

Oct 17, 2023

Version 1

hsqc_metab.nan V.1

Forked from a private protocol



DOI

<https://dx.doi.org/10.17504/protocols.io.5jyl8pd2dg2w/v1>

NAN KB¹, John Glushka², Mario Uchimiya², Saraa Al Jawad², Christopher Esselman², Leandro Ponce², Laura Morris², Arthur Edison²

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

Saraa Al Jawad: Protocol review;

Christopher Esselman: Protocol review

Leandro Ponce: Protocol review



NAN-KB UGA

Network for Advanced NMR

Create & collaborate more with a free account

Edit and publish protocols, collaborate in communities, share insights through comments, and track progress with run records.

Create free account

OPEN  ACCESS



DOI: <https://dx.doi.org/10.17504/protocols.io.5jyl8pd2dg2w/v1>

Protocol Citation: NAN KB, John Glushka, Mario Uchimiya, Saraa Al Jawad, Christopher Esselman, Leandro Ponce, Laura Morris, Arthur Edison 2023. hsqc_metab.nan. protocols.io <https://dx.doi.org/10.17504/protocols.io.5jyl8pd2dg2w/v1>

License: This is an open access protocol distributed under the terms of the [Creative Commons Attribution License](#), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited

Protocol status: Working

We use this protocol and it's working

Created: September 13, 2023

Last Modified: October 17, 2023

Protocol Integer ID: 87728

Keywords: NAN, NMR, HSQC, Metabolomics, hsqcetgpsisp2, bruker pulse program, pulse program, protocol, bruker

Funders Acknowledgements:

National Science Foundation

Grant ID: 194670

Disclaimer

This protocol is developed and maintained by Network for Advanced NMR (NAN). The protocol content here is for informational purposes only and does not constitute legal, medical, clinical, or safety advice, or otherwise; content added to this protocol is not peer reviewed and may not have undergone a formal approval of any kind. Information presented in this protocol should not substitute for independent professional judgment, advice, diagnosis, or treatment. Any action you take or refrain from taking using or relying upon the information presented here is strictly at your own risk. You agree that neither the Company nor any of the authors, contributors, administrators, or anyone else associated with this protocol, can be held responsible for your use of the information contained in or linked to this protocol or any of our Sites/Apps and Services.

Abstract

This is a protocol for running the Bruker pulse program "hsqcetgpsisp2".

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.

Before start

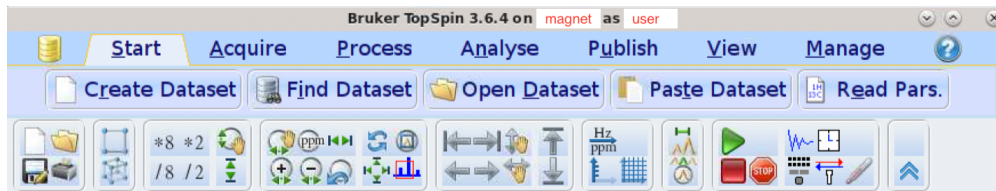
This protocol assumes:

- 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

EXPNO

Directory

☐ Open in new window

Parameters

☐ Use current parameters

☒ Read parameterset

☒ Set solvent

Additional action

☒ No additional action

☐ Execute getprosol

☐ Keep parameters

Advanced

Number of datasets (receivers)

Title

Note

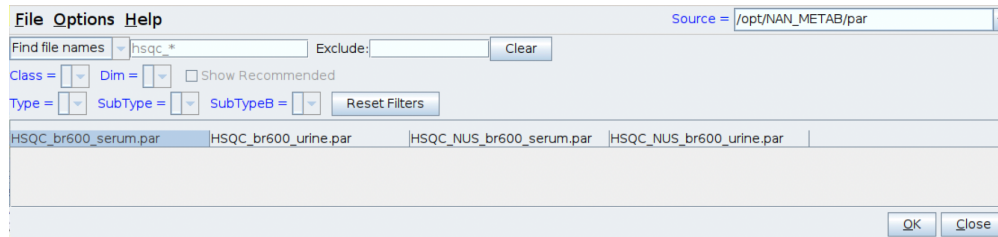
Your new dataset will be stored in **Directory/NAME/EXPNO**

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:

- **HSQC_br600_serum.par**: Parameter set using an acquisition mode "traditional planes"
- **HSQC_NUS_br600_serum.par**: Parameter set using an acquisition mode "non-uniform sampling (NUS)". Higher resolution on the indirect dimension

For urine samples:

- **HSQC_br600_urine.par**: Parameter set using an acquisition mode "traditional planes"
- **HSQC_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.



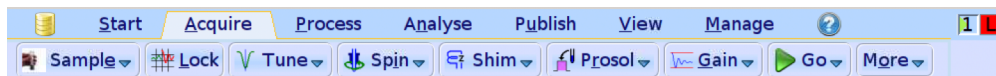
```
getprosol 1H [calibrated P1 value] [power level for P1]
```

(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".