# Acceptance Manual

- Bruker NMR Product Test (NMRPT) for Avance NMR Systems with “Topspin Version 4.1.4” Software

Version 042

Innovation with Integrity

NMR

This manual was modified by

Bruker BioSpin - Docu Group

© October 01 2021: Bruker Corporation

Rheinstetten, Germany

P/N: ZUEP0102
DWG-Nr.:

# Summary of Contents

# Contents

# Contents

# Contents

# Contents

# Contents

# Contents

# 1 Introduction

## 1.1 Purpose

This manual describes the NMR tests, which have been scheduled logically to efficiently demonstrate the full **installation and operational qualification (IQ/OQ)** of a Bruker AVANCE-series instrument. It includes basic specification tests such as line shape, resolution and signal-to-noise ratio for 1H and 13C as well as signal-to-noise ratio tests for other nuclei. Additional tests will show the high stability and precision of the electronics as well as that of the magnet and the probes.

**NOTICE**

**Test procedures and Tests:**

Please note that Bruker Service Engineers are not responsible for, nor are they trained to run, any extra tests or test spectra in addition to those described in the NMR Product Test manual ZUEP0102.

The aforementioned NMR Product Test procedure constitutes the agreed tests for demon-strating the correct function and performance of the instrument.

Upon successful completion of the tests, both the customer and the Bruker service engineer shall sign the acceptance report ZFPT0008 and the instrument shall be deemed to have been accepted in full according to the terms of the sales agreement.

=> All test procedures and typical performance values are subject to change without notice.

**Additional Tests:**

Any tests additional to those described in this document must be agreed upon at the time of sale and must be documented in the sales agreement. They will be performed by the Bruker application expert subsequent to the installation and they do not form part of the technical acceptance (IQ/OQ) of the instrument.

Some experiments of the NMR Product Test procedure are also used when installing a probe or accessories on an existing spectrometer. For the IQ/OQ procedure of such components, the acceptance reports ZFPT0009 (for probes) and ZFPT0014 (for accessories) will be generated automatically from the NMRPT software.

## 1.2 Area of application

With any installation of an NMR system, the customer will receive an introduction and basic training from the Bruker service engineer. The goal of this demonstration is to familiarize the user with safety requirements, system features, and the handling of the OEM products. In addition to the installation procedure, a list of technical demonstrations is outlined in order to provide an effective introduction to the NMR system.

## 1.3 Warning / Notice Signs

Safety instructions in this manual and labels of devices are marked with symbols. The safety instructions are introduced using indicative words which express the extent of the hazard.

In order to avoid accidents, personal injury or damage to property, always observe safety instructions and proceed with care.

**WARNING**

**WARNING indicates a hazardous situation, which, if not avoided, could result in death or serious injury.**

This is the consequence of not following the warning.

1. This is the safety condition.

**=>** This is the safety instruction.

**NOTICE**

**NOTICE indicates a property damage message.**

This is the consequence of not following the notice.

1. This is the safety condition.

**=>** This is the safety instruction.

This symbol highlights useful tips and recommendations as well as information designed to ensure efficient and smooth operation.

## 1.4 Referenced documents

### 1.4.1 Test procedures, Test protocols and Test report (forms)

| | |
|---|---|
| ZUEP0103 | Test procedures for final test of Avance NMR systems |
| ZFPT0008 | Acceptance test protocol for systems |
| ZFPT0009 | Accpetance test protocol for probes (add-on installation) |
| ZFPT0014 | Acceptance test protocol for accessories (add-on installation) |
| ANAPH011 | LC-NMR Acceptance test description |
| FBAPH009 | LC-NMR Acceptance test report |

### 1.4.2 Installation Manuals and Service Manuals

| | |
|---|---|
| Z31555 | CryoProbe System Installation Manual |
| Z31984 | CryoProbe Prodigy Installation Manual |
| H9153 | Diffusion Installation and User Manual |
| Z31750 | SampleJet Installation Manual |
| Z31973 | SampleMail / SampleCase Installation Manual |
| Z31901 | SampleXpress Service Manual |
| Z31942 | DNP-NMR Control System Console Service Manual |

### 1.4.3 User Manuals

| | |
|---|---|
| Z31836 | General Safety Considerations User Manual (English version). Note: This manual is also available in other languages. |
| Z31633e | Avance SGU Based Frequency Generation Beginners Guide (English version). Note: This manual is also available in other languages. |
| H9775SA3 | Acquisition Reference Manual – TopSpin online help |
| Z31326 | User manual for NMR magnet systems and refilling procedures |
| Z33092 | Liquid Handler SamplePro Tube |
| Z33075 | Micro Imaging for AVANCE III Systems User Manual |
| Z33117 | BSNL (Bruker Smart Nitrogen Liquefier) |
| Z33119 | BCU I User Manual |
| Z33120 | BCU II User Manual |
| W153895 | LT-MAS (Low temperature MAS equipment) |
| Z31943 | DNP-NMR Control System Console User Manual |
| H146901 | MAS III Pneumatic Unit User Manual |
| Z33045 | CryoProbe Prodigy Order Information |

# 2 Installation Qualification (IQ)

The system must first be installed and certain initial tests must be performed to ensure general functionality before the operational qualification can be started. The installation qualification includes the following steps.

## 2.1 General setup of the console

The engineer checks that all cables in the console and also all cables leading to peripherals are firmly connected and not bent in an unfavourable way that may compromise the functionality of the connected device or otherwise negatively influence the performance of the system. Next, the computer controlling the system, the console, and all peripherals are connected to power and turned on. The engineer makes sure that all power supplies work correctly and that all hardware components including the peripherals show no error indicators.

In particular, the following connections to site-specific supply lines or installations must be checked. Together with the system owner and local authorities it must be made sure that these connections comply with local regulations. The following list serves as a guideline, but the check is not limited to these devices. Instead, all site-specific connections need to be validated.

=> Check the correct **grounding** of the console, preamplifier and magnet in accordance with the descriptions given in the “General Safety Considerations” User Manual Z31836 (available in several languages) on the BASH-CD-ROM. This applies also to the following checks.

=> Check all **electrical connections** together with a local electrician. If a UPS is installed, make sure that it’s connected properly to the wall outlet and that proper grounding of the UPS is established.

=> Check all **gas connectors** (to nitrogen, air, or helium gas supply or air-cooled compressors) and make sure that the required pressure and flow is delivered. This applies to the magnet stands, automation devices, the console, the cryo platform, and possibly additional devices.

=> Check all connections to **water supplies** (e.g. for water-cooled compressors).

=> Check any other connections to local infrastructural devices.

Upon signing the acceptance documents, the future responsibility for these connections now lies with the system owner.

Topspin is started and some basic software checks are performed as outlined in the next chapters.

## 2.2 Firmware check

The engineer checks the firmware version on all devices and makes sure that the appropriate version is installed.

Engineers are provided with a Bruker internal document describing the download procedures:

=> **Firmware_Updates.pptx**
Customers can be provided with this document upon request.

## 2.3 Cortab

The engineer checks together with the customer that all necessary Cortab tables (linearization tables of the NMR spectrometer) for the required nuclei and routings are present on the system.

The cortab handling is explained in the acquisition manual H9775SA3 which is part of the TopSpin online documentation.

## 2.4 Sample Lift and Spin calibration

The engineer sets up the sample lift and checks the sample spinning.

## 2.5 Software license installed

Bruker supports different types of software licenses for all computers such as:

**a) Floating licenses**

Floating licenses allow the user to run the licensed program on any host in the licensed network. The number of programs that can run simultaneously on any host in this network is limited by the number of available floating licenses only.

**b) Spectrometer routing license (up to TopSpin3.5)**

TopSpin offers one additional license type: the spectrometer routing license. On a host computer that controls a spectrometer, TopSpin will always work even if no dedicated TopSpin license is available. This spectrometer routing license allows basic operation of the spectrometer, but some advanced features may not be available.

Please note that the spectrometer routing license is just a security feature that will be used only if for any reason (e.g. hardware problems) a regular license is temporarily unavailable.If a regular license (floating, node-locked, demo) is available, TopSpin will always use the regular license and not the spectrometer routing license.

**c) Demo licenses**

Demo licenses are node-locked licenses that expire after three months. They are availa-ble for all TopSpin versions. In addition, they can be used as an emergency license for TopSpin4 as a replacement of the spectrometer routing license (see point b above).

The Bruker engineer should see to it that an appropriate license has been installed.

To request any type of license, please use the Bruker license request form.

*https://www.bruker.com/service/support-upgrades/license-requests/nmr-license-requests.html*

For further information please refer to the Software Release Letter of your TopSpin version or see *www.bruker.com* for more information on software packages and license types.

## 2.6 Helium and Nitrogen level log files active

The procedures that write log files for the Helium level measurement and, if installed, the Nitrogen level measurement must be set up and checked.

## 2.7 MICS installed

The Magnet Information and Control System software (MICS) must be installed and the correct magnet BIS file must be in place. The alarm settings must be explained to the customer. All details are described in the MICS manual, which is part of the MICS software online documentation.

You can configure your system to allow remote monitoring of your system health by Bruker. Remote monitoring allows us to take preventive action prior to system failure and help you obtain maximum uptime. This remote monitoring service is free of charge.

If you have subscribed on a **LabScape** Agreement, or if you are within 12 months of system acceptance, Bruker will, in the event that we detect any potential issue with your system, analyze the situation after which we will contact you from the local office to plan remedial action. Additional responsibilities covered by Bruker will depend on the type of **LabScape** Agreement.

In addition, you will also receive emails at approximately three month intervals reporting upon the status of your magnet and summarizing events that have taken place (e.g. warnings, number of refilling operations etc.) during this period.

For further information, visit our website at *www.bruker.com/LabScape* or contact your local office.

## 2.8 Special precautions if a Prodigy Cryoprobe will be installed

If a Prodigy CryoProbe will be installed with the system, special precautions are required. The Prodigy CryoProbe will be cooled through evaporation of liquid nitrogen. Approximately 10 liters of liquid nitrogen will be evaporated during 24 hours of operation. This results in approximately 7000 liters (7 $m^3$) of nitrogen gas in the atmosphere of the spectrometer room. The ventilation system must be capable to replace this additional nitrogen gas with air.

**NOTICE**

**Use of Oxygen Sensors:**

Bruker strongly recommends installing oxygen sensors in the spectrometer room to detect a possible drop in the oxygen level.

=> Consult the CryoProbe Prodigy Order Information Z33045 for details.

## 2.9 Customer Information

The Customer Information must be entered in TopSpin with the edcstm command.

It is recommended to print the resulting file and to keep it with the installation documentation.

The system is now ready and the operational qualification (OQ) can be started.

# 3 Operational qualification (OQ) and customer training

The operational qualification of the system is performed through the execution of NMR measurements outlined in subsequent chapters of this manual. The type and number of experiments is determined through the type and number of probes that will be used with the NMR system. A protocol with the results from these NMR measurements will be presented to and discussed with the customer.

The goal of this demonstration is to familiarize the user with the safety requirements, with the system features, and with the handling of the peripherals and, if present, additional OEM products.

At the end of the demonstration, the acceptance protocol will be signed.

## 3.1 Basic safety precautions

**NOTICE**

**Prevention of hazards:**

The installation and operation of a superconducting magnet system presents a number of hazards that all laboratory staff must be aware of.

=> The Service Engineer will explain the effects of the magnetic field on magnetic materials such as tools, cell phones, watches, magnetic tapes, credit cards, and surgical implants.

=> **The customer is responsible after this training to forward these instructions to all laboratory staff, also to new employees in the future.**

=> Be aware that during normal operation only 3-5m3/day of nitrogen is evaporated, but during a quench 50-100m3 of helium gas is produced within a short time. Because of that a magnet system must not be installed in an airtight room.

=> Normal-sized windows and doors are usually sufficient for ventilation even during and after a quench.

For more details consult the magnet manual specific for your magnet system. Also refer to the “General Safety Considerations” User Manual Z31836 (available in several languages) on the BASH-CD-ROM.

### 3.1.1 Magnet safety

**NOTICE**

**Before charging of the magnet:**

The appropriate warning signs must be posted by the customer at each entrance to any room containing an NMR-System.

=> If the magnet is placed in an open setting, warning signs have to be posted at least 5 m from the magnetic center such that people cannot approach without first seeing the signs.

=> Also post the warning signs at rooms above and below the magnet, if the lines of 5G (0.5 mT) and 30 G (3.0 mT) penetrate into these areas.

=> Ensure that all loose ferromagnetic objects are removed from within the 5G (0.5 mT) area.

=> The customer should be aware of the fact that the operation of other equipment may be affected by the presence of large magnetic fields above 30 G (3.0 mT).

=> Items such as watches, cell phones, tape recorders and cameras may be magnetized and irreparably damaged if they are exposed to fields above 100 G (10.0 mT).

=> **The customer must provide on-site training about magnetic field hazards to people who may be exposed to 5G (0.5mT) or higher magnetic fields.**

=> The vertical and horizontal stray field plots are available in the Bruker site planning manuals and in the magnet manual specific for your magnet system.

### 3.1.2 Handling of cryogenic liquids and magnet refilling

The safe handling of cryogenic liquids requires some knowledge of the physical properties of these liquids, common sense, and sufficient understanding to predict the reactions of such liquids under certain physical conditions.

**NOTICE**

**Prevention of hazards:**

The very large increase in volume accompanying the vaporization of the liquid into gas and the subsequent process of warming up is approx. 700:1 for helium and nitrogen.

=> Therefore, we recommend that containers for cryogenic liquids must not be closed completely to avoid a large pressure build-up.
This will present an explosion hazard and may lead to large product losses.

**WARNING**

**Risk of injury during refilling procedure**

Risk of blindness if cryogenic liquids come into contact with the eyes!
Risk of severe cold-burns if skin comes into contact with cryogenic fluids!
Risk of skin adhesion with cooled metal parts.

1. Always wear protective goggles when carrying out the refilling procedure.
2. Always wear protective gloves and closed clothing when carrying out the refilling procedure.
3. Read the user manual for NMR magnet systems Z31326 for more details on the refilling procedures.
4. Refer to the Bruker movies explaining the correct helium and nitrogen refilling procedures. Movies to these topics are available for registered customers on *www.bruker.com* here: *https://www.bruker.com/service/information-communication/bruker-academy-videos.html.*

**NOTICE**

**Refilling of liquid Nitrogen:**

The nitrogen tank of the magnet (if present) should be refilled once a week or as often as described in the magnet manual.

=> Never apply a transfer pressure of more than 350 mbar (5.0 psi) to the nitrogen vessel.

=> Make sure that during the transfer all nitrogen neck tubes are fully open.

=> Before refilling the helium tank of the magnet, the level in the refill vessel must be checked with the dip-stick.

**Liquid Nitrogen:**

For the refilling procedure of **liquid nitrogen** follow the description in the user manual for NMR magnet systems Z31326 or refer to the **nitrogen refill movie** on *www.bruker.com* or on the BASH-CD-ROM.

**NOTICE**

**Refilling of liquid Helium:**

=> Always refill nitrogen (see above) before refilling helium.

=> Never insert a "warm helium transfer line" into the cryostat, the warm helium gas could lead to a quench of the magnet.

=> Never use any extensions on the helium transfer line because they might reach the siphon.

=> Never apply a transfer pressure of more than 100 mbar (1.45 psi) to the helium vessel.

=> Always make sure that the outlet of the helium manifold is fully open to the atmosphere or to a helium recovery system.

=> After refilling of helium, check that all nitrogen neck tubes are free of any ice blockages.

**Liquid Helium:**

For the refilling procedure of **liquid helium** follow the description in the user manual for NMR magnet systems Z31326 or refer to the **helium refill movie** on *www.bruker.com* or on the BASH-CD-ROM.

### 3.1.3 Control of nitrogen and helium level

The NMR instrument measures the helium level once a day at 04.15 am (in TopSpin2.x and older versions it was measured at 03:00 am). This level is recorded by software…

**Windows:** c:\bruker\diskless\prog\logfiles\heliumlog

or

**Linux:** /usr/diskless/prog/logfiles/heliumlog)

…and can be checked manually on the BSMS Keyboard (He-Level) or in the BSMS display.

This level must be recorded at least once a week. You can find prepared sheets at the end of the magnet manual.

The MICS software (see above) can be configured such that it will read the levels recorded in the heliumlog file.

With this information, MICS can provide graphical presentations of helium and nitrogen boil-off.

We recommend that the helium vessel is refilled within the specified hold time period and certainly before the level falls below the allowed minimum level (check the user manual for NMR magnet systems Z31326).

### 3.1.4 Homogeneity and stability disturbance

**Ferromagnetic Material**

The presence of any ferromagnetic materials in the immediate vicinity of the magnet will decrease the magnet homogeneity. The site-planning manuals on the BASH-CD-ROM provide guidelines for minimum requirements.

**Electromagnetic Interferences**

Large electromagnetic interference can affect the long term stability of an NMR system. Possible sources of electromagnetic interference may be produced, for instance, by elevators, trams, subways, mass spectrometers, centrifuges, large electric motors, air conditioning systems, heavy duty transformers etc.

The site planning manuals contain detailed information on the tolerated limits.

### 3.1.5 Earthquake precautions

If the system is placed in a territory with higher seismic activities, we recommend securing the magnet system either with ropes from a ceiling hook or with non-magnetic brackets around the magnet stand.

### 3.1.6 Refilling of the nitrogen vessel for Prodigy CryoProbes

The refilling of the nitrogen vessel for Prodigy CryoProbes and necessary precautions will be explained in cases where such a probe will be installed on the system.

## 3.2 Hardware overview

The Service Engineer will outline the function of the NMR system. The individual hardware units are explained to familiarize the customer with all system features.

Detailed circuit descriptions will not be covered. Special customer training courses are offered by Bruker here:

*https://www.bruker.com/service/education-training/training-courses/magnetic-resonance.html*

**NOTICE**

**Damage to the probe because of excessive power:**

Applying too much power may damage the probe and will most likely lead to an expensive probe repair.

=> Each probe has a maximum power limit for every possible nucleus.

=> For probes that are delivered with a PICS module (probe information control system), these values are directly imported with the command “edprobe”.

=> The maximum RF power values for the corresponding nuclei are also provided in the “Customer Certificate” that is delivered with the probe.

=> Make sure this maximum power is never exceeded in any experiment.

=> If possible always turn powercheck on in Topspin.

### 3.2.1 Console on/off operation

The customer will be trained on the different procedures of how to power down a console carefully (like RF power down, computer power down, and main power down) as well as how to start it up again. Also the reset functions will be shown on all units.

The customer will be trained to do some basic system tests like DRU and ELCB tests through the respective web interfaces (TopSpin command “ha”).

Bruker offers periodically scheduled training courses for operation and troubleshooting of spectrometers especially for technicians and engineers. See here:

*https://www.bruker.com/service/education-training/training-courses/magnetic-resonance.html*

**NOTICE**

**Safety Demonstration of power down:**

For safety reasons a fast power down will be demonstrated.

**The customer is warned that only trained service staff should open the units because of hazardous voltages.**

### 3.2.2 Basic operation

An introduction to standard measurements on 1H- and X-nuclei is given by the Bruker service engineer. A demonstration of peripheral units like temperature control, gradient control, gradient amplifiers, or solids accessories will be performed (including mechanical operations like probe change).

**NOTICE**

**Read Manual before Demonstation:**

We recommend that the customer reviews the operation manuals before attending the demonstration in order to benefit most.

A general guide to shimming as well as tuning and matching will be part of the introduction. Engineers are provided with a presentation explaining the basic features of TopSpin.

**=> TopSpin3.5_introduction_3h.pptx**

Customers can be provided with this document upon request.

A basic introduction is provided with the Beginners’ Guide Z31633e, which is available in several languages on the BASH-CD-ROM as well as on the Bruker website at

*https://www.bruker.com/service/information-communication/user-manuals/nmr.html*

Bruker offers periodically scheduled training courses for operation and usage of the TopSpin and IconNMR software packages for users of the spectrometers. See here:

*https://www.bruker.com/service/education-training/training-courses/magnetic-resonance.html*

## NOTICE

**Installation and Operation of products from other sources:**

Bruker service engineers are not responsible for, nor are they trained to install, locally ordered OEM-products from other sources but Bruker.

### 3.2.3 Troubleshooting

The complete range of software service tools such as web tools, BSMS, HPPR, and IPSO software tools will be demonstrated.

### 3.2.4 Backup (nmr_save, Images)

The TopSpin software provides functionality to periodically archive the current spectrometer configuration to a file. In case of computer hardware problems, this archive can be used to restore a computer to the last known spectrometer status.

Bruker also provides a software tool to create a complete computer system disk image. The customer will be informed about these possibilities.

### 3.2.5 Introduction to IconNMR

The basic functionality of IconNMR should be presented and explained to the customer, especially if a sample changer is installed on the system. An example run should be started and the quality of the results should be verified.

Engineers are provided with a presentation explaining the basic features of IconNMR.
**=> IconNMR-acquisition-overview.pptx**
Customers can be provided with this document upon request.

### 3.2.6 AssureSST / Performance check

AssureSST (System Suitabilty Test) is a part of IconNMR to check system performance on a regular basis (e.g. for instruments that are installed in a GxP environment). AssureSST should be setup and demonstrated.

Engineers are provided with a presentation explaining the basic features of AssureSST.
**=> AssureSST_overview.pptx**
Customers can be provided with this document upon request.

## 3.3 Optional Components

The customer will be informed about the handling and documentation of optional or addional components like…:

=> Sample Changer
=> MAS controller
=> High power equipment
=> LC-NMR
=> Liquid Handler SamplePro Tube
=> Micro-Imaging

=> Diffusion
=> CryoProbe / Cryoplatform
=> BSNL
=> Additional cooling/heating units (like BCU1 / BCU2)
=> LT-MAS (Low Temperature MAS equipment)
=> Gyrotron magnet and DNP console

### 3.3.1 Sample Changer

The Sample Changer will be installed in accordance with its corresponding service or user manual. If the device may be installed by the customer, then the instructions are contained in the user manual. Otherwise, the instructions are contained in the service manual.

An acceptance protocol for the device is part of the installation instructions. The engineer will complete this acceptance protocol together with the customer and both will sign this acceptance document.

#### 3.3.1.1 SampleJet

The installation manual Z31750 contains the installation instructions and the acceptance protocol.

#### 3.3.1.2 SampleMail / SampleCase

The installation manual Z31973 contains the installation instructions and the acceptance protocol.

#### 3.3.1.3 SampleXpress / SampleXpress Lite

The service manual Z31901 contains the installation instructions and the acceptance protocol.

### 3.3.2 MAS Controller

The MAS Controller will be installed in accordance with its corresponding user manual (H146901), which also covers the installation.

The successful installation will be shown through the measurement of relevant samples that show the proper functionality in combination with the spectroscopic test results obtained with a suitable MAS probe.

### 3.3.3 High power equipment

High power equipment refers to special amplifiers that provide high power output typically for solid-state applications. The basic functionality of these amplifiers is tested during the Cortab procedure (see above 2.3).

The proper functionality will be shown through the measurement of relevant samples in combination with the spectroscopic test results obtained with a suitable MAS probe.

### 3.3.4 LC-NMR

The LC-NMR equipment will be installed in accordance with the document ANAPH011 and the acceptance test report will be documented in FBAPH009.

The proper functionality will be shown through the measurement of relevant samples in combination with the spectroscopic test results obtained with a suitable probe.

### 3.3.5 Liquid Handler SamplePro Tube

The basic installation of the Liquid Handler SamplePro Tube will be done in accordance with the document Z33092.

**NOTICE**

**Application-specific Tests**

Additional application-specific tests and adjustments are not part of the basic installation. They are part of, and defined for, an application specific installation.

### 3.3.6 Micro-Imaging

The Micro-Imaging equipment will be installed in accordance with the document Z33075.

The proper functionality will be shown through the measurement of relevant samples in combination with the spectroscopic test results obtained with a suitable Micro-Imaging probe.

### 3.3.7 Diffusion

The Diffusion equipment will be installed in accordance with the document H9153.

The proper functionality will be shown through the measurement of relevant samples in combination with the spectroscopic test results obtained with a suitable Diffusion probe.

### 3.3.8 CryoProbe / Cryoplatform

The Cryoprobe equipment will be installed in accordance with the documents listed be-low.

The proper functionality will be shown through the measurement of relevant samples in combination with the spectroscopic test results obtained through the NMRPT procedure.

#### 3.3.8.1 Helium-cooled cryoprobes

The CryoProbe / Cryoplatform will be installed in accordance with the document Z31555.

#### 3.3.8.2 Nitrogen-cooled CryoProbes (Prodigy probes)

The CryoProbe / Cryoplatform will be installed in accordance with the document Z31984.

### 3.3.9 BSNL (Bruker Smart Nitrogen Liquefier)

The BSNL unit will be installed in accordance with the document Z33117.

### 3.3.10 Additional cooling/heating units (like BCU1 / BCU2)

The additional cooling units will be installed in accordance with the documents Z33119 and Z33120, respectively.

### 3.3.11 LT-MAS (Low Temperature MAS equipment)

The LT-MAS (Low Temperature MAS equipment) will be installed in accordance with the document W153895.

The proper functionality will be shown through the measurement of relevant samples in combination with the spectroscopic test results obtained with a suitable MAS probe.

### 3.3.12 Gyrotron magnet and DNP console

The Gyrotron equipment will be installed in accordance with the document Z31942. The operation of the system is described in the user manual Z31943.

The proper functionality will be shown through the measurement of relevant samples in combination with the spectroscopic test results obtained with a suitable probe.

## 3.4 Acceptance and warranty

### 3.4.1 Explanation of warranty

**NOTICE**

The customer will be informed that the warranty will begin with the acceptance of the instrument. The warranty period will be in accordance with the terms of sale and must be inserted in the acceptance report ZFPT0008.

The items covered under warranty are also described in the sales agreement and normally include all defects in material and workmanship.Glassware and parts, subject to wear and tear, are not included.

In the case of parts delivered late, the warranty for these parts will begin on the acceptance of these parts.

### 3.4.2 System documentation

For each Bruker NMR-System a whole set of operation and reference manuals is provided either in printed form, or stored on CD/DVD, or as online help in the respective software packages.

The service engineer will give a short introduction on how to use this documentation.

### 3.4.3 Customer support hotlines

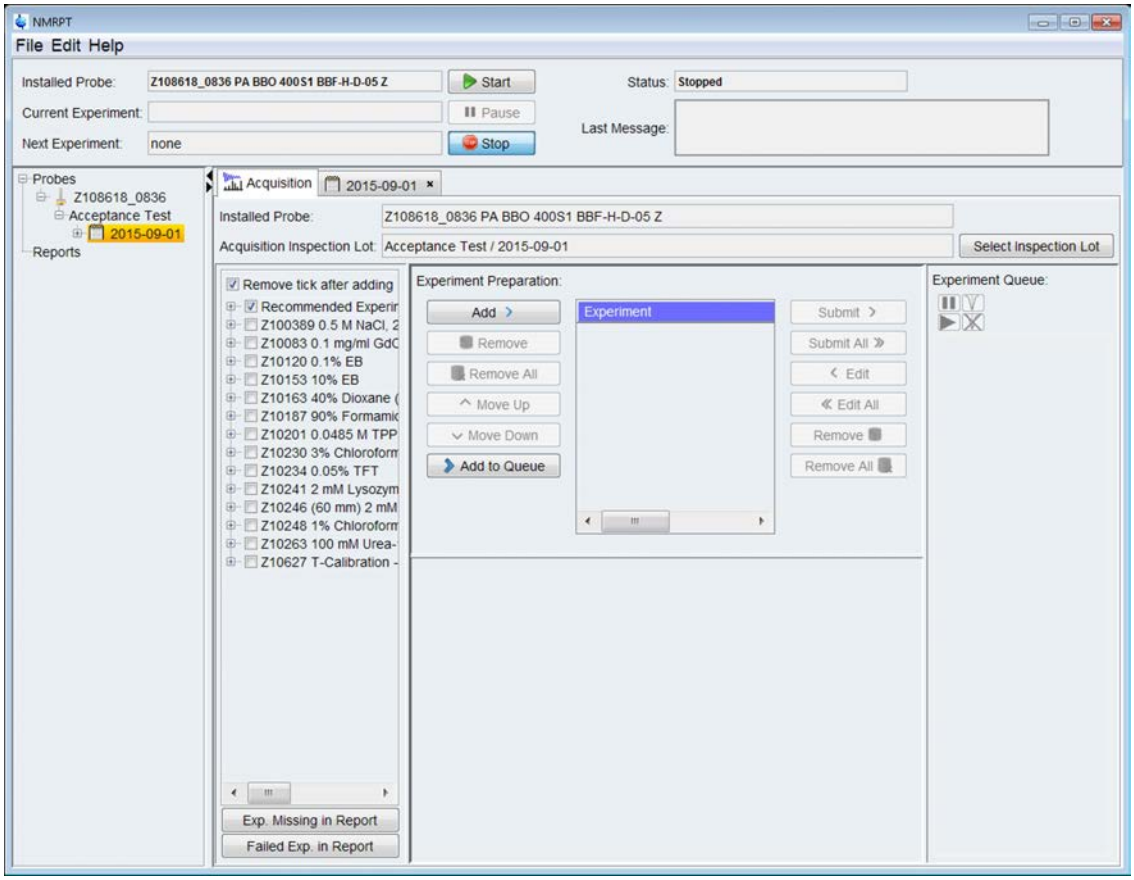
Customer support hotlines will be entered in the corresponding software interfaces.

General contact information is provided in the Contact chapter of this manual.

# Operational qualification (OQ) and customer training

# 4 NMR Product Test (NMRPT)

*NMRPT* software provides an automated Acceptance Test and Service Test procedure of spectrometers and probes.




This software is generating all necessary acquisition and processing parameters for Acceptance and Service Testing of all kind of probes and consoles (AVIII and newer). Evaluation of the results is provided. Customer information, spectrometer and probe information is collected by the *NMRPT* software for documentation and acquisition purposes. All processing and plotting parameters are created and applied automatically. Measurement results can be explored individually and selected measurements of each experiment are collected into one spectra PDF. The collected spectra and a Test Certificate are the two parts of the Test Report. The type of Test Report depends on the selected test mode. This Test Report is created by the Service Engineer after all measurements are finished. If the results meet the specifications according to the Customer Certificate (ZFUT0015), the Service Engineer can finalize this Test Report to obtain an official Bruker Test Document.

*NMRPT* automatically stores a shimfile for the Lineshape Nonspinning and the Water Suppression experiments.These shim file names are composed of the part number and serial number as well as an extension containing the experiment type, e.g. the file Z104275_0118_1H_ls_nrot is a shimfile of the 5 mm BBO probe Z104275_0118 shimmed on 1H for Line Shape Nonspinning experiment.

Note: All probe specifications (Line Shape, Resolution, Sensitivity, Hump and Splitting) will automatically be evaluated from measurement by *NMRPT*. The *NMRPT* software therefore always calculates the 1H Sensitivity for each, a noise region of 2 ppm and a noise region of 200 Hertz. See the probe specifications (Customer Certificate ZFUT0015) for the corresponding values ("Rated Specification", "Rated Sample" and "Conditions") of the respective nuclei.

# 5 NMRPT Experiments

## 5.1 Introduction

All standardized experiments provided by *NMRPT* are described in this chapter. But the user can select only from the subset feasible to the current hardware (combination of probe, console, and routing). The datasets included with the *NMRPT* are automatically adjusted and optimized to the current hardware. Therefor the parameters shown in this chapter are only example values and may differ depending on the hardware to be tested. If user interaction is necessary, the software will guide the user (e.g. through the parameter optimization).
A PDF file documents the results and spectra for each successful measurement. *NMRPT* collates the results and spectra of all acquired experiments (one measurement per experiment) in a report. This report is the test document for the acceptance or a service of a spectrometer, parts of a spectrometer, a probe, or accessories.

**Receiver Gain (RG)**

The value for RG is predefined in each experiment. It is adjusted for each probe during setup. The usual standard values are $RG_{min}$ or $RG_{max}$. In first case, *NMRPT* executes RGA to set the optimum value. In second case, *NMRPT* adopts the value. For a user controlled RG, set RG in the Preparation Panel of *NMRPT* Acquisition page. $RG_{min}$ and $RG_{max}$ are derived from TopSpin configuration information (after execution of cf, see TopSpin manual). In *NMRPT* the maximum value of $RG_{max}$ is limited to 203. If the $RG_{max}$ value of the TopSpin configuration is lower, this value will be used.

**Carrier Frequencies (O1 and O2)**

The carrier frequency offset can be changed in all experiments where *NMRPT* does not optimize these settings. It is not recommended to change this except for the water suppression experiments when using specific options of L23 (see subsequent section of watersuppression experiment).

**Loopcounter Parameter L23**

The loopcounter L23 is used to apply special conditions in *NMRPT* experiments. The allowed values for each experiment are provided in the experiment description in this chapter. For some experiments (e.g. L23=27 in watersuppression experiment) changing the L23 value results in a non-standard experiment without a regular experiment output.

**Gradient Strength (GPZx)**

The used gradient strength (given in %) of all experiments is related to a maximum gradient current of the probe. If the maximum current of a gradient amplifier differs from the one of the probe, the gradient strength is recalculated accordingly.

**Pre-Scan Delay (DE)**

The value of DE is set during execution of getprosol. For a user controlled DE, set DE and the option ‘Skip Getprosol’ in the Preparation Panel of NMRPT Acquisition Page or change the DE entry in the Prosol table. For the following experiments this handling is overruled by setting DE explicitly after getprosol: NPT_1H_cosydfphpr, NPT_1H_noesyphpr, NPT_13C_ringing_dec1h, NPT_prep_fieldsetting_d, NPT_prep_lineshape_wrot

## 5.2 Experiments for High Resolution Probes (HR)

**Sample Rotation Frequency (RO)**

The sample rotation frequency is set and interpreted by NMRPT as provided in sample state in the experiment descriptions of this chapter. Selected experiments (e.g. 2D experiments) are measured always with RO = 0. For all the other experiments RO is set according the following rules:

Sample diameter <= 1.7mm => RO = 0
Sample diameter = 3.0mm => RO = 0 (RT probes)

Sample diameter = 3.0mm => RO = 20 (CRP probes)
Sample diameter = 5mm => RO = 20
Sample diameter = 8mm => RO = 18
Sample diameter = 10mm => RO = 14

**Probes with the same nucleus on multiple channels (13C, 15N, 31P, 19F)**

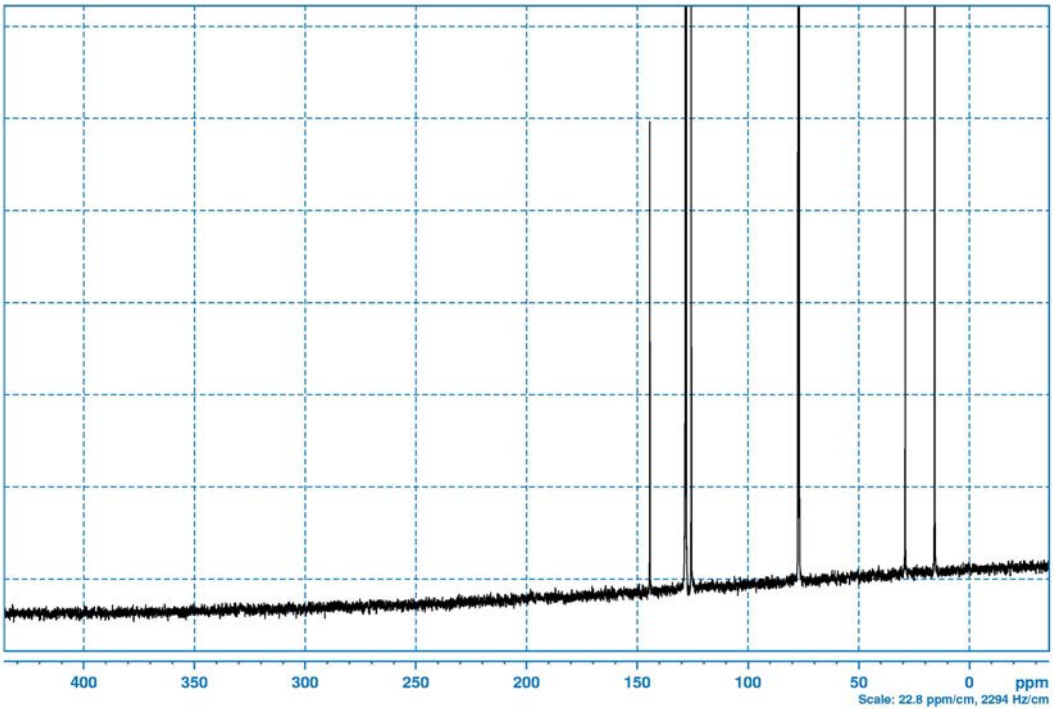
When a nucleus occurs twice on a probe, different experiments are used for each probe channel. The standard experiment (e.g. NPT_13C_sensitivity) is measured on the selective probe channel (excluding 1H/19F channel). The second experiment, labeled with "_2nd" (e.g. NPT_13C_sensitivity_2nd) is measured on the broadband channel. The "_2nd" experiments are not documented in this chapter, since they are similar to the corresponding standard experiments.

**Probes with 19F tuneable on 1H channel**

In case of 19F measurements on a 1H/19F channel the experiments need special handling for certain hardware. Therefore the experiment names for 19F measurements on the 1H/19F channel are indicated with "_hcoil".

### 5.2.1 13C background with sample (NPT_13C_backgr_withsample)

**Test Sample:** 10% Ethylbenzene (EB) in Chloroform-D
Z10153, Z10154, Z10034, Z10253, Z10292, Z10723
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

13C Background signal spectrum with sample. Sharp signals arise from sample and solvent, broad signal could arise from solid compound in the probe.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PULPROG | npt_zg0dc | | |
| NS | 1000 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | 199.988 | ppm | |
| O2P | 5.000 | ppm | |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| SW | 496.855 | ppm | |
| TD | 65536 | | |
| AQ | 0.655 | s | field dependent |
| FIDRES | 1.526 | Hz | field dependent |
| D 1 | 1.430 | s | AQ+D1=const |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 40.2 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| DIGMOD | 3 | | baseopt |
| TE | 298.000 | K | default |

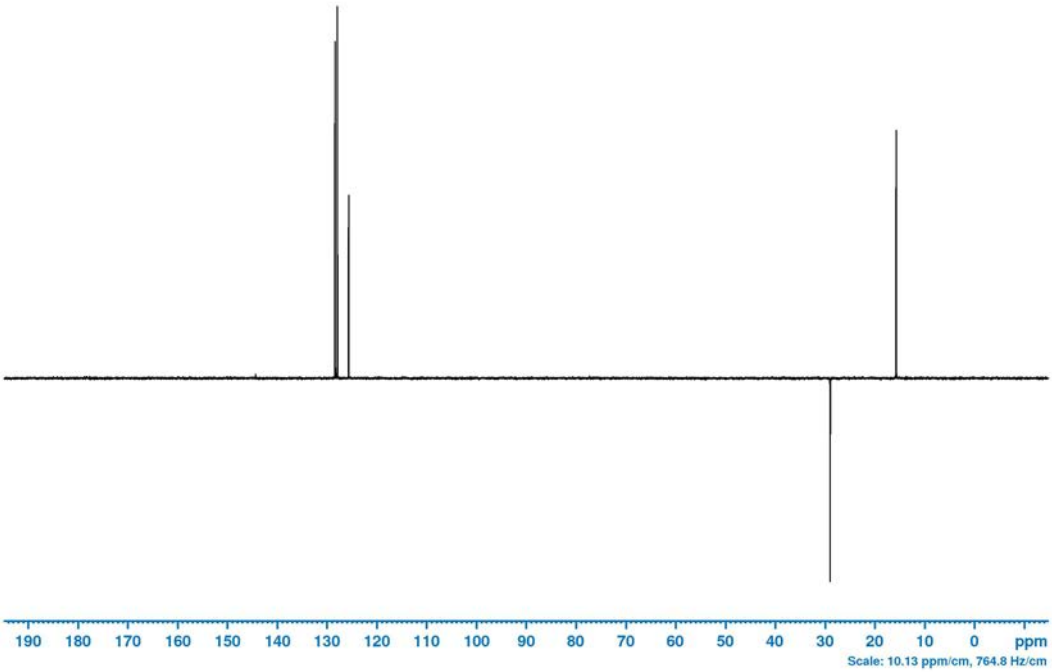
| | | | |
|---|---|---|---|
| CNST 10 | 20.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 65536 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| PC | 1.400 | | |
| F1P | 180.000 | ppm | |
| F2P | -20.000 | ppm | |

### Experiment Description

Background signal measurements are executed using a small flip angle due to two reasons. First, to get more efficient excitation bandwidth, secondly to compensate for usually long T1 relaxation time of solid signals.
Full spectrum is normally printed without any baseline correction.

### 5.2.2 DEPT135 (NPT_13C_dept135)

**Test Sample:** 10% Ethylbenzene (EB) in Chloroform-D
Z10153, Z10154, Z10034, Z10253, Z10292, Z10723
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

DEPT ('Distortionless Enhancement of Polarization Transfer') using a 135 degree decoupler pulse. The experiment shows carbon-13 signals where one (CH) or three protons (CH3) are attached with positive sign, whereas the negative signals in the spectrum arise from carbon with two protons (CH2). Carbons with no protons attached are virtually suppressed, as well as carbon signals from solvent molecules.

**Control Option for Acquisition (L23)**

1 default

## Parameters

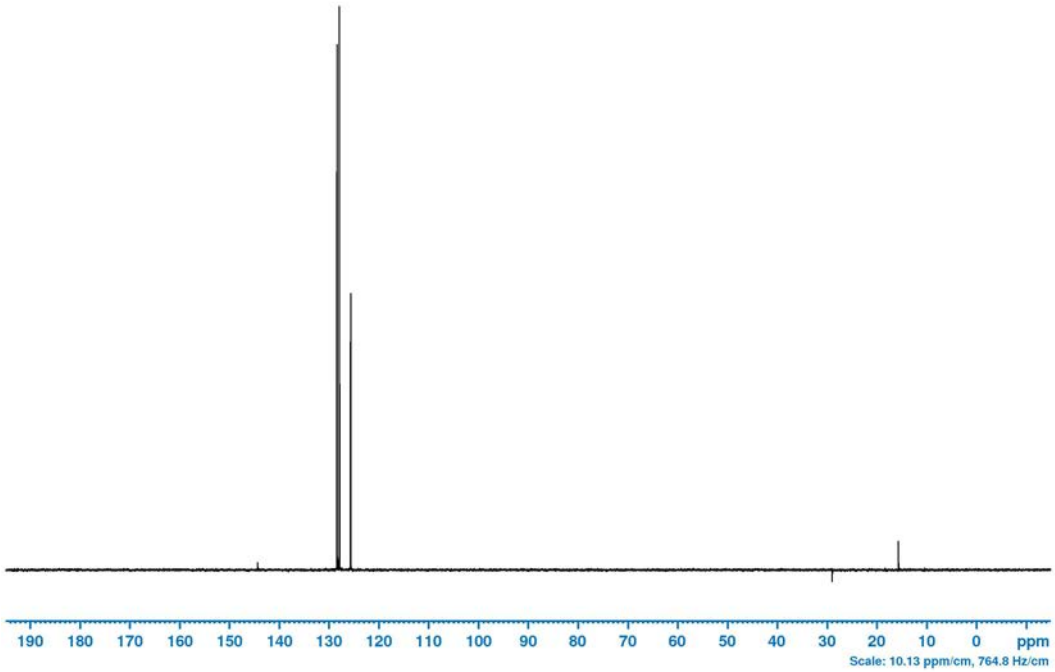
| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PULPROG | deptsp135 | | |
| NS | 128 | | RT: 128, Cryo: 8 |
| DS | 8 | | |
| RG | 101.000 | | no optim. |
| O1P | 89.981 | ppm | |
| O2P | 5.000 | ppm | |
| SW | 216.048 | ppm | |
| TD | 130434 | | field dependent |
| AQ | 3.000 | s | |
| FIDRES | 0.333 | Hz | field dependent |
| D 1 | 4.000 | s | |
| D 2 | 0.003 | s | 1s/(CNST2*2) |
| CPDPRG2 | waltz65 | | decoupl. sequence |
| CNST 2 | 145.000 | Hz | J[XH] coupling |
| P 1 | 11.0 | us | 90deg NUC1 |
| P 3 | 14.0 | us | 90deg NUC2 |
| P 4 | 28.0 | us | 180deg NUC2 |
| PCPD 2 | 115.0 | us | 90deg CPD |
| P 13 | 2000.0 | us | 180deg shaped pulse |
| PLW 1 | 19.3 | W | Pow@90deg(Specs) NUC1 |
| PLW 2 | 5.6 | W | Pow@90deg(Specs) NUC2 |
| PLW 12 | 0.08 | W | Pow@90deg(CPD) |
| SPNAM5 | Gaus1.1000 | | shape name |
| SPOAL 5 | 0.500 | | phase align. |
| SPOFFS 5 | 0.000 | Hz | offset freq. |
| SPW 5 | 3.6 | W | Pow@Shape |
| TE | 298.000 | K | default |
| **F1 PROC** | | | Parameters |
| SI | 131072 | | |
| WDW | 0 | | |
| LB | 1.000 | Hz | |
| PC | 1.400 | | |
| F1P | 175.000 | ppm | |
| F2P | -5.000 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 48 | 1.000 | | SN_WSUP(res.) |

## Experiment Description

DEPT experiments are executed as integral and functional test of the system. The outcome of this experiment is strongly dependend on correct decoupler pulses (1H). The pulse sequence version used in NMRPT is using shaped pulses for 180 degree carbon refocussing pulse to suppress off-resonance effects which are often responsible for phase distortions at higher field strengths.
The evaluation of the experiment is based on the comparison of the signal integral at ~126 ppm (reference) and ~29 ppm (check). For the DEPT135 the integral ratio should be close to 100%.

### 5.2.3 DEPT90 (NPT_13C_dept90)

**Test Sample:** 10% Ethylbenzene (EB) in Chloroform-D
Z10153, Z10154, Z10034, Z10253, Z10292, Z10723
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

DEPT ('Distortionless Enhancement of Polarization Transfer') using a 90 degree decoupler pulse. The experiment shows only carbon-13 signals where one proton (CH) is attached. All other carbon signals including signals from solvent molecules are virtually suppressed.

**Control Option for Acquisition (L23)**

1 default

## Parameters

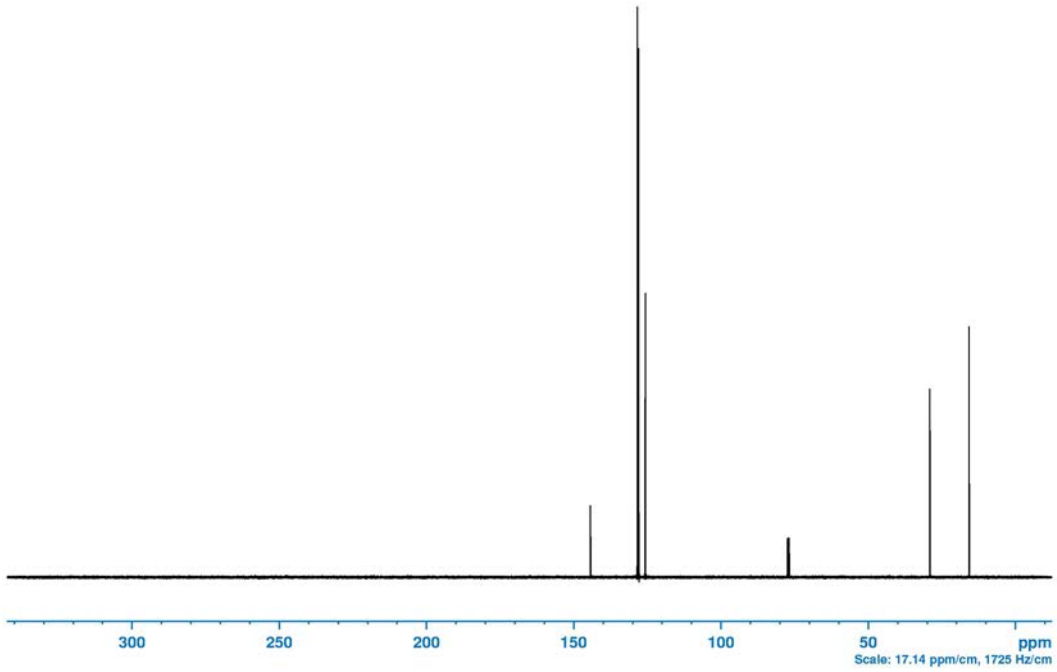
| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PULPROG | deptsp90 | | |
| NS | 128 | | RT: 128, Cryo: 8 |
| DS | 8 | | |
| RG | 101.000 | | no optim. |
| O1P | 89.981 | ppm | |
| O2P | 5.000 | ppm | |
| SW | 216.048 | ppm | |
| TD | 130434 | | field dependent |
| AQ | 3.000 | s | |
| FIDRES | 0.333 | Hz | field dependent |
| D 1 | 4.000 | s | |
| D 2 | 0.003 | s | 1s/(CNST2*2) |
| CPDPRG2 | waltz65 | | decoupl. sequence |
| CNST 2 | 145.000 | Hz | J[XH] coupling |
| P 1 | 11.0 | us | 90deg NUC1 |
| P 3 | 14.0 | us | 90deg NUC2 |
| P 4 | 28.0 | us | 180deg NUC2 |
| PCPD 2 | 115.0 | us | 90deg CPD |
| P 13 | 2000.0 | us | 180deg shaped pulse |
| PLW 1 | 19.3 | W | Pow@90deg(Specs) NUC1 |
| PLW 2 | 5.6 | W | Pow@90deg(Specs) NUC2 |
| PLW 12 | 0.08 | W | Pow@90deg(CPD) |
| SPNAM5 | Gaus1.1000 | | shape name |
| SPOAL 5 | 0.500 | | phase align. |
| SPOFFS 5 | 0.000 | Hz | offset freq. |
| SPW 5 | 3.6 | W | Pow@Shape |
| TE | 298.000 | K | default |
| **F1 PROC** | | | Parameters |
| SI | 131072 | | |
| WDW | 0 | | |
| LB | 1.000 | Hz | |
| PC | 1.400 | | |
| F1P | 175.000 | ppm | |
| F2P | -5.000 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 48 | 1.000 | | SN_WSUP(res.) |

## Experiment Description

DEPT experiments are executed as integral and functional test of the system. The outcome of this experiment is strongly dependend on correct decoupler pulses (1H). The pulse sequence version used in NMRPT is using shaped pulses for 180 degree carbon refocussing pulse to suppress off-resonance effects which are often responsible for phase distortions at higher field strengths.
The evaluation of the experiment is based on the comparison of the signal integral at ~126 ppm (reference) and ~29 ppm (check). For the DEPT90 the integral ratio should be close to 0%.

### 5.2.4 13C test for artifacts with 1H decoupling (NPT_13C_fullsw_dec1h)

**Test Sample:** 10% Ethylbenzene (EB) in Chloroform-D
Z10153, Z10154, Z10034, Z10253, Z10292, Z10723
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Full range 13C spectrum with 1H decoupling.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PULPROG | npt_zg0dc | | |
| NS | 64 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | 164.987 | ppm | |
| O2P | 5.000 | ppm | |
| SW | 354.909 | ppm | |
| TD | 262144 | | |
| AQ | 3.670 | s | field dependent |
| FIDRES | 0.272 | Hz | field dependent |
| D 1 | 1.230 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 40.2 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| DIGMOD | 3 | | baseopt |
| TE | 298.000 | K | default |

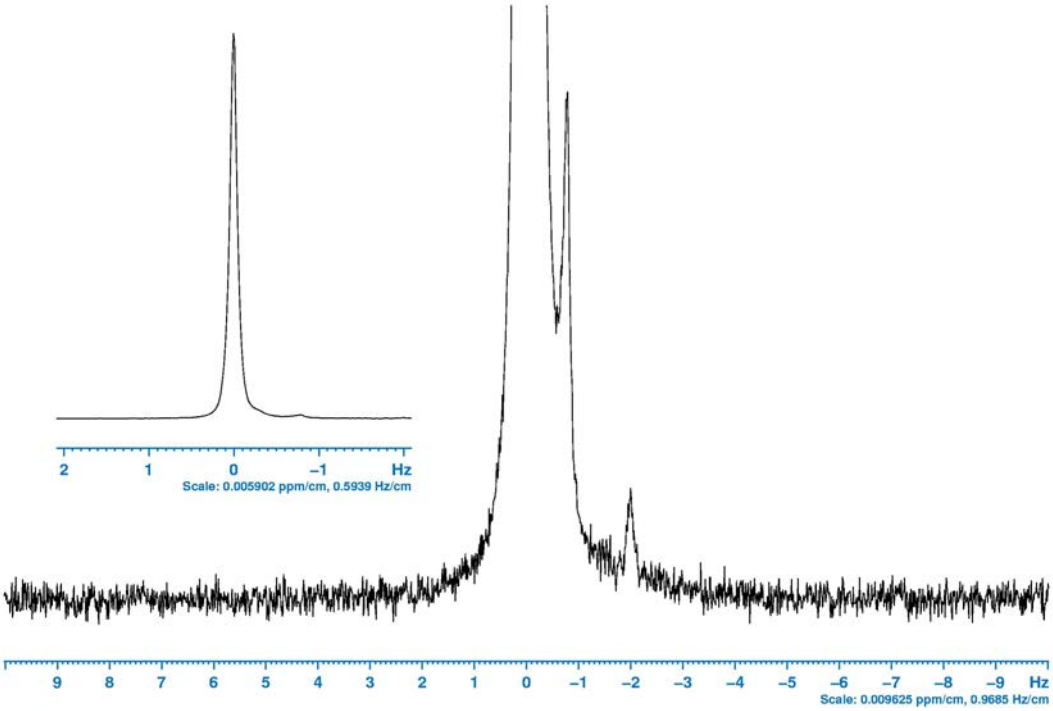
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 524288 | | |
| WDW | 1 | | |
| LB | 0.300 | Hz | |
| PC | 1.400 | | |
| F1P | 180.000 | ppm | |
| F2P | -20.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Full range spectra (spectroscopically useful range) are acquired as test for RF artifacts (spikes). Currently no evaluation is provided and visual inspection of the data is required. Data are treated with baseline correction.

## 5.2.5 13C lineshape without sample rotation (NPT_13C_lineshape_nrot)

**Test Sample:** 40% Dioxane in Benzene-D6 (ASTM)
Z10163, Z100929, Z10164, Z10035, Z10255, Z10242, Z10724
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Carbon-13 line shape spectrum from +10.0 Hz to -10.0 Hz as overview spectrum. The expansion plot scaled to full intensity on the left shows the dioxane (1,4-dioxane) signal with higher resolution (+2.0 Hz, -2.0 Hz).

**Control Option for Acquisition (L23)**

1 Broad band decoupling using waltz65, PULPROG=zgpg
11 CW decoupling based on PLW12, automatic O2 optimization, PULPROG=zgcw
21 CW decoupling based on PLW12, O2 from parameter set, no optimization, PULPROG=zgcw

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PULPROG | zgpg | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 66.488 | ppm | |
| O2P | 3.474 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 32768 | | |
| AQ | 41.288 | s | |
| FIDRES | 0.024 | Hz | |
| D 1 | 33.712 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PCPD 2 | 120.0 | us | CPD NUC2 |
| PLW 1 | 39.3 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| PLW 13 | 0.05 | W | Pow@CPD NOE NUC2 |
| CPDPRG2 | waltz65 | | decoupl. sequence |
| TE | 298.000 | K | default |

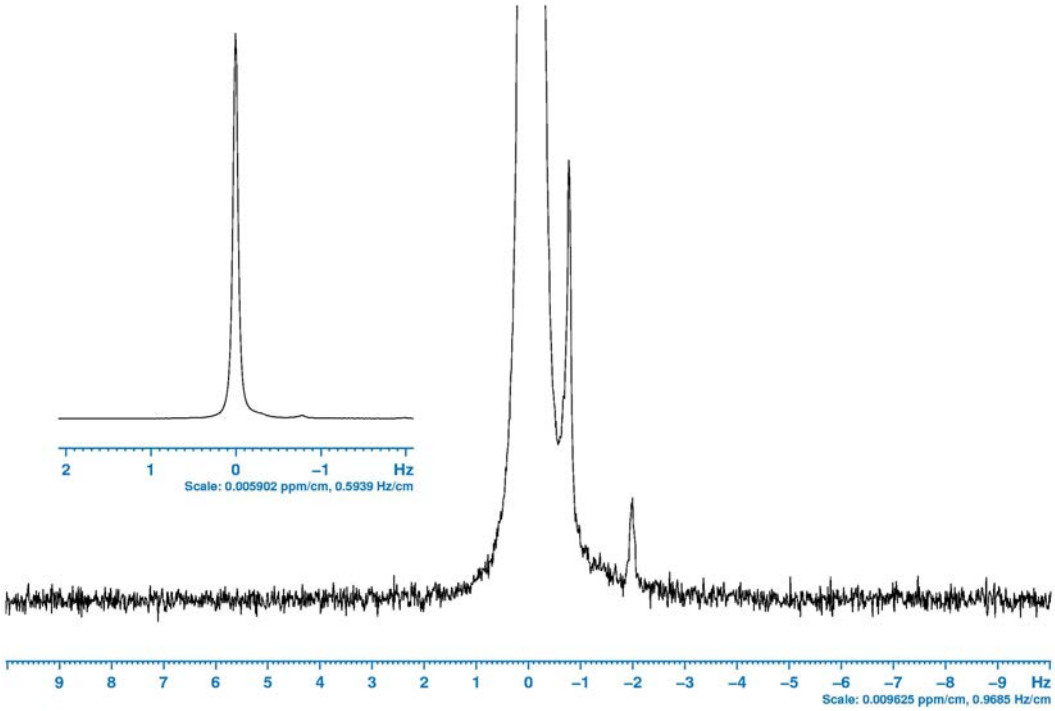
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.400 | | |
| F1P | 0.099 | ppm | |
| F2P | -0.099 | ppm | |
| CY | 1000.000 | cm | |

## Experiment Description

The Carbon-13 line shape experiment with 1H decoupling using as default waltz65 and decoupler pulse length (PCPD2) of 120 us. The corresponding decoupling powers (PLW12 and PLW13) are calculated from prosol entries for P12 and PLW12.
The exact signal position is determined with NS=1 prior to the line shape measurement. The carrier position is afterwards set to this position
O1 optimized = peakFreqHz - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.

## 5.2.6 13C lineshape with sample rotation (NPT_13C_lineshape_wrot)

**Test Sample:** 40% Dioxane in Benzene-D6 (ASTM)
Z10163, Z100929, Z10164, Z10035, Z10255, Z10242, Z10724
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Carbon-13 line shape spectrum from +10.0 Hz to -10.0 Hz as overview spectrum. The expansion plot scaled to full intensity on the left shows the dioxane (1,4-dioxane) signal with higher resolution (+2.0 Hz, -2.0 Hz).
The PDF comprises a second page (not shown in documentation) which shows carbon-13 line shape spectrum with a printing range from +45.0 Hz to -45.0 Hz (including spinning side bands).

**Control Option for Acquisition (L23)**

1 Broad band decoupling using waltz65, PULPROG=zgpg
11 CW decoupling based on PLW12, automatic O2 optimization, PULPROG=zgcw
21 CW decoupling based on PLW12, O2 from parameter set, no optimization, PULPROG=zgcw

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PULPROG | zgpg | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 66.488 | ppm | |
| O2P | 3.474 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 32768 | | |
| AQ | 41.288 | s | |
| FIDRES | 0.024 | Hz | |
| D 1 | 33.712 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PCPD 2 | 120.0 | us | CPD NUC2 |
| PLW 1 | 39.3 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| PLW 13 | 0.05 | W | Pow@CPD NOE NUC2 |
| CPDPRG2 | waltz65 | | decoupl. sequence |
| TE | 298.000 | K | default |

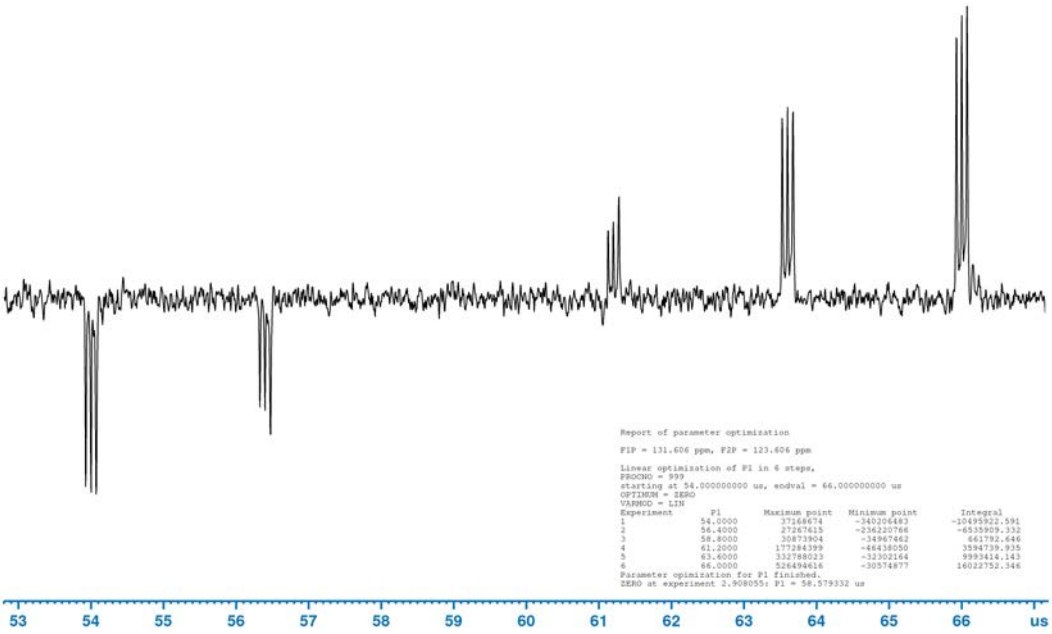
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.400 | | |
| F1P | 0.099 | ppm | |
| F2P | -0.099 | ppm | |
| CY | 1000.000 | cm | |

## Experiment Description

The Carbon-13 line shape experiment with 1H decoupling using as default waltz65 and decoupler pulse length (PCPD2) of 120 us. The corresponding decoupling powers (PLW12 and PLW13) are calculated from prosol entries for P12 and PLW12.
The exact signal position is determined with NS=1 prior to the line shape measurement. The carrier position is afterwards set to this position
O1 optimized = peakFreqHz - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.

### 5.2.7 P90 13C pulse calibration (NPT_13C_p90det_astm_13c)

**Test Sample:** 40% Dioxane in Benzene-D6 (ASTM)
Z10163, Z100929, Z10164, Z10035, Z10255, Z10242, Z10724
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments arround 360 deg.

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| SWH | 2000.000 | Hz | |
| TD | 1048 | | |
| AQ | 0.262 | s | |
| FIDRES | 3.817 | Hz | |
| O1P | 127.000 | ppm | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| DIGMOD | 3 | | baseopt |
| DSPFIRM | 4 | | rectangle |
| TE | 298.000 | K | default |

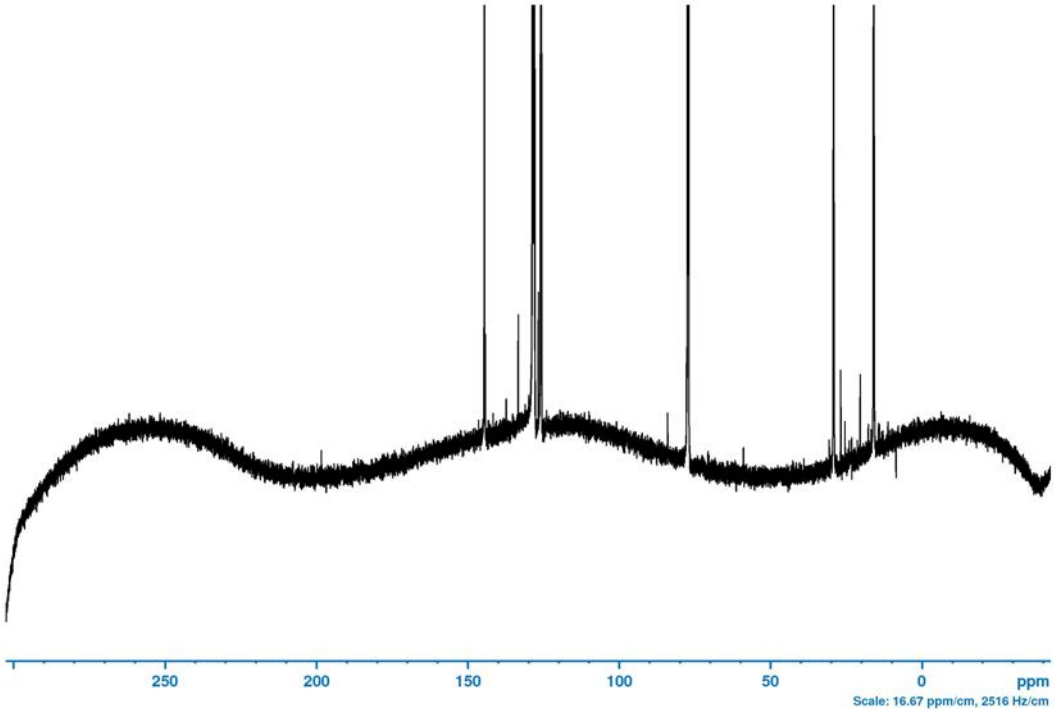
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 1024 | | |
| LB | 3.500 | Hz | |
| F1P | 130.975 | ppm | |
| F2P | 123.025 | ppm | |
| CY | 5.500 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).

## 5.2.8 13C ringing test with 1H decoupling (NPT_13C_ringing_dec1h)

**Test Sample:** 10% Ethylbenzene (EB) in Chloroform-D
Z10153, Z10154, Z10034, Z10253, Z10292, Z10723
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
13C spectrum of 10% ethyl benzene in CDCl3 scaled to show baseline distortions.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PULPROG | npt_zg0dc | | |
| NS | 500 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | 130.000 | ppm | |
| O2P | 5.000 | ppm | |
| SW | 354.922 | ppm | |
| TD | 262144 | | |
| AQ | 3.670 | s | field dependent |
| FIDRES | 0.272 | Hz | field dependent |
| D 1 | 1.230 | s | AQ+D1=const |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 40.2 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| TE | 298.000 | K | default |
| DIGMOD | 3 | | baseopt |
| DE | 42.000 | us | set after getprosol |

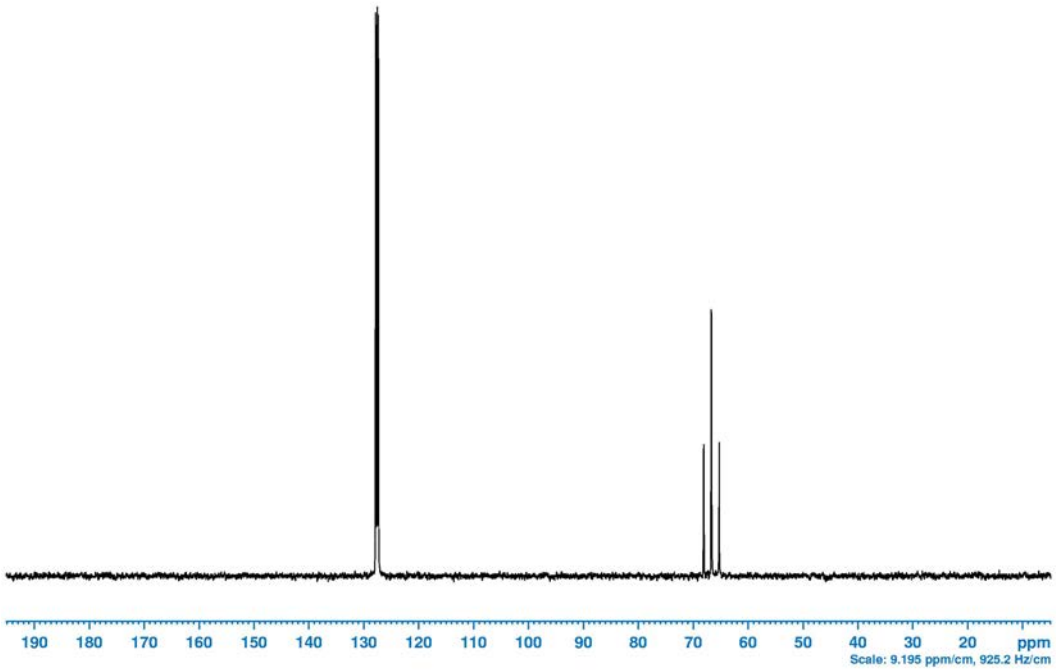
| | | | |
|---|---|---|---|
| CNST 10 | 45.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 524288 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| PC | 1.400 | | |
| F1P | 180.000 | ppm | |
| F2P | -20.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

13C-ringing test full range spectrum. The fullrange spectrum is first baseline corrected before being fitted, without the peaks, with a polynomial function. The ratio distortion/noise=(max(fit)-min(fit))/noise(250 to 210 ppm) gives a measure of the baseline distortion due to ringing. Procno 2 is used for noise determination, procno 3 contains the baseline where all the peaks have been replaced with piece-wise linear noisy sections, whereas procno 4 contains the fit itself.

## 5.2.9 13C sensitivity (NPT_13C_sensitivity)

**Test Sample:** 40% Dioxane in Benzene-D6 (ASTM)
Z10163, Z100929, Z10164, Z10035, Z10255, Z10242, Z10724, Z142224
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Carbon-13 sensitivity test.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 99.987 | ppm | |
| SW | 198.762 | ppm | |
| TD | 65536 | | |
| AQ | 1.638 | s | field dependent |
| FIDRES | 0.610 | Hz | field dependent |
| D 1 | 828.362 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 39.6 | W | Pow@90deg(Specs) NUC1 |
| DIGMOD | 3 | | baseopt |
| TE | 298.000 | K | default |

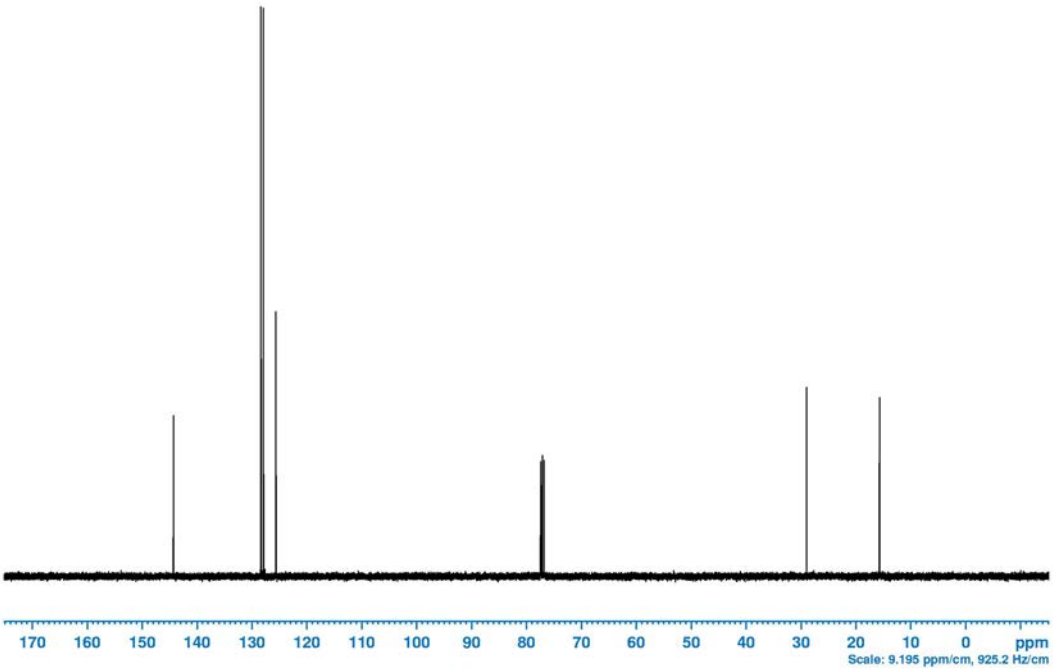
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 1 | | |
| LB | 3.500 | Hz | |
| PC | 1.400 | | |
| F1P | 140.000 | ppm | |
| F2P | 60.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Carbon-13 sensitivity test (no 1H decoupling). Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from 140.0 to 124.0 ppm, while the best 40 ppm noise region is determined over the range from 124.0 to 80.0 ppm.

## 5.2.10 13C sensitivity with 1H decoupling (NPT_13C_sensitivity_dec1h)

**Test Sample:** 10% Ethylbenzene (EB) in Chloroform-D
Z10153, Z100929, Z10154, Z10034, Z10253, Z10292, Z10723
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Carbon-13 sensitivity test with 1H decoupling.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PULPROG | zgpg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 79.987 | ppm | |
| O2P | 4.000 | ppm | |
| SW | 198.766 | ppm | |
| TD | 262144 | | |
| AQ | 6.554 | s | field dependent |
| FIDRES | 0.153 | Hz | field dependent |
| D 1 | 132.446 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 39.6 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| PLW 13 | 0.05 | W | Pow@CPD NOE NUC2 |
| DIGMOD | 3 | | baseopt |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| TE | 298.000 | K | default |

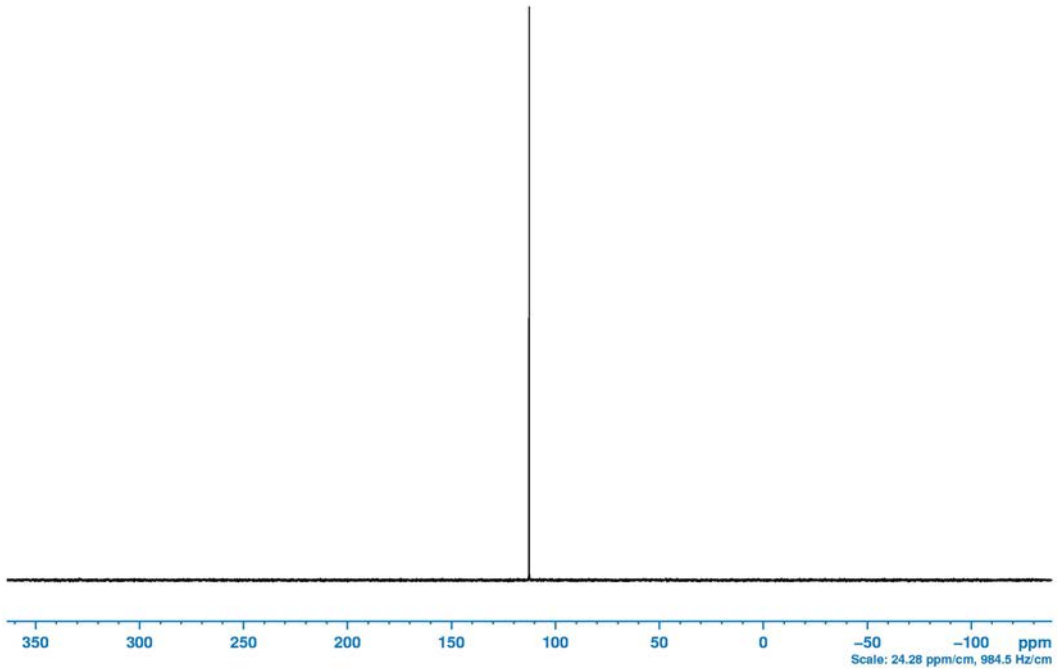
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 524288 | | |
| WDW | 1 | | |
| LB | 0.300 | Hz | |
| PC | 1.400 | | |
| F1P | 180.000 | ppm | |
| F2P | -20.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Carbon-13 sensitivity test with 1H decoupling. Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from 140.0 to 124.0 ppm, while the best 40 ppm noise region is determined over the range from 124.0 to 80.0 ppm.

### 5.2.11 15N test for artifacts (NPT_15N_fullsw_inept)

**Test Sample:** 90% Formamide (HCONH2) in Dimethyl Sulfoxide-D6
Z10187, Z10188, Z10039, Z10256, Z10136, Z142227
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Full range 15N spectrum with 1H decoupling.

**Control Option for Acquisition (L23)**
1 default

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PULPROG | ineptrd | | |
| NS | 32 | | |
| DS | 2 | | |
| RG | 101.000 | | no optim. |
| O1P | 112.421 | ppm | |
| O2P | 7.300 | ppm | |
| SW | 493.226 | ppm | |
| TD | 65536 | | |
| AQ | 1.638 | s | field dependent |
| FIDRES | 0.610 | Hz | field dependent |
| D 1 | 2.862 | s | AQ+D1=const |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 82.034 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz65 | | decoupl. sequence |
| TE | 298.000 | K | default |

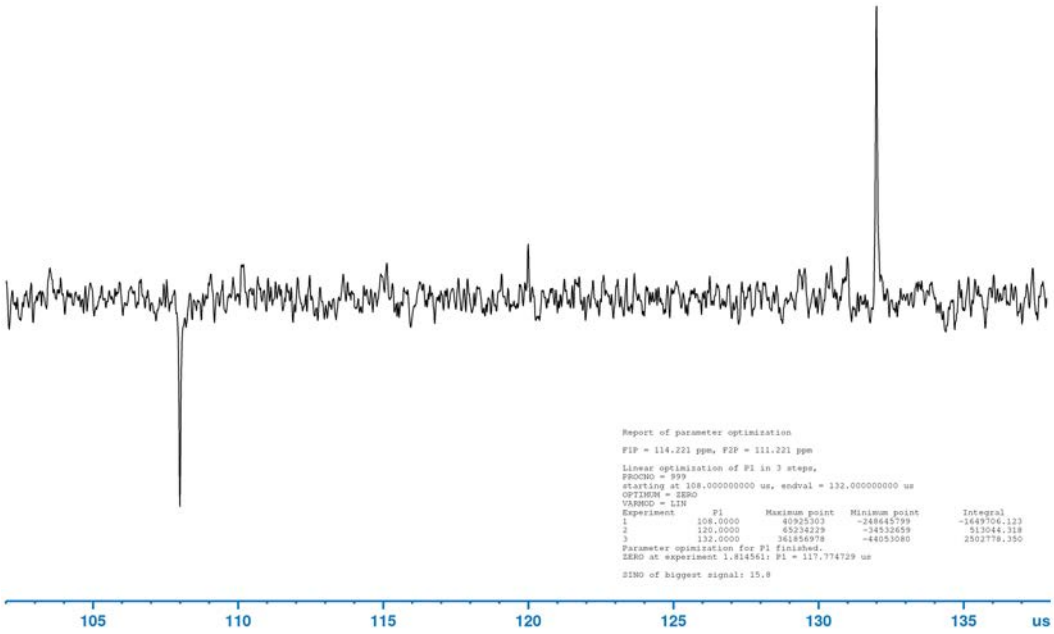
| | | | |
|---|---|---|---|
| CNST 10 | 45.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 131072 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 122.000 | ppm | |
| F2P | 104.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

Full range spectra (spectroscopically useful range) are acquired as test for RF artifacts (spikes). Currently no evaluation is provided and visual inspection of the data is required. Data are treated with baseline correction.

### 5.2.12 P90 15N pulse calibration (NPT_15N_p90det_formamide_15n)

**Test Sample:** 90% Formamide (HCONH2) in Dimethyl Sulfoxide-D6
Z10187, Z10188, Z10039, Z10256, Z10136, Z142227
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows three experiments arround 360 deg.

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zgig | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| SWH | 526.316 | Hz | |
| TD | 4192 | | |
| AQ | 3.982 | s | |
| FIDRES | 0.251 | Hz | |
| O1P | 112.000 | ppm | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| O2P | 7.200 | ppm | |
| PCPD 2 | 90.0 | us | PCPD2 NUC2 |
| PLW 12 | 0.13 | W | Pow@90deg(Specs) |
| DIGMOD | 3 | | baseopt |
| DSPFIRM | 4 | | rectangle |
| TE | 298.000 | K | default |

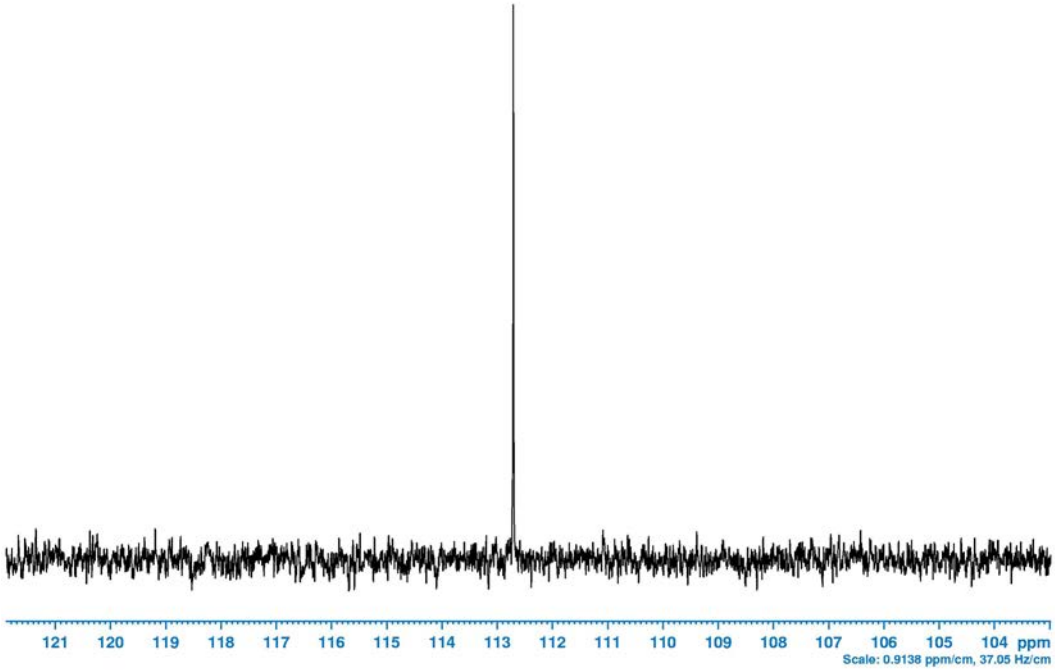
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.500 | Hz | |
| F1P | 113.233 | ppm | |
| F2P | 110.767 | ppm | |
| CY | 5.500 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 8 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).

### 5.2.13 15N sensitivity with 1H decoupling (NPT_15N_sensitivity_dec1h)

**Test Sample:** 90% Formamide (HCONH2) in Dimethyl Sulfoxide-D6
Z10187, Z10188, Z10039, Z10256, Z10136, Z142227
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Nitrogen-15 sensitivity test with 1H decoupling.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PULPROG | zgig | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 112.421 | ppm | |
| O2P | 7.300 | ppm | |
| SW | 20.214 | ppm | |
| TD | 32768 | | |
| AQ | 19.988 | s | field dependent |
| FIDRES | 0.050 | Hz | field dependent |
| D 1 | 110.011 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 84.4 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.2 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| TE | 298.000 | K | default |

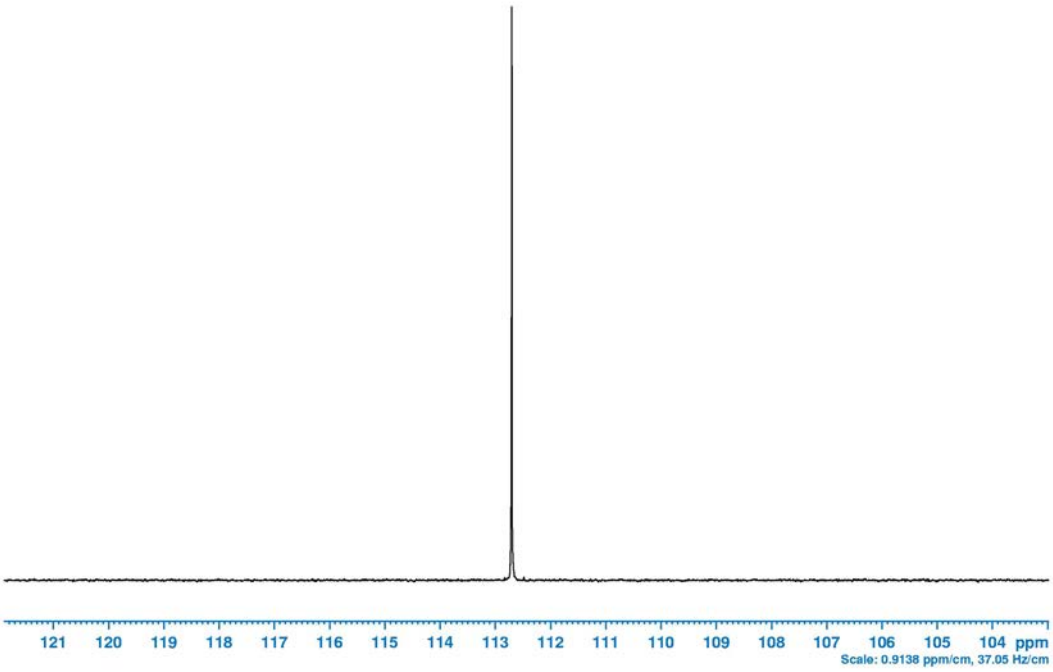
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 0.300 | Hz | |
| PC | 1.000 | | |
| F1P | 122.000 | ppm | |
| F2P | 104.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Nitrogen-15 sensitivity test with 1H decoupling. Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from 113.0 to 111.0 ppm, while the best 2 ppm noise region is determined over the range from 122.0 to 113.0 ppm.
Before the acquisition, the proton 90 degrees pulse is calibrated using pulscal, which result is stored in the corresponding derived dataset.The pulse determination is skiped if experiment is measured with option 'Skip Getprosol'.

### 5.2.14 15N sensitivity (INEPT) with 1H decoupling (NPT_15N_sensitivity_inept)

**Test Sample:** 90% Formamide (HCONH2) in Dimethyl Sulfoxide-D6
Z10187, Z10188, Z10039, Z10256, Z10136, Z142227
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Nitrogen-15 sensitivity test based on INEPT (with 1H decoupling).

**Control Option for Acquisition (L23)**

1 default
2 no decoupling during acquisition

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PULPROG | ineptrd | | |
| NS | 8 | | |
| DS | 2 | | |
| RG | 101.000 | | no optim. |
| O1P | 112.421 | ppm | |
| O2P | 7.300 | ppm | |
| SW | 20.214 | ppm | |
| TD | 4918 | | field dependent |
| AQ | 3.000 | s | |
| FIDRES | 0.333 | Hz | field dependent |
| D 1 | 10.500 | s | |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| CNST 2 | 88.000 | Hz | J(NH) coupling |
| CNST 11 | 6.000 | | 6=all NH[n] pos. |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| PLW 1 | 84.4 | W | Pow@90deg(Specs) NUC1 |
| PLW 2 | 19.3 | W | Pow@90deg(Specs) NUC2 |
| PLW 12 | 0.08 | W | Pow@CPD NUC2 |
| TE | 298.000 | K | default |

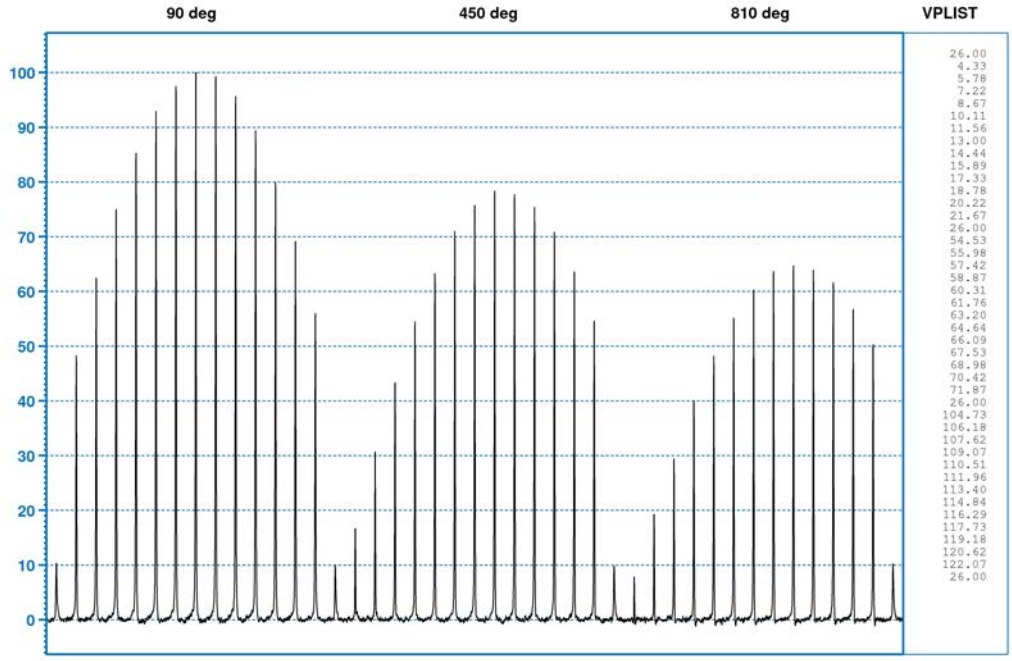
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | field dependent |
| WDW | 1 | | |
| LB | 0.300 | Hz | |
| PC | 1.000 | | |
| F1P | 122.000 | ppm | |
| F2P | 104.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Nitrogen-15 sensitivity test based on INEPT pulse sequence with 1H decoupling during acquisition. Signal enhancement compared to 15N{1H} experiment should be ~ BF1[1H]/BF1[15N]=10*sqrt(NS=8).
Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from 113.0 to 111.0 ppm, while the best 2 ppm noise region is determined over the range from 122.0 to 113.0 ppm.
Before the acquisition, the proton 90 degrees pulse is calibrated using pulscal, which result is stored in the corresponding derived dataset.The pulse determination is skiped if experiment is measured with option 'Skip Getprosol'.
Option L23=1 is standard whereas option L23=2 is non-standard and will not be considered as regular test from the 'NMRPT Control Structure'.

## 5.2.15 19F B1 homogeneity integral (NPT_19F_b1homogeneityInt_19f)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a fraction around signal maximum (-60 deg, +60 deg) is acquired and shown in the figure. The variable pulse list which is used for acquisition is shown to the right.
The B1-homogeneities based on amplitudes and integrals are computed from the peak-picking list amplitudes and the magnitude of the second complex FID data point respectively.

**Control Option for Acquisition (L23)**

1 default PLW 1 is used for determination of B1 homogeneity.
2 PLW 1 will be set to CNST 10 and resultant pulses are used for determination of B1 homogeneity. Experiment will be set to irregular.
3 PLW 1 will be set to power corresponding to specified customer pulses and resultant pulses are used for determination of B1 homogeneity.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 19F | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1b1hom2d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | -62.766 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 1024 | | |
| AQ | 1.290 | s | |
| FIDRES | 0.775 | Hz | |
| D 1 | 23.527 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

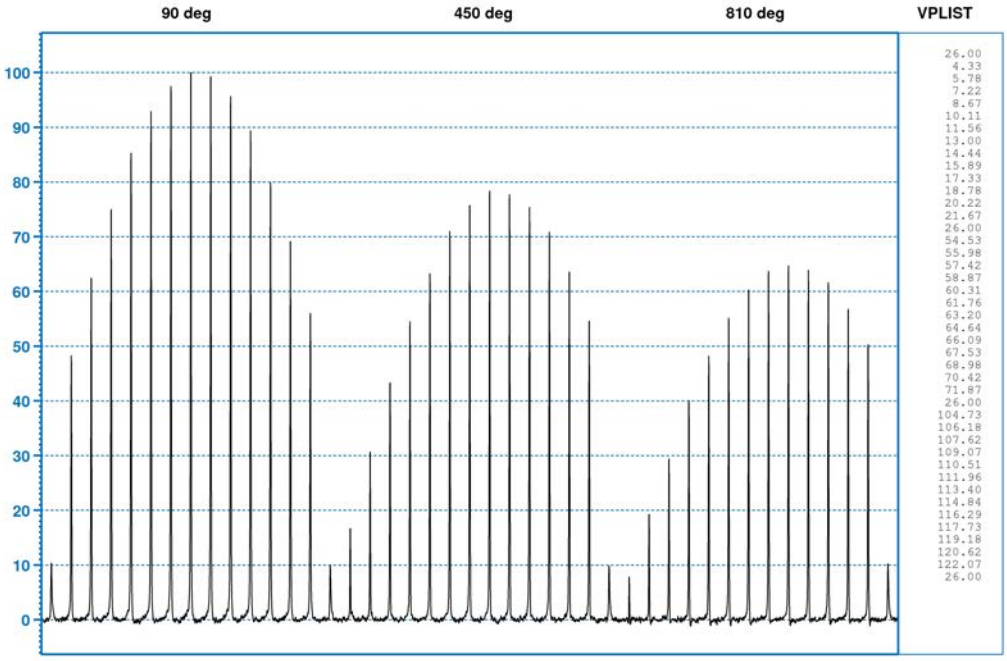
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | -62.574 | ppm | |
| F2P | -62.874 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 19F | | |
| TD | 43 | | No of incr. |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |
| **NMRPT** | | | Parameters |
| L 4 | 6 | | integ. fraction of 90deg |
| L 5 | 8 | | # of step per maxima |

## Experiment Description

The B1 homogeneity measurement is normally acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range is from 90 to 810 degree. In order to speed up the measurements NMRPT is acquiring only the partial ranges around the positive signal maxima for the pulse angles 90, 450, and 810 degree.
By this approach it is possible to get a better incremental resolution and a shorter overall measuring time.
Prior to the main acquisition O1P (PROCNO=2) and phase correction (PROCNO=3) will be optimized.
Intermediate results of the CONVTO1D routine is stored in PROCNO=998, result of CONVTO1D in PROCNO=999.
As control of stability, reproducability and 90 degree calibration a spectrum with 180 degree pulse is acquired before and after each maxima. If relaxation conditions and instrument stability is sufficient, the result should not differ among them.
For the predicition of the signal maxima at 450 and 810 degree the propagation delay is included in the calculation of the VP list. (PDelay is calculated as difference of 360 and 180 degree pulse lengths during the corresponding 90 degree pulse determination experiment.) In this measurement O1 is determined before the main acquisition is started. Evaluation is achieved after processing the data in F2 only (XF2) by peak picking and integral determination of the most intense signal per maxima.

## 5.2.16 19F B1 homogeneity integral on H-coil (NPT_19F_b1homogeneityInt_hcoil)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a fraction around signal maximum (-60 deg, +60 deg) is acquired and shown in the figure. The variable pulse list which is used for acquisition is shown to the right.
The B1-homogeneities based on amplitudes and integrals are computed from the peak-picking list amplitudes and the magnitude of the second complex FID data point respectively.

**Control Option for Acquisition (L23)**

1 default PLW 1 is used for determination of B1 homogeneity.
2 PLW 1 will be set to CNST 10 and resultant pulses are used for determination of B1 homogeneity. Experiment will be set to irregular.
3 PLW 1 will be set to power corresponding to specified customer pulses and resultant pulses are used for determination of B1 homogeneity.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 19F | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1b1hom2d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | -62.766 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 1024 | | |
| AQ | 1.290 | s | |
| FIDRES | 0.775 | Hz | |
| D 1 | 23.527 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

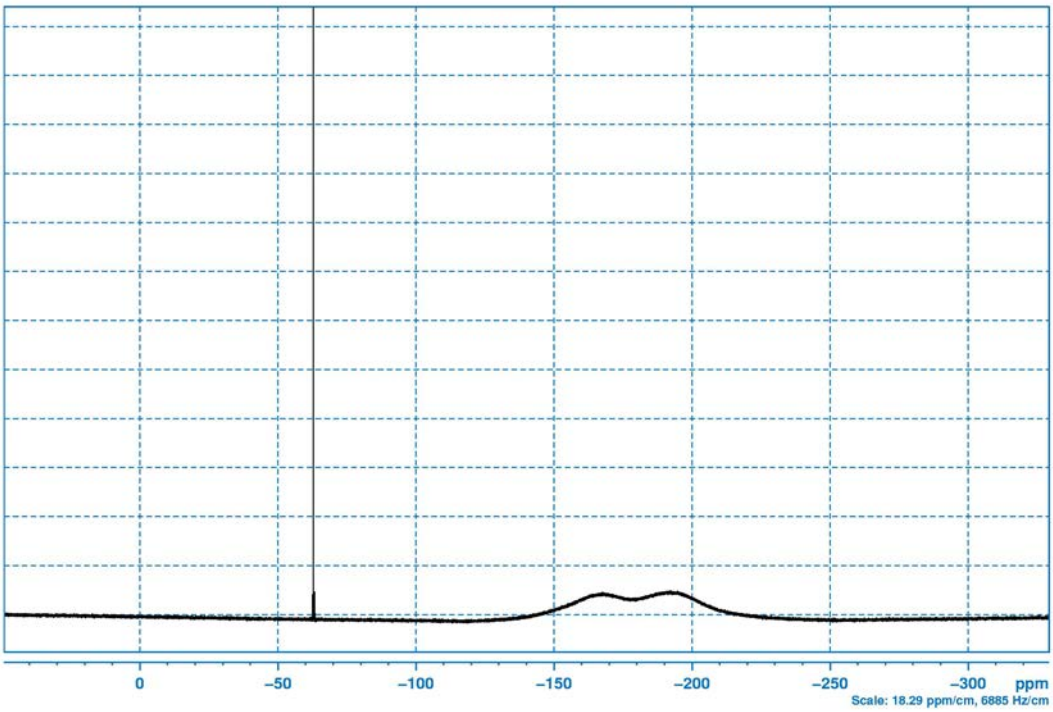
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | -62.574 | ppm | |
| F2P | -62.874 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 19F | | |
| TD | 43 | | No of incr. |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |
| **NMRPT** | | | Parameters |
| L 4 | 6 | | integ. fraction of 90deg |
| L 5 | 8 | | # of step per maxima |

## Experiment Description

The B1 homogeneity measurement is normally acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range is from 90 to 810 degree. In order to speed up the measurements NMRPT is acquiring only the partial ranges around the positive signal maxima for the pulse angles 90, 450, and 810 degree.
By this approach it is possible to get a better incremental resolution and a shorter overall measuring time.
Prior to the main acquisition O1P (PROCNO=2) and phase correction (PROCNO=3) will be optimized.
Intermediate results of the CONVTO1D routine is stored in PROCNO=998, result of CONVTO1D in PROCNO=999.
As control of stability, reproducability and 90 degree calibration a spectrum with 180 degree pulse is acquired before and after each maxima. If relaxation conditions and instrument stability is sufficient, the result should not differ among them.
For the predicition of the signal maxima at 450 and 810 degree the propagation delay is included in the calculation of the VP list. (PDelay is calculated as difference of 360 and 180 degree pulse lengths during the corresponding 90 degree pulse determination experiment.) In this measurement O1 is determined before the main acquisition is started. Evaluation is achieved after processing the data in F2 only (XF2) by peak picking and integral determination of the most intense signal per maxima.

## 5.2.17 19F background with sample and 1H decoupling (NPT_19F_backgr_withsample)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

19F Background signal spectrum with sample. Sharp signal arises from sample, broad signal around -175 ppm arises from solid compound in the probe.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 19F | | |
| NUC2 | 1H | | |
| PULPROG | npt_zg0ig | | |
| NS | 1000 | | |
| DS | 0 | | |
| RG | 32.000 | | no optim. |
| O1P | -139.998 | ppm | |
| O2P | 5.000 | ppm | |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| SWH | 147058.828 | Hz | |
| TD | 131072 | | |
| AQ | 0.446 | s | |
| FIDRES | 2.244 | Hz | |
| D 1 | 1.000 | s | AQ+D1=const |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 25.1 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.23 | W | Pow@CPD NUC2 |
| TE | 298.000 | K | default |

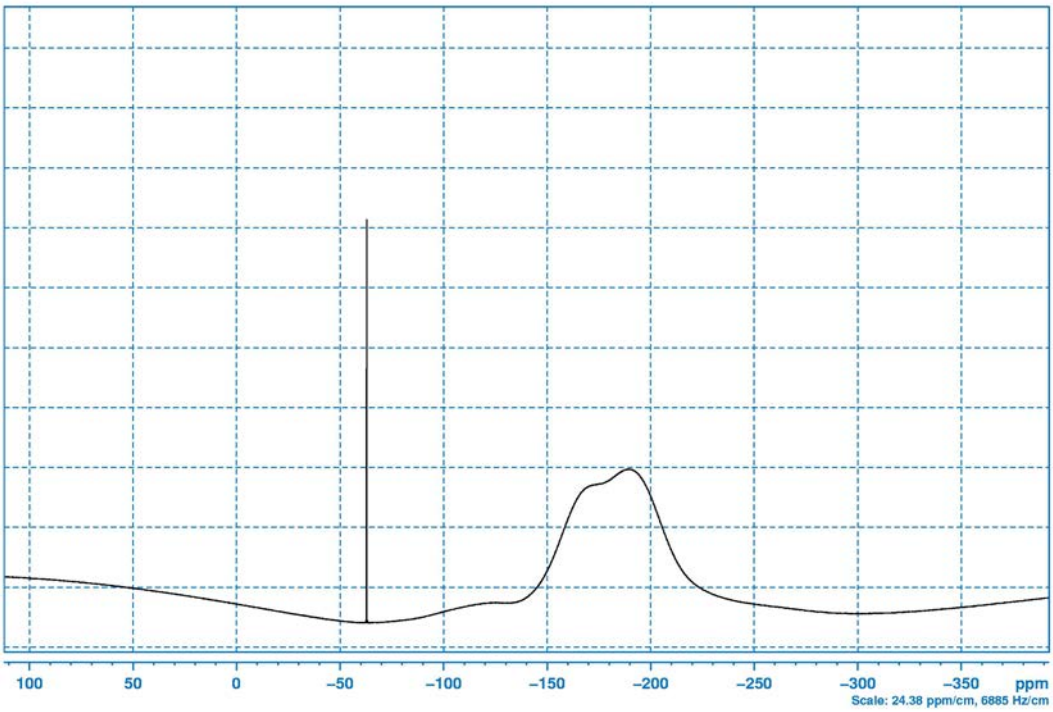
| | | | |
|---|---|---|---|
| CNST 10 | 45.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 131072 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| PC | 1.000 | | |
| F1P | 24.747 | ppm | |
| F2P | -150.759 | ppm | |

### Experiment Description

Background signal measurements are executed using a small flip angle due to two reasons. First, to get more efficient excitation bandwidth, secondly to compensate for usually long T1 relaxation time of solid signals.
Full spectrum is normally printed without any baseline correction.
Spectrum is processed with MC always.

## 5.2.18 19F background with sample on H-coil (NPT_19F_backgr_withsample_hcoil)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

19F Background signal spectrum with sample. Sharp signal arises from sample, broad signal around -175 ppm arises from solid compound in the probe.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 19F | | |
| NUC2 | off | | |
| PULPROG | npt_zg0 | | |
| NS | 1000 | | |
| DS | 0 | | |
| RG | 32.000 | | no optim. |
| O1P | -139.998 | ppm | |
| O2P | -139.998 | ppm | |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| SWH | 147058.828 | Hz | |
| TD | 131072 | | |
| AQ | 0.446 | s | |
| FIDRES | 2.244 | Hz | |
| D 1 | 1.000 | s | AQ+D1=const |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 15.0 | us | 90deg NUC1 |
| PLW 1 | 10.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

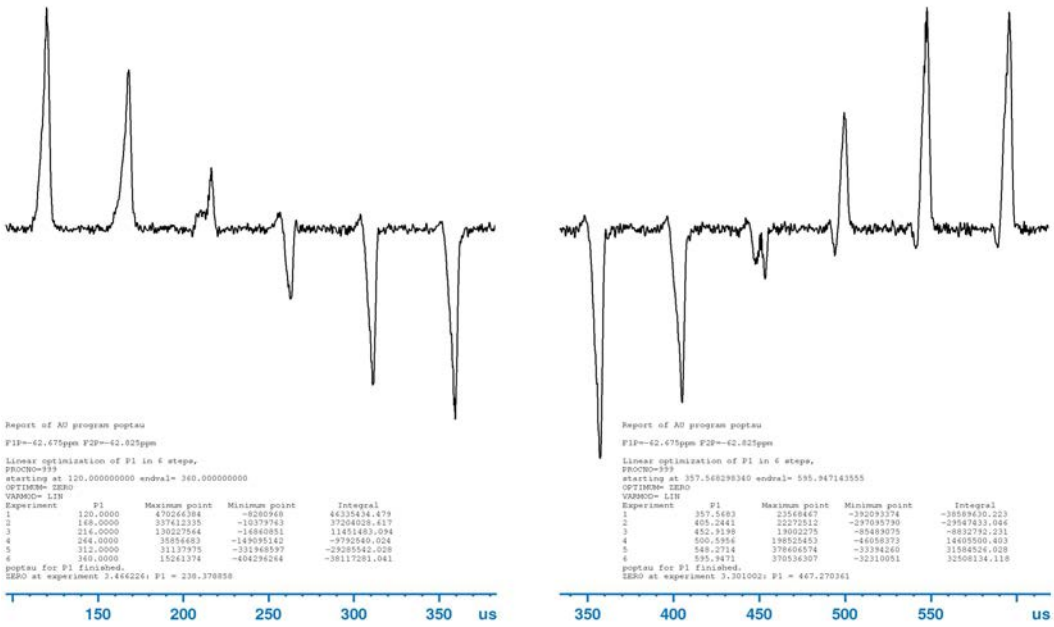
| | | | |
|---|---|---|---|
| CNST 10 | 45.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 131072 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| PC | 1.000 | | |
| F1P | 24.747 | ppm | |
| F2P | -150.759 | ppm | |

## Experiment Description

Background signal measurements are executed using a small flip angle due to two reasons. First, to get more efficient excitation bandwidth, secondly to compensate for usually long T1 relaxation time of solid signals.
Full spectrum is normally printed without any baseline correction.
Spectrum is processed with MC always.

## 5.2.19 CPD 19F pulse calibration (NPT_19F_cpddeterminationf1_19f)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | -62.800 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 1000 | | |
| AQ | 1.260 | s | |
| FIDRES | 0.794 | Hz | |
| D 1 | 4.300 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

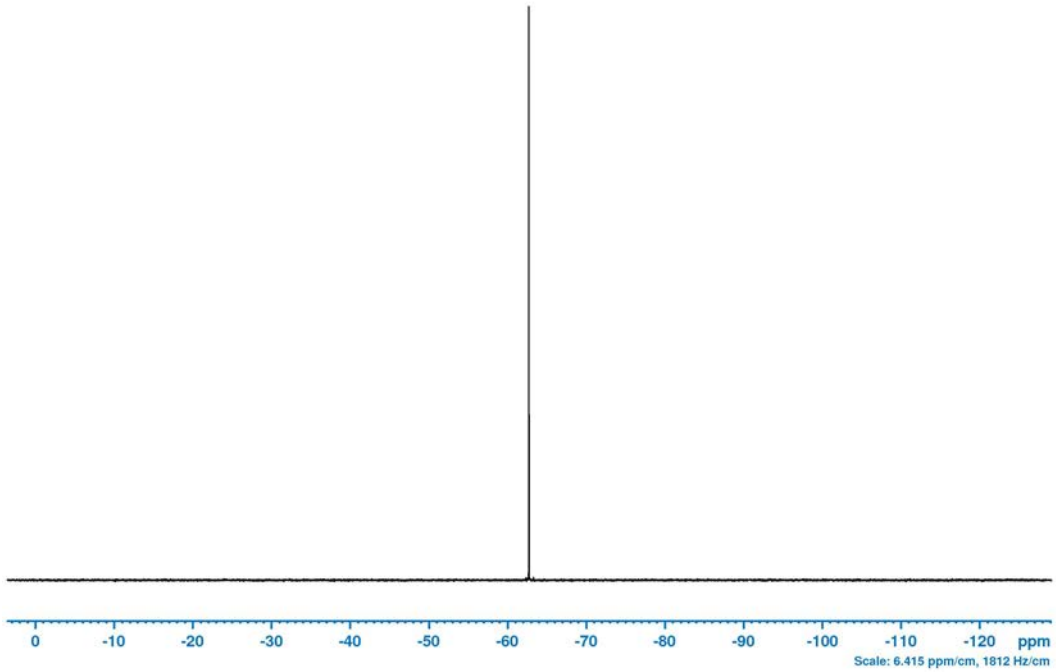
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 3 | | |
| LB | 2.000 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | -57.199 | ppm | |
| ABSF2 | -68.200 | ppm | |
| F1P | -57.700 | ppm | |
| F2P | -67.700 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

### 5.2.20 19F test for artifacts (NPT_19F_fullsw_dec1h)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Full range 19F spectrum with 1H decoupling.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| NUC2 | 1H | | |
| PULPROG | npt_zg0ig | | |
| NS | 64 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | -62.766 | ppm | |
| O2P | 5.000 | ppm | |
| SW | 132.811 | ppm | |
| TD | 65536 | | |
| AQ | 0.655 | s | field dependent |
| FIDRES | 1.526 | Hz | field dependent |
| D 1 | 0.545 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 22.473 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| PC | 1.000 | | |
| F1P | 24.747 | ppm | |
| F2P | -150.759 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Full range spectra (spectroscopically useful range) are acquired as test for RF artifacts (spikes). Currently no evaluation is provided and visual inspection of the data is required. Data are treated with baseline correction.

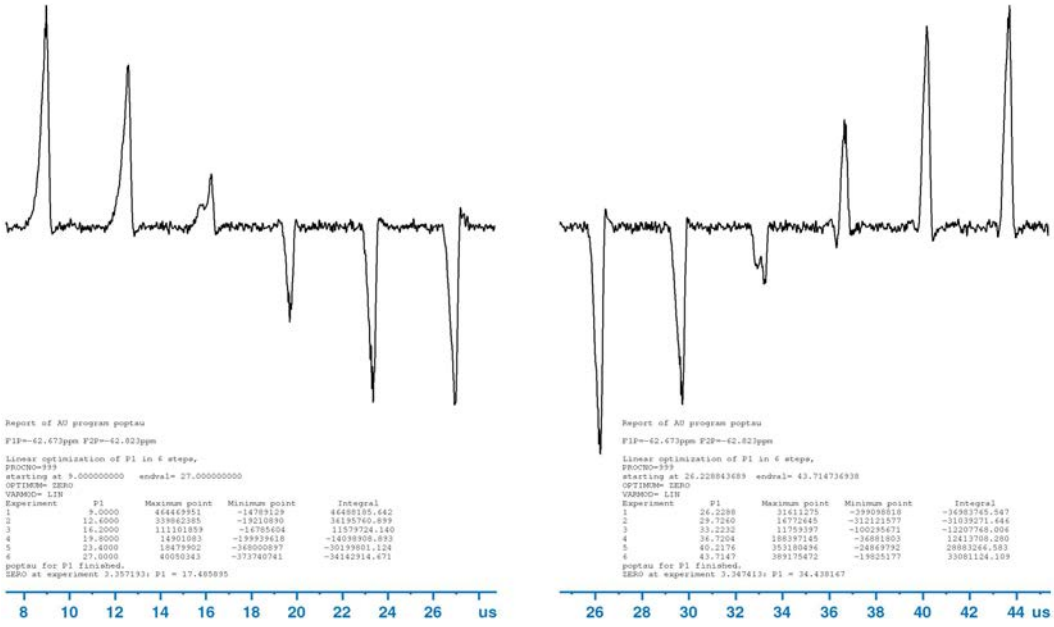
## 5.2.21 P90 19F pulse calibration (NPT_19F_p90determinationf1_19f)

**Test Sample:** (a) 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
(b) 45% Chloroform-D (CDCl3) and 45% Chloroform (CHCl3) in 10% Hexafluorobenzene (C6F6).
Z10234, Z100937, Z10235, Z10040, Z10728, Z10079, Z142228

**Solvent:** (a) CDCl3
(b) C6F6

**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table

**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | -62.800 | ppm | (TFT Sample) |
| O1P | -162.2 | ppm | (Fluor Lock Sample) |
| SWH | 396.825 | Hz | |
| TD | 1000 | | (TFT Sample) |
| TD | 4096 | | (Fluor Lock Sample) |
| AQ | 1.260 | s | |
| FIDRES | 0.794 | Hz | |
| D 1 | 4.300 | s | AQ+D1=const (TFT Sample) |
| D1 | 1.0 | s | (Fluor Lock Sample) |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

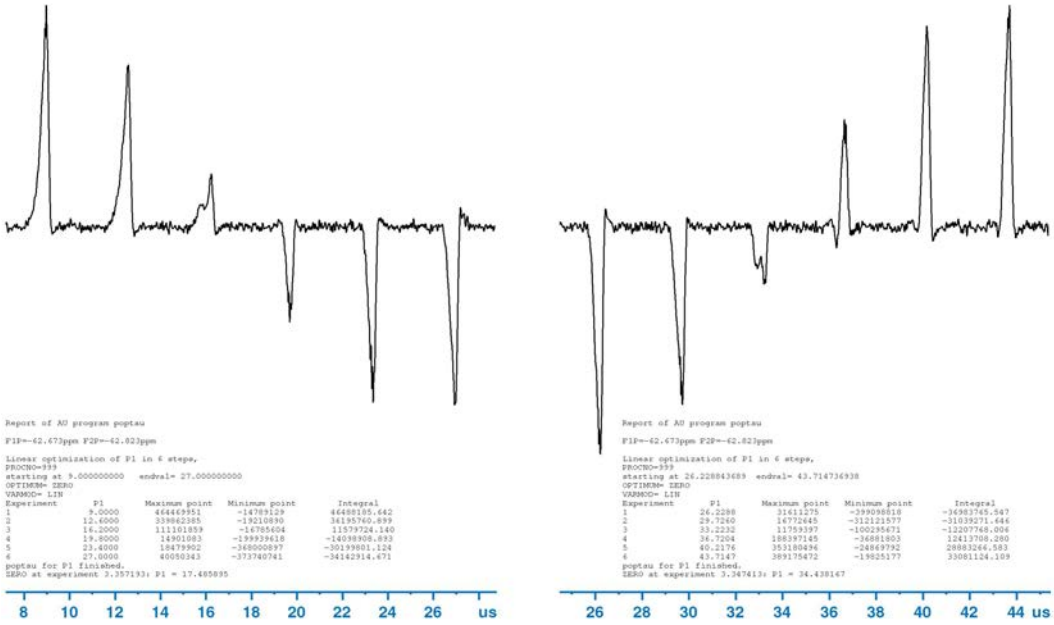
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 3 | | (TFT Sample) |
| WDW | 1 | | (Fluor Lock Sample) |
| LB | 2.000 | Hz | (TFT Sample) |
| LB | 1.0 | Hz | (Fluor Lock Sample) |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | -57.199 | ppm | |
| ABSF2 | -68.200 | ppm | |
| F1P | -57.700 | ppm | |
| F2P | -67.700 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.22 19F P90 pulse calibration on H-coil (NPT_19F_p90determinationf1_hcoil)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | -62.800 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 1000 | | |
| AQ | 1.260 | s | |
| FIDRES | 0.794 | Hz | |
| D 1 | 4.300 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

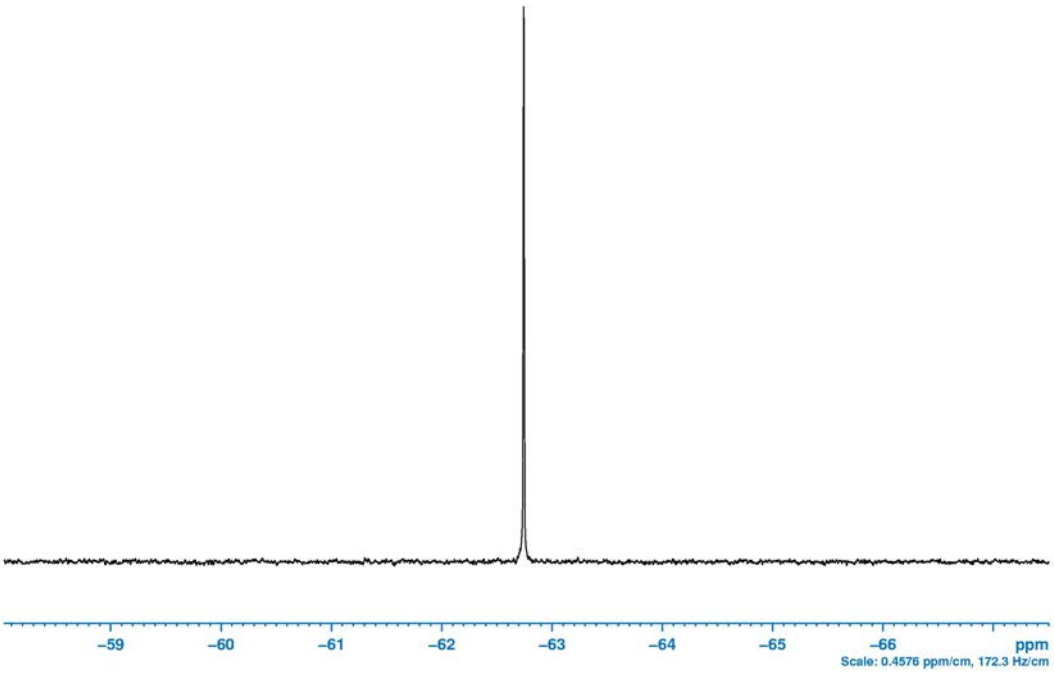
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 3 | | |
| LB | 2.000 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | -57.199 | ppm | |
| ABSF2 | -68.200 | ppm | |
| F1P | -57.700 | ppm | |
| F2P | -67.700 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

### 5.2.23 19F sensitivity (NPT_19F_sensitivity)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Fluorine-19 sensitivity test.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | -62.766 | ppm | |
| SW | 9.838 | ppm | |
| TD | 32768 | | |
| AQ | 4.424 | s | field dependent |
| FIDRES | 0.226 | Hz | field dependent |
| D 1 | 30.576 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 25.1 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

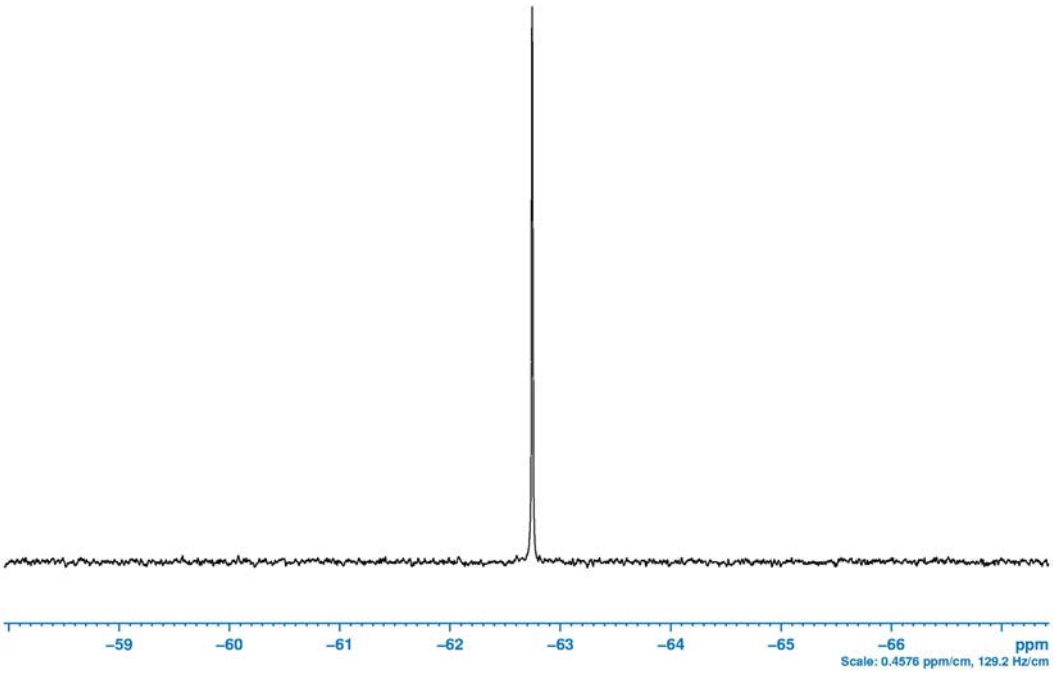
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| PC | 1.000 | | |
| F1P | -58.015 | ppm | |
| F2P | -67.985 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Fluorine-19 sensitivity test (no 1H decoupling). Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from -61.0 to -65.0 ppm, while the best 1 ppm noise region is determined over the range from -58.5 to -63.0 ppm.

### 5.2.24 19F sensitivity on H-coil (NPT_19F_sensitivity_hcoil)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Fluorine-19 sensitivity test on 1H-coil tuned to 19F.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | -62.766 | ppm | |
| SW | 9.838 | ppm | |
| TD | 32768 | | |
| AQ | 4.424 | s | field dependent |
| FIDRES | 0.226 | Hz | field dependent |
| D 1 | 30.576 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 25.1 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

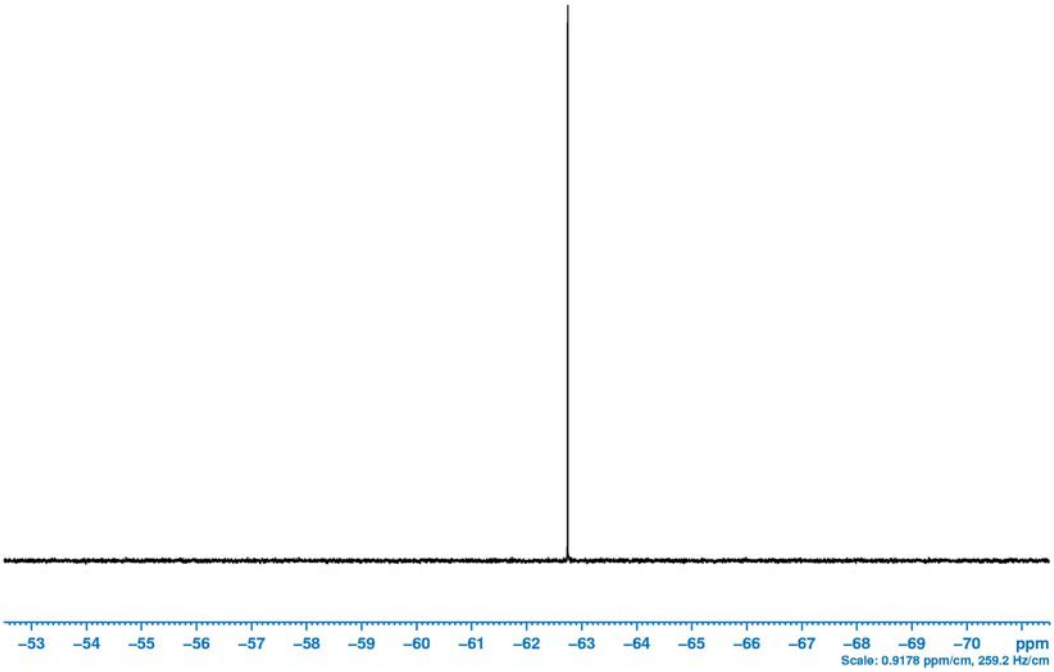
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| PC | 1.000 | | |
| F1P | -58.015 | ppm | |
| F2P | -67.985 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Fluorine-19 sensitivity test (no 1H decoupling). Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from -61.0 to -65.0 ppm, while the best 1 ppm noise region is determined over the range from -58.5 to -63.0 ppm.

### 5.2.25 19F sensitivity with 1H decoupling and LB=0.5 (NPT_19F_sensitivity_lb05_dec1h)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Fluorine-19 sensitivity test (LB = 0.5) with 1H decoupling.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| NUC2 | 1H | | |
| PULPROG | zgig | | |
| NS | 1 | | |
| DS | 0 | | |
| SW | 19.823 | ppm | |
| RG | 101.000 | | no optim. |
| O1P | -62.000 | ppm | |
| O2P | 8.000 | ppm | |
| SW | 19.823 | ppm | |
| TD | 44776 | | |
| AQ | 3.000 | s | field dependent |
| FIDRES | 0.333 | Hz | field dependent |
| D 1 | 35.000 | s | |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 22.5 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| TE | 298.000 | K | default |

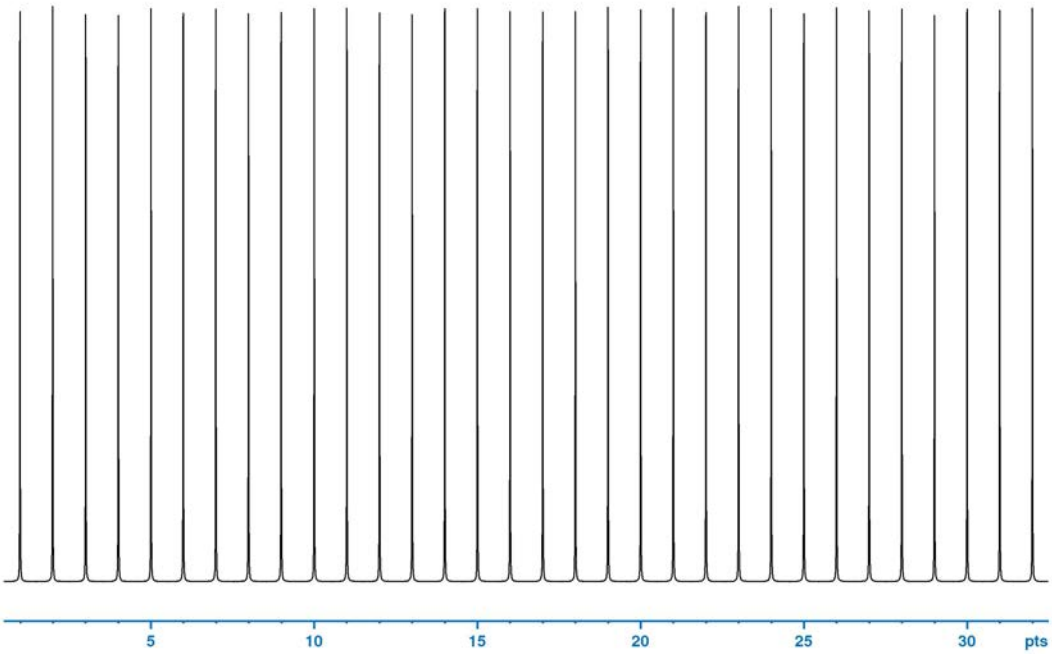
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.500 | Hz | |
| PC | 1.000 | | |
| F1P | -58.015 | ppm | |
| F2P | -67.985 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Fluorine-19 sensitivity test with 1H decoupling. Processing is using line broadening (LB) of 0.5 Hz and baseline correction (ABS). Evaluation is carried out by the AU `hwcal` to determine the line width at 50% of signal height and by the AU `sinocal`. The signal is searched over the range from -62.0 to -63.0 ppm, while the best 1 ppm noise region is determined over the range from -53.0 to -62.0 ppm.

### 5.2.26 13 degree pulse stability test (NPT_1H_13degtest)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** Lockregulation based on LGAIN=80 dB
**Sample State:** Rotation off




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the residual water signal of the sample.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | sys13deg | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.704 | ppm | |
| SW | 9.917 | ppm | |
| TD | 8192 | | |
| AQ | 1.032 | s | field dependent |
| FIDRES | 0.969 | Hz | field dependent |
| D 1 | 2.000 | s | |
| D 20 | 0.001 | s | |
| P 1 | 11.0 | us | 90deg NUC1 |
| PLW 1 | 19.3 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |
| **F2 PROC** | | | Parameters F2 |
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| F1P | 5.204 | ppm | |
| F2P | 4.204 | ppm | |

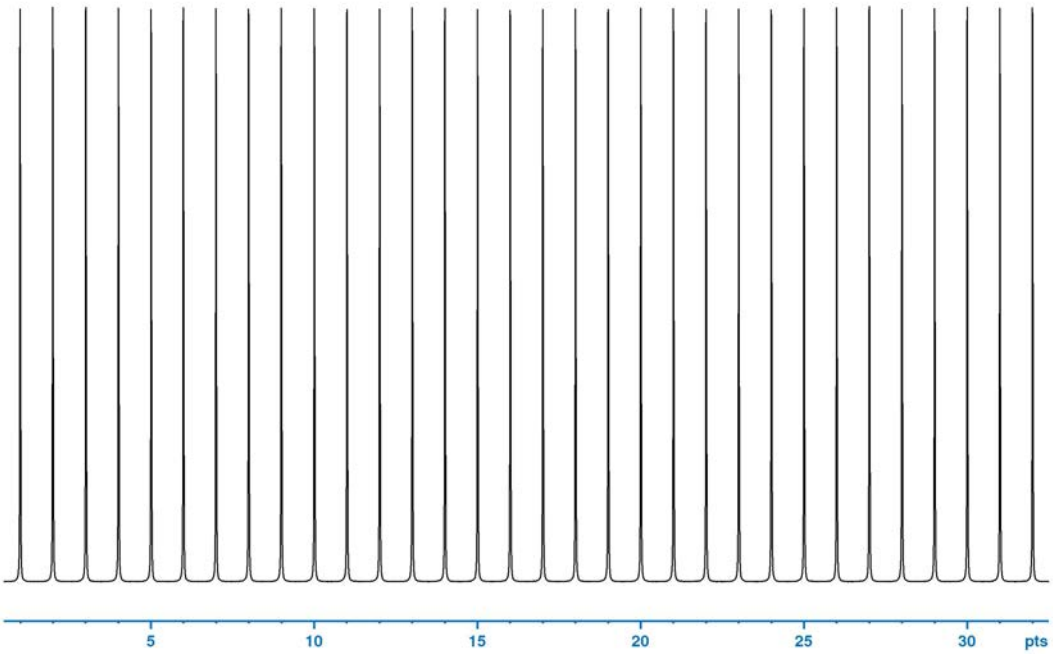
| | | |
|---|---|---|
| **F1 ACQU** | | Parameters F1 |
| NUC1 | 1H | |
| TD | 32 | |
| **F1 PROC** | | Parameters F1 |
| SI | 32 | |
| **NMRPT** | | Parameters |
| CNST 45 | -1.000 | Return Mean Value |
| CNST 46 | -1.000 | Return Std Dev |

## Experiment Description

Purpose of this experiment is the measurement of overall pulse stability of the spectrometer, according to the methods described in 'Assessment of Spectrometer Pulse Reproducibility' by G.A. Morris, JMR, 78, 281ff (1988).
For this hardware test (HWT) some experimental preparation is needed. Initially the exact resonance position of the residual water signal is determined after receiver gain adjustment based on a single scan acquisition followed by processing with FT, MC, PP. The processed data are stored in PROCNO=2.
The setting of special LOCK settings is executed prior to the start of the main acquisition.
Data are processed with LB and no baseline correction. Evaluation is based on peak picking after conversion of the processed data to 1D-mode using CONVTO1D procedure.

### 5.2.27 30 degree pulse stability test (NPT_1H_30degtest)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** Lockregulation based on LGAIN=80 dB
**Sample State:** Rotation off




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the residual water signal of the sample.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_zg2dp0 | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.704 | ppm | |
| SW | 9.917 | ppm | |
| TD | 8192 | | |
| AQ | 1.032 | s | field dependent |
| FIDRES | 0.969 | Hz | field dependent |
| D 1 | 2.000 | s | |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 11.0 | us | 90deg NUC1 |
| PLW 1 | 19.3 | W | Pow@90deg(Specs) NUC1 |
| CNST 10 | 30.000 | deg | flip angle |
| TE | 298.000 | K | default |
| **F2 PROC** | | | Parameters F2 |
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| F1P | 5.204 | ppm | |
| F2P | 4.204 | ppm | |

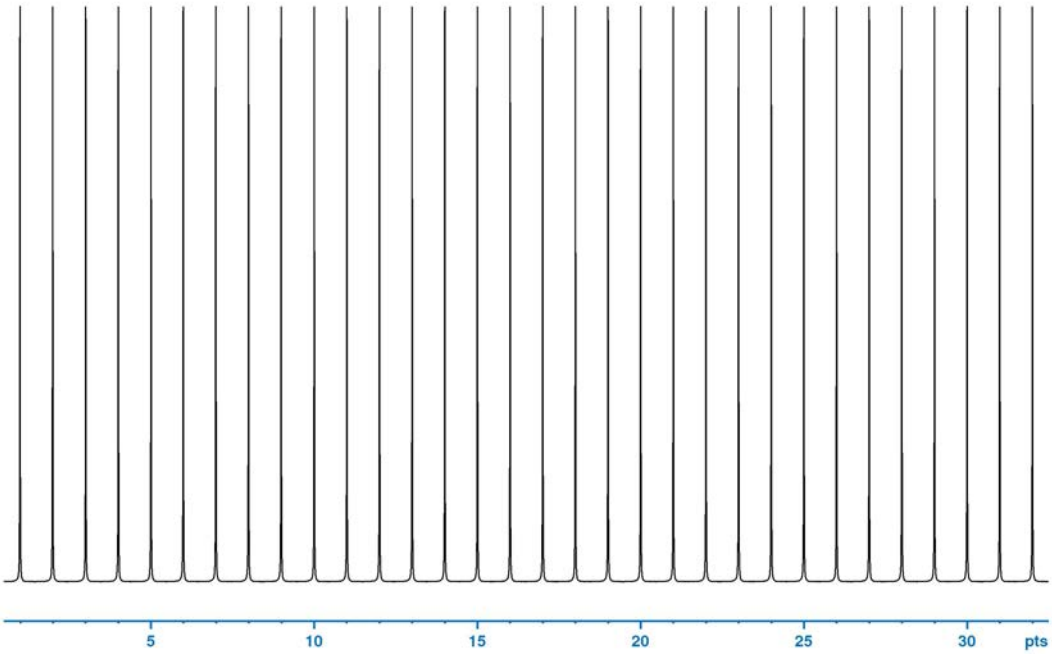
| | | |
|---|---|---|
| **F1 ACQU** | | Parameters F1 |
| NUC1 | 1H | |
| TD | 32 | |
| **F1 PROC** | | Parameters F1 |
| SI | 32 | |
| **NMRPT** | | Parameters |
| CNST 45 | -1.000 | Return Mean Value |
| CNST 46 | -1.000 | Return Std Dev |

## Experiment Description

Purpose of this experiment is the measurement of overall amplitude stability of the spectrometer using a 30degree excitation pulse.
For this hardware test (HWT) some experimental preparation is needed. Initially the exact resonance position of the residual water signal is determined after receiver gain adjustment based on a single scan acquisition followed by processing with FT, MC, PP. The processed data are stored in PROCNO=2.
The setting of special LOCK settings is executed prior to the start of the main acquisition.
Data are processed with LB and no baseline correction. Evaluation is based on peak picking after conversion of the processed data to 1D-mode using CONVTO1D procedure.

### 5.2.28 90 degree pulse stability test (NPT_1H_90degtest)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** Lockregulation based on LGAIN=80 dB
**Sample State:** Rotation off




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the residual water signal of the sample.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_zg2dp0 | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.704 | ppm | |
| SW | 9.917 | ppm | |
| TD | 8192 | | |
| AQ | 1.032 | s | field dependent |
| FIDRES | 0.969 | Hz | field dependent |
| D 1 | 2.000 | s | |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 11.0 | us | 90deg NUC1 |
| PLW 1 | 19.3 | W | Pow@90deg(Specs) NUC1 |
| CNST 10 | 90.000 | deg | flip angle |
| TE | 298.000 | K | default |
| **F2 PROC** | | | Parameters F2 |
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| F1P | 5.204 | ppm | |
| F2P | 4.204 | ppm | |

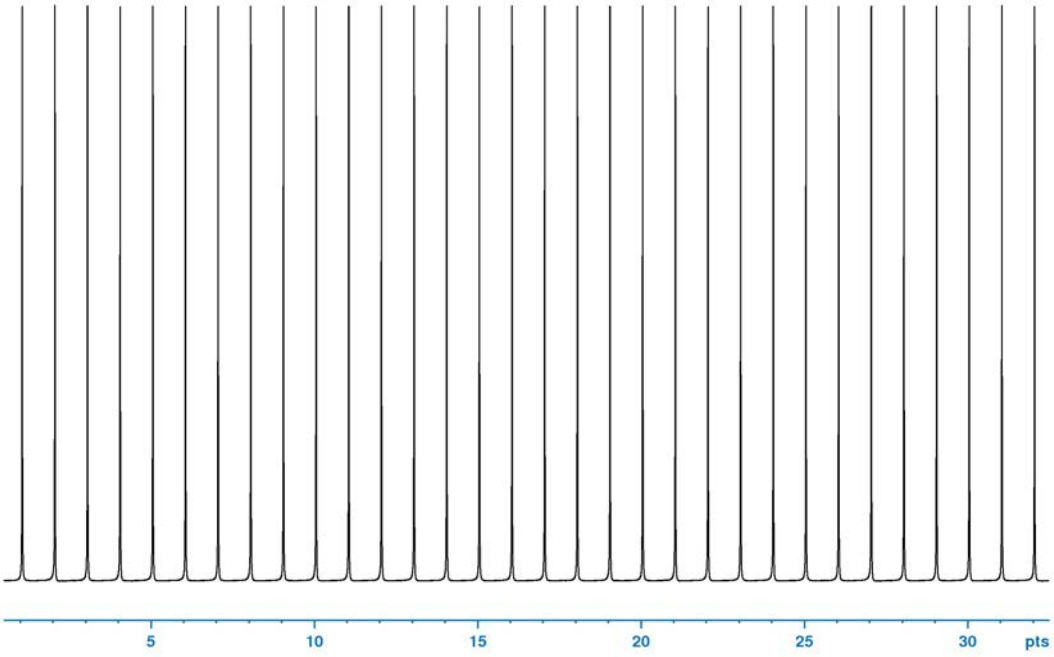
| | | |
|---|---|---|
| **F1 ACQU** | | Parameters F1 |
| NUC1 | 1H | |
| TD | 32 | |
| **F1 PROC** | | Parameters F1 |
| SI | 32 | |
| **NMRPT** | | Parameters |
| CNST 45 | -1.000 | Return Mean Value |
| CNST 46 | -1.000 | Return Std Dev |

## Experiment Description

Purpose of this experiment is the measurement of overall amplitude stability of the spectrometer using a 90 degree excitation pulse.
For this hardware test (HWT) some experimental preparation is needed. Initially the exact resonance position of the residual water signal is determined after receiver gain adjustment based on a single scan acquisition followed by processing with FT, MC, PP. The processed data are stored in PROCNO=2.
The setting of special LOCK settings is executed prior to the start of the main acquisition.
Data are processed with LB and no baseline correction. Evaluation is based on peak picking after conversion of the processed data to 1D-mode using CONVTO1D procedure.

### 5.2.29 Amplitude stability after gradient echo with strong gradient pulses (NPT_1H_ampStabGradientEchoStrong)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode, showing the residual water peak after a gradient echo.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | syszggegp2d | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.697 | ppm | |
| SW | 16.442 | ppm | |
| TD | 8192 | | |
| AQ | 0.623 | s | field dependent |
| FIDRES | 1.606 | Hz | field dependent |
| D 1 | 0.200 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPNAM2 | RECT.1 | | |
| GPZ 1 | 60.000 | % | |
| GPZ 2 | -60.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |
| **F2 PROC** | | | Parameters F2 |
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 0 | | pk |
| F1P | 5.250 | ppm | |
| F2P | 4.250 | ppm | |

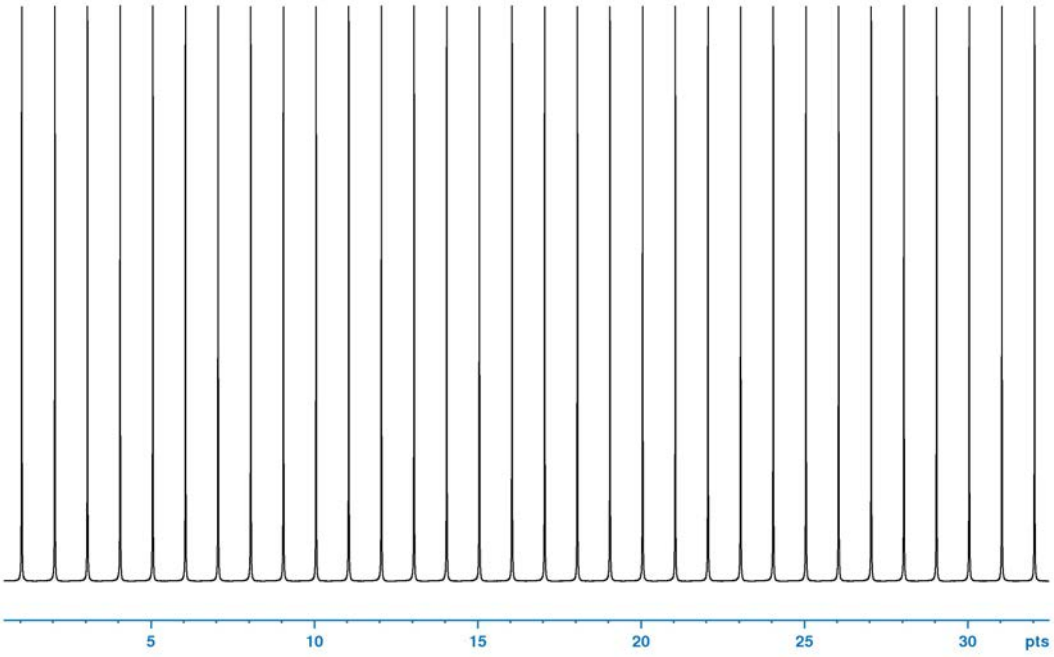
| | | |
|---|---|---|
| **F1 ACQU** | | Parameters F1 |
| NUC1 | 1H | |
| TD | 32 | |
| **F1 PROC** | | Parameters F1 |
| SI | 32 | |

## Experiment Description

The purpose of this test is the assessment of the amplitude stability after a gradient echo. After a 90 degree pulse, the generated coherence is first defocused and subsequently refocused by a pair of gradient pulses with equal but opposite strengths separated by a delay D16=500 us. The gradient echo which builds up after another delay D16 is finally recorded.
The quality criteria of this test are defined by the mean relative amplitude and the standard deviation of the relative amplitude, both in percent, of a series of identical experiments.
In this test, the pair of gradient pulse strengths are +/-60% of the maximum strength of the probe gradient.

### 5.2.30 Amplitude stability after gradient echo with weak gradient pulses (NPT_1H_ampStabGradientEchoWeak)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode, showing the residual water peak after a gradient echo.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | syszggegp2d | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.697 | ppm | |
| SW | 16.442 | ppm | |
| TD | 8192 | | |
| AQ | 0.623 | s | field dependent |
| FIDRES | 1.606 | Hz | field dependent |
| D 1 | 0.200 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPNAM2 | RECT.1 | | |
| GPZ 1 | 20.000 | % | |
| GPZ 2 | -20.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |
| **F2 PROC** | | | Parameters F2 |
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 0 | | pk |
| F1P | 5.250 | ppm | |
| F2P | 4.250 | ppm | |

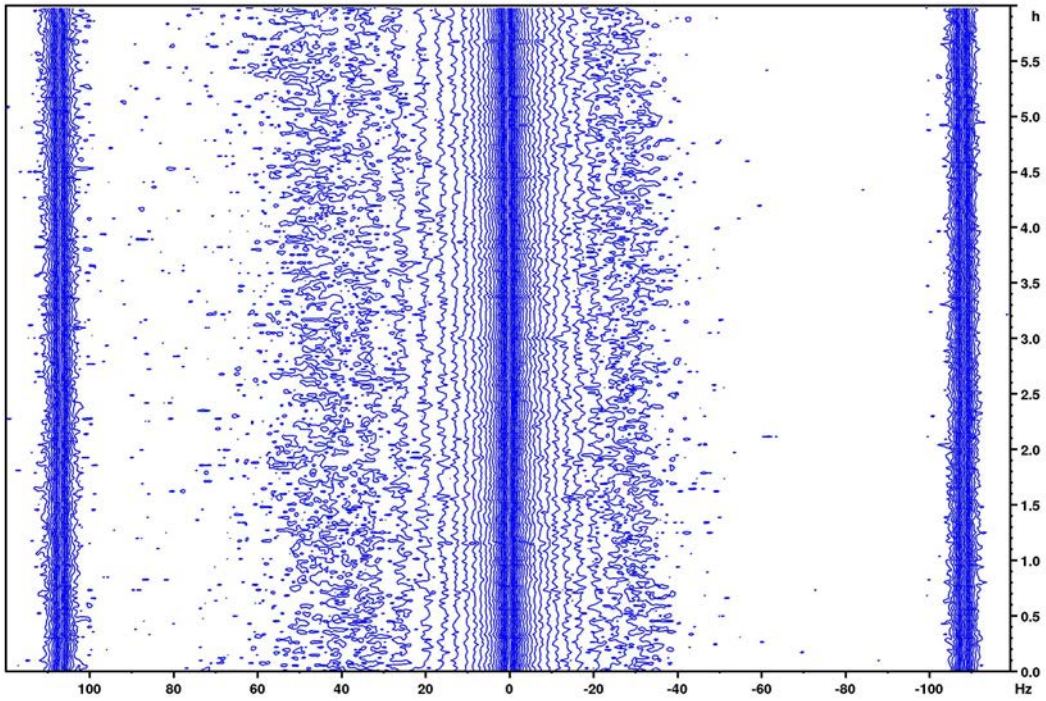
| | | |
|---|---|---|
| **F1 ACQU** | | Parameters F1 |
| NUC1 | 1H | |
| TD | 32 | |
| **F1 PROC** | | Parameters F1 |
| SI | 32 | |

## Experiment Description

The purpose of this test is the assessment of the amplitude stability after a gradient echo. After a 90 degree pulse, the generated coherence is first defocused and subsequently refocused by a pair of gradient pulses with equal but opposite strengths separated by a delay D16=500 us. The gradient echo which builds up after another delay D16 is finally recorded.
The quality criteria of this test are defined by the mean relative amplitude and the standard deviation of the relative amplitude, both in percent, of a series of identical experiments.
In this test, the pair of gradient pulse strengths are +/-20% of the maximum strength of the probe gradient.

### 5.2.31 B0 magnet drift experiment (NPT_1H_b0drifttest)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z10248, Z10701, Z100926, Z10250, Z10031, Z10030, Z10029, Z10260, Z10249, Z10275, Z10272, Z10717
**Solvent:** Acetone
**Lock parameter:** LOCK is off during main acquisition
**Sample State:** Rotation off




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the chloroform signal.

**Control Option for Acquisition (L23)**

1 duration of drift test according to specification for minimal drift time, 6 hours if not specified
10- duration of drift test in minutes
6000

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_zgp02d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 8.000 | ppm | |
| SWH | 8196.722 | Hz | |
| TD | 65536 | | |
| AQ | 3.998 | s | |
| FIDRES | 0.250 | Hz | |
| D 1 | 59.500 | s | |
| D 20 | 337.500 | s | time per scan |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 5.6 | W | Pow@90deg(Specs) |
| CNST 10 | 45.000 | deg | flip angle |
| TE | 298.000 | K | default |

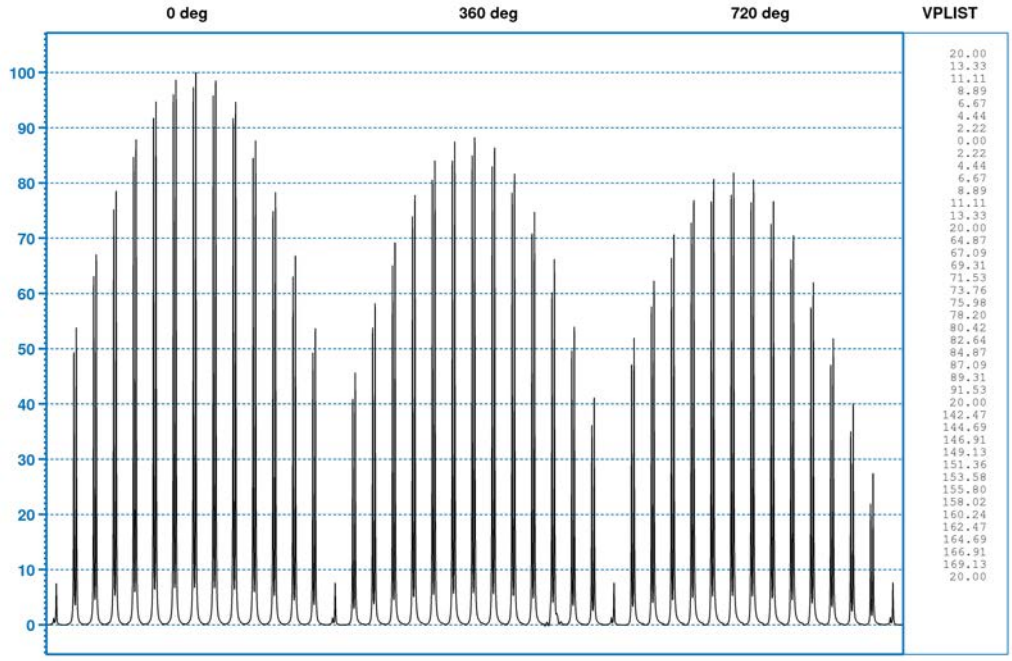
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 65536 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| F1P | 11.004 | ppm | |
| F2P | 8.502 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 256 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 256 | | |

### Experiment Description

Purpose of this experiment is the measurement of the magnet drift rate in unlocked state, but the experiment starts in locked state.
For this hardware test some experimental preparation is needed. Initially the exact resonance position of the chloroform signal is determined after receiver gain adjustment based on a single scan acquisition followed by processing with FT, MC, PP. The data are stored in the derived dataset with EXPNO=1. Data are processed with LB and no baseline correction. Evaluation is based on peak picking of the first and the last acquisition. The printing includes all measurements in pseudo-2D mode.

## 5.2.32 13C B1 homogeneity integral (NPT_1H_b1homogeneityInt_13c)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721, Z142223
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a fraction around signal maximum (-60 deg, +60 deg) is acquired and shown in the figure. The variable pulse list which is used for acquisition is shown to the right.
The B1-homogeneities based on amplitudes and integrals are computed from the peak-picking list amplitudes and the magnitude of the second complex FID data point respectively.

**Control Option for Acquisition (L23)**

1 default PLW 2 is used for determination of B1 homogeneity.
2 PLW 2 will be set to CNST 10 and resultant pulses are used for determination of B1 homogeneity. Experiment will be set to irregular.
3 PLW 2 will be set to power corresponding to specified customer pulses and resultant pulses are used for determination of B1 homogeneity.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p3b1hom2d | | |
| NS | 1 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 3.080 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 1024 | | |
| AQ | 2.219 | s | |
| FIDRES | 0.451 | Hz | |
| D 1 | 8.804 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| P 3 | 9.0 | us | 90deg NUC1 |
| PLW 2 | 42.0 | W | Pow@90deg(Specs) NUC2 |
| TE | 298.000 | K | default |

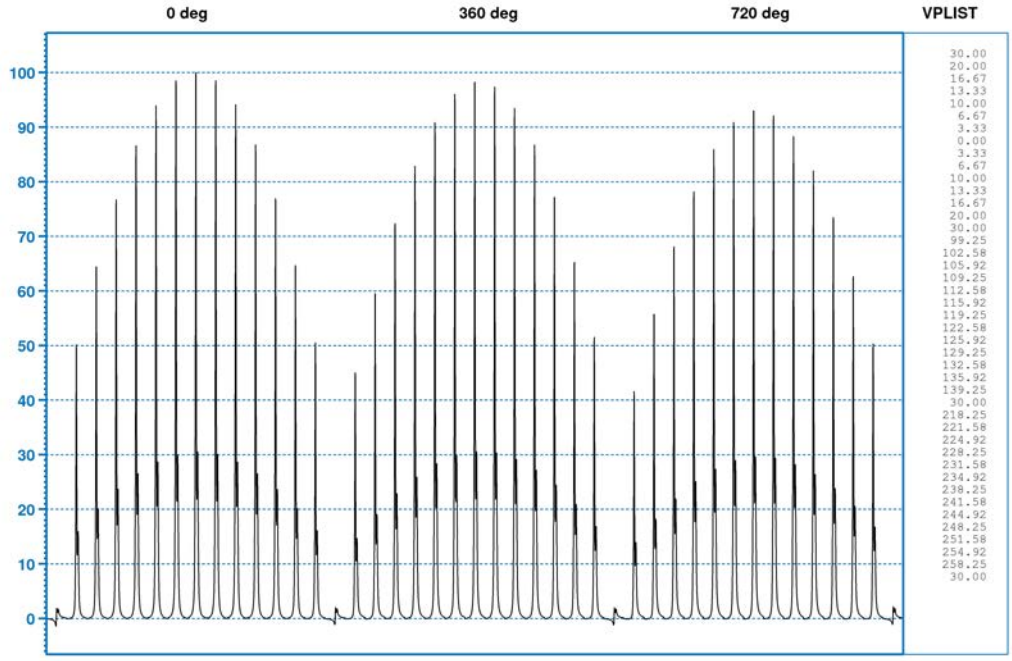
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| NCOEF | 0 | | |
| ABSF1 | 3.150 | ppm | |
| ABSF2 | 2.850 | ppm | |
| F1P | 3.150 | ppm | |
| F2P | 2.850 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 43 | | No of incr. |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |
| **NMRPT** | | | Parameters |
| L 4 | 6 | | integ. fraction of 90deg |
| L 5 | 8 | | # of step per maxima |

## Experiment Description

The B1 homogeneity measurement is normally acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range is from 0 to 720 degree. In order to speed up the measurements NMRPT is acquiring only the partial ranges around the positive signal maxima for the pulse angles 0, 360, and 720 degree.
By this approach it is possible to get a better incremental resolution and a shorter overall measuring time.
Prior to the main acquisition O1P (PROCNO=2) and phase correction (PROCNO=3) will be optimized.
Intermediate results of the CONVTO1D routine is stored in PROCNO=998, result of CONVTO1D in PROCNO=999.
As control of stability, reproducability and 90 degree calibration a spectrum with 180 degree pulse is acquired before and after each maxima. If relaxation conditions and instrument stability is sufficient, the result should not differ among them.
For the predicition of the signal maxima at 360 and 720 degree the propagation delay is included in the calculation of the VP list. (PDelay is calculated as difference of 270 and 90 degree pulse lengths during the corresponding 90 degree pulse determination experiment.) In this measurement O1 is determined before the main acquisition is started. Evaluation is achieved after processing the data in F2 only (XF2) by peak picking and integral determination of the most intense signal per maxima.

## 5.2.33 15N B1 homogeneity integral (NPT_1H_b1homogeneityInt_15n)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721, Z142223
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a fraction around signal maximum (-60 deg, +60 deg) is acquired and shown in the figure. The variable pulse list which is used for acquisition is shown to the right.
The B1-homogeneities based on amplitudes and integrals are computed from the peak-picking list amplitudes and the magnitude of the second complex FID data point respectively.

**Control Option for Acquisition (L23)**

1 default PLW 2 is used for determination of B1 homogeneity.
2 PLW 2 will be set to CNST 10 and resultant pulses are used for determination of B1 homogeneity. Experiment will be set to irregular.
3 PLW 2 will be set to power corresponding to specified customer pulses and resultant pulses are used for determination of B1 homogeneity.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p3b1hom2d | | |
| NS | 1 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 5.500 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 1024 | | |
| AQ | 2.219 | s | |
| FIDRES | 0.451 | Hz | |
| D 1 | 0.381 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| P 3 | 14.0 | us | 90deg NUC1 |
| PLW 2 | 86.0 | W | Pow@90deg(Specs) NUC2 |
| TE | 298.000 | K | default |

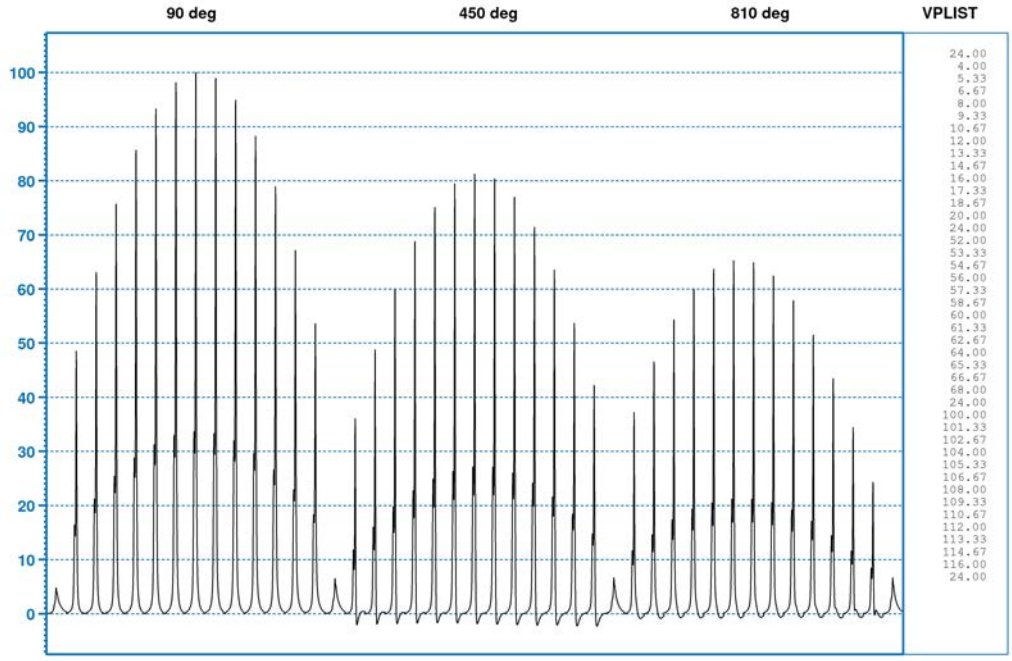
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 43 | | No of incr. |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |
| **NMRPT** | | | Parameters |
| L 4 | 6 | | integ. fraction of 90deg |
| L 5 | 8 | | # of step per maxima |

## Experiment Description

The B1 homogeneity measurement is normally acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range is from 0 to 720 degree. In order to speed up the measurements NMRPT is acquiring only the partial ranges around the positive signal maxima for the pulse angles 0, 360, and 720 degree.
By this approach it is possible to get a better incremental resolution and a shorter overall measuring time.
Prior to the main acquisition O1P (PROCNO=2) and phase correction (PROCNO=3) will be optimized.
Intermediate results of the CONVTO1D routine is stored in PROCNO=998, result of CONVTO1D in PROCNO=999.
As control of stability, reproducability and 90 degree calibration a spectrum with 180 degree pulse is acquired before and after each maxima. If relaxation conditions and instrument stability is sufficient, the result should not differ among them.
For the predicition of the signal maxima at 360 and 720 degree the propagation delay is included in the calculation of the VP list. (PDelay is calculated as difference of 270 and 90 degree pulse lengths during the corresponding 90 degree pulse determination experiment.) In this measurement O1 is determined before the main acquisition is started. Evaluation is achieved after processing the data in F2 only (XF2) by peak picking and integral determination of the most intense signal per maxima.

## 5.2.34 1H B1 homogeneity integral (NPT_1H_b1homogeneityInt_1h)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721, Z142223
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a fraction around signal maximum (-60 deg, +60 deg) is acquired and shown in the figure. The variable pulse list which is used for acquisition is shown to the right.
The B1-homogeneities based on amplitudes and integrals are computed from the peak-picking list amplitudes and the magnitude of the second complex FID data point respectively.

**Control Option for Acquisition (L23)**

1 default PLW 1 is used for determination of B1 homogeneity.
2 PLW 1 will be set to CNST 10 and resultant pulses are used for determination of B1 homogeneity. Experiment will be set to irregular.
3 PLW 1 will be set to power corresponding to specified customer pulses and resultant pulses are used for determination of B1 homogeneity.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1b1hom2d | | |
| NS | 1 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 5.500 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 1024 | | |
| AQ | 2.219 | s | |
| FIDRES | 0.451 | Hz | |
| D 1 | 6.531 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

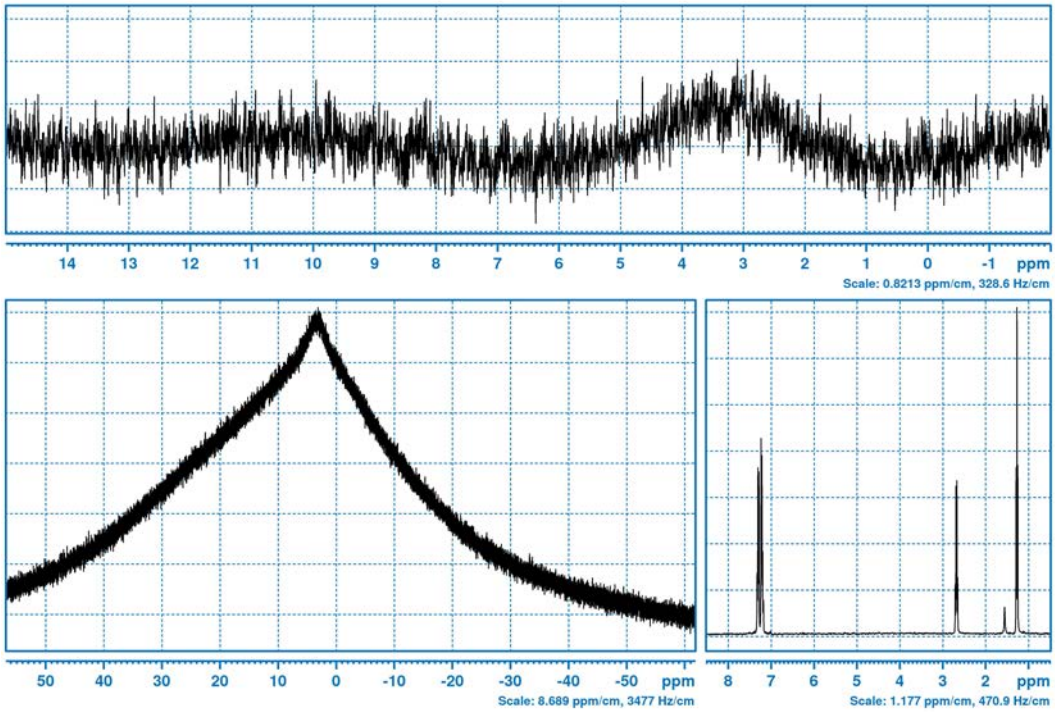
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 43 | | No of incr. |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |
| **NMRPT** | | | Parameters |
| L 4 | 6 | | integ. fraction of 90deg |
| L 5 | 8 | | # of step per maxima |

## Experiment Description

The B1 homogeneity measurement is normally acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range is from 90 to 810 degree. In order to speed up the measurements NMRPT is acquiring only the partial ranges around the positive signal maxima for the pulse angles 90, 450, and 810 degree.
By this approach it is possible to get a better incremental resolution and a shorter overall measuring time.
Prior to the main acquisition O1P (PROCNO=2) and phase correction (PROCNO=3) will be optimized.
Intermediate results of the CONVTO1D routine is stored in PROCNO=998, result of CONVTO1D in PROCNO=999.
As control of stability, reproducability and 90 degree calibration a spectrum with 180 degree pulse is acquired before and after each maxima. If relaxation conditions and instrument stability is sufficient, the result should not differ among them.
For the predicition of the signal maxima at 450 and 810 degree the propagation delay is included in the calculation of the VP list. (PDelay is calculated as difference of 360 and 180 degree pulse lengths during the corresponding 90 degree pulse determination experiment.) In this measurement O1 is determined before the main acquisition is started. Evaluation is achieved after processing the data in F2 only (XF2) by peak picking and integral determination of the most intense signal per maxima.

## 5.2.35 1H background without sample (NPT_1H_backgr_nosample)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10121, Z10033, Z10270, Z10718
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

1H Background signal spectrum without sample (bottom left spectrum). No sharp signal should be present. Broad signal could arise from solid compound in the probe. Top spectrum shows expansion from 15.0 ppm to -2.0 ppm. CY is reduced by scaling factor (CNST50) compared to bottom left spectrum.
1H spectrum with sample to inspect phase correction (bottom right spectrum). Same phase correction values used for spectra with and without sample.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 1H | | |
| PULPROG | npt_zg0 | | |
| NS | 100 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | -2.500 | ppm | |
| SWH | 50000.000 | Hz | |
| TD | 32768 | | |
| AQ | 0.328 | s | |
| FIDRES | 3.052 | Hz | |
| D 1 | 0.872 | s | AQ+D1=const |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

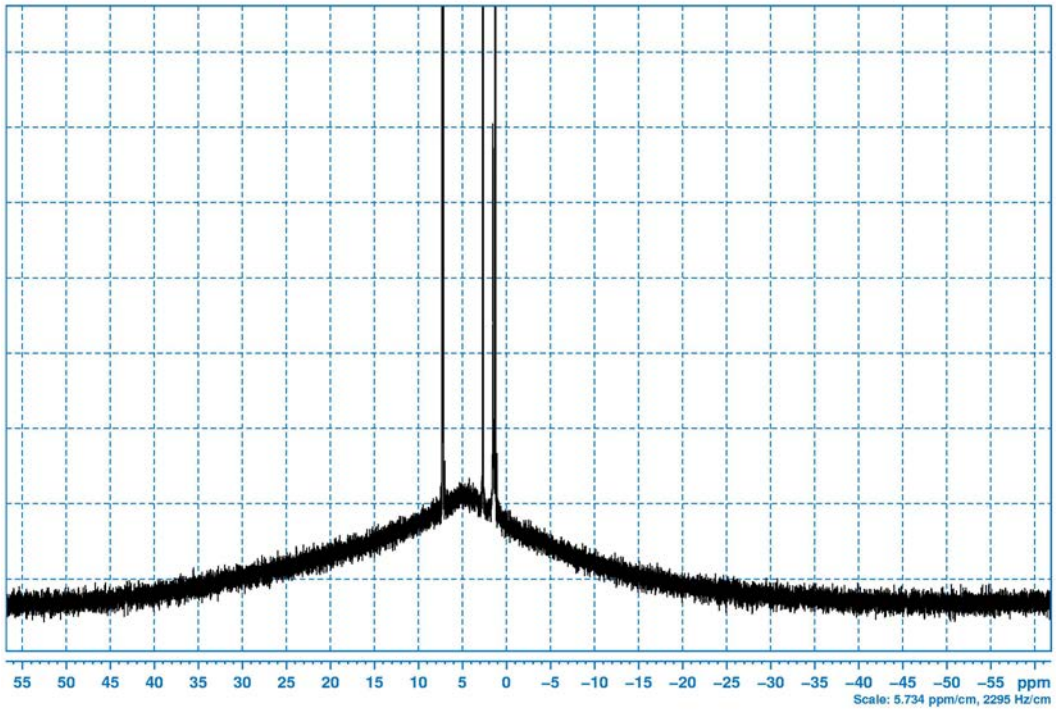
| | | | |
|---|---|---|---|
| CNST 10 | 45.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 66.605 | ppm | |
| F2P | -58.605 | ppm | |
| CY | 6.500 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 0.500 | | Scaling factor for CY |

### Experiment Description

Background signal measurements are executed using a small flip angle due to two reasons. First, to get more efficient excitation bandwidth, secondly to compensate for usually long T1 relaxation time of solid signals.
Full spectrum is normally printed without any baseline correction (bottom spectrum). Using CNST 50, it is possible to scale CY for the top spectrum and adjust print out.
Experiment will be set to irregular if one or both of the options 'Skip Tuning/Matching' or 'Skip HNUC Tuning/Matching' are selected.

## 5.2.36 1H background with sample (NPT_1H_backgr_withsample)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10121, Z10033, Z10270, Z10718, Z142221
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

1H Background signal spectrum with sample. Sharp signal arises from sample, broad signal could arise from solid compound in the probe.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 1H | | |
| PULPROG | npt_zg0 | | |
| NS | 10 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | -2.500 | ppm | |
| SWH | 50000.000 | Hz | |
| TD | 32768 | | |
| AQ | 0.328 | s | |
| FIDRES | 3.052 | Hz | |
| D 1 | 3.837 | s | AQ+D1=const |
| P 0 | 7,9 | us | P 1 * CNST 10 / 90 |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

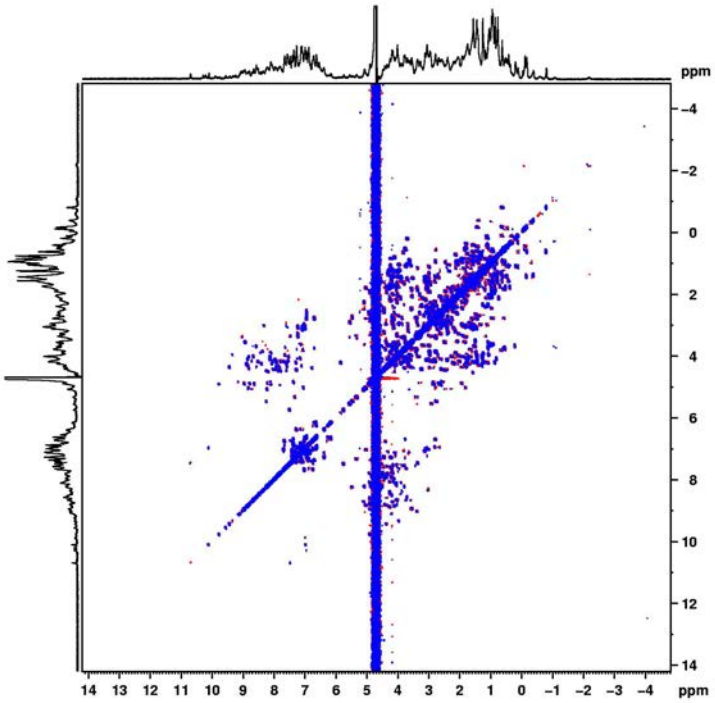
| | | | |
|---|---|---|---|
| CNST 10 | 45.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 63.434 | ppm | |
| F2P | -55.775 | ppm | |
| CY | 200.000 | cm | |

### Experiment Description

Background signal measurements are executed using a small flip angle due to two reasons. First, to get more efficient excitation bandwidth, secondly to compensate for usually long T1 relaxation time of solid signals.
Full spectrum is normally printed without any baseline correction.

## 5.2.37 2D COSY (NPT_1H_cosydfphpr)

**Test Sample:** 2 mM Lysozyme in 90% H2O + 10% D2O
Z10241
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Double quantum filtered, phase sensitive COSY with presaturation during relaxation delay. 1D watersuppression experiment is shown at the left and at the top of the 2D.

**Control Option for Acquisition (L23)**

1 default, with O1 optimization
2 no O1 optimization, the optimization of O1 is enforced, if O1 was not determined during a previous measurement.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| FnMODE | 5 | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_cosydfphpr | | |
| NS | 8 | | |
| DS | 16 | | |
| RG | 0.250 | | optim. by RGA |
| TD0 | 1 | | |
| SW | 20.485 | ppm | |
| TD | 4096 | | |
| AQ | 0.250 | s | field dependent |
| FIDRES | 4.002 | Hz | field dependent |
| D 1 | 2.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |
| DSPFIRM | 4 | | rectangle |
| DIGMOD | 3 | | baseopt |
| DE | 40.000 | us | set after getprosol |

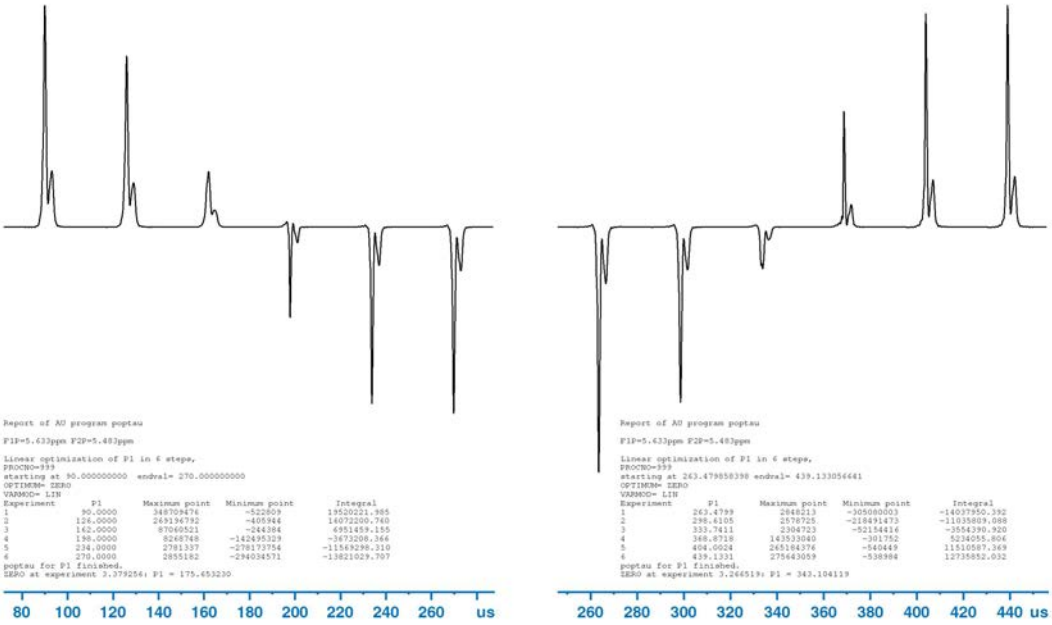
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 2048 | | |
| WDW | 4 | | |
| SSB | 4.000 | | |
| PH_mod | 1 | | pk |
| F1P | 24.732 | ppm | |
| F2P | -15.316 | ppm | |
| LEV0 | 4.250 | | |
| TOPLEV | 50.000 | % | |
| NLEV | 20 | | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| FnMODE | 5 | | |
| O1P | 4.708 | ppm | |
| SW | 20.485 | ppm | |
| TD | 1024 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 2048 | | |
| WDW | 4 | | |
| SSB | 4.000 | | |
| PH_mod | 1 | | pk |
| PHC0 | 90.000 | deg | 90deg (default) |
| PHC1 | -180.000 | deg | 180deg (default) |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

Double quantum filtered, phase sensitive COSY with presaturation.
Presaturation requires the exact determination of the irradiation position (O1P). The determination is executed in a derived data set using the parameter set 'NPT_1H_watersuppression_recflow'.
Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
Option L23=2 will skip the procedure just outlined above.
RG can be set in the Preparation Panel. If RG <= 1 RGA will be exectued after O1 determination in the derived data set.
Processing is achieved using the phase correction values from the preparation experiment.
Contour levels for 2D spectrum are obtained by command levcalc. Levcalc sets the lowest contour level to LEV0*S_DEV, where S_DEV (standard deviation) is a processing status parameter.

## 5.2.38 CPD 1H pulse calibration (NPT_1H_cpddeterminationf1_1h)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 5.500 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 300 | | |
| AQ | 0.650 | s | |
| FIDRES | 1.538 | Hz | |
| D 1 | 1.225 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

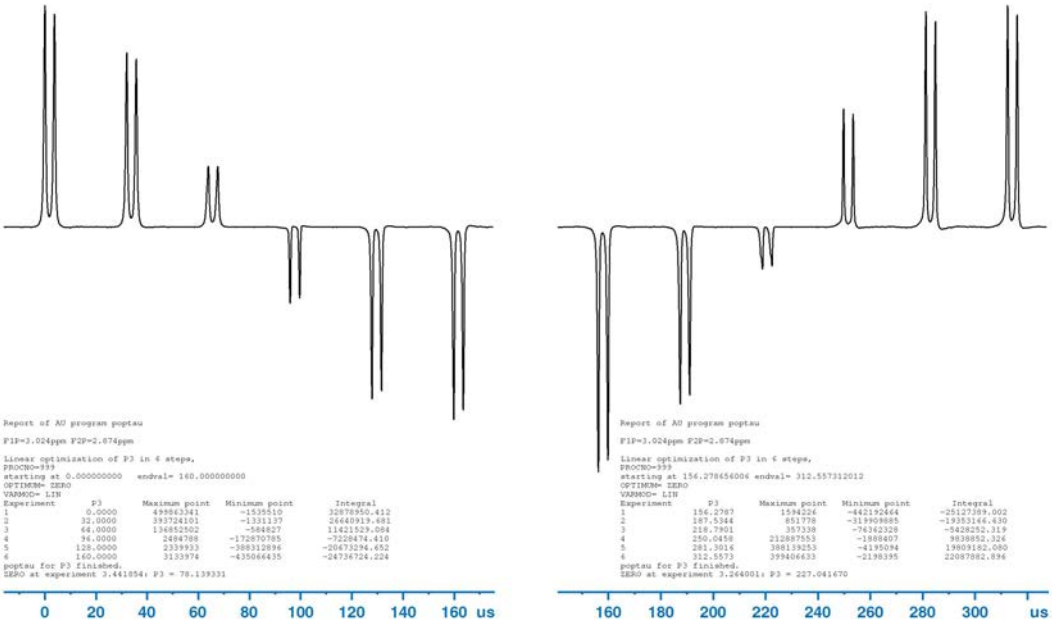
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 3 | | |
| LB | 0.750 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.496 | ppm | |
| F2P | 5.096 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.39 Indirect CPD 13C pulse calibration (NPT_1H_cpddeterminationf2_13c)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the decoupler pulse. On the left side the result of a CONVTO1D routine shows six experiments from 0 to 180 deg (PROCNO 100). On the right side the series goes from 180 to 360 deg (PROCNO 200).

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | decp90 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 3.012 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 1000 | | |
| AQ | 2.167 | s | |
| FIDRES | 0.462 | Hz | |
| D 1 | 1.710 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| P 3 | 9.0 | us | 90deg NUC1 |
| PLW 2 | 42.0 | W | Pow@90deg(Specs) NUC2 |
| TE | 298.000 | K | default |

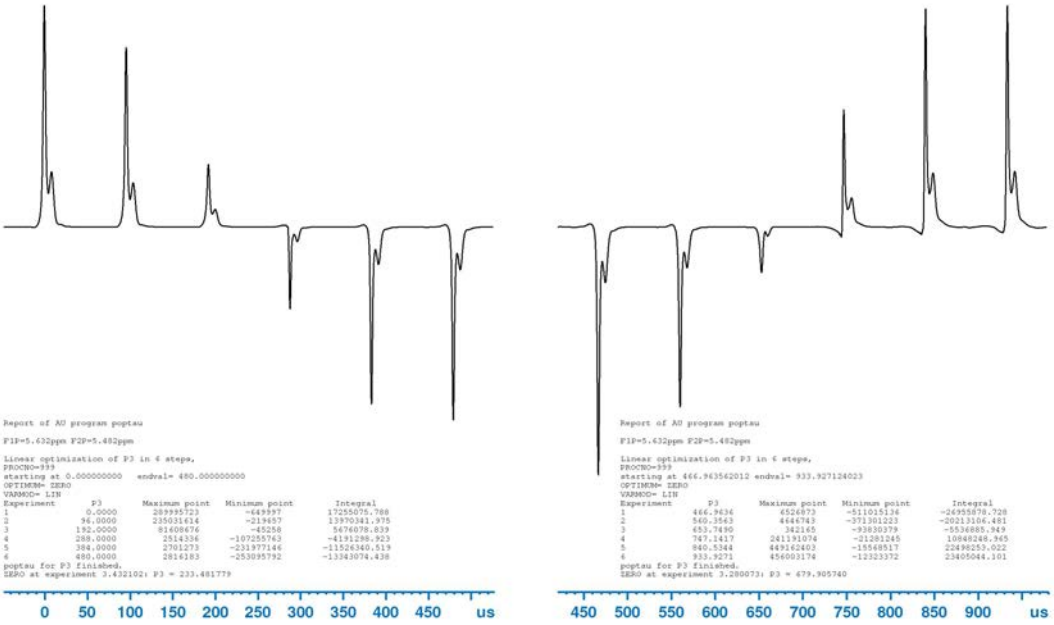
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 1 | | |
| LB | 0.500 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 3.150 | ppm | |
| F2P | 2.850 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 270 and 90 degree pulse lengths and memorised for further use in B1 homogeneity experiments.

## 5.2.40 Indirect CPD 15N pulse calibration (NPT_1H_cpddeterminationf2_15n)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the decoupler pulse. On the left side the result of a CONVTO1D routine shows six experiments from 0 to 180 deg (PROCNO 100). On the right side the series goes from 180 to 360 deg (PROCNO 200).

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | decp90 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 5.500 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 200 | | |
| AQ | 0.433 | s | |
| FIDRES | 2.308 | Hz | |
| D 1 | 0.433 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| P 3 | 14.0 | us | 90deg NUC1 |
| PLW 2 | 86.0 | W | Pow@90deg(Specs) NUC2 |
| TE | 298.000 | K | default |

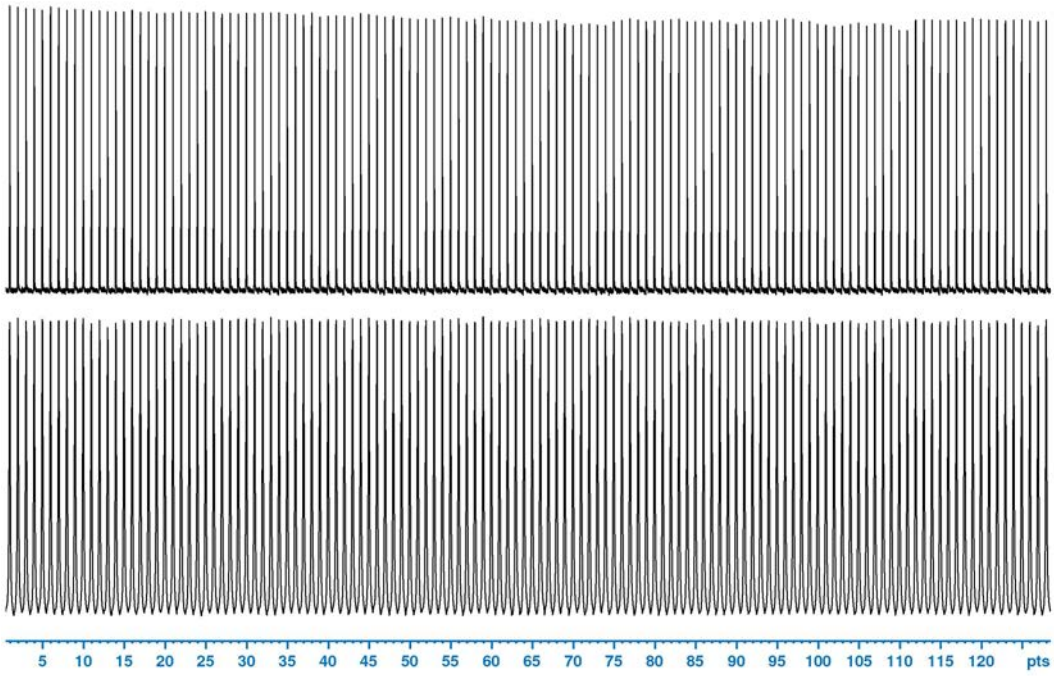
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 3 | | |
| LB | 0.750 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.667 | ppm | |
| F2P | 5.367 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 270 and 90 degree pulse lengths and memorised for further use in B1 homogeneity experiments.

### 5.2.41 13C CPMG test (NPT_1H_cpmgtestf2_13c)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the signal used for evaluation.
Top: Processing with WDW=QSINE and SSB=2, sharp signals which are sensitive to shim effects.
Bottom: Processing with WDW=EM and LB=10.0 Hz, broadend signals which are sensitive to tuning effects.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_decp90f2cpmg2d | | |
| NS | 1 | | |
| DS | 16 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 3.200 | ppm | |
| SW | 0.753 | ppm | |
| TD | 1024 | | |
| AQ | 1.700 | s | field dependent |
| FIDRES | 0.588 | Hz | field dependent |
| D 1 | 0.800 | s | |
| D 21 | 0.000 | s | interpulse delay/2 |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| P 3 | 14.0 | us | 90deg Pulse |
| PLW 2 | 89.0 | W | Pow@90deg(Specs) |
| P 30 | 80.0 | us | 180deg Pulse |
| PLW 20 | 10.9 | W | Pow@90deg(P30) |
| VCLIST | npt_cpmg13c | | |
| TE | 298.000 | K | default |
| WDW | LB | | 1st processing |
| LB | 10 | Hz | 1st processing |
| WDW | QSINE | | 2nd processing |
| SSB | 2 | | 2nd processing |

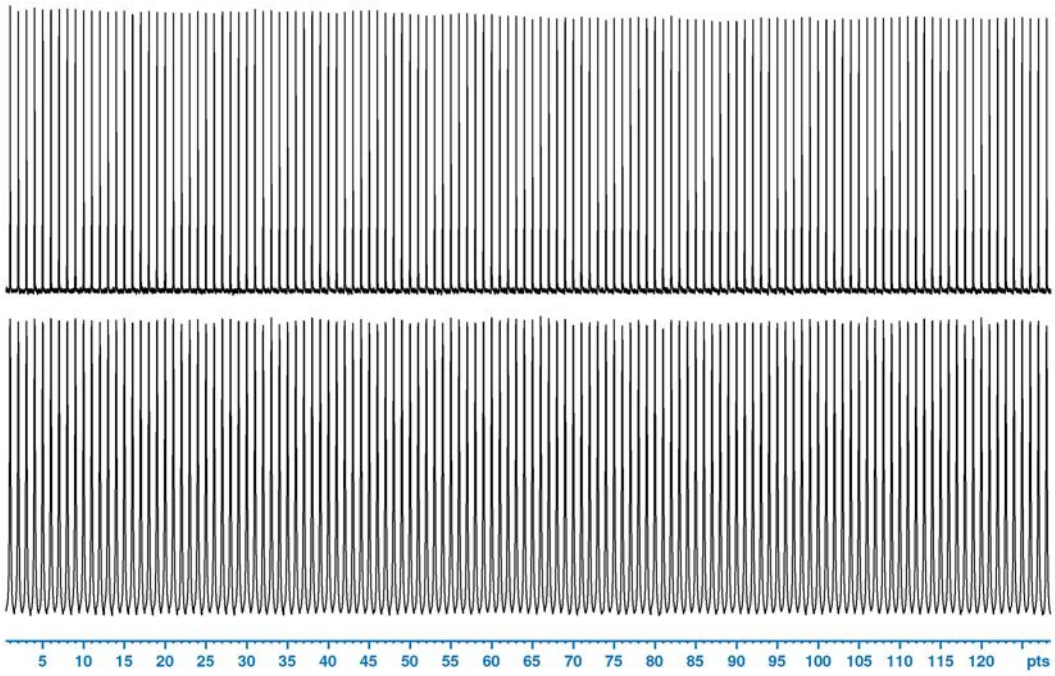
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| ABSF1 | 20.000 | ppm | |
| ABSF2 | 0.000 | ppm | |
| F1P | 3.096 | ppm | |
| F2P | 3.049 | ppm | |
| CY | 13.500 | cm | |

## Experiment Description

Pseudo 2D experiment with CPMG sequence. The interpulse delay is d21*2. The number of repetions of the CPMG sequence and hence the CPMG duration is given by VCLIST.
For evaluation the ratio of the average intensity from signals 99 to 128 and 1 to 30 is deteremined for two different sets of processing parameters. Using WDW=QSINE and SSB=2 will result in sharp signals, i.e. the determined ratio is sensitive for shim effects. Using WDW==EM and LB=10.0 Hz will result in broadend signals, i.e. the determined ratio is sensitive for tuning effects.

### 5.2.42 15N CPMG test (NPT_1H_cpmgtestf2_15n)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the signal used for evaluation.
Top: Processing with WDW=QSINE and SSB=2, sharp signals which are sensitive to shim effects.
Bottom: Processing with WDW=EM and LB=10.0 Hz, broadend signals which are sensitive to tuning effects.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_decp90f2cpmg2d | | |
| NS | 1 | | |
| DS | 16 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 5.400 | ppm | |
| SW | 0.753 | ppm | |
| TD | 1024 | | |
| AQ | 1.700 | s | field dependent |
| FIDRES | 0.588 | Hz | field dependent |
| D 1 | 0.800 | s | |
| D 21 | 0.000 | s | interpulse delay/2 |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| P 3 | 14.0 | us | 90deg Pulse |
| PLW 2 | 89.0 | W | Pow@90deg(Specs) |
| P 30 | 80.0 | us | 180deg Pulse |
| PLW 20 | 10.9 | W | Pow@90deg(P30) |
| VCLIST | npt_cpmg15n | | |
| TE | 298.000 | K | default |
| WDW | LB | | 1st processing |
| LB | 10 | Hz | 1st processing |
| WDW | QSINE | | 2nd processing |
| SSB | 2 | | 2nd processing |

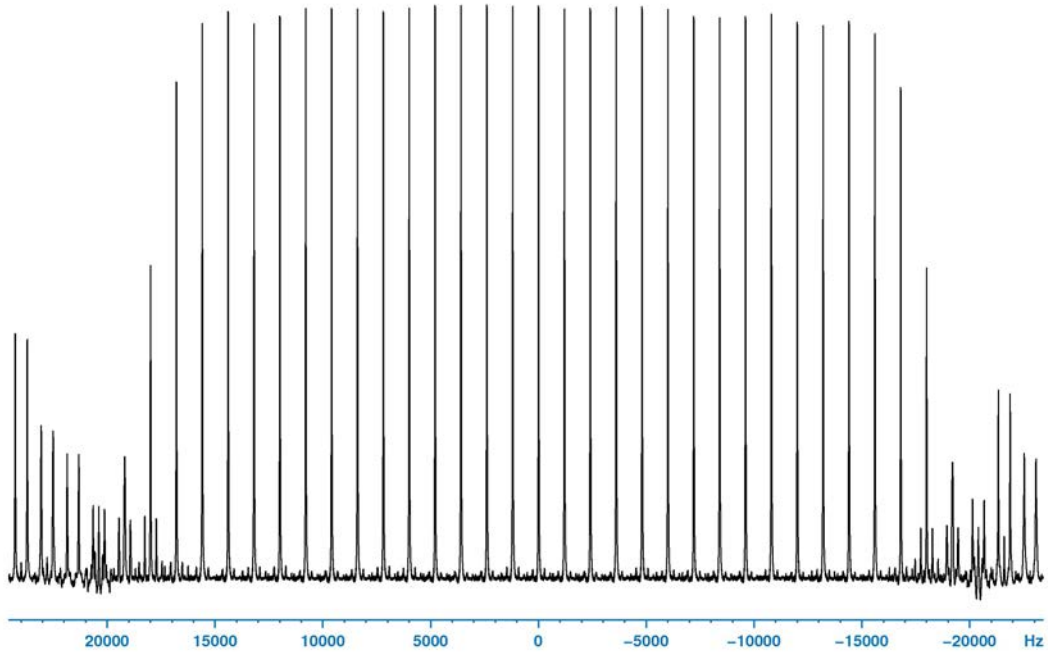
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| ABSF1 | 20.000 | ppm | |
| ABSF2 | 0.000 | ppm | |
| F1P | 5.517 | ppm | |
| F2P | 5.424 | ppm | |
| CY | 13.500 | cm | |

## Experiment Description

Pseudo 2D experiment with CPMG sequence. The interpulse delay is d21*2. The number of repetions of the CPMG sequence and hence the CPMG duration is given by VCLIST.
For evaluation the ratio of the average intensity from signals 99 to 128 and 1 to 30 is deteremined for two different sets of processing parameters. Using WDW=QSINE and SSB=2 will result in sharp signals, i.e. the determined ratio is sensitive for shim effects. Using WDW==EM and LB=10.0 Hz will result in broadend signals, i.e. the determined ratio is sensitive for tuning effects.

### 5.2.43 13C decoupler profile Chirp (NPT_1H_decProfile_chirp_13c)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Decoupling profile of the methanol doublet as a function of the decoupling offset.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | sysdecpro | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 101.000 | | no optim. |
| O1P | 3.260 | ppm | |
| O2P | 49.200 | ppm | |
| SWH | 5000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.205 | s | |
| FIDRES | 4.883 | Hz | |
| D 1 | 2.813 | s | |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| PCPD2 | 1500.0 | us | PCPD NUC2 |
| PLW 1 | 6.7 | W | Pow@90deg(Specs) NUC1 |
| PLW 2 | 26.5 | W | Pow@90deg(Specs) NUC2 |
| PLW 12 | 0.56 | W | Pow@CPD NUC2 |
| SPNAM15 | crp40,1.5.hwt | | shaped pulse |
| CPDPRG2 | p5m4sp180 | | decoupl. sequence |
| FQ2LIST | | | Offset List, gen. dynamically. |
| TE | 298.000 | K | default |

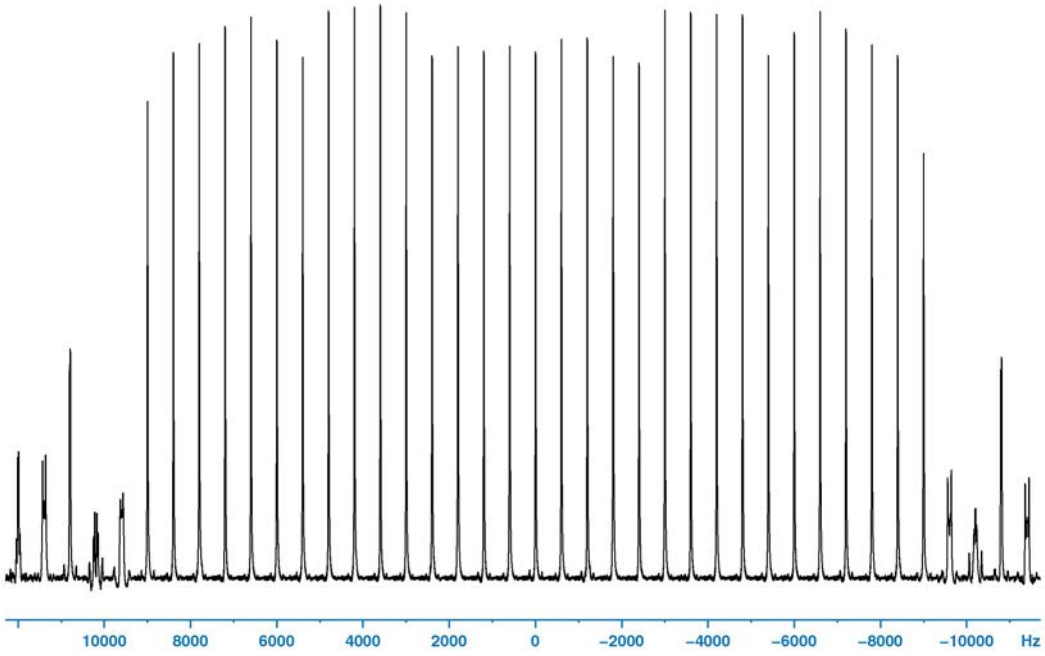
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| PH_mod | 0 | | mc |
| F1P | 3.760 | ppm | |
| F2P | 2.760 | ppm | |
| **NMRPT** | | | Parameters |
| CNST 24 | 48000.0 | Hz | Total Offset Range |
| CNST 41 | 1.000 | | Return Value Evaluation |

### Experiment Description

The purpose of this test is the assessment of the 13C-decoupling efficiency on the methanol doublet as a function of the decoupling offset at constant decoupling power. The amplitude of the resulting singlet peak should be as high as possible over the largest offset range.
The decoupling scheme used in this experiment is chirp.

## 5.2.44 13C decoupler profile Garp (NPT_1H_decProfile_garp_13c)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Decoupling profile of the methanol doublet as a function of the decoupling offset.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | sysdecpro | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 101.000 | | no optim. |
| O1P | 3.260 | ppm | |
| O2P | 49.200 | ppm | |
| SWH | 5000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.205 | s | |
| FIDRES | 4.883 | Hz | |
| D 1 | 2.813 | s | |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| PCPD2 | 70.0 | us | PCPD NUC2 |
| PLW 1 | 6.7 | W | Pow@90deg(Specs) NUC1 |
| PLW 2 | 26.5 | W | Pow@90deg(Specs) NUC2 |
| PLW 12 | 0.56 | W | Pow@CPD NUC2 |
| CPDPRG2 | garp | | decoupl. sequence |
| FQ2LIST | | | Offset List, gen. dynamically. |
| TE | 298.000 | K | default |

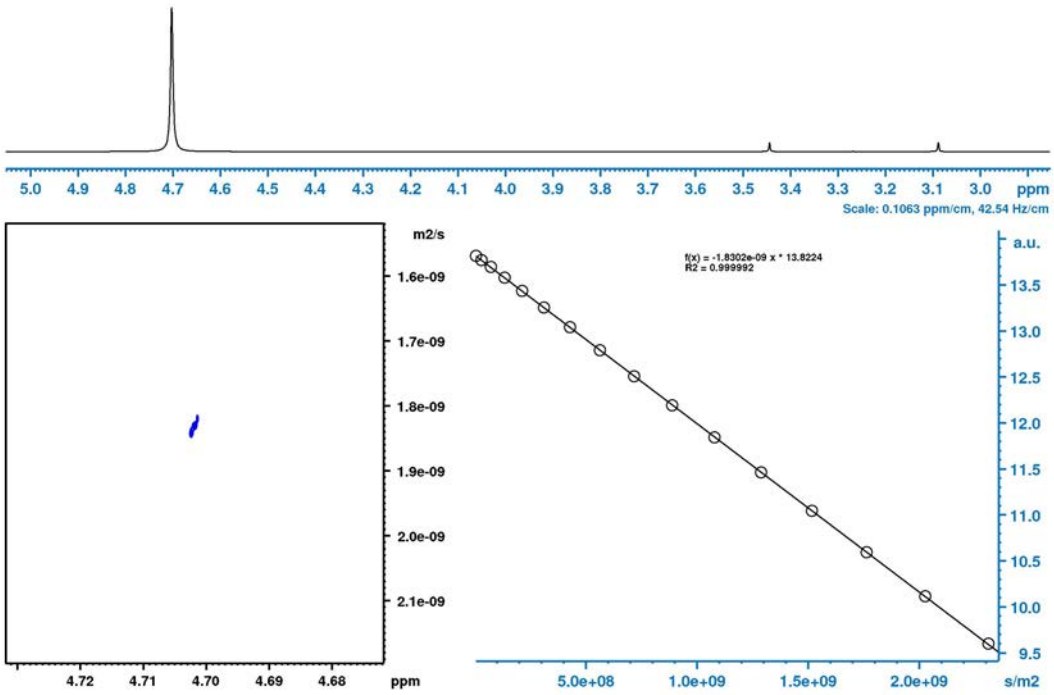
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| PH_mod | 0 | | mc |
| F1P | 3.760 | ppm | |
| F2P | 2.760 | ppm | |
| **NMRPT** | | | Parameters |
| CNST 24 | 24000.0 | Hz | Total Offset Range |
| CNST 41 | 1.000 | | Return Value Evaluation |

## Experiment Description

The purpose of this test is the assessment of the 13C-decoupling efficiency on the methanol doublet as a function of the decoupling offset at constant decoupling power. The amplitude of the resulting singlet peak should be as high as possible over the largest offset range.
The decoupling scheme used in this experiment is garp.

## 5.2.45 Low Current Diffusion Test for Z-direction (NPT_1H_diffusionLowCurrentZ)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O Z10083
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top: Phase corrected first row of the pseudo 2D experiment.
Bottom left: Dosy plot.
Bottom right: Logarithmic plot of the intensities against b-values along with a linear fit.

**Control Option for Acquisition (L23)**

1 default, execute O1P determination
2 skip O1P determination.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | diffSte -DLOCK | | |
| ZGOPTNS | -Dspoil -DSINE | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SW | 13.884 | ppm | |
| TD | 16666 | | field dependent |
| AQ | 1.500 | s | |
| FIDRES | 0.667 | Hz | field dependent |
| D 1 | 1.450 | s | |
| D 2 | 0.001 | s | gradient stabilistation time |
| D 5 | 0.014 | s | big delta remainder |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPZ 5 | 2.41 | % | 41.8 gauss/cm |
| GPNAM5 | SINE.100 | | |
| P 19 | 2000.000 | us | spoil gradient pulse |
| GPNAM31 | npt_diffusion | | |
| CNST 3 | 7.40 | % | 128.3 gauss/cm |
| D 16 | 0.000 | s | ramp down time |
| D 18 | 0.002 | s | gradient on time |
| D 60 | 300.000 | s | temperature stabilisation |
| TE | 298.200 | K | default |

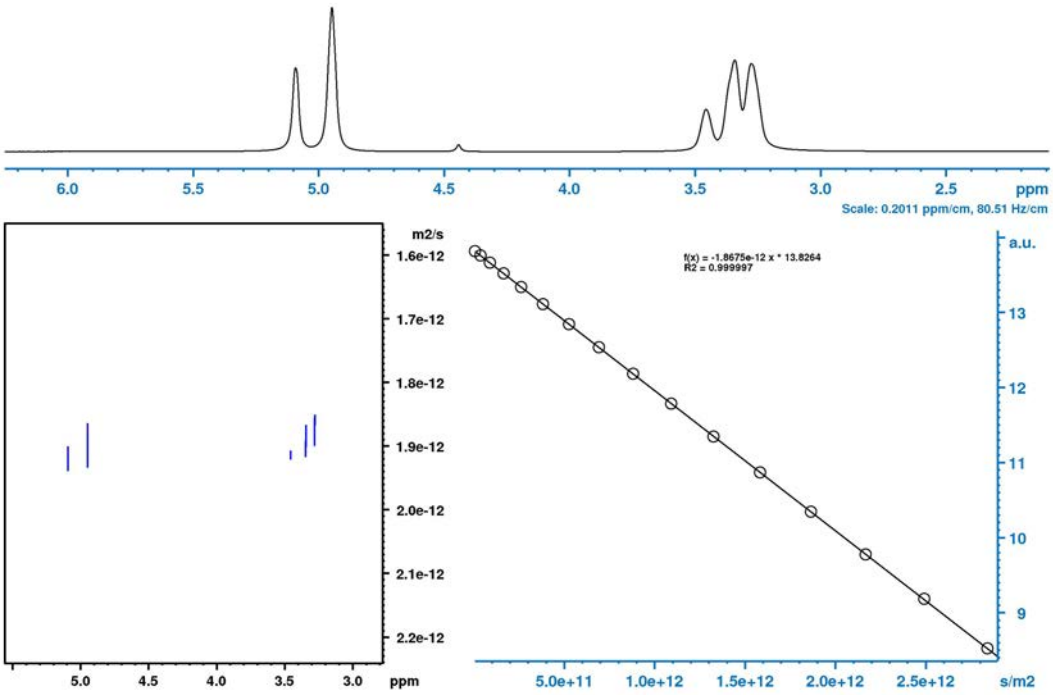
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 16 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 16 | | |

## Experiment Description

Purpose of this experiment is the measurement of the diffusion constant by varying the strength of the applied field gradients.
Low current diffusion experiment using the ste method. The experiment is only implemented for the gradient shape sine. The following parameters are used: gmax=128.33 gauss/cm, delta=1.0 ms, DELTA=20.0 ms, repetition time=3.0 s, ZGOPTNS=-DLOCK -Dspoil -DSINE
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the first experiment of the series using APK0 as default and applied to the series. The diffusion constant is fitted using the Steijskal-Tanner Equation. Therefor the signal intensities are determined from PROCNO 999.
The dosy plot is created with the AU programm setdiffparm and the command dosy2d.
Attention: Before running the diffusion experiment the DC offset of the gradient amplifier must be calibrated.

## 5.2.46 High Current Diffusion Test for Z-direction (NPT_1H_diffusionHighCurrentZ)

**Test Sample:** Dry Glycerol
Z10650
**Solvent:** None
**Lock parameter:** None
**Sample State:** Rotation off




**Example Printout**

Top: Phase corrected first row of the pseudo 2D experiment.
Bottom left: Dosy plot.
Bottom right: Logarithmic plot of the intensities against b-values along with a linear fit.

**Control Option for Acquisition (L23)**

1 default, execute O1P and pulse determination
2 skip O1P determination and exectue pulse determination.
10 execute O1P determination and skip pulse determination.
12 skip O1P and pulse determination.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | diffSte -Dspoil - | | |
| ZGOPTNS | DLED - DSINE | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SW | 13.884 | ppm | |
| TD | 16666 | | field dependent |
| AQ | 1.500 | s | |
| FIDRES | 0.667 | Hz | field dependent |
| D 1 | 1.290 | s | |
| D 2 | 0.001 | s | gradient stabilistation time |
| D 5 | 0.092 | s | big delta remainder |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPZ 5 | 3.06 | % | 53.0 gauss/cm |
| GPNAM5 | SINE.100 | | |
| P 19 | 2000.000 | us | spoil gradient pulse |
| GPNAM31 | npt_diffusion | | |
| CNST 3 | 57.67 | % | 1000.0 gauss/cm |
| D 16 | 0.000 | s | ramp down time |
| D 18 | 0.003 | s | gradient on time |
| D 60 | 300.000 | s | temperature stabilisation |
| TE | 298.200 | K | default |

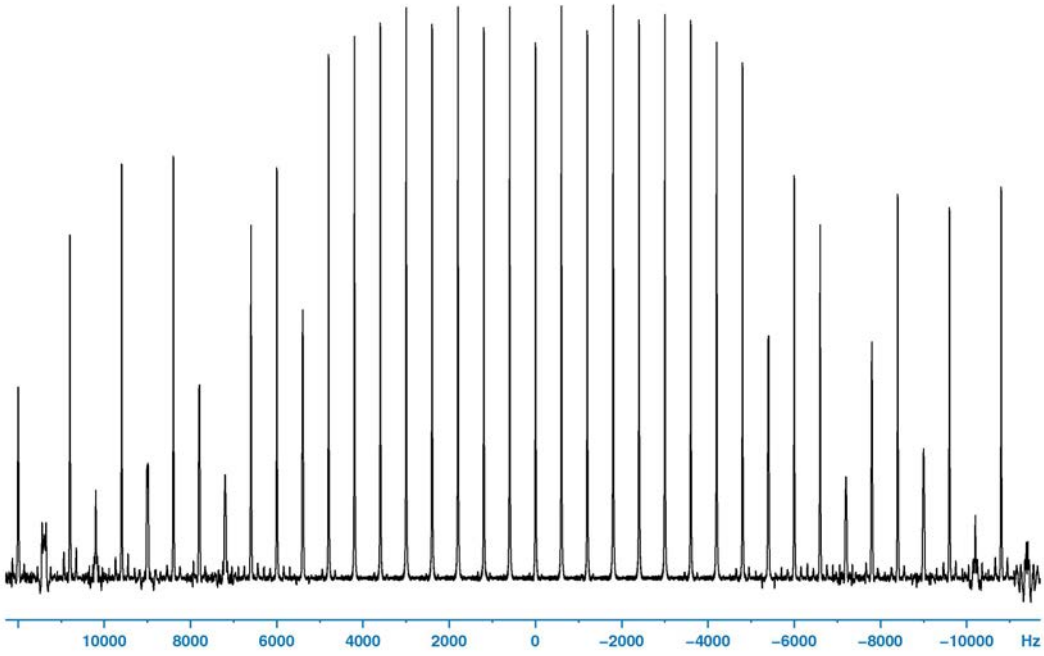
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 16 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 16 | | |

## Experiment Description

Purpose of this experiment is the measurement of the diffusion constant by varying the strength of the applied field gradients.
High current diffusion experiment using the ste method. The experiment is only implemented for the gradient shape sine. The following parameters are used: gmax=1000.00 gauss/cm, delta=2.0 ms, DELTA=100.0 ms, repetition time=3.0 s, ZGOPTNS=-Dspoil -DLED -DSINE
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
L23 dependent pulse determination using pulsecal.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the first experiment of the series using APK0 as default and applied to the series. The diffusion constant is fitted using the Steijskal-Tanner Equation. Therefor the signal intensities are determined from PROCNO 999.
The dosy plot is created with the AU programm setdiffparm and the command dosy2d.
Attention: Before running the diffusion experiment the DC offset of the gradient amplifier must be calibrated.

## 5.2.47 13C decoupler profile Waltz (NPT_1H_decProfile_waltz_13c)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Decoupling profile of the methanol doublet as a function of the decoupling offset.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | sysdecpro | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 101.000 | | no optim. |
| O1P | 3.260 | ppm | |
| O2P | 49.200 | ppm | |
| SWH | 5000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.205 | s | |
| FIDRES | 4.883 | Hz | |
| D 1 | 2.813 | s | |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| PCPD2 | 70.0 | us | PCPD NUC2 |
| PLW 1 | 6.7 | W | Pow@90deg(Specs) NUC1 |
| PLW 2 | 26.5 | W | Pow@90deg(Specs) NUC2 |
| PLW 12 | 0.56 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| FQ2LIST | | | Offset List, gen. dynamically. |
| TE | 298.000 | K | default |

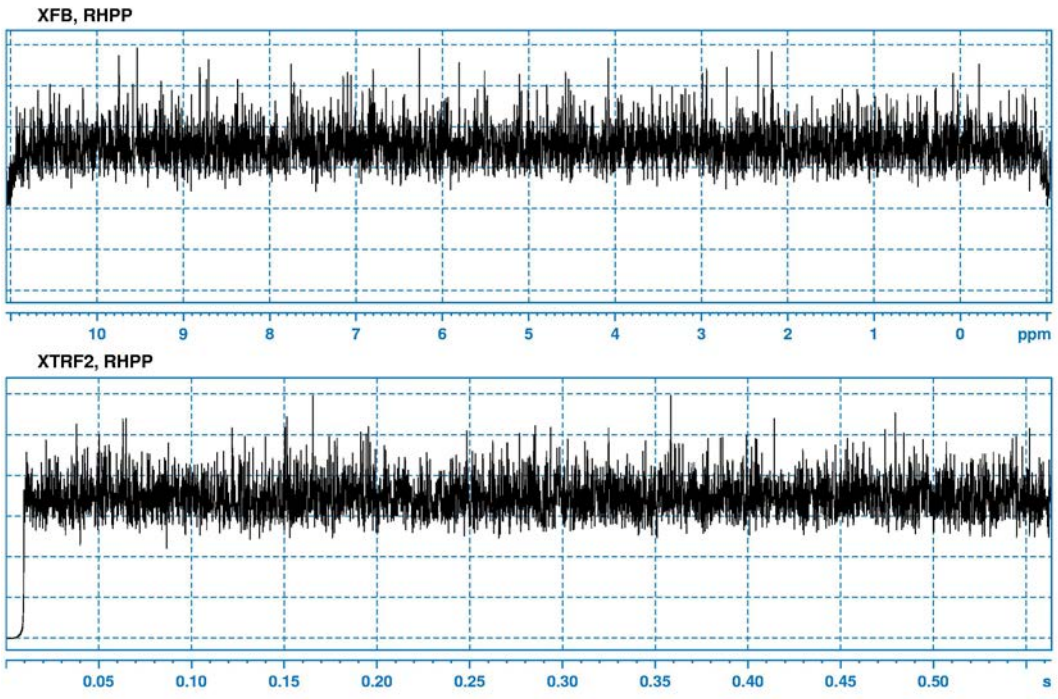
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| PH_mod | 0 | | mc |
| F1P | 3.760 | ppm | |
| F2P | 2.760 | ppm | |
| **NMRPT** | | | Parameters |
| CNST 24 | 24000.0 | Hz | Total Offset Range |
| CNST 41 | 1.000 | | Return Value Evaluation |

## Experiment Description

The purpose of this test is the assessment of the 13C-decoupling efficiency on the methanol doublet as a function of the decoupling offset at constant decoupling power. The amplitude of the resulting singlet peak should be as high as possible over the largest offset range.
The decoupling scheme used in this experiment is waltz64.

## 5.2.48 1H detection with 13C garp decoupling (NPT_1H_garpdectestf2_13c)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10033, Z10270, Z10718, Z10121
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

Top spectrum shows 2D projection (XFB, RHPP).
Bottom spectrum shows 2D projection (XTRF2, RHPP).

### Control Option for Acquisition (L23)

70 PLW12[apparent]=PLW12[prosol], default
80 PLW12[apparent]=PLW12[prosol], 6 h waiting time before execution
71 PLW12[apparent]=PLW12[prosol]*1.5849 (-2 dB)
81 PLW12[apparent]=PLW12[prosol]*1.5849 (-2 dB), 6 h waiting time before execution
72 PLW12[apparent]=PLW12[prosol]*2.0 (-3 dB)
82 PLW12[apparent]=PLW12[prosol]*2.0 (-3 dB), 6 h waiting time before execution

## Parameters

| F2 ACQU | | | Parameters F2 |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_garptest | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| TD0 | 1 | | |
| SW | 12.132 | ppm | |
| TD | 8192 | | |
| AQ | 0.844 | s | |
| FIDRES | 1.185 | Hz | field dependent |
| D 1 | 2.109 | s | 2.5*AQ |
| P 1 | 14.0 | us | 90deg NUC1 |
| PCPD 2 | 80.0 | us | CPD 90deg |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.5 | W | Pow@CPD(Specs) |
| CPDPRG2 | garp | | default CPD Seq. |
| TE | 298.000 | K | default |

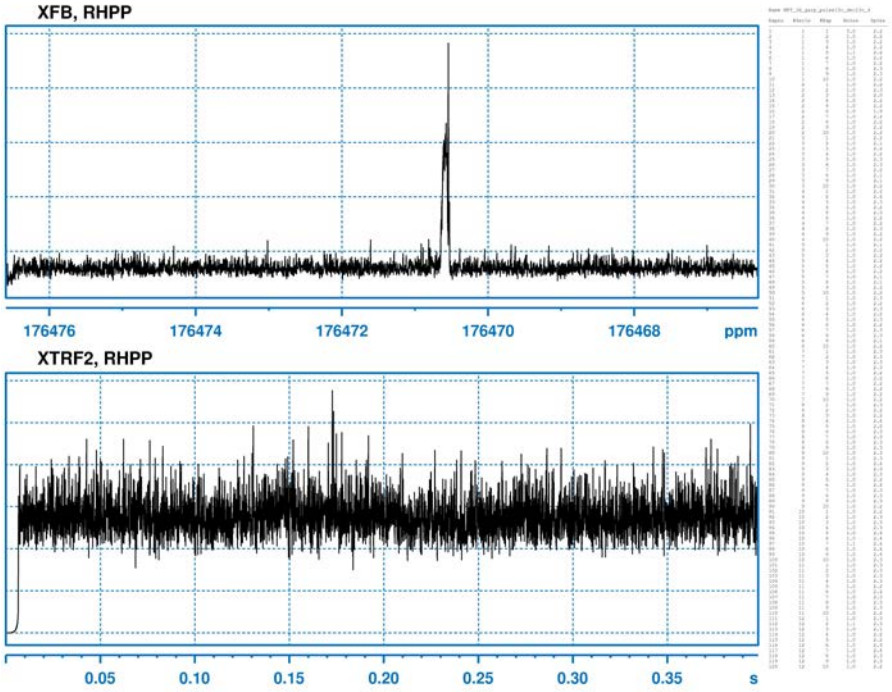
| F2 PROC | | | Parameters F2 |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| BC_mod | 0 | | |
| ME_mod | 0 | | |
| FT_mod | 0 | | |
| F1P | 8.500 | ppm | |
| F2P | 0.500 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 13C | | |
| TD | 256 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 256 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| BC_mod | 0 | | |
| ME_mod | 0 | | |
| FT_mod | 0 | | |

## Experiment Description

The GARP decoupling test indicates the reliability of the probe with respect to decoupling. No excitation pulse is applied, only decoupling takes place during acquisition of the noise. The acquisition time is splitted up according to the scheme 25%-50%-25% thereby only during the 50% decoupling power is applied. D1 is set to 2.5*AQ, so that the duty cycle is 15%
The different options for the experiment are self-explanatory.
The first evaluation is done by processing with XFB using the standard Fourier transform features of the TopSpin software. The horizontal positive projection (RHPP) is then evaluated by searching for the minimal and maximal intensity and forming the ratio of the two. Interpreation of the result is only possible in relation to the second evaluation.
A value close to 1.0 is optimal, higher values are worse, values < 1.0 are only meaningful, if the second evaluation results in small values, too.
The second evaluation is done by processing with XTRF2 using parameters as outlined below resulting in time domain data. The horizontal positive projection (RHPP) is then used to determine a 'noise factor' between the average noise of the decoupled and the coupled region. If the ratio is close to 1.0 the decoupling efficiency is optimal.
Options L23=70 and 80 are standard whereas all other L23 options are non-standard and will not be considered as regular test from the 'NMRPT Control Structure'.

## 5.2.49 1H detection with 13C hard pulse and 13C garp decoupling (NPT_1H_garp_pulse13c_dec13c)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10033, Z10270, Z10718, Z10121
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top spectrum shows 2D projection (XFB, RHPP).
Bottom spectrum shows 2D projection (XTRF2, RHPP).
Both projections are from the 2D experiment of the last series with the highest noise factor.

**Control Option for Acquisition (L23)**

1 default

### Parameters

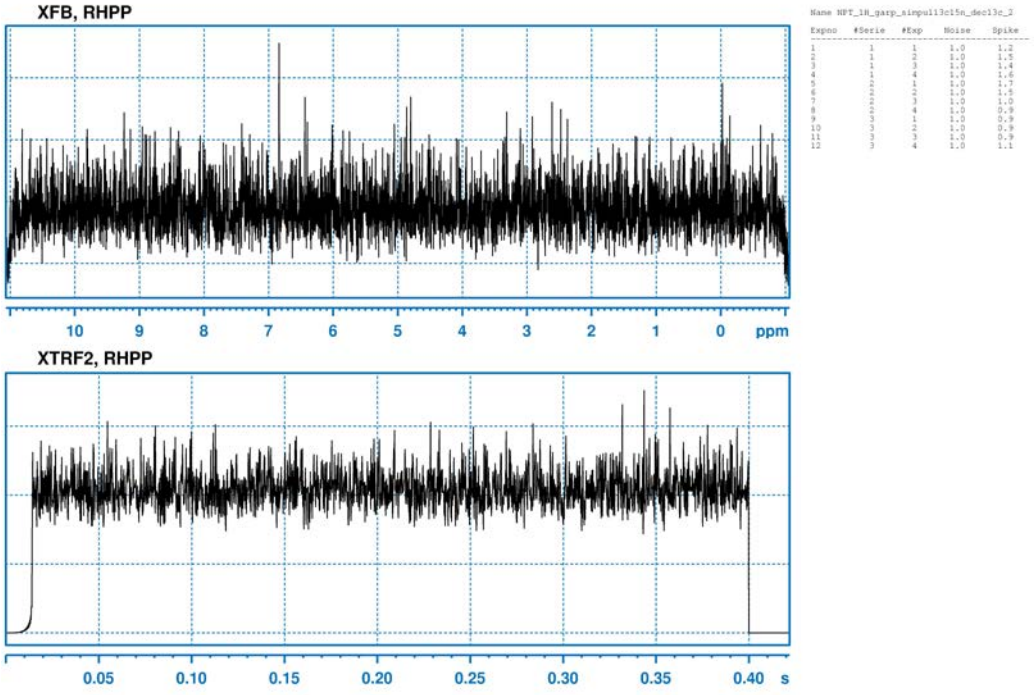
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 | **F2 PROC** | | | Parameters F2 |
| NUC1 | 1H | | | SI | 4096 | | |
| NUC2 | 13C | | | WDW | 0 | | |
| PARMODE | 1 | | Data Dimension | PH_mod | 0 | | |
| PULPROG | npt_garptest | | | BC_mod | 0 | | |
| NS | 1 | | | ME_mod | 0 | | |
| DS | 0 | | | FT_mod | 0 | | |
| RG | 101.000 | | no optim. | F1P | 8.500 | ppm | |
| TD0 | 1 | | | F2P | 0.500 | ppm | |
| SW | 12.132 | ppm | | **F1 ACQU** | | | Parameters F1 |
| TD | 3882 | | | NUC1 | 13C | | |
| AQ | 0.400 | s | | TD | 256 | | |
| FIDRES | 2.501 | Hz | field dependent | **F1 PROC** | | | Parameters F1 |
| D 1 | 1.000 | s | 2.5*AQ | SI | 256 | | |
| P 4 | 24.0 | us | 180deg NUC2 | WDW | 0 | | |
| PLW 2 | 86.0 | W | Pow@90deg(Specs) NUC2 | PH_mod | 0 | | |
| PCPD 2 | 80.0 | us | CPD 90deg | BC_mod | 0 | | |
| PLW 12 | 0.5 | W | Pow@CPD(Specs) | ME_mod | 0 | | |
| CPDPRG2 | garp | | default CPD Seq. | FT_mod | 0 | | |
| TE | 298.000 | K | default | | | | |

### Experiment Description

Garp series experiment with 13C hard pulse, 13C decoupling and 1H detection.
The garp series experiment has the following structure [n * (2D Garp Experiment) - (Delay T)] * m
The parameters m, n, and T are set via specifications. If not specified following default values will be used: m=2, n=2, and T=30 min. WRPA is used to copy each acquired experiment into a derived data set.
The results for Noise Factor and Spike Ratio are taken from the 2D experiment of the last series with the highest noise factor.
The GARP decoupling test indicates the reliability of the probe with respect to decoupling. No excitation pulse is applied, only decoupling takes place during acquisition of the noise. The acquisition time is splitted up according to the scheme 50%-25%-25% thereby only during the 50% decoupling power is applied. D1 is set to 2.5*AQ, so that the duty cycle is 15%
The first evaluation is done by processing with XFB using the standard Fourier transform features of the TopSpin software. The horizontal positive projection (RHPP) is then evaluated by searching for the minimal and maximal intensity and forming the ratio of the two. Interpreation of the result is only possible in relation to the second evaluation.
A value close to 1.0 is optimal, higher values are worse, values < 1.0 are only meaningful, if the second evaluation results in small values, too.
The second evaluation is done by processing with XTRF2 using parameters as outlined below resulting in time domain data. The horizontal positive projection (RHPP) is then used to determine a 'noise factor' between the average noise of the decoupled and the coupled region. If the ratio is close to 1.0 the decoupling efficiency is optimal.

## 5.2.50 1H detection with 13C and 15N hard pulses and 13C garp decoupling (NPT_1H_garp_simpul13c15n_dec13c)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10033, Z10270, Z10718, Z10121
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

Top spectrum shows 2D projection (XFB, RHPP).
Bottom spectrum shows 2D projection (XTRF2, RHPP).
Both projections are from the 2D experiment of the last series with the highest noise factor.

### Control Option for Acquisition (L23)

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| NUC3 | 15N | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_garptest | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| TD0 | 1 | | |
| SW | 12.132 | ppm | |
| TD | 3882 | | |
| AQ | 0.400 | s | |
| FIDRES | 2.501 | Hz | field dependent |
| D 1 | 1.000 | s | 2.5*AQ |
| P 4 | 24.0 | us | 180deg NUC2 |
| PLW 2 | 86.0 | W | Pow@90deg(Specs) NUC2 |
| P 6 | 50.0 | us | 180deg NUC3 |
| PLW 3 | 155.5 | W | Pow@CPD(Specs) |
| PCPD 2 | 80.0 | us | CPD 90deg |
| PLW 12 | 0.5 | W | Pow@CPD(Specs) |
| CPDPRG2 | garp | | default CPD Seq. |
| TE | 298.000 | K | default |

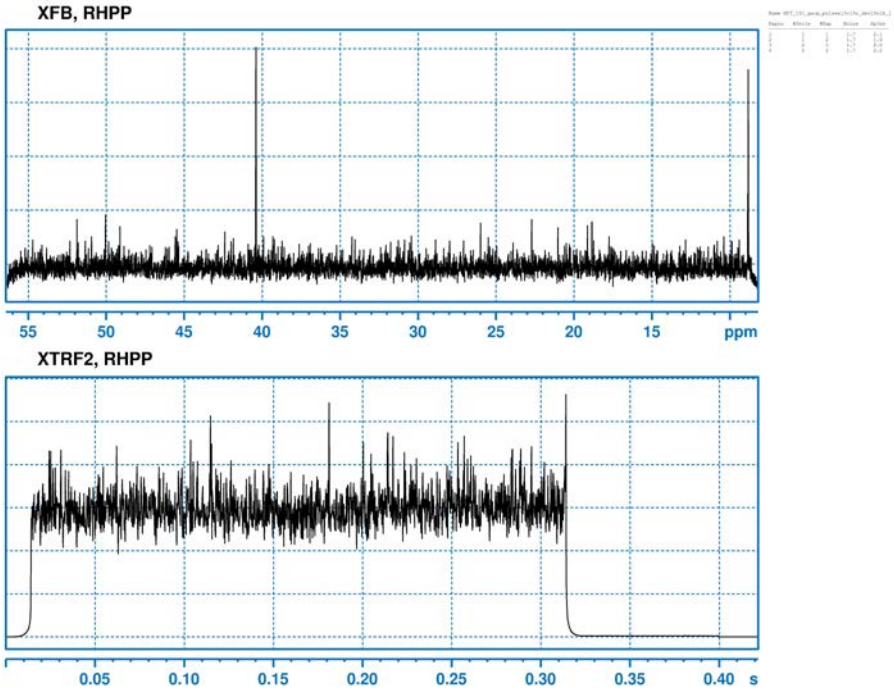
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| BC_mod | 0 | | |
| ME_mod | 0 | | |
| FT_mod | 0 | | |
| F1P | 8.500 | ppm | |
| F2P | 0.500 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 13C | | |
| TD | 256 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 256 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| BC_mod | 0 | | |
| ME_mod | 0 | | |
| FT_mod | 0 | | |

### Experiment Description

Garp series experiment with simultanieus 13C and 15N hard pulses, 13C decoupling and 1H detection.
The garp series experiment has the following structure [n * (2D Garp Experiment) - (Delay T)] * m
The parameters m, n, and T are set via specifications. If not specified following default values will be used: m=2, n=2, and T=30 min. WRPA is used to copy each acquired experiment into a derived data set. The results for Noise Factor and Spike Ratio are taken from the 2D experiment of the last series with the highest noise factor.
The GARP decoupling test indicates the reliability of the probe with respect to decoupling. No excitation pulse is applied, only decoupling takes place during acquisition of the noise. The acquisition time is splitted up according to the scheme 50%-25%-25% thereby only during the 50% decoupling power is applied. D1 is set to 2.5*AQ, so that the duty cycle is 15%
The first evaluation is done by processing with XFB using the standard Fourier transform features of the TopSpin software. The horizontal positive projection (RHPP) is then evaluated by searching for the minimal and maximal intensity and forming the ratio of the two. Interpreation of the result is only possible in relation to the second evaluation.
A value close to 1.0 is optimal, higher values are worse, values < 1.0 are only meaningful, if the second evaluation results in small values, too.
The second evaluation is done by processing with XTRF2 using parameters as outlined below resulting in time domain data. The horizontal positive projection (RHPP) is then used to determine a 'noise factor' between the average noise of the decoupled and the coupled region. If the ratio is close to 1.0 the decoupling efficiency is optimal.

## 5.2.51 13C detection with 13C and 15N hard pulses and 15N and 1H garp decoupling (NPT_13C_garp_pulses13c15n_dec15n1h)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10033, Z10270, Z10718, Z10121
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top spectrum shows 2D projection (XFB, RHPP).
Bottom spectrum shows 2D projection (XTRF2, RHPP).
Both projections are from the 2D experiment of the last series with the highest noise factor.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 13C | | |
| NUC2 | 15N | | |
| NUC3 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_garptest | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| TD0 | 1 | | |
| SW | 48.246 | ppm | |
| TD | 3882 | | |
| AQ | 0.400 | s | |
| FIDRES | 2.501 | Hz | field dependent |
| D 1 | 1.000 | s | 2.5*AQ |
| P 2 | 24.0 | us | 180deg NUC2 |
| PLW 1 | 86.0 | W | Pow@90deg(Specs) NUC2 |
| P 4 | 50.0 | us | 180deg NUC3 |
| PLW 2 | 155.5 | W | Pow@CPD(Specs) |
| PCPD 2 | 200.0 | us | CPD 90deg |
| PLW 12 | 2.5 | W | Pow@CPD(Specs) |
| CPDPRG2 | garp | | default CPD Seq. |
| PCPD 3 | 80.0 | us | CPD 90deg |
| PLW 16 | 0.5 | W | Pow@CPD(Specs) |
| CPDPRG3 | garp | | default CPD Seq. |
| TE | 298.000 | K | default |

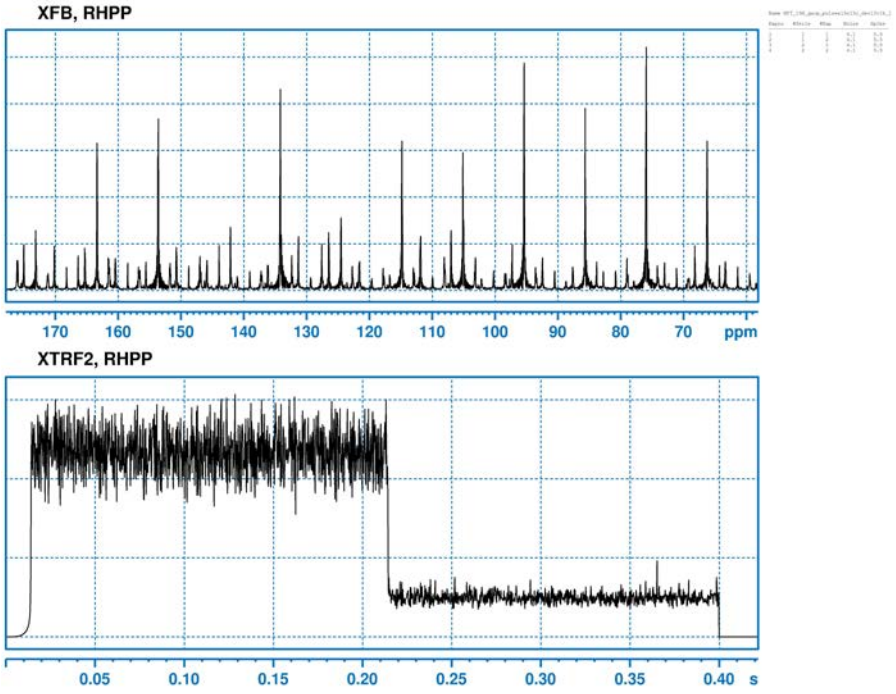
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| BC_mod | 0 | | |
| ME_mod | 0 | | |
| FT_mod | 0 | | |
| F1P | 8.500 | ppm | |
| F2P | 0.500 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 13C | | |
| TD | 256 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 256 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| BC_mod | 0 | | |
| ME_mod | 0 | | |
| FT_mod | 0 | | |

## Experiment Description

Garp series experiment with serial 13C and 15N hard pulses, 15N and 1H decoupling and 13C detection.
The garp series experiment has the following structure [n * (2D Garp Experiment) - (Delay T)] * m
The parameters m, n, and T are set via specifications. If not specified following default values will be used: m=2, n=2, and T=30 min. WRPA is used to copy each acquired experiment into a derived data set. The results for Noise Factor and Spike Ratio are taken from the 2D experiment of the last series with the highest noise factor.
The GARP decoupling test indicates the reliability of the probe with respect to decoupling. No excitation pulse is applied, only decoupling takes place during acquisition of the noise. The acquisition time is splitted up according to the scheme 50%-25%-25% thereby only during the 50% decoupling power is applied. D1 is set to 2.5*AQ, so that the duty cycle is 15%
The first evaluation is done by processing with XFB using the standard Fourier transform features of the TopSpin software. The horizontal positive projection (RHPP) is then evaluated by searching for the minimal and maximal intensity and forming the ratio of the two. Interpreation of the result is only possible in relation to the second evaluation.
A value close to 1.0 is optimal, higher values are worse, values < 1.0 are only meaningful, if the second evaluation results in small values, too.
The second evaluation is done by processing with XTRF2 using parameters as outlined below resulting in time domain data. The horizontal positive projection (RHPP) is then used to determine a 'noise factor' between the average noise of the decoupled and the coupled region. If the ratio is close to 1.0 the decoupling efficiency is optimal.

## 5.2.52 15N detection with 15N and 13C hard pulses and 13C and 1H garp decoupling (NPT_15N_garp_pulses15n13c_dec13c1h)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10033, Z10270, Z10718, Z10121
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top spectrum shows 2D projection (XFB, RHPP).
Bottom spectrum shows 2D projection (XTRF2, RHPP).
Both projections are from the 2D experiment of the last series with the highest noise factor.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 15N | | |
| NUC2 | 13C | | |
| NUC3 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_garptest | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| TD0 | 1 | | |
| SW | 119.714 | ppm | |
| TD | 3882 | | |
| AQ | 0.400 | s | |
| FIDRES | 2.501 | Hz | field dependent |
| D 1 | 1.000 | s | 2.5*AQ |
| P 2 | 50.0 | us | 180deg NUC3 |
| PLW 1 | 155.5 | W | Pow@CPD(Specs) |
| P 4 | 24.0 | us | 180deg NUC2 |
| PLW 2 | 86.0 | W | Pow@90deg(Specs) NUC2 |
| PCPD 2 | 65.0 | us | CPD 90deg |
| PLW 12 | 3.3 | W | Pow@CPD(Specs) |
| CPDPRG2 | garp | | default CPD Seq. |
| PCPD 3 | 80.0 | us | CPD 90deg |
| PLW 16 | 0.5 | W | Pow@CPD(Specs) |
| CPDPRG3 | garp | | default CPD Seq. |
| TE | 298.000 | K | default |

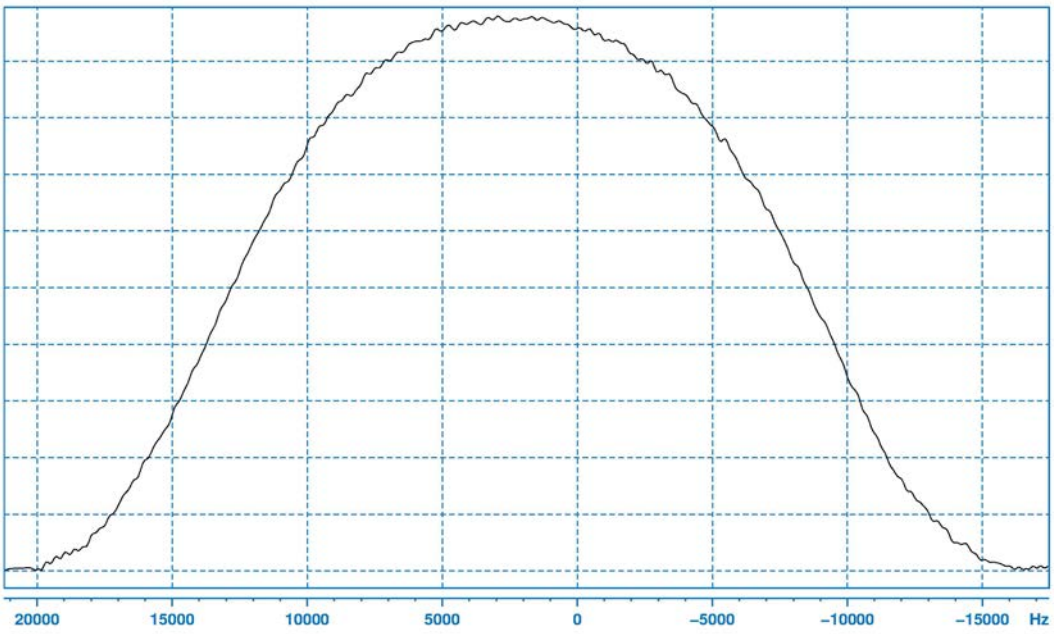
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| BC_mod | 0 | | |
| ME_mod | 0 | | |
| FT_mod | 0 | | |
| F1P | 8.500 | ppm | |
| F2P | 0.500 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 13C | | |
| TD | 256 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 256 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| BC_mod | 0 | | |
| ME_mod | 0 | | |
| FT_mod | 0 | | |

## Experiment Description

Garp series experiment with serial 15N and 13C hard pulses, 13C and 1H decoupling and 15N detection.
The garp series experiment has the following structure [n * (2D Garp Experiment) - (Delay T)] * m
The parameters m, n, and T are set via specifications. If not specified following default values will be used: m=2, n=2, and T=30 min. WRPA is used to copy each acquired experiment into a derived data set. The results for Noise Factor and Spike Ratio are taken from the 2D experiment of the last series with the highest noise factor.
The GARP decoupling test indicates the reliability of the probe with respect to decoupling. No excitation pulse is applied, only decoupling takes place during acquisition of the noise. The acquisition time is splitted up according to the scheme 50%-25%-25% thereby only during the 50% decoupling power is applied. D1 is set to 2.5*AQ, so that the duty cycle is 15%
The first evaluation is done by processing with XFB using the standard Fourier transform features of the TopSpin software. The horizontal positive projection (RHPP) is then evaluated by searching for the minimal and maximal intensity and forming the ratio of the two. Interpreation of the result is only possible in relation to the second evaluation.
A value close to 1.0 is optimal, higher values are worse, values < 1.0 are only meaningful, if the second evaluation results in small values, too.
The second evaluation is done by processing with XTRF2 using parameters as outlined below resulting in time domain data. The horizontal positive projection (RHPP) is then used to determine a 'noise factor' between the average noise of the decoupled and the coupled region. If the ratio is close to 1.0 the decoupling efficiency is optimal.

### 5.2.53 1H Z-gradient profile [-] (NPT_1H_gradientprofile_neg)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719, Z142222
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Proton Z-gradient profile.

**Control Option for Acquisition (L23)**

1 default
2 skip gradient functionality check during processing

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 81967.211 | Hz | |
| TD | 1024 | | |
| AQ | 0.006 | s | |
| FIDRES | 160.092 | Hz | |
| D 1 | 0.500 | s | |
| D 15 | 0.005 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 2.0 | us | Cryo=1deg, RT=5deg |
| PLW 0 | | W | adjusted power |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | gauss | | |
| GPNAM2 | gauss | | |
| GPZ 1 | -4.843 | % | |
| GPZ 2 | 6.053 | % | |
| TE | 298.000 | K | default |

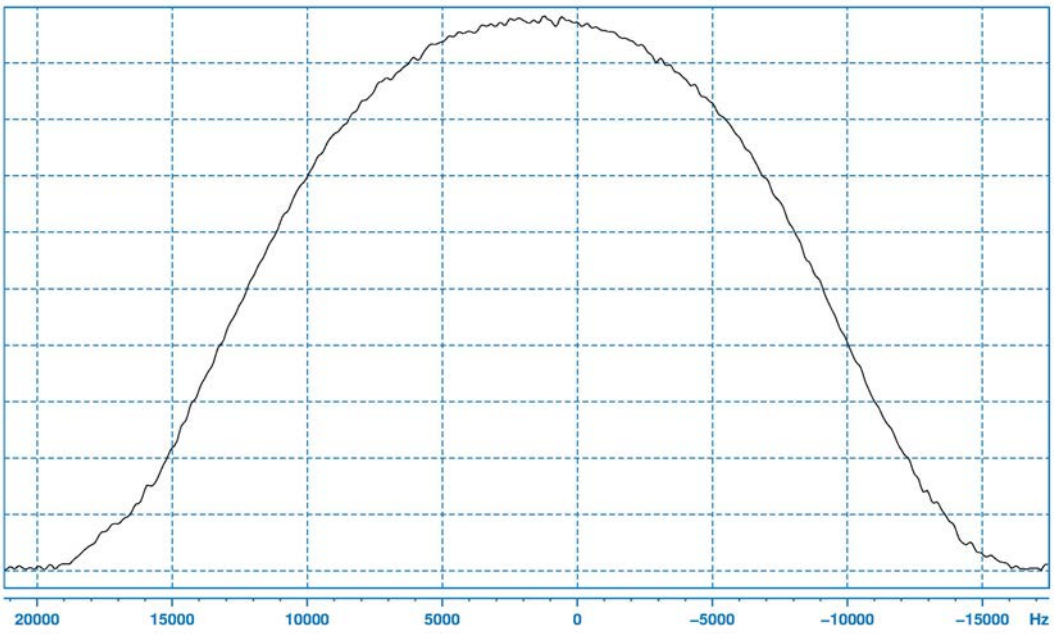
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 54.559 | ppm | |
| F2P | -45.159 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 1.000 | G/cm*A | gradient strength |
| CNST 37 | 19.400 | mm | active sample size |

## Experiment Description

Z-gradient profile is acquired with negative gradient in order to check the basic functionality of gradient. GPZ 2 is calculated to obtain a profilewidth of 25000 Hz.
The profile width is determined at 50% (HR) and 15% (HRMAS) of the maximum profile intensity respectively.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

### 5.2.54 1H Z-gradient profile [+] (NPT_1H_gradientprofile_pos)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719, Z142222
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Proton Z-gradient profile.

**Control Option for Acquisition (L23)**

1 default
2 skip gradient functionality check during processing

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 81967.211 | Hz | |
| TD | 1024 | | |
| AQ | 0.006 | s | |
| FIDRES | 160.092 | Hz | |
| D 1 | 0.500 | s | |
| D 15 | 0.005 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 2.0 | us | Cryo=1deg, RT=5deg |
| PLW 0 | | W | adjusted power |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | gauss | | |
| GPNAM2 | gauss | | |
| GPZ 1 | 4.843 | % | |
| GPZ 2 | -6.053 | % | |
| TE | 298.000 | K | default |

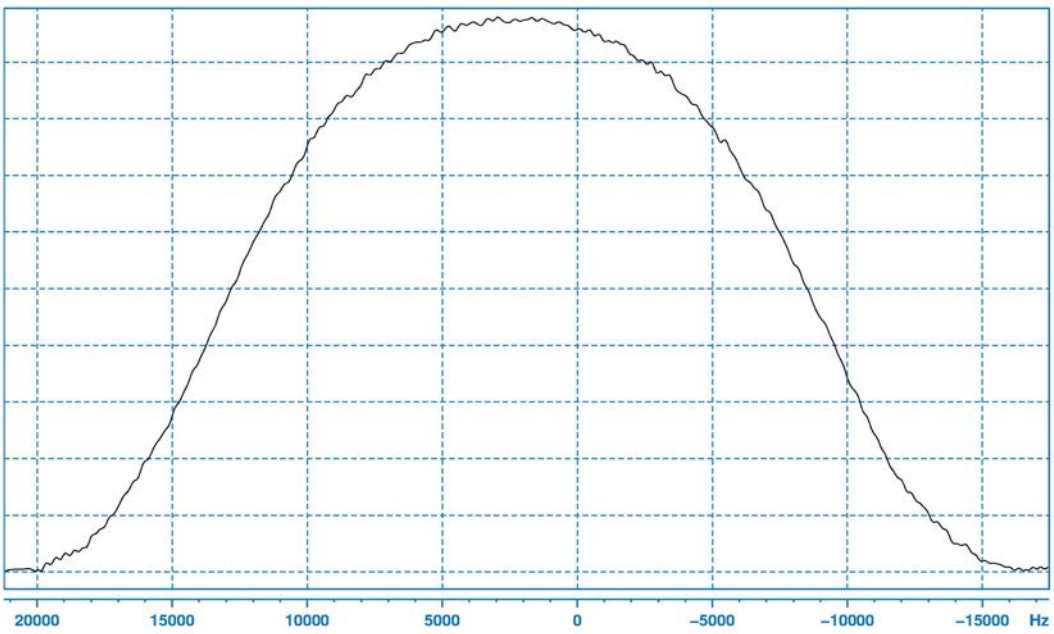
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 54.559 | ppm | |
| F2P | -45.159 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 1.000 | G/cm*A | gradient strength |
| CNST 37 | 19.400 | mm | active sample size |

## Experiment Description

Z-gradient profile is acquired with positive gradient in order to check the basic functionality of gradient.
GPZ 2 is calculated to obtain a profilewidth of 25000 Hz.
The profile width is determined at 50% (HR) and 15% (HRMAS) of the maximum profile intensity respectively.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

### 5.2.55 1H X-gradient profile [-] (NPT_1H_gradprofX_neg)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**
Proton X-gradient profile.

**Control Option for Acquisition (L23)**
1 default
2 skip gradient functionality check during processing

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 81967.211 | Hz | |
| TD | 1024 | | |
| AQ | 0.006 | s | |
| FIDRES | 160.092 | Hz | |
| D 1 | 0.500 | s | |
| D 15 | 0.005 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 2.0 | us | Cryo=1deg, RT=5deg |
| PLW 0 | | W | adjusted power |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | gauss | | |
| GPNAM2 | gauss | | |
| GPX 1 | -0.000 | % | |
| GPX 2 | 0.000 | % | |
| TE | 298.000 | K | default |

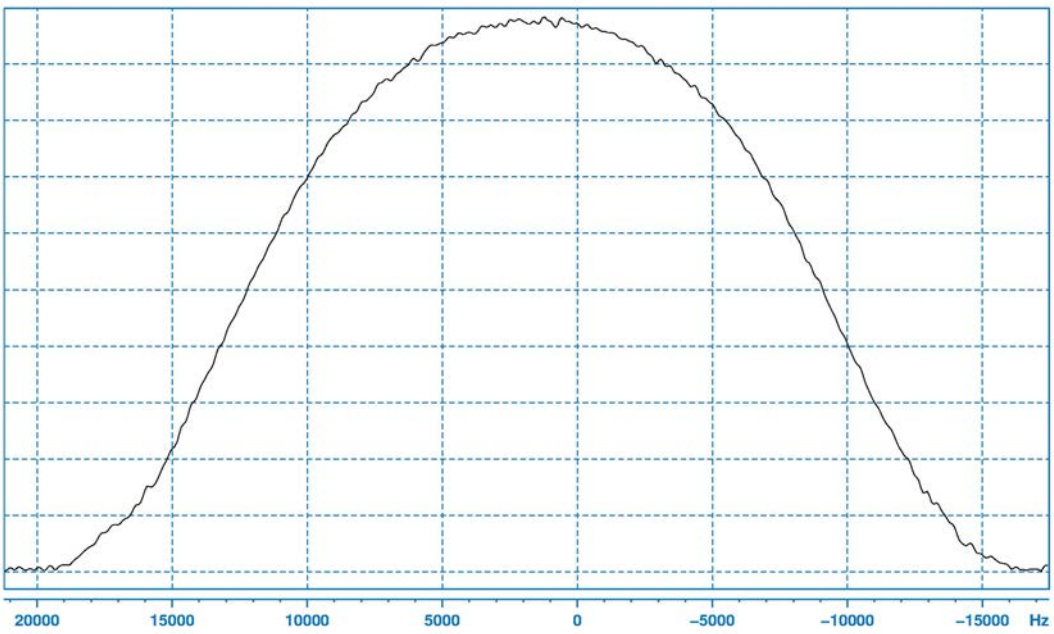
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 54.559 | ppm | |
| F2P | -45.159 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 1.000 | G/cm*A | gradient strength |
| CNST 37 | 4.240 | mm | active sample size |

## Experiment Description

X-gradient profile is acquired with negative gradient in order to check the basic functionality of gradient. GPX 2 is calculated to obtain a profilewidth of 25000 Hz.
The profile width is determined at 15% of the maximum profile intensity.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

### 5.2.56 1H X-gradient profile [+] (NPT_1H_gradprofX_pos)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**
Proton X-gradient profile.

**Control Option for Acquisition (L23)**
1 default
2 skip gradient functionality check during processing

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 81967.211 | Hz | |
| TD | 1024 | | |
| AQ | 0.006 | s | |
| FIDRES | 160.092 | Hz | |
| D 1 | 0.500 | s | |
| D 15 | 0.005 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 2.0 | us | Cryo=1deg, RT=5deg |
| PLW 0 | | W | adjusted power |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | gauss | | |
| GPNAM2 | gauss | | |
| GPX 1 | 0.000 | % | |
| GPX 2 | -0.000 | % | |
| TE | 298.000 | K | default |

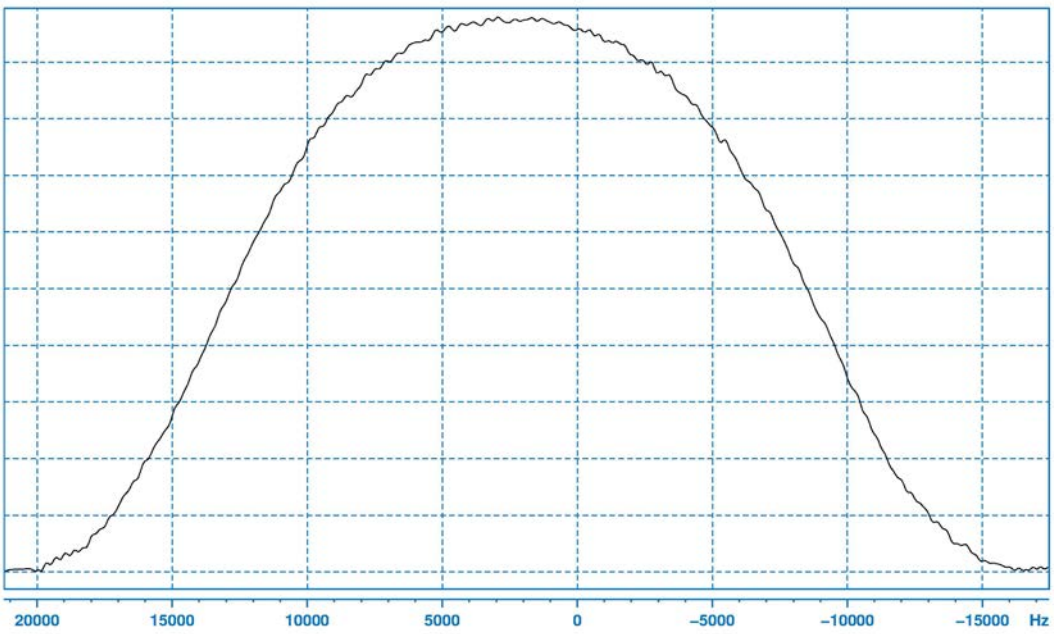
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 54.559 | ppm | |
| F2P | -45.159 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 1.000 | G/cm*A | gradient strength |
| CNST 37 | 4.240 | mm | active sample size |

## Experiment Description

X-gradient profile is acquired with positive gradient in order to check the basic functionality of gradient.
GPX 2 is calculated to obtain a profilewidth of 25000 Hz.
The profile width is determined at 15% of the maximum profile intensity.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

### 5.2.57 1H Y-gradient profile [-] (NPT_1H_gradprofY_neg)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**
Proton Y-gradient profile.

**Control Option for Acquisition (L23)**
1 default
2 skip gradient functionality check during processing

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 81967.211 | Hz | |
| TD | 1024 | | |
| AQ | 0.006 | s | |
| FIDRES | 160.092 | Hz | |
| D 1 | 0.500 | s | |
| D 15 | 0.005 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 2.0 | us | Cryo=1deg, RT=5deg |
| PLW 0 | | W | adjusted power |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | gauss | | |
| GPNAM2 | gauss | | |
| GPY 1 | -0.000 | % | |
| GPY 2 | 0.000 | % | |
| TE | 298.000 | K | default |

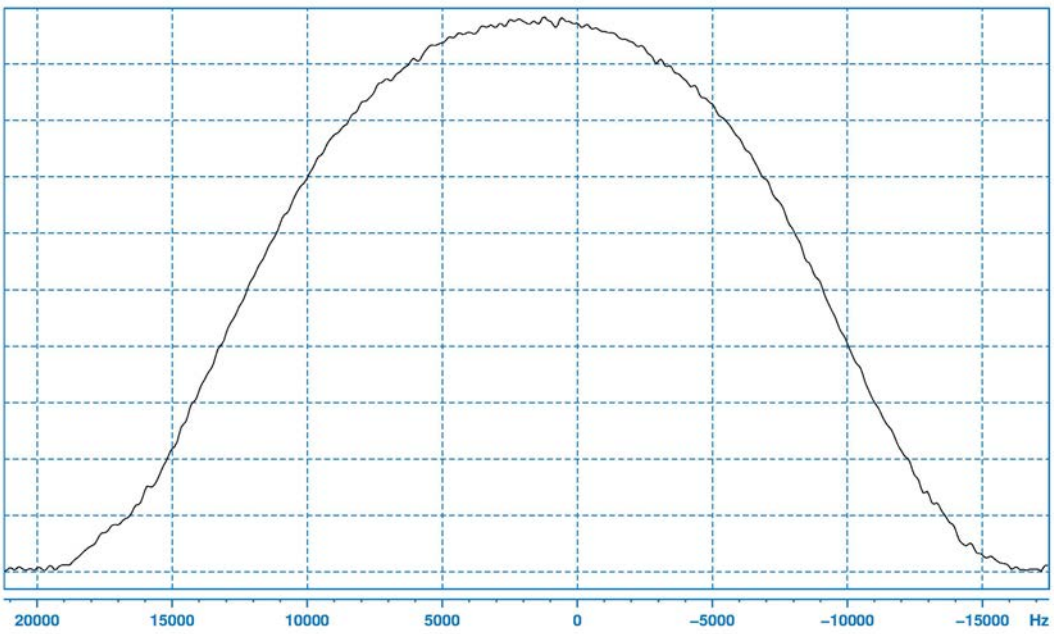
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 54.559 | ppm | |
| F2P | -45.159 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 1.000 | G/cm*A | gradient strength |
| CNST 37 | 4.240 | mm | active sample size |

## Experiment Description

Y-gradient profile is acquired with negative gradient in order to check the basic functionality of gradient. GPY 2 is calculated to obtain a profilewidth of 25000 Hz.
The profile width is determined at 15% of the maximum profile intensity.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

### 5.2.58 1H Y-gradient profile [+] (NPT_1H_gradprofY_pos)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**
Proton Y-gradient profile.

**Control Option for Acquisition (L23)**
1 default
2 skip gradient functionality check during processing

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 81967.211 | Hz | |
| TD | 1024 | | |
| AQ | 0.006 | s | |
| FIDRES | 160.092 | Hz | |
| D 1 | 0.500 | s | |
| D 15 | 0.005 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 2.0 | us | Cryo=1deg, RT=5deg |
| PLW 0 | | W | adjusted power |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | gauss | | |
| GPNAM2 | gauss | | |
| GPY 1 | 0.000 | % | |
| GPY 2 | -0.000 | % | |
| TE | 298.000 | K | default |

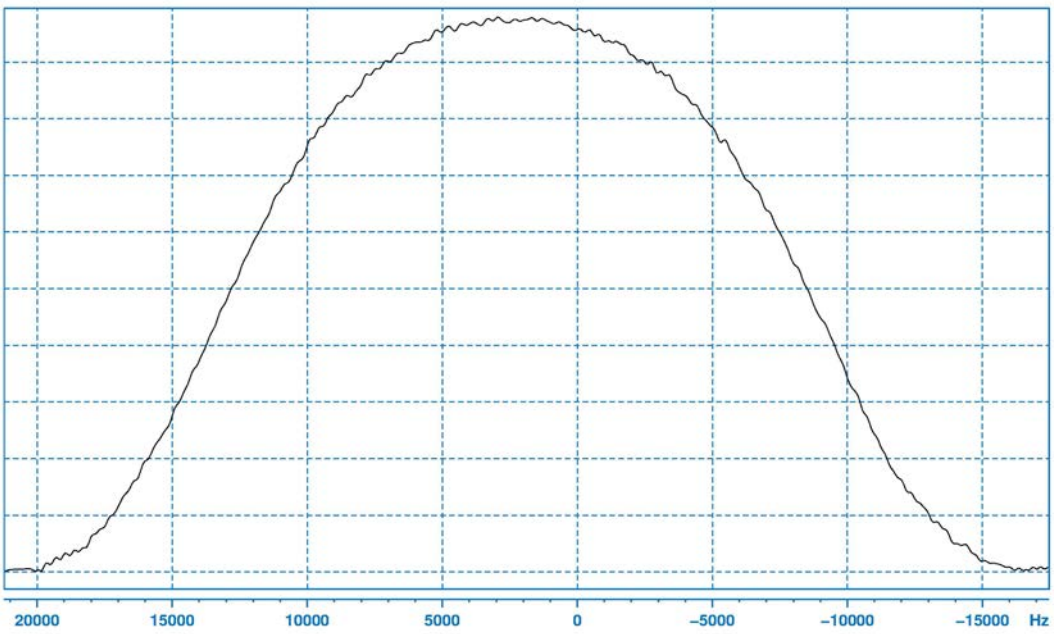
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 54.559 | ppm | |
| F2P | -45.159 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 1.000 | G/cm*A | gradient strength |
| CNST 37 | 4.240 | mm | active sample size |

## Experiment Description

Y-gradient profile is acquired with positive gradient in order to check the basic functionality of gradient.
GPY 2 is calculated to obtain a profilewidth of 25000 Hz.
The profile width is determined at 15% of the maximum profile intensity.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

### 5.2.59 1H Z-gradient profile [-] (NPT_1H_gradprofZ_neg)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Proton Z-gradient profile.

**Control Option for Acquisition (L23)**
1 default
2 skip gradient functionality check during processing

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 81967.211 | Hz | |
| TD | 1024 | | |
| AQ | 0.006 | s | |
| FIDRES | 160.092 | Hz | |
| D 1 | 0.500 | s | |
| D 15 | 0.005 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 2.0 | us | Cryo=1deg, RT=5deg |
| PLW 0 | | W | adjusted power |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | gauss | | |
| GPNAM2 | gauss | | |
| GPZ 1 | -4.843 | % | |
| GPZ 2 | 6.053 | % | |
| TE | 298.000 | K | default |

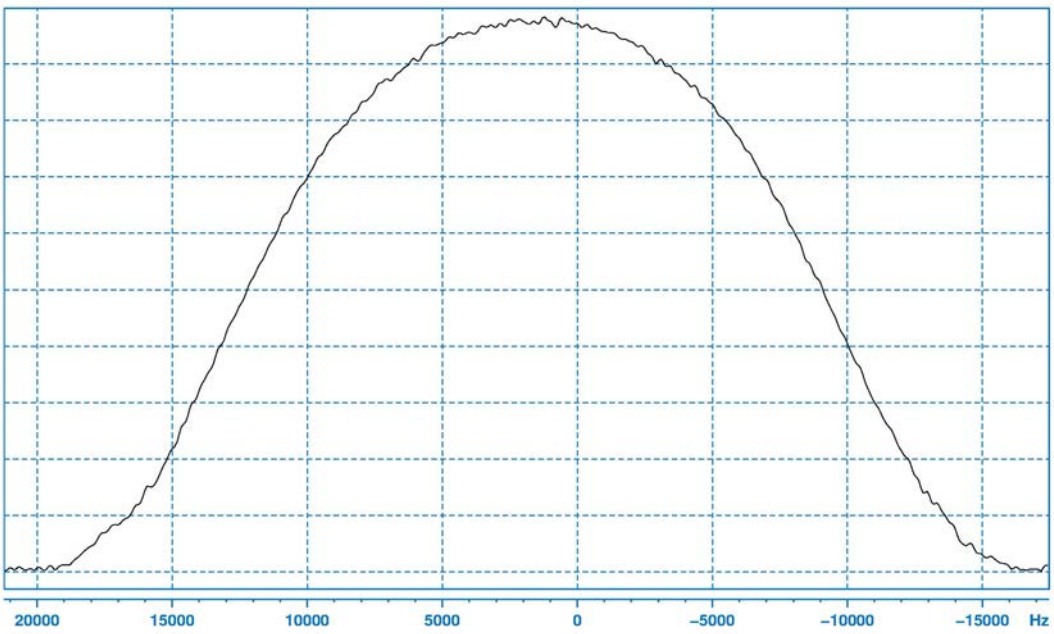
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 54.559 | ppm | |
| F2P | -45.159 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 1.000 | G/cm*A | gradient strength |
| CNST 37 | 19.400 | mm | active sample size |

## Experiment Description

Z-gradient profile is acquired with negative gradient in order to check the basic functionality of gradient. GPZ 2 is calculated to obtain a profilewidth of 25000 Hz.
The profile width is determined at 50% (HR) and 15% (HRMAS) of the maximum profile intensity respectively.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

### 5.2.60 1H Z-gradient profile [+] (NPT_1H_gradprofZ_pos)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Proton Z-gradient profile.

**Control Option for Acquisition (L23)**
1 default
2 skip gradient functionality check during processing

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 81967.211 | Hz | |
| TD | 1024 | | |
| AQ | 0.006 | s | |
| FIDRES | 160.092 | Hz | |
| D 1 | 0.500 | s | |
| D 15 | 0.005 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 2.0 | us | Cryo=1deg, RT=5deg |
| PLW 0 | | W | adjusted power |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | gauss | | |
| GPNAM2 | gauss | | |
| GPZ 1 | 4.843 | % | |
| GPZ 2 | -6.053 | % | |
| TE | 298.000 | K | default |

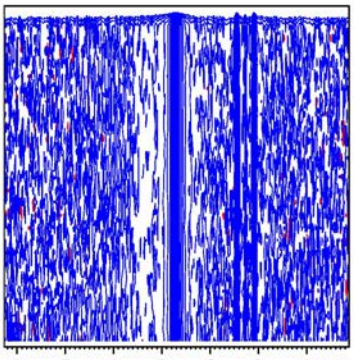
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 54.559 | ppm | |
| F2P | -45.159 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 1.000 | G/cm*A | gradient strength |
| CNST 37 | 19.400 | mm | active sample size |

## Experiment Description

Z-gradient profile is acquired with positive gradient in order to check the basic functionality of gradient.
GPZ 2 is calculated to obtain a profilewidth of 25000 Hz.
The profile width is determined at 50% (HR) and 15% (HRMAS) of the maximum profile intensity respectively.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

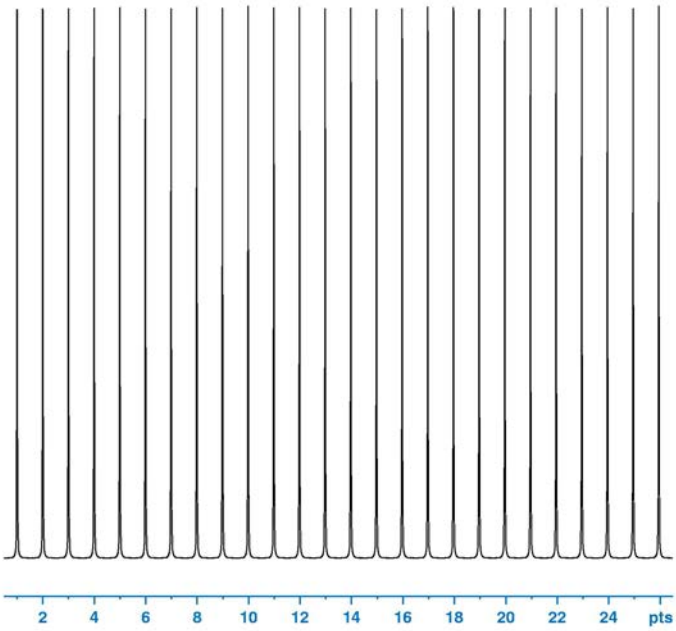
## 5.2.61 Gradient recovery stability test (NPT_1H_gradrec_stest_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727, Z142231
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[dl6] | Scal.Int.[#26] | BO-Shift[Hz] | +APK0[APK #26] |
|---|---|---|---|---|
| 1 | 10.00 us | 99.86 | 4.56 | 1.0 |
| 2 | 15.85 us | 99.89 | 4.39 | 0.0 |
| 3 | 25.12 us | 99.87 | 4.22 | 0.0 |
| 4 | 39.81 us | 99.86 | 4.01 | 0.0 |
| 5 | 63.10 us | 99.90 | 3.84 | 1.0 |
| 6 | 100.0 us | 99.87 | 3.63 | 1.0 |
| 7 | 158.5 us | 99.87 | 3.46 | 0.5 |
| 8 | 251.2 us | 99.91 | 3.30 | 1.0 |
| 9 | 398.1 us | 99.85 | 3.09 | 1.0 |
| 10 | 630.9 us | 99.94 | 2.96 | 1.0 |
| 11 | 1.000 ms | 99.86 | 2.71 | 1.0 |
| 12 | 1.585 ms | 99.91 | 2.58 | 0.0 |
| 13 | 2.512 ms | 99.91 | 2.37 | 0.0 |
| 14 | 3.981 ms | 99.92 | 2.20 | 0.0 |
| 15 | 6.310 ms | 99.87 | 1.99 | 0.0 |
| 16 | 10.00 ms | 99.88 | 1.82 | 0.5 |
| 17 | 15.85 ms | 99.92 | 1.61 | -0.5 |
| 18 | 25.12 ms | 99.93 | 1.48 | 0.0 |
| 19 | 39.81 ms | 99.87 | 1.27 | 0.0 |
| 20 | 63.10 ms | 99.93 | 1.10 | 0.0 |
| 21 | 0.100 s | 99.92 | 0.89 | 0.5 |
| 22 | 0.158 s | 99.95 | 0.72 | 0.5 |
| 23 | 0.251 s | 99.96 | 0.51 | 0.0 |
| 24 | 0.398 s | 99.89 | 0.34 | 0.5 |
| 25 | 0.631 s | 99.95 | 0.13 | 1.0 |
| 26 | 1.000 s | 100.00 | 0.00 | 0.0 |




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the residual water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrec | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPZ 1 | 0.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

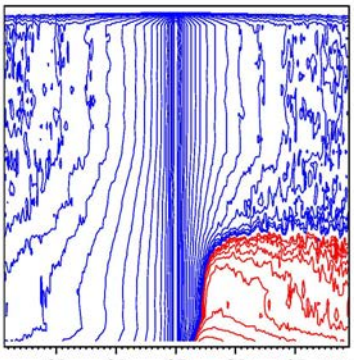
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 26 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

## Experiment Description

Purpose of this experiment is the measurement of the basic instrument stability under the same conditions as used for the gradient recovery test. The experiment is normally executed just prior or after the series of gradient experiments.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

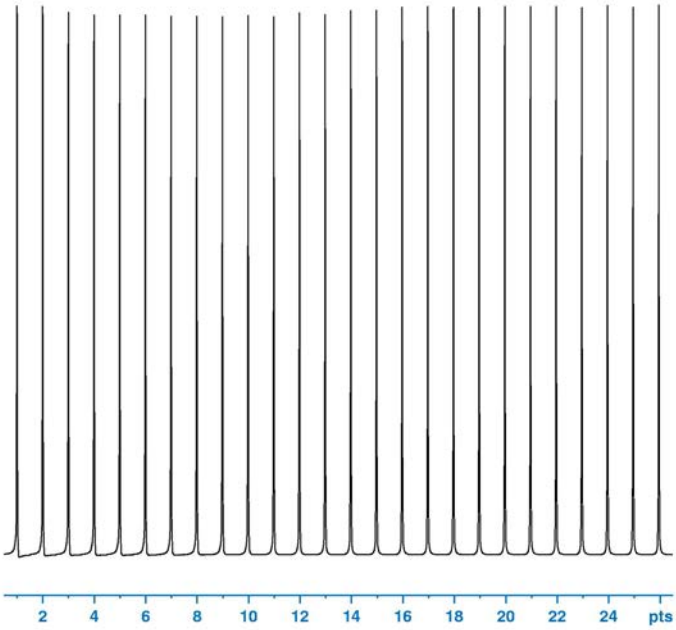
## 5.2.62 Gradient recovery test for X-direction [-] (NPT_1H_gradrecX_sqn_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[dl6] | Scal.Int.[#26] | BO-Shift[Hz] | +APK0[APK #26] |
|---|---|---|---|---|
| 1 | 10.00 us | 99.30 | 4.68 | 4.0 |
| 2 | 15.85 us | 99.17 | 4.51 | 2.5 |
| 3 | 25.12 us | 98.28 | 4.30 | 2.0 |
| 4 | 39.81 us | 97.73 | 4.13 | 2.0 |
| 5 | 63.10 us | 97.76 | 3.92 | 2.0 |
| 6 | 100.0 us | 97.70 | 3.75 | 1.5 |
| 7 | 158.5 us | 97.62 | 3.54 | 1.5 |
| 8 | 251.2 us | 97.66 | 3.38 | 1.0 |
| 9 | 398.1 us | 97.64 | 3.17 | 0.5 |
| 10 | 630.9 us | 97.85 | 3.00 | 0.0 |
| 11 | 1.000 ms | 97.93 | 2.79 | 0.0 |
| 12 | 1.585 ms | 98.29 | 2.62 | -0.5 |
| 13 | 2.512 ms | 98.60 | 2.41 | 1.0 |
| 14 | 3.981 ms | 98.78 | 2.24 | 0.0 |
| 15 | 6.310 ms | 99.18 | 2.03 | 0.0 |
| 16 | 10.00 ms | 99.56 | 1.86 | 0.5 |
| 17 | 15.85 ms | 99.75 | 1.65 | -0.5 |
| 18 | 25.12 ms | 99.77 | 1.48 | 0.0 |
| 19 | 39.81 ms | 99.85 | 1.31 | -0.5 |
| 20 | 63.10 ms | 99.82 | 1.10 | -0.5 |
| 21 | 0.100 s | 99.95 | 0.93 | 0.5 |
| 22 | 0.158 s | 99.92 | 0.72 | -0.5 |
| 23 | 0.251 s | 99.90 | 0.55 | 0.0 |
| 24 | 0.398 s | 99.97 | 0.38 | 0.0 |
| 25 | 0.631 s | 99.96 | 0.21 | 0.0 |
| 26 | 1.000 s | 100.00 | 0.00 | 0.0 |




### Example Printout

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

### Control Option for Acquisition (L23)

1 default
10 skip sino check and gradient amplifier functioning test

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrec | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPX 1 | -75.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 26 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

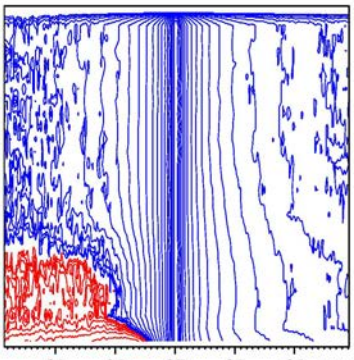
## Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of range one, needs to be specified.

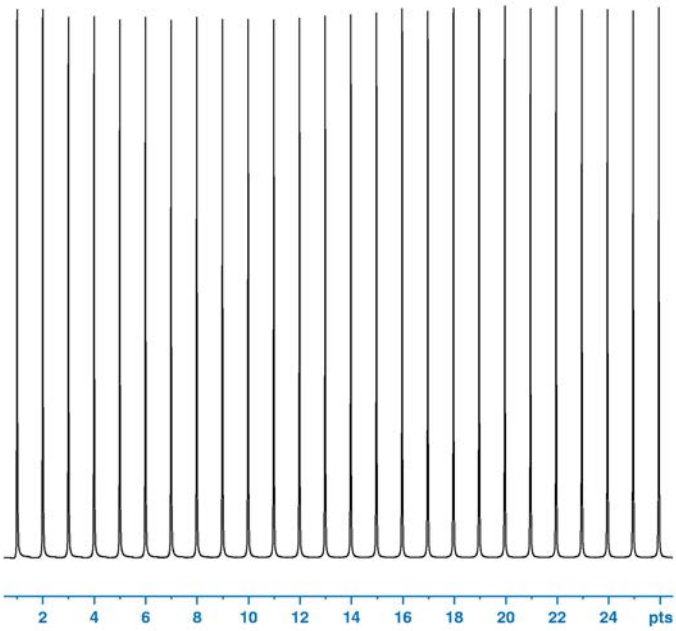
## 5.2.63 Gradient recovery test for X-direction [+] (NPT_1H_gradrecX_sqp_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[dl6] | Scal.Int.[#26] | BO-Shift[Hz] | *APK0[APK #26] |
|---|---|---|---|---|
| 1 | 10.00 us | 99.46 | 4.60 | -3.5 |
| 2 | 15.85 us | 99.62 | 4.43 | -2.0 |
| 3 | 25.12 us | 98.61 | 4.26 | -1.0 |
| 4 | 39.81 us | 98.34 | 4.05 | -1.5 |
| 5 | 63.10 us | 98.31 | 3.92 | -2.0 |
| 6 | 100.0 us | 98.24 | 3.71 | -1.5 |
| 7 | 158.5 us | 98.16 | 3.54 | -1.5 |
| 8 | 251.2 us | 98.10 | 3.34 | -1.5 |
| 9 | 398.1 us | 98.16 | 3.31 | -1.0 |
| 10 | 630.9 us | 98.04 | 2.96 | -0.5 |
| 11 | 1.000 ms | 98.25 | 2.79 | 0.0 |
| 12 | 1.585 ms | 98.46 | 2.62 | -0.5 |
| 13 | 2.512 ms | 98.70 | 2.41 | -0.5 |
| 14 | 3.981 ms | 99.04 | 2.24 | -0.5 |
| 15 | 6.310 ms | 99.38 | 2.07 | -0.5 |
| 16 | 10.00 ms | 99.72 | 1.86 | 0.0 |
| 17 | 15.85 ms | 99.83 | 1.69 | -0.5 |
| 18 | 25.12 ms | 99.93 | 1.48 | -0.5 |
| 19 | 39.81 ms | 99.93 | 1.35 | -0.5 |
| 20 | 63.10 ms | 99.99 | 1.10 | -0.5 |
| 21 | 0.100 s | 99.97 | 1.01 | -0.5 |
| 22 | 0.158 s | 100.00 | 0.76 | 0.0 |
| 23 | 0.251 s | 99.92 | 0.59 | 0.0 |
| 24 | 0.398 s | 99.95 | 0.42 | -0.5 |
| 25 | 0.631 s | 99.98 | 0.25 | 0.0 |
| 26 | 1.000 s | 100.00 | 0.00 | 0.0 |




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

**Control Option for Acquisition (L23)**

1 default
10 skip sino check and gradient amplifier functioning test

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrec | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPX 1 | 75.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 26 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

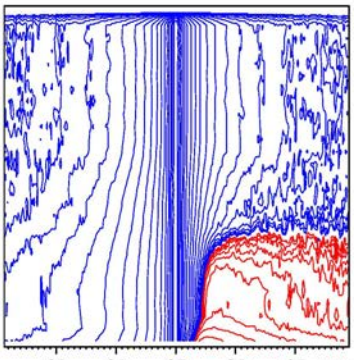
### Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of range one, needs to be specified.

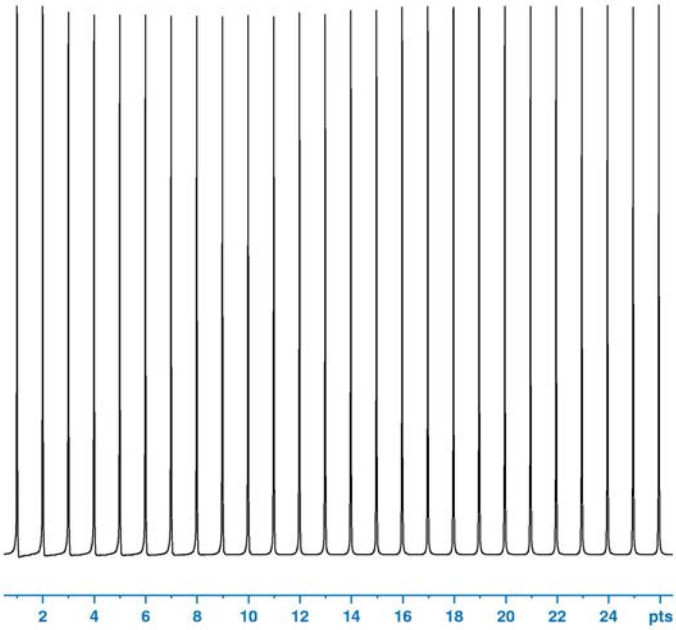
## 5.2.64 Gradient recovery test for Y-direction [-] (NPT_1H_gradrecY_sqn_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[dl6] | Scal.Int.[#26] | BO-Shift[Hz] | +APK0[APK #26] |
|---|---|---|---|---|
| 1 | 10.00 us | 99.30 | 4.68 | 4.0 |
| 2 | 15.85 us | 99.17 | 4.51 | 2.5 |
| 3 | 25.12 us | 98.28 | 4.30 | 2.0 |
| 4 | 39.81 us | 97.73 | 4.13 | 2.0 |
| 5 | 63.10 us | 97.76 | 3.92 | 2.0 |
| 6 | 100.0 us | 97.70 | 3.75 | 1.5 |
| 7 | 158.5 us | 97.62 | 3.54 | 1.5 |
| 8 | 251.2 us | 97.66 | 3.38 | 1.0 |
| 9 | 398.1 us | 97.64 | 3.17 | 0.5 |
| 10 | 630.9 us | 97.85 | 3.00 | 0.0 |
| 11 | 1.000 ms | 97.93 | 2.79 | 0.0 |
| 12 | 1.585 ms | 98.29 | 2.62 | -0.5 |
| 13 | 2.512 ms | 98.60 | 2.41 | 1.0 |
| 14 | 3.981 ms | 98.78 | 2.24 | 0.0 |
| 15 | 6.310 ms | 99.18 | 2.03 | 0.0 |
| 16 | 10.00 ms | 99.56 | 1.86 | 0.5 |
| 17 | 15.85 ms | 99.75 | 1.65 | -0.5 |
| 18 | 25.12 ms | 99.77 | 1.48 | 0.0 |
| 19 | 39.81 ms | 99.85 | 1.31 | -0.5 |
| 20 | 63.10 ms | 99.82 | 1.10 | -0.5 |
| 21 | 0.100 s | 99.95 | 0.93 | 0.5 |
| 22 | 0.158 s | 99.92 | 0.72 | -0.5 |
| 23 | 0.251 s | 99.90 | 0.55 | 0.0 |
| 24 | 0.398 s | 99.97 | 0.38 | 0.0 |
| 25 | 0.631 s | 99.96 | 0.21 | 0.0 |
| 26 | 1.000 s | 100.00 | 0.00 | 0.0 |




### Example Printout

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

### Control Option for Acquisition (L23)

1 default
10 skip sino check and gradient amplifier functioning test

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrec | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPY 1 | -75.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 26 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

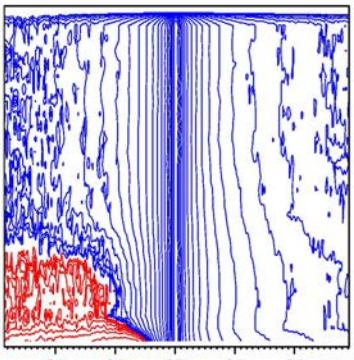
## Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of range one, needs to be specified.

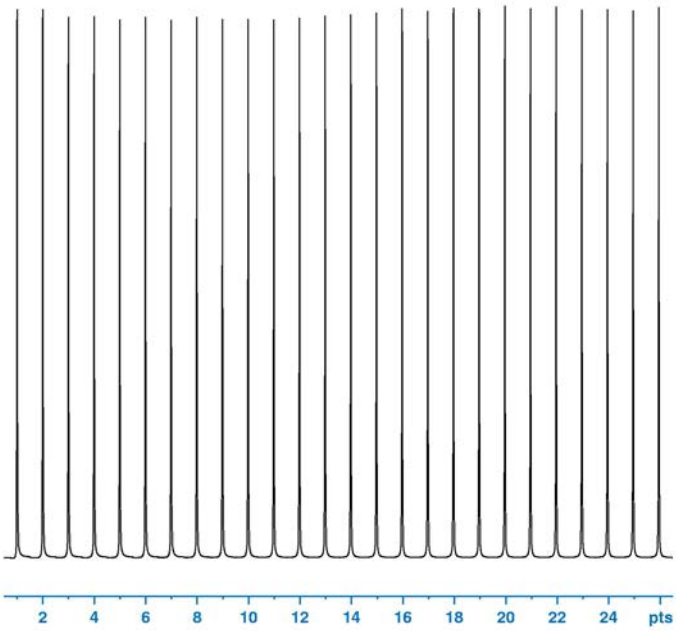
## 5.2.65 Gradient recovery test for Y-direction [+] (NPT_1H_gradrecY_sqp_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[dl6] | Scal.Int.[#26] | BO-Shift[Hz] | *APK0[APK #26] |
|---|---|---|---|---|
| 1 | 10.00 us | 99.46 | 4.60 | -3.5 |
| 2 | 15.85 us | 99.62 | 4.43 | -2.0 |
| 3 | 25.12 us | 98.61 | 4.26 | -1.0 |
| 4 | 39.81 us | 98.34 | 4.05 | -1.5 |
| 5 | 63.10 us | 98.31 | 3.92 | -2.0 |
| 6 | 100.0 us | 98.24 | 3.71 | -1.5 |
| 7 | 158.5 us | 98.16 | 3.54 | -1.5 |
| 8 | 251.2 us | 98.10 | 3.34 | -1.5 |
| 9 | 398.1 us | 98.16 | 3.31 | -1.0 |
| 10 | 630.9 us | 98.04 | 2.96 | -0.5 |
| 11 | 1.000 ms | 98.25 | 2.79 | 0.0 |
| 12 | 1.585 ms | 98.46 | 2.62 | -0.5 |
| 13 | 2.512 ms | 98.70 | 2.41 | -0.5 |
| 14 | 3.981 ms | 99.04 | 2.24 | -0.5 |
| 15 | 6.310 ms | 99.38 | 2.07 | -0.5 |
| 16 | 10.00 ms | 99.72 | 1.86 | 0.0 |
| 17 | 15.85 ms | 99.83 | 1.69 | -0.5 |
| 18 | 25.12 ms | 99.93 | 1.48 | -0.5 |
| 19 | 39.81 ms | 99.93 | 1.35 | -0.5 |
| 20 | 63.10 ms | 99.99 | 1.10 | -0.5 |
| 21 | 0.100 s | 99.97 | 1.01 | -0.5 |
| 22 | 0.158 s | 100.00 | 0.76 | 0.0 |
| 23 | 0.251 s | 99.92 | 0.59 | 0.0 |
| 24 | 0.398 s | 99.95 | 0.42 | -0.5 |
| 25 | 0.631 s | 99.98 | 0.25 | 0.0 |
| 26 | 1.000 s | 100.00 | 0.00 | 0.0 |




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

**Control Option for Acquisition (L23)**

1 default
10 skip sino check and gradient amplifier functioning test

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrec | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPY 1 | 75.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 26 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

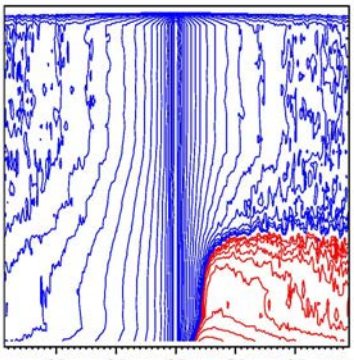
## Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of range one, needs to be specified.

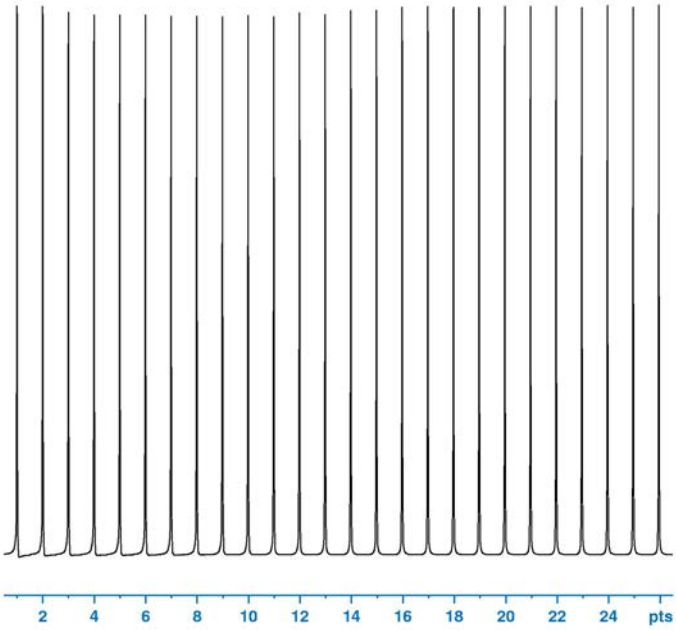
## 5.2.66 Gradient recovery test for Z-direction [-] (NPT_1H_gradrecZ_sqn_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727, Z142231
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[dl6] | Scal.Int.[#26] | BO-Shift[Hz] | +APK0[APK #26] |
|---|---|---|---|---|
| 1 | 10.00 us | 99.30 | 4.68 | 4.0 |
| 2 | 15.85 us | 99.17 | 4.51 | 2.5 |
| 3 | 25.12 us | 98.28 | 4.30 | 2.0 |
| 4 | 39.81 us | 97.73 | 4.13 | 2.0 |
| 5 | 63.10 us | 97.76 | 3.92 | 2.0 |
| 6 | 100.0 us | 97.70 | 3.75 | 1.5 |
| 7 | 158.5 us | 97.62 | 3.54 | 1.5 |
| 8 | 251.2 us | 97.66 | 3.38 | 1.0 |
| 9 | 398.1 us | 97.64 | 3.17 | 0.5 |
| 10 | 630.9 us | 97.85 | 3.00 | 0.0 |
| 11 | 1.000 ms | 97.93 | 2.79 | 0.0 |
| 12 | 1.585 ms | 98.29 | 2.62 | -0.5 |
| 13 | 2.512 ms | 98.60 | 2.41 | 1.0 |
| 14 | 3.981 ms | 98.78 | 2.24 | 0.0 |
| 15 | 6.310 ms | 99.18 | 2.03 | 0.0 |
| 16 | 10.00 ms | 99.56 | 1.86 | 0.5 |
| 17 | 15.85 ms | 99.75 | 1.65 | -0.5 |
| 18 | 25.12 ms | 99.77 | 1.48 | 0.0 |
| 19 | 39.81 ms | 99.85 | 1.31 | -0.5 |
| 20 | 63.10 ms | 99.82 | 1.10 | -0.5 |
| 21 | 0.100 s | 99.95 | 0.93 | 0.5 |
| 22 | 0.158 s | 99.92 | 0.72 | -0.5 |
| 23 | 0.251 s | 99.90 | 0.55 | 0.0 |
| 24 | 0.398 s | 99.97 | 0.38 | 0.0 |
| 25 | 0.631 s | 99.96 | 0.21 | 0.0 |
| 26 | 1.000 s | 100.00 | 0.00 | 0.0 |




### Example Printout

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

### Control Option for Acquisition (L23)

1 default
10 skip sino check and gradient amplifier functioning test

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrec | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPZ 1 | -75.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 26 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

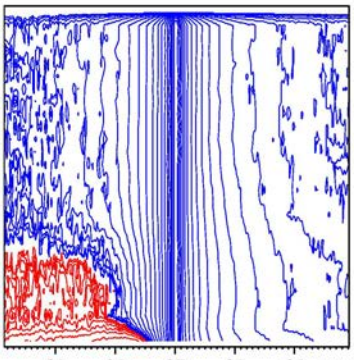
## Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of range one, needs to be specified.

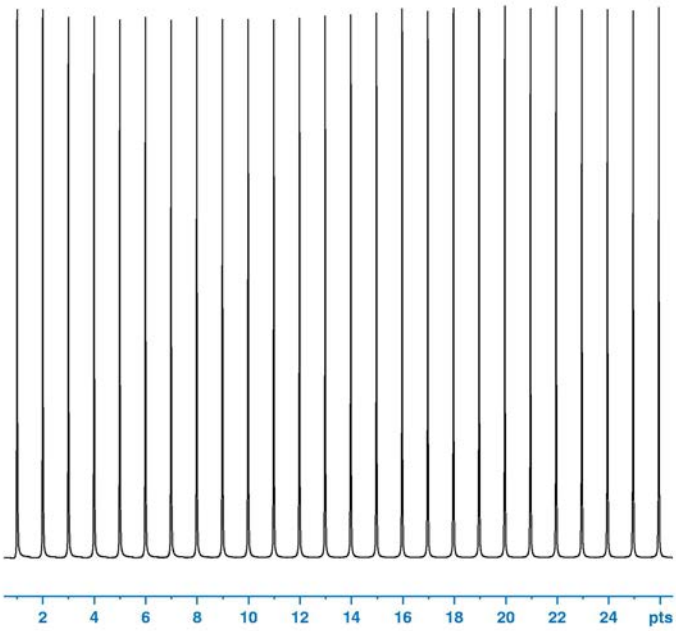
## 5.2.67 Gradient recovery test for Z-direction [+] (NPT_1H_gradrecZ_sqp_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727, Z142231
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[dl6] | Scal.Int.[#26] | BO-Shift[Hz] | *APK0[APK #26] |
|---|---|---|---|---|
| 1 | 10.00 us | 99.46 | 4.60 | -3.5 |
| 2 | 15.85 us | 99.62 | 4.43 | -2.0 |
| 3 | 25.12 us | 98.61 | 4.26 | -1.0 |
| 4 | 39.81 us | 98.34 | 4.05 | -1.5 |
| 5 | 63.10 us | 98.31 | 3.92 | -2.0 |
| 6 | 100.0 us | 98.24 | 3.71 | -1.5 |
| 7 | 158.5 us | 98.16 | 3.54 | -1.5 |
| 8 | 251.2 us | 98.10 | 3.34 | -1.5 |
| 9 | 398.1 us | 98.16 | 3.31 | -1.0 |
| 10 | 630.9 us | 98.04 | 2.96 | -0.5 |
| 11 | 1.000 ms | 98.25 | 2.79 | 0.0 |
| 12 | 1.585 ms | 98.46 | 2.62 | -0.5 |
| 13 | 2.512 ms | 98.70 | 2.41 | -0.5 |
| 14 | 3.981 ms | 99.04 | 2.24 | -0.5 |
| 15 | 6.310 ms | 99.38 | 2.07 | -0.5 |
| 16 | 10.00 ms | 99.72 | 1.86 | 0.0 |
| 17 | 15.85 ms | 99.83 | 1.69 | -0.5 |
| 18 | 25.12 ms | 99.93 | 1.48 | -0.5 |
| 19 | 39.81 ms | 99.93 | 1.35 | -0.5 |
| 20 | 63.10 ms | 99.99 | 1.10 | -0.5 |
| 21 | 0.100 s | 99.97 | 1.01 | -0.5 |
| 22 | 0.158 s | 100.00 | 0.76 | 0.0 |
| 23 | 0.251 s | 99.92 | 0.59 | 0.0 |
| 24 | 0.398 s | 99.95 | 0.42 | -0.5 |
| 25 | 0.631 s | 99.98 | 0.25 | 0.0 |
| 26 | 1.000 s | 100.00 | 0.00 | 0.0 |




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

**Control Option for Acquisition (L23)**

1 default
10 skip sino check and gradient amplifier functioning test

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrec | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | RECT.1 | | |
| GPZ 1 | 75.000 | % | |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 26 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

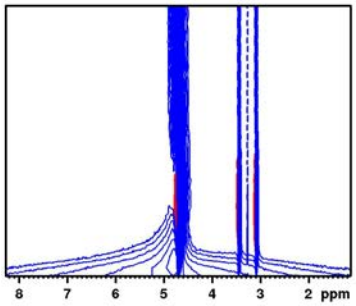
## Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of range one, needs to be specified.

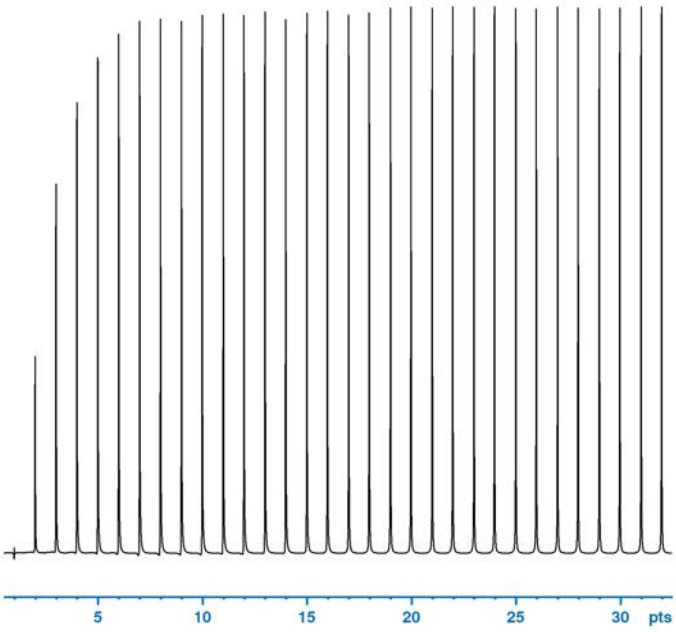
## 5.2.68 Gradient recovery test for X-direction [-] with trapezoid pulses (NPT_1H_gradrecX_trapezoid_neg_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z10085, Z10084
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[d16] | Scal.Int.[#32] | B0-Shift[Hz] | +APK0[APK #32] |
|---|---|---|---|---|
| 1 | 0.10 ms | ---- | ---- | ---- |
| 2 | 0.13 ms | 36.03 | -1.09 | 16.86 |
| 3 | 0.16 ms | 67.80 | -1.16 | 8.70 |
| 4 | 0.24 ms | 83.06 | -1.06 | 5.64 |
| 5 | 0.33 ms | 91.67 | -1.20 | -0.24 |
| 6 | 0.44 ms | 95.54 | -1.00 | 0.08 |
| 7 | 0.59 ms | 97.31 | -1.30 | 0.66 |
| 8 | 0.80 ms | 97.89 | -0.90 | 0.48 |
| 9 | 1.08 ms | 98.09 | -1.42 | -0.12 |
| 10 | 1.45 ms | 98.51 | -0.77 | -0.20 |
| 11 | 1.95 ms | 98.80 | -1.52 | 0.22 |
| 12 | 2.63 ms | 98.78 | -0.61 | -0.44 |
| 13 | 3.54 ms | 99.05 | -1.67 | -0.02 |
| 14 | 4.76 ms | 98.98 | -0.47 | 0.08 |
| 15 | 6.40 ms | 99.29 | -1.81 | 0.10 |
| 16 | 8.62 ms | 99.54 | -0.24 | -0.12 |
| 17 | 11.60 ms | 99.63 | -1.96 | -0.16 |
| 18 | 15.62 ms | 99.74 | -0.09 | 0.10 |
| 19 | 21.02 ms | 99.95 | -2.01 | -0.14 |
| 20 | 28.29 ms | 100.00 | -0.01 | -0.14 |
| 21 | 38.08 ms | 99.94 | -2.01 | -0.12 |
| 22 | 51.25 ms | 99.99 | -0.00 | -0.14 |
| 23 | 68.98 ms | 100.00 | -2.02 | -0.16 |
| 24 | 92.84 ms | 100.00 | -0.01 | -0.12 |
| 25 | 124.96 ms | 99.94 | -2.00 | 0.24 |
| 26 | 168.19 ms | 99.95 | 0.03 | -0.18 |
| 27 | 226.38 ms | 100.01 | -2.03 | 0.04 |
| 28 | 304.70 ms | 99.96 | 0.02 | 0.04 |
| 29 | 410.11 ms | 99.94 | -2.00 | 0.14 |
| 30 | 552.00 ms | 99.97 | 0.02 | 0.00 |
| 31 | 742.96 ms | 99.99 | -2.04 | -0.08 |
| 32 | 1.0 s | 100.00 | 0.00 | 0.00 |




### Example Printout

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

### Control Option for Acquisition (L23)

1 default
10 skip sino check and gradient amplifier functioning test

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrectrvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrecTrapezoid | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | GRADREC5m | | |
| GPX 1 | 0.000 | % | 7.5 A |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 32 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

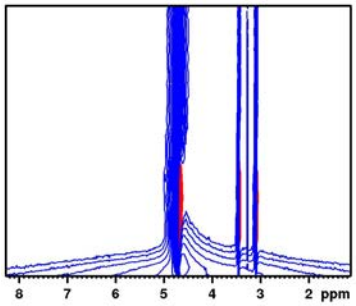
## Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of evaluation range, needs to be specified.

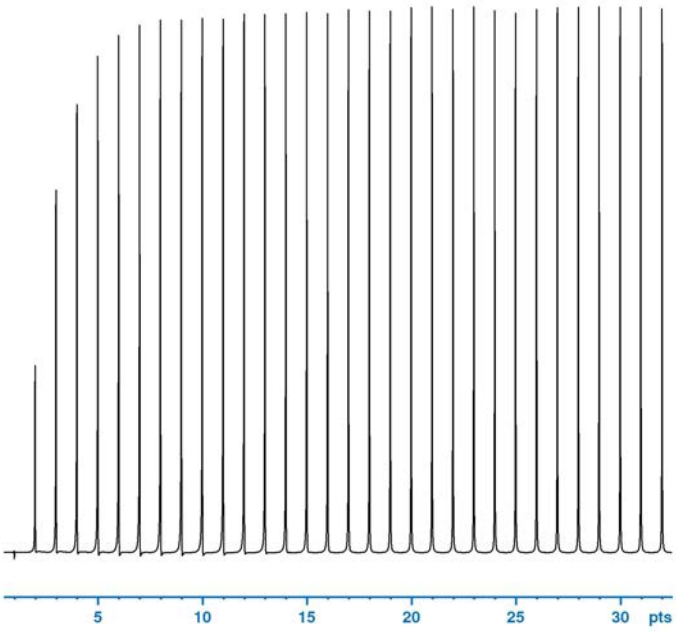
## 5.2.69 Gradient recovery test for X-direction [+] with trapezoid pulses (NPT_1H_gradrecX_trapezoid_pos_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z10085, Z10084
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[d16] | Scal.Int.[#32] | B0-Shift[Hz] | +APK0[APK #32] |
|---|---|---|---|---|
| 1 | 0.10 ms | ----- | ----- | ----- |
| 2 | 0.13 ms | 34.33 | 0.86 | 7.36 |
| 3 | 0.18 ms | 66.55 | 0.90 | 3.10 |
| 4 | 0.24 ms | 82.21 | 0.85 | 1.54 |
| 5 | 0.33 ms | 90.99 | 0.89 | 0.58 |
| 6 | 0.44 ms | 94.86 | 0.88 | -0.02 |
| 7 | 0.59 ms | 94.71 | 0.88 | -0.50 |
| 8 | 0.80 ms | 97.70 | 0.90 | -0.14 |
| 9 | 1.08 ms | 97.89 | 0.84 | 0.14 |
| 10 | 1.45 ms | 98.07 | 0.91 | 0.24 |
| 11 | 1.95 ms | 98.14 | 0.83 | 0.24 |
| 12 | 2.63 ms | 98.69 | 0.88 | 0.06 |
| 13 | 3.54 ms | 98.79 | 0.85 | -0.18 |
| 14 | 4.76 ms | 99.06 | 0.84 | -0.12 |
| 15 | 6.40 ms | 99.30 | 0.84 | 0.22 |
| 16 | 8.62 ms | 99.64 | 0.76 | -0.08 |
| 17 | 11.60 ms | 99.77 | 0.84 | -0.24 |
| 18 | 15.62 ms | 99.90 | 0.75 | -0.20 |
| 19 | 21.02 ms | 99.90 | 0.82 | 0.04 |
| 20 | 28.29 ms | 100.03 | 0.67 | 0.10 |
| 21 | 38.08 ms | 100.09 | 0.89 | -0.08 |
| 22 | 51.25 ms | 100.01 | 0.64 | 0.02 |
| 23 | 68.98 ms | 100.09 | 0.87 | 0.10 |
| 24 | 92.84 ms | 99.99 | 0.57 | -0.12 |
| 25 | 124.96 ms | 99.95 | 0.96 | -0.10 |
| 26 | 168.19 ms | 100.01 | 0.46 | -0.12 |
| 27 | 226.38 ms | 100.05 | 1.09 | -0.04 |
| 28 | 304.70 ms | 100.08 | 0.30 | -0.02 |
| 29 | 410.11 ms | 100.08 | 1.25 | 0.02 |
| 30 | 552.00 ms | 100.07 | 0.12 | 0.08 |
| 31 | 742.96 ms | 100.07 | 1.41 | 0.08 |
| 32 | 1.0 s | 100.00 | 0.00 | 0.00 |




### Example Printout

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

### Control Option for Acquisition (L23)

1 default
10 skip sino check and gradient amplifier functioning test

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrectrvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrecTrapezoid | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | GRADREC5m | | |
| GPX 1 | 0.000 | % | 7.5 A |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 32 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

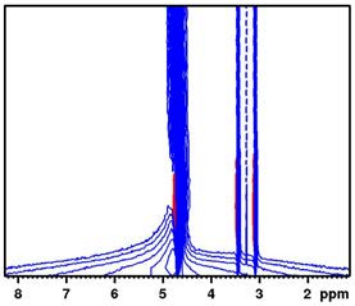
### Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of evaluation range, needs to be specified.

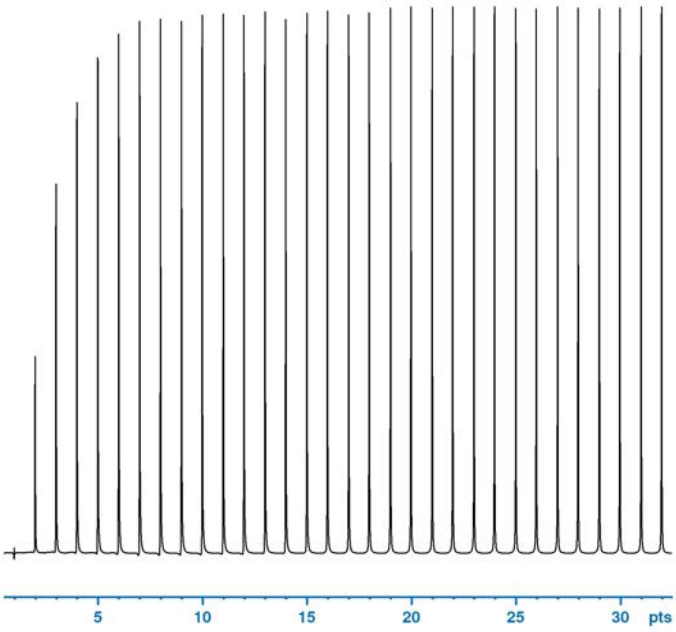
## 5.2.70 Gradient recovery test for Y-direction [-] with trapezoid pulses (NPT_1H_gradrecY_trapezoid_neg_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z10085, Z10084
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[d16] | Scal.Int.[#32] | B0-Shift[Hz] | +APK0[APK #32] |
|---|---|---|---|---|
| 1 | 0.10 ms | ---- | ---- | ---- |
| 2 | 0.13 ms | 36.03 | -1.09 | 16.86 |
| 3 | 0.16 ms | 67.80 | -1.16 | 8.70 |
| 4 | 0.24 ms | 83.06 | -1.06 | 5.64 |
| 5 | 0.33 ms | 91.67 | -1.20 | -0.24 |
| 6 | 0.44 ms | 95.54 | -1.00 | 0.08 |
| 7 | 0.59 ms | 97.31 | -1.30 | 0.46 |
| 8 | 0.80 ms | 97.89 | -0.90 | 0.48 |
| 9 | 1.08 ms | 98.09 | -1.42 | -0.12 |
| 10 | 1.45 ms | 98.51 | -0.77 | -0.20 |
| 11 | 1.95 ms | 98.80 | -1.52 | 0.22 |
| 12 | 2.63 ms | 98.78 | -0.61 | -0.44 |
| 13 | 3.54 ms | 99.05 | -1.67 | -0.02 |
| 14 | 4.76 ms | 98.98 | -0.47 | 0.08 |
| 15 | 6.40 ms | 99.29 | -1.81 | 0.10 |
| 16 | 8.62 ms | 99.54 | -0.24 | -0.12 |
| 17 | 11.60 ms | 99.43 | -1.96 | -0.16 |
| 18 | 15.62 ms | 99.74 | -0.09 | 0.10 |
| 19 | 21.02 ms | 99.95 | -2.01 | -0.14 |
| 20 | 28.29 ms | 100.00 | -0.01 | -0.14 |
| 21 | 38.08 ms | 99.94 | -2.01 | -0.12 |
| 22 | 51.25 ms | 99.99 | -0.00 | -0.14 |
| 23 | 68.98 ms | 100.00 | -2.02 | -0.16 |
| 24 | 92.84 ms | 100.00 | -0.01 | -0.12 |
| 25 | 124.96 ms | 99.94 | -2.00 | 0.24 |
| 26 | 168.19 ms | 99.95 | 0.03 | -0.18 |
| 27 | 226.38 ms | 100.01 | -2.03 | 0.04 |
| 28 | 304.70 ms | 99.96 | 0.02 | 0.04 |
| 29 | 410.11 ms | 99.94 | -2.00 | 0.14 |
| 30 | 552.00 ms | 99.97 | 0.02 | 0.00 |
| 31 | 742.96 ms | 99.99 | -2.04 | -0.08 |
| 32 | 1.0 s | 100.00 | 0.00 | 0.00 |




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

**Control Option for Acquisition (L23)**

1 default
10 skip sino check and gradient amplifier functioning test

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrectrvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrecTrapezoid | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | GRADREC5m | | |
| GPY 1 | 0.000 | % | 7.5 A |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 32 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

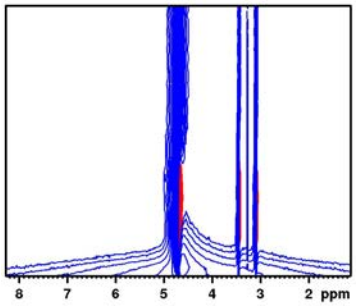
### Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of evaluation range, needs to be specified.

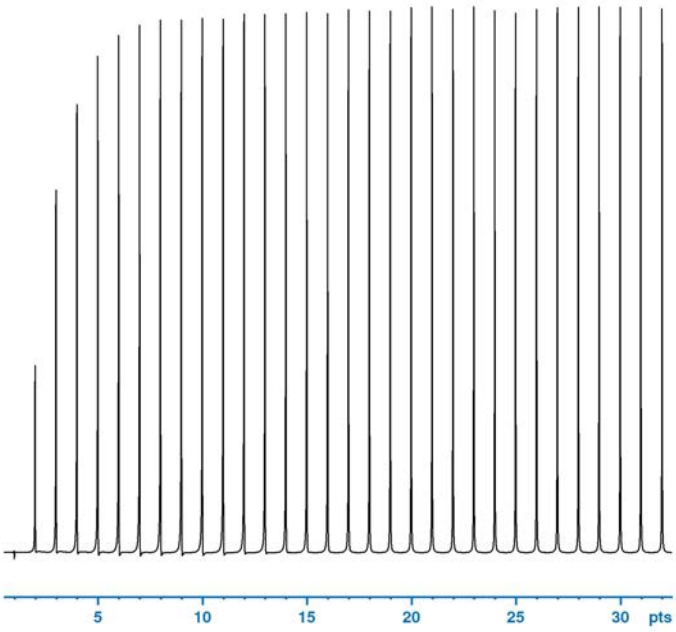
## 5.2.71 Gradient recovery test for Y-direction [+] with trapezoid pulses (NPT_1H_gradrecY_trapezoid_pos_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O Z10083, Z10085, Z10084
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[d16] | Scal.Int.[#32] | B0-Shift[Hz] | +APK0[APK #32] |
|---|---|---|---|---|
| 1 | 0.10 ms | ----- | ----- | ----- |
| 2 | 0.13 ms | 34.33 | 0.86 | 7.36 |
| 3 | 0.16 ms | 66.55 | 0.90 | 3.10 |
| 4 | 0.24 ms | 82.21 | 0.85 | 1.54 |
| 5 | 0.33 ms | 90.99 | 0.89 | 0.58 |
| 6 | 0.44 ms | 94.86 | 0.88 | -0.02 |
| 7 | 0.59 ms | 94.71 | 0.88 | -0.50 |
| 8 | 0.80 ms | 97.70 | 0.90 | -0.14 |
| 9 | 1.08 ms | 97.89 | 0.84 | 0.14 |
| 10 | 1.45 ms | 98.07 | 0.91 | 0.24 |
| 11 | 1.95 ms | 98.14 | 0.83 | 0.24 |
| 12 | 2.63 ms | 98.69 | 0.88 | 0.06 |
| 13 | 3.54 ms | 98.79 | 0.85 | -0.18 |
| 14 | 4.76 ms | 99.06 | 0.84 | -0.12 |
| 15 | 6.40 ms | 99.30 | 0.84 | 0.22 |
| 16 | 8.62 ms | 99.64 | 0.76 | -0.08 |
| 17 | 11.60 ms | 99.77 | 0.84 | -0.24 |
| 18 | 15.62 ms | 99.90 | 0.75 | -0.20 |
| 19 | 21.02 ms | 99.90 | 0.82 | 0.04 |
| 20 | 28.29 ms | 100.03 | 0.67 | 0.10 |
| 21 | 38.08 ms | 100.09 | 0.89 | -0.08 |
| 22 | 51.25 ms | 100.01 | 0.64 | 0.02 |
| 23 | 68.98 ms | 100.09 | 0.87 | 0.10 |
| 24 | 92.84 ms | 99.99 | 0.57 | -0.12 |
| 25 | 124.96 ms | 99.95 | 0.96 | -0.10 |
| 26 | 168.19 ms | 100.01 | 0.46 | -0.12 |
| 27 | 226.38 ms | 100.05 | 1.09 | -0.04 |
| 28 | 304.70 ms | 100.08 | 0.30 | -0.02 |
| 29 | 410.11 ms | 100.08 | 1.25 | 0.02 |
| 30 | 552.00 ms | 100.07 | 0.12 | 0.08 |
| 31 | 742.96 ms | 100.07 | 1.41 | 0.08 |
| 32 | 1.0 s | 100.00 | 0.00 | 0.00 |




### Example Printout

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

### Control Option for Acquisition (L23)

1 default
10 skip sino check and gradient amplifier functioning test

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrectrvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrecTrapezoid | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | GRADREC5m | | |
| GPY 1 | 0.000 | % | 7.5 A |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 32 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

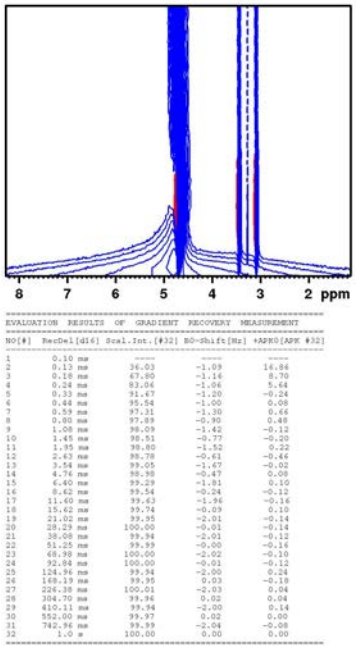
## Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of evaluation range, needs to be specified.

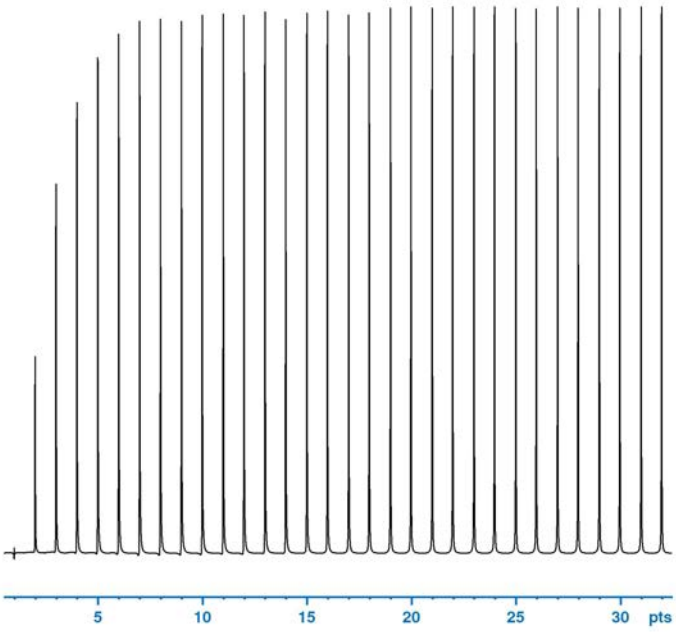
## 5.2.72 Gradient recovery test for Z-direction [-] with trapezoid pulses (NPT_1H_gradrecZ_trapezoid_neg_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O Z10083, Z10085, Z10084
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[d16] | Scal.Int.[#32] | B0-Shift[Hz] | +APK0[APK #32] |
|---|---|---|---|---|
| 1 | 0.10 ms | ----- | ----- | ----- |
| 2 | 0.13 ms | 36.03 | -1.09 | 16.86 |
| 3 | 0.16 ms | 67.80 | -1.16 | 8.70 |
| 4 | 0.24 ms | 83.06 | -1.06 | 5.64 |
| 5 | 0.33 ms | 91.67 | -1.20 | -0.24 |
| 6 | 0.44 ms | 95.54 | -1.00 | 0.08 |
| 7 | 0.59 ms | 97.31 | -1.30 | 0.46 |
| 8 | 0.80 ms | 97.89 | -0.90 | 0.48 |
| 9 | 1.08 ms | 98.09 | -1.42 | -0.12 |
| 10 | 1.45 ms | 98.51 | -0.77 | -0.20 |
| 11 | 1.95 ms | 98.80 | -1.52 | 0.22 |
| 12 | 2.63 ms | 98.78 | -0.61 | -0.44 |
| 13 | 3.54 ms | 99.05 | -1.67 | -0.02 |
| 14 | 4.76 ms | 98.98 | -0.47 | 0.08 |
| 15 | 6.40 ms | 99.29 | -1.81 | 0.10 |
| 16 | 8.62 ms | 99.54 | -0.24 | -0.12 |
| 17 | 11.60 ms | 99.43 | -1.96 | -0.16 |
| 18 | 15.62 ms | 99.74 | -0.09 | 0.10 |
| 19 | 21.02 ms | 99.95 | -2.01 | -0.14 |
| 20 | 28.29 ms | 100.00 | -0.01 | -0.14 |
| 21 | 38.08 ms | 99.94 | -2.01 | -0.12 |
| 22 | 51.25 ms | 99.99 | -0.00 | -0.16 |
| 23 | 68.98 ms | 100.00 | -2.02 | -0.16 |
| 24 | 92.84 ms | 100.00 | -0.01 | -0.12 |
| 25 | 124.96 ms | 99.94 | -2.00 | 0.24 |
| 26 | 168.19 ms | 99.95 | 0.03 | -0.18 |
| 27 | 226.38 ms | 100.01 | -2.03 | 0.04 |
| 28 | 304.70 ms | 99.96 | 0.02 | 0.04 |
| 29 | 410.11 ms | 99.94 | -2.00 | 0.14 |
| 30 | 552.00 ms | 99.97 | 0.02 | 0.00 |
| 31 | 742.96 ms | 99.99 | -2.04 | -0.08 |
| 32 | 1.0 s | 100.00 | 0.00 | 0.00 |




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

**Control Option for Acquisition (L23)**

1 default
10 skip sino check and gradient amplifier functioning test

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrectrvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrecTrapezoid | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | GRADREC5m | | |
| GPZ 1 | -75.000 | % | 7.5 A |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 32 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

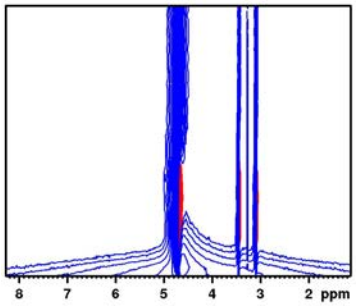
### Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of evaluation range, needs to be specified.

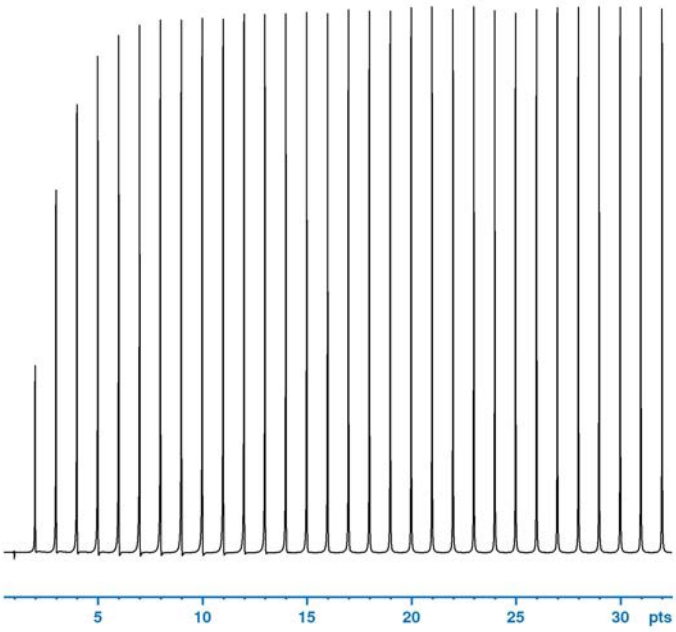
## 5.2.73 Gradient recovery test for Z-direction [+] with trapezoid pulses (NPT_1H_gradrecZ_trapezoid_pos_1h)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O Z10083, Z10085, Z10084
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| NO[#] | RecDel[d16] | Scal.Int.[#32] | B0-Shift[Hz] | +APK0[APK #32] |
|---|---|---|---|---|
| 1 | 0.10 ms | ----- | ----- | ----- |
| 2 | 0.13 ms | 34.33 | 0.86 | 7.36 |
| 3 | 0.16 ms | 66.55 | 0.90 | 3.10 |
| 4 | 0.24 ms | 82.21 | 0.85 | 1.54 |
| 5 | 0.33 ms | 90.99 | 0.89 | 0.58 |
| 6 | 0.44 ms | 94.86 | 0.88 | -0.02 |
| 7 | 0.59 ms | 94.71 | 0.88 | -0.50 |
| 8 | 0.80 ms | 97.70 | 0.90 | -0.14 |
| 9 | 1.08 ms | 97.89 | 0.84 | 0.14 |
| 10 | 1.45 ms | 98.07 | 0.91 | 0.24 |
| 11 | 1.95 ms | 98.14 | 0.83 | 0.24 |
| 12 | 2.63 ms | 98.69 | 0.88 | 0.06 |
| 13 | 3.54 ms | 98.79 | 0.85 | -0.18 |
| 14 | 4.76 ms | 99.06 | 0.84 | -0.12 |
| 15 | 6.40 ms | 99.30 | 0.84 | 0.22 |
| 16 | 8.62 ms | 99.64 | 0.76 | -0.08 |
| 17 | 11.60 ms | 99.77 | 0.84 | -0.24 |
| 18 | 15.62 ms | 99.90 | 0.75 | -0.20 |
| 19 | 21.02 ms | 99.90 | 0.82 | 0.04 |
| 20 | 28.29 ms | 100.03 | 0.67 | 0.10 |
| 21 | 38.08 ms | 100.09 | 0.89 | -0.08 |
| 22 | 51.25 ms | 100.01 | 0.64 | 0.02 |
| 23 | 68.98 ms | 100.09 | 0.87 | 0.10 |
| 24 | 92.84 ms | 99.99 | 0.57 | -0.12 |
| 25 | 124.96 ms | 99.95 | 0.96 | -0.10 |
| 26 | 168.19 ms | 100.01 | 0.46 | -0.12 |
| 27 | 226.38 ms | 100.05 | 1.09 | -0.04 |
| 28 | 304.70 ms | 100.08 | 0.30 | -0.02 |
| 29 | 410.11 ms | 100.08 | 1.25 | 0.02 |
| 30 | 552.00 ms | 100.07 | 0.12 | 0.08 |
| 31 | 742.96 ms | 100.07 | 1.41 | 0.08 |
| 32 | 1.0 s | 100.00 | 0.00 | 0.00 |




### Example Printout

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, signal intensity, signal shift (B0), phase deviation (apk0).

### Control Option for Acquisition (L23)

1 default
10 skip sino check and gradient amplifier functioning test

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrectrvd | | |
| NS | 1 | | |
| DS | 2 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.697 | ppm | |
| SW | 7.528 | ppm | |
| TD | 16506 | | field dependent |
| AQ | 2.740 | s | |
| FIDRES | 0.365 | Hz | |
| D 1 | 0.300 | s | |
| VDLIST | npt_gradrecTrapezoid | | default |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| GPNAM1 | GRADREC5m | | |
| GPZ 1 | 75.000 | % | 7.5 A |
| P 16 | 5000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 32 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |

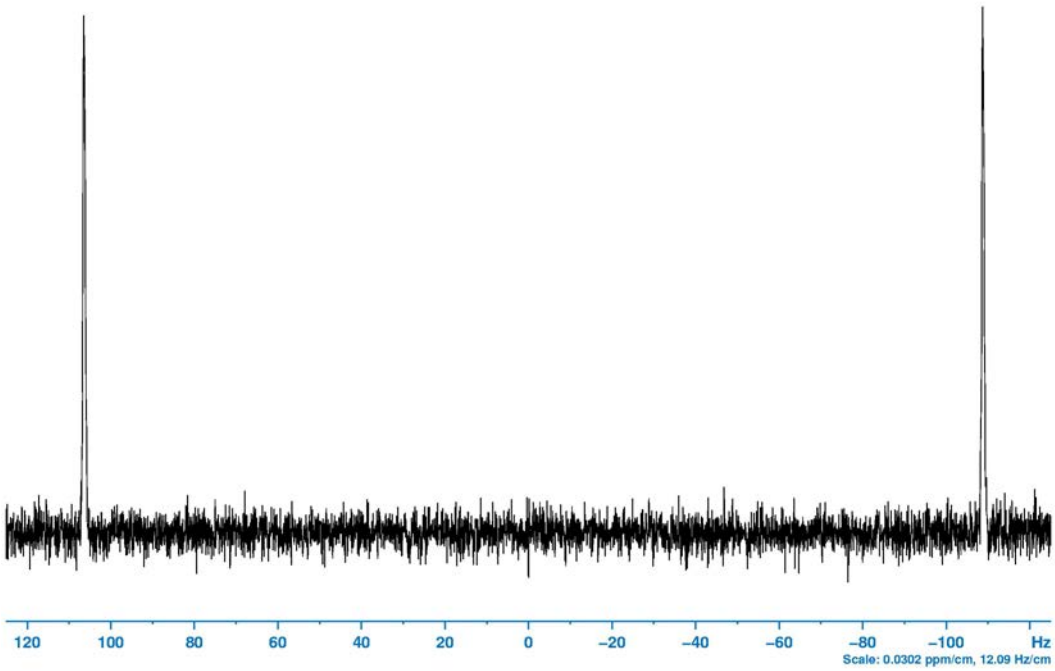
### Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
The next step is a gradient echo experiment on a derived data set to check the functioning of the gradient amplifier.
SINO check and gradient amplifier functioning test can be skiped with L23=10
After successful SINO and gradient checks, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of the determination of the zero-order phase correction difference to the reference experiment (last of the series) and the determination of the intensity deviation again referenced to the last experiment.
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of evaluation range, needs to be specified.

## 5.2.74 Inverse spin echo difference (NPT_1H_hmqc1df2_13c)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z10248, Z10701, Z100926, Z10250, Z10031, Z10030, Z10029, Z10260, Z10249, Z10275, Z10272, Z10717
**Solvent:** Acetone
**Lock parameter:** Lockregulation based on LGAIN=80 dB and default LOCKPOWER
**Sample State:** Rotation off




**Example Printout**

Inverse spin echo difference spectrum (1H) of the 13C satellites of chloroform. Printing range is centered around the suppressed proton signal of chloroform attached to 12C (no coupling).

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| PARMODE | 0 | | Data Dimension |
| TD0 | 1 | | |
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| PULPROG | hmqcndrd1d | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | 8.000 | ppm | CHCl3 (1H) |
| O2P | 76.987 | ppm | CDCl3 (13C) |
| SWH | 1000.000 | Hz | |
| TD | 16384 | | |
| AQ | 8.192 | s | |
| FIDRES | 0.122 | Hz | |
| D 1 | 14.000 | s | |
| CNST 2 | 216.000 | Hz | J[CH] |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| PLW 1 | 6.6 | W | Pow@P90(Specs) |
| PLW 2 | 26.5 | W | Pow@P90(Specs) |
| TE | 298.000 | K | default |

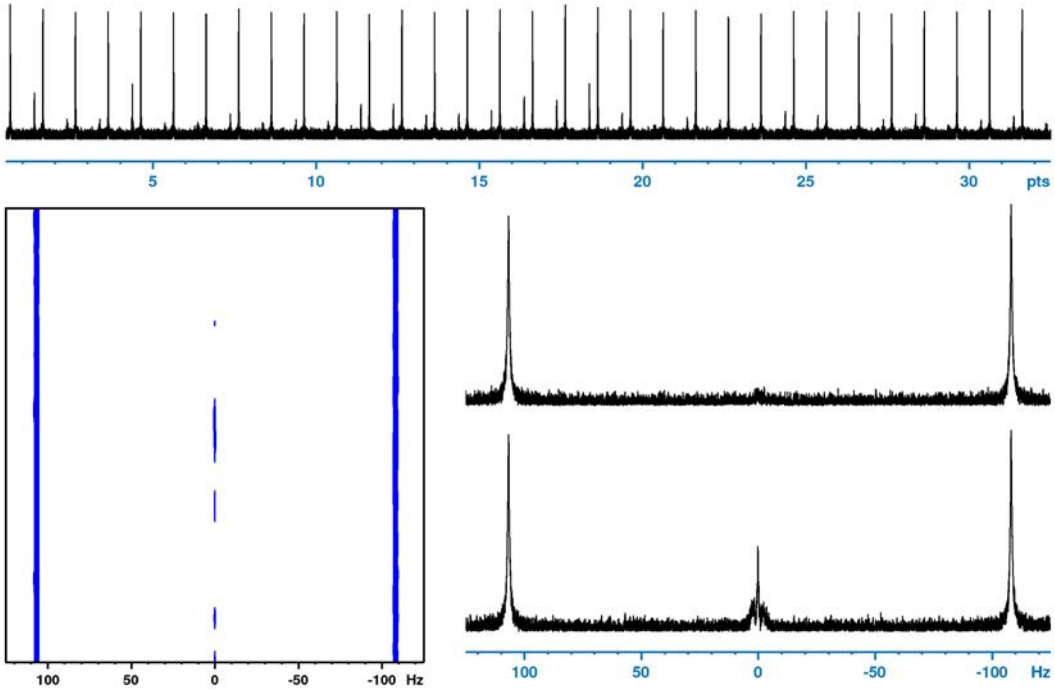
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | |
| F1P | 2475.044 | ppm | |
| F2P | 2345.044 | ppm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 2.000 | min | Waittime for AQ |

## Experiment Description

Purpose of this experiment is to show phase stabilitiy of the spectrometer. The central signal (1H attached to 12C) should ideally be suppressed. Influencing variables are lock stability, instrument environment and sample temperature besides the electronic stability and quality of the instrument itself. It is very important, that the sample is sufficiently relaxed before starting the experiment.
NMRPT is doing an O1 opimization, followed by a delay of 600 s before the main experiment.
Processing is accomplished with no line broadening. Data evaluation consists of the comparison of the intensity ratio satellite signal versus central signal under consideration of potential unlike sign.

## 5.2.75 Inverse spin echo difference experiment [2D] (NPT_1H_hmqc2df2_13c)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z10248, Z10701, Z100926, Z10250, Z10031, Z10030, Z10029, Z10260, Z10249, Z10275, Z10272, Z10717
**Solvent:** Acetone
**Lock parameter:** Lockregulation based on LGAIN=80 dB and default LOCKPOWER
**Sample State:** Rotation off




**Example Printout**

Inverse spin echo difference spectrum (1H) of the 13C satellites of chloroform.
The top spectrum shows a series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the left satellite and the suppresed proton signal of chloroform attached to 12C (no coupling). For all other spectra the printing range is centered around the suppressed proton signal.
The bottom spectrum to the left shows the pseudo-2D transformed with XF2 in maginitude mode. The middle spectrum to the right shows the row with highest suppression of the central peak. The bottom spectrum to the right shows the row with lowest suppression.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| PARMODE | 1 | | Data Dimension |
| TD0 | 1 | | |
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| PULPROG | npt_hmqcndrd2d | | |
| NS | 2 | | |
| DS | 8 | | |
| RG | 101.000 | | no optim. |
| O1P | 8.000 | ppm | CHCl3 (1H) |
| O2P | 76.988 | ppm | CDCl3 (13C) |
| SWH | 1000.000 | Hz | |
| TD | 32768 | | |
| AQ | 16.384 | s | |
| FIDRES | 0.061 | Hz | |
| D 1 | 10.000 | s | |
| CNST 2 | 214.900 | Hz | J[CH] |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| PLW 1 | 6.6 | W | Pow@P90(Specs) |
| PLW 2 | 26.5 | W | Pow@P90(Specs) |
| TE | 298.000 | K | default |

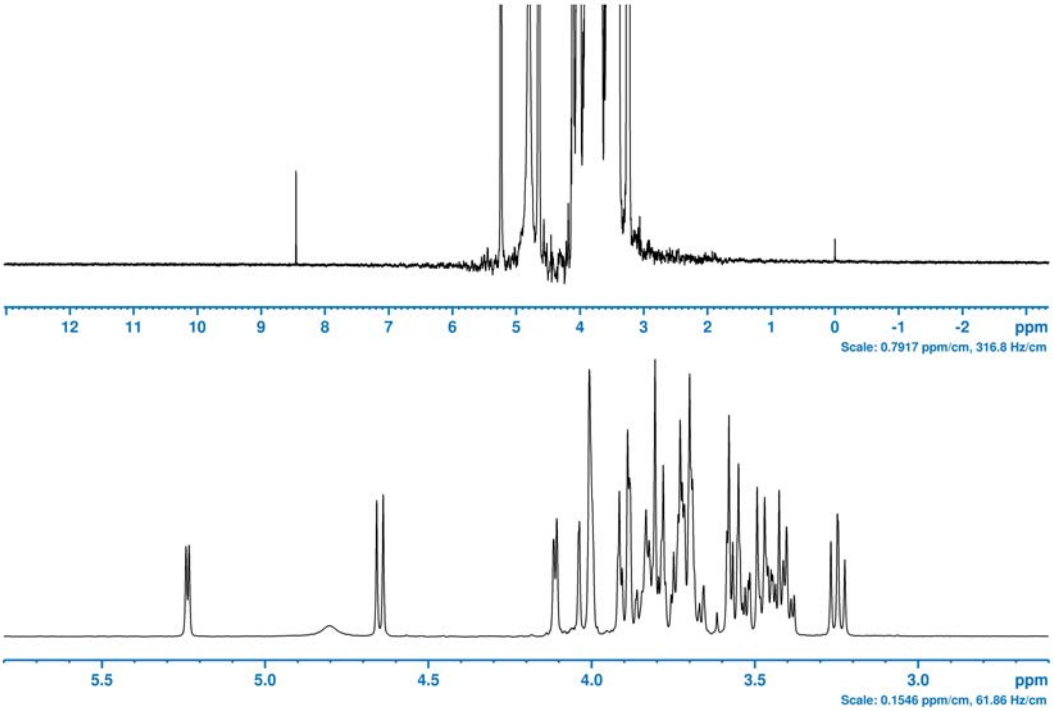
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 65536 | | |
| WDW | 0 | | no |
| LB | 0.000 | Hz | 0=default |
| PH_mod | 2 | | mc |
| F1P | 2475.044 | ppm | |
| F2P | 2345.044 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| TD | 32 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 32 | | |
| **NMRPT** | | | Parameters |
| CNST 50 | 5.000 | min | Waittime for AQ |

## Experiment Description

Purpose of this experiment is to show phase stabilitiy of the spectrometer over extended time periods. The central signal (1H attached to 12C) should ideally be suppressed. Influencing variables are lock stability, instrument environment and sample temperature besides the electronic stability and quality of the instrument itself.
NMRPT is going through the preparative steps:
1) LOCK optimization (regulation, lockgain, lockphase, lockgain)
2) Exact O1P determination
3) Waiting time for sample temperature stabilisation (CNST50, in minutes)
4) Main acquisition
Processing is accomplished with no line broadening. For each row the intensity ratio is calculated as ratio of the intensity of central peak versus the average intensity of the two satellites. For calculation of the average intensity ratio first the intensities of central peak and the average intensities of the two satellites of each row are added separately. Maximal, minimal, and average intensity ratio are stated in the experiment title.

## 5.2.76 1H of pseudo honey with noesy for solvent suppression (NPT_1H_honeyNoesy)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
H177072
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Bottom & Top: 1H noesy overview spectrum of pseudo honey sample with different scaling.

**Control Option for Acquisition (L23)**

1 default, GPZ1=50, GPZ2=-10
2 GPZ1=-10, GPZ2=50
3 GPZ1=0, GPZ2=0
4 GPZ1 and GPZ2 can be set by user

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | noesygppr1d | | |
| NS | 32 | | |
| DS | 4 | | |
| RG | 16.000 | | |
| O1P | 4.702 | ppm | |
| SWH | 8196.722 | Hz | |
| TD | 65536 | | |
| AQ | 3.998 | s | |
| FIDRES | 0.250 | Hz | field dependent |
| D 1 | 4.000 | s | |
| D 8 | 0.010 | s | |
| D 16 | 0.000 | s | |
| P 0 | 14.0 | us | 90deg Pulse |
| P 1 | 14.0 | us | 90deg Pulse |
| P 16 | 1000.000 | us | gradient pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.015 | mW | Pow@90deg(25 Hz) |
| GPNAM1 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 2 | -10.000 | % | |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| LB | 0.300 | Hz | |
| CY | 5.500 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 1000.000 | | Scaling factor for CY |

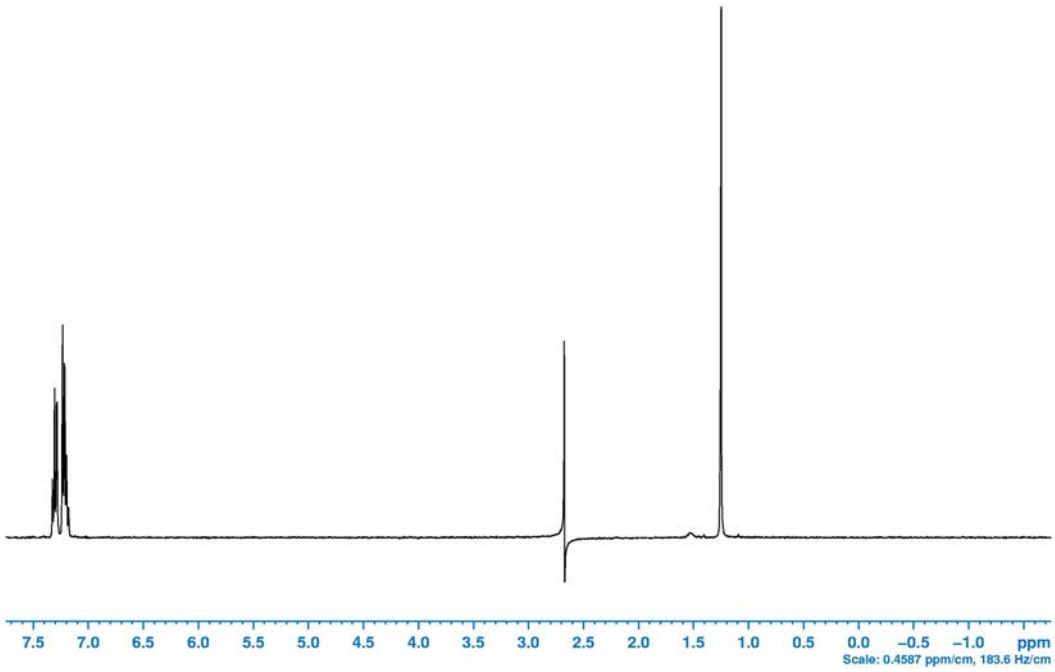
## Experiment Description

1H spectrum with presaturation and noesy for solvent suppression.
Before the acquisition, the proton 90 degrees pulse is calibrated using pulscal, which result is stored in the corresponding derived dataset.The pulse determination is skiped if experiment is measured with option 'Skip Getprosol'.
After pulsecal PLW 9 is calculated and set for excitation bandwidth of 25 Hz.
Processing of spectrum with window funktion EM and zero order phase correction followed by a lortentzian baseline correction.

For evaluation the RMSD ratio of baseline to noise is determined. RMSD per point of baseline is determined over the whole spectrum excluding signal regions and spectrum edges. RMSD per point of noise is determined from 14.0 to 13.0 ppm after baseline correction (ABSF) to minimize baseline offset.

## 5.2.77 1H homodecoupling (NPT_1H_homodec)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10121, Z10033, Z10270, Z10718
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Proton spectrum of 0.1% Ethylbenzene with homodecoupled methyl group at 1.26 ppm.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | npt_zghdp0.2 | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | 3.000 | ppm | |
| O1P | 3.000 | ppm | |
| SW | 9.917 | ppm | |
| TD | 32768 | | |
| AQ | 4.129 | s | field dependent |
| FIDRES | 0.242 | Hz | field dependent |
| D 1 | 10.871 | s | AQ+D1=constant |
| DIGMOD | 1 | | default |
| HDDUTY | 20.000 | % | hd duty cycle |
| HDRATE | 20.000 | | oversampl. hd |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 24 | 0.004 | W | Pow@hd(Specs) NUC2 |
| CNST 10 | 30.000 | deg | flip angle |
| TE | 298.000 | K | default |

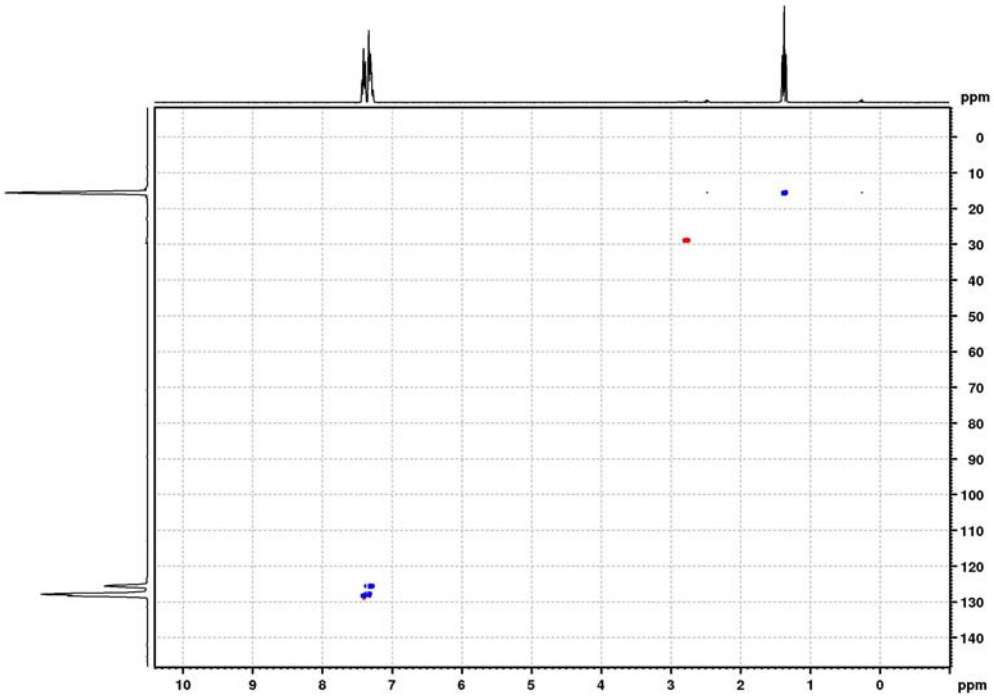
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 8.000 | ppm | |
| F2P | -2.000 | ppm | |
| SIGF1 | 1.500 | ppm | |
| SIGF2 | 0.250 | ppm | |
| NOISF1 | 0.200 | ppm | |
| NOISF2 | -1.800 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Homodecoupling test is performed to check apparent spectrometer performance with respect to switching times. The irradiation power is proportional to ~2 ms pulse length. The experimental setup consists of the exact determination of the irradiation position (O2). The processed data are stored in PROCNO=2. Processing is accomplished with exponential multiplication using line broadening. Evaluation consists of signal-to-noise determination using fixed noise region.

## 5.2.78 2D 1H-13C HSQC (NPT_1H_hsqc_10EB_13c_2d)

**Test Sample:** 10% Ethylbenzene (EB) in Chloroform-D
Z10153, Z10154, Z10034, Z10253, Z10292, Z10723
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

2D 1H-13C HSQC of 10% ethyl benzene in CDCl3. The F2 projection is shown at the top, the F1 projection at the left.

**Control Option for Acquisition (L23)**

1 default
2 use gradients with inverted sign (GPZ 1 = -80.0%, GPZ 2 = -20.1%)

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| PARMODE | 1 | | Data Dimension |
| TD0 | 1 | | |
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| PULPROG | hsqcedetgpsp.3 | | |
| NS | 1 | | |
| DS | 32 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | 1H |
| O2P | 70.000 | ppm | 13C) |
| SW | 12.132 | ppm | |
| TD | 2912 | | field dependent |
| AQ | 0.300 | s | |
| FIDRES | 3.334 | Hz | |
| D 1 | 2.000 | s | |
| CNST 2 | 145.000 | Hz | J[CH] |
| D 1 | 2.000 | s | |
| D 16 | 0.000 | s | gradrec del. |
| D 21 | 0.004 | s | 1/2 J[CH] |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| P 14 | 500.0 | us | sh.pul.invers. |
| P 24 | 2000.0 | us | sh.pul.refoc. |
| P 28 | 0.1 | us | trimpul. |
| PLW 1 | 16.2 | W | Pow@P90(Specs) |
| PLW 2 | 54.35 | W | Pow@P90(Specs) |
| PLW 12 | 0.8 | W | Pow@CPD(Specs) |
| PCPD 2 | 80 | us | 90deg CPD NUC2 |
| CPDPRG2 | p5m4sp180.2 | | > 600 MHz |
| CPDPRG2 | garp4 | | <= 600 MHz |
| SPNAM3 | Crp60,0.5,20.1 | | |
| SPOAL 3 | 0.500 | | 0.5 |
| SPW 3 | 8.3 | W | default |
| SPNAM18 | Crp60_xfilt.2 | | |
| SPOAL 18 | 0.500 | | |
| SPW 18 | 1.6 | W | default |
| SPNAM31 | Crp32,1.5,20.2 | | |
| SPOAL 31 | 0.500 | | |
| SPW 31 | 0.9 | W | default |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 80.000 | % | |
| GPZ 2 | 20.100 | % | |
| P 16 | 1000 | us | grad.pulse |
| TE | 298.000 | K | default |

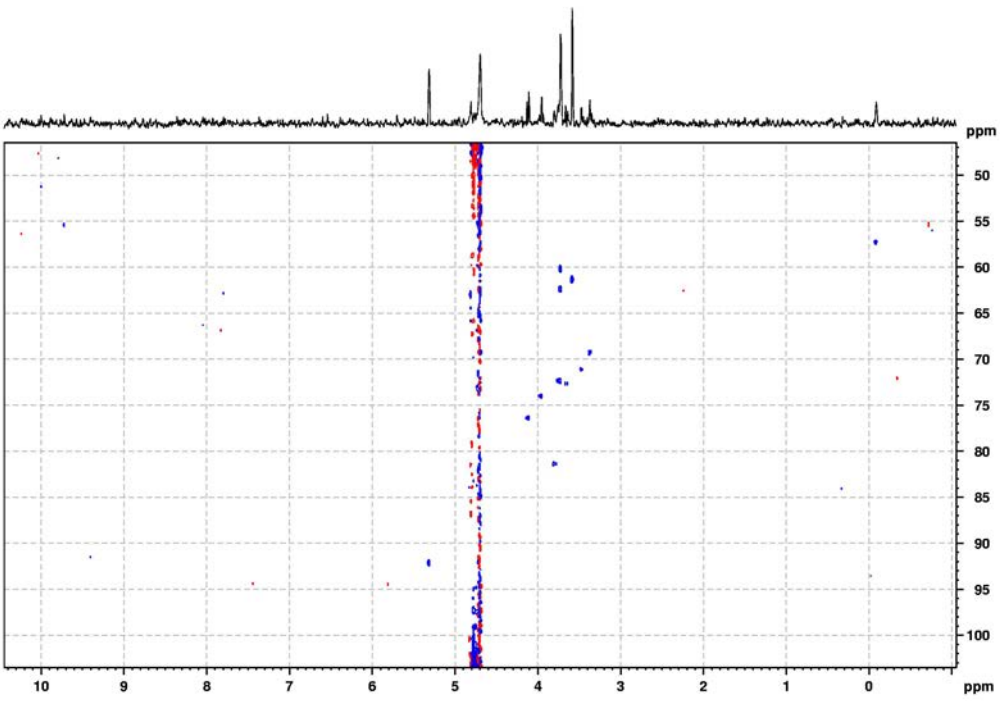
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 4 | | QSINE |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| F1P | 10.707 | ppm | |
| F2P | -1.307 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 13C | | |
| FnMODE | 6 | | |
| SW | 165.000 | ppm | |
| TD | 256 | | |
| O1P | 70.000 | ppm | 13C |
| **F1 PROC** | | | Parameters F1 |
| SI | 1024 | | |
| WDW | 4 | | QSINE |
| SSB | 2.000 | | |
| PH_mod | 0 | | |
| F1P | 152.405 | ppm | |
| F2P | -12.405 | ppm | |

## Experiment Description

2D 1H-13C HSQC is acquired phase-sensitive using shaped pulses for all 180 degree 13C pulses. Before the acquisition, the proton 90 degrees pulse is calibrated using pulscal, which result is stored in the corresponding derived dataset.The pulse determination is skiped if experiment is measured with option 'Skip Getprosol'.
Contour levels for 2D spectrum are obtained by command levcalc. Levcalc sets the lowest contour level to LEV0*S_DEV, where S_DEV (standard deviation) is a processing status parameter.

## 5.2.79 2D 1H-13C HSQC (NPT_1H_hsqc_etsisp_13c_2d)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

2D 1H-13C HSQC of 2 mM sucrose in 90%/10% H2O/D2O. The F2 projection from 95 to 50 ppm is shown at the top.

**Control Option for Acquisition (L23)**

1 default
20 no decoupling during acquisition (PLW12=0)

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| PARMODE | 1 | | Data Dimension |
| TD0 | 1 | | |
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| PULPROG | hsqcetgpsisp.2 | | |
| NS | 4 | | |
| DS | 64 | | |
| RG | 101.000 | | no optim. |
| TD | 2048 | | |
| O1P | 4.700 | ppm | 1H |
| O2P | 74.987 | ppm | 13C) |
| SW | 12.132 | ppm | |
| TD | 2048 | | |
| AQ | 0.211 | s | field dependent |
| FIDRES | 4.741 | Hz | field dependent |
| D 1 | 1.189 | s | |
| CNST 2 | 145.000 | Hz | J[CH] |
| CNST 17 | -0.500 | | -0.5, Crp60comp.4 |
| D 1 | 1.189 | s | |
| D 16 | 0.000 | s | gradrec del. |
| D 24 | 0.001 | s | 1/8*J[CH] |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| P 14 | 500.0 | us | sh.pul.invers. |
| P 24 | 2000.0 | us | sh.pul.refoc. |
| P 28 | 0.1 | us | trimpul. |
| PLW 1 | 6.6 | W | Pow@P90(Specs) |
| PLW 2 | 26.8 | W | Pow@P90(Specs) |
| PLW 12 | 0.3 | W | Pow@CPD(Specs) |
| PCPD 2 | 102.5 | us | 90deg CPD NUC2 |
| CPDPRG2 | garp | | cpd seq. |
| SPNAM3 | Crp60,0.5,20.1 | | |
| SPOAL 3 | 0.500 | | 0.5 |
| SPW 3 | 0.000 | W | default |
| SPNAM7 | Crp60comp.4 | | |
| SPOAL 7 | 0.500 | | 0.5 |
| SPW 7 | 0.000 | W | default |
| GPNAM1 | SINE.100 | | |
| GPNAM2 | SINE.100 | | |
| GPZ 1 | 80.000 | % | |
| GPZ 2 | 20.100 | % | |
| P 16 | 0.000 | us | grad.pulse |
| TE | 298.000 | K | default |

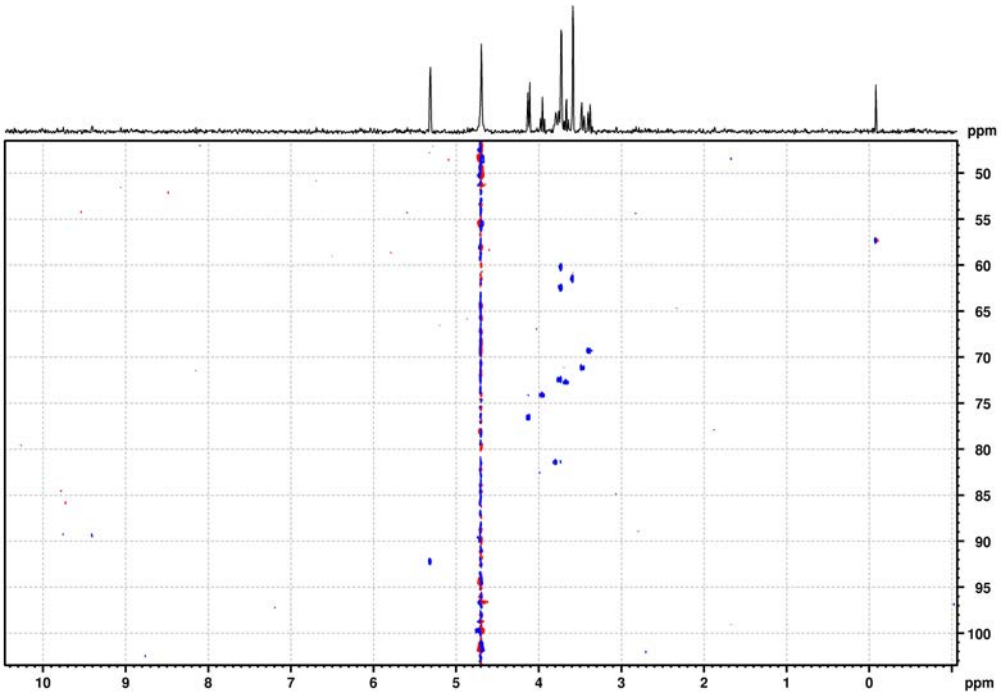
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 2048 | | |
| WDW | 4 | | QSINE |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| SIGF1 | 5.500 | ppm | |
| SIGF2 | 5.100 | ppm | |
| NOISF1 | 9.580 | ppm | |
| NOISF2 | 6.560 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 13C | | |
| FnMODE | 6 | | |
| SW | 60.008 | ppm | |
| TD | 256 | | |
| O1P | 74.987 | ppm | 13C |
| **F1 PROC** | | | Parameters F1 |
| SI | 512 | | |
| WDW | 4 | | QSINE |
| SSB | 2.000 | | |
| PH_mod | 0 | | no=default |
| SIGF1 | 93.000 | ppm | |
| SIGF2 | 91.000 | ppm | |
| NOISF1 | 81.600 | ppm | |
| NOISF2 | 66.700 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

2D 1H-13C HSQC is acquired phase-sensitive using shaped pulses for all 180 degree 13C pulses. Evaluation is achieved by determining the 2-dimensional signal-to-noise ratio according to the parameters section. The evaluation routine is part of the NMRPT package.
Option L23=1 is standard whereas option L23=20 is non-standard and will not be considered as regular test from the 'NMRPT Control Structure'.
Contour levels for 2D spectrum are obtained by command levcalc. Levcalc sets the lowest contour level to LEV0*S_DEV, where S_DEV (standard deviation) is a processing status parameter.

## 5.2.80 2D 1H-13C HSQC with adiabatic 13C decoupling (NPT_1H_hsqc_etsisp_adia13c_2d)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z100930, Z10268, Z10036, Z10247, Z10267, Z10719, Z10720
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

2D 1H-13C HSQC of 2 mM sucrose in 90%/10% H2O/D2O. The F2 projection from 95 to 50 ppm is shown at the top.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| PARMODE | 1 | | Data Dimension |
| TD0 | 1 | | |
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| PULPROG | hsqcetgpsisp.2 | | |
| NS | 4 | | |
| DS | 64 | | |
| RG | 101.000 | | no optim. |
| TD | 2426 | | |
| O1P | 4.700 | ppm | 1H |
| O2P | 74.987 | ppm | 13C) |
| SW | 12.132 | ppm | |
| TD | 2426 | | |
| AQ | 0.250 | s | field dependent |
| FIDRES | 4.002 | Hz | field dependent |
| D 1 | 1.150 | s | |
| CNST 2 | 145.000 | Hz | J[CH] |
| CNST 17 | -0.500 | | -0.5, Crp60comp.4 |
| D 1 | 1.150 | s | |
| D 16 | 0.000 | s | gradrec del. |
| D 24 | 0.001 | s | 1/8*J[CH] |
| P 1 | 14.0 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| P 14 | 500.0 | us | sh.pul.invers. |
| P 24 | 2000.0 | us | sh.pul.refoc. |
| P 28 | 0.1 | us | trimpul. |
| PLW 1 | 6.6 | W | Pow@P90(Specs) |
| PLW 2 | 26.8 | W | Pow@P90(Specs) |
| PLW 12 | 0.3 | W | Pow@CPD(Specs) |
| PCPD 2 | 102.5 | us | 90deg CPD NUC2 |
| CPDPRG2 | bi_p5m4sp_4sp.2 | | cpd seq. |
| SPNAM3 | Crp60,0.5,20.1 | | |
| SPOAL 3 | 0.500 | | 0.5 |
| SPW 3 | 0.000 | W | default |
| SPNAM7 | Crp60comp.4 | | |
| SPOAL 7 | 0.500 | | 0.5 |
| SPW 7 | 0.000 | W | default |
| GPNAM1 | SINE.100 | | |
| GPNAM2 | SINE.100 | | |
| GPZ 1 | 80.000 | % | |
| GPZ 2 | 20.100 | % | |
| P 16 | 0.000 | us | grad.pulse |
| TE | 298.000 | K | default |

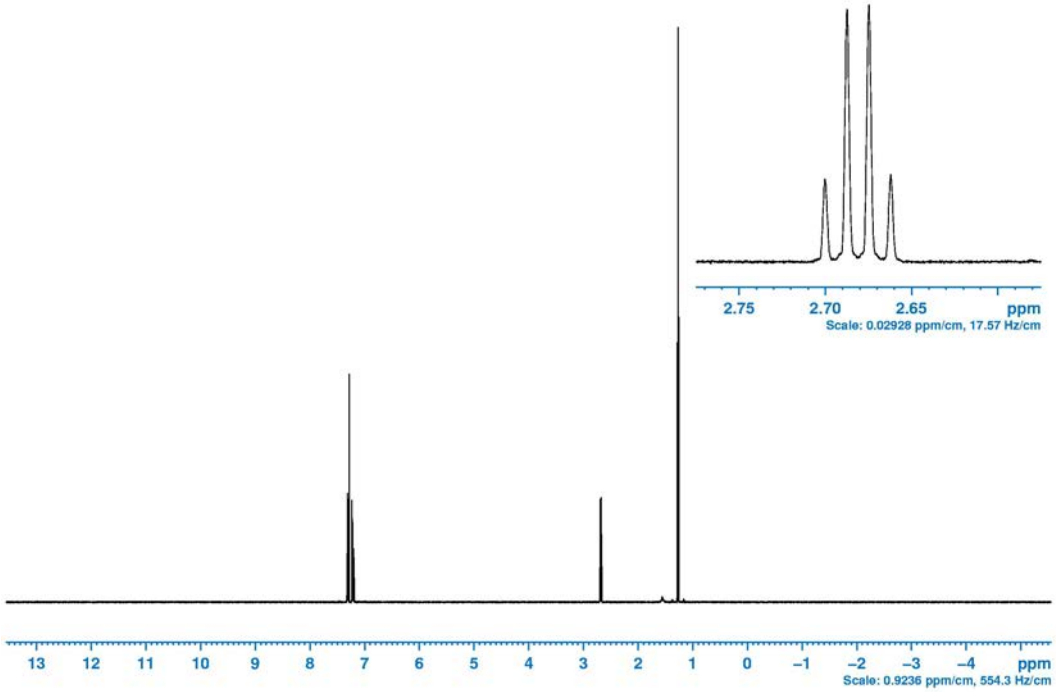
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 2048 | | |
| WDW | 4 | | QSINE |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| SIGF1 | 5.500 | ppm | |
| SIGF2 | 5.100 | ppm | |
| NOISF1 | 9.580 | ppm | |
| NOISF2 | 6.560 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 13C | | |
| FnMODE | 6 | | |
| SW | 60.008 | ppm | |
| TD | 256 | | |
| O1P | 74.987 | ppm | 13C |
| **F1 PROC** | | | Parameters F1 |
| SI | 512 | | |
| WDW | 4 | | QSINE |
| SSB | 2.000 | | |
| PH_mod | 0 | | no=default |
| SIGF1 | 93.000 | ppm | |
| SIGF2 | 91.000 | ppm | |
| NOISF1 | 81.600 | ppm | |
| NOISF2 | 66.700 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

2D 1H-13C HSQC is acquired phase-sensitive using shaped pulses for all 180 degree 13C pulses.
For decoupling adiabatic sequence bi_p5m4sp_4sp.2 is used.
Evaluation is achieved by determining the 2-dimensional signal-to-noise ratio according to the parameters section. The evaluation routine is part of the NMRPT package.
Contour levels for 2D spectrum are obtained by command levcalc. Levcalc sets the lowest contour level to LEV0*S_DEV, where S_DEV (standard deviation) is a processing status parameter.

## 5.2.81 1H integral sensitivity (NPT_1H_inno)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10121, Z10033, Z10270, Z10718, Z142221
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

1H spectrum of ethylbenzene processed without line broadening. Top right shows the methylene (CH2) group used in evaluation for signal-to-noise and integral-to-noise ratio.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.000 | ppm | |
| SW | 20.485 | ppm | |
| TD | 264292 | | |
| AQ | 16.122 | s | field dependent |
| FIDRES | 0.062 | Hz | field dependent |
| D 1 | 113.574 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

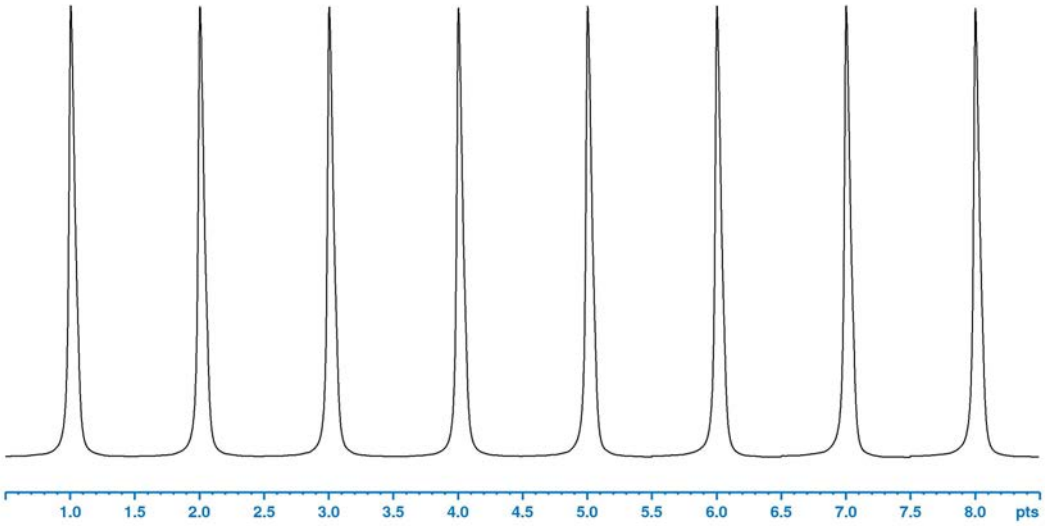
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 8.520 | ppm | |
| F2P | 0.480 | ppm | |
| CY | 100.000 | cm | |

## Experiment Description

The experiment determines SINO and INNO (Integral-to-noise ratio, I/N). The determination of I/N allows to obtain a measure for the sensitivity of the probe independent of the actual shim.

## 5.2.82 Linearity test with constant flip angle (NPT_1H_linearityConstFlipAngle)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




| Exp # | Pulse Length [us] | Power | Intensity [%] |
|---|---|---|---|
| 1 | 14.0 | 7.24 W | 99.97 |
| 2 | 28.0 | 1.81 W | 99.85 |
| 3 | 56.0 | 452 mW | 99.70 |
| 4 | 112.0 | 113 mW | 99.53 |
| 5 | 224.0 | 28.3 mW | 99.88 |
| 6 | 448.0 | 7.07 mW | 99.94 |
| 7 | 896.0 | 1.77 mW | 100.00 |
| 8 | 1792.0 | 442 uW | 99.46 |

**Example Printout**

Plot of the water peak intensities corresponding to increasing pulse lengths while keeping a constant flip angle of 90 degrees.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | syszg4 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.688 | ppm | |
| SW | 16.442 | ppm | |
| TD | 8192 | | |
| AQ | 0.623 | s | field dependent |
| FIDRES | 1.606 | Hz | field dependent |
| D 1 | 0.200 | s | |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

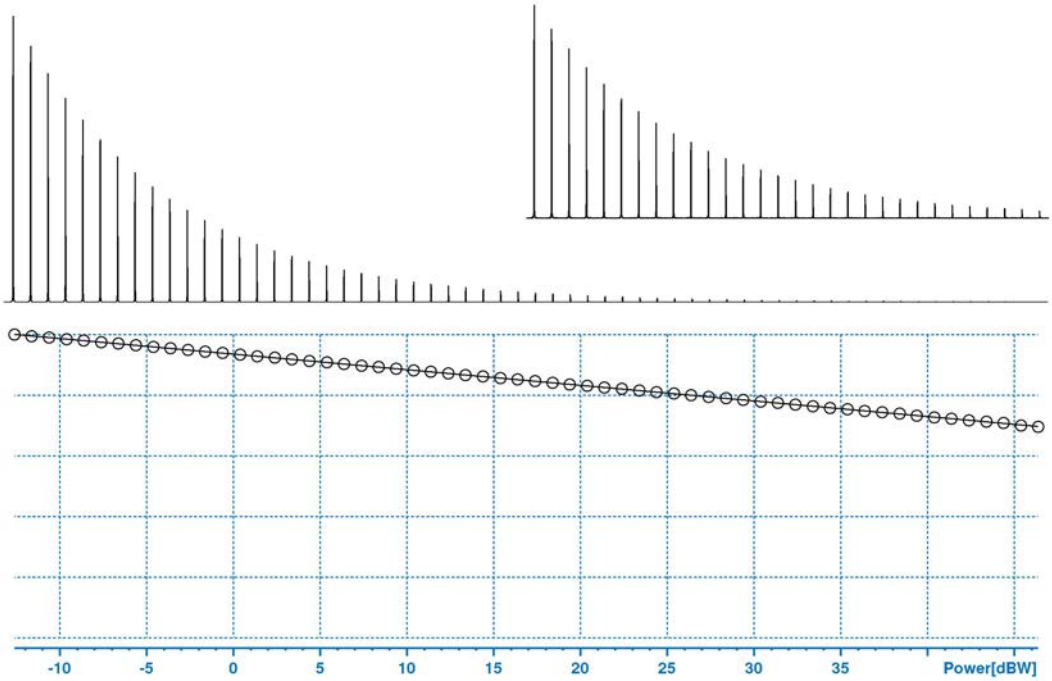
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 5.250 | ppm | |
| F2P | 4.250 | ppm | |
| CY | 15.000 | cm | |

## Experiment Description

The purpose of this test is the assessment of the spectrometer response to a series of pulses of increasing length and constant flip angle of 90 degrees.
The experiment starts with the pulse length and power level from prosol. The offset O1 is first optimized (PROCNOs 10 and 11).
Afterwards, a series of experiments where the pulse length is successively doubled and the power level divided by four is acquired, processed and stored in PROCNO 999.
The quality criterion of the test is the minimum peak intensity relative to the maximum peak intensity (normalized to 100 percent) and should be as high as possible.

### 5.2.83 Linearity test with decreasing power (NPT_1H_linearityDecreasingPower)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top: Plot of the water peak intensities as a function of the logarithmically decreasing power level (dBW) for a constant pulse length.
Top detail: 50% width zoom plot of the lower intensities to the right.
Bottom: Logarithmic plot of the upper plot along with a linear fit.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | syszg4 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.688 | ppm | |
| SW | 16.442 | ppm | |
| TD | 8192 | | |
| AQ | 0.623 | s | field dependent |
| FIDRES | 1.606 | Hz | field dependent |
| D 1 | 0.200 | s | |
| P 1 | 3.1 | us | 20deg Pulse |
| PLW 1 | | W | adjusted power |
| TE | 298.000 | K | default |

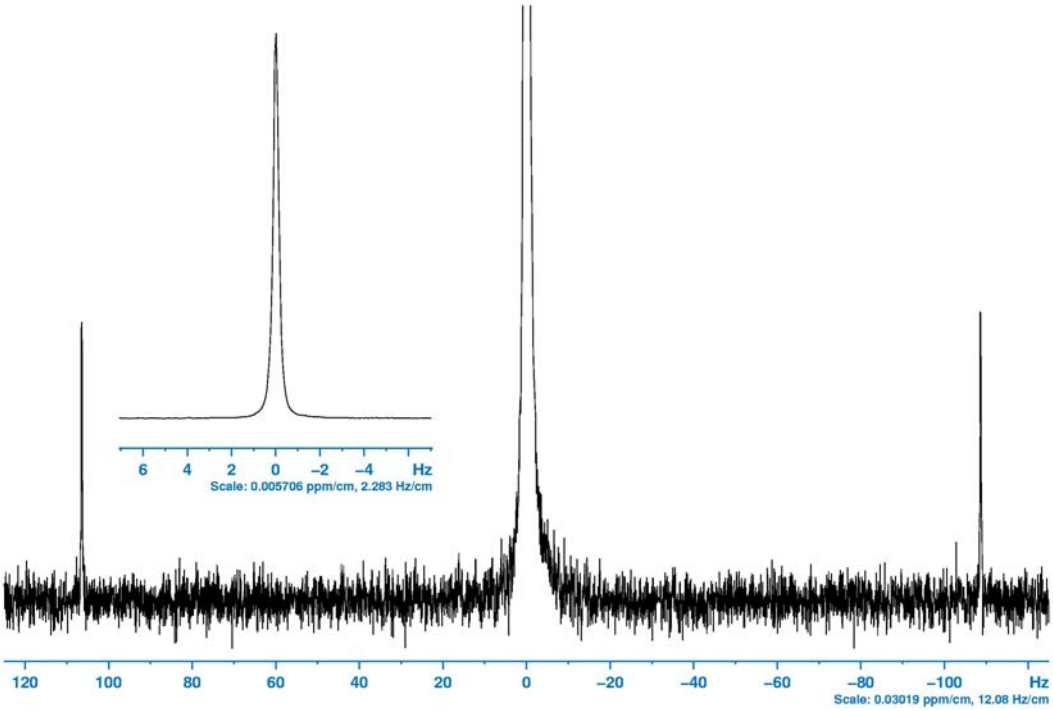
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 5.250 | ppm | |
| F2P | 4.250 | ppm | |
| CY | 15.000 | cm | |

## Experiment Description

Purpose of this test is the assessment of the spectrometer response to a series of pulses of constant duration and logarithmically decreasing power.
The experiment starts with the power level from prosol and a pulse length corresponding to a 20 degrees pulse. The offset O1 is first optimized (PROCNOs 10 and 11). Second, a series of experiments with decreasing power level (1dB-steps) is acquired, processed and stored in PROCNO 999.
Simfit is then used to obtain a linear fit of log10(peak amplitude) as a function of the power level in dBW. The quality criterion of the test is the standard deviation of the linear fit which should be as small as possible.

## 5.2.84 1H lineshape without sample rotation (NPT_1H_lineshape_nrot)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z10248, Z10701, Z100926, Z10250, Z10702, Z10031, Z10030, Z10029, Z10249, Z10275, Z10272, Z10717
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Proton line shape spectrum with offset calibration to O1P as overview spectrum. Printing is from +125.0 Hz to -125.0 Hz. The expansion plot to the left shows chloroform signal with higher resolution (+7.0 Hz, -7.0 Hz).

**Control Option for Acquisition (L23)**

1 default
2 write default shimfile, in case of successful evaluation

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg30 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 7.700 | ppm | |
| SWH | 1000.000 | Hz | |
| TD | 32768 | | |
| AQ | 16.384 | s | |
| FIDRES | 0.061 | Hz | |
| D 1 | 9.116 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

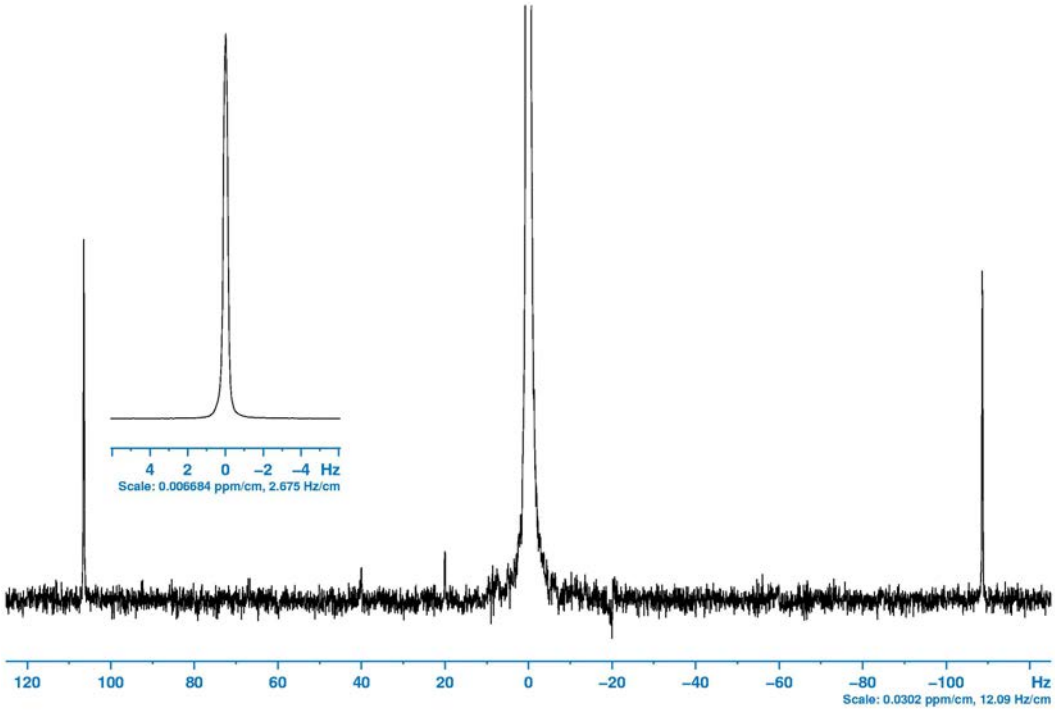
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 8.640 | ppm | |
| F2P | 7.440 | ppm | |
| CY | 1000.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 0.200 | | Scaling factor for CY |

### Experiment Description

Before acquiring the final spectrum, the exact signal position is determined with NS=1. The carrier position is afterwards set to the position
optimized O1 = peak frequency [Hz] - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.
Setting L23=2, it is possible to store the standard shimfile provided the evaluation of the experiment is successful. This event takes place during acquisition only. During regular processing of the data no shimfile is stored.

## 5.2.85 1H lineshape with sample rotation and NS = 4 (NPT_1H_lineshape_wrot)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z10248, Z10701, Z100926, Z10250, Z10702, Z10031, Z10030, Z10029, Z10249, Z10275, Z10272, Z10717
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Proton line shape spectrum with offset calibration to O1P as overview spectrum. Printing is from +125.0 Hz to -125.0 Hz. The expansion plot to the left shows chloroform signal with higher resolution (+7.0 Hz, -7.0 Hz).

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg30 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 7.700 | ppm | |
| SWH | 1000.000 | Hz | |
| TD | 32768 | | |
| AQ | 16.384 | s | |
| FIDRES | 0.061 | Hz | |
| D 1 | 9.116 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

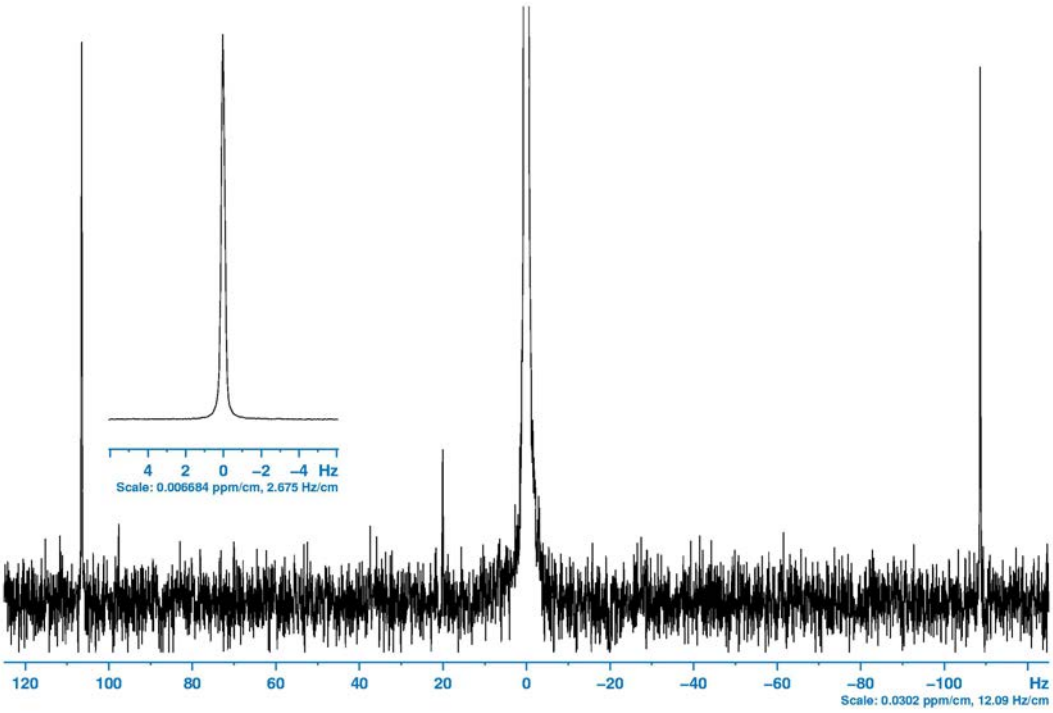
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 8.640 | ppm | |
| F2P | 7.440 | ppm | |
| CY | 1000.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 0.200 | | Scaling factor for CY |

## Experiment Description

Before acquiring the final spectrum, the exact signal position is determined with NS=1. The carrier position is afterwards set to the position
optimized O1 = peak frequency [Hz] - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.

## 5.2.86 1H lineshape with sample rotation and NS = 1 (NPT_1H_lineshape_wrot_ns1)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z10248, Z10701, Z100926, Z10031, Z10030, Z10029, Z10249, Z10275, Z10717
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Proton line shape spectrum with offset calibration to O1P as overview spectrum. Printing is from +125.0 Hz to -125.0 Hz. The expansion plot to the left shows chloroform signal with higher resolution (+7.0 Hz, -7.0 Hz).

**Control Option for Acquisition (L23)**

1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg30 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 7.700 | ppm | |
| SWH | 1000.000 | Hz | |
| TD | 32768 | | |
| AQ | 16.384 | s | |
| FIDRES | 0.061 | Hz | |
| D 1 | 9.116 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

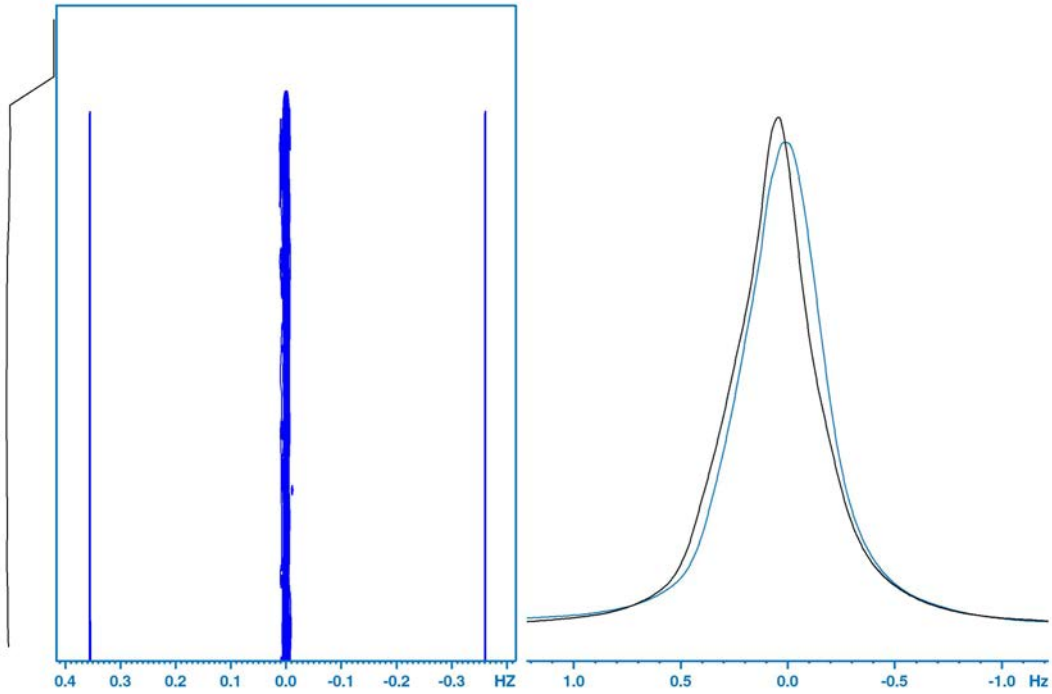
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 8.640 | ppm | |
| F2P | 7.440 | ppm | |
| CY | 1000.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 0.200 | | Scaling factor for CY |

### Experiment Description

Before acquiring the final spectrum, the exact signal position is determined with NS=1. The carrier position is afterwards set to the position
optimized O1 = peak frequency [Hz] - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.
In order to get better statistics for spinning sideband values, the number of scans is reduced to 1.
Evaluation is the same as for the standard experiment.

## 5.2.87 1H lineshape stability test (NPT_1H_lineshapeStability)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z10248, Z10701, Z100926, Z10250, Z10702, Z10031, Z10030, Z10029, Z10249, Z10275, Z10272, Z10717
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

The 2D plot to the left shows all measured line shape experiments as pseudo 2D and their F1 projection. The plot to the right shows the experiment with the highest (black) and lowest (blue) resolution.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg2d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 8.000 | ppm | |
| SWH | 1315.789 | Hz | |
| TD | 65536 | | |
| AQ | 24.904 | s | |
| FIDRES | 0.040 | Hz | |
| D 20 | 600.000 | s | repetition rate |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

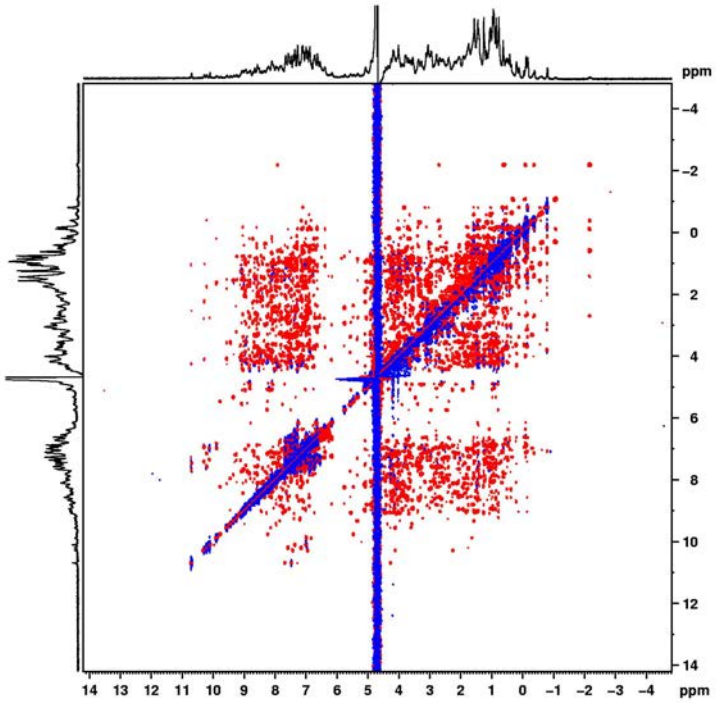
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 262144 | | |
| LB | 0.000 | Hz | |
| F1P | 5.201 | ppm | |
| F2P | 4.201 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

In the line shape stability test a certain number of 1D spectra will be acquired on a CHCl3 sample. The repetion rate, given by delay D20, must be high enough (10 min) to gurantee complete relaxation.

## 5.2.88 2D NOESY (NPT_1H_noesyphpr)

**Test Sample:** 2 mM Lysozyme in 90% H2O + 10% D2O
Z10241
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Phase sensitive NOESY with presaturation during mixing and relaxation delay. 1D watersuppression experiment is shown at the left and at the top of the 2D.

**Control Option for Acquisition (L23)**

1 default, with O1 optimization
2 no O1 optimization, the optimization of O1 is enforced, if O1 was not determined during a previous measurement.

## Parameters

| **F2 ACQU** | | | Parameters F2 |
|---|---|---|---|
| NUC1 | 1H | | |
| FnMODE | 5 | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | noesyphpr | | |
| NS | 8 | | |
| DS | 16 | | |
| RG | 0.250 | | optim. by RGA |
| TD0 | 1 | | |
| SW | 20.485 | ppm | |
| TD | 4096 | | |
| AQ | 0.250 | s | field dependent |
| FIDRES | 4.002 | Hz | field dependent |
| D 1 | 2.000 | s | |
| D 8 | 0.150 | s | mixing time |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |
| DSPFIRM | 4 | | rectangle |
| DIGMOD | 3 | | baseopt |
| DE | 40.000 | us | set after getprosol |

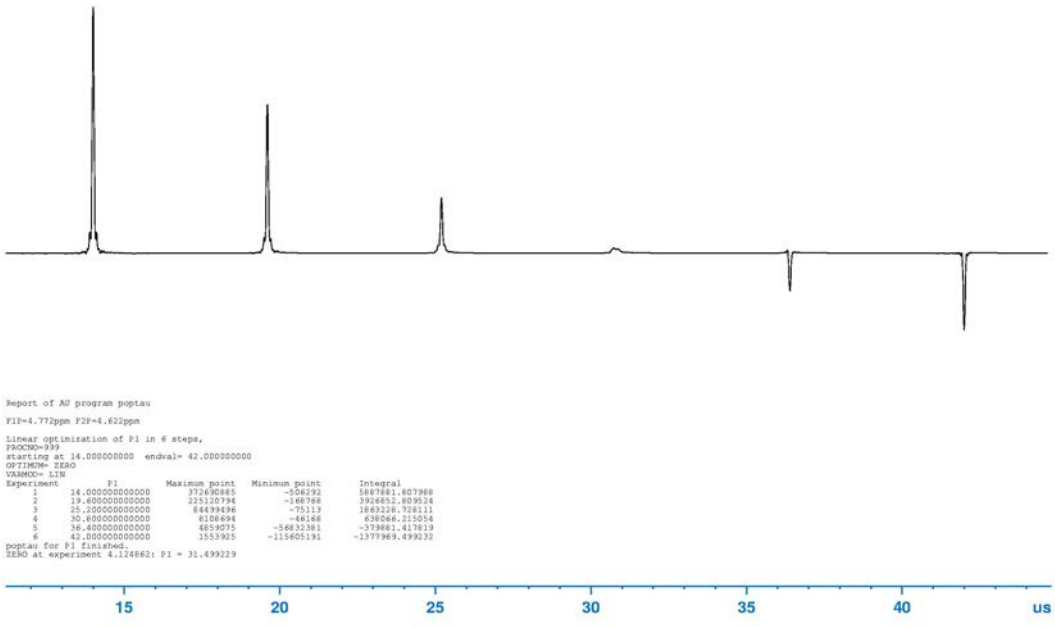
| **F2 PROC** | | | Parameters F2 |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 4 | | |
| SSB | 4.000 | | |
| PH_mod | 1 | | pk |
| F1P | 24.732 | ppm | |
| F2P | -15.316 | ppm | |
| LEV0 | 4.250 | | |
| TOPLEV | 50.000 | % | |
| NLEV | 20 | | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| FnMODE | 5 | | |
| O1P | 4.708 | ppm | |
| SW | 20.485 | ppm | |
| TD | 512 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 2048 | | |
| WDW | 4 | | |
| SSB | 4.000 | | |
| PH_mod | 1 | | pk |
| PHC0 | 90.000 | deg | 90deg (default) |
| PHC1 | -180.000 | deg | 180deg (default) |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

Phase sensitive NOESY with presaturation.
Presaturation requires the exact determination of the irradiation position (O1P). The determination is executed in a derived data set using the parameter set 'NPT_1H_watersuppression_recflow'.
Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
Option L23=2 will skip the procedure just outlined above.
RG can be set in the Preparation Panel. If RG <= 1 RGA will be exectued after O1 determination in the derived data set.
Processing is achieved using the phase correction values from the preparation experiment.
Contour levels for 2D spectrum are obtained by command levcalc. Levcalc sets the lowest contour level to LEV0*S_DEV, where S_DEV (standard deviation) is a processing status parameter.

## 5.2.89 P90 1H pulse calibration 0.5M NaCl (NPT_1H_p90_05M_NaCl_1h)

**Test Sample:** 0.5 M Sodium Chloride (NaCl) in D2O
Z10288, Z101716, Z101712, Z100376, Z100372, Z10730
**Solvent:** D2O_salt
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg.

### Control Option for Acquisition (L23)

1 default
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 300 | | |
| AQ | 0.650 | s | |
| FIDRES | 1.538 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

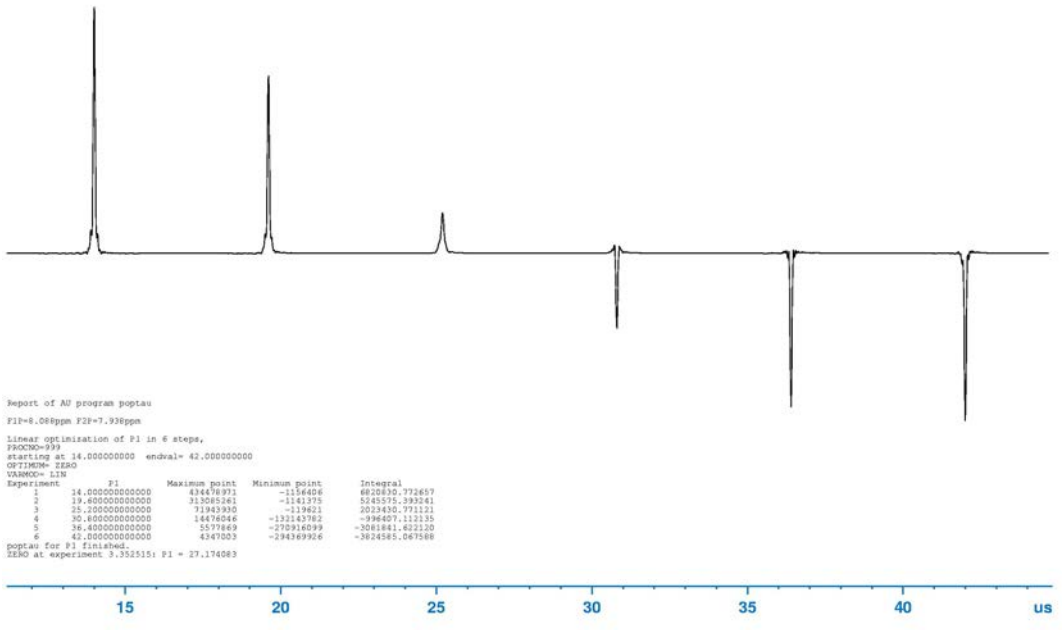
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 3 | | |
| LB | 0.750 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.496 | ppm | |
| F2P | 5.096 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL generic table. Prior to the execution of P90 determination for a given solvent, the standard p90 experiment on the urea sample must be executed.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. The information about O1, RG, PHC0, PHC1 is stored to a separate file to be used during the a possible repetition of the determination.
Before the acquisition, the proton 90 degrees pulse is calibrated using POPT, which result is stored in the corresponding derived dataset. The calibrated pulse, which is not set in prosol, is written in the acquisition title along with the starting pulse length and power from prosol.
The determination of the pulse is executed once in six steps. For the determined pulse at the used power the PROSOL table for the given solvent is updated.Results are stored under PROCNO 999.

## 5.2.90 P90 1H pulse calibration acetone (NPT_1H_p90_acetone_1h)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z100926, Z10031, Z10030, Z10029, Z10249, Z10275, Z10717
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg.

### Control Option for Acquisition (L23)

1 default
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 8.020 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 300 | | |
| AQ | 0.650 | s | |
| FIDRES | 1.538 | Hz | |
| D 1 | 255.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

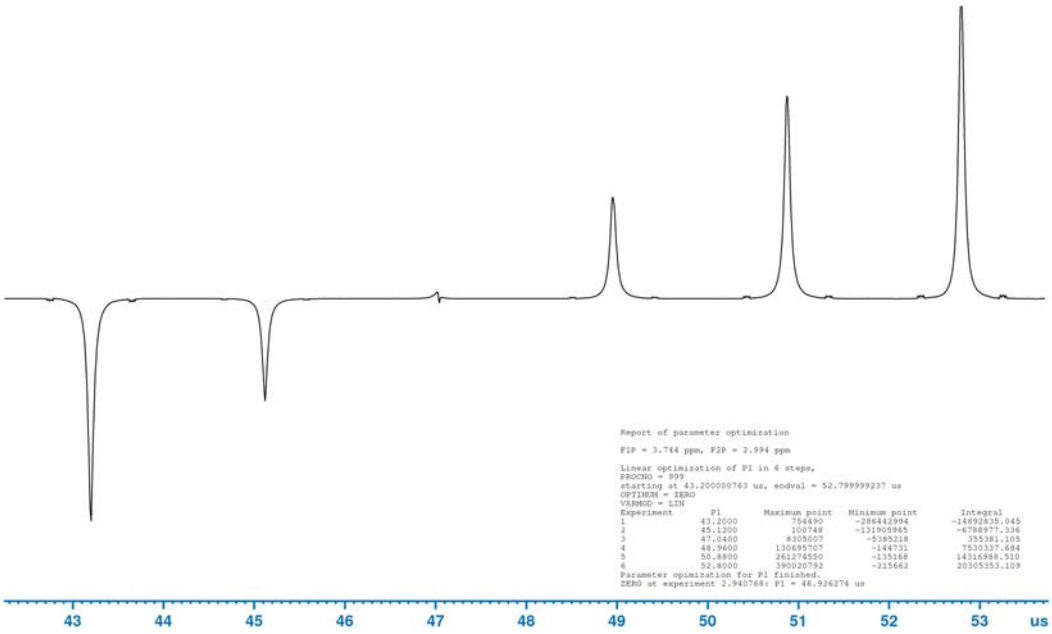
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 3 | | |
| LB | 0.750 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.496 | ppm | |
| F2P | 5.096 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL generic table. Prior to the execution of P90 determination for a given solvent, the standard p90 experiment on the urea sample must be executed.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. The information about O1, RG, PHC0, PHC1 is stored to a separate file to be used during the a possible repetition of the determination.
The determination of the pulse is executed once in six steps. For the determined pulse at the used power the PROSOL table for the given solvent is updated.Results are stored under PROCNO 999.

## 5.2.91 P90 1H pulse calibration (NPT_1H_p90det_astm_1h)

**Test Sample:** 40% Dioxane in Benzene-D6 (ASTM)
Z10163, Z100929, Z10164, Z10035, Z10255, Z10242, Z10724
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments arround 360 deg.

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| SWH | 1250.000 | Hz | |
| TD | 1048 | | |
| AQ | 0.419 | s | |
| FIDRES | 2.385 | Hz | |
| O1P | 3.375 | ppm | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| DIGMOD | 3 | | baseopt |
| DSPFIRM | 4 | | rectangle |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 1024 | | |
| LB | 2.000 | Hz | |
| F1P | 3.625 | ppm | |
| F2P | 3.125 | ppm | |
| CY | 5.500 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).

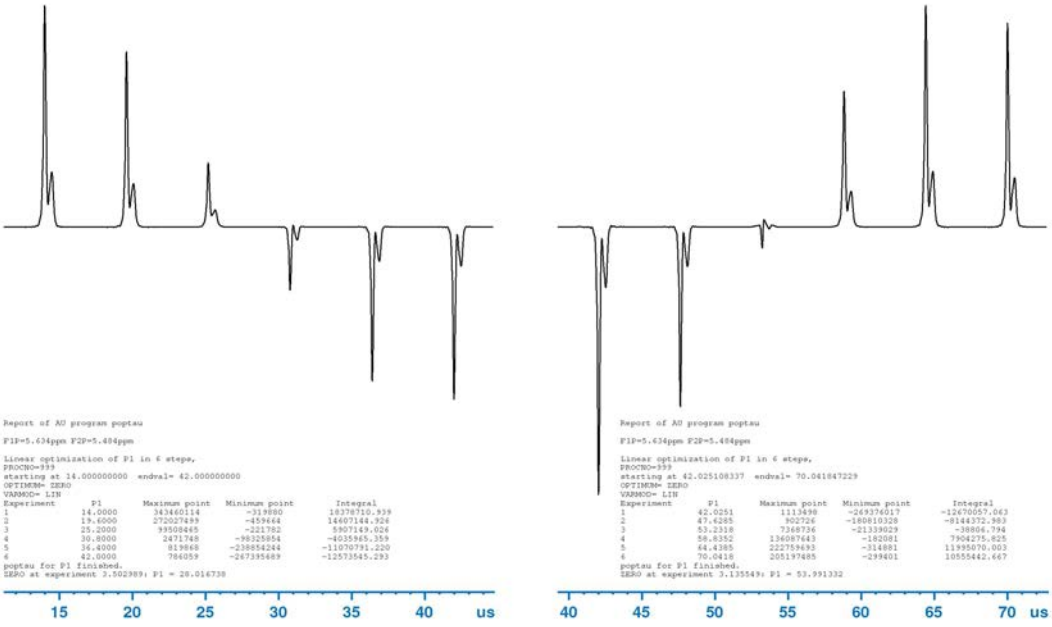
## 5.2.92 P90 1H pulse calibration (NPT_1H_p90determinationf1_1h)

**Test Sample:** (a) 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
(b) 40% Dioxane in Benzene-D6 (ASTM)
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721, Z142223

**Solvent:** (a) DMSO
(b) C6D6

**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table

**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 5.500 | ppm | (Urea Sample) |
| O1P | 3.38 | ppm | (Dioxane Sample) |
| SWH | 230.766 | Hz | (Urea Sample) |
| SWH | 1500.0 | Hz | (Dioxane Sample) |
| TD | 300 | | (Urea Sample) |
| TD | 1024 | | (Dioxane Sample) |
| AQ | 0.650 | s | (Urea Sample) |
| AQ | 0.341 | s | (Dioxane Sample) |
| FIDRES | 1.538 | Hz | (Urea Sample) |
| FIDRES | 2.93 | Hz | (Dioxane Sample) |
| D 1 | 1.225 | s | AQ+D1=const (Urea) |
| D1 | 30.0 | s | (Dioxane Sample) |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

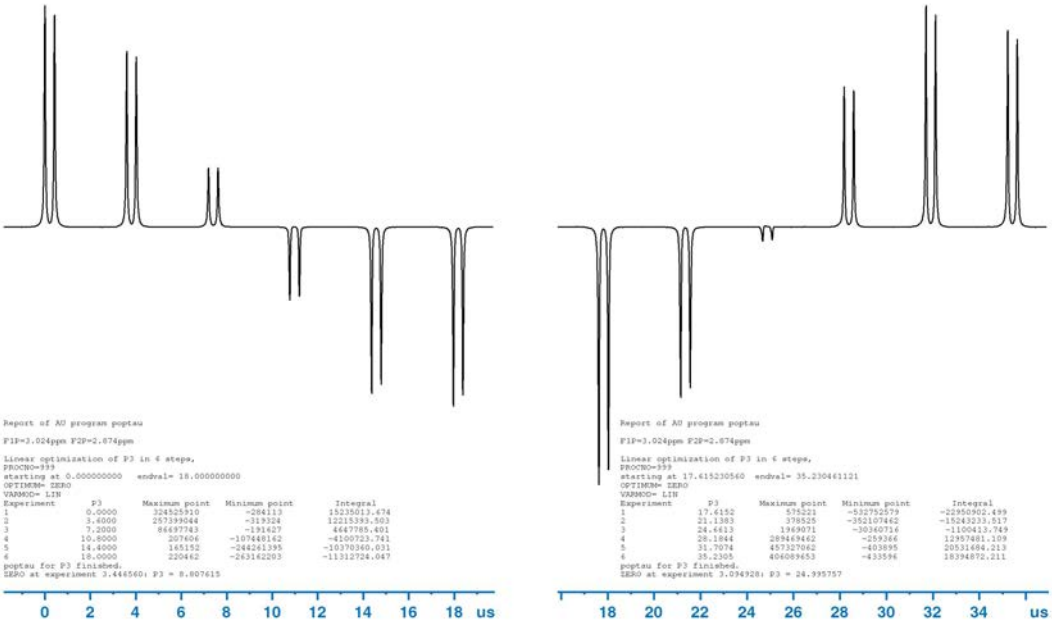
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 3 | | (Urea Sample) |
| WDW | 1 | | (Dioxane Sample) |
| LB | 0.750 | Hz | (Urea Sample) |
| LB | 10.0 | Hz | (Dioxane Sample) |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.496 | ppm | |
| F2P | 5.096 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.93 Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721, Z142223
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the decoupler pulse. On the left side the result of a CONVTO1D routine shows six experiments from 0 to 180 deg (PROCNO 100). On the right side the series goes from 180 to 360 deg (PROCNO 200).

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | decp90 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 3.012 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 1000 | | |
| AQ | 2.167 | s | |
| FIDRES | 0.462 | Hz | |
| D 1 | 1.710 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| P 3 | 9.0 | us | 90deg NUC1 |
| PLW 2 | 42.0 | W | Pow@90deg(Specs) NUC2 |
| TE | 298.000 | K | default |

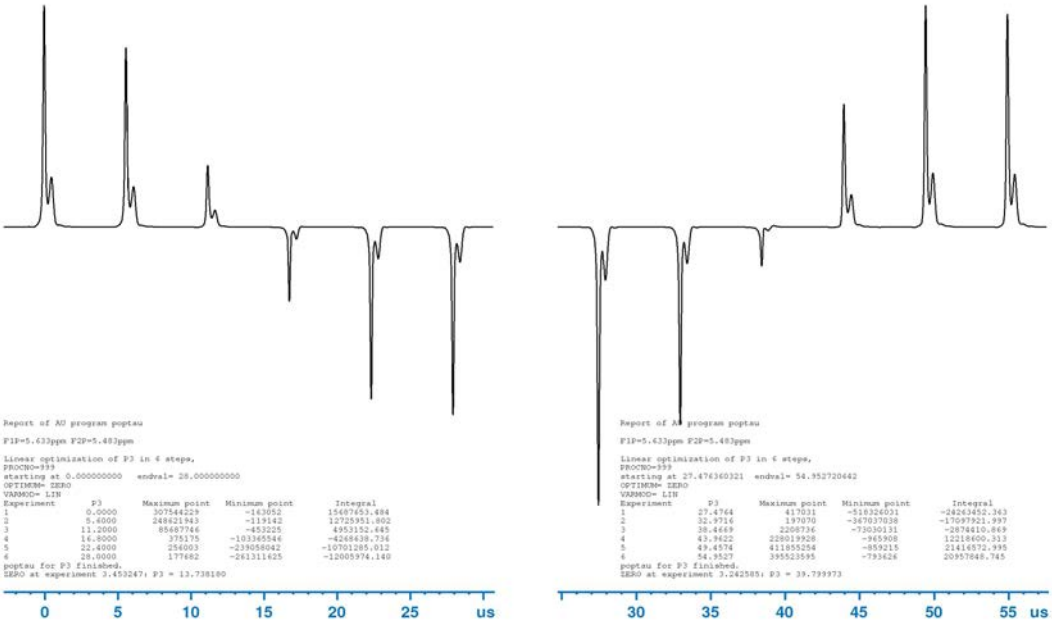
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 1 | | |
| LB | 0.500 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 3.150 | ppm | |
| F2P | 2.850 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 270 and 90 degree pulse lengths and memorised for further use in B1 homogeneity experiments.

## 5.2.94 Indirect P90 15N pulse calibration (NPT_1H_p90determinationf2_15n)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721, Z142223
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the decoupler pulse. On the left side the result of a CONVTO1D routine shows six experiments from 0 to 180 deg (PROCNO 100). On the right side the series goes from 180 to 360 deg (PROCNO 200).

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | decp90 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 5.500 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 200 | | |
| AQ | 0.433 | s | |
| FIDRES | 2.308 | Hz | |
| D 1 | 0.433 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| P 3 | 14.0 | us | 90deg NUC1 |
| PLW 2 | 86.0 | W | Pow@90deg(Specs) NUC2 |
| TE | 298.000 | K | default |

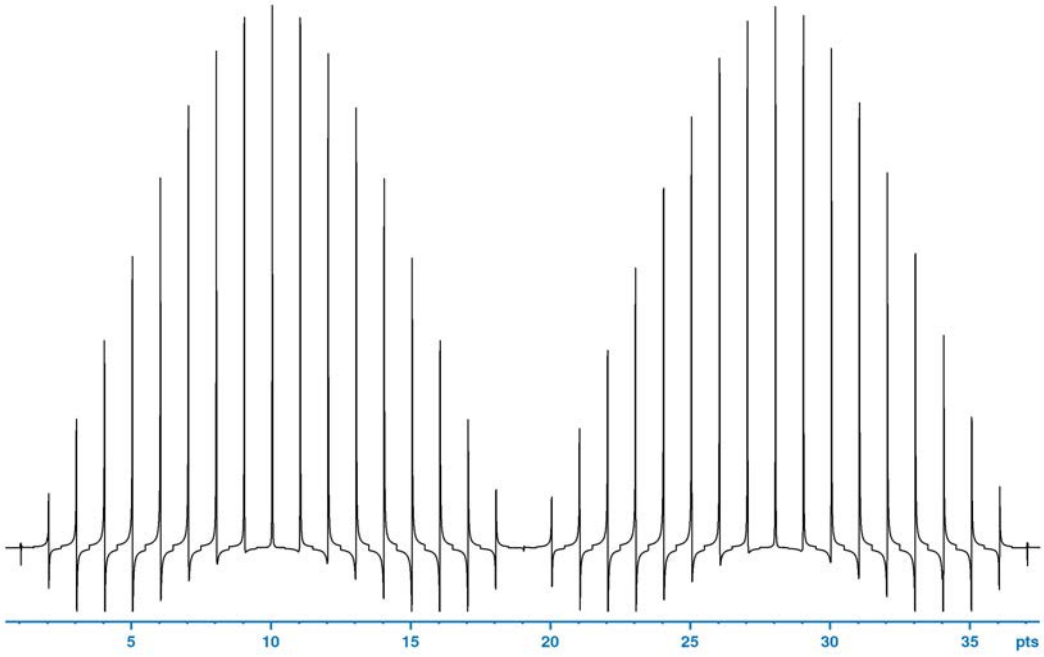
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 3 | | |
| LB | 0.750 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.667 | ppm | |
| F2P | 5.367 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 270 and 90 degree pulse lengths and memorised for further use in B1 homogeneity experiments.

## 5.2.95 Phase propagation test (NPT_1H_phase_propagation)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Series of spectra showing the water peak where, while maintaining the phase of the first pulse of the receiver to 0 degree, the phase of the second pulse is varied from 0 degree to 360 degrees in 10 degree steps.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | sysphas2f1 | | |
| NS | 1 | | |
| DS | 4 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 4.698 | ppm | |
| SW | 16.442 | ppm | |
| TD | 8192 | | |
| AQ | 0.623 | s | field dependent |
| FIDRES | 1.606 | Hz | field dependent |
| D 1 | 0.200 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

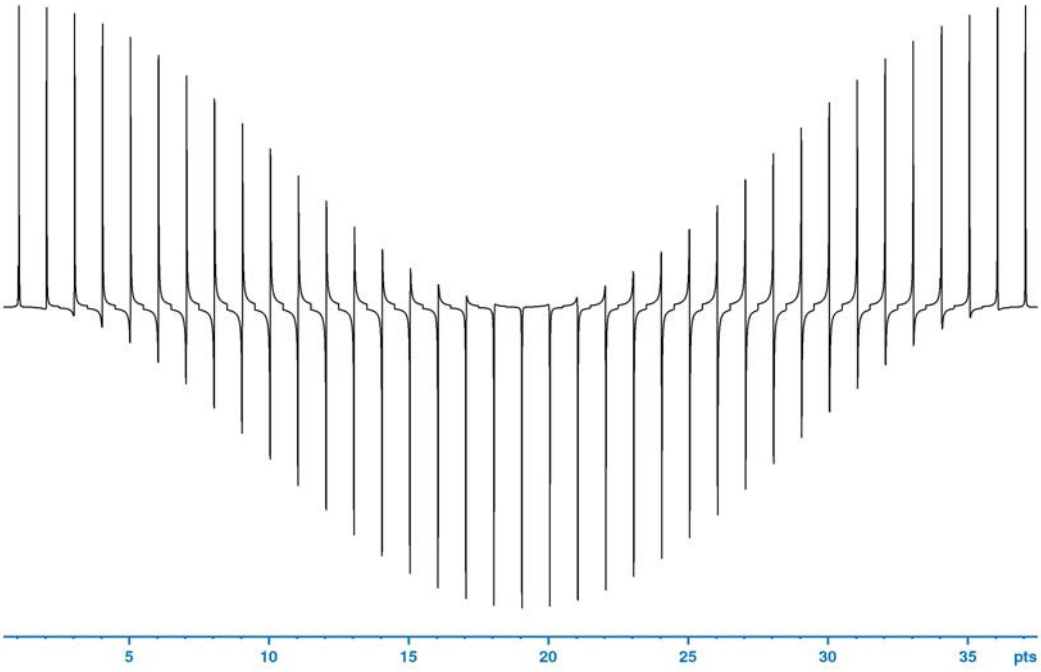
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 5.250 | ppm | |
| F2P | 4.250 | ppm | |
| CY | 15.000 | cm | |

## Experiment Description

This test consists in a series of pairs of 90 degree pulses of constant power and duration recorded in a two-dimensional fashion. The phase of the second pulse is varied from 0 to 360 degrees in 10 degree steps, while maintaining the phases of the first pulse and of the receiver set to zero degree. The 2D-spectrum is stored in procno 1 and the result as a series of 1D spectra in procno 999.

## 5.2.96 Phase shifting test (NPT_1H_phase_shifting)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Series of spectra showing the water peak where the phase of the pulse is varied from 0 degree to 360 degrees in 10 degree steps, while maintaining the phase of the receiver to 0 degree.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | sysphasf1 | | |
| NS | 1 | | |
| DS | 4 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 4.698 | ppm | |
| SW | 16.442 | ppm | |
| TD | 8192 | | |
| AQ | 0.623 | s | field dependent |
| FIDRES | 1.606 | Hz | field dependent |
| D 1 | 0.200 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

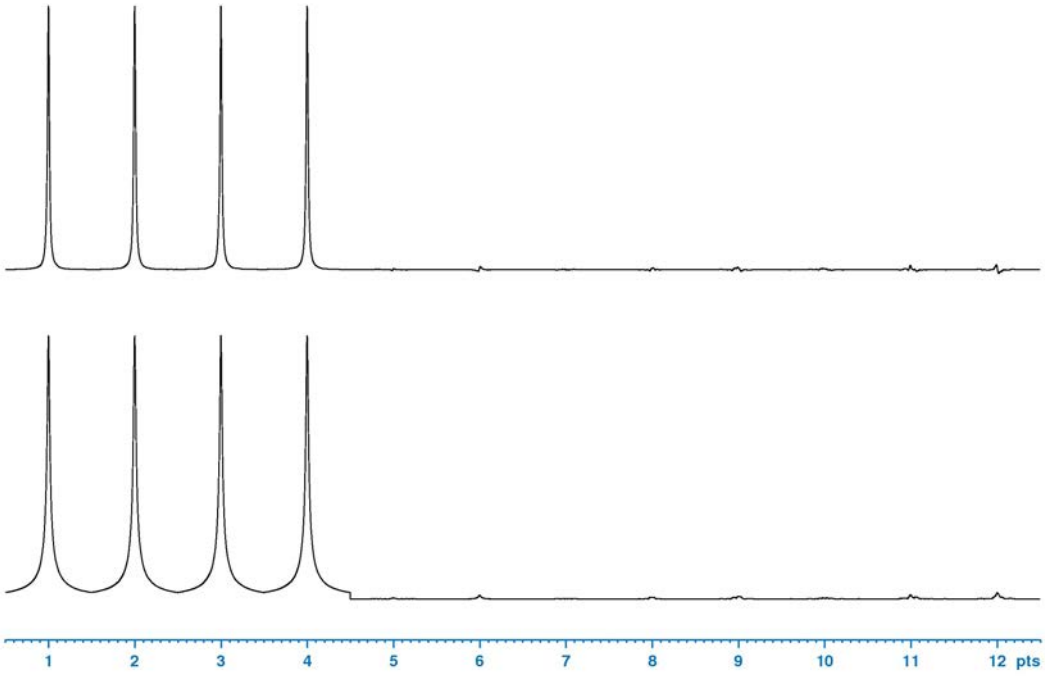
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 5.250 | ppm | |
| F2P | 4.250 | ppm | |
| CY | 15.000 | cm | |

## Experiment Description

This test consists in a series of 90 degree pulses of constant power and duration recorded in a two-dimensional fashion. The phase of the pulse is varied from 0 to 360 degrees in 10 degree steps, while maintaining the phase of the receiver set to zero degree. The 2D-spectrum is stored in procno 1 and the result as a series of 1D spectra in procno 999.

## 5.2.97 Phase cycle cancelation (NPT_1H_phaseCycleCancelation)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top: Series of twelve spectra showing the residual water peak in phase-sensitive mode with NS=1,1,1,1,2,2,2,2,4,4,4 and 4.
Bottom: Same series as the top but in magnitude mode.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | syscancel | | |
| NS | | | varied parameter |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.697 | ppm | |
| SW | 16.442 | ppm | |
| TD | 8192 | | |
| AQ | 0.623 | s | field dependent |
| FIDRES | 1.606 | Hz | field dependent |
| D 1 | 0.200 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

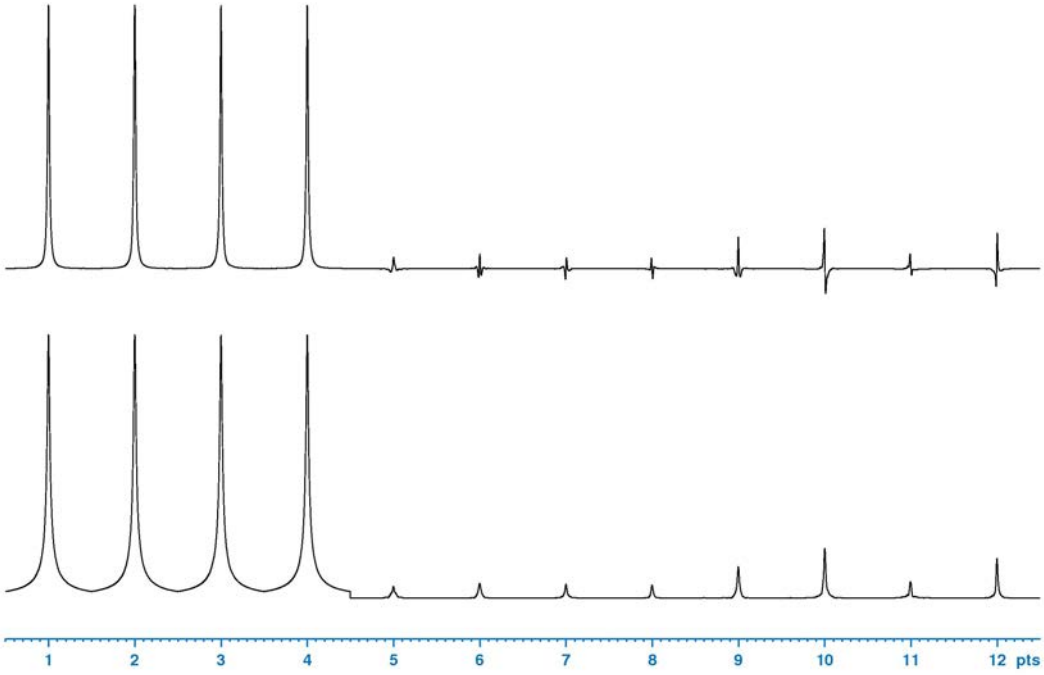
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 5.250 | ppm | |
| F2P | 4.250 | ppm | |
| CY | 15.000 | cm | |

## Experiment Description

The aim of this test is the assessment of the signal cancelation by a two-steps and a four-steps phase cycle. The test consists of a 90 degree pulse which is phase-cycled, while maintaining the receiver phase set to zero.
The test comprises twelve experiments. The first four are recorded with NS=1, i.e. without phase cycling suppression. The average signal intensity of these four experiments is set to 100 percent. The next four experiments are acquired with NS=2, meaning a two-steps phase cycle (0 and 180 degrees). Finally, the last four experiments are recorded with NS=4 which corresponds to a four-steps phase-cycling (0, 180, 90 and 270 degrees).

## 5.2.98 Phase cycle cancelation after gradient pulse (NPT_1H_phaseCycleCancelationGrad)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top: Series of twelve spectra showing the residual water peak in phase-sensitive mode with NS=1,1,1,1,2,2,2,2,4,4,4 and 4.
Bottom: Same series as the top but in magnitude mode.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | sysgrcan | | |
| NS | | | varied parameter |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.697 | ppm | |
| SW | 16.442 | ppm | |
| TD | 8192 | | |
| AQ | 0.623 | s | field dependent |
| FIDRES | 1.606 | Hz | field dependent |
| D 1 | 0.200 | s | |
| GPNAM1 | RECT.1 | | |
| GPZ 1 | 14.286 | % | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

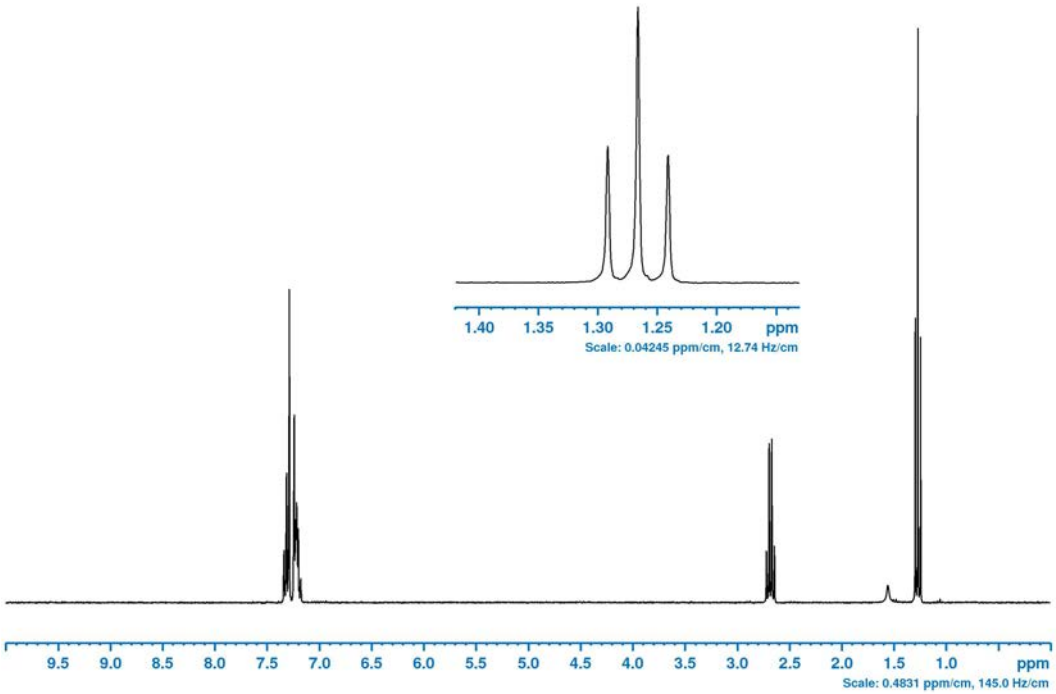
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PC | 1.000 | | |
| F1P | 5.250 | ppm | |
| F2P | 4.250 | ppm | |
| CY | 15.000 | cm | |

## Experiment Description

The aim of this test is the assessment of the signal cancelation by a two-steps and a four-steps phase cycle following a gradient pulse. The test consists of a Z-gradient pulse followed by a delay D16=100 us and finally a 90 degree pulse which is phase-cycled, while maintaining the receiver phase set to zero. The test comprises twelve experiments. The first four are recorded with NS=1, i.e. without phase cycling suppression. The average signal intensity of these four experiments is set to 100 percent. The next four experiments are acquired with NS=2, meaning a two-steps phase cycle (0 and 180 degrees). Finally, the last four experiments are recorded with NS=4 which corresponds to a four-steps phase-cycling (0, 180, 90 and 270 degrees).

## 5.2.99 1H quantification reference (NPT_1H_quant_ref)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10121, Z10033, Z10270, Z10718, Z142221
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

1H overview spectrum of ethylbenzene.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg30 | | |
| NS | 16 | | |
| DS | 2 | | |
| RG | 32.000 | | no optim. |
| O1P | 6.175 | ppm | |
| SW | 20.485 | ppm | |
| TD | 65536 | | |
| AQ | 3.998 | s | field dependent |
| FIDRES | 0.250 | Hz | field dependent |
| D 1 | 30.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

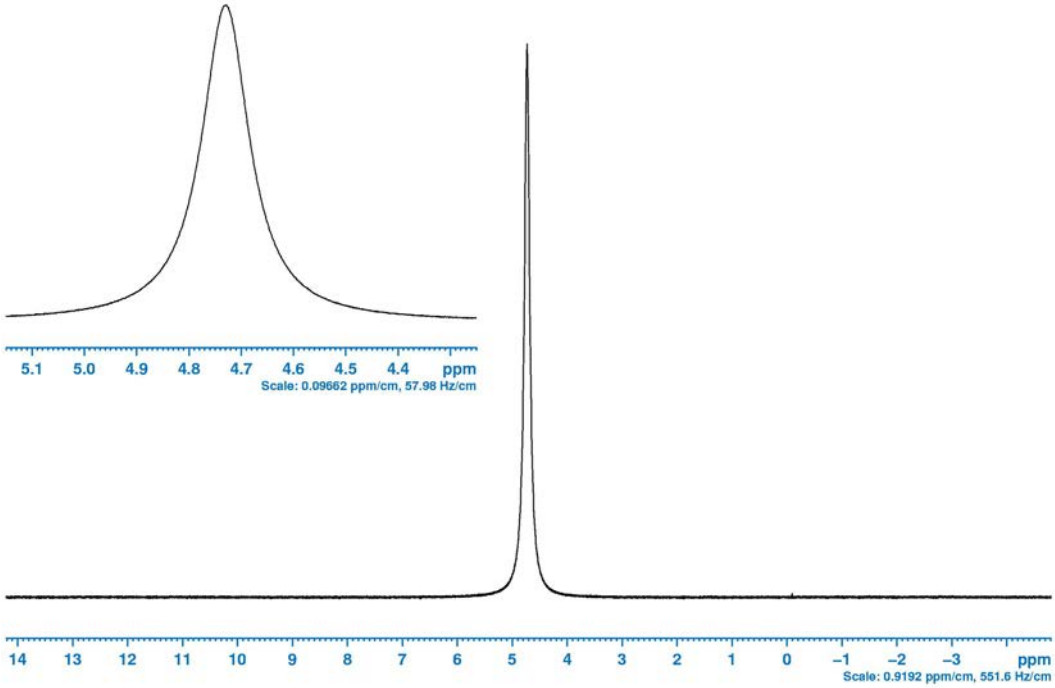
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 65536 | | |
| WDW | 1 | | |
| LB | 0.300 | Hz | |
| PC | 1.000 | | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

Quantification experiment using the ethylbenzen sample. This experiment is used as default reference by the eretic procedure. The expansion plot shows the quantified signal with higher resolution
Processing is done by the AU program cmc_proc1h_usup. For this reason the NMRPT processing options are ignored.

## 5.2.100 1H low flipangle single scan experiment (NPT_1H_rd)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

1H spectrum of H2O signal showing radiation damping effect (line broadening). Top left shows H2O signal expanded.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg0 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 2.000 | | no optim. |
| O1P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 5.000 | s | |
| P 0 | 1.0 | us | 1 us=1 deg |
| PLW 1 | 0.005 | W | Pow@1 deg=1 us NUC1 |
| TE | 298.000 | K | default |

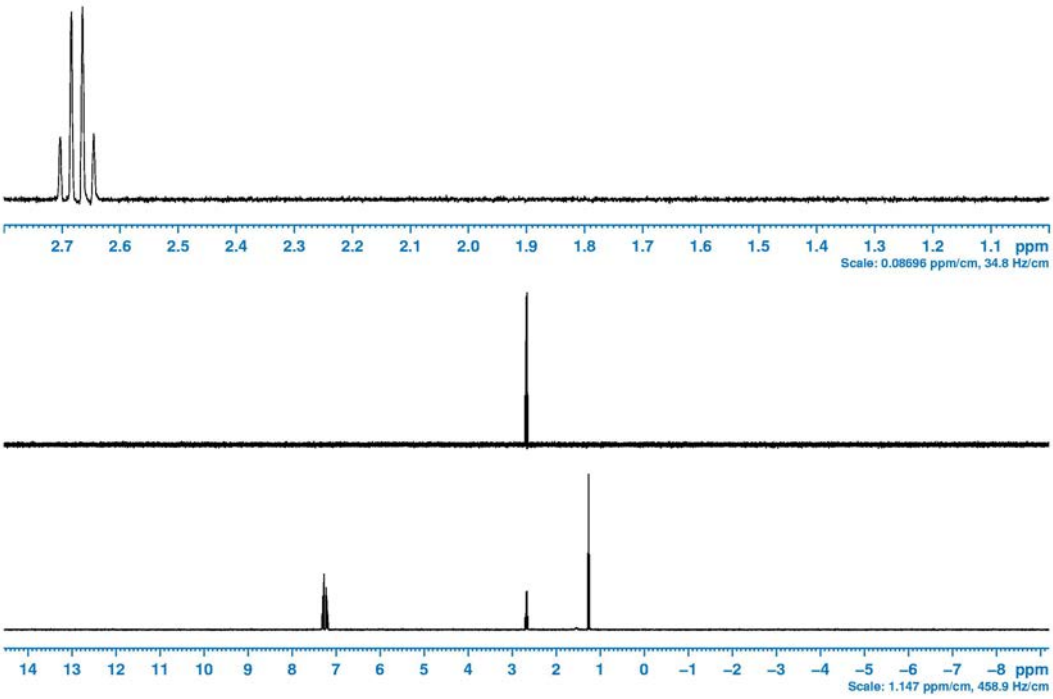
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| F1P | 10.806 | ppm | |
| F2P | -1.227 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Radiation damping experiment is executed with small flip angle as single scan experiment. NMRPT is calculating PLW1 according to the equation 1deg=1us. Processing is achieved with Fourier transformation without line broadening (LB=0). Evaluation consists of line width determination at 50% of signal height using the TopSpin AU program 'hwcal'.

## 5.2.101 1H selective excitation (NPT_1H_selex)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10121, Z10033, Z10270, Z10718
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Bottom: 1H overview spectrum of ethylbenzene using hard pulse. Center: 1H signal of methylene signal using selective excitation. Top: Selectively excitated 1H signal expanded including the noise region for evaluation.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | selzg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 2.673 | ppm | |
| SW | 24.992 | ppm | |
| TD | 65536 | | |
| AQ | 3.277 | s | field dependent |
| FIDRES | 0.305 | Hz | field dependent |
| D 1 | 119.000 | s | |
| P 11 | 20000.000 | us | P90 selective |
| SPW 1 | 0.000 | W | Pow@P90 sel. NUC1 |
| SPNAM1 | Gaus1.1000 | | shape |
| SPOAL 1 | 0.500 | | shape |
| SPOFFS 1 | 0.000 | | shape |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

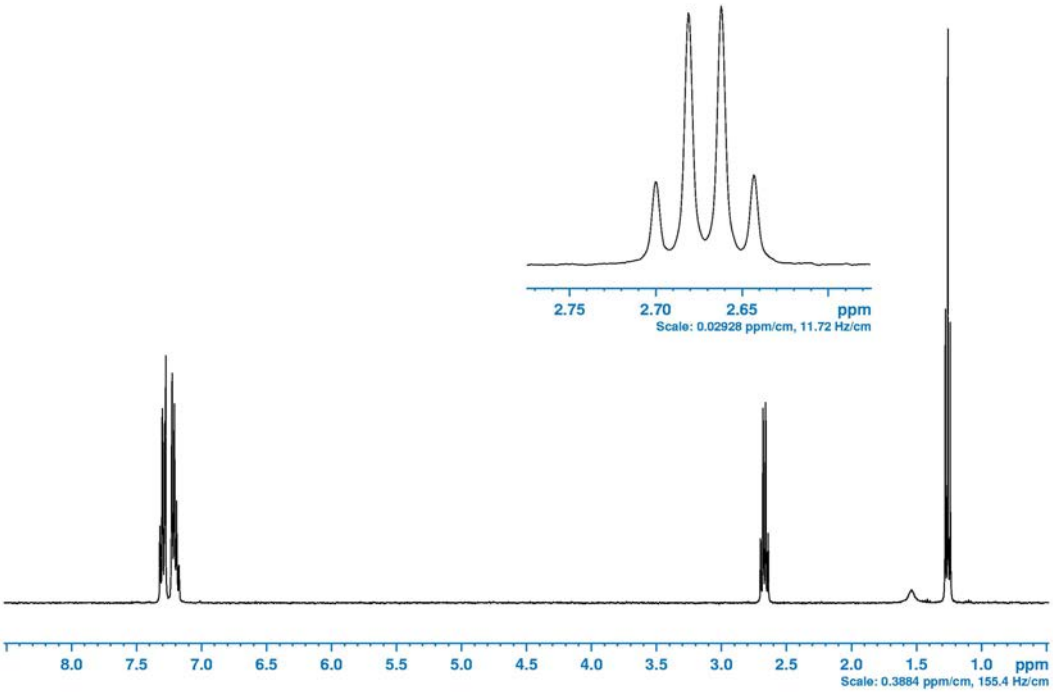
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 65536 | | |
| LB | 0.000 | Hz | |
| SIGF1 | 3.500 | ppm | |
| SIGF2 | 2.000 | ppm | |
| NOISF1 | 0.000 | ppm | |
| NOISF2 | -9.000 | ppm | |
| F1P | 8.000 | ppm | |
| F2P | -9.200 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Selective excitation experiment is carried out to show the quality with respect to selectivity of the frequency generation and the noise excitation of the amplifier. The experiment consists of two parts:
1) Reference acquisition using hard pulse, stored in derived dataset (EXPNO=1).
2) Selectively excited methylene signal using the same spectral parameters as for 1), stored in the main dataset.
Processing is for both spectra the same. Evaluation consists of signal-to-noise determinations for both experiments and the formation of the ratio of the two. The noise range (9 ppm) is fixed thereby the comparison becomes possible.

## 5.2.102 1H sensitivity (NPT_1H_sensitivity)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10121, Z10033, Z10270, Z10718, Z142221
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Bottom: 1H overview spectrum of ethylbenzene.
Top right: Expanded region showing the methylene signal used for evaluation.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.000 | ppm | |
| SW | 10.159 | ppm | |
| TD | 32768 | | |
| AQ | 4.030 | s | field dependent |
| FIDRES | 0.248 | Hz | field dependent |
| D 1 | 113.574 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

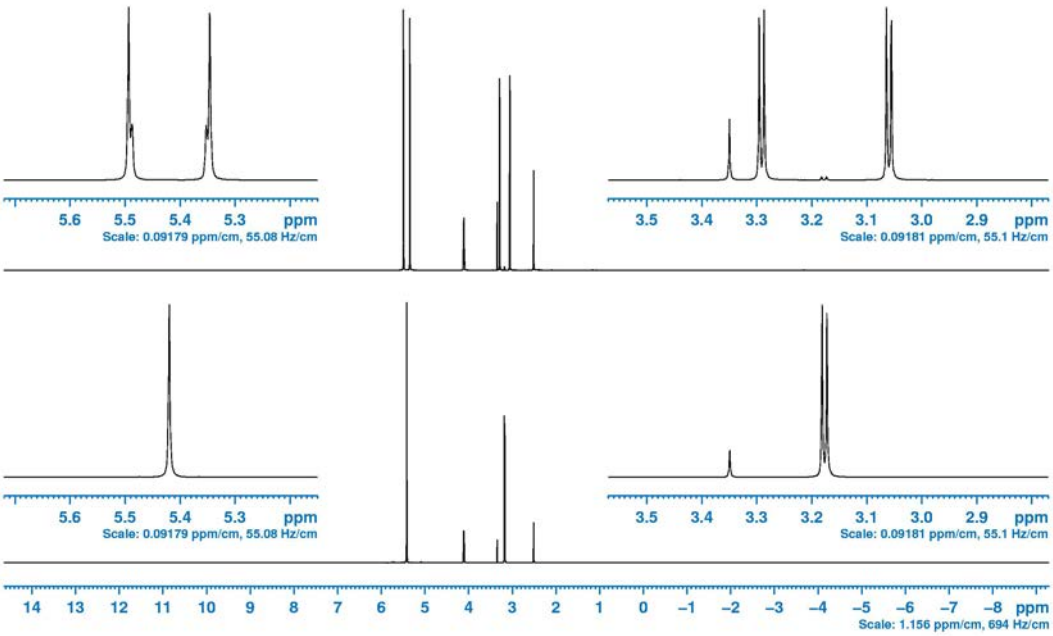
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 1.000 | Hz | 1.0 |
| SIGF1 | 3.000 | ppm | |
| SIGF2 | 2.000 | ppm | |
| NOISF1 | 7.000 | ppm | |
| NOISF2 | 2.800 | ppm | |
| F1P | 8.520 | ppm | |
| F2P | 0.480 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 57 | 1.000 | | Return Value Intensity InnoSinoShim |
| CNST 58 | 1.000 | | Return Value Integral InnoSinoShim |

## Experiment Description

Proton sensitivity is measured using the ethylbenzene sample. Processing is using LB. The signal-to-noise is determined using the methylene signal (CH2) of the molecule. The signal is searched over the range from 3.0 to 2.0 ppm, while the best 2 ppm or 200 Hz noise region is determined over the range from 7.0 to 2.8 ppm.

## 5.2.103 Triple resonance (NPT_1H_sensitivity_dec13c15n)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

1H spectra of 100 mM 15N labelled urea and 100 mM 13C labelled methanol. Spectra at the top without decoupling, spectra at the bottom with simultaneous 13C and 15N decoupling. The extensions on the left show the urea signals, the extensions on the rigth th methanol signals.

### Control Option for Acquisition (L23)

1 default

## Parameters

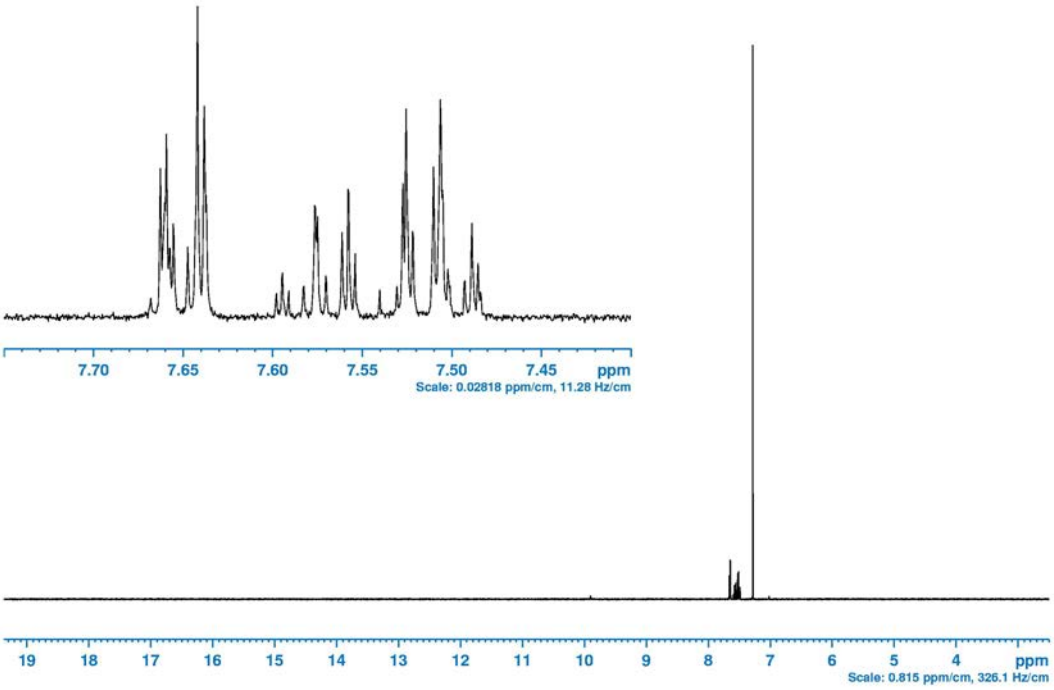
| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| NUC3 | 15N | | |
| PULPROG | npt_zg0fbig | | |
| NS | 8 | | |
| DS | 2 | | |
| RG | 1.000 | | no optim. |
| O1P | 2.670 | ppm | |
| O2P | 49.487 | ppm | |
| O3P | 75.986 | ppm | |
| SW | 24.992 | ppm | |
| TD | 32768 | | |
| AQ | 1.638 | s | field dependent |
| FIDRES | 0.610 | Hz | field dependent |
| D 1 | 30.000 | s | >10*T1 |
| P 0 | 6.0 | us | P 1 * CNST 10 / 90 |
| P 1 | 10.0 | us | 90deg NUC1 |
| PLW 1 | 15.0 | W | Pow@P90(Specs) |
| PLW 12 | 9.0 | W | Pow@CPD(Specs) NUC2 |
| PLW 16 | 8.2 | W | Pow@CPD(Specs) NUC3 |
| PCPD 2 | 50.0 | us | 90deg CPD NUC2 |
| CPDPRG2 | garp | | cpd seq. |
| PCPD 3 | 200.0 | us | 90deg CPD NUC3 |
| CPDPRG3 | garp | | cpd seq. |
| TE | 298.000 | K | default |
| CNST 10 | 60.000 | | flip angle |
| **F1 PROC** | | | Parameters |
| SI | 32768 | | |
| LB | 0.750 | Hz | |
| SIGF1 | 0.000 | ppm | |
| SIGF2 | 0.000 | ppm | |
| NOISF1 | 0.000 | ppm | |
| NOISF2 | -9.000 | ppm | |
| F1P | 6.500 | ppm | |
| F2P | 1.500 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |

## Experiment Description

Simultaneous decoupling on two nuclei (13C, 15N) is executed with the 15N-urea/13C-methanol sample. Two spectra are acquired (coupled, decoupled) using derived dataset with EXNPO=1 for the coupled spectrum and the current dataset for the decoupled spectrum.
Processing is executed with LB. Evaluation is comparing the signal-to-noise ratios (coupled/decoupled) for methylene group (13C, 3.6 to 2.8 ppm) and amino group (15N, 6.8 to 5.0 ppm) and the noise region from 0.0 to -9.0 ppm.

## 5.2.104 1H sensitivity with 19F GARP decoupling (NPT_1H_sensitivity_dec19f)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Bottom: 1H overview spectrum of trifluorotoluene with 19F decoupling.
Top left: Expanded region showing the signal region of the aromatic part of the molecule used for evaluation.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 19F | | |
| PULPROG | zgig | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 7.500 | ppm | |
| O2P | -62.498 | ppm | |
| SW | 24.992 | ppm | |
| TD | 32768 | | 32768 <500MHz, 65536 >=500 MHz |
| AQ | 1.638 | s | field dependent |
| FIDRES | 0.610 | Hz | field dependent |
| D 1 | 52.500 | s | |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.5 | W | Pow@P90(Specs) |
| PLW 12 | 0.064 | W | Pow@CPD(Specs) |
| CPDPRG2 | garp4 | | cpd seq. |
| TE | 298.000 | K | default |

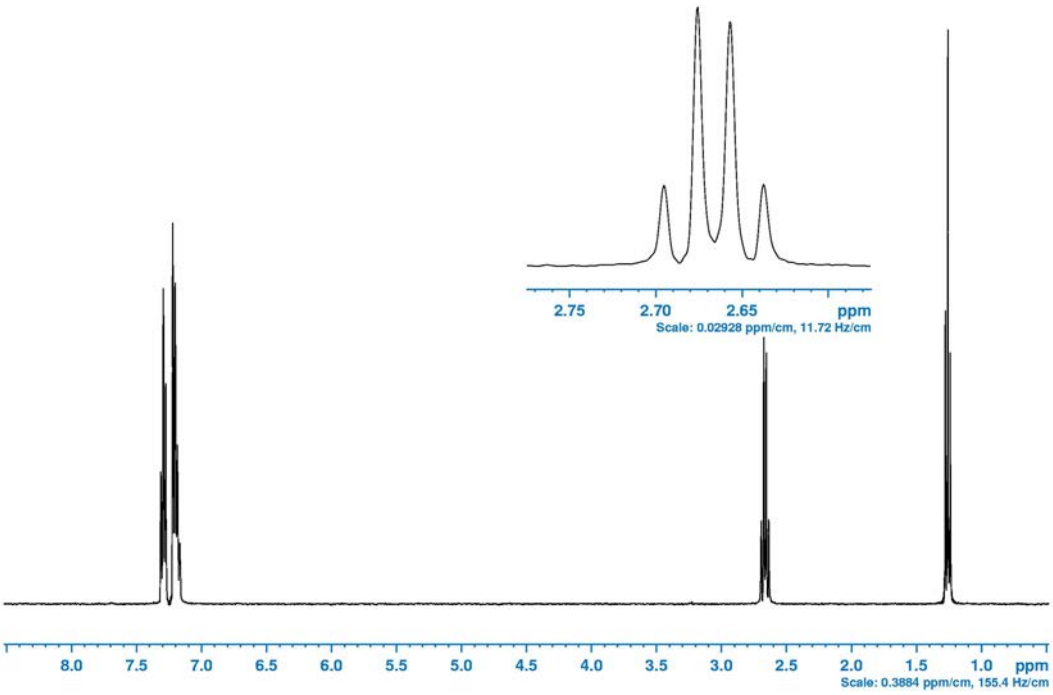
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| SIGF1 | 8.000 | ppm | |
| SIGF2 | 7.400 | ppm | |
| NOISF1 | 18.200 | ppm | |
| NOISF2 | 9.200 | ppm | |
| F1P | 19.000 | ppm | |
| F2P | 0.500 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton sensitivity with 19F decoupling is measured using the trifluorotoluene sample. Processing is using no LB. The signal-to-noise is determined using the highest signalof the aromatic region (~7.64 ppm). The noise region is fixed from 18.2 to 9.2 ppm.

## 5.2.105 1H sensitivity with HSQC selection and 13C garp decoupling (NPT_1H_sensitivity_hsqc13c)

**Test Sample:** 10% Ethylbenzene (EB) in Chloroform-D
Z10153, Z10154, Z10034, Z10253, Z10292, Z10723
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Bottom: 1D 1H-13C HSQC overview spectrum of ethylbenzene with 13C decoupling.
Top left: Expanded region showing the signal region of the methylene group (CH2) used for evaluation.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| PULPROG | hsqcetgpsisp2.2 | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.000 | ppm | |
| O2P | 79.987 | ppm | |
| SW | 10.159 | ppm | |
| TD | 4096 | | |
| AQ | 0.504 | s | field dependent |
| FIDRES | 1.985 | Hz | field dependent |
| D 1 | 35.196 | s | AQ+D1=const |
| D 16 | 0.001 | s | gradrec del. |
| D 24 | 0.001 | s | 1/8*J[CH] |
| P 1 | 12.9 | us | 90deg NUC1 |
| P 3 | 11.0 | us | 90deg NUC2 |
| P 14 | 500.0 | us | 180deg NUC2 Inversion |
| P 24 | 2000.0 | us | 180deg NUC2 Refocussing |
| P 28 | 0.1 | us | trimpul. |
| PLW 1 | 7.0 | W | Pow@P90(Specs) |
| PLW 2 | 27.3 | W | Pow@P90(Specs) |
| PLW 12 | 0.24 | W | Pow@CPD(Specs) |
| PCPD 2 | 102.5 | us | 90deg CPD NUC2 |
| CPDPRG2 | garp4 | | cpd seq. |
| CNST 2 | 135.000 | Hz | J[CH] |
| CNST 17 | -0.500 | | -0.5 for SPNAM7 |
| SPNAM3 | Gaus1.1000 | | Crp60,0.5,20.1 |
| SPOAL 3 | 0.500 | | phase align. |
| SPOFFS 3 | 0.000 | | offset freq. |
| SPW 3 | 0.000 | W | default |
| SPNAM7 | Gaus1.1000 | | Crp60comp.4 |
| SPOAL 7 | 0.500 | | phase align. |
| SPOFFS 7 | 0.000 | | offset freq. |
| SPW 7 | 0.000 | W | default |

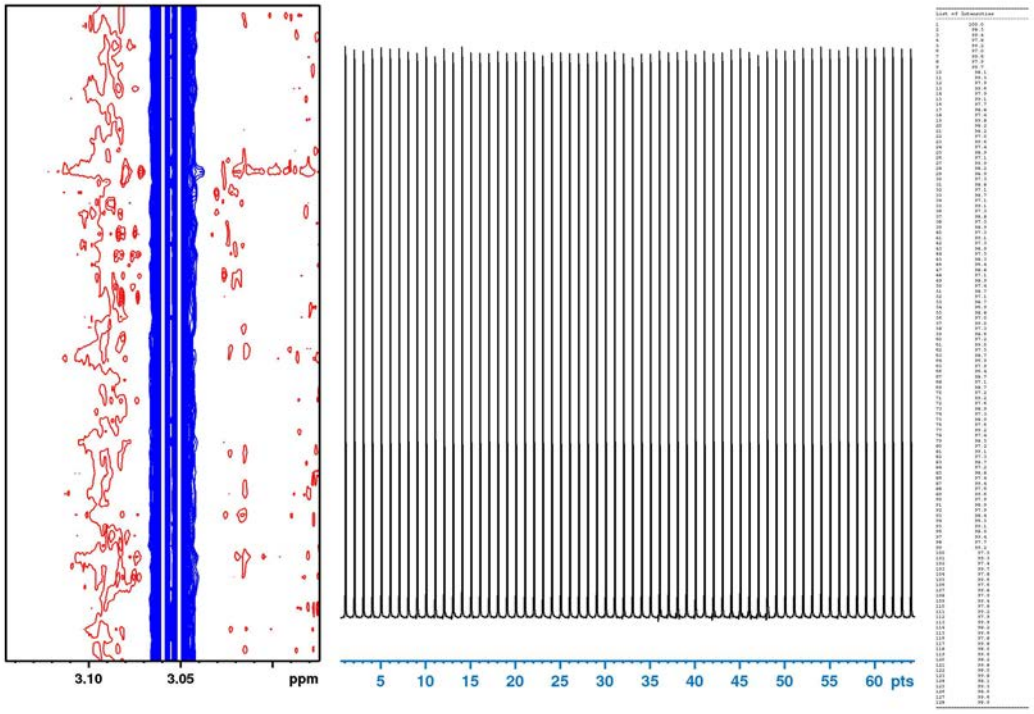
| | | | |
|---|---|---|---|
| GPNAM1 | SMSQ10.32 | | |
| GPNAM2 | SMSQ10.32 | | |
| GPNAM3 | SMSQ10.32 | | |
| GPNAM4 | SMSQ10.32 | | |
| GPZ 1 | 80.000 | % | |
| GPZ 2 | 20.100 | % | |
| GPZ 3 | 11.000 | % | |
| GPZ 4 | -5.000 | % | |
| P 16 | 0.000 | us | grad.pulse |
| P 19 | 0.000 | us | grad.pulse2 |
| TE | 298.000 | K | default |
| **F1 PROC** | | | Parameters |
| SI | 16384 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 3.000 | ppm | |
| SIGF2 | 2.000 | ppm | |
| NOISF1 | 7.000 | ppm | |
| NOISF2 | 2.800 | ppm | |
| F1P | 8.520 | ppm | |
| F2P | 0.480 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton sensitivity with 13C decoupling is measured using the ethylbenzene sample. Method used: Phase sensitive HSQC with echo/antiecho TPPI gradient selection.
Before the acquisition, the proton 90 degrees pulse is calibrated using pulscal, which result is stored in the corresponding derived dataset.The pulse determination is skiped if experiment is measured with option 'Skip Getprosol'.
Processing is using LB. The signal-to-noise is determined using the methylene signal (CH2) of the molecule. The signal is searched over the range from 3.0 to 2.0 ppm, whereas the best 2 ppm region over the range from 7.0 to 2.8 ppm.

## 5.2.106 Simultaneous hard pulses on 13C and 15N (NPT_1H_simpul_13c15n)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Left: Pseudo-2D showing expanded region of the methyl group of methanol. Experiment consists of a modified decp90 method using 360 deg (13C) and 180 deg (15N) giving in-phase signal for the methyl group.
Right: 1D representation of the pseudo-2D, generated with CONVTO1D procedure.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F2 ACQU | | | Parameters F2 |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| NUC3 | 15N | | |
| PULPROG | npt_simpul13c15n | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 3.080 | ppm | |
| O2P | 49.430 | ppm | |
| O3P | 75.921 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 1000 | | |
| AQ | 2.167 | s | |
| FIDRES | 0.462 | Hz | |
| D 1 | 1.710 | s | AQ+D1=const |
| P 1 | 9.5 | us | 90deg NUC1 |
| P 3 | 14.0 | us | 90deg NUC2 |
| P 21 | 30.0 | us | 90deg NUC3 |
| PLW 1 | 0.7 | W | Pow@P90(Specs) |
| PLW 2 | 72.2 | W | Pow@P90(Specs) |
| PLW 3 | 158.4 | W | Pow@P90(Specs) |
| CNST 2 | 139.000 | Hz | J[XH] |
| TE | 298.000 | K | default |

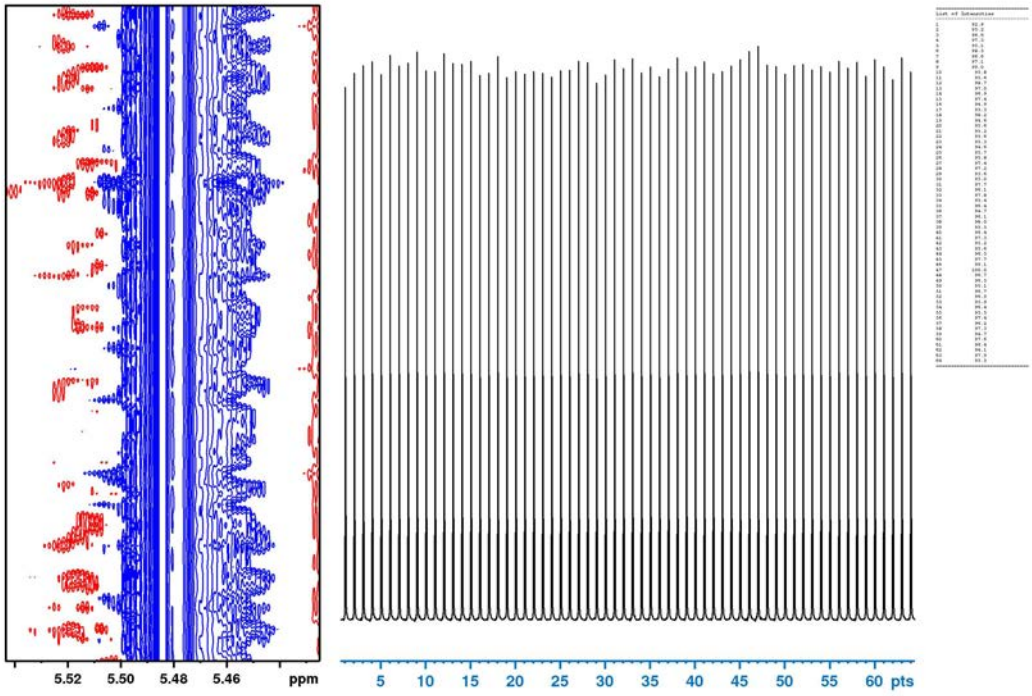
| F2 PROC | | | Parameters F2 |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.500 | Hz | |
| SIGF1 | 0.000 | ppm | |
| SIGF2 | 0.000 | ppm | |
| NOISF1 | 0.000 | ppm | |
| NOISF2 | 0.000 | ppm | |
| F1P | 3.200 | ppm | |
| F2P | 2.950 | ppm | |
| CY | 11.000 | cm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 64 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |

## Experiment Description

Simultaneous application of pulses are common especially in multi-dimensional and multi-nuclear applications. The simultaneous pulse test checks the stability of the probe under these conditions by repetitively applying pulses concurrently on two decoupling channels.
Processing is using LB. Evaluation consist of determination of intensity deviation based on peak picking intensities.

## 5.2.107 Simultaneous hard pulses on 15N and 13C (NPT_1H_simpul_15n13c)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Left: Pseudo-2D showing expanded region of the amino group of urea. Experiment consists of a modified decp90 method using 360 deg (15N) and 180 deg (13C) giving in-phase signal for the amino group.
Right: 1D representation of the pseudo-2D, generated with CONVTO1D procedure.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F2 ACQU | | | Parameters F2 |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 13C | | |
| NUC3 | 15N | | |
| PULPROG | npt_simpul15n13c | | |
| NS | 1 | | |
| DS | 8 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 5.500 | ppm | |
| O2P | 49.430 | ppm | |
| O3P | 75.921 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 200 | | |
| AQ | 0.433 | s | |
| FIDRES | 2.308 | Hz | |
| D 1 | 0.433 | s | AQ+D1=const |
| P 1 | 9.5 | us | 90deg NUC1 |
| P 3 | 14.0 | us | 90deg NUC2 |
| P 21 | 30.0 | us | 90deg NUC3 |
| PLW 1 | 0.7 | W | Pow@P90(Specs) |
| PLW 2 | 72.2 | W | Pow@P90(Specs) |
| PLW 3 | 158.4 | W | Pow@P90(Specs) |
| CNST 2 | 88.500 | Hz | J[XH] |
| TE | 298.000 | K | default |

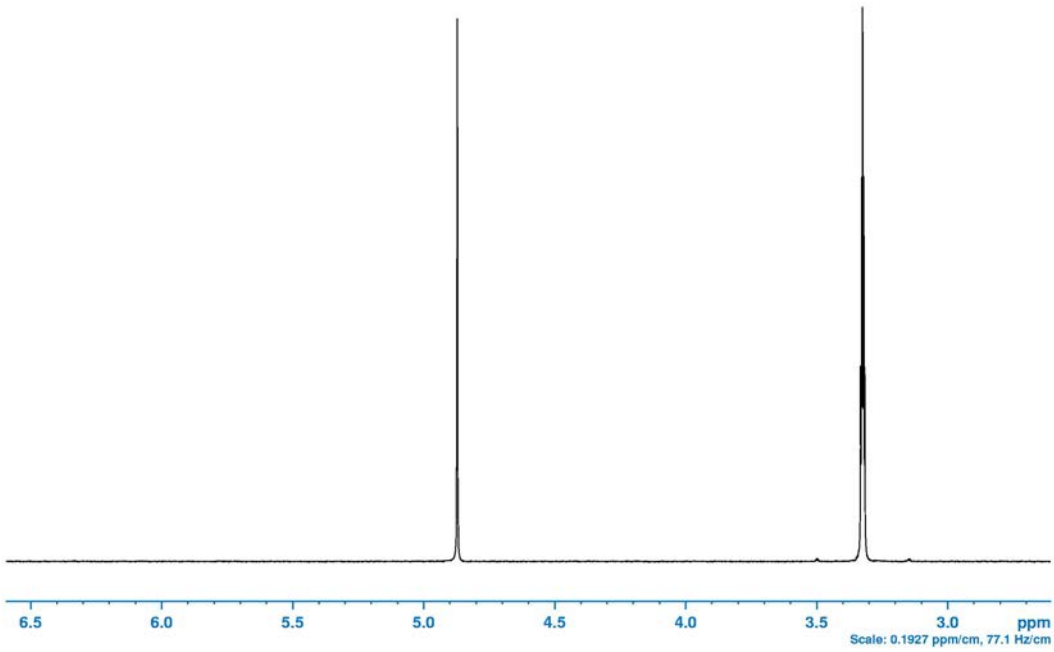
| F2 PROC | | | Parameters F2 |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.500 | Hz | |
| SIGF1 | 0.000 | ppm | |
| SIGF2 | 0.000 | ppm | |
| NOISF1 | 0.000 | ppm | |
| NOISF2 | 0.000 | ppm | |
| F1P | 5.670 | ppm | |
| F2P | 5.370 | ppm | |
| CY | 11.000 | cm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 64 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |

## Experiment Description

Simultaneous application of pulses are common especially in multi-dimensional and multi-nuclear applications. The simultaneous pulse test checks the stability of the probe under these conditions by repetitively applying pulses concurrently on two decoupling channels.
Processing is using LB. Evaluation consist of determination of intensity deviation based on peak picking intensities.

## 5.2.108 1H temperature calibration with 99.8% MeOD (NPT_1H_tempcalib_998meod)

**Test Sample:** Temperature Calibration 99.8% Methanol-D4
Z10627, Z10628, Z10053, Z10734
**Solvent:** MeOD
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Spectrum of 0.2% MeOH at standard probe temperature.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg30 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.600 | ppm | |
| SW | 4.165 | ppm | |
| TD | 8192 | | |
| AQ | 2.458 | s | field dependent |
| FIDRES | 0.407 | Hz | field dependent |
| D 1 | 2.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

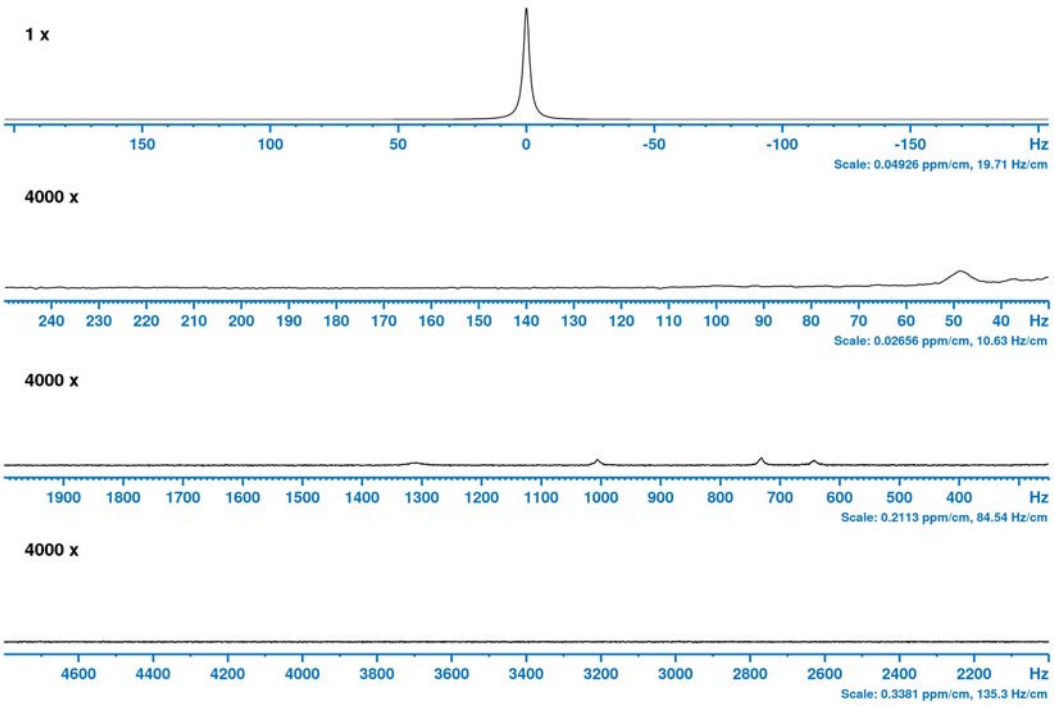
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.500 | Hz | 0.5 |
| SIGF1 | 0.000 | ppm | |
| SIGF2 | 0.000 | ppm | |
| NOISF1 | 0.000 | ppm | |
| NOISF2 | 0.000 | ppm | |
| F1P | 5.501 | ppm | |
| F2P | 2.499 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 1.000 | K | min TE for calibr. |
| CNST 51 | 1.000 | K | max TE for calibr. |
| CNST 52 | 1.000 | | no. points TE calibr. |

## Experiment Description

Temperature calibration experiment expects a temperature unit. The procedure is calibrating at least two TE settings according to the entries in the parameter set (CNST 50 to 53).
The result of the experiment is the determination of the offset and slope of the correction curve (y=ax +b). For a BSVT the correction will be set in the temperature unit if the experiment was not measured with option 'Skip FLow'.
CNST 50: lowest TE used for calibration, default value of 1 means that the standard temperature will be used.
CNST 51: highest TE used for calibration, default value of 1 means that lowest TE + 10 K will be used.
CNST 52: number of points (TE settings) used for calibration. The default is 2.

## 5.2.109 Vibration Test using Doped Water Sample (NPT_1H_vibration_doped_water)

**Test Sample:** 0.1 mg/ml Gadolinium Chloride (GdCl3), 0.1% Methanol-13C, and 1% H2O in D2O
Z10083, Z100933, Z10085, Z10046, Z10084, Z10082, Z10727, Z142231
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top: Expansion plot of the arithmetic Mean Projection of pseudo-2D data.
Other Plots: Calculated symmetrized standard deviation for the different frequency ranges.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | zg2d_random | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| TD0 | 1 | | |
| SWH | 10000.000 | Hz | |
| TD | 32768 | | |
| AQ | 1.638 | s | |
| FIDRES | 0.610 | Hz | |
| D 1 | 1.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

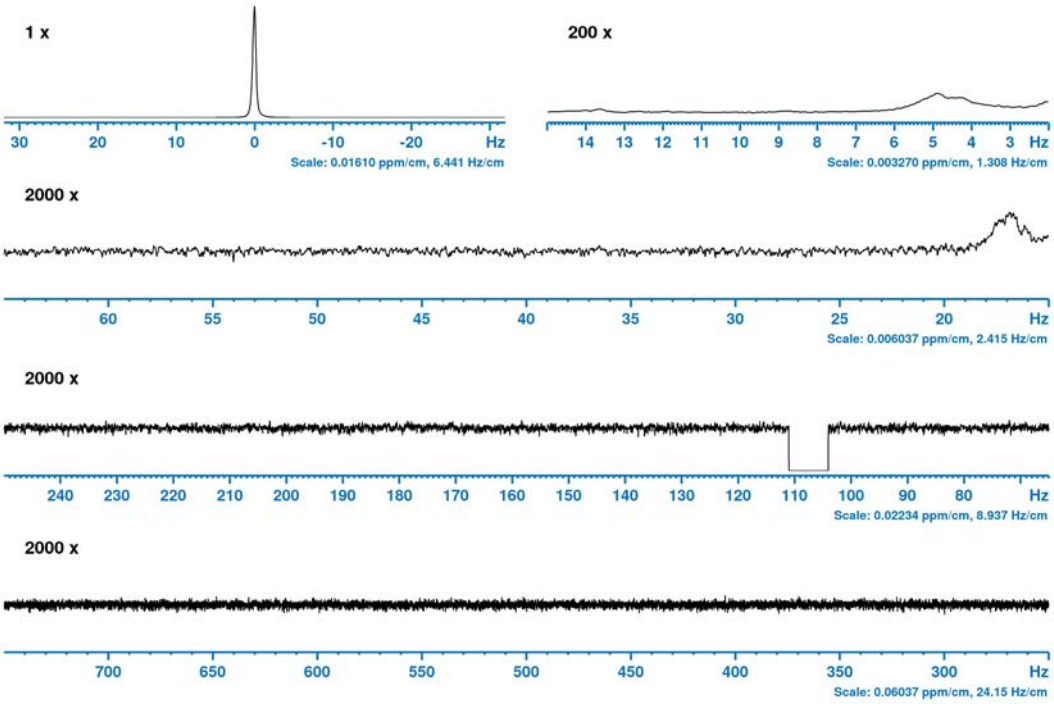
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 32768 | | |
| WDW | 1 | | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| PHC0 | 0.000 | deg | |
| PHC1 | 0.000 | deg | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 256 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 256 | | |

### Experiment Description

The standard deviation is computed from the rows of the pseudo 2D spectrum. The first 8 largest peaks are listed for each frequency range in the tables on the right.

## 5.2.110 Vibration Test using Lineshape Sample (NPT_1H_vibration_lineshape)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
Z10230, Z10248, Z10701, Z100926, Z10031, Z10030, Z10029, Z10249, Z10275, Z10717, Z142220
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top Right: Expansion plot of the arithmetic Mean Projection of pseudo-2D data.
Other Plots: Calculated symmetrized standard deviation for the different frequency ranges.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | zg2d_random | | |
| NS | 1 | | |
| DS | 6 | | |
| RG | 0.250 | | optim. by RGA |
| TD0 | 1 | | |
| SWH | 1612.903 | Hz | |
| TD | 65536 | | |
| AQ | 20.316 | s | |
| FIDRES | 0.049 | Hz | |
| D 1 | 1.000 | s | |
| P 1 | 8.6 | us | 55deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

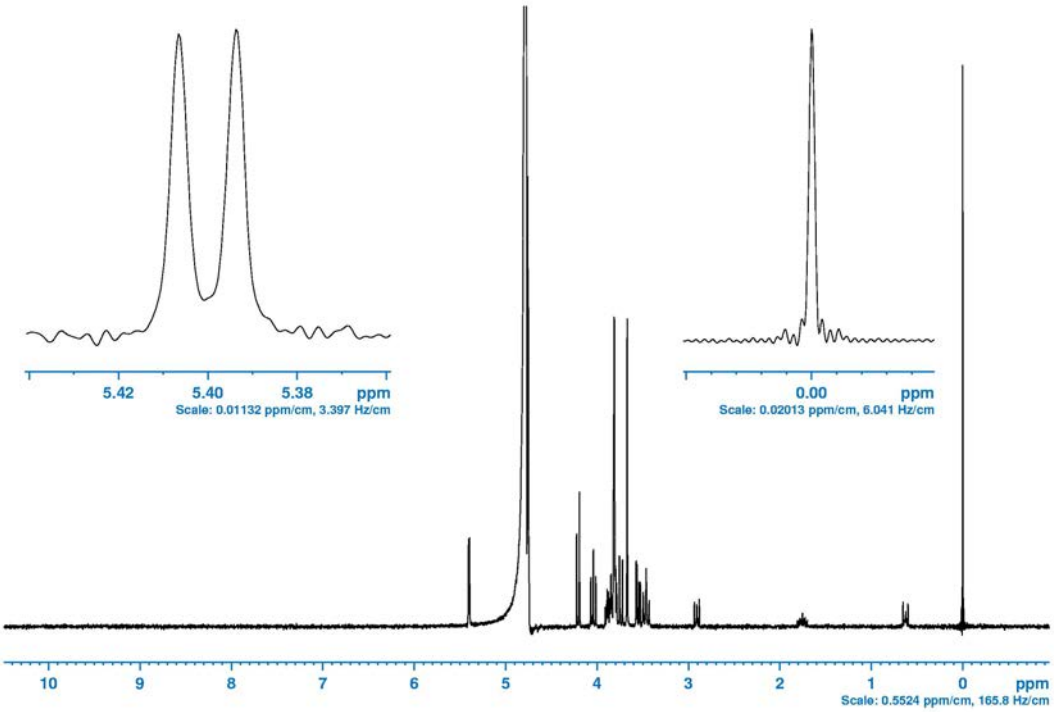
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 65536 | | |
| WDW | 1 | | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| PHC0 | 0.000 | deg | |
| PHC1 | 0.000 | deg | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 128 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 128 | | |

## Experiment Description

The standard deviation is computed from the rows of the pseudo 2D spectrum. The first 8 largest peaks are listed for each frequency range in the tables on the right.

## 5.2.111 Watersuppression NaCl with recommended gas flow (NPT_1H_watersupp_NaCl_recflow)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O with salt Z100384, Z100385, Z100386, Z100387, Z100388, Z100389, Z107150, Z107151, Z107152
**Solvent:** H2O+D2O_salt
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Water suppression spectrum printed from 10.5 ppm to -1.0 ppm as overview spectrum. The expansion plot to the right shows the DSS (sodium 2,2-dimethyl-2-silapentane-5-sulphonate) signal, indicative for the quality of the spectral resolution. The quality of the water suppression is determined as linewidth of the residual water signal using the 10% and 50% intensity of the DSS signal.
The expansion plot to the left shows the signal of the anomeric proton (alpha-C1) of the sucrose (2-beta-D-fructofuranosyl-1-alpha- D-glucopyranosid). The anomeric proton intensity is used for the signal-to-noise calculation and the splitting of the signal is analysed to give a measure for spectral resolution.

**Control Option for Acquisition (L23)**

1 with O1 optimization, with PULPROG=zgpr
20 O1 from parameter set, no optimization, with PULPROG=zgpr
23 O1 from parameter set, no optimization, with PULPROG=npt_zggppr
25 O1 from parameter set, no optimization, with PULPROG=zgcppr
27 O1 from parameter set, no optimization, with PULPROG=zgcpgppr

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zgpr | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by NMRPT |
| O1P | 4.699 | ppm | |
| SW | 12.132 | ppm | |
| TD | 10194 | | field dependent |
| AQ | 1.050 | s | |
| FIDRES | 0.952 | Hz | field dependent |
| D 1 | 5.000 | s | |
| P 1 | 14.0 | us | 90deg |
| PLW 1 | 7.5 | W | Pow@90deg(Specs) |
| PLW 9 | 0.00006 | W | Pow@90deg(5000u) |
| TE | 298.000 | K | default |

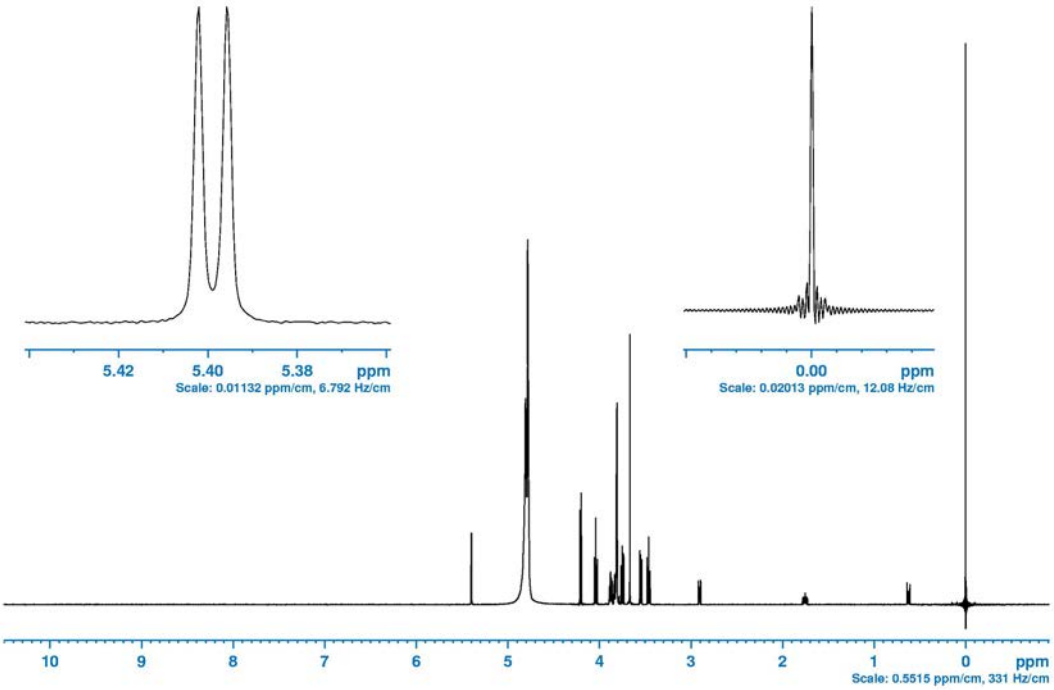
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.100 | | |
| F1P | 10.806 | ppm | |
| F2P | -1.227 | ppm | |
| CY | 111.000 | cm | |

## Experiment Description

For the watersuppression experiment the carrier offset O1 needs to be very carefully adjusted. Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
RG adjustment is executed by running experiments with DS=0, NS=4 and a reduced PLW1. The highest RG without signal overflow in these experiments will be used.
Before the acquisition, the proton 90 degrees pulse is calibrated using POPT, which result is stored in the corresponding derived dataset. The calibrated pulse, which is not set in prosol, is written in the acquisition title along with the starting pulse length and power from prosol.
The pulse determination is skiped if experiment is measured with option 'Skip Getprosol'.
Options L23=1, 20 and 30 are standard whereas Options L23=23, 25, 27, 33, 35, and 37 are non-standard and will not be considered as regular test from the 'NMRPT Control Structure'. Their existence is purely diagnostic.
Experiment will be set to irregular if option 'Skip Temperature' is selected.

## 5.2.112 Watersuppression with 270 l/h gas flow (NPT_1H_watersuppression_270l)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z100930, Z10268, Z10036, Z10267, Z10719, Z10720
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Water suppression spectrum printed from 10.5 ppm to -1.0 ppm as overview spectrum. The expansion plot to the right shows the DSS (sodium 2,2-dimethyl-2-silapentane-5-sulphonate) signal, indicative for the quality of the spectral resolution. The quality of the water suppression is determined as linewidth of the residual water signal using the 10% and 50% intensity of the DSS signal.
The expansion plot to the left shows the signal of the anomeric proton (alpha-C1) of the sucrose (2-beta-D-fructofuranosyl-1-alpha- D-glucopyranosid). The anomeric proton intensity is used for the signal-to-noise calculation and the splitting of the signal is analysed to give a measure for spectral resolution.

**Control Option for Acquisition (L23)**

1 with O1 optimization, with PULPROG=zgpr
20 O1 from parameter set, no optimization, with PULPROG=zgpr
23 O1 from parameter set, no optimization, with PULPROG=npt_zggppr
25 O1 from parameter set, no optimization, with PULPROG=zgcppr
27 O1 from parameter set, no optimization, with PULPROG=zgcpgppr
30 O1 from previous watersuppression, no optimization[*], with PULPROG=zgpr
33 O1 from previous watersuppression, no optimization[*], with PULPROG=npt_zggppr
35 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcppr
37 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcpgppr
[*] The optimization of O1 is enforced, if O1 was not determined during a previous measurement.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zgpr | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by NMRPT |
| O1P | 4.699 | ppm | |
| SW | 12.132 | ppm | |
| TD | 10194 | | field dependent |
| AQ | 1.050 | s | |
| FIDRES | 0.952 | Hz | field dependent |
| D 1 | 5.000 | s | |
| P 1 | 14.0 | us | 90deg |
| PLW 1 | 7.5 | W | Pow@90deg(Specs) |
| PLW 9 | 0.00006 | W | Pow@90deg(5000u) |
| TE | 298.000 | K | default |

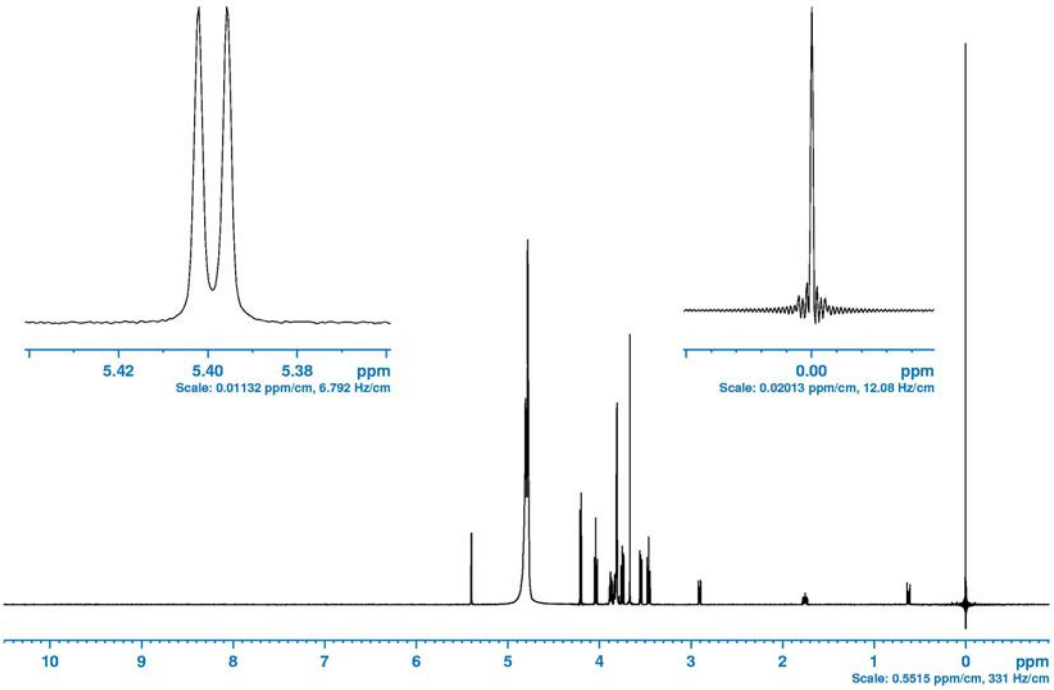
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.100 | | |
| F1P | 10.806 | ppm | |
| F2P | -1.227 | ppm | |
| CY | 111.000 | cm | |

## Experiment Description

For the watersuppression experiment the carrier offset O1 needs to be very carefully adjusted. Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
RG adjustment is executed by running experiments with DS=0, NS=4 and a reduced PLW1. The highest RG without signal overflow in these experiments will be used.
Options L23=1 and 20 are standard whereas Options L23=23, 25, and 27 are non-standard and will not be considered as regular test from the 'NMRPT Control Structure'. Their existence is purely diagnostic. Experiment will be set to irregular if one or both of the options 'Skip Flow' or 'Skip Temperature' are selected.

## 5.2.113 Watersuppression with 400 l/h gas flow (NPT_1H_watersuppression_400l)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z100930, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Water suppression spectrum printed from 10.5 ppm to -1.0 ppm as overview spectrum. The expansion plot to the right shows the DSS (sodium 2,2-dimethyl-2-silapentane-5-sulphonate) signal, indicative for the quality of the spectral resolution. The quality of the water suppression is determined as linewidth of the residual water signal using the 10% and 50% intensity of the DSS signal.
The expansion plot to the left shows the signal of the anomeric proton (alpha-C1) of the sucrose (2-beta-D-fructofuranosyl-1-alpha- D-glucopyranosid). The anomeric proton intensity is used for the signal-to-noise calculation and the splitting of the signal is analysed to give a measure for spectral resolution.

**Control Option for Acquisition (L23)**

1 with O1 optimization, with PULPROG=zgpr
20 O1 from parameter set, no optimization, with PULPROG=zgpr
23 O1 from parameter set, no optimization, with PULPROG=npt_zggppr
25 O1 from parameter set, no optimization, with PULPROG=zgcppr
27 O1 from parameter set, no optimization, with PULPROG=zgcpgppr
30 O1 from previous watersuppression, no optimization[*], with PULPROG=zgpr
33 O1 from previous watersuppression, no optimization[*], with PULPROG=npt_zggppr
35 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcppr
37 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcpgppr
[*] The optimization of O1 is enforced, if O1 was not determined during a previous measurement.

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zgpr | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by NMRPT |
| O1P | 4.699 | ppm | |
| SW | 12.132 | ppm | |
| TD | 10194 | | field dependent |
| AQ | 1.050 | s | |
| FIDRES | 0.952 | Hz | field dependent |
| D 1 | 5.000 | s | |
| P 1 | 14.0 | us | 90deg |
| PLW 1 | 7.5 | W | Pow@90deg(Specs) |
| PLW 9 | 0.00006 | W | Pow@90deg(5000u) |
| TE | 298.000 | K | default |

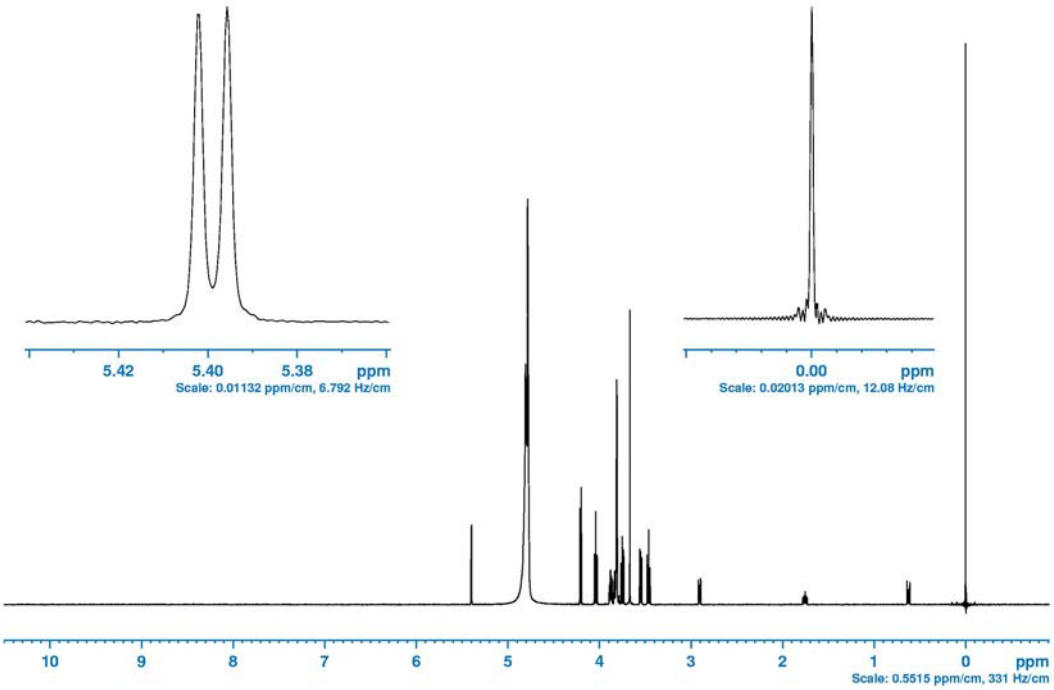
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.100 | | |
| F1P | 10.806 | ppm | |
| F2P | -1.227 | ppm | |
| CY | 111.000 | cm | |

### Experiment Description

For the watersuppression experiment the carrier offset O1 needs to be very carefully adjusted. Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
RG adjustment is executed by running experiments with DS=0, NS=4 and a reduced PLW1. The highest RG without signal overflow in these experiments will be used.
Options L23=1 and 20 are standard whereas Options L23=23, 25, and 27 are non-standard and will not be considered as regular test from the 'NMRPT Control Structure'. Their existence is purely diagnostic. Experiment will be set to irregular if one or both of the options 'Skip Flow' or 'Skip Temperature' are selected.

## 5.2.114 Watersuppression with 535 l/h gas flow (NPT_1H_watersuppression_535l)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z100930, Z10268, Z10036, Z10267, Z10719, Z10720
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Water suppression spectrum printed from 10.5 ppm to -1.0 ppm as overview spectrum. The expansion plot to the right shows the DSS (sodium 2,2-dimethyl-2-silapentane-5-sulphonate) signal, indicative for the quality of the spectral resolution. The quality of the water suppression is determined as linewidth of the residual water signal using the 10% and 50% intensity of the DSS signal.
The expansion plot to the left shows the signal of the anomeric proton (alpha-C1) of the sucrose (2-beta-D-fructofuranosyl-1-alpha- D-glucopyranosid). The anomeric proton intensity is used for the signal-to-noise calculation and the splitting of the signal is analysed to give a measure for spectral resolution.

**Control Option for Acquisition (L23)**

1 with O1 optimization, with PULPROG=zgpr
20 O1 from parameter set, no optimization, with PULPROG=zgpr
23 O1 from parameter set, no optimization, with PULPROG=npt_zggppr
25 O1 from parameter set, no optimization, with PULPROG=zgcppr
27 O1 from parameter set, no optimization, with PULPROG=zgcpgppr
30 O1 from previous watersuppression, no optimization[*], with PULPROG=zgpr
33 O1 from previous watersuppression, no optimization[*], with PULPROG=npt_zggppr
35 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcppr
37 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcpgppr
[*] The optimization of O1 is enforced, if O1 was not determined during a previous measurement.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zgpr | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by NMRPT |
| O1P | 4.699 | ppm | |
| SW | 12.132 | ppm | |
| TD | 10194 | | field dependent |
| AQ | 1.050 | s | |
| FIDRES | 0.952 | Hz | field dependent |
| D 1 | 5.000 | s | |
| P 1 | 14.0 | us | 90deg |
| PLW 1 | 7.5 | W | Pow@90deg(Specs) |
| PLW 9 | 0.00006 | W | Pow@90deg(5000u) |
| TE | 298.000 | K | default |

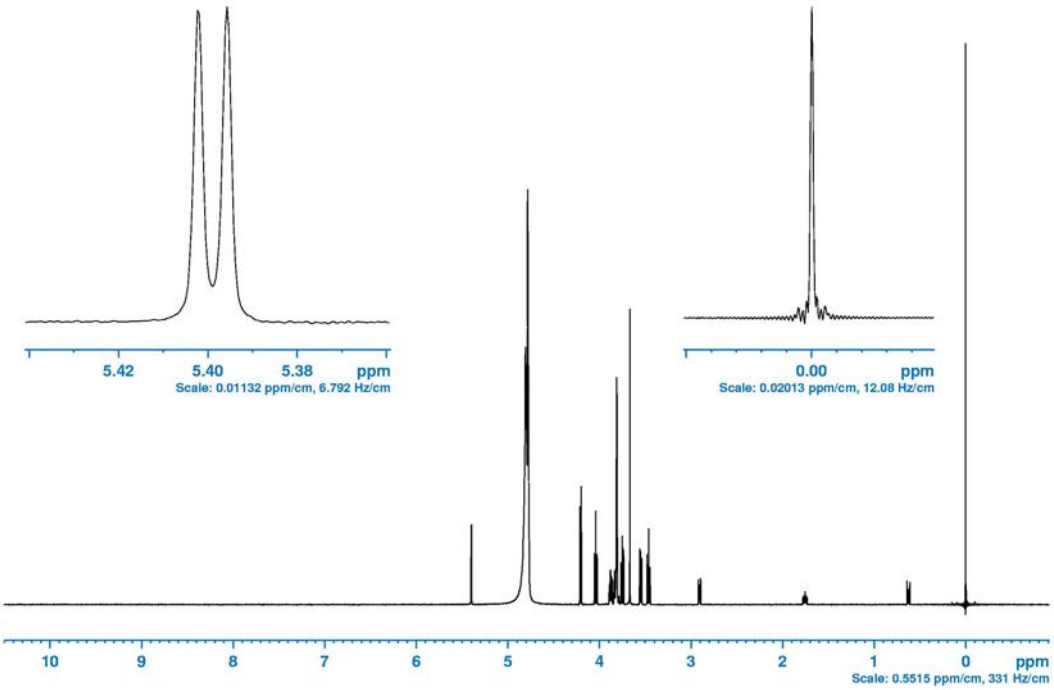
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.100 | | |
| F1P | 10.806 | ppm | |
| F2P | -1.227 | ppm | |
| CY | 111.000 | cm | |

## Experiment Description

For the watersuppression experiment the carrier offset O1 needs to be very carefully adjusted. Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
RG adjustment is executed by running experiments with DS=0, NS=4 and a reduced PLW1. The highest RG without signal overflow in these experiments will be used.
Options L23=1 and 20 are standard whereas Options L23=23, 25, and 27 are non-standard and will not be considered as regular test from the 'NMRPT Control Structure'. Their existence is purely diagnostic. Experiment will be set to irregular if one or both of the options 'Skip Flow' or 'Skip Temperature' are selected.

## 5.2.115 Watersuppression with 670 l/h gas flow (NPT_1H_watersuppression_670l)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z100930, Z10268, Z10036, Z10247, Z10267, Z10719, Z10720
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Water suppression spectrum printed from 10.5 ppm to -1.0 ppm as overview spectrum. The expansion plot to the right shows the DSS (sodium 2,2-dimethyl-2-silapentane-5-sulphonate) signal, indicative for the quality of the spectral resolution. The quality of the water suppression is determined as linewidth of the residual water signal using the 10% and 50% intensity of the DSS signal.
The expansion plot to the left shows the signal of the anomeric proton (alpha-C1) of the sucrose (2-beta-D-fructofuranosyl-1-alpha- D-glucopyranosid). The anomeric proton intensity is used for the signal-to-noise calculation and the splitting of the signal is analysed to give a measure for spectral resolution.

**Control Option for Acquisition (L23)**

1 with O1 optimization, with PULPROG=zgpr
20 O1 from parameter set, no optimization, with PULPROG=zgpr
23 O1 from parameter set, no optimization, with PULPROG=npt_zggppr
25 O1 from parameter set, no optimization, with PULPROG=zgcppr
27 O1 from parameter set, no optimization, with PULPROG=zgcpgppr
30 O1 from previous watersuppression, no optimization[*], with PULPROG=zgpr
33 O1 from previous watersuppression, no optimization[*], with PULPROG=npt_zggppr
35 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcppr
37 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcpgppr
[*] The optimization of O1 is enforced, if O1 was not determined during a previous measurement.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zgpr | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by NMRPT |
| O1P | 4.699 | ppm | |
| SW | 12.132 | ppm | |
| TD | 10194 | | field dependent |
| AQ | 1.050 | s | |
| FIDRES | 0.952 | Hz | field dependent |
| D 1 | 5.000 | s | |
| P 1 | 14.0 | us | 90deg |
| PLW 1 | 7.5 | W | Pow@90deg(Specs) |
| PLW 9 | 0.00006 | W | Pow@90deg(5000u) |
| TE | 298.000 | K | default |

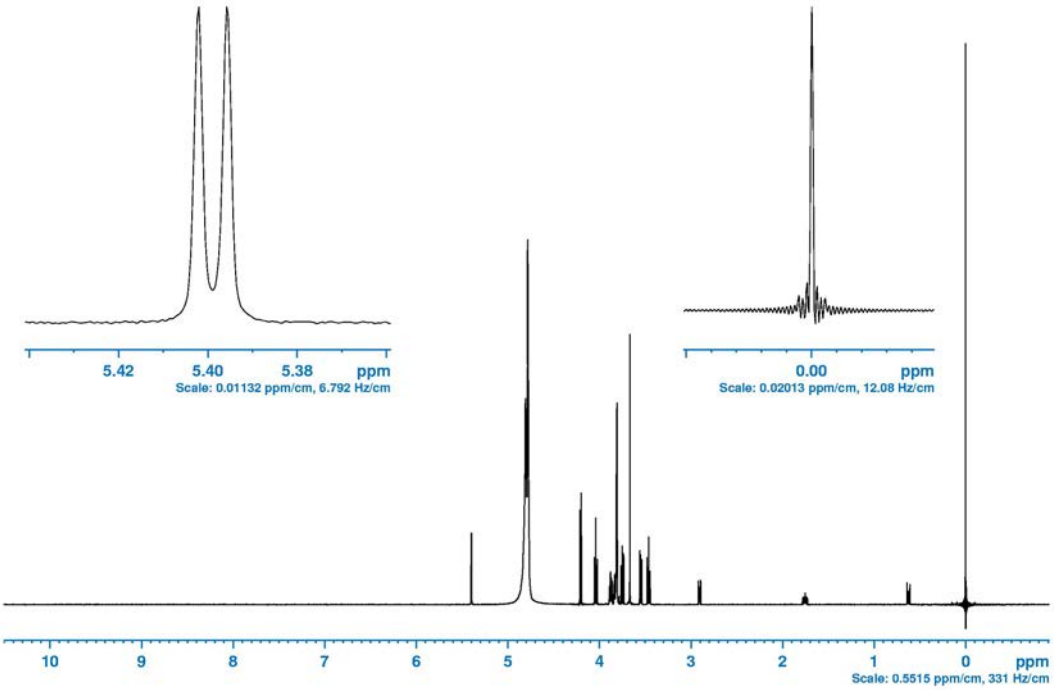
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.100 | | |
| F1P | 10.806 | ppm | |
| F2P | -1.227 | ppm | |
| CY | 111.000 | cm | |

## Experiment Description

For the watersuppression experiment the carrier offset O1 needs to be very carefully adjusted. Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
RG adjustment is executed by running experiments with DS=0, NS=4 and a reduced PLW1. The highest RG without signal overflow in these experiments will be used.
Options L23=1 and 20 are standard whereas Options L23=23, 25, and 27 are non-standard and will not be considered as regular test from the 'NMRPT Control Structure'. Their existence is purely diagnostic.
Experiment will be set to irregular if one or both of the options 'Skip Flow' or 'Skip Temperature' are selected.

## 5.2.116 Watersuppression with recommended gas flow (NPT_1H_watersuppression_recflow)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z180181, Z100930, Z10268, Z10036, Z10247, Z10267, Z10719, Z10720, Z142222
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Water suppression spectrum printed from 10.5 ppm to -1.0 ppm as overview spectrum. The expansion plot to the right shows the DSS (sodium 2,2-dimethyl-2-silapentane-5-sulphonate) signal, indicative for the quality of the spectral resolution. The quality of the water suppression is determined as linewidth of the residual water signal using the 10% and 50% intensity of the DSS signal.
The expansion plot to the left shows the signal of the anomeric proton (alpha-C1) of the sucrose (2-beta-D-fructofuranosyl-1-alpha- D-glucopyranosid). The anomeric proton intensity is used for the signal-to-noise calculation and the splitting of the signal is analysed to give a measure for spectral resolution.

**Control Option for Acquisition (L23)**

1 with O1 optimization, with PULPROG=zgpr
20 O1 from parameter set, no optimization, with PULPROG=zgpr
23 O1 from parameter set, no optimization, with PULPROG=npt_zggppr
25 O1 from parameter set, no optimization, with PULPROG=zgcppr
27 O1 from parameter set, no optimization, with PULPROG=zgcpgppr
30 O1 from previous watersuppression, no optimization[*], with PULPROG=zgpr
33 O1 from previous watersuppression, no optimization[*], with PULPROG=npt_zggppr
35 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcppr
37 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcpgppr
[*] The optimization of O1 is enforced, if O1 was not determined during a previous measurement.

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zgpr | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by NMRPT |
| O1P | 4.699 | ppm | |
| SW | 12.132 | ppm | |
| TD | 10194 | | field dependent |
| AQ | 1.050 | s | |
| FIDRES | 0.952 | Hz | field dependent |
| D 1 | 5.000 | s | |
| P 1 | 14.0 | us | 90deg |
| PLW 1 | 7.5 | W | Pow@90deg(Specs) |
| PLW 9 | 0.00006 | W | Pow@90deg(5000u) |
| TE | 298.000 | K | default |

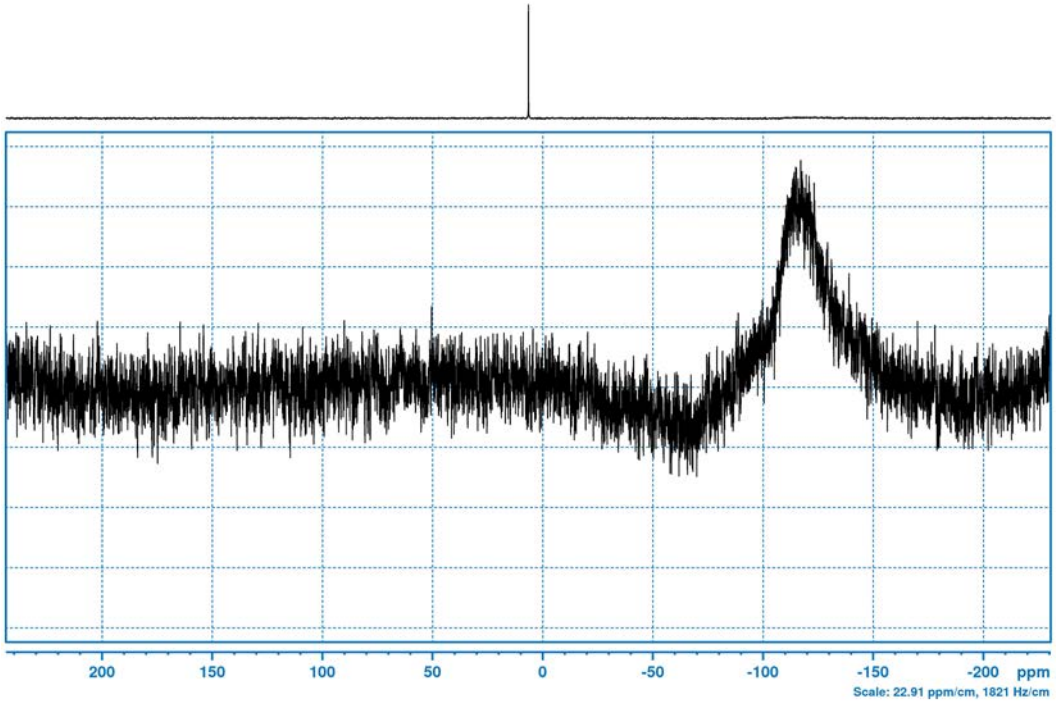
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.100 | | |
| F1P | 10.806 | ppm | |
| F2P | -1.227 | ppm | |
| CY | 111.000 | cm | |

### Experiment Description

For the watersuppression experiment the carrier offset O1 needs to be very carefully adjusted. Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
RG adjustment is executed by running experiments with DS=0, NS=4 and a reduced PLW1. The highest RG without signal overflow in these experiments will be used.
Options L23=1 and 20 are standard whereas Options L23=23, 25, and 27 are non-standard and will not be considered as regular test from the 'NMRPT Control Structure'. Their existence is purely diagnostic.
Experiment will be set to irregular if option 'Skip Temperature' is selected.

## 5.2.117 29Si background without sample (NPT_29Si_backgr_nosample)

**Test Sample:** 85% Hexamethyldisiloxane (HMDSO, [[CH3]3Si]2O) in Benzene-D6
Z10209, Z10210
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Top: 29Si spectrum with sample to estimate spectrum quality.
Bottom: 29Si Background signal spectrum without sample. No sharp signal should be present. Broad signal could arise from solid compound in the probe.

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on experiment with sample

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 29Si | | |
| PULPROG | zgig30 | | |
| NS | 500 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 6.518 | ppm | |
| SW | 499.182 | ppm | |
| TD | 65536 | | |
| D 1 | 4.874 | s | AQ+D1=const |
| P 1 | 20.0 | us | 90deg NUC1 |
| PLW 1 | 14.3 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@90deg(CPD) |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| TE | 298.000 | K | default |

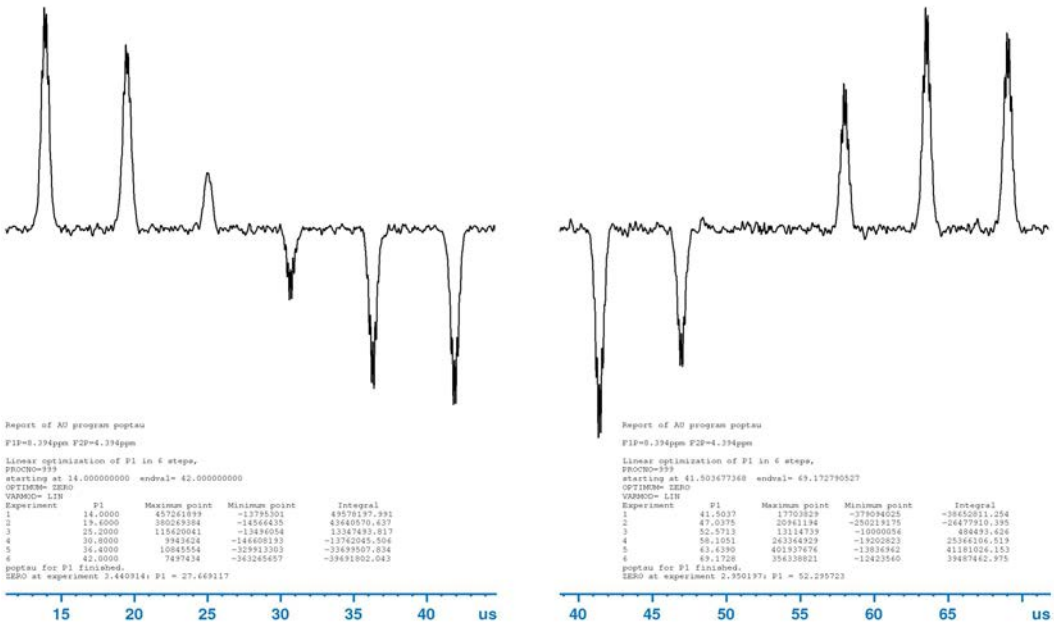
| | | | |
|---|---|---|---|
| PLW 2 | 6.6 | W | Pow@90deg(Specs) NUC2 |
| **F1 PROC** | | | Parameters |
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| PC | 1.400 | | |
| F1P | 10.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 8.000 | cm | |

### Experiment Description

Background signal measurements are executed using a small flip angle due to two reasons. First, to get more efficient excitation bandwidth, secondly to compensate for usually long T1 relaxation time of solid signals.
Experiment will be set to irregular if one or both of the options 'Skip Tuning/Matching' or 'Skip XNUC Tuning/Matching' are selected.
A spectrum with sample and NS=1 will be acquired on a derived data set. This experiment can be used to estimate the spectrum quality.After phase correction SINO will be executed on the spectrum with sample. The experiment will be aborted, if a minimal SINO of 20 is not achieved. SINO check can be skiped with L23=2.

## 5.2.118 P90 29Si pulse calibration (NPT_29Si_p90determination_29si)

**Test Sample:** 85% Hexamethyldisiloxane (HMDSO, [[CH3]3Si]2O) in Benzene-D6
Z10209, Z142229, Z10210
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 29Si | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 6.512 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 1000 | | |
| AQ | 1.260 | s | |
| FIDRES | 0.794 | Hz | |
| D 1 | 62.415 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

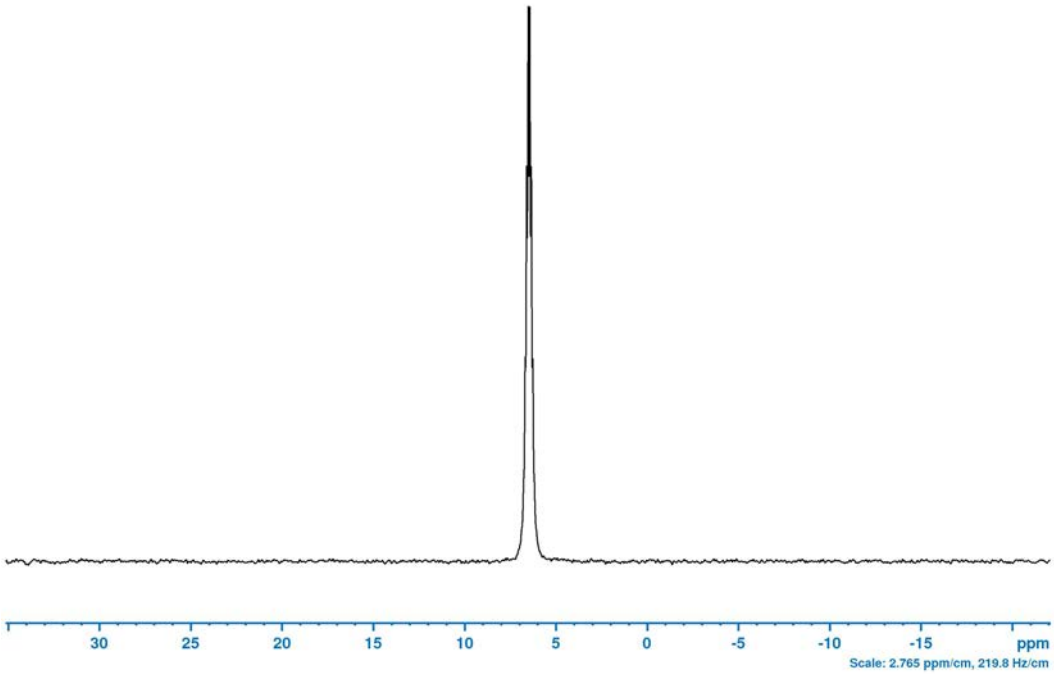
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 10.000 | ppm | |
| F2P | -38.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.119 29Si sensitivity (NPT_29Si_sensitivity)

**Test Sample:** 85% Hexamethyldisiloxane (HMDSO, [[CH3]3Si]2O) in Benzene-D6
Z10209, Z142229, Z10210
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Silicon-29 sensitivity test.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 29Si | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 6.512 | ppm | |
| SW | 61.065 | ppm | |
| TD | 32768 | | |
| AQ | 3.375 | s | field dependent |
| FIDRES | 0.296 | Hz | field dependent |
| D 1 | 415.525 | s | AQ+D1=const |
| P 1 | 20.0 | us | 90deg NUC1 |
| PLW 1 | 14.3 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

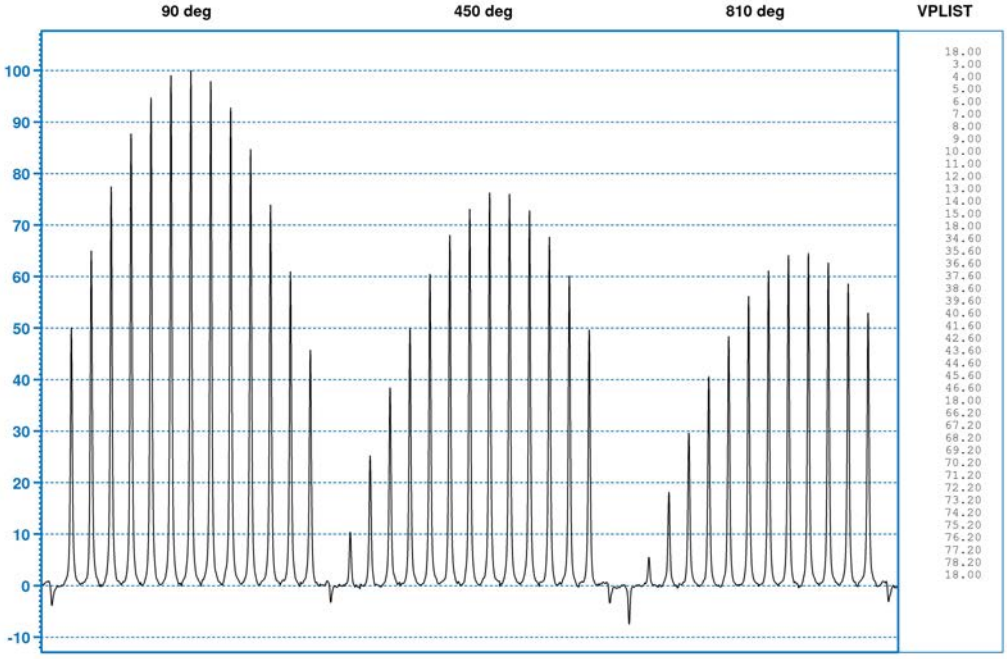
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 65536 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| PC | 1.400 | | |
| F1P | 10.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Silicon-29 sensitivity test (no 1H decoupling). Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from 10.0 to 0.0 ppm, while the best 10 ppm noise region is determined over the range from 37.0 to 9.0 ppm.

## 5.2.120 31P B1 homogeneity integral (NPT_31P_b1homogeneityInt_31p)

**Test Sample:** 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10201, Z100934, Z10202, Z10038, Z10257, Z10276, Z10722, Z142226
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a fraction around signal maximum (-60 deg, +60 deg) is acquired and shown in the figure. The variable pulse list which is used for acquisition is shown to the right.
The B1-homogeneities based on amplitudes and integrals are computed from the peak-picking list amplitudes and the magnitude of the second complex FID data point respectively.

**Control Option for Acquisition (L23)**

1 default PLW 1 is used for determination of B1 homogeneity.
2 PLW 1 will be set to CNST 10 and resultant pulses are used for determination of B1 homogeneity. Experiment will be set to irregular.
3 PLW 1 will be set to power corresponding to specified customer pulses and resultant pulses are used for determination of B1 homogeneity.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 31P | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1b1hom2d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | -17.609 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 1024 | | |
| AQ | 1.290 | s | |
| FIDRES | 0.775 | Hz | |
| D 1 | 83.727 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

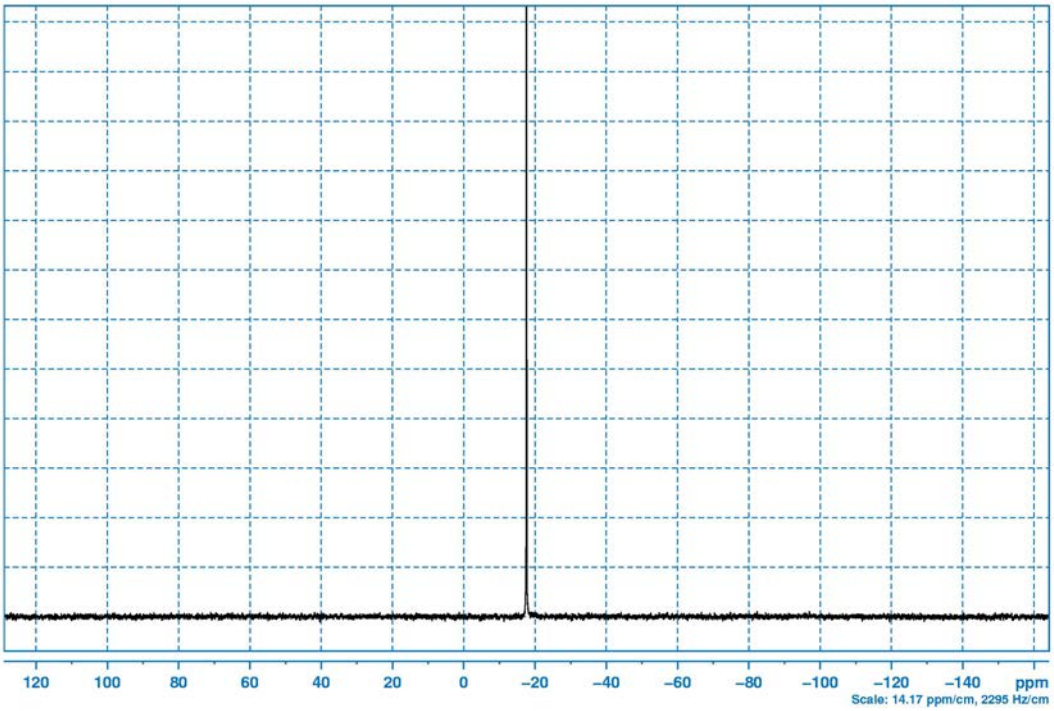
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 31P | | |
| TD | 43 | | No of incr. |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |
| **NMRPT** | | | Parameters |
| L 4 | 15 | | integ. fraction of 90deg |
| L 5 | 4 | | # of step per maxima |

## Experiment Description

The B1 homogeneity measurement is normally acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range is from 90 to 810 degree. In order to speed up the measurements NMRPT is acquiring only the partial ranges around the positive signal maxima for the pulse angles 90, 450, and 810 degree.
By this approach it is possible to get a better incremental resolution and a shorter overall measuring time.
Prior to the main acquisition O1P (PROCNO=2) and phase correction (PROCNO=3) will be optimized.
Intermediate results of the CONVTO1D routine is stored in PROCNO=998, result of CONVTO1D in PROCNO=999.
As control of stability, reproducability and 90 degree calibration a spectrum with 180 degree pulse is acquired before and after each maxima. If relaxation conditions and instrument stability is sufficient, the result should not differ among them.
For the predicition of the signal maxima at 450 and 810 degree the propagation delay is included in the calculation of the VP list. (PDelay is calculated as difference of 360 and 180 degree pulse lengths during the corresponding 90 degree pulse determination experiment.) In this measurement O1 is determined before the main acquisition is started. Evaluation is achieved after processing the data in F2 only (XF2) by peak picking and integral determination of the most intense signal per maxima.

## 5.2.121 31P background with sample (NPT_31P_backgr_withsample)

**Test Sample:** 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10201, Z100934, Z10202, Z10038, Z10257, Z10276, Z10722
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

31P Background signal spectrum with sample. Sharp signal arises from sample, broad signal could arise from solid compound in the probe.

**Control Option for Acquisition (L23)**

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PULPROG | npt_zg0ig | | |
| NS | 1000 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | -17.609 | ppm | |
| O2P | 5.000 | ppm | |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| SW | 308.694 | ppm | |
| TD | 32768 | | |
| AQ | 0.328 | s | field dependent |
| FIDRES | 3.052 | Hz | field dependent |
| D 1 | 1.487 | s | AQ+D1=const |
| P 0 | | us | P 1 * CNST 10 / 90 |
| P 1 | 11.0 | us | 90deg NUC1 |
| PLW 1 | 15.5 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.1 | W | Pow@CPD NUC2 |
| TE | 298.000 | K | default |

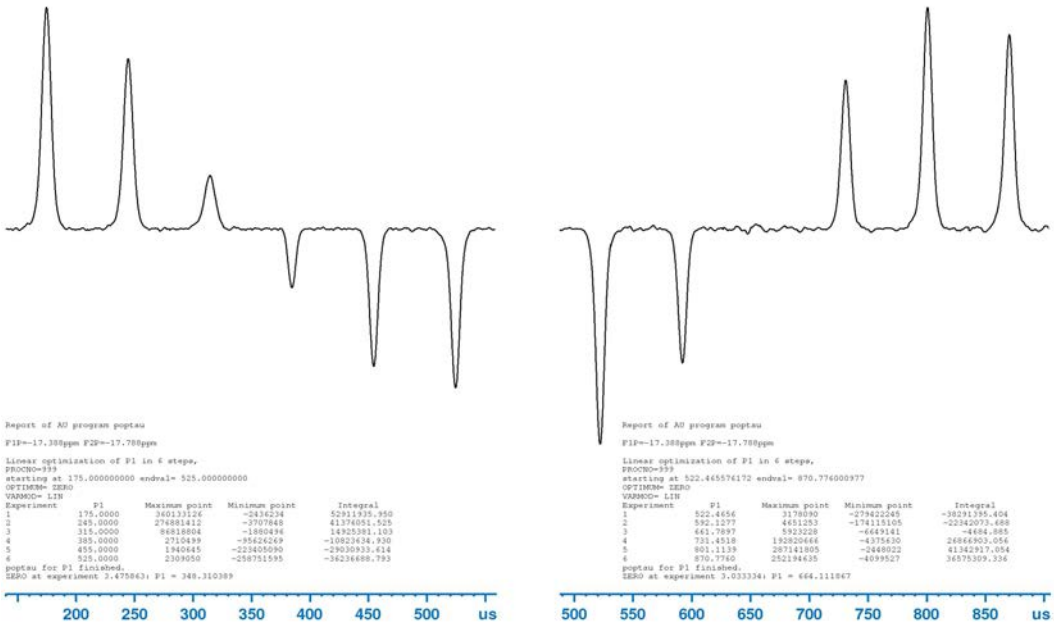
| | | | |
|---|---|---|---|
| CNST 10 | 20.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| PC | 1.400 | | |
| F1P | 24.747 | ppm | |
| F2P | -150.759 | ppm | |

### Experiment Description

Background signal measurements are executed using a small flip angle due to two reasons. First, to get more efficient excitation bandwidth, secondly to compensate for usually long T1 relaxation time of solid signals.
Full spectrum is normally printed without any baseline correction.

## 5.2.122 CPD 31P pulse calibration (NPT_31P_cpddeterminationf1_31p)

**Test Sample:** 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10201, Z100934, Z10202, Z10038, Z10257, Z10276, Z10722
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | -17.609 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 1000 | | |
| AQ | 1.260 | s | |
| FIDRES | 0.794 | Hz | |
| D 1 | 17.200 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

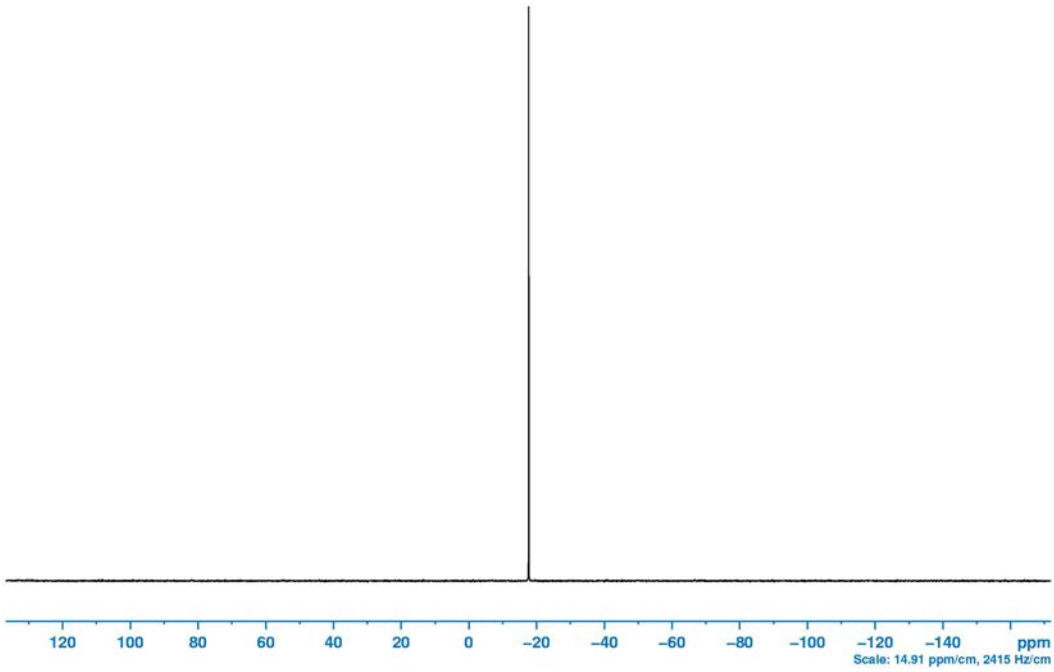
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 10.000 | ppm | |
| F2P | -38.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.123 31P test for artifacts (NPT_31P_fullsw_dec1h)

**Test Sample:** 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10201, Z100934, Z10202, Z10038, Z10257, Z10276, Z10722
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Full range 31P spectrum with 1H decoupling.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PULPROG | npt_zg0ig | | |
| NS | 64 | | |
| DS | 4 | | |
| RG | 101.000 | | no optim. |
| O1P | -17.609 | ppm | |
| O2P | 5.000 | ppm | |
| SW | 308.694 | ppm | |
| TD | 65536 | | |
| AQ | 0.655 | s | field dependent |
| FIDRES | 1.526 | Hz | field dependent |
| D 1 | 3.545 | s | AQ+D1=const |
| P 1 | 11.0 | us | 90deg NUC1 |
| PLW 1 | 18.0 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.2 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| TE | 298.000 | K | default |

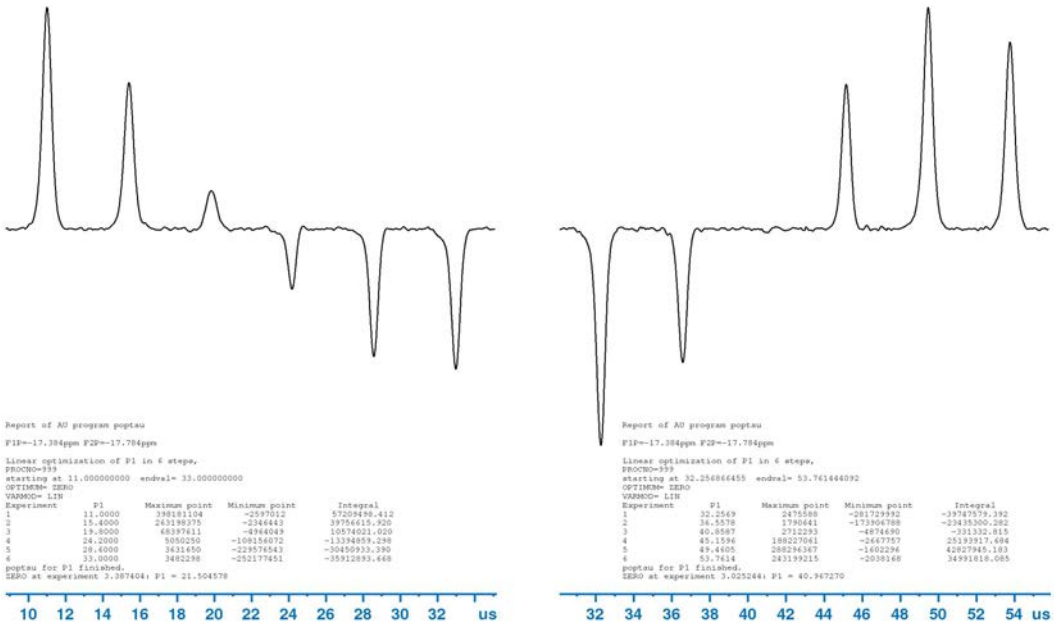
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| PC | 1.400 | | |
| F1P | 24.747 | ppm | |
| F2P | -150.759 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Full range spectra (spectroscopically useful range) are acquired as test for RF artifacts (spikes). Currently no evaluation is provided and visual inspection of the data is required. Data are treated with baseline correction.

## 5.2.124 P90 31P pulse calibration (NPT_31P_p90determinationf1_31p)

**Test Sample:** 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10201, Z100934, Z10202, Z10038, Z10257, Z10276, Z10722, Z142226
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | -17.609 | ppm | |
| SWH | 396.825 | Hz | |
| TD | 1000 | | |
| AQ | 1.260 | s | |
| FIDRES | 0.794 | Hz | |
| D 1 | 17.200 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

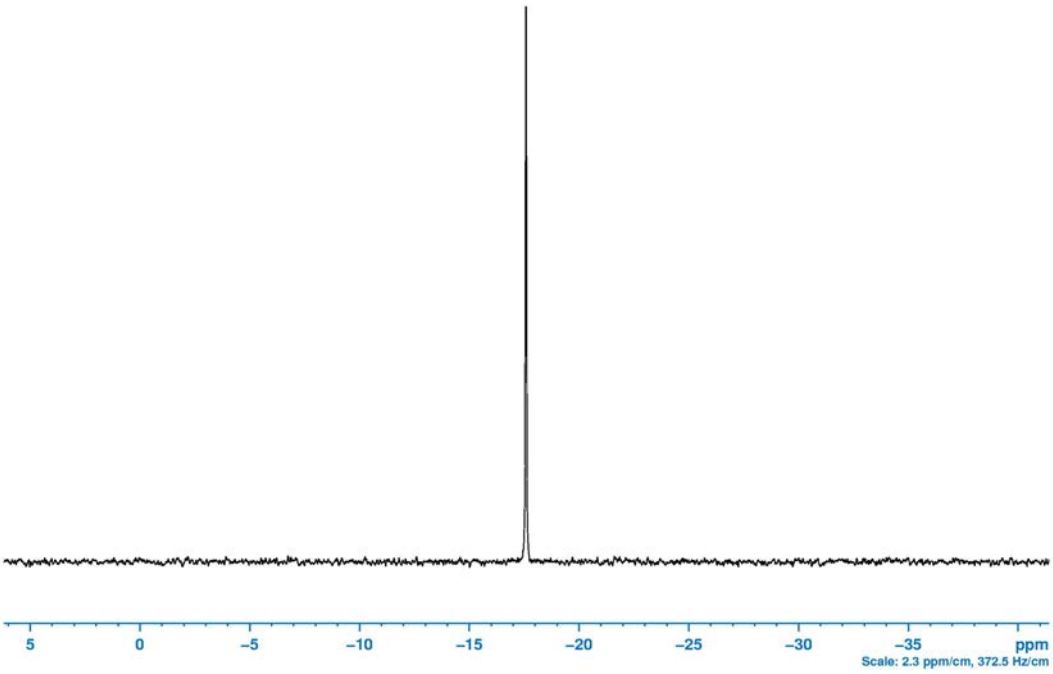
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 10.000 | ppm | |
| F2P | -38.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.125 31P sensitivity (NPT_31P_sensitivity)

**Test Sample:** 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10201, Z100934, Z10202, Z10038, Z10257, Z10276, Z10722, Z142226
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Phosphorous-31 sensitivity test.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | -17.609 | ppm | |
| SW | 50.606 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 119.001 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 27.4 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

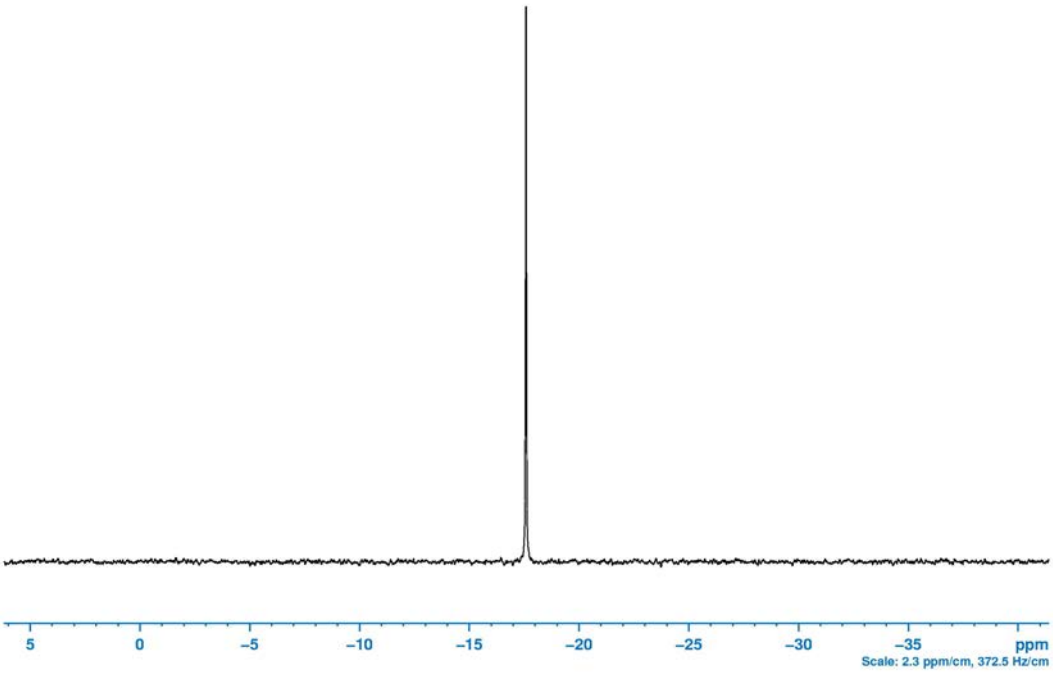
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| PC | 1.400 | | |
| F1P | 6.168 | ppm | |
| F2P | -43.919 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Phosphorous-31 sensitivity test (no 1H decoupling). Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from -15.0 to -18.0 ppm, while the best 5 ppm noise region is determined over the range from 7.0 to -15.0 ppm.

## 5.2.126 31P sensitivity with 1H decoupling (NPT_31P_sensitivity_dec1h)

**Test Sample:** 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10201, Z100934, Z10202, Z10038, Z10257, Z10276, Z10722, Z142226
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Phosphorous-31 sensitivity test with 1H decoupling.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PULPROG | zgig | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | -17.609 | ppm | |
| O2P | 5.000 | ppm | |
| SW | 50.606 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 119.001 | s | AQ+D1=const |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 27.4 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.35 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| TE | 298.000 | K | default |

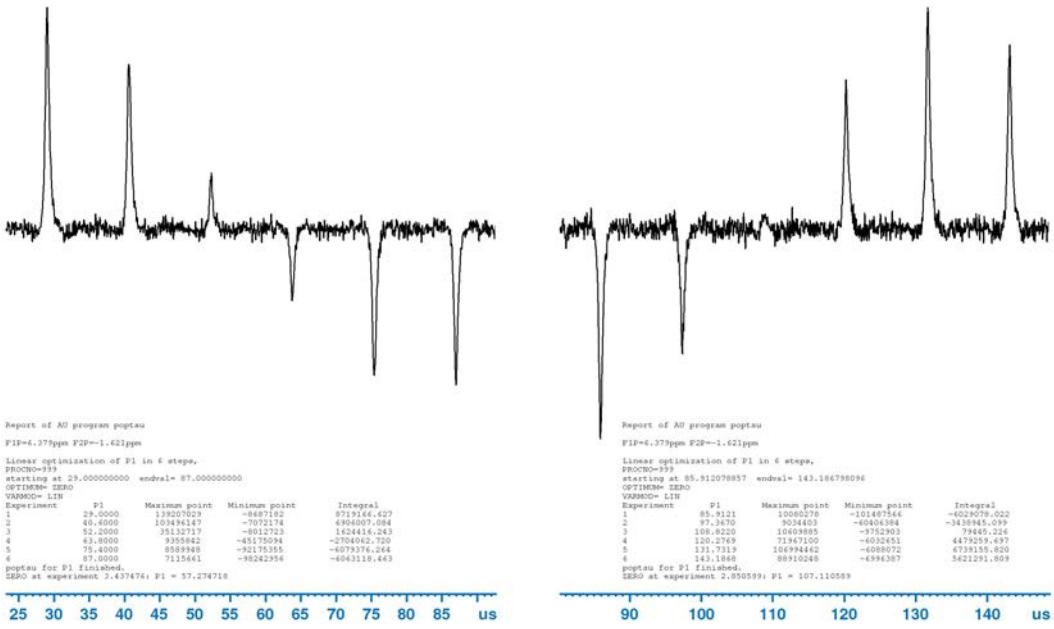
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 5.000 | Hz | |
| PC | 1.400 | | |
| F1P | 6.168 | ppm | |
| F2P | -43.919 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Phosphorous-31 sensitivity test with 1H decoupling. Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from -15.0 to -18.0 ppm, while the best 5 ppm noise region is determined over the range from 7.0 to -15.0 ppm.

## 5.2.127 P90 39K pulse calibration (NPT_39K_p90determination_39k)

**Test Sample:** 1 M Potassium Chloride (KCl) in D2O
Z10075, Z10076
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 39K | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 1.341 | ppm | |
| SWH | 588.235 | Hz | |
| TD | 1000 | | |
| AQ | 0.850 | s | |
| FIDRES | 1.176 | Hz | |
| D 1 | 0.250 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

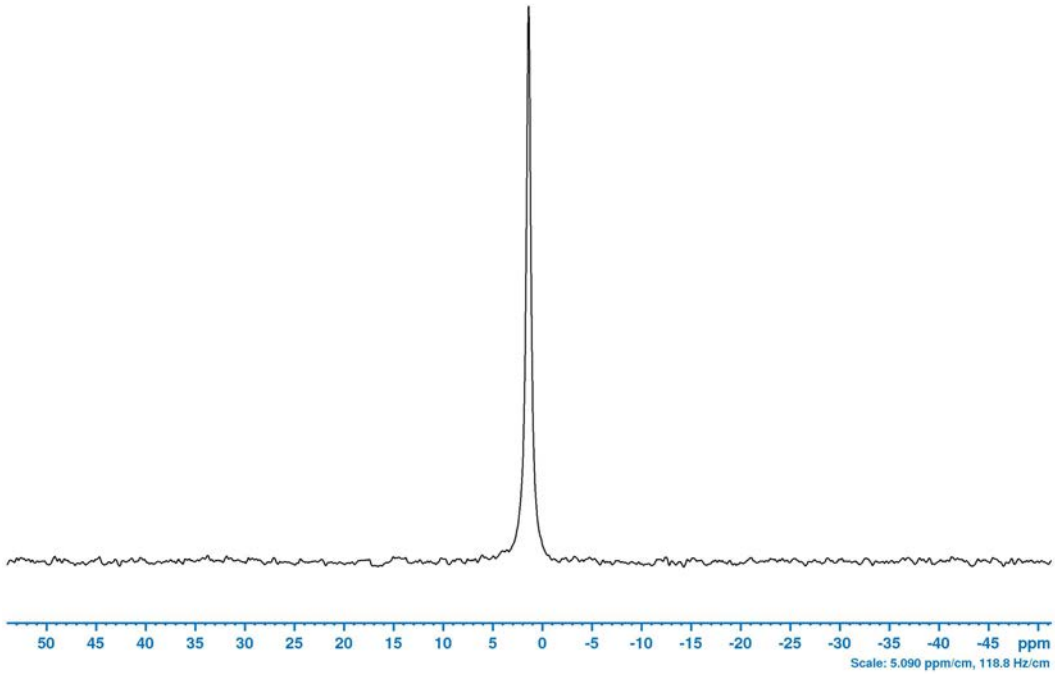
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| WDW | 3 | | |
| LB | 6.000 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 2.652 | ppm | |
| ABSF2 | -1.964 | ppm | |
| F1P | 2.907 | ppm | |
| F2P | -2.221 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.128 39K sensitivity (NPT_39K_sensitivity)

**Test Sample:** 1 M Potassium Chloride (KCl) in D2O
Z10075, Z10076
**Solvent:** D2O_salt
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**
Potassium-39 sensitivity test.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 39K | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 1.341 | ppm | |
| SW | 111.578 | ppm | |
| TD | 4096 | | |
| AQ | 0.983 | s | field dependent |
| FIDRES | 1.017 | Hz | field dependent |
| D 1 | 5.000 | s | AQ+D1=const |
| P 1 | 35.0 | us | 90deg NUC1 |
| PLW 1 | 70.2 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

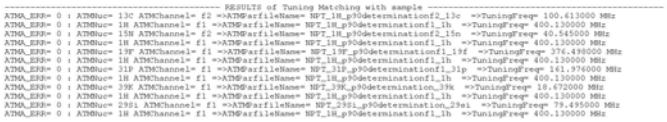
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 6.000 | Hz | |
| PC | 1.000 | | |
| F1P | 50.100 | ppm | |
| F2P | -50.100 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Potassium-39 sensitivity test. Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from 10.0 to -10.0 ppm, while the best 40 ppm noise region is determined over the range from 50.0 to 10.0 ppm.

## 5.2.129 Atma test (NPT_prep_atma_test)

**Test Sample:** Water Sample with 0.0, 0.25, or 1.0 M Sodium Chloride (NaCl).
Z142222, Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10719, Z10720, Z10191, Z101717, Z101714, Z100377, Z10731, Z10284, Z101715, Z10285, Z100375, Z101710, Z10192, Z10729, Z10288, Z101716, Z101712, Z100376, Z100372, Z10730
**Solvent:** H2O+D2O or D2O_salt
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**
List of ATM events.

**Control Option for Acquisition (L23)**
1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_zgnopul | | |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| CY | 11.000 | cm | |

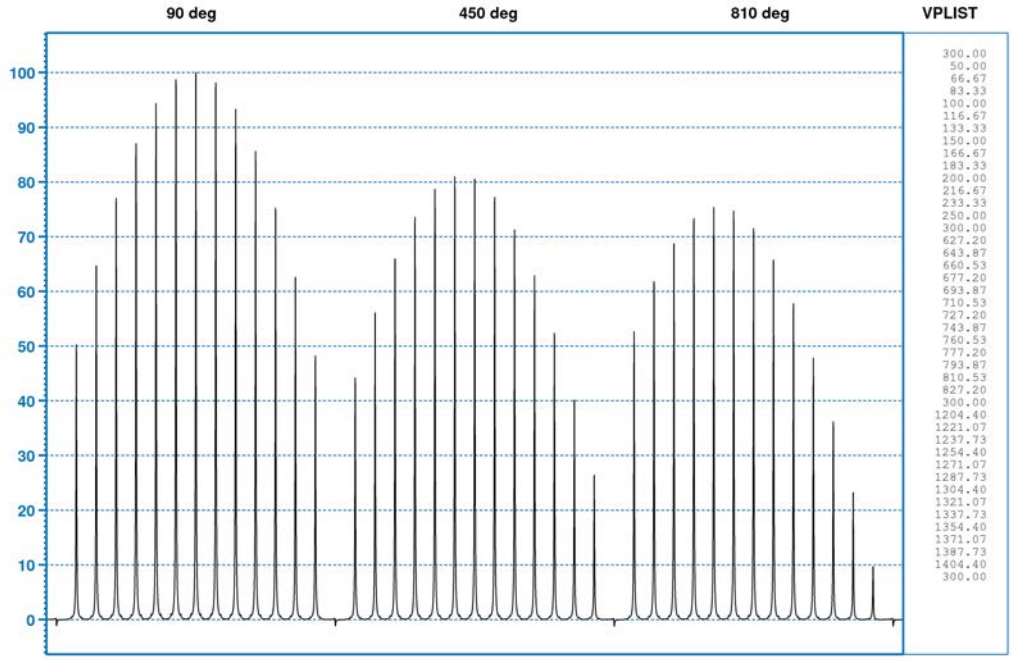
### Experiment Description

ATM test is executed for nuclei 1H, 2H, 13C, 15N, 19F, 29Si, 31P, 39K and 79Br, if specified for the given probe.
The tuning/matching order is defined by the ATMA_SEQUENCE specified.
The tuning/matching frequency is always referenced to the standard basic proton frequency of BF.13 MHz.
The probe will be tuned and matched to (standard frequency - 0.5 * specified value).
The wobble curves will be stored with procno 700 + number of atma attempt.

Requirements: Ratios for nuclei to be tested need to be specified.

## 5.2.130 2H B1 homogeneity integral (NPT_prep_b1homogeneityInt_d)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721, Z142223
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a fraction around signal maximum (-60 deg, +60 deg) is acquired and shown in the figure. The variable pulse list which is used for acquisition is shown to the right.
The B1-homogeneities based on amplitudes and integrals are computed from the peak-picking list amplitudes and the magnitude of the second complex FID data point respectively.

**Control Option for Acquisition (L23)**

1 default PLW 1 is used for determination of B1 homogeneity.
2 PLW 1 will be set to CNST 10 and resultant pulses are used for determination of B1 homogeneity. Experiment will be set to irregular.
3 PLW 1 will be set to power corresponding to specified customer pulses and resultant pulses are used for determination of B1 homogeneity.

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 2H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1b1hom2h2d | | |
| NS | 1 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.056 | ppm | |
| SWH | 230.766 | Hz | |
| TD | 1024 | | |
| AQ | 2.219 | s | |
| FIDRES | 0.451 | Hz | |
| D 1 | 3.683 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

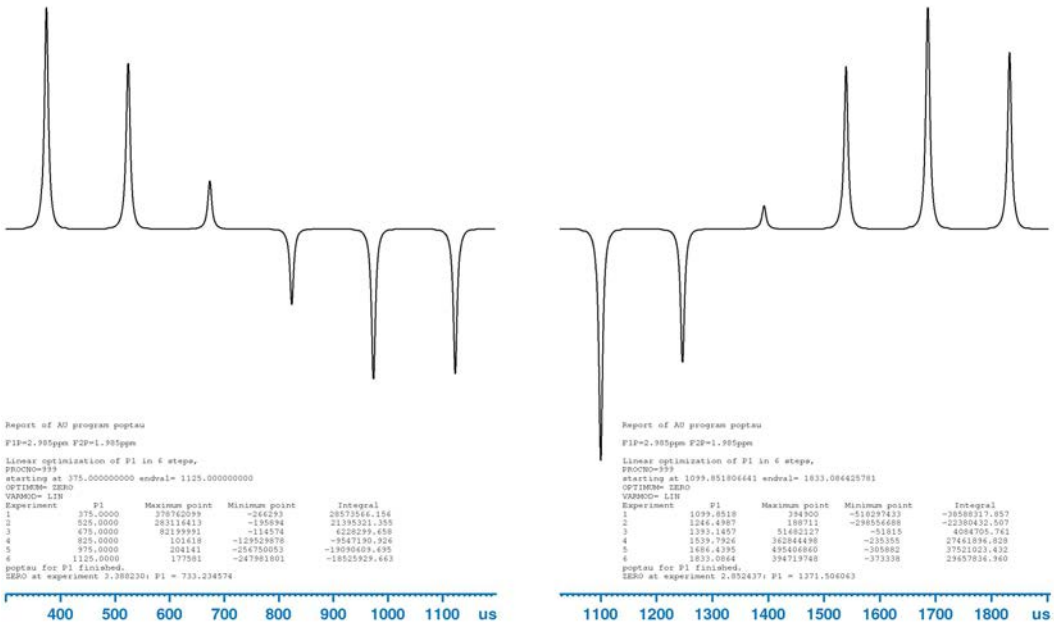
| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 4096 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 2H | | |
| TD | 43 | | No of incr. |
| **F1 PROC** | | | Parameters F1 |
| SI | 64 | | |
| **NMRPT** | | | Parameters |
| L 4 | 6 | | integ. fraction of 90deg |
| L 5 | 8 | | # of step per maxima |

## Experiment Description

The B1 homogeneity measurement is normally acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range is from 90 to 810 degree. In order to speed up the measurements NMRPT is acquiring only the partial ranges around the positive signal maxima for the pulse angles 90, 450, and 810 degree.
By this approach it is possible to get a better incremental resolution and a shorter overall measuring time.
Prior to the main acquisition O1P (PROCNO=2) and phase correction (PROCNO=3) will be optimized.
Intermediate results of the CONVTO1D routine is stored in PROCNO=998, result of CONVTO1D in PROCNO=999.
As control of stability, reproducability and 90 degree calibration a spectrum with 180 degree pulse is acquired before and after each maxima. If relaxation conditions and instrument stability is sufficient, the result should not differ among them.
For the predicition of the signal maxima at 450 and 810 degree the propagation delay is included in the calculation of the VP list. (PDelay is calculated as difference of 360 and 180 degree pulse lengths during the corresponding 90 degree pulse determination experiment.) In this measurement O1 is determined before the main acquisition is started. Evaluation is achieved after processing the data in F2 only (XF2) by peak picking and integral determination of the most intense signal per maxima.

## 5.2.131 CPD 2H pulse calibration (NPT_prep_cpddeterminationf1_d)

**Test Sample:** 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721
**Solvent:** DMSO
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | npt_zg2h | | |
| LOCNUC | off | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | optim. by RGA |
| O1P | 2.509 | ppm | |
| SWH | 326.797 | Hz | |
| TD | 1024 | | |
| AQ | 1.567 | s | |
| FIDRES | 0.638 | Hz | |
| D 1 | 0.350 | s | AQ+D1=const |
| P 1 | 180.0 | us | 90deg NUC1 |
| PLW 1 | 6.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

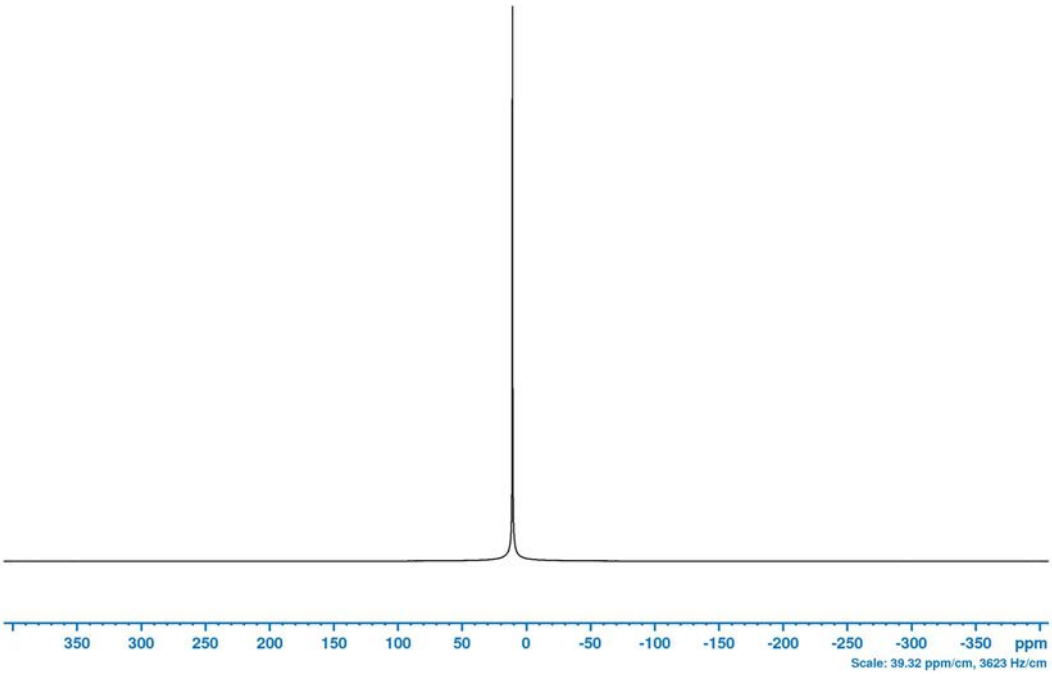
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.132 Optimization of 2H frequency (NPT_prep_fieldsetting_d)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10719, Z10720, Z142222
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

2H spectrum after field optimization

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | npt_zg2h | | |
| LOCNUC | off | | |
| NS | 8 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 0.000 | ppm | |
| SWH | 74626.867 | Hz | |
| TD | 131072 | | |
| AQ | 0.878 | s | |
| FIDRES | 1.139 | Hz | |
| D 1 | 0.500 | s | |
| P 1 | 180.0 | us | 90deg NUC1 |
| PLW 1 | 6.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |
| DE | 100.000 | us | set after getprosol |

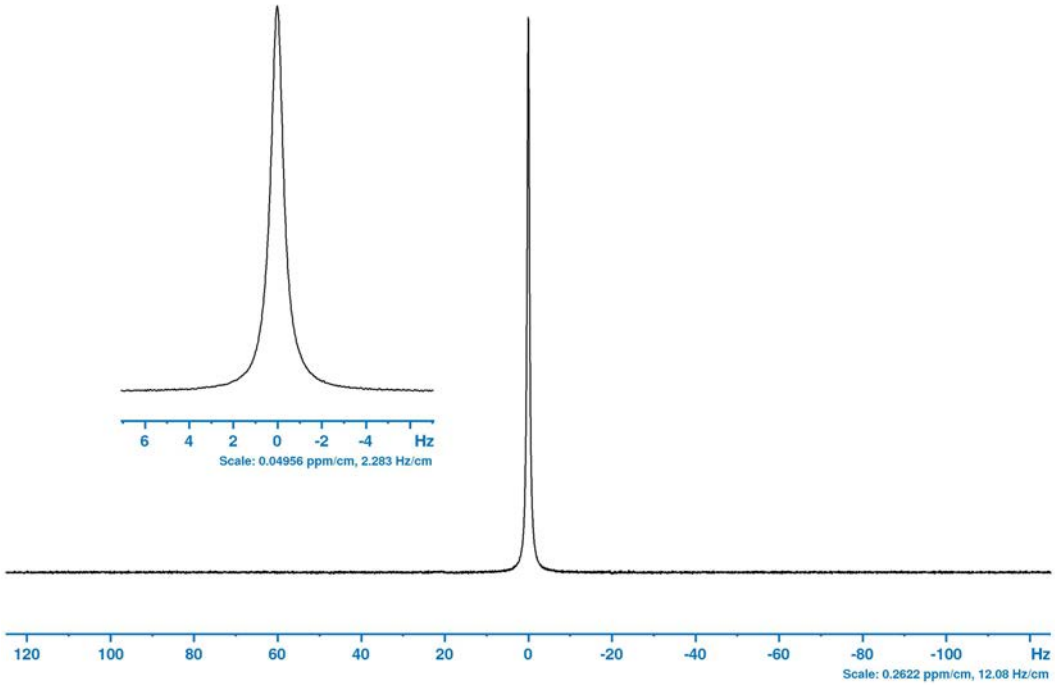
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 1 | | |
| PH_mod | 2 | | MC |
| F1P | 813.947 | ppm | |
| F2P | -813.947 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 0.450 | | LOCK(sweep rate) |
| CNST 51 | 2.500 | | LOCK(sweep amplitude) |
| CNST 52 | -75.000 | dB | LOCKDC (default) |
| CNST 53 | -59.900 | dB | min LOCKPOWER |
| CNST 54 | -500.000 | | delta FIELD for determ. |
| CNST 55 | 105.000 | dB | LOCKGAIN reference |

## Experiment Description

The experiment is used for determination of the current FIELD value based on the SOLVENT which is defined.
The experimental procedure includes two 2H acquisitions with constant 01 and LOCKSHIFT at two known FIELD positions. Using 4.7 ppm as chemical shift of 2H in H20+D2O the correct FIELD value can be calculated from these measurements.
NMRPT stores the resulting FIELD value in the BSMS.

## 5.2.133 2H linseshape with sample rotation (NPT_prep_lineshape_wrot)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z10268, Z10247
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Deuterium line shape spectrum with offset calibration to O1P as overview spectrum. Printing is from +125.0 Hz to -125.0 Hz. The expansion plot to the left shows deuterium signal with higher resolution (+7.0 Hz, -7.0 Hz).

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PULPROG | zg2h | | |
| LOCNUC | off | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 0.642 | ppm | |
| SWH | 1000.000 | Hz | |
| TD | 16384 | | |
| AQ | 8.192 | s | |
| FIDRES | 0.122 | Hz | |
| D 1 | 10.000 | s | |
| P 1 | 20.0 | us | 90deg NUC1 |
| PLW 1 | 64.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |
| DE | 100.000 | us | set after getprosol |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 0.400 | | |
| F1P | 14.693 | ppm | |
| F2P | -5.305 | ppm | |
| CY | 1000.000 | cm | |

## Experiment Description

Before acquiring the final spectrum, the exact signal position is determined. The carrier position is afterwards set to the position
optimized O1 = peak frequency [Hz] - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.

## 5.2.134 Optimization of 19F locksetting (NPT_prep_locksettings_19f)

**Test Sample:** 45% Chloroform-D (CDCl3) and 45% Chloroform (CHCl3) in 10% Hexafluorobenzene (C6F6).
Z10078, Z10079
**Solvent:** C6F6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off

Current LOCK Settings (according to 19Flock)

| Solvent | FIELD | LOCKPOWER | LOOPGAIN | LOOPTIME | LOOPFILTER | LOCKPHASE |
|---|---|---|---|---|---|---|
| C6F6 | 5763.0 | -50.0 | -3.4 | 0.3122 | 96.3 | 169.3 |

**Example Printout**

Listing of entries from edlock (TopSpin configuration file, accessible by edlock).

**Control Option for Acquisition (L23)**

1 Update LOCK control parameters for current SOLVENT (locked after experiment, default)
11 same as L23=1 but enforces a more complex phase optimization algorithm

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PULPROG | zg2h | | |
| LOCNUC | 19F | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | optim. by RGA |
| O1P | 7.000 | ppm | |
| SWH | 7462.687 | Hz | |
| TD | 74626 | | |
| AQ | 5.000 | s | |
| FIDRES | 0.200 | Hz | |
| D 1 | 1.000 | s | |
| P 1 | 14 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| WDW | 1 | | |
| PH_mod | 1 | | |
| F1P | 14.693 | ppm | |
| F2P | -5.305 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment is used for the initial setup of the LOCK environment and the update of the lock table of individual SOLVENT.
In case of successful LOCK and after AUTOGAIN the LOCKGAIN is memorized. The best LOCKGAIN value must be nearest to the optimal LOCKPHASE. Using these settings the AUTOPHASE routine determines the exact LOCKPHASE.
The final task of the experiment after storage of all information is the execution of a regular LOCK procedure.

## 5.2.135 Optimization of 2H locksetting (NPT_prep_locksettings_d)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z100930, Z10268, Z10036, Z10247, Z10267, Z10719, Z10720, Z142222
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off

Current LOCK Settings (according to 2Hlock)

| Solvent | FIELD | LOCKPOWER | LOOPGAIN | LOOPTIME | LOOPFILTER | LOCKPHASE |
|---|---|---|---|---|---|---|
| H2O+D2O | 7855.0 | -18.0 | -9.4 | 0.4640 | 50.0 | 33.2 |
| D2O_S0 | 7856.0 | -18.0 | 5.9 | 0.1256 | 334.3 | 32.5 |
| D2O | 7859.0 | -18.0 | 5.4 | 0.1329 | 312.4 | 32.7 |
| CDCl3 | 7849.0 | -30.0 | -9.4 | 0.4640 | 50.0 | 32.4 |
| C6D6 | 7861.0 | -26.0 | -1.5 | 0.2670 | 122.9 | 32.5 |
| DMSO | 7880.0 | -20.0 | -9.4 | 0.4640 | 50.0 | 32.2 |
| D2O_S1000 | 7851.0 | -18.0 | 5.7 | 0.1285 | 325.4 | 32.2 |
| Acetone | 7891.0 | -38.0 | 2.1 | 0.1925 | 195.4 | 27.0 |
| MeOD | 7886.0 | -35.0 | 2.0 | 0.1943 | 193.0 | 32.7 |

**Example Printout**

Listing of entries from edlock (TopSpin configuration file, accessible by edlock).

**Control Option for Acquisition (L23)**

1 Update LOCK control parameters for current SOLVENT (locked after experiment, default)
11 same as L23=1 but enforces a more complex phase optimization algorithm

### Parameters

| F1 ACQU | | Parameters |
|---|---|---|
| NUC1 | 1H | |
| PULPROG | npt_zgnopul | |
| LOCNUC | 2H | |
| RG | 101.000 | no optim. |

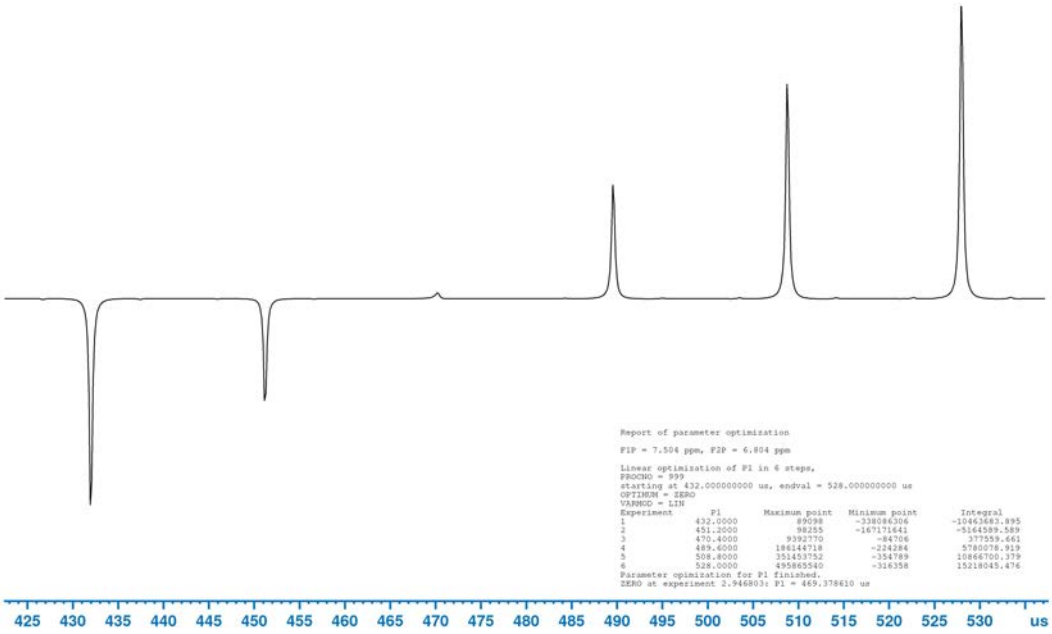
| F1 PROC | | | Parameters |
|---|---|---|---|
| CY | 11.000 | cm | |

### Experiment Description

This experiment is used for the initial setup of the LOCK environment and the update of the lock table of individual SOLVENT.
In case of successful LOCK and after AUTOGAIN the LOCKGAIN is memorized. The best LOCKGAIN value must be nearest to the optimal LOCKPHASE. Using these settings the AUTOPHASE routine determines the exact LOCKPHASE.
NMRPT stores the resulting LOCKPHASE value in the edlock of TopSpin.
The final task of the experiment after storage of all information is the execution of a regular LOCK procedure.

## 5.2.136 P90 2H pulse calibration (NPT_prep_p90det_astm_d)

**Test Sample:** 40% Dioxane in Benzene-D6 (ASTM)
Z10163, Z100929, Z10164, Z10035, Z10255, Z10242, Z10724
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments arround 360 deg.

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | npt_zg2h | | |
| LOCNUC | off | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| SWH | 357.143 | Hz | |
| TD | 1048 | | |
| AQ | 1.467 | s | |
| FIDRES | 0.682 | Hz | |
| O1P | 7.200 | ppm | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| DIGMOD | 3 | | baseopt |
| DSPFIRM | 4 | | rectangle |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 1024 | | |
| LB | 0.500 | Hz | |
| F1P | 8.095 | ppm | |
| F2P | 6.305 | ppm | |
| CY | 5.500 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).

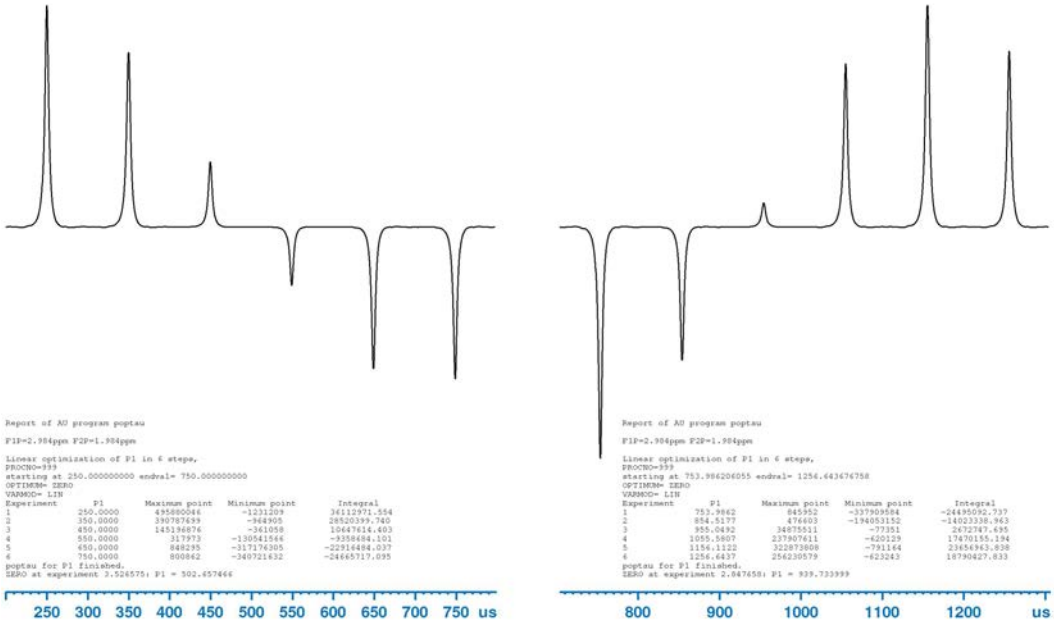
## 5.2.137 P90 2H pulse calibration (NPT_prep_p90det_d)

**Test Sample:** (a) 100 mM Urea-15N ([15NH2]2CO) and 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
(b) 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10263, Z100932, Z10265, Z10037, Z10264, Z10274, Z10721, Z142223

**Solvent:** (a) DMSO
(b) H2O+D2O

**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table

**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. On the left side the result of a CONVTO1D routine shows six experiments from 90 to 270 deg. On the right side the series goes from 270 deg to 450 deg.

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | npt_zg2h | | |
| LOCNUC | off | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.509 | ppm | (Urea Sample) |
| O1P | 4.7 | ppm | (Sucrose Sample) |
| SWH | 326.797 | Hz | |
| TD | 1024 | | |
| AQ | 1.567 | s | |
| FIDRES | 0.638 | Hz | |
| D 1 | 0.350 | s | AQ+D1=const |
| P 1 | 180.0 | us | 90deg NUC1 |
| PLW 1 | 6.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

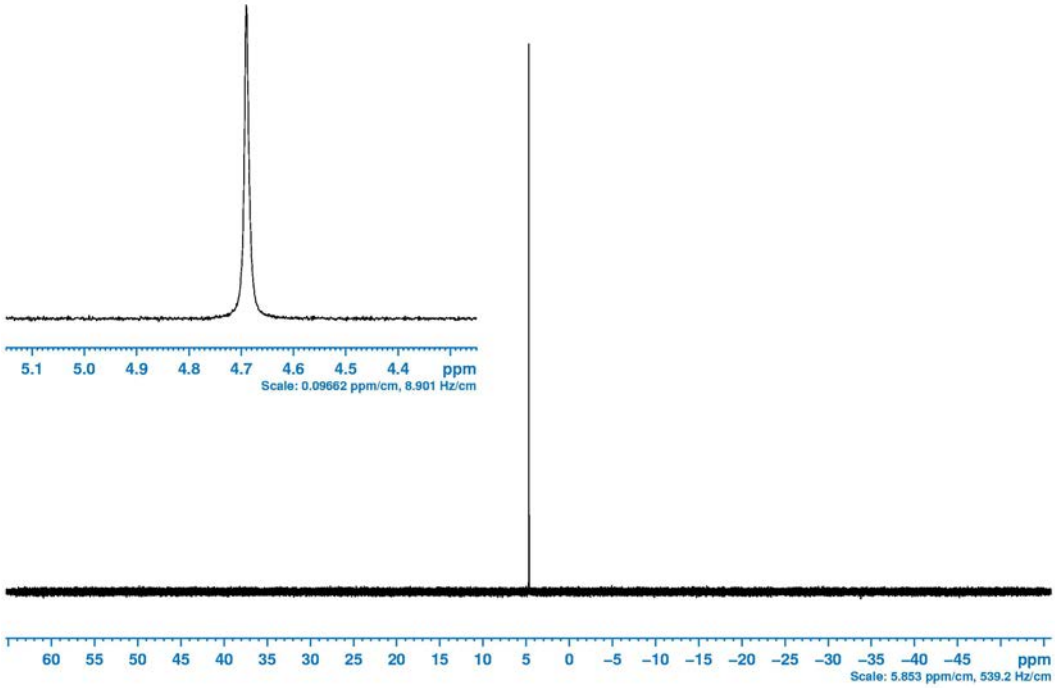
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).
PDelay (propagation delay) is calculated as difference of 360 and 180 degree pulse lengths- and memorised for further use in B1 homogeneity experiments.

## 5.2.138 2H sensitivity, 1% D2O (NPT_prep_sensitivity_1_d)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 99% H2O + 1% D2O
Z10908, Z10610, Z10056
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Deuterium sensitivity test.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PULPROG | zg2h | | |
| LOCNUC | off | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.716 | ppm | |
| SW | 121.497 | ppm | |
| AQ | 5.000 | s | |
| FIDRES | 0.200 | Hz | |
| D 1 | 10.000 | s | |
| P 1 | 180.0 | us | 90deg NUC1 |
| PLW 1 | 6.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

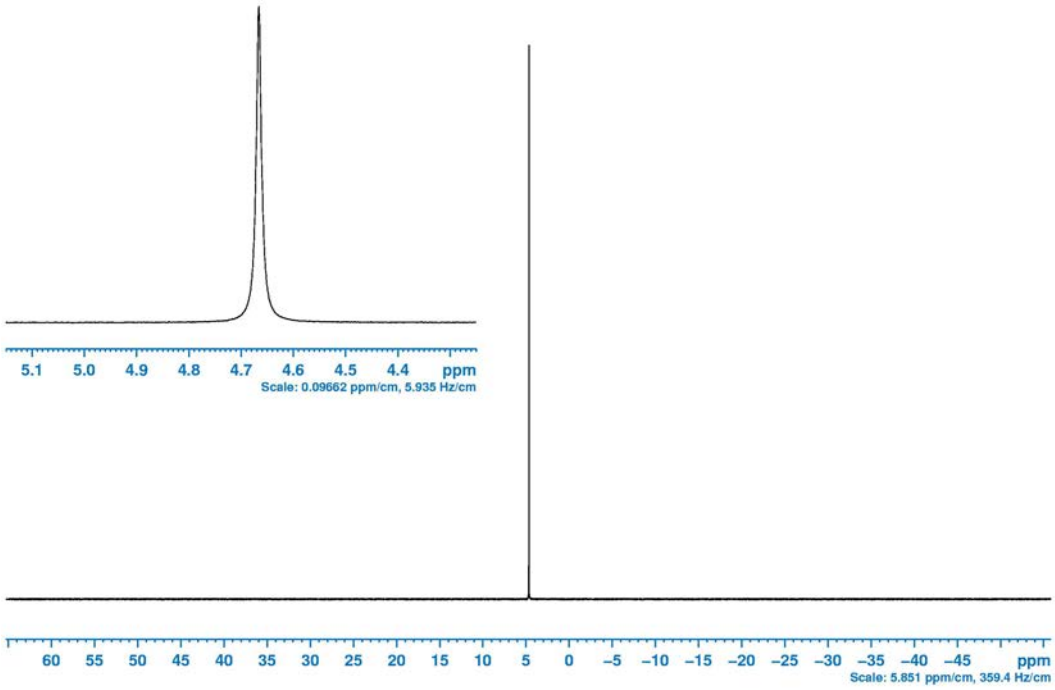
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 262144 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.400 | | |
| F1P | 14.693 | ppm | |
| F2P | -5.305 | ppm | |
| SIGF1 | 5.000 | ppm | |
| SIGF2 | 4.000 | ppm | |
| NOISF1 | 60.000 | ppm | |
| NOISF2 | 10.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Deuterium sensitivity test. Processing is using no line broadening (LB=0) and baseline correction (ABS). Evaluation is carried out by the command SINO. The signal is searched over the range from 5.0 to 4.0 ppm. For HR probes the noise region is determined over the range from 60.0 to 10.0 ppm, while for CMP and HRMAS probes a noise region of 2000 Hz will be used to exclude spinning side bands .

## 5.2.139 2H sensitivity, 10% D2O (NPT_prep_sensitivity_10_d)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10902, Z10246, Z142222, Z100930, Z10268, Z10036, Z10247, Z10719, Z10720
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**
Deuterium sensitivity test.

**Control Option for Acquisition (L23)**
1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PULPROG | zg2h | | |
| LOCNUC | off | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.716 | ppm | |
| SW | 121.497 | ppm | |
| AQ | 5.000 | s | |
| FIDRES | 0.200 | Hz | |
| D 1 | 10.000 | s | |
| P 1 | 180.0 | us | 90deg NUC1 |
| PLW 1 | 6.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

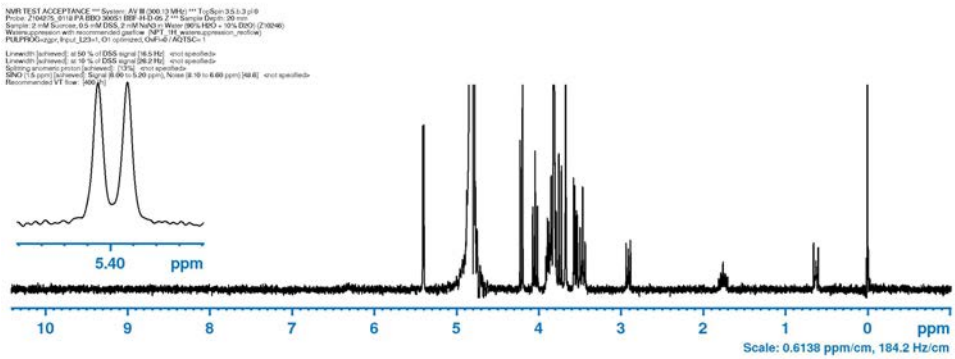
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 262144 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.400 | | |
| F1P | 14.693 | ppm | |
| F2P | -5.305 | ppm | |
| SIGF1 | 5.000 | ppm | |
| SIGF2 | 4.000 | ppm | |
| NOISF1 | 60.000 | ppm | |
| NOISF2 | 10.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

Deuterium sensitivity test. Processing is using no line broadening (LB=0) and baseline correction (ABS). Evaluation is carried out by the command SINO. The signal is searched over the range from 5.0 to 4.0 ppm. For HR probes the noise region is determined over the range from 60.0 to 10.0 ppm, while for CMP and HRMAS probes a noise region of 2000 Hz will be used to exclude spinning side bands .

## 5.2.140 Automated shim optimization (NPT_prep_tsopt)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O
Z10246, Z10902, Z180181, Z100930, Z10268, Z10036, Z10247, Z10267, Z10720, Z10719
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation according to RO




**Example Printout**

Top: Result of last water suppression experiment
Bottom: Protocol of shim sequences used

**Control Option for Acquisition (L23)**

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 1H | | |
| PULPROG | npt_zgnopul | | |
| TE | 298.000 | K | default |
| **F1 PROC** | | | Parameters |
| CY | 11.000 | cm | |

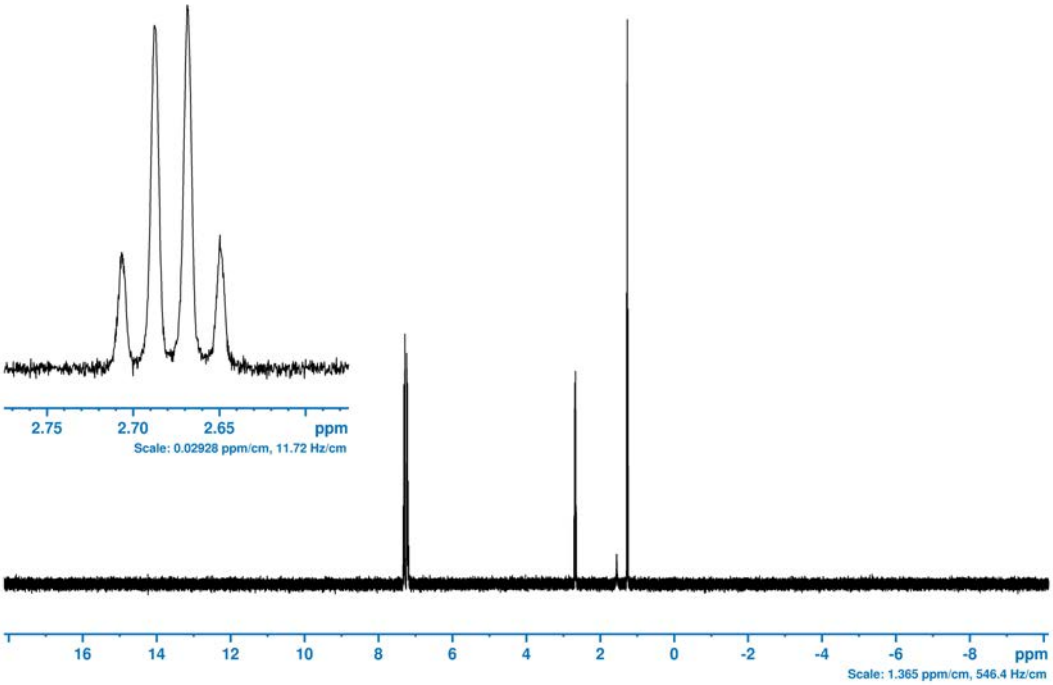
| | | |
|---|---|---|
| **NMRPT** | | Parameters |
| CNST 55 | 1.000 | L23 watersuppr. |

### Experiment Description

This experiment is used to initialize some settings at the beginning of nmrpt. As pre-condition the 1H pulse must be set with edprosol.
The composite experiment consists of the following steps:
1) For BB probes the BB channel will be tuned and matched.
2) The correct FIELD value will be determined using the experiment NPT_prep_fieldsetting_d and stored into the BSMS.
3) Shimming by TopShim. As default 'topshim initial cal' will be used.
4) LOCK parameters are optimized using NPT_prep_locksettings.
5) Watersuppression experiment is executed (including O1 and RG optimization) and evaluated. Evaluation is based on the interpretation of the splitting which is obtained in the water suppression experiment.

## 5.2.141 1H inno (NPT_1H_sensitivity_inno)

**Test Sample:** 0.1% Ethylbenzene (EB) in Chloroform-D
Z10120, Z100927, Z10121, Z10033, Z10270, Z10718, Z142221
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Bottom: 1H overview spectrum of ethylbenzene processed without line broadening.
Top left: Expanded region showing the methylene group used for evaluation.

**Control Option for Acquisition (L23)**

1- number of cycles of phase and base line correction
10

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 4.000 | ppm | |
| SWH | 11904.762 | Hz | |
| TD | 262144 | | |
| AQ | 11.010 | s | |
| FIDRES | 0.091 | Hz | |
| D 1 | 113.574 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

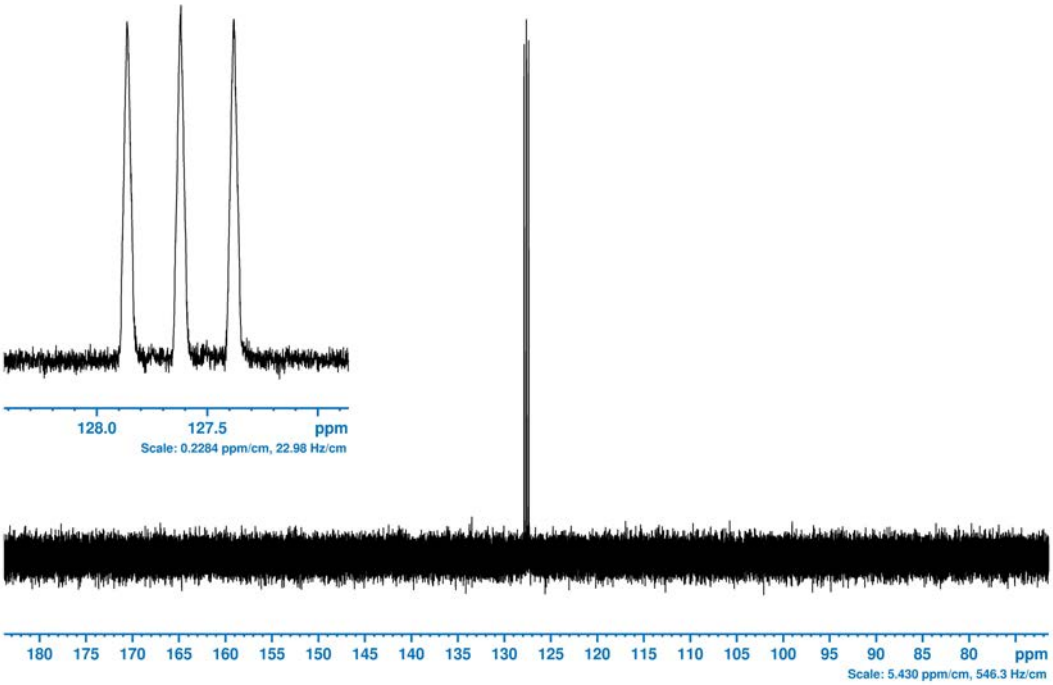
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

The experiment determines INNO (Integral-to-noise ratio, I/N). Before the INNO determination baseline and phase correction is executed in an iterative manner. The noise is determined over the whole spectrum, excluding signals und spectrum edges. The determination of I/N allows to obtain a measure for the sensitivity of the probe independent of the actual shim. The noise (and integral) determination is execute after scaling the data stored as intergers in 1r with pow(2.0, NC_proc).

## 5.2.142 13C inno (NPT_13C_sensitivity_inno)

**Test Sample:** 40% Dioxane in Benzene-D6 (ASTM)
Z10163, Z100929, Z10164, Z10035, Z10255, Z10242, Z10724, Z142224
**Solvent:** C6D6
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Bottom: 13C overview spectrum of benzene-d6 (no 1H decoupling) processed without line broadening.
Top left: Expanded region showing the CH group used for evaluation.

**Control Option for Acquisition (L23)**

1- number of cycles of phase and base line correction
10

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 127.620 | ppm | |
| SWH | 11904.762 | Hz | |
| TD | 262144 | | |
| AQ | 11.010 | s | |
| FIDRES | 0.091 | Hz | |
| D 1 | 828.899 | s | |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 39.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

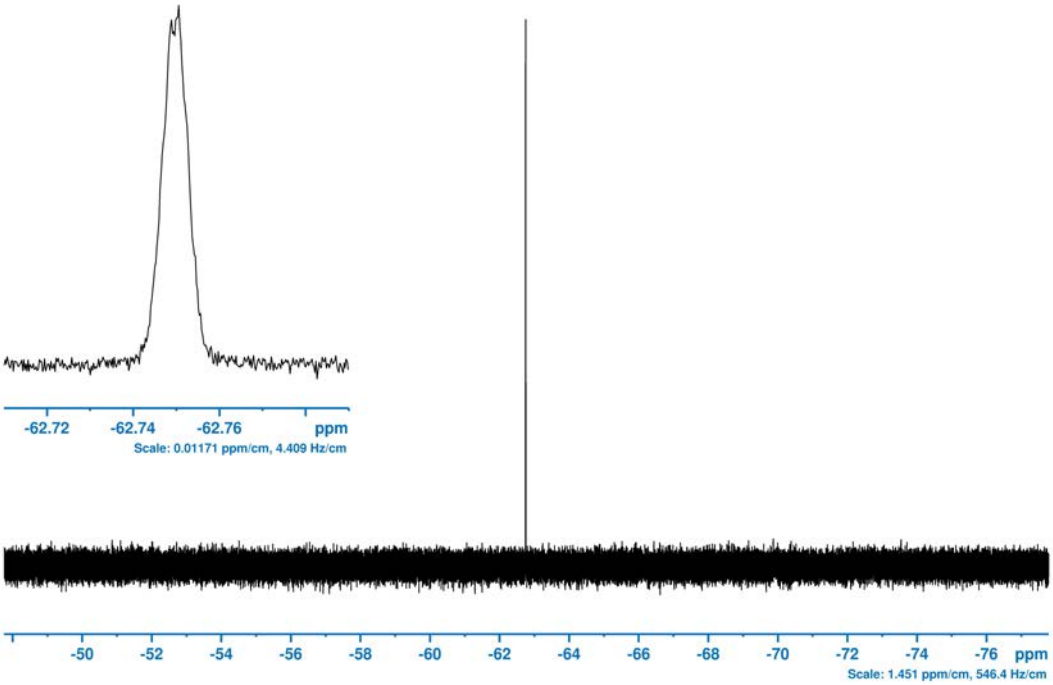
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.400 | | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

The experiment determines INNO (Integral-to-noise ratio, I/N). Before the INNO determination baseline and phase correction is executed in an iterative manner. The noise is determined over the whole spectrum, excluding signals und spectrum edges. The determination of I/N allows to obtain a measure for the sensitivity of the probe independent of the actual shim. The noise (and integral) determination is execute after scaling the data stored as intergers in 1r with pow(2.0, NC_proc).

## 5.2.143 19F inno (NPT_19F_sensitivity_inno)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Bottom: 19F overview spectrum of trifluorotoluene (no 1H decoupling) processed without line broadening.
Top left: Expanded region showing the CF3 group used for evaluation.

**Control Option for Acquisition (L23)**

1- number of cycles of phase and base line correction
10

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | -62.766 | ppm | |
| SWH | 11904.762 | Hz | |
| TD | 262144 | | |
| AQ | 11.010 | s | |
| FIDRES | 0.091 | Hz | |
| D 1 | 32.090 | s | |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 25.1 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

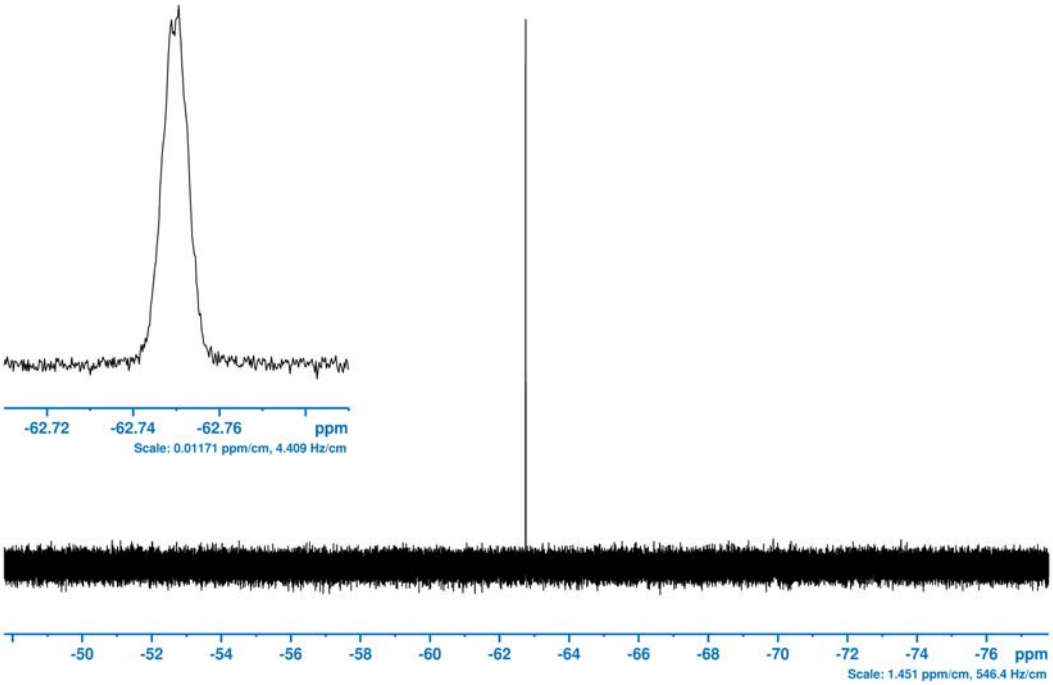
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

The experiment determines INNO (Integral-to-noise ratio, I/N). Before the INNO determination baseline and phase correction is executed in an iterative manner. The noise is determined over the whole spectrum, excluding signals und spectrum edges. The determination of I/N allows to obtain a measure for the sensitivity of the probe independent of the actual shim. The noise (and integral) determination is execute after scaling the data stored as intergers in 1r with pow(2.0, NC_proc).

## 5.2.144 19F inno on 1H/19F-coil (NPT_19F_sensitivity_inno_hcoil)

**Test Sample:** 0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10234, Z100937, Z10235, Z10040, Z10728, Z142228
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Bottom: 19F overview spectrum of trifluorotoluene (no 1H decoupling) processed without line broadening.
Top left: Expanded region showing the CF3 group used for evaluation.

**Control Option for Acquisition (L23)**

1- number of cycles of phase and base line correction
10

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | -62.766 | ppm | |
| SWH | 11904.762 | Hz | |
| TD | 262144 | | |
| AQ | 11.010 | s | |
| FIDRES | 0.091 | Hz | |
| D 1 | 32.090 | s | |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 25.1 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

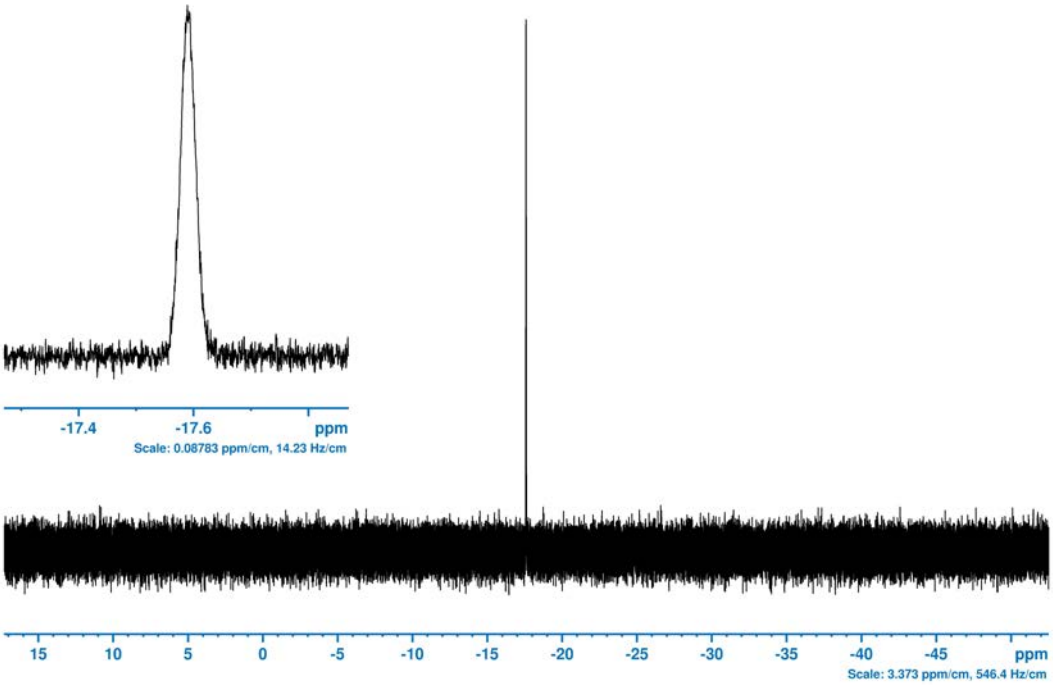
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

The experiment determines INNO (Integral-to-noise ratio, I/N). Before the INNO determination baseline and phase correction is executed in an iterative manner. The noise is determined over the whole spectrum, excluding signals und spectrum edges. The determination of I/N allows to obtain a measure for the sensitivity of the probe independent of the actual shim. The noise (and integral) determination is execute after scaling the data stored as intergers in 1r with pow(2.0, NC_proc).

## 5.2.145 31P inno (NPT_31P_sensitivity_inno)

**Test Sample:** 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10201, Z100934, Z10202, Z10038, Z10257, Z10276, Z10722, Z142226
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**

Bottom: 31P overview spectrum of triphenyl phosphate (no 1H decoupling) processed without line broadening.
Top left: Expanded region showing the PO4 group used for evaluation.

**Control Option for Acquisition (L23)**

1- number of cycles of phase and base line correction
10

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | -17.609 | ppm | |
| SWH | 11904.762 | Hz | |
| TD | 262144 | | |
| AQ | 11.010 | s | |
| FIDRES | 0.091 | Hz | |
| D 1 | 119.654 | s | |
| P 1 | 9.0 | us | 90deg NUC1 |
| PLW 1 | 27.4 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

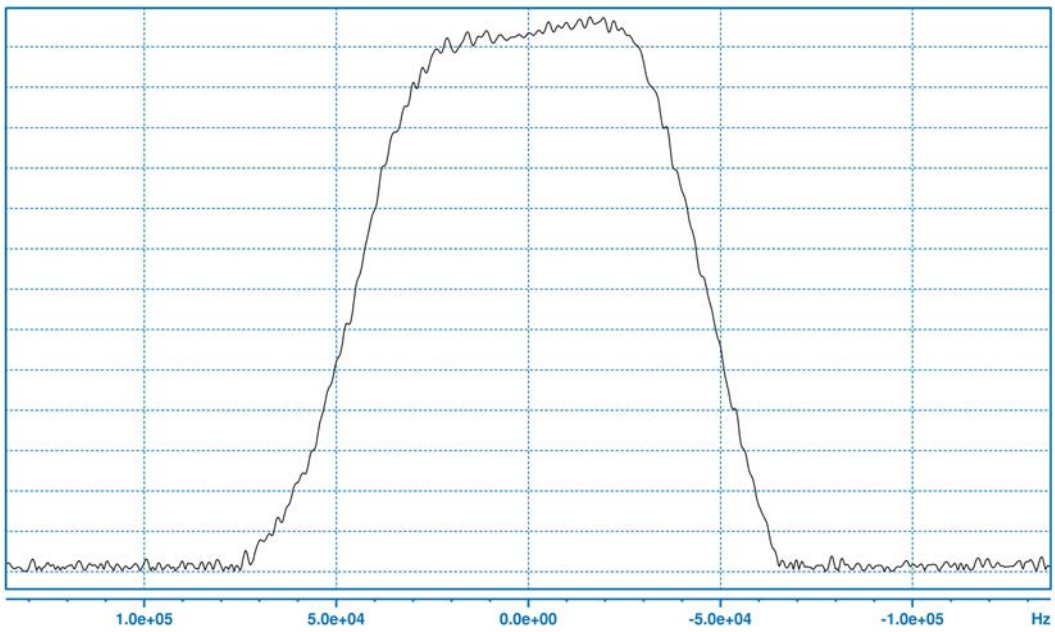
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.400 | | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

The experiment determines INNO (Integral-to-noise ratio, I/N). Before the INNO determination baseline and phase correction is executed in an iterative manner. The noise is determined over the whole spectrum, excluding signals und spectrum edges. The determination of I/N allows to obtain a measure for the sensitivity of the probe independent of the actual shim. The noise (and integral) determination is execute after scaling the data stored as intergers in 1r with pow(2.0, NC_proc).

## 5.2.146 1H Z-gradient profile [+] (NPT_1H_CMR_gradientprofile_pos)

**Test Sample:** 5% H2O, 0.6mM CuSO4 in D2O
Z10688
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**
Proton Z-gradient profile.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 16 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 4.700 | ppm | |
| SWH | 2500000.000 | Hz | |
| TD | 1024 | | |
| AQ | 0.000 | s | |
| FIDRES | 4882.812 | Hz | |
| D 1 | 10.000 | s | |
| D 15 | 0.015 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 11.0 | us | 90 degree |
| PLW 0 | 1.1 | W | Pow@90deg(Specs) NUC1 |
| P 1 | 11.0 | us | 90deg NUC1 |
| PLW 1 | 1.1 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | | | |
| GPNAM2 | | | |
| GPZ 1 | 25.000 | % | |
| GPZ 2 | -100.000 | % | |
| TE | 298.000 | K | default |

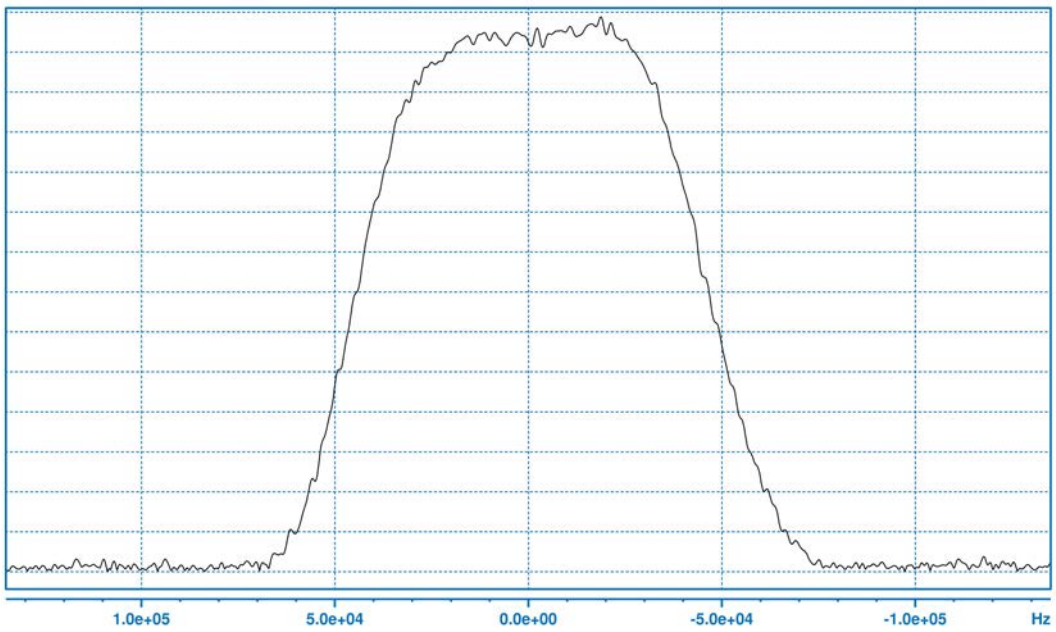
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 16.243 | ppm | |
| F2P | -3.893 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 37 | 19.400 | mm | active sample size |

## Experiment Description

Z-gradient profile is acquired with positive gradient in order to check the basic functionality of gradient. The profile width is determined at 50% of the maximum profile intensity respectively.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

## 5.2.147 1H Z-gradient profile [-] (NPT_1H_CMR_gradientprofile_neg)

**Test Sample:** 5% H2O, 0.6mM CuSO4 in D2O
Z10688
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




**Example Printout**
Proton Z-gradient profile.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | npt_imgegp1d | | |
| NS | 16 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 4.700 | ppm | |
| SWH | 2500000.000 | Hz | |
| TD | 1024 | | |
| AQ | 0.000 | s | |
| FIDRES | 4882.812 | Hz | |
| D 1 | 10.000 | s | |
| D 15 | 0.015 | s | Echo time |
| D 21 | 0.000 | s | Grad. stab. |
| D 27 | 0.002 | s | Dephas. grad. |
| P 0 | 11.0 | us | 90 degree |
| PLW 0 | 1.1 | W | Pow@90deg(Specs) NUC1 |
| P 1 | 11.0 | us | 90deg NUC1 |
| PLW 1 | 1.1 | W | Pow@90deg(Specs) NUC1 |
| GPNAM1 | | | |
| GPNAM2 | | | |
| GPZ 1 | -25.000 | % | |
| GPZ 2 | 100.000 | % | |
| TE | 298.000 | K | default |

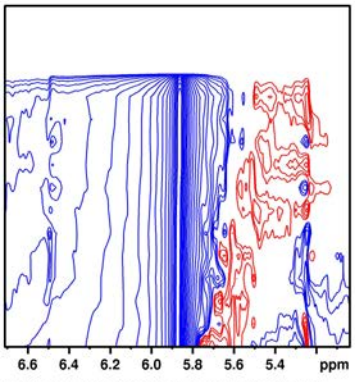
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 16.243 | ppm | |
| F2P | -3.893 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 37 | 19.400 | mm | active sample size |

## Experiment Description

Z-gradient profile is acquired with negative gradient in order to check the basic functionality of gradient. The profile width is determined at 50% of the maximum profile intensity respectively.
Together with the length of the RF coil and gyromagnetic ratio of the observed nuclei the gradient strength (G/cm*A) is calculated. Processing is always executed with magnitude correction (PH_mod=MC).

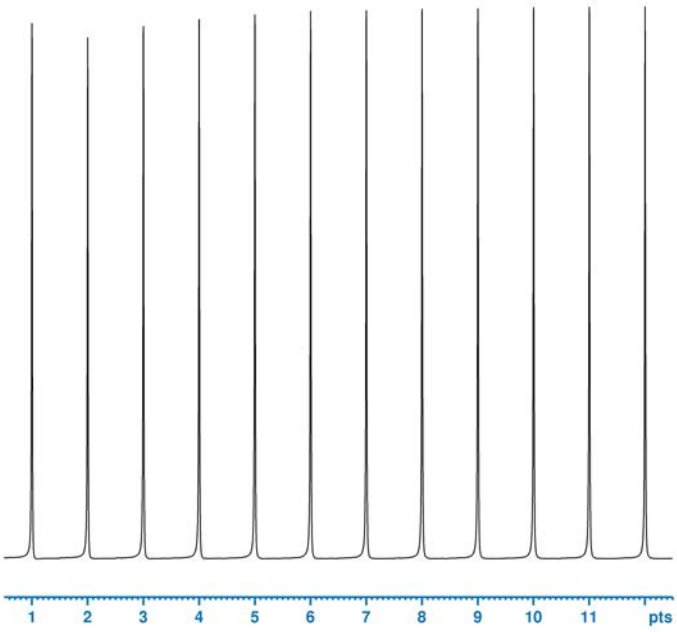
## 5.2.148 Gradient recovery test for Z-direction [+] (NPT_1H_CMR_gradientrecovery_pos)

**Test Sample:** 5% H2O, 0.6mM CuSO4 in D2O
Z10688
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| Experiment Number | Recovery Delay | Scaled Intensity |
|---|---|---|
| 1 | 100.0 us | 96.88% |
| 2 | 200.0 us | 94.31% |
| 3 | 300.0 us | 96.36% |
| 4 | 400.0 us | 97.64% |
| 5 | 500.0 us | 98.53% |
| 6 | 600.0 us | 99.11% |
| 7 | 700.0 us | 99.42% |
| 8 | 800.0 us | 99.63% |
| 9 | 900.0 us | 99.73% |
| 10 | 1.0 ms | 99.87% |
| 11 | 1.1 ms | 99.89% |
| 12 | 1.2 ms | 100.00% |




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, and signal intensity.

**Control Option for Acquisition (L23)**

1 default
10 skip sino check

## Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 3.000 | ppm | |
| SW | 20.485 | ppm | |
| TD | 16384 | | field dependent |
| AQ | 0.999 | s | |
| FIDRES | 1.001 | Hz | |
| D 1 | 10.000 | s | |
| VDLIST | npt_gradrecCMR | | default |
| P 1 | 11.0 | us | 90deg Pulse |
| PLW 1 | 1.1 | W | Pow@90deg(Specs) |
| GPNAM1 | SINE.100 | | |
| GPZ 1 | 100.000 | % | 7.5 A |
| P 16 | 1000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 12 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 12 | | |

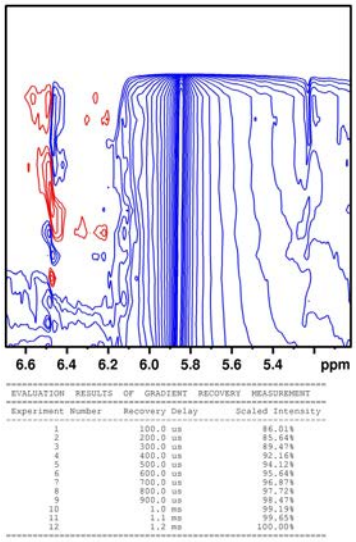
## Experiment Description

Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
SINO check can be skiped with L23=10
After successful SINO check, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of he determination of the intensity deviation to the reference experiment (last of the series)
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of range where specified intensity must be reached, needs to be specified.

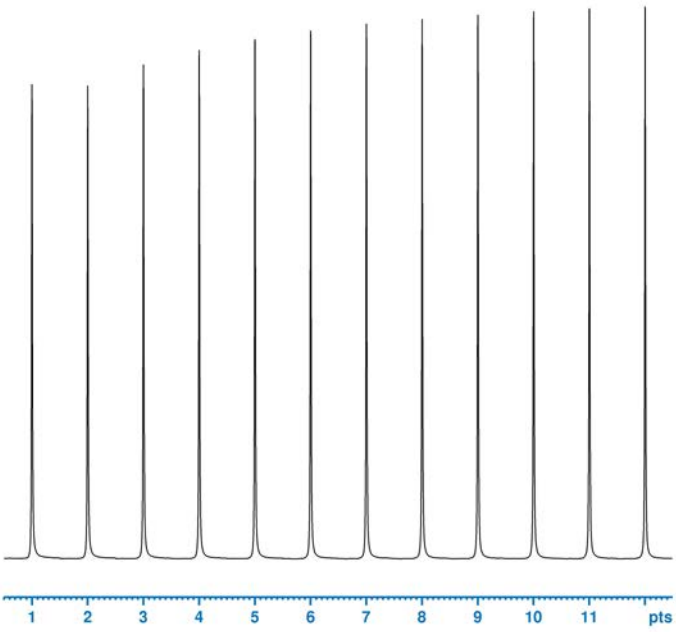
## 5.2.149 Gradient recovery test for Z-direction [-] (NPT_1H_CMR_gradientrecovery_neg)

**Test Sample:** 5% H2O, 0.6mM CuSO4 in D2O
Z10688
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Rotation off




EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT

| Experiment Number | Recovery Delay | Scaled Intensity |
|---|---|---|
| 1 | 100.0 us | 86.01% |
| 2 | 200.0 us | 85.64% |
| 3 | 300.0 us | 89.47% |
| 4 | 400.0 us | 92.16% |
| 5 | 500.0 us | 94.12% |
| 6 | 600.0 us | 95.64% |
| 7 | 700.0 us | 96.87% |
| 8 | 800.0 us | 97.72% |
| 9 | 900.0 us | 98.47% |
| 10 | 1.0 ms | 99.19% |
| 11 | 1.1 ms | 99.65% |
| 12 | 1.2 ms | 100.00% |




**Example Printout**

Series of 1D spectra acquired in pseudo-2D mode. The printed segment shows the water signal of the sample. Top left side shows the same spectra in 2D mode. Bottom left side shows table output of the evaluation, containing experiment number, recovery delay, and signal intensity.

**Control Option for Acquisition (L23)**

1 default
10 skip sino check

### Parameters

| | | | |
|---|---|---|---|
| **F2 ACQU** | | | Parameters F2 |
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_gradrecvd | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 3.000 | ppm | |
| SW | 20.485 | ppm | |
| TD | 16384 | | field dependent |
| AQ | 0.999 | s | |
| FIDRES | 1.001 | Hz | |
| D 1 | 10.000 | s | |
| VDLIST | npt_gradrecCMR | | default |
| P 1 | 11.0 | us | 90deg Pulse |
| PLW 1 | 1.1 | W | Pow@90deg(Specs) |
| GPNAM1 | SINE.100 | | |
| GPZ 1 | -100.000 | % | 7.5 A |
| P 16 | 1000.000 | us | gradient pulse |
| TE | 298.000 | K | default |

| | | | |
|---|---|---|---|
| **F2 PROC** | | | Parameters F2 |
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| PH_mod | 1 | | pk |
| F1P | 5.720 | ppm | |
| F2P | 5.320 | ppm | |
| **F1 ACQU** | | | Parameters F1 |
| NUC1 | 1H | | |
| TD | 12 | | |
| **F1 PROC** | | | Parameters F1 |
| SI | 12 | | |

### Experiment Description

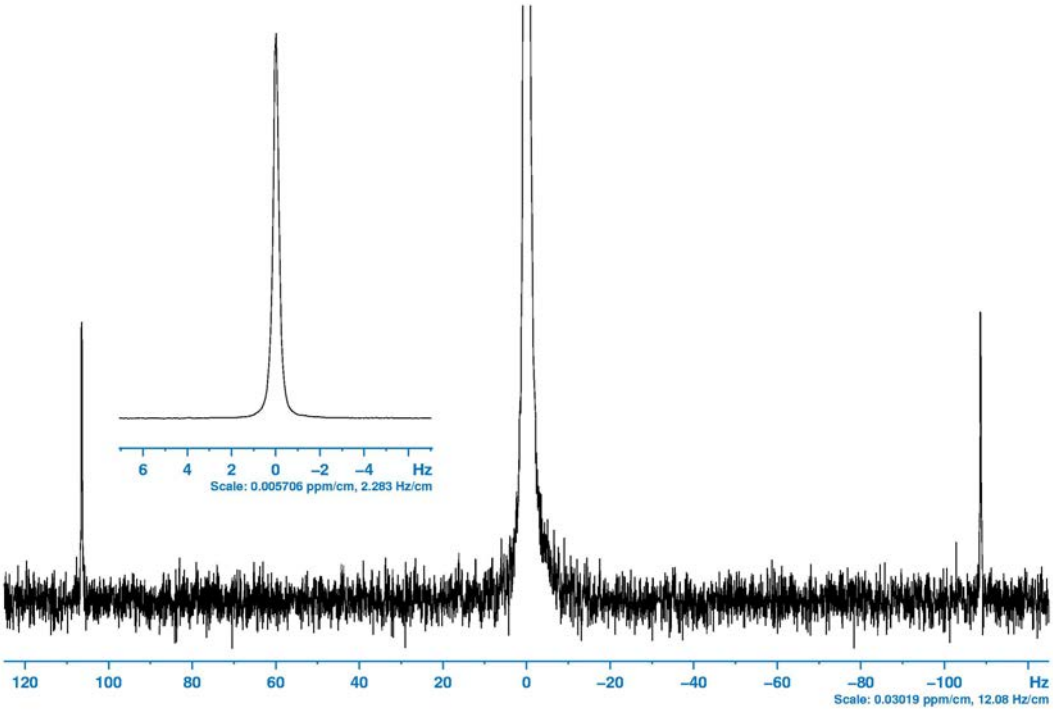
Purpose of this experiment is the measurement of the recovery delay after applying a field gradient.
The exact signal offset (O1P) is first determined with a recovery delay of 1 s. The resulting spectrum is stored in PROCNO 2, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved.
SINO check can be skiped with L23=10
After successful SINO check, the pseudo 2D gradient recovery experiment will be acquired.
Processing is accomplished by Fourier transformation in observation domain only (XF2). Phase correction is determined on the last experiment of the series and applied to the series.
Evaluation consists of he determination of the intensity deviation to the reference experiment (last of the series)
The results are summarized in the text file printed together with spectrum (bottom left).

Requirements: At least time of recovery delay, which defines start point of range where specified intensity must be reached, needs to be specified.

## 5.3 Experiments for HR-Probes with Flow Inserts (LC)

### 5.3.1 1H lineshape (NPT_1H_LC_lineshape)

**Test Sample:** 0.5%, 1.0% or 3.0% Chloroform in Acetone-D6
H7284, H7284-01, H7284-02
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton line shape spectrum with offset calibration to O1P as overview spectrum. Printing is from +125.0 Hz to -125.0 Hz. The expansion plot to the left shows chloroform signal with higher resolution (+7.0 Hz, -7.0 Hz).

**Control Option for Acquisition (L23)**

1 default
2 write default shimfile, in case of successful evaluation

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg30 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 7.700 | ppm | |
| SWH | 1000.000 | Hz | |
| TD | 32768 | | |
| AQ | 16.384 | s | |
| FIDRES | 0.061 | Hz | |
| D 1 | 9.116 | s | AQ+D1=const |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

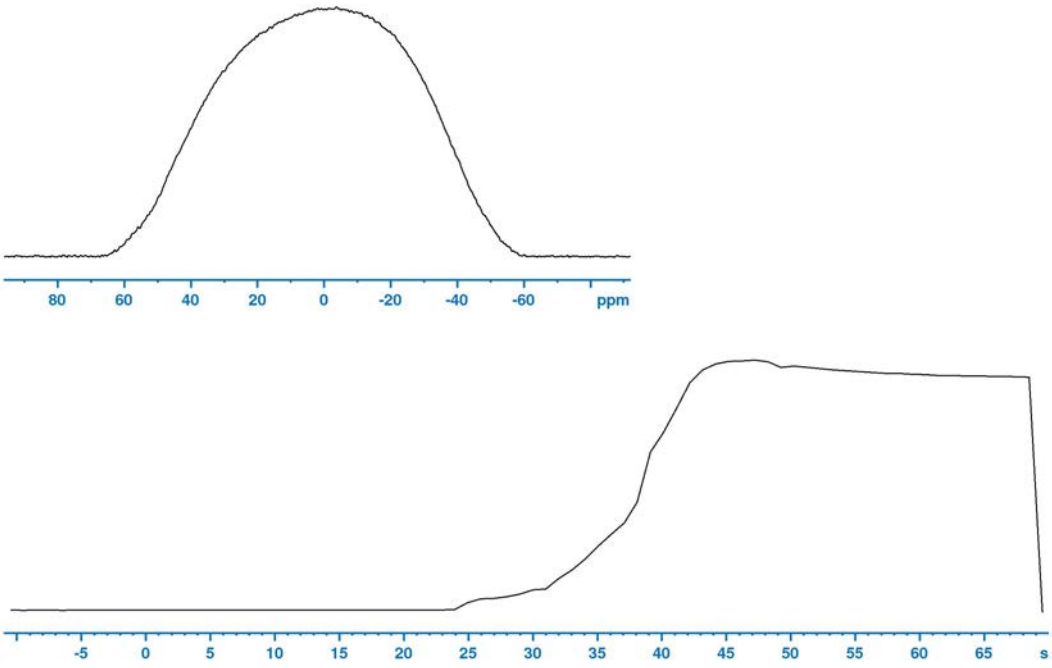
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 8.640 | ppm | |
| F2P | 7.440 | ppm | |
| CY | 1000.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 0.200 | | Scaling factor for CY |

### Experiment Description

Before acquiring the final spectrum, the exact signal position is determined with NS=1. The carrier position is afterwards set to the position
optimized O1 = peak frequency [Hz] - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.
Setting L23=2, it is possible to store the standard shimfile provided the evaluation of the experiment is successful. This event takes place during acquisition only. During regular processing of the data no shimfile is stored.

### 5.3.2 loop transfer time determination starting with empty cell (NPT_1H_LC_loopTransferTimeEmptyCell)

**Test Sample:** Mixture of solvents Acetonitrile and D2O
CH3CN_D2O
**Solvent:** CH3CN+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Bottom: Time curve of the integral of the proton Z gradient profile. At time=0 s transfer was started. Top: Proton Z gradient profile, row where the maximum integral/broadest gradient profile was observed.

**Control Option for Acquisition (L23)**

1 Execution of preparation steps (shimming, lock, tuning/matching)
2 Skip preparation steps

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | off | | |
| PULPROG | imgegp2d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 2.000 | ppm | |
| SW | 204.851 | ppm | |
| TD | 1024 | | |
| AQ | 0.006 | s | field dependent |
| FIDRES | 160.092 | Hz | field dependent |
| D 1 | 0.250 | s | |
| D 20 | 1.000 | s | time per row |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

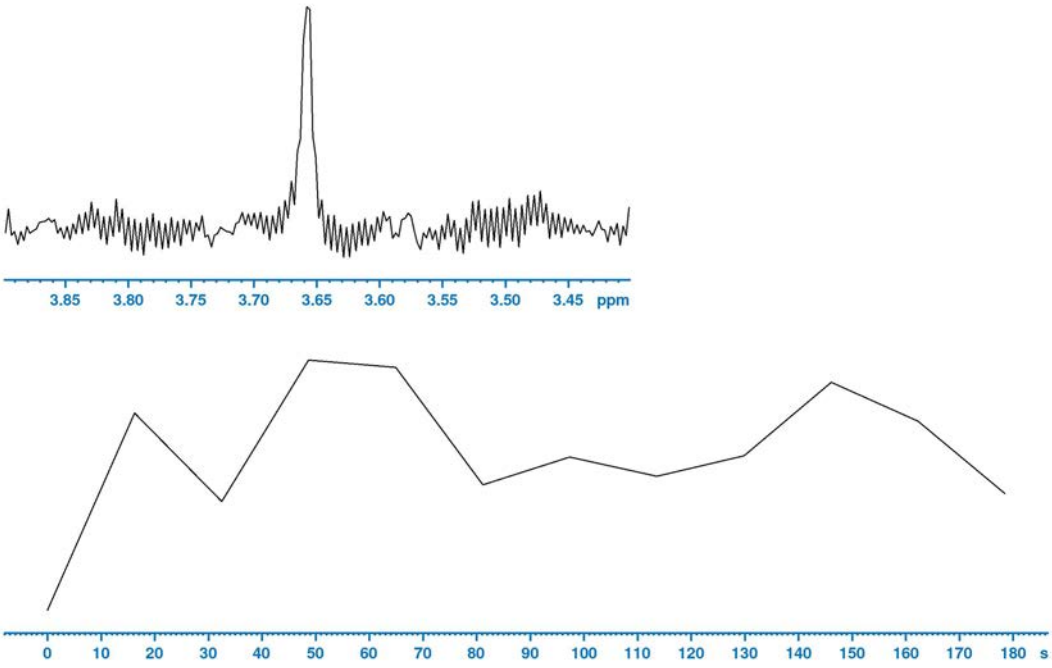
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 1024 | | |
| LB | 1.000 | Hz | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 0.000 | | used flow rate |
| L 27 | 0 | | row of UV detection |
| L 28 | 0 | | row with maximum integral |

## Experiment Description

Experiment to determine the transfer time from the BPSU Loop starting with an empty flow cell by continious acquisition of proton gradient profiles into a 2D file. The preparation of the experiment (temperature equilibration, tuning/matching, locking, shimming, and RGA) is executed after BPSU transfer is finished and the flow cell is filled with solvent. After the preparation the user will be guided to empty the flow cell, so that the main NMR experiment starts with an empty flow cell and to execute the transfer. The row at which 'Valve Position/Transfer to Probehead' was executed will be saved in L 27. The flow rate will be saved in CNST 20. After the user reports that BPSU transfer finished or the flow cell is completely filled NMR experiment will be stopped.
The time resolution of the experiment (time per row) depends on parameter D20.
The row at which the flow cell is filled completely will be saved in L 28. If L 28 equals 0 (e.g. first execution of processing) the user will be asked to manually determine the row where flow cell is filled completely. If neccessary the user may change parameters L 27, and L 28 in procno 1 before reprocessing the experiment.

### 5.3.3 loop transfer time determination starting with filled cell (NPT_1H_LC_loopTransferTimeFilledCell)

**Test Sample:** 5 ug/ul of 1,3,5-Trimethoxybenzene in Acetonitrile/D2O 70/30 H5798
**Solvent:** CH3CN+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Bottom: Time curve of the integral of the Tri-methoxy benzene signal. At time=0 s theBPSU switched to transfer. Top: 1H signal of Tri-methoxy benzene, row where the maximum integral was observed.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc2prf2 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 8192 | | |
| AQ | 0.500 | s | field dependent |
| FIDRES | 2.001 | Hz | field dependent |
| D 1 | 0.468 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000020 | W | Pow@90deg(10000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| TE | 298.000 | K | default |

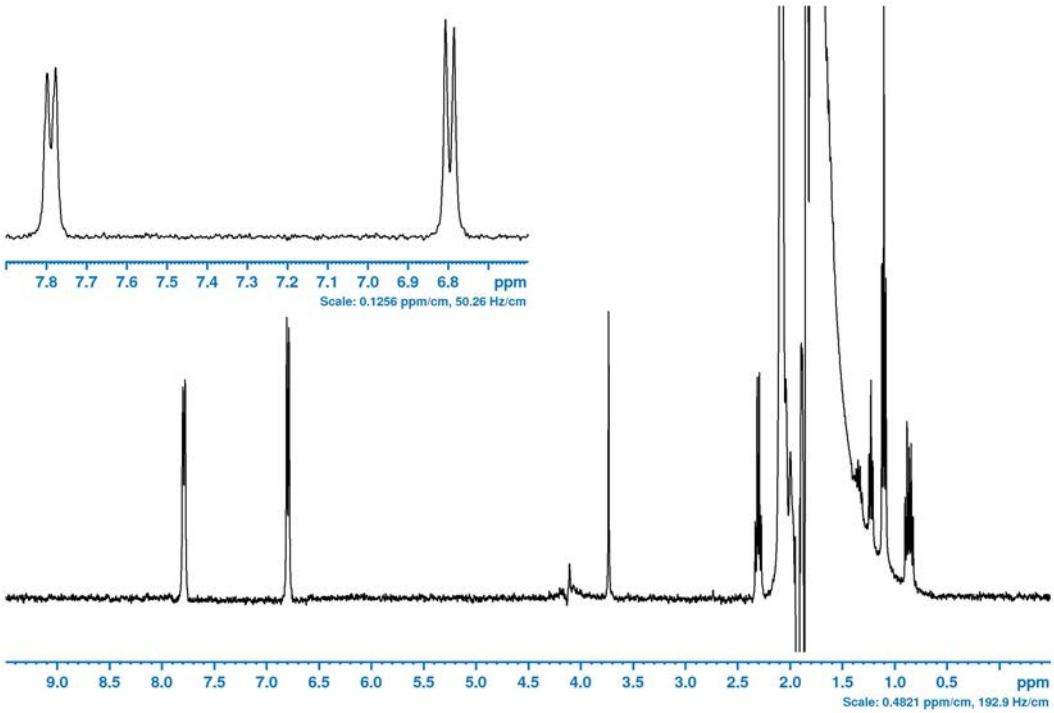
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| LB | 2.000 | Hz | |
| SIGF1 | 7.200 | ppm | |
| SIGF2 | 5.800 | ppm | |
| NOISF1 | -2.000 | ppm | |
| NOISF2 | -3.000 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 0.000 | | used flow rate |
| CNST 21 | 1.000 | | time per row |
| L 27 | 0 | | row where BPSU switched to transfer |
| L 28 | 0 | | row with maximum integral |

## Experiment Description

Experiment to determine the loop transfer time starting with a filled flow cell. The preparation of the experiment is executed after the user started the LC-pump and the flow cell is filled with solvent. The flow rate will be saved in CNST 20. After the preparation the user will be prompted to report the time at which the BPSU switches to transfer. The preflow time must be large enough to encounter preparation of the NMR (temperature equilibration, tuning/matching, locking, shimming, O1- and 02-determination, and RGA). The main NMR experiment starts automatically after these preparation steps. The row at which BPSU switched to transfer will be saved in L 27. After the user reports that the substance has passed the flow cell NMR experiment will be stopped.
The time resolution of the loop transfer time determination (time per row) depends mainly on the parameters NS, TD and D1. The default time per row is around one second.
The time resolution of the experiment (time per row) depends mainly on the parameters NS, TD and D1. The default time per row is around one second.
The row at which the flow cell is filled completely will be saved in L 28. If L 28 equals 0 (e.g. first execution of processing) the user will be asked to manually determine the row where flow cell is filled completely. If neccessary the user may change parameters L 27, and L 28 in procno 1 before reprocessing the experiment.

### 5.3.4 1H integrated system performance peak multi-trapping/transfe (NPT_1H_LC_multiTrappingTransfer_spe)

**Test Sample:** Mixture of 4 PHBA Esters in CH3CN/D2O separated by HPLC (i.e. only one of these esters is present in the spectrum)
H5799-SPE, H5799-SPE-5, H5799-SPE-3, H5799-SPE-1.7
**Solvent:** CD3CN_SPE
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton spectrum with double solvent suppression as overview spectrum.
The expansion plot to the left shows the aromatic signals of the PHBA ester of selected chromatographic fraction.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc1pngpf2 | | |
| NS | 24 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000005 | W | Pow@90deg(20000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPZ 2 | -10.000 | % | |
| P 16 | | us | gradient pulse |
| TE | 298.000 | K | default |

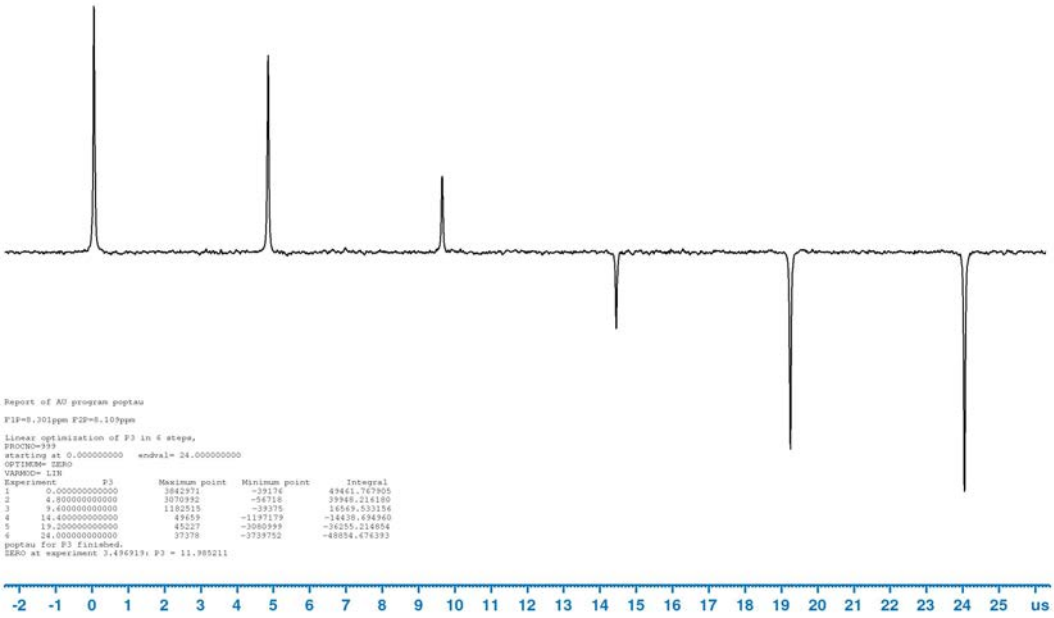
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 8.700 | ppm | |
| SIGF2 | 6.000 | ppm | |
| NOISF1 | -1.000 | ppm | |
| NOISF2 | -7.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton Sensititvity test with cw presaturation on channels F1 and F2. A preparation experiment is acquired for referencing and the search of the two biggest solvent signals (O1 and O2 optimization). For basline correction AU program lcabsf is used.
Integrated system performance is proofed with this test. In advance to this test the mixture of four PHBA esters is separated twice by LC and trapped on the same spe cartrdiges (multi trapping).
The resulting sensitivity should be around twice the sensitivity observed in NPT_1H_LC_performanceTransfer_spe_peak_A or NPT_1H_LC_performanceTransfer_spe_peak_B experiment.

## 5.3.5 Indirect P90 13C pulse calibration, LC (NPT_1H_LC_p90det_13c)

**Test Sample:** 0.3%, 1.0% or 3.0% Chloroform in Acetone-D6
H7284, H7284-01, H7284-02
**Solvent:** CDCl3
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




### Example Printout

P90 pulse determination using 1D method by varying the decoupler pulse. The result of a CONVTO1D routine shows five experiments from 45 to 135 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | decp90 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 8.000 | ppm | |
| SWH | 5000.000 | Hz | |
| TD | 16384 | | |
| AQ | 1.638 | s | |
| FIDRES | 0.610 | Hz | |
| D 1 | 60.000 | s | |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| P 3 | 9.0 | us | 90deg NUC1 |
| PLW 2 | 42.0 | W | Pow@90deg(Specs) NUC2 |
| TE | 298.000 | K | default |

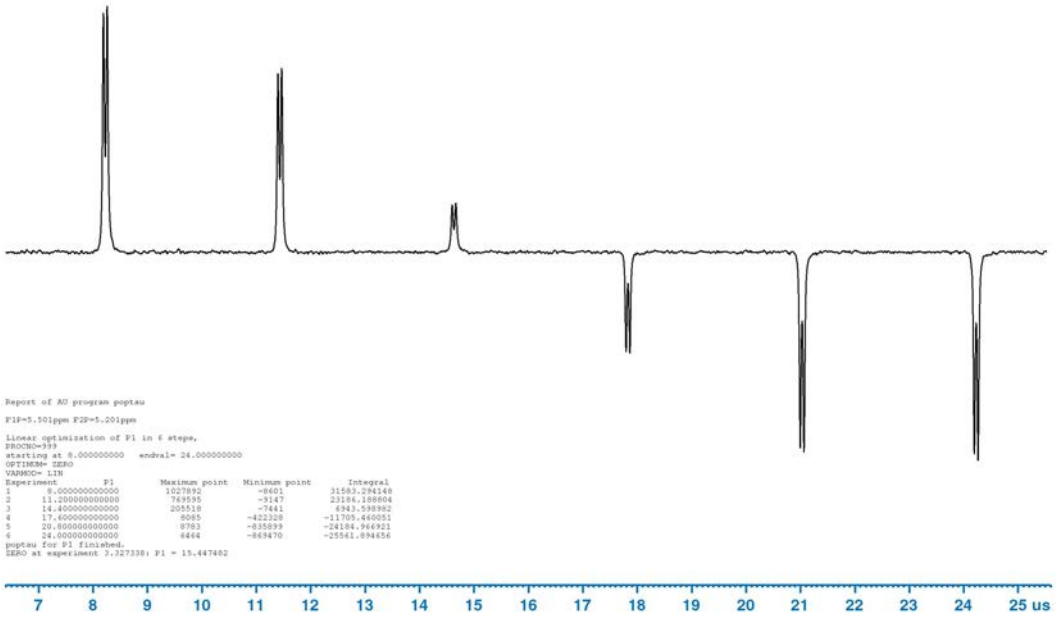
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.500 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 8.340 | ppm | |
| F2P | 8.190 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase with absf using the corrected O1P. F1P, F2P, ABSF1 and ABSF2 are set symmetrically around the phase corrected Signal. The result is stored in PROCNO 11, the FID is discarded.
The pulse will be determined on the signal(s) between F1P and F2P, i.e the left 13C satellite. The pulse determination may be erroneous if the solpe of the main signal is included in the plot region. If so, please select a smaller plot region by setting F1P and F2P while the experiment is in the preparation queue.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates based on the specified pulse length a new power value, updates the PROSOL table and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n.
The PROSOL table is then updated with the determined pulse and the used power.Results are stored under PROCNO 999.

## 5.3.6 P90 1H pulse calibration, LC (NPT_1H_LC_p90det_1h)

**Test Sample:** 2 mM Sucrose in D2O
H7285
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 11904.762 | Hz | |
| TD | 65536 | | |
| AQ | 2.753 | s | |
| FIDRES | 0.363 | Hz | |
| D 1 | 30.000 | s | |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

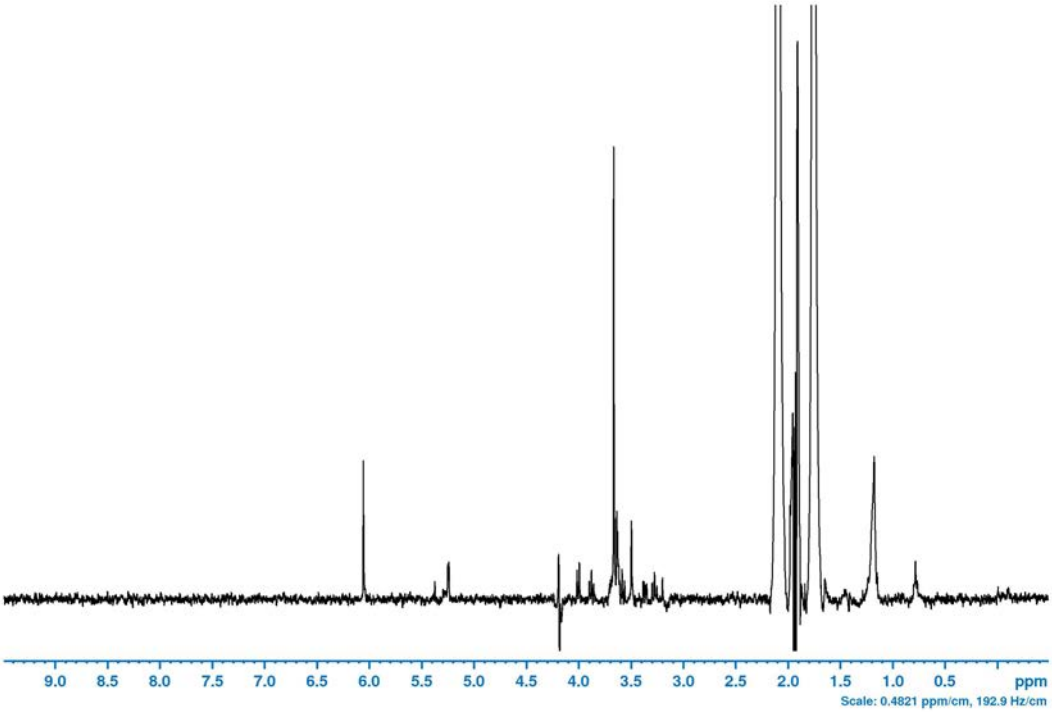
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| NCOEF | 0 | | |
| ABSF1 | 5.600 | ppm | |
| ABSF2 | 5.100 | ppm | |
| F1P | 5.500 | ppm | |
| F2P | 5.200 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase with absf using the corrected O1P. F1P, F2P, ABSF1 and ABSF2 are set symmetrically around the phase corrected Signal. The result is stored in PROCNO 11, the FID is discarded.
The pulse will be determined on the signal(s) between F1P and F2P, i.e the anomeric proton.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates based on the specified pulse length a new power value, updates the PROSOL table and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n.
The PROSOL table is then updated with the determined pulse and the used power.Results are stored under PROCNO 999.

## 5.3.7 1H system performance, LC (NPT_1H_LC_performance)

**Test Sample:** 800 ng of 1,3,5-Trimethoxybenzene in Acetonitrile/D2O 50/50 (concentration depends on flowcell size)
H9630, H9630-01, H9630-02, H9630-06
**Solvent:** CH3CN+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton spectrum with double solvent suppression as overview spectrum.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc1pngpf2 | | |
| NS | 16 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000020 | W | Pow@90deg(10000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPZ 2 | -10.000 | % | |
| P 16 | | us | gradient pulse |
| TE | 298.000 | K | default |

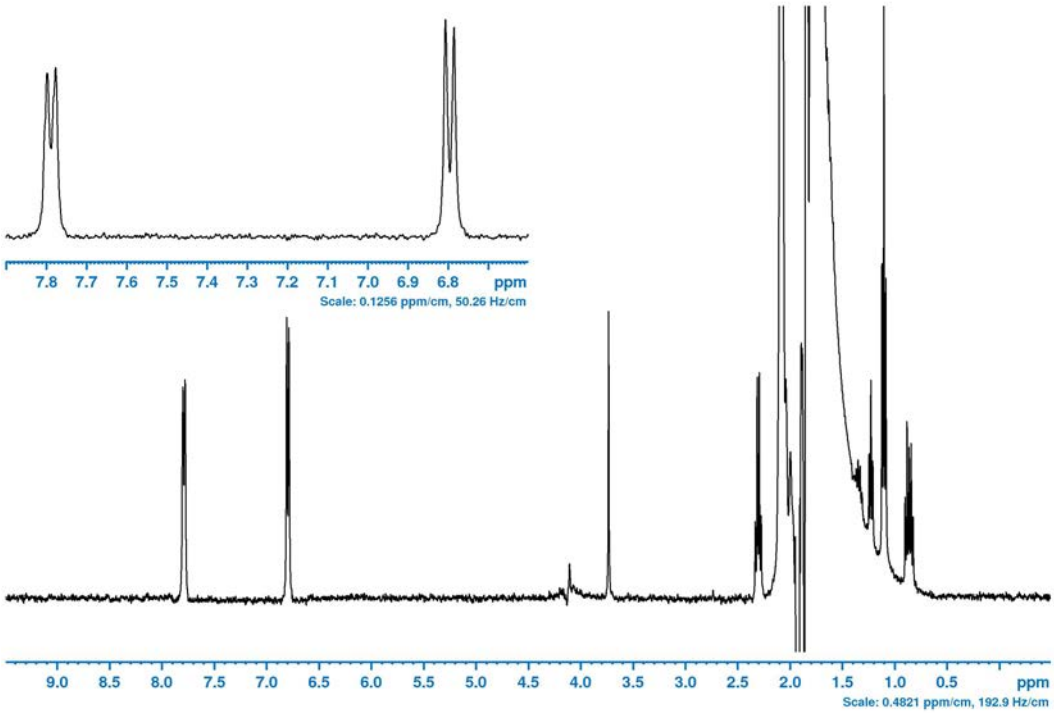
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 3.900 | ppm | |
| SIGF2 | 3.400 | ppm | |
| NOISF1 | -1.000 | ppm | |
| NOISF2 | -7.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton Sensititvity test with cw presaturation on channels F1 and F2. A preparation experiment is acquired for referencing and the search of the two biggest solvent signals (O1 and O2 optimization). For basline correction AU program lcabsf is used.
Performance of FlowProbe/CryoFit is proofed with this test. A defined sample is injected directly into the flow cell (without LC purification).

### 5.3.8 1H integrated system performance stop-flow peak A (NPT_1H_LC_performanceStopFlow_d2o_peak_A)

**Test Sample:** Mixture of 4 PHBA Esters in CH3CN/D2O separated by HPLC (i.e. only one of these esters is present in the spectrum)
H5799-D2O
**Solvent:** CH3CN+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton spectrum with double solvent suppression as overview spectrum.
The expansion plot to the left shows the aromatic signals of the PHBA ester of selected chromatographic fraction.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc1pngpf2 | | |
| NS | 24 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000020 | W | Pow@90deg(10000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPZ 2 | -10.000 | % | |
| P 16 | | us | gradient pulse |
| TE | 298.000 | K | default |

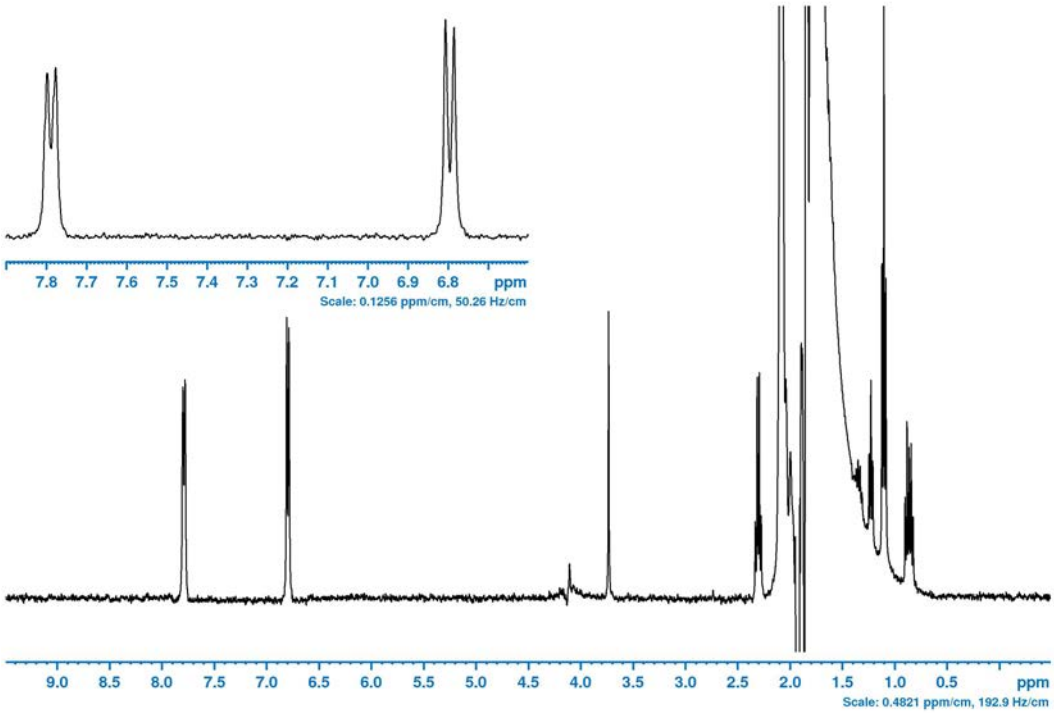
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 8.700 | ppm | |
| SIGF2 | 6.000 | ppm | |
| NOISF1 | -1.000 | ppm | |
| NOISF2 | -7.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton Sensititvity test with cw presaturation on channels F1 and F2. A preparation experiment is acquired for referencing and the search of the two biggest solvent signals (O1 and O2 optimization). For basline correction AU program lcabsf is used.
Integrated system performance is proofed with this test. A mixture of four PHBA esters is separated by LC in stop-flow mode.
The resulting sensitivities observed in NPT_1H_LC_performanceStopFlow_d2o_peak_A and NPT_1H_LC_performanceStopFlow_d2o_peak_B should be equal.

### 5.3.9 1H integrated system performance stop-flow peak B (NPT_1H_LC_performanceStopFlow_d2o_peak_B)

**Test Sample:** Mixture of 4 PHBA Esters in CH3CN/D2O separated by HPLC (i.e. only one of these esters is present in the spectrum)
H5799-D2O
**Solvent:** CH3CN+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton spectrum with double solvent suppression as overview spectrum.
The expansion plot to the left shows the aromatic signals of the PHBA ester of selected chromatographic fraction.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc1pngpf2 | | |
| NS | 24 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000020 | W | Pow@90deg(10000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPZ 2 | -10.000 | % | |
| P 16 | | us | gradient pulse |
| TE | 298.000 | K | default |

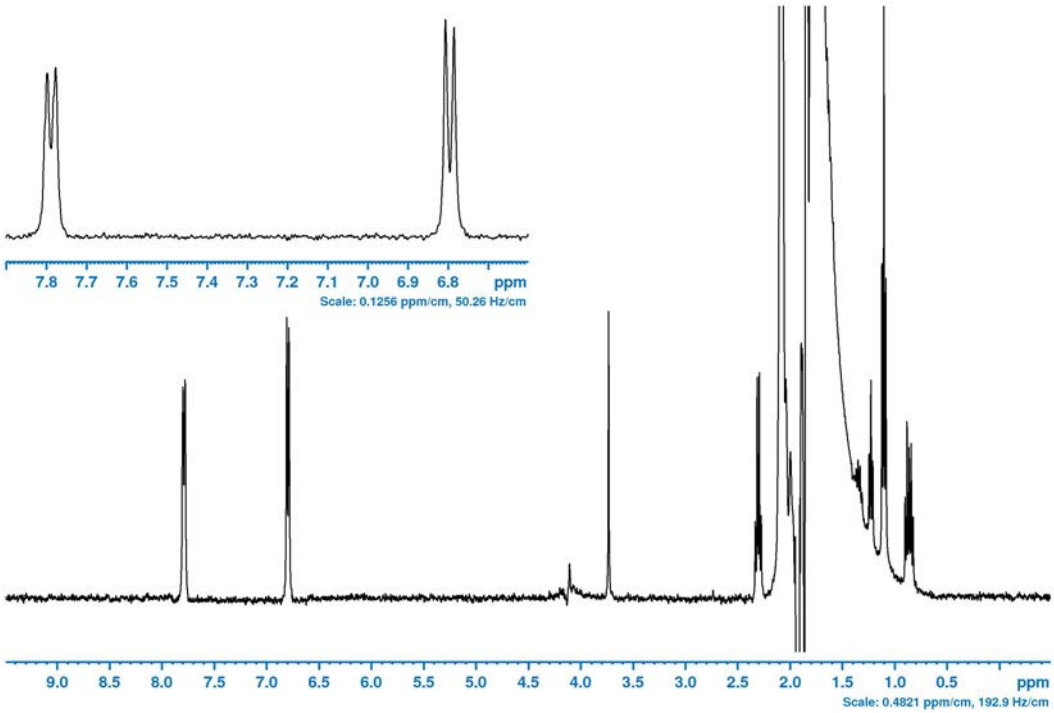
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 8.700 | ppm | |
| SIGF2 | 6.000 | ppm | |
| NOISF1 | -1.000 | ppm | |
| NOISF2 | -7.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton Sensititvity test with cw presaturation on channels F1 and F2. A preparation experiment is acquired for referencing and the search of the two biggest solvent signals (O1 and O2 optimization). For basline correction AU program lcabsf is used.
Integrated system performance is proofed with this test. A mixture of four PHBA esters is separated by LC in stop-flow mode.
The resulting sensitivities observed in NPT_1H_LC_performanceStopFlow_d2o_peak_A and NPT_1H_LC_performanceStopFlow_d2o_peak_B should be equal.

### 5.3.10 1H integrated system performance loop-sapmling/transfer peak A (NPT_1H_LC_performanceTransfer_d2o_peak_A)

**Test Sample:** Mixture of 4 PHBA Esters in CH3CN/D2O separated by HPLC (i.e. only one of these esters is present in the spectrum)
H5799-D2O
**Solvent:** CH3CN+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton spectrum with double solvent suppression as overview spectrum.
The expansion plot to the left shows the aromatic signals of the PHBA ester of selected chromatographic fraction.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc1pngpf2 | | |
| NS | 24 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000020 | W | Pow@90deg(10000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPZ 2 | -10.000 | % | |
| P 16 | | us | gradient pulse |
| TE | 298.000 | K | default |

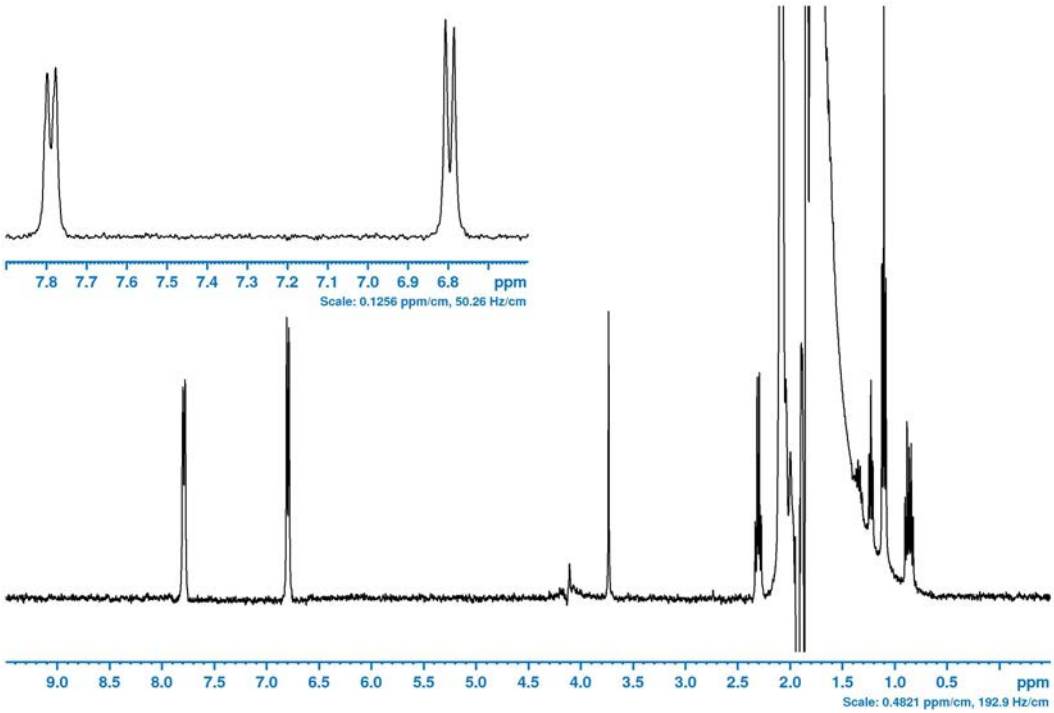
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 8.700 | ppm | |
| SIGF2 | 6.000 | ppm | |
| NOISF1 | -1.000 | ppm | |
| NOISF2 | -7.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton Sensititvity test with cw presaturation on channels F1 and F2. A preparation experiment is acquired for referencing and the search of the two biggest solvent signals (O1 and O2 optimization). For basline correction AU program lcabsf is used.
Integrated system performance is proofed with this test. In advance to this test the mixture of four PHBA esters is separated by LC and stored in loops.
The resulting sensitivities observed in NPT_1H_LC_performanceTransfer_d2o_peak_A and NPT_1H_LC_performanceTransfer_d2o_peak_B should be equal.

### 5.3.11 1H integrated system performance loop-sapmling/transfer peak B (NPT_1H_LC_performanceTransfer_d2o_peak_B)

**Test Sample:** Mixture of 4 PHBA Esters in CH3CN/D2O separated by HPLC (i.e. only one of these esters is present in the spectrum)
H5799-D2O
**Solvent:** CH3CN+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton spectrum with double solvent suppression as overview spectrum.
The expansion plot to the left shows the aromatic signals of the PHBA ester of selected chromatographic fraction.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc1pngpf2 | | |
| NS | 24 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000020 | W | Pow@90deg(10000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPZ 2 | -10.000 | % | |
| P 16 | | us | gradient pulse |
| TE | 298.000 | K | default |

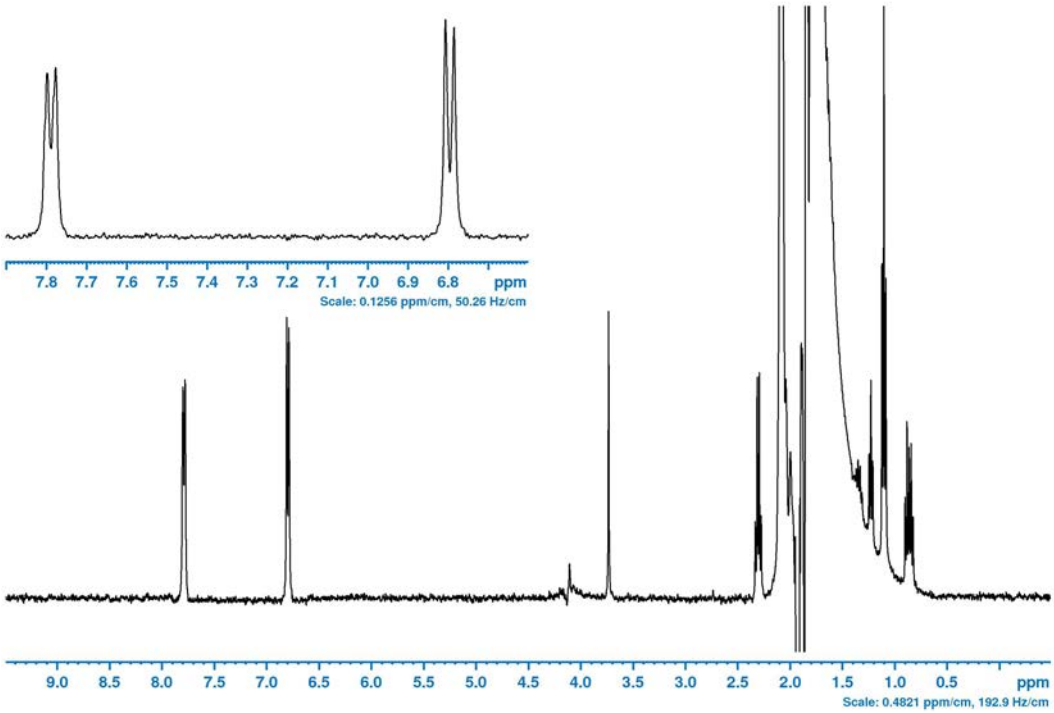
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 8.700 | ppm | |
| SIGF2 | 6.000 | ppm | |
| NOISF1 | -1.000 | ppm | |
| NOISF2 | -7.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton Sensititvity test with cw presaturation on channels F1 and F2. A preparation experiment is acquired for referencing and the search of the two biggest solvent signals (O1 and O2 optimization). For basline correction AU program lcabsf is used.
Integrated system performance is proofed with this test. In advance to this test the mixture of four PHBA esters is separated by LC and stored in loops.
The resulting sensitivities observed in NPT_1H_LC_performanceTransfer_d2o_peak_A and NPT_1H_LC_performanceTransfer_d2o_peak_B should be equal.

### 5.3.12 1H integrated system performance peak-trapping/transfer peak A (NPT_1H_LC_performanceTransfer_spe_peak_A)

**Test Sample:** Mixture of 4 PHBA Esters in CH3CN/D2O separated by HPLC (i.e. only one of these esters is present in the spectrum)
H5799-SPE, H5799-SPE-5, H5799-SPE-3, H5799-SPE-1.7
**Solvent:** CD3CN_SPE
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton spectrum with double solvent suppression as overview spectrum.
The expansion plot to the left shows the aromatic signals of the PHBA ester of selected chromatographic fraction.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc1pngpf2 | | |
| NS | 24 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000005 | W | Pow@90deg(20000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPZ 2 | -10.000 | % | |
| P 16 | | us | gradient pulse |
| TE | 298.000 | K | default |

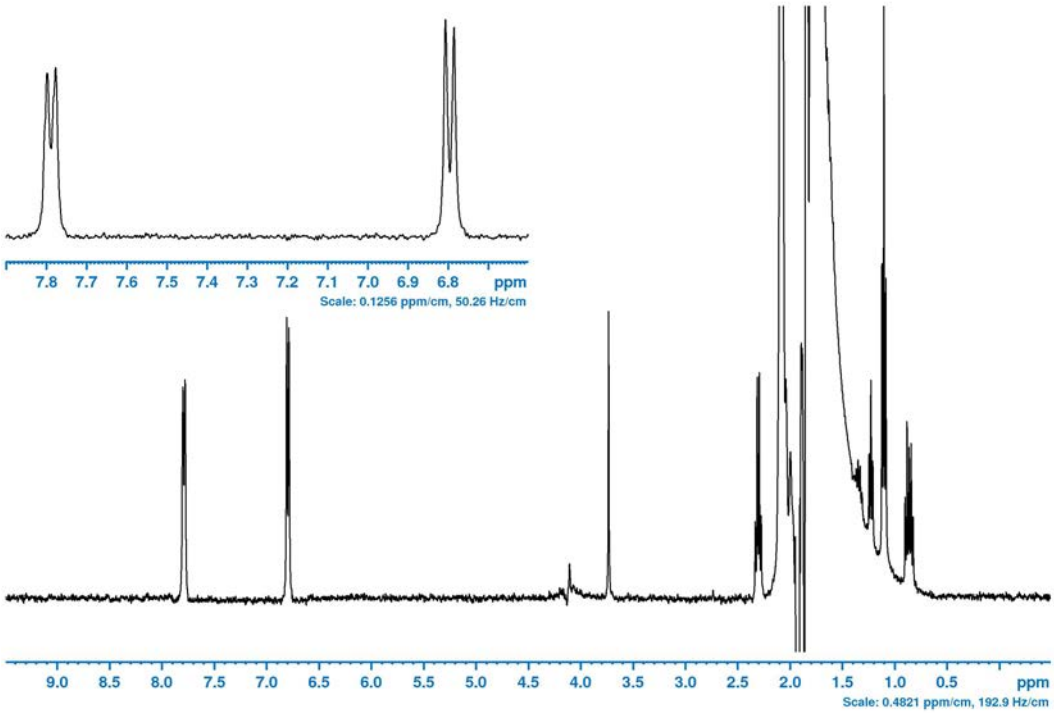
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 8.700 | ppm | |
| SIGF2 | 6.000 | ppm | |
| NOISF1 | -1.000 | ppm | |
| NOISF2 | -7.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton Sensititvity test with cw presaturation on channels F1 and F2. A preparation experiment is acquired for referencing and the search of the two biggest solvent signals (O1 and O2 optimization). For basline correction AU program lcabsf is used.
Integrated system performance is proofed with this test. In advance to this test the mixture of four PHBA esters is separated by LC and trapped on spe cartrdiges.
The resulting sensitivities observed in NPT_1H_LC_performanceTransfer_spe_peak_A and NPT_1H_LC_performanceTransfer_spe_peak_B should be equal.

### 5.3.13 1H integrated system performance peak-trapping/transfer peak B (NPT_1H_LC_performanceTransfer_spe_peak_B)

**Test Sample:** Mixture of 4 PHBA Esters in CH3CN/D2O separated by HPLC (i.e. only one of these esters is present in the spectrum)
H5799-SPE, H5799-SPE-5, H5799-SPE-3, H5799-SPE-1.7
**Solvent:** CD3CN_SPE
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Proton spectrum with double solvent suppression as overview spectrum.
The expansion plot to the left shows the aromatic signals of the PHBA ester of selected chromatographic fraction.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc1pngpf2 | | |
| NS | 24 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 32768 | | |
| AQ | 1.999 | s | field dependent |
| FIDRES | 0.500 | Hz | field dependent |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000005 | W | Pow@90deg(20000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| GPNAM1 | SMSQ10.100 | | |
| GPNAM2 | SMSQ10.100 | | |
| GPZ 1 | 50.000 | % | |
| GPZ 2 | -10.000 | % | |
| P 16 | | us | gradient pulse |
| TE | 298.000 | K | default |

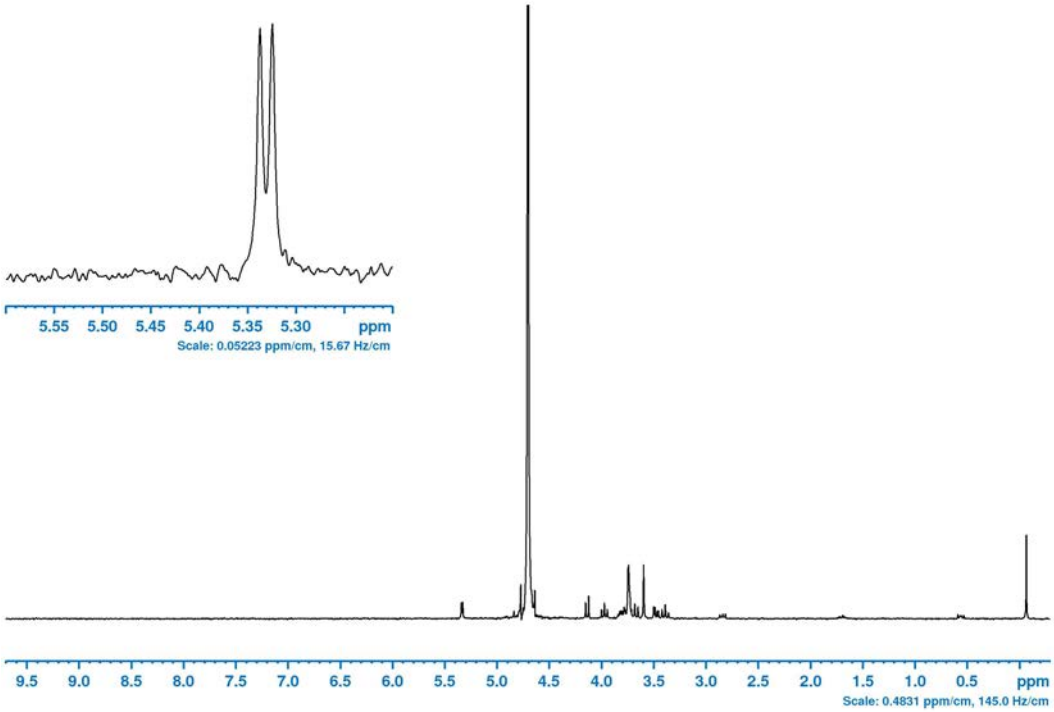
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 1.000 | Hz | |
| SIGF1 | 8.700 | ppm | |
| SIGF2 | 6.000 | ppm | |
| NOISF1 | -1.000 | ppm | |
| NOISF2 | -7.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Proton Sensititvity test with cw presaturation on channels F1 and F2. A preparation experiment is acquired for referencing and the search of the two biggest solvent signals (O1 and O2 optimization). For basline correction AU program lcabsf is used.
Integrated system performance is proofed with this test. In advance to this test the mixture of four PHBA esters is separated by LC and trapped on spe cartrdiges.
The resulting sensitivities observed in NPT_1H_LC_performanceTransfer_spe_peak_A and NPT_1H_LC_performanceTransfer_spe_peak_B should be equal.

## 5.3.14 1H sensitivity, LC (NPT_1H_LC_sensitivity)

**Test Sample:** 2 mM Sucrose in D2O
H7285
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Bottom: 1H overview spectrum of sucrose.
Top left: Expanded region showing the anomeric proton used for evaluation.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SW | 29.752 | ppm | |
| TD | 65536 | | |
| AQ | 2.753 | s | field dependent |
| FIDRES | 0.363 | Hz | field dependent |
| D 1 | 30.000 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

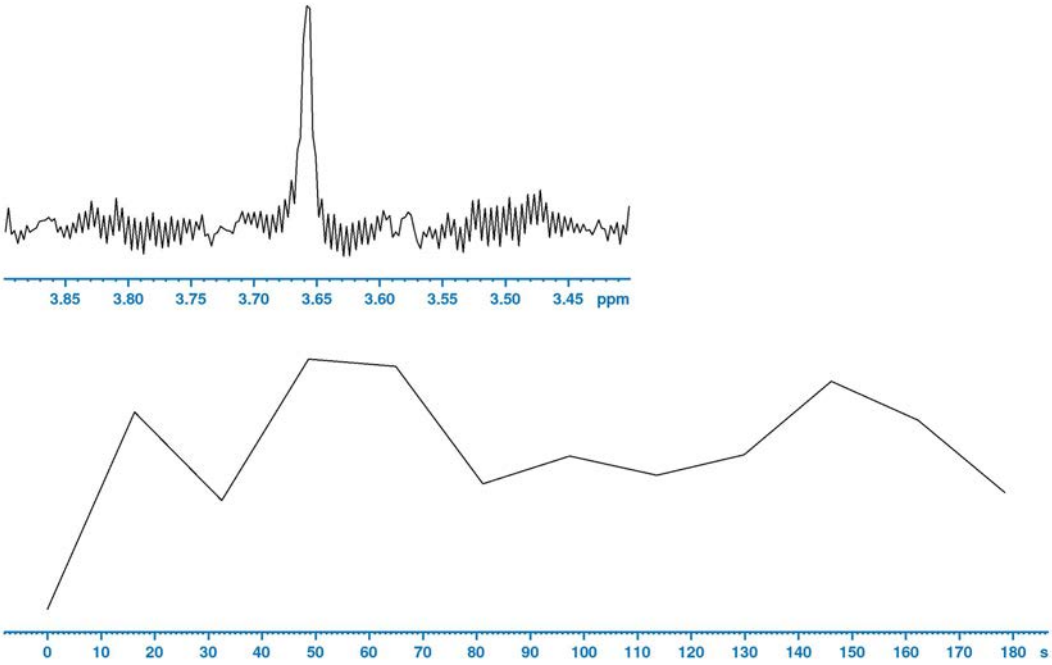
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 65536 | | |
| LB | 1.000 | Hz | 1.0 |
| SIGF1 | 3.000 | ppm | |
| SIGF2 | 2.000 | ppm | |
| NOISF1 | 6.000 | ppm | |
| NOISF2 | 4.000 | ppm | |
| F1P | 8.520 | ppm | |
| F2P | 0.480 | ppm | |
| CY | 100.000 | cm | |

## Experiment Description

Proton sensitivity is measured using the sucrose in D2O sample. Processing is using LB. The signal-to-noise is determined using the singnal of the anomeric proton. The signal is searched over the range from 5.6 to 5.3 ppm, while the best 200 Hz noise region is determined over the complete spectrum.

## 5.3.15 stop-flow time determination (NPT_1H_LC_stopFlowTime)

**Test Sample:** 5 ug/ul of 1,3,5-Trimethoxybenzene in Acetonitrile/D2O 70/30 H5798
**Solvent:** CH3CN+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Bottom: Time curve of the integral of the Tri-methoxy benzene signal. At time=0 s the UV maximum was detected. Top: 1H signal of Tri-methoxy benzene, row where the maximum integral was observed.

**Control Option for Acquisition (L23)**

1 Optimization of O1 and O2 for solvent suppression
2 No optimization of O1 and O2 for solvent suppression

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| NUC2 | 1H | | |
| PULPROG | lc2prf2 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 4.700 | ppm | |
| SW | 20.485 | ppm | |
| TD | 8192 | | |
| AQ | 0.500 | s | field dependent |
| FIDRES | 2.001 | Hz | field dependent |
| D 1 | 0.468 | s | |
| P 1 | 14.0 | us | 90deg Pulse |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) |
| PLW 9 | 0.000020 | W | Pow@90deg(10000u) |
| PLW 21 | 0.000005 | W | Pow@90deg(20000u) |
| TE | 298.000 | K | default |

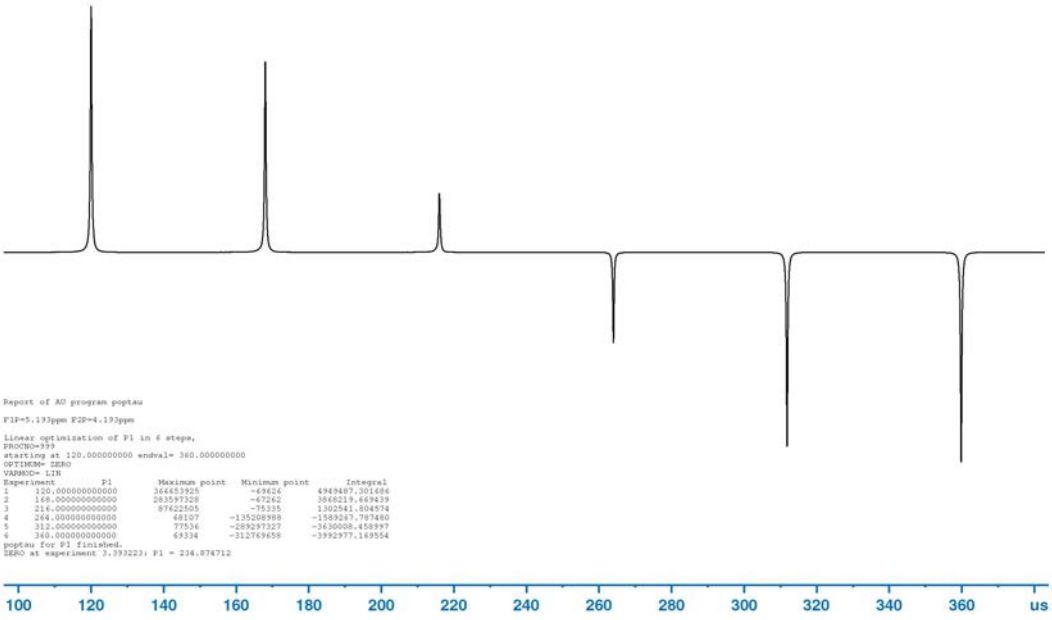
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| LB | 2.000 | Hz | |
| SIGF1 | 7.200 | ppm | |
| SIGF2 | 5.800 | ppm | |
| NOISF1 | -2.000 | ppm | |
| NOISF2 | -3.000 | ppm | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 0.000 | | used flow rate |
| CNST 21 | 1.000 | | time per row |
| L 27 | 0 | | row of UV detection |
| L 28 | 0 | | row with maximum integral |

## Experiment Description

Experiment to determine the stop-flow time. The preparation of the experiment (temperature equilibration, tuning/matching, locking, shimming, O1- and O2-determination, and RGA) is executed after the user started the LC-pump and the flow cell is filled with solvent. The flow rate will be saved in CNST 20. After the preparation the user will be prompted to inject the sample and to report the time at which the peak appears at the UV detector. The main NMR experiment starts at time of sample injection. The row at which UV maximum was observed will be saved in L 27. After the user reports that the substance has passed the flow cell NMR experiment will be stopped.
The time resolution of the experiment (time per row) depends mainly on the parameters NS, TD and D1. The default time per row is around one second.
The row at which the flow cell is filled completely will be saved in L 28. If L 28 equals 0 (e.g. first execution of processing) the user will be asked to manually determine the row where flow cell is filled completely. If neccessary the user may change parameters L 27, and L 28 in procno 1 before reprocessing the experiment.

## 5.3.16 P90 2H pulse calibration, LC (NPT_prep_LC_p90det_d)

**Test Sample:** 2 mM Sucrose in D2O
H7285
**Solvent:** D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg2h | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 4.700 | ppm | |
| SWH | 1000.000 | Hz | |
| TD | 4096 | | |
| AQ | 2.048 | s | |
| FIDRES | 0.488 | Hz | |
| D 1 | 10.000 | s | |
| P 1 | 14.0 | us | 90deg NUC1 |
| PLW 1 | 6.6 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

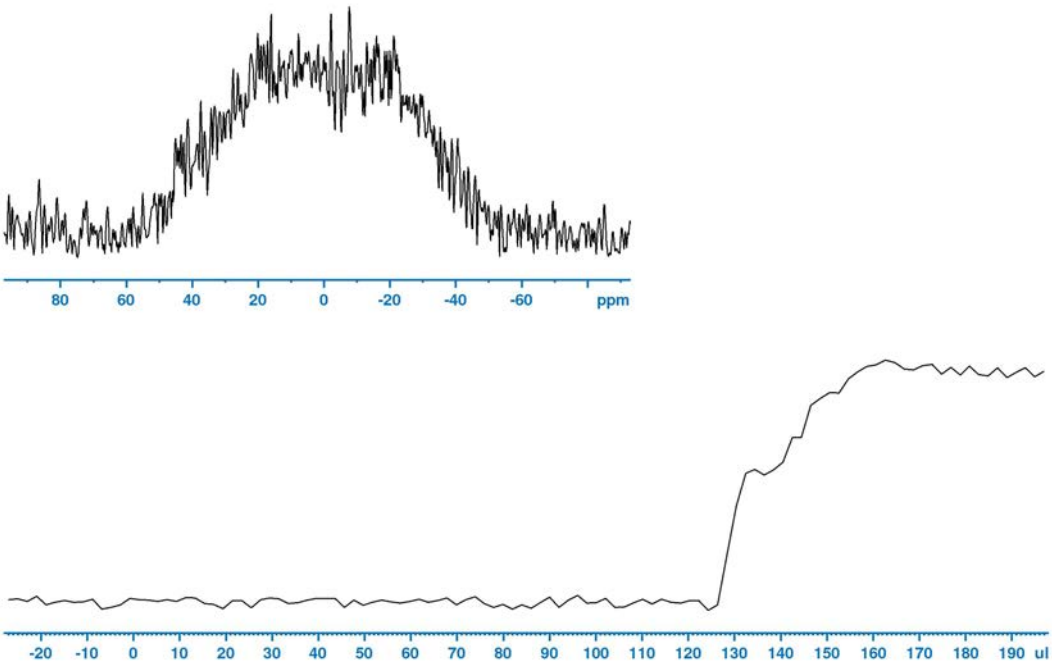
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| NCOEF | 0 | | |
| ABSF1 | 10.000 | ppm | |
| ABSF2 | 0.000 | ppm | |
| F1P | 5.200 | ppm | |
| F2P | 4.200 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase with absf using the corrected O1P. F1P, F2P, ABSF1 and ABSF2 are set symmetrically around the phase corrected Signal. The result is stored in PROCNO 11, the FID is discarded.
The pulse will be determined on the signal(s) between F1P and F2P.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates based on the specified pulse length a new power value, updates the PROSOL table and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n.
The PROSOL table is then updated with the determined pulse and the used power.Results are stored under PROCNO 999.

### 5.3.17 peak transfer volume determination starting with empty cell (NPT_prep_LC_peakTransferVolume)

**Test Sample:** Solvent Acetonitrile-D3 or Methanol-D4
MeOD, CD3CN
**Solvent:** CD3OD_SPE or CD3CN_SPE
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Flow cell




**Example Printout**

Bottom: Time curve of the integral of the deuterium Z gradient profile. At volume=0 ul transfer was started. Top: Deuterium Z gradient profile, row where the maximum integral/broadest gradient profile was observed.

**Control Option for Acquisition (L23)**

1 Execution of preparation steps (shimming, lock, tuning/matching)
2 Skip preparation steps

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 2H | | |
| NUC2 | off | | |
| PULPROG | imgegp2d2h | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 0.250 | | optim. by RGA |
| O1P | 2.000 | ppm | |
| O2P | 2.000 | ppm | |
| SW | 203.508 | ppm | |
| TD | 1024 | | |
| AQ | 0.041 | s | field dependent |
| FIDRES | 24.414 | Hz | field dependent |
| D 1 | 0.750 | s | |
| D 20 | 1.000 | s | time per row |
| P 1 | 180.0 | us | 90deg NUC1 |
| PLW 1 | 6.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 1024 | | |
| LB | 1.000 | Hz | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 20 | 0.000 | | used flow rate |
| L 27 | 0 | | row where BPSU switched to transfer |
| L 28 | 0 | | row with maximum integral |

### Experiment Description

Experiment to determine the peak transfer volume from SPE to flow cell by continious acquisition of deuterium gradient profiles into a 2D file. The preparation of the experiment (temperature equilibration, tuning/matching, shimming, and RGA) is executed after HyStar transfer is finished and the flow cell is filled with solvent. After the preparation the user will be prompted to start another transfer. The transfer step includes probe drying, so that the main NMR experiment starts with an empty flow cell. The row at which HyStar shows TRANSFER will be saved in L 27. The flow rate will be saved in CNST 20. After the user reports that HyStar transfer finished or the flow cell is completely filled NMR experiment will be stopped. The time resolution of the experiment (time per row) depends on parameter D20.
The row at which the flow cell is filled completely will be saved in L 28. If L 28 equals 0 (e.g. first execution of processing) the user will be asked to manually determine the row where flow cell is filled completely. If neccessary the user may change parameters L 27, and L 28 in procno 1 before reprocessing the experiment.

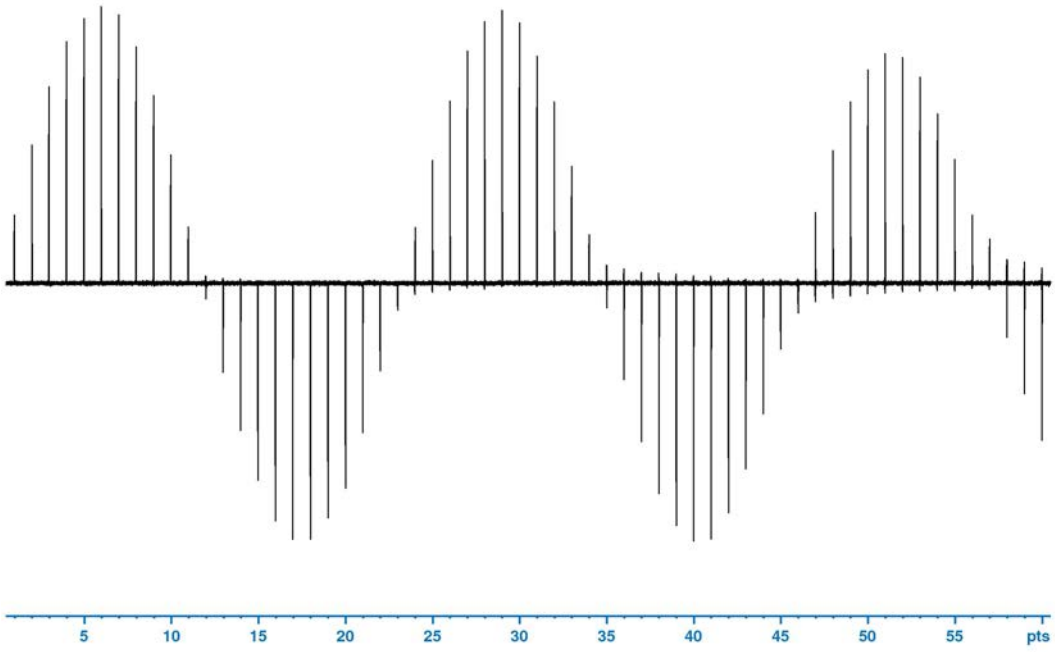
## 5.4 Experiments for Magic Angle Spinning Probes (Solids)

In *NMRPT* the default rotational spinning frequency of the rotors depends on sample, experiments and base frequency of the magnet. The default values for each experiment are provided in the experiment description in this chapter.

It is recommended to adjust the FIELD value of the spectrometer using KBr or Adamantane sample. If using KBr for field adjustement, set the 79Br signal to 59.70 ppm. If using Adamantane set the 13C methylene (low field) signal to 38.48 ppm. With this FIELD value calibration done, carrier frequency optimisation (O1P and O2P) during experiment setup should not be necessary.

### 5.4.1 13C B1 homogeneity, MAS (NPT_13C_MAS_b1homogeneity_13c)

**Test Sample:** Adamantane
Z151221, Z151271, Z151261, Z151251, Z151231, Z151241, Z151211, Z163274, Z183104
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a region around each main signal is shown in the figure.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1nuthpdec2d | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 34.000 | ppm | |
| O2P | 2.460 | ppm | |
| SWH | 10000.000 | Hz | |
| TD | 19998 | | |
| AQ | 1.000 | s | |
| FIDRES | 1.000 | Hz | |
| D 1 | 15.000 | s | |
| CPDPRG2 | cw | | decoupl. sequence |
| P 1 | 4.0 | us | 90deg NUC1 |
| PCPD2 | 17.0 | us | PCPD NUC2 |
| PLW 1 | 125 | W | Pow@90deg NUC1 |
| PLW 12 | 0.2 | W | B1(NUC2) = MASR/4 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| CY | 11.000 | cm | |

## Experiment Description

The B1 homogeneity measurement is acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range reaches from 15 to approx. 810 degrees. The B1-homogeneities based on integrals are computed from the magnitude of the second complex FID data point in PROCNO=2.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined for decoupling by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
The result of CONVTO1D is stored in PROCNO=999. This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Requirements: The corresponding 90° pulse determination experiment (NPT_X_MAS_p90det_YZ) is mandatory for B1 homogeneity measurement.

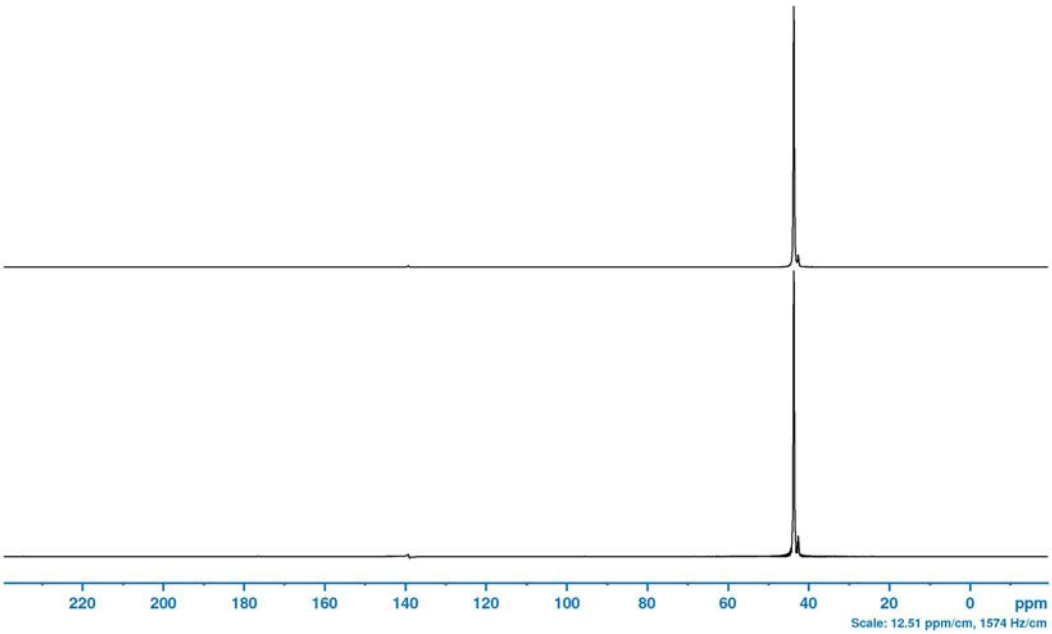
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

### 5.4.2 Double CP 1H-15N-13C, MAS (NPT_13C_MAS_double_cp1h15n_13c)

**Test Sample:** Alpha-crystalline 2-13C, 15N Glycine
Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Top: 13C spectrum with 1H 15N double cross polarization. Bottom: 13C spectrum with 1H cross polarization.

**Control Option for Acquisition (L23)**

1 default, automatic parameter optimization
11 Several manual user interaction steps for parameter optimization

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| NUC3 | 15N | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | doubcp | | |
| NS | 16 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 110.000 | ppm | |
| O2P | 6.200 | ppm | |
| O3P | 35.000 | ppm | |
| SW | 299.337 | ppm | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| CNST 9 | 110.000 | ppm | 13C carrier pos. |
| CNST 10 | 20.000 | ppm | 13C carrier pos. (optimized) |
| CNST 53 | 5.50 | us | 90 deg. 15N pulse |
| CNST 54 | 42 | W | max. Pow@90deg 1H |
| P 1 | 8.33 | us | 90deg 13C |
| P 3 | 2.27 | us | 1H max. dec. field |
| P 15 | 4000.0 | us | 1H 15N contact time (optimized) |
| P 16 | 10000.0 | us | 15N 13C contact time (optimized) |
| PCPD 2 | 4.2 | us | PCPD2 1H |
| PLW 1 | 20.5 | W | Pow@90deg 13C |
| PLW 3 | 162.0 | W | Pow@90deg 15N |
| PLW 5 | 140.9 | W | Pow@90deg 15N |
| PLW 11 | 20.5 | W | Pow@90degCP(Specs) 13C |
| PLW 12 | 230.0 | W | Pow@90deg 1H |
| PLW 13 | 230.0 | W | Pow@90deg 1H (optimized) |
| SPW 0 | 100.0 | W | Pow 1H contact (optimized) |
| SPW 1 | 27.5 | W | Pow 13C contact (optimized) |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp.100 | | |
| SPNAM 1 | tacn80 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 96.013 | ppm | |
| ABSF2 | -8.769 | ppm | |
| F1P | 91.249 | ppm | |
| F2P | -4.011 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

13C sensitivity experiment with 1H 15n double cross polarization including automatic paramter optimization.
First step: parameter optimization for 1H 15N cross polarization in a derived 15N 1H data set (expno=1, NS=4).
Second step: 1H 13C cross polarization are optimized in a derived 13C 1H data set (expno=2, NS=4).
Third step: acquisition of the 1H 13C cross polarization experiment as reference for evaluating the efficiency of the double cross polarization (NS=16).
Fourth step: parameter optimization of the 15N 13C cross polarization using the double cross polarization experiment (NS=4, optimized parameters from first step).
Fifth step: acquisition of the 1H 15N 13C double cross polarization experiment (NS=16).
The transfer efficiency in percent is determined as ratio of sino of 1H 15N 13C double cross polaristaion and 1H 13C cross polarization (derived data set, expno=2).

For MASR < 20000 the start values of SPW1 and PLW5 are calculated for B1(NUC1) = (5/2 * MASR) and B1(NUC3) = (7/2 * MASR) respectively.
For MASR >= 20000 the start values of SPW1 and PLW5 are calculated for B1(NUC1) = (1/3 * MASR) and B1(NUC3) = (2/3 * MASR) respectively.
Start value of SPW0 is calculated for absolute value of B1(NUC2) = (B1(NUC1) + sideBandCondition * MASR) * rampFactor.
For MASR < 60000 sideBandCondition = 1, for MASR >=60000 sideBandCondition = -1 is used.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.

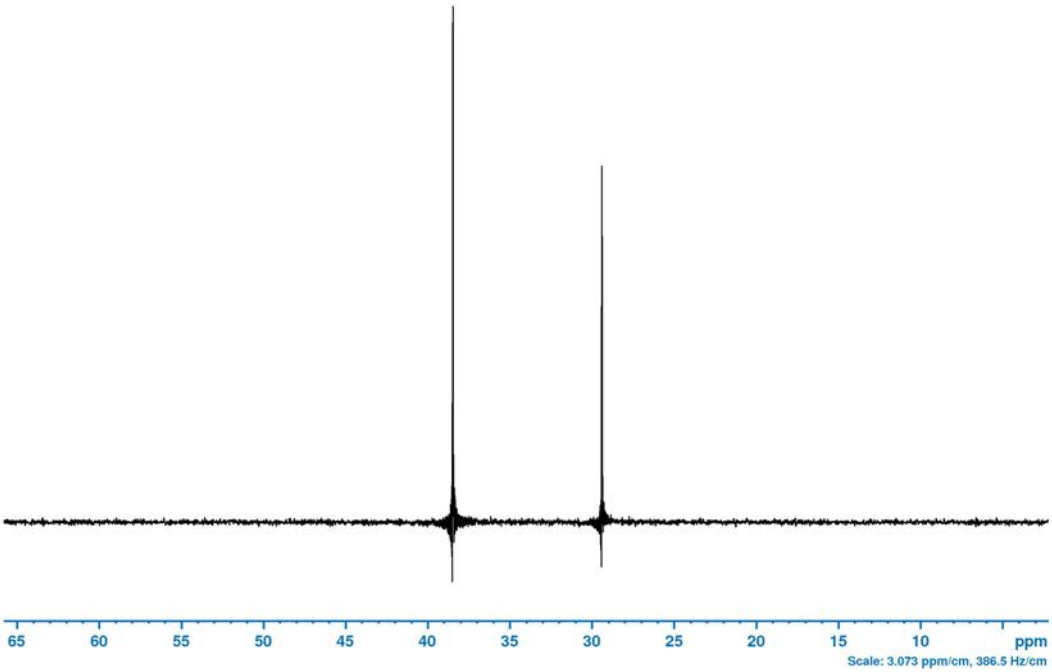
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 400 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 500 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 600 | 111000 | 11000 | 11000 | 11000 | 11000 | 11000 | 7000 |
| 700 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 750 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 800 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 850 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 900 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 950 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |
| 1000 | 111000 | 12000 | 12000 | 12000 | 12000 | 12000 | 7000 |

### 5.4.3 Optimization of 13C frequency (NPT_13C_MAS_fieldsetting_dec1h)

**Test Sample:** Adamantane
Z151221, Z151271, Z151261, Z151251, Z151231, Z151241, Z151211, Z163274, Z183104
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

13C spectrum with 1H CW decoupling after field optimization

**Control Option for Acquisition (L23)**

1 default
2 skip SINO and line width check on PROCNO 2

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | hpdec | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 34.000 | ppm | |
| O2P | 2.460 | ppm | |
| SWH | 10000.000 | Hz | |
| TD | 4000 | | |
| AQ | 0.200 | s | |
| FIDRES | 5.000 | Hz | |
| D 1 | 15.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| CPDPRG2 | cw | | decoupl. sequence |
| PLW 1 | 52 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.05 | W | B1(NUC2) = MASR/4 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| WDW | 0 | | |
| PH_mod | 0 | | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 100.000 | cm | |

## Experiment Description

The experimental procedure includes two 13C acquisitions with constant 01 at two known FIELD positions. Using 38.46 ppm as 13C chemical shift of the CH2 groups Adamantane the correct FIELD value can be calculated from these measurements.
O2P is determined for each FIELD position by acquisition and processing of a spectrum of NUC 2 in a derived data set.
After acquisition of the first 13C spectrum SINO and line width determination will be executed. The experiment will be aborted, if a minimal SINO of 10 and a minimal line width of 15 Hz are not achieved. SINO and line width check can be skiped with L23=2.
Before acquisition of the final nmr spectrum NMRPT stores the resulting FIELD value in the BSMS.

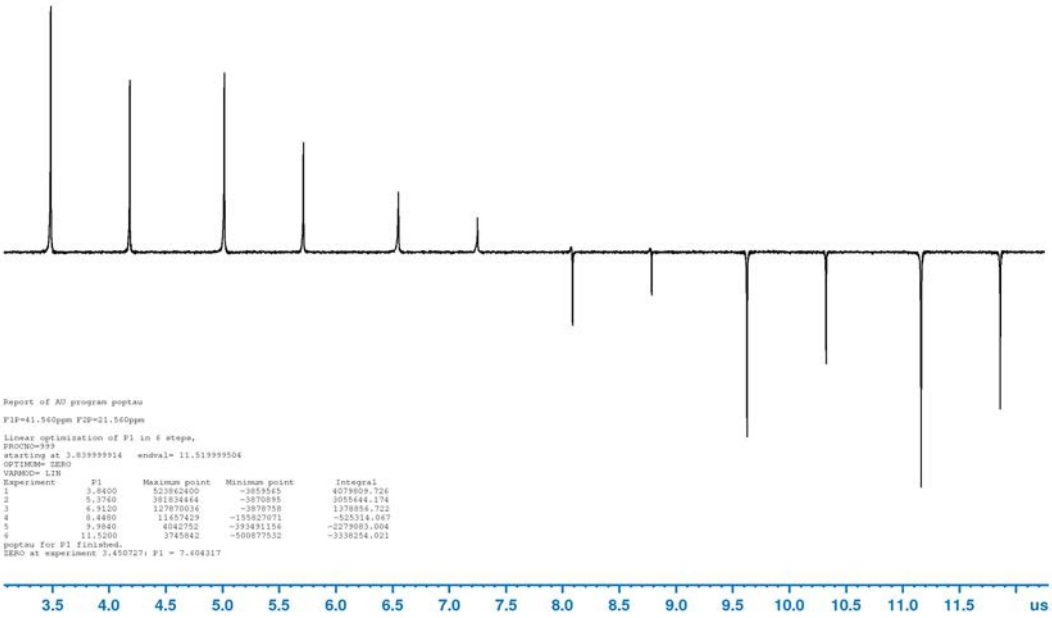
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

### 5.4.4 P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c)

**Test Sample:** Adamantane
Z151221, Z151271, Z151261, Z151251, Z151231, Z151241, Z151211, Z163274, Z183104
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | hpdec | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 34.000 | ppm | |
| O2P | 2.460 | ppm | |
| SWH | 10000.000 | Hz | |
| TD | 4000 | | |
| AQ | 0.200 | s | |
| FIDRES | 5.000 | Hz | |
| D 1 | 15.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| CPDPRG2 | cw | | decoupl. sequence |
| PLW 1 | 125 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.2 | W | B1(NUC2) = MASR/4 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
O2P is determined for decoupling by acquisition and processing of a spectrum of NUC 2 in a derived data set.
Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n. The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

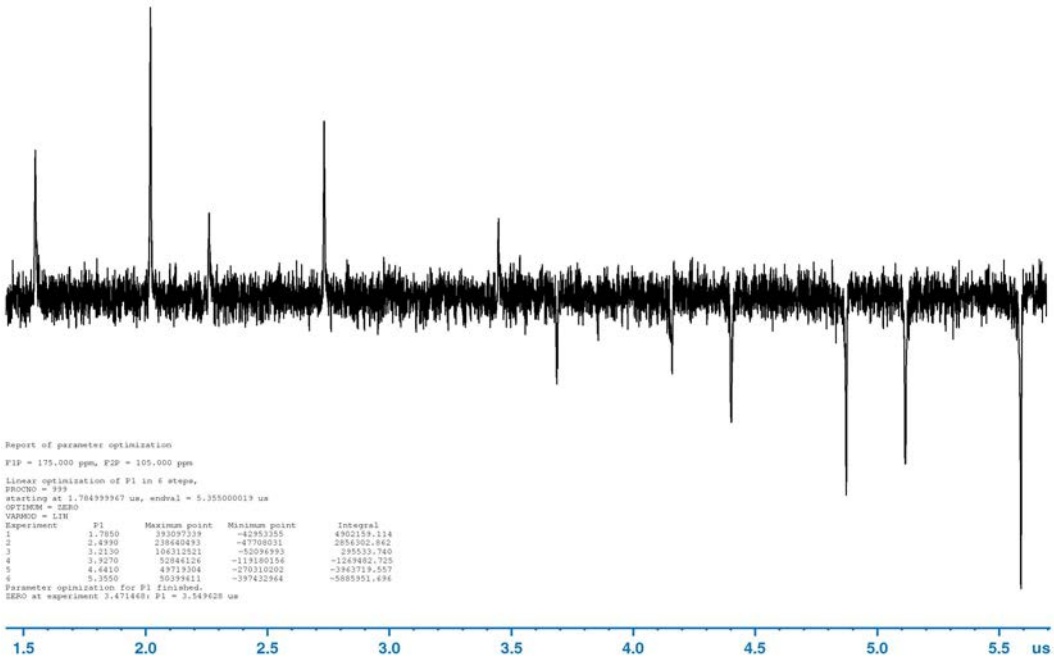
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

## 5.4.5 P90 13C 19F-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp19f_13c)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

P90 CP pulse determination using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows six experiments P1*0.5 to P1*1.5 (PROCNO 999).

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 140.000 | ppm | |
| O2P | -74.000 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 2.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 5000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 49.0 | W | Pow@90deg NUC2 |
| SPW 0 | 49.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will not be updated during this experiment.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

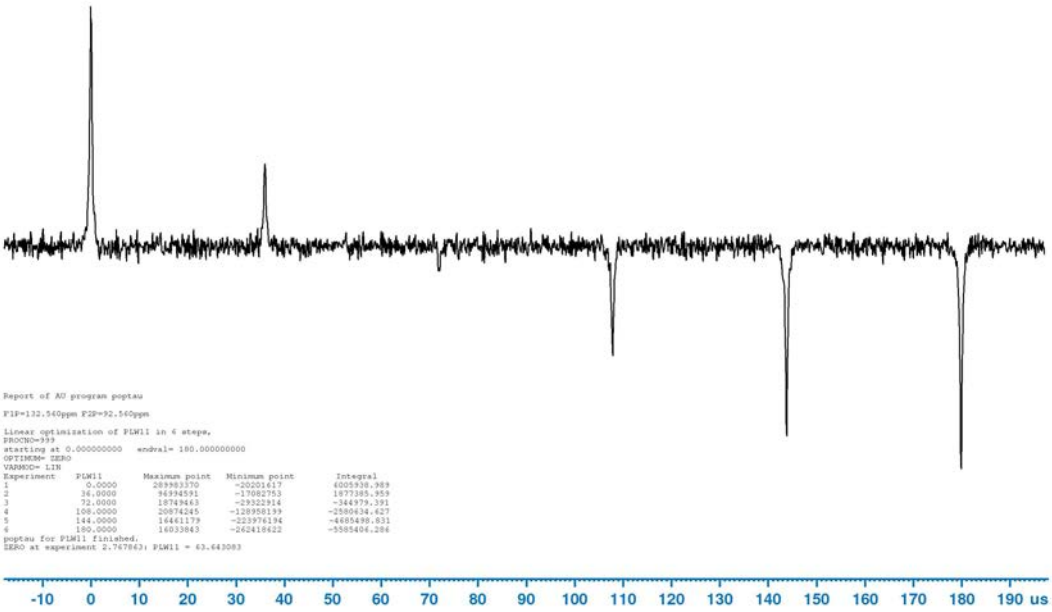
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.6 P90 13C 19F-13C CP pulse calibration using H-coil, MAS (NPT_13C_MAS_p90det_cp19f_13c_hcoil)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

P90 CP pulse determination using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows six experiments P1*0.5 to P1*1.5 (PROCNO 999).

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 140.000 | ppm | |
| O2P | -74.000 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 2.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 5000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 49.0 | W | Pow@90deg NUC2 |
| SPW 0 | 49.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will not be updated during this experiment.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

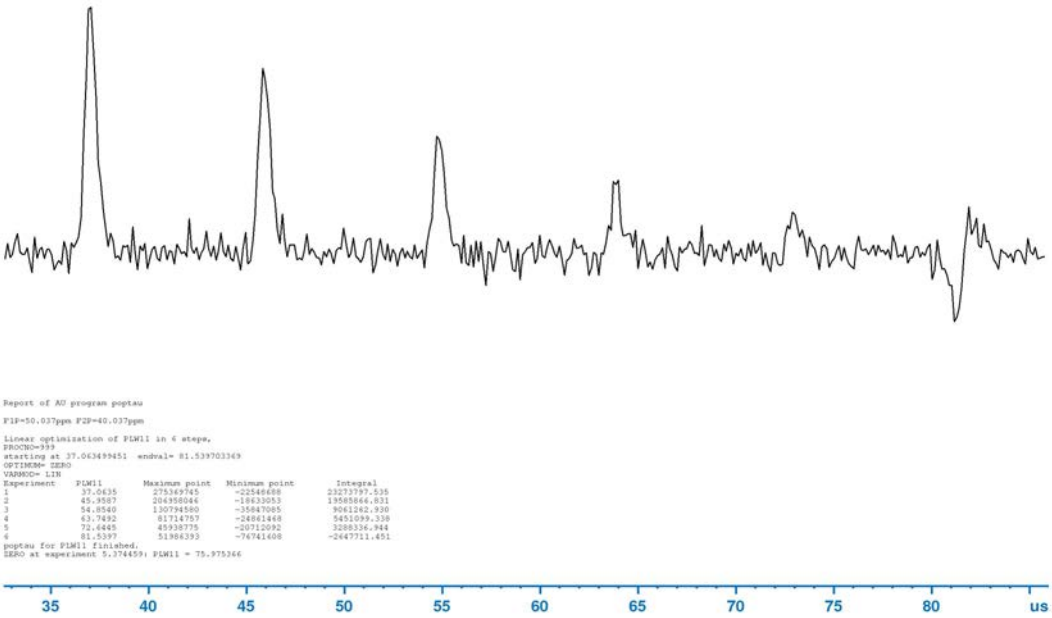
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.7 P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c)

**Test Sample:** Alpha-crystalline Glycine (not isotope-labeled or 2-13C, 15N Glycine) Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z183105, Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 CP pulse determination using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows six experiments P1*0.5 to P1*1.5 (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 43.000 | ppm | |
| O2P | 6.200 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 2000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will be updated with the determined pulse and the power used.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

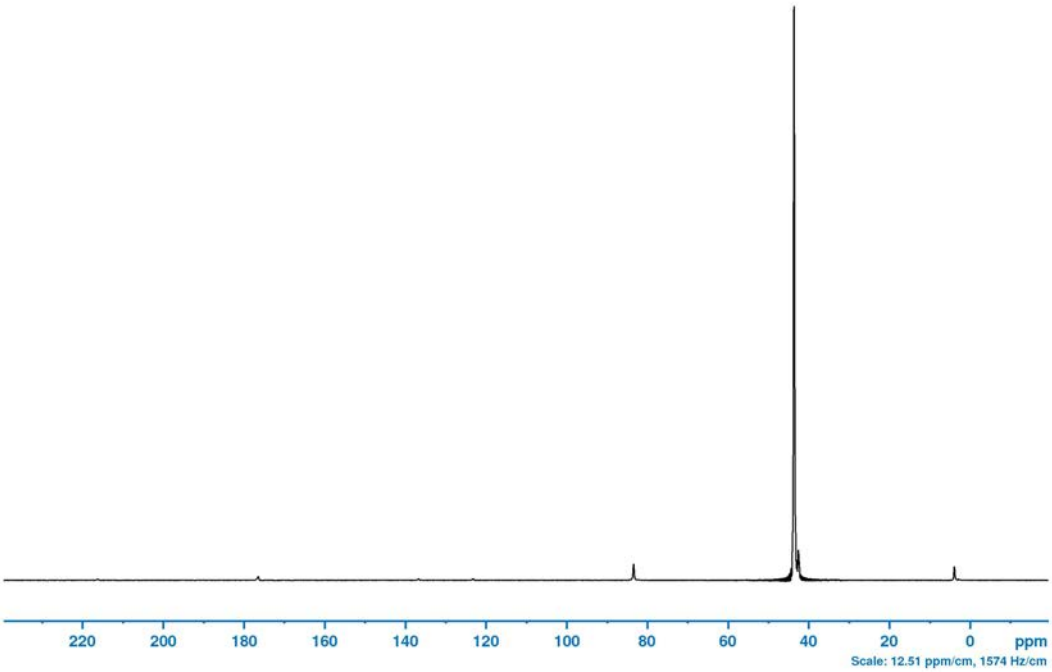
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

## 5.4.8 CP 1H-13C parameter optimization, MAS (NPT_13C_MAS_paropt_cp1h_13c)

**Test Sample:** Alpha-crystalline 2-13C, 15N Glycine
Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp | | |
| NS | 4 | | set according specs |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 110.000 | ppm | |
| O2P | 6.200 | ppm | |
| SW | 299.337 | ppm | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 2000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| TDeff | 2048 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Experiment for parameter optimization (PLW12 and SPW0) for mas experiments with cp. Signal to noise value is calculated using noise range of 20 ppm. All ranges are provided in plot title.
L23 dependent offset optimization: Prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
Start value of SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.

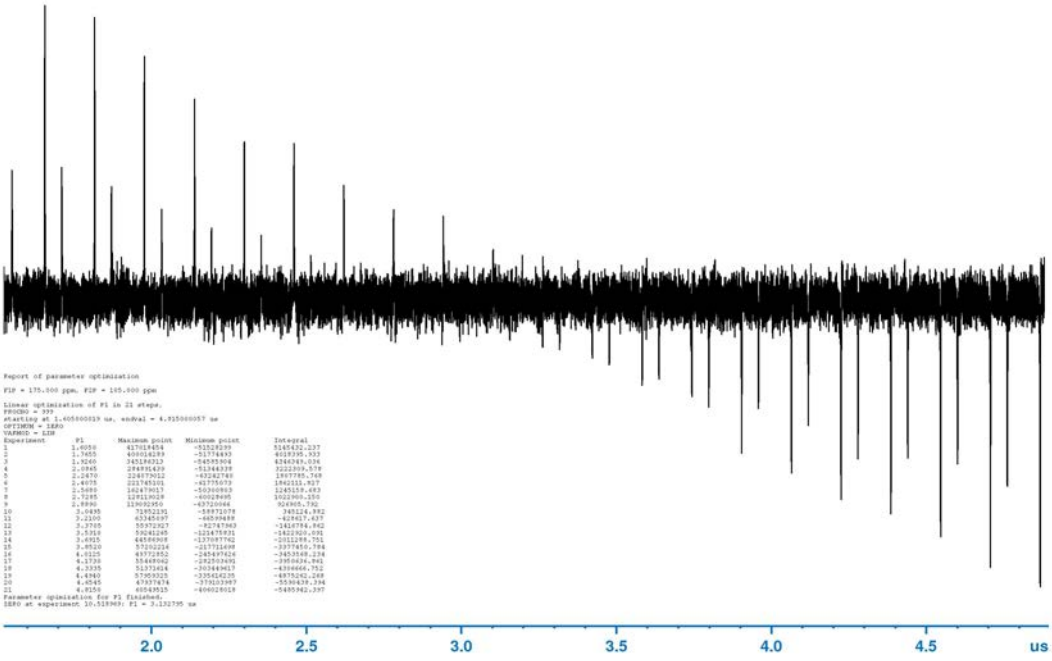
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

## 5.4.9 P90 13C 19F-13C CP shortest pulse calibration, MAS (NPT_13C_MAS_shortestPulse_cp19f_13c)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

Shortest pulse determination with CP using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows 21 experiments P1*0.5 to P1*1.5(PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 140.000 | ppm | |
| O2P | -74.000 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 2.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 5000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 49.0 | W | Pow@90deg NUC2 |
| SPW 0 | 49.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will not be updated during this experiment.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

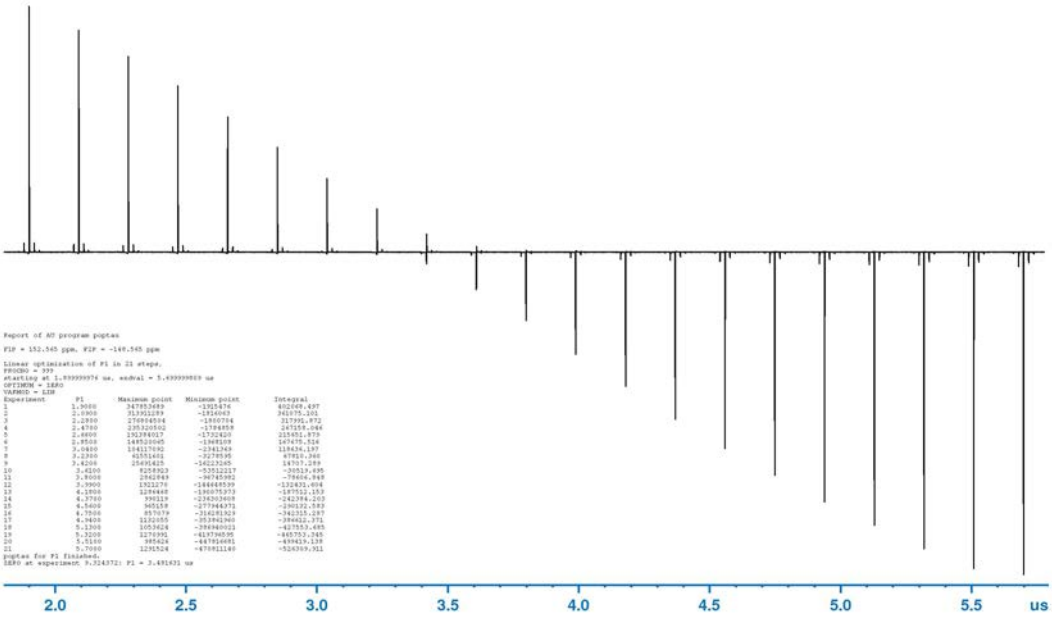
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.10 P90 13C 19F-13C CP shortest pulse calibration using H-coil, MAS (NPT_13C_MAS_shortestPulse_cp19f13c_hcoil)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

Shortest pulse determination with CP using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows 21 experiments P1*0.5 to P1*1.5(PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 140.000 | ppm | |
| O2P | -74.000 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 2.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 5000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 49.0 | W | Pow@90deg NUC2 |
| SPW 0 | 49.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will not be updated during this experiment.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

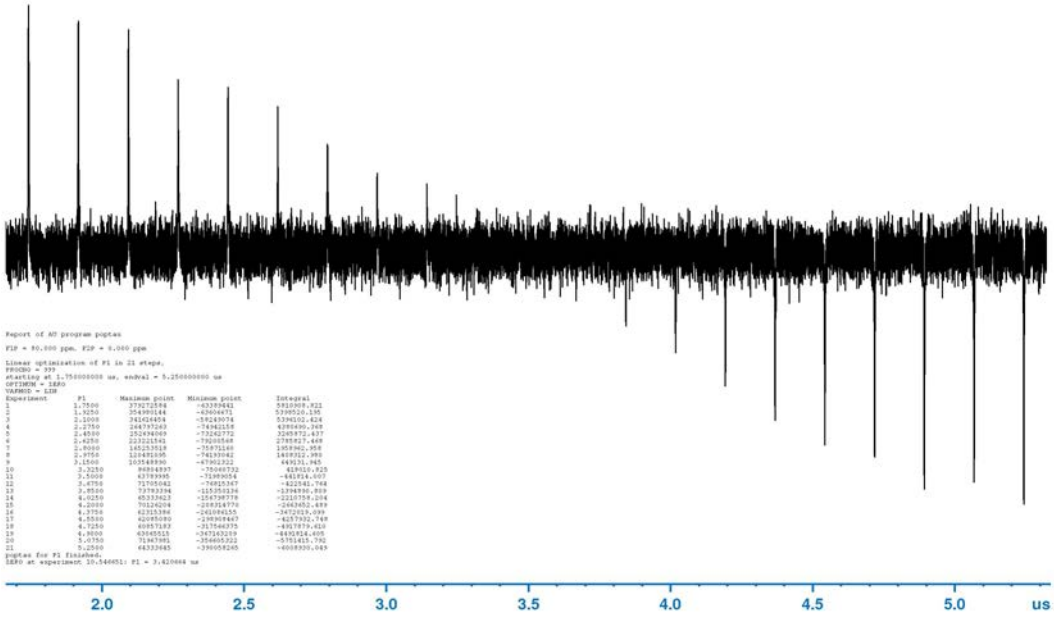
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

### 5.4.11 P90 13C 1H-13C CP shortest pulse calibration, MAS (NPT_13C_MAS_shortestPulse_cp1h_13c)

**Test Sample:** Alpha-crystalline Glycine (not isotope-labeled or 2-13C, 15N Glycine) Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z183105, Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Shortest pulse determination with CP using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows 21 experiments P1*0.5 to P1*1.5(PROCNO 999).

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 43.000 | ppm | |
| O2P | 6.200 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 2000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will not be updated during this experiment.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

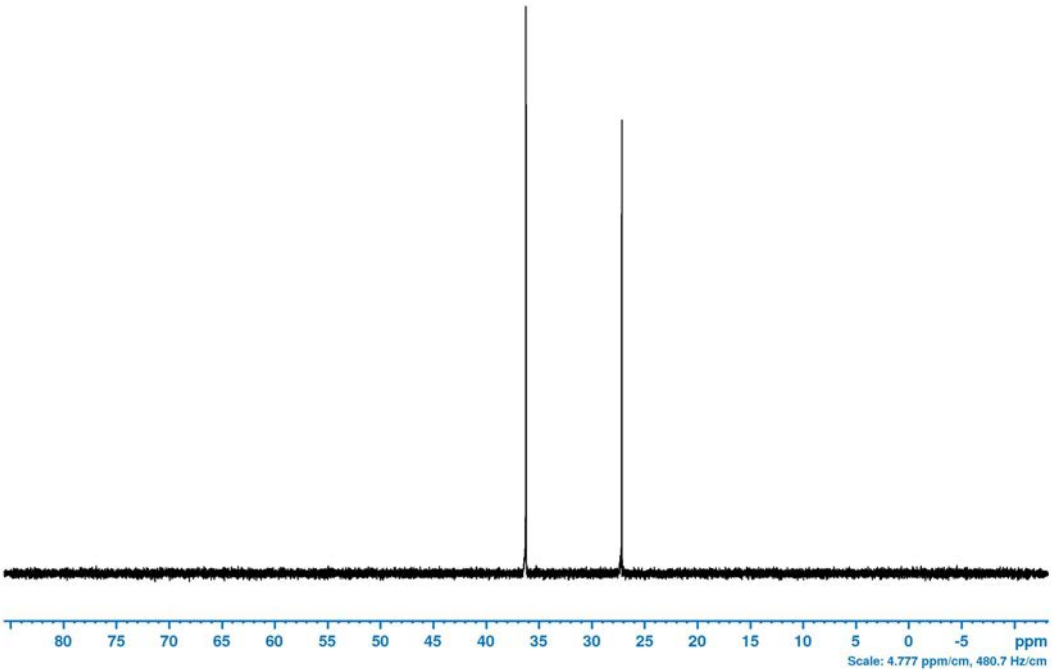
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

## 5.4.12 13C sensitivity, MAS (NPT_13C_MAS_sino_13c)

**Test Sample:** Adamantane
Z151221, Z151271, Z151261, Z151251, Z151231, Z151241, Z151211, Z163274, Z183104
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity and line width determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | hpdec | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 34.000 | ppm | |
| O2P | 2.460 | ppm | |
| SWH | 10000.000 | Hz | |
| TD | 19998 | | |
| AQ | 1.000 | s | |
| FIDRES | 1.000 | Hz | |
| D 1 | 15.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| CPDPRG2 | cw | | decoupl. sequence |
| PLW 1 | 125 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.2 | W | B1(NUC2) = MASR/4 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Sensitivity determination on solid probes including line width determination. Signal to noise value is calculated using noise range of 20 ppm set apart possible MAS spinning side bands. All ranges are provided in plot title.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined for decoupling by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

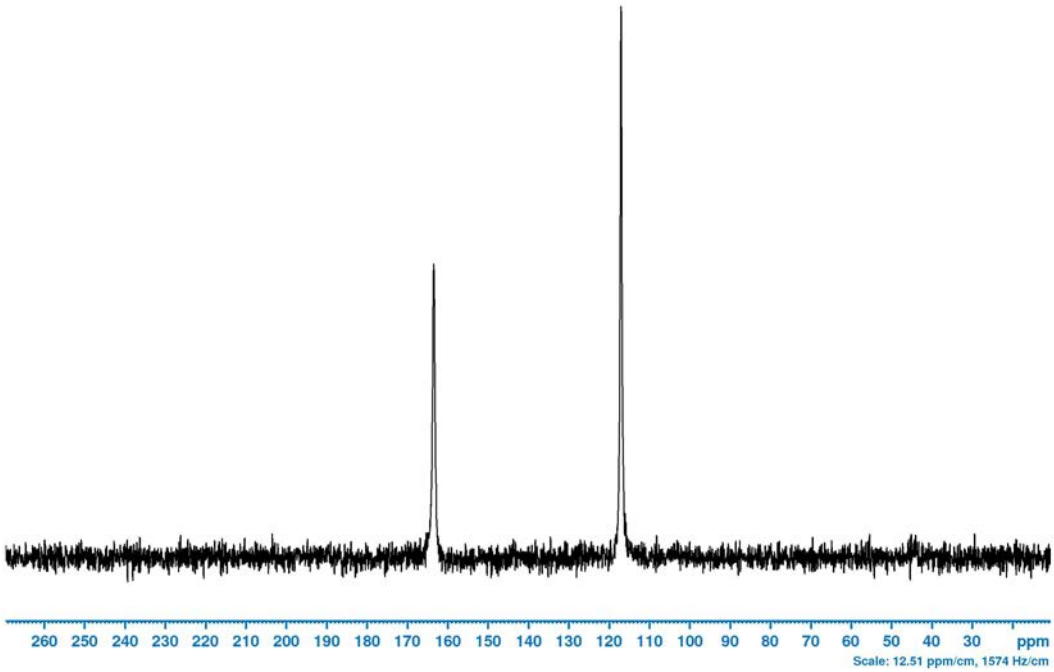
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

### 5.4.13 CP 19F-13C sensitivity, MAS (NPT_13C_MAS_sino_cp19f_13c)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**
Spectrum of sensitivity determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12
21 Same as 1 but with forced automatic optimization of SPW0 and PLW12
22 Same as 2 but with forced automatic optimization of SPW0 and PLW12
23 Same as 3 but with forced automatic optimization of SPW0 and PLW12
24 Same as 4 but with forced automatic optimization of SPW0 and PLW12
25 Same as 5 but with forced automatic optimization of SPW0 and PLW12

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp | | |
| NS | 64 | | set according specs |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 140.000 | ppm | |
| O2P | -74.000 | ppm | |
| SW | 299.328 | ppm | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 5000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 49.0 | W | Pow@90deg NUC2 |
| SPW 0 | 49.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Sensitivity determination on solid probes including steps for optimization of PLW12 and SPW0. Signal to noise value is calculated using noise range of 20 ppm. All ranges are provided in plot title.
If number of scans is specified, NS will be set accordingly during acquisition.
L23 dependent offset optimization: Prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 = 1, 2, 3, 4, and 5 the values of SPW0 and PLW12 will be taken from an allready acquired sino experiment.
For L23 = 11, 12, 13, 14 and 15 or if the sino experiment has not been measured a manual user interaction part to set or optimize SPW0, and PLW12 is included.
For L23 = 21, 22, 23, 24 and 25 the optimization of SPW0 and PLW12 will be enforced.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

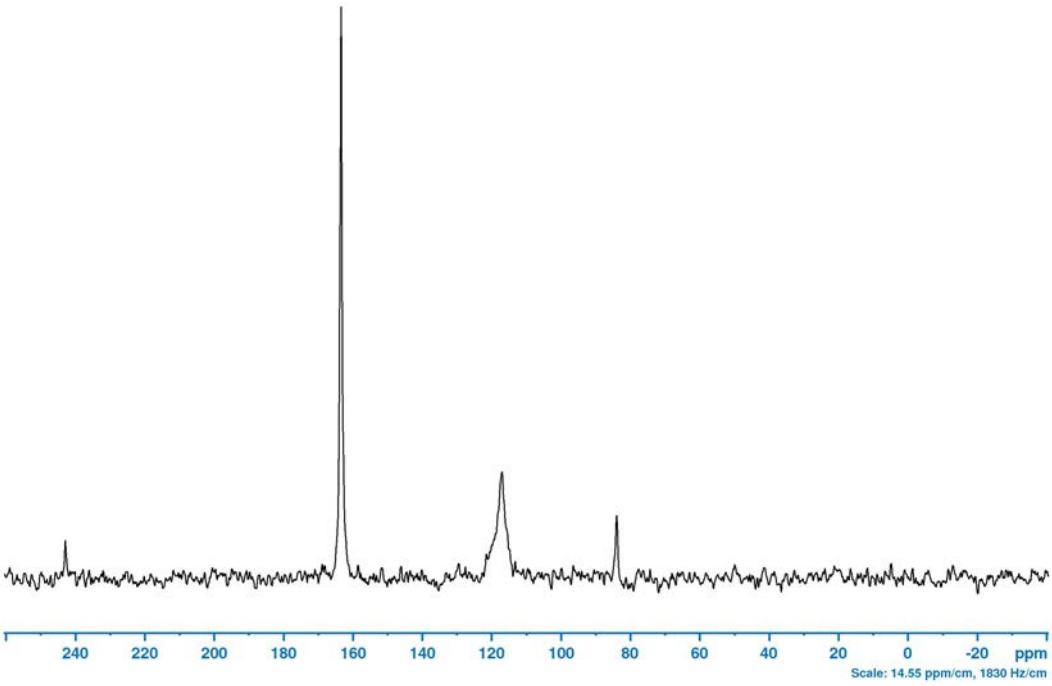
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.14 CP 19F-13C sensitivity using H-coil, MAS (NPT_13C_MAS_sino_cp19f_13c_hcoil)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12
21 Same as 1 but with forced automatic optimization of SPW0 and PLW12
22 Same as 2 but with forced automatic optimization of SPW0 and PLW12
23 Same as 3 but with forced automatic optimization of SPW0 and PLW12
24 Same as 4 but with forced automatic optimization of SPW0 and PLW12
25 Same as 5 but with forced automatic optimization of SPW0 and PLW12

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp | | |
| NS | 64 | | set according specs |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 140.000 | ppm | |
| O2P | -74.000 | ppm | |
| SW | 299.328 | ppm | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 5000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 49.0 | W | Pow@90deg NUC2 |
| SPW 0 | 49.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

Sensitivity determination on solid probes including steps for optimization of PLW12 and SPW0. Signal to noise value is calculated using noise range of 20 ppm. All ranges are provided in plot title.
If number of scans is specified, NS will be set accordingly during acquisition.
L23 dependent offset optimization: Prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 = 1, 2, 3, 4, and 5 the values of SPW0 and PLW12 will be taken from an allready acquired sino experiment.
For L23 = 11, 12, 13, 14 and 15 or if the sino experiment has not been measured a manual user interaction part to set or optimize SPW0, and PLW12 is included.
For L23 = 21, 22, 23, 24 and 25 the optimization of SPW0 and PLW12 will be enforced.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

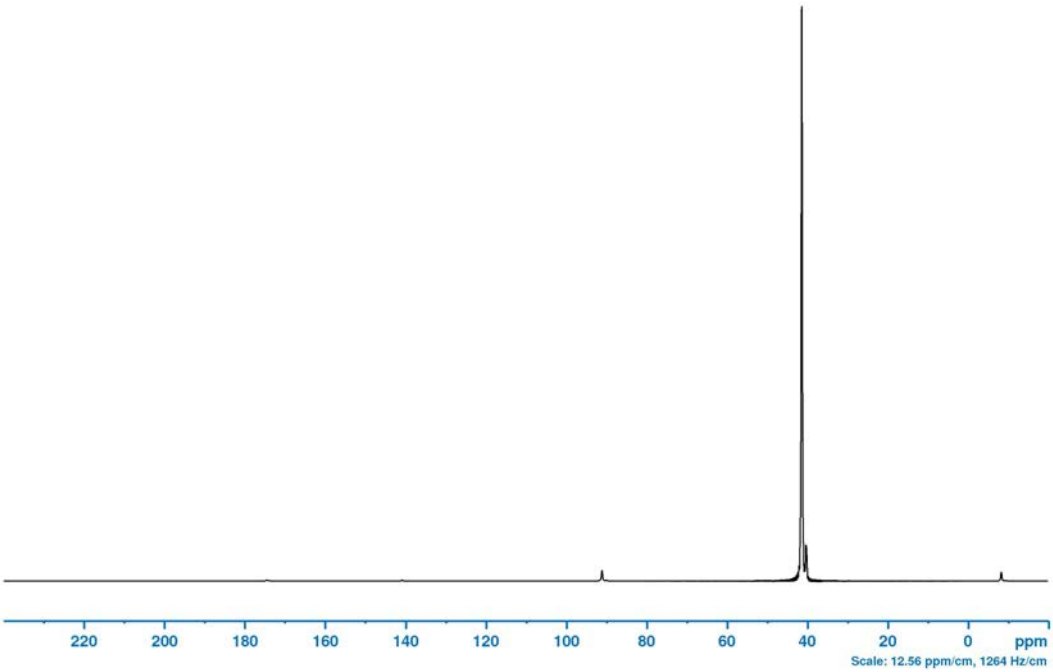
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

### 5.4.15 CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c)

**Test Sample:** Alpha-crystalline Glycine (weighted sample depending on rotor diameter) Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z163275, Z183105
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12
21 Same as 1 but with forced automatic optimization of SPW0 and PLW12
22 Same as 2 but with forced automatic optimization of SPW0 and PLW12
23 Same as 3 but with forced automatic optimization of SPW0 and PLW12
24 Same as 4 but with forced automatic optimization of SPW0 and PLW12
25 Same as 5 but with forced automatic optimization of SPW0 and PLW12

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp | | |
| NS | 64 | | set according specs |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 110.000 | ppm | |
| O2P | 6.200 | ppm | |
| SW | 299.337 | ppm | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 2000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| TDeff | 2048 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Sensitivity determination on solid probes including steps for optimization of PLW12 and SPW0. Signal to noise value is calculated using noise range of 20 ppm. All ranges are provided in plot title.
If number of scans is specified, NS will be set accordingly during acquisition.
L23 dependent offset optimization: Prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 = 1, 2, 3, 4, and 5 the values of SPW0 and PLW12 will be taken from an allready acquired paropt_cp1h experiment.
For L23 = 11, 12, 13, 14 and 15 or if the paropt_cp1h experiment has not been measured a manual user interaction part to set or optimize SPW0, and PLW12 is included.
For L23 = 21, 22, 23, 24 and 25 the optimization of SPW0 and PLW12 will be enforced.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

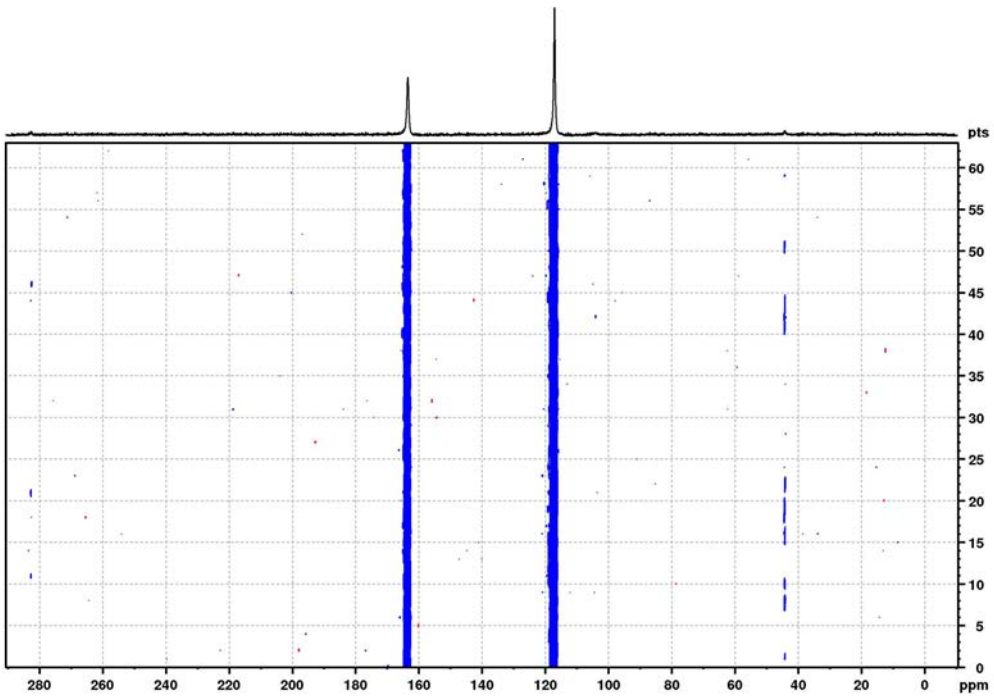
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

### 5.4.16 CP 19F-13C power stability MAS (NPT_13C_MAS_stab_cp19f_13c)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Pseudo 2D CP spectrum to observe power stability.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 19F | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_cp2d | | |
| NS | 16 | | |
| DS | 32 | | |
| RG | 101.000 | | no optim. |
| O1P | 140.000 | ppm | |
| O2P | -74.000 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 8500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 49.0 | W | Pow@90deg NUC2 |
| SPW 0 | 49.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

Determination of power stability for CP experiments on solid probes using maximum decoupling field and maximum acquisition time provided as mandatory specifications. The average signal-to-noise ratio (20 ppm noise range)
is evaluated considering all rows of the pseudo-2D measurement. Also the maximum deviation of the results is determined, along with the rows of maximum and minimum result.
For power stability measurement the specs for acquisition time and decoupling pulse length must be specified.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 < 10 the values of SPW0 and PLW12 will be taken from the corresponding sino experiment. PLW12 will be optimized if the specified PCPD2 pulse differs from PCPD2 used in the corresponding sino experiment.
For L23 > 10 or if the corresponding sino experiment has not been measured a manual user interaction part to set or optimize SPW0 and PLW12 is included.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.

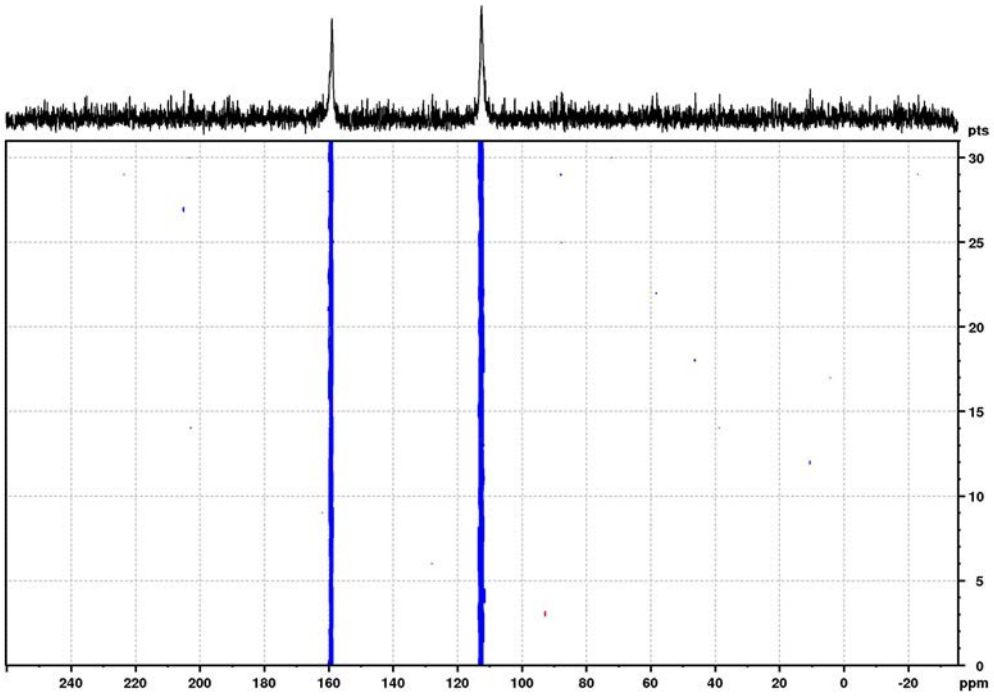
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.17 CP 19F-13C power stability using H-coil, MAS (NPT_13C_MAS_stab_cp19f_13c_hcoil)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Pseudo 2D CP spectrum to observe power stability.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 19F | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_cp2d | | |
| NS | 16 | | |
| DS | 32 | | |
| RG | 101.000 | | no optim. |
| O1P | 140.000 | ppm | |
| O2P | -74.000 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 8500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 49.0 | W | Pow@90deg NUC2 |
| SPW 0 | 49.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

Determination of power stability for CP experiments on solid probes using maximum decoupling field and maximum acquisition time provided as mandatory specifications. The average signal-to-noise ratio (20 ppm noise range)
is evaluated considering all rows of the pseudo-2D measurement. Also the maximum deviation of the results is determined, along with the rows of maximum and minimum result.
For power stability measurement the specs for acquisition time and decoupling pulse length must be specified.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 < 10 the values of SPW0 and PLW12 will be taken from the corresponding sino experiment. PLW12 will be optimized if the specified PCPD2 pulse differs from PCPD2 used in the corresponding sino experiment.
For L23 > 10 or if the corresponding sino experiment has not been measured a manual user interaction part to set or optimize SPW0 and PLW12 is included.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + 2*MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition 1, -1, and -2 until power is in limits.
The selection of a certain side band condition can be forced by setting CNST 50 to 2, 1, -1, or -2.

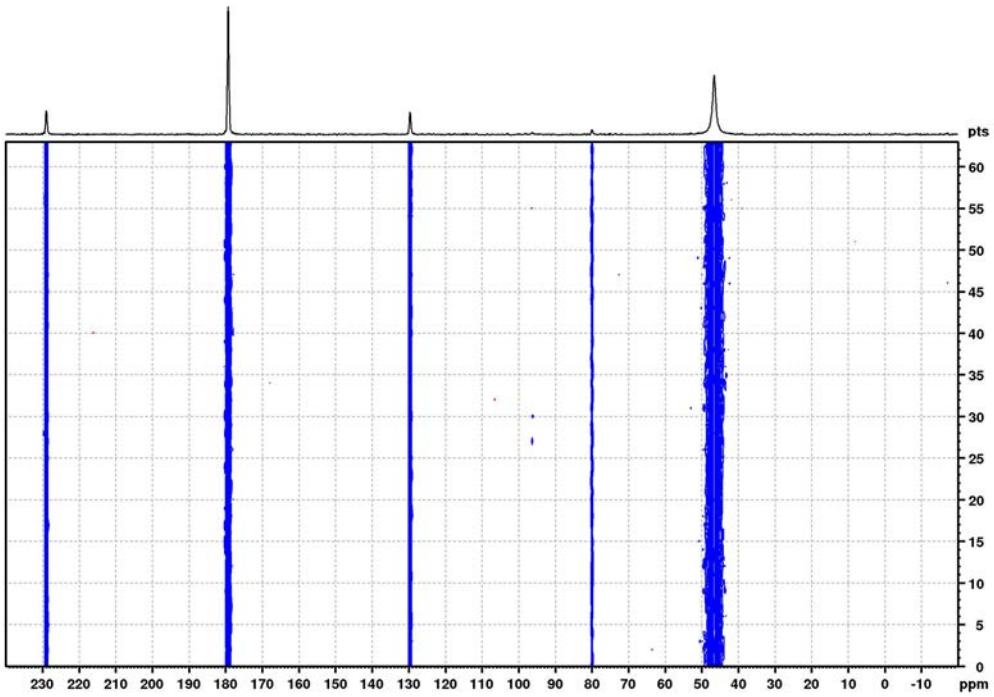
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

### 5.4.18 CP 1H-13C power stability MAS (NPT_13C_MAS_stab_cp1h_13c)

**Test Sample:** Alpha-crystalline Glycine (not isotope-labeled or 2-13C, 15N Glycine)
Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z183105, Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Pseudo 2D CP spectrum to observe power stability.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_cp2d | | |
| NS | 1 | | |
| DS | 32 | | |
| RG | 101.000 | | no optim. |
| O1P | 110.000 | ppm | |
| O2P | 6.200 | ppm | |
| SWH | 30120.482 | Hz | |
| TD | 3012 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 10000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 125.0 | W | Pow@90deg NUC1 |
| PLW 11 | 125.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

Determination of power stability for CP experiments on solid probes using maximum decoupling field and maximum acquisition time provided as mandatory specifications. The average signal-to-noise ratio (20 ppm noise range)
is evaluated considering all rows of the pseudo-2D measurement. Also the maximum deviation of the results is determined, along with the rows of maximum and minimum result.
For power stability measurement the specs for acquisition time and decoupling pulse length must be specified.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 < 10 the values of SPW0 and PLW12 will be taken from the corresponding paropt_cp1h experiment.
PLW12 will be optimized if the specified PCPD2 pulse differs from PCPD2 used in the corresponding paropt_cp1h experiment.
For L23 > 10 or if the corresponding sino experiment has not been measured a manual user interaction part to set or optimize SPW0 and PLW12 is included.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.

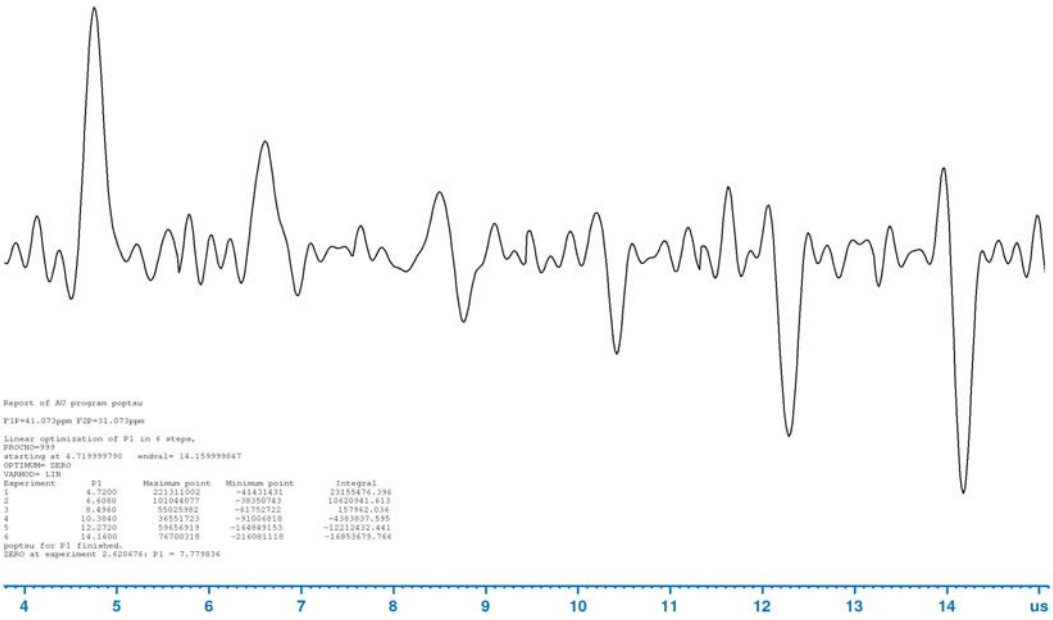
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

### 5.4.19 P90 15N pulse calibration, MAS (NPT_15N_MAS_p90det_15n)

**Test Sample:** Alpha-crystalline Glycine (not isotope-labeled or 2-13C, 15N Glycine) Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z183105, Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | hpdec | | |
| NS | 128 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 35.000 | ppm | |
| O2P | 6.200 | ppm | |
| SWH | 38461.539 | Hz | |
| TD | 1510 | | |
| AQ | 0.020 | s | |
| FIDRES | 50.942 | Hz | |
| D 1 | 15.000 | s | |
| P 1 | 4.5 | us | 90deg NUC1 |
| CPDPRG2 | spinal64 | | decoupl. sequence |
| PCPD2 | 8.3 | us | PCPD NUC2 |
| PLW 1 | 236.0 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 54.0 | W | |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.300 | Hz | |
| PH_mod | 1 | | pk |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
O2P is determined for decoupling by acquisition and processing of a spectrum of NUC 2 in a derived data set.
Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n. The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

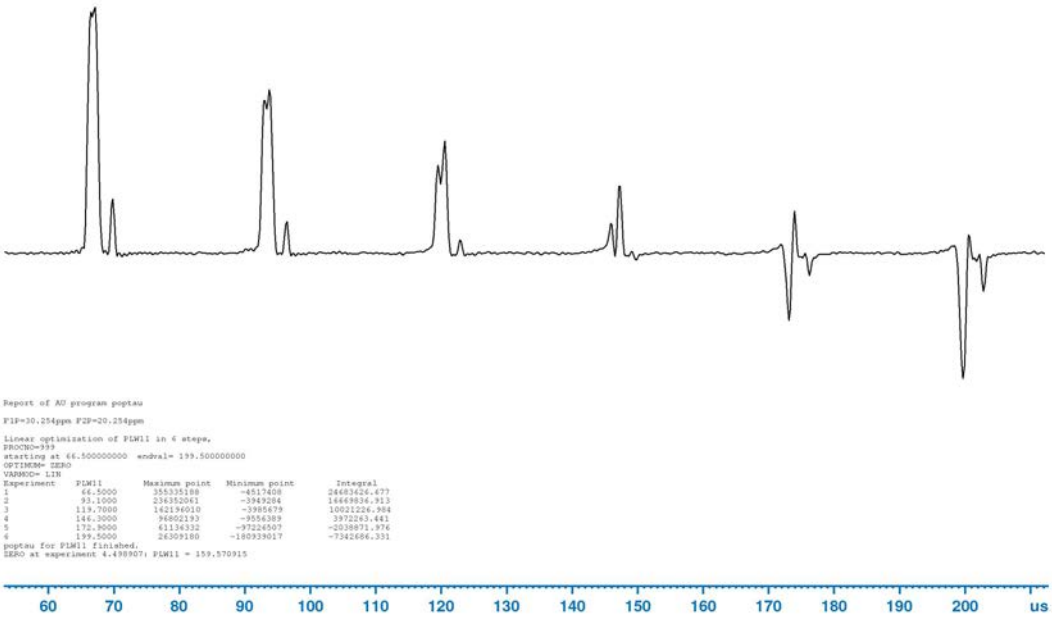
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

## 5.4.20 P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n)

**Test Sample:** Alpha-crystalline Glycine (not isotope-labeled or 2-13C, 15N Glycine) Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z183105, Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 CP pulse determination using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows six experiments P1*0.5 to P1*1.5 (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 35.000 | ppm | |
| O2P | 6.200 | ppm | |
| SWH | 16129.032 | Hz | |
| TD | 1612 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.011 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.5 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 3500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 236.0 | W | Pow@90deg NUC1 |
| PLW 11 | 236.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 26.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will be updated with the determined pulse and the power used.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

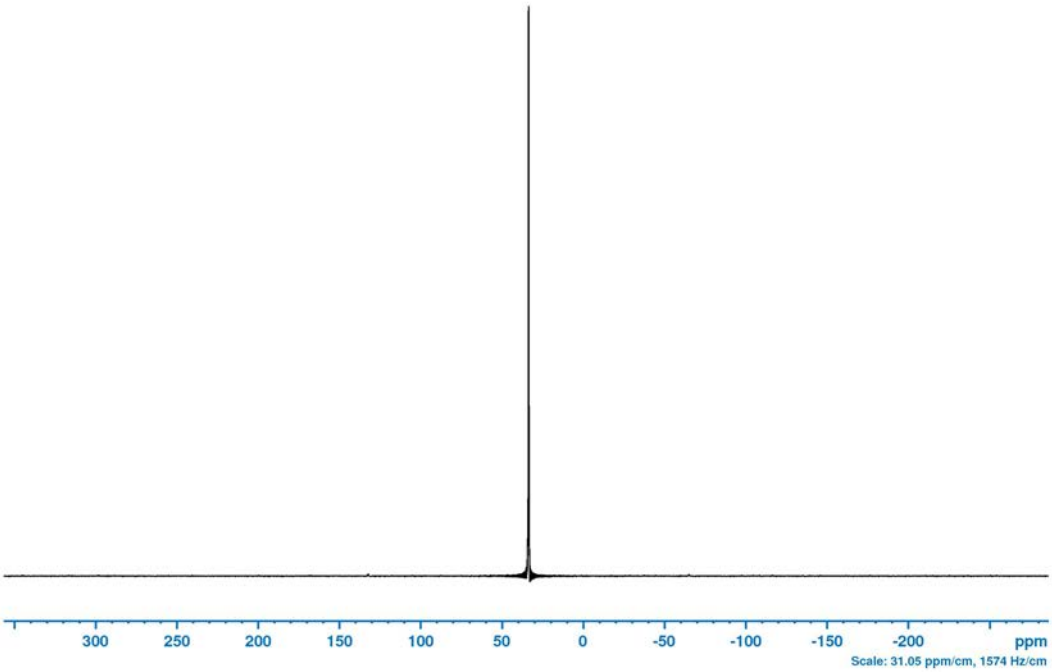
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

## 5.4.21 CP 1H-15N parameter optimization, MAS (NPT_15N_MAS_paropt_cp1h_15n)

**Test Sample:** Alpha-crystalline 2-13C, 15N Glycine
Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp | | |
| NS | 4 | | set according specs |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 35.000 | ppm | |
| O2P | 6.200 | ppm | |
| SW | 742.867 | ppm | |
| TD | 3012 | | field dependent |
| AQ | 0.050 | s | |
| FIDRES | 20.000 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.5 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 3500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 236.0 | W | Pow@90deg NUC1 |
| PLW 11 | 236.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 26.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Experiment for parameter optimization (PLW12 and SPW0) for mas experiments with cp. Signal to noise value is calculated using noise range of 20 ppm. All ranges are provided in plot title.
L23 dependent offset optimization: Prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
Start value of SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.

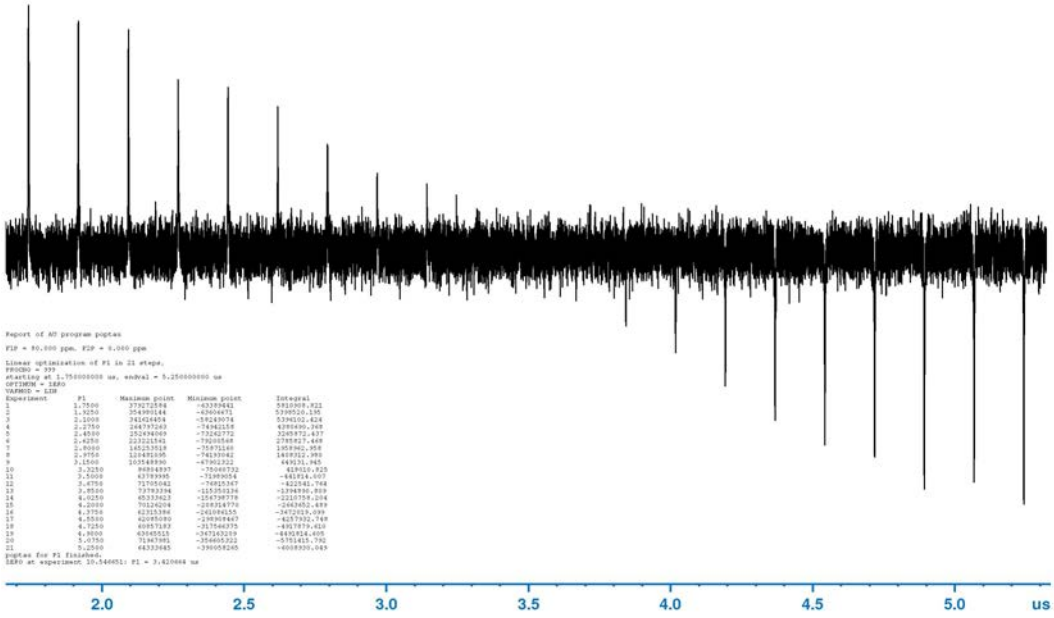
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

### 5.4.22 P90 15N 1H-15N CP shortest pulse calibration, MAS (NPT_15N_MAS_shortestPulse_cp1h_15n)

**Test Sample:** Alpha-crystalline Glycine (not isotope-labeled or 2-13C, 15N Glycine) Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z183105, Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Shortest pulse determination with CP using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows 21 experiments P1*0.5 to P1*1.5(PROCNO 999).

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 35.000 | ppm | |
| O2P | 6.200 | ppm | |
| SWH | 16129.032 | Hz | |
| TD | 1612 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.011 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.5 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 3500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 236.0 | W | Pow@90deg NUC1 |
| PLW 11 | 236.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 26.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will not be updated during this experiment.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

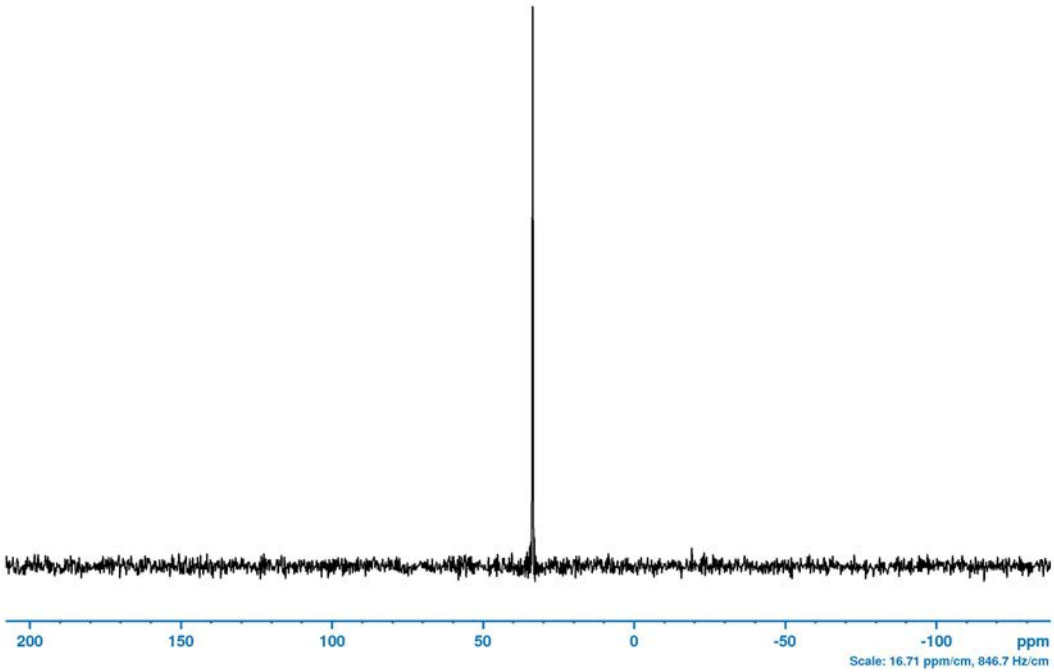
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

### 5.4.23 CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n)

**Test Sample:** Alpha-crystalline Glycine (weighted sample depending on rotor diameter) Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z163275, Z183105
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12
21 Same as 1 but with forced automatic optimization of SPW0 and PLW12
22 Same as 2 but with forced automatic optimization of SPW0 and PLW12
23 Same as 3 but with forced automatic optimization of SPW0 and PLW12
24 Same as 4 but with forced automatic optimization of SPW0 and PLW12
25 Same as 5 but with forced automatic optimization of SPW0 and PLW12

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp | | |
| NS | 64 | | set according specs |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 35.000 | ppm | |
| O2P | 6.200 | ppm | |
| SW | 397.794 | ppm | |
| TD | 1612 | | field dependent |
| AQ | 0.050 | s | |
| FIDRES | 20.011 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.5 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 3500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 236.0 | W | Pow@90deg NUC1 |
| PLW 11 | 236.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 26.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Sensitivity determination on solid probes including steps for optimization of PLW12 and SPW0. Signal to noise value is calculated using noise range of 20 ppm. All ranges are provided in plot title.
If number of scans is specified, NS will be set accordingly during acquisition.
L23 dependent offset optimization: Prior to the main acquisition O1P (PROCNO=10) will be optimized.
O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 = 1, 2, 3, 4, and 5 the values of SPW0 and PLW12 will be taken from an allready acquired paropt_cp1h experiment.
For L23 = 11, 12, 13, 14 and 15 or if the paropt_cp1h experiment has not been measured a manual user interaction part to set or optimize SPW0, and PLW12 is included.
For L23 = 21, 22, 23, 24 and 25 the optimization of SPW0 and PLW12 will be enforced.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

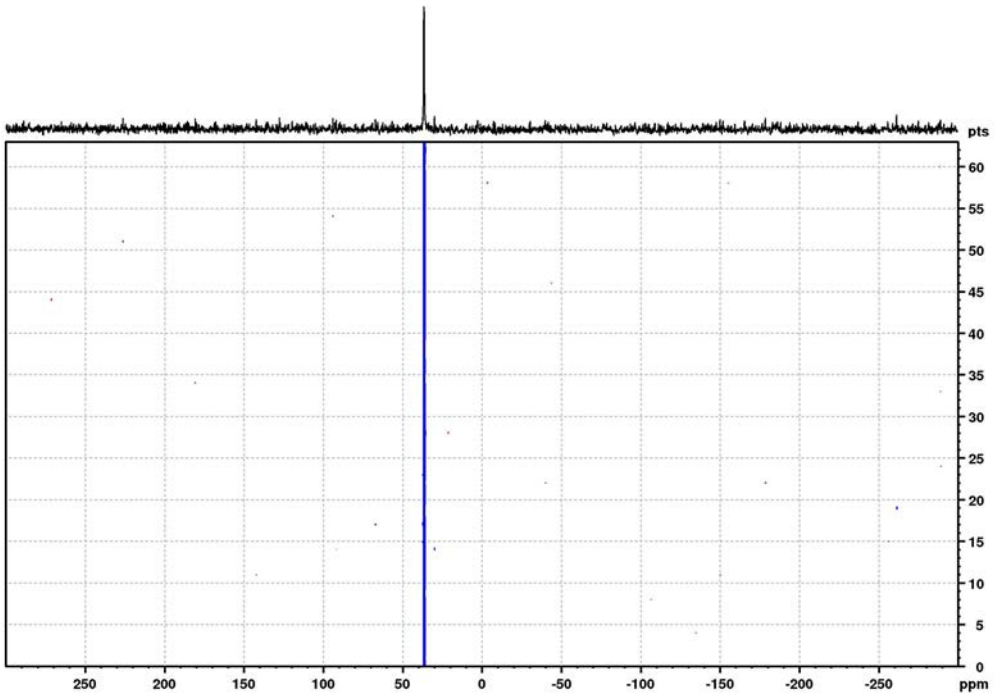
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

### 5.4.24 CP 1H-15N power stability MAS (NPT_15N_MAS_stab_cp1h_15n)

**Test Sample:** Alpha-crystalline Glycine (not isotope-labeled or 2-13C, 15N Glycine)
Z151222, Z151272, Z151262, Z151252, Z151232, Z151242, Z151212, Z183105, Z151223, Z151273, Z151263, Z151253, Z151233, Z151243, Z151213, Z163276, Z183106
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Pseudo 2D CP spectrum to observe power stability.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 15N | | |
| NUC2 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_cp2d | | |
| NS | 1 | | |
| DS | 32 | | |
| RG | 101.000 | | no optim. |
| O1P | 35.000 | ppm | |
| O2P | 6.200 | ppm | |
| SWH | 16129.032 | Hz | |
| TD | 1612 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.011 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.5 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 10000.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 236.0 | W | Pow@90deg NUC1 |
| PLW 11 | 236.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 26.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

Determination of power stability for CP experiments on solid probes using maximum decoupling field and maximum acquisition time provided as mandatory specifications. The average signal-to-noise ratio (20 ppm noise range)
is evaluated considering all rows of the pseudo-2D measurement. Also the maximum deviation of the results is determined, along with the rows of maximum and minimum result.
For power stability measurement the specs for acquisition time and decoupling pulse length must be specified.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 < 10 the values of SPW0 and PLW12 will be taken from the corresponding paropt_cp1h experiment.
PLW12 will be optimized if the specified PCPD2 pulse differs from PCPD2 used in the corresponding paropt_cp1h experiment.
For L23 > 10 or if the corresponding sino experiment has not been measured a manual user interaction part to set or optimize SPW0 and PLW12 is included.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.

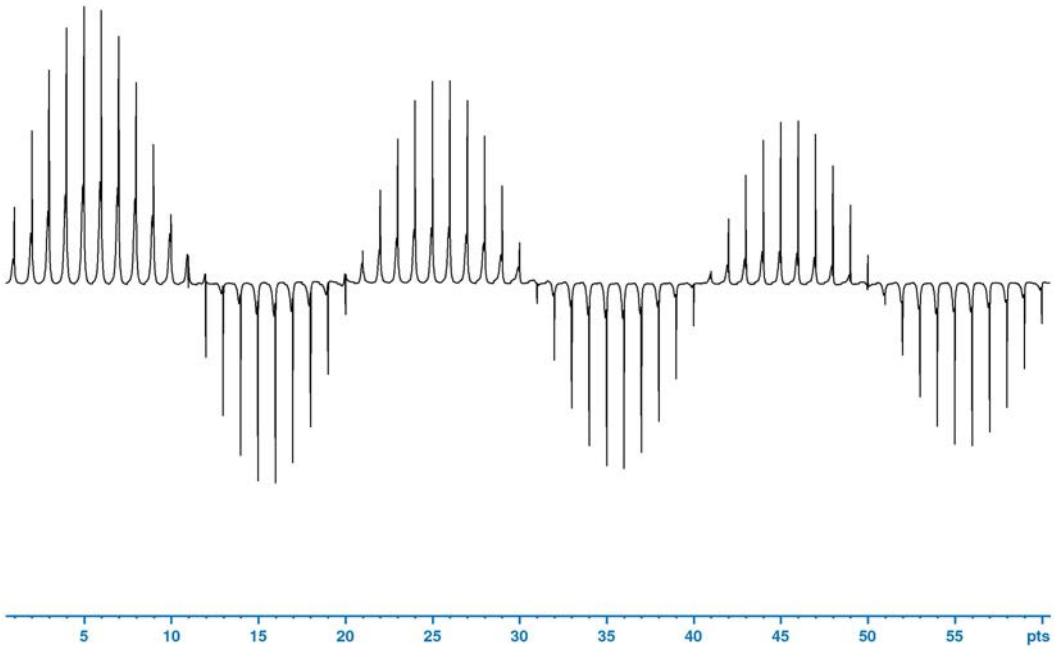
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 3000 |
| 400 | 40000 | 8000 | 5000 | 4800 | 4000 | 4000 | 4000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 6000 | 6000 | 6000 | 6000 | 6000 |
| 700 | 40000 | 8000 | 7000 | 7000 | 7000 | 7000 | 7000 |
| 750 | 40000 | 8000 | 7500 | 7500 | 7500 | 7500 | 7000 |
| 800 | 40000 | 8000 | 8000 | 8000 | 8000 | 8000 | 7000 |
| 850 | 40000 | 8500 | 8500 | 8500 | 8500 | 8500 | 7000 |
| 900 | 40000 | 9000 | 9000 | 9000 | 9000 | 9000 | 7000 |
| 950 | 40000 | 9500 | 9500 | 9500 | 9500 | 9500 | 7000 |
| 1000 | 40000 | 10000 | 10000 | 10000 | 10000 | 10000 | 7000 |

## 5.4.25 19F B1 homogeneity, MAS (NPT_19F_MAS_b1homogeneity_19f)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a region around each main signal is shown in the figure.

**Control Option for Acquisition (L23)**

1 default, skip O1P determination.
2 execute O1P determination.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1b1hom2d_sol | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 16.000 | | no optim. |
| O1P | -74.000 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.010 | s | |
| FIDRES | 97.656 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 68.0 | W | Pow@90deg NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| CY | 11.000 | cm | |

## Experiment Description

The B1 homogeneity measurement is acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range reaches from 15 to approx. 810 degrees. The B1-homogeneities based on integrals are computed from the magnitude of the second complex FID data point in PROCNO=2.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. With the option L23 = 1 O1P determination step can be skipped to apply manually set value, i.e. value will be taken from data set.
The result of CONVTO1D is stored in PROCNO=999. This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Requirements: The corresponding 90° pulse determination experiment (NPT_X_MAS_p90det_YZ) is mandatory for B1 homogeneity measurement.

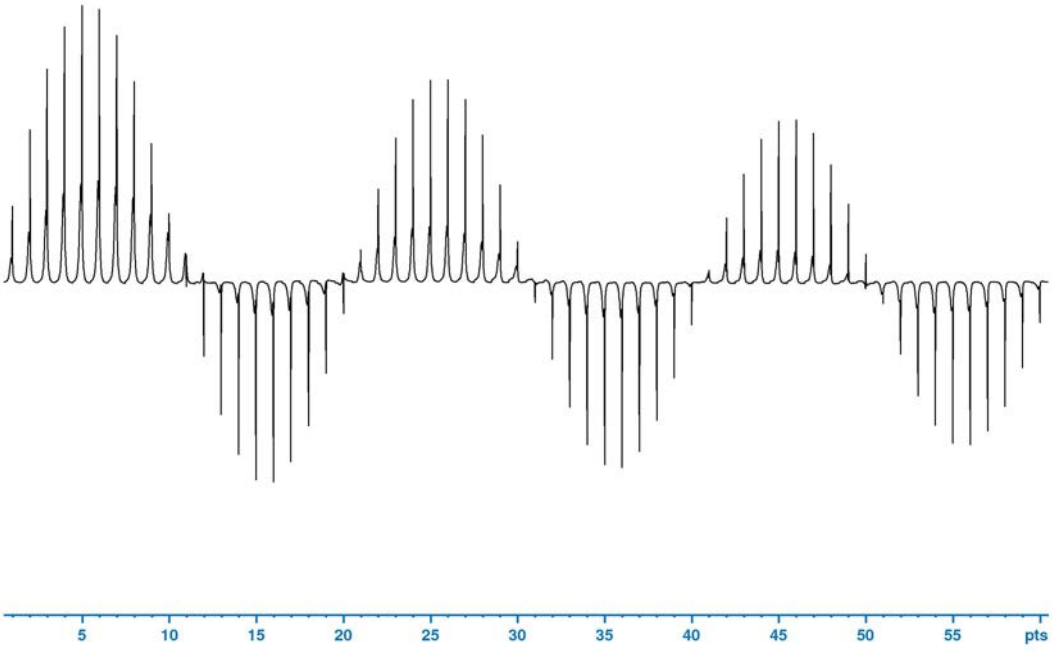
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.26 19F B1 homogeneity on H-coil, MAS (NPT_19F_MAS_b1homogeneity_19f_hcoil)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a region around each main signal is shown in the figure.

**Control Option for Acquisition (L23)**

1 default, skip O1P determination.
2 execute O1P determination.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1b1hom2d_sol | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 16.000 | | no optim. |
| O1P | -74.000 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.010 | s | |
| FIDRES | 97.656 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 68.0 | W | Pow@90deg NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| CY | 11.000 | cm | |

## Experiment Description

The B1 homogeneity measurement is acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range reaches from 15 to approx. 810 degrees. The B1-homogeneities based on integrals are computed from the magnitude of the second complex FID data point in PROCNO=2.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. With the option L23 = 1 O1P determination step can be skipped to apply manually set value, i.e. value will be taken from data set.
The result of CONVTO1D is stored in PROCNO=999. This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Requirements: The corresponding 90° pulse determination experiment (NPT_X_MAS_p90det_YZ) is mandatory for B1 homogeneity measurement.

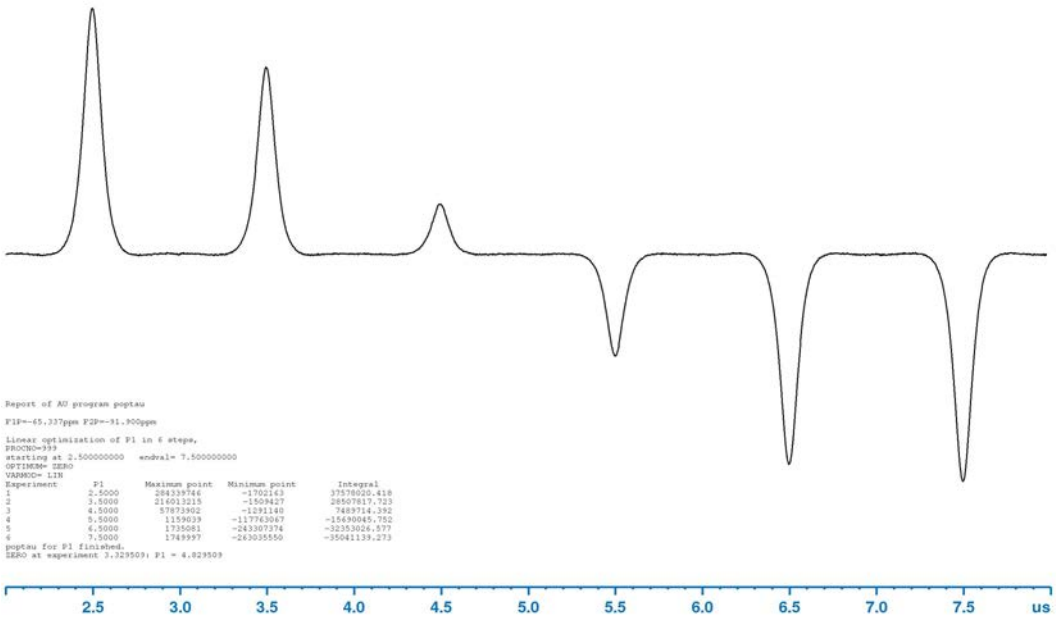
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.27 P90 19F pulse calibration, MAS (NPT_19F_MAS_p90det_19f)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P determination.
2 execute O1P determination.
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 16.000 | | no optim. |
| O1P | -74.000 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2988 | | |
| AQ | 0.015 | s | |
| FIDRES | 66.934 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 68.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Phase correction is done applying APK as default method. With the option L23 = 2 and 12 O1P determination step can be skipped to apply manually set values. The options L23 = 11 and 12 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n. The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

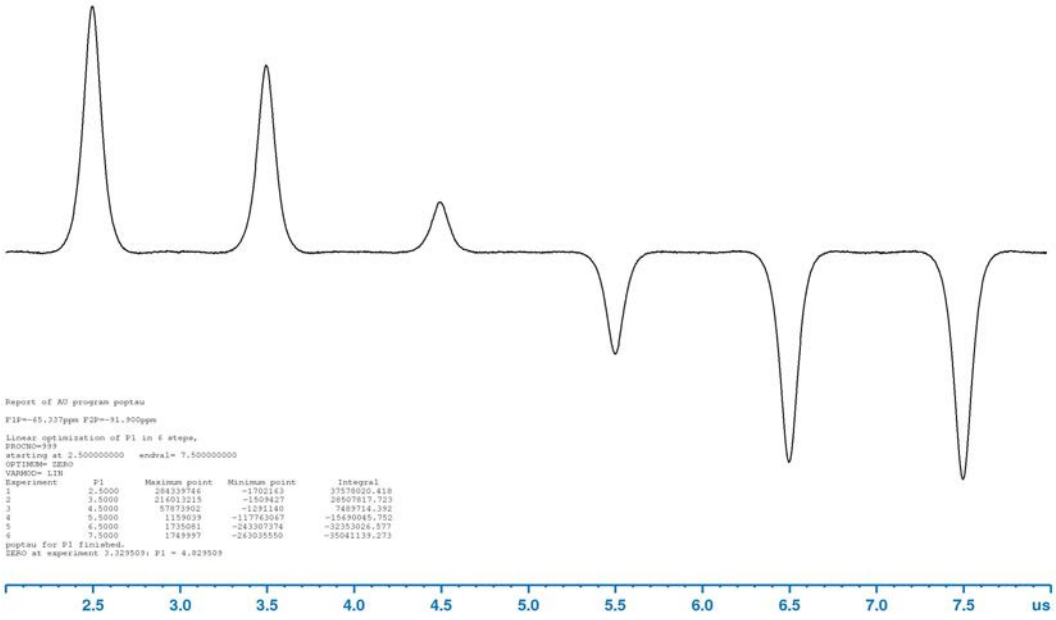
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.28 P90 19F pulse calibration on h-coil, MAS (NPT_19F_MAS_p90det_19f_hcoil)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P determination.
2 execute O1P determination.
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 16.000 | | no optim. |
| O1P | -74.000 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2988 | | |
| AQ | 0.015 | s | |
| FIDRES | 66.934 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 68.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Phase correction is done applying APK as default method. With the option L23 = 2 and 12 O1P determination step can be skipped to apply manually set values. The options L23 = 11 and 12 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n. The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

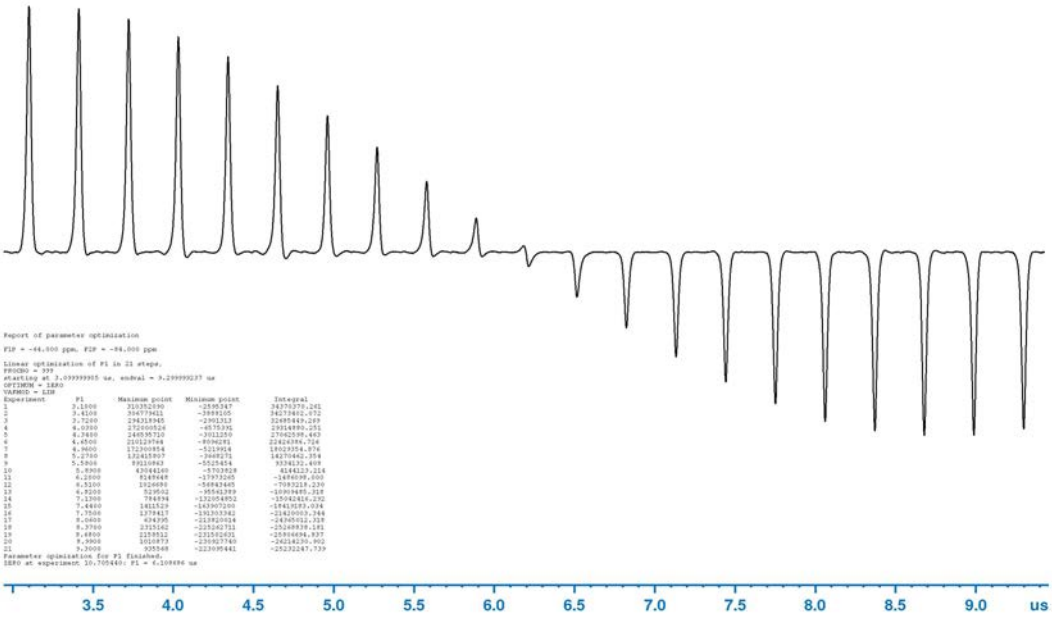
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.29 P90 19F shortest pulse calibration, MAS (NPT_19F_MAS_shortestPulse_19f)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows 21 experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P determination.
2 execute O1P determination.
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 16.000 | | no optim. |
| O1P | -74.000 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2988 | | |
| AQ | 0.015 | s | |
| FIDRES | 66.934 | Hz | |
| D 1 | 5.000 | s | |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Phase correction is done applying APK as default method. With the option L23 = 2 and 12 O1P determination step can be skipped to apply manually set values. The options L23 = 11 and 12 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n.
The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

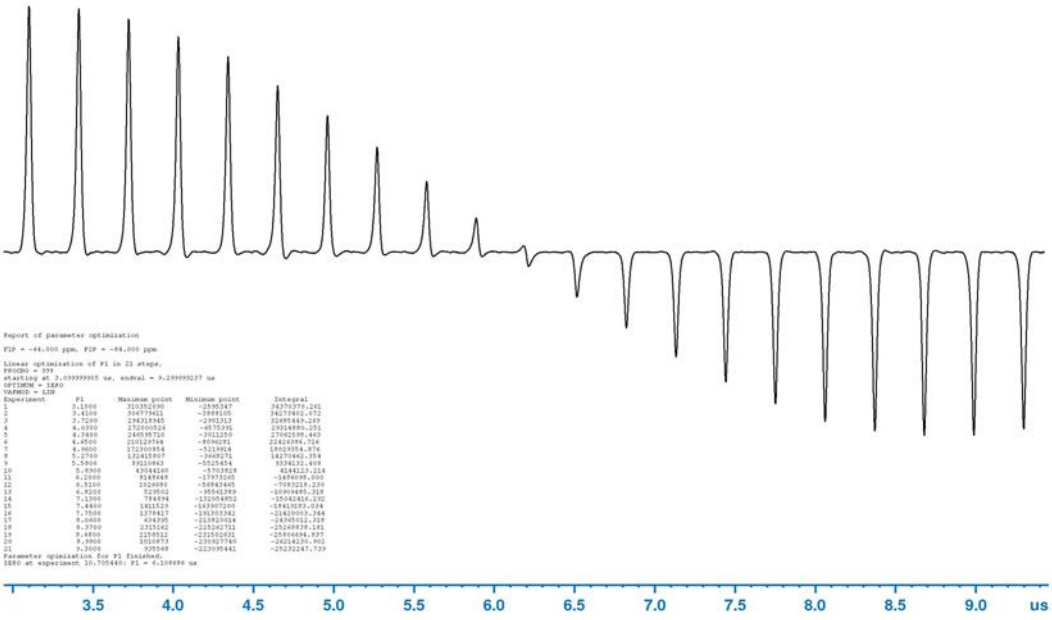
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.30 P90 19F shortest pulse calibration on h-coil, MAS (NPT_19F_MAS_shortestPulse_19f_hcoil)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows 21 experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P determination.
2 execute O1P determination.
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 16.000 | | no optim. |
| O1P | -74.000 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2988 | | |
| AQ | 0.015 | s | |
| FIDRES | 66.934 | Hz | |
| D 1 | 5.000 | s | |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Phase correction is done applying APK as default method. With the option L23 = 2 and 12 O1P determination step can be skipped to apply manually set values. The options L23 = 11 and 12 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n.
The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

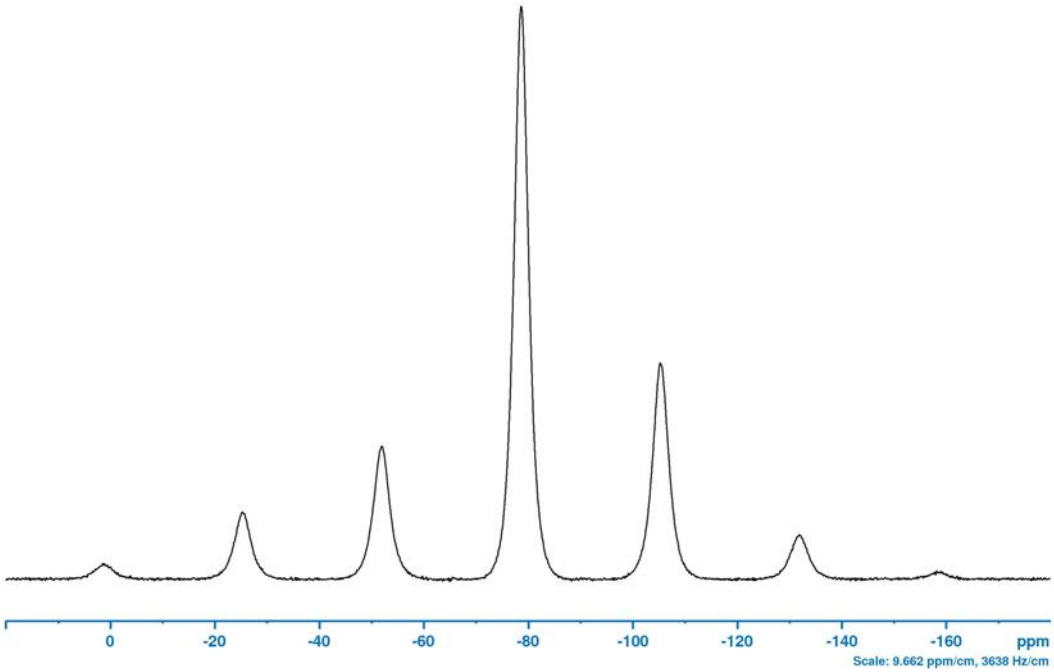
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.31 19F sensitivity, MAS (NPT_19F_MAS_sino_19f)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity and line width determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P determination.
2 execute O1P determination.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 16.000 | | no optim. |
| O1P | -74.000 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.010 | s | |
| FIDRES | 97.656 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 68.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.300 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 156.761 | ppm | |
| F2P | -140.761 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Sensitivity determination on solid probes including line width determination. Signal to noise value is calculated using noise range of 20 ppm set apart possible MAS spinning side bands. All ranges are provided in plot title.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. With the option L23 = 1 O1P determination step can be skipped to apply manually set value, i.e. value will be taken from data set.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

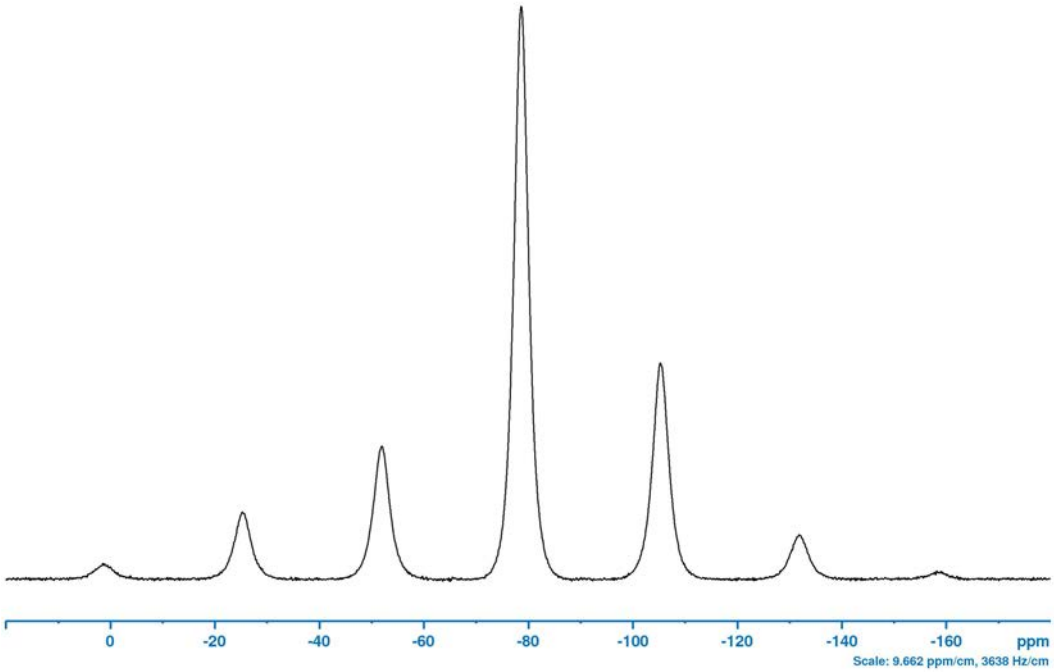
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.32 19F sensitivity on h-coil, MAS (NPT_19F_MAS_sino_19f_hcoil)

**Test Sample:** Ammonium Trifluoroacetate (CF3CO2NH4)
Z151226, Z151276, Z151266, Z151256, Z151236, Z151246, Z151216, Z163278
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity and line width determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P determination.
2 execute O1P determination.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 19F | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 16.000 | | no optim. |
| O1P | -74.000 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.010 | s | |
| FIDRES | 97.656 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 68.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.300 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 156.761 | ppm | |
| F2P | -140.761 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Sensitivity determination on solid probes including line width determination. Signal to noise value is calculated using noise range of 20 ppm set apart possible MAS spinning side bands. All ranges are provided in plot title.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. With the option L23 = 1 O1P determination step can be skipped to apply manually set value, i.e. value will be taken from data set.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

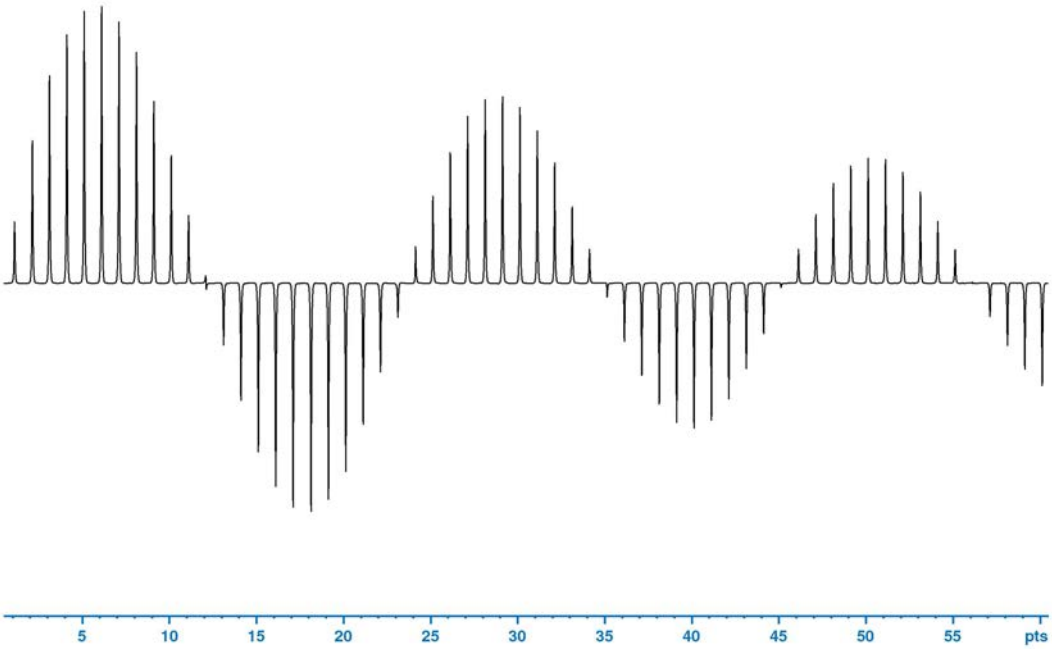
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 400 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 500 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 600 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 700 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 750 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 800 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 850 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 900 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 950 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |
| 1000 | 40000 | 24000 | 24000 | 24000 | 24000 | 15000 | 7000 |

## 5.4.33 1H B1 homogeneity, MAS (NPT_1H_MAS_b1homogeneity_1h)

**Test Sample:** Adamantane
Z151221, Z151271, Z151261, Z151251, Z151231, Z151241, Z151211, Z163274, Z183104
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

B1 homogeneity determination using a pseudo 2D method. Only a region around each main signal is shown in the figure.

**Control Option for Acquisition (L23)**

1 default, skip O1P determination.
2 execute O1P determination.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_p1b1hom2d_sol | | |
| NS | 1 | | |
| DS | 4 | | |
| RG | 8.000 | | no optim. |
| O1P | 2.460 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.010 | s | |
| FIDRES | 97.656 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 74.0 | W | Pow@90deg NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| CY | 11.000 | cm | |

## Experiment Description

The B1 homogeneity measurement is acquired by a series of 1D spectra whereby the excitation pulse is step-by-step incremented. The acquired range reaches from 15 to approx. 810 degrees. The B1-homogeneities based on integrals are computed from the magnitude of the second complex FID data point in PROCNO=2.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. With the option L23 = 1 O1P determination step can be skipped to apply manually set value, i.e. value will be taken from data set.
The result of CONVTO1D is stored in PROCNO=999. This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Requirements: The corresponding 90° pulse determination experiment (NPT_X_MAS_p90det_YZ) is mandatory for B1 homogeneity measurement.

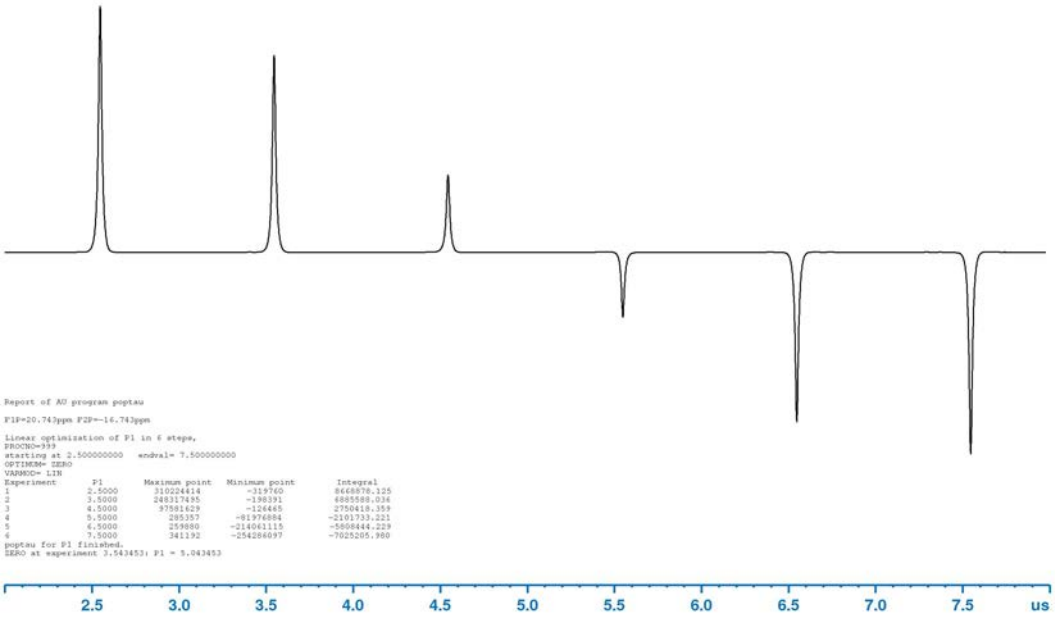
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

## 5.4.34 P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h)

**Test Sample:** Adamantane
Z151221, Z151271, Z151261, Z151251, Z151231, Z151241, Z151211, Z163274, Z183104
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P determination.
2 execute O1P determination.
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 8.000 | | no optim. |
| O1P | 2.460 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2988 | | |
| AQ | 0.015 | s | |
| FIDRES | 66.934 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 74.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Phase correction is done applying APK as default method. With the option L23 = 2 and 12 O1P determination step can be skipped to apply manually set values. The options L23 = 11 and 12 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n. The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

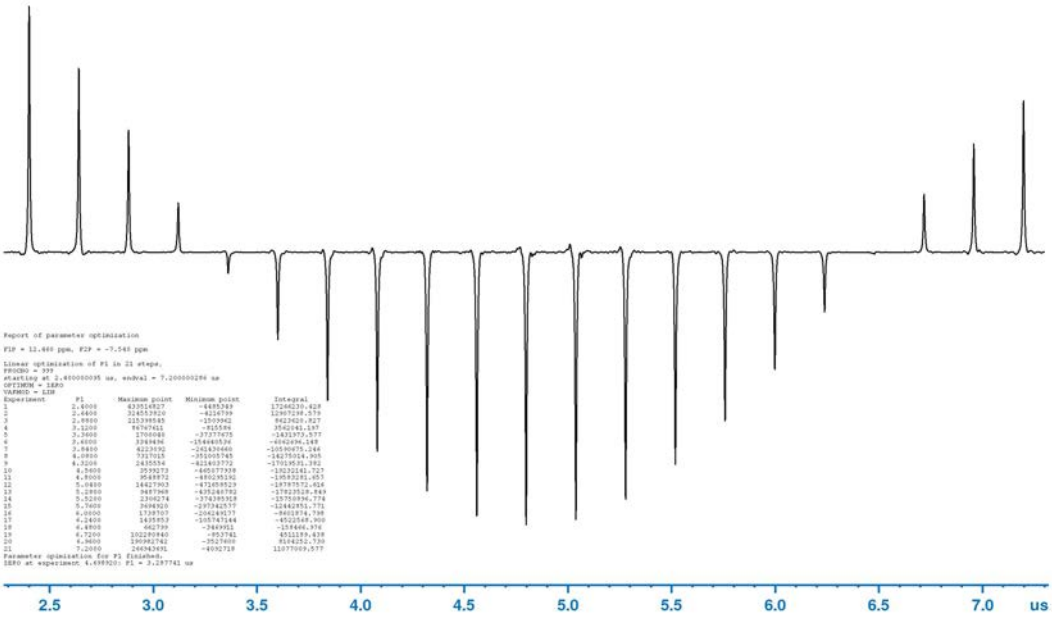
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

## 5.4.35 P90 1H shortest pulse calibration, MAS (NPT_1H_MAS_shortestPulse_1h)

**Test Sample:** Adamantane
Z151221, Z151271, Z151261, Z151251, Z151231, Z151241, Z151211, Z163274, Z183104
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows 21 experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P determination.
2 execute O1P determination.
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 8.000 | | no optim. |
| O1P | 2.460 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2988 | | |
| AQ | 0.015 | s | |
| FIDRES | 66.934 | Hz | |
| D 1 | 5.000 | s | |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Phase correction is done applying APK as default method. With the option L23 = 2 and 12 O1P determination step can be skipped to apply manually set values. The options L23 = 11 and 12 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n.
The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

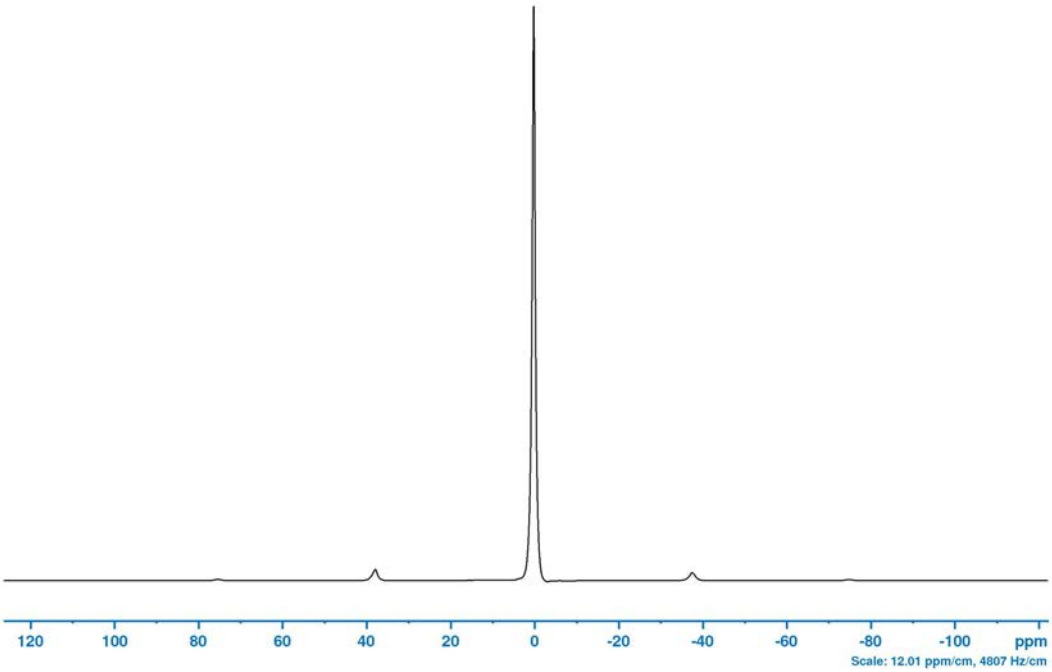
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

### 5.4.36 1H sensitivity, MAS (NPT_1H_MAS_sino_1h)

**Test Sample:** Adamantane
Z151221, Z151271, Z151261, Z151251, Z151231, Z151241, Z151211, Z163274, Z183104
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity and line width determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P determination.
2 execute O1P determination.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 8.000 | | no optim. |
| O1P | 2.460 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.010 | s | |
| FIDRES | 97.656 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 3.5 | us | 90deg NUC1 |
| PLW 1 | 74.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 156.761 | ppm | |
| F2P | -140.761 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Sensitivity determination on solid probes including line width determination. Signal to noise value is calculated using noise range of 20 ppm set apart possible MAS spinning side bands. All ranges are provided in plot title.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. With the option L23 = 1 O1P determination step can be skipped to apply manually set value, i.e. value will be taken from data set.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

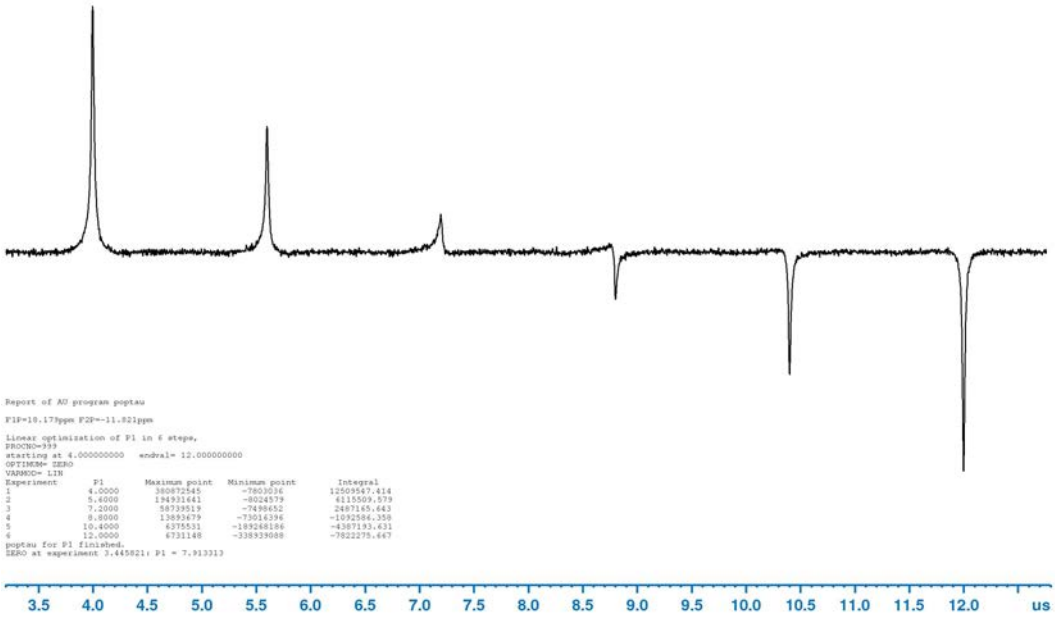
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

## 5.4.37 P90 31P pulse calibration, MAS (NPT_31P_MAS_p90det_31p)

**Test Sample:** Ammonium Dihydrogenphosphate (NH4H2PO4)
Z151224, Z151274, Z151264, Z151254, Z151234, Z151244, Z151214, Z163277
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | hpdec | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 2.000 | ppm | |
| O2P | 7.200 | ppm | |
| SWH | 40650.406 | Hz | |
| TD | 3256 | | |
| AQ | 0.040 | s | |
| FIDRES | 24.970 | Hz | |
| D 1 | 10.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| CPDPRG2 | spinal64 | | decoupl. sequence |
| PCPD2 | 8.3 | us | PCPD NUC2 |
| PLW 1 | 135 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 54.0 | W | |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| LB | 0.300 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
O2P is determined for decoupling by acquisition and processing of a spectrum of NUC 2 in a derived data set.
Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n. The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

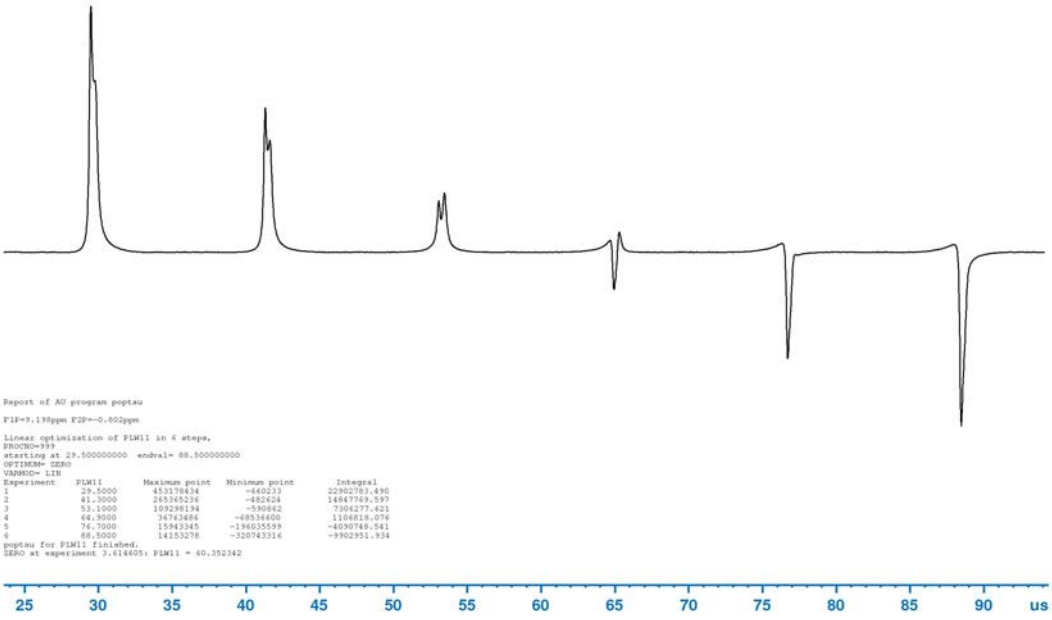
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 400 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 500 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 600 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 700 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 750 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 800 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 850 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 900 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 950 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 1000 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |

## 5.4.38 P90 31P 1H-31P CP pulse calibration, MAS (NPT_31P_MAS_p90det_cp1h_31p)

**Test Sample:** Ammonium Dihydrogenphosphate (NH4H2PO4)
Z151224, Z151274, Z151264, Z151254, Z151234, Z151244, Z151214, Z163277
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

P90 CP pulse determination using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows six experiments P1*0.5 to P1*1.5 (PROCNO 999).

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 2.000 | ppm | |
| O2P | 7.200 | ppm | |
| SWH | 48543.688 | Hz | |
| TD | 4854 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.002 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 3500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 135.0 | W | Pow@90deg NUC1 |
| PLW 11 | 135.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will be updated with the determined pulse and the power used.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

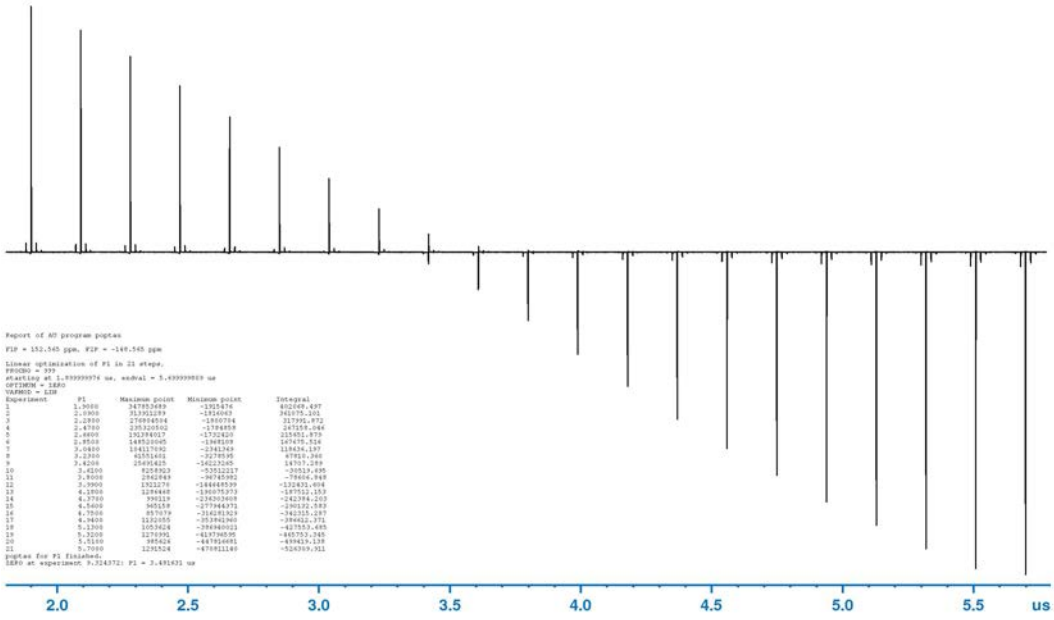
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 400 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 500 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 600 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 700 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 750 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 800 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 850 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 900 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 950 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 1000 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |

## 5.4.39 P90 31P 1H-31P CP shortest pulse calibration, MAS (NPT_31P_MAS_shortestPulse_cp1h_31p)

**Test Sample:** Ammonium Dihydrogenphosphate (NH4H2PO4)
Z151224, Z151274, Z151264, Z151254, Z151234, Z151244, Z151214, Z163277
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Shortest pulse determination with CP using 1D method by varying the excitation pulse P1. The result of a CONVTO1D routine shows 21 experiments P1*0.5 to P1*1.5(PROCNO 999).

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
13 skip automatic phase correction and apply manually set values, execute O2P determination.
14 skip automatic phase correction and apply manually set values, execute O1P and O2P determination.
15 Same as 14 but with RGA during O2P determination
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp90 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 2.000 | ppm | |
| O2P | 7.200 | ppm | |
| SWH | 48543.688 | Hz | |
| TD | 4854 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.002 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 3500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 135.0 | W | Pow@90deg NUC1 |
| PLW 11 | 135.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal (maximum intensity) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set. Phase correction is done applying APK as default method. With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set. The options L23 = 11, 12, 13, 14 and 15 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.
The results of the parameter optimization for PLW11 are stored under PROCNO 100.
Experiment results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
The PROSOL table will not be updated during this experiment.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

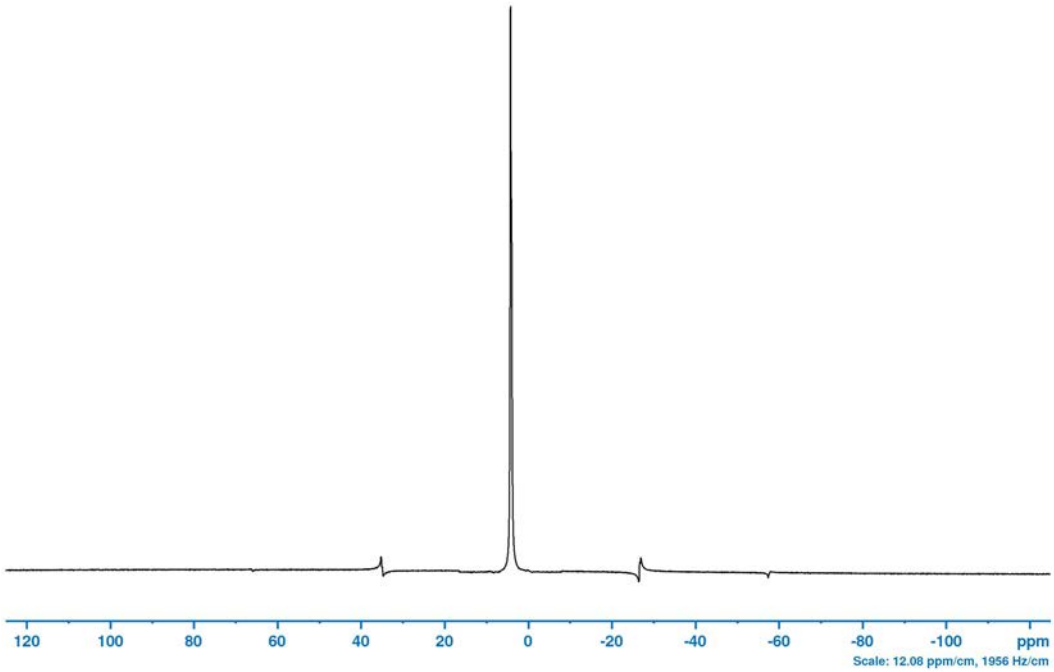
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 400 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 500 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 600 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 700 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 750 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 800 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 850 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 900 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 950 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 1000 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |

## 5.4.40 CP 1H-31P sensitivity, MAS (NPT_31P_MAS_sino_cp1h_31p)

**Test Sample:** Ammonium Dihydrogenphosphate (NH4H2PO4)
Z151224, Z151274, Z151264, Z151254, Z151234, Z151244, Z151214, Z163277
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Spectrum of sensitivity determination.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12
21 Same as 1 but with forced automatic optimization of SPW0 and PLW12
22 Same as 2 but with forced automatic optimization of SPW0 and PLW12
23 Same as 3 but with forced automatic optimization of SPW0 and PLW12
24 Same as 4 but with forced automatic optimization of SPW0 and PLW12
25 Same as 5 but with forced automatic optimization of SPW0 and PLW12

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | cp | | |
| NS | 4 | | set according specs |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 2.000 | ppm | |
| O2P | 7.200 | ppm | |
| SW | 299.697 | ppm | |
| TD | 4854 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.002 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 3500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 135.0 | W | Pow@90deg NUC1 |
| PLW 11 | 135.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

### Experiment Description

Sensitivity determination on solid probes including steps for optimization of PLW12 and SPW0. Signal to noise value is calculated using noise range of 20 ppm. All ranges are provided in plot title.
If number of scans is specified, NS will be set accordingly during acquisition.
L23 dependent offset optimization: Prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, and 3 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 = 1, 2, 3, 4, and 5 the values of SPW0 and PLW12 will be taken from an allready acquired sino experiment.
For L23 = 11, 12, 13, 14 and 15 or if the sino experiment has not been measured a manual user interaction part to set or optimize SPW0, and PLW12 is included.
For L23 = 21, 22, 23, 24 and 25 the optimization of SPW0 and PLW12 will be enforced.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.

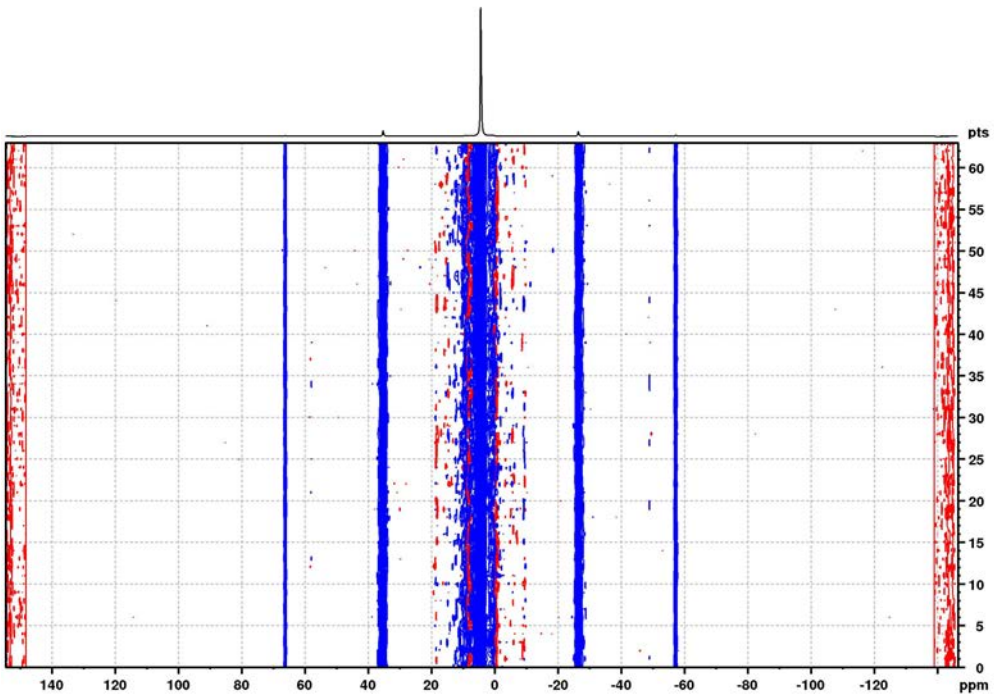
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 400 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 500 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 600 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 700 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 750 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 800 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 850 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 900 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 950 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 1000 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |

## 5.4.41 CP 1H-31P power stability MAS (NPT_31P_MAS_stab_cp1h_31p)

**Test Sample:** Ammonium Dihydrogenphosphate (NH4H2PO4)
Z151224, Z151274, Z151264, Z151254, Z151234, Z151244, Z151214, Z163277
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Pseudo 2D CP spectrum to observe power stability.

**Control Option for Acquisition (L23)**

1 default, skip O1P and O2P determination.
2 execute O1P determination.
3 execute O2P determination.
4 execute O1P and O2P determination.
5 Same as 4 but with RGA during O2P determination
11 Same as 1 but with manual user interaction to set SPW0 and PLW12
12 Same as 2 but with manual user interaction to set SPW0 and PLW12
13 Same as 3 but with manual user interaction to set SPW0 and PLW12
14 Same as 4 but with manual user interaction to set SPW0 and PLW12
15 Same as 5 but with manual user interaction to set SPW0 and PLW12

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PARMODE | 1 | | Data Dimension |
| PULPROG | npt_cp2d | | |
| NS | 1 | | |
| DS | 32 | | |
| RG | 101.000 | | no optim. |
| O1P | 2.000 | ppm | |
| O2P | 7.200 | ppm | |
| SWH | 48543.688 | Hz | |
| TD | 4854 | | |
| AQ | 0.050 | s | |
| FIDRES | 20.002 | Hz | |
| D 1 | 5.000 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| P 3 | 3.5 | us | max. dec. field |
| P 15 | 3500.0 | us | HH NUC2-NUC1 |
| PCPD 2 | 6.8 | us | PCPD2 NUC2 |
| PLW 1 | 135.0 | W | Pow@90deg NUC1 |
| PLW 11 | 135.0 | W | Pow@90degCP(Specs) NUC1 |
| PLW 12 | 54.0 | W | Pow@90deg NUC2 |
| SPW 0 | 54.0 | W | Pow@HHshaped NUC2 |
| TE | 298.000 | K | default |
| SPNAM 0 | ramp50100.100 | | |
| CPDPRG 2 | spinal64 | | |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |

## Experiment Description

Determination of power stability for CP experiments on solid probes using maximum decoupling field and maximum acquisition time provided as mandatory specifications. The average signal-to-noise ratio (10 ppm noise range)
is evaluated considering all rows of the pseudo-2D measurement. Also the maximum deviation of the results is determined, along with the rows of maximum and minimum result.
For power stability measurement the specs for acquisition time and decoupling pulse length must be specified.
L23 dependent offset optimization: prior to the main acquisition O1P (PROCNO=10) will be optimized. O2P is determined by acquisition and processing of a spectrum of NUC 2 in a derived data set.
With the option L23 = 1, 2, 3, 11, 12, and 13 O1P and O2P determination steps can be skipped to apply manually set values, i.e. values will be taken from data set.
For L23 < 10 the values of SPW0 and PLW12 will be taken from the corresponding sino experiment. PLW12 will be optimized if the specified PCPD2 pulse differs from PCPD2 used in the corresponding sino experiment.
For L23 > 10 or if the corresponding sino experiment has not been measured a manual user interaction part to set or optimize SPW0 and PLW12 is included.
SPW0 is calculated for B1(NUC2) = (B1(NUC1) + MASR) * rampFactor.
If the resulting power SPW0 exceeds the power limits of the probe, SPW0 will be recalculated for side band condition -1.
The selection of a certain side band condition can be forced by setting CNST 50 to 1 or -1.

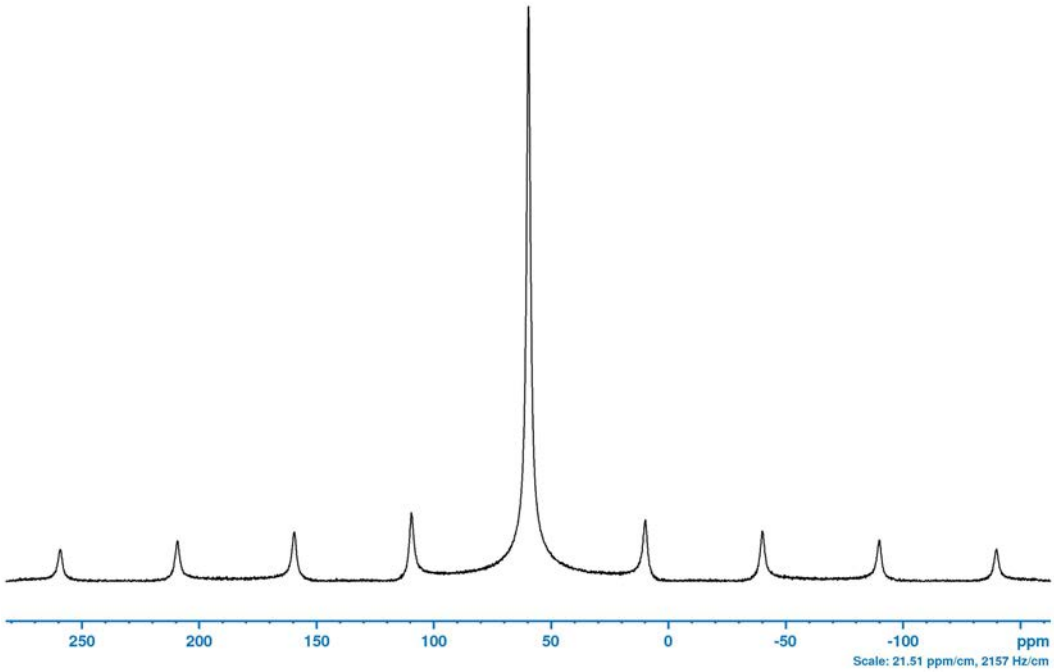
**Spinrate**

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 400 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 500 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 600 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 700 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 750 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 800 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 850 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 900 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 950 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |
| 1000 | 40000 | 15000 | 15000 | 10000 | 10000 | 5000 | 4000 |

## 5.4.42 Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting)

**Test Sample:** Potassium Bromide (KBr)
Z151220, Z151270, Z151260, Z151250, Z151230, Z151240, Z151210, Z163271, Z183103
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**
79Br spectrum after field optimization

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 44247.789 | Hz | |
| TD | 4096 | | |
| AQ | 0.046 | s | |
| FIDRES | 21.605 | Hz | |
| D 1 | 0.500 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| PLW 1 | 72.0 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| WDW | 0 | | |
| PH_mod | 2 | | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

The experimental procedure includes two 79Br acquisitions with constant 01 at two known FIELD positions. Using 59.7 ppm as chemical shift of 79Br in KBr the correct FIELD value can be calculated from these measurements. The determined field is only an approximation due to the temperature dependence of the chemical shift of 79Br in KBr.
Before acquisition of the final nmr spectrum NMRPT stores the resulting FIELD value in the BSMS.

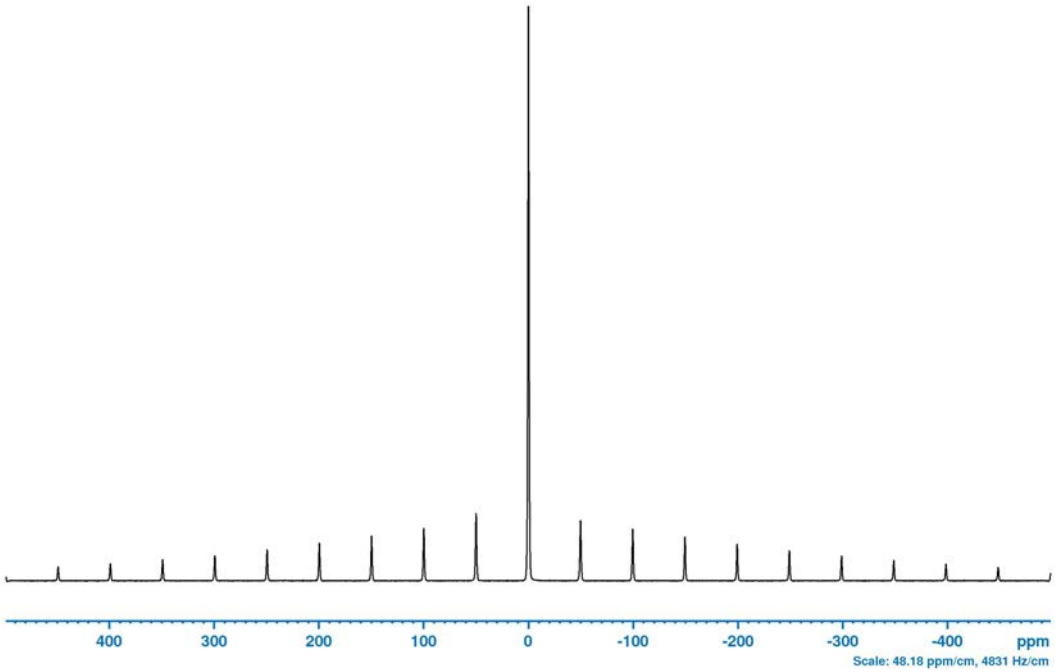
## Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 400 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 700 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 750 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 800 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 850 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 900 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 950 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 1000 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |

### 5.4.43 Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle)

**Test Sample:** Potassium Bromide (KBr)
Z151220, Z151270, Z151260, Z151250, Z151230, Z151240, Z151210, Z163271, Z183103
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

79Br spectrum of KBr with spinning side bands - documentation of magic angle adjustment.

**Control Option for Acquisition (L23)**

1 default
2 manual adjustment of magic angle for probes with stator controlled by ATM

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PULPROG | onepulse | | |
| NS | 16 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 8192 | | |
| AQ | 0.041 | s | |
| FIDRES | 24.414 | Hz | |
| D 1 | 0.250 | s | |
| P 1 | 4.0 | us | 90deg Pulse |
| PLW 1 | 126.0 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 10.000 | cm | |

### Experiment Description

The experiment proves the accuracy of the magic angle which is to be optimized within first step. The line width of the main signal is calculated. Further spinning side bands to be analyzed may be specified by their side band number. A spectrum is plotted for documentation.

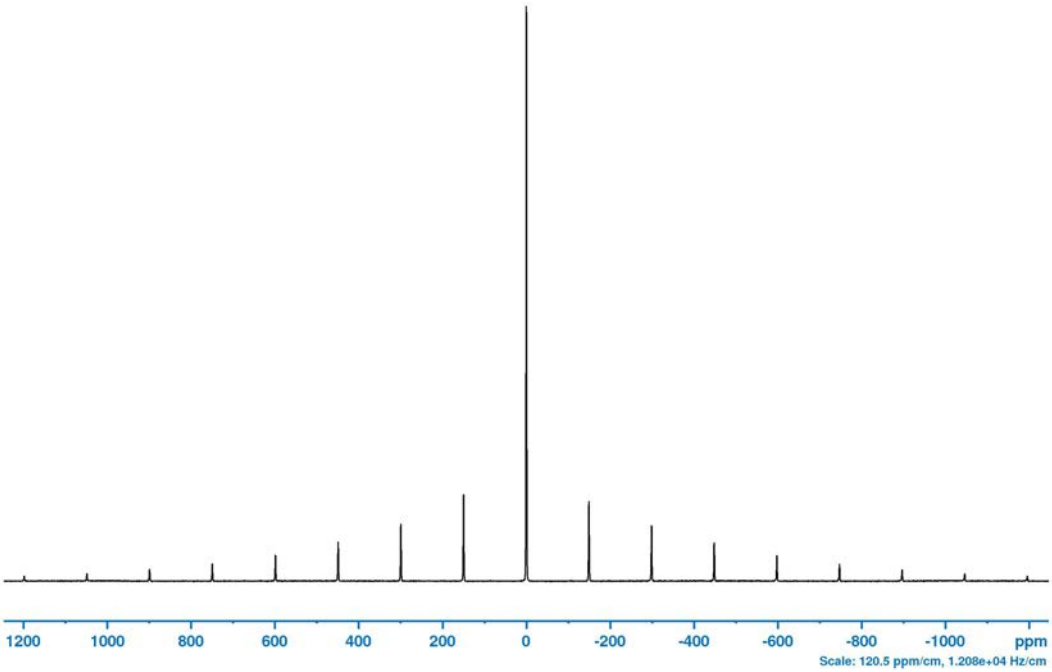
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 400 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 700 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 750 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 800 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 850 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 900 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 950 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 1000 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |

### 5.4.44 Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate)

**Test Sample:** Potassium Bromide (KBr)
Z151220, Z151270, Z151260, Z151250, Z151230, Z151240, Z151210, Z163271, Z183103
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

79Br spectrum of KBr with spinning side bands for documentation of maximum rotation frequency

**Control Option for Acquisition (L23)**

1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PULPROG | onepulse | | |
| NS | 16 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 250000.000 | Hz | |
| TD | 16384 | | |
| AQ | 0.033 | s | |
| FIDRES | 30.518 | Hz | |
| D 1 | 0.250 | s | |
| P 1 | 4.0 | us | 90deg Pulse |
| PLW 1 | 126.0 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 10.000 | cm | |

### Experiment Description

The experiment proves that maximum rotation frequency (default or as specified) can be reached. If the maximum rotation frequency is stable, maximum deviation during a period of about 3 minutes is evaluated and a spectrum is acquired. A spectrum showing the rotation side bands is plotted for documentation.

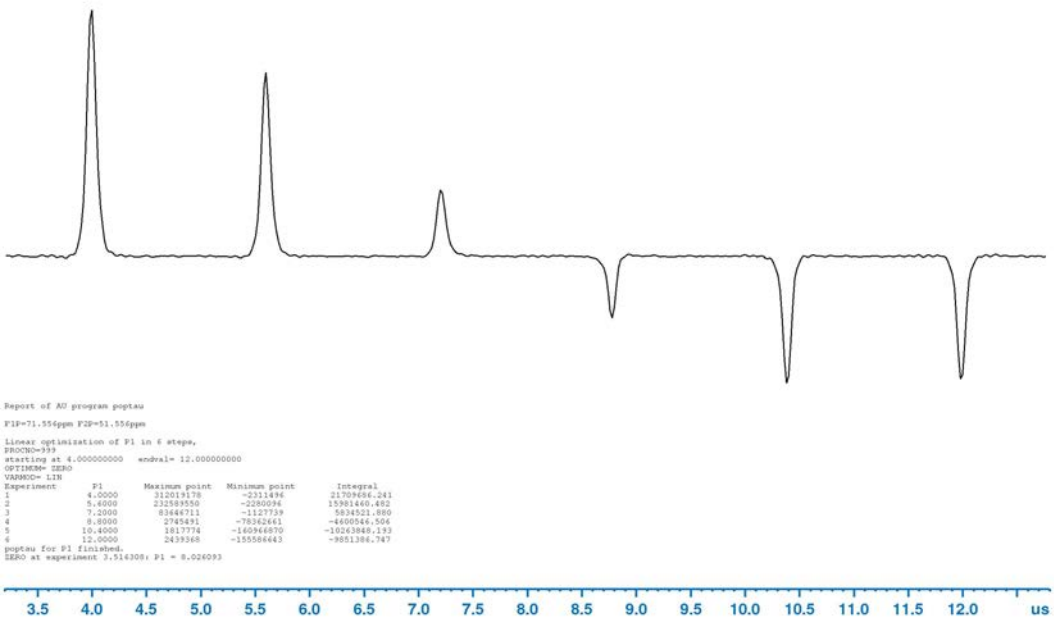
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 400 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 500 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 600 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 700 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 750 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 800 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 850 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 900 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 950 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |
| 1000 | 111000 | 67000 | 42000 | 35000 | 24000 | 15000 | 7000 |

## 5.4.45 P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br)

**Test Sample:** Potassium Bromide (KBr)
Z151220, Z151270, Z151260, Z151250, Z151230, Z151240, Z151210, Z163271, Z183103
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P determination.
2 execute O1P determination.
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | onepulse | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.010 | s | |
| FIDRES | 97.656 | Hz | |
| D 1 | 0.250 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| PLW 1 | 106 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Phase correction is done applying APK as default method. With the option L23 = 2 and 12 O1P determination step can be skipped to apply manually set values. The options L23 = 11 and 12 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n. The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.

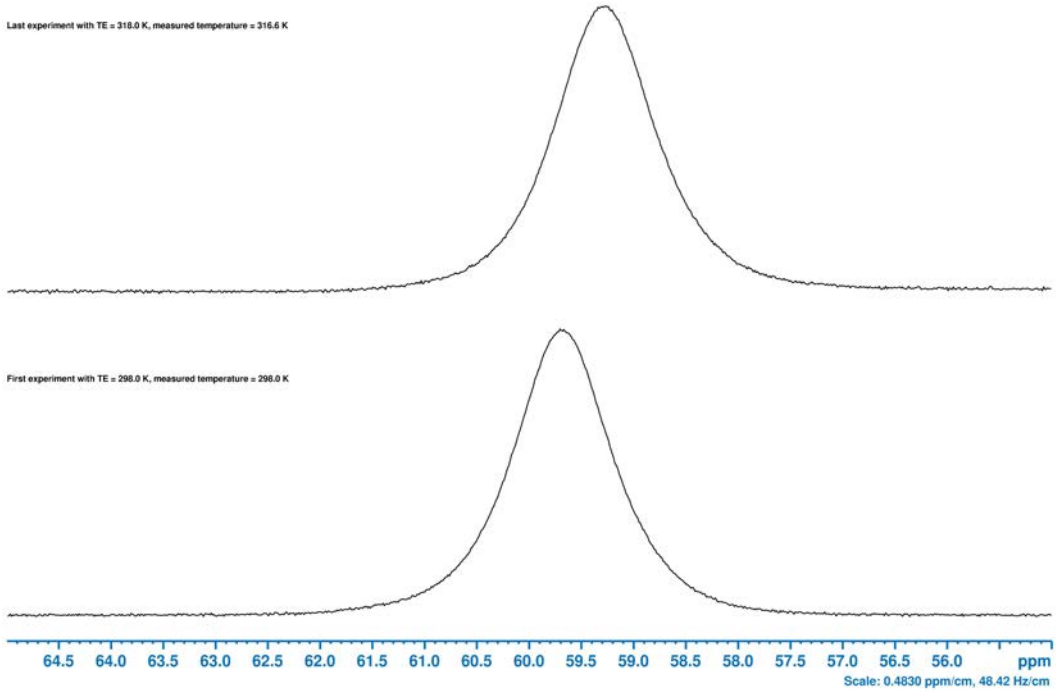
### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 400 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 700 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 750 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 800 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 850 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 900 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 950 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 1000 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |

## 5.4.46 Temperature controll test on KBr, MAS (NPT_79Br_MAS_temperatureTestKBr)

**Test Sample:** Potassium Bromide (KBr)
Z151220, Z151270, Z151260, Z151250, Z151230, Z151240, Z151210, Z163271, Z183103
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

Top: 79Br spectrum of KBr with spinning side bands at lowest measured temperature.
Bottom: 79Br spectrum of KBr with spinning side bands at highest measured temperature.

### Control Option for Acquisition (L23)

1 default
2 ignore specifications and take parameters from D 60, CNST 50, 51, and 52 instead
11 activation of newly determined temperature correction in the BSVT
12 ignore specification and activation of newly determined temperature correction in the BSVT

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PULPROG | onepulse | | |
| NS | 8 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 5000.000 | Hz | |
| TD | 4096 | | |
| AQ | 0.410 | s | |
| FIDRES | 2.441 | Hz | |
| D 1 | 0.250 | s | |
| D 60 | 180.000 | s | teready waiting time |
| P 1 | 4.0 | us | 90deg Pulse |
| PLW 1 | 126.0 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| PH_mod | 1 | | pk |
| F1P | 65.000 | ppm | |
| F2P | 55.000 | ppm | |
| CY | 10.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 1.000 | K | min TE for calibr. |
| CNST 51 | 1.000 | K | max TE for calibr. |
| CNST 52 | 1.000 | | no. points TE calibr. |

### Experiment Description

Temperature test expects a temperature unit. The procedure is acquiring at least two experiments with different TE settings according to the specifications or for L23==2 entries in the parameter set (CNST 50 to 53).
The result of the experiment is the determination of the offset and slope of the correction curve (y=ax+b). The correction will not be set in the temperature unit.
Due to the fact that only the chemical shift is used for temperature determination, the true temperature can not be determined with this experiment. Hence, this is no temperature calibration experiment.
Temperature correction will not be disabled during the experiments. If L23==1 or L23==2 the original values will be retained in the BSVT at the end of the test. If L23==11 odr L23==12 the newly determined correction values will be activated in the BSVT.
If L23==2 or L23==12 the specifications for highest and lowest TE and number of points are ignored and will be taken from the following constants:
CNST 50: lowest TE used for calibration.
CNST 51: highest TE used for calibration.
CNST 52: number of points (TE settings) used for calibration.
If no specifications are given and L23==1 the following default values will be used:
Three experiments with 298, 308, and 318 K are acquired.

### Spinrate

MASR [Hz] as function of sample diamter and spectrometer frequency

| | 0.7 | 1.3 | 1.9 | 2.5 | 3.2 | 4.0 | 7.0 |
|---|---|---|---|---|---|---|---|
| 300 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 400 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 500 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 600 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 700 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 750 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 800 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 850 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 900 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 950 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |
| 1000 | 40000 | 8000 | 5000 | 5000 | 5000 | 5000 | 5000 |

## 5.5 Experiments for High Resolution Magic Angle Spinning Probes (HRMAS)

### Sample Rotation Frequency

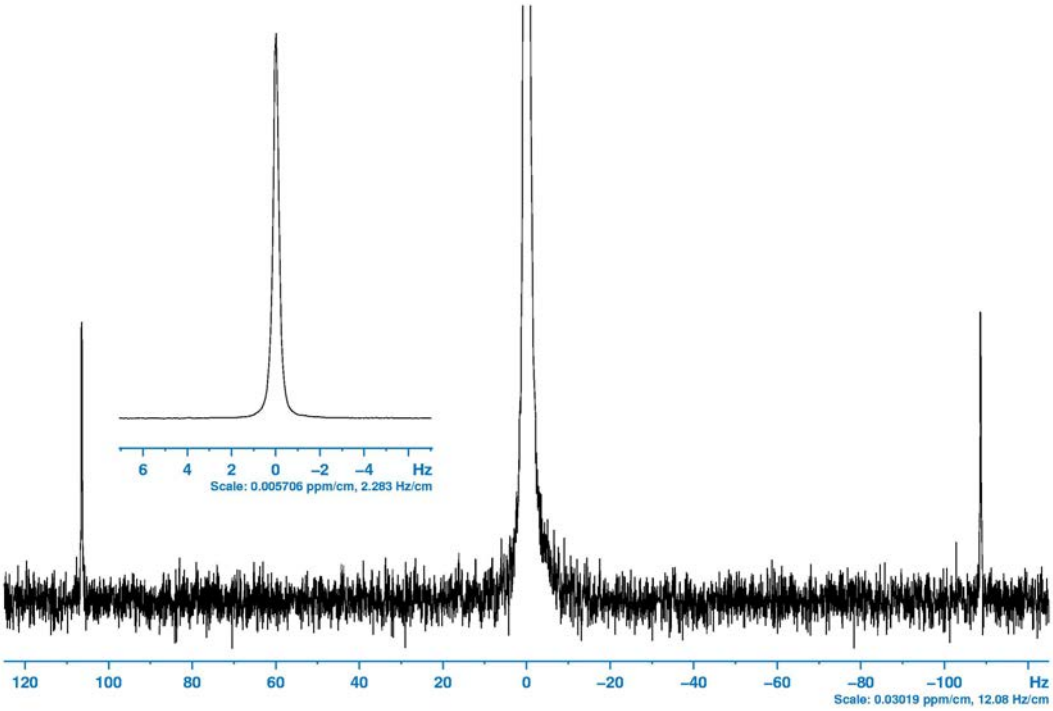
The parameter MASR is set to 4 kHz by *NMRPT*. The parmater RO is set to zero, commands ROTON and ROTOFF are ignored.

The experiments described in this section as well as the follwing HR experiments are provided for HRMAS probes:

NPT_13C_sensitivity
NPT_13C_sensitivity_inno
NPT_15N_fullsw_inept
NPT_15N_sensitivity_dec1h
NPT_15N_sensitivity_inept
NPT_1H_b1homogeneityInt_13c
NPT_1H_b1homogeneityInt_15n
NPT_1H_b1homogeneityInt_1h
NPT_1H_backgr_withsample
NPT_1H_cpmgtestf2_13c
NPT_1H_cpmgtestf2_15n
NPT_1H_gradientprofile_neg
NPT_1H_gradientprofile_pos
NPT_1H_gradrec_stest_1h
NPT_1H_gradrecZ_sqn_1h
NPT_1H_gradrecZ_sqp_1h
NPT_1H_inno
NPT_1H_inno
NPT_1H_p90determinationf1_1h
NPT_1H_p90determinationf2_13c
NPT_1H_p90determinationf2_15n
NPT_1H_quant_ref
NPT_1H_sensitivity
NPT_1H_sensitivity_dec19f
NPT_1H_sensitivity_inno
NPT_1H_vibration_doped_water
NPT_1H_vibration_lineshape
NPT_19F_b1homogeneityInt_19f
NPT_19F_backgr_withsample
NPT_19F_fullsw_dec1h
NPT_19F_p90determinationf1_19f
NPT_19F_sensitivity
NPT_19F_sensitivity_inno
NPT_19F_sensitivity_lb05_dec1h
NPT_31P_b1homogeneityInt_31p
NPT_31P_p90determinationf1_31p
NPT_31P_sensitivity
NPT_31P_sensitivity_dec1h
NPT_31P_sensitivity_inno
NPT_prep_atma_test
NPT_prep_fieldsetting_d
NPT_prep_locksettings_d
NPT_prep_b1homogeneityInt_d
NPT_prep_p90det_d
NPT_prep_sensitivity_10_d
NPT_29Si_p90determination_29si
NPT_29Si_sensitivity

### 5.5.1 1H lineshape with magic angle spinning (NPT_1H_HRMAS_lineshape)

**Test Sample:** 1.0% Chloroform in Acetone-D6
Z142220
**Solvent:** Acetone
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Magic Angle Spinning




**Example Printout**

Proton line shape spectrum with offset calibration to O1P as overview spectrum. Printing is from +125.0 Hz to -125.0 Hz. The expansion plot to the left shows chloroform signal with higher resolution (+7.0 Hz, -7.0 Hz).

**Control Option for Acquisition (L23)**

1 default
2 write default shimfile, in case of successful evaluation

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg30 | | |
| NS | 4 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 7.700 | ppm | |
| SWH | 1000.000 | Hz | |
| TD | 32768 | | |
| AQ | 16.384 | s | |
| FIDRES | 0.061 | Hz | |
| D 1 | 9.116 | s | AQ+D1=const |
| P 1 | 4.5 | us | 90deg Pulse |
| PLW 1 | 16.6 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

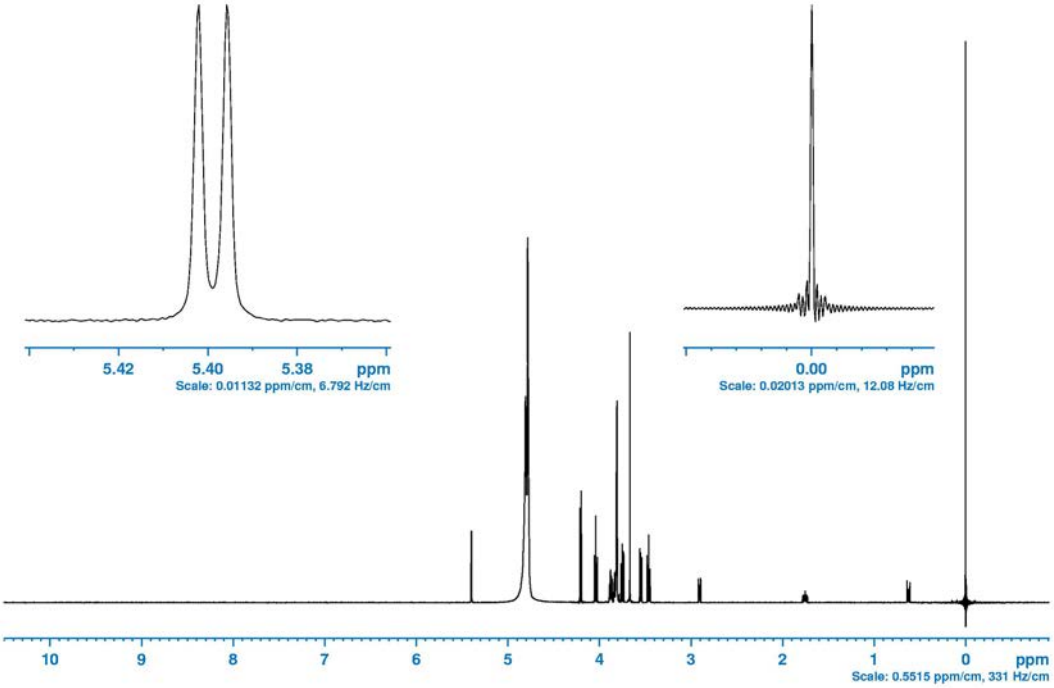
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 8.640 | ppm | |
| F2P | 7.440 | ppm | |
| CY | 1000.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 0.200 | | Scaling factor for CY |

## Experiment Description

Before acquiring the final spectrum, the exact signal position is determined with NS=1. The carrier position is afterwards set to the position
optimized O1 = peak frequency [Hz] - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.
Setting L23=2, it is possible to store the standard shimfile provided the evaluation of the experiment is successful. This event takes place during acquisition only. During regular processing of the data no shimfile is stored.

## 5.5.2 Watersuppression (NPT_1H_HRMAS_watersuppression)

**Test Sample:** 2 mM Sucrose, 0.5 mM DSS, and 2 mM NaN3 in 90% H2O + 10% D2O Z142222
**Solvent:** H2O+D2O
**Lock parameter:** AUTOGAIN, lock regulation according to actual Edlock Table
**Sample State:** Magic Angle Spinning




**Example Printout**

Water suppression spectrum printed from 10.5 ppm to -1.0 ppm as overview spectrum. The expansion plot to the right shows the DSS (sodium 2,2-dimethyl-2-silapentane-5-sulphonate) signal, indicative for the quality of the spectral resolution. The quality of the water suppression is determined as linewidth of the residual water signal using the 10% and 50% intensity of the DSS signal.
The expansion plot to the left shows the signal of the anomeric proton (alpha-C1) of the sucrose (2-beta-D-fructofuranosyl-1-alpha- D-glucopyranosid). The anomeric proton intensity is used for the signal-to-noise calculation and the splitting of the signal is analysed to give a measure for spectral resolution.

**Control Option for Acquisition (L23)**

1 with O1 optimization, with PULPROG=zgpr
20 O1 from parameter set, no optimization, with PULPROG=zgpr
23 O1 from parameter set, no optimization, with PULPROG=npt_zggppr
25 O1 from parameter set, no optimization, with PULPROG=zgcppr
27 O1 from parameter set, no optimization, with PULPROG=zgcpgppr
30 O1 from previous watersuppression, no optimization[*], with PULPROG=zgpr
33 O1 from previous watersuppression, no optimization[*], with PULPROG=npt_zggppr
35 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcppr
37 O1 from previous watersuppression, no optimization[*], with PULPROG=zgcpgppr
[*] The optimization of O1 is enforced, if O1 was not determined during a previous measurement.

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zgpr | | |
| NS | 8 | | |
| DS | 4 | | |
| RG | 0.250 | | optim. by NMRPT |
| O1P | 4.699 | ppm | |
| SW | 12.132 | ppm | |
| TD | 10194 | | field dependent |
| AQ | 1.050 | s | |
| FIDRES | 0.952 | Hz | field dependent |
| D 1 | 5.000 | s | |
| P 1 | 14.0 | us | 90deg |
| PLW 1 | 7.5 | W | Pow@90deg(Specs) |
| PLW 9 | 0.00006 | W | Pow@90deg(5000u) |
| TE | 298.000 | K | default |

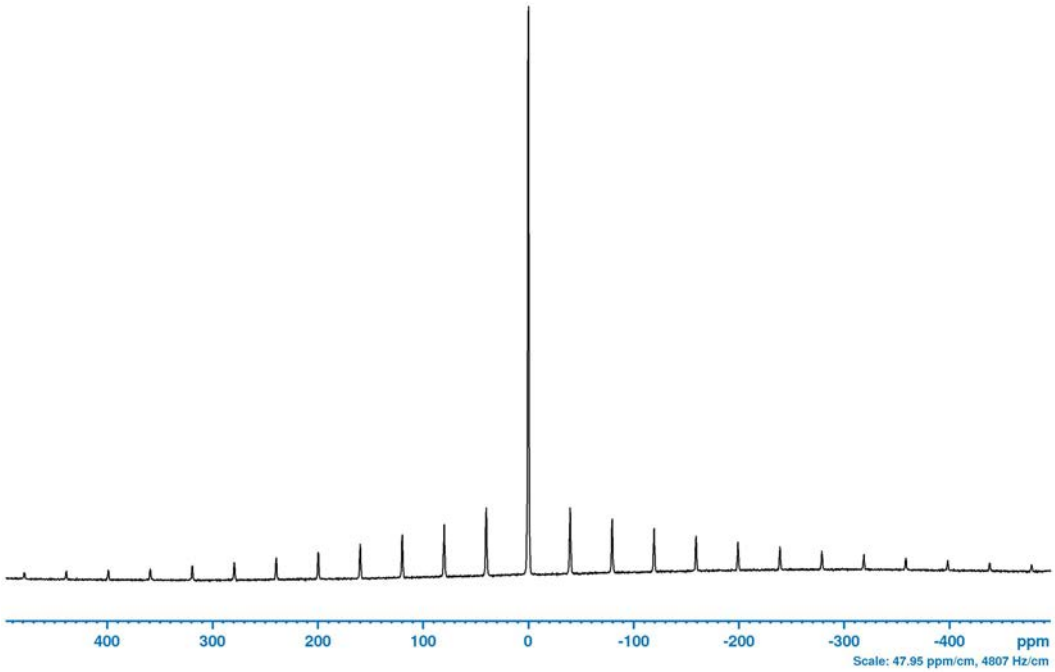
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.000 | Hz | |
| PC | 0.100 | | |
| F1P | 10.806 | ppm | |
| F2P | -1.227 | ppm | |
| CY | 111.000 | cm | |

## Experiment Description

For the watersuppression experiment the carrier offset O1 needs to be very carefully adjusted. Using the control option for acquisition L23=1, O1 is determined by an intensity profile(second point of FID) over a range of 16 Hz in 0.4 Hz steps around submitted O1.
RG adjustment is executed by running experiments with DS=0, NS=4 and a reduced PLW1. The highest RG without signal overflow in these experiments will be used.
Options L23=1 and 20 are standard whereas Options L23=23, 25, and 27 are non-standard and will not be considered as regular test from the 'NMRPT Control Structure'. Their existence is purely diagnostic.
Experiment will be set to irregular if option 'Skip Temperature' is selected.

### 5.5.3 Magic Angle setting, HRMAS (NPT_79Br_HRMAS_magicAngle)

**Test Sample:** Potassium Bromide (KBr)
Z151220
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

79Br spectrum of KBr with spinning side bands - documentation of magic angle adjustment.

**Control Option for Acquisition (L23)**

1 default
2 manual adjustment of magic angle for probes with stator controlled by ATM

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PULPROG | zg | | |
| NS | 16 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 8192 | | |
| AQ | 0.041 | s | |
| FIDRES | 24.414 | Hz | |
| D 1 | 0.250 | s | |
| P 1 | 4.0 | us | 90deg Pulse |
| PLW 1 | 126.0 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

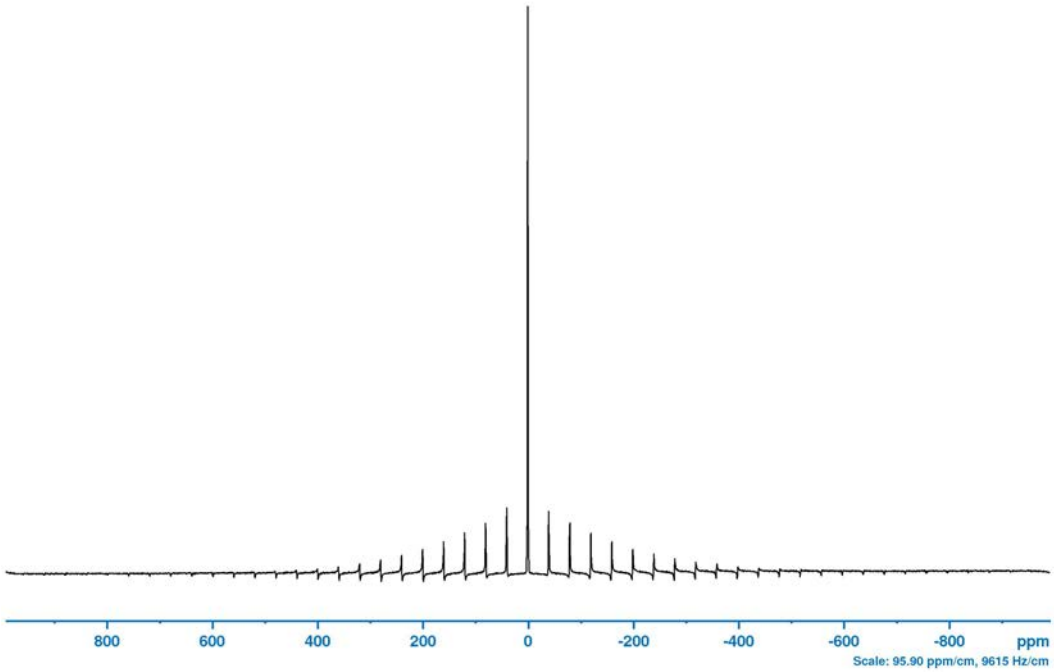
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 131072 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 10.000 | cm | |

### Experiment Description

The experiment proves the accuracy of the magic angle which is to be optimized within first step. The line width of the main signal is calculated. Further spinning side bands to be analyzed may be specified by their side band number. A spectrum is plotted for documentation.
LOCNUC is set to off as a default.

### 5.5.4 Maximum spin rate testing, HRMAS (NPT_79Br_HRMAS_maxSpinRate)

**Test Sample:** Potassium Bromide (KBr) Z151220
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

79Br spectrum of KBr with spinning side bands for documentation of maximum rotation frequency

**Control Option for Acquisition (L23)**

1 default

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PULPROG | zg | | |
| NS | 16 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 200000.000 | Hz | |
| TD | 8192 | | |
| AQ | 0.020 | s | |
| FIDRES | 48.828 | Hz | |
| D 1 | 0.250 | s | |
| P 1 | 4.0 | us | 90deg Pulse |
| PLW 1 | 126.0 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

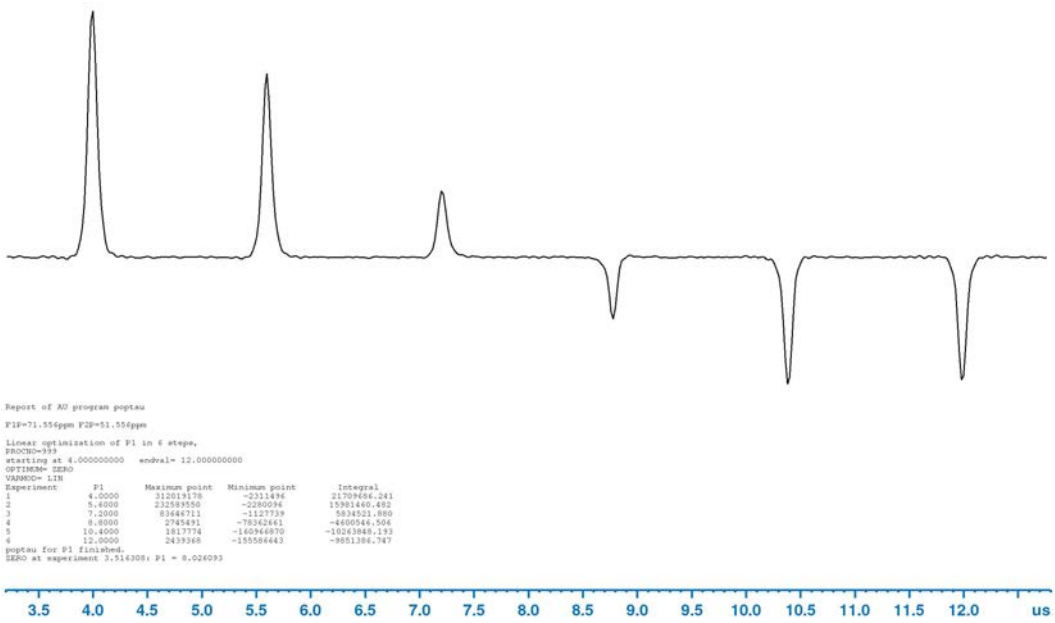
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 0.000 | ppm | |
| F2P | 0.000 | ppm | |
| CY | 10.000 | cm | |

### Experiment Description

The experiment proves that maximum rotation frequency (default or as specified) can be reached. If the maximum rotation frequency is stable, maximum deviation during a period of about 3 minutes is evaluated and a spectrum is acquired. A spectrum showing the rotation side bands is plotted for documentation. LOCNUC is set to off as a default.

## 5.5.5 P90 79Br pulse calibration, HRMAS (NPT_79Br_HRMAS_p90det_79br)

**Test Sample:** Potassium Bromide (KBr)
Z151220
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 999).

### Control Option for Acquisition (L23)

1 default, skip O1P determination.
2 execute O1P determination.
11 skip automatic phase correction and apply manually set values, skip O1P and O2P determination.
12 skip automatic phase correction and apply manually set values, execute O1P determination.
100 same as xx but skip of SINO check on PROCNO 11
+xx
1000 same as xxx but ignore specifications (optimize power for pulse length from prosol)
+xxx

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 100000.000 | Hz | |
| TD | 2048 | | |
| AQ | 0.010 | s | |
| FIDRES | 97.656 | Hz | |
| D 1 | 0.250 | s | |
| P 1 | 4.0 | us | 90deg NUC1 |
| PLW 1 | 106 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

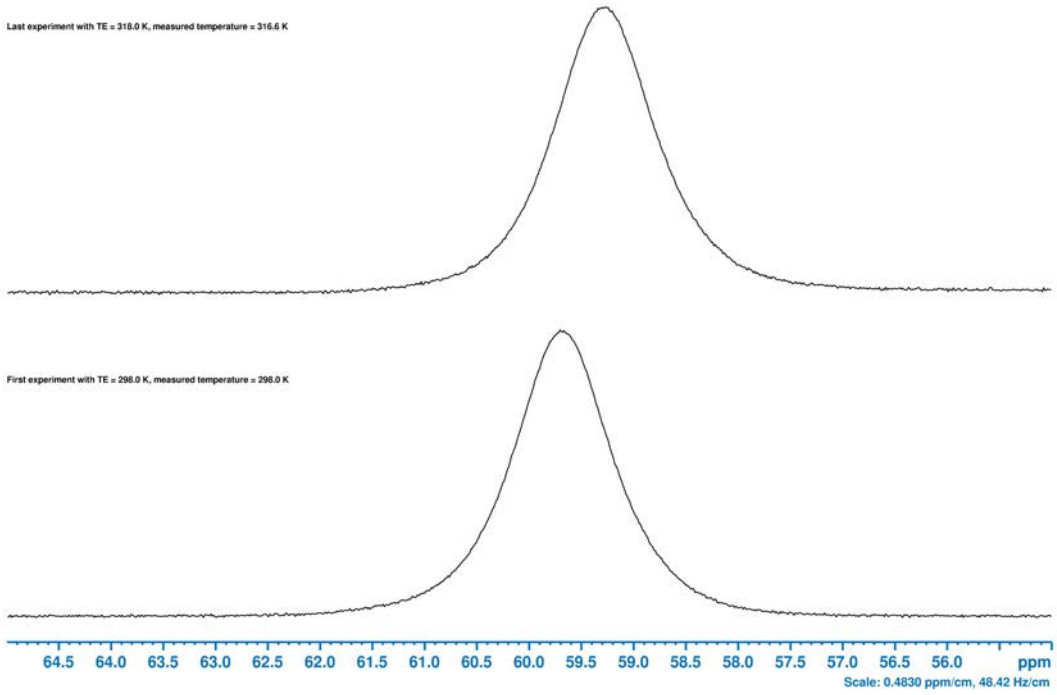
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| LB | 0.000 | Hz | |
| PH_mod | 1 | | pk |

### Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
L23 dependent offset optimization: the exact signal offset (O1P) of the main signal is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
Phase correction is done applying APK as default method. With the option L23 = 2 and 12 O1P determination step can be skipped to apply manually set values. The options L23 = 11 and 12 skip automatic phase correction for manual settings to be applied.
After phase correction the resulting spectrum is stored in PROCNO 12, the FID is discarded. SINO will be executed on PROCNO 11. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped using the corrsponding L23 options.
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [90%, 100%], it calculates a new power value based on the specified pulse length and repeats the measurement with the new power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n. The PROSOL table will be updated updated with the determined pulse and the power used. Results are stored under PROCNO 999.
This experiment includes a manual user interaction part, e.g. to manual match/tune or prepare acquisition as required.
Phase correction is applied during acquisition and will not take any effect if experiment is reprocessed.
LOCNUC is set to off as a default.

## 5.5.6 Temperature controll test on KBr, HRMAS (NPT_79Br_HRMAS_temperatureTestKBr)

**Test Sample:** Potassium Bromide (KBr)
Z151220
**Solvent:** None
**Lock parameter:** None
**Sample State:** Magic Angle Spinning




**Example Printout**

Top: 79Br spectrum of KBr with spinning side bands at lowest measured temperature.
Bottom: 79Br spectrum of KBr with spinning side bands at highest measured temperature.

**Control Option for Acquisition (L23)**

1 default
2 ignore specifications and take parameters from D 60, CNST 50, 51, and 52 instead
11 activation of newly determined temperature correction in the BSVT
12 ignore specification and activation of newly determined temperature correction in the BSVT

### Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 79Br | | |
| PULPROG | zg | | |
| NS | 8 | | |
| DS | 0 | | |
| RG | 101.000 | | no optim. |
| O1P | 59.700 | ppm | |
| SWH | 5000.000 | Hz | |
| TD | 4096 | | |
| AQ | 0.410 | s | |
| FIDRES | 2.441 | Hz | |
| D 1 | 0.250 | s | |
| D 60 | 180.000 | s | teready waiting time |
| P 1 | 4.0 | us | 90deg Pulse |
| PLW 1 | 126.0 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 4096 | | |
| PH_mod | 1 | | pk |
| F1P | 65.000 | ppm | |
| F2P | 55.000 | ppm | |
| CY | 10.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 1.000 | K | min TE for calibr. |
| CNST 51 | 1.000 | K | max TE for calibr. |
| CNST 52 | 1.000 | | no. points TE calibr. |

### Experiment Description

Temperature test expects a temperature unit. The procedure is acquiring at least two experiments with different TE settings according to the specifications or for L23==2 entries in the parameter set (CNST 50 to 53).
The result of the experiment is the determination of the offset and slope of the correction curve (y=ax+b). The correction will not be set in the temperature unit.
Due to the fact that only the chemical shift is used for temperature determination, the true temperature can not be determined with this experiment. Hence, this is no temperature calibration experiment.
Temperature correction will not be disabled during the experiments. If L23==1 or L23==2 the original values will be retained in the BSVT at the end of the test. If L23==11 odr L23==12 the newly determined correction values will be activated in the BSVT.
If L23==2 or L23==12 the specifications for highest and lowest TE and number of points are ignored and will be taken from the following constants:
CNST 50: lowest TE used for calibration.
CNST 51: highest TE used for calibration.
CNST 52: number of points (TE settings) used for calibration.
If no specifications are given and L23==1 the following default values will be used:
Three experiments with 298, 308, and 318 K are acquired.
LOCNUC is set to off as a default.

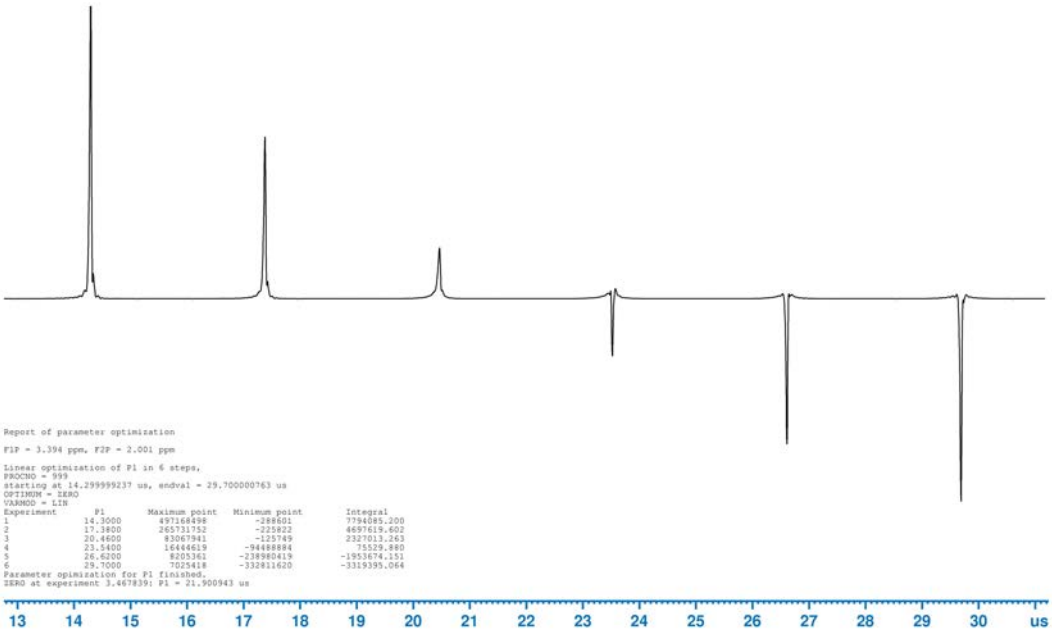
## 5.6 Experiments for Fourier Spectrometer (CMR)

As a prerequisit for NMRPT the system must be shimmed and the probe must be locked with the external lock. Experiments are acquired without sample rotation.

Experiments for Fourier Spectrometer are only implemented for TopSpin 4.1.0 and higher.

## 5.6.1 P90 1H pulse calibration (NPT_1H_CMR_p90determination_1h)

**Test Sample:** 1 M Methanol-13C in D2O
Z10692
**Solvent:** D2O
**Lock parameter:** External Lock
**Sample State:** Rotation off




**Example Printout**

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 100).

**Control Option for Acquisition (L23)**

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 3.416 | ppm | |
| SWH | 230.766 | Hz | |
| AQ | 0.650 | s | |
| FIDRES | 1.538 | Hz | |
| D 1 | 15.318 | s | AQ+D1=const |
| P 1 | 11.0 | us | 90deg NUC1 |
| PLW 1 | 1.1 | W | Pow@90deg(Specs) NUC1 |
| TE | 298.000 | K | default |

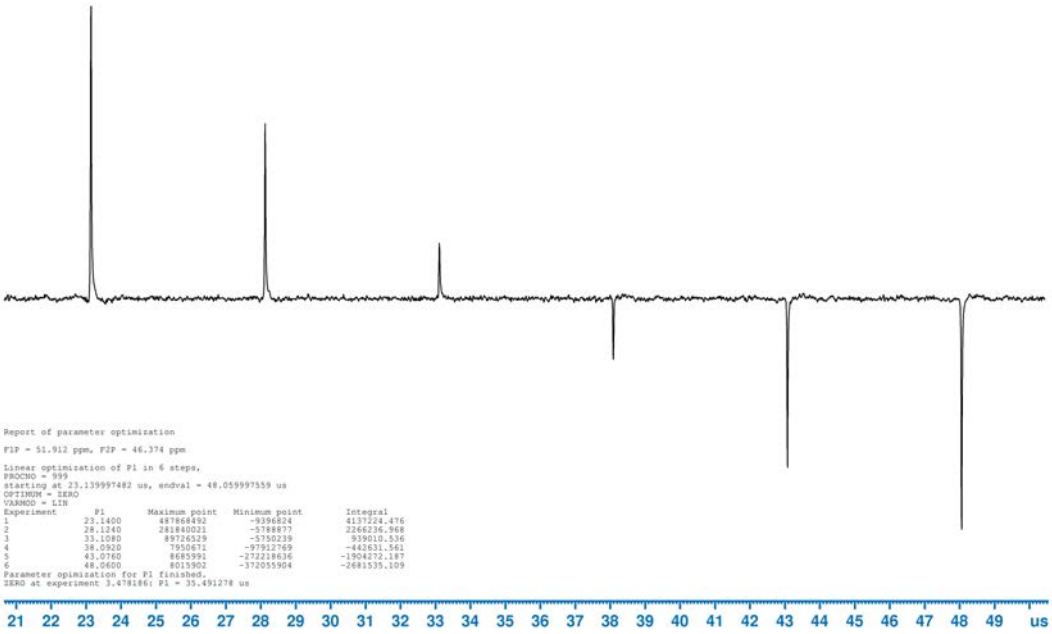
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 2048 | | |
| WDW | 3 | | |
| LB | 0.750 | Hz | |
| SSB | 2.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 2 | | LPfc |
| NCOEF | 20 | | |
| ABSF1 | 1000.000 | ppm | |
| ABSF2 | -1000.000 | ppm | |
| F1P | 5.496 | ppm | |
| F2P | 5.096 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).

## 5.6.2 P90 13C pulse calibration (NPT_13C_CMR_p90determination_13c)

**Test Sample:** 1 M Methanol-13C in D2O
Z10692
**Solvent:** D2O
**Lock parameter:** External Lock
**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 100).

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zgpg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 49.435 | ppm | |
| O2P | 3.590 | ppm | |
| SWH | 8196.722 | Hz | |
| AQ | 0.500 | s | |
| FIDRES | 2.001 | Hz | |
| D 1 | 29.500 | s | AQ+D1=const |
| P 1 | 17.2 | us | 90deg NUC1 |
| PCPD 2 | 120.0 | W | PCPD NUC2 |
| PLW 1 | 4.8 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.018 | W | Pow@CPD NUC2 |
| PLW 13 | 0.009 | W | Pow@CPD NOE NUC2 |
| TE | 298.000 | K | default |

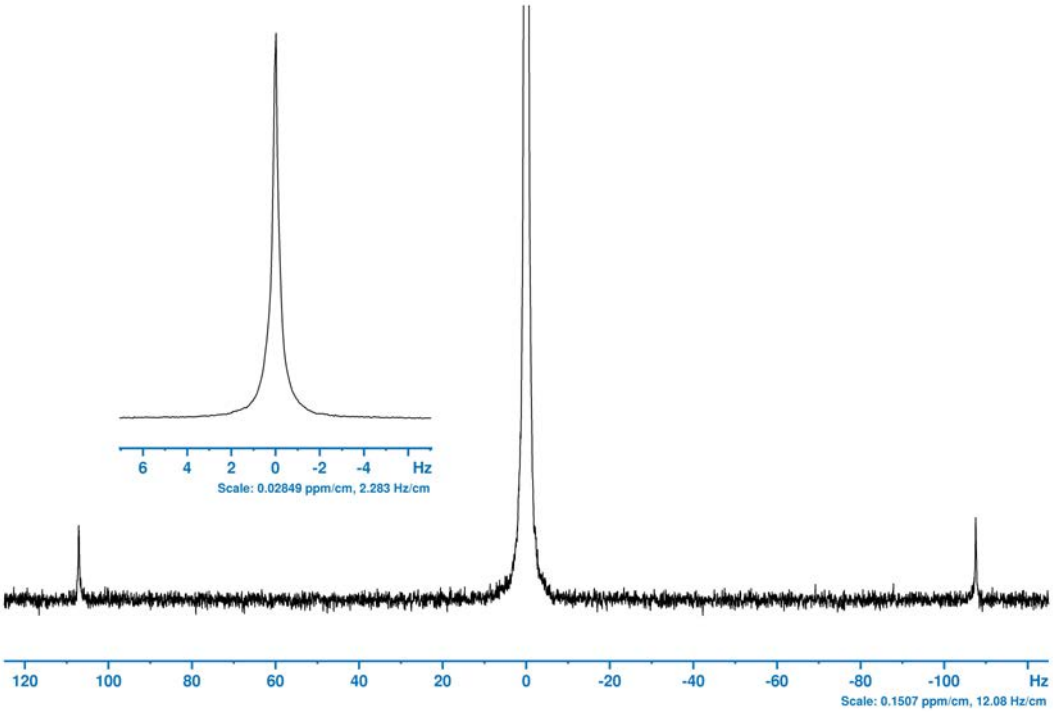
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 8192 | | |
| WDW | 1 | | |
| LB | 0.300 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| NCOEF | 0 | | |
| ABSF1 | 240.000 | ppm | |
| ABSF2 | -10.000 | ppm | |
| F1P | 180.000 | ppm | |
| F2P | -20.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).

### 5.6.3 1H lineshape (NPT_1H_CMR_lineshape)

**Test Sample:** 20% Chloroform in Acetone-D6
Z10689
**Solvent:** Acetone
**Lock parameter:** External Lock
**Sample State:** Rotation off




**Example Printout**

Proton line shape spectrum with offset calibration to O1P as overview spectrum. Printing is from +125.0 Hz to -125.0 Hz. The expansion plot to the left shows chloroform signal with higher resolution (+7.0 Hz, -7.0 Hz).

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg30 | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 7.410 | ppm | |
| SWH | 1000.000 | Hz | |
| TD | 32768 | | |
| AQ | 16.384 | s | |
| FIDRES | 0.061 | Hz | |
| D 1 | 9.116 | s | AQ+D1=const |
| P 1 | 11.0 | us | 90deg Pulse |
| PLW 1 | 1.1 | W | Pow@90deg(Specs) |

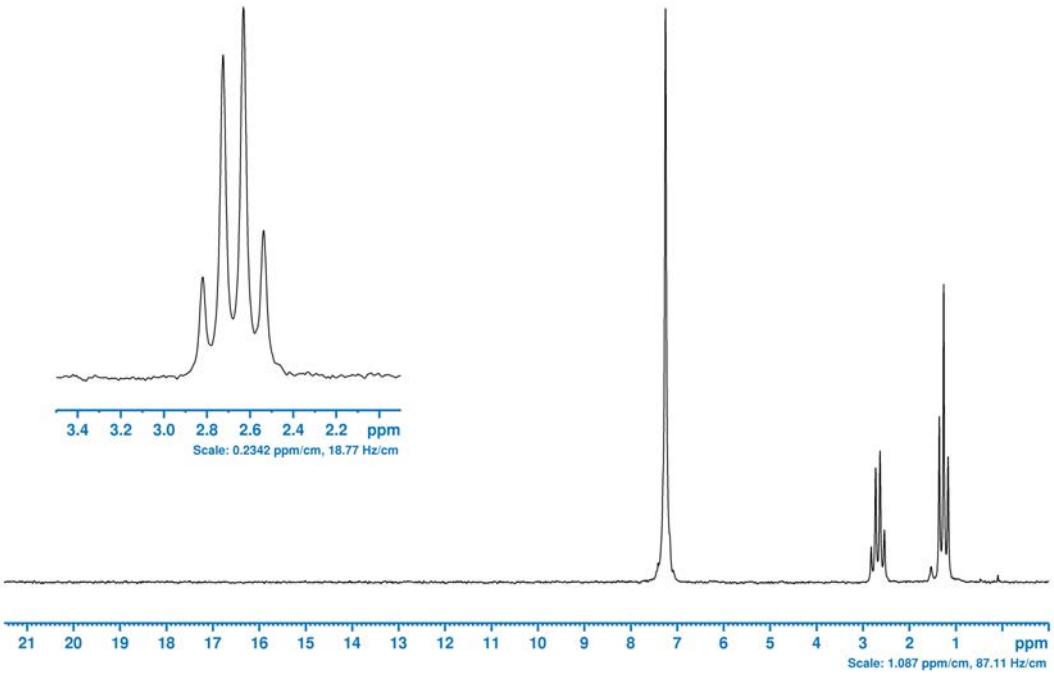
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| WDW | 0 | | |
| LB | 0.000 | Hz | |
| PC | 1.000 | | |
| F1P | 8.640 | ppm | |
| F2P | 7.440 | ppm | |
| CY | 1000.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 0.200 | | Scaling factor for CY |

## Experiment Description

Before acquiring the final spectrum, the exact signal position is determined with NS=1. The carrier position is afterwards set to the position
optimized O1 = peak frequency [Hz] - (SWH/4)
This procedure allows the application of a strip transformation with the parameters STSR=0, STSI=SI/2 resulting in the signal position on-resonance and in most cases resulting in an optimal automatic phase correction.

## 5.6.4 1H sensitivity (NPT_1H_CMR_sensitivity)

**Test Sample:** 1% Ethylbenzene (EB) in Chloroform-D Z10690
**Solvent:** CDCl3
**Lock parameter:** External Lock
**Sample State:** Rotation off




**Example Printout**

Bottom: 1H overview spectrum of ethylbenzene.
Top right: Expanded region showing the methylene signal used for evaluation.

**Control Option for Acquisition (L23)**

1 default

## Parameters

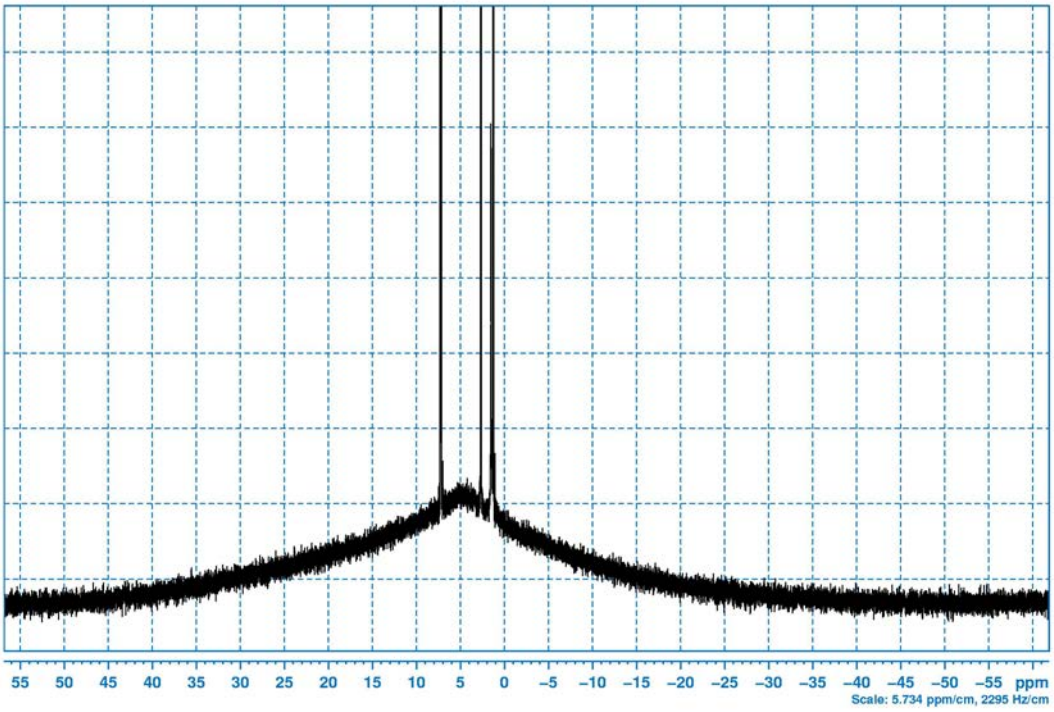
| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 1H | | |
| PULPROG | zg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 4.000 | ppm | |
| SW | 36.753 | ppm | |
| TD | 16384 | | |
| AQ | 0.557 | s | field dependent |
| FIDRES | 1.795 | Hz | field dependent |
| D 1 | 113.574 | s | |
| P 1 | 11.0 | us | 90deg Pulse |
| PLW 1 | 1.1 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 16384 | | |
| LB | 1.000 | Hz | 1.0 |
| SIGF1 | 3.500 | ppm | |
| SIGF2 | 1.900 | ppm | |
| NOISF1 | 20.000 | ppm | |
| NOISF2 | 8.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

## 5.6.5 1H background with sample (NPT_1H_CMR_background)

**Test Sample:** 1% Ethylbenzene (EB) in Chloroform-D Z10690
**Solvent:** CDCl3
**Lock parameter:** External Lock
**Sample State:** Rotation off




**Example Printout**

Top: 1H Background signal spectrum with sample. Sharp signal arises from sample, broad signal could arise from solid compound in the probe.
Bottom: Same spectrum scaled to see baseline distortions

**Control Option for Acquisition (L23)**

1 default

### Parameters

| | | | |
|---|---|---|---|
| **F1 ACQU** | | | Parameters |
| NUC1 | 1H | | |
| PULPROG | npt_zg0 | | |
| NS | 32 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 4.000 | ppm | |
| SWH | 7812.500 | Hz | |
| TD | 16384 | | |
| AQ | 1.049 | s | |
| FIDRES | 0.954 | Hz | |
| D 1 | 3.116 | s | AQ+D1=const |
| P 0 | 5.5 | us | P 1 * CNST 10 / 90 |
| P 1 | 11.0 | us | 90deg Pulse |
| PLW 1 | 1.1 | W | Pow@90deg(Specs) |
| TE | 298.000 | K | default |

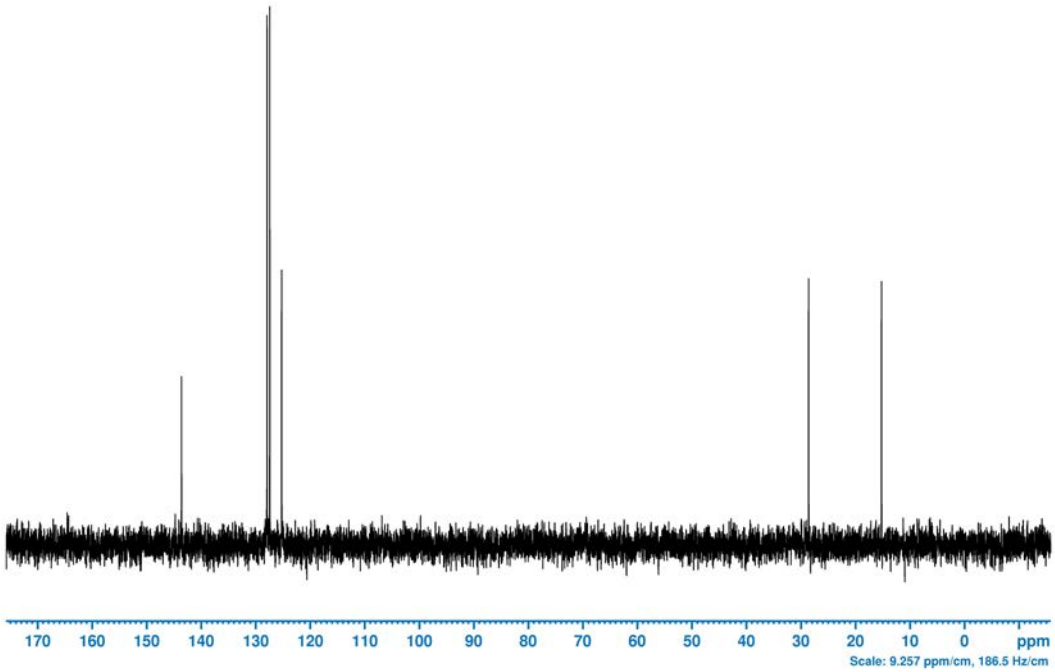
| | | | |
|---|---|---|---|
| CNST 10 | 45.000 | | Flip angle for P90 |
| **F1 PROC** | | | Parameters |
| SI | 16384 | | |
| WDW | 1 | | |
| LB | 1.000 | Hz | |
| CY | 11.000 | cm | |
| **NMRPT** | | | Parameters |
| CNST 50 | 10.000 | | Scaling factor for CY |

### Experiment Description

Background signal measurements are executed using a small flip angle to compensate for usually long T1 relaxation time of solid signals.
Full spectrum is normally printed without any baseline correction.

## 5.6.6 13C sensitivity with 1H decoupling (NPT_13C_CMR_sensitivity_dec1h)

**Test Sample:** 100% Ethylbenzene (EB)
Z10694
**Solvent:** None
**Lock parameter:** External Lock
**Sample State:** Rotation off




**Example Printout**
Carbon-13 sensitivity test with 1H decoupling.

**Control Option for Acquisition (L23)**
1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 13C | | |
| PULPROG | zgpg | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 80.000 | ppm | |
| O2P | 19.970 | ppm | |
| SW | 198.766 | ppm | |
| TD | 262144 | | |
| AQ | 6.554 | s | field dependent |
| FIDRES | 0.153 | Hz | field dependent |
| D 1 | 823.446 | s | AQ+D1=const |
| P 1 | 17.2 | us | 90deg NUC1 |
| PCPD 2 | 120.0 | W | PCPD NUC2 |
| PLW 1 | 4.8 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.018 | W | Pow@CPD NUC2 |
| PLW 13 | 0.009 | W | Pow@CPD NOE NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| DIGMOD | 3 | | baseopt |
| TE | 298.000 | K | default |

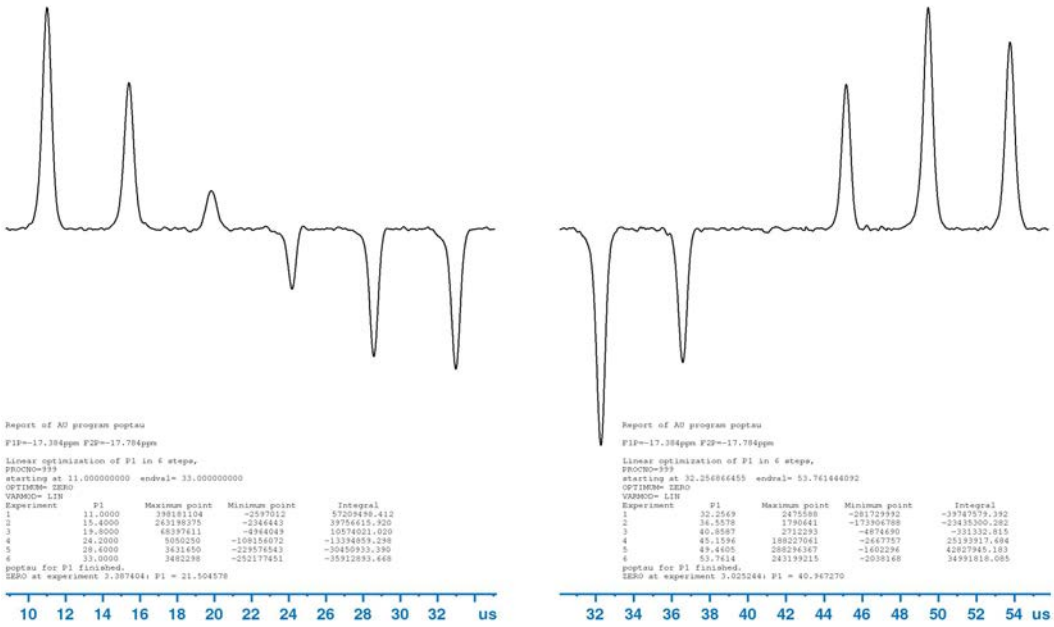
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 262144 | | |
| WDW | 1 | | |
| LB | 0.300 | Hz | |
| PC | 1.400 | | |
| F1P | 180.000 | ppm | |
| F2P | -20.000 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Carbon-13 sensitivity test with 1H decoupling. Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from 140.0 to 124.0 ppm, while the best 40 ppm noise region is determined over the range from 124.0 to 80.0 ppm.

## 5.6.7 P90 31P pulse calibration (NPT_31P_CMR_p90determination_31p)

**Test Sample:** 0.485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
CMR_TPP
**Solvent:** Acetone
**Lock parameter:** External Lock
**Sample State:** Rotation off




### Example Printout

P90 pulse determination using 1D method by varying the excitation pulse. The result of a CONVTO1D routine shows six experiments from 90 to 270 deg (PROCNO 100).

### Control Option for Acquisition (L23)

1 default
2 skip SINO check on PROCNO 11
11 ignore specifications (optimize power for pulse length from prosol)
12 ignore specifications and skip SINO check on PROCNO 11
21 ignore specifications and optimize pulse length for power from prosol
22 ignore specs, skip SINO check, and optimize pulse length for power from prosol
100 Same as xx but skip automatic phase correction and apply manually set values.
+xx
1000 Same as xxx but skip automatic O1P determination
+xxx

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PARMODE | 0 | | Data Dimension |
| PULPROG | zgig | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | 0.000 | ppm | |
| O2P | 5.000 | ppm | |
| SWH | 8196.722 | Hz | |
| AQ | 0.393 | s | |
| FIDRES | 2.542 | Hz | |
| D 1 | 17.757 | s | AQ+D1=const |
| P 1 | 10.5 | us | 90deg NUC1 |
| PCPD 2 | 120.0 | W | PCPD NUC2 |
| PLW 1 | 5.0 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.016 | W | Pow@CPD NUC2 |
| TE | 298.000 | K | default |

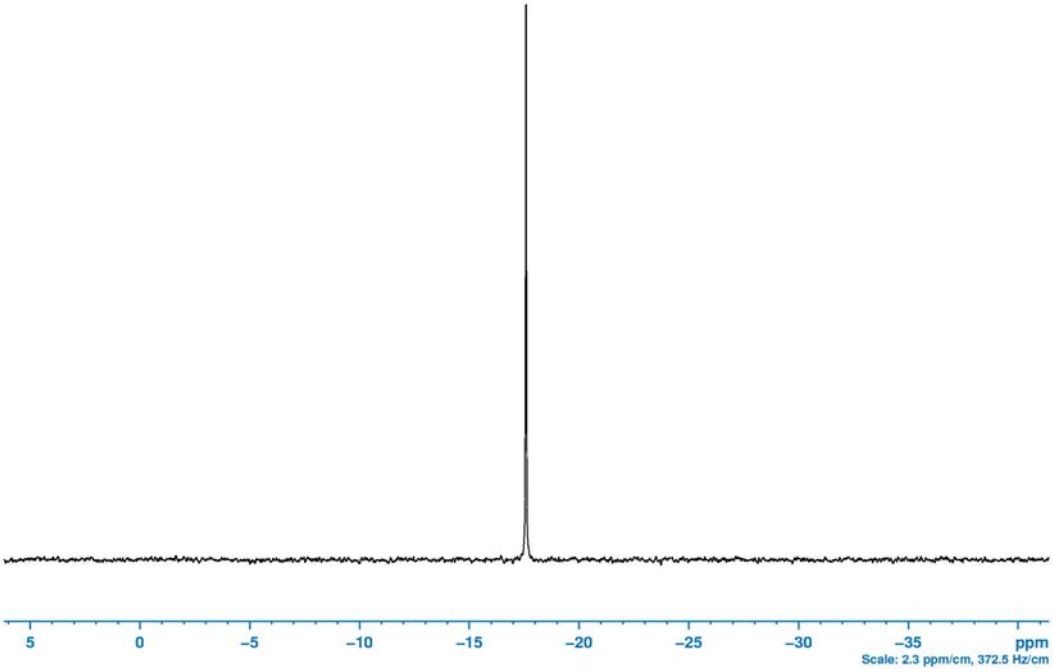
| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 2.000 | Hz | |
| SSB | 0.000 | | |
| PH_mod | 1 | | pk |
| ME_mod | 0 | | LPfc |
| NCOEF | 0 | | |
| ABSF1 | -17.332 | ppm | |
| ABSF2 | -17.860 | ppm | |
| F1P | -17.357 | ppm | |
| F2P | -17.835 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

This experiment depends on the entry of the 90 degree pulse in the PROSOL table.
As usual for pulse determinations the exact signal offset (O1P) is first determined. The resulting spectrum is stored in PROCNO 10 in magnitude mode, the FID is discarded.
The next step is the determination of the correct phase of the signal using the corrected O1P. The result is stored in PROCNO 11, the FID is discarded. After phase correction SINO will be executed. The experiment will be aborted, if a minimal SINO of 10 is not achieved. SINO check can be skiped with L23=2, 12, or 22
If the evaluation shows a deviation for the 90 degree pulse which is not in the interval [97%, 100%], a new power value will be calculated based on the specified pulse length, followed by the update of the PROSOL table and a new execution of the measurement with the newly set power. This cycle can be repeated up to six times and its results are stored under PROCNO 100+n and 200, 201.
A protocol is shown on the lower right side of the printout, containing a table with PLW90, P90, P90[det], Deviation (%).

### 5.6.8 31P sensitivity with 1H decoupling (NPT_31P_CMR_sensitivity_dec1h)

**Test Sample:** 0.485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
CMR_TPP
**Solvent:** Acetone
**Lock parameter:** External Lock
**Sample State:** Rotation off




**Example Printout**

Phosphorous-31 sensitivity test with 1H decoupling.

**Control Option for Acquisition (L23)**

1 default

## Parameters

| F1 ACQU | | | Parameters |
|---|---|---|---|
| NUC1 | 31P | | |
| NUC2 | 1H | | |
| PULPROG | zgig | | |
| NS | 1 | | |
| DS | 0 | | |
| RG | 1.000 | | no optim. |
| O1P | -17.000 | ppm | |
| O2P | 5.000 | ppm | |
| SW | 50.606 | ppm | |
| TD | 6450 | | |
| AQ | 0.393 | s | field dependent |
| FIDRES | 2.542 | Hz | field dependent |
| D 1 | 120.607 | s | AQ+D1=const |
| P 1 | 10.5 | us | 90deg NUC1 |
| PCPD 2 | 120.0 | W | PCPD NUC2 |
| PLW 1 | 5.0 | W | Pow@90deg(Specs) NUC1 |
| PLW 12 | 0.016 | W | Pow@CPD NUC2 |
| CPDPRG2 | waltz64 | | decoupl. sequence |
| DIGMOD | 1 | | baseopt |
| TE | 298.000 | K | default |

| F1 PROC | | | Parameters |
|---|---|---|---|
| SI | 32768 | | |
| WDW | 1 | | |
| LB | 0.500 | Hz | |
| PC | 1.400 | | |
| F1P | -17.357 | ppm | |
| F2P | -17.835 | ppm | |
| CY | 11.000 | cm | |

## Experiment Description

Phosphorous-31 sensitivity test with 1H decoupling. Processing is using line broadening (LB) and baseline correction (ABS). Evaluation is carried out by the AU `sinocal`. The signal is searched over the range from -15.0 to -21.0 ppm, while the best 5 ppm noise region is determined over the range from 0.0 to -36.0 ppm.

# 6 Appendix

## 6.1 Sample List

| Sample ID | Diameter | Description |
|---|---|---|
| CD3CN | n.a. | Acetonitrile-$D_3$ |
| CH3CN_D2O | n.a. | Acetonitrile/$D_2O$ |
| CMR_TPP | 5.0 | 0.485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ |
| H177072 | 5.0 | Pseudo Honey |
| H5798 | n.a. | 5 ug/ul of 1,3,5-Trimethoxybenzene ($C_6H_3(OCH_3)_3$) in Acetonitrile/ $D_2O$ 70/30 |
| H5799-D2O | n.a. | Methyl-, Ethyl-, Propyl- and Butyl-Ester of para-Hydroxybenzoic Acid, 6.57 mM each in Acetonitrile/$D_2O$ 30/70 |
| H5799-SPE | n.a. | Methyl-, Ethyl-, Propyl- and Butyl-Ester of para-Hydroxybenzoic Acid, 6.57 mM each in Acetonitrile/$D_2O$ 30/70 |
| H5799-SPE-1.7 | 1.7 | Methyl-, Ethyl-, Propyl- and Butyl-Ester of para-Hydroxybenzoic Acid, 6.57 mM each in Acetonitrile/$D_2O$ 30/70 |
| H5799-SPE-3 | 3.0 | Methyl-, Ethyl-, Propyl- and Butyl-Ester of para-Hydroxybenzoic Acid, 6.57 mM each in Acetonitrile/$D_2O$ 30/70 |
| H5799-SPE-5 | 5.0 | Methyl-, Ethyl-, Propyl- and Butyl-Ester of para-Hydroxybenzoic Acid, 6.57 mM each in Acetonitrile/$D_2O$ 30/70 |
| H7284 | n.a. | 0.5% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| H7284-01 | n.a. | 1% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| H7284-02 | n.a. | 3% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| H7285 | n.a. | 2nM Sucrose in $D_2O$ |
| H9630 | n.a. | 800 ng of 1,3,5-Trimethoxybenzene ($C_6H_3(OCH_3)_3$) in 30 ul Acetonitrile/$D_2O$ 50/50 |
| H9630-01 | n.a. | 800 ng of 1,3,5-Trimethoxybenzene ($C_6H_3(OCH_3)_3$) in 60 ul Acetonitrile/$D_2O$ 50/50 |
| H9630-02 | n.a. | 800 ng of 1,3,5-Trimethoxybenzene ($C_6H_3(OCH_3)_3$) in 120 ul Acetonitrile/$D_2O$ 50/50 |
| H9630-06 | n.a. | 800 ng of 1,3,5-Trimethoxybenzene ($C_6H_3(OCH_3)_3$) in 10 ul Acetonitrile/$D_2O$ 50/50 |
| MeOD | n.a. | Methanol-D4 |
| Z10029 | 3.0 | 0.3% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10030 | 3.0 | 1% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10031 | 3.0 | 3% Chloroform ($CHCl_3$), 0.2% TMS in Acetone-$D_6$ |
| Z10033 | 3.0 | 0.1% Ethylbenzene (EB) in Chloroform-D |
| Z10034 | 3.0 | 10% Ethylbenzene (EB) in Chloroform-D |
| Z10035 | 3.0 | 40% Dioxane in Benzene-$D_6$ (ASTM) |
| Z10036 | 3.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z10037 | 3.0 | 100 mM Urea-$^{15}N$ ($[^{15}NH_2]_2CO$), 100 mM Methanol-$^{13}C$ ($^{13}CH_3OH$) in Dimethyl Sulfoxide-$D_6$ |

| Sample ID | Diameter | Description |
|---|---|---|
| Z100372 | 2.5 | 0.5 M Sodium Chloride (NaCl) in $D_2O$ |
| Z100375 | 3.0 | 0.25 M Sodium Chloride (NaCl) in $D_2O$ |
| Z100376 | 3.0 | 0.5 M Sodium Chloride (NaCl) in $D_2O$ |
| Z100377 | 3.0 | 1 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10038 | 3.0 | 0.0485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ |
| Z100384 | 5.0 | 0.05 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z100385 | 5.0 | 0.1 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z100386 | 5.0 | 0.15 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z100387 | 5.0 | 0.2 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z100388 | 5.0 | 0.25 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z100389 | 5.0 | 0.5 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z10039 | 3.0 | 90% Formamide ($HCONH_2$) in Dimethyl Sulfoxide-$D_6$ |
| Z10040 | 3.0 | 0.05% Trifluorotoluene (TFT, a,a,a-$CF_3C_6H_5$) in Chloroform-D |
| Z10046 | 3.0 | 0.1 mg/ml Gadolinium Chloride ($GdCl_3$), 0.1% Methanol-$^{13}C$ ($^{13}CH_3OH$), 1% $H_2O$ in $D_2O$ |
| Z10053 | 3.0 | Temperature Calibration - 99.8% Methanol-$D_4$ |
| Z10056 | 3.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 99% $H_2O$ + 1% $D_2O$ |
| Z10075 | 5.0 | 1 M Potassium Chloride (KCl) in $D_2O$ |
| Z10076 | 10.0 | 1 M Potassium Chloride (KCl) in $D_2O$ |
| Z10078 | 5.0 | 45% Chloroform-D ($CDCl_3$), 45% Chloroform ($CHCl_3$) in 10% Hexafluorobenzene ($C_6F_6$) |
| Z10079 | 10.0 | 45% Chloroform-D ($CDCl_3$), 45% Chloroform ($CHCl_3$) in 10% Hexafluorobenzene ($C_6F_6$) |
| Z10082 | 2.5 | 0.1 mg/ml Gadolinium Chloride ($GdCl_3$), 0.1% Methanol-$^{13}C$ ($^{13}CH_3OH$), 1% $H_2O$ in $D_2O$ |
| Z10083 | 5.0 | 0.1 mg/ml Gadolinium Chloride ($GdCl_3$), 0.1% Methanol-$^{13}C$ ($^{13}CH_3OH$), 1% $H_2O$ in $D_2O$ |
| Z10084 | 8.0 | 0.1 mg/ml Gadolinium Chloride ($GdCl_3$), 0.1% Methanol-$^{13}C$ ($^{13}CH_3OH$), 1% $H_2O$ in $D_2O$ |
| Z10085 | 10.0 | 0.1 mg/ml Gadolinium Chloride ($GdCl_3$), 0.1% Methanol-$^{13}C$ ($^{13}CH_3OH$), 1% $H_2O$ in $D_2O$ |
| Z100926 | 1.0 | 3% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z100927 | 1.0 | 0.1% Ethylbenzene (EB) in Chloroform-D |
| Z100929 | 1.0 | 40% Dioxane in Benzene-$D_6$ (ASTM) |
| Z100930 | 1.0 | 10 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |

| Sample ID | Diameter | Description |
|---|---|---|
| Z100932 | 1.0 | 100 mM Urea-$^{15}$N ($[^{15}NH_2]_2CO$), 100 mM Methanol-$^{13}$C ($^{13}CH_3OH$) in Dimethyl Sulfoxide-$D_6$ |
| Z100933 | 1.0 | 0.1 mg/ml Gadolinium Chloride ($GdCl_3$), 0.1% Methanol-$^{13}$C ($^{13}CH_3OH$), 1% $H_2O$ in $D_2O$ |
| Z100934 | 1.0 | 0.485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ |
| Z100937 | 1.0 | 0.05% Trifluorotoluene (TFT, a,a,a-$CF_3C_6H_5$) in Chloroform-D |
| Z10120 | 5.0 | 0.1% Ethylbenzene (EB) in Chloroform-D |
| Z10121 | 10.0 | 0.1% Ethylbenzene (EB) in Chloroform-D |
| Z10136 | 2.5 | 90% Formamide ($HCONH_2$) in Dimethyl Sulfoxide-$D_6$ |
| Z10153 | 5.0 | 10% Ethylbenzene (EB) in Chloroform-D |
| Z10154 | 10.0 | 10% Ethylbenzene (EB) in Chloroform-D |
| Z10163 | 5.0 | 40% Dioxane in Benzene-$D_6$ (ASTM) |
| Z10164 | 10.0 | 40% Dioxane in Benzene-$D_6$ (ASTM) |
| Z101710 | 8.0 | 0.25 M Sodium Chloride (NaCl) in $D_2O$ |
| Z101712 | 10.0 | 0.5 M Sodium Chloride (NaCl) in $D_2O$ |
| Z101714 | 10.0 | 1 M Sodium Chloride (NaCl) in $D_2O$ |
| Z101715 | 1.0 | 0.25 M Sodium Chloride (NaCl) in $D_2O$ |
| Z101716 | 1.0 | 0.5 M Sodium Chloride (NaCl) in $D_2O$ |
| Z101717 | 1.0 | 1 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10187 | 5.0 | 90% Formamide ($HCONH_2$) in Dimethyl Sulfoxide-$D_6$ |
| Z10188 | 10.0 | 90% Formamide ($HCONH_2$) in Dimethyl Sulfoxide-$D_6$ |
| Z10191 | 5.0 | 1 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10192 | 2.5 | 0.25 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10201 | 5.0 | 0.0485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ |
| Z10202 | 10.0 | 0.0485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ |
| Z10209 | 5.0 | 85% Hexamethyldisiloxane (HMDSO, $[[CH_3]_3Si]_2O$) in Benzene-$D_6$ |
| Z10210 | 10.0 | 85% Hexamethyldisiloxane (HMDSO, $[[CH_3]_3Si]_2O$) in Benzene-$D_6$ |
| Z10230 | 5.0 | 3% Chloroform ($CHCl_3$), 0.2% TMS in Acetone-$D_6$ |
| Z10234 | 5.0 | 0.05% Trifluorotoluene (TFT, a,a,a-$CF_3C_6H_5$) in Chloroform-D |
| Z10235 | 10.0 | 0.05% Trifluorotoluene (TFT, a,a,a-$CF_3C_6H_5$) in Chloroform-D |
| Z10241 | 5.0 | 2 mM Lysozyme in 90% $H_2O$ + 10% $D_2O$ |
| Z10242 | 2.5 | 40% Dioxane in Benzene-$D_6$ (ASTM) |
| Z10246 | 5.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ (60 mm filling height) |
| Z10247 | 8.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z10248 | 5.0 | 1% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10249 | 8.0 | 1% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10250 | 10.0 | 1% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10253 | 8.0 | 10% Ethylbenzene (EB) in Chloroform-D |
| Z10255 | 8.0 | 40% Dioxane in Benzene-$D_6$ (ASTM) |

| Sample ID | Diameter | Description |
|---|---|---|
| Z10256 | 8.0 | 90% Formamide ($HCONH_2$) in Dimethyl Sulfoxide-$D_6$ |
| Z10257 | 8.0 | 0.0485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ |
| Z10260 | 8.0 | 3% Chloroform ($CHCl_3$), 0.2% TMS in Acetone-$D_6$ |
| Z10263 | 5.0 | 100 mM Urea-$^{15}N$ ($[^{15}NH_2]_2CO$), 100 mM Methanol-$^{13}C$ ($^{13}CH_3OH$) in Dimethyl Sulfoxide-$D_6$ |
| Z10264 | 8.0 | 100 mM Urea-$^{15}N$ ($[^{15}NH_2]_2CO$), 100 mM Methanol-$^{13}C$ ($^{13}CH_3OH$) in Dimethyl Sulfoxide-$D_6$ |
| Z10265 | 10.0 | 100 mM Urea-$^{15}N$ ($[^{15}NH_2]_2CO$), 100 mM Methanol-$^{13}C$ ($^{13}CH_3OH$) in Dimethyl Sulfoxide-$D_6$ |
| Z10267 | 2.5 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z10268 | 10.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z10270 | 2.5 | 0.1% Ethylbenzene (EB) in Chloroform-D |
| Z10272 | 2.5 | 1% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10274 | 2.5 | 100 mM Urea-$^{15}N$ ($[^{15}NH_2]_2CO$), 100 mM Methanol-$^{13}C$ ($^{13}CH_3OH$) in Dimethyl Sulfoxide-$D_6$ |
| Z10275 | 2.5 | 3% Chloroform ($CHCl_3$), 0.2% TMS in Acetone-$D_6$ |
| Z10276 | 2.5 | 0.0485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ |
| Z10284 | 5.0 | 0.25 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10285 | 10.0 | 0.25 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10288 | 5.0 | 0.5 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10292 | 2.5 | 10% Ethylbenzene (EB) in Chloroform-D |
| Z10610 | 10.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 99% $H_2O$ + 1% $D_2O$ |
| Z10627 | 5.0 | Temperature Calibration - 99.8% Methanol-$D_4$ |
| Z10628 | 10.0 | Temperature Calibration - 99.8% Methanol-$D_4$ |
| Z10650 | 5.0 | Diffusion Dry Glycerol |
| Z10688 | 5.0 | 5% $H_2O$, 0.6 mM $CuSO_4$in $D_2O$ |
| Z10689 | 5.0 | 20% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10690 | 5.0 | 1% Ethylbenzene (EB) in Chloroform-D |
| Z10692 | 5.0 | 1 M Methanol-$^{13}C$ ($^{13}CH_3OH$) in $D_2O$ |
| Z10694 | 5.0 | 100% Ethylbenzene (EB) |
| Z10701 | 5.0 | 0.3% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10702 | 10.0 | 0.3% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z107150 | 5.0 | 0.15 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ (shaped tube) |
| Z107151 | 5.0 | 0.25 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ (shaped tube) |
| Z107152 | 5.0 | 0.5 M Sodium Chloride (NaCl), 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ (shaped tube) |
| Z10717 | 1.7 | 1% Chloroform ($CHCl_3$) in Acetone-$D_6$ |
| Z10718 | 1.7 | 0.1% Ethylbenzene (EB) in Chloroform-D |
| Z10719 | 1.7 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |

| Sample ID | Diameter | Description |
|---|---|---|
| Z10720 | 1.7 | 10 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ |
| Z10721 | 1.7 | 100 mM Urea-$^{15}N$ ($[^{15}NH_2]_2CO$), 100 mM Methanol-$^{13}C$ ($^{13}CH_3OH$) in Dimethyl Sulfoxide-$D_6$ |
| Z10722 | 1.7 | 0.0485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ |
| Z10723 | 1.7 | 10% Ethylbenzene (EB) in Chloroform-D |
| Z10724 | 1.7 | 40% Dioxane in Benzene-$D_6$ (ASTM) |
| Z10727 | 1.7 | 0.1 mg/ml Gadolinium Chloride ($GdCl_3$), 0.1% Methanol-$^{13}C$ ($^{13}CH_3OH$), 1% $H_2O$ in $D_2O$ |
| Z10728 | 1.7 | 0.05% Trifluorotoluene (TFT, a,a,a-$CF_3C_6H_5$) in Chloroform-D |
| Z10729 | 1.7 | 0.25 M Sodium Chloride (NaCl) in Deuterium Oxide ($D_2O$) |
| Z10730 | 1.7 | 0.5 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10731 | 1.7 | 1 M Sodium Chloride (NaCl) in $D_2O$ |
| Z10734 | 1.7 | Temperature Calibration - 99.8% Methanol-$D_4$ |
| Z10902 | 5.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ (40 mm filling height) |
| Z10908 | 5.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 99% $H_2O$ + 1% $D_2O$ |
| Z142220 | 4.0 | Chloroform ($CHCl_3$) in Acetone-$D_6$ (50 ul) |
| Z142221 | 4.0 | 0.1% Ethylbenzene (EB) in Chloroform-D (50 ul) |
| Z142222 | 4.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ (50 ul) |
| Z142223 | 4.0 | 100 mM Urea-$^{15}N$ ($[^{15}NH_2]_2CO$), 100 mM Methanol-$^{13}C$ ($^{13}CH_3OH$) in Dimethyl Sulfoxide-$D_6$ (50 ul) |
| Z142224 | 4.0 | 40% Dioxane in Benzene-$D_6$ (ASTM, 50 ul) |
| Z142226 | 4.0 | 0.0485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-$D_6$ (50 ul) |
| Z142227 | 4.0 | 90% Formamide ($HCONH_2$) in Dimethyl Sulfoxide-$D_6$ (50 ul) |
| Z142228 | 4.0 | 0.05% Trifluorotoluene (TFT, a,a,a-$CF_3C_6H_5$) in Chloroform-D |
| Z142229 | 4.0 | 85% Hexamethyldisiloxane (HMDSO, $[[CH_3]_3Si]_2O$) in Benzene-$D_6$ (50 ul) |
| Z142231 | 4.0 | 0.1 mg/ml Gadolinium Chloride ($GdCl_3$), 0.1% Methanol-$^{13}C$ ($^{13}CH_3OH$), 1% $H_2O$ in $D_2O$ (50 ul) |
| Z151210 | 7.0 | Potassium Bromide (KBr, 234 ul) |
| Z151211 | 7.0 | Adamantane (234 ul) |
| Z151212 | 7.0 | Alpha-glycine (234 ul) |
| Z151213 | 7.0 | 2-$^{13}C$, $^{15}N$ alpha-glycine (234 ul) |
| Z151214 | 7.0 | Ammonium Dihydrogenphosphate ($NH_4H_2PO_4$, 80 ul) |
| Z151216 | 7.0 | Ammonium Trifluoroacetate ($CF_3CO_2NH_4$, 80 ul) |
| Z151220 | 4.0 | Potassium Bromide (KBr, 80 ul) |
| Z151221 | 4.0 | Adamantane (50 ul) |
| Z151222 | 4.0 | Alpha-glycine (50 ul) |
| Z151223 | 4.0 | 2-$^{13}C$, $^{15}N$ alpha-glycine (50 ul) |

| Sample ID | Diameter | Description |
|---|---|---|
| Z151224 | 4.0 | Ammonium Dihydrogenphosphate ($NH_4H_2PO_4$, 50 ul) |
| Z151226 | 4.0 | Ammonium Trifluoroacetate ($CF_3CO_2NH_4$, 50 ul) |
| Z151230 | 3.2 | Potassium Bromide (KBr, 34 ul) |
| Z151231 | 3.2 | Adamantane (34 ul) |
| Z151232 | 3.2 | Alpha-glycine (34 ul) |
| Z151233 | 3.2 | 2-$^{13}C$, $^{15}N$ alpha-glycine (34 ul) |
| Z151234 | 3.2 | Ammonium Dihydrogenphosphate ($NH_4H_2PO_4$, 34 ul) |
| Z151236 | 3.2 | Ammonium Trifluoroacetate ($CF_3CO_2NH_4$, 34 ul) |
| Z151240 | 3.2 | Thinwalled Potassium Bromide (KBr, 45.5 ul) |
| Z151241 | 3.2 | Thinwalled Adamantane (45.5 ul) |
| Z151242 | 3.2 | Thinwalled Alpha-glycine (45.5 ul) |
| Z151243 | 3.2 | Thinwalled 2-$^{13}C$, $^{15}N$ alpha-glycine (45.5 ul) |
| Z151244 | 3.2 | Thinwalled Ammonium Dihydrogenphosphate ($NH_4H_2PO_4$, 45.5 ul) |
| Z151246 | 3.2 | Thinwalled Ammonium Trifluoroacetate ($CF_3CO_2NH_4$, 45.5 ul) |
| Z151250 | 2.5 | Potassium Bromide (KBr, 13.6 ul) |
| Z151251 | 2.5 | Adamantane (13.6 ul) |
| Z151252 | 2.5 | Alpha-glycine (12 mg, 13.6 ul) |
| Z151253 | 2.5 | 2-$^{13}C$, $^{15}N$ alpha-glycine (12 mg, 13.6 ul) |
| Z151254 | 2.5 | Ammonium Dihydrogenphosphate ($NH_4H_2PO_4$, 13.6 ul) |
| Z151256 | 2.5 | Ammonium Trifluoroacetate ($CF_3CO_2NH_4$, 13.6 ul) |
| Z151260 | 1.9 | Potassium Bromide (KBr, 13.1 ul) |
| Z151261 | 1.9 | Adamantane (13.1 ul) |
| Z151262 | 1.9 | Alpha-glycine (10 mg, 13.1 ul) |
| Z151263 | 1.9 | 2-$^{13}C$, $^{15}N$ alpha-glycine (10 mg, 13.1 ul) |
| Z151264 | 1.9 | Ammonium Dihydrogenphosphate ($NH_4H_2PO_4$, 13.1 ul) |
| Z151266 | 1.9 | Ammonium Trifluoroacetate ($CF_3CO_2NH_4$, 13.1 ul) |
| Z151270 | 1.3 | Potassium Bromide (KBr, 3.0 ul) |
| Z151271 | 1.3 | Adamantane (3.0 ul) |
| Z151272 | 1.3 | Alpha-glycine (2 mg, 3.0 ul) |
| Z151273 | 1.3 | 2-$^{13}C$, $^{15}N$ alpha-glycine (2 mg, 3.0 ul) |
| Z151274 | 1.3 | Ammonium Dihydrogenphosphate ($NH_4H_2PO_4$, 3.0 ul) |
| Z151276 | 1.3 | Ammonium Trifluoroacetate ($CF_3CO_2NH_4$, 3.0 ul) |
| Z163271 | 0.7 | Potassium Bromide (KBr, 0.5 ull) |
| Z163274 | 0.7 | Adamantane (0.5 ul) |
| Z163275 | 0.7 | Alpha-glycine 0.5 ul) |
| Z163276 | 0.7 | 2-$^{13}C$, $^{15}N$ alpha-glycine (0.5 ul) |
| Z163277 | 0.7 | Ammonium Dihydrogenphosphate ($NH_4H_2PO_4$, 0.5 ul) |
| Z163278 | 0.7 | Ammonium Trifluoroacetate ($CF_3CO_2NH_4$, 0.5 ul) |
| Z180181 | 5.0 | 2 mM Sucrose, 0.5 mM DSS, 2 mM $NaN_3$ in 90% $H_2O$ + 10% $D_2O$ (40 mm filling height, AvCo Sample Autocal) |

# Appendix

| Sample ID | Diameter | Description |
|---|---|---|
| Z183103 | 3.2 | Potassium Bromide |
| Z183104 | 3.2 | Adamantane |
| Z183105 | 3.2 | Alpha-glycine |
| Z183106 | 3.2 | 2-$^{13}$C, $^{15}$N alpha-glycine |

# 7 Contact

## 7.1 Manufacturer

Bruker BioSpin GmbH
Silberstreifen 4
D-76287 Rheinstetten
Germany

*http://www.bruker.com*

WEEE DE43181702

## 7.2 NMR Hotlines

Contact our NMR service centers.

Bruker BioSpin NMR provides dedicated hotlines and service centers, so that our specialists can respond as quickly as possible to all your service requests, applications questions, software or technical needs.

Please select the NMR service center or hotline you wish to contact from our list available at: *https://www.bruker.com/service/information-communication/helpdesk.html*

Phone: +49 721-5161-6155

E-mail: *nmr-support@bruker.com*

Bruker Corporation

info@bruker.com
www.bruker.com