NMR Product Test

- Release Letter NMR Product Test

Version: TopSpin 4.1.4

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NMRPT

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1 Introduction

1.1 For Guidance

About the Release Letter

The Release Letter describes the latest developments of NMRPT. The Release letter is not available as a hardcopy. This allows Bruker to provide an up-to-date version of the Release Letter.

Target Audience

The Release Letter for NMR Product Test in TopSpin 4.1.4 supports all Bruker engineers who work with NMRPT.

How to get the Release Letter

This document is only electronically available in PDF format directly in the Help menu of NMRPT in the installed TopSpin program.

2 NMRPT Basics

2.1 About NMRPT

NMRPT in TopSpin 4.1.4 is for all AVANCE NEO spectrometers. Compared to NMRPT in TopSpin 4.1.3 it is a minor update containing many improvements, new features, and bug fixes.

2.2 Program Versions

NMRPT is part of the installed TopSpin version for TopSpin 4.1.3 and later.

3 Bug Fixes in NMRPT

3.1 Truncation of Long Shim Commands in PDF

Long shim commands will no longer be truncated in table shim sequence of spectrum PDF.

3.2 Plot of TopShim Tune Results Contains Empty Plots

Shim results of “topshim tune" now only shows two plots instead of four in former NMRPT versions, since TopShim does provide fewer results.

3.3 NPT_29Si_backgr_nosample with Option Skip HNUC Tuning/Matching as Default

Experiment NPT_29Si_backgr_nosample must execute tuning and matching of ^{1}H as default, since experiment applies ^{1}H decoupling during acquisition of FID.

3.4 Acquisition Order of NPT_19F_MAS_shortestPulse_19f

NPT_19F_MAS_p90det_19f should be measured before NPT_19F_MAS_shortestPulse_19f.

3.5 PICS Probe Type LTMAS

Probes with PICS probe type LTMAS are now supported in NMRPT.

4 New Experiments in NMRPT

4.1 2D ^{1}H ^{13}C HSQC with Adiabatic Decoupling

New 2D ^{1}H ^{13}C HSQC with adiabatic decoupling using sucrose sample. Experiment uses a fixed AQ of 250 ms.

4.2 Series Experiments $^{13}C(^{15}N, ^{1}H)$ and $^{15}N(^{13}C, ^{1}H)$

Two new garp series experiments without sample with ^{13}C and ^{15}N hard pulse before detection of the FID:
- $^{13}C(^{15}N, ^{1}H)$ experiment with ^{13}C detection and simultaneous ^{15}N and ^{1}H decoupling
- $^{15}N(^{13}N, ^{1}H)$ experiment with ^{15}N detection and simultaneous ^{13}C and ^{1}H decoupling.

4.3 MAS Temperature Functionality Test on KBr Sample

New temperature functionality test on KBr sample for HRMAS and MAS probes. Since the test only uses the shift of the ^{79}Br signal no absolute calibration of the temperature is possible. Only temperature changes between the different experiments can be observed. For further details see NMRPT experiment manual.

4.4 F80/CMR: Gradient Profile Experiments

^{1}H gradient profile Experiments for Fourier 80 spectrometer with positive and negative gradient direction.

4.5 F80/CMR: Gradient Recovery Experiments

^{1}H gradient recovery experiments for Fourier 80 spectrometer with positive and negative gradient direction.

4.6 F80/CMR: ^{1}H Background Experiment

^{1}H background experiment with sample for Fourier 80 spectrometer.

4.7 F80/CMR: ^{31}P Experiments

^{31}P pulse determination and sensitivity experiments for Fourier 80 spectrometer.

5 Changes in Experiments

5.1 Garp Series Experiments

In the garp series experiments NPT_1H_garp_pulse13C_dec13c and NPT_1H_garp_simpul13c15n_dec13c a delay of 1 ms is introduced between hard pulses and acquisition of FID.

5.2 Gradient Recovery Experiments

Improved algorithm for evaluation of zero order phase correction to get more reliable results.

5.3 Evaluation of NPT_1H_honeyNoesy Experiment

Evaluation of baseline distortion of NPT_1H_honeyNoesy experiment implemented.

5.4 NPT_13C_MAS_p90det_13c for 1.3 and 0.7 mm Probes

For probes with sample diameters <= 1.3 mm the direct ^{13}C pulse determination on adamantane is no longer a mandatory experiment. For these probes only the indirect ^{13}C pulse determination on glycine is mandatory.

5.5 Shortest Pulse Experiments with CP

In shortest pulse experiments with cross polarization the minimum of 2 μs and (pulse specification * 0.5) will be used as start pulse to avoid that the start pulse is bigger than the 90-degree pulse with the maximum power of this nucleus taken from PICS.

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6 New Features in NMRPT

6.1 TopShim Report Available in Result Panel

The TopShim Report for each experiment is now available in the window “Show Additional Information” of the Result Panel.

6.2 Setting of Z2 Shim Correction

Z2 shim correction can now be set in Probe Setup Tab. For further information concerning Z/Z2 shim correction set NMRPT GUI manual.

6.3 Skip Experiments in Experiment Queue

In Experiment Queue a new state “skip experiments” is introduced.

7 Changes in NMRPT

7.1 Shim Command List

Shim commands are regrouped for improved manageability.

7.2 New Default Shim Commands with Option ws30 for Water Suppression and Gradient Recovery Experiments

For water suppression experiment shim command 215 (ro off wait; topshim fine ws30 seriousws tunea ordmax=8) will be used as new default.
For gradient recovery experiments shim command 205 (ro off wait; topshim fine ws30 tunea ordmax=8) will be used as new default.

7.3 Lock Handling

Instead of BSMS_LOCK_LOST the parameter BSMS_DEF_ELCB_LOCK will be interpreted by NMRPT to check if sample is locked.
ATMA will no be executed before the lock handling, since sometimes LOCK will be lost during ATMA and to avoid negative effect of lock due to tuning and matching

7.4 NMRPT Reports

Coil and Dewar in NMRPT protocol are renamed to Magnet and Cryostat respectively to use the same naming convention as MICS and magnets.

7.5 Handling of Sample Changer Errors

In case of sample changer error NMRPT set all experiments of this holder to status “skip experiment” in experiment. If possible NMRPT will continue with the experiments of the next holder.
After fixing the sample changer problem of a certain holder the skipped experiments can be set for measurement again. All settings made in Preparation Queue will be retained.

7.6 ZG with Options -d20 and -cd0

NMRPT now calls ZG with two additional options -d20 and cd0 to print more debug information into the log files.

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