topspin

Bruker BioSpin

TopSpin NUS Parameter

Software Manual
Version: 3.1.0

think forward

NMR Spectroscopy

TopSpin

Version: 3.1.0

Software Manual

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Bruker software support is available via phone, fax, e-mail, Internet, or ISDN. Please contact your local office, or directly:

Address: Bruker BioSpin GmbH
Service & Support Department
Silberstreifen
D-76287 Rheinstetten
Germany

E-mail: nmr-software-support@bruker.de

WWW: *www.bruker-biospin.com*

FTP: ftp.bruker.de / ftp.bruker.com

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1 Introduction

1.1 About this manual

This manual is a short description of non-uniformly sampled (**NUS**) multidimensional NMR available in **TopSpin 3** and its processing with „MDDNMR”.

„MDDNMR” is a program especially for processing of **NUS** multidimensional NMR data developed by Orekhov et al. and implemented in **TopSpin**. (MDD means Multi Dimensional Decomposition)

For detailed information about this program please refer to the original papers.[1,2,3,4,5,6)]

1.2 Conventions

Bold Arial: commands to type in command line

Cursive Arial: path names and directories

`Courier new`: web-server addresses

Introduction

2 General Concept

Traditionally multi-dimensional NMR-data sets are collected using a linear incrementation of evolution times and require a FTT algorithm for processing. The data points acquired in the indirect dimension(s) form a grid where the distance between the points on the grid is given by the sweep width and the number of points by the TD for each dimension respectively

The principle of **NUS** is to acquire only a subset of data points in a random manner while still using the same grid. Such data are generally processed by other methods. These can be:

[1] **Multi Dimensional Decomposition** (MDD-NMR) by Orekhov et al. [1,3,4)]

[2] **Maximum Entropy** (MaxEnt) methods
Rowland Toolkit by Hoch et al. [7,8,9,10)]
Forward Maximum Entropy by Wagner et al.[11)]
Azara (CCPN) by Laue et al. [12)]

[3] **Multidimensional Fourier Transformation** (MFT) by Kozminski et al. [13,14,15)]

Bruker decided to use the MDD-NMR. Among others this program produces quantifiable results.

Recording of data in **NUS** mode can save a lot of time, especially for nD datasets.

After a spectrum is recorded and stored to a disk, it has to be processed. The processing of a regular NMR spectrum includes the following steps:

a) Fourier transformation in the directly detected dimension

b) Fourier transformation in all indirect dimensions, viewing of the result and, if necessary, fine tuning of the processing parameters

If a spectrum is recorded in the **NUS** mode, the indirect dimensions cannot be Fourier transformed right away. Here ‚MDDNMR' software intervenes after step a). It replenishes the complete data matrix in all indirect dimensions with reconstructed points, which means resorting of recorded data points and extrapolation of the miss-

ing ones. Then the steps b) is performed.

For a regularly acquired dataset one point after the other (from beginning to end of the whole matrix) has to be recorded according to the sampling. Spectra recorded in **NUS** mode may be obtained for two and higher dimensional experiments where only a small amount of data points will be acquired which is randomly spread over the whole data space (see figure 2.1). Therefore it is possible to process the dataset after only a few percent of the data is recorded to obtain a spectrum with the final resolution, provided S/N the is sufficient.

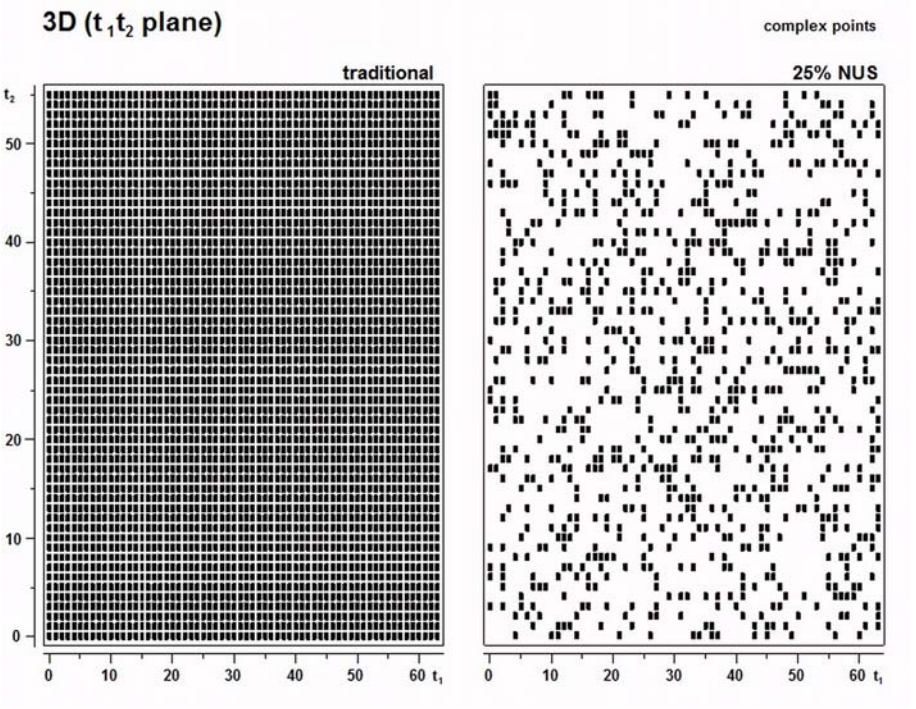

Figure 2.1 Distribution of complex points in traditional and NUS experiment

- Note: If prior knowledge about T2 or J-coupling is available, the position of the sampling points can be optimized (attach more weight to the strong parts of the FID)

2.1 Parameter setup for NUS experiments

First of all the parameters for the chosen experiment will be set as usually in the ‚eda' table. You can select the ‚FnType' which will set the nD acquisition mode. For a **NUS** experiment it is set to ‚non-uniform_sampling' as shown in figure 2.2

- Note**:** Former **TopSpin** versions (all versions before **TopSpin 3.0**) require modified pulsprograms.

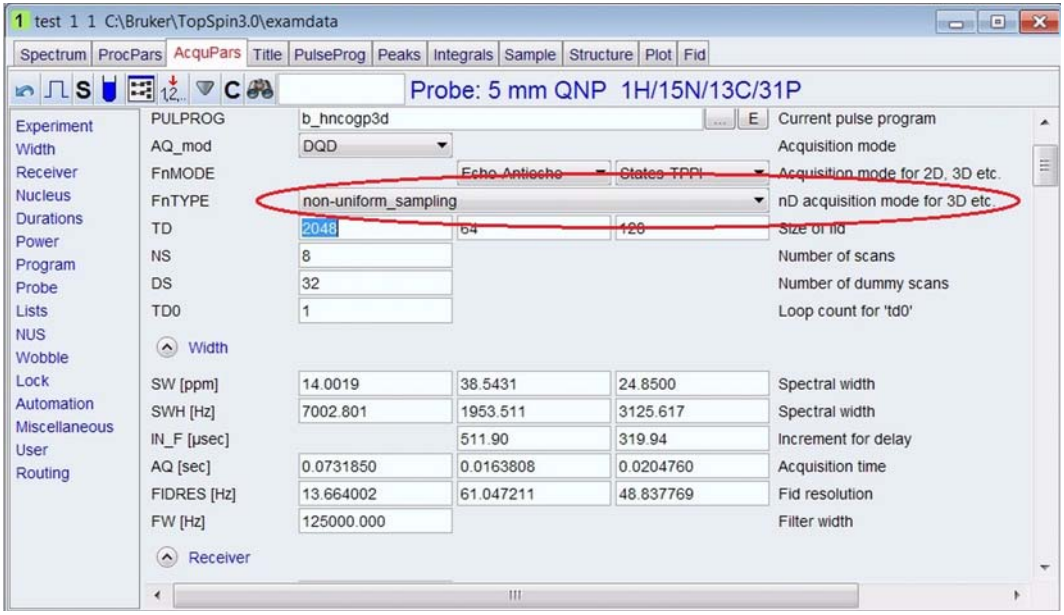

Figure 2.2 ‚eda' table for setup of a NUS experiment

After setting the ‚FnTYPE' to non-uniform_sampling, click NUS from the listing on the left side of the ‚eda' table to get the additional acquisition parameters for a NUS experiment. They are shown in figure 2.3

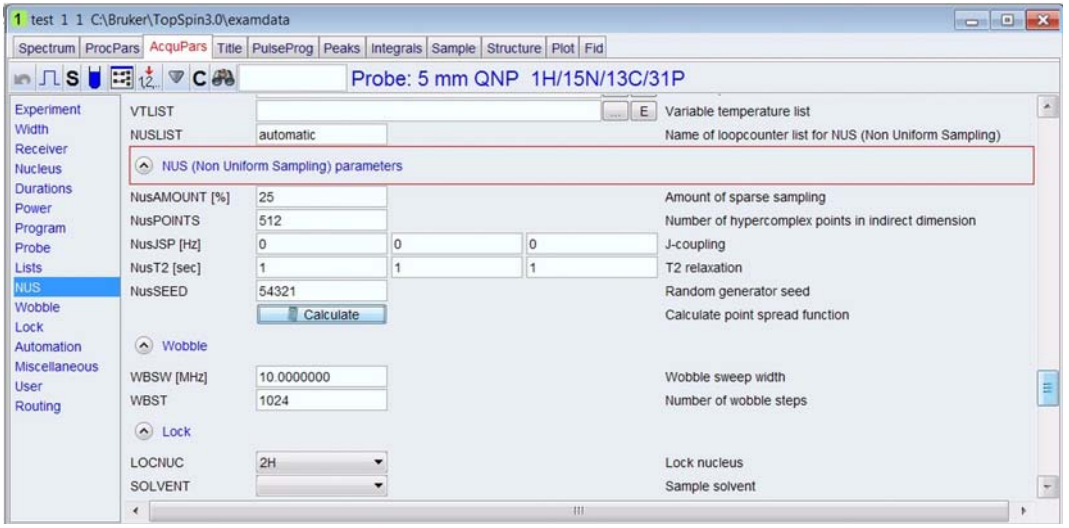

Figure 2.3 NUS acquisition parameter block

[1] Acquisition parameters:

NusAMOUNT[%] - percentage amount of sparse sampling, default is 25

NusPOINTS - number of complex data points to be recorded, for nD experiment it is [(td1*td2 ...*tdn) *amount/100] / $2^{(n-1)}$

- Note: As a rule of thumb the number of hypercomplex points should be at least the same as the number of frequencies (signals in the spectrum).

Jsp [Hz] - J coupling, default is 0. In the case of J evolution in an indirect dimension the points acquired can be matched to the maxima of such a FID by setting this coupling constant.

T2 [s] - T2 relaxation time, default is 1. For indirect dimensions with so called real time evolution the FID in the indirect dimension will decay according to the T2 relaxation time of the spins evolving in this dimension.

By setting the T2 parameter according to the relaxation time, parts of the FID with more intensity will be strengthened (exponential weighting of sampling scheme)

- Note: If an evolution period is implemented as constant time in the pulse program, exponential weighting must not be used!

  seed - random number generator seed, responsible for the different distribution of data points, default is 54321

  Calculate - allows to calculate and then view the distribution of points without starting the experiment.

Now make sure, that the NUSLIST is called ‚automatic' (loopcounter list for NUS). You will find it together with other lists above the NUS parameter block (Fig. 2.2).

The processing parameters for a NUS experiment will be found in the ‚edp' table. Click NUS in the listing on the left side and the edp parameter list is scrolled to the NUS parameter block (Fig. 2.3).

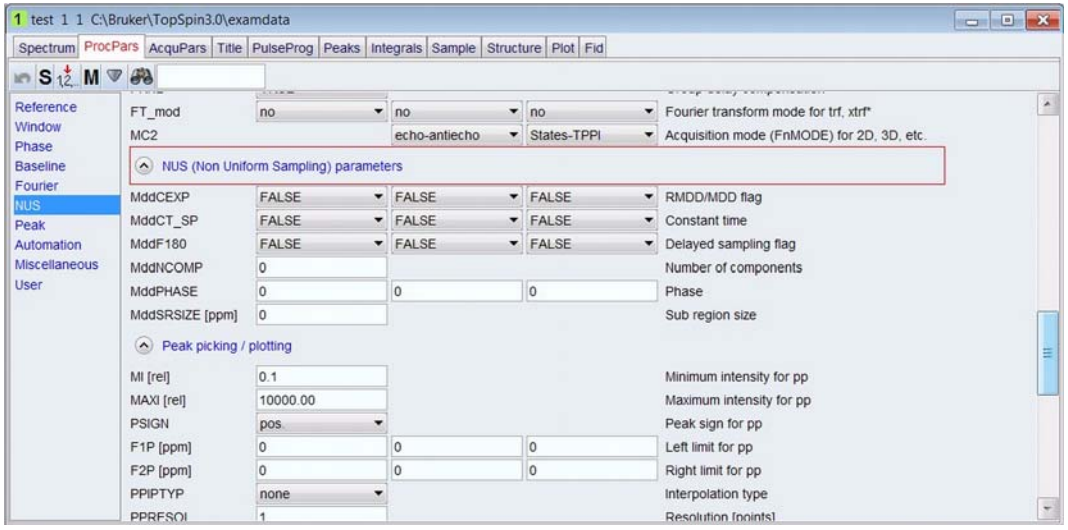

Figure 2.4 NUS processing parameter block

MddCEXP - recursive MDD/MDD flag, default is false in all dimensions (true = recursive), selecting true takes more time, for 2D spectra recursive MDD is mandatory in F1

MddCT_SP - allows to specify constant time direction, used as in the original MDD, false = non constant time direction, true = constant time direction, default is false in all dimensions, in the case of being true mirror image processing is used

MddF180 - delayed sampling flag, default is false in all dimensions; false = no delayed sampling, true = delayed sampling (first value for delay = 1/2 increment or T1(0) = IN/2

MddNCOMP - number of components, default is 0 which uses the internal default of 15 components, if peaks are missing NCOMP should be increased

- Note: The increase of NCOMP leads to disproportional increase of calculating time

MddPHASE - zero order phase for correction for indirect dimension, default is 0 in all dimensions

MddSRSIZE [ppm] - sub region size, for ^{1}H 0,15 ppm are sufficient, for other nuclei the value might be larger. The default of 0 uses the internal default of 0,15 ppm.

3 Contact

Manufacturer:

Address:	Bruker BioSpin GmbH Service & Support Department Silberstreifen D-76287 Rheinstetten Germany
E-mail:	nmr-software-support@bruker.de
WWW:	http://www.bruker-biospin.com

Appendix A

A.1 Warning Signs

A.2 Figures

A.3 Tables

A.4 Glossar

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