

NMR Test Spectrometer

Report Name: 1.9mm_TriG_Install

AV NEO (1000 MHz) 408457

Content:

- Configuration Information ([uxnmr.info](#))
- IP Config Information
- Probe: H171375_0001 / 1.9mm_TriG_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 TRANSCIEVER 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 TRANSCIEVER 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 TRANSCIEVER 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 TRANSCIEVER 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 TRANSCIEVER 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 = BOS33-SB
- SGB channels = 40
- Shim matrix file: 292722dd.dat
- Active shims: Z Z2 Z3 Z4 Z5 X XZ X2 (X2-Y2) XY Y ZY2 (X2-Y2)Z X24 X23 Z6 (X2-Y2)Z YZ4 YZ3 XY22 XYZ X32 X3
- Magnet polarity: SN (Bruker), uses standard H0 polarity
- L-TRX = BSMS/2 LOCK TRANSCIEVER 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 TRANSCIEVER 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 17764746 bytes 5231757722 (4.8 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 21882250 bytes 3888676409 (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 1044031 bytes 193502115 (184.5 MiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 511458 bytes 93529192 (89.1 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 30144640 bytes 5097654991 (4.7 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 30144640 bytes 5097654991 (4.7 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
```

PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E

1000 MHz

Probe ID: H171375_0001

Inspection Lot: 1.9mm_TriG_Install

● Probe NMR Test Data: PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E

Probe Related Information

EC-Level _____ 0
 Gas Compensation _____ nitrogen
 Gradient System _____ unknown
 ATM Accessory _____ false
 Temperature Sensor Type _____ unknown
 Proton Frequency [MHz] _____ 1000
 Diameter [mm] _____ 1.9

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

H171375_0001.ph

```
H171375_0001.ph
=====
$Bis,1,20200124,2048,PICS,5#
$Production,H171375,0001,0.00,0,BDE,20200107#
$Name,PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E#
$ProbeCompatibility,1.0,SB,6,1000#
$ProbeType,1.0,MAS#
$ProbeSample,1.0,1.9,#
$ProbeTemperature,1.0,Type_T,-50,80#
$HeatTemp,1.0,Type_K,-270,600#
$GasFlow,1.0,,,600,,,#
$ProbeAllCoils,1.1,1,1,1#
$ProbeCoil,1.0,1,,3,BB,BB,1H#
$ProbeChannel,1.0,1H,,,120,,,FALSE#
$ProbeMas,1.0,8000,42000,0,1,0,0,0,0,0#
$ProbeBB,1.0,3,31P-15N,,,#
$ProbeBBSets,1.0,31P,,120,,,#
$ProbeBBSets,1.0,13C,,120,,,#
$ProbeBBSets,1.0,79Br,,120,,,#
$ProbeBBSets,1.0,15N,,280,,,#
$EndBis,69,AD#
```

● **Required Samples** PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E

Z151260	Potassium Bromide (KBr, 13.1 ul)
Z151261	Adamantane (13.1 ul)
Z151262	Alpha-glycine (10 mg, 13.1 ul)
Z151263	2-13C, 15N alpha-glycine (10 mg, 13.1 ul)
Z151264	Ammonium Dihydrogenphosphate (13.1 ul)

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: Potassium Bromide (KBr, 13.1 ul) (Z151260)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 8000 Hz)

Line width main [achieved]: [181] <n/a>



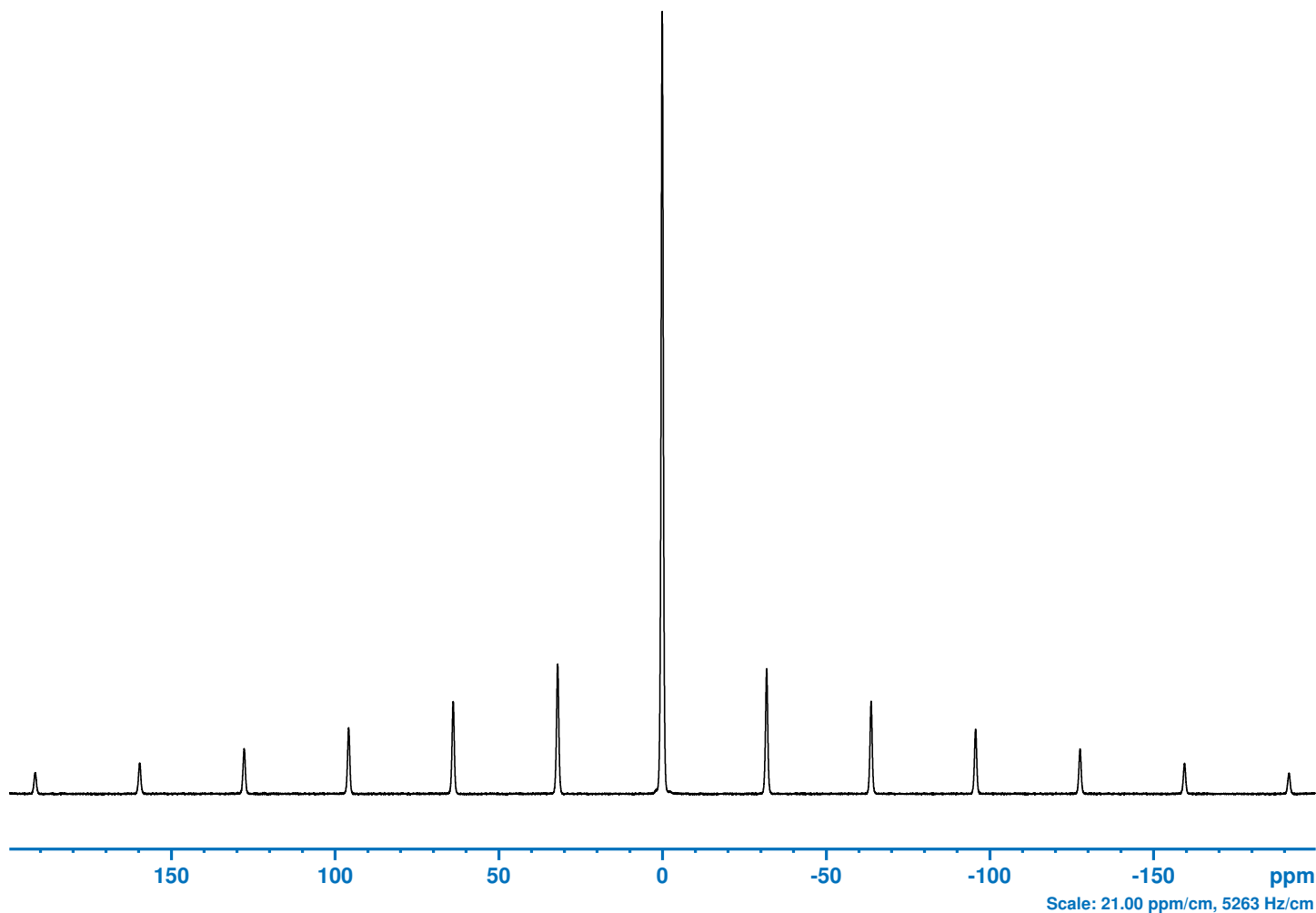
Bruker BioSpin

NPT_79Br_MAS_magicAngle

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

F2 - Acquisition Parameters
Date_     20201202
Time      10.57 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171375_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         308.0 K
D1         0.25000000 sec
SFO1      250.6547463 MHz
NUC1       79Br
P1         5.00 usec
PLW1       81.45999908 W

F2 - Processing parameters
SI         131072
SF         250.6547463 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: Potassium Bromide (KBr, 13.1 ul) (Z151260)
Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 42000 Hz)
Determination of spinning stability for 180 s
Pressure values in mbar: DrivePressure=3851/BearingPressure=3156/BearingSensePressure=3078/SupplyPressure=7034/SystemPressure=7236

Spin rate at maximum deviation [measured]: @ MASR 42000 Hz [42008 Hz]
Maximum deviation [achieved/rated]: @ MASR 42000 Hz [8 Hz <= 42 Hz] <pass>



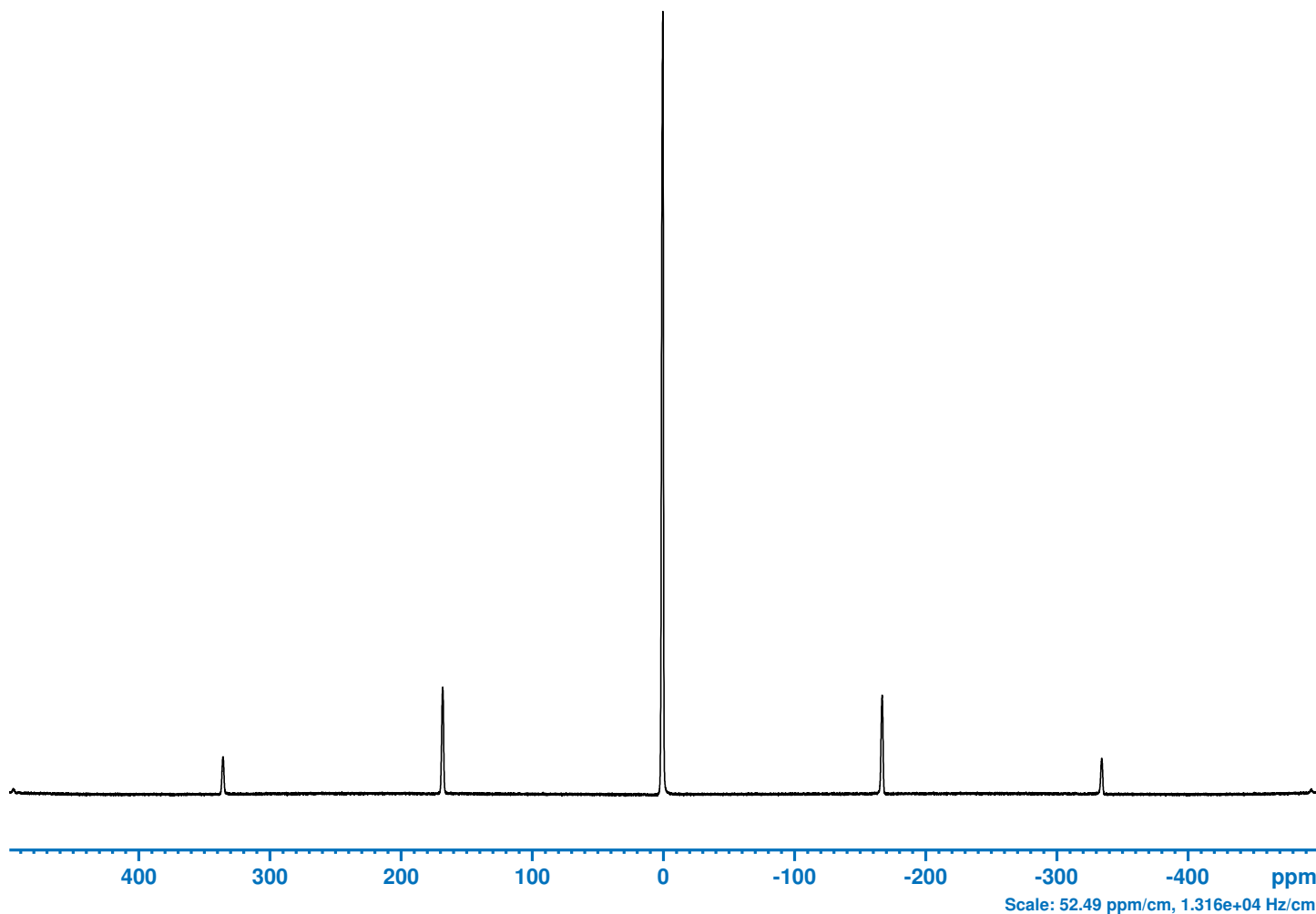
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

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

F2 - Acquisition Parameters
Date_     20201202
Time      11.12 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171375_0001 (
PULPROG   onepulse
TD        16384
SOLVENT   CDCl3
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        308.0 K
D1        0.2500000 sec
SFO1      250.6547505 MHz
NUC1      79Br
P1        5.00 usec
PLW1      81.45999908 W

F2 - Processing parameters
SI        32768
SF        250.6547505 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: Potassium Bromide (KBr, 13.1 ul) (Z151260)
Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting, spin rate 8000 Hz)
FIELD was set to 2064.4 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0069 ppm.



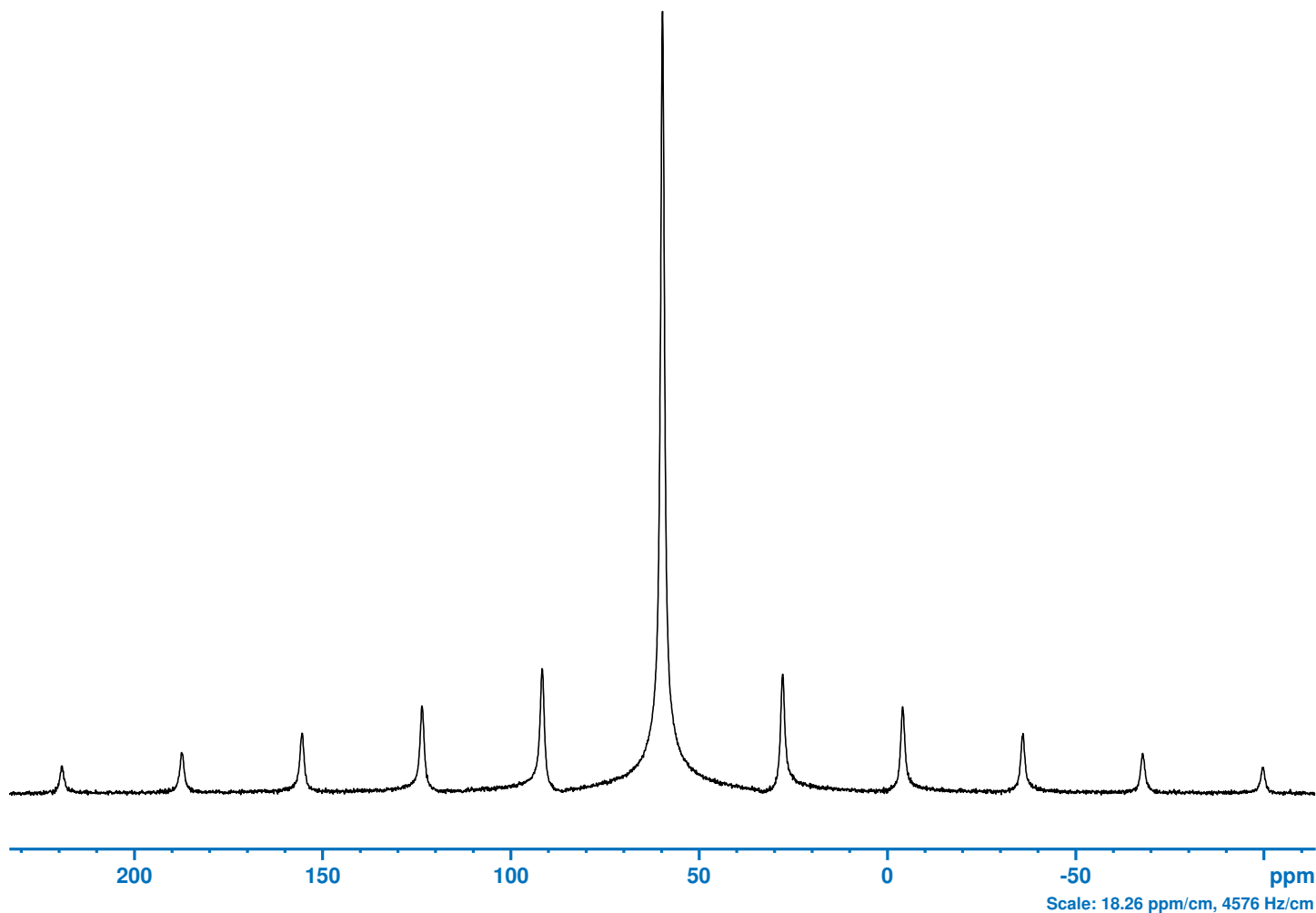
Bruker BioSpin

NPT_79Br_MAS_fieldsetting

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

F2 - Acquisition Parameters
Date_     20201202
Time      10.57 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171375_0001 (
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         308.0 K
D1         0.5000000 sec
SFO1      250.6549791 MHz
NUC1       79Br
P1         5.00 usec
PLW1      81.45999908 W

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



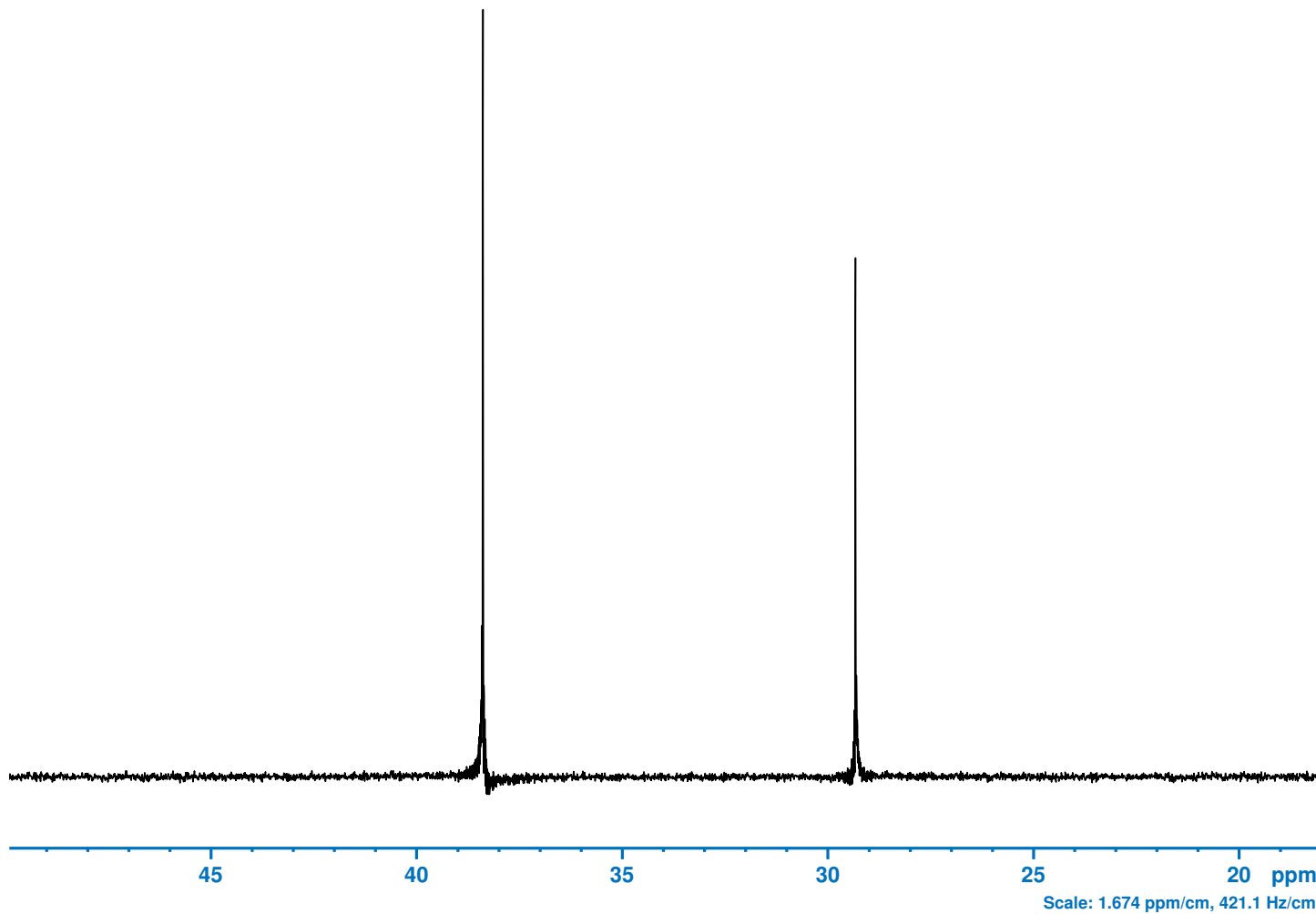
SHIM SEQUENCE
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: Adamantane (13.1 ul) (Z151261)
 Optimization of 13C frequency (NPT_13C_MAS_fieldsetting_dec1h, spin rate 10000 Hz)
 FIELD was set to 2001.0 for 13C chemical shift of 38.460 ppm. One field unit corresponds to 0.0073 ppm.



Bruker BioSpin

NPT_13C_MAS_fieldsetting_dec1h



```

Current Data Parameters
NAME      NPT_13C_MAS_fieldsetting_dec1h
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20201202
Time      12.49 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171375_0001 (
PULPROG   hpdec
TD         4000
SOLVENT   CDC13
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         308.0 K
D1         15.0000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1      251.5593320 MHz
NUC1       13C
P1         5.00 usec
PLW1       74.00499725 W
SFO2      1000.4023186 MHz
NUC2       1H
CPDPRG[2]  cw
PLW2       99.00299835 W
PLW12      0.03960120 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
-----
  
```

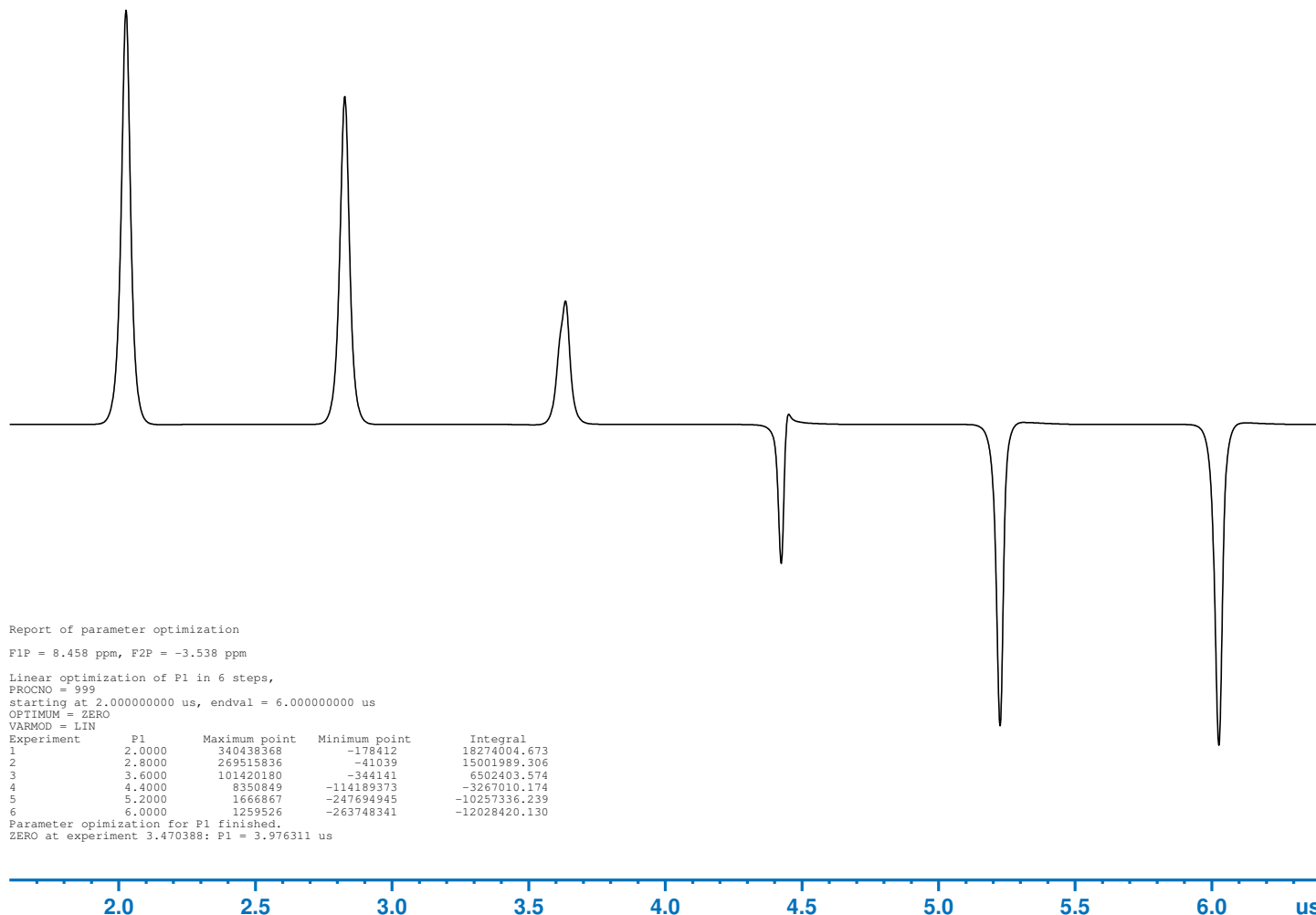
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: Adamantane (13.1 ul) (Z151261)
 P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 12000 Hz)
 ATTENTION: Updated PROSOL Tables with [2.00 us @ 99.0 W].

P90 MAS 1H pulse [achieved/rated]: @ 100 W [1.99 us <= 2.00 us] <pass>



Bruker BioSpin

NPT_1H_MAS_p90det_1h



```
Current Data Parameters
NAME      NPT_1H_MAS_p90det_1h
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201202
Time      12.23 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171375_0001 (
PULPROG   onepulse
TD        2988
SOLVENT   CDC13
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        308.0 K
D1        5.00000000 sec
SFO1      1000.4024610 MHz
NUC1      1H
P1        6.00 usec
PLW1      100.00000000 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
-----
100 W    2.00 us    1.99 us    -0.5%
```

Report of parameter optimization

F1P = 8.458 ppm, F2P = -3.538 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	340438368	-178412	18274004.673
2	2.8000	269515836	-41039	15001989.306
3	3.6000	101420180	-344141	6502403.574
4	4.4000	8350849	-114189373	-3267010.174
5	5.2000	1666867	-247694945	-10257336.239
6	6.0000	1259526	-263748341	-12028420.130

Parameter optimization for P1 finished.

ZERO at experiment 3.470388: P1 = 3.976311 us

 SHIM SEQUENCE

skip shimming

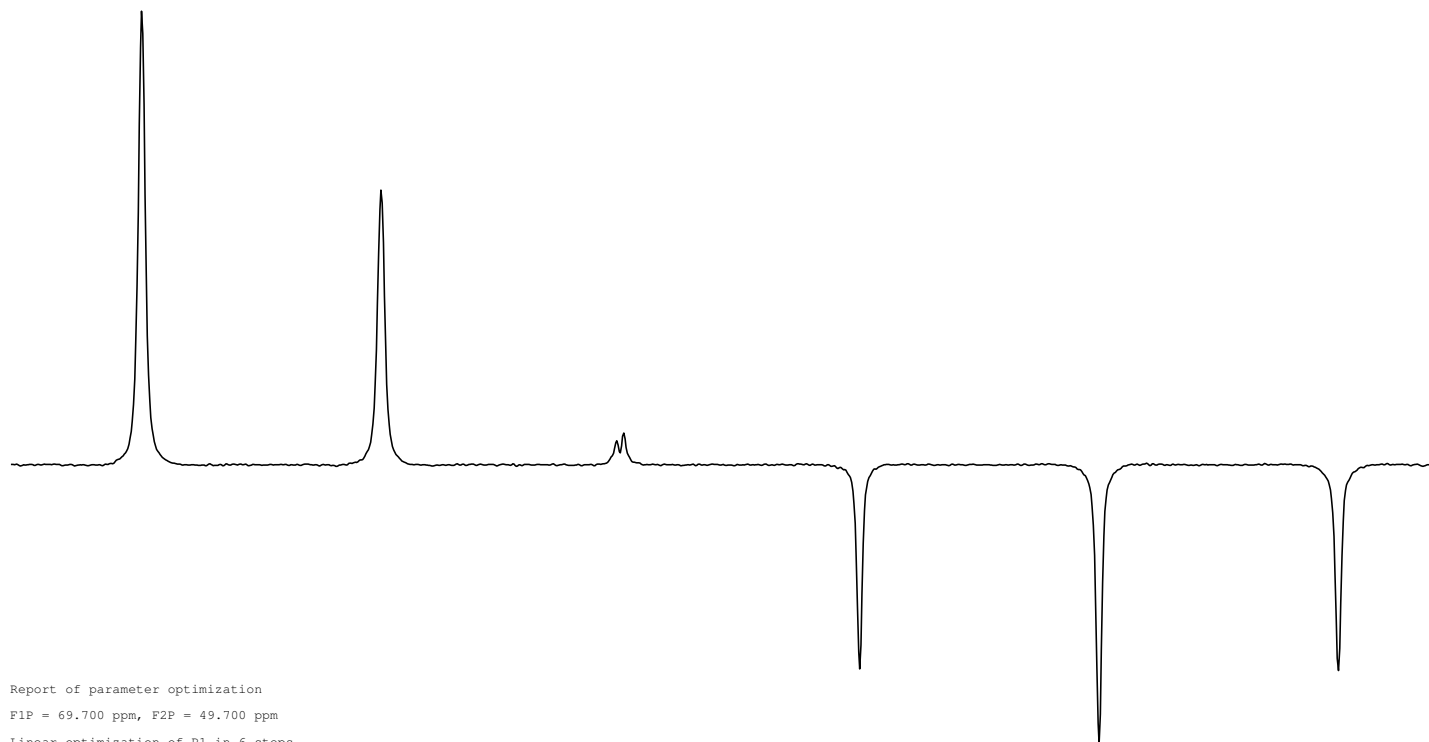
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: Potassium Bromide (KBr, 13.1 ul) (Z151260)
 P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br, spin rate 8000 Hz)
 ATTENTION: Updated PROSOL Tables with [5.00 us @ 81.5 W].

P90 MAS 79Br pulse [achieved/rated]: @ 95.0 W [4.63 us <= 5.00 us] <pass>



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 5.000000000 us, endval = 15.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	5.0000	293719658	-807664	12279597.034
2	7.0000	177903970	-975230	7666884.773
3	9.0000	20489028	-1017462	1022102.087
4	11.0000	764324	-132179016	-4417797.512
5	13.0000	1007742	-180607515	-6497748.024
6	15.0000	830128	-133163446	-5102952.242

Parameter optimization for P1 finished.

ZERO at experiment 3.134206: P1 = 9.268413 us

Current Data Parameters
 NAME NPT_79Br_MAS_p90det_79br
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20201202
 Time 10.53 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171375_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 308.0 K
 D1 0.25000000 sec
 SFO1 250.6549791 MHz
 NUC1 79Br
 P1 15.00 usec
 PLW1 95.00000000 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
95.0 W	5.00 us		
95.0 W	5.00 us	4.63 us	-7.4%

 SHIM SEQUENCE

 skip shimming



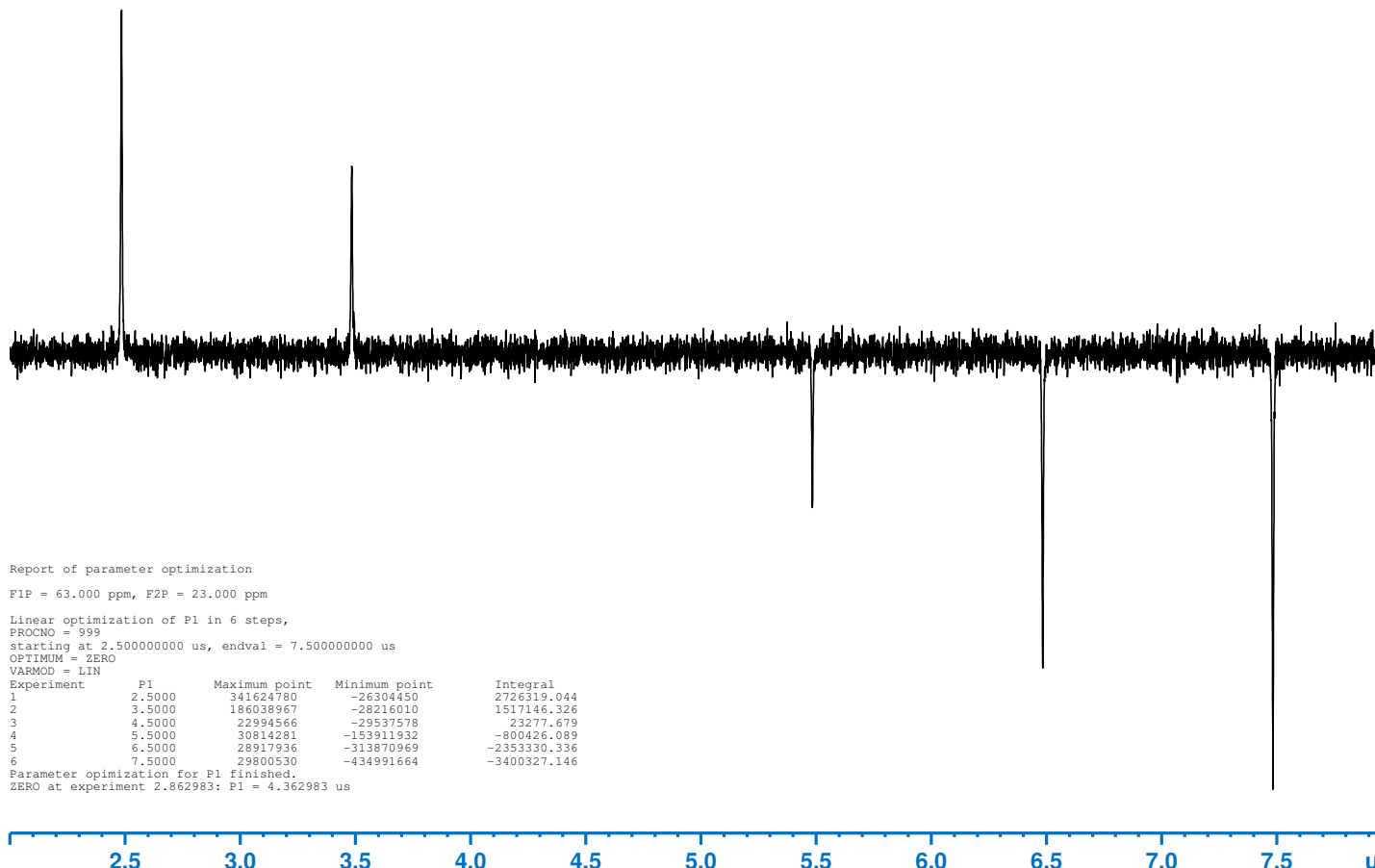
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: 2-13C, 15N alpha-glycine (10 mg, 13.1 ul) (Z151263)
 P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [5.00 us @ 56.3 W].



Bruker BioSpin

P90_MAS_CP 1H13C power (PLW 11) [achieved]: [74.0 W] <n/a>
 P90_MAS_CP 1H13C pulse (P 1) [achieved/rated]: [4.36 us <= 5.00 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_ 20201202
 Time 14.15 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171375_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 308.0 K
 D1 5.00000000 sec
 ZGPGTNS
 SFO1 251.5615968 MHz
 NUC1 13C
 P1 7.50 usec
 P15 2000.00 usec
 PLW1 74.00499725 W
 PLW11 74.00499725 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 2.00 usec
 PCPD2 3.80 usec
 PLW2 99.00299835 W
 PLW12 99.00299835 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 55.19527054 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

 74.0 W 5.00 us
 74.0 W 5.00 us 4.36 us -12.8%

Report of parameter optimization

F1P = 63.000 ppm, F2P = 23.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 2.500000000 us, endval = 7.500000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.5000	341624780	-26304450	2726319.044
2	3.5000	186038967	-28216010	1517146.326
3	4.5000	22994566	-29537578	23277.679
4	5.5000	30814281	-153911932	-800426.089
5	6.5000	28917936	-313870969	-2353330.336
6	7.5000	29800530	-434991664	-3400327.146

Parameter optimization for P1 finished.

ZERO at experiment 2.862983: P1 = 4.362983 us

 SHIM SEQUENCE

 skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: Adamantane (13.1 ul) (Z151261)
 P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c, spin rate 12000 Hz)
 ATTENTION: Updated PROSOL Tables with [5.00 us @ 74.0 W].



Bruker BioSpin

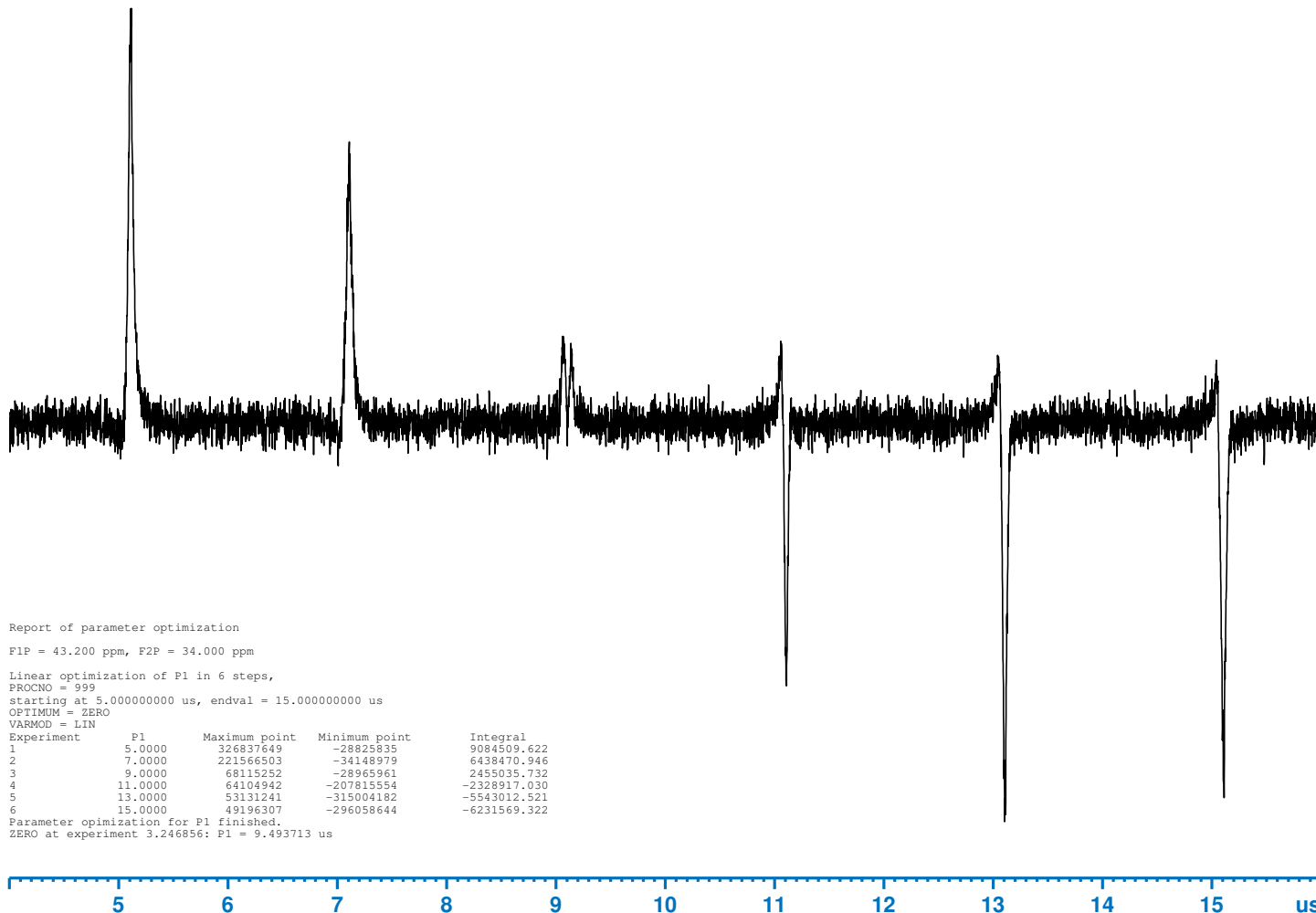
P90 MAS 13C pulse [achieved/rated]: @ 82.0 W [4.75 us <= 5.00 us] <pass>

NPT_13C_MAS_p90det_13c

```
Current Data Parameters
NAME      NPT_13C_MAS_p90det_13c
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201202
Time      12.32 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171375_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         308.0 K
D1         15.00000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1      251.5593328 MHz
NUC1       13C
P1         15.00 usec
PLW1       82.00000000 W
SFO2       1000.4024610 MHz
NUC2        1H
CPDPRG[2]  cw
PLW2       99.00299835 W
PLW12      0.05702572 W

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



Report of parameter optimization

F1P = 43.200 ppm, F2P = 34.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 5.000000000 us, endval = 15.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	5.0000	326837649	-28825835	9084509.622
2	7.0000	221566503	-34148979	6438470.946
3	9.0000	68115252	-28965961	2455035.732
4	11.0000	64104942	-207815554	-2328917.030
5	13.0000	53131241	-315004182	-5543012.521
6	15.0000	49196307	-296058644	-6231569.322

Parameter optimization for P1 finished.

ZERO at experiment 3.246856: P1 = 9.493713 us

```
***** P90 Pulse Determination History *****
PLW90   P90   P90[det]   Deviation
-----
82.0 W   5.00 us
82.0 W   5.00 us   4.75 us   -5.0%
```

 SHIM SEQUENCE

skip shimming

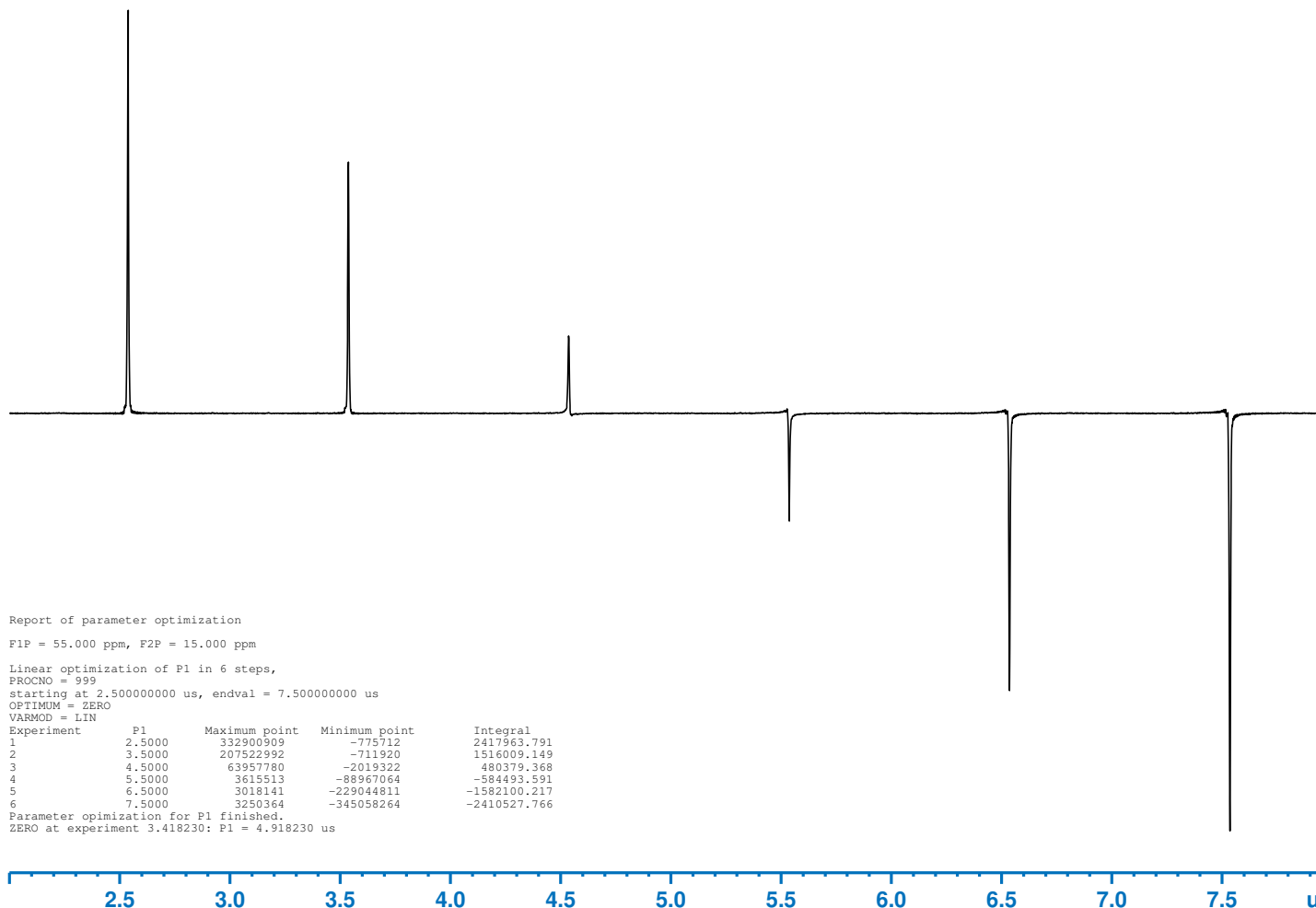
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: 2-13C, 15N alpha-glycine (10 mg, 13.1 ul) (Z151263)
 P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [5.00 us @ 271 W].



Bruker BioSpin

P90_MAS_CP 1H15N power (PLW 11) [achieved]: [280.0 W] <n/a>
 P90_MAS_CP 1H15N pulse (P 1) [achieved/rated]: [4.92 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_ 20201202
 Time 14.33 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171375_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 308.0 K
 D1 5.00000000 sec
 ZGPTNS
 SF01 101.3731996 MHz
 NUC1 15N
 P1 7.50 usec
 P15 3500.00 usec
 PLW1 280.0000000 W
 PLW11 280.0000000 W
 SF02 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 2.00 usec
 PCPD2 3.80 usec
 PLW2 99.00299835 W
 PLW12 99.00299835 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 40.55162811 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

 280 W 5.00 us
 280 W 5.00 us 4.92 us -1.6%

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	332900909	-775712	2417963.791
2	3.5000	207522992	-711920	1516009.149
3	4.5000	63957780	-2019322	480379.368
4	5.5000	3615513	-88967064	-584493.591
5	6.5000	3018141	-229044811	-1582100.217
6	7.5000	3250364	-345058264	-2410527.766

Parameter optimization for P1 finished.

ZERO at experiment 3.418230: P1 = 4.918230 us

 SHIM SEQUENCE

 skip shimming

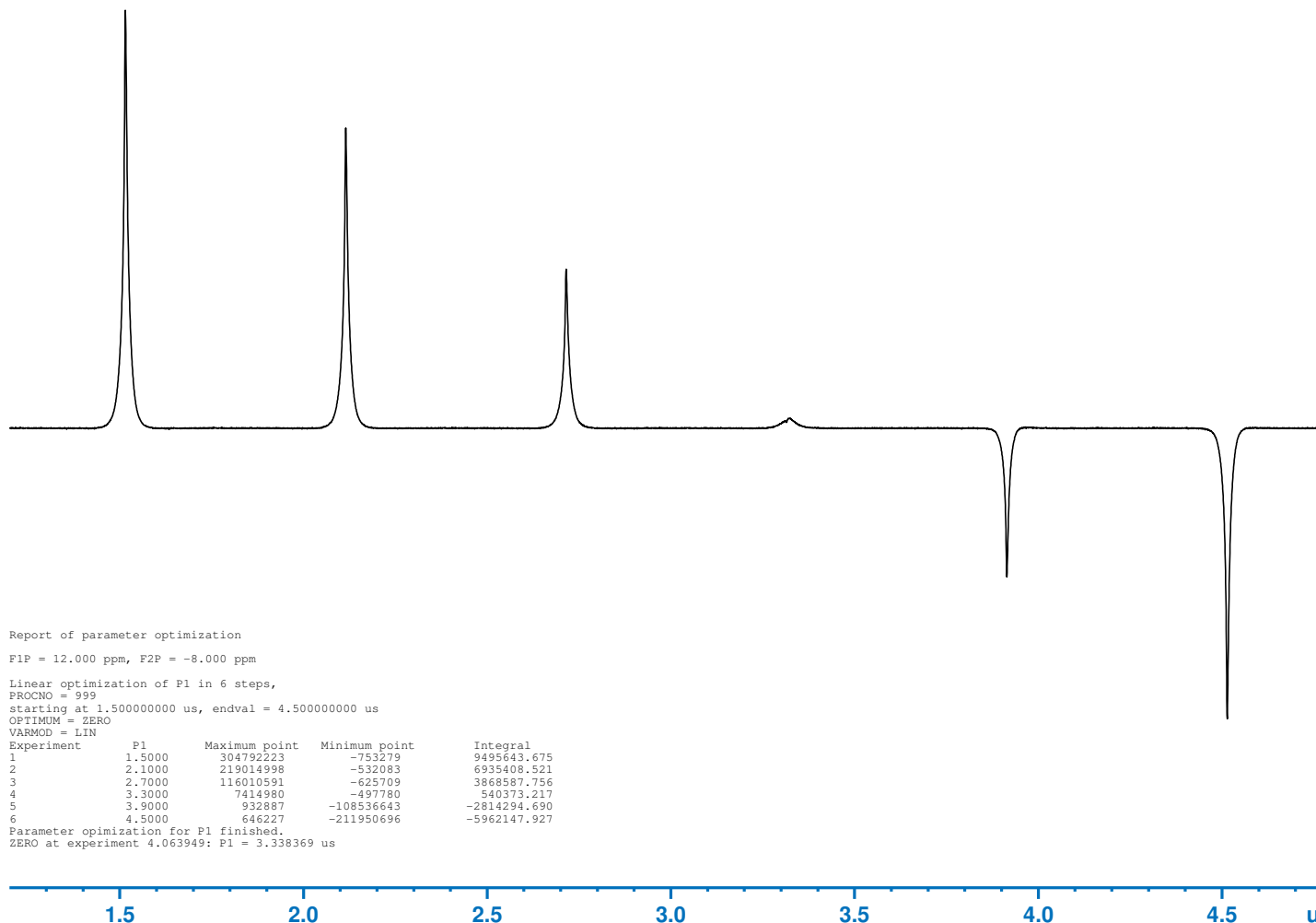
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: Ammonium Dihydrogenphosphate (13.1 ul) (Z151264)
 P90 31P 1H-31P CP pulse calibration, MAS (NPT_31P_MAS_p90det_cp1h_31p, spin rate 15000 Hz)
 ATTENTION: Update PROSOL Tables (31P) failed.



Bruker BioSpin

P90_MAS_CP 1H31P power (PLW 11) [achieved]: [119.4 W] <n/a>
 P90_MAS_CP 1H31P pulse (P 1) [achieved/rated]: [3.34 us <= 3.50 us] <pass>

NPT_31P_MAS_p90det_cp1h_31p



Current Data Parameters
 NAME NPT_31P_MAS_p90det_cp1h_31p
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20201203
 Time 11.51 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171375_0001 ()
 PULPROG cp90
 TD 11904
 SOLVENT CDCl3
 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 311.0 K
 D1 5.00000000 sec
 ZGPGTNS
 SFO1 404.9701529 MHz
 NUC1 31P
 P1 4.50 usec
 P15 3500.00 usec
 PLW1 100.0000000 W
 PLW11 119.40000153 W
 SFO2 1000.4072029 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 2.00 usec
 PCPD2 3.80 usec
 PLW2 99.00299835 W
 PLW12 99.00299835 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 108.91989899 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
100 W	3.00 us		
100 W	3.00 us	3.61 us	20.3%
119 W	3.00 us	3.34 us	11.3%

 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 1.500000000 us, endval = 4.500000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	1.5000	304792223	-753279	9495643.675
2	2.1000	219014998	-532083	6935408.521
3	2.7000	116010591	-625709	3868587.756
4	3.3000	7414980	-497780	540373.217
5	3.9000	932887	-108536643	-2814294.690
6	4.5000	646227	-211950696	-5962147.927

Parameter optimization for P1 finished.

ZERO at experiment 4.063949: P1 = 3.338369 us

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: Alpha-glycine (10 mg, 13.1 ul) (Z151262)
CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c, spin rate 10000 Hz)

SINO (20.0 ppm) [achieved/rated]: Signal (43.57 ppm), Noise (2.46 to -17.54 ppm) [157.5 >= 120.0] <pass>
Number of scans (NS) [achieved]: [64] <n/a>
Processed with TDef=2048



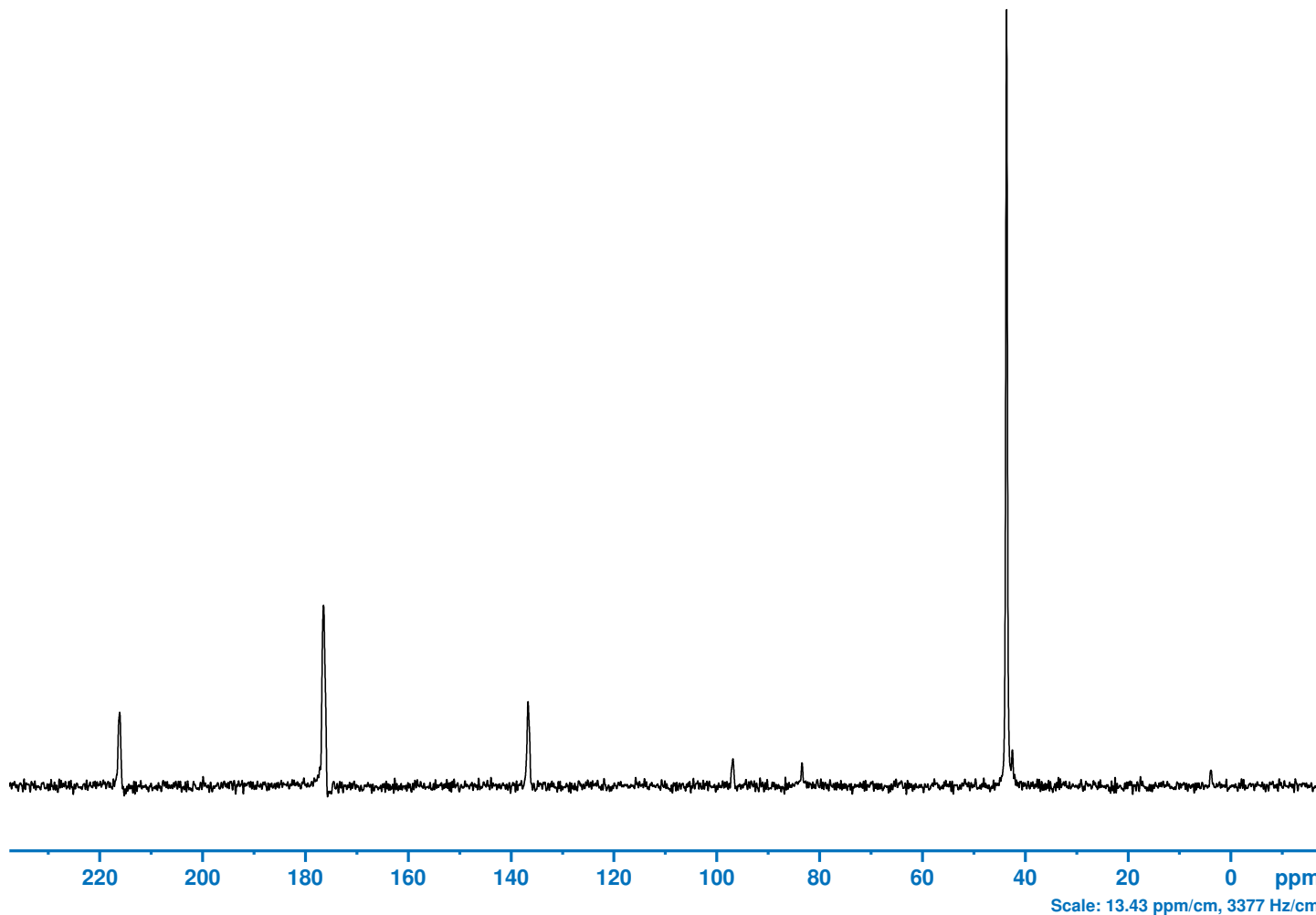
Bruker BioSpin

NPT_13C_MAS_sino_cp1h_13c

Current Data Parameters
NAME NPT_13C_MAS_sino_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201203
Time 10.07 h
INSTRUM Avance Neo 1GHz
PROBHD H171375_0001 (cp
PULPROG cp
TD 7462
SOLVENT CDC13
NS 64
DSH 0
SWH 74626.867 Hz
FIDRES 20.001841 Hz
AQ 0.0499954 sec
RG 101
DW 6.700 usec
DE 6.50 usec
TE 308.0 K
D1 5.0000000 sec
ZGPTNS
SFO1 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 56.27199936 W
SFO2 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.00 usec
PCPD2 3.80 usec
PLW2 99.00299835 W
PLW12 94.55999756 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 56.75000000 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: Alpha-glycine (10 mg, 13.1 ul) (Z151262)
CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n, spin rate 10000 Hz)

SINO (20.0 ppm) [achieved/rated]: Signal (33.42 ppm), Noise (-24.15 to -44.15 ppm) [19.6 >= 10.0] <pass>
Number of scans (NS) [achieved]: [64] <n/a>



Bruker BioSpin

NPT_15N_MAS_sino_cp1h_15n

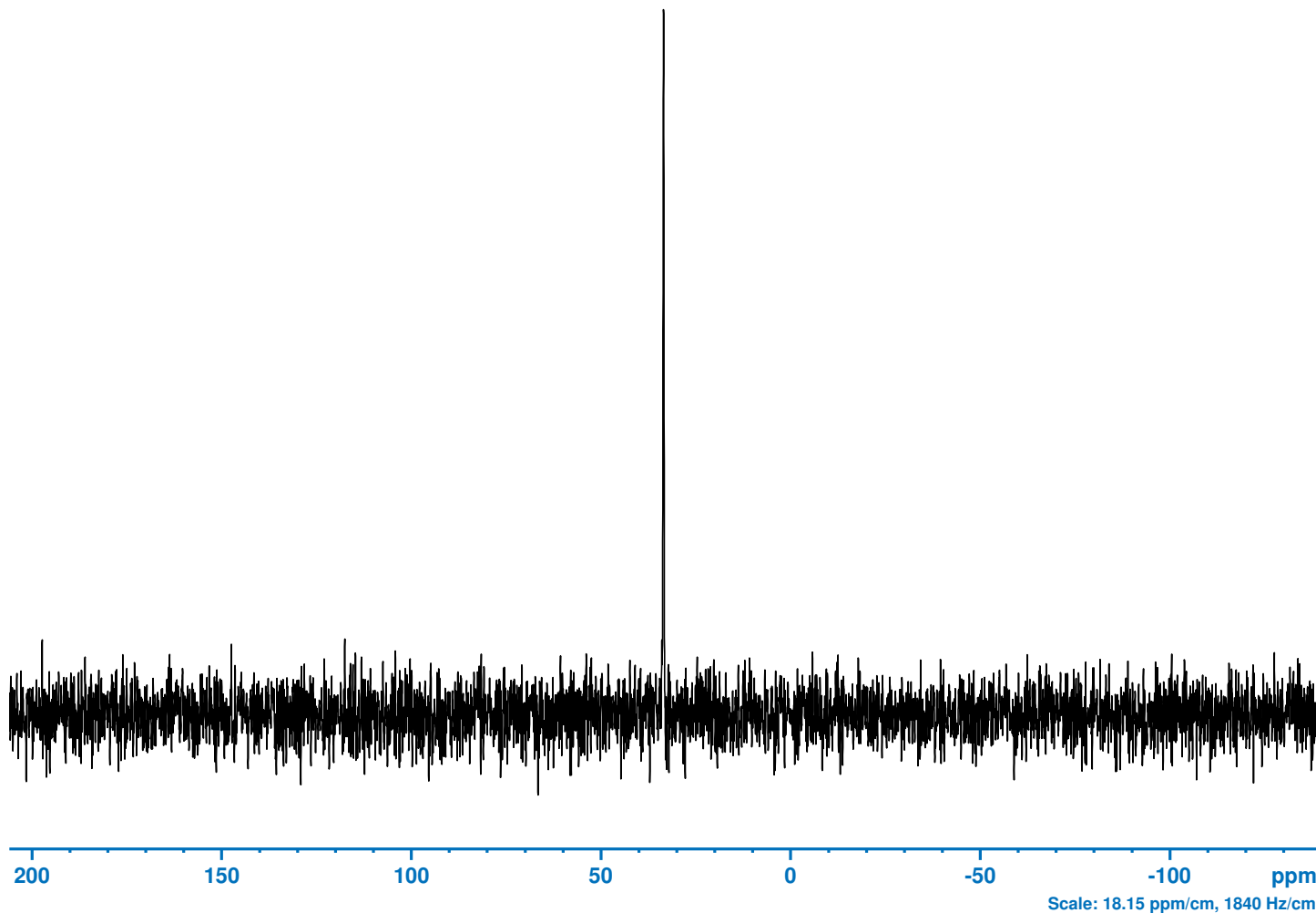
Current Data Parameters
NAME NPT_15N_MAS_sino_cp1h_15n
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201203
Time 10.45 h
INSTRUM Avance Neo 1GHz
PROBHD H171375_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 308.0 K
D1 5.0000000 sec
ZGPTNS
SF01 101.3730500 MHz
NUC1 15N
P15 3500.00 usec
PLW1 271.10998535 W
SF02 1000.4093580 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.00 usec
PCPD2 3.80 usec
PLW2 99.00299835 W
PLW12 83.04000092 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 44.59999847 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: Ammonium Dihydrogenphosphate (13.1 ul) (Z151264)
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 (-84.06 to -94.06 ppm) [2327.2] <n/a>
Number of scans (NS) [achieved]: [4] <n/a>



Bruker BioSpin

NPT_31P_MAS_sino_cp1h_31p

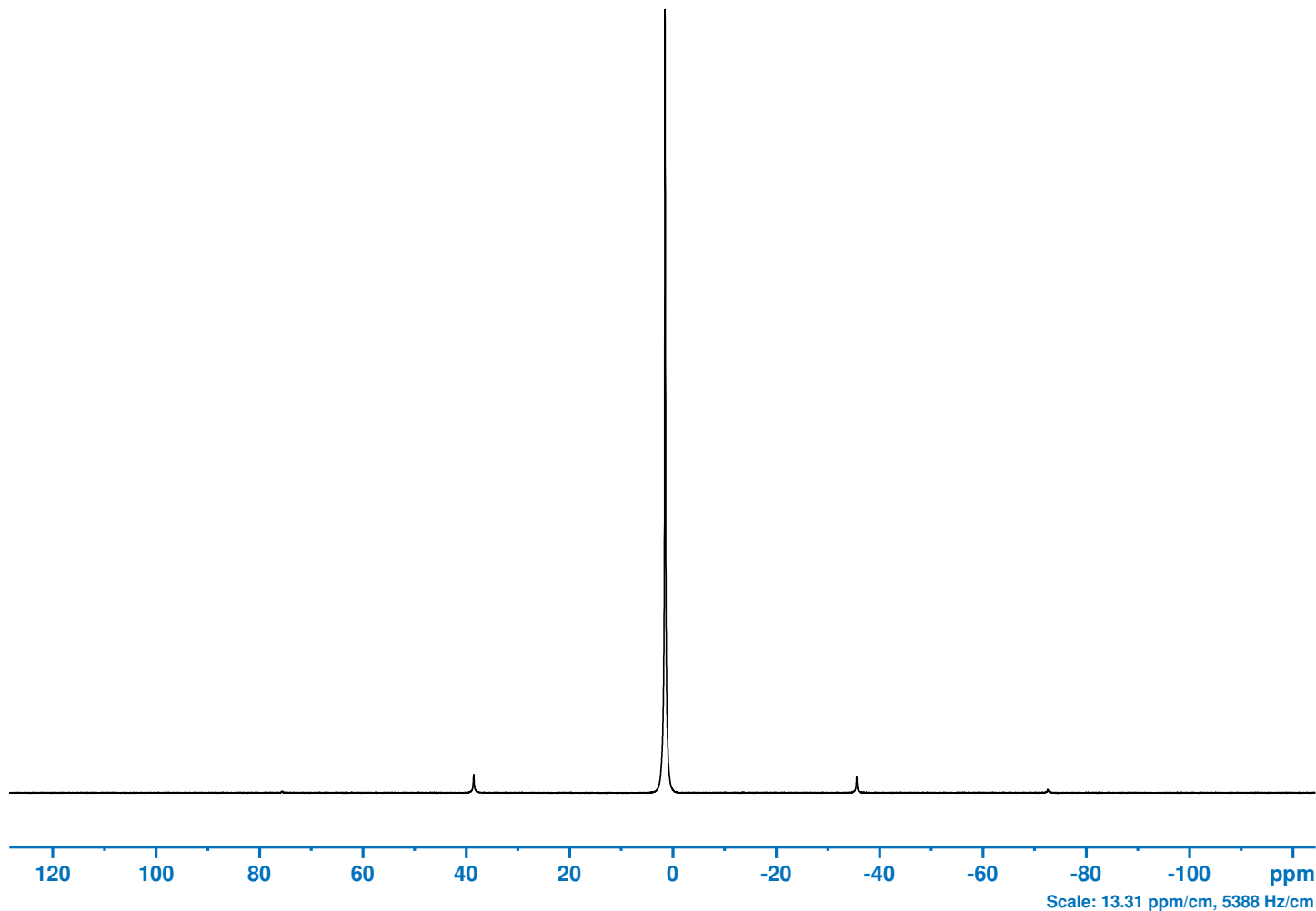
Current Data Parameters
NAME NPT_31P_MAS_sino_cp1h_31p
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201203
Time 12.02 h
INSTRUM Avance Neo 1GHz
PROBHD H171375_0001 (cp
PULPROG cp
TD 11904
SOLVENT CDC13
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 311.0 K
D1 5.0000000 sec
ZGPTNS
SF01 404.9701529 MHz
NUC1 31P
P15 3500.00 usec
PLW1 100.0000000 W
SF02 1000.4072029 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.00 usec
PCPD2 3.80 usec
PLW2 99.00299835 W
PLW12 117.59999847 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 117.59999847 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: Adamantane (13.1 ul) (Z151261)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 28000 Hz)

SINO (20.0 ppm) [achieved]: Signal (38.46 ppm), Noise (34.22 to 14.22 ppm) [24.6] <n/a>
Linewidth [achieved/rated]: at 50% of signal height [3.5 Hz <= 7.0 Hz] <pass>
Number of scans (NS) [achieved]: [1] <n/a>



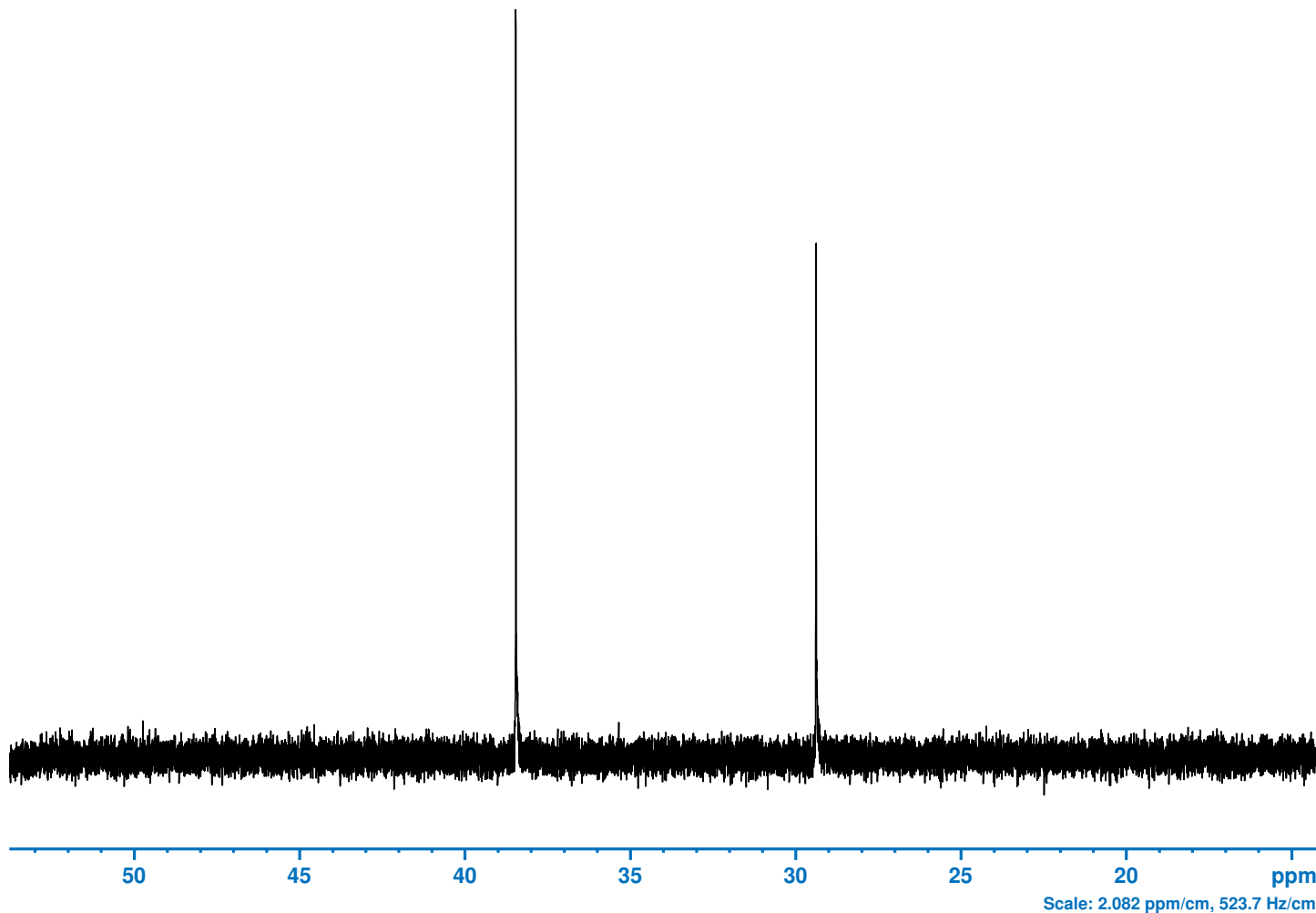
Bruker BioSpin

NPT_13C_MAS_sino_13c

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

F2 - Acquisition Parameters
Date_     20201202
Time      14.02 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171375_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         308.0 K
D1         15.00000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1      251.5593320 MHz
NUC1       13C
P1         5.00 usec
PLW1       74.00499725 W
SFO2      1000.4024610 MHz
NUC2       1H
CPDPRG[2]  cw
PLW2       99.00299835 W
PLW12      0.31047341 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: Adamantane (13.1 ul) (Z151261)
 13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 28000 Hz)



Bruker BioSpin

NPT_13C_MAS_sino_13c

```
# Wed Dec 2 14:02:25 2020
##$PROBEIDENTIFIER=H171375_0001
##$PROBENAME=PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
##$SHIMID=292722
#
# Active Shim Gradients
#
Z -39000
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 2001.037
LOCKPHASE 186.600
LOCKPOWER -17.000
LOCKGAIN 130.455
```

```
LOCKDC -75.000
LOCKSHIFT 7.240
LOOPGAIN -9.400
LOOPTIME 0.464
LOOPFILTER 50.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1] -18915.00000504
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] -18953.56432404
SHIM_SETTING [ 4] -0.00000000
SHIM_SETTING [ 5] -6827.25356706
SHIM_SETTING [ 6] 6827.25356706
SHIM_SETTING [ 7] 18953.56432404
SHIM_SETTING [ 8] -18953.56432404
SHIM_SETTING [ 9] -1032.71415246
SHIM_SETTING [10] 1032.71415246
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] -0.00000046
SHIM_SETTING [22] -0.00000046
SHIM_SETTING [23] -0.00000072
SHIM_SETTING [24] -0.00000072
SHIM_SETTING [25] -0.00000028
SHIM_SETTING [26] -0.00000028
SHIM_SETTING [27] -0.00000000
SHIM_SETTING [28] 0.00000472
SHIM_SETTING [29] 0.00000000
SHIM_SETTING [30] 0.00000000
SHIM_SETTING [31] 0.00000523
SHIM_SETTING [32] 0.00000472
SHIM_SETTING [33] 0.00000000
SHIM_SETTING [34] 0.00000000
SHIM_SETTING [35] 0.00000000
SHIM_SETTING [36] -0.00000000
SHIM_SETTING [37] 0.00000247
SHIM_SETTING [38] 0.00000247
SHIM_SETTING [39] 0.00000523
SHIM_SETTING [40] 0.00000000
```

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

F2 - Acquisition Parameters
Date_ 20201202
Time 14.02 h
INSTRUM Avance Neo 1GHz
PROBHD H171375_0001 (
PULPROG hpdec
TD 19998
SOLVENT CDC13
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 1.000100 Hz
AQ 0.9999000 sec
RG 401
DW 50.000 usec
DE 6.50 usec
TE 308.0 K
D1 15.00000000 sec
P15 0 usec
ZGPTNS -D1acq
SFO1 251.559328 MHz
NUC1 13C
P1 5.00 usec
PLW1 74.00499725 W
SFO2 1000.4024610 MHz
NUC2 1H
CPDPRG2 cw
PLW2 99.00299835 W
PLW12 0.31047341 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: Adamantane (13.1 ul) (Z151261)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 28000 Hz)

SINO (20.0 ppm) [achieved]: Signal (2.36 ppm), Noise (-4.09 to -24.09 ppm) [8586.8] <n/a>
Linewidth [achieved]: at 50% of signal height [236.8 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>



Bruker BioSpin

NPT_1H_MAS_sino_1h

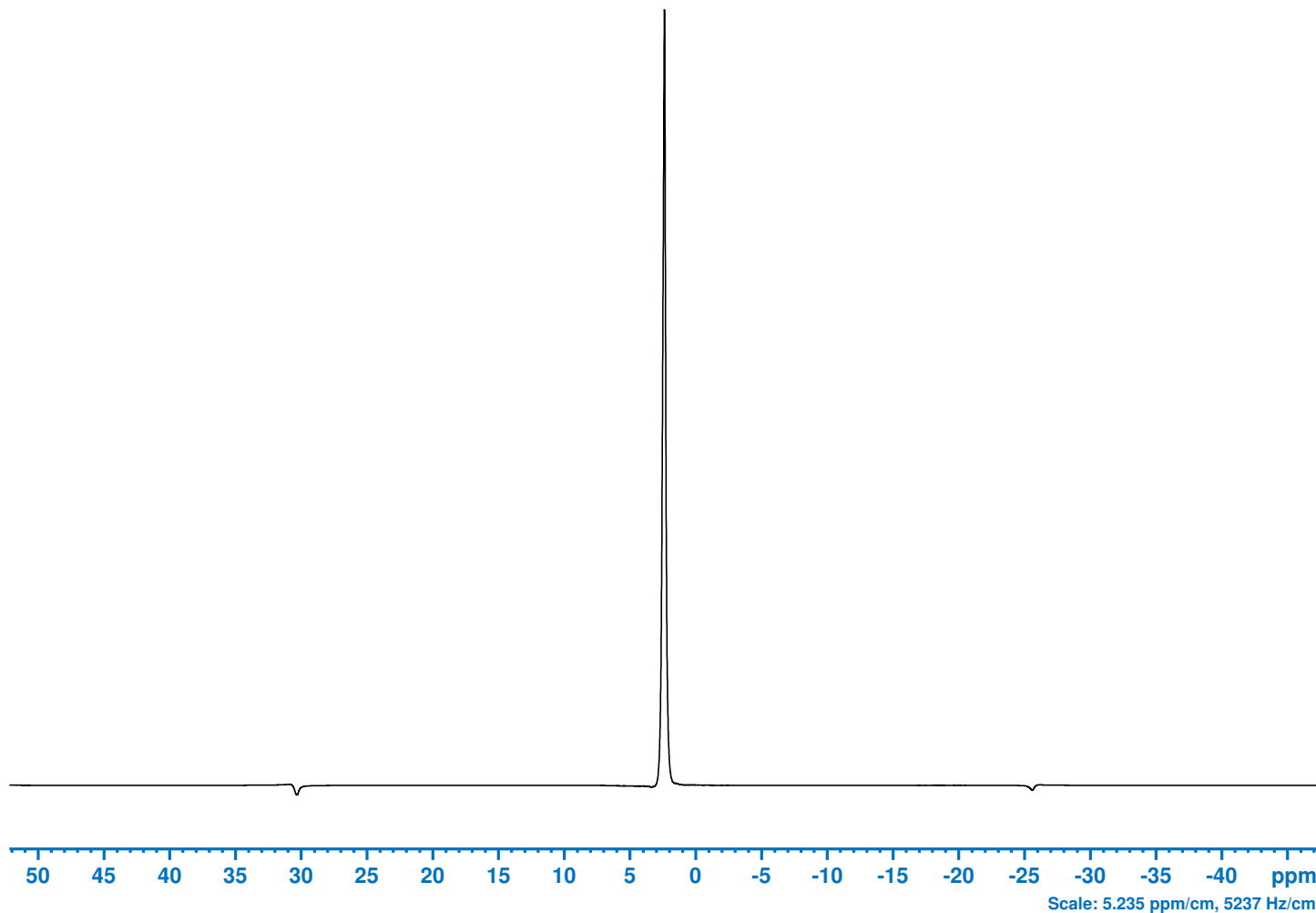
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Current Data Parameters
NAME      NPT_1H_MAS_sino_1h
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201202
Time      14.01 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171375_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          308.0 K
D1          5.00000000 sec
SFO1       1000.4024610 MHz
NUC1       1H
P1          2.00 usec
PLW1       99.00299835 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
 Sample: 2-13C, 15N alpha-glycine (10 mg, 13.1 ul) (Z151263)
 Double CP 1H-15N-13C, MAS (NPT_13C_MAS_double_cp1h15n_13c, spin rate 12000 Hz)



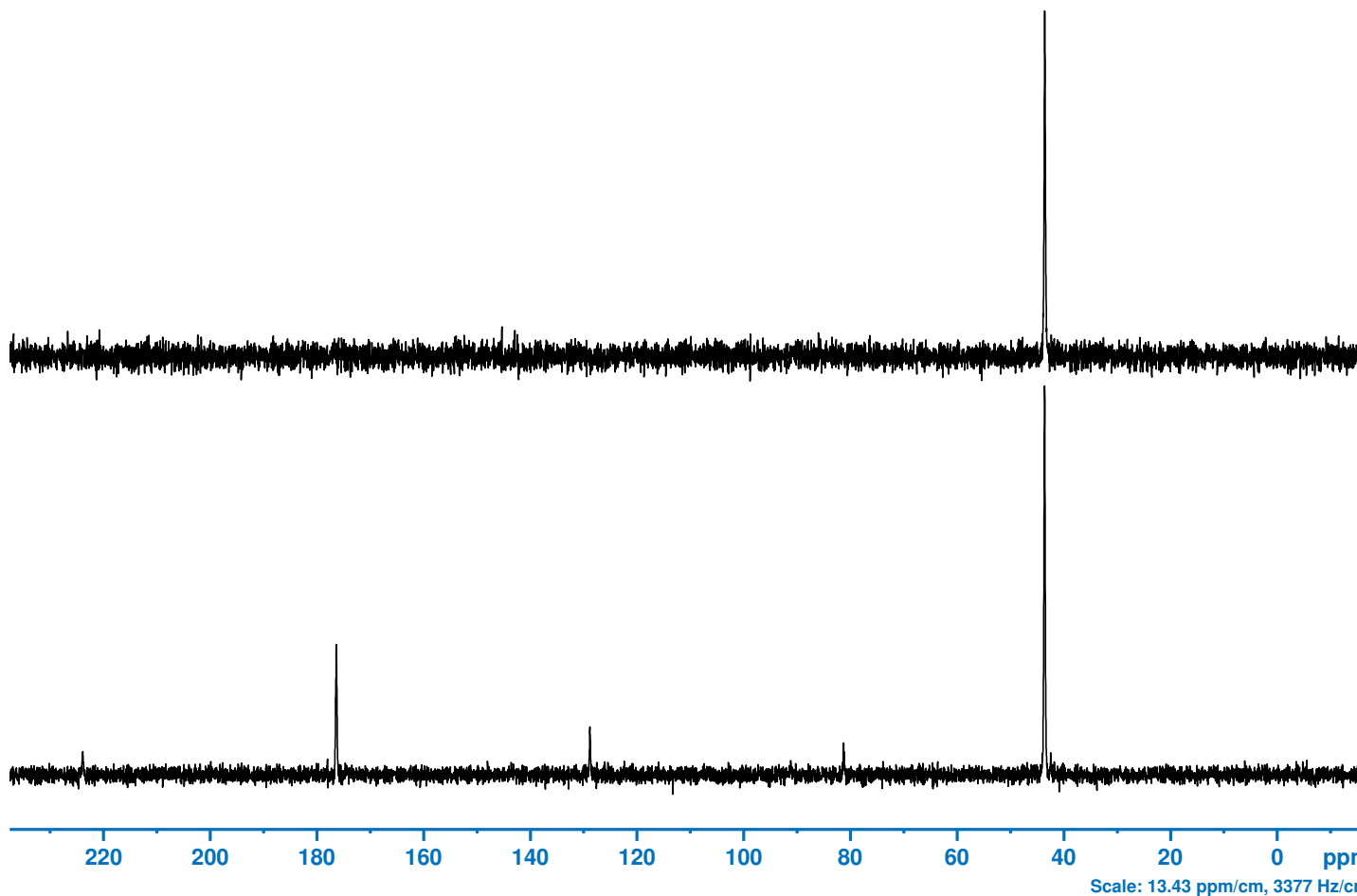
Bruker BioSpin

Contact time P15: [8000.0 us]
 Contact time P16: [9000.0 us]
 Transfer efficiency for C-alpha of double CP vs. 1H 13C CP experiment [achieved]: [54.3%] <n/a>
 Double CP C-alpha: SINO (20.0 ppm) = 28.3, Signal (43.52 ppm), Noise (22.05 to 2.05 ppm)
 1H 13 CP C-alpha: SINO (20.0 ppm) = 52.1, Signal (43.54 ppm), Noise (31.85 to 11.85 ppm)
 Double CP carboxyl: SINO (20.0 ppm) = 1.5, Signal (85 to 65 ppm), Noise (22.05 to 2.05 ppm)
 1H 13 CP carboxyl: SINO (20.0 ppm) = 17.4, Signal (85 to 65 ppm), Noise (31.85 to 11.85 ppm)

NPT_13C_MAS_double_cp1h15n_13c

Current Data Parameters
 NAME NPT_13C_MAS_double_cp1h15n_13c
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201203
 Time 9.53 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171375_0001 ()
 PULPROG doubcp
 TD 7462
 SOLVENT CDC13
 NS 16
 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 308.0 K
 CNST11 1.0000000
 DQ 0.00000300 sec
 D1 5.00000000 sec
 INO 0 sec
 LO 0
 SFO1 251.5784507 MHz
 NUC1 13C
 CNST9 110.0000000
 CNST10 20.0000000
 P1 8.33 usec
 P2 16.67 usec
 P16 9000.00 usec
 PLW1 20.25791931 W
 PLW11 20.25791931 W
 SPNAM[1] tacn80
 SPOAL1 0.500
 SPOFFS1 0 Hz
 SPW1 33.98667145 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 0
 CNST24 1.0000000
 CPDPRG[2] spinal64
 P3 2.00 usec
 P15 8000.00 usec
 PCPD2 3.80 usec
 PLW2 0 W
 PLW12 99.00299835 W
 PLW13 79.19999695 W
 SPNAM[0] ramp.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 60.66999817 W
 SFO3 101.3731996 MHz
 NUC3 15N
 PLW3 271.10998535 W
 PLW5 191.29519653 W



 SHIM SEQUENCE

 skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: 2-13C, 15N alpha-glycine (10 mg, 13.1 ul) (Z151263)
CP 1H-13C parameter optimization, MAS (NPT_13C_MAS_paropt_cp1h_13c, spin rate 10000 Hz)

SINO (20.0 ppm): Signal (43.59 ppm), Noise (2.46 to -17.54 ppm) [62.8]
Processed with TDef=2048



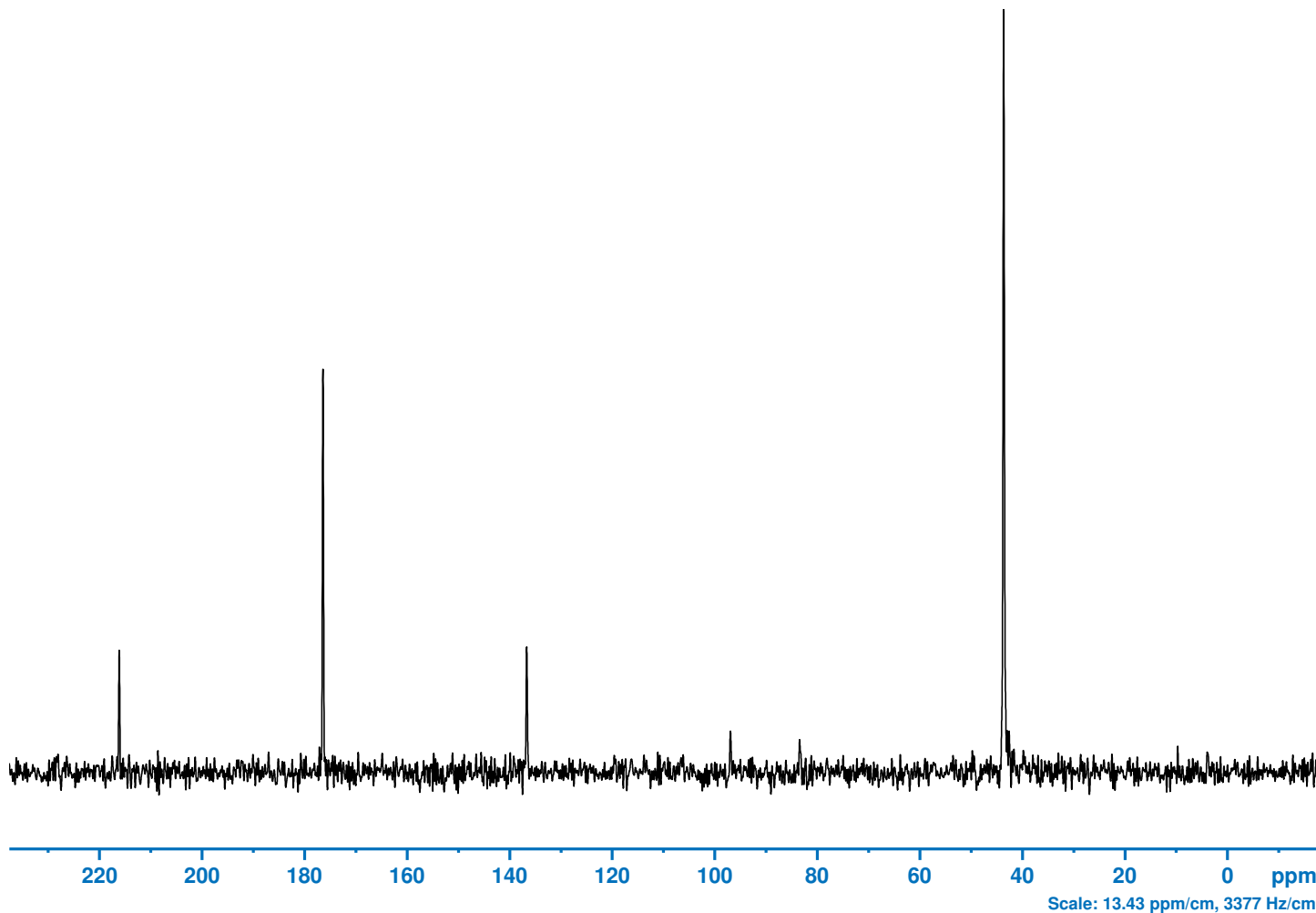
Bruker BioSpin

NPT_13C_MAS_paropt_cp1h_13c

Current Data Parameters
NAME NPT_13C_MAS_paropt_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201202
Time 14.24 h
INSTRUM Avance Neo 1GHz
PROBHD H171375_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 308.0 K
D1 5.0000000 sec
ZGPTNS
SFO1 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 56.27199936 W
SFO2 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.00 usec
PCPD2 3.80 usec
PLW2 99.00299835 W
PLW12 94.55999756 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 56.75000000 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: H171375_0001 PH MASDVT1000S6 BL1.9 X/Y/H TRIG2 NO_I/E
Sample: 2-13C, 15N alpha-glycine (10 mg, 13.1 ul) (Z151263)
CP 1H-15N parameter optimization, MAS (NPT_15N_MAS_paropt_cp1h_15n, spin rate 10000 Hz)

SINO (20.0 ppm): Signal (33.38 ppm), Noise (223.83 to 203.83 ppm) [1674.6]



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_ 20201202
Time 14.47 h
INSTRUM Avance Neo 1GHz
PROBHD H171375_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 308.0 K
D1 5.0000000 sec
ZGPTNS
SF01 101.3731996 MHz
NUC1 15N
P15 3500.00 usec
PLW1 271.10998535 W
SFO2 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.00 usec
PCPD2 3.80 usec
PLW2 99.00299835 W
PLW12 102.23999786 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 48.65000153 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

