

NMR Test Spectrometer

Report Name: 1.3mm_HX_Install

AV NEO (1000 MHz) 408457

Content:

- Configuration Information ([uxnmr.info](#))
- IP Config Information
- Probe: H144137_0002 / 1.3mm_HX_Install

Dec 22, 2020

NMR TEST ACCEPTANCE



● 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 = BSMS/2 LOCK TRANSCEIVER 1000: Z109897/00202 ECL 01.01

BSMS: BSMS/2 connected to ethernet
- TCP/IP address = 192.168.99.15
- ELCB firmware version = 20191111
- ELCB = BSMS/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 = BSMS/2 LOCK TRANSCEIVER 1000: Z109897/00202 ECL 01.01
- Lock: on L-TRX board, supports 2H
- VTU_SFB = BSMS/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 BSMS/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

```
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::9e7b:efff:fe38:65cc prefixlen 64 scopeid 0x20<link>
ether 9c:7b:ef:38:65:cc txqueuelen 1000 (Ethernet)
RX packets 17769918 bytes 5233355142 (4.8 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 21888104 bytes 3890595459 (3.6 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
device interrupt 16 memory 0x90200000-90220000

en02: 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 1044226 bytes 193525006 (184.5 MiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 511527 bytes 93534454 (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 30154051 bytes 5100710937 (4.7 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 30154051 bytes 5100710937 (4.7 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
```

PH MAS DVT1000S6 BL1.3 X/H NO_I/E

1000 MHz

Probe ID: H144137_0002

Inspection Lot: 1.3mm_HX_Install

● Probe NMR Test Data: PH MAS DVT1000S6 BL1.3 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] _____ 1.3

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

H144137_0002.ph

```
H144137_0002.ph
=====
$Bis,1,20201126,2048,PICS,5#
$Production,H144137,0002,00.00,,BNMRDE,20201126#
$Name,PH MAS DVT1000S6 Bt1.3 X/H NO_I/E#
$ProbeCompatibility,1.0,SB,6,1000#
$ProbeType,1.1,MAS,0,0#
$ProbeSample,1.0,1.3,0#
$ProbeTemperature,1.0,TypeT,-30,70#
$ProbeHeaterTemperature,1.0,TypeK,-274,600#
$ProbeGasFlow,1.0,,,600,50,2000,,,#
$ProbeAllCoils,1.1,,1#
$ProbeCoil,1.0,1,2.5,2,BB,1H#
$ProbeChannel,1.1,1H,,,150,,,,FALSE,,,#
$ProbeBB,2.0,2,31P-15N,,,,,,#
$ProbeBBSets,1.0,31P,,,150,,,#
$ProbeBBSets,1.0,79Br/13C,,,200,,,#
$ProbeBBSets,1.0,15N,,,400,,,#
$ProbeMas,1.0,8000,67000,0,0,0,0,0,0,0#
$EndBis,77,A5#
```

● **Required Samples** PH MAS DVT1000S6 BL1.3 X/H NO_I/E

Z151270	Potassium Bromide (KBr, 3.0 ul)
Z151271	Adamantane (3.0 ul)
Z151272	Alpha-glycine (2 mg, 3.0 ul)
Z151273	2-13C, 15N alpha-glycine (2 mg, 3.0 ul)
Z151274	Ammonium Dihydrogenphosphate (3.0 ul)

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: Potassium Bromide (KBr, 3.0 ul) (Z151270)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 8000 Hz)

Line width main [achieved]: [265] <n/a>



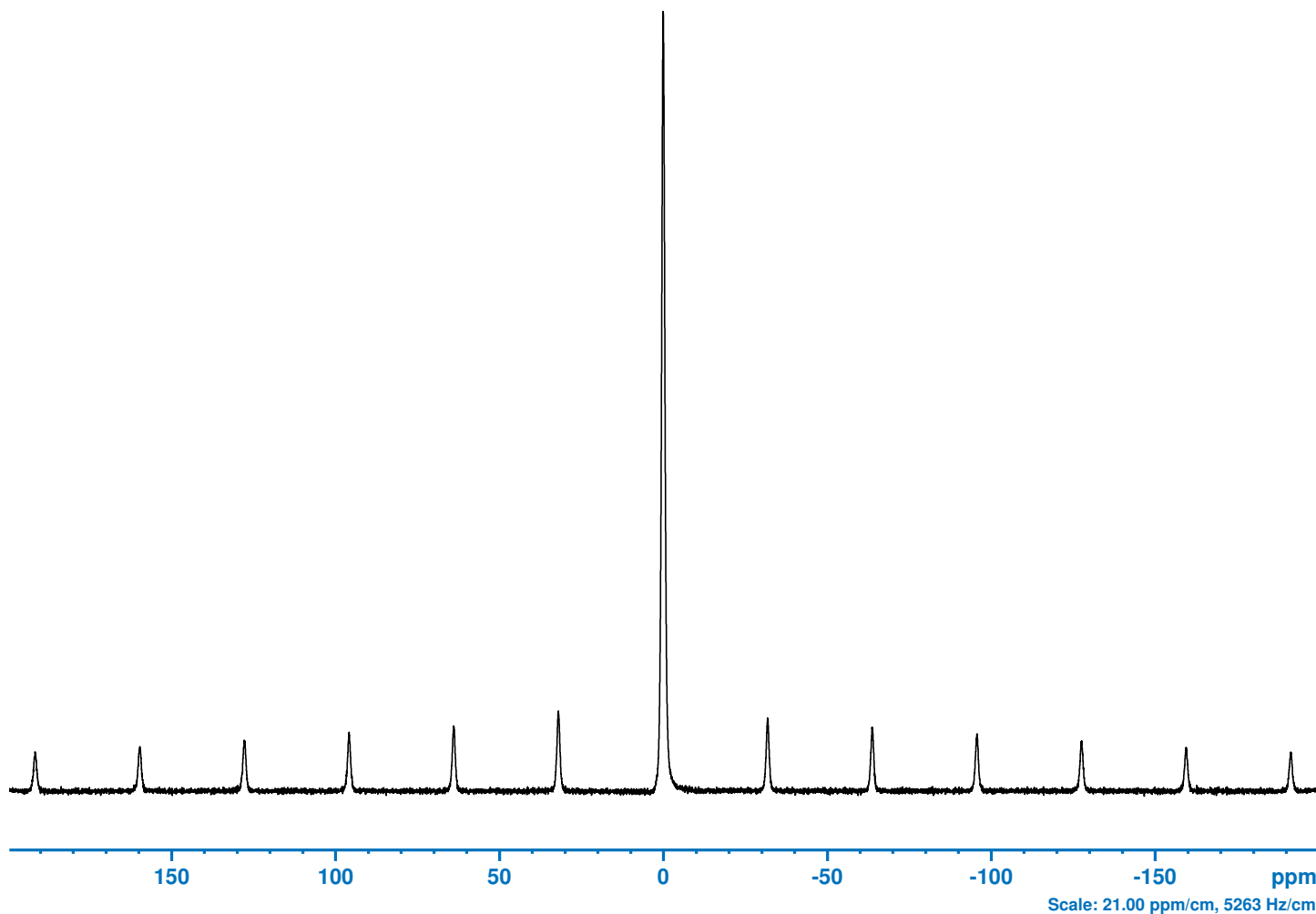
Bruker BioSpin

NPT_79Br_MAS_magicAngle

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

F2 - Acquisition Parameters
Date_     20201218
Time      13.51 h
INSTRUM   Avance Neo 1GHz
PROBHD    H144137_0002 (
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         298.0 K
D1         0.2500000 sec
SFO1      250.6552759 MHz
NUC1       79Br
P1         2.50 usec
PLW1       48.95700073 W

F2 - Processing parameters
SI         131072
SF         250.6552759 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
 Sample: Potassium Bromide (KBr, 3.0 ul) (Z151270)
 Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 67000 Hz)
 Determination of spinning stability for 180 s
 Pressure values in mbar: DrivePressure=3829/BearingPressure=3167/BearingSensePressure=3100/SupplyPressure=6936/SystemPressure=7131

Spin rate at maximum deviation [measured]: @ MASR 67000 Hz [66994 Hz]
 Maximum deviation [achieved/rated]: @ MASR 67000 Hz [6 Hz <= 67 Hz] <pass>



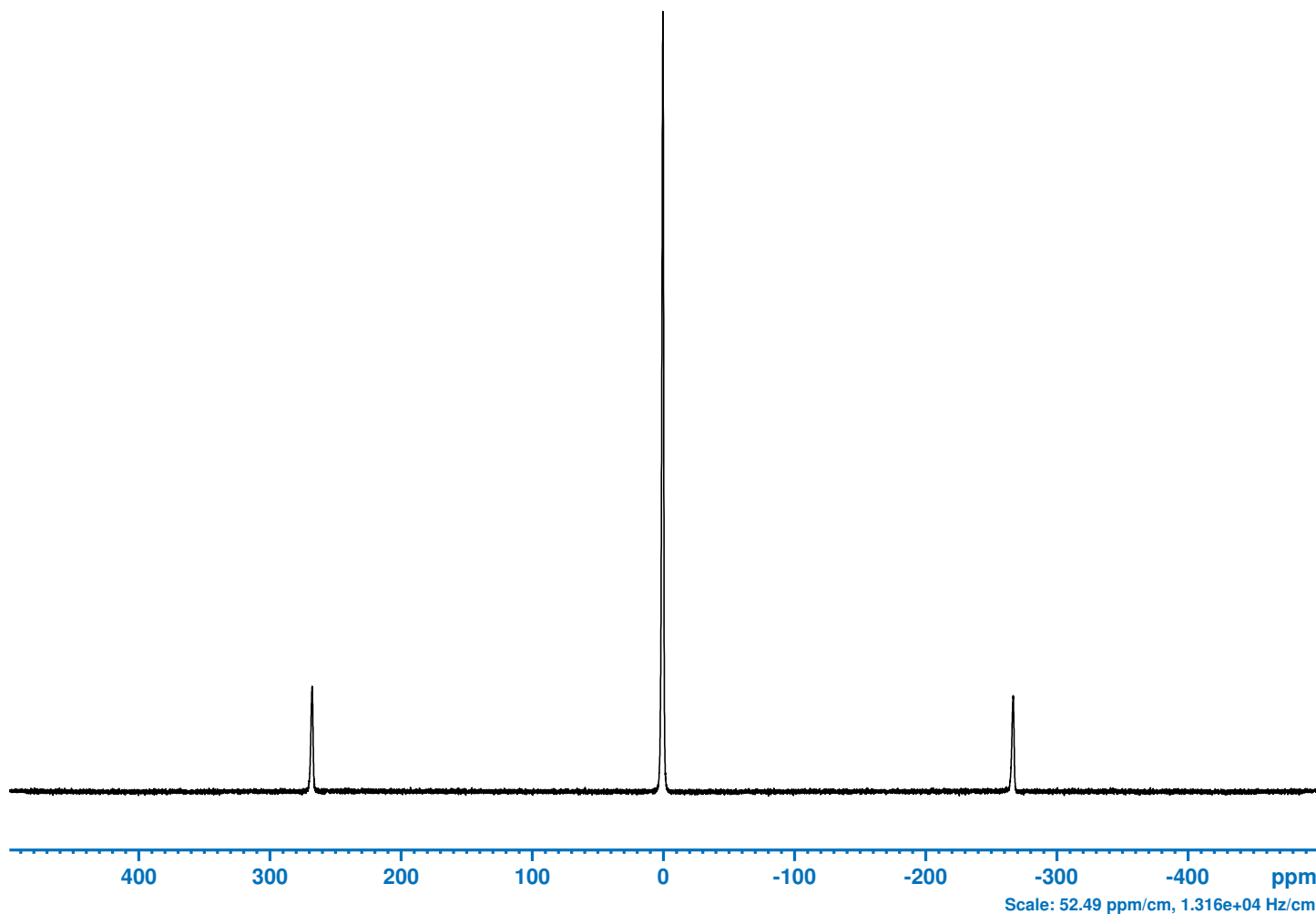
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

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

F2 - Acquisition Parameters
Date_     20201218
Time      14.05 h
INSTRUM   Avance Neo 1GHz
PROBHD    H144137_0002 (
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         298.0 K
D1         0.2500000 sec
SFO1       250.6546516 MHz
NUC1       79Br
P1         2.50 usec
PLW1       48.95700073 W

F2 - Processing parameters
SI         32768
SF         250.6546516 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0
PC         0.20
```



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

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: Potassium Bromide (KBr, 3.0 ul) (Z151270)
Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting, spin rate 8000 Hz)
FIELD was set to 2783.9 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0070 ppm.



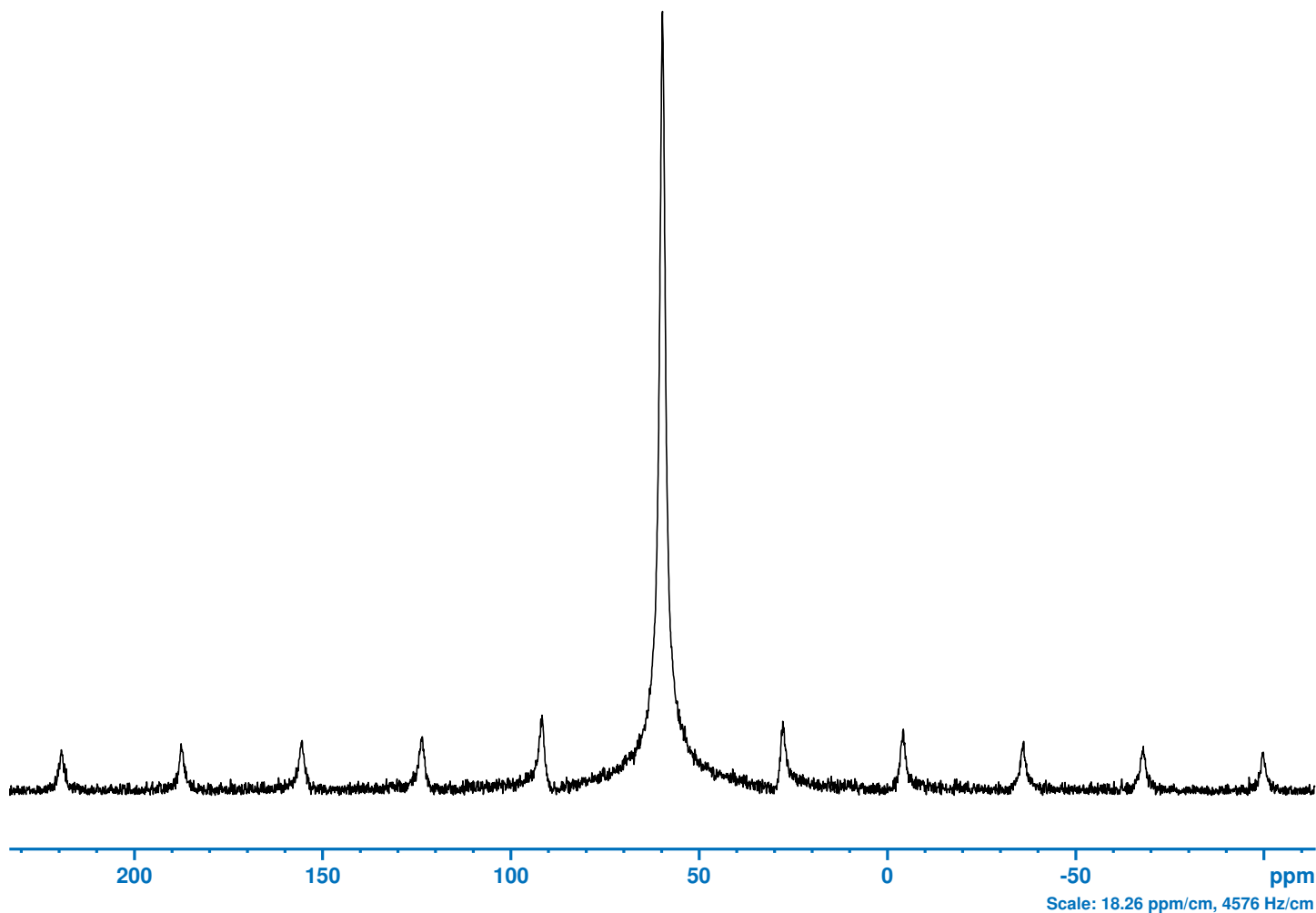
Bruker BioSpin

NPT_79Br_MAS_fieldsetting

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

F2 - Acquisition Parameters
Date_     20201218
Time      13.52 h
INSTRUM   Avance Neo 1GHz
PROBHD    H144137_0002 (
PULPROG   onepulse
TD         4096
SOLVENT   CDC13
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         298.0 K
D1         0.50000000 sec
SFO1      250.6549791 MHz
NUC1       79Br
P1         2.50 usec
PLW1       48.95700073 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: Adamantane (3.0 ul) (Z151271)
Optimization of 13C frequency (NPT_13C_MAS_fieldsetting_dec1h, spin rate 30000 Hz)
FIELD was set to 2844.1 for 13C chemical shift of 38.460 ppm. One field unit corresponds to 0.0071 ppm.



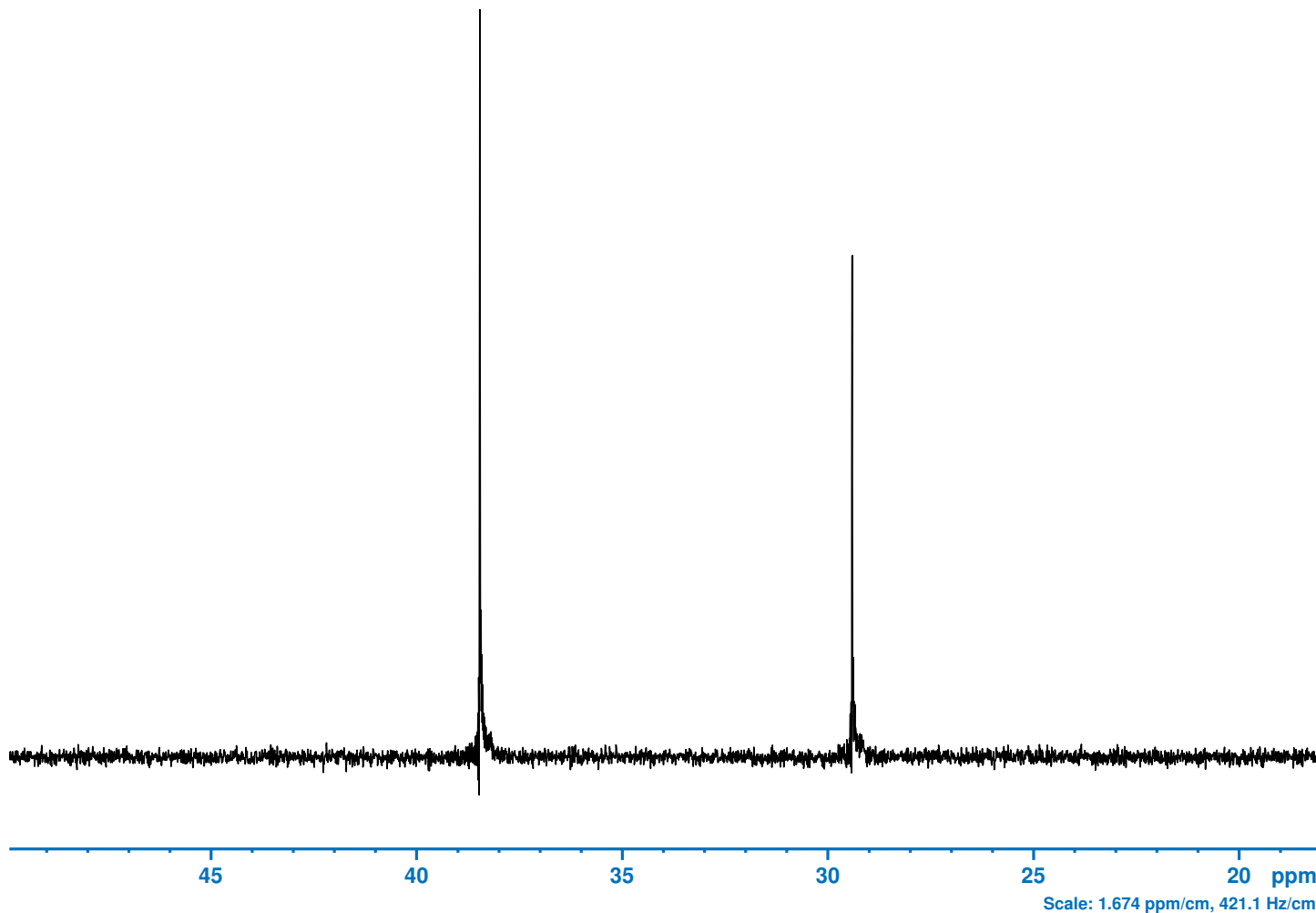
Bruker BioSpin

NPT_13C_MAS_fieldsetting_dec1h

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

F2 - Acquisition Parameters
Date_     20201221
Time      11.59 h
INSTRUM   Avance Neo 1GHz
PROBHD    H144137_0002 (
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        303.0 K
D1        15.0000000 sec
P15       0 usec
ZGPTNS    -D1acq
SFO1      251.5593328 MHz
NUC1       13C
P1         2.50 usec
PLW1      38.72999954 W
SFO2      1000.4023807 MHz
NUC2       1H
CPDPRG2   cw
PLW2      49.34000015 W
PLW12     0.12833340 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

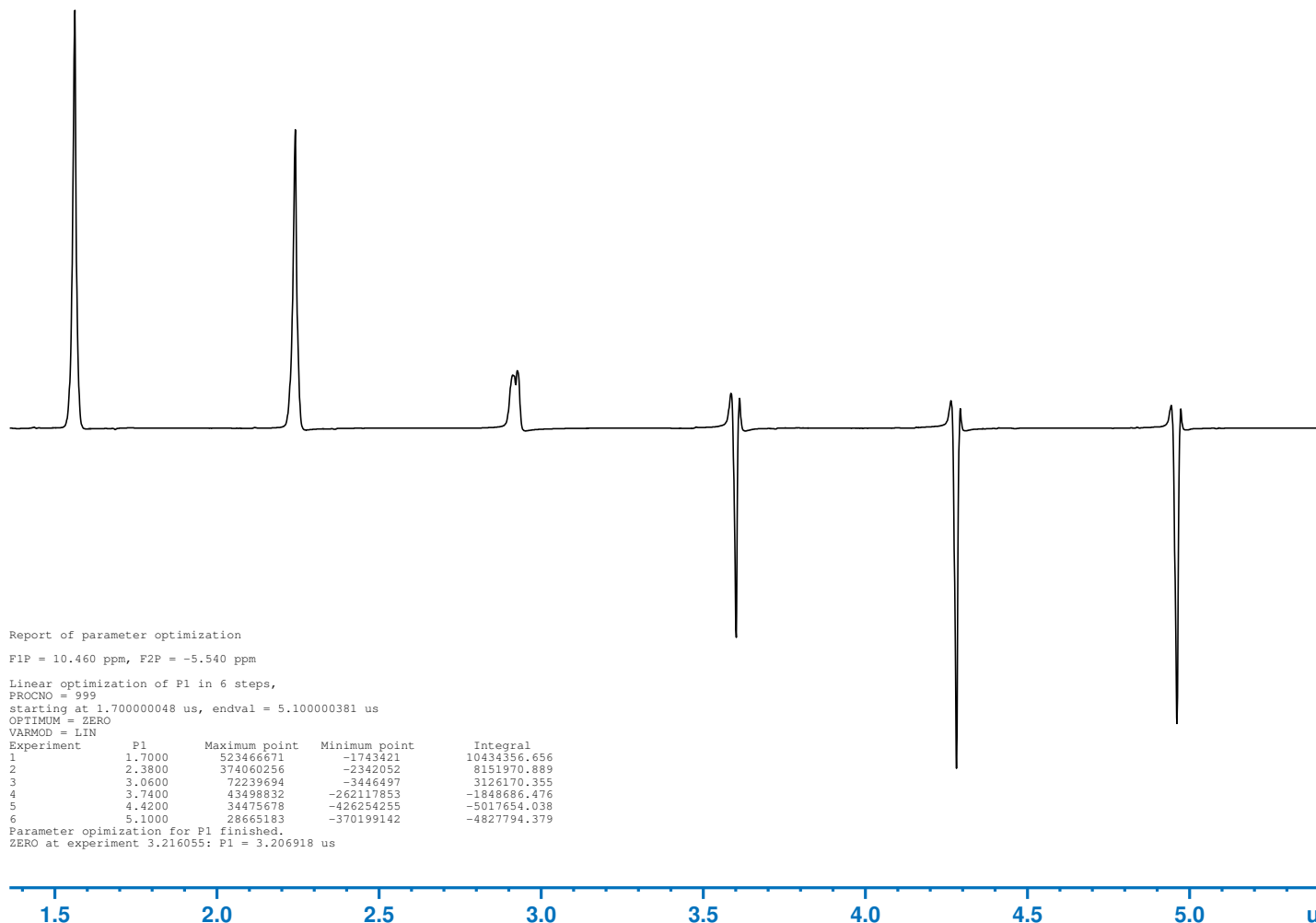
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
 Sample: Adamantane (3.0 ul) (Z151271)
 P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 30000 Hz)
 ATTENTION: Updated PROSOL Tables with [1.70 us @ 49.3 W].



Bruker BioSpin

P90 MAS 1H pulse [achieved/rated]: @ 55.7 W [1.60 us <= 1.70 us] <pass>

NPT_1H_MAS_p90det_1h



Current Data Parameters
 NAME NPT_1H_MAS_p90det_1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201221
 Time 11.45 h
 INSTRUM Avance Neo 1GHz
 PROBHD H144137_0002 ()
 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 6.500 usec
 TE 303.0 K
 D1 5.00000000 sec
 SFO1 1000.4024610 MHz
 NUC1 1H
 P1 5.10 usec
 PLW1 55.70000076 W

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

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

 55.7 W 1.70 us
 55.7 W 1.70 us 1.60 us -5.9%

Report of parameter optimization

F1P = 10.460 ppm, F2P = -5.540 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 1.700000048 us, endval = 5.100000381 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	1.7000	523466671	-1743421	10434356.656
2	2.3800	374060256	-2342052	8151970.889
3	3.0600	72239694	-3446497	3126170.355
4	3.7400	43498832	-262117853	-1848686.476
5	4.4200	34475678	-426254255	-5017654.038
6	5.1000	28665183	-370199142	-4827794.379

Parameter optimization for P1 finished.

ZERO at experiment 3.216055: P1 = 3.206918 us

 SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
 Sample: Potassium Bromide (KBr, 3.0 ul) (Z151270)
 P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br, spin rate 8000 Hz)
 ATTENTION: Updated PROSOL Tables with [2.50 us @ 49.0 W].

P90 MAS 79Br pulse [achieved/rated]: @ 50.6 W [2.46 us <= 2.50 us] <pass>



Bruker BioSpin

NPT_79Br_MAS_p90det_79br



Current Data Parameters
 NAME NPT_79Br_MAS_p90det_79br
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201218
 Time 13.51 h
 INSTRUM Avance Neo 1GHz
 PROBHD H144137_0002 ()
 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 298.0 K
 D1 0.25000000 sec
 SFO1 250.6549791 MHz
 NUC1 79Br
 P1 7.50 usec
 PLW1 50.56206894 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
48.0 W	2.50 us	2.51 us	0.4%
48.0 W	2.50 us	2.46 us	-1.6%

Report of parameter optimization

F1P = 69.700 ppm, F2P = 49.700 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	359420405	-3213036	22750629.889
2	3.5000	238931109	-3247745	14975521.536
3	4.5000	62677964	-5018461	3978928.990
4	5.5000	5828414	-89413178	-4154888.213
5	6.5000	5438806	-143665526	-6934936.652
6	7.5000	5393321	-101754360	-4610440.242

Parameter optimization for P1 finished.

ZERO at experiment 3.412108: P1 = 4.912108 us

 SHIM SEQUENCE

skip shimming

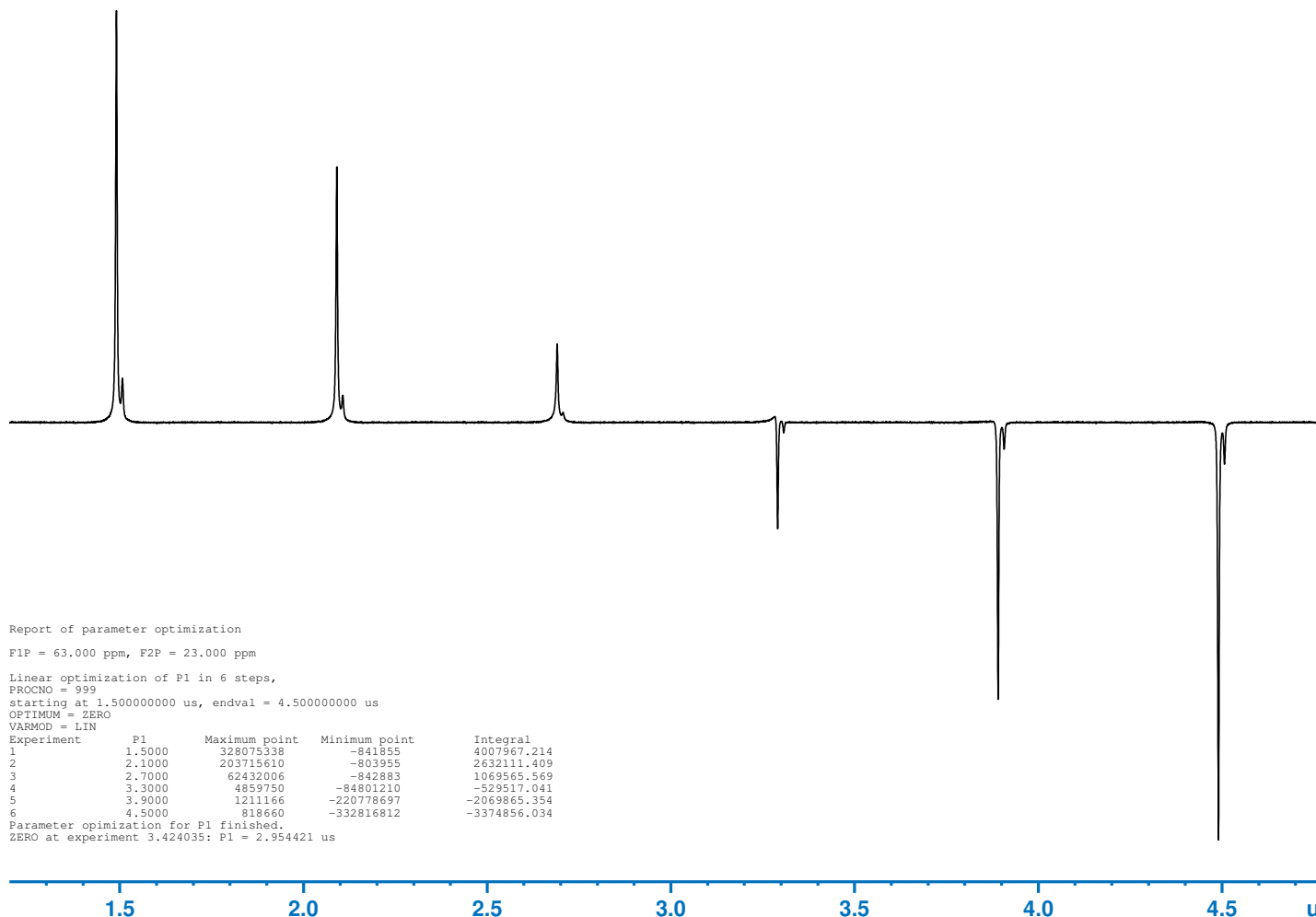
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)
 P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.00 us @ 26.0 W].

P90_MAS_CP 1H13C power (PLW 11) [achieved]: [26.9 W] <n/a>
 P90_MAS_CP 1H13C pulse (P 1) [achieved/rated]: [2.95 us <= 3.00 us] <pass>



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_ 20201221
 Time 12.12 h
 INSTRUM Avance Neo 1GHz
 PROBHD H144137_0002 ()
 PULPROG cp90
 TD 7462
 SOLVENT H2O+D2O
 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 303.0 K
 D1 5.00000000 sec
 ZGPTNS
 SFO1 251.5615968 MHz
 NUC1 13C
 P1 4.50 usec
 P15 2000.00 usec
 PLW1 26.89583015 W
 PLW11 26.89583015 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 1.70 usec
 PCPD2 3.20 usec
 PLW2 49.34000015 W
 PLW12 49.34000015 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 58.40594101 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

 38.7 W 2.50 us
 26.9 W 3.00 us 2.95 us -1.7%

 SHIM SEQUENCE

 skip shimming

Report of parameter optimization

F1P = 63.000 ppm, F2P = 23.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 1.500000000 us, endval = 4.500000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	1.5000	328075338	-841855	4007967.214
2	2.1000	203715610	-803955	2632111.409
3	2.7000	62432006	-842883	1069565.569
4	3.3000	4859750	-84801210	-529517.041
5	3.9000	1211166	-220778697	-2069865.354
6	4.5000	818660	-332816812	-3374856.034

Parameter optimization for P1 finished.

ZERO at experiment 3.424035: P1 = 2.954421 us

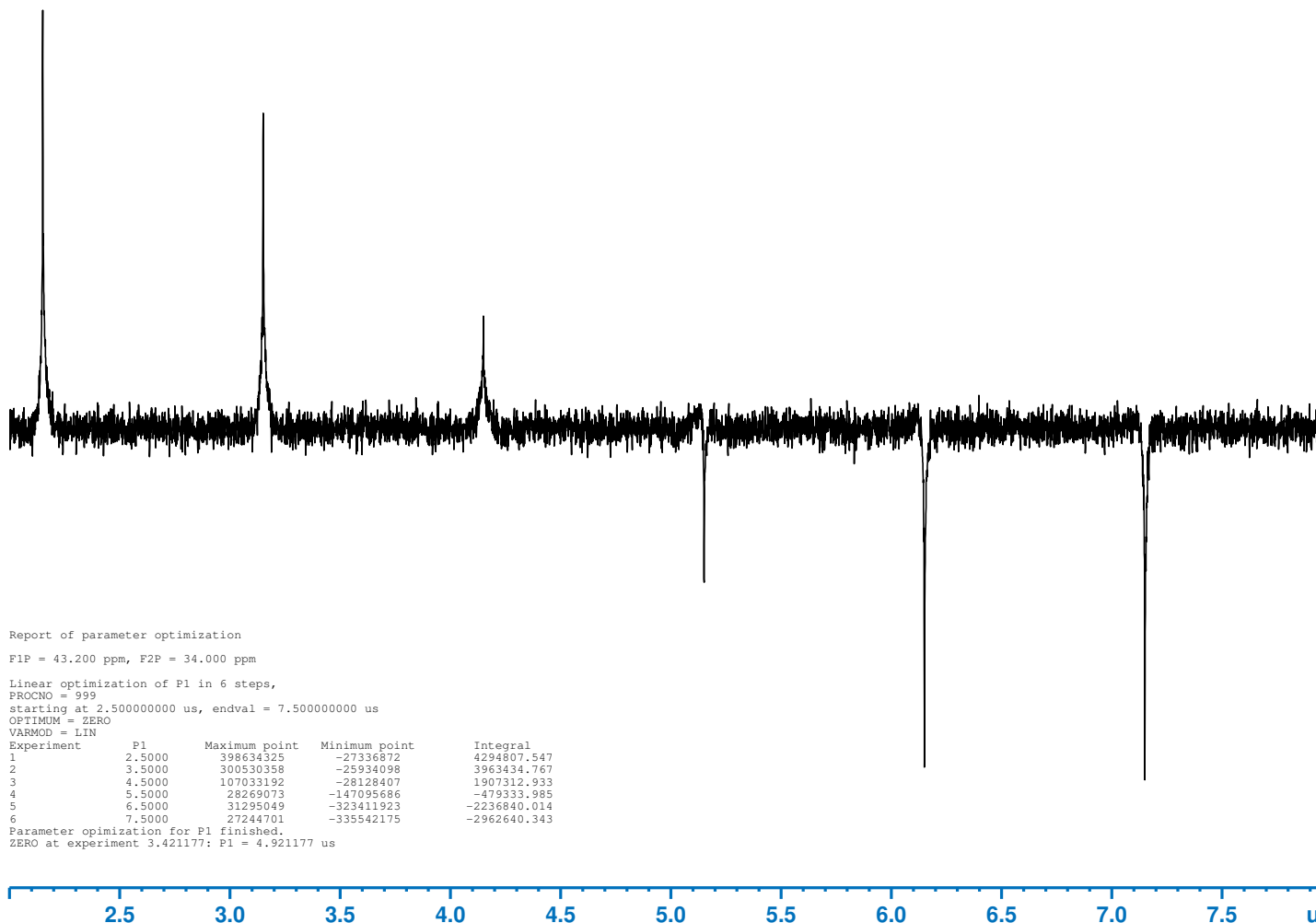
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
 Sample: Adamantane (3.0 ul) (Z151271)
 P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c, spin rate 30000 Hz)
 ATTENTION: Updated PROSOL Tables with [2.50 us @ 38.7 W].



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P90 MAS 13C pulse [achieved/rated]: @ 40.0 W [2.46 us <= 2.50 us] <pass>

NPT_13C_MAS_p90det_13c



Current Data Parameters
 NAME NPT_13C_MAS_p90det_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201221
 Time 11.53 h
 INSTRUM Avance Neo 1GHz
 PROBHD H144137_0002 ()
 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 303.0 K
 D1 15.00000000 sec
 P15 0 usec
 ZGPTNS -D1acq
 SFO1 251.5593328 MHz
 NUC1 13C
 P1 7.50 usec
 PLW1 40.00000000 W
 SFO2 1000.4024610 MHz
 NUC2 1H
 CPDPRG[2] cw
 PLW2 49.34000015 W
 PLW12 0.12833340 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
40.0 W	2.50 us		
40.0 W	2.50 us	2.46 us	-1.6%

Report of parameter optimization

F1P = 43.200 ppm, F2P = 34.000 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	398634325	-27336872	4294807.547
2	3.5000	300530358	-25934098	3963434.767
3	4.5000	107033192	-28128407	1907312.933
4	5.5000	28269073	-147095686	-479333.985
5	6.5000	31295049	-323411923	-2236840.014
6	7.5000	27244701	-335542175	-2962640.343

Parameter optimization for P1 finished.

ZERO at experiment 3.421177: P1 = 4.921177 us

 SHIM SEQUENCE

 skip shimming

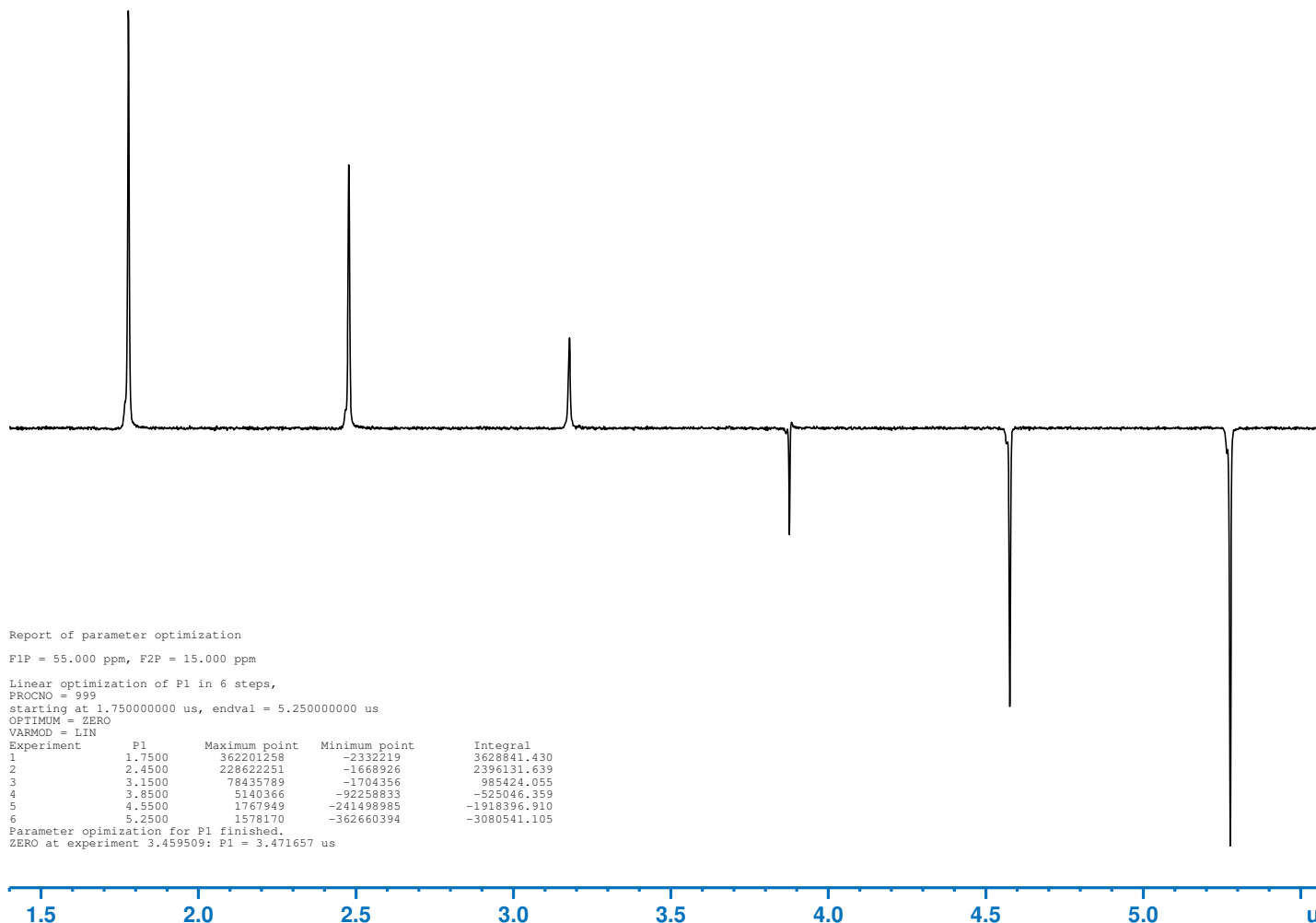
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)
 P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.50 us @ 83.2 W].



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P90_MAS_CP 1H15N power (PLW 11) [achieved]: [84.6 W] <n/a>
 P90_MAS_CP 1H15N pulse (P 1) [achieved/rated]: [3.47 us <= 3.50 us] <pass>

NPT_15N_MAS_p90det_cp1h_15n



Current Data Parameters
 NAME NPT_15N_MAS_p90det_cp1h_15n
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201221
 Time 12.34 h
 INSTRUM Avance Neo 1GHz
 PROBHD H144137_0002 (cp90)
 PULPROG cp90
 TD 4064
 SOLVENT H2O+D2O
 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 303.0 K
 D1 5.00000000 sec
 ZGPGTNS
 SFO1 101.3731996 MHz
 NUC1 15N
 P1 5.25 usec
 P15 3500.00 usec
 PLW1 54.91427994 W
 PLW11 84.61421204 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 1.70 usec
 PCPD2 3.20 usec
 PLW2 49.34000015 W
 PLW12 49.34000015 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 33.32604980 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
70.0 W	3.10 us		
54.9 W	3.50 us	4.25 us	21.4%
84.6 W	3.50 us	3.47 us	-0.9%

Report of parameter optimization

F1P = 55.000 ppm, F2P = 15.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 1.750000000 us, endval = 5.250000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	1.7500	362201258	-2332219	3628841.430
2	2.4500	228622251	-1668926	2396131.639
3	3.1500	78435789	-1704356	985424.055
4	3.8500	5140366	-92258833	-525046.359
5	4.5500	1767949	-241498985	-1918396.910
6	5.2500	1578170	-362660394	-3080541.105

Parameter optimization for P1 finished.

ZERO at experiment 3.459509: P1 = 3.471657 us

 SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO I/E
 Sample: Ammonium Dihydrogenphosphate (3.0 ul) (Z151274)
 P90 31P 1H-31P CP pulse calibration, MAS (NPT_31P_MAS_p90det_cp1h_31p, spin rate 15000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.50 us @ 23.8 W].



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P90_MAS_CP 1H31P power (PLW 11) [achieved]: [30.0 W] <n/a>
 P90_MAS_CP 1H31P pulse (P 1) [achieved/rated]: [3.12 us <= 3.50 us] <pass>

NPT_31P_MAS_p90det_cp1h_31p

Current Data Parameters
 NAME NPT_31P_MAS_p90det_cp1h_31p
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201221
 Time 14.09 h
 INSTRUM Avance Neo 1GHz
 PROBHD H144137_0002 ()
 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
 ZGPTNS
 SFO1 404.9701529 MHz
 NUC1 31P
 P1 5.25 usec
 P15 3500.00 usec
 PLW1 30.00000000 W
 PLW11 30.00000000 W
 SFO2 1000.4072029 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 1.70 usec
 PCPD2 3.20 usec
 PLW2 49.34000015 W
 PLW12 49.34000015 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 30.29766083 W

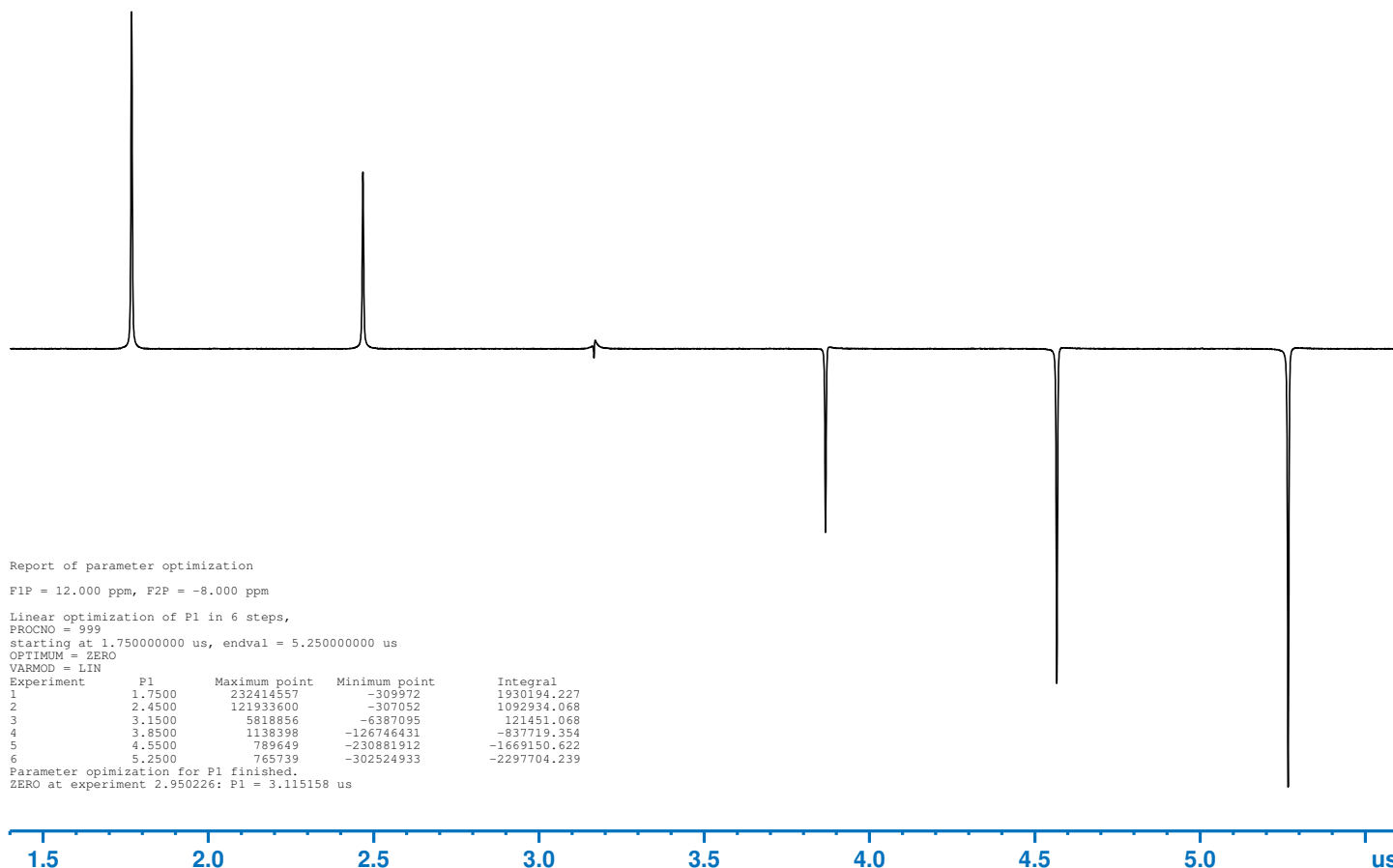
F2 - Processing parameters
 SI 16384
 SF 404.9693430 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

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

 30.0 W 3.50 us
 30.0 W 3.50 us 3.12 us -10.9%

 SHIM SEQUENCE

 skip shimming



NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: Alpha-glycine (2 mg, 3.0 ul) (Z151272)
CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c, spin rate 10000 Hz)

SINO (20.0 ppm) [achieved]: Signal (43.63 ppm), Noise (129.81 to 109.81 ppm) [83.1] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>
Processed with TDef=2048



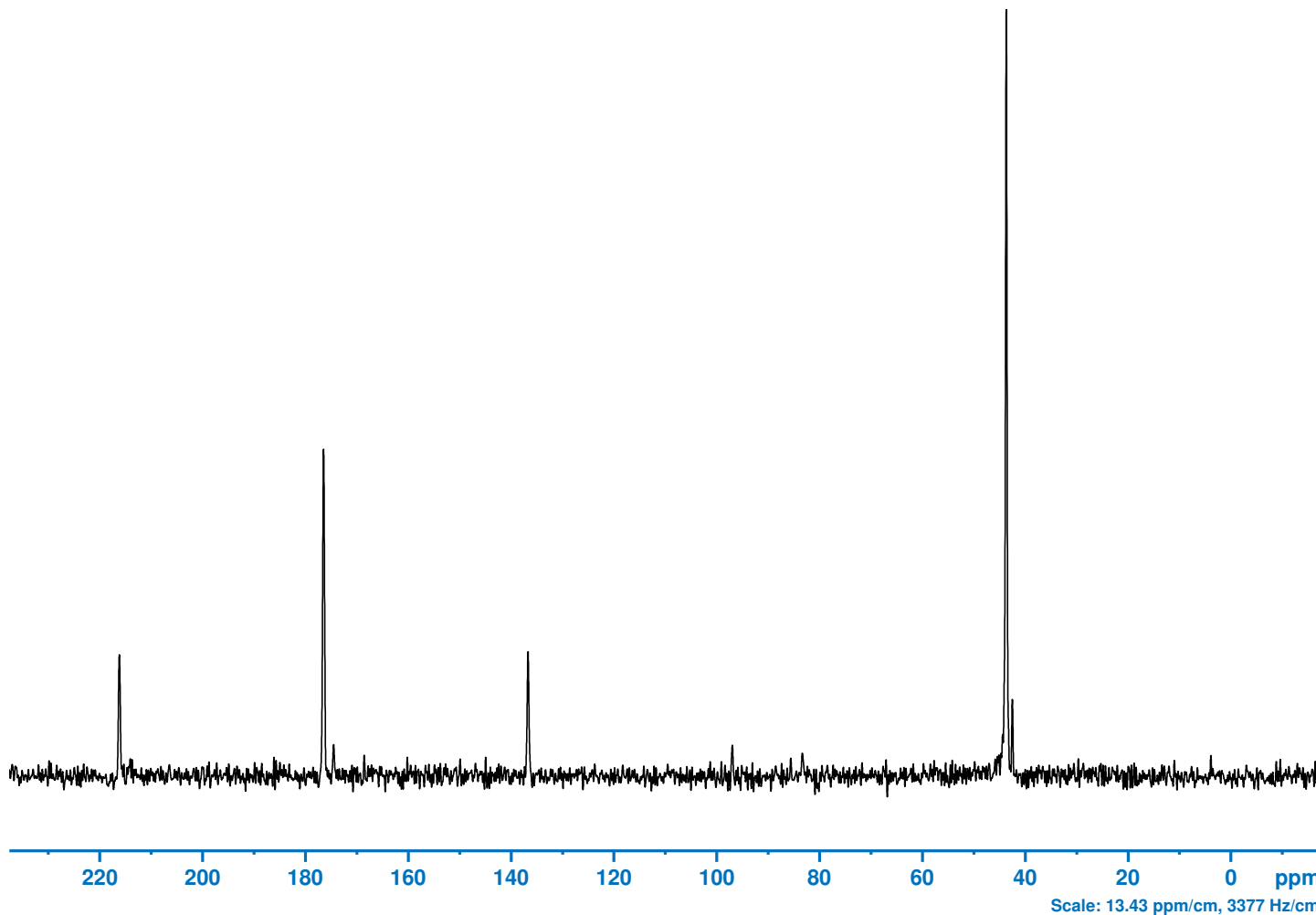
Bruker BioSpin

NPT_13C_MAS_sino_cp1h_13c

Current Data Parameters
NAME NPT_13C_MAS_sino_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201221
Time 13.53 h
INSTRUM Avance Neo 1GHz
PROBHD H144137_0002 (cp
PULPROG cp
TD 7462
SOLVENT H2O+D2O
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 303.0 K
D1 5.0000000 sec
ZGPTNS
SF01 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 26.00699997 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 1.70 usec
PCPD2 3.20 usec
PLW2 49.34000015 W
PLW12 59.20000076 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 38.88000107 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: Alpha-glycine (2 mg, 3.0 ul) (Z151272)
CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n, spin rate 10000 Hz)

SINO (20.0 ppm) [achieved]: Signal (33.28 ppm), Noise (-76.81 to -96.81 ppm) [8.1] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>



Bruker BioSpin

NPT_15N_MAS_sino_cp1h_15n

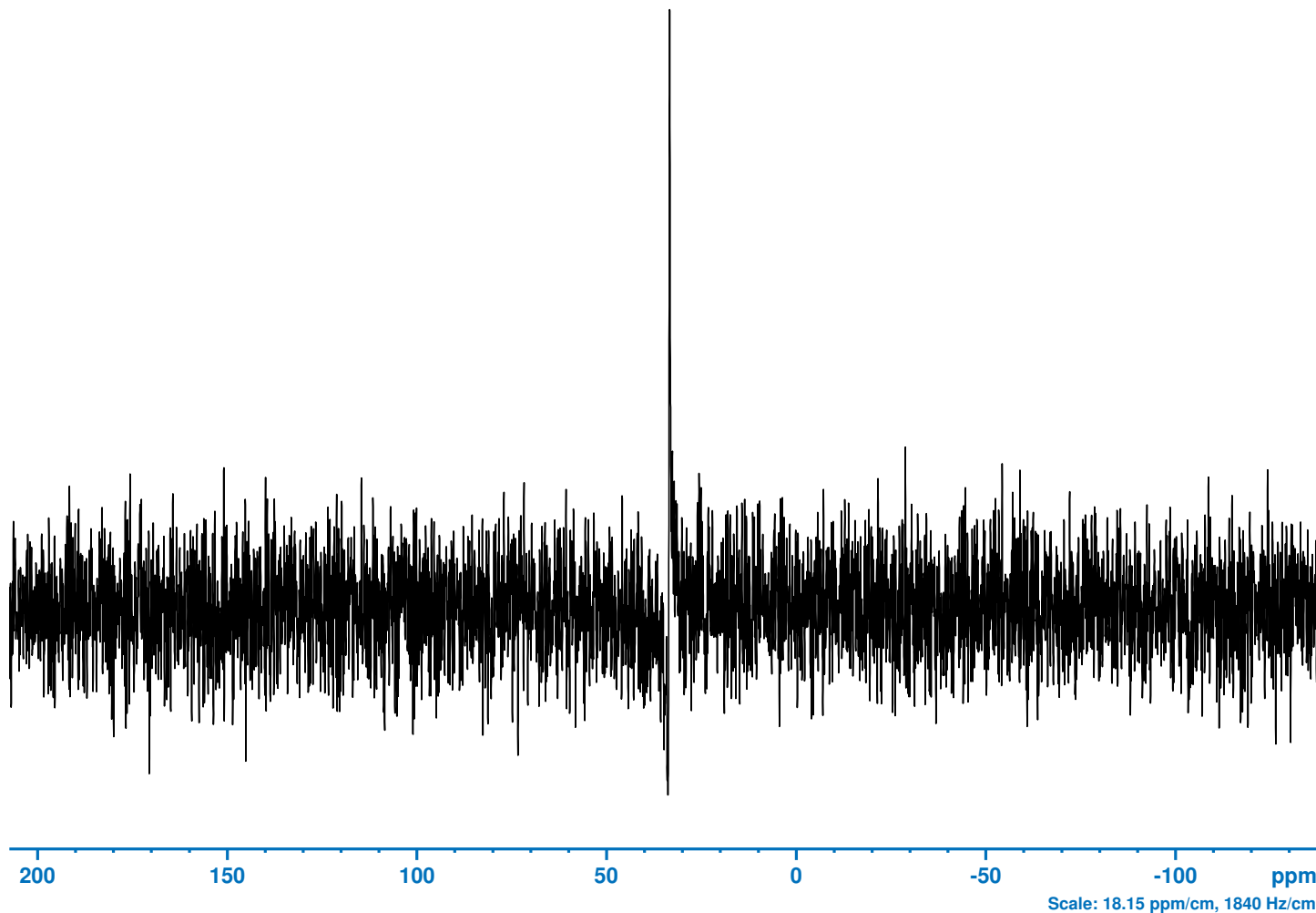
Current Data Parameters
NAME NPT_15N_MAS_sino_cp1h_15n
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201221
Time 13.17 h
INSTRUM Avance Neo 1GHz
PROBHD H144137_0002 (cp
PULPROG cp
TD 4064
SOLVENT H2O+D2O
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 303.0 K
D1 5.0000000 sec
ZGPTNS
SF01 101.3731996 MHz
NUC1 15N
P15 3500.00 usec
PLW1 83.16999817 W
SFO2 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 1.70 usec
PCPD2 3.20 usec
PLW2 49.34000015 W
PLW12 41.47000122 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 18.78000069 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO I/E
Sample: Ammonium Dihydrogenphosphate (3.0 ul) (Z151274)
CP 1H-31P sensitivity, MAS (NPT_31P_MAS_sino_cp1h_31p, spin rate 15000 Hz)

SINO (10.0 ppm) [achieved]: Signal (1.47 ppm), Noise (-94.18 to -104.18 ppm) [2593.2] <n/a>
Number of scans (NS) [achieved]: [4] <n/a>



Bruker BioSpin

NPT_31P_MAS_sino_cp1h_31p

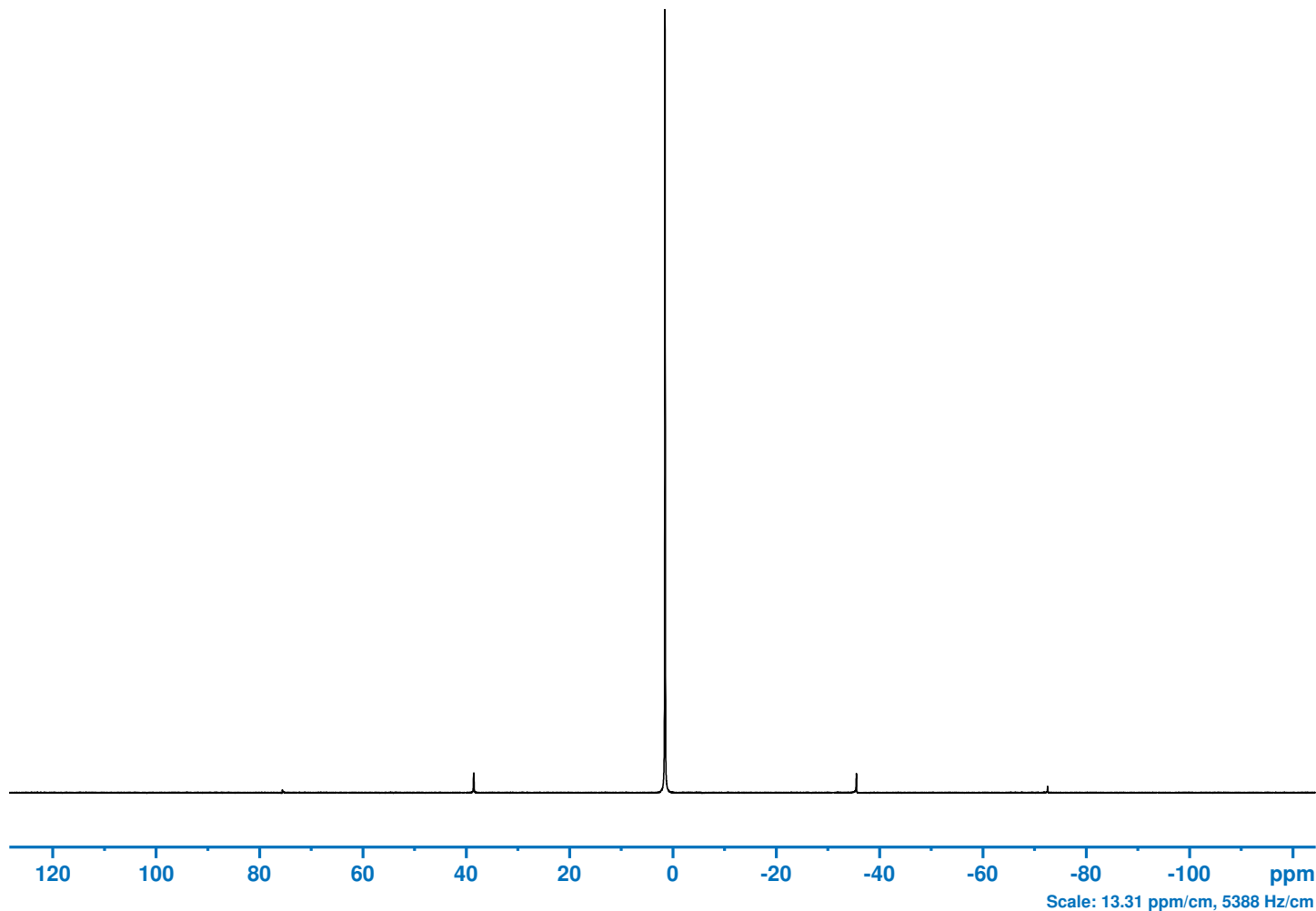
Current Data Parameters
NAME NPT_31P_MAS_sino_cp1h_31p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201221
Time 14.20 h
INSTRUM Avance Neo 1GHz
PROBHD H144137_0002 (cp
PULPROG cp
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 5.0000000 sec
ZGPTNS
SF01 404.9701529 MHz
NUC1 31P
P15 3500.00 usec
PLW1 23.83900070 W
SF02 1000.4072029 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 1.70 usec
PCPD2 3.20 usec
PLW2 49.34000015 W
PLW12 55.25999832 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 45.40000153 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: Adamantane (3.0 ul) (Z151271)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 30000 Hz)

SINO (20.0 ppm) [achieved]: Signal (38.46 ppm), Noise (35.85 to 15.85 ppm) [28.4] <n/a>
Linewidth [achieved/rated]: at 50% of signal height [1.6 Hz <= 7.0 Hz] <pass>
Number of scans (NS) [achieved]: [1] <n/a>



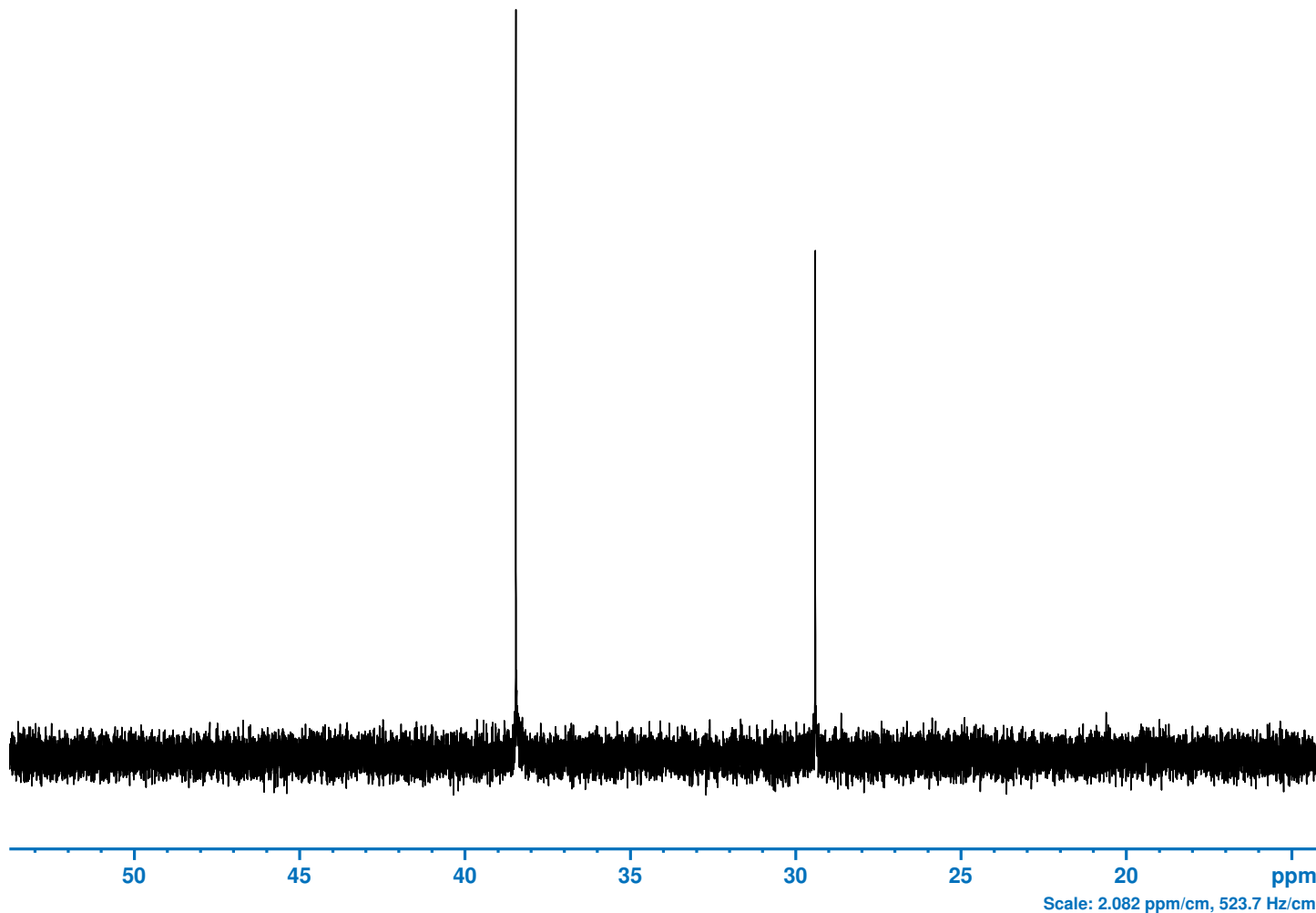
Bruker BioSpin

NPT_13C_MAS_sino_13c

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

F2 - Acquisition Parameters
Date_     20201221
Time      12.02 h
INSTRUM   Avance Neo 1GHz
PROBHD    H144137_0002 (
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        303.0 K
D1        15.00000000 sec
P15       0 usec
ZGPTNS    -D1acq
SFO1      251.5593320 MHz
NUC1      13C
P1        2.50 usec
PLW1      38.72999954 W
SFO2      1000.4024610 MHz
NUC2      1H
CPDPRG2   cw
PLW2      49.34000015 W
PLW12     0.12833340 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
 Sample: Adamantane (3.0 ul) (Z151271)
 13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 30000 Hz)



Bruker BioSpin

NPT_13C_MAS_sino_13c

```
# Mon Dec 21 12:02:15 2020
$$$PROBEIDENTIFIER=H144137_0002
$$$PROBENAME=PH MAS DVT1000S6 BL1.3 X/H NO_I/E
$$$SHIMID=292722
#
# Active Shim Gradients
#
Z -53000
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 2844.085
LOCKPHASE 180.000
LOCKPOWER -8.000
LOCKGAIN 129.629
```

```
LOCKDC -75.000
LOCKSHIFT 4.700
LOOPGAIN -9.400
LOOPTIME 0.464
LOOPFILTER 50.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1] -25705.00000000
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] -25757.40800000
SHIM_SETTING [ 4] -0.00000000
SHIM_SETTING [ 5] -9278.06300000
SHIM_SETTING [ 6] 9278.06300000
SHIM_SETTING [ 7] 25757.40800000
SHIM_SETTING [ 8] -25757.40800000
SHIM_SETTING [ 9] -1403.43200000
SHIM_SETTING [10] 1403.43200000
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_ 20201221
Time 12.02 h
INSTRUM Avance Neo 1GHz
PROBHD H144137_0002 (
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 303.0 K
D1 15.00000000 sec
P15 0 usec
ZGPTNS -D1acq
SFO1 251.5593328 MHz
NUC1 13C
P1 2.50 usec
PLW1 38.72999954 W
SFO2 1000.4024610 MHz
NUC2 1H
CPDPRG2 cw
PLW2 49.34000015 W
PLW12 0.12833340 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: Adamantane (3.0 ul) (Z151271)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 30000 Hz)

SINO (20.0 ppm) [achieved]: Signal (2.38 ppm), Noise (-4.09 to -24.09 ppm) [6368.3] <n/a>
Linewidth [achieved]: at 50% of signal height [244.1 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>



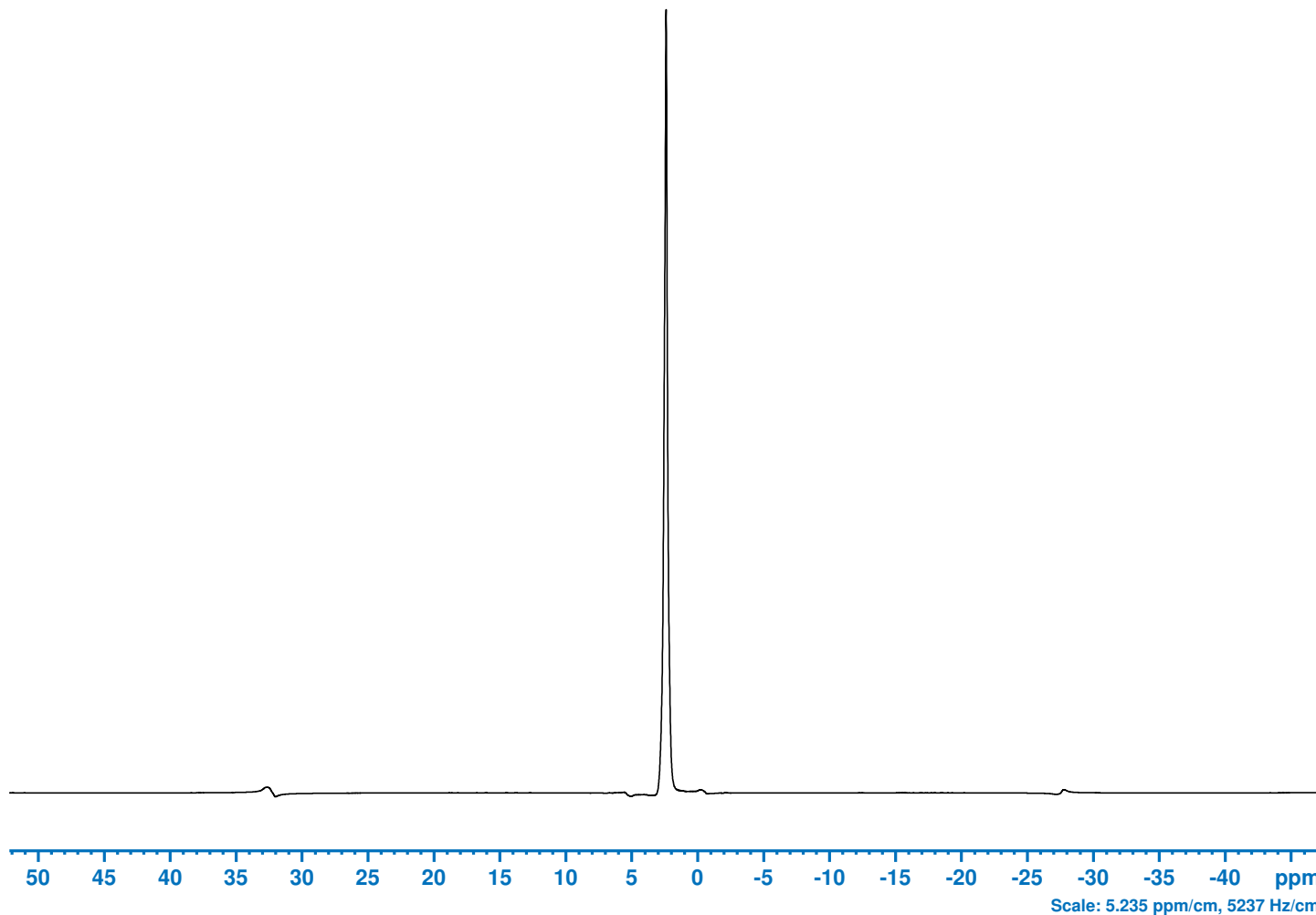
Bruker BioSpin

NPT_1H_MAS_sino_1h

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

F2 - Acquisition Parameters
Date_     20201221
Time      12.01 h
INSTRUM   Avance Neo 1GHz
PROBHD    H144137_0002 (
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         303.0 K
D1         5.00000000 sec
SFO1       1000.4024610 MHz
NUC1       1H
P1         1.70 usec
PLW1       49.34000015 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)
CP 1H-13C parameter optimization, MAS (NPT_13C_MAS_paropt_cp1h_13c, spin rate 10000 Hz)

SINO (20.0 ppm): Signal (43.57 ppm), Noise (208.18 to 188.18 ppm) [2173.2]
Processed with TDef=2048



Bruker BioSpin

NPT_13C_MAS_paropt_cp1h_13c

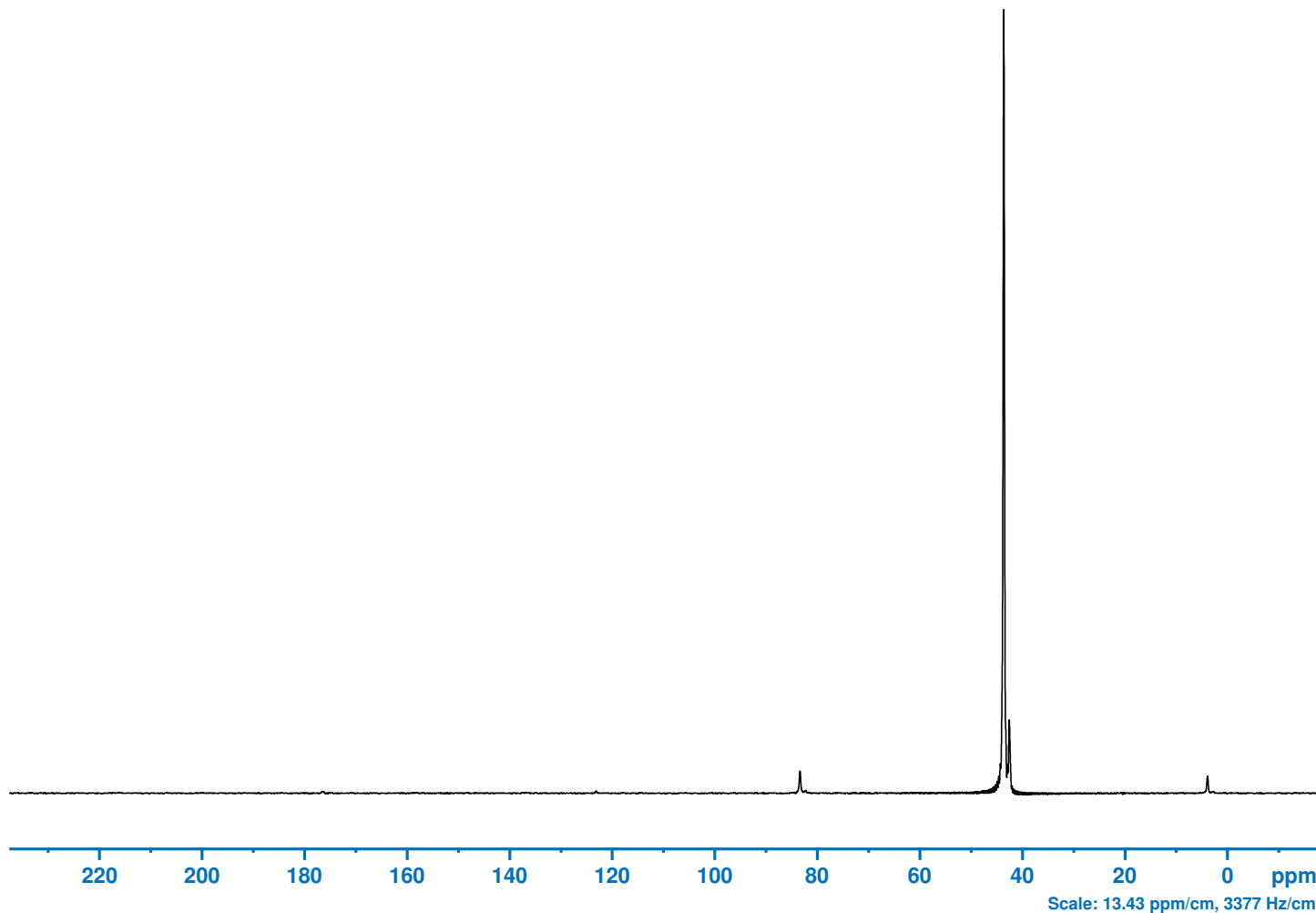
Current Data Parameters
NAME NPT_13C_MAS_paropt_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201221
Time 12.22 h
INSTRUM Avance Neo 1GHz
PROBHD H144137_0002 (cp)
PULPROG cp
TD 7462
SOLVENT H2O+D2O
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 303.0 K
D1 5.0000000 sec
ZGPTNS
SF01 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 26.00699997 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 1.70 usec
PCPD2 3.20 usec
PLW2 49.34000015 W
PLW12 59.20000076 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 38.88000107 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: H144137_0002 PH MAS DVT1000S6 BL1.3 X/H NO_I/E
Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)
CP 1H-15N parameter optimization, MAS (NPT_15N_MAS_paropt_cp1h_15n, spin rate 10000 Hz)

SINO (20.0 ppm): Signal (33.37 ppm), Noise (-6.08 to -26.08 ppm) [747.6]



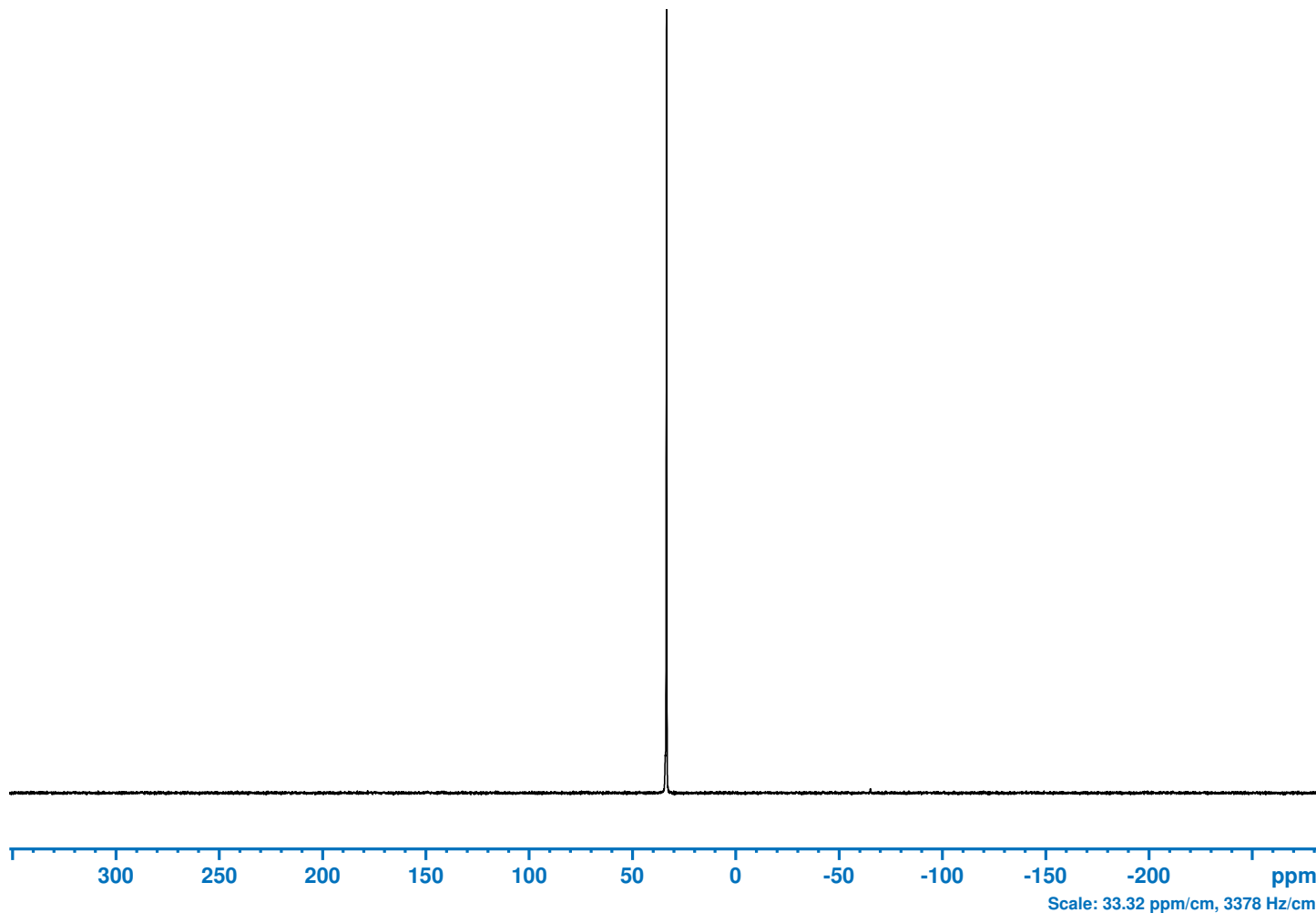
Bruker BioSpin

NPT_15N_MAS_paropt_cp1h_15n

```
Current Data Parameters
NAME      NPT_15N_MAS_paropt_cp1h_15n
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201221
Time      12.44 h
INSTRUM   Avance Neo 1GHz
PROBHD    H144137_0002 (
PULPROG   cp
TD         7462
SOLVENT   H2O+D2O
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         303.0 K
D1         5.0000000 sec
ZGPGTNS
SF01      101.3731996 MHz
NUC1       15N
P15        3500.00 usec
PLW1       83.16999817 W
SFO2       1000.4062025 MHz
NUC2       1H
CNST21     1.0000000
CPDPRG[2]  spinal64
P3         1.70 usec
PCPD2      3.20 usec
PLW2       49.34000015 W
PLW12      41.47000122 W
SPNAM[0]   ramp50100.100
SPOAL0     0.500
SPOFFS0    0 Hz
SPW0       18.78000069 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
