

NMR Test Spectrometer

Report Name: 2021-10-20

AV NEO (750 MHz) HCAB-76_00003

Content:

- Configuration Information (uxnmr.info)
- IP Config Information
- Probe: H11833_0001 / 2021-10-19



● Configuration Information uxnmr.info

CONFIGURATION INFORMATION

=====

```
Path      : /opt/topspin/conf/instr/spect/uxnmr.info
Date      : Tue Oct 19 09:17:26 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 900 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 = BOSS-WB
- SCB channels = 40
- Shim matrix file: 272623fa.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 X3Z 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
```

```
- Firmware version = 20210503.1702
MAS Control Unit: MAS_H139288.0479
- TCP/IP address = 192.168.98.5
```

Line Distribution Units at the spectrometer subnet:

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

● Configuration Information uxnmr.info

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

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 LABBB1000 15-600 W144060/000235 at TCP/IP 192.168.99.12)
TRX2 AUX  output -> open
TRX3 NORM output -> input 1 of transmitter 1 (AV4 LABBB1000 15-600 W144060/000236 at TCP/IP 192.168.99.13)
TRX3 AUX  output -> open

Blanking cable connections (detected)
-----
transmitter 1 = AV4 LABBB1000 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 LABBB1000 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 4686717 bytes 2612610071 (2.4 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 5231681 bytes 1050643840 (1001.9 MiB)
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 393180 bytes 134687158 (128.4 MiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 125387 bytes 16103872 (15.3 MiB)
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 1720317 bytes 736173795 (702.0 MiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 1720317 bytes 736173795 (702.0 MiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
```

PH MASDVT 750W4 EFREE2 BL3.2 C/N/H

750 MHz

Probe ID: H11833_0001

Inspection Lot: 2021-10-19

Oct 20, 2021

NMR TEST SERVICE

● Probe NMR Test Data: PH MASDVT 750W4 EFREE2 BL3.2 C/N/H

Probe Related Information

EC-Level	0
Gas Compensation	air
Gradient System	unknown
ATM Accessory	false
Temperature Sensor Type	TypeT
Proton Frequency [MHz]	750
Diameter [mm]	3.2

Spectrometer Related Information

Type	AV NEO
CF Frequency [MHz]	750.30
Shim System	BOSS-WB
Shim System Offset	Standard
Software	TopSpin 4.1.3
OS	CentOS Linux release 7.9.2009 (Core)
Host Name	CZC1228YHM
Magnet System	WB
Magnet Coil No	BR.091075110
Dewar No	BD228972
Helium Level	61%
System Number	HCAB-76_00003

● PICS Data

H11833_0001.ph

```
H11833_0001.ph
=====
$Bis,1,20190116,2048,PICS,5#
$Production,H11833,0001,0.00,0,BDE,20160202#
$Name,PH MASDVT 750W4 EFREE2 BL3.2 C/N/H#
$ProbeCompatibility,1.0,WB,4,750#
$ProbeType,1.0,MAS#
$ProbeSample,1.0,3.2,#
$ProbeTemperature,1.0,TypeT,-180,30#
$ProbeHeaterTemperature,1.0,TypeK,-273,+600#
$GasFlow,1.0,,,,600,50,3000,,,#
$ProbeMas,1.0,1000,24000,0,1,0,0,0,0,0#
$ProbeAllCoils,1.1,2,0#
$ProbeCoil,1.0,1,,1,1H#
$ProbeCoil,1.0,2,,2,15N,13C/79Br#
$ProbeChannel,1.0,1H,,,,,300,,,,FALSE#
$ProbeChannel,1.0,15N,,,,,450,,,,0#
$ProbeChannel,1.0,13C/79Br,,,,,300,,,,0#
$EndBis,3E,46#
```

● **Required Samples** PH MASDVT 750W4 EFREE2 BL3.2 C/N/H

Z151230	Potassium Bromide (KBr, 34 ul)
Z151231	Adamantane (34 ul)
Z151232	Alpha-glycine (34 ul)

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 5000 Hz)

Line width main [achieved]: [135] <n/a>



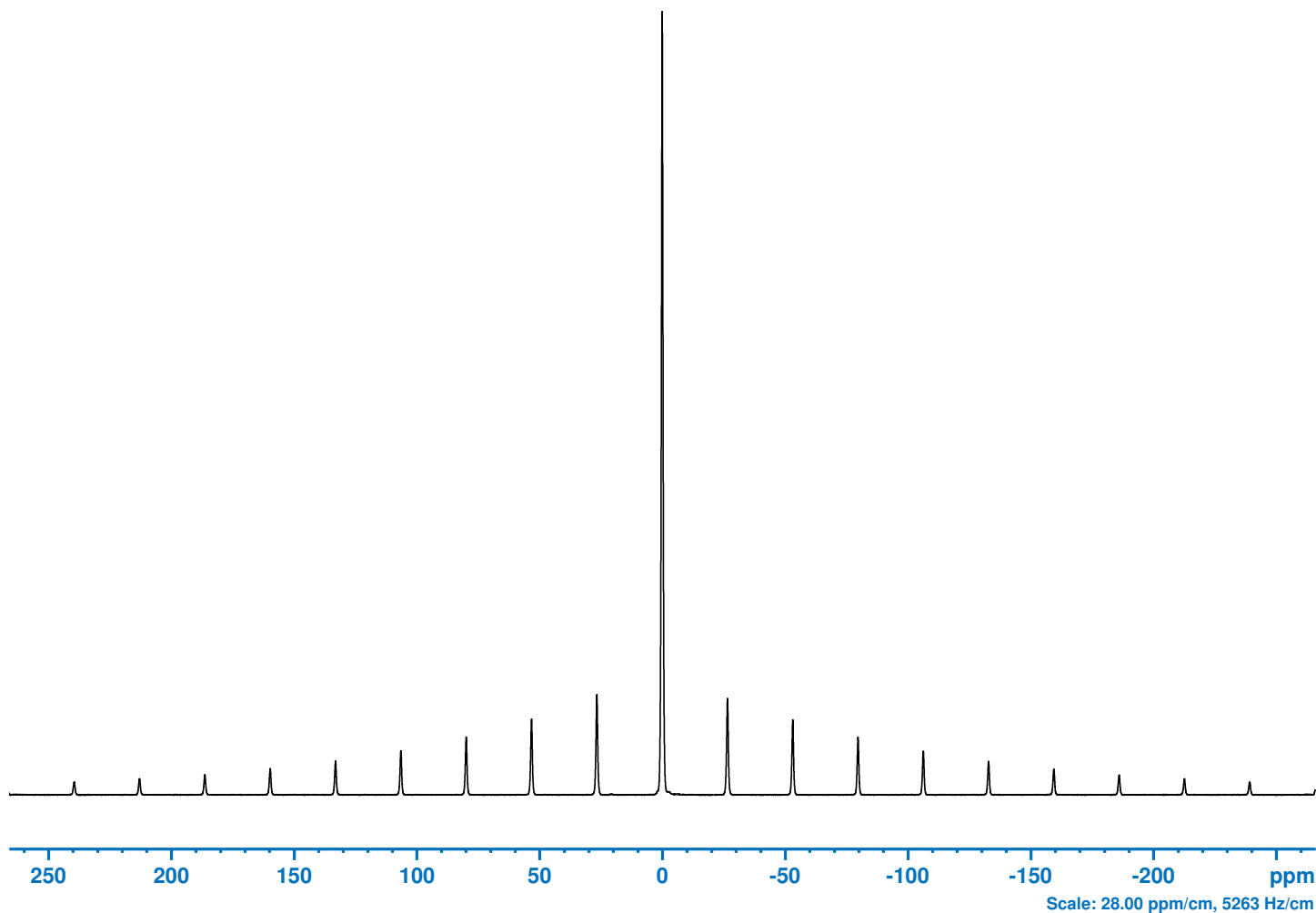
Bruker BioSpin

NPT_79Br_MAS_magicAngle

Current Data Parameters
NAME NPT_79Br_MAS_magicAngle
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 12.31 h
INSTRUM Avance
PROBHD H11833_0001 (P)
PULPROG onepulse
TD 8192
SOLVENT H2O+D2O
NS 16
DS 0
SWH 100000.000 Hz
FIDRES 24.414062 Hz
AQ 0.0409600 sec
RG 101
DW 5.000 usec
DE 6.50 usec
TE 298.0 K
D1 0.25000000 sec
SFO1 187.9912362 MHz
NUC1 79Br
P1 2.60 usec
PLW1 187.50000000 W

F2 - Processing parameters
SI 131072
SF 187.9912362 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20



SHIM SEQUENCE
skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3

Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H

Sample: Potassium Bromide (KBr, 34 ul) (Z151230)

Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 23000 Hz)

Determination of spinning stability for 180 s

Pressure values in mbar: DrivePressure=2396/BearingPressure=3164/BearingSensePressure=3164/SupplyPressure=6521/SystemPressure=6625

Spin rate at maximum deviation [measured]: @ MASR 23000 Hz [23003 Hz]

Maximum deviation [achieved]: @ MASR 23000 Hz [3 Hz] <n/a>



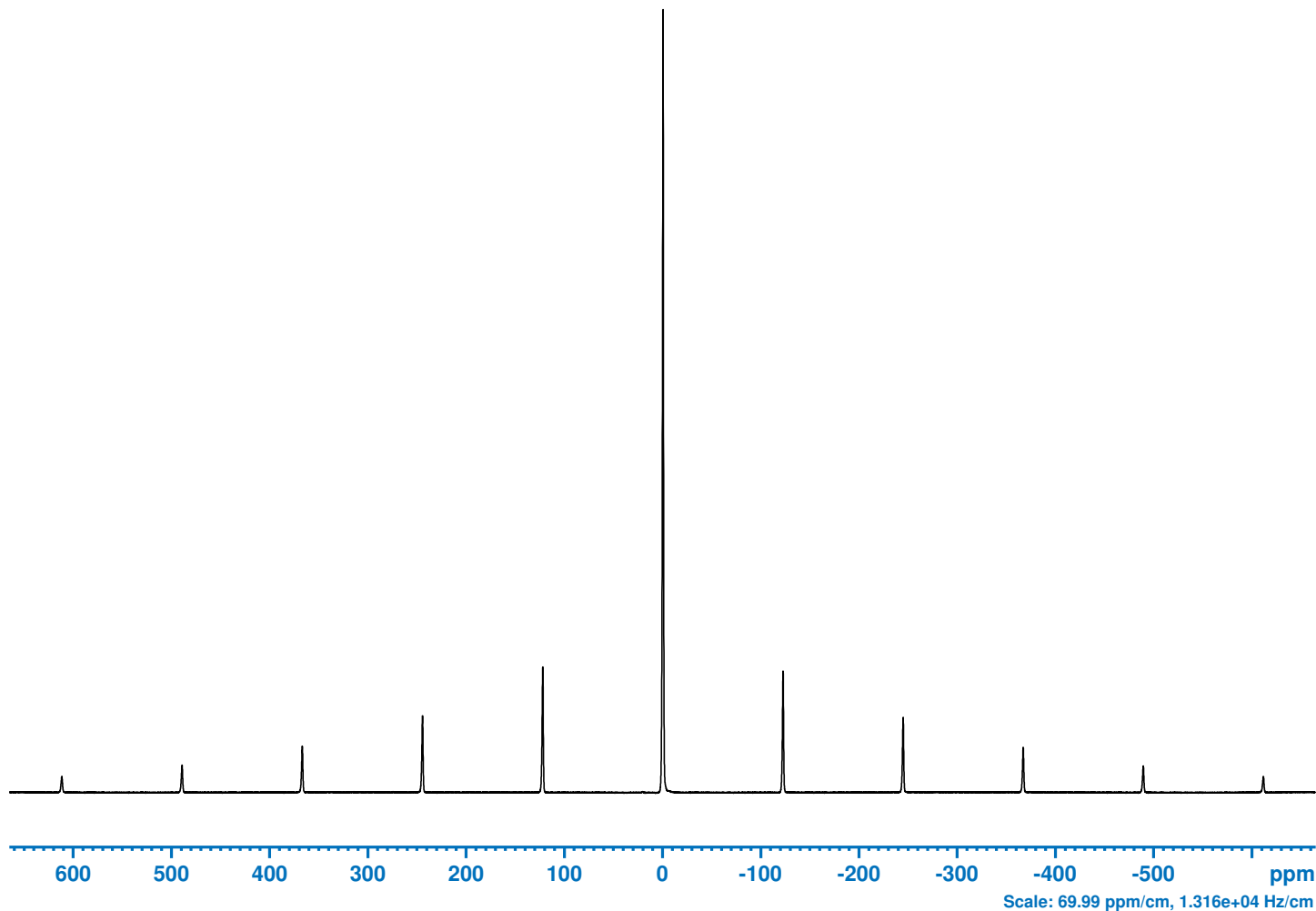
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

Current Data Parameters
NAME NPT_79Br_MAS_maxSpinRate
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 12.49 h
INSTRUM Avance
PROBHD H11833_0001 (P)
PULPROG onepulse
TD 16384
SOLVENT H2O+D2O
NS 16
DS 0
SWH 250000.000 Hz
FIDRES 30.517578 Hz
AQ 0.0327680 sec
RG 401
DW 2.000 usec
DE 6.50 usec
TE 297.8 K
D1 0.25000000 sec
SFO1 187.9912201 MHz
NUC1 79Br
P1 2.60 usec
PLW1 187.5000000 W

F2 - Processing parameters
SI 32768
SF 187.9912201 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20



SHIM SEQUENCE
skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting, spin rate 5000 Hz)
FIELD was set to 3172.9 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0065 ppm.



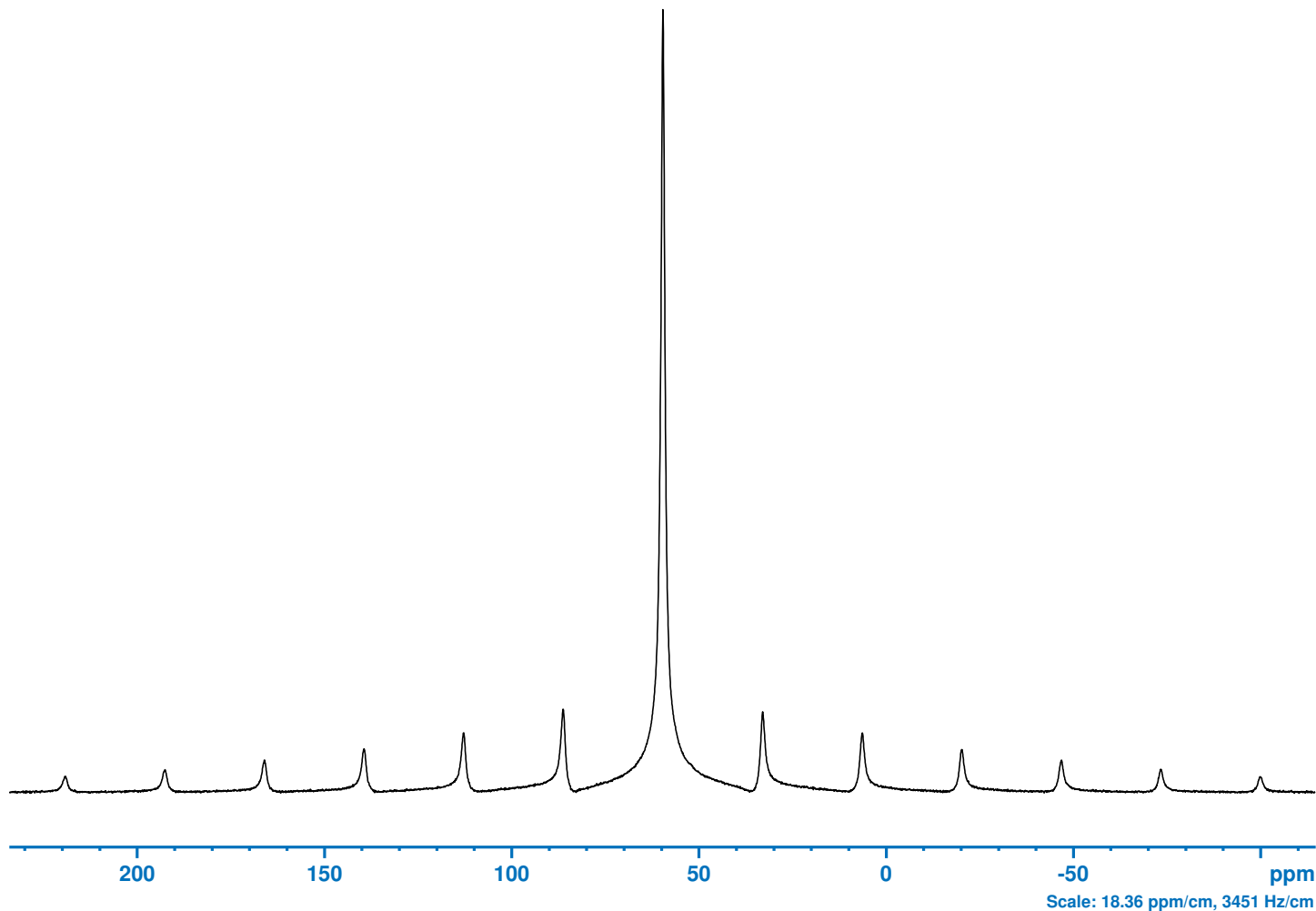
Bruker BioSpin

NPT_79Br_MAS_fieldsetting

Current Data Parameters
NAME NPT_79Br_MAS_fieldsetting
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 12.16 h
INSTRUM Avance
PROBHD H11833_0001 (P)
PULPROG onepulse
TD 4096
SOLVENT H2O+D2O
NS 1
DS 0
SWH 81967.211 Hz
FIDRES 40.023052 Hz
AQ 0.0249856 sec
RG 101
DW 6.100 usec
DE 6.50 usec
TE 296.3 K
D1 0.50000000 sec
SFO1 187.9912343 MHz
NUC1 79Br
P1 2.60 usec
PLW1 120.0000000 W

F2 - Processing parameters
SI 8192
SF 187.9800119 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 0.50



SHIM SEQUENCE
skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
 Sample: Adamantane (34 ul) (Z151231)
 P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 24000 Hz)
 ATTENTION: Updated PROSOL Tables with [2.50 us @ 175.3 W]. Calculation based on ==> [3.59 us @ 85.0 W]

P90 MAS 1H pulse [achieved]: @ 85.0 W [3.59 us] <n/a>



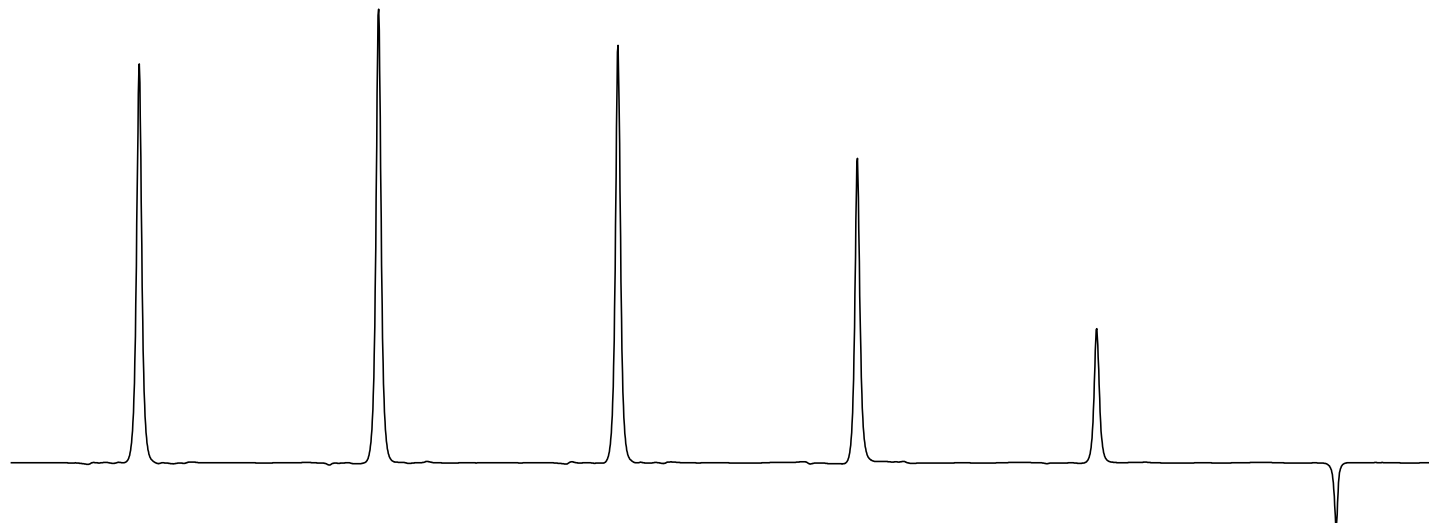
Bruker BioSpin

NPT_1H_MAS_p90det_1h

Current Data Parameters
 NAME NPT_1H_MAS_p90det_1h
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211019
 Time 13.31 h
 INSTRUM Avance
 PROBHD H11833_0001 (P)
 PULPROG onepulse
 TD 2988
 SOLVENT H2O+D2O
 NS 1
 DS 0
 SWH 100000.000 Hz
 FIDRES 66.934402 Hz
 AQ 0.0149400 sec
 RG 8
 DW 5.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 5.00000000 sec
 SFO1 750.3018457 MHz
 NUC1 1H
 P1 7.50 usec
 PLW1 85.00000000 W

F2 - Processing parameters
 SI 4096
 SF 750.3000000 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.20



Report of parameter optimization

F1P = 10.460 ppm, F2P = -5.540 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 2.500000000 us, endval = 7.500000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.5000	413149279	-1652166	11230451.245
2	3.5000	469913065	-2343122	12525297.513
3	4.5000	432533622	-1269690	11458210.282
4	5.5000	315261941	-1143553	8376457.217
5	6.5000	138858756	-904335	3810999.152
6	7.5000	403318	-66116779	-1310916.797

Parameter optimization for P1 finished.
 ZERO at experiment 5.677441: P1 = 7.177441 us

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

PLW90	P90	P90[det]	Deviation
85.0 W	2.50 us		
85.0 W	2.50 us	3.59 us	43.6%

 SHIM SEQUENCE

 skip shimming



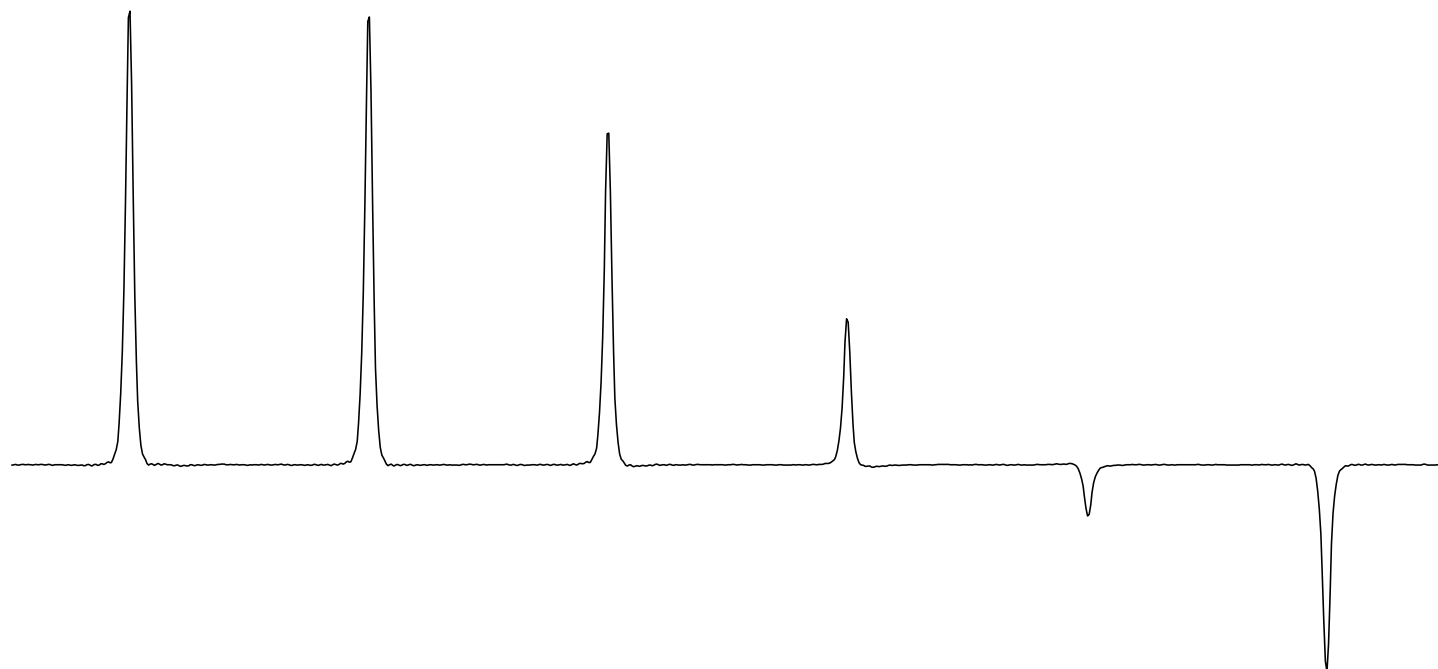
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
 Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
 P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br, spin rate 5000 Hz)
 ATTENTION: Updated PROSOL Tables with [2.60 us @ 187.5 W]. Calculation based on ==> [3.25 us @ 120.0 W]

P90 MAS 79Br pulse [achieved]: @ 120.0 W [3.25 us] <n/a>



Bruker BioSpin

NPT_79Br_MAS_p90det_79br



Report of parameter optimization

F1P = 69.700 ppm, F2P = 49.700 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 2.599999905 us, endval = 7.799999714 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.6000	419848749	-1425672	18310115.484
2	3.6400	414598904	-1027477	17959372.987
3	4.6800	307086741	-1776897	13063159.774
4	5.7200	135218484	-2288900	5369454.729
5	6.7600	1396463	-47268098	-2053898.684
6	7.8000	820802	-191626390	-8036908.948

Parameter optimization for P1 finished.
 ZERO at experiment 4.740978: P1 = 6.490617 us

Current Data Parameters
 NAME NPT_79Br_MAS_p90det_79br
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211019
 Time 12.18 h
 INSTRUM Avance
 PROBHD H11833_0001 (P)
 PULPROG onepulse
 TD 2048
 SOLVENT H2O+D2O
 NS 1
 DS 0
 SWH 100000.000 Hz
 FIDRES 97.656250 Hz
 AQ 0.0102400 sec
 RG 101
 DW 5.000 usec
 DE 6.50 usec
 TE 297.2 K
 D1 0.25000000 sec
 SFO1 187.9912343 MHz
 NUC1 79Br
 P1 7.80 usec
 PLW1 120.00000000 W

F2 - Processing parameters
 SI 4096
 SF 187.9800119 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.20

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

PLW90	P90	P90[det]	Deviation
120.0 W	2.60 us		
120.0 W	2.60 us	3.25 us	25.0%

 SHIM SEQUENCE

 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
 Sample: Alpha-glycine (34 ul) (Z151232)
 P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c, spin rate 7500 Hz)
 ATTENTION: Updated PROSOL Tables with [3.50 us @ 99.8 W].

P90_MAS_CP 1H13C power (PLW 11) [achieved]: [91.7 W] <n/a>
 P90_MAS_CP 1H13C pulse (P 1) [achieved]: [3.65 us] <n/a>



Bruker BioSpin

NPT_13C_MAS_p90det_cp1h_13c

Current Data Parameters
 NAME NPT_13C_MAS_p90det_cp1h_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211019
 Time 14.40 h
 INSTRUM Avance
 PROBHD H11833_0001 (P)
 PULPROG cp90
 TD 5554
 SOLVENT H2O+D2O
 NS 4
 DS 0
 SWH 55555.555 Hz
 FIDRES 20.005602 Hz
 AQ 0.0499860 sec
 RG 101
 DW 9.000 usec
 DE 6.50 usec
 TE 298.1 K
 D1 5.00000000 sec
 ZGPGTNS
 SFO1 188.6711976 MHz
 NUC1 13C
 P1 5.25 usec
 P15 2000.00 usec
 PLW1 91.72799683 W
 PLW11 91.72799683 W
 SFO2 750.3046519 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG2 spinal64
 P3 2.50 usec
 PCPD2 4.80 usec
 PLW2 175.27999878 W
 PLW12 175.27999878 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 232.76870728 W

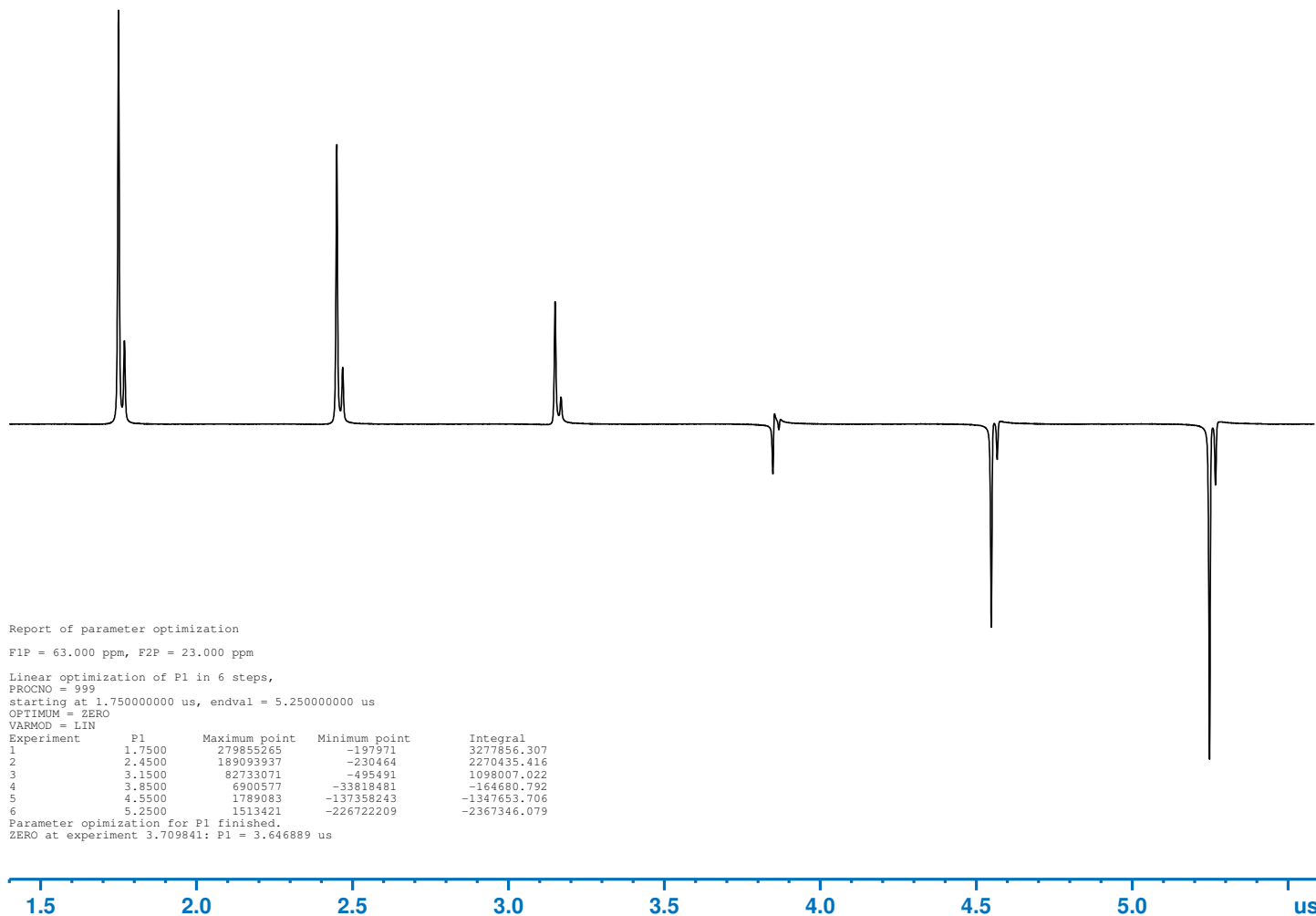
F2 - Processing parameters
 SI 8192
 SF 188.6630851 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.20

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

PLW90	P90	P90[det]	Deviation
91.7 W	3.50 us		
91.7 W	3.50 us	3.65 us	4.3%

SHIM SEQUENCE

skip shimming



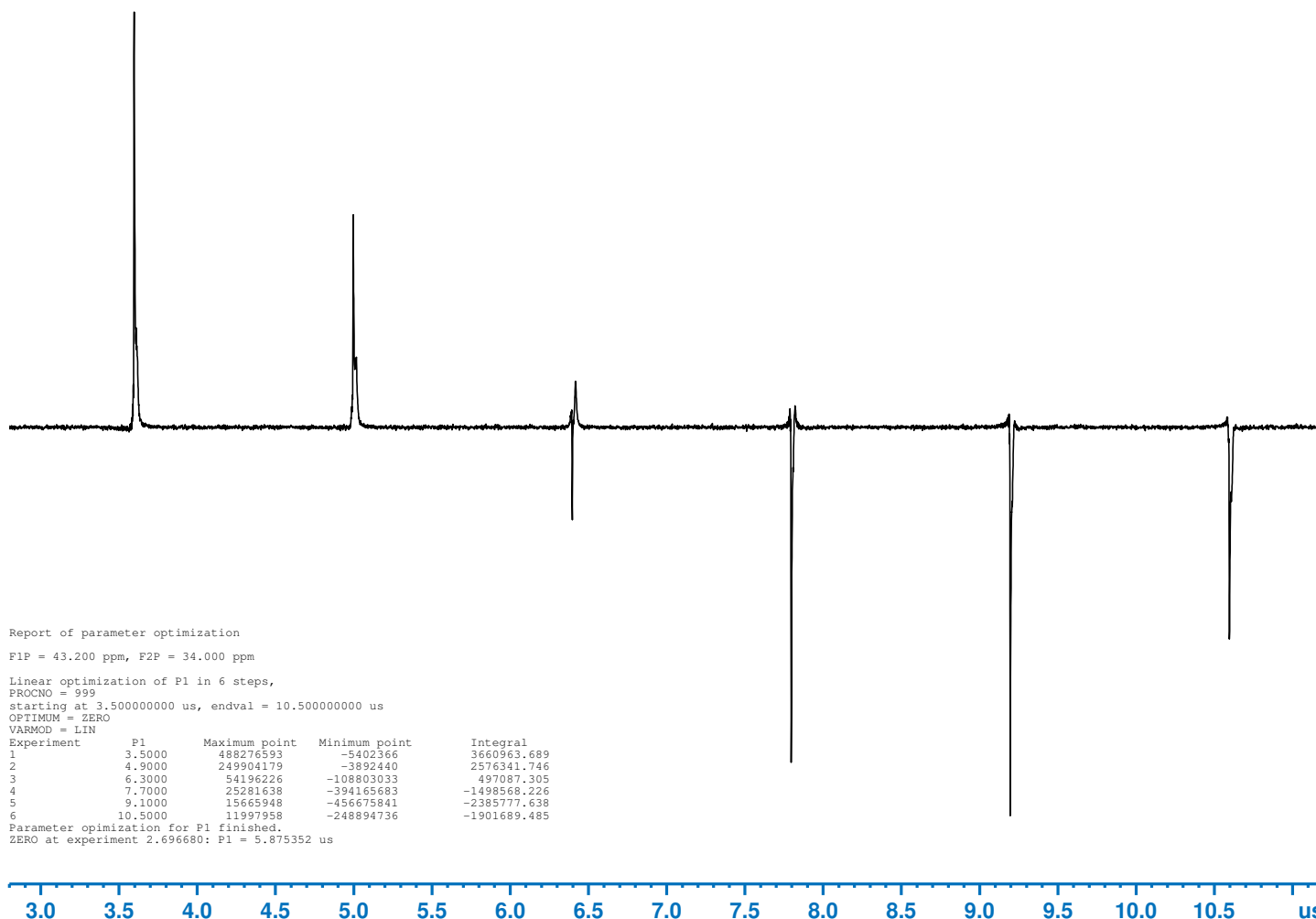
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
 Sample: Adamantane (34 ul) (Z151231)
 P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c, spin rate 24000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.50 us @ 91.7 W]. Calculation based on ==> [2.94 us @ 130.0 W]

P90 MAS 13C pulse [achieved]: @ 130.0 W [2.94 us] <n/a>



Bruker BioSpin

NPT_13C_MAS_p90det_13c



Current Data Parameters
 NAME NPT_13C_MAS_p90det_13c
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211019
 Time 14.09 h
 INSTRUM Avance
 PROBHD H11833_0001 (P)
 PULPROG hpdec
 TD 4000
 SOLVENT H2O+D2O
 NS 4
 DS 0
 SWH 10000.000 Hz
 FIDRES 5.000000 Hz
 AQ 0.2000000 sec
 RG 101
 DW 50.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 15.00000000 sec
 P15 0 usec
 ZGPTNS -Dlacq
 SFO1 188.6694996 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 130.00000000 W
 SFO2 750.3018457 MHz
 NUC2 1H
 CPDPRG[2] cw
 PLW2 175.27999878 W
 PLW12 0.63100803 W

F2 - Processing parameters
 SI 8192
 SF 188.6630851 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 FC 0.50

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

PLW90	P90	P90[det]	Deviation
130.0 W	3.50 us		
130.0 W	3.50 us	2.94 us	-16.0%

SHM SEQUENCE

skip shimming

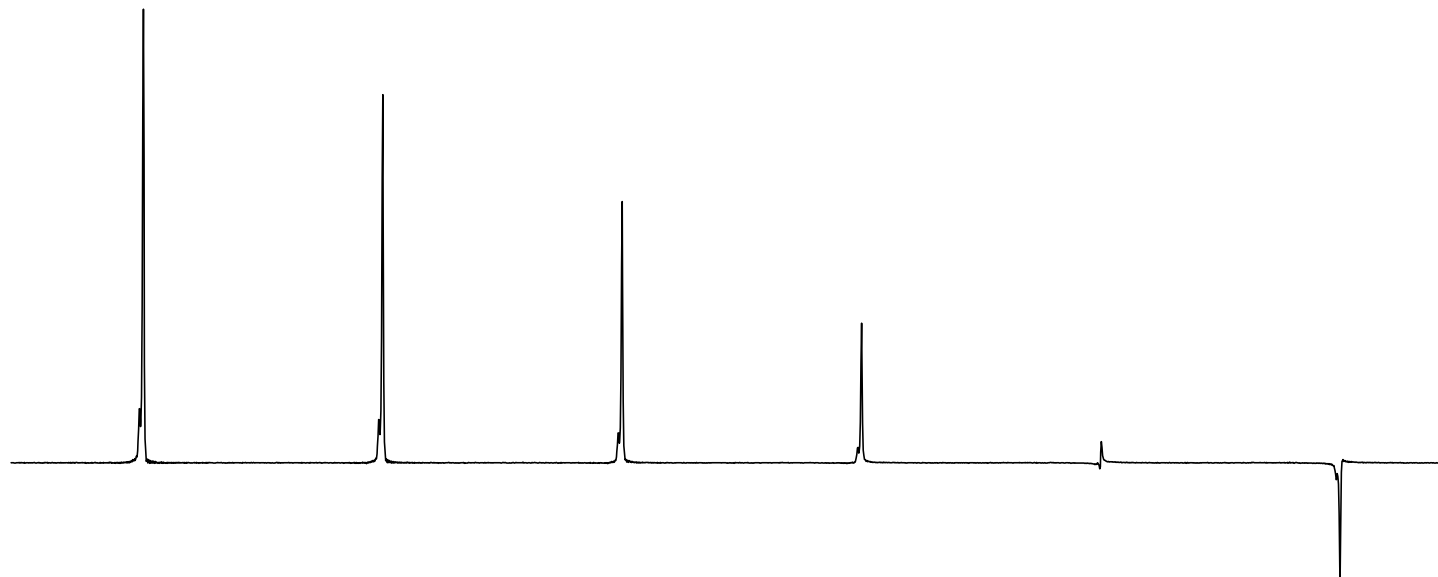
NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
 Sample: Alpha-glycine (34 ul) (Z151232)
 P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n, spin rate 7500 Hz)
 ATTENTION: Updated PROSOL Tables with [4.50 us @ 318.9 W].

P90_MAS_CP 1H15N power (PLW 11) [achieved]: [180.0 W] <n/a>
 P90_MAS_CP 1H15N pulse (P 1) [achieved]: [5.99 us] <n/a>



Bruker BioSpin

NPT_15N_MAS_p90det_cp1h_15n



Report of parameter optimization

F1P = 55.000 ppm, F2P = 15.000 ppm

Linear optimization of P1 in 6 steps,
 PROCNO = 999
 starting at 2.250000000 us, endval = 6.750000000 us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.2500	377551055	-595104	3566014.899
2	3.1500	306468557	-617379	2882888.458
3	4.0500	217472410	-643885	2049439.836
4	4.9500	116285429	-626375	1110058.728
5	5.8500	17684533	-5002705	115480.858
6	6.7500	2798058	-97253203	-894047.063

Parameter optimization for P1 finished.
 ZERO at experiment 5.153862: P1 = 5.988476 us

Current Data Parameters
 NAME NPT_15N_MAS_p90det_cp1h_15n
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211019
 Time 15.08 h
 INSTRUM Avance
 PROBHD H11833_0001 (P)
 PULPROG cp90
 TD 3012
 SOLVENT H2O+D2O
 NS 4
 DS 0
 SWH 30120.482 Hz
 FIDRES 20.000320 Hz
 AQ 0.0499992 sec
 RG 101
 DW 16.600 usec
 DE 6.50 usec
 TE 298.2 K
 D1 5.00000000 sec
 ZGPTNS
 SFO1 76.0298997 MHz
 NUC1 15N
 P1 6.75 usec
 P15 3500.00 usec
 PLW1 180.00000000 W
 PLW11 180.00000000 W
 SFO2 750.3046519 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG2 spinal64
 P3 2.50 usec
 PCPD2 4.80 usec
 PLW2 175.27999878 W
 PLW12 175.27999878 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 123.89579773 W

F2 - Processing parameters
 SI 4096
 SF 76.0272387 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

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

PLW90	P90	P90[det]	Deviation
180.0 W	4.50 us		
180.0 W	4.50 us	5.99 us	33.1%

 SHM SEQUENCE

 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
 Sample: Alpha-glycine (34 ul) (Z151232)
 CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c, spin rate 7500 Hz)

SINO (20.0 ppm) [achieved/rated]: Signal (42.79 ppm), Noise (118.79 to 98.78 ppm) [673.2 >= 500.0] <pass>
 Number of scans (NS) [achieved/rated]: [64 <= 64] <pass>
 Processed with TDef=2048



Bruker BioSpin

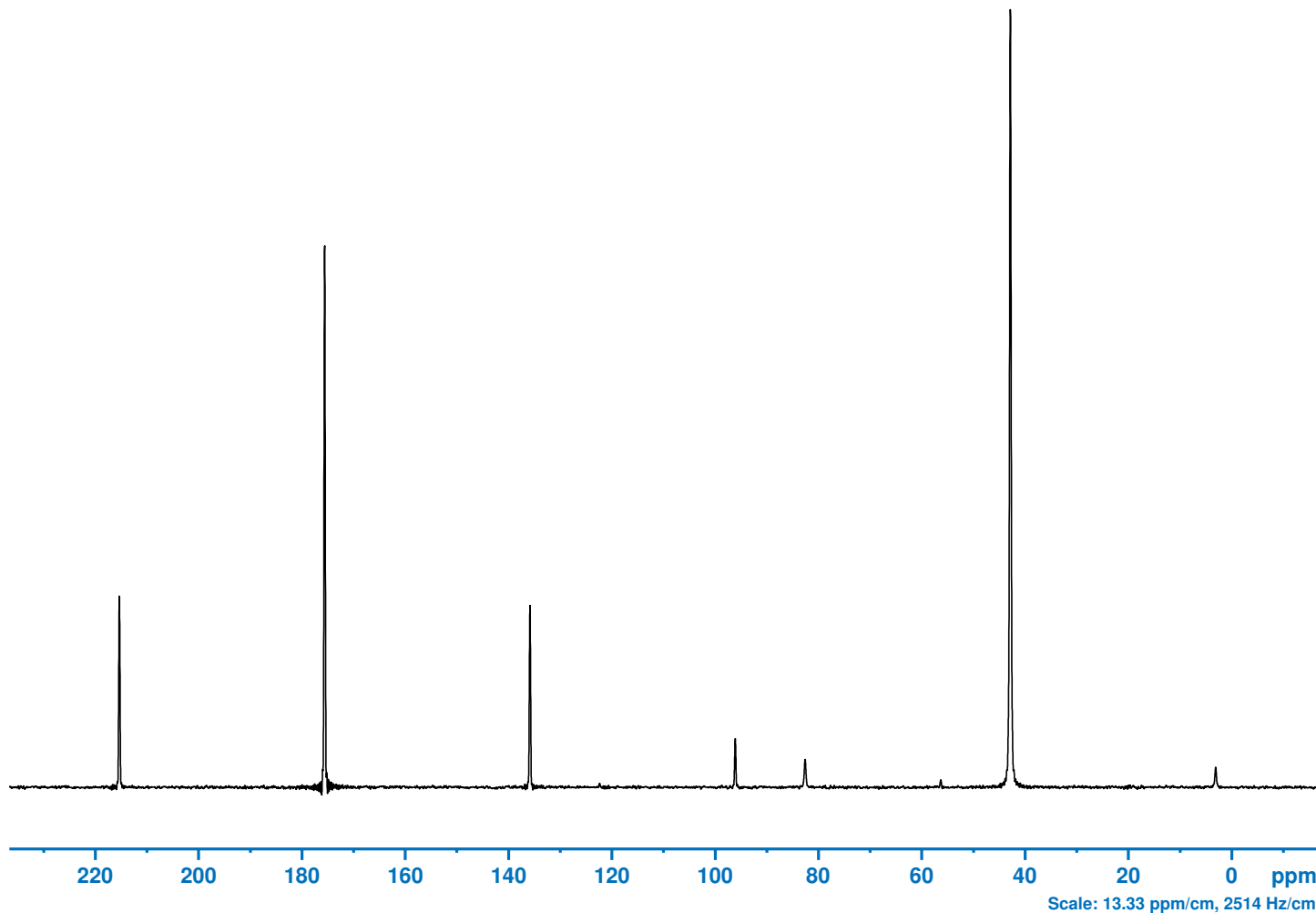
NPT_13C_MAS_sino_cp1h_13c

Current Data Parameters
 NAME NPT_13C_MAS_sino_cp1h_13c
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211020
 Time 10.43 h
 INSTRUM Avance
 PROBHD H11833_0001 (P)
 PULPROG cp
 TD 5554
 SOLVENT H2O+D2O
 NS 64
 DS 0
 SWH 55555.555 Hz
 FIDRES 20.005602 Hz
 AQ 0.0499860 sec
 RG 101
 DW 9.000 usec
 DE 6.50 usec
 TE 298.0 K
 D1 5.00000000 sec
 ZGPGTNS
 SFO1 188.6838380 MHz
 NUC1 13C
 P15 2000.00 usec
 PLW1 99.75900269 W
 SFO2 750.3046519 MHz
 NUC2 1H
 CNST21 1.00000000
 CPDPRG[2] spinal64
 P3 2.50 usec
 PCPD2 4.80 usec
 PLW2 175.27999878 W
 PLW12 182.25999451 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 194.14999390 W

F2 - Processing parameters
 SI 32768
 SF 188.6630851 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 FC 0.20

SHIM SEQUENCE
 skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
 Sample: Alpha-glycine (34 ul) (Z151232)
 CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n, spin rate 7500 Hz)

SINO (20.0 ppm) [achieved/rated]: Signal (32.61 ppm), Noise (25.64 to 5.63 ppm) [84.4 >= 80.0] <pass>
 Number of scans (NS) [achieved/rated]: [64 <= 64] <pass>



Bruker BioSpin

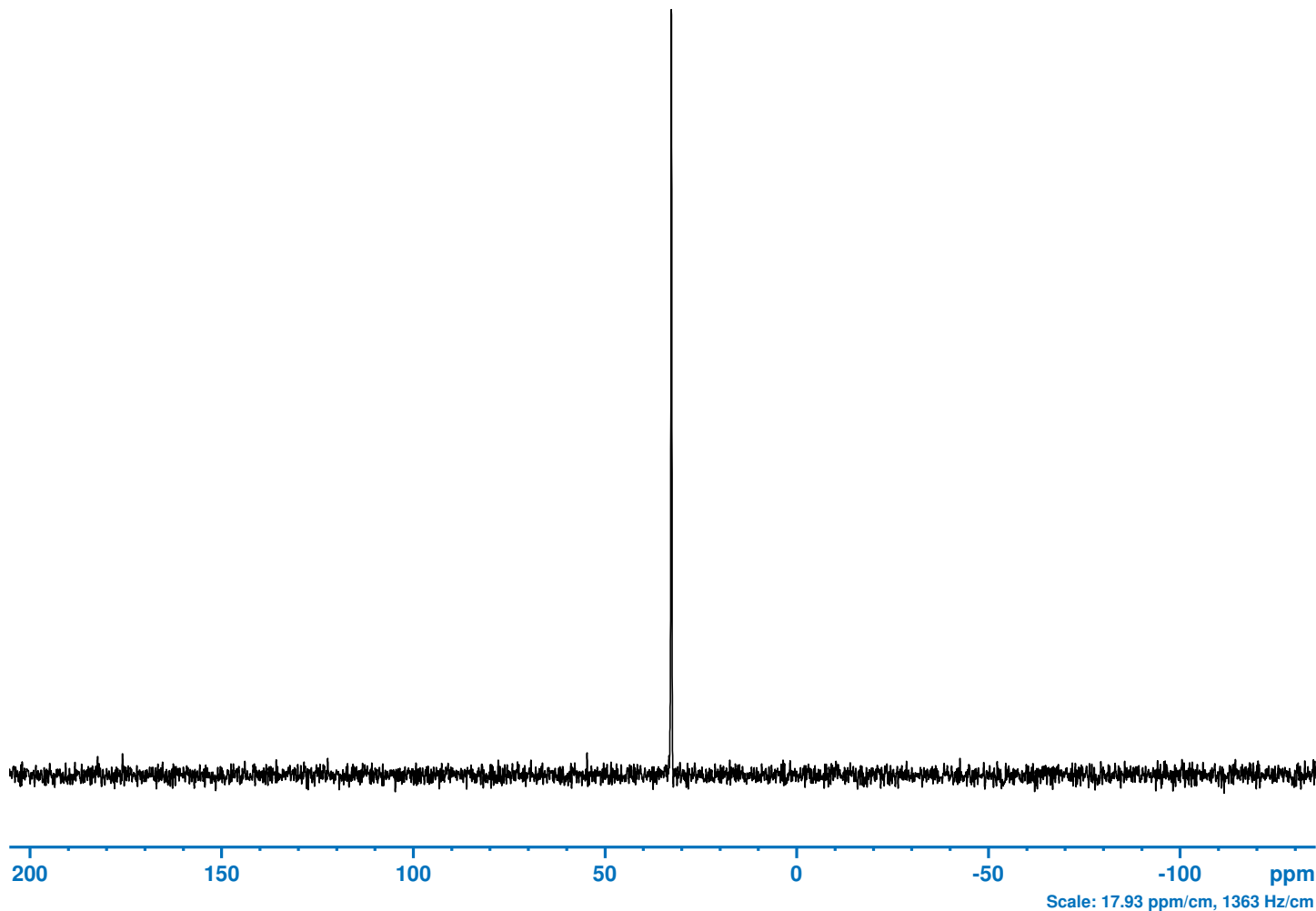
NPT_15N_MAS_sino_cp1h_15n

Current Data Parameters
 NAME NPT_15N_MAS_sino_cp1h_15n
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20211020
 Time 11.20 h
 INSTRUM Avance
 PROBHD H11833_0001 (P)
 PULPROG cp
 TD 3012
 SOLVENT H2O+D2O
 NS 64
 DS 0
 SWH 30120.482 Hz
 FIDRES 20.000320 Hz
 AQ 0.0499992 sec
 RG 101
 DW 16.600 usec
 DE 6.50 usec
 TE 298.0 K
 D1 5.0000000 sec
 ZGPGTNS
 SFO1 76.0298997 MHz
 NUC1 15N
 P15 3500.00 usec
 PLW1 318.92999268 W
 SFO2 750.3046519 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG2 spinal64
 P3 2.50 usec
 PCPD2 4.80 usec
 PLW2 175.27999878 W
 PLW12 161.22999573 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 111.45999908 W

F2 - Processing parameters
 SI 32768
 SF 76.0272387 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

SHIM SEQUENCE
 skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Adamantane (34 ul) (Z151231)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 23980 Hz)

SINO (20.0 ppm) [achieved]: Signal (37.93 ppm), Noise (60.36 to 40.36 ppm) [52.4] <n/a>
Linewidth [achieved]: at 50% of signal height [5.3 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>



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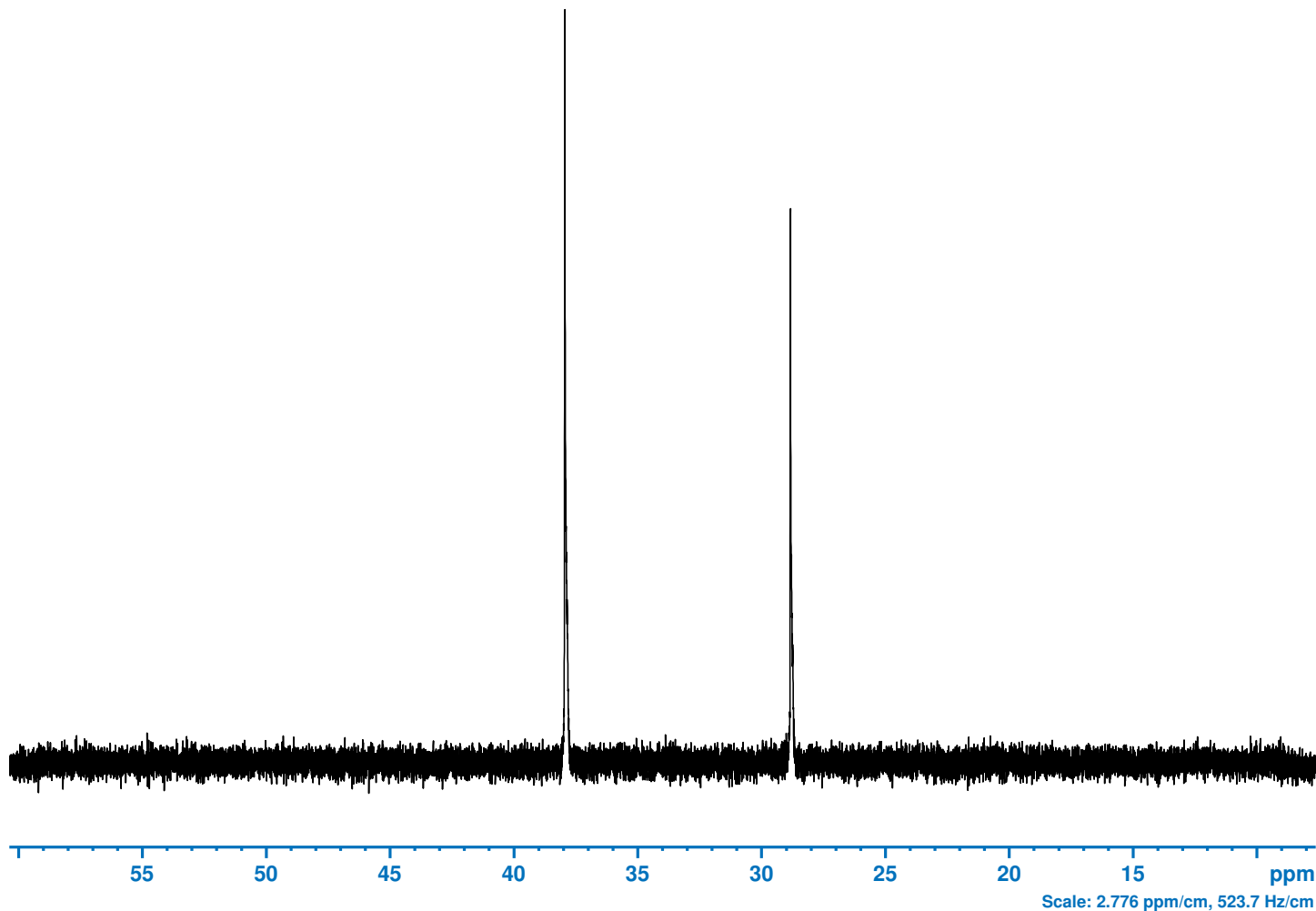
NPT_13C_MAS_sino_13c

Current Data Parameters
NAME NPT_13C_MAS_sino_13c
EXPNO 501
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 14.24 h
INSTRUM Avance
PROBHD H11833_0001 (P)
PULPROG hpdcc
TD 19998
SOLVENT H2O+D2O
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 1.000100 Hz
AQ 0.9999000 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 15.00000000 sec
P15 0 usec
ZGPGTNS -Dlacq
SFO1 188.6694996 MHz
NUC1 13C
P1 3.50 usec
PLW1 91.72799683 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG2 cw
PLW2 175.27999878 W
PLW12 0.62995678 W

F2 - Processing parameters
SI 32768
SF 188.6630851 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 0.20

SHIM SEQUENCE
skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
 Sample: Adamantane (34 ul) (Z151231)
 13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 23980 Hz)



Bruker BioSpin

NPT_13C_MAS_sino_13c

```
# Tue Oct 19 12:24:28 2021
##$PROBEIDENTIFIER=H11833_0001
##$PROBENAME=PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
##$SHIMID=272623
#
# Active Shim Gradients
#
Z -32510
Z2 0
Z3 0
Z4 0
Z5 0
Z6 0
X -350
XZ 0
XZ2 0
XZ3 0
XZ4 0
Y 2300
YZ -2800
YZ2 0
YZ3 0
YZ4 0
XY 0
XYZ 0
XYZ2 0
XYZ3 0
(X2-Y2) 0
(X2-Y2) Z 0
(X2-Y2) Z2 0
(X2-Y2) Z3 0
X3 0
X3Z 0
Y3 0
Y3Z 0
#
# Lock Parameter
#
FIELD 3172.873
LOCKPHASE 30.000
LOCKPOWER -8.000
LOCKGAIN 109.219
LOCKDC -70.000
LOCKSHIFT 4.700
LOOPGAIN -5.000
LOOPTIME 0.350
LOOPFILTER 100.000
#
IEEE64_VERSION_CODE 1
#
```

```
# Shim currents
#
SHIM_SETTING [ 1] -8127.49987255
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] 0.00000000
SHIM_SETTING [ 4] 1132.02262374
SHIM_SETTING [ 5] -1131.89943035
SHIM_SETTING [ 6] -249.63718606
SHIM_SETTING [ 7] 249.51399609
SHIM_SETTING [ 8] 19.21606552
SHIM_SETTING [ 9] -19.69548428
SHIM_SETTING [10] 2636.55242012
SHIM_SETTING [11] -2636.30130789
SHIM_SETTING [12] 0.00000000
SHIM_SETTING [13] 0.00000000
SHIM_SETTING [14] 0.00000000
SHIM_SETTING [15] -79.01924802
SHIM_SETTING [16] -79.01924802
SHIM_SETTING [17] 87.50027464
SHIM_SETTING [18] 87.50027464
SHIM_SETTING [19] -41.41112998
SHIM_SETTING [20] -41.41112998
SHIM_SETTING [21] 0.00000000
SHIM_SETTING [22] 0.00000000
SHIM_SETTING [23] 0.00000000
SHIM_SETTING [24] 0.00000000
SHIM_SETTING [25] 0.00000000
SHIM_SETTING [26] 0.00000000
SHIM_SETTING [27] 0.00000000
SHIM_SETTING [28] -180.72969409
SHIM_SETTING [29] 0.00000000
SHIM_SETTING [30] 0.00000000
SHIM_SETTING [31] -239.71010748
SHIM_SETTING [32] 1219.26973051
SHIM_SETTING [33] 0.00000000
SHIM_SETTING [34] 0.00000000
SHIM_SETTING [35] 0.00000000
SHIM_SETTING [36] 0.00000000
SHIM_SETTING [37] 396.12871413
SHIM_SETTING [38] 148.13581605
SHIM_SETTING [39] -910.28983188
SHIM_SETTING [40] 0.00000000
```

```
Current Data Parameters
NAME NPT_13C_MAS_sino_13c
EXPNO 501
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 14.24 h
INSTRUM Avance
PROBHD H11833_0001 (P
PULPROG hpdec
TD 19998
SOLVENT H2O+D2O
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 1.000100 Hz
AQ 0.9999000 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 15.00000000 sec
P15 0 usec
ZGPGTNS -Dlacq
SFO1 188.6694996 MHz
NUC1 13C
P1 3.50 usec
PLW1 91.72799683 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG2 cw
PLW2 175.27999878 W
PLW12 0.62995678 W

F2 - Processing parameters
SI 32768
SF 188.6630851 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 0.20
```

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Adamantane (34 ul) (Z151231)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 23990 Hz)

SINO (20.0 ppm) [achieved]: Signal (1.81 ppm), Noise (63.99 to 43.98 ppm) [29517.0] <n/a>
Linewidth [achieved]: at 50% of signal height [264.3 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>



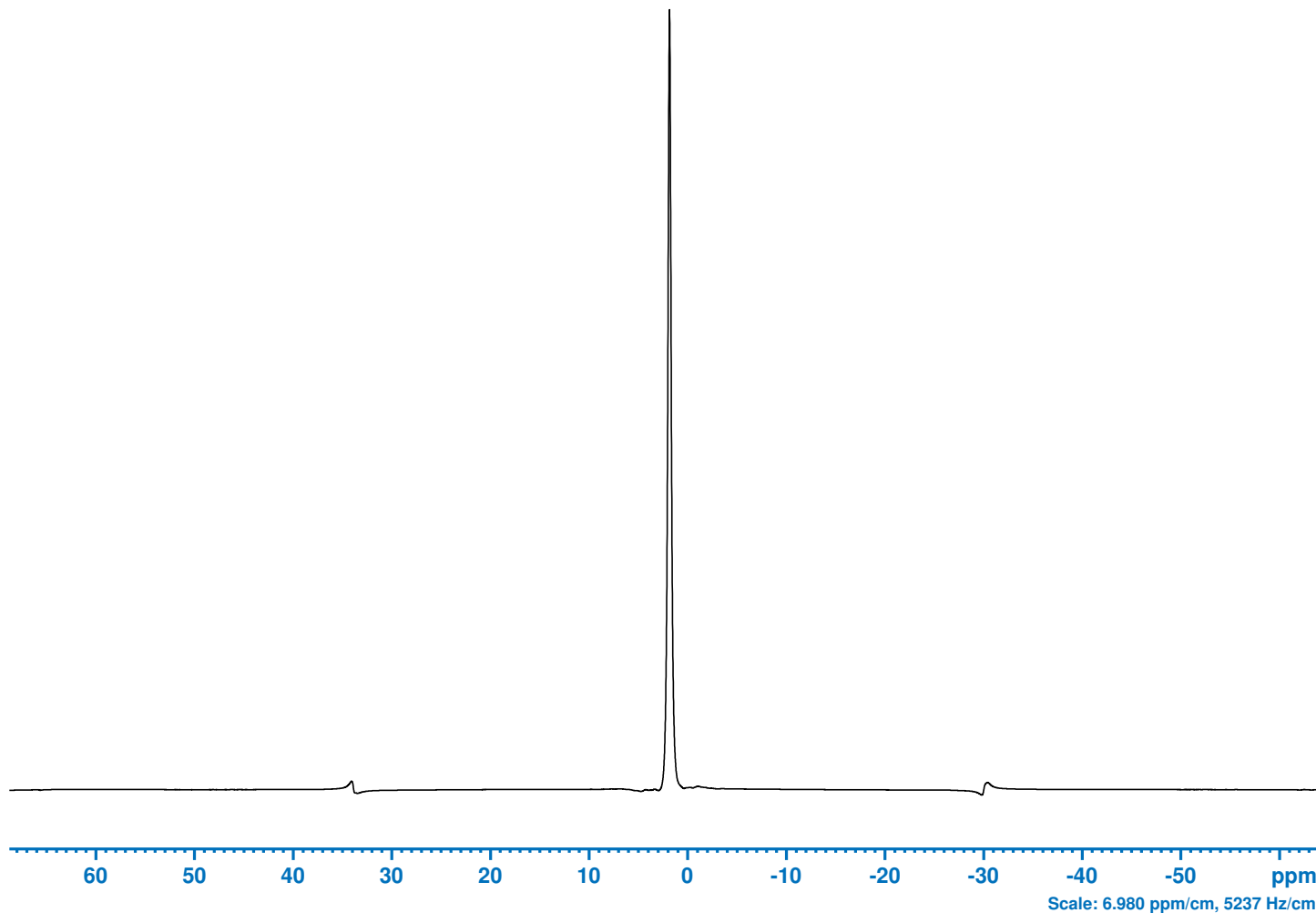
Bruker BioSpin

NPT_1H_MAS_sino_1h

Current Data Parameters
NAME NPT_1H_MAS_sino_1h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 14.12 h
INSTRUM Avance
PROBHD H11833_0001 (P)
PULPROG onepulse
TD 2048
SOLVENT H2O+D2O
NS 1
DS 0
SWH 100000.000 Hz
FIDRES 97.656250 Hz
AQ 0.0102400 sec
RG 8
DW 5.000 usec
DE 6.50 usec
TE 298.0 K
D1 5.00000000 sec
SFO1 750.3018457 MHz
NUC1 1H
P1 2.50 usec
PLW1 175.27999878 W

F2 - Processing parameters
SI 16384
SF 750.3000000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



SHIM SEQUENCE
skip shimming