

NMR Test Spectrometer

Report Name: 3.2mm_HX_Install

AV NEO (1000 MHz) 408457

Content:

- Configuration Information ([uxnmr.info](#))
- IP Config Information
- Probe: H177324_0001 / 3.2mm_HX_Install



● Configuration Information uxnmr.info

CONFIGURATION INFORMATION

=====

```
Path      : /opt/topspin/conf/instr/spect/uxnmr.info
Date      : Thu Dec 17 10:06:33 2020
Release   : TopSpin 4.0.9
Installed in : /opt/topspin
Host      : BladeEpu
OS        : CentOS Linux release 7.2.1511 (Core)
SPECTR-OS : Version 4.1.146.20200805
CPU       : Intel(R) Core(TM) i7-4700EQ CPU @ 2.40GHz (8 cores at 2362 MHz with Hyperthreading)
User      : root (root)
System    : Avance Neo 1000 NMR spectrometer
1H-frequency : 1000.40 Mhz
Description : Avance Neo 1GHZ
Bruker Order : 408457
Configured in: BladeEpu:/opt/topspin/conf/instr/spect

AQ-Rack:
- EPU/2: AV4 EPU/2 Embedded Processing Unit H153448F1/01415 ECL 01.04
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/04540 ECL 02.03
Location: slot 1 in rack 1
Connection: at IP 192.168.180.14 via PCIe #3
Firmware Version: 20190906112554
Devices: MTD at /dev/mtd2, DRX at /dev/bbu/drx3.5, RTD at /dev/bbu/rtd3.4
Sequencer: FCube
- FCube1
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/04541 ECL 02.03
Location: slot 2 in rack 1
Connection: at IP 192.168.180.18 via PCIe #4
Firmware Version: 20190906112554
Devices: MTD at /dev/mtd11, DRX at /dev/bbu/drx4.5, RTD at /dev/bbu/rtd4.4
Sequencer: FCube
- FCube2
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/04542 ECL 02.03
Location: slot 3 in rack 1
Connection: at IP 192.168.180.22 via PCIe #5
Firmware Version: 20190906112554
Devices: MTD at /dev/mtd20, DRX at /dev/bbu/drx5.5, RTD at /dev/bbu/rtd5.4
Sequencer: FCube
- FCube3
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/04543 ECL 02.03
Location: slot 4 in rack 1
Connection: at IP 192.168.180.26 via PCIe #6
Firmware Version: 20190906112554
Devices: MTD at /dev/mtd29, DRX at /dev/bbu/drx6.5, RTD at /dev/bbu/rtd6.4
Sequencer: FCube
- FCube4
- GTU: AV4 GT-CONTROLLER UNIT Z148393/01463 ECL 01.02
Location: slot 6 in rack 1
Connection: at IP 192.168.180.38 via PCIe #9
Firmware Version: 20190906085855
Devices: MTD at /dev/mtd37, RTD at /dev/bbu/rtd9.4, GPROC at /dev/bbu/gproc9.7
Sequencer: GCube, TCube
- GCube1
- TCube1
- BSM-A: AV4 PSM-A Z149510/01853 ECL 03.01
- HPPR/2 COVER2: HPPR/2 Cover2 Z124567/03490 ECL 00.05
HPPR2: - HPPR/2 preamplifier connected via AgRack
Type      : HPPR/2
Controller: Cover/2
no LED display for tuning and matching
Module 1 : HPLNA 19FH (virtual 50 Ohm reference: 101.0%/-0.2deg, reflection meter without CRP-Bias capability)
PN=Z103210, SN=00209 from 20190703
Module 2 : 2H
```

```
PN=Z109356, SN=00204 from 20190627
Module 3 : HPLNA BB31P (reflection meter without CRP-Bias capability)
PN=Z111100, SN=00208 from 20190913
Module 4 : 13C/79Br
PN=Z109357, SN=00205 from 20190710
Module 5 : HPLNA BB31P (reflection meter without CRP-Bias capability)
PN=Z111100, SN=00212 from 20190621
Module 6 : 15N
PN=Z109358, SN=00205 from 20190606
```

```
- HPLNA 19FH: HPLNA 1H MODULE 1000 Z103210/00209 ECL 06.02
- 2H: HPPR/2 2H MODULE 1000 Z109356/00204 ECL 07.00
- HPLNA BB31P: HPLNA XBB 31P MODULE 1000 Z111100/00208 ECL 04.04
- 13C/79Br: HPPR/2 13C MODULE 1000 Z109357/00205 ECL 08.00
- HPLNA BB31P: HPLNA XBB 31P MODULE 1000 Z111100/00212 ECL 04.04
- 15N: HPPR/2 15N MODULE 1000 Z109358/00205 ECL 07.01
- RACK: AV4 AQS CHASSIS Z149500/01433 ECL 02.00
- PSM-4BV: AV4 PSM-4BV Z149850/03257 ECL 01.02
- PSM-D: AV4 PSM-D Z149520/01837 ECL 01.01
- FANTRAY: AV4 AQS FAN TRAY Z149501/01486 ECL 00.02
- REF 1200: AV4 REFERENCE 1200 Z148270/01580 ECL 02.02
```

Transmitters at the spectrometer subnet:

```
-----
BLA-W144060-000152 W144060/000152 ECL 40:
- TCP/IP address = 192.168.99.13
- Firmware VS = 20181126
- Amplifier = AV4 BLABB1000 15-600: W144060/000152 ECL 40
- Controller = BLA CONTROL BOARD 7: W133936/022502 ECL 21
BLA-W162904-000018 W162904/000018 ECL 00:
- TCP/IP address = 192.168.99.12
- Firmware VS = 20181126
- Amplifier = BLA2H 950-1200: W162904/000018 ECL 00
- Controller = BLA CONTROL BOARD 7: W133936/022213 ECL 21
BLA-W144271-000013 W144271/000013 ECL 01:
- TCP/IP address = 192.168.99.11
- Firmware VS = 20181126
- Amplifier = AV4 BLAH1000 950-1000: W144271/000013 ECL 01
- Controller = BLA CONTROL BOARD 7: W133936/022599 ECL 21
BLA-W144059-000401 W144059/000401 ECL 10:
- TCP/IP address = 192.168.99.10
- Firmware VS = 20181126
- Amplifier = AV4 BLABB500 15-600: W144059/000401 ECL 10
- Controller = BLA CONTROL BOARD 7: W133936/022507 ECL 21
LTRX Z109897/00202 ECL 01.01:
- TCP/IP address = 192.168.99.15
- Amplifier = BSM5/2 LOCK TRANSCEIVER 1000: Z109897/00202 ECL 01.01

BSMS: BSM5/2 connected to ethernet
- TCP/IP address = 192.168.99.15
- ELCB firmware version = 20191111
- ELCB = BSM5/2 ELCB: Z100818/08512 ECL 07.02
- GAB current limits = 0.0/X, 0.0/Y, 10.0/Z (in A)
- Shim System = B0SS3-SB
- SGB channels = 40
- Shim matrix file: 292722dd.dat
- Active shims: Z Z2 Z3 Z4 Z5 X XZ X22 (X2-Y2) XY YZ Y22 (X2-Y2)Z X24 X23 Z6 (X2-Y2)Z Y24 Y23 XY22 XYZ X32 X3
- Magnet polarity: SN (Bruker), uses standard H0 polarity
- L-TRX = BSM5/2 LOCK TRANSCEIVER 1000: Z109897/00202 ECL 01.01
- Lock: on L-TRX board, supports 2H
- VTU_SFB = BSM5/2 SFB SENSOR & PNEUMATIC BD: Z115191/05625 ECL 05.04
- VTU_VPSB1 = AV4 VARIABLE POWER SUPPLY BD DC: Z139305/01462 ECL 01.02

VTU: in BSM5/2 connected to ethernet
```

● Configuration Information uxnmr.info

```
- TCP/IP address = 192.168.99.15
MAS Control Unit: MAS_H139288_0799
- TCP/IP address = 192.168.98.3
- Firmware version = 20200617_1039

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

Gradient Controller cable connections
-----

RF cable connections (detected)
-----
TRX1 NORM output -> input 1 of transmitter 3 (AV4 BLAH1000 950-1000 W144271/000013 at TCP/IP 192.168.99.11)
TRX1 AUX output -> open
TRX2 NORM output -> input 1 of transmitter 2 (BLA2H 950-1200 W162904/000018 at TCP/IP 192.168.99.12)
TRX2 AUX output -> open
TRX3 NORM output -> input 1 of transmitter 4 (AV4 BLABB500 15-600 W144059/000401 at TCP/IP 192.168.99.10)
TRX3 AUX output -> open
TRX4 NORM output -> input 1 of transmitter 1 (AV4 BLABB1000 15-600 W144060/000152 at TCP/IP 192.168.99.13)
TRX4 AUX output -> open

Blanking cable connections (detected)
-----
transmitter 1 = AV4 BLABB1000 15-600 W144060/000152 at TCP/IP 192.168.99.13:
- amplifier B-1000W uses blanking 4
- amplifier B-100W uses blanking 4

transmitter 2 = BLA2H 950-1200 W162904/000018 at TCP/IP 192.168.99.12:
- amplifier 2H-250W uses blanking 2

transmitter 3 = AV4 BLAH1000 950-1000 W144271/000013 at TCP/IP 192.168.99.11:
- amplifier 1H-1000W uses blanking 1
- amplifier 1H-100W uses blanking 1

transmitter 4 = AV4 BLABB500 15-600 W144059/000401 at TCP/IP 192.168.99.10:
- amplifier B-500W uses blanking 3

transmitter 5 = BSMS/2 LOCK TRANSCEIVER 1000 Z109897/00202 at TCP/IP 192.168.99.15:
- amplifier 2H-5W needs no blanking

Preamplifier connections (detected)
-----
Tune-TRX1 -> HPLNA 19F1H -> REC1
Tune-TRX2 -> ZH -> REC2
Tune-TRX3 -> HPLNA BB31P -> REC3
Tune-TRX3 -> 13C/79Br -> REC3
Tune-TRX4 -> HPLNA BB31P -> REC4
Tune-TRX4 -> 15N -> REC4
```

● IP Config Information

```
eno1: 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::9e7b:efff:fe38:65cc prefixlen 64 scopeid 0x20<link>
ether 9c:7b:ef:38:65:cc txqueuelen 1000 (Ethernet)
RX packets 17779007 bytes 5236260545 (4.8 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 21898407 bytes 3894115812 (3.6 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 137.205.214.25 netmask 255.255.255.0 broadcast 137.205.214.255
inet6 fe80::383:4909:2087:a495 prefixlen 64 scopeid 0x20<link>
ether 9c:7b:ef:38:65:cd txqueuelen 1000 (Ethernet)
RX packets 1044627 bytes 193572919 (184.6 MiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 511622 bytes 93541680 (89.2 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 30168133 bytes 5104994250 (4.7 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 30168133 bytes 5104994250 (4.7 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
```

PH MASDVT1000S6 BL3.2 X/H NO_I/E

1000 MHz

Probe ID: H177324_0001

Inspection Lot: 3.2mm_HX_Install

Dec 22, 2020

NMR TEST ACCEPTANCE

● Probe NMR Test Data: PH MASDVT1000S6 BL3.2 X/H NO_I/E

Probe Related Information

EC-Level _____ 0
 Gas Compensation _____ nitrogen
 Gradient System _____ unknown
 ATM Accessory _____ false
 Temperature Sensor Type _____ TypeT
 Proton Frequency [MHz] _____ 1000
 Diameter [mm] _____ 3.2

Spectrometer Related Information

Type _____ AV NEO
 CF Frequency [MHz] _____ 1000.40
 Shim System _____ BOSS3-SB
 Shim System Offset _____ 59 mm
 Software _____ TopSpin 4.0.9
 Operating System _____ CentOS Linux release 7.8.2003 (Core)
 Host Name _____ CZC018C67F
 Magnet System _____ SB
 Magnet Coil No _____
 Dewar No _____
 Helium Level _____ 80%
 System Number _____ 408457

● PICS Data

H177324_0001.ph

```
H177324_0001.ph
=====
$Bis,1,20201221,2048,PICS,5#
$Production,H177324,0001,00,00,,BNMRDE,20201126#
$Name,PH MASEDVT1000S6 BLS.2 X/H NO.1/E#
$ProbeCompatibility,1.0,SB,6,1000#
$ProbeType,1.1,MAS,0,0#
$ProbeSample,1.0,3.2,0#
$ProbeTemperature,1.0,TypeT,-50,80#
$ProbeHeaterTemperature,1.0,TypeK,-274,600#
$ProbeGasFlow,1.0,,,,,600,50,2000,,,#
$ProbeAllCoils,1.1,,1#
$ProbeCoil,1.0,1,7.9,2,BB,1H#
$ProbeChannel,1.1,1H,,,250,,,,,FALSE,,,,#
$ProbeBB,2.0,2,31P-15N,,,,,,#
$ProbeBBSets,1.0,31P,,,200,,,#
$ProbeBBSets,1.0,79Br/13C,,,300,,,#
$ProbeBBSets,1.0,15N,,,500,,,#
$ProbeMas,1.0,1800,24000,0,1,0,0,0,0,500#
$EndBis,7P,51#
```

● **Required Samples PH MASDVT1000S6 BL3.2 X/H NO_I/E**

Z151230	Potassium Bromide (KBr, 34 ul)
Z151231	Adamantane (34 ul)
Z151232	Alpha-glycine (34 ul)
Z151233	2-13C, 15N alpha-glycine (34 ul)
Z151234	Ammonium Dihydrogenphosphate (34 ul)

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 5000 Hz)

Line width main [achieved]: [215] <n/a>



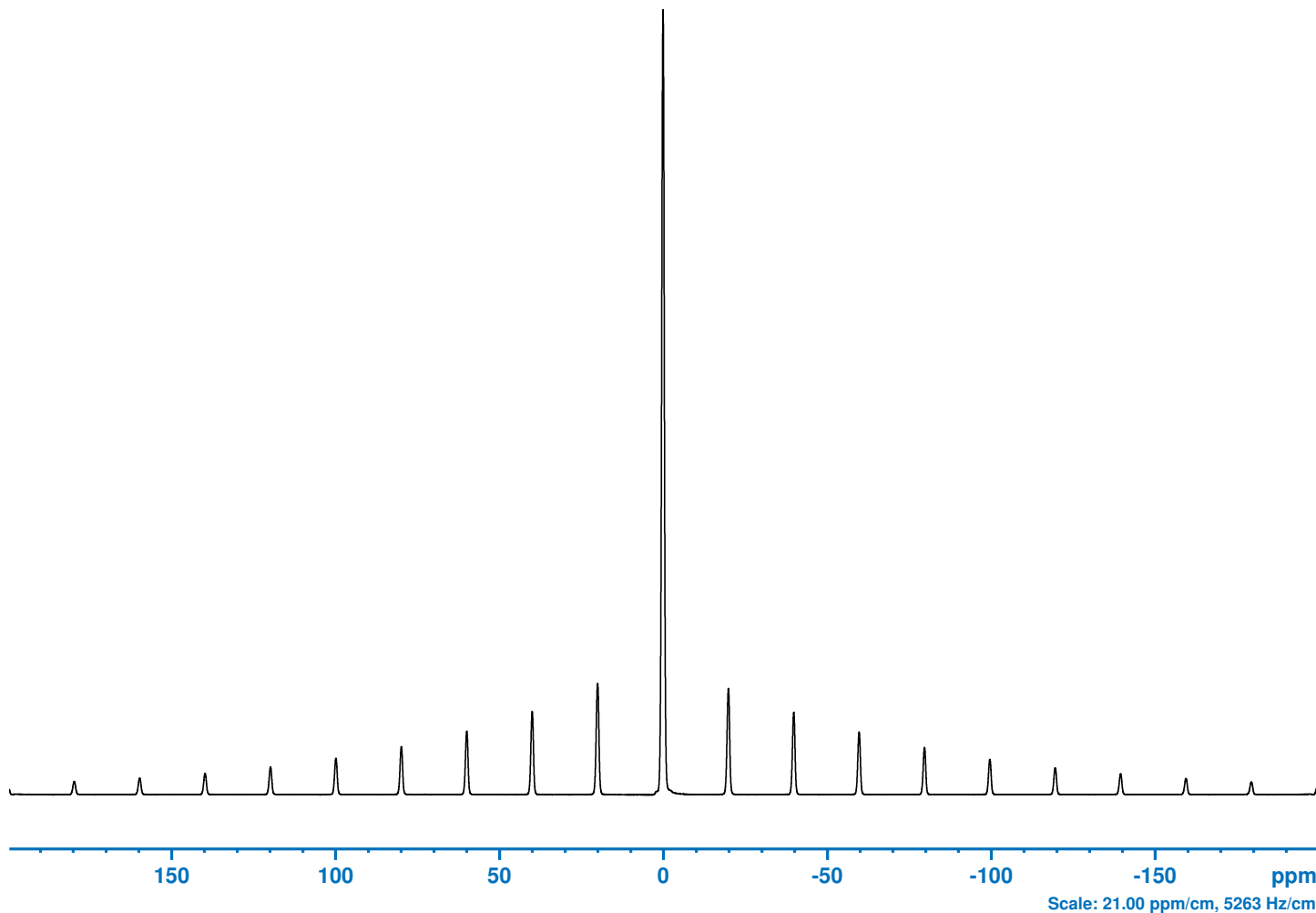
Bruker BioSpin

NPT_79Br_MAS_magicAngle

```
Current Data Parameters
NAME      NPT_79Br_MAS_magicAngle
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201217
Time      16.03 h
INSTRUM   Avance Neo 1GHz
PROBHD    H177324_0001 (
PULPROG   onepulse
TD        8192
SOLVENT   CDC13
NS        16
DS        0
SWH       100000.000 Hz
FIDRES    24.414062 Hz
AQ        0.0409600 sec
RG        401
DW        5.000 usec
DE        6.50 usec
TE        307.9 K
D1        0.25000000 sec
SFO1      250.6551693 MHz
NUC1      79Br
P1        4.00 usec
PLW1      121.97000122 W

F2 - Processing parameters
SI        131072
SF        250.6551693 MHz
WDW       no
SSB       0
LB        0 Hz
GB        0
PC        0.20
```



SHIM SEQUENCE
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
 Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
 Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 24000 Hz)
 Determination of spinning stability for 180 s
 Pressure values in mbar: DrivePressure=2564/BearingPressure=3176/BearingSensePressure=3133/SupplyPressure=6961/SystemPressure=7158

Spin rate at maximum deviation [measured]: @ MASR 24000 Hz [23997 Hz]
 Maximum deviation [achieved/rated]: @ MASR 24000 Hz [3 Hz <= 24 Hz] <pass>



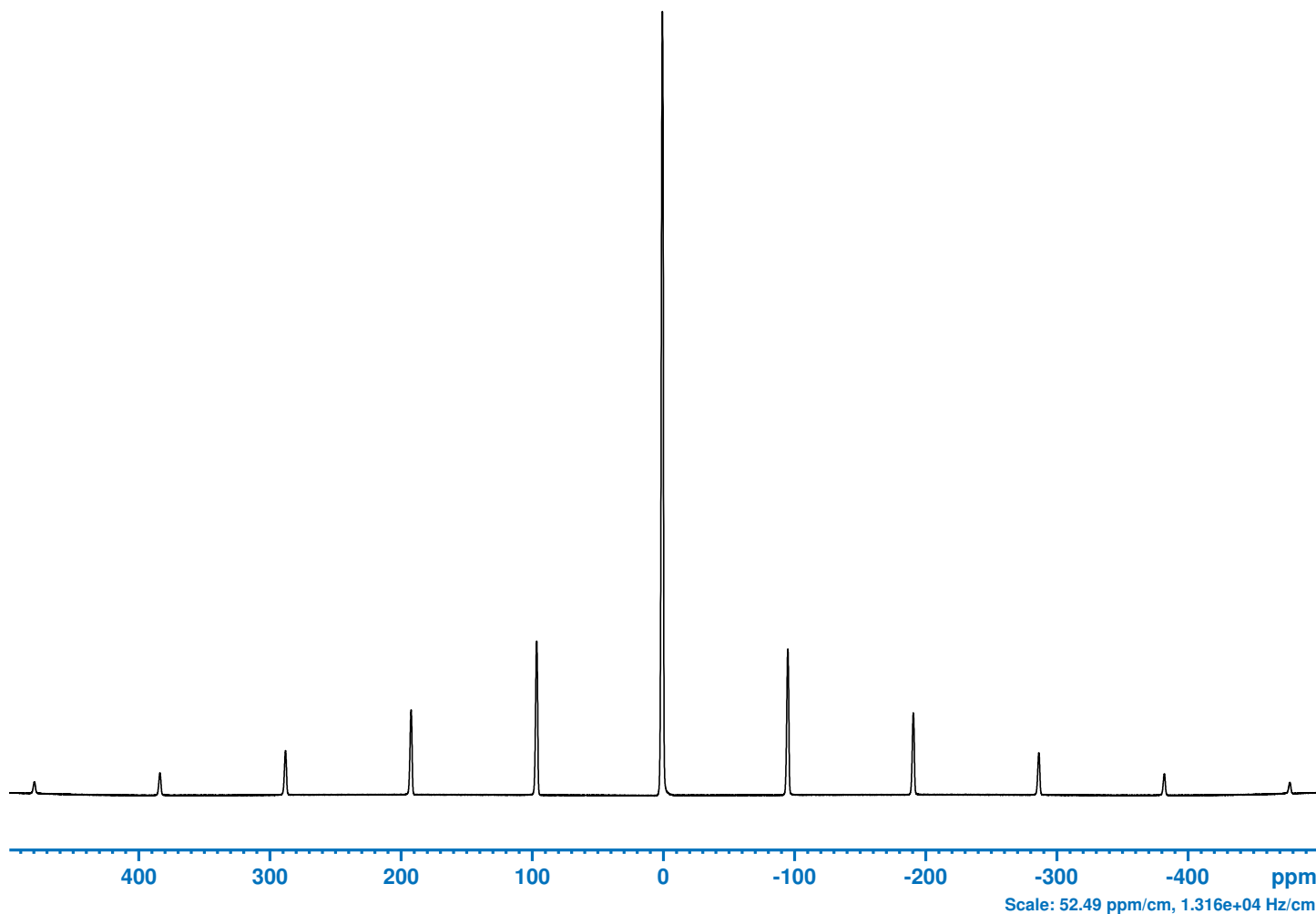
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

```
Current Data Parameters
NAME      NPT_79Br_MAS_maxSpinRate
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20201217
Time      16.18 h
INSTRUM   Avance Neo 1GHz
PROBHD    H177324_0001 (
PULPROG   onepulse
TD         16384
SOLVENT   CDC13
NS         16
DS         0
SWH        250000.000 Hz
FIDRES     30.517578 Hz
AQ         0.0327880 sec
RG         401
DW         2.000 usec
DE         6.50 usec
TE         301.7 K
D1         0.2500000 sec
SFO1       250.6546121 MHz
NUC1       79Br
P1         4.00 usec
PLW1       121.97000122 W

F2 - Processing parameters
SI         32768
SF         250.6546121 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0
PC         0.20
```



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

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting, spin rate 5000 Hz)
FIELD was set to 2654.7 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0069 ppm.



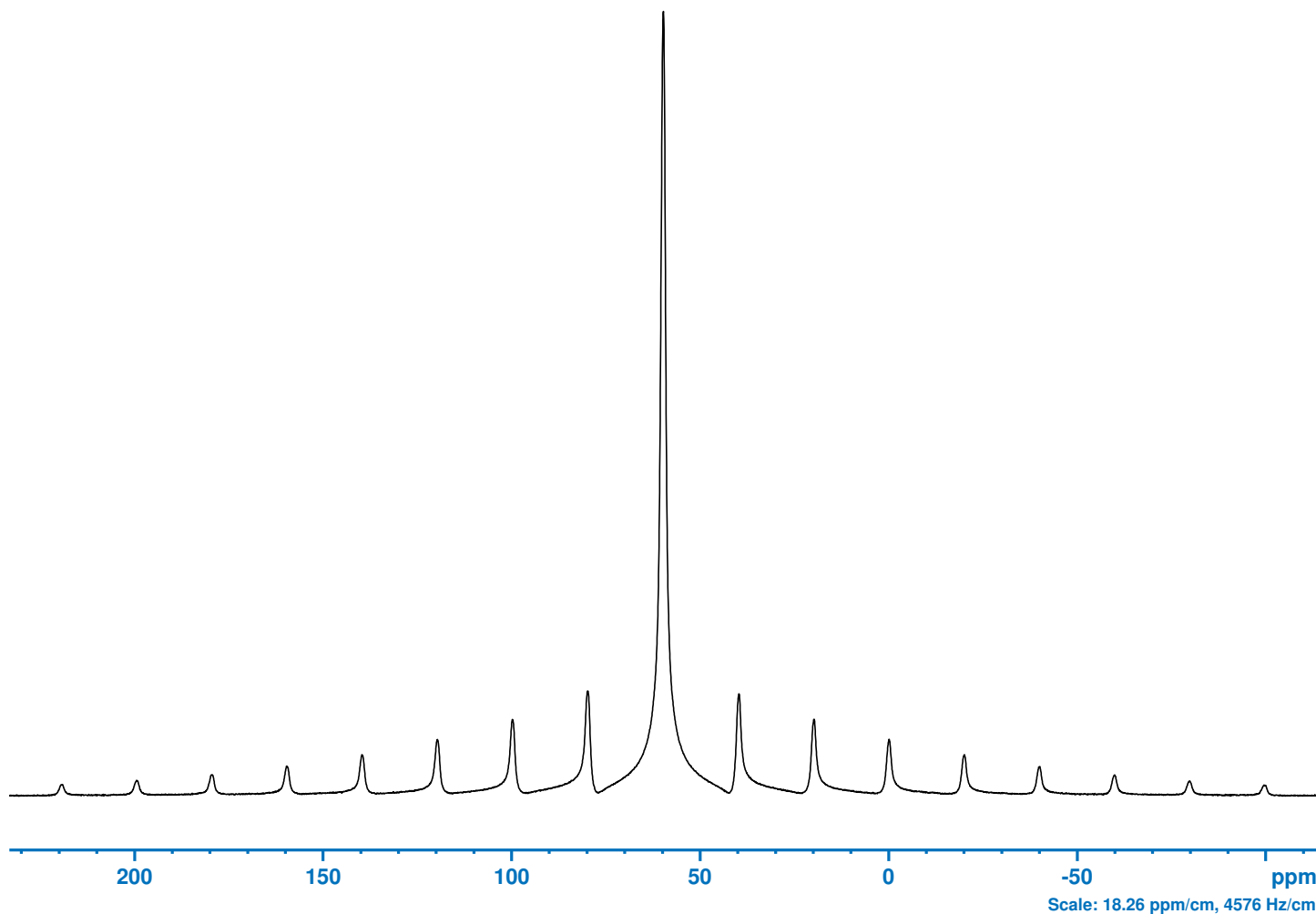
Bruker BioSpin

NPT_79Br_MAS_fieldsetting

```
Current Data Parameters
NAME      NPT_79Br_MAS_fieldsetting
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201217
Time      16.03 h
INSTRUM   Avance Neo 1GHz
PROBHD    H177324_0001 (
PULPROG   onepulse
TD        4096
SOLVENT   CDCl3
NS         1
DS         0
SWH       108695.648 Hz
FIDRES    53.074047 Hz
AQ        0.0188416 sec
RG         101
DW         4.600 usec
DE         6.50 usec
TE         307.5 K
D1         0.5000000 sec
SFO1      250.6549791 MHz
NUC1       79Br
P1         4.00 usec
PLW1      121.97000122 W

F2 - Processing parameters
SI         8192
SF         250.6400159 MHz
WDW        EM
SSB         0
LB          0 Hz
GB          0
PC          0.50
```



SHIM SEQUENCE
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: Adamantane (34 ul) (Z151231)
Optimization of 13C frequency (NPT_13C_MAS_fieldsetting_dec1h, spin rate 10000 Hz)
FIELD was set to 2618.7 for 13C chemical shift of 38.460 ppm. One field unit corresponds to 0.0071 ppm.



Bruker BioSpin

NPT_13C_MAS_fieldsetting_dec1h

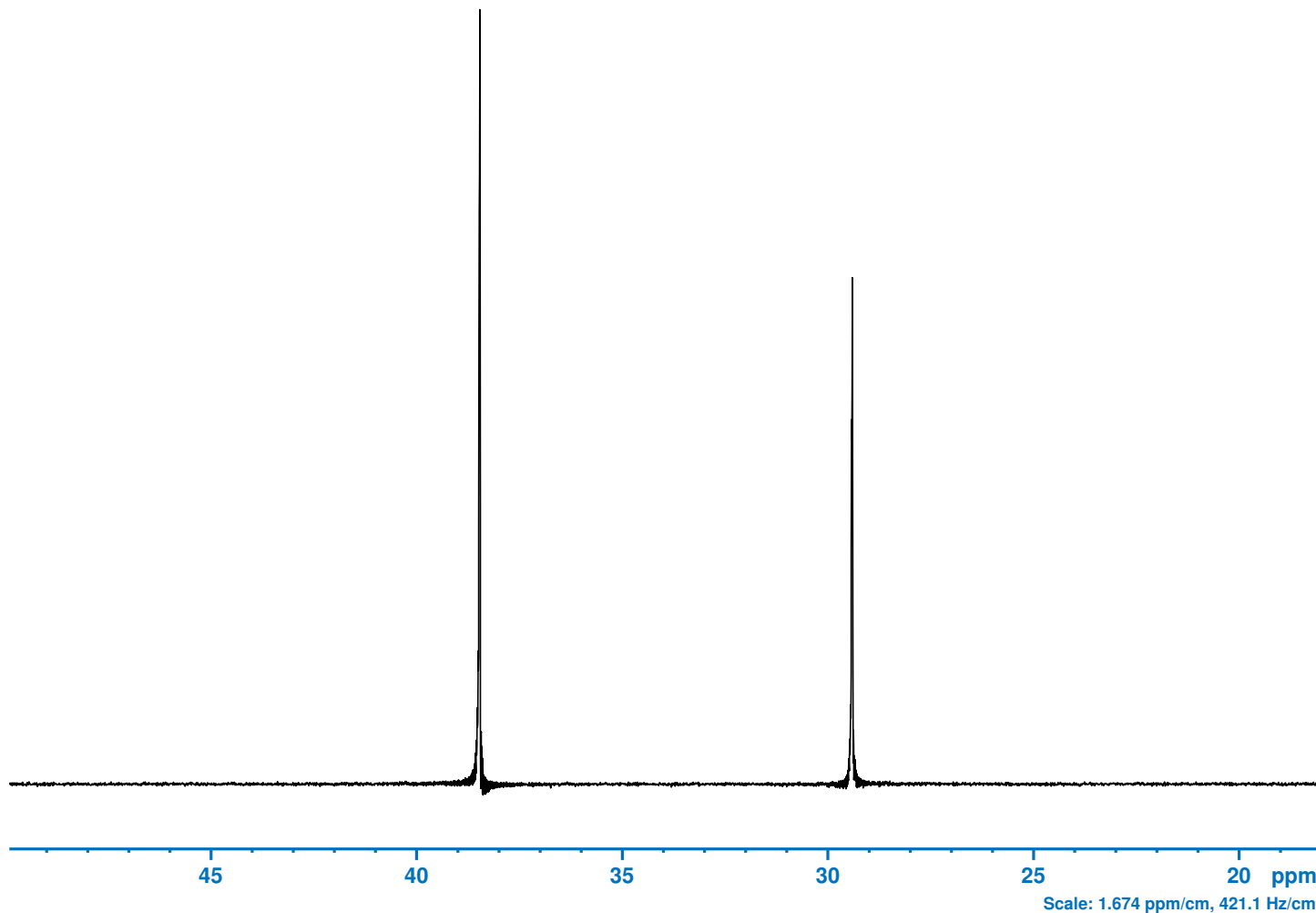
```
Current Data Parameters
NAME      NPT_13C_MAS_fieldsetting_dec1h
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201217
Time      20.40 h
INSTRUM   Avance Neo 1GHz
PROBHD    H177324_0001 (
PULPROG   hpdec
TD         4000
SOLVENT   CDCl3
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         15.0000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1      251.5593320 MHz
NUC1       13C
P1         3.50 usec
PLW1       146.30999756 W
SFO2      1000.4024064 MHz
NUC2       1H
CPDPRG[2] cw
PLW2       114.33999634 W
PLW12      0.14006650 W

F2 - Processing parameters
SI         8192
SF         251.5507801 MHz
WDW        no
SSB         0
LB          0 Hz
GB          0
PC          0.50
```

SHIM SEQUENCE

skip shimming



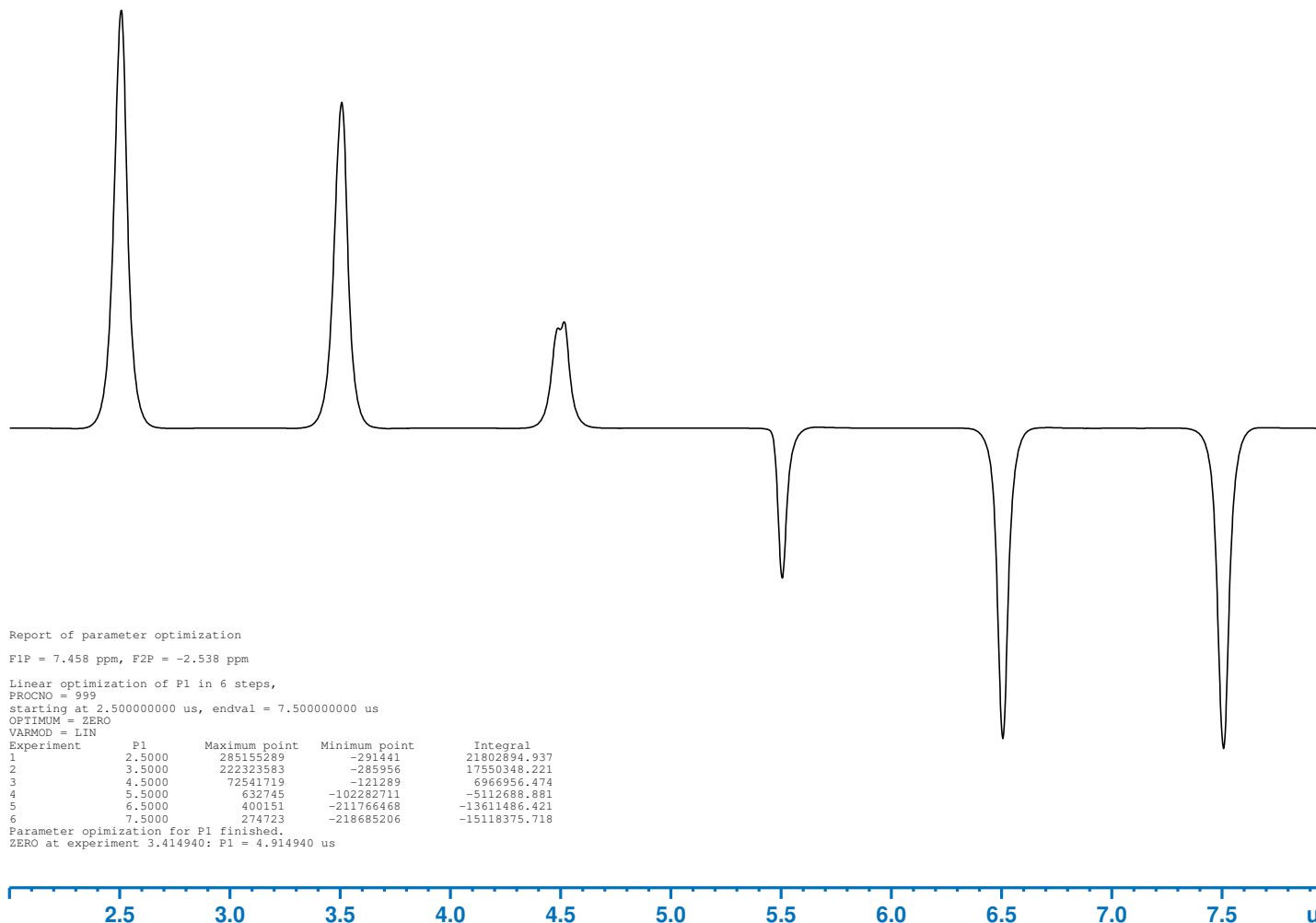
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
 Sample: Adamantane (34 ul) (Z151231)
 P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [2.50 us @ 237 W].



Bruker BioSpin

P90 MAS 1H pulse [achieved/rated]: @ 244 W [2.46 us <= 2.50 us] <pass>

NPT_1H_MAS_p90det_1h



Current Data Parameters
 NAME NPT_1H_MAS_p90det_1h
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201222
 Time 10.03 h
 INSTRUM Avance Neo 1GHz
 PROBHD H177324_0001 ()
 PULPROG onepulse
 TD 2988
 SOLVENT H2O+D2O
 NS 1
 DS 0
 SWH 100000.000 Hz
 FIDRES 66.934402 Hz
 AQ 0.0149400 sec
 RG 1
 DW 5.000 usec
 DE 6.50 usec
 TE 282.1 K
 D1 5.00000000 sec
 SFO1 1000.4024610 MHz
 NUC1 1H
 P1 7.50 usec
 PLW1 244.35490417 W

F2 - Processing parameters
 SI 4096
 SF 1000.4000000 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.20

Report of parameter optimization

F1P = 7.458 ppm, F2P = -2.538 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	285155289	-291441	21802894.937
2	3.5000	222323583	-285956	17550348.221
3	4.5000	72541719	-121289	6966956.474
4	5.5000	632745	-102282711	-5112688.881
5	6.5000	400151	-211766468	-13611486.421
6	7.5000	274723	-218685206	-15118375.718

Parameter optimization for P1 finished.

ZERO at experiment 3.414940: P1 = 4.914940 us

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

PLW90	P90	P90[det]	Deviation
223 W	2.50 us	2.56 us	2.4%
223 W	2.50 us	2.46 us	-1.6%

 SHIM SEQUENCE

 skip shimming

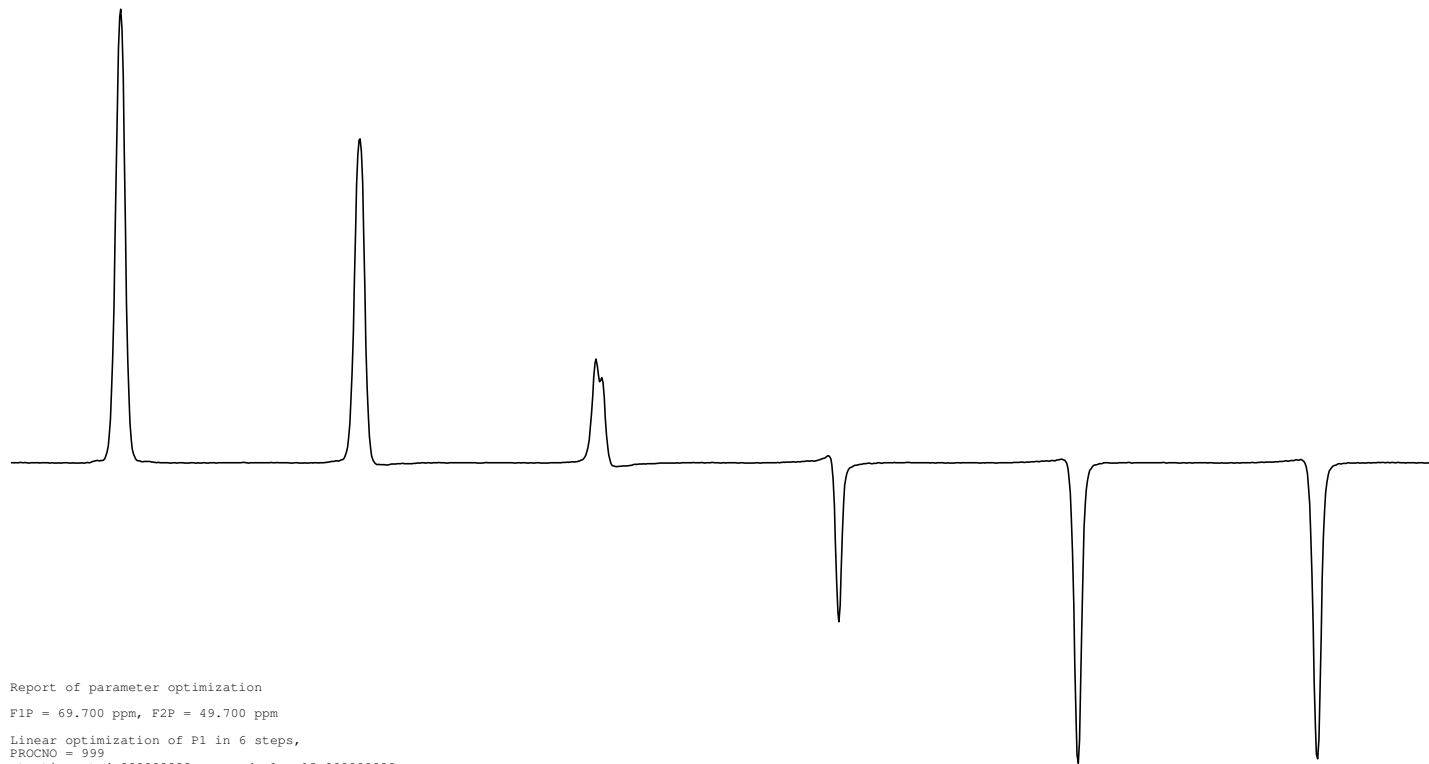
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
 Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
 P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br, spin rate 5000 Hz)
 ATTENTION: Updated PROSOL Tables with [4.00 us @ 122 W].



Bruker BioSpin

P90 MAS 79Br pulse [achieved/rated]: @ 127 W [3.92 us <= 4.00 us] <pass>

NPT_79Br_MAS_p90det_79br



Current Data Parameters
 NAME NPT_79Br_MAS_p90det_79br
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201217
 Time 16.02 h
 INSTRUM Avance Neo 1GHz
 PROBHD H177324_0001 ()
 PULPROG onepulse
 TD 2048
 SOLVENT CDC13
 NS 1
 DS 0
 SWH 100000.000 Hz
 FIDRES 97.656250 Hz
 AQ 0.0102400 sec
 RG 101
 DW 5.000 usec
 DE 6.500 usec
 TE 308.9 K
 D1 0.25000000 sec
 SFO1 250.6549791 MHz
 NUC1 79Br
 P1 12.000 usec
 PLW1 127.00000000 W

F2 - Processing parameters
 SI 4096
 SF 250.6400159 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.20

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

PLW90	P90	P90[det]	Deviation
127 W	4.00 us	3.92 us	-2.0%
127 W	4.00 us	3.92 us	-2.0%

Report of parameter optimization

F1P = 69.700 ppm, F2P = 49.700 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 4.000000000 us, endval = 12.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	4.0000	297198454	-263544	14106889.860
2	5.6000	212376093	-1480910	10427266.111
3	7.2000	67952002	-2491878	3537602.787
4	8.8000	4637561	-104084292	-2949787.092
5	10.4000	2405637	-196919987	-7214463.676
6	12.0000	2102685	-193974444	-7757879.377

Parameter optimization for P1 finished.

ZERO at experiment 3.394986: P1 = 7.831978 us

 SHIM SEQUENCE

skip shimming

3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0 8.5 9.0 9.5 10.0 10.5 11.0 11.5 12.0 us

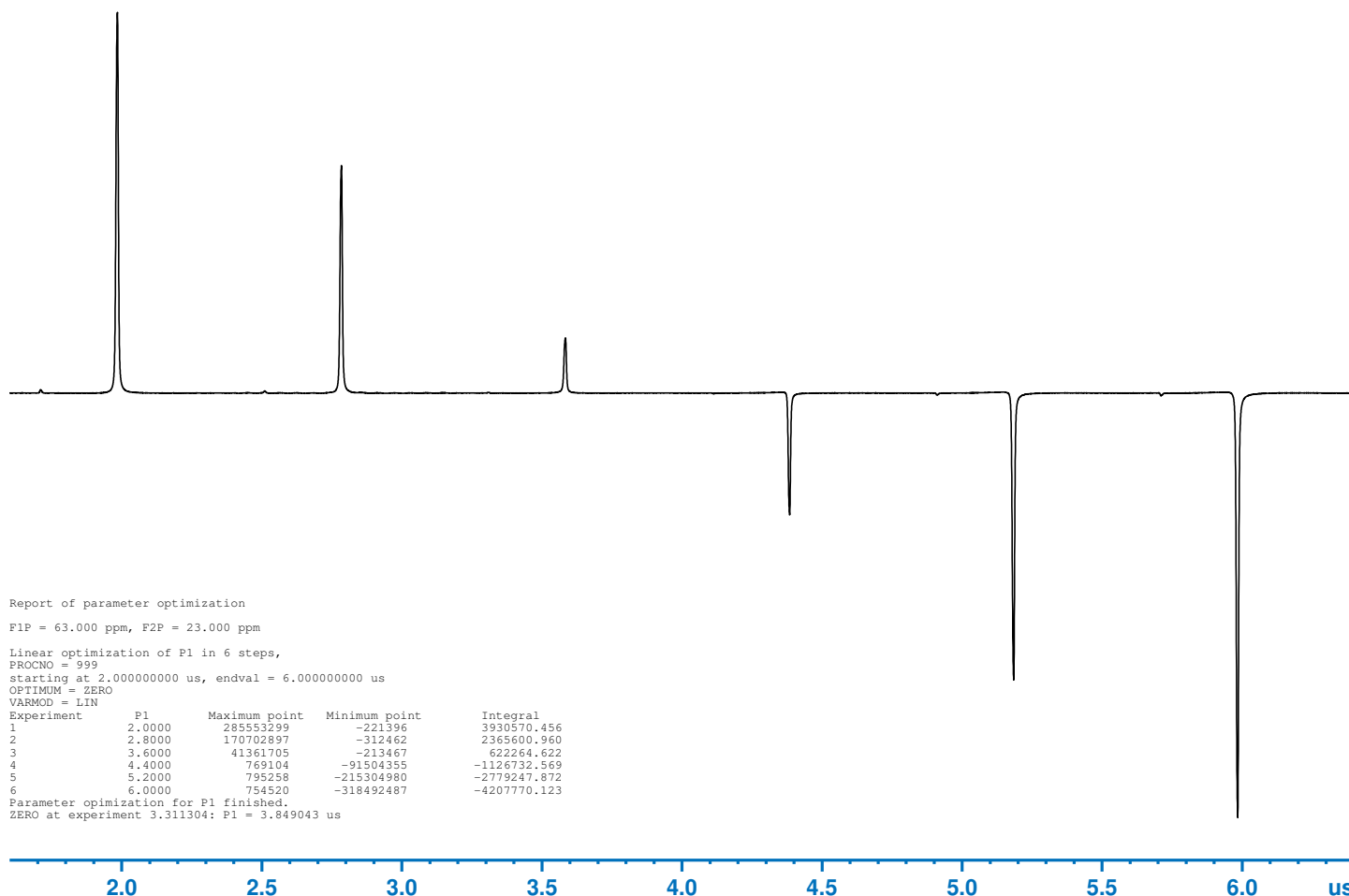
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (34 ul) (Z151233)
 P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [4.00 us @ 104 W].



Bruker BioSpin

P90_MAS_CP 1H13C power (PLW 11) [achieved]: [112.0 W] <n/a>
 P90_MAS_CP 1H13C pulse (P 1) [achieved/rated]: [3.85 us <= 4.00 us] <pass>

NPT_13C_MAS_p90det_cp1h_13c



Current Data Parameters
 NAME NPT_13C_MAS_p90det_cp1h_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201218
 Time 10.12 h
 INSTRUM Avance Neo 1GHz
 PROBHD H177324_0001 ()
 PULPROG cp90
 TD 7462
 SOLVENT CDC13
 NS 4
 DS 0
 SWH 74626.867 Hz
 FIDRES 20.001841 Hz
 AQ 0.0499954 sec
 RG 101
 DW 6.700 usec
 DE 6.50 usec
 TE 298.0 K
 D1 5.00000000 sec
 ZGPTNS
 SFO1 251.5615968 MHz
 NUC1 13C
 P1 6.00 usec
 P15 2000.00 usec
 PLW1 112.01860046 W
 PLW11 112.01860046 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 2.50 usec
 PCPD2 4.80 usec
 PLW2 223.00000000 W
 PLW12 223.00000000 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 92.61000061 W

F2 - Processing parameters
 SI 16384
 SF 251.5507801 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.20

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation

 146 W 3.50 us
 112 W 4.00 us 3.85 us -3.8%

Report of parameter optimization

F1P = 63.000 ppm, F2P = 23.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 2.000000000 us, endval = 6.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.0000	285553299	-221396	3930570.456
2	2.8000	170702897	-312462	2365600.960
3	3.6000	41361705	-213467	622264.622
4	4.4000	769104	-91504355	-1126732.569
5	5.2000	795258	-215304980	-2779247.872
6	6.0000	754520	-318492487	-4207770.123

Parameter optimization for P1 finished.

ZERO at experiment 3.311304: P1 = 3.849043 us

 SHIM SEQUENCE

 skip shimming

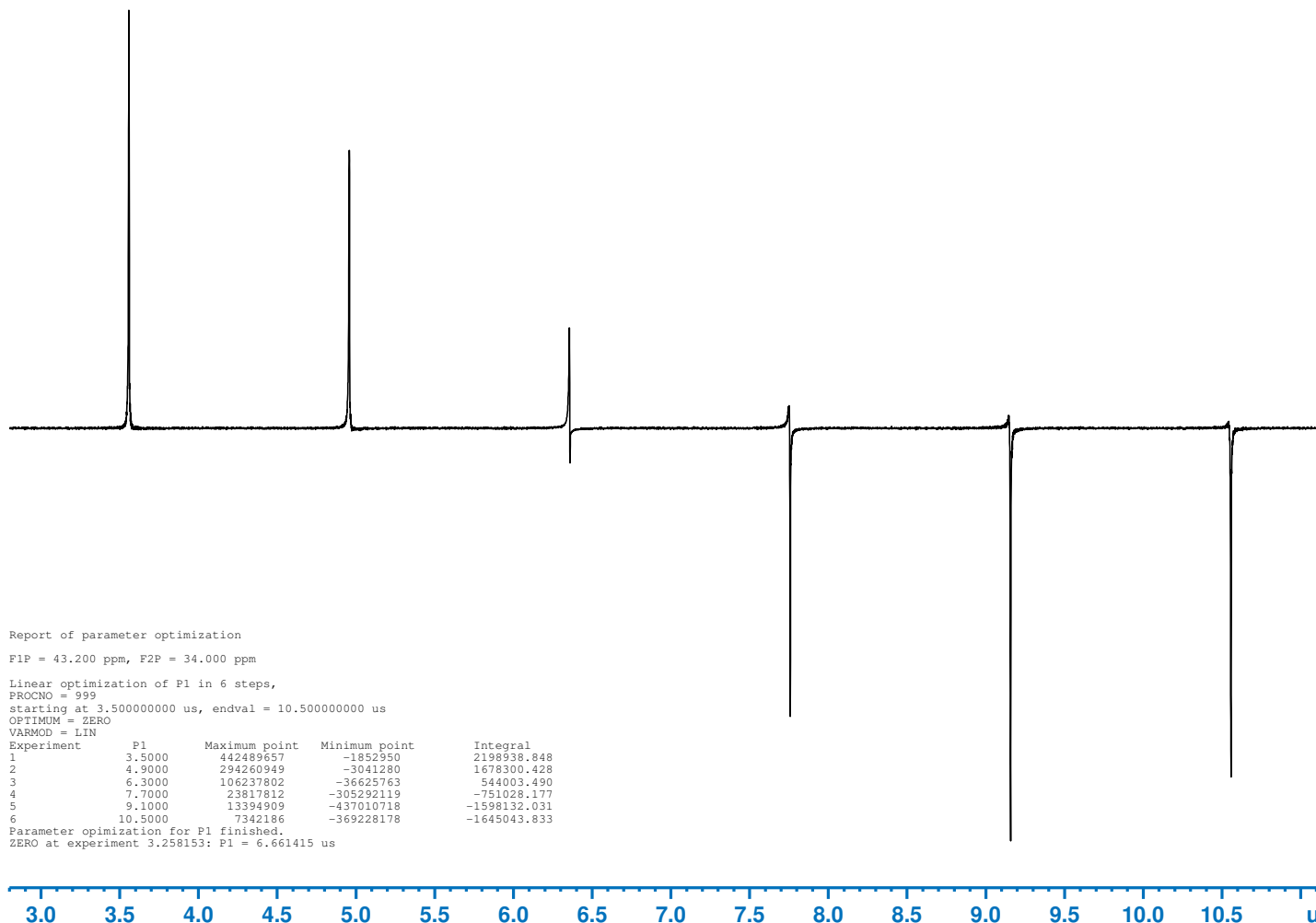
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
 Sample: Adamantane (34 ul) (Z151231)
 P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.50 us @ 146 W].



Bruker BioSpin

P90 MAS 13C pulse [achieved/rated]: @ 162 W [3.33 us <= 3.50 us] <pass>

NPT_13C_MAS_p90det_13c



Current Data Parameters
 NAME NPT_13C_MAS_p90det_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201217
 Time 20.35 h
 INSTRUM Avance Neo 1GHz
 PROBHD H177324_0001 ()
 PULPROG hpdec
 TD 4000
 SOLVENT CDCl3
 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 -D1acq
 SFO1 251.5593328 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 161.63270569 W
 SFO2 1000.4024610 MHz
 NUC2 1H
 CPDPRG[2] cw
 PLW2 114.33999634 W
 PLW12 0.14006650 W

F2 - Processing parameters
 SI 8192
 SF 251.5507801 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.50

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation

 220 W 3.00 us
 162 W 3.50 us 3.33 us -4.9%

Report of parameter optimization

F1P = 43.200 ppm, F2P = 34.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 3.500000000 us, endval = 10.500000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	3.5000	442489657	-1852950	2198938.848
2	4.9000	294260949	-3041280	1678300.428
3	6.3000	106237802	-36625763	544003.490
4	7.7000	23817812	-305292119	-751028.177
5	9.1000	13394909	-437010718	-1598132.031
6	10.5000	7342186	-369228178	-1645043.833

Parameter optimization for P1 finished.

ZERO at experiment 3.258153: P1 = 6.661415 us

 SHIM SEQUENCE

skip shimming

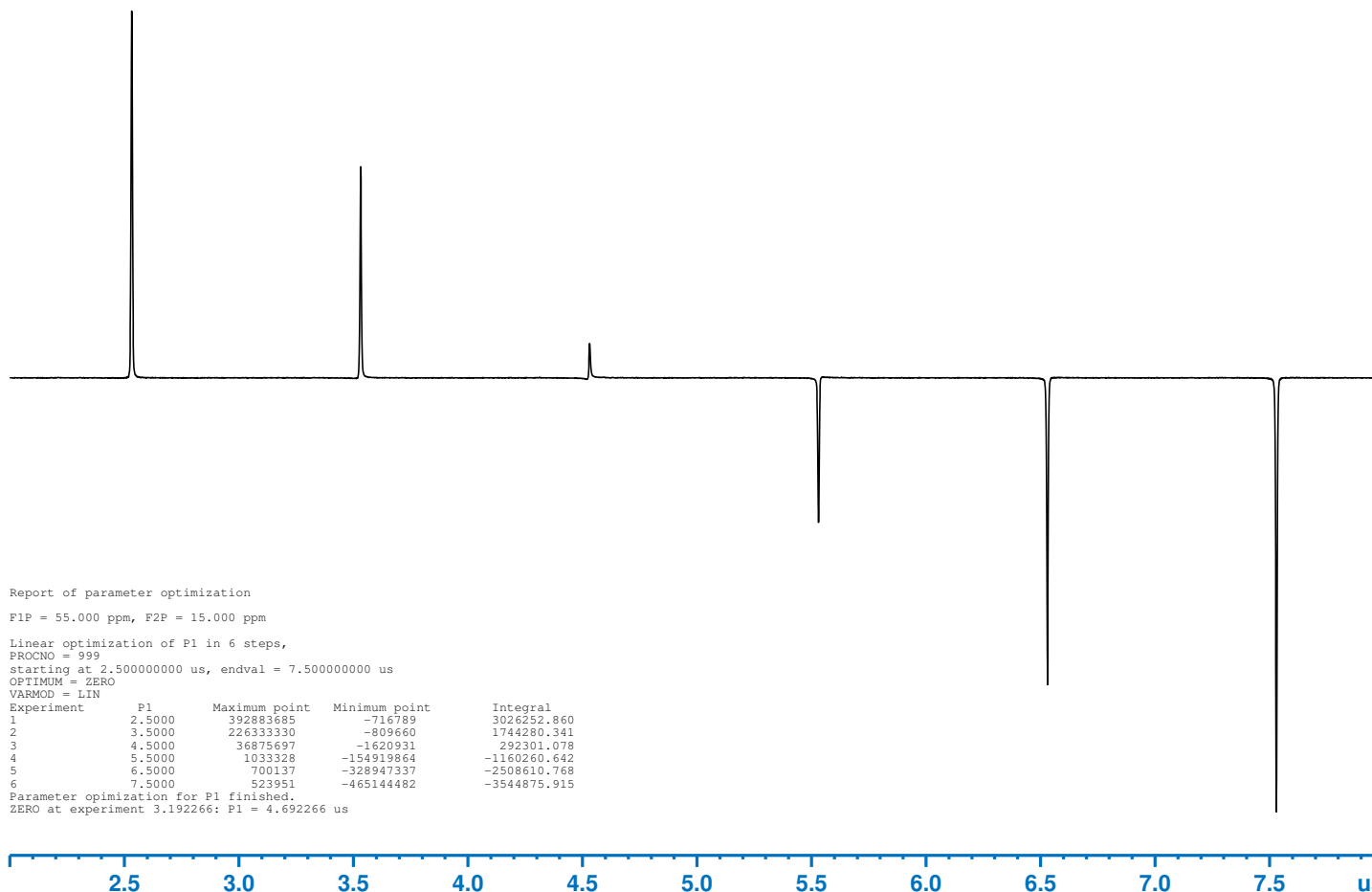
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (34 ul) (Z151233)
 P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [5.00 us @ 275 W].



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P90_MAS_CP 1H15N power (PLW 11) [achieved]: [313.0 W] <n/a>
 P90_MAS_CP 1H15N pulse (P 1) [achieved/rated]: [4.69 us <= 5.00 us] <pass>

NPT_15N_MAS_p90det_cp1h_15n



Current Data Parameters
 NAME NPT_15N_MAS_p90det_cp1h_15n
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201218
 Time 10.34 h
 INSTRUM Avance Neo 1GHz
 PROBHD H177324_0001 ()
 PULPROG cp90
 TD 4064
 SOLVENT CDC13
 NS 4
 DS 0
 SWH 40650.406 Hz
 FIDRES 20.005121 Hz
 AQ 0.0499972 sec
 RG 101
 DW 12.300 usec
 DE 6.50 usec
 TE 298.0 K
 D1 5.00000000 sec
 ZGPTNS
 SF01 101.3731996 MHz
 NUC1 15N
 P1 7.50 usec
 P15 3500.00 usec
 PLW1 313.0000000 W
 PLW11 313.0000000 W
 SF02 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 2.50 usec
 PCPD2 4.80 usec
 PLW2 223.0000000 W
 PLW12 223.0000000 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 63.43112183 W

F2 - Processing parameters
 SI 8192
 SF 101.3696516 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation

 313 W 5.00 us
 313 W 5.00 us 4.69 us -6.2%

Report of parameter optimization

F1P = 55.000 ppm, F2P = 15.000 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	392883685	-716789	3026252.860
2	3.5000	226333330	-809660	1744280.341
3	4.5000	36875697	-1620931	292301.078
4	5.5000	1033328	-154919864	-1160260.642
5	6.5000	700137	-328947337	-2508610.768
6	7.5000	523951	-465144482	-3544875.915

Parameter optimization for P1 finished.

ZERO at experiment 3.192266: P1 = 4.692266 us

 SHIM SEQUENCE

skip shimming

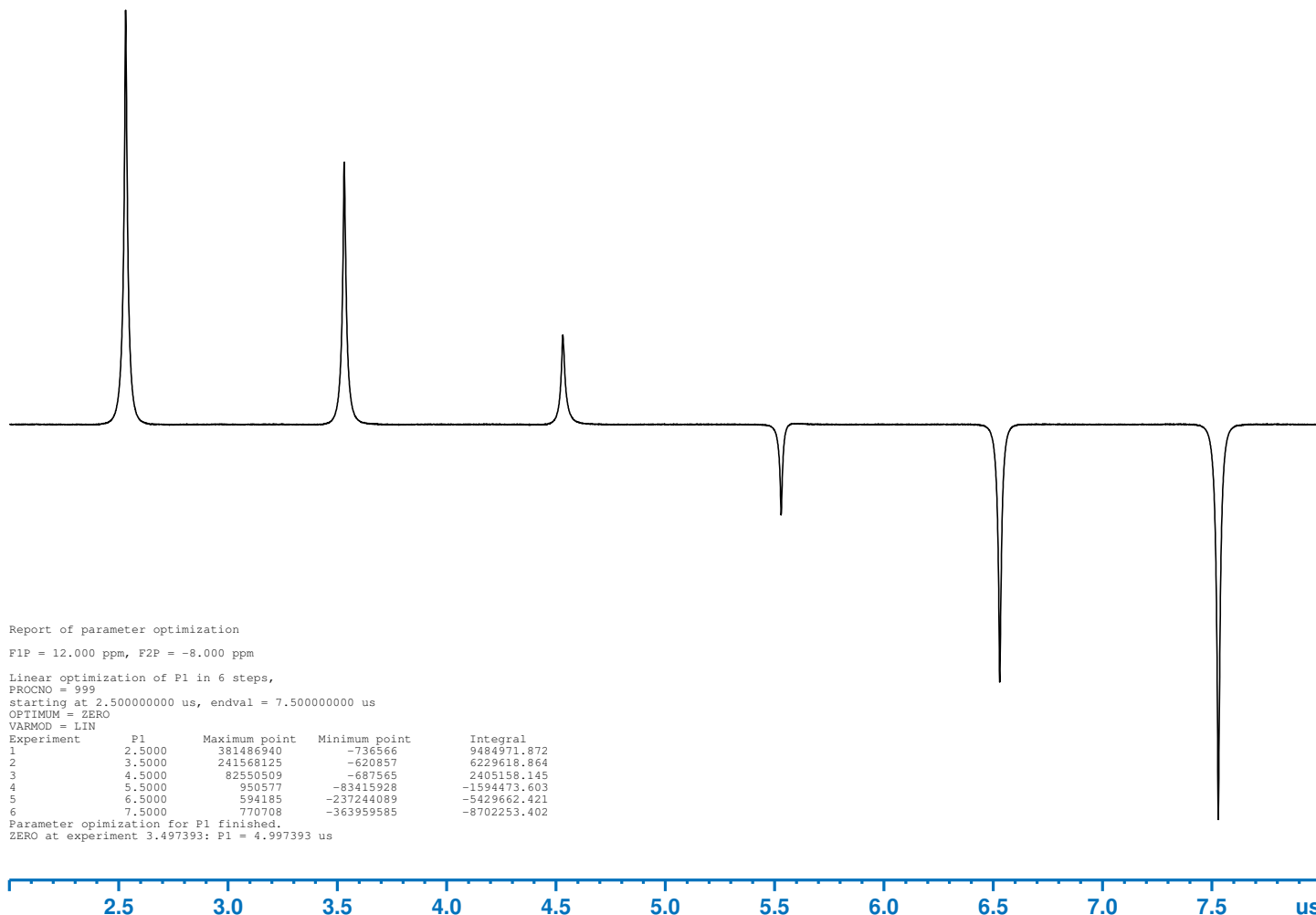
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO I/E
 Sample: Ammonium Dihydrogenphosphate (34 ul) (Z151234)
 P90 31P 1H-31P CP pulse calibration, MAS (NPT_31P_MAS_p90det_cp1h_31p, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [5.00 us @ 174 W].



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P90_MAS_CP 1H31P power (PLW 11) [achieved]: [174.4 W] <n/a>
 P90_MAS_CP 1H31P pulse (P 1) [achieved/rated]: [5.00 us <= 5.00 us] <pass>

NPT_31P_MAS_p90det_cp1h_31p



Current Data Parameters
 NAME NPT_31P_MAS_p90det_cp1h_31p
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201221
 Time 15.22 h
 INSTRUM Avance Neo 1GHz
 PROBHD H177324_0001 ()
 PULPROG cp90
 TD 11904
 SOLVENT H2O+D2O
 NS 4
 DS 0
 SWH 119047.617 Hz
 FIDRES 20.001280 Hz
 AQ 0.0499968 sec
 RG 101
 DW 4.200 usec
 DE 6.50 usec
 TE 303.0 K
 D1 5.00000000 sec
 ZGPGTNS
 SF01 404.9701529 MHz
 NUC1 31P
 P1 7.50 usec
 P15 3500.00 usec
 PLW1 174.41999817 W
 PLW11 174.41999817 W
 SF02 1000.4072029 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 2.50 usec
 PCPD2 4.80 usec
 PLW2 223.00000000 W
 PLW12 223.00000000 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 142.72000122 W

F2 - Processing parameters
 SI 16384
 SF 404.9693430 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation

 174 W 5.00 us
 174 W 5.00 us 5.00 us 0.0%

 SHIM SEQUENCE

 skip shimming

Report of parameter optimization

F1P = 12.000 ppm, F2P = -8.000 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	381486940	-736566	9484971.872
2	3.5000	241568125	-620857	6229618.864
3	4.5000	82550509	-687565	2405158.145
4	5.5000	950577	-83415928	-1594473.603
5	6.5000	594185	-237244089	-5429662.421
6	7.5000	770708	-363959585	-8702253.402

Parameter optimization for P1 finished.

ZERO at experiment 3.497393: P1 = 4.997393 us

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: Alpha-glycine (34 ul) (Z151232)
CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c, spin rate 10000 Hz)

SINO (20.0 ppm) [achieved]: Signal (43.86 ppm), Noise (120.02 to 100.02 ppm) [420.4] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>
Processed with TDef=2048



Bruker BioSpin

NPT_13C_MAS_sino_cp1h_13c

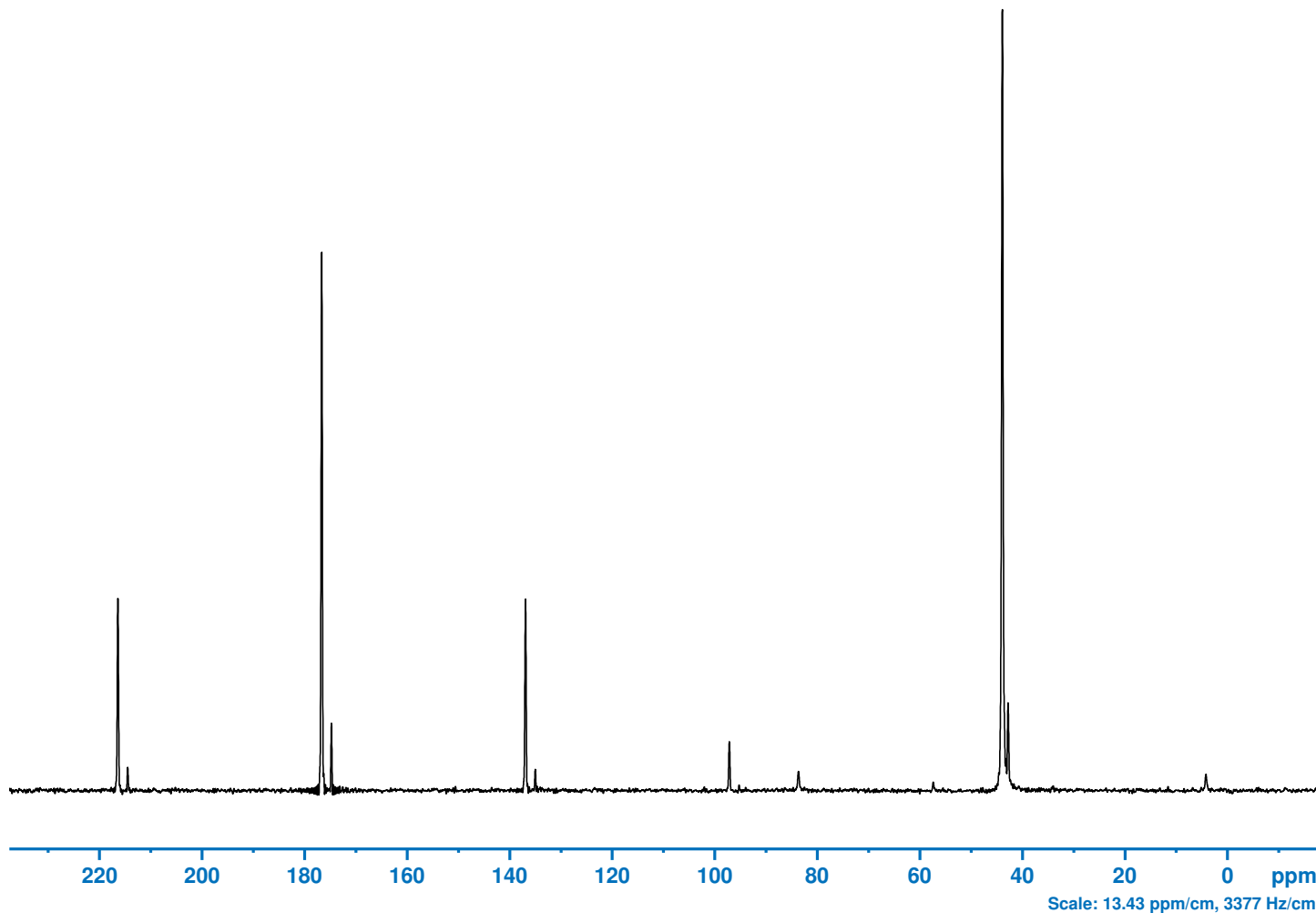
Current Data Parameters
NAME NPT_13C_MAS_sino_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201218
Time 11.21 h
INSTRUM Avance Neo 1GHz
PROBHD H177324_0001 (cp
PULPROG cp
TD 7462
SOLVENT CDC13
NS 64
DS 0
SWH 74626.867 Hz
FIDRES 20.001841 Hz
AQ 0.0499954 sec
RG 101
DW 6.700 usec
DE 6.50 usec
TE 298.0 K
D1 5.0000000 sec
ZGPTNS
SF01 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 103.76999664 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 223.00000000 W
PLW12 178.39999390 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 92.59999847 W

F2 - Processing parameters
SI 32768
SF 251.5507801 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20

SHIM SEQUENCE

skip shimming



NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: Alpha-glycine (34 ul) (Z151232)
CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n, spin rate 10000 Hz)

SINO (20.0 ppm) [achieved]: Signal (33.70 ppm), Noise (207.44 to 187.44 ppm) [56.9] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>



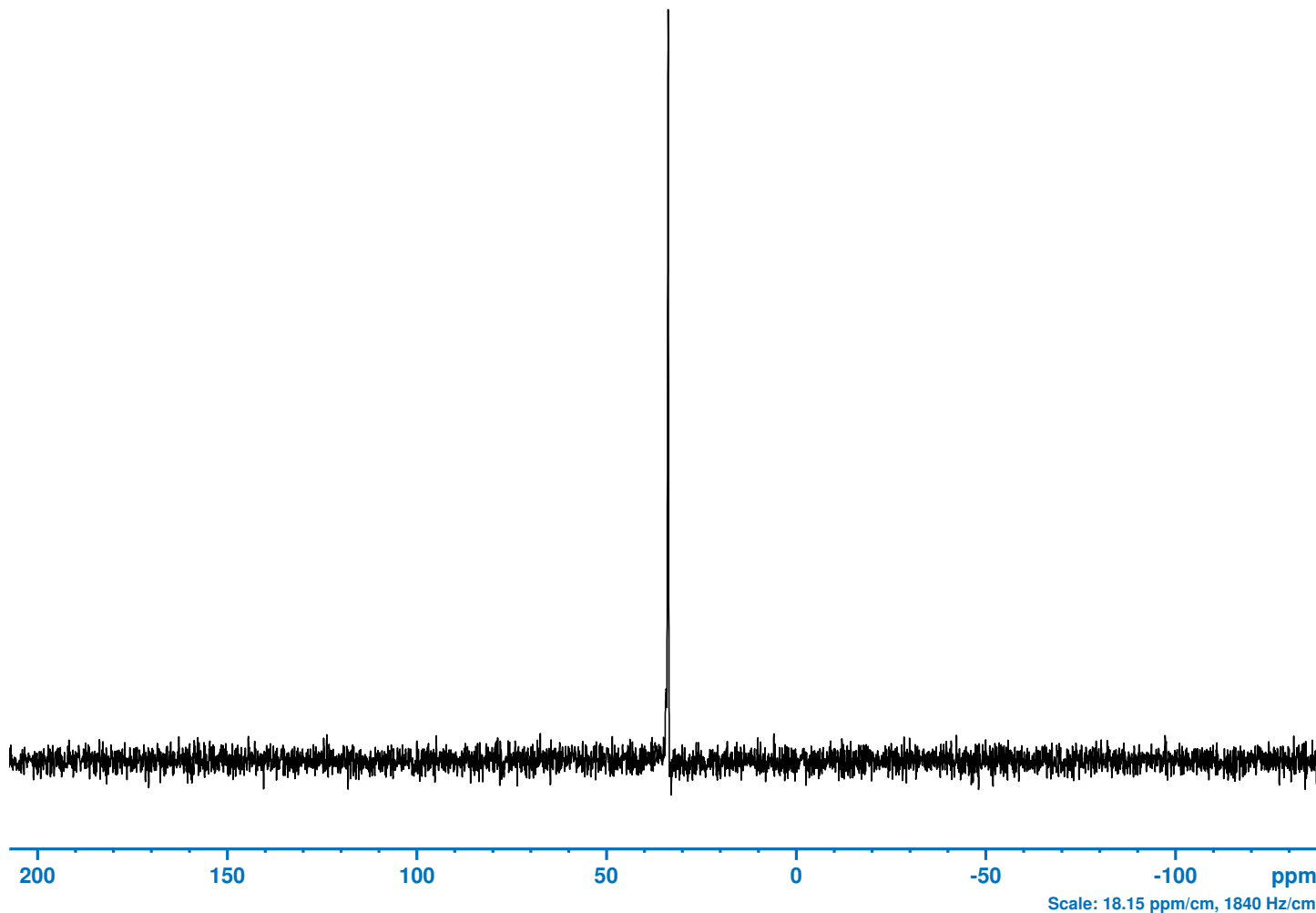
Bruker BioSpin

NPT_15N_MAS_sino_cp1h_15n

Current Data Parameters
NAME NPT_15N_MAS_sino_cp1h_15n
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201218
Time 11.12 h
INSTRUM Avance Neo 1GHz
PROBHD H177324_0001 (cp
PULPROG cp
TD 4064
SOLVENT CDC13
NS 64
DS 0
SWH 40650.406 Hz
FIDRES 20.005121 Hz
AQ 0.0499972 sec
RG 101
DW 12.300 usec
DE 6.50 usec
TE 298.0 K
D1 5.0000000 sec
ZGPTNS
SF01 101.3731996 MHz
NUC1 15N
P15 3500.00 usec
PLW1 275.39001465 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 223.00000000 W
PLW12 178.39999390 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 92.59999847 W

F2 - Processing parameters
SI 32768
SF 101.3696516 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



SHIM SEQUENCE
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO I/E
Sample: Ammonium Dihydrogenphosphate (34 ul) (Z151234)
CP 1H-31P sensitivity, MAS (NPT_31P_MAS_sino_cp1h_31p, spin rate 10000 Hz)

SINO (10.0 ppm) [achieved]: Signal (1.31 ppm), Noise (-94.18 to -104.18 ppm) [880.7] <n/a>
Number of scans (NS) [achieved]: [4] <n/a>



Bruker BioSpin

NPT_31P_MAS_sino_cp1h_31p

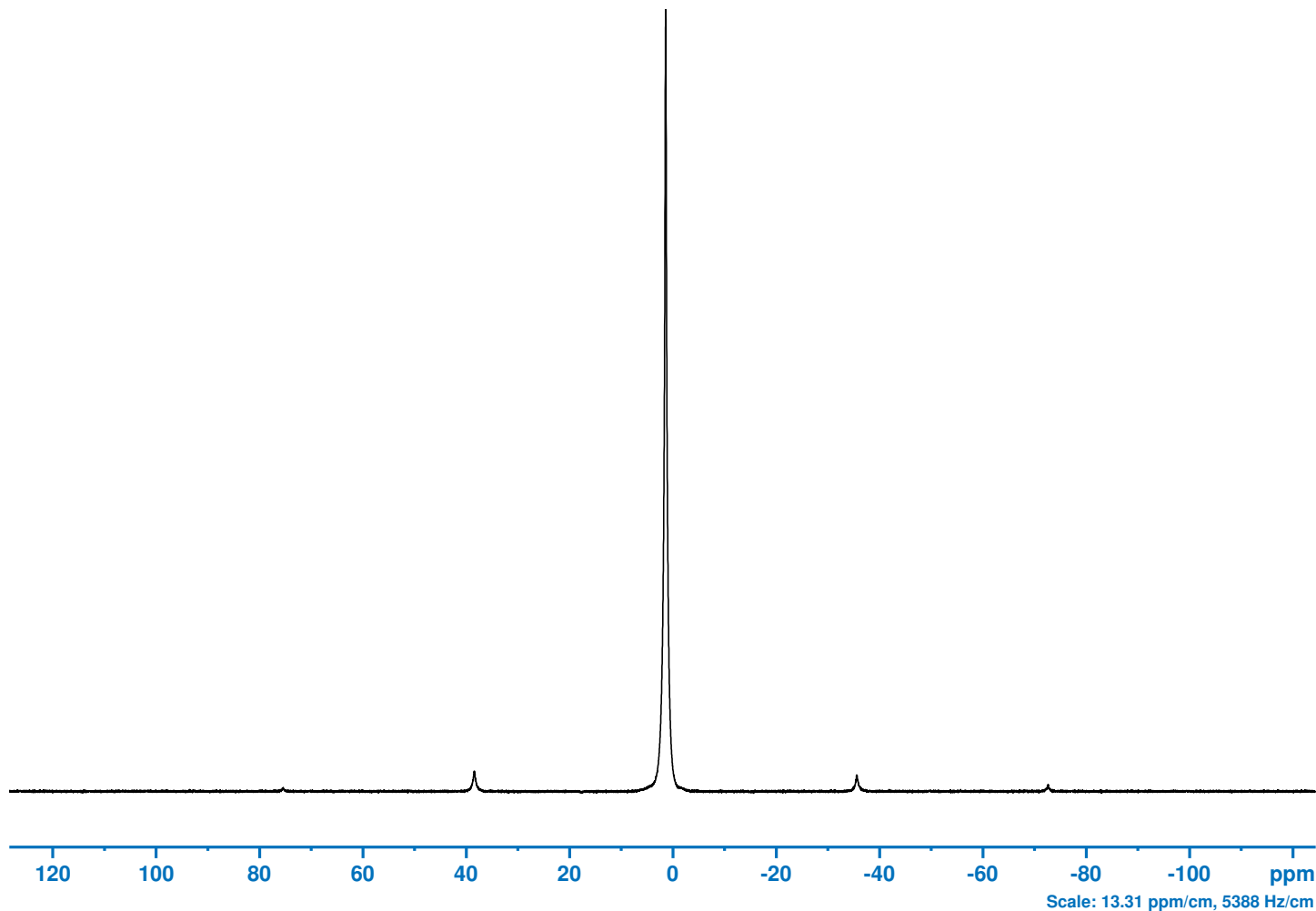
Current Data Parameters
NAME NPT_31P_MAS_sino_cp1h_31p
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201221
Time 15.23 h
INSTRUM Avance Neo 1GHz
PROBHD H177324_0001 (cp
PULPROG cp
TD 11904
SOLVENT H2O+D2O
NS 4
DSH 0
SWH 119047.617 Hz
FIDRES 20.001280 Hz
AQ 0.0499968 sec
RG 101
DW 4.200 usec
DE 6.50 usec
TE 303.0 K
D1 5.0000000 sec
ZGPTNS
SF01 404.9701529 MHz
NUC1 31P
P15 3500.00 usec
PLW1 174.41999817 W
SF02 1000.4072029 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 223.00000000 W
PLW12 156.41999817 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 138.30000305 W

F2 - Processing parameters
SI 32768
SF 404.9693430 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

SHIM SEQUENCE

skip shimming



NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: Adamantane (34 ul) (Z151231)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 10000 Hz)

SINO (20.0 ppm) [achieved]: Signal (38.45 ppm), Noise (34.22 to 14.22 ppm) [25.7] <n/a>
Linewidth [achieved/rated]: at 50% of signal height [5.8 Hz <= 7.0 Hz] <pass>
Number of scans (NS) [achieved]: [1] <n/a>



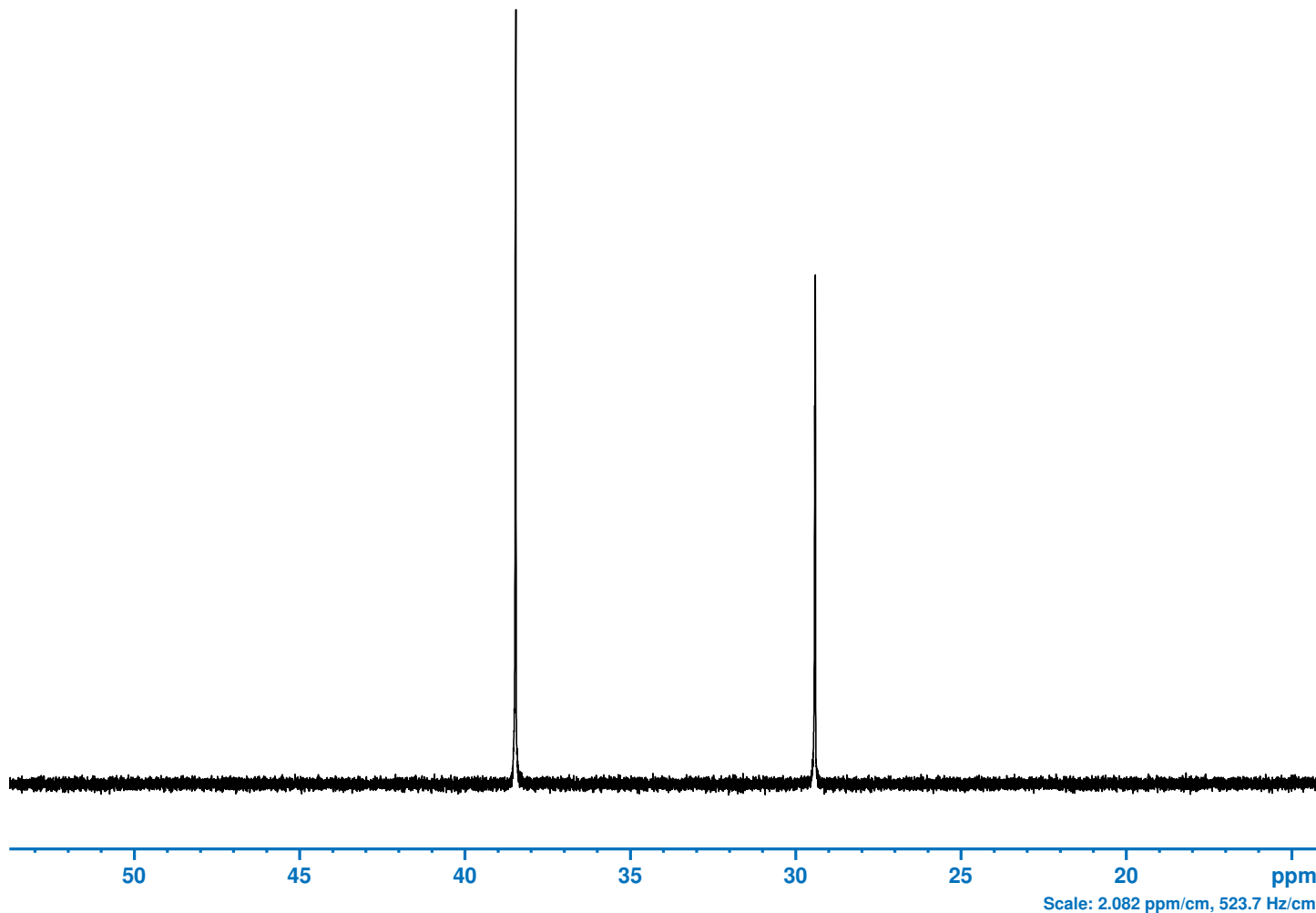
Bruker BioSpin

NPT_13C_MAS_sino_13c

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

F2 - Acquisition Parameters
Date_     20201217
Time      20.41 h
INSTRUM   Avance Neo 1GHz
PROBHD    H177324_0001 (
PULPROG   hpdec
TD         19998
SOLVENT   CDC13
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         15.0000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1       251.5593320 MHz
NUC1        13C
P1          3.50 usec
PLW1       146.30999756 W
SFO2       1000.4024610 MHz
NUC2        1H
CPDPRG[2]  cw
PLW2       114.33999634 W
PLW12      0.14006650 W

F2 - Processing parameters
SI         32768
SF         251.5507801 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         0.20
```



SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
 Sample: Adamantane (34 ul) (Z151231)
 13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 10000 Hz)



Bruker BioSpin

NPT_13C_MAS_sino_13c

```
# Thu Dec 17 20:41:02 2020
$$$PROBEIDENTIFIER=H177324_0001
$$$PROBENAME=PH MASDVT1000S6 BL3.2 X/H NO_I/E
$$$SHIMID=292722
#
# Active Shim Gradients
#
Z -34000
Z2 0
Z3 0
Z4 0
Z5 0
Z6 0
Z7 0
Z8 0
X 0
XZ 0
XZ2 0
XZ3 0
XZ4 0
XZ5 0
Y 0
YZ 0
YZ2 0
YZ3 0
YZ4 0
YZ5 0
XY 0
XYZ 0
XYZ2 0
XYZ3 0
XYZ4 0
XYZ5 0
(X2-Y2) 0
(X2-Y2) Z 0
(X2-Y2) Z2 0
(X2-Y2) Z3 0
(X2-Y2) Z4 0
(X2-Y2) Z5 0
X3 0
X3Z 0
Y3 0
Y3Z 0
#
# Lock Parameter
#
FIELD 2618.700
LOCKPHASE 154.400
LOCKPOWER -17.000
LOCKGAIN 132.300
```

```
LOCKDC -75.000
LOCKSHIFT 7.240
LOOPGAIN -9.400
LOOPTIME 0.464
LOOPFILTER 50.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1] -16489.99996000
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] -16523.61981645
SHIM_SETTING [ 4] -0.00000000
SHIM_SETTING [ 5] -5951.96506694
SHIM_SETTING [ 6] 5951.96506694
SHIM_SETTING [ 7] 16523.61981645
SHIM_SETTING [ 8] -16523.61981645
SHIM_SETTING [ 9] -900.31474754
SHIM_SETTING [10] 900.31474754
SHIM_SETTING [11] 0.00000000
SHIM_SETTING [12] 0.00000000
SHIM_SETTING [13] -0.00000000
SHIM_SETTING [14] -0.00000000
SHIM_SETTING [15] -0.00000000
SHIM_SETTING [16] 0.00000000
SHIM_SETTING [17] 0.00000000
SHIM_SETTING [18] -0.00000000
SHIM_SETTING [19] -0.00000000
SHIM_SETTING [20] 0.00000000
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] 0.00000000
SHIM_SETTING [29] 0.00000000
SHIM_SETTING [30] 0.00000000
SHIM_SETTING [31] 0.00000000
SHIM_SETTING [32] 0.00000000
SHIM_SETTING [33] 0.00000000
SHIM_SETTING [34] 0.00000000
SHIM_SETTING [35] 0.00000000
SHIM_SETTING [36] -0.00000000
SHIM_SETTING [37] 0.00000000
SHIM_SETTING [38] 0.00000000
SHIM_SETTING [39] 0.00000000
SHIM_SETTING [40] 0.00000000
```

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

F2 - Acquisition Parameters
Date_ 20201217
Time 20.41 h
INSTRUM Avance Neo 1GHz
PROBHD H177324_0001 (
PULPROG hpdec
TD 19998
SOLVENT CDC13
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
ZGPTNS -D1acq
SFO1 251.559328 MHz
NUC1 13C
P1 3.50 usec
PLW1 146.30999756 W
SFO2 1000.4024610 MHz
NUC2 1H
CPDPRG2 cw
PLW2 114.33999634 W
PLW12 0.14006650 W

F2 - Processing parameters
SI 32768
SF 251.5507801 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 0.20
```

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: Adamantane (34 ul) (Z151231)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 10000 Hz)

SINO (20.0 ppm) [achieved]: Signal (2.41 ppm), Noise (52.19 to 32.19 ppm) [4751.1] <n/a>
Linewidth [achieved]: at 50% of signal height [488.3 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>



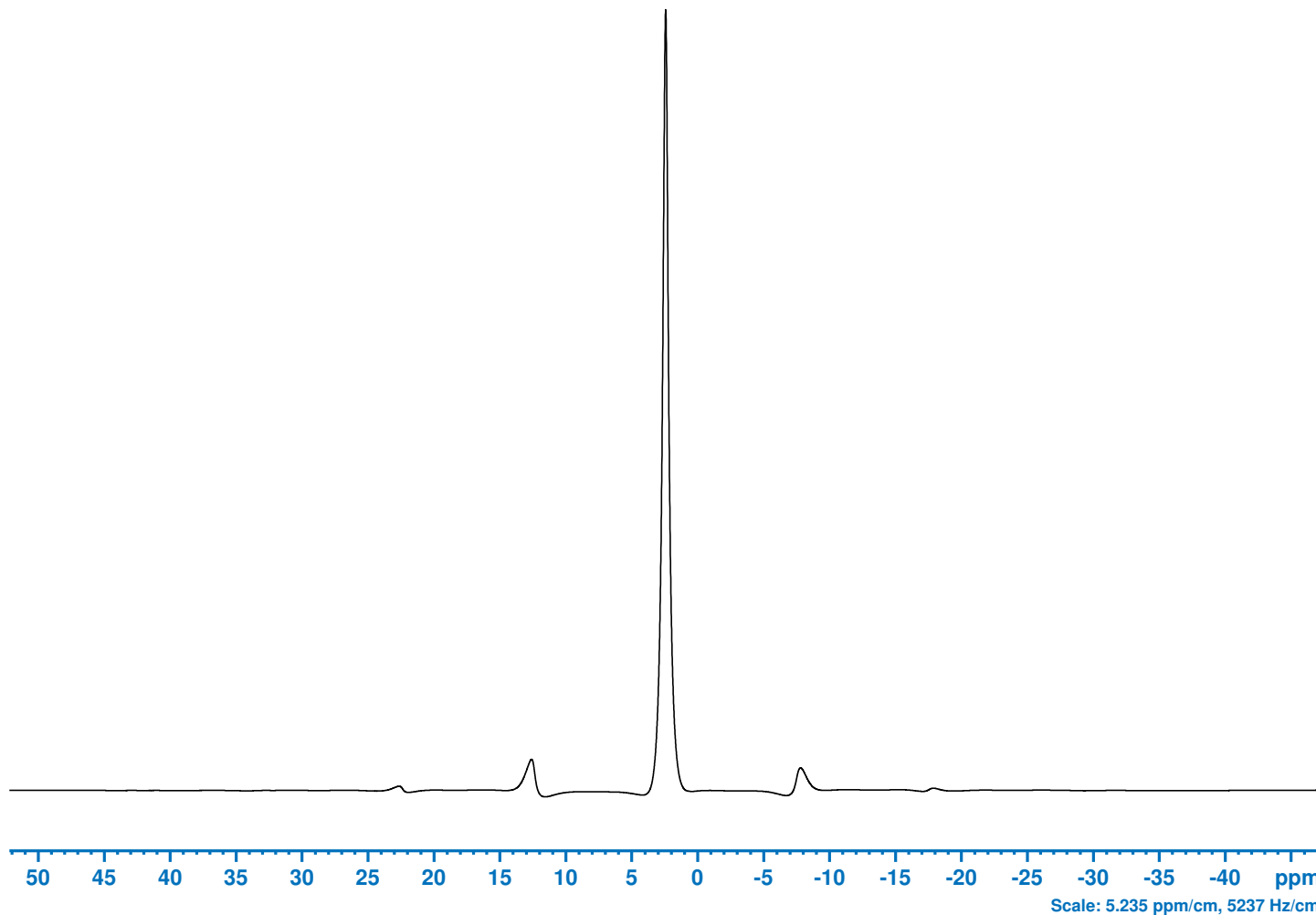
Bruker BioSpin

NPT_1H_MAS_sino_1h

```
Current Data Parameters
NAME      NPT_1H_MAS_sino_1h
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201217
Time      20.40 h
INSTRUM   Avance Neo 1GHz
PROBHD    H177324_0001 (
PULPROG   onepulse
TD         2048
SOLVENT   CDC13
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      1000.4024610 MHz
NUC1       1H
P1         3.50 usec
PLW1      114.33999634 W

F2 - Processing parameters
SI         16384
SF         1000.4000000 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         1.00
```



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


NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: 2-13C, 15N alpha-glycine (34 ul) (Z151233)
CP 1H-13C parameter optimization, MAS (NPT_13C_MAS_paropt_cp1h_13c, spin rate 10000 Hz)

SINO (20.0 ppm): Signal (43.77 ppm), Noise (80.83 to 60.83 ppm) [5782.6]
Processed with TDef=2048



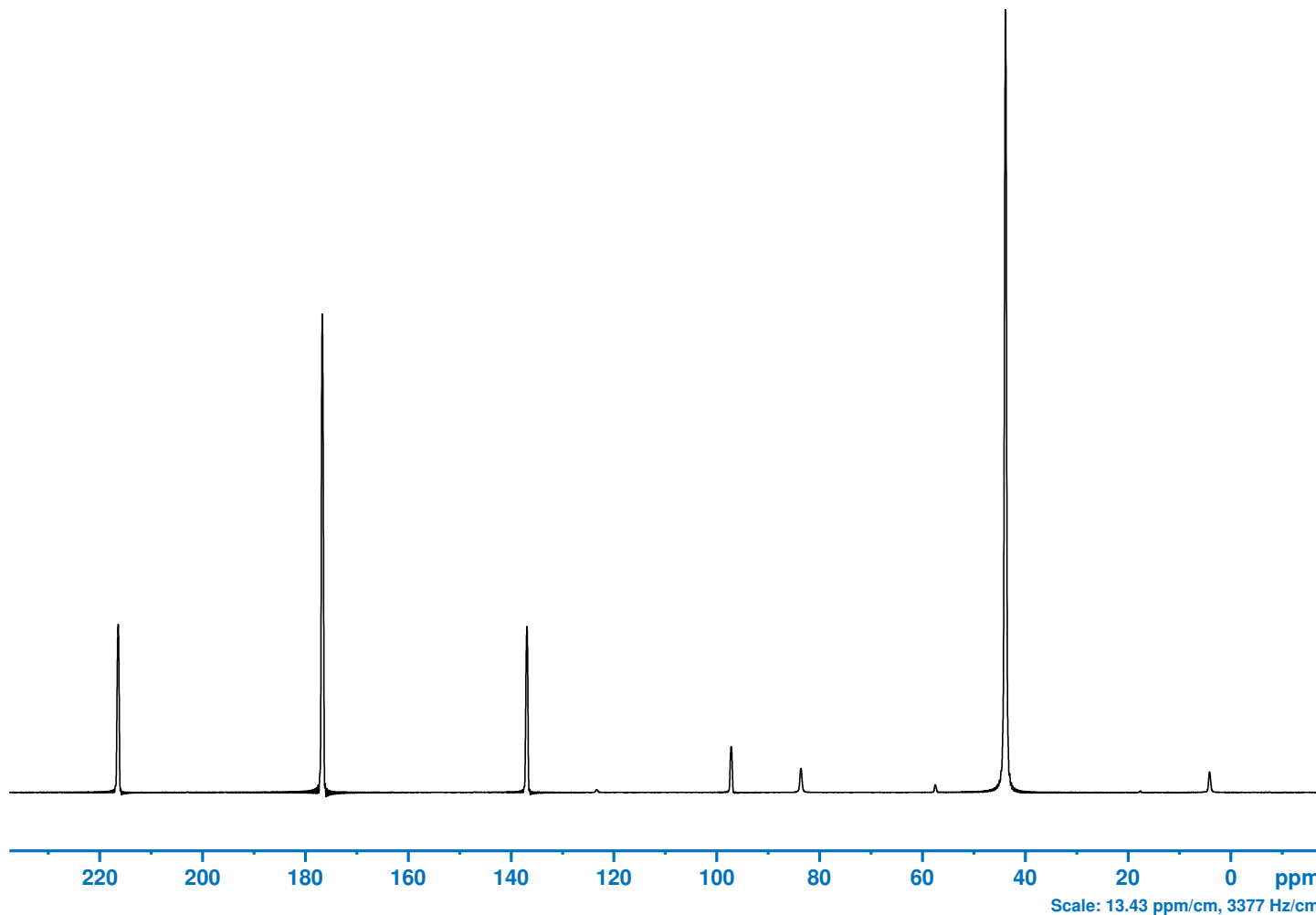
Bruker BioSpin

NPT_13C_MAS_paropt_cp1h_13c

Current Data Parameters
NAME NPT_13C_MAS_paropt_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201218
Time 10.22 h
INSTRUM Avance Neo 1GHz
PROBHD H177324_0001 (cp
PULPROG 7462
TD CDC13
SOLVENT 4
NS 0
DSH 74626.867 Hz
SWH 20.001841 Hz
FIDRES 0.0499954 sec
AQ 101
RG 6.700 usec
DW 6.50 usec
DE 298.0 K
TE 5.0000000 sec
D1 ZGPTNS
SF01 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 103.76999664 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 223.00000000 W
PLW12 178.39999390 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 92.59999847 W

F2 - Processing parameters
SI 32768
SF 251.5507801 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20



SHIM SEQUENCE
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H177324_0001 PH MASDVT1000S6 BL3.2 X/H NO_I/E
Sample: 2-13C, 15N alpha-glycine (34 ul) (Z151233)
CP 1H-15N parameter optimization, MAS (NPT_15N_MAS_paropt_cp1h_15n, spin rate 10000 Hz)

SINO (20.0 ppm): Signal (33.66 ppm), Noise (19.46 to -0.54 ppm) [3465.1]



Bruker BioSpin

NPT_15N_MAS_paropt_cp1h_15n

Current Data Parameters
NAME NPT_15N_MAS_paropt_cp1h_15n
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201218
Time 10.44 h
INSTRUM Avance Neo 1GHz
PROBHD H177324_0001 (cp)
PULPROG cp
TD 7462
SOLVENT CDC13
NS 4
DS 0
SWH 74626.867 Hz
FIDRES 20.001841 Hz
AQ 0.0499954 sec
RG 101
DW 6.700 usec
DE 6.50 usec
TE 298.0 K
D1 5.0000000 sec
ZGPTNS
SF01 101.3731996 MHz
NUC1 15N
P15 3500.00 usec
PLW1 275.39001465 W
SFO2 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 223.00000000 W
PLW12 178.39999390 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 92.59999847 W

F2 - Processing parameters
SI 32768
SF 101.3696516 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

SHIM SEQUENCE

skip shimming

