

NMR Test Spectrometer

Report Name: 2025-11-21

AV III (400 MHz) Z133003_00028

Content:

- Configuration Information (uxnmr.info)
- IP Config Information
- Probe: Z108618_0547 / 2025-11-21



● Configuration Information uxnmr.info

CONFIGURATION INFORMATION

=====

Path : C:/Bruker/TopSpin3.5p17/conf/instr/spect/uxnmr.info
Date : Wed Oct 29 17:21:12 2025
Release : TopSpin 3.5 pl 7
Installed in : C:/Bruker/TopSpin3.5p17
Host : CZC2157P94
OS : Windows 7 (Vs 6.2)
CPU : 12th Gen Intel(R) Core(TM) i5-12400 (12 cores at 2496 MHz with Hyperthreading)
User : root
System : Avance III 400 NMR spectrometer
1H-frequency : 400.17 MHz
Description : Avance Nanobay V3-I 400MHz
Location : Suzhou China
Bruker Order : Z133003_00028
Configured in: CZC2157P94:C:/Bruker/TopSpin3.5p17/conf/instr/spect

IPSO: connected to spectrometer subnet
- TCP/IP address = 149.236.99.250
- IPSO type: AQS
- Tctrl : 1
- Fctrls: 2
- Gctrl1: without digital preemphasis
- Rctrl : 1
- FREDs : none
- DPP : none

DRU1: AQS DRU Z100977/02014 ECL 07.01
- TCP/IP address = 149.236.99.89
- Firmware Version = 151014
- DRU1 controls AQS-Rack and HPPR/2

AQS: connected to 149.236.99.89:/dev/tty10

Number	Addr	Type	HW-VS	FW-VS	ID	ECL Name	Description
2	0x10 0x43	0x5	CD	R	0.0 REC-1	AQS RXAD/2 600 Z130588/115 ECL 00.00	
3	0x34 0xd6	0x1	X	5.2 REF-1	REF/3-600 Reference Board for AQS/3 Receiver		
4	0x24 0x32	0	S	2.0 SGU-1	AQS SGU/3 600 (2CH) Z117129/00179 ECL 02.00	FPGA-Vs=20131031	
8	0x36 0x5	0	A	9.1 BLA-1	BLA2BB 150/60 20-400 W1345049/3052 ECL 09.01		
14	0xa0 0x90	0	V	2.0 PS-1	AQS PSM-A Power Supply Module		
15	0xa1 0x91	0	V	1.1 PS-2	AQS PSM-D Power Supply Module		
--	0x20 0xd9	0	B	0.2 MASTER			
1	0x20 0x7	0	B	MASTER AQS Rack Master			

Logical Receiver/SGU configuration:

Router: 1 AQS-Minirouter

Amplifiers (AQS configuration):

RO	Amplifier	Module	Nucleus	Power/W	Switchbox	Name	PN/SN/FW
1	1	1	B	150	N	BLA2BB 150/60 20-400 W1345049/3052/-	
2	1	2	B	60	N	BLA2BB 150/60 20-400 W1345049/3052/-	

Transmitters at the spectrometer subnet:

LTRX Z109888/00781 ECL 03.00:
- TCP/IP address = 149.236.99.20
- Amplifier = BSMS/2 LOCK TRANSCEIVER 400: Z109888/00781 ECL 03.00

BSMS: BSMS/2 connected to ethernet
- TCP/IP address = 149.236.99.20
- ELCB firmware version = 20161026

- GAB current limits = 0.0/X, 0.0/Y, 10.0/Z (in A)
- SCB channels = 20
- Shim System = BOSS1-SB
- L-TRX = BSMS/2 LOCK TRANSCEIVER 400: Z109888/00781 ECL 03.00
- Lock: on L-TRX board
- VTU_SFB = BSMS/2 SFB SENSOR & PNEUMATIC BD: Z115191/07999 ECL 05.05
- VTU_VFSB1 = BSMS/2 VARIABLE POWER SUPPLY BD: Z115193/04146 ECL 01.05

VTU: in BSMS/2 connected to ethernet
- TCP/IP address = 149.236.99.20

Bruker Automatic Changer: device connected to 149.236.99.250:/dev/tty01
- Capacity: 60 holders
- Firmware: 20120525
- use BACS air = yes
- BACS sx delay = 1 s
- Sample Rail fast changer mode = no

Preamplifiers :
HPPR2: - HPPR/2 preamplifier connected to 149.236.99.89:/dev/tty10
Type : HPPR/2
Controller: no Cover, with Application firmware = aq
no LED display for tuning and matching
Module 1 : 1H/2H 1H (virtual 50 Ohm reference: 280.7%/93.5deg)
PN=Z128274, SN=00035 from 20120706
Module 2 : 1H/2H 2H (virtual 50 Ohm reference: 118.5%/67.3deg)
PN=Z128274, SN=00035 from 20120706
Module 3 : XBB19F 2HS
PN=Z128143, SN=00039 from 20120710

Gradient Controller cable connections

GCtrl1: connected to GAB in BSMS

RF cable connections (detected)

SGU1 NORM output -> input 1 of transmitter 1 (BLA2BB 150/60 20-400 W1345049/3052)
SGU1 AUX output -> input 1 of transmitter 2 (BSMS/2 LOCK TRANSCEIVER 400 Z109888/00781 at TCP/IP 149.236.99.20)
SGU2 NORM output -> input 2 of transmitter 1 (BLA2BB 150/60 20-400 W1345049/3052)
SGU2 AUX output -> TUNE signal input of HPPR

Blanking cable connections (detected)

transmitter 1 = BLA2BB 150/60 20-400 W1345049/3052:
- amplifier B-150W uses blanking 1
- amplifier B-60W uses blanking 2

transmitter 2 = BSMS/2 LOCK TRANSCEIVER 400 Z109888/00781 at TCP/IP 149.236.99.20:
- amplifier 2H-5W uses blanking 8

● IP Config Information

```
Windows IP Configuration

Host Name . . . . . : CZC2157P94
Primary Dns Suffix . . . . . :
Node Type . . . . . : Hybrid
IP Routing Enabled. . . . . : No
WINS Proxy Enabled. . . . . : No
DNS Suffix Search List. . . . . : lan

Ethernet adapter Ethernet 2:

Media State . . . . . : Media disconnected
Connection-specific DNS Suffix . :
Description . . . . . : Realtek PCIe GbE Family Controller
Physical Address. . . . . : 48-5F-08-AC-87-48
DHCP Enabled. . . . . : No
Autoconfiguration Enabled . . . . : Yes

Ethernet adapter Ethernet:

Connection-specific DNS Suffix . :
Description . . . . . : Realtek Gaming 2.5GbE Family Controller
Physical Address. . . . . : 08-2E-5F-05-40-4B
DHCP Enabled. . . . . : No
Autoconfiguration Enabled . . . . : Yes
Link-local IPv6 Address . . . . . : fe80::f532:ca97:2f02:7b82%10 (Preferred)
IPv4 Address. . . . . : 149.236.99.1 (Preferred)
Subnet Mask . . . . . : 255.255.255.0
Default Gateway . . . . . :
DHCPv6 IAID . . . . . : 151568312
DHCPv6 Client DUID. . . . . : 00-01-00-01-2C-5E-F9-07-C8-5A-CF-0C-0D-DD
DNS Servers . . . . . : fec0:0:0:ffff::1%1
fec0:0:0:ffff::2%1
fec0:0:0:ffff::3%1
NetBIOS over Tcpip. . . . . : Enabled

Wireless LAN adapter Wi-Fi:

Connection-specific DNS Suffix . : lan
Description . . . . . : TP-LINK Wireless USB Adapter
Physical Address. . . . . : 78-60-5B-DD-4A-B4
DHCP Enabled. . . . . : Yes
Autoconfiguration Enabled . . . . : Yes
Link-local IPv6 Address . . . . . : fe80::7983:944a:5b18:3119%16 (Preferred)
IPv4 Address. . . . . : 192.168.110.118 (Preferred)
Subnet Mask . . . . . : 255.255.255.0
Lease Obtained. . . . . : Wednesday, October 29, 2025 5:15:56 PM
Lease Expires . . . . . : Friday, November 21, 2025 5:37:37 PM
Default Gateway . . . . . : 192.168.110.1
DHCP Server . . . . . : 192.168.110.1
DHCPv6 IAID . . . . . : 544759899
DHCPv6 Client DUID. . . . . : 00-01-00-01-2C-5E-F9-07-C8-5A-CF-0C-0D-DD
DNS Servers . . . . . : 192.168.110.1
NetBIOS over Tcpip. . . . . : Enabled
```

PA BBO 400S1 BBF-H-D-05 Z PLUS

400 MHz

Probe ID: Z108618_0547

Inspection Lot: 2025-11-21

Nov 21, 2025

NMR TEST SERVICE

● Probe NMR Test Data: **PA BBO 400S1 BBF-H-D-05 Z PLUS**

Probe Related Information

EC-Level	1.05
Sample Depth (standard) [mm]	20
Sample Depth (water-based Solvents) [mm]	20
Gas Compensation	air
Gradient System	Z
ATM Accessory	true
Temperature Sensor Type	Type_T
Proton Frequency [MHz]	400
Diameter [mm]	5.0

Spectrometer Related Information

Type	AV III
CF Frequency [MHz]	400.17
Shim System	BOSS1-SB
Shim System Offset	37
Software	TopSpin 3.5 pl 7
Operating System	Windows 7 (Vs 6.2)
Host Name	CZC2157P94
Magnet System	SB
Magnet Coil No	
Dewar No	
Helium Level	0%
System Number	Z133003_00028

● PICS Data

Z108618_0547.ph

```
Z108618_0547.ph
=====
$BIS, 1, 20120625, 2048, PICS, 3#
$Production, Z108618, 0547, 1.05, , BCH, 20120622#
$Name, PA BBO 400S1 BBF-H-D-05 Z PLUS#
$ProbeCompatibility, 1.0, SB, 1, 400#
$ProbeType, 1.1, HR, 0, 0#
$ProbeSample, 1.0, 05, 20#
$ProbeTemperature, 1.0, TypeT, -150, +150#
$ProbeAllCoils, 1.1, 2, 0#
$ProbeCoil, 1.0, 1, 19.4, 1, BB, , , , #
$ProbeCoil, 1.0, 2, 19.4, 2, 1H, D, , , #
$PHeatTemp, 1.0, TypeT, , 400#
$ProbeChannel, 1.0, 1H, 1/-/F, 2/+F, 6.00, 40, 5, 0.4, 0.1, FALSE#
$ProbeChannel, 1.0, D, -1, -1, , 30, 5, 0.4, 0.1, 0#
$ProbeZ-Grad, 1.0, , , 5.00, 10, , , , , #
$ProbeGradInfo, 1.0, Z114117, , , , 13#
$ProbeBB, 2.0, 2, 19F-109Ag, 8.00, 34.286, 6/+8, 7/+9, 8/+9, 9/-/F, 5/+9, 4/+9, 3/+F#
$ProbeBBSets, 1.0, 19F, 899.0054, 99.0324, 50, , 0.4, 0.1#
$ProbeBBSets, 1.0, 31P, 799.0059, 99.0270, 70, , 0.4, 0.1#
$ProbeBBSets, 1.0, 87Rb, 799.0204, 99.0230, 70, , 0.4, 0.1#
$ProbeBBSets, 1.0, 13C, 796.0171, 98.0269, 100, , 0.4, 0.1#
$ProbeBBSets, 1.0, 17O, 779.0097, 87.0145, 100, , 0.4, 0.1#
$ProbeBBSets, 1.0, 15N, 758.0204, 83.0177, 150, , 0.4, 0.1#
$ProbeBBSets, 1.0, 14N, 681.0151, 74.0179, 150, , 0.4, 0.1#
$ProbeBBSets, 1.0, 109Ag, 498.0155, 48.0288, 150, , 0.4, 0.1#
$ProbeElec, 1.0, Z003615, 04974, 03.00, 2.2#
$ProbeATMA, 1.1, 1H/BB, 2.6#
$EndBis, 45, E2#
```

● **Required Samples PA BBO 400S1 BBF-H-D-05 Z PLUS**

Z10120	0.1% Ethylbenzene (EB) in Chloroform-D
Z10153	10% Ethylbenzene (EB) in Chloroform-D
Z10163	40% Dioxane in Benzene-D6 (ASTM)
Z10187	90% Formamide in Dimethyl Sulfoxide-D6
Z10201	0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6
Z10234	0.05% Trifluorotoluene (TFT, a,a,a-CF3C6H5) in Chloroform-D
Z10248	1% Chloroform in Acetone-D6
Z10263	100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6

NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 1% Chloroform in Acetone-D6 (Z10248)
 1H lineshape with sample rotation and NS = 4 (NPT_1H_lineshape_wrot, spin rate 20 Hz)

Line width [achieved/rated]: at 0.11% of signal height [4.9 Hz <= 12.0 Hz] <pass>
 Line width [achieved/rated]: at 0.55% of signal height [2.2 Hz <= 6.0 Hz] <pass>
 Line width [achieved/rated]: at 50% of signal height [0.34 Hz <= 0.60 Hz] <pass>
 Spinning side band [achieved]: at -20 Hz [0.3%] <n/a>



Bruker BioSpin

NPT_1H_lineshape_wrot

Current Data Parameters
 NAME NPT_1H_lineshape_wrot
 EXPNO 1
 PROCNO 1

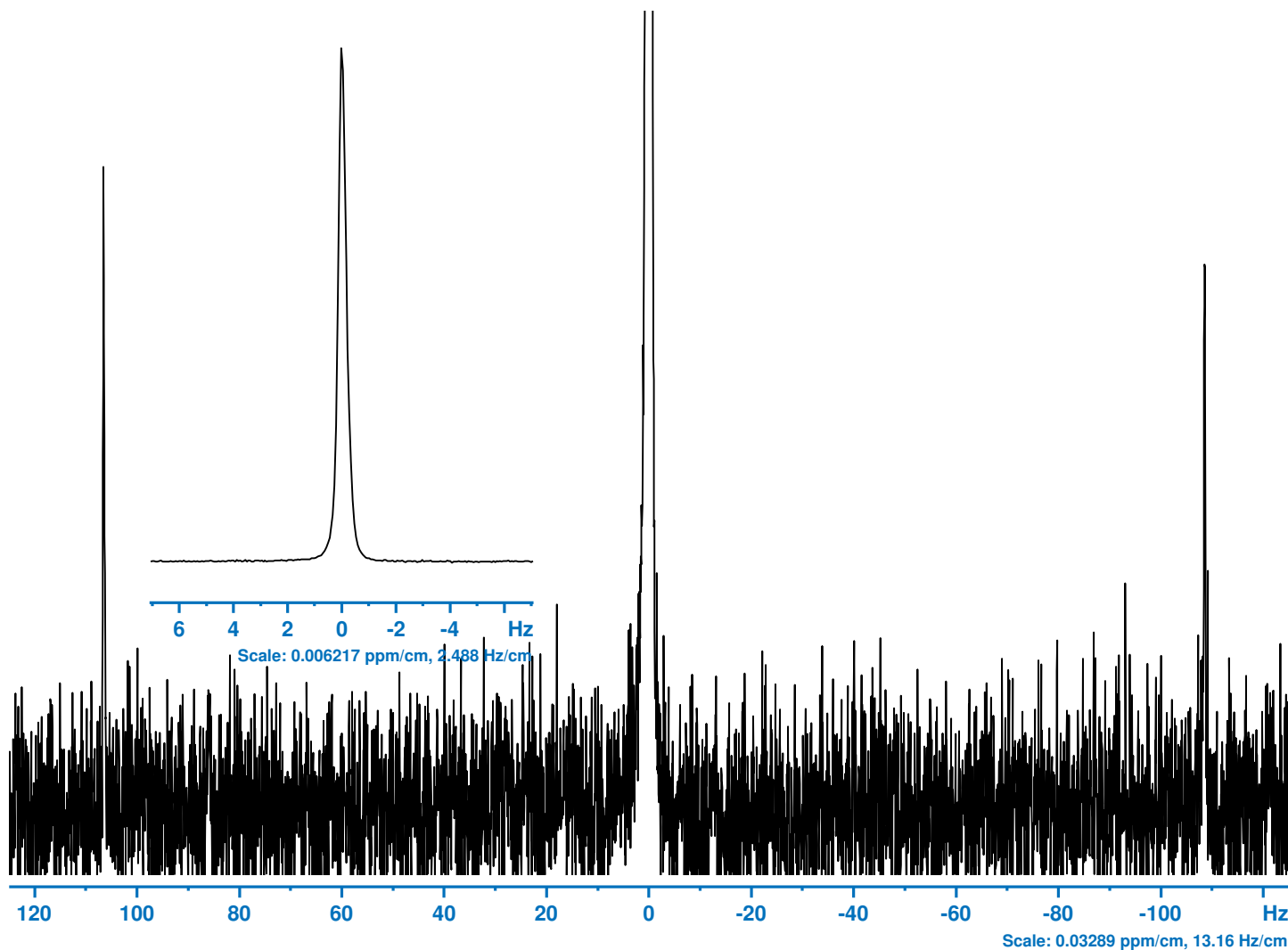
F2 - Acquisition Parameters
 Date_ 20251121
 Time 15.47 h
 INSTRUM spect
 PROBHD Z108618_0547 ()
 PULPROG zg30
 TD 32768
 SOLVENT Acetone
 NS 4
 DS 0
 SWH 1001.201 Hz
 FIDRES 0.061108 Hz
 AQ 16.3643398 sec
 RG 202.77
 DW 499.400 usec
 DE 6.50 usec
 TE 294.9 K
 D1 9.13566208 sec
 TDO 1
 SFO1 400.1729651 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 17.20400047 W

Additional Parameters
 Field 2240.180
 Lock Phase 230.276
 Lock Power -38.000
 Lock Gain 98.749
 Lock DC -75.000
 Lock Shift 2.040
 Loop Gain 15.133
 Loop Time 0.047
 Loop Filter 1468.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 8192
 SF 400.1732154 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 4.00

SHIM SEQUENCE

topshim 1d ss ordmax=6 convcomp <pass>



NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 1% Chloroform in Acetone-D6 (Z10248)
 1H lineshape with sample rotation and NS = 4 (NPT_1H_lineshape_wrot, spin rate 20 Hz)



Bruker BioSpin

NPT_1H_lineshape_wrot

```
# Fri Nov 21 15:47:14 2025
##$PROBEIDENTIFIER=Z108618_0547
##$PROBENAME=PA BBO 400S1 BBF-H-D-05 Z PLUS
##$SHIMID=313232
```

```
#
# Active Shim Gradients
#
Z          11265
Z2         -146
Z3          71
Z4        -15380
Z5         -2517
Z6         16407
X         -3315
XZ         15827
XZ2        14906
XZ3        -197
Y         -5117
YZ        -67369
YZ2        -4945
YZ3         4482
XY         12434
XYZ         2829
(X2-Y2)     1996
(X2-Y2) Z   -15440
X3          7772
Y3         -9643
```

```
#
# Lock Parameter
#
FIELD      2240.180
LOCKPHASE   230.276
LOCKPOWER  -38.000
LOCKGAIN    98.749
LOCKDC     -75.000
LOCKSHIFT   2.040
LOOPGAIN    15.133
LOOPTIME    0.047
LOOPFILTER  1468.000
```

```
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [1 ] 5463.46313686
SHIM_SETTING [2 ] -72.27977975
SHIM_SETTING [3 ] 37.49874643
SHIM_SETTING [4 ] -8090.00872162
SHIM_SETTING [5 ] -1323.91380717
SHIM_SETTING [6 ] -1743.70900000
```

```
SHIM_SETTING [7 ] 8325.15700000
SHIM_SETTING [8 ] 7840.34100000
SHIM_SETTING [9 ] 1049.82000000
SHIM_SETTING [10] 6540.31300000
SHIM_SETTING [11] -2691.44900000
SHIM_SETTING [12] -35436.23100000
SHIM_SETTING [13] -2601.29300000
SHIM_SETTING [14] 2357.48900000
SHIM_SETTING [15] 8629.88063220
SHIM_SETTING [16] -8121.60600000
SHIM_SETTING [17] -103.84400000
SHIM_SETTING [18] 1488.26300000
SHIM_SETTING [19] 4088.04500000
SHIM_SETTING [20] -5072.34700000
```

```
Current Data Parameters
NAME      NPT_1H_lineshape_wrot
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20251121
Time      15.47 h
INSTRUM   spect
PROBHD    Z108618_0547 (
PULPROG   zg30
TD         32768
SOLVENT    Acetone
NS         4
DS         0
SWH        1001.201 Hz
FIDRES     0.061108 Hz
AQ         16.3643398 sec
RG         202.77
DW         499.400 usec
DE         6.50 usec
TE         294.9 K
D1         9.13566208 sec
TD0        1
SF01       400.1729651 MHz
NUC1       1H
P1         12.00 usec
PLW1       17.20400047 W

F2 - Processing parameters
SI         8192
SF         400.1732154 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0
PC         4.00
```

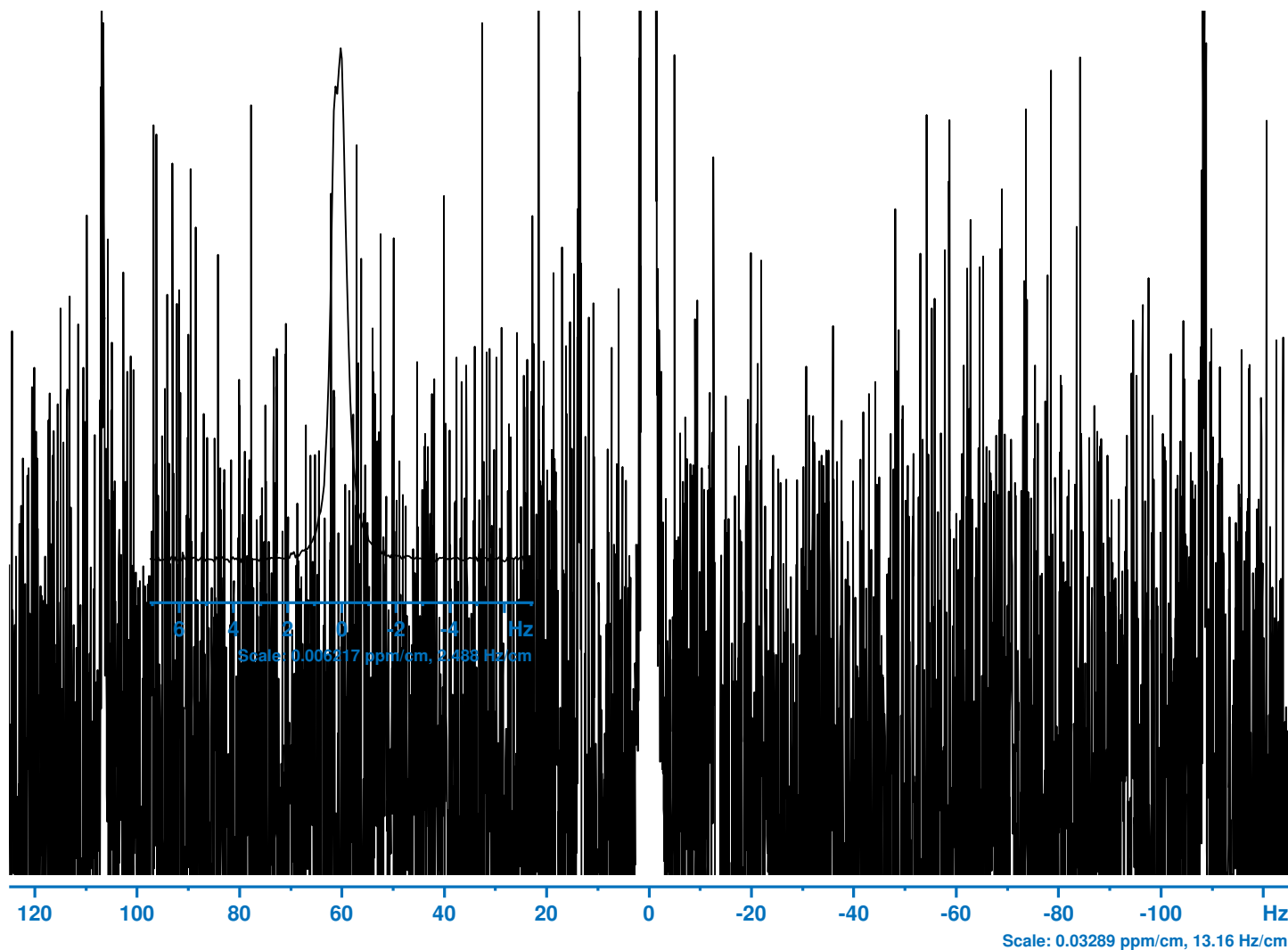
NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 1% Chloroform in Acetone-D6 (Z10248)
 1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)

Line width [achieved/rated]: at 0.11% of signal height [5.7 Hz <= 14.0 Hz] <pass>
 Line width [achieved/rated]: at 0.55% of signal height [3.8 Hz <= 7.0 Hz] <pass>
 Line width [achieved/rated]: at 50% of signal height [0.63 Hz <= 0.80 Hz] <pass>



Bruker BioSpin

NPT_1H_lineshape_nrot



```
Current Data Parameters
NAME      NPT_1H_lineshape_nrot
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20251121
Time      15.43 h
INSTRUM   spect
PROBHD    Z108618_0547 (
PULPROG   zg30
TD        32768
SOLVENT   Acetone
NS         1
DS         0
SWH       1001.201 Hz
FIDRES    0.061108 Hz
AQ        16.3643398 sec
RG         202.77
DW        499.400 usec
DE         6.50 usec
TE        294.9 K
D1        9.13566208 sec
TD0        1
SF01      400.1729650 MHz
NUC1       1H
P1        12.00 usec
PLW1      17.20400047 W

Additional Parameters
Field      2239.866
Lock Phase 230.276
Lock Power -38.000
Lock Gain  100.406
Lock DC    -75.000
Lock Shift 2.040
Loop Gain  15.133
Loop Time  0.047
Loop Filter 1468.000
Gas Flow   400 l/h

F2 - Processing parameters
SI         8192
SF         400.1732153 MHz
WDW        no
SSB         0
LB         0 Hz
GB         0
PC          4.00
```

```
SHIM SEQUENCE
ro off wait <pass>
topshim ld ss ordmax=6 convcomp <pass>
topshim tune tunea <pass>
```

NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 1% Chloroform in Acetone-D6 (Z10248)
 1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)



Bruker BioSpin

NPT_1H_lineshape_nrot

```
# Fri Nov 21 15:43:33 2025
##$PROBEIDENTIFIER=Z108618_0547
##$PROBENAME=PA BBO 400S1 BBF-H-D-05 Z PLUS
##$SHIMID=313232
```

```
#
# Active Shim Gradients
#
Z          11258
Z2         -133
Z3          26
Z4        -15470
Z5         -2396
Z6         17145
X          -3315
XZ         15903
XZ2        14906
XZ3        -197
Y          -5124
YZ         -67515
YZ2        -4945
YZ3         4482
XY         12434
XYZ        2829
(X2-Y2)    1996
(X2-Y2) Z  -15440
X3         7772
Y3        -9643
```

```
#
# Lock Parameter
#
FIELD      2239.866
LOCKPHASE  230.276
LOCKPOWER  -38.000
LOCKGAIN   100.406
LOCKDC     -75.000
LOCKSHIFT  2.040
LOOPGAIN   15.133
LOOPTIME   0.047
LOOPFILTER 1468.000
```

```
#
IEEE64_VERSION_CODE 1
```

```
#
# Shim currents
#
SHIM_SETTING [1 ] 5460.24469597
SHIM_SETTING [2 ] -65.99722104
SHIM_SETTING [3 ] 13.53197906
SHIM_SETTING [4 ] -8137.04435780
SHIM_SETTING [5 ] -1260.21260177
SHIM_SETTING [6 ] -1743.70900000
```

```
SHIM_SETTING [7 ] 8365.13300000
SHIM_SETTING [8 ] 7840.34100000
SHIM_SETTING [9 ] 1049.82000000
SHIM_SETTING [10] 6540.31300000
SHIM_SETTING [11] -2695.13100000
SHIM_SETTING [12] -35513.02700000
SHIM_SETTING [13] -2601.29300000
SHIM_SETTING [14] 2357.48900000
SHIM_SETTING [15] 9018.36986521
SHIM_SETTING [16] -8121.60600000
SHIM_SETTING [17] -103.84400000
SHIM_SETTING [18] 1488.26300000
SHIM_SETTING [19] 4088.04500000
SHIM_SETTING [20] -5072.34700000
```

```
Current Data Parameters
NAME      NPT_1H_lineshape_nrot
EXPNO     1
PROCNO    1
```

```
F2 - Acquisition Parameters
Date_     20251121
Time      15.43 h
INSTRUM    spect
PROBHD     Z108618_0547 (
PULPROG    zg30
TD          32768
SOLVENT     Acetone
NS          1
DS          0
SWH         1001.201 Hz
FIDRES      0.061108 Hz
AQ          16.3643398 sec
RG          202.77
DW          499.400 usec
DE          6.50 usec
TE          294.9 K
D1          9.13566208 sec
TD0         1
SF01        400.1729650 MHz
NUC1        1H
P1          12.00 usec
PLW1        17.20400047 W
```

```
F2 - Processing parameters
SI          8192
SF          400.1732153 MHz
WDW         no
SSB         0
LB          0 Hz
GB          0
PC          4.00
```

NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 P90 1H pulse calibration (NPT_1H_p90determinationf1_1h, spin rate 0 Hz)
 Result: [180/2] = 12.1 us @ 16.9 W [360] = 47.4 us ==> [PDelay = 2*180 - 360] = 1.0 us
 ATTENTION: Updated PROSOL Tables with [12.0 us @ 17.2 W]
 Deviation from pulse target value (= 12.0 us): 0.8%

P90 1H pulse [achieved]: @ 16.9 W [12.1 us] <n/a>



Bruker BioSpin

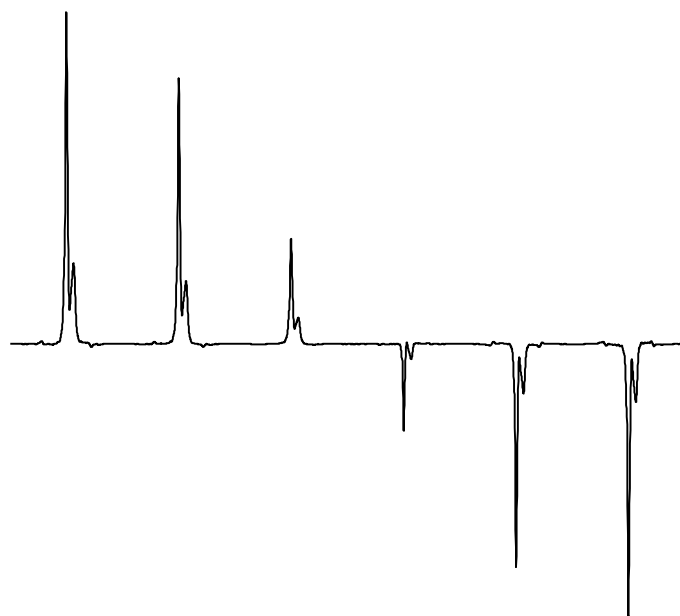
NPT_1H_p90determinationf1_1h

Current Data Parameters
 NAME NPT_1H_p90determinationf1_1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 15.31 h
 INSTRUM spect
 PROBHD Z108618_0547 ()
 PULPROG zg
 TD 300
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 142.045 Hz
 FIDRES 0.946970 Hz
 AQ 1.056000 sec
 RG 64.11
 DW 3520.000 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.0801197 sec
 TD0 1
 SF01 400.1722147 MHz
 NUC1 1H
 P1 60.50 usec
 PLW1 16.92099953 W

Additional Parameters
 Field 2215.815
 Lock Phase 211.219
 Lock Power -20.000
 Lock Gain 97.079
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 2048
 SF 400.1700000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00



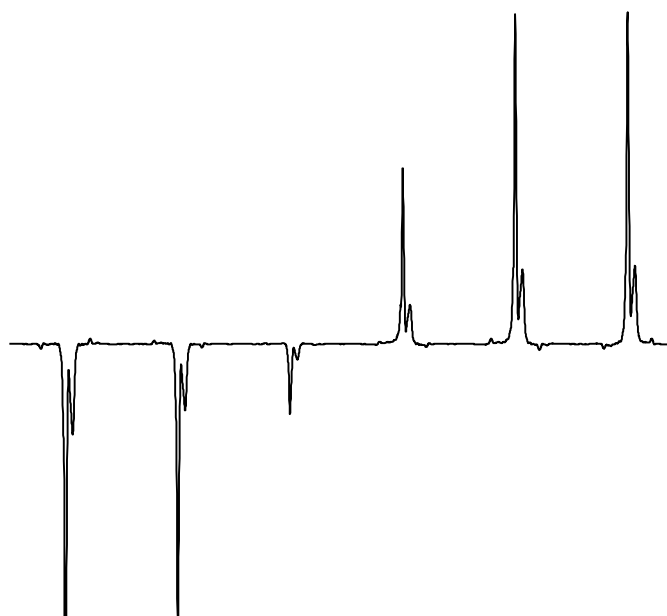
Report of parameter optimization

F1P = 5.609 ppm, F2P = 5.459 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 12.000000000 us, endval = 36.000000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	12.0000	454431061	-4388157	17667951.003
2	16.8000	363864570	-3786835	14128044.472
3	21.6000	143820776	-1163840	6234196.903
4	26.4000	2336372	-118993327	-2849641.292
5	31.2000	3166264	-305488890	-10234568.210
6	36.0000	3622098	-375064369	-12569108.890

Parameter optimization for P1 finished.
 ZERO at experiment 3.547234: P1 = 24.226723 us



Report of parameter optimization

F1P = 5.609 ppm, F2P = 5.459 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 36.300003052 us, endval = 60.500000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	36.3000	5248814	-376461583	-12893588.723
2	41.1400	3156846	-271424942	-9455453.268
3	45.9800	1118337	-65754924	-2280142.631
4	50.8200	164228472	-2743717	5958820.051
5	55.6600	308395534	-5659847	11193336.582
6	60.5000	310364993	-4305939	11395382.254

Parameter optimization for P1 finished.
 ZERO at experiment 3.285912: P1 = 47.363814 us



***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 16.9 W 12.0 us
 16.9 W 12.0 us 12.1 us 0.8%

 SHIM SEQUENCE
 topshim ld ss ordmax=6 convcomp <pass>

NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 0.1% Ethylbenzene (EB) in Chloroform-D (Z10120)
 1H sensitivity (NPT_1H_sensitivity, spin rate 20 Hz)

SINO (2.0 ppm) [achieved]: Signal (3.00 to 2.00 ppm), Noise (6.45 to 4.45 ppm) [366.1] <n/a>
 SINO (200.0 Hz) [achieved/rated]: Signal (3.00 to 2.00 ppm), Noise (5.46 to 4.96 ppm) [402.6 >= 300.0] <pass>



Bruker BioSpin

NPT_1H_sensitivity

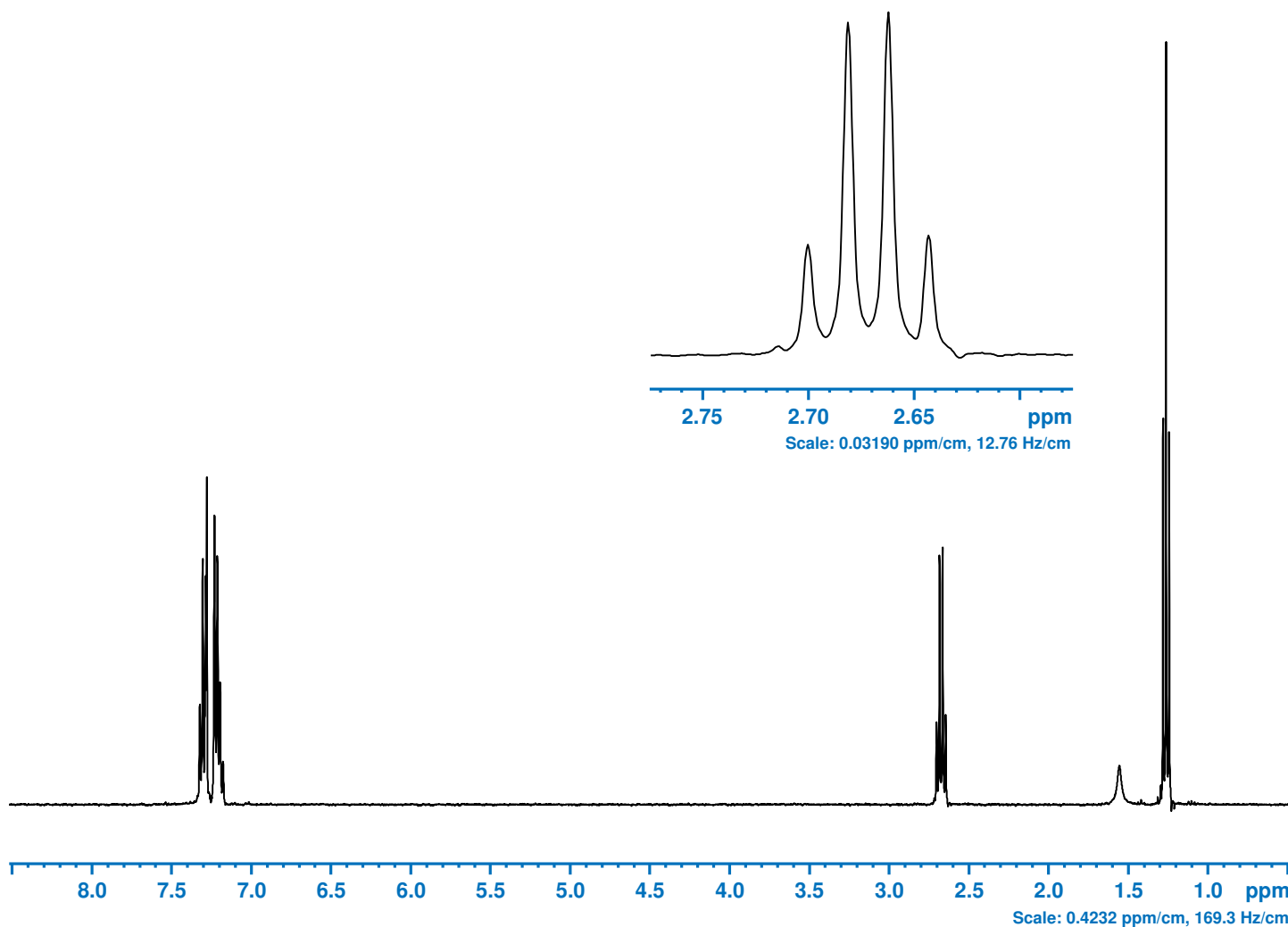
Current Data Parameters
 NAME NPT_1H_sensitivity
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 15.53 h
 INSTRUM spect
 PROBHD Z108618_0547 ()
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 4025.765 Hz
 FIDRES 0.245713 Hz
 AQ 4.0697856 sec
 RG 202.77
 DW 124.200 usec
 DE 6.50 usec
 TE 294.9 K
 D1 113.57360077 sec
 TDO 1
 SFO1 400.1716007 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 17.20400047 W

Additional Parameters
 Field 2183.400
 Lock Phase 223.325
 Lock Power -30.000
 Lock Gain 115.746
 Lock DC -75.000
 Lock Shift 7.240
 Loop Gain -12.000
 Loop Time 0.400
 Loop Filter 100.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 16384
 SF 400.1700028 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

SHIM SEQUENCE
 topshim 1d ss ordmax=6 <pass>



NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 40% Dioxane in Benzene-D6 (ASTM) (Z10163)
 13C lineshape with sample rotation (NPT_13C_lineshape_wrot, spin rate 20 Hz)
 Decoupling power PLW12=172 mW, PLW13=86.0 mW

Line width [achieved/rated]: at 0.11% of signal height [3.1 Hz <= 4.0 Hz] <pass>
 Line width [achieved/rated]: at 0.55% of signal height [1.2 Hz <= 2.0 Hz] <pass>
 Line width [achieved/rated]: at 50% of signal height [0.07 Hz <= 0.20 Hz] <pass>
 Spinning side band [achieved]: at +20 Hz [0.1%] <n/a>



Bruker BioSpin

NPT_13C_lineshape_wrot

Current Data Parameters
 NAME NPT_13C_lineshape_wrot
 EXPNO 2
 PROCNO 1

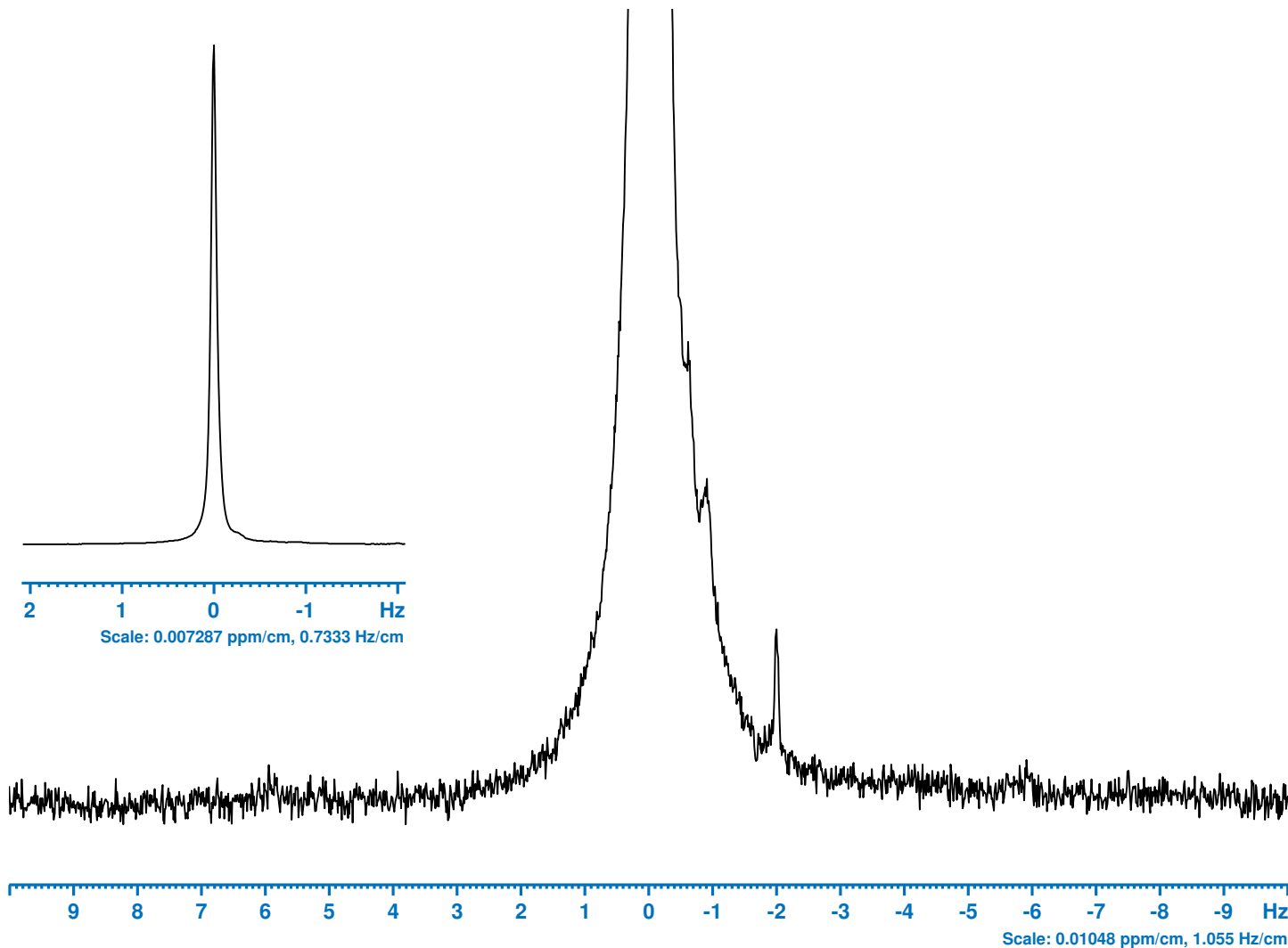
F2 - Acquisition Parameters
 Date_ 20251121
 Time 17.17 h
 INSTRUM spect
 PROBHD Z108618_0547 ()
 PULPROG zgpg
 TD 32768
 SOLVENT C6D6
 NS 4
 DS 0
 SWH 401.070 Hz
 FIDRES 0.024479 Hz
 AQ 40.8507729 sec
 RG 202.77
 DW 1246.667 usec
 DE 6.50 usec
 TE 295.4 K
 D1 34.14923096 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6294372 MHz
 NUC1 13C
 F1 8.66 usec
 PLW1 76.59700012 W
 SFO2 400.1713901 MHz
 NUC2 1H
 CPDPRG2 waltz65
 PCPD2 120.00 usec
 PLW2 17.20400047 W
 PLW12 0.17204060 W
 PLW13 0.08602031 W

Additional Parameters
 Field 2201.176
 Lock Phase 194.021
 Lock Power -26.000
 Lock Gain 103.119
 Lock DC -75.000
 Lock Shift 7.160
 Loop Gain 15.133
 Loop Time 0.047
 Loop Filter 1468.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 16384
 SF 100.6295375 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 4.00

SHIM SEQUENCE

topshim 1d ss ordmax=6 <pass>



NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 40% Dioxane in Benzene-D6 (ASTM) (Z10163)
 13C lineshape with sample rotation (NPT_13C_lineshape_wrot, spin rate 20 Hz)
 Decoupling power PLW12=172 mW, PLW13=86.0 mW



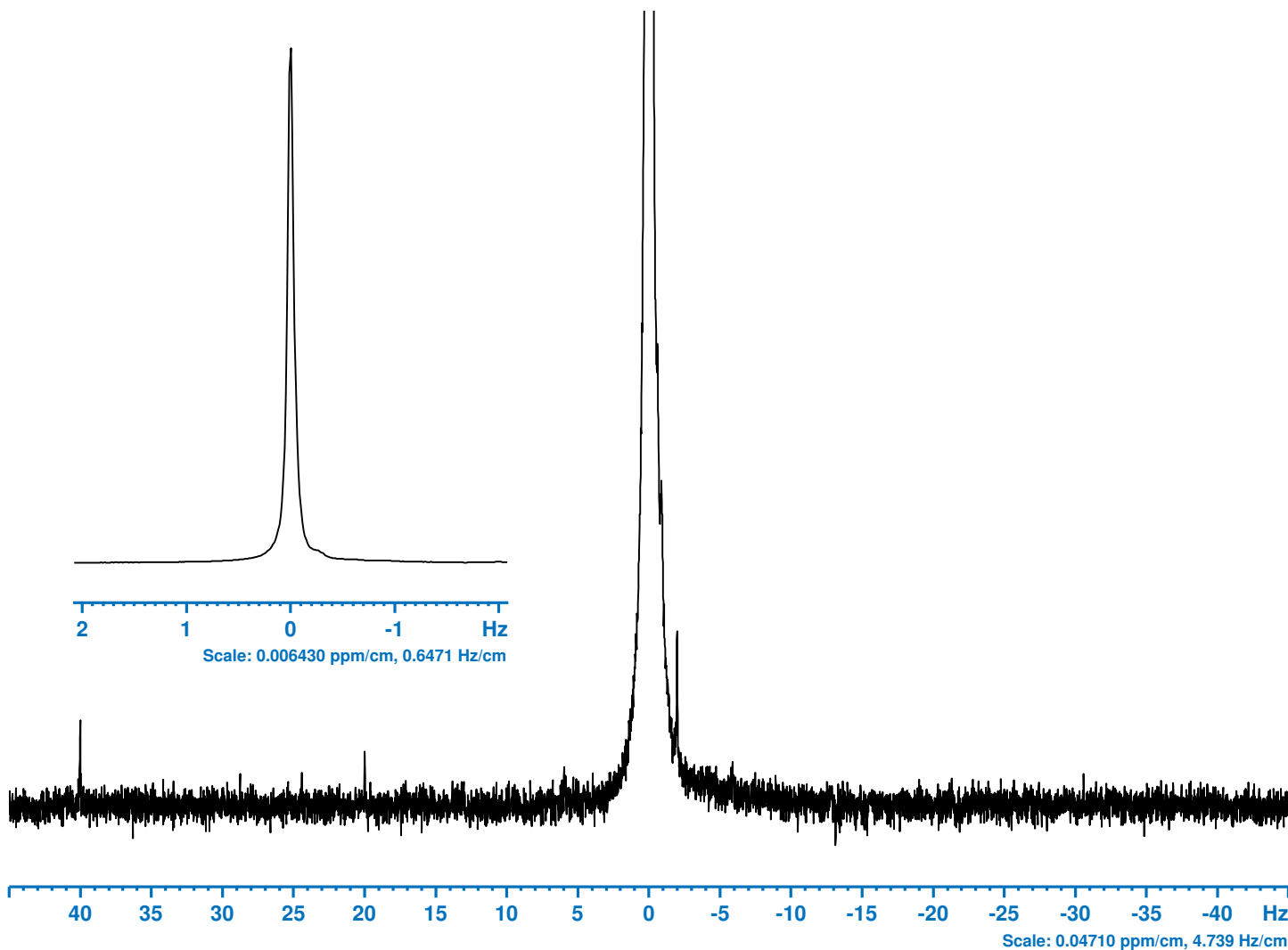
Bruker BioSpin

NPT_13C_lineshape_wrot

Current Data Parameters
 NAME NPT_13C_lineshape_wrot
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 17.17 h
 INSTRUM spect
 PROBHD Z108618_0547 (Z10163)
 PULPROG zgpg30
 TD 32768
 SOLVENT C6D6
 NS 4
 DS 0
 SWH 401.070 Hz
 FIDRES 0.024479 Hz
 AQ 40.8507729 sec
 RG 202.77
 DW 1246.667 usec
 DE 6.50 usec
 TE 295.4 K
 D1 34.14923096 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 100.6294372 MHz
 NUC1 13C
 P1 8.66 usec
 PLW1 76.59700012 W
 SFO2 400.1713901 MHz
 NUC2 1H
 CPDPRG2 waltz65
 PCPD2 120.00 usec
 PLW2 17.20400047 W
 PLW12 0.17204060 W
 PLW13 0.08602031 W

F2 - Processing parameters
 SI 16384
 SF 100.6295375 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 4.00



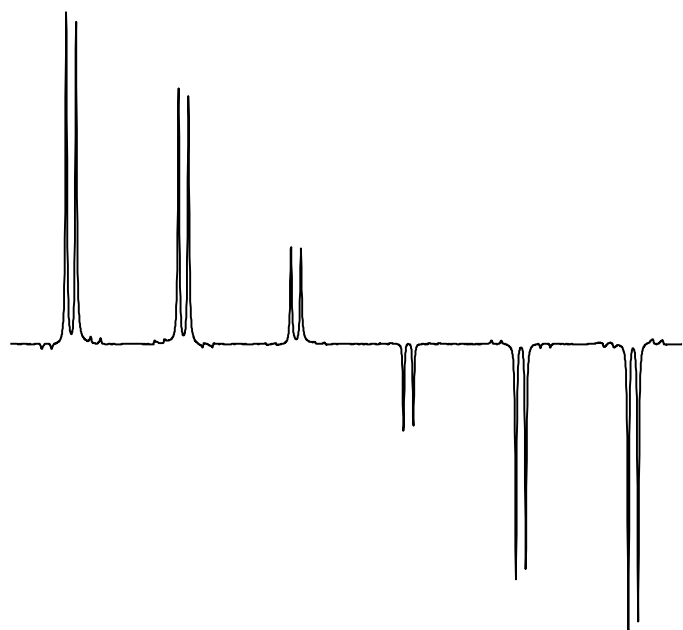
NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c, spin rate 0 Hz)
 Result: [90] = 8.8 us @ 74.2 W [270] = 26.0 us ==> [PDelay = 3*90 - 270] = 0.4 us
 ATTENTION: Updated PROSOL Tables with [8.7 us @ 76.6 W]
 Deviation from pulse target value (= 8.7 us): 1.1%



Bruker BioSpin

P90 13C pulse [achieved]: @ 74.2 W [8.8 us] <n/a>

NPT_1H_p90determinationf2_13c



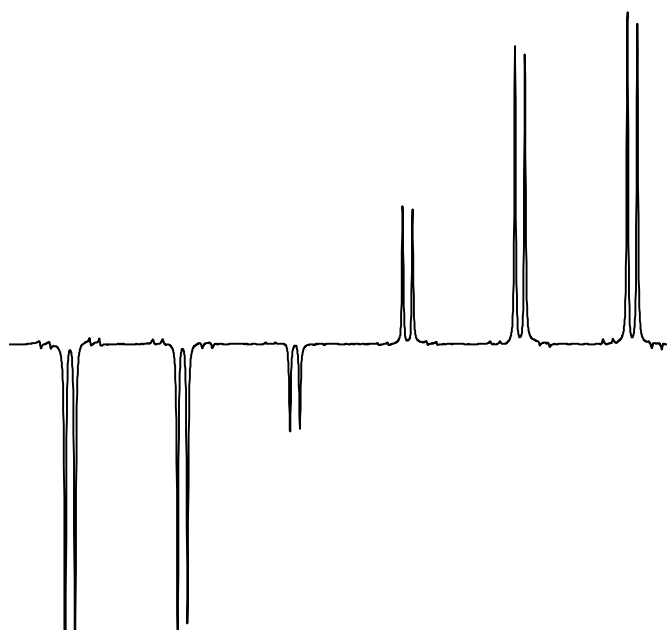
Report of parameter optimization

F1P = 3.079 ppm, F2P = 2.929 ppm

Linear optimization of P3 in 6 steps,
 PROCNO = 999
 starting at 0.000000000 us, endval = 17.319999695 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P3	Maximum point	Minimum point	Integral
1	0.0000	340534952	-5143523	15099046.830
2	3.4640	262776574	-3549452	11818573.526
3	6.9280	99433734	-1096307	4879949.488
4	10.3920	1197989	-88813828	-2992807.950
5	13.8560	3709095	-241531226	-9433792.879
6	17.3200	5039461	-296598969	-11583734.000

Parameter optimization for P3 finished.
 ZERO at experiment 3.528207: P3 = 8.757710 us



Report of parameter optimization

F1P = 3.079 ppm, F2P = 2.929 ppm

Linear optimization of P3 in 6 steps,
 PROCNO = 999
 starting at 17.600000381 us, endval = 35.200000763 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P3	Maximum point	Minimum point	Integral
1	17.6000	4570340	-297784469	-11735676.438
2	21.1200	3689850	-226332221	-9024415.621
3	24.6400	1127322	-68333759	-2914015.529
4	28.1600	107615354	-943457	4275410.106
5	31.6800	233127046	-2414944	9407879.942
6	35.2000	259433806	-4084094	10359166.363

Parameter optimization for P3 finished.
 ZERO at experiment 3.388372: P3 = 26.007071 us



Current Data Parameters
 NAME NPT_1H_p90determinationf2_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 15.35 h
 INSTRUM spect
 PROBHD Z108618_0547
 PULPROG decp90
 TD 1000
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 205.052 Hz
 FIDRES 0.410105 Hz
 AQ 2.4384000 sec
 RG 64.11
 DW 2438.400 usec
 DE 6.50 usec
 TE 294.8 K
 CNST2 139.0000000
 D1 1.73610795 sec
 D2 0.00359712 sec
 TD0 1
 SFO1 400.1712020 MHz
 NUC1 1H
 P1 6.00 usec
 PLW1 17.20400047 W
 SFO2 100.6278008 MHz
 NUC2 13C
 P3 35.20 usec
 PLW2 74.17900085 W

Additional Parameters
 Field 2215.856
 Lock Phase 211.219
 Lock Power -20.000
 Lock Gain 97.079
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 2048
 SF 400.1700000 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 0.10

***** P90 Pulse Determination History *****
 FLW90 P90 P90[det] Deviation
 74.2 W 8.7 us
 74.2 W 8.7 us 8.8 us 1.1%

SHIM SEQUENCE
 topshim ld ss ordmax=6 convcomp <pass>

NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 40% Dioxane in Benzene-D6 (ASTM) (Z10163)
 13C sensitivity (NPT_13C_sensitivity, spin rate 20 Hz)

SINO (40.0 ppm) [achieved/rated]: Signal (127.62 ppm), Noise (120.17 to 80.17 ppm) [214.3 >= 190.0] <pass>



Bruker BioSpin

NPT_13C_sensitivity

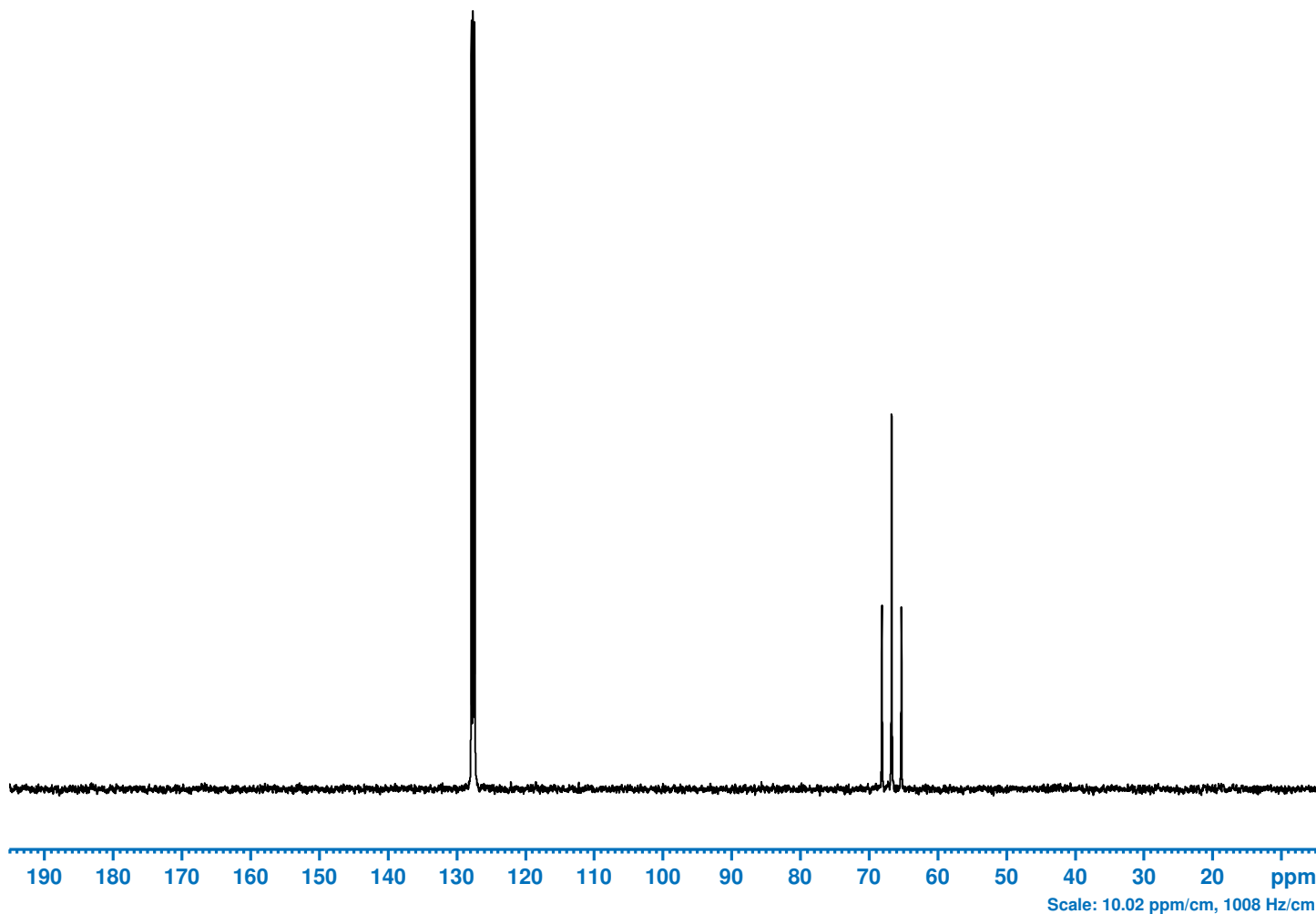
Current Data Parameters
 NAME NPT_13C_sensitivity
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 17.09 h
 INSTRUM spect
 PROBHD Z108618_0547 ()
 PULPROG zg
 TD 65536
 SOLVENT C6D6
 NS 1
 DS 0
 SWH 20161.291 Hz
 FIDRES 0.615274 Hz
 AQ 1.6252928 sec
 RG 202.77
 DW 24.800 usec
 DE 8.41 usec
 TE 294.9 K
 D1 120.00000000 sec
 TDO 1
 SFO1 100.6328876 MHz
 NUC1 13C
 P1 8.66 usec
 PLW1 76.59700012 W

Additional Parameters
 Field 2201.116
 Lock Phase 194.021
 Lock Power -26.000
 Lock Gain 103.119
 Lock DC -75.000
 Lock Shift 7.160
 Loop Gain -0.000
 Loop Time 0.200
 Loop Filter 300.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 131072
 SF 100.6228270 MHz
 WDW EM
 SSB 0
 LB 3.50 Hz
 GB 0
 PC 1.40

SHIM SEQUENCE
 topshim 1d ss ordmax=6 <pass>



NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 10% Ethylbenzene (EB) in Chloroform-D (Z10153)
 13C sensitivity with 1H decoupling (NPT_13C_sensitivity_dec1h, spin rate 20 Hz)

SINO (40.0 ppm) [achieved/rated]: Signal (127.96 ppm), Noise (120.00 to 80.00 ppm) [264.3 >= 190.0] <pass>



Bruker BioSpin

NPT_13C_sensitivity_dec1h

```

Current Data Parameters
NAME      NPT_13C_sensitivity_dec1h
EXPNO     2
PROCNO    1

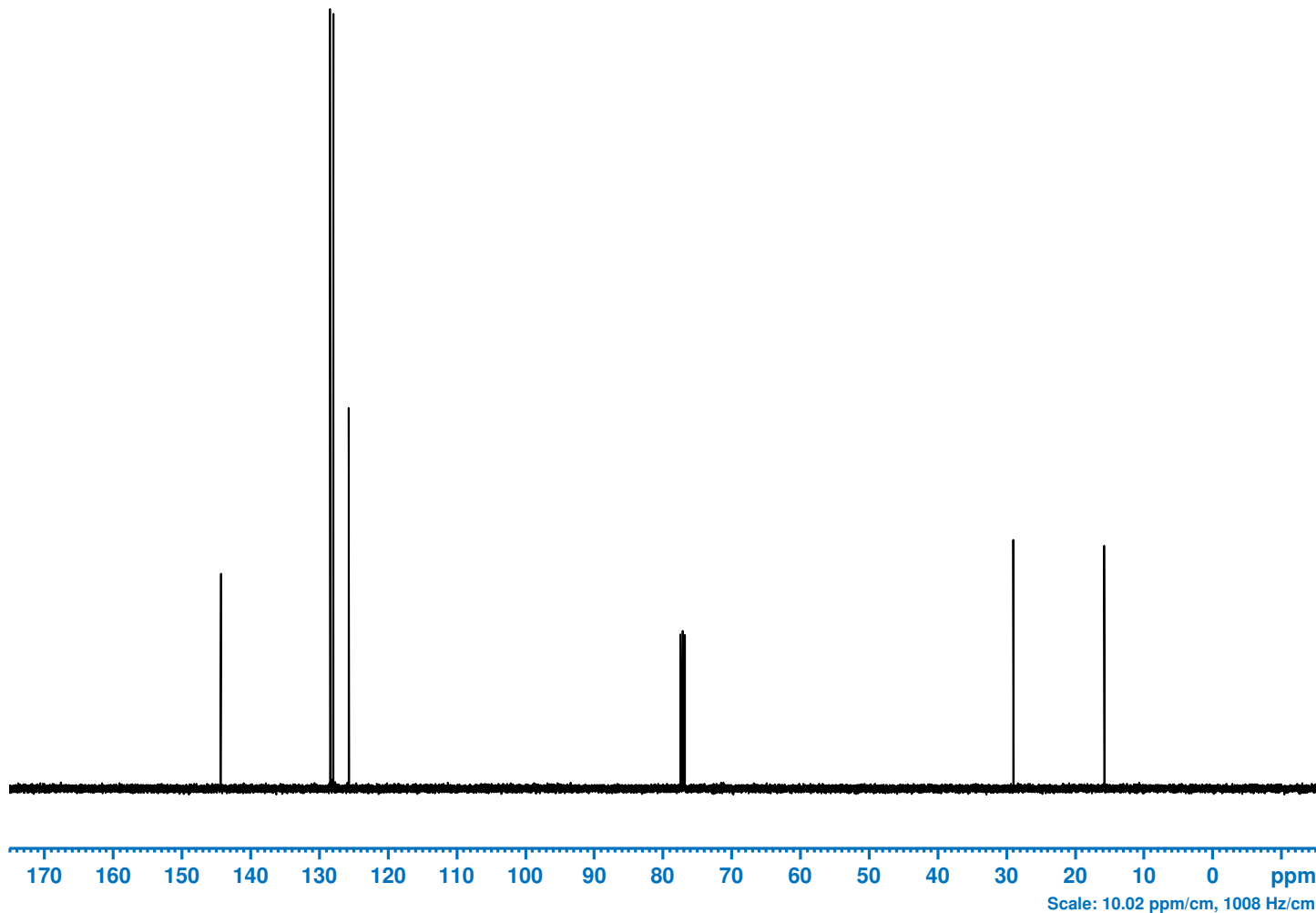
F2 - Acquisition Parameters
Date_     20251121
Time      17.04 h
INSTRUM    spect
PROBHD     Z108618_0547 (
PULPROG    zgpg
TD         262144
SOLVENT     CDCl3
NS         1
DS         0
SWH        20161.291 Hz
FIDRES     0.153818 Hz
AQ         6.5011711 sec
RG         202.77
DW         24.800 usec
DE         8.41 usec
TE         295.4 K
D1         132.49879456 sec
D11        0.03000000 sec
TD0        1
SFO1       100.6308751 MHz
NUC1       13C
F1         8.66 usec
PLW1       76.59700012 W
SFO2       400.1716007 MHz
NUC2       1H
CPDPRG[2]  waltz64
PCPD2      90.00 usec
PLW2       17.20400047 W
PLW12      0.30585000 W
PLW13      0.15384001 W

Additional Parameters
Field      2178.791
Lock Phase 212.208
Lock Power -30.000
Lock Gain  116.614
Lock DC    -75.000
Lock Shift 7.240
Loop Gain  -12.000
Loop Time  0.400
Loop Filter 100.000
Gas Flow   400 l/h

F2 - Processing parameters
SI         524288
SF         100.6228270 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.40
  
```

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-----
SHIM SEQUENCE
topshim ld ss ordmax=6 <pass>
-----
  
```



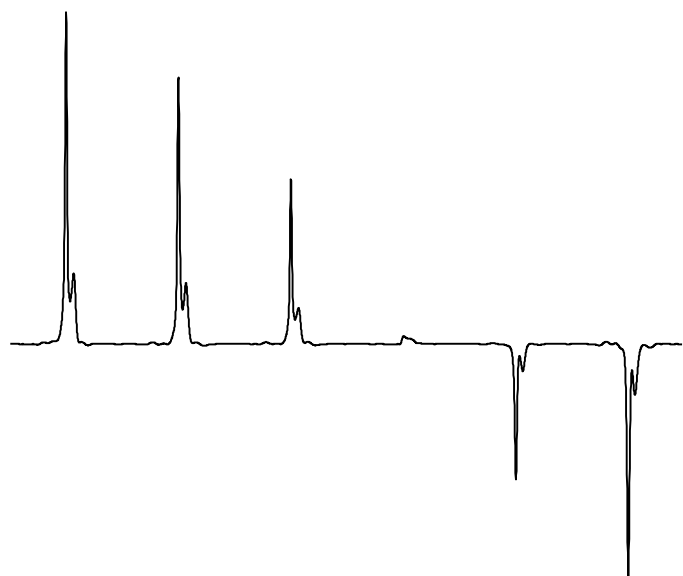
NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 Indirect P90 15N pulse calibration (NPT_1H_p90determinationf2_15n, spin rate 0 Hz)
 Result: [90] = 17.1 us @ 110 W [270] = 50.7 us ==> [PDelay = 3*90 - 270] = 0.6 us
 ATTENTION: Update PROSOL Tables (15N) failed
 Deviation (< 3.0%) from pulse target value (= 14.0 us): 22.1%



Bruker BioSpin

P90 15N pulse [achieved]: @ 110 W [17.1 us] <n/a>

NPT_1H_p90determinationf2_15n



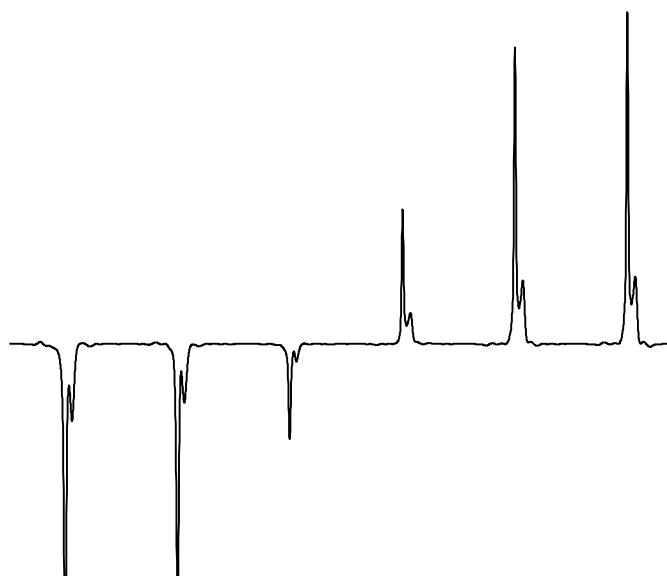
Report of parameter optimization

F1P = 5.606 ppm, F2P = 5.456 ppm

Linear optimization of P3 in 6 steps,
 PROCNO = 999
 starting at 0.000000000 us, endval = 28.000000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P3	Maximum point	Minimum point	Integral
1	0.0000	366513721	-1572303	14413911.847
2	5.6000	294509275	-2087492	11981371.561
3	11.2000	182106727	-1487699	7401686.610
4	16.8000	8634825	-501498	756485.464
5	22.4000	970334	-149935131	-5765405.111
6	28.0000	2607924	-257777446	-10808241.965

Parameter optimization for P3 finished.
 ZERO at experiment 4.054454: P3 = 17.104944 us



Report of parameter optimization

F1P = 5.606 ppm, F2P = 5.456 ppm

Linear optimization of P3 in 6 steps,
 PROCNO = 999
 starting at 34.200000763 us, endval = 68.400001526 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P3	Maximum point	Minimum point	Integral
1	34.2000	1741312	-321717513	-12548146.943
2	41.0400	1445108	-228979655	-9484124.597
3	47.8800	499346	-80681631	-3080368.622
4	54.7200	114210331	-784159	4255802.195
5	61.5600	251339767	-1666456	9088727.529
6	68.4000	281064907	-2368354	10027454.983

Parameter optimization for P3 finished.
 ZERO at experiment 3.413981: P3 = 50.711633 us



Current Data Parameters
 NAME NPT_1H_p90determinationf2_15n
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 15.38 h
 INSTRUM spect
 PROBHD Z108618_0547
 PULPROG decp90
 TD 200
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 142.045 Hz
 FIDRES 1.420455 Hz
 AQ 0.704000 sec
 RG 64.11
 DW 3520.000 usec
 DE 6.50 usec
 TE 294.9 K
 CNST2 88.5000000
 D1 0.33651409 sec
 D2 0.00564972 sec
 TD0 1
 SFO1 400.1722134 MHz
 NUC1 1H
 P1 8.00 usec
 PLW1 17.20400047 W
 SFO2 40.5519525 MHz
 NUC2 15N
 P3 68.40 usec
 PLW2 110.00000000 W

Additional Parameters
 Field 2216.031
 Lock Phase 211.219
 Lock Power -20.000
 Lock Gain 97.079
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 2048
 SF 400.1700000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 FC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 110 W 14.0 us
 110 W 14.0 us 17.1 us 22.1%

SHIM SEQUENCE

topshim 1d ss ordmax=6 convcomp <pass>

NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 90% Formamide in Dimethyl Sulfoxide-D6 (Z10187)
 15N sensitivity with 1H decoupling (NPT_15N_sensitivity_dec1h, spin rate 20 Hz)
 PCPD2 1H pulse determined using pulsecal: 85.42 us @ 306 mW



Bruker BioSpin

SINO (2.0 ppm) [achieved/rated]: Signal (112.79 ppm), Noise (118.50 to 116.50 ppm) [33.6 >= 20.0] <pass>

NPT_15N_sensitivity_dec1h

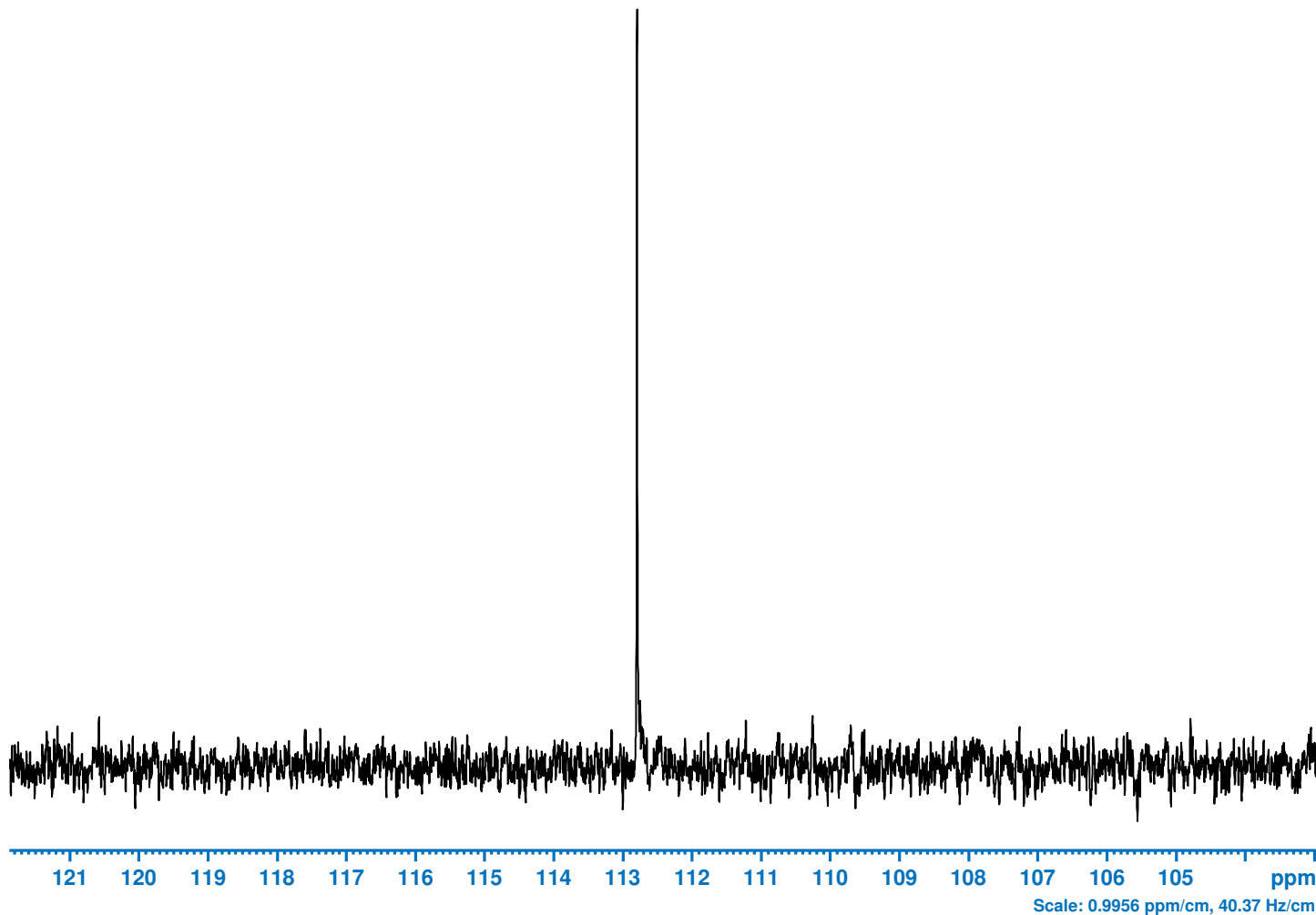
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Current Data Parameters
NAME      NPT_15N_sensitivity_dec1h
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20251121
Time      16.22 h
INSTRUM   spect
PROBHD    Z108618_0547 (
PULPROG   zgpg
TD         32768
SOLVENT   DMSO
NS         1
DS         0
SWH        807.494 Hz
FIDRES     0.049285 Hz
AQ         20.2899456 sec
RG         202.77
DW         619.200 usec
DE         6.50 usec
TE         295.1 K
D1         109.71009827 sec
D11        0.03000000 sec
TD0        1
SFO1       40.5534325 MHz
NUC1       15N
P1         14.00 usec
PLW1       110.00000000 W
SFO2       400.1729212 MHz
NUC2       1H
CPDPRG[2] waltz64
PCPD2      85.42 usec
PLW2       17.20400047 W
PLW12      0.30585000 W

Additional Parameters
Field      2224.959
Lock Phase 193.153
Lock Power -20.000
Lock Gain  119.434
Lock DC    -75.000
Lock Shift 2.490
Loop Gain  5.000
Loop Time  0.250
Loop Filter 500.000
Gas Flow   400 l/h

F2 - Processing parameters
SI         16384
SF         40.5488740 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```



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SHIM SEQUENCE
topshim ld ss ordmax=6 <pass>
-----
  
```

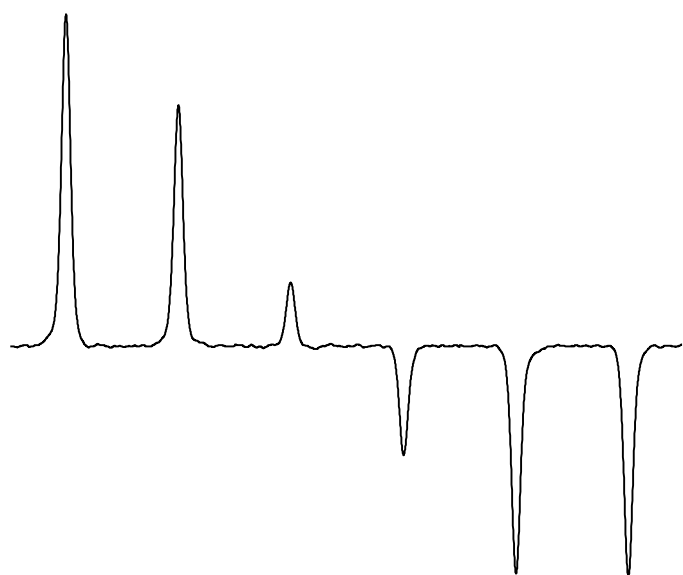
NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6 (Z10201)
 P90 31P pulse calibration (NPT_31P_p90determinationf1_31p, spin rate 0 Hz)
 Result: [180/2] = 14.6 us @ 13.9 W [360] = 55.6 us ==> [PDelay = 2*180 - 360] = 2.8 us
 ATTENTION: Updated PROSOL Tables with [15.0 us @ 13.2 W]
 Deviation from pulse target value (= 15.0 us): -2.7%



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P90 31P pulse [achieved/rated]: @ 13.9 W [14.6 us <= 15.0 us] <pass>

NPT_31P_p90determinationf1_31p



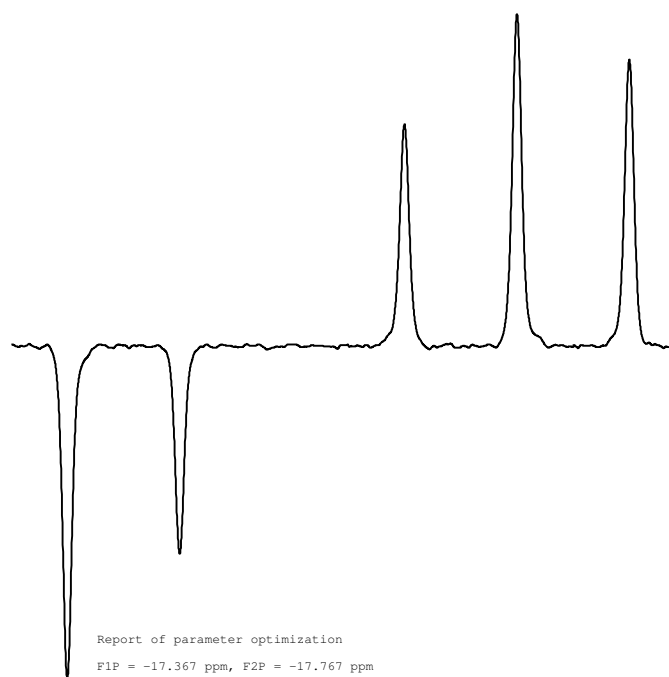
Report of parameter optimization

F1P = -17.367 ppm, F2P = -17.767 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 15.000000000 us, endval = 45.000000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	15.0000	275680338	-1620659	29220343.727
2	21.0000	200037251	-916744	21472394.701
3	27.0000	52706341	-2702749	5085907.344
4	33.0000	1356665	-90710627	-9210182.383
5	39.0000	1037585	-189064920	-20423565.195
6	45.0000	1210682	-191868268	-19914583.259

Parameter optimization for P1 finished.
 ZERO at experiment 3.367504: P1 = 29.205025 us



Report of parameter optimization

F1P = -17.367 ppm, F2P = -17.767 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 43.800003052 us, endval = 73.000000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	43.8000	2799514	-428321622	-46113162.873
2	49.6400	2034217	-266994697	-27444026.424
3	55.4800	2403739	-4369175	-215333.774
4	61.3200	285380874	-4189228	30966252.228
5	67.1600	426457496	-2314770	46201058.534
6	73.0000	368341611	-2574686	38864966.712

Parameter optimization for P1 finished.
 ZERO at experiment 3.015079: P1 = 55.568064 us



Current Data Parameters
 NAME NPT_31P_p90determinationf1_31p
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 16.32 h
 INSTRUM spect
 PROBHD Z108618_0547 ()
 PULPROG zg
 TD 1000
 SOLVENT Acetone
 NS 1
 DS 0
 SWH 401.070 Hz
 FIDRES 0.802139 Hz
 AQ 1.2466667 sec
 RG 202.77
 DW 1246.667 usec
 DE 6.50 usec
 TE 294.9 K
 D1 17.21400070 sec
 TDO 1
 SFO1 161.9889392 MHz
 NUC1 31P
 P1 73.00 usec
 PLW1 13.88996029 W

Additional Parameters
 Field 2239.856
 Lock Phase 226.078
 Lock Power -38.000
 Lock Gain 102.419
 Lock DC -75.000
 Lock Shift 2.040
 Loop Gain -2.000
 Loop Time 0.100
 Loop Filter 200.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 4096
 SF 161.9917850 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 14.2 W 15.0 us 14.2 us -5.3%
 14.8 W 15.0 us 14.2 us -2.7%
 13.9 W 15.0 us 14.6 us -2.7%

SHIM SEQUENCE
 topshim ld ss ordmax=6 convcomp <pass>

NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 0.0485 M Triphenyl Phosphate (TPP, [C₆H₅]₃PO₄) in Acetone-D₆ (Z10201)
 31P sensitivity (NPT_31P_sensitivity, spin rate 20 Hz)

SINO (5.0 ppm) [achieved]: Signal (-17.57 ppm), Noise (-4.33 to -9.33 ppm) [235.6] <n/a>



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NPT_31P_sensitivity

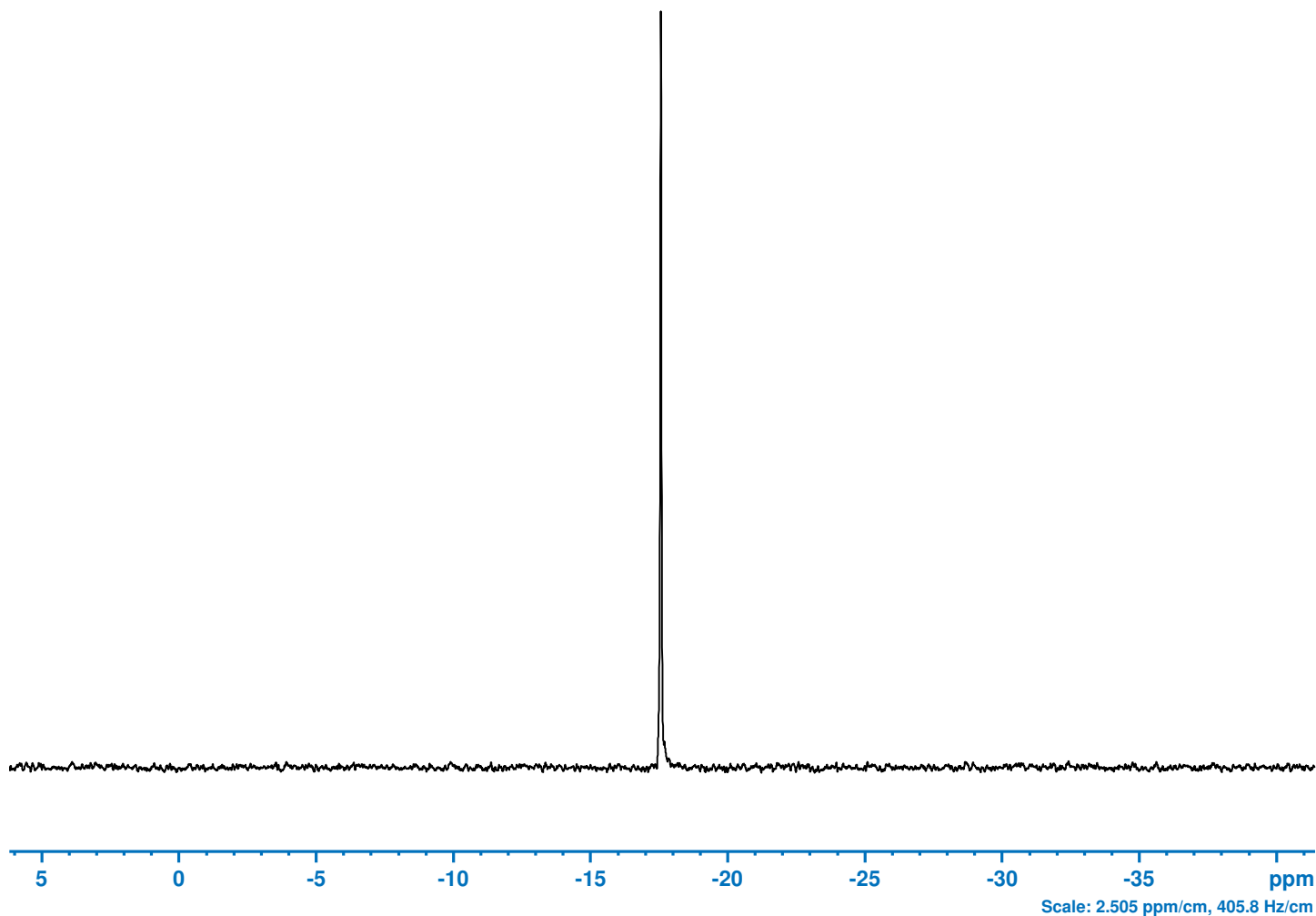
Current Data Parameters
 NAME NPT_31P_sensitivity
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 16.36 h
 INSTRUM spect
 PROBHD Z108618_0547 ()
 PULPROG zg
 TD 32768
 SOLVENT Acetone
 NS 1
 DS 0
 SWH 8116.883 Hz
 FIDRES 0.495415 Hz
 AQ 2.0185089 sec
 RG 202.77
 DW 61.600 usec
 DE 6.50 usec
 TE 294.9 K
 D1 118.98149872 sec
 TDO 1
 SFO1 161.9889328 MHz
 NUC1 31P
 P1 15.00 usec
 PLW1 13.15900040 W

Additional Parameters
 Field 2240.092
 Lock Phase 226.078
 Lock Power -38.000
 Lock Gain 100.211
 Lock DC -75.000
 Lock Shift 2.040
 Loop Gain -2.000
 Loop Time 0.100
 Loop Filter 200.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 16384
 SF 161.9917850 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

SHIM SEQUENCE
 topshim ld ss ordmax=6 convcomp <pass>



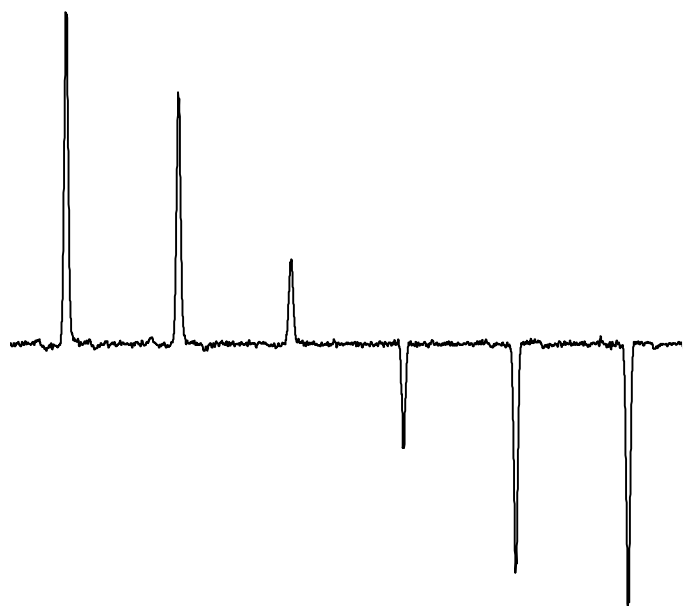
NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 0.05% Trifluorotoluene (TFT, a,a,a-CF₃CH₃) in Chloroform-D (Z10234)
 P90 19F pulse calibration (NPT_19F_p90determinationf1_19f, spin rate 0 Hz)
 Result: [180/2] = 14.8 us @ 22.8 W [360] = 57.9 us ==> [PDelay = 2*180 - 360] = 1.3 us
 ATTENTION: Updated PROSOL Tables with [15.0 us @ 22.2 W]
 Deviation from pulse target value (= 15.0 us): -1.3%



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P90 19F pulse [achieved/rated]: @ 22.8 W [14.8 us <= 15.0 us] <pass>

NPT_19F_p90determinationf1_19f



Report of parameter optimization

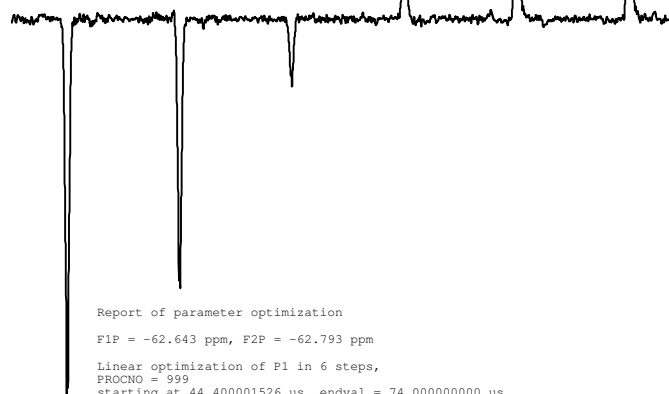
F1P = -62.643 ppm, F2P = -62.793 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 15.000000000 us, endval = 45.000000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	15.0000	437051001	-8913369	18554628.904
2	21.0000	332123736	-8901425	14297524.508
3	27.0000	111808612	-5563260	5197820.811
4	33.0000	6578562	-137409711	-4778478.450
5	39.0000	6987271	-301722399	-12039986.982
6	45.0000	10069958	-348491096	-14461018.354

Parameter optimization for P1 finished.
 ZERO at experiment 3.448637: P1 = 29.691823 us

15 20 25 30 35 40 45 us



Report of parameter optimization

F1P = -62.643 ppm, F2P = -62.793 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 44.400001526 us, endval = 74.000000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	44.4000	6255384	-381858667	-15088991.982
2	50.3200	8530774	-271899822	-10788379.547
3	56.2400	6072725	-68098882	-2644772.778
4	62.1600	174396842	-7560096	6489714.856
5	68.0800	322915700	-8172223	13163620.362
6	74.0000	334704031	-5135468	13885322.149

Parameter optimization for P1 finished.
 ZERO at experiment 3.280825: P1 = 57.902485 us

45 50 55 60 65 70 us

Current Data Parameters
 NAME NPT_19F_p90determinationf1_19f
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20251121
 Time 16.58 h
 INSTRUM spect
 PROBHD Z108618_0547 ()
 PULPROG zg
 TD 1000
 SOLVENT CDCl₃
 NS 1
 DS 0
 SWH 401.070 Hz
 FIDRES 0.802139 Hz
 AQ 1.2466667 sec
 RG 64.11
 DW 1246.667 usec
 DE 6.50 usec
 TE 294.9 K
 D1 4.31400013 sec
 TDO 1
 SF01 376.5123886 MHz
 NUC1 19F
 P1 74.00 usec
 PLW1 22.79875946 W

Additional Parameters
 Field 2184.584
 Lock Phase 199.415
 Lock Power -30.000
 Lock Gain 116.918
 Lock DC -75.000
 Lock Shift 7.240
 Loop Gain -12.000
 Loop Time 0.400
 Loop Filter 100.000
 Gas Flow 400 l/h

F2 - Processing parameters
 SI 16384
 SF 376.5360040 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 21.8 W 15.0 us
 22.8 W 15.0 us 14.8 us -1.3%

SHIM SEQUENCE

topshim 1d ss ordmax=6 convcomp <pass>

NMR TEST SERVICE *** System: AV III (400.17 MHz) *** TopSpin 3.5 pl 7
 Probe: Z108618_0547 PA BBO 400S1 BBF-H-D-05 Z PLUS *** Sample Depth: 20 mm
 Sample: 0.05% Trifluorotoluene (TFT, a,a,a-CF₃C₆H₅) in Chloroform-D (Z10234)
 19F sensitivity with 1H decoupling and LB=0.5 (NPT_19F_sensitivity_lb05_dec1h, spin rate 20 Hz)

SINO (1.0 ppm) [achieved/rated]: Signal (-62.00 to -63.00 ppm), Noise (-57.00 to -58.00 ppm) [487.2 >= 275.0] <pass>
 Line width [achieved]: at 50% of signal height [0.80 Hz] <n/a>



Bruker BioSpin

NPT_19F_sensitivity_lb05_dec1h

```
Current Data Parameters
NAME      NPT_19F_sensitivity_lb05_dec1h
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20251121
Time      16.54 h
INSTRUM   spect
PROBHD    Z108618_0547 (
PULPROG   zgpg30
TD        45178
SOLVENT    CDCl3
NS         1
DS         0
SWH        7530.121 Hz
FIDRES     0.333353 Hz
AQ         2.9998193 sec
RG         202.77
DW         66.400 usec
DE         6.50 usec
TE         294.9 K
D1         35.00000000 sec
D11        0.03000000 sec
D12        0.00002000 sec
TD0        1
SFO1       376.5126588 MHz
NUC1       19F
P1         15.00 usec
PLW1       21.81699944 W
SFO2       400.1732014 MHz
NUC2       1H
CPDPRG2    waltz64
PCPD2      90.00 usec
PLW2       17.20400047 W
PLW12      0.30585000 W

Additional Parameters
Field      2184.516
Lock Phase 199.415
Lock Power -30.000
Lock Gain  116.918
Lock DC    -75.000
Lock Shift 7.240
Loop Gain  -12.000
Loop Time  0.400
Loop Filter 100.000
Gas Flow   400 l/h

F2 - Processing parameters
SI         65536
SF         376.5360040 MHz
WDW        EM
SSB        0
LB         0.50 Hz
GB         0
PC         4.00
```

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SHIM SEQUENCE
topshim ld ss ordmax=6 convcomp <pass>
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```

