catalogue. 1D/2D" for the details about the pulse program used in this protocol.

Troubleshooting



Before start

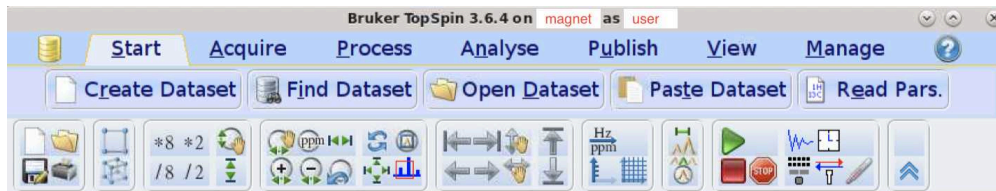
This protocol assumes:

- Your sample is loaded, locked, tuned for both proton and carbon channels, and shimmed in the magnet
- The calibrated 90° pulse value for proton (i.e., P1) for the sample has been collected

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: HMBC_NUS_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

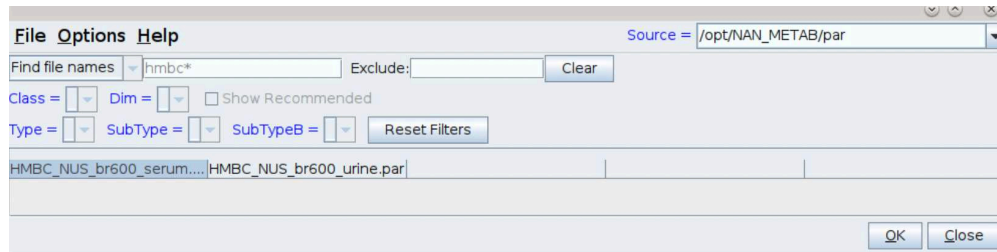
Your new dataset will be stored in **Directory/NAME/EXPNO**

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:

For serum and plasma samples:

- **HMBC_NUS_br600_serum.par**: Parameter set using an acquisition mode "non-uniform sampling (NUS)". Higher resolution on the indirect dimension

For urine samples:

- **HMBC_NUS_br600_urine.par**: Parameter set using an acquisition mode "non-uniform sampling (NUS)". Higher resolution on the indirect dimension

Note

Parameter set names in the list vary between spectrometers (e.g., HSQC_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.

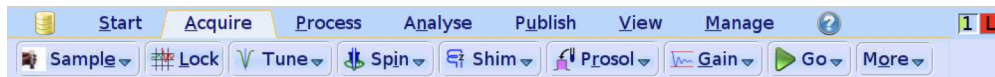
```
getprosol 1H [calibrated P1 value] [power level for P1]
```

(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 After the run, 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 the step case "**MODIFY PAR**".