

NMR Test Spectrometer

Report Name: 2021-09-30

AV NEO (750 MHz) HCAB-76_00003

Content:

- Configuration Information (uxnmr.info)
- IP Config Information
- Probe: Z5663_0001 / 2021-09-22
- Probe: Z5661_0001 / 2021-09-29



● Configuration Information uxnmr.info

CONFIGURATION INFORMATION

=====

```
Path      : /opt/topspin/conf/instr/spect/uxnmr.info
Date      : Tue Sep 14 10:13:53 2021
Release   : TopSpin 4.1.3
Installed in : /opt/topspin
Host      : BladeEpu
OS        : CentOS Linux release 7.2.1511 (Core)
SPECTR-OS : Version 4.1.156.20210628
CPU       : Intel(R) Core(TM) i5-8400H CPU @ 2.50GHz (8 cores at 3766 MHz with Hyperthreading)
User      : root (root)
System    : Avance Neo 750 NMR spectrometer
1H-frequency : 750.3 MHz
Description : Avance
Bruker Order : HCAB-76_00003
Configured in: BladeEpu:/opt/topspin/conf/instr/spect
```

AQ-Rack:

```
- SCU: AV4I SCU SYSTEM CONTROL UNIT Z162978/00387 ECL 02.00
- {EPU}: AV4I SCU SYSTEM CONTROL UNIT Z162978/00387 ECL 02.00
- {GTU}: AV4I SCU SYSTEM CONTROL UNIT Z162978/00387 ECL 02.00
Location: slot 7 in rack 1
Connection: at IP 192.168.180.18 via PCIe #4
Firmware Version: 20210312125813
- Gradient resolution: 1.0 us
Devices: MTD at /dev/mtdd2, RTD at /dev/bbu/rtdd4.4, GPROC at /dev/bbu/gproc4.7
Sequencer: GCube, TCube
- GCube1
- TCube1
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/06700 ECL 02.05
Location: slot 3 in rack 1
Connection: at IP 192.168.180.38 via PCIe #9
Firmware Version: 20210312121750
Devices: MTD at /dev/mtdd11, DRX at /dev/bbu/drxd9.5, RTD at /dev/bbu/rtdd9.4
Sequencer: FCube
- FCube1
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/06699 ECL 02.05
Location: slot 4 in rack 1
Connection: at IP 192.168.180.46 via PCIe #11
Firmware Version: 20210312121750
Devices: MTD at /dev/mtdd20, DRX at /dev/bbu/drxd11.5, RTD at /dev/bbu/rtdd11.4
Sequencer: FCube
- FCube2
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/06698 ECL 02.05
Location: slot 5 in rack 1
Connection: at IP 192.168.180.54 via PCIe #13
Firmware Version: 20210312121750
Devices: MTD at /dev/mtdd29, DRX at /dev/bbu/drxd13.5, RTD at /dev/bbu/rtdd13.4
Sequencer: FCube
- FCube3
- PSM-A: AV4 PSM-A Z149510/02732 ECL 03.01
- HPR2: - HPR2/2 Cover2: HPR2/2 Cover2N Z178831/00167 ECL 00.00
HPR2: - HPR2/2 preamplifier connected via AqRack
Type : HPR2/2
Controller: Cover2
no LED display for tuning and matching
Module 1 : HPLNA 1H19F (reflection meter with CRP-Bias capability)
PN=Z103207, SN=00209 from 20210618
Module 2 : 2H
PN=Z003475, SN=00210 from 20190312
Module 3 : HPLNA BB31P (reflection meter without CRP-Bias capability)
PN=Z111095, SN=00223 from 20190705
Module 4 : 13C/79Br
PN=Z003526, SN=00207 from 20180612
```

```
Module 5 : HPLNA BB31P (reflection meter without CRP-Bias capability)
PN=Z111095, SN=00221 from 20190315
Module 6 : 31P
PN=Z102451, SN=00200 from 20210622
```

```
- HPLNA 1H19F: HPLNA 1H MODULE 750 Z103207/00209 ECL 06.05
- 2H: HPR2/2 2H MODULE 750 Z003475/00210 ECL 07.00
- HPLNA BB31P: HPLNA XBB 31P MODULE 750 Z111095/00223 ECL 04.04
- 13C/79Br: HPR2/2 13C MODULE 750 Z003526/00207 ECL 08.00
- HPLNA BB31P: HPLNA XBB 31P MODULE 750 Z111095/00221 ECL 04.04
- 31P: HPR2/2 31P MODULE 750 Z102451/00200 ECL 07.01
- RACK: AV4I AQS CHASSIS Z175600/00370 ECL 00.00
- PSM-48V: AV4 PSM-48V Z149850/04474 ECL 01.02
- PSM-D: AV4 PSM-D Z149520/02583 ECL 01.01
- FANTRAY: AV4I AQS FAN TRAY Z175900/00312 ECL 00.00
- REF 1200: AV4 REFERENCE 1200 Z148270/02367 ECL 02.02
```

Transmitters at the spectrometer subnet:

```
BLA-W144060-000236 W144060/000236 ECL 41:
- TCP/IP address = 192.168.99.13
- Firmware VS = 20210223
- Amplifier = AV4 BLABB1000 15-600: W144060/000236 ECL 41
- Controller = BLA CONTROL BOARD 7: W133936/025326 ECL 40
BLA-W144060-000235 W144060/000235 ECL 41:
- TCP/IP address = 192.168.99.12
- Firmware VS = 20210223
- Amplifier = AV4 BLABB1000 15-600: W144060/000235 ECL 41
- Controller = BLA CONTROL BOARD 7: W133936/025302 ECL 40
BLA-W144058-000036 W144058/000036 ECL 02:
- TCP/IP address = 192.168.99.11
- Firmware VS = 20201119
- Amplifier = AV4 BLAH1000 700-900: W144058/000036 ECL 02
- Controller = BLA CONTROL BOARD 7: W133936/023492 ECL 40
LTX Z109892/00208 ECL 02.02:
- TCP/IP address = 192.168.99.10
- Amplifier = BSMS/2 LOCK TRANSCEIVER 750: Z109892/00208 ECL 02.02

BSMS: BSMS/2 connected to ethernet
- TCP/IP address = 192.168.99.10
- ELCB firmware version = 20210212
- ELCB = BSMS/2 ELCB: Z100818/09250 ECL 07.03
- GAB current limits = 0.0/X, 0.0/Y, 10.0/Z (in A)
- Shim System = BOSS3-SB
- SCB channels = 40
- Shim matrix file: 292721aa.dat
- Active shims: Z Z2 Z3 Z4 Z5 X XZ XZ2 (X2-Y2) XY Y YZ YZ2 (X2-Y2)Z2 XZ4 XZ3 Z6 (X2-Y2)Z YZ4 YZ3 XYZ2 XYZ XZ3 X3
- Magnet polarity: SN (Bruker), uses standard H0 polarity
- L-TRX = BSMS/2 LOCK TRANSCEIVER 750: Z109892/00208 ECL 02.02
- Lock: on L-TRX board, supports 2H
- VTU_SPB = BSMS/2 SPB-E SENSOR & PNEUMATIC BD: Z115192/00870 ECL 05.05
- VTU_VPSB1 = AV4 VARIABLE POWER SUPPLY BD DC-E: Z140144/00301 ECL 01.02
```

```
VTU: in BSMS/2 connected to ethernet
- TCP/IP address = 192.168.99.10
```

Line Distribution Units at the spectrometer subnet:

```
Line Distribution Unit 1: PDU1
- TCP/IP address = 192.168.99.99
Line Distribution Unit 2: PDU2
- TCP/IP address = 192.168.99.101
```

● Configuration Information uxnmr.info

```
RF cable connections (detected)
-----
TRX1 NORM output -> input 1 of transmitter 3 (AV4 BLAH1000 700-900 W144058/000036 at TCP/IP 192.168.99.11)
TRX1 AUX output -> input 1 of transmitter 4 (BSMS/2 LOCK TRANSCEIVER 750 Z109892/00208 at TCP/IP 192.168.99.10)
TRX2 NORM output -> input 1 of transmitter 2 (AV4 BLABB1000 15-600 W144060/000235 at TCP/IP 192.168.99.12)
TRX2 AUX output -> open
TRX3 NORM output -> input 1 of transmitter 1 (AV4 BLABB1000 15-600 W144060/000236 at TCP/IP 192.168.99.13)
TRX3 AUX output -> open

Blanking cable connections (detected)
-----
transmitter 1 = AV4 BLABB1000 15-600 W144060/000236 at TCP/IP 192.168.99.13:
- amplifier B-1000W uses blanking 3
- amplifier B-100W uses blanking 3

transmitter 2 = AV4 BLABB1000 15-600 W144060/000235 at TCP/IP 192.168.99.12:
- amplifier B-1000W uses blanking 2
- amplifier B-100W uses blanking 2

transmitter 3 = AV4 BLAH1000 700-900 W144058/000036 at TCP/IP 192.168.99.11:
- amplifier 1H-1000W uses blanking 1
- amplifier 1H-100W uses blanking 1

transmitter 4 = BSMS/2 LOCK TRANSCEIVER 750 Z109892/00208 at TCP/IP 192.168.99.10:
- amplifier 2H-5W uses blanking 9

Preamplifier connections (detected)
-----
Tune-TRX1 -> HPLNA 1H19F -> REC1
Tune-TRX1 -> 2H -> REC1
Tune-TRX2 -> HPLNA BB31P -> REC2
Tune-TRX2 -> 13C/79Br -> REC2
Tune-TRX3 -> HPLNA BB31P -> REC3
Tune-TRX3 -> 31P -> REC3
```

● IP Config Information

```
en01: flags=4163<UP,BROADCAST,RUNNING,MULTICAST> mtu 1500
inet 149.236.99.1 netmask 255.255.255.0 broadcast 149.236.99.255
inet6 fe80::bee9:2fff:fea0:537c prefixlen 64 scopeid 0x20<link>
ether bc:e9:2f:a0:53:7c txqueuelen 1000 (Ethernet)
RX packets 2526350746 bytes 3704559932092 (3.3 TiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 698848627 bytes 53990698181 (50.2 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
device interrupt 16 memory 0x90200000-90220000

eno2: flags=4163<UP,BROADCAST,RUNNING,MULTICAST> mtu 1500
inet 132.229.125.41 netmask 255.255.255.0 broadcast 132.229.125.255
inet6 fe80::88d8:b392:8bfa:f470 prefixlen 64 scopeid 0x20<link>
ether bc:e9:2f:a0:53:7d txqueuelen 1000 (Ethernet)
RX packets 15670460 bytes 5044569948 (4.6 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 24983825 bytes 5071985199 (4.7 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
device memory 0x90100000-9017ffff

lo: flags=73<UP,LOOPBACK,RUNNING> mtu 65536
inet 127.0.0.1 netmask 255.0.0.0
inet6 ::1 prefixlen 128 scopeid 0x10<host>
loop txqueuelen 1000 (Local Loopback)
RX packets 260513993 bytes 171724482399 (159.9 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 260513993 bytes 171724482399 (159.9 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
```

BBI 750WB H-BB-D-05 Z

750 MHz

Probe ID: Z5663_0001

Inspection Lot: 2021-09-22

Oct 1, 2021

NMR TEST SERVICE

● Probe NMR Test Data: **BBI 750WB H-BB-D-05 Z**

Probe Related Information

EC-Level	0
Sample Depth (standard) [mm]	20
Sample Depth (water-based Solvents) [mm]	20
Gas Compensation	unknown
Gradient System	Z
ATM Accessory	false
Temperature Sensor Type	BTO2000
Proton Frequency [MHz]	750
Diameter [mm]	5.0

Spectrometer Related Information

Type	AV NEO
CF Frequency [MHz]	750.30
Shim System	BOSS3-SB
Shim System Offset	Standard
Software	TopSpin 4.1.3
OS	CentOS Linux release 7.9.2009 (Core)
Host Name	CZC1228YHM
Magnet System	SB
Magnet Coil No	BR.091075110
Dewar No	BD228972
Helium Level	91%
System Number	HCAB-76_00003

● PICS Data

Z5663_0001.ph

```
Z5663_0001.ph
=====
$Bis,1,20210909,2048,PICS,1#
$Production,Z5663,0001,0.00,,BCH,19990219#
$Name,BBI 750WB H-BB-D-05 2#
$ProbeCompatibility,1.0,WB,5,750#
$ProbeType,1.0,HR#
$ProbeSample,1.0,5,20#
$ProbeTemperature,1.0,BTO2000,-150,180#
$ProbeAllCoils,1.0,2#
$ProbeCoil,1.0,1,18.0,2,1H,D#
$ProbeCoil,1.0,2,22.0,1,BB#
$ProbeChannel,1.0,1H,,0,30,,0.4,0.1,FALSE#
$ProbeChannel,1.0,D,-1,-1,0,28,,0.4,0.1,0#
$ProbeZ-Grad,1.0,,5.00,10#
$ProbeXYZ-Grad,1.0,,5.00,5.00,5.03,10,10,10#
$ProbeBB,2.0,2,31P-15N,0,0.000,,,,#
$ProbeBBSets,1.0,31P,,210,5,0.4,0.1#
$ProbeBBSets,1.0,13C,,300,5,0.4,0.1#
$ProbeBBSets,1.0,15N,,600,5,0.4,0.1#
$ProbeElec,1.0,0,0,0.0,0.0#
$EndBis,4F,10#
```

● Required Samples **BBI 750WB H-BB-D-05 Z**

Z10120	0.1% Ethylbenzene (EB) in Chloroform-D
Z10201	0.0485 M Triphenyl Phosphate (TPP, $[C_6H_5]_3PO_4$) in Acetone-D6
Z10263	100 mM Urea- ^{15}N , 100 mM Methanol- ^{13}C in Dimethyl Sulfoxide-D6
Z10701	0.3% Chloroform in Acetone-D6

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)

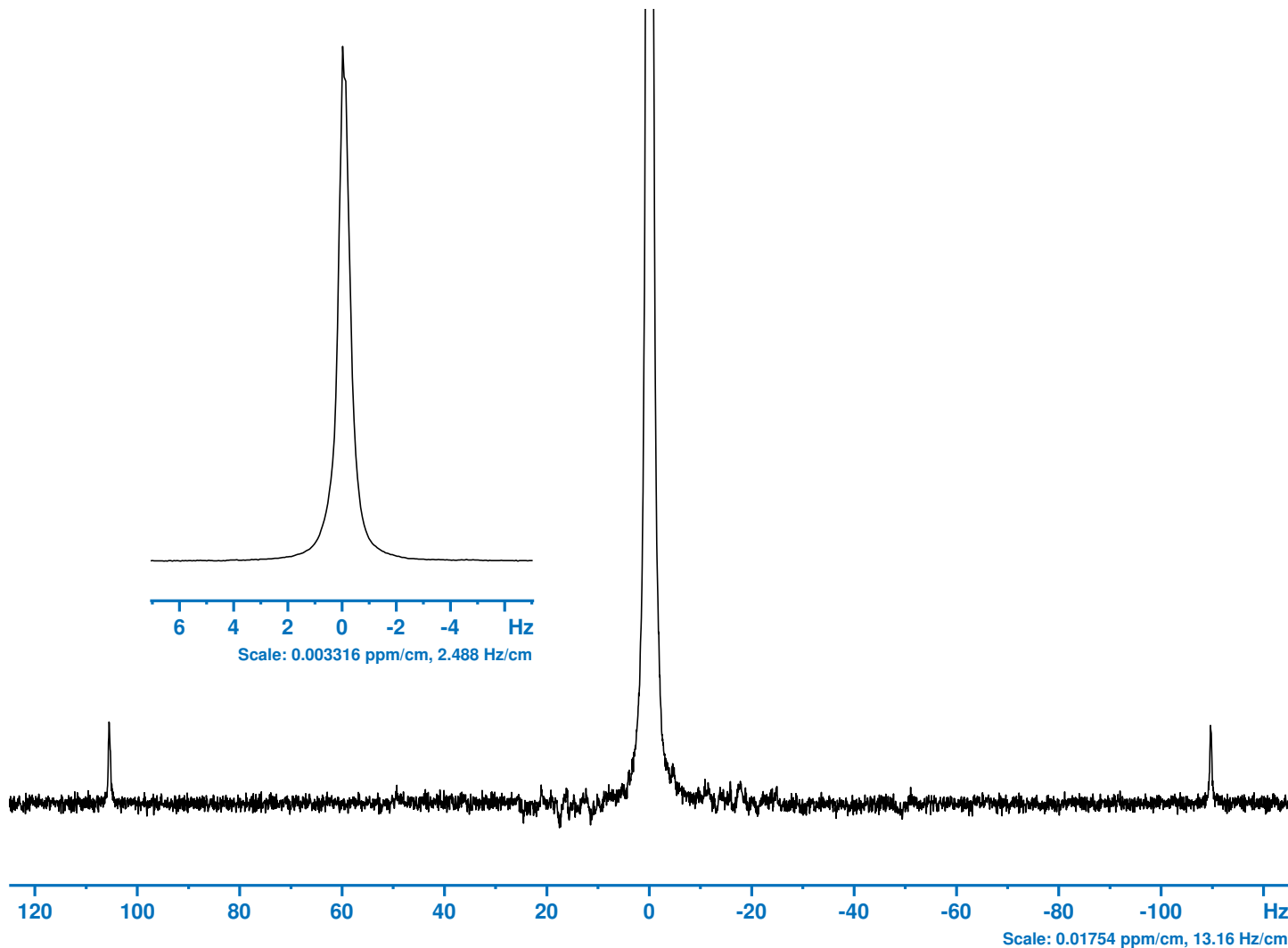
Line width [achieved]: at 0.11% of signal height [11.2 Hz] <n/a>
 Line width [achieved]: at 0.55% of signal height [5.0 Hz] <n/a>
 Line width [achieved]: at 50% of signal height [0.48 Hz] <n/a>



Bruker BioSpin

NPT_1H_lineshape_nrot

Current Data Parameters	
NAME	NPT_1H_lineshape_nrot
EXPNO	5
PROCNO	1
F2 - Acquisition Parameters	
Date_	20210928
Time	8.57 h
INSTRUM	Avance
PROBHD	Z5663_0001 (BB)
PULPROG	zg30
TD	32768
SOLVENT	Acetone
NS	1
DS	0
SWH	1000.000 Hz
FIDRES	0.061035 Hz
AQ	16.3840008 sec
RG	101
DW	500.000 usec
DE	6.50 usec
TE	295.0 K
D1	9.11600113 sec
TD0	1
SFO1	750.3057787 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
PLW1	14.90600014 W
F2 - Processing parameters	
SI	8192
SF	750.3060287 MHz
WDW	no
SSB	0
LB	0 Hz
GB	0
PC	4.00
Additional Parameters	
Field	1887.448
Lock Phase	30.000
Lock Power	-34.000
Lock Gain	92.414
Lock DC	-70.000
Lock Shift	2.040
Loop Gain	15.133
Loop Time	0.047
Loop Filter	1468.000
Gas Flow	670 l/h



SHIM SEQUENCE
 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)



Bruker BioSpin

NPT_1H_lineshape_nrot

```
# Tue Sep 28 06:57:40 2021
##$PROBEIDENTIFIER=Z5663_0001
##$PROBENAME=BBI 750WB H-BB-D-05 Z
##$SHIMID=292721
#
# Active Shim Gradients
#
Z -6180
Z2 4046
Z3 123
Z4 -3167
Z5 919
Z6 4297
Z7 -28718
Z8 21744
X -3703
XZ 1940
XZ2 178
XZ3 -6611
XZ4 8461
XZ5 2363
Y 1660
YZ 987
YZ2 3994
YZ3 638
YZ4 -2766
YZ5 1084
XY -17669
XYZ 169
XYZ2 47
XYZ3 1693
XYZ4 -983
XYZ5 269
(X2-Y2) 6710
(X2-Y2) Z 1947
(X2-Y2) Z2 -605
(X2-Y2) Z3 4427
(X2-Y2) Z4 -2701
(X2-Y2) Z5 568
X3 -381
X3Z -1095
Y3 1350
Y3Z -1011
#
# Lock Parameter
#
FIELD 1887.448
LOCKPHASE 30.000
LOCKPOWER -34.000
LOCKGAIN 92.414
```

```
LOCKDC -70.000
LOCKSHIFT 2.040
LOOPGAIN 15.133
LOOPTIME 0.047
LOOPFILTER 1468.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1] -6489.11173822
SHIM_SETTING [ 2] -7669.25056769
SHIM_SETTING [ 3] 17377.91006390
SHIM_SETTING [ 4] 19789.49943361
SHIM_SETTING [ 5] -5229.37641819
SHIM_SETTING [ 6] -14910.70834103
SHIM_SETTING [ 7] -4706.22477518
SHIM_SETTING [ 8] 50987.54553669
SHIM_SETTING [ 9] -3634.71844628
SHIM_SETTING [10] 8763.74677454
SHIM_SETTING [11] 0.00000000
SHIM_SETTING [12] 2360.83400000
SHIM_SETTING [13] 338.32700000
SHIM_SETTING [14] 346.37300007
SHIM_SETTING [15] -1238.52325110
SHIM_SETTING [16] 5195.84876422
SHIM_SETTING [17] -4211.64208382
SHIM_SETTING [18] -20347.44791000
SHIM_SETTING [19] 2741.48944029
SHIM_SETTING [20] 6671.93679152
SHIM_SETTING [21] 7866.86000690
SHIM_SETTING [22] -2902.21299714
SHIM_SETTING [23] 8617.96199830
SHIM_SETTING [24] 11090.74500024
SHIM_SETTING [25] 6267.62500276
SHIM_SETTING [26] -4591.45899390
SHIM_SETTING [27] -715.85600013
SHIM_SETTING [28] 5751.42567541
SHIM_SETTING [29] -5632.47200877
SHIM_SETTING [30] -9630.57800779
SHIM_SETTING [31] 1924.22792401
SHIM_SETTING [32] 1871.06267218
SHIM_SETTING [33] -10341.36301039
SHIM_SETTING [34] -13337.54701195
SHIM_SETTING [35] -17582.45199864
SHIM_SETTING [36] -15859.17799840
SHIM_SETTING [37] -4267.12934436
SHIM_SETTING [38] -847.19396406
SHIM_SETTING [39] 1769.42507446
SHIM_SETTING [40] 0.00000000
```

```
Current Data Parameters
NAME NPT_1H_lineshape_nrot
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210928
Time 8.57 h
INSTRUM Avance
PROBHD Z5663_0001 (BB)
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 1
DS 0
SWH 1000.000 Hz
FIDRES 0.061035 Hz
AQ 16.3840008 sec
RG 101
DW 500.000 usec
DE 6.50 usec
TE 295.0 K
D1 9.11600113 sec
TD0 1
SF01 750.3057787 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 14.90600014 W

F2 - Processing parameters
SI 8192
SF 750.3060287 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 4.00
```

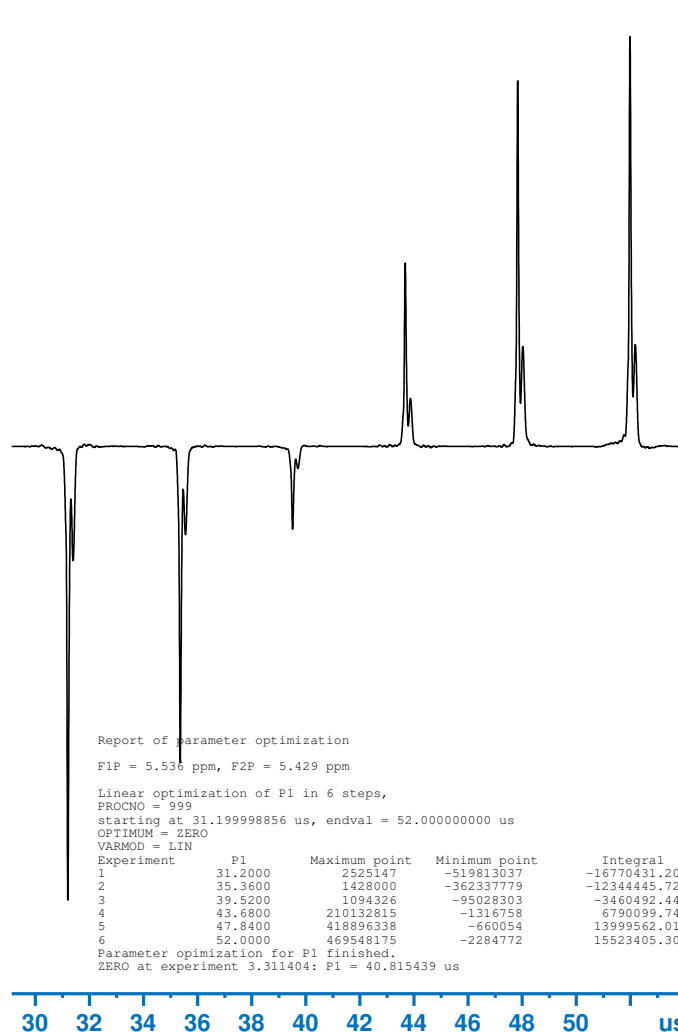
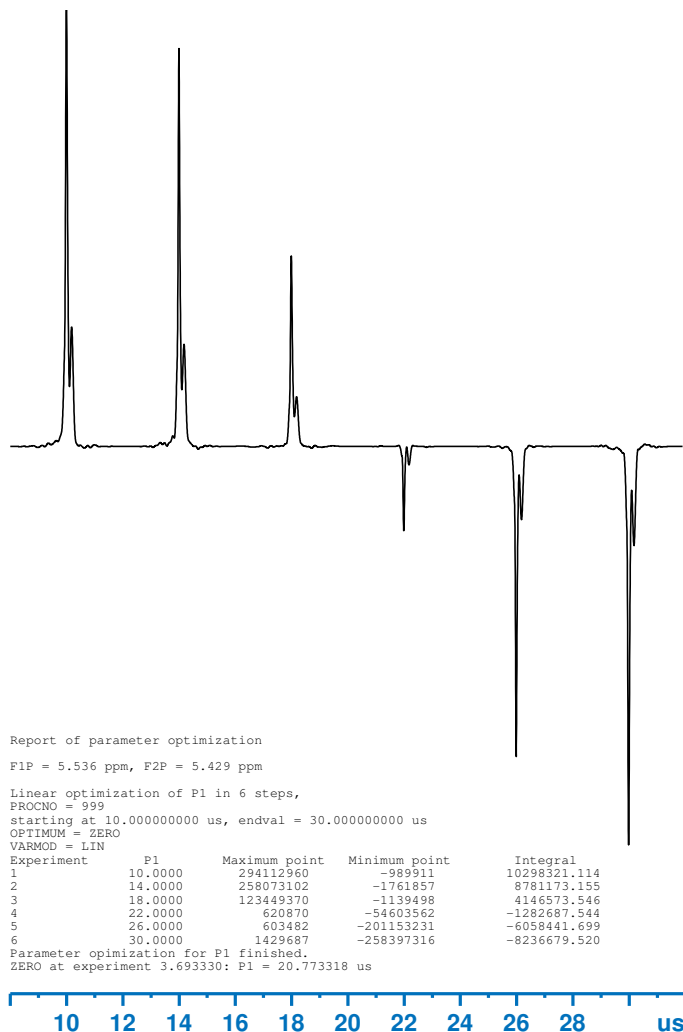
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** Sample Depth: 20 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 P90 1H pulse calibration (NPT_1H_p90determinationf1_1h, spin rate 0 Hz)
 Result: [180/2] = 10.4 us @ 14.9 W [360] = 40.8 us ==> [PDelay = 2*180 - 360] = 0.8 us
 ATTENTION: Updated PROSOL Tables with [10.0 us @ 16.1 W]. Calculation based on ==> [10.4 us @ 14.9 W]
 Deviation from pulse target value (= 10.0 us): 4.0%

P90 1H pulse [achieved]: @ 14.9 W [10.4 us] <n/a>



Bruker BioSpin

NPT_1H_p90determinationf1_1h



Current Data Parameters
 NAME NPT_1H_p90determinationf1_1h
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210930
 Time 11.22 h
 INSTRUM Avance
 PROBHD Z5663_0001 (BB)
 PULPROG zg
 TD 300
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 230.766 Hz
 FIDRES 1.538438 Hz
 AQ 0.6500100 sec
 RG 45.2
 DW 2166.700 usec
 DE 6.50 usec
 TE 295.0 K
 D1 1.45500004 sec
 TD0 1
 SFO1 750.3041136 MHz
 NUC1 1H
 P1 52.00 usec
 PLW1 14.90600014 W

Additional Parameters
 Field 1857.235
 Lock Phase 30.000
 Lock Power -19.000
 Lock Gain 89.966
 Lock DC -70.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 2048
 SF 750.3000000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 14.9 W 10.0 us
 14.9 W 10.0 us 10.4 us 4.0%

SHIM SEQUENCE
 ro off wait <pass>
 topshim fine tunea ordmax=8 <pass>

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** 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 (5.43 to 3.43 ppm) [1161.7] <n/a>
 SINO (200.0 Hz) [achieved]: Signal (3.00 to 2.00 ppm), Noise (5.51 to 5.24 ppm) [1324.4] <n/a>



Bruker BioSpin

NPT_1H_sensitivity

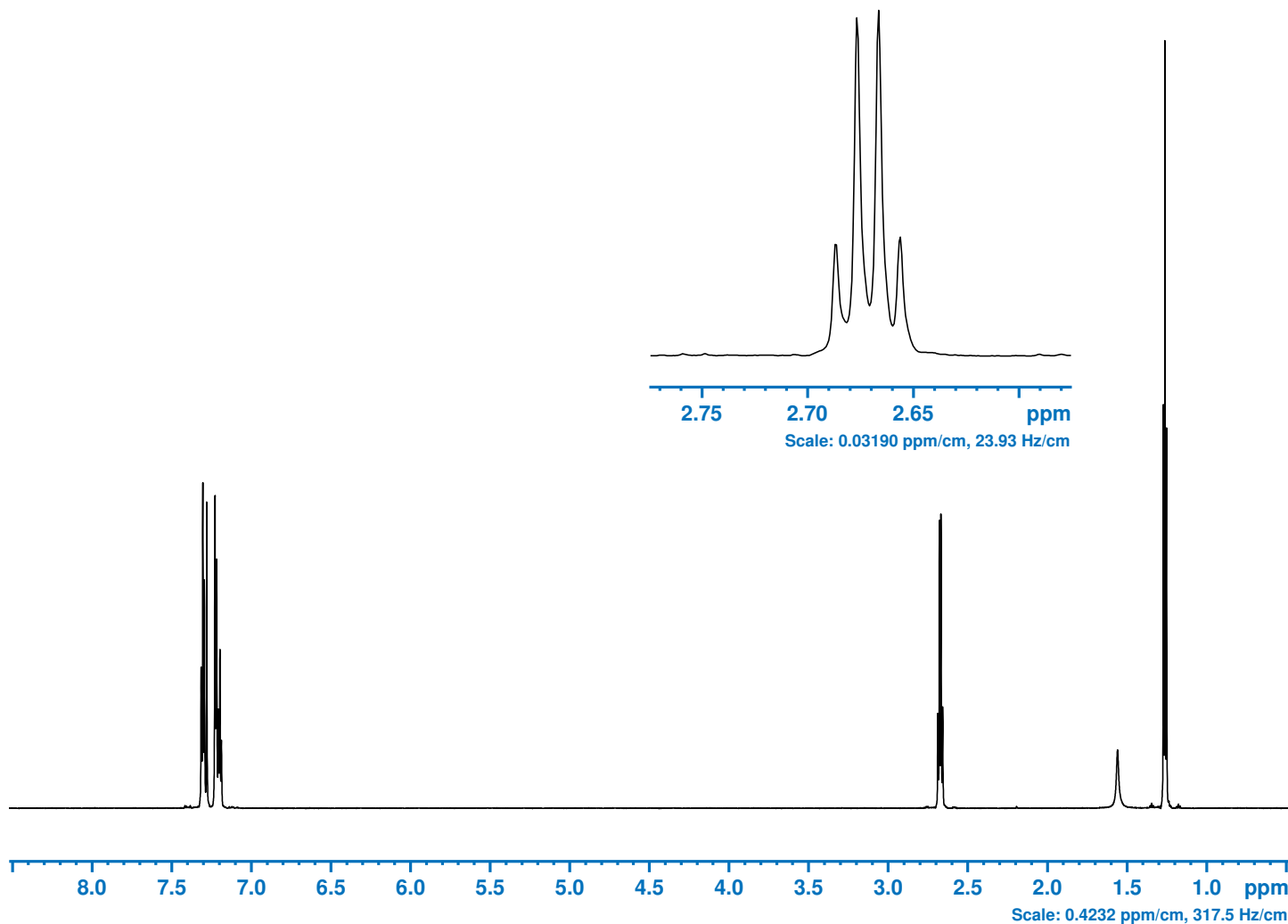
Current Data Parameters
 NAME NPT_1H_sensitivity
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210928
 Time 12.48 h
 INSTRUM Avance
 PROBHD Z5663_0001 (BB)
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 1
 DS 0
 SWH 7462.687 Hz
 FIDRES 0.455496 Hz
 AQ 2.1954560 sec
 RG 101
 DW 67.000 usec
 DE 6.50 usec
 TE 295.0 K
 D1 113.57360077 sec
 TD0 1
 SFO1 750.3030012 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 14.90600014 W

Additional Parameters
 Field 1793.674
 Lock Phase 30.000
 Lock Power -27.000
 Lock Gain 111.511
 Lock DC -70.000
 Lock Shift 7.240
 Loop Gain -12.000
 Loop Time 0.400
 Loop Filter 100.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 16384
 SF 750.3000051 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

SHIM SEQUENCE
 topshim fine ordmax=8 <pass>



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** 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)
 No ZERO crossing found for 90/180 degree pulse optimization
 ATTENTION: Update PROSOL Tables (13C) failed
 Deviation from pulse target value (= 12.0 us): 100.0%
 Experiment failed (no zero crossing or popt protocol missing)

P90 13C pulse was not determinable (-> failed)



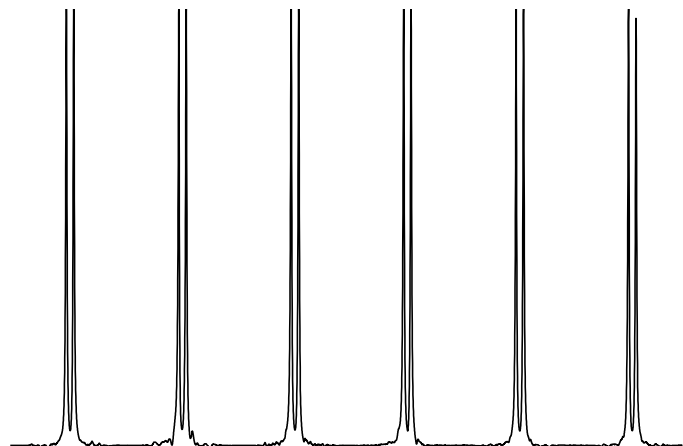
Bruker BioSpin

NPT_1H_p90determinationf2_13c

Current Data Parameters
 NAME NPT_1H_p90determinationf2_13c
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters		Additional Parameters	
Date_	20210930	Field	1857.217
Time	11.23 h	Lock Phase	30.000
INSTRUM	Avance	Lock Power	-19.000
PROBHD	Z5663_0001 (BB)	Lock Gain	89.966
PULPROG	decpg90	Lock DC	-70.000
TD	1000	Lock Shift	2.490
SOLVENT	DMSO	Loop Gain	5.000
NS	0	Loop Time	0.250
DS	0	Loop Filter	500.000
SWH	230.766 Hz	Gas Flow	670 l/h
FIDRES	0.461531 Hz		
AQ	2.1666999 sec		
RG	32		
DW	2166.700 usec		
DE	6.50 usec		
TE	295.0 K		
CNST2	139.0000000		
D1	2.56970811 sec		
D2	0.00359712 sec		
TD0	1		
SFO1	750.3023118 MHz		
NUC1	1H		
P1	5.00 usec		
PLW1	16.12199974 W		
SFO2	188.6724116 MHz		
NUC2	13C		
P3	24.00 usec		
PLW2	300.0000000 W		

F2 - Processing parameters
 SI 2048
 SF 750.3000000 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 FC 0.10



Report of parameter optimization

F1P = 3.135 ppm, F2P = 3.028 ppm

Linear optimization of P3 in 6 steps,

PROCNO = 999

starting at 0.000000000 us, endval = 24.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P3	Maximum point	Minimum point	Integral
1	0.0000	315965886	-2567767	11478376.364
2	4.8000	307057659	-1393135	11749888.975
3	9.6000	309188032	-1695166	11594977.194
4	14.4000	311954906	-808361	11592954.394
5	19.2000	310383022	-1145488	11289601.969
6	24.0000	304186615	-1133236	11059409.165

Parameter optimization for P3 finished.
 ZERO : No zero crossing found.

Skipped 270/360 degree pulse optimization after detection
 of NO ZERO crossing in 90/180 degree pulse optimization.

***** P90 Pulse Determination History *****

FLW90	P90	P90[det]	Deviation
300.0 W	12.0 us		
300.0 W	12.0 us	0.0 us	100.0%

SHIM SEQUENCE

skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** 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] = 23.2 us @ 300.0 W [270] = 72.3 us ==> [PDelay = 3*90 - 270] = -2.7 us
 ATTENTION: Updated PROSOL Tables with [35.0 us @ 131.8 W]. Calculation based on ==> [23.2 us @ 300.0 W])
 Deviation from pulse target value (= 35.0 us): -33.7%



Bruker BioSpin

P90 15N pulse [achieved]: @ 300.0 W [23.2 us] <n/a>

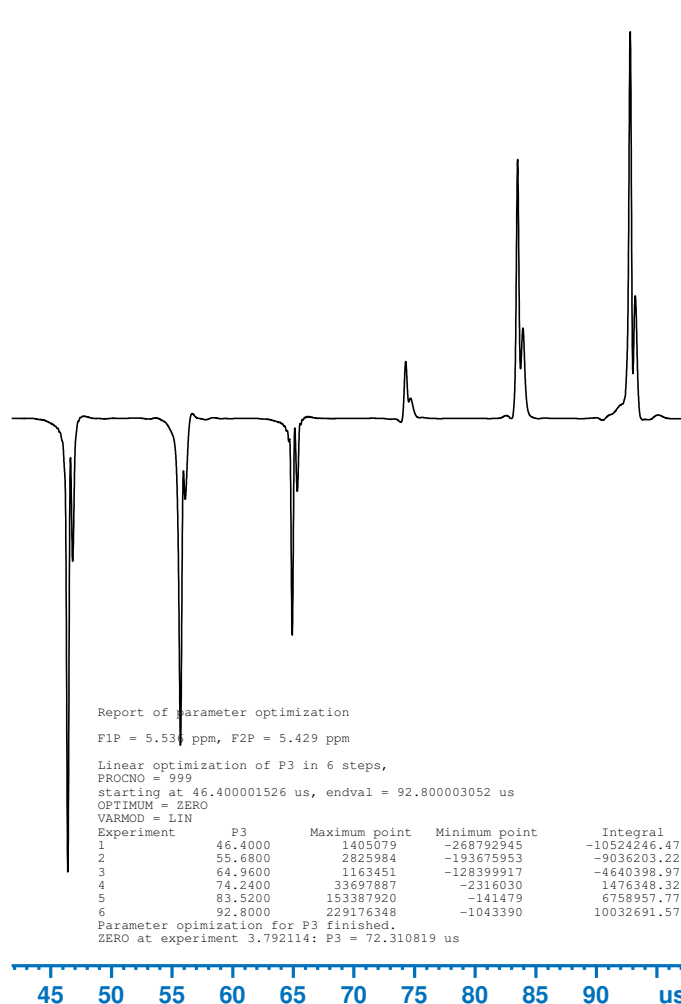
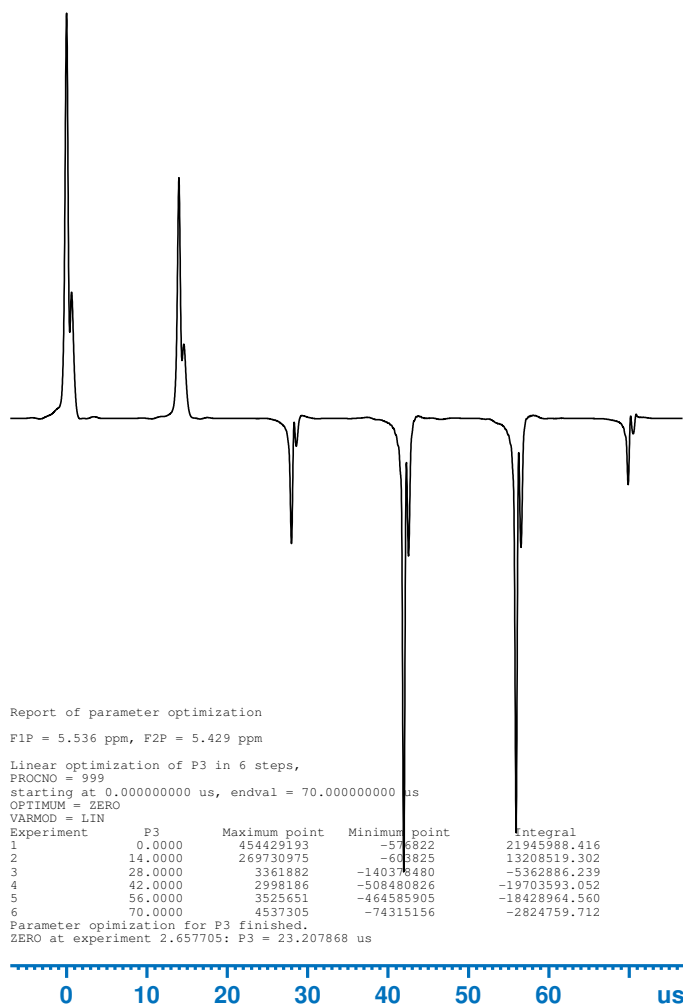
NPT_1H_p90determinationf2_15n

Current Data Parameters
 NAME NPT_1H_p90determinationf2_15n
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210928
 Time 11.53 h
 INSTRUM Avance
 PROBHD Z5663_0001 (BB)
 PULPROG decp90
 TD 200
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 230.766 Hz
 FIDRES 2.307657 Hz
 AQ 0.4333400 sec
 RG 32
 DW 2166.700 usec
 DE 6.50 usec
 TE 295.0 K
 CNST2 88.5000000
 D1 0.58643401 sec
 D2 0.00564972 sec
 TD0 1
 SFO1 750.3041134 MHz
 NUC1 1H
 P1 6.67 usec
 PLW1 14.90600014 W
 SFO2 76.0330108 MHz
 NUC2 15N
 P3 92.80 usec
 PLW2 300.0000000 W

Additional Parameters
 Field 1848.335
 Lock Phase 30.000
 Lock Power -19.000
 Lock Gain 93.011
 Lock DC -70.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 2048
 SF 750.3000000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00



***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 300.0 W 35.0 us
 300.0 W 35.0 us 23.2 us -33.7%

SHIM SEQUENCE
 skip shimming

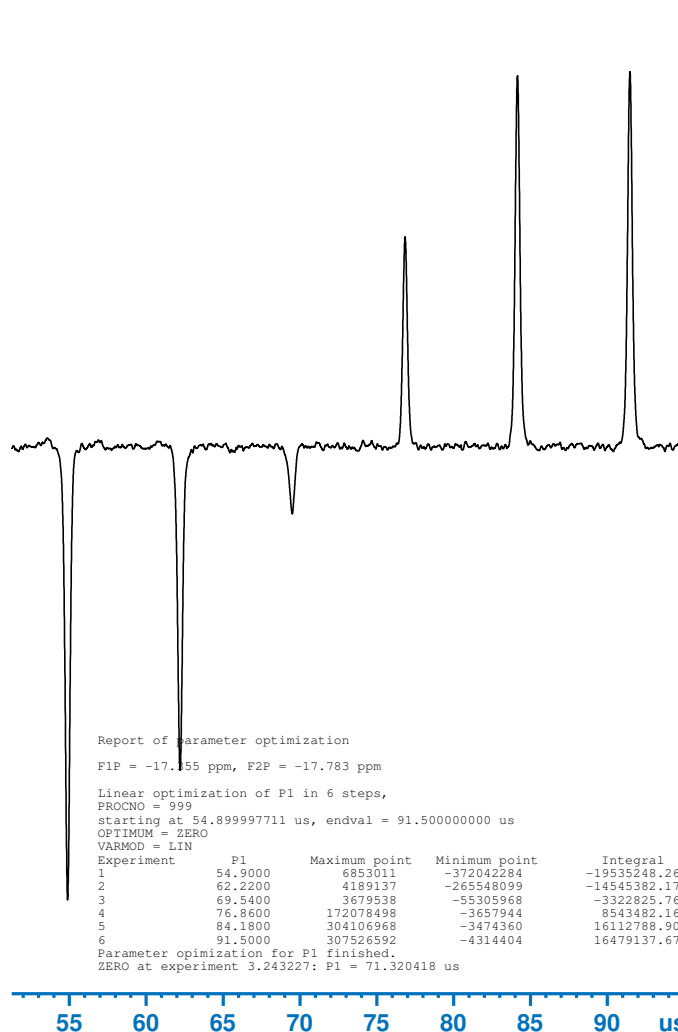
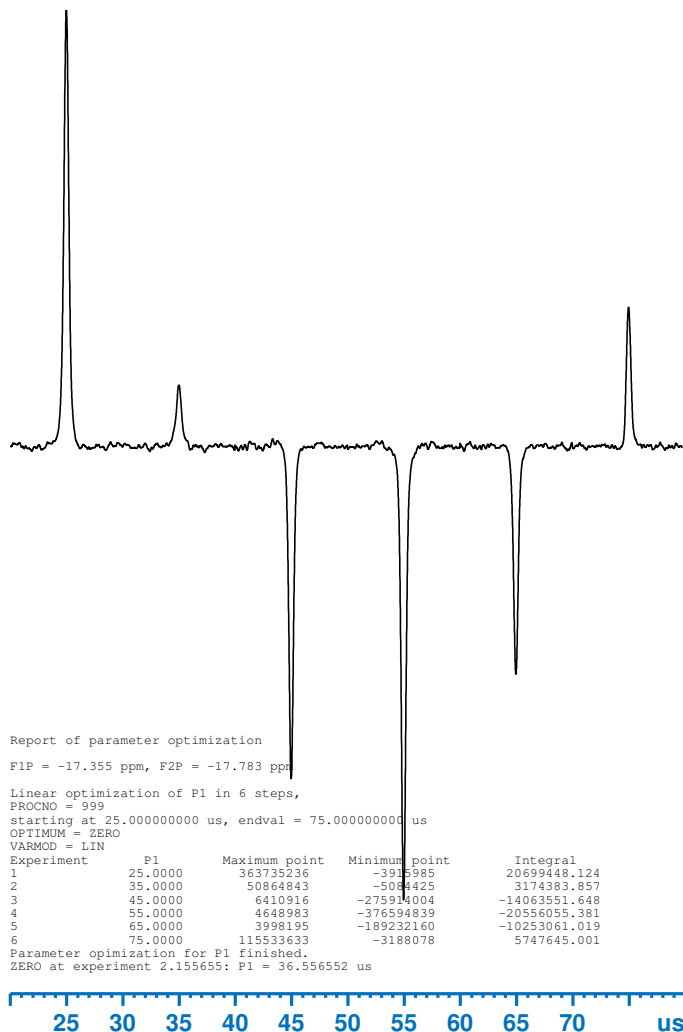
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** Sample Depth: 20 mm
 Sample: 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6 (Z10201)
 P90 31P pulse calibration (NPT_31P_p90determinationf1_31p, spin rate 0 Hz)
 Result: [180/2] = 18.3 us @ 200.0 W [360] = 71.3 us ==> [PDelay = 2*180 - 360] = 1.9 us
 ATTENTION: Updated PROSOL Tables with [25.0 us @ 107.2 W]. Calculation based on ==> [18.3 us @ 200.0 W]
 Deviation from pulse target value (= 25.0 us): -26.8%



Bruker BioSpin

P90 31P pulse [achieved]: @ 200.0 W [18.3 us] <n/a>

NPT_31P_p90determinationf1_31p



Current Data Parameters
 NAME NPT_31P_p90determinationf1_31p
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters		Additional Parameters	
Date_	20210928	Field	1891.771
Time	14.50 h	Lock Phase	30.000
INSTRUM	Avance	Lock Power	-34.000
PROBHD	Z5663_0001 (BB)	Lock Gain	93.532
PULPROG	zg	Lock DC	-70.000
TD	1000	Lock Shift	2.040
SOLVENT	Acetone	Loop Gain	-2.000
NS	1	Loop Time	0.100
DS	0	Loop Filter	200.000
SWH	396.825 Hz	Gas Flow	670 l/h
FIDRES	0.793651 Hz		
AQ	1.2600000 sec		
RG	101		
DW	1260.000 usec		
DE	6.50 usec		
TE	295.0 K		
D1	17.64999962 sec		
TD0	1		
SFO1	303.7216712 MHz		
NUC1	31P		
P1	91.50 usec		
PLW1	200.00000000 W		

F2 - Processing parameters
 SI 4096
 SF 303.7270072 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****

PLW90	P90	P90[det]	Deviation
200.0 W	25.0 us		
200.0 W	25.0 us	18.3 us	-26.8%

SHIM SEQUENCE
 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** 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 (2.75 to -2.26 ppm) [156.9] <n/a>



Bruker BioSpin

NPT_31P_sensitivity

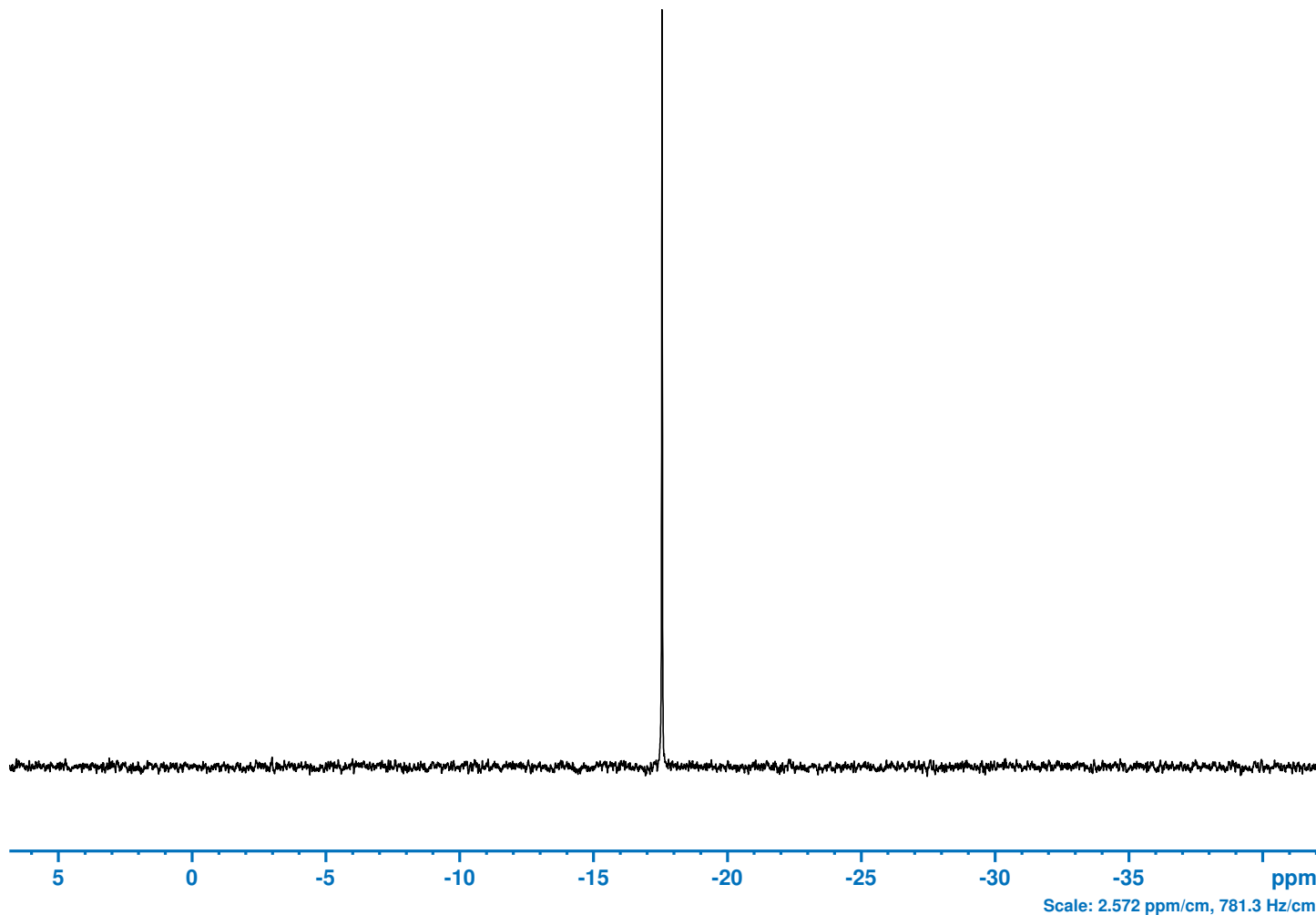
Current Data Parameters
 NAME NPT_31P_sensitivity
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210928
 Time 14.53 h
 INSTRUM Avance
 PROBHD Z5663_0001 (BB)
 PULPROG zg
 TD 32768
 SOLVENT Acetone
 NS 1
 DS 0
 SWH 15625.000 Hz
 FIDRES 0.953674 Hz
 AQ 1.0485760 sec
 RG 101
 DW 32.000 usec
 DE 6.50 usec
 TE 295.0 K
 D1 119.95140076 sec
 TD0 1
 SFO1 303.7216590 MHz
 NUC1 31P
 P1 25.00 usec
 PLW1 107.16000366 W

Additional Parameters
 Field 1891.746
 Lock Phase 30.000
 Lock Power -34.000
 Lock Gain 93.532
 Lock DC -70.000
 Lock Shift 2.040
 Loop Gain -2.000
 Loop Time 0.100
 Loop Filter 200.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 16384
 SF 303.7270072 MHz
 WDW EM
 SSB 0
 LB 5.00 Hz
 GB 0
 PC 1.40

SHIM SEQUENCE
 skip shimming



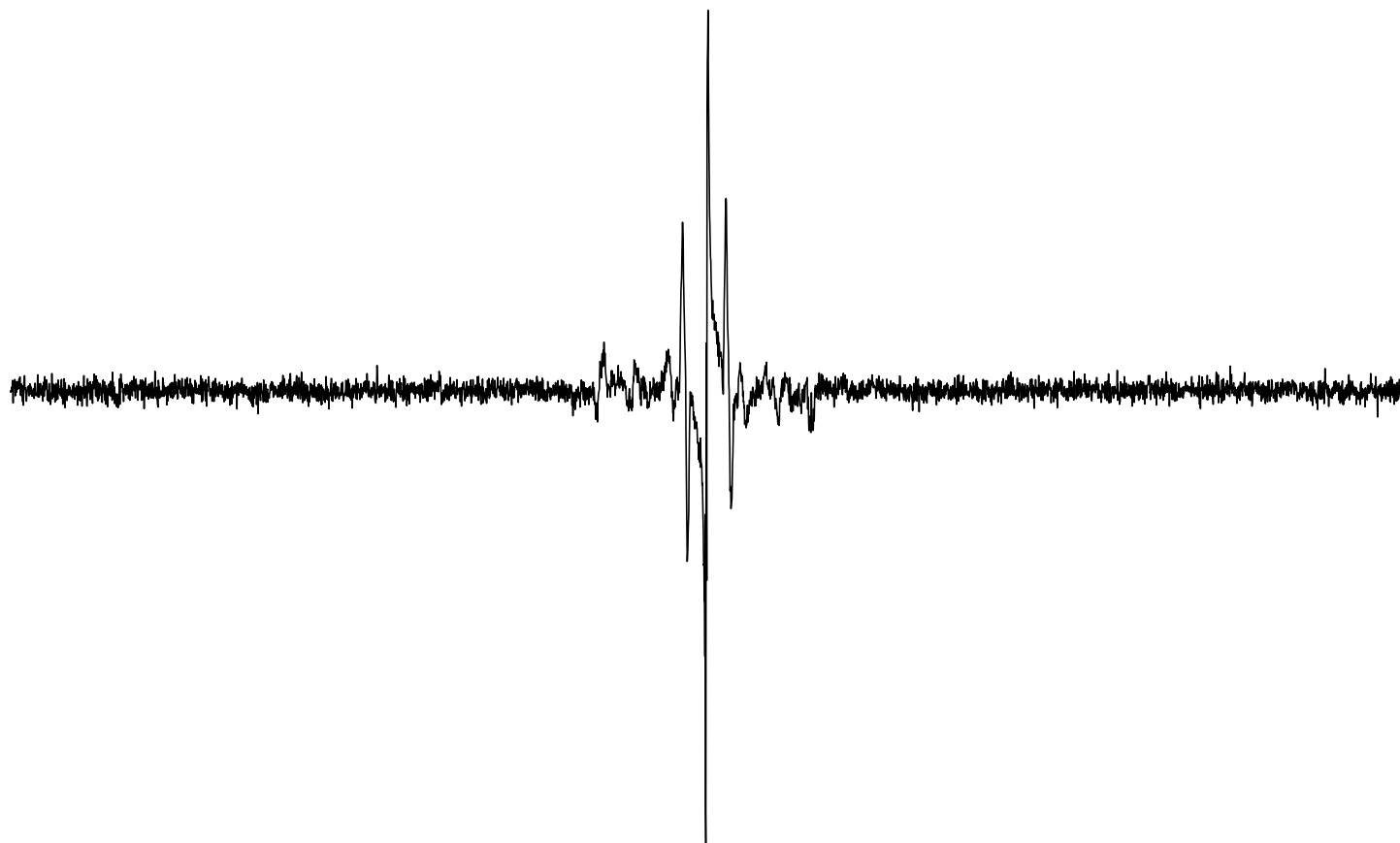
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 Inverse spin echo difference (NPT_1H_hmqc1df2_13c, spin rate 0 Hz)

Ratio [achieved]: Satellite (-110.99 Hz), Central Peak (0.18 Hz) [0.04] <n/a>



Bruker BioSpin

NPT_1H_hmqc1df2_13c



Current Data Parameters			
NAME	NPT_1H_hmqc1df2_13c		
EXPNO	2		
PROCNO	1		
F2 - Acquisition Parameters		Additional Parameters	
Date_	20210928	Field	1893.524
Time	15.27 h	Lock Phase	30.000
INSTRUM	Avance	Lock Power	-34.000
PROBHD	Z5663_0001 (BB)	Lock Gain	92.073
PULPROG	hmqcndrld	Lock DC	-70.000
TD	16384	Lock Shift	2.040
SOLVENT	Acetone	Loop Gain	-2.000
NS	8	Loop Time	0.100
DS	4	Loop Filter	200.000
SWH	1000.000 Hz	Gas Flow	670 l/h
FIDRES	0.122070 Hz		
AQ	8.1920004 sec		
RG	101		
DW	500.000 usec		
DE	6.50 usec		
TE	295.0 K		
CNST2	216.0000000		
D1	14.00000000 sec		
D2	0.00231482 sec		
D13	0.00000400 sec		
TD0	1		
SFO1	750.3060289 MHz		
NUC1	1H		
F1	10.00 usec		
P2	20.00 usec		
PLW1	14.90600014 W		
SFO2	188.6776097 MHz		
NUC2	13C		
P3	12.00 usec		
PLW2	300.00000000 W		
F2 - Processing parameters			
SI	16384		
SF	750.3060289 MHz		
WDW	no		
SSB	0		
LB	0 Hz		
GB	0		
PC	0.50		

 SHIM SEQUENCE

 skip shimming

120 100 80 60 40 20 0 -20 -40 -60 -80 -100 Hz
 Scale: 0.01755 ppm/cm, 13.17 Hz/cm

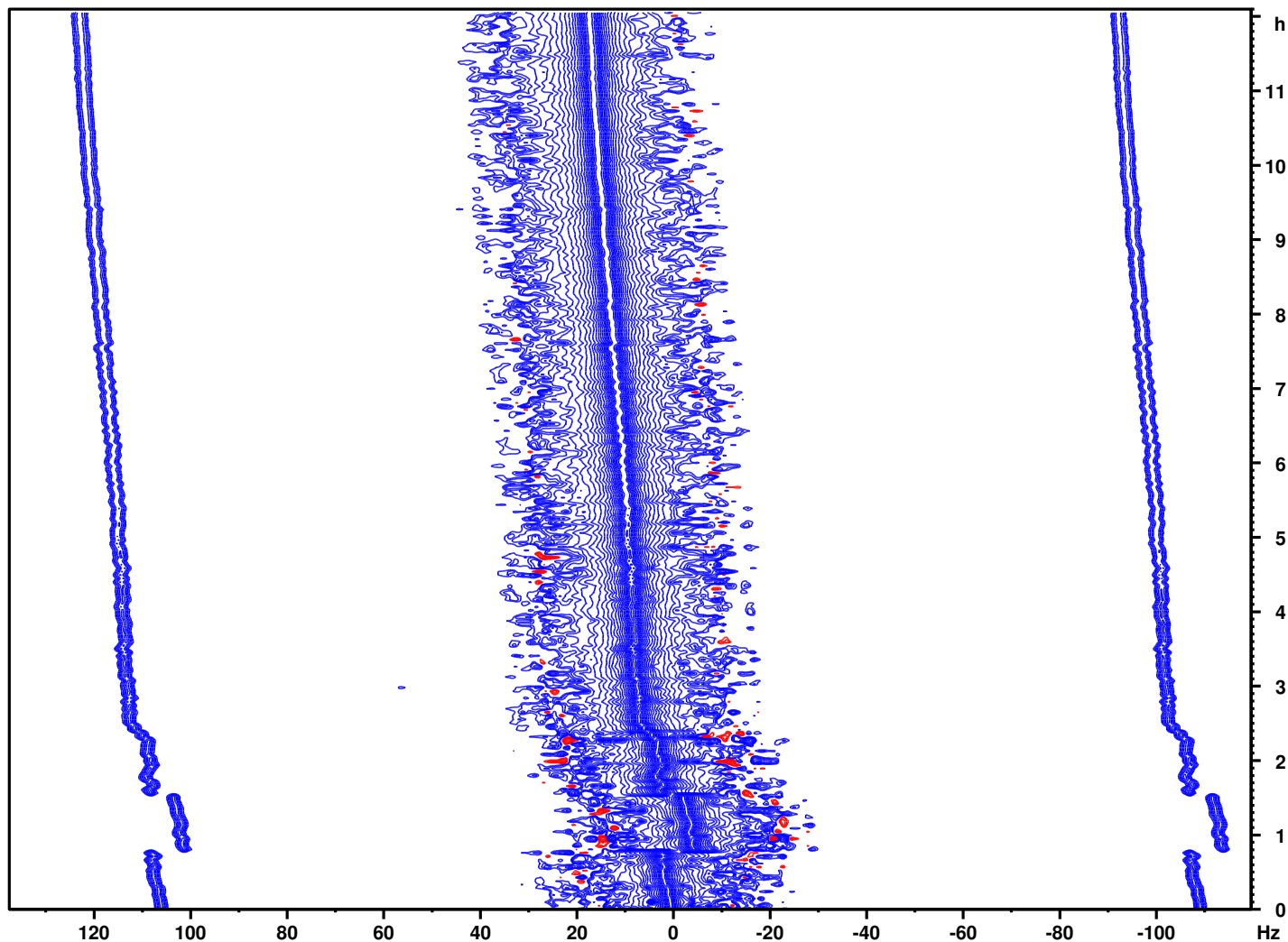
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5663_0001 BBI 750WB H-BB-D-05 Z *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 B0 magnet drift experiment (NPT_1H_b0drifftest, spin rate 0 Hz)

Average positive drift rate [achieved]: [1.41 Hz/h] <n/a>
 Drift measure time [achieved/rated]: [12 h >= 12 h] <pass>



Bruker BioSpin

NPT_1H_b0drifftest



```
Current Data Parameters
NAME      NPT_1H_b0drifftest
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20210929
Time      3.31 h
INSTRUM   Avance
PROBHD    Z5663_0001 (BB
PULPROG   npt_zgp02d
TD         65536
SOLVENT   Acetone
NS         1
DS         0
SWH        8196.722 Hz
FIDRES     0.250144 Hz
AQ         3.9976959 sec
RG         101
DW         61.000 usec
DE         6.50 usec
TE         295.0 K
D1         59.50000000 sec
D20        169.41180420 sec
SF01       750.3060300 MHz
NUC1       1H
CNST10     45.0000000
P0         5.00 usec
P1         10.00 usec
PLW1       14.90600014 W

===== F1 INDIRECT DIMENSION =====
td1        256
sw_F1      0

F1 - Acquisition parameters
TD          256
SF01        0 MHz
FIDRES       0 Hz
SW           0 ppm
FnMODE      QF (no-frequency)

F2 - Processing parameters
SI           65536
SF           750.3060300 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           0.50

F1 - Processing parameters
SI           256
MC2          QF (no-frequency)
SF           750.3000000 MHz
WDW          no
SSB          0
LB           0 Hz
GB           0
```

```
-----
SHIM SEQUENCE
-----
skip shimming
-----
```

PATXI

750 MHz

Probe ID: Z5661_0001

Inspection Lot: 2021-09-29

Oct 1, 2021

NMR TEST SERVICE

● Probe NMR Test Data: PATXI

Probe Related Information

EC-Level	0
Sample Depth (standard) [mm]	20
Sample Depth (water-based Solvents) [mm]	20
Gas Compensation	nitrogen
Gradient System	Z
ATM Accessory	false
Temperature Sensor Type	BTO2000
Proton Frequency [MHz]	750
Diameter [mm]	5.0

Spectrometer Related Information

Type	AV NEO
CF Frequency [MHz]	750.30
Shim System	BOSS3-SB
Shim System Offset	Standard
Software	TopSpin 4.1.3
OS	CentOS Linux release 7.9.2009 (Core)
Host Name	CZC1228YHM
Magnet System	SB
Magnet Coil No	BR.091075110
Dewar No	BD228972
Helium Level	91%
System Number	HCAB-76_00003

● Required Samples **PATXI**

Z10120	0.1% Ethylbenzene (EB) in Chloroform-D
Z10263	100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6
Z10701	0.3% Chloroform in Acetone-D6
Z10902	2 mM Sucrose, 0.5 mM DSS, 2 mM NaN3 in 90% H2O + 10% D2O (40 mm filling height)

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)

Line width [achieved]: at 0.11% of signal height [12.2 Hz] <n/a>
 Line width [achieved]: at 0.55% of signal height [6.4 Hz] <n/a>
 Line width [achieved]: at 50% of signal height [0.71 Hz] <n/a>



Bruker BioSpin

NPT_1H_lineshape_nrot

Current Data Parameters
 NAME NPT_1H_lineshape_nrot
 EXPNO 2
 PROCNO 1

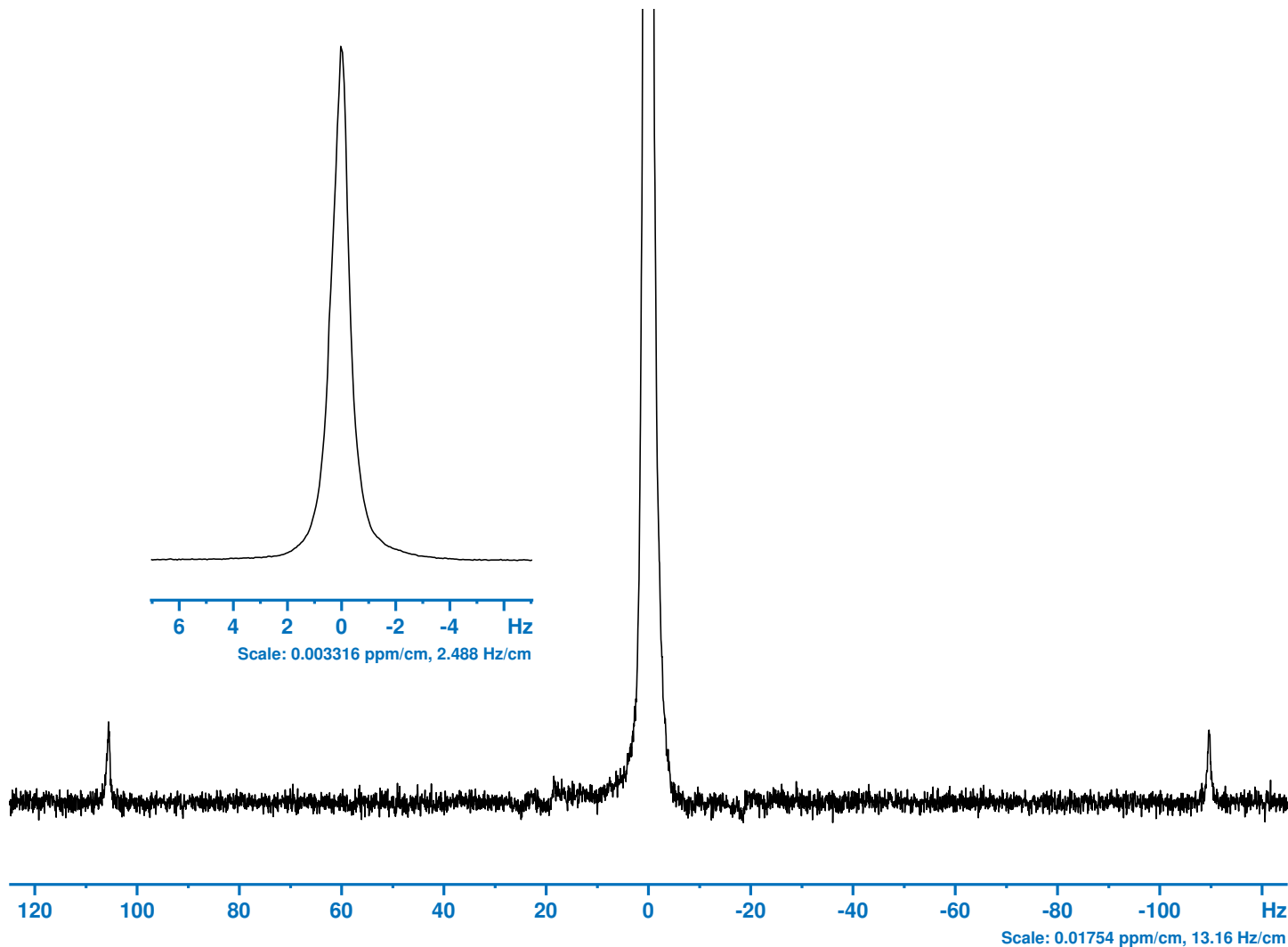
F2 - Acquisition Parameters
 Date_ 20210929
 Time 20.21 h
 INSTRUM Avance
 PROBHD Z5661_0001 (PA)
 PULPROG zg30
 TD 32768
 SOLVENT Acetone
 NS 1
 DS 0
 SWH 1000.000 Hz
 FIDRES 0.061035 Hz
 AQ 16.3840008 sec
 RG 101
 DW 500.000 usec
 DE 6.50 usec
 TE 295.0 K
 D1 9.11600113 sec
 TD0 1
 SFO1 750.3057780 MHz
 NUC1 1H
 P0 2.67 usec
 P1 8.00 usec
 PLW1 22.04999924 W

Additional Parameters
 Field 1938.285
 Lock Phase 30.000
 Lock Power -34.000
 Lock Gain 90.548
 Lock DC -70.000
 Lock Shift 2.040
 Loop Gain 15.133
 Loop Time 0.047
 Loop Filter 1468.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 8192
 SF 750.3060280 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 4.00

SHIM SEQUENCE

ro off wait <pass>
 topshim fine tunea ordmax=8 <pass>



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)



Bruker BioSpin

NPT_1H_lineshape_nrot

```
# Wed Sep 29 18:21:06 2021
##$PROBEIDENTIFIER=Z5661_0001
##$PROBENAME=PATXI
##$SHIMID=292721
#
# Active Shim Gradients
#
Z -8367
Z2 4252
Z3 -764
Z4 -967
Z5 1062
Z6 4810
Z7 -31341
Z8 23795
X -3704
XZ 580
XZ2 985
XZ3 -4564
XZ4 8461
XZ5 2363
Y 1504
YZ 872
YZ2 4127
YZ3 1180
YZ4 -2766
YZ5 1084
XY -17997
XYZ 1079
XYZ2 528
XYZ3 1693
XYZ4 -983
XYZ5 269
(X2-Y2) 6133
(X2-Y2) Z 1495
(X2-Y2) Z2 407
(X2-Y2) Z3 4427
(X2-Y2) Z4 -2701
(X2-Y2) Z5 568
X3 158
X3Z -1003
Y3 1655
Y3Z -1564
#
# Lock Parameter
#
FIELD 1938.285
LOCKPHASE 30.000
LOCKPOWER -34.000
LOCKGAIN 90.548
```

```
LOCKDC -70.000
LOCKSHIFT 2.040
LOOPGAIN 15.133
LOOPTIME 0.047
LOOPFILTER 1468.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1] -7942.50587111
SHIM_SETTING [ 2] -8230.68542549
SHIM_SETTING [ 3] 18025.19965879
SHIM_SETTING [ 4] 19740.18942617
SHIM_SETTING [ 5] -5099.73254539
SHIM_SETTING [ 6] -15384.48276916
SHIM_SETTING [ 7] -2886.49183001
SHIM_SETTING [ 8] 58595.74901769
SHIM_SETTING [ 9] -3220.06688593
SHIM_SETTING [10] 10633.24849385
SHIM_SETTING [11] 0.00000000
SHIM_SETTING [12] 3219.34600000
SHIM_SETTING [13] 90.40700000
SHIM_SETTING [14] 563.29900008
SHIM_SETTING [15] 59.33993532
SHIM_SETTING [16] 5511.58694290
SHIM_SETTING [17] -7432.62611613
SHIM_SETTING [18] -18171.63087925
SHIM_SETTING [19] 3701.35838624
SHIM_SETTING [20] 5220.14518110
SHIM_SETTING [21] 8053.58300482
SHIM_SETTING [22] -1810.96899822
SHIM_SETTING [23] 6980.67899877
SHIM_SETTING [24] 10091.07299994
SHIM_SETTING [25] 5677.30800204
SHIM_SETTING [26] -4979.63299566
SHIM_SETTING [27] -409.55600006
SHIM_SETTING [28] 6119.25737754
SHIM_SETTING [29] -5682.38800686
SHIM_SETTING [30] -10087.30200572
SHIM_SETTING [31] 1084.39792402
SHIM_SETTING [32] 1488.29537401
SHIM_SETTING [33] -9163.24300800
SHIM_SETTING [34] -13979.75200915
SHIM_SETTING [35] -17620.59699931
SHIM_SETTING [36] -17180.49899855
SHIM_SETTING [37] -4744.52288040
SHIM_SETTING [38] -598.84449961
SHIM_SETTING [39] 2124.34607470
SHIM_SETTING [40] 0.00000000
```

```
Current Data Parameters
NAME NPT_1H_lineshape_nrot
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210929
Time 20.21 h
INSTRUM Avance
PROBHD Z5661_0001 (PA
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 1
DS 0
SWH 1000.000 Hz
FIDRES 0.061035 Hz
AQ 16.3840008 sec
RG 101
DW 500.000 usec
DE 6.50 usec
TE 295.0 K
D1 9.11600113 sec
TD0 1
SF01 750.3057780 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 22.04999924 W

F2 - Processing parameters
SI 8192
SF 750.3060280 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 4.00
```

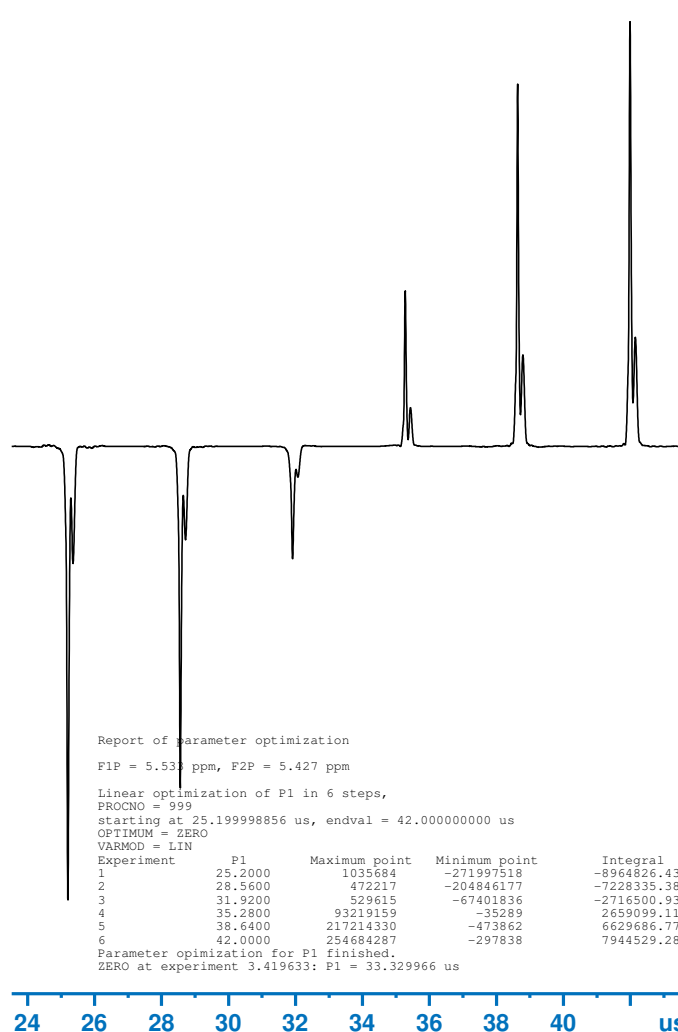
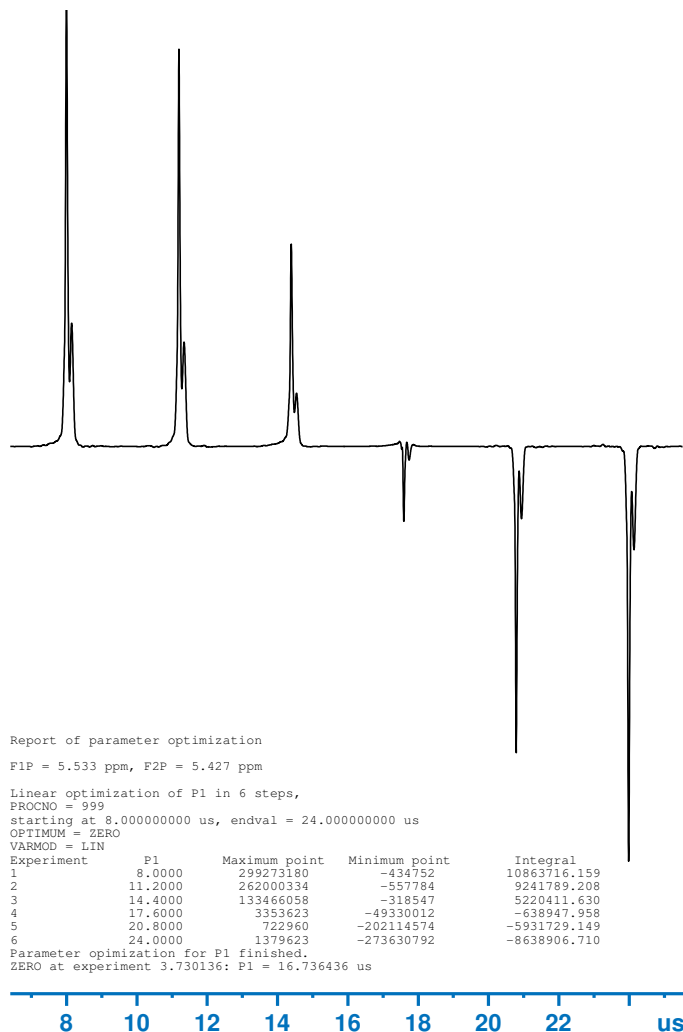
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 P90 1H pulse calibration (NPT_1H_p90determinationf1_1h, spin rate 0 Hz)
 Result: [180/2] = 8.4 us @ 20.0 W [360] = 33.3 us ==> [PDelay = 2*180 - 360] = 0.3 us
 ATTENTION: Updated PROSOL Tables with [8.0 us @ 22.0 W]. Calculation based on ==> [8.4 us @ 20.0 W]
 Deviation from pulse target value (= 8.0 us): 5.0%



Bruker BioSpin

P90 1H pulse [achieved]: @ 20.0 W [8.4 us] <n/a>

NPT_1H_p90determinationf1_1h



Current Data Parameters
 NAME NPT_1H_p90determinationf1_1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210929
 Time 12.32 h
 INSTRUM Avance
 PROBHD Z5661_0001 (PA)
 PULPROG zg
 TD 300
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 230.766 Hz
 FIDRES 1.538438 Hz
 AQ 0.6500100 sec
 RG 45.2
 DW 2166.700 usec
 DE 6.50 usec
 TE 295.0 K
 D1 1.45500004 sec
 TD0 1
 SFO1 750.3041117 MHz
 NUC1 1H
 P1 42.00 usec
 PLW1 20.00000000 W

Additional Parameters
 Field 1894.766
 Lock Phase 30.000
 Lock Power -19.000
 Lock Gain 86.806
 Lock DC -70.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 2048
 SF 750.3000000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 20.0 W 8.0 us
 20.0 W 8.0 us 8.4 us 5.0%

 SHIM SEQUENCE
 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 0.1% Ethylbenzene (EB) in Chloroform-D (Z10120)
 1H sensitivity (NPT_1H_sensitivity, spin rate 0 Hz)

SINO (2.0 ppm) [achieved]: Signal (3.00 to 2.00 ppm), Noise (6.44 to 4.44 ppm) [1304.3] <n/a>
 SINO (200.0 Hz) [achieved]: Signal (3.00 to 2.00 ppm), Noise (4.94 to 4.67 ppm) [1535.9] <n/a>



Bruker BioSpin

NPT_1H_sensitivity

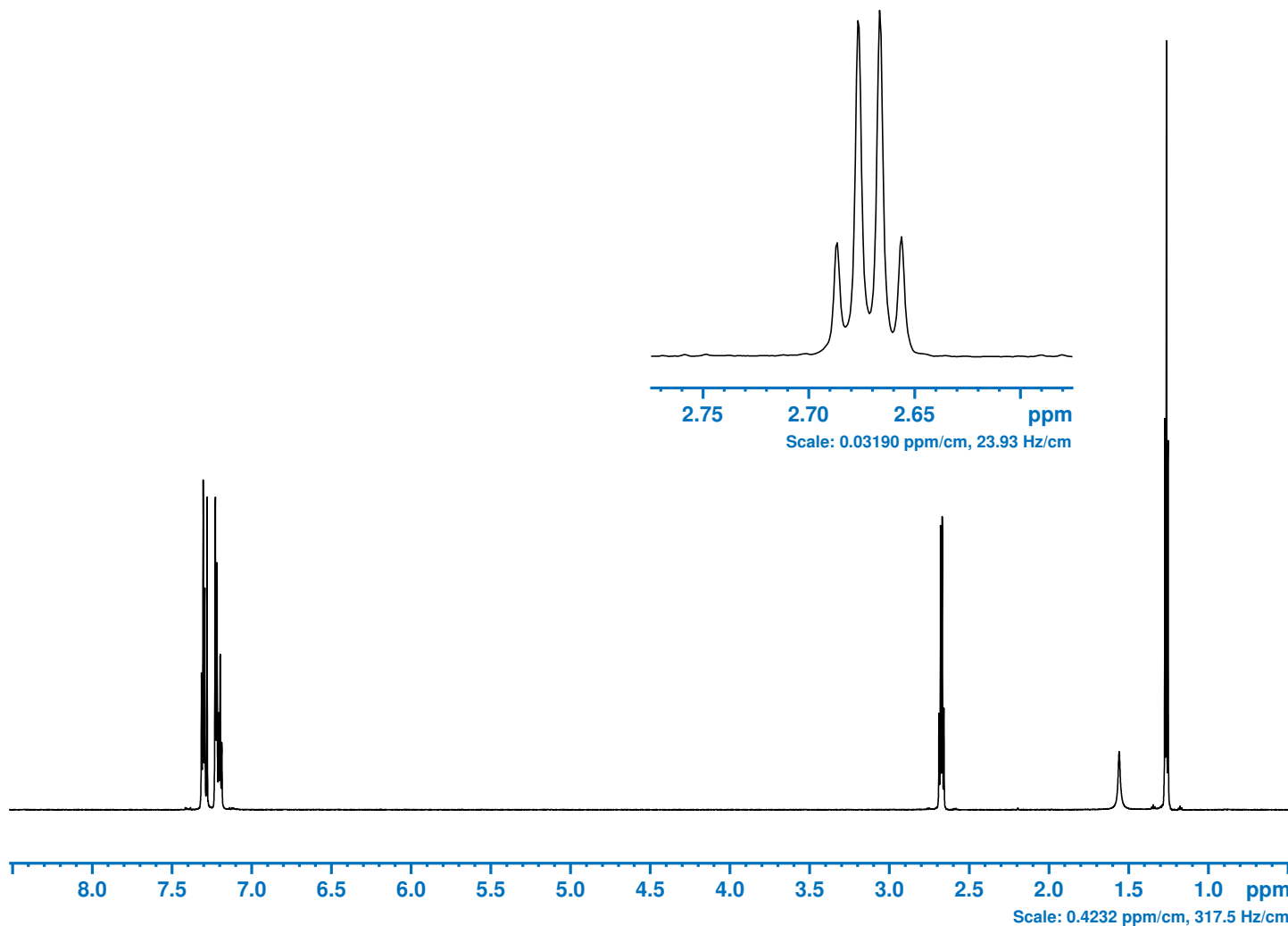
Current Data Parameters
 NAME NPT_1H_sensitivity
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210929
 Time 13.01 h
 INSTRUM Avance
 PROBHD Z5661_0001 (PA)
 PULPROG zg
 TD 32768
 SOLVENT CDC13
 NS 1
 DS 0
 SWH 7462.687 Hz
 FIDRES 0.455486 Hz
 AQ 2.1954560 sec
 RG 101
 DW 67.000 usec
 DE 6.50 usec
 TE 295.0 K
 D1 113.57360077 sec
 TD0 1
 SFO1 750.3030012 MHz
 NUC1 1H
 P1 8.00 usec
 PLW1 22.04999924 W

Additional Parameters
 Field 1840.649
 Lock Phase 30.000
 Lock Power -27.000
 Lock Gain 108.953
 Lock DC -70.000
 Lock Shift 7.240
 Loop Gain -12.000
 Loop Time 0.400
 Loop Filter 100.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 16384
 SF 750.3000037 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

SHIM SEQUENCE
 topshim fine ordmax=8 <pass>



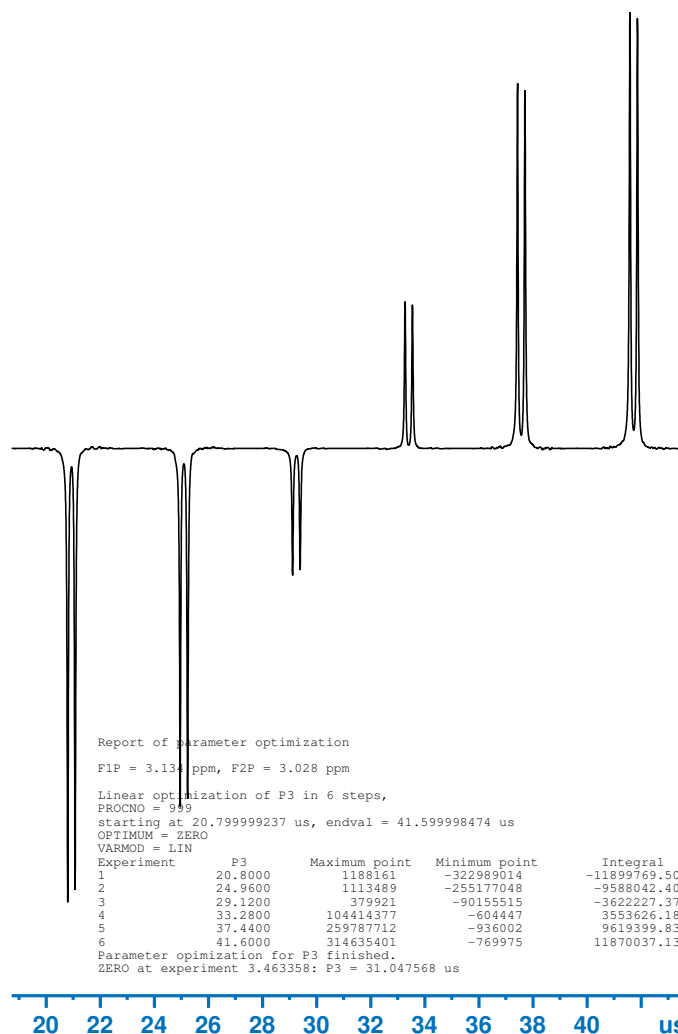
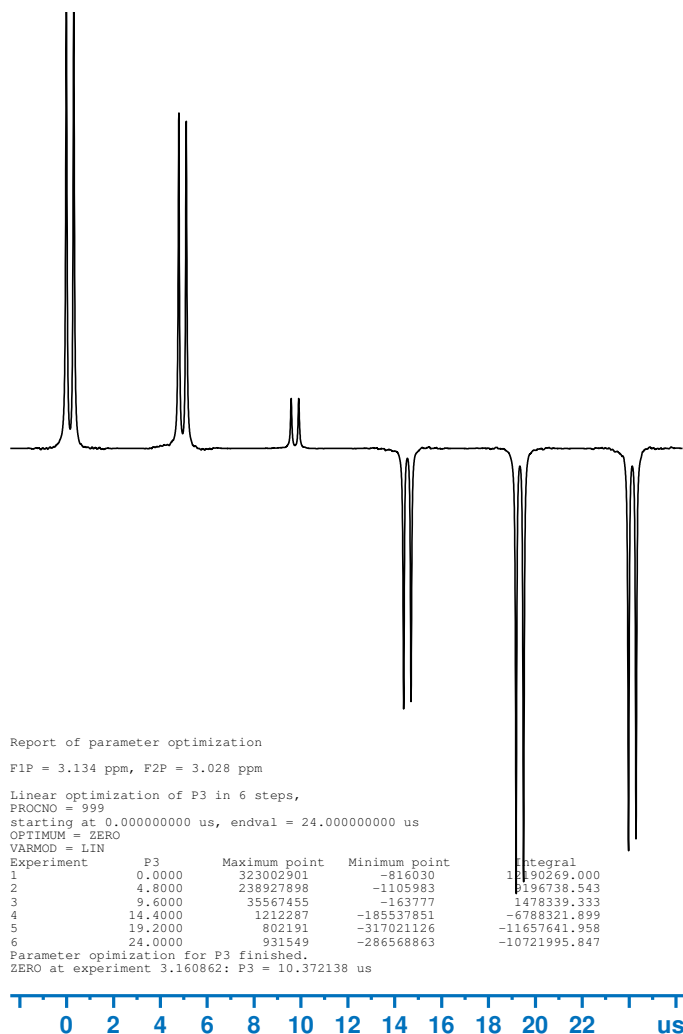
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c, spin rate 0 Hz)
 Result: [90] = 10.4 us @ 300.0 W [270] = 31.0 us ==> [PDelay = 3*90 - 270] = 0.2 us
 ATTENTION: Updated PROSOL Tables with [12.0 us @ 225.3 W]. Calculation based on ==> [10.4 us @ 300.0 W]
 Deviation from pulse target value (= 12.0 us): -13.3%



Bruker BioSpin

P90 13C pulse [achieved]: @ 300.0 W [10.4 us] <n/a>

NPT_1H_p90determinationf2_13c



Current Data Parameters
 NAME NPT_1H_p90determinationf2_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210929
 Time 12.35 h
 INSTRUM Avance
 PROBHD Z5661_0001 (PA)
 PULPROG decp90
 TD 1000
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 230.766 Hz
 FIDRES 0.461531 Hz
 AQ 2.1666999 sec
 RG 32
 DW 2166.700 usec
 DE 6.50 usec
 TE 295.0 K
 CNST2 139.0000000
 D1 2.56970811 sec
 D2 0.00359712 sec
 TD0 1
 SFO1 750.3023117 MHz
 NUC1 1H
 P1 4.00 usec
 PLW1 22.04999924 W
 SFO2 188.6724116 MHz
 NUC2 13C
 P3 41.60 usec
 PLW2 300.0000000 W

Additional Parameters
 Field 1894.791
 Lock Phase 30.000
 Lock Power -19.000
 Lock Gain 86.806
 Lock DC -70.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 2048
 SF 750.3000000 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 FC 0.10

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 300.0 W 12.0 us
 300.0 W 12.0 us 10.4 us -13.3%

 SHIM SEQUENCE
 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** 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] = 36.9 us @ 300.0 W [270] = 116.1 us ==> [PDelay = 3*90 - 270] = -5.4 us
 ATTENTION: Updated PROSOL Tables with [37.0 us @ 298.4 W]
 Deviation from pulse target value (= 37.0 us): -0.3%

P90 15N pulse [achieved]: @ 300.0 W [36.9 us] <n/a>



Bruker BioSpin

NPT_1H_p90determinationf2_15n

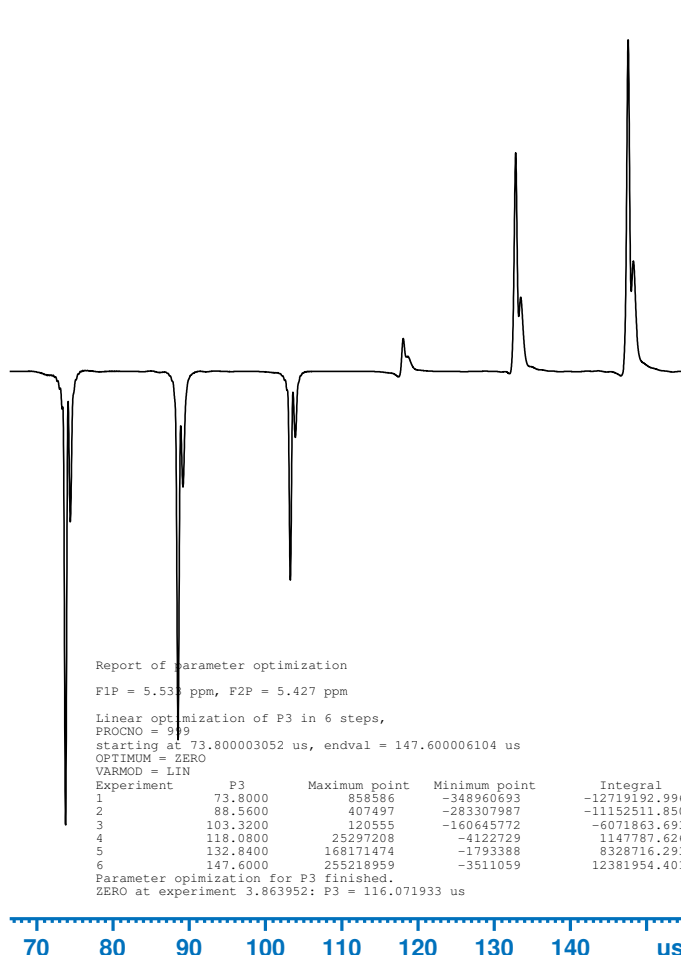
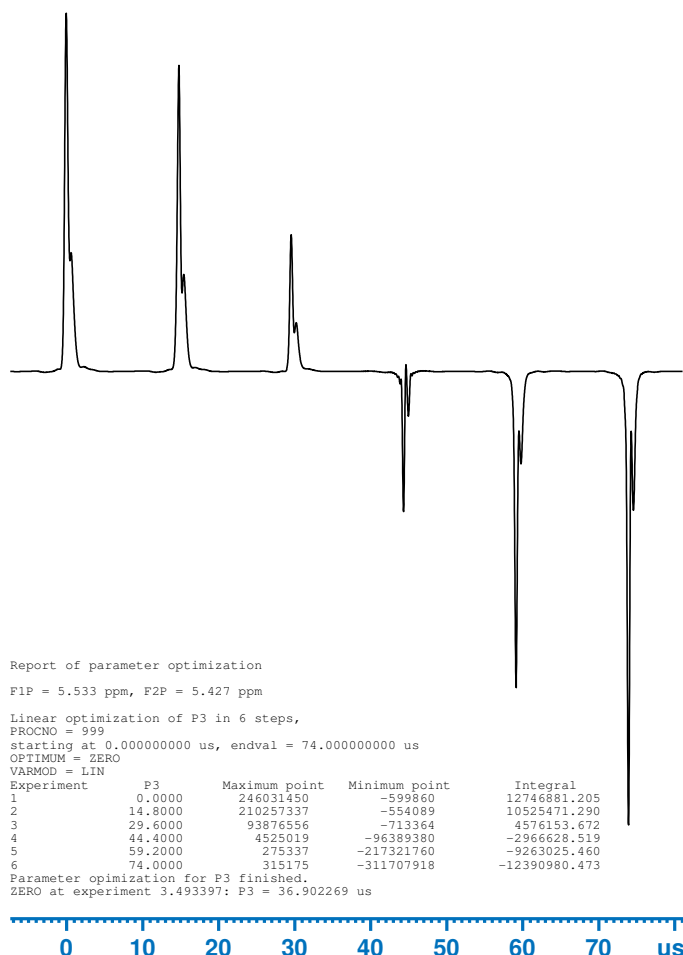
Current Data Parameters
 NAME NPT_1H_p90determinationf2_15n
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210929
 Time 12.36 h
 INSTRUM Avance
 PROBHD Z5661_0001 (PA)
 PULPROG decp90
 TD 200
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 230.766 Hz
 FIDRES 2.307657 Hz
 AQ 0.4333400 sec
 RG 32
 DW 2166.700 usec
 DE 6.50 usec
 TE 295.0 K
 CNST2 88.5000000
 D1 0.58643401 sec
 D2 0.00564972 sec
 TD0 1
 SFO1 750.3041116 MHz
 NUC1 1H
 F1 5.33 usec
 PLW1 22.04999924 W
 SFO2 76.0330108 MHz
 NUC2 15N
 P3 147.60 usec
 PLW2 300.0000000 W

Additional Parameters
 Field 1894.800
 Lock Phase 30.000
 Lock Power -19.000
 Lock Gain 86.806
 Lock DC -70.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 670 l/h

F2 - Processing parameters
 SI 2048
 SF 750.3000000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 FC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 300.0 W 37.0 us
 300.0 W 37.0 us 36.9 us -0.3%



 SHIM SEQUENCE
 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 2 mM Sucrose, 0.5 mM DSS, 2 mM NaN3 in 90% H2O + 10% D2O (40 mm filling height) (Z10902)
 2H sensitivity, 10% D2O (NPT_prep_sensitivity_10_d, spin rate 0 Hz)

SINO (50.0 ppm) [achieved]: Signal (5.00 to 4.00 ppm), Noise (60.00 to 10.00 ppm) [3018.9] <n/a>
 Linewidth at 50 % of signal height [achieved]: [0.75 Hz] <n/a>



Bruker BioSpin

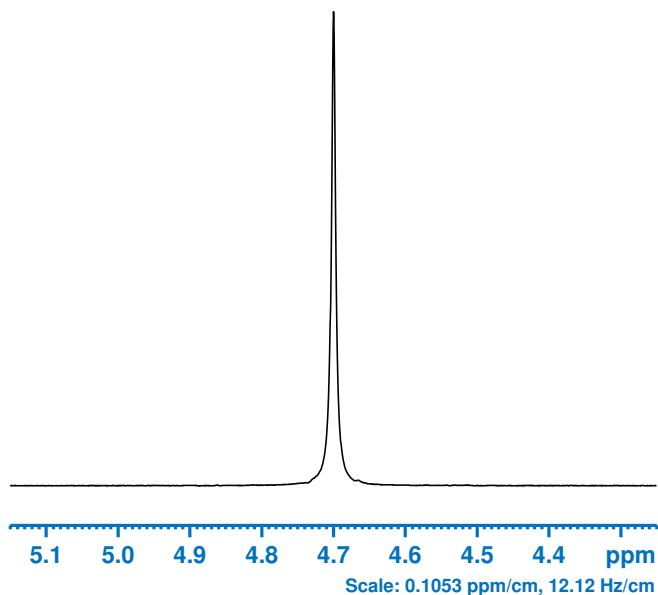
NPT_prep_sensitivity_10_d

Current Data Parameters
 NAME NPT_prep_sensitivity_10_d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210929
 Time 11.27 h
 INSTRUM Avance
 PROBHD Z5661_0001 (PA)
 PULPROG zg2h
 TD 138888
 SOLVENT H2O+D2O
 NS 1
 DS 0
 SWH 13888.889 Hz
 FIDRES 0.200001 Hz
 AQ 4.9999681 sec
 RG 101
 DW 36.000 usec
 DE 6.50 usec
 TE 295.0 K
 D1 10.00000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 115.1761591 MHz
 NUC1 2H
 P1 150.00 usec
 PLW1 5.00000000 W

F2 - Processing parameters
 SI 262144
 SF 115.1756178 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.40

SHIM SEQUENCE
 ro off wait <pass>
 topshim fine tunea ordmax=8 <pass>



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 Inverse spin echo difference (NPT_1H_hmqc1df2_13c, spin rate 0 Hz)

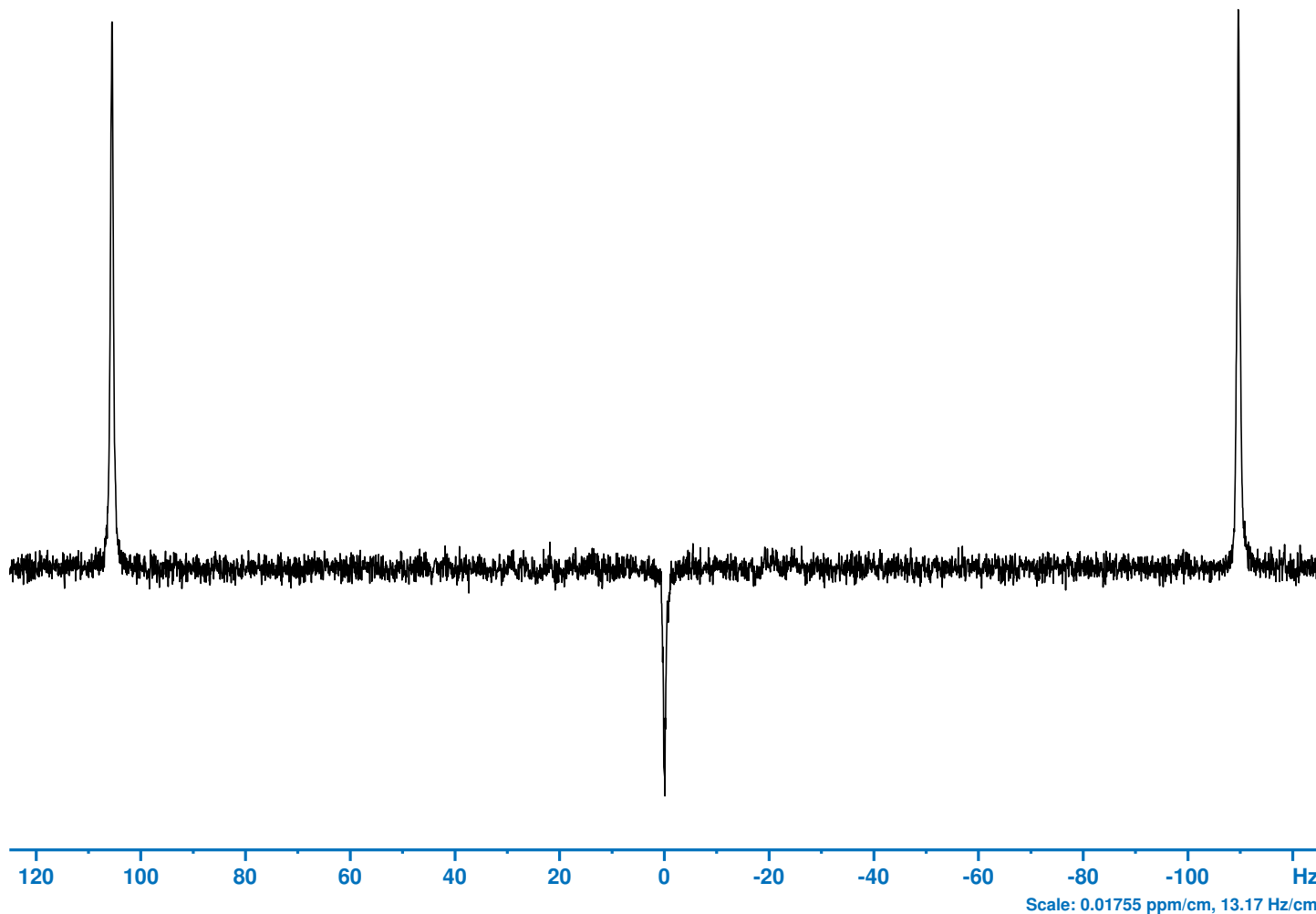
Ratio [achieved]: Satellite (-109.61 Hz), Central Peak (-0.07 Hz) [2.42] <n/a>



Bruker BioSpin

NPT_1H_hmqc1df2_13c

Current Data Parameters		
NAME	NPT_1H_hmqc1df2_13c	
EXPNO	1	
PROCNO	1	
F2 - Acquisition Parameters		Additional Parameters
Date_	20210930	Field
Time	0.05 h	1938.115
INSTRUM	Avance	Lock Phase
PROBHD	Z5661_0001 (PA)	30.000
PULPROG	hmqcndruid	Lock Power
TD	16384	-34.000
SOLVENT	Acetone	Lock Gain
NS	8	89.893
DS	4	Lock DC
SWH	1000.000 Hz	-70.000
FIDRES	0.122070 Hz	Lock Shift
AQ	8.1920004 sec	2.040
RG	101	Loop Gain
DW	500.000 usec	15.133
DE	6.50 usec	Loop Time
TE	295.0 K	0.047
CNST2	216.0000000	Loop Filter
D1	14.00000000 sec	1468.000
D2	0.00231482 sec	Gas Flow
D13	0.00000400 sec	670 l/h
TD0	1	
SFO1	750.3060281 MHz	
NUC1	1H	
F1	8.00 usec	
P2	16.00 usec	
PLW1	22.04999924 W	
SFO2	188.6776097 MHz	
NUC2	13C	
P3	12.00 usec	
PLW2	225.33000183 W	
F2 - Processing parameters		
SI	16384	
SF	750.3060281 MHz	
WDW	no	
SSB	0	
LB	0 Hz	
GB	0	
PC	0.50	



SHIM SEQUENCE

ro off wait <pass>

topshim fine tunea ordmax=8 <pass>

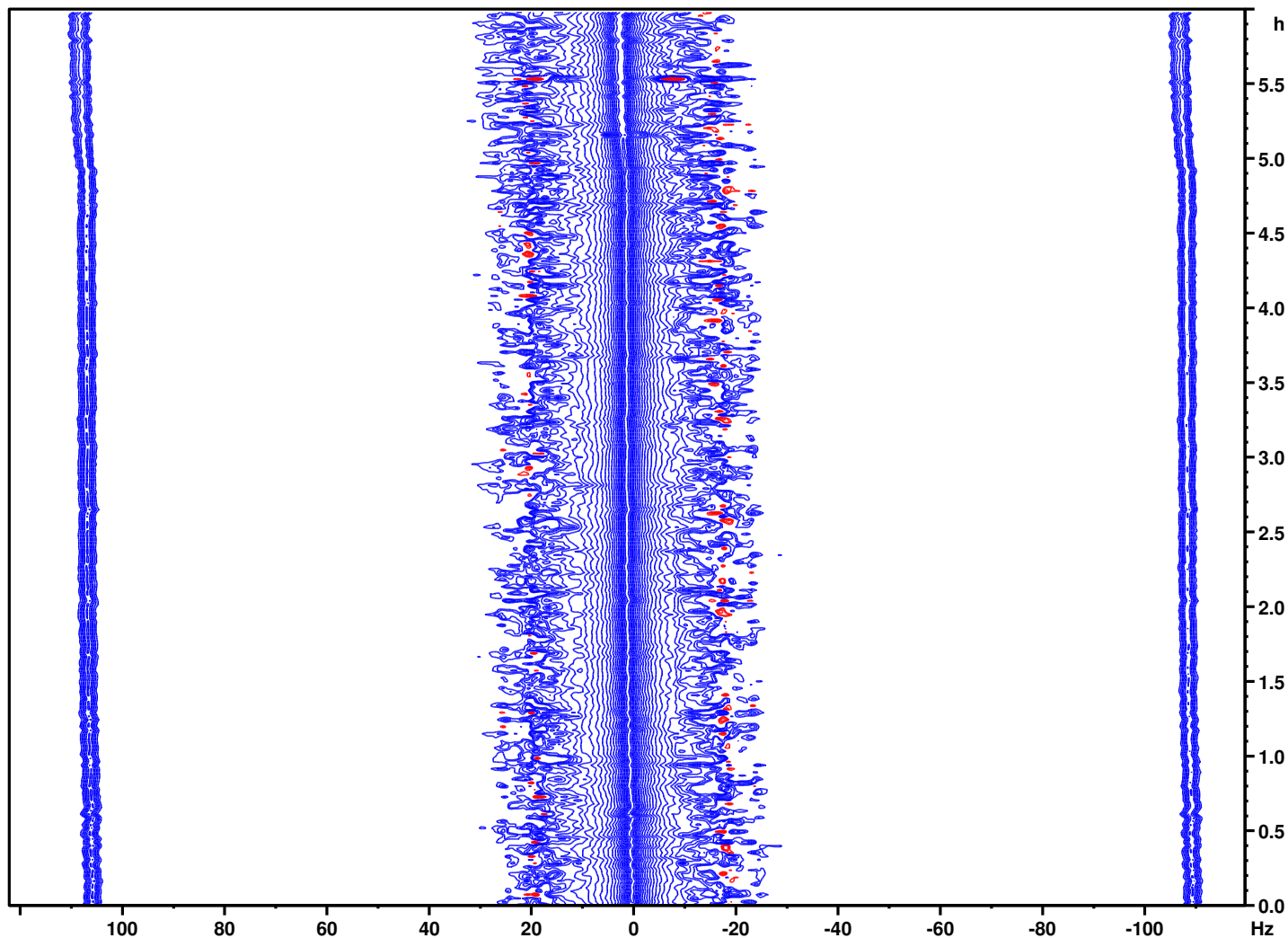
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 B0 magnet drift experiment (NPT_1H_b0drifftest, spin rate 0 Hz)

Average positive drift rate [achieved]: [0.25 Hz/h] <n/a>
 Drift measure time [achieved]: [6 h] <n/a>



Bruker BioSpin

NPT_1H_b0drifftest



```
Current Data Parameters
NAME      NPT_1H_b0drifftest
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20210930
Time      6.08 h
INSTRUM   Avance
PROBHD    Z5661_0001 (PA
PULPROG   npt_zgp02d
TD        65536
SOLVENT   Acetone
NS         1
DS         0
SWH       8196.722 Hz
FIDRES    0.250144 Hz
AQ        3.9976959 sec
RG         101
DW        61.000 usec
DE         6.50 usec
TE        295.0 K
D1         59.50000000 sec
D20       84.70587921 sec
SF01      750.3060266 MHz
NUC1       1H
CNST10    45.0000000
P0         4.00 usec
P1         8.00 usec
PLW1      22.04999924 W

===== F1 INDIRECT DIMENSION =====
td1       256
sw_F1     0

F1 - Acquisition parameters
TD        256
SF01      0 MHz
FIDRES    0 Hz
SW         0 ppm
FnMODE    QF (no-frequency)

F2 - Processing parameters
SI        65536
SF        750.3060266 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.50

F1 - Processing parameters
SI        256
MC2       QF (no-frequency)
SF        750.3000000 MHz
WDW       no
SSB       0
LB        0 Hz
GB        0
```

SHIM SEQUENCE
 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: Z5661_0001 PATXI *** Sample Depth: 20 mm
 Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
 1H lineshape stability test (NPT_1H_lineshapeStability, spin rate 0 Hz)
 Repetition rate: 10 min, total experiment time: 3 h 20 min



Bruker BioSpin

SINO (200.0 Hz) [achieved]: Signal (-0.20 to 0.20 ppm), Noise (0.26 to -0.01 ppm) [-0.0] <n/a>
 Deviation of Linewidth [achieved]: at 0.11% of signal height [4.50 Hz] <n/a>
 Deviation of Linewidth [achieved]: at 0.55% of signal height [0.90 Hz] <n/a>
 Deviation of Linewidth [achieved]: at 50.0% of signal height [0.29 Hz] <n/a>

NPT_1H_lineshapeStability

```
Current Data Parameters
NAME      NPT_1H_lineshapeStability
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20210929
Time      23.45 h
INSTRUM   Avance
PROBHD    Z5661_0001 (PA)
PULPROG   zg2d
TD        65536
SOLVENT   Acetone
NS         1
DS         0
SWH        2500.000 Hz
FIDRES     0.076294 Hz
AQ         13.1071997 sec
RG         101
DW         200.000 usec
DE         6.50 usec
TE         295.0 K
D1         2.00000000 sec
D20        600.00000000 sec
SF01       750.3054031 MHz
NUC1       1H
P1         8.00 usec
PLW1       22.04999924 W

Additional Parameters
Field      1938.274
Lock Phase 30.000
Lock Power -34.000
Lock Gain  90.548
Lock DC    -70.000
Lock Shift 2.040
Loop Gain  15.133
Loop Time  0.047
Loop Filter 1468.000
Gas Flow   670 l/h

===== F1 INDIRECT DIMENSION =====
td1      20
sw_F1    0

F1 - Acquisition parameters
TD        20
SF01       0 MHz
FIDRES     0 Hz
SW         0 ppm
FnMODE     QF (no-frequency)

F2 - Processing parameters
SI         262144
SF         750.3060281 MHz
WDW         no
SSB         0
LB         0 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         32
MC2         QF (no-frequency)
SF         750.3000000 MHz
WDW         no
SSB         0
LB         0 Hz
GB         0
```

```
-----
SHIM SEQUENCE
ro off wait <pass>
topshim fine tunea ordmax=8 <pass>
-----
```

