

NMR Test Spectrometer

Report Name: 1.3mm_NCHD_Install

AV NEO (1000 MHz) 408457

Content:

- Configuration Information ([uxnmr.info](#))
- IP Config Information
- Probe: H170062_0001 / 1.3mm_NCH_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 = B0SS3-SB
- SGB channels = 40
- Shim matrix file: 292722dd.dat
- Active shims: Z Z2 Z3 Z4 Z5 X XZ X22 (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 17765739 bytes 5232004863 (4.8 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 21883349 bytes 3889040787 (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 1044074 bytes 193507349 (184.5 MiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 511478 bytes 93530732 (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 30147452 bytes 5098629539 (4.7 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 30147452 bytes 5098629539 (4.7 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
```

PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E

1000 MHz

Probe ID: H170062_0001

Inspection Lot: 1.3mm_NCH_Install

● Probe NMR Test Data: **PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E**

Probe Related Information

EC-Level _____ 0
 Gas Compensation _____ nitrogen
 Gradient System _____ none
 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

H170062_0001.ph

```
H170062_0001.ph
=====
$Bis,1,20201020,2048,PICS,5#
$Production,H170062,0001,00,00,,BNMRDE,20201020#
$Name,PH MAS DVT 1000S6 EL1.3 N/C/H NO_I/E#
$ProbeCompatibility,1.0,WB,6,1000#
$ProbeType,1.1,MAS,0,0#
$ProbeSample,1.0,1.3,0#
$ProbeTemperature,1.0,TypeT,-50,80#
$ProbeHeaterTemperature,1.0,TypeK,-274,600#
$ProbeGasFlow,1.0,,,,,600,50,3000,,,#
$ProbeAllCoils,1.1,1,1#
$ProbeCoil,1.0,1,2.5,3,15N,13C/79Br,1H#
$ProbeChannel,1.1,1H,,,,,50,,,FALSE,,,#
$ProbeChannel,1.1,13C/79Br,,,,,40,,,,,0,,,#
$ProbeChannel,1.1,15N,,,,,90,,,,,0,,,#
$ProbeMas,1.0,8000,67000,0,0,0,0,0,0,0#
$EndBis,D0,29#
```

● **Required Samples** PH MAS DVT 1000S6 BL1.3 N/C/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)

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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]: [185] <n/a>



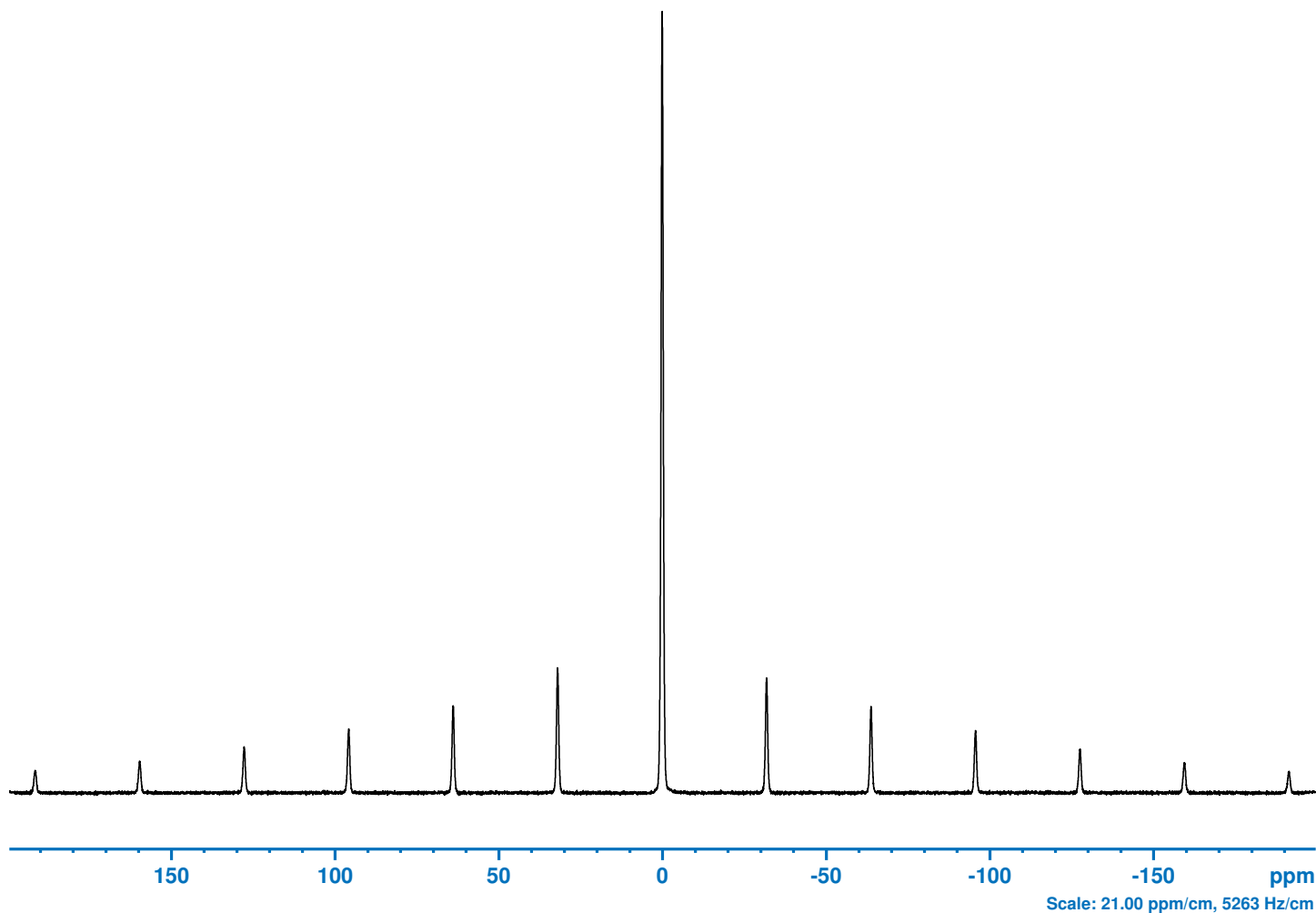
Bruker BioSpin

NPT_79Br_MAS_magicAngle

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

F2 - Acquisition Parameters
Date_     20201130
Time      14.32 h
INSTRUM   Avance Neo 1GHz
PROBHD    H170062_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         307.4 K
D1         0.2500000 sec
SFO1       250.6558776 MHz
NUC1       79Br
P1         3.50 usec
PLW1       33.22299957 W

F2 - Processing parameters
SI         131072
SF         250.6558776 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: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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=3785/BearingPressure=3162/BearingSensePressure=3127/SupplyPressure=7046/SystemPressure=7273

Spin rate at maximum deviation [measured]: @ MASR 67000 Hz [67020 Hz]
Maximum deviation [achieved/rated]: @ MASR 67000 Hz [20 Hz <= 67 Hz] <pass>



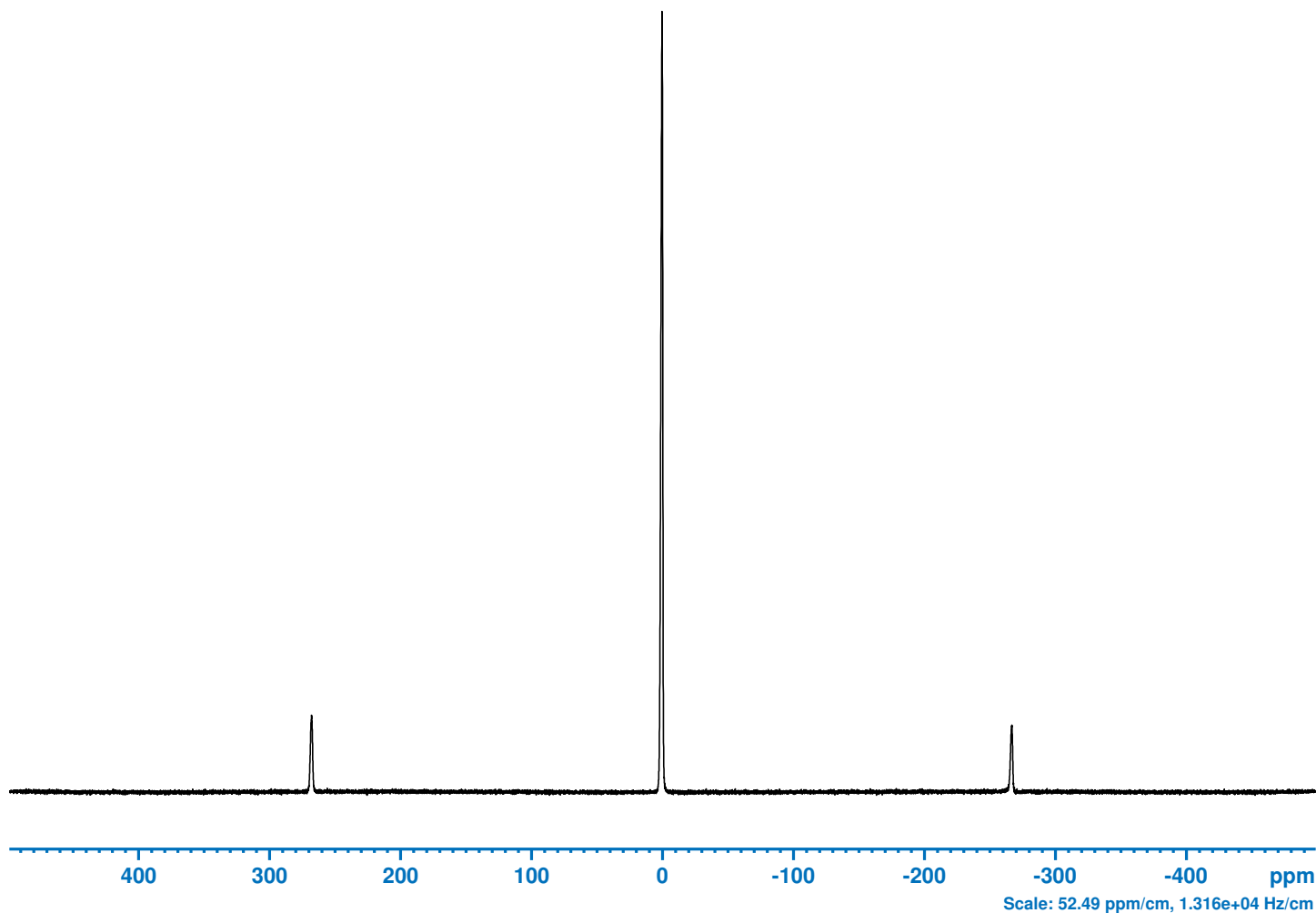
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

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

F2 - Acquisition Parameters
Date_     20201130
Time      14.48 h
INSTRUM   Avance Neo 1GHz
PROBHD    H170062_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         301.8 K
D1         0.25000000 sec
SFO1       250.6546967 MHz
NUC1       79Br
P1         3.50 usec
PLW1       33.22299957 W

F2 - Processing parameters
SI         32768
SF         250.6546967 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0
PC         0.20
```



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

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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 2232.7 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0070 ppm.



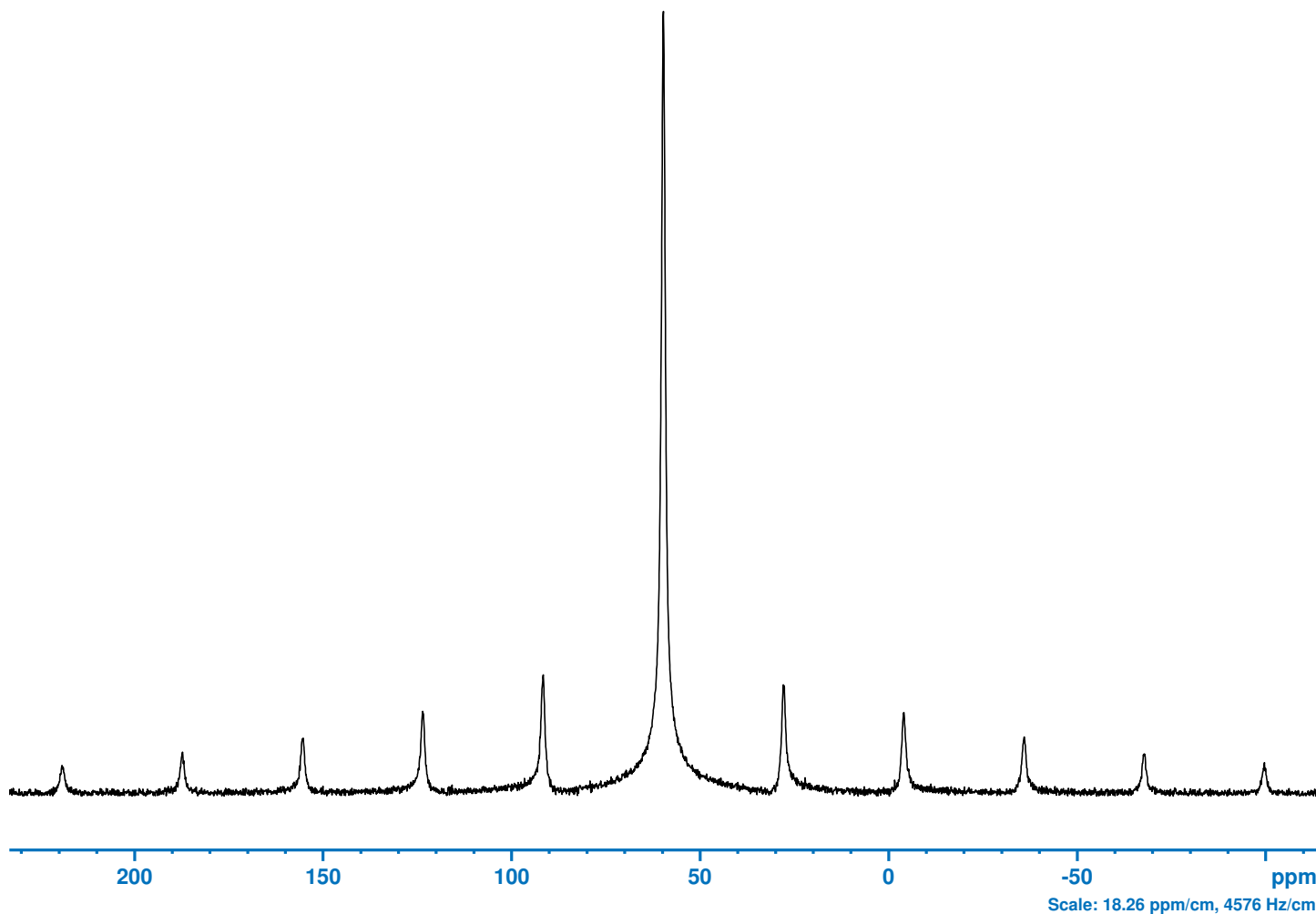
Bruker BioSpin

NPT_79Br_MAS_fieldsetting

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

F2 - Acquisition Parameters
Date_     20201130
Time      14.32 h
INSTRUM   Avance Neo 1GHz
PROBHD    H170062_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         307.1 K
D1         0.50000000 sec
SFO1       250.6549791 MHz
NUC1       79Br
P1         3.50 usec
PLW1       33.22299957 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: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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 2201.7 for 13C chemical shift of 38.460 ppm. One field unit corresponds to 0.0071 ppm.



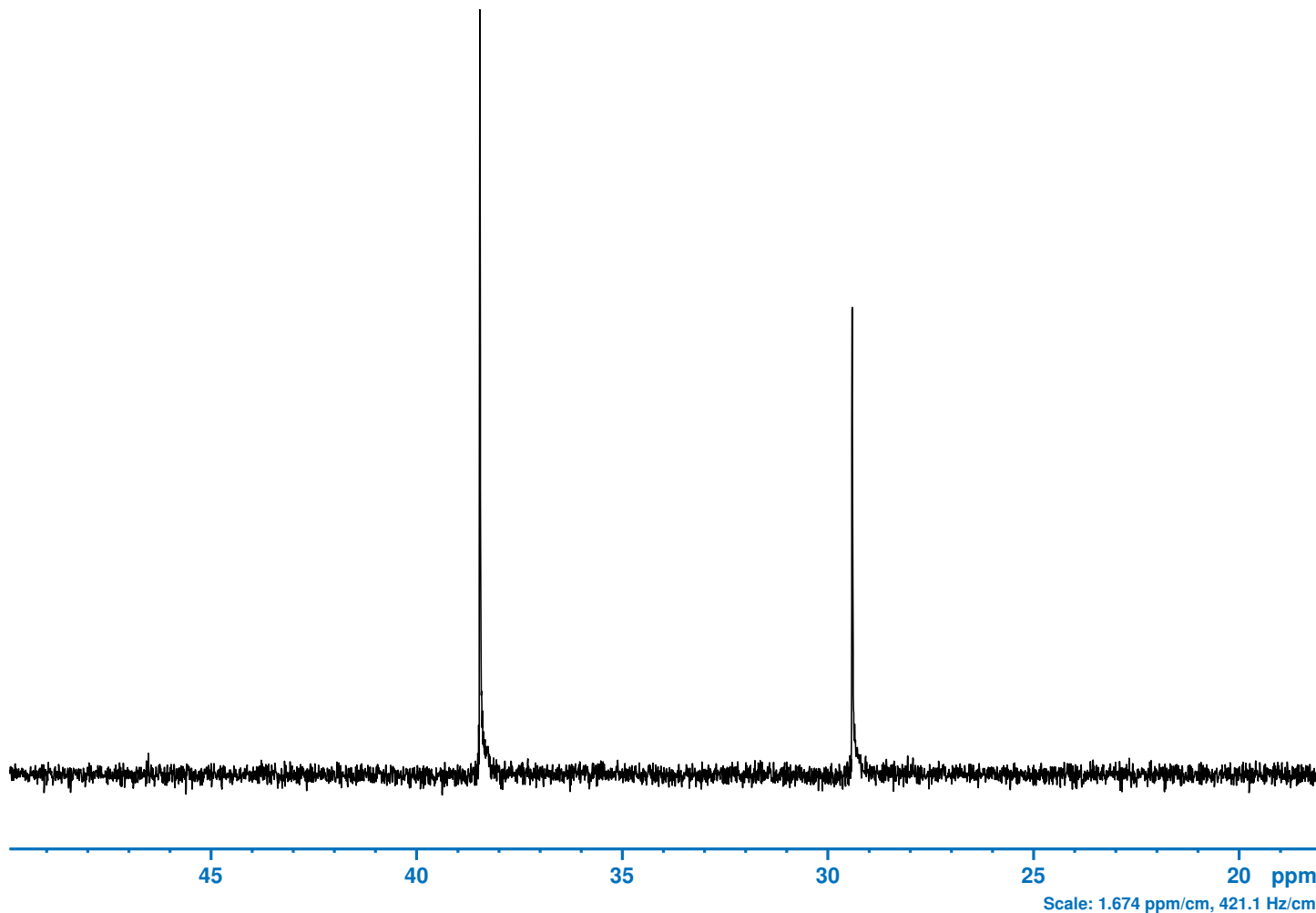
Bruker BioSpin

NPT_13C_MAS_fieldsetting_dec1h

```
Current Data Parameters
NAME      NPT_13C_MAS_fieldsetting_dec1h
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20201130
Time      15.32 h
INSTRUM   Avance Neo 1GHz
PROBHD    H170062_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         300.0 K
D1         15.0000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1      251.5593320 MHz
NUC1       13C
P1         3.00 usec
PLW1      36.09999847 W
SFO2      1000.4023777 MHz
NUC2       1H
CPDPRG2   cw
PLW2      44.50099945 W
PLW12     0.12976490 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

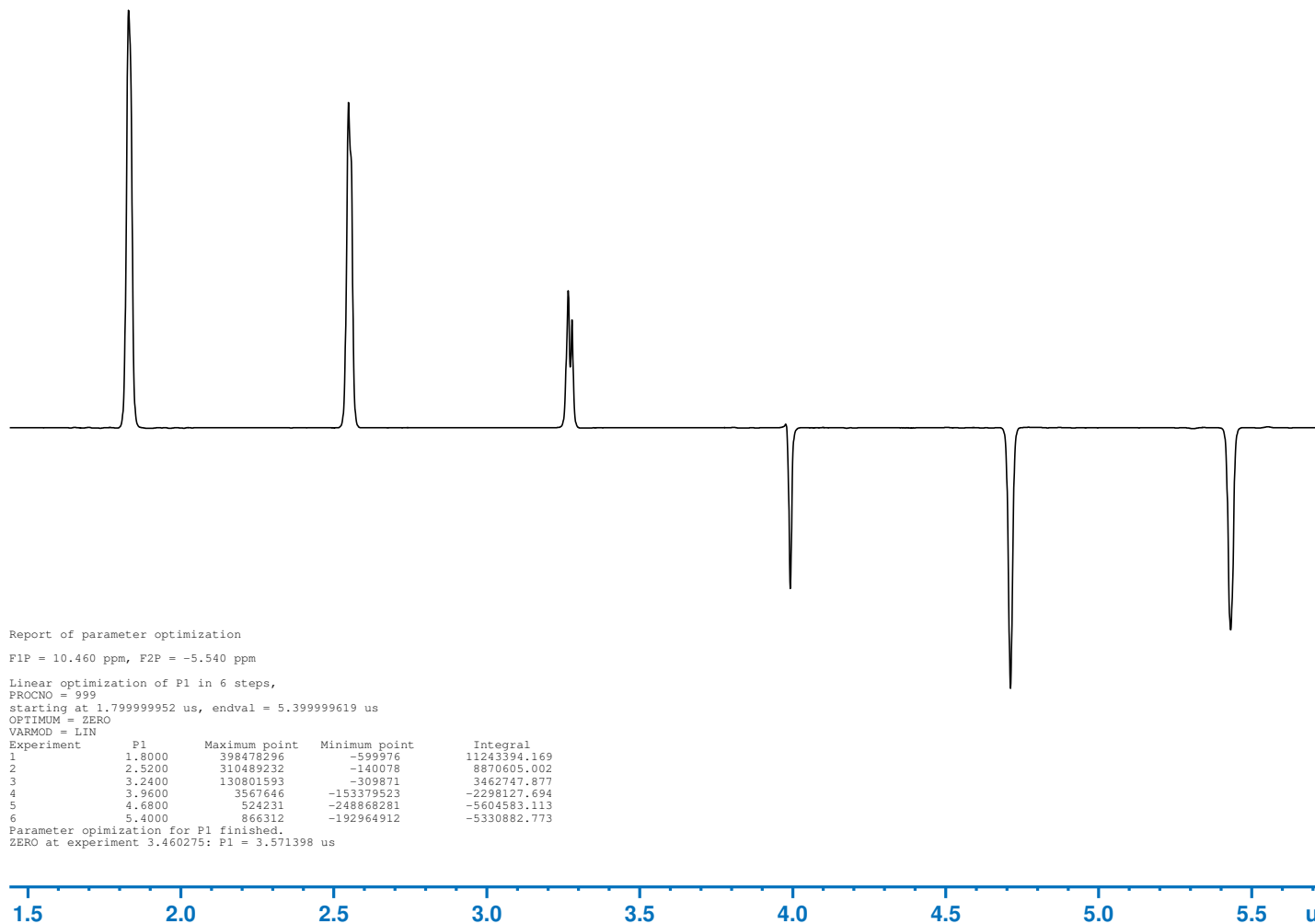
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
 Sample: Adamantane (3.0 ul) (Z151271)
 P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 30000 Hz)
 ATTENTION: Updated PROSOL Tables with [1.80 us @ 44.5 W].



Bruker BioSpin

P90 MAS 1H pulse [achieved/rated]: @ 45.0 W [1.79 us <= 1.80 us] <pass>

NPT_1H_MAS_p90det_1h



```
Current Data Parameters
NAME      NPT_1H_MAS_p90det_1h
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20201130
Time      15.05 h
INSTRUM   Avance Neo 1GHz
PROBHD    H170062_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        6.500 usec
TE        300.4 K
DI        5.00000000 sec
SFO1      1000.4024610 MHz
NUC1      1H
P1        5.40 usec
PLW1      45.00000000 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
-----
45.0 W   1.80 us   1.79 us   -0.6%
```

Report of parameter optimization

F1P = 10.460 ppm, F2P = -5.540 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 1.799999952 us, endval = 5.3999999619 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	1.8000	398478296	-599976	11243394.169
2	2.5200	310489232	-140078	8870605.002
3	3.2400	130801593	-309871	3462747.877
4	3.9600	3567646	-153379523	-2298127.694
5	4.6800	524231	-248868281	-5604583.113
6	5.4000	866312	-192964912	-5330882.773

Parameter optimization for P1 finished.

ZERO at experiment 3.460275: P1 = 3.571398 us

 SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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 [3.50 us @ 33.2 W].

P90 MAS 79Br pulse [achieved/rated]: @ 33.8 W [3.47 us <= 3.50 us] <pass>



Bruker BioSpin

NPT_79Br_MAS_p90det_79br



Current Data Parameters
 NAME NPT_79Br_MAS_p90det_79br
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201130
 Time 14.31 h
 INSTRUM Avance Neo 1GHz
 PROBHD H170062_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 10.50 usec
 PLW1 33.79999924 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
33.8 W	3.50 us		
33.8 W	3.50 us	3.47 us	-0.9%

Report of parameter optimization

F1P = 69.700 ppm, F2P = 49.700 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	318203749	-3018650	13289312.783
2	4.9000	226786415	-3043917	9558550.343
3	6.3000	74196913	-4364355	2773709.565
4	7.7000	2318701	-88796168	-2988348.560
5	9.1000	1325422	-149391516	-5536326.870
6	10.5000	1498631	-117763407	-4312045.773

Parameter optimization for P1 finished.

ZERO at experiment 3.455215: P1 = 6.937301 us

 SHIM SEQUENCE

skip shimming

3.0 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 us

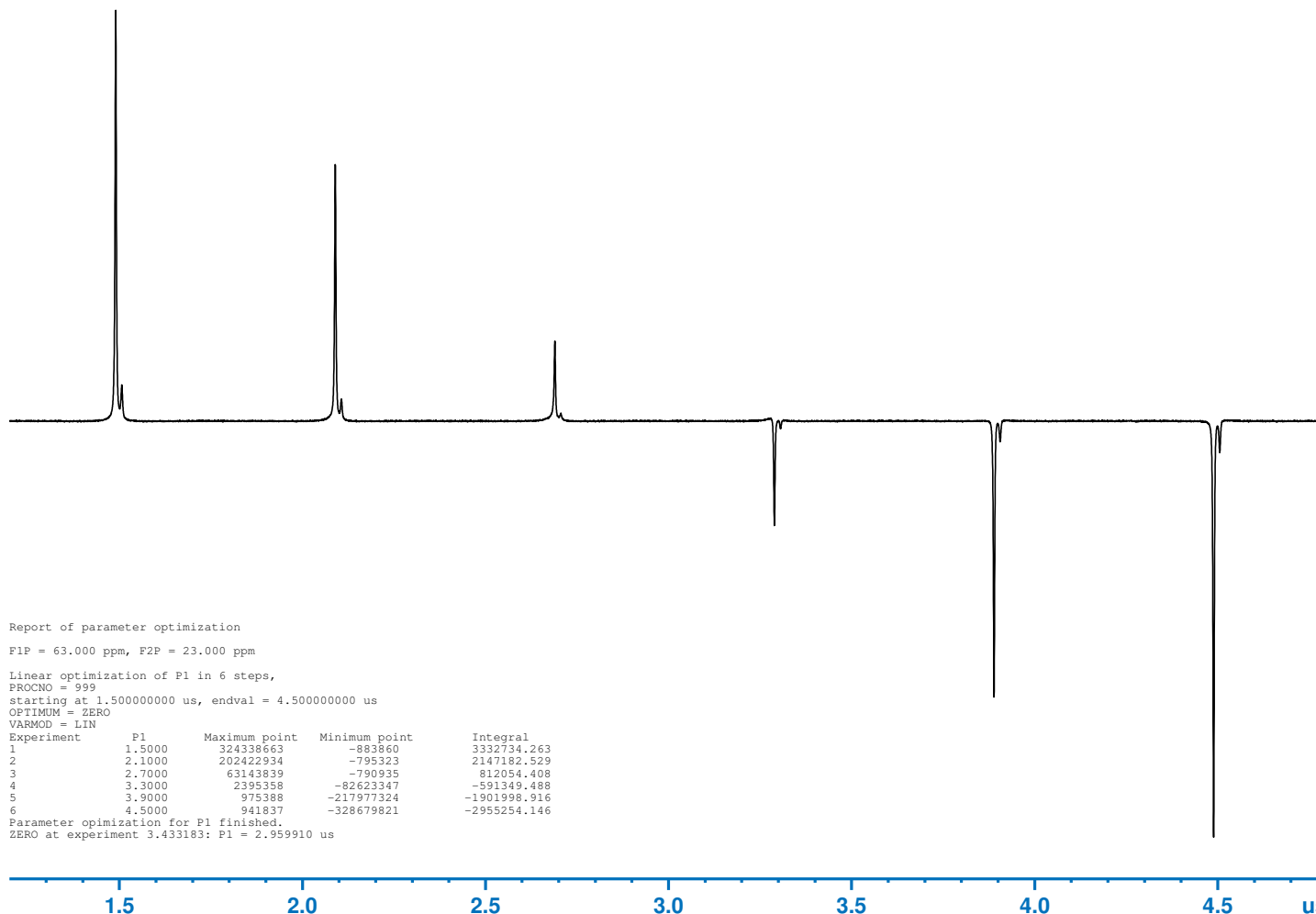
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)
 P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.00 us @ 35.1 W].

P90_MAS_CP 1H13C power (PLW 11) [achieved]: [36.1 W] <n/a>
 P90_MAS_CP 1H13C pulse (P 1) [achieved/rated]: [2.96 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_ 20201130
 Time 16.46 h
 INSTRUM Avance Neo 1GHz
 PROBHD H170062_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 307.0 K
 D1 5.00000000 sec
 ZGPGTNS
 SFO1 251.5615968 MHz
 NUC1 13C
 P1 4.50 usec
 P15 2000.00 usec
 PLW1 36.09999847 W
 PLW11 36.09999847 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 1.80 usec
 PCPD2 3.40 usec
 PLW2 44.50099945 W
 PLW12 44.50099945 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 43.79182053 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

 36.1 W 3.00 us
 36.1 W 3.00 us 2.96 us -1.3%

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	324338663	-883860	3332734.263
2	2.1000	202422934	-795323	2147182.529
3	2.7000	63143839	-790935	812054.408
4	3.3000	2395358	-82623347	-591349.488
5	3.9000	975388	-217977324	-1901998.916
6	4.5000	941837	-328679821	-2955254.146

Parameter optimization for P1 finished.

ZERO at experiment 3.433183: P1 = 2.959910 us

 SHIM SEQUENCE

skip shimming

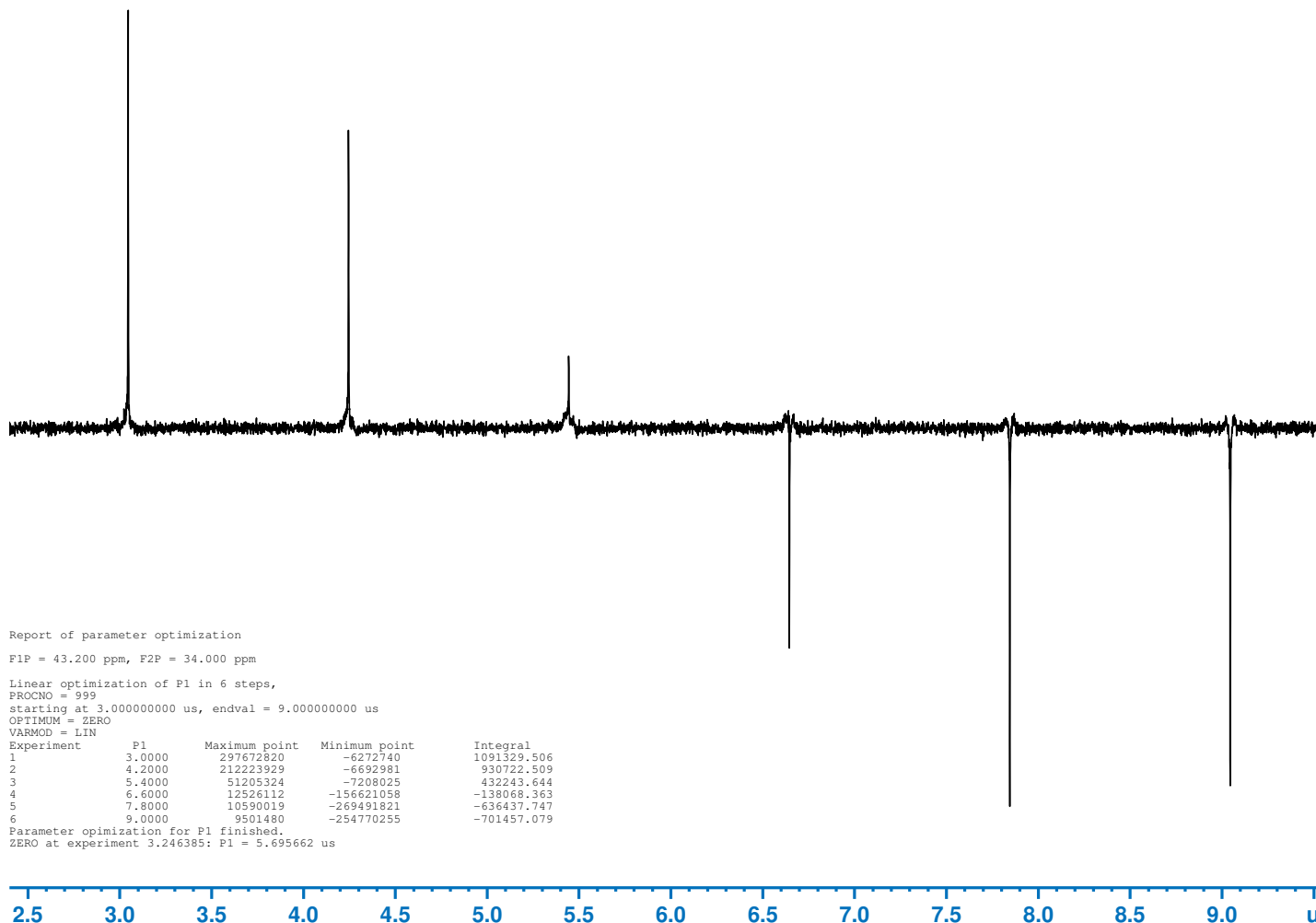
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
 Sample: Adamantane (3.0 ul) (Z151271)
 P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c, spin rate 30000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.00 us @ 36.1 W].



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P90 MAS 13C pulse [achieved/rated]: @ 40.0 W [2.85 us <= 3.00 us] <pass>

NPT_13C_MAS_p90det_13c



Current Data Parameters
 NAME NPT_13C_MAS_p90det_13c
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201130
 Time 15.28 h
 INSTRUM Avance Neo 1GHz
 PROBHD H170062_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 300.0 K
 D1 15.00000000 sec
 P15 0 usec
 ZGPTNS -D1acq
 SFO1 251.5593328 MHz
 NUC1 13C
 P1 9.00 usec
 PLW1 40.00000000 W
 SFO2 1000.4024610 MHz
 NUC2 1H
 CPDPRG2 cw
 PLW2 44.50099945 W
 PLW12 0.12976490 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 3.00 us
 40.0 W 3.00 us 2.85 us -5.0%

Report of parameter optimization

F1P = 43.200 ppm, F2P = 34.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 3.000000000 us, endval = 9.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	3.0000	297672820	-6272740	1091329.506
2	4.2000	212223929	-6692981	930722.509
3	5.4000	51205324	-7208025	432243.644
4	6.6000	12526112	-156621058	-138068.363
5	7.8000	10590019	-269491821	-636437.747
6	9.0000	9501480	-254770255	-701457.079

Parameter optimization for P1 finished.

ZERO at experiment 3.246385: P1 = 5.695662 us

 SHIM SEQUENCE

 skip shimming

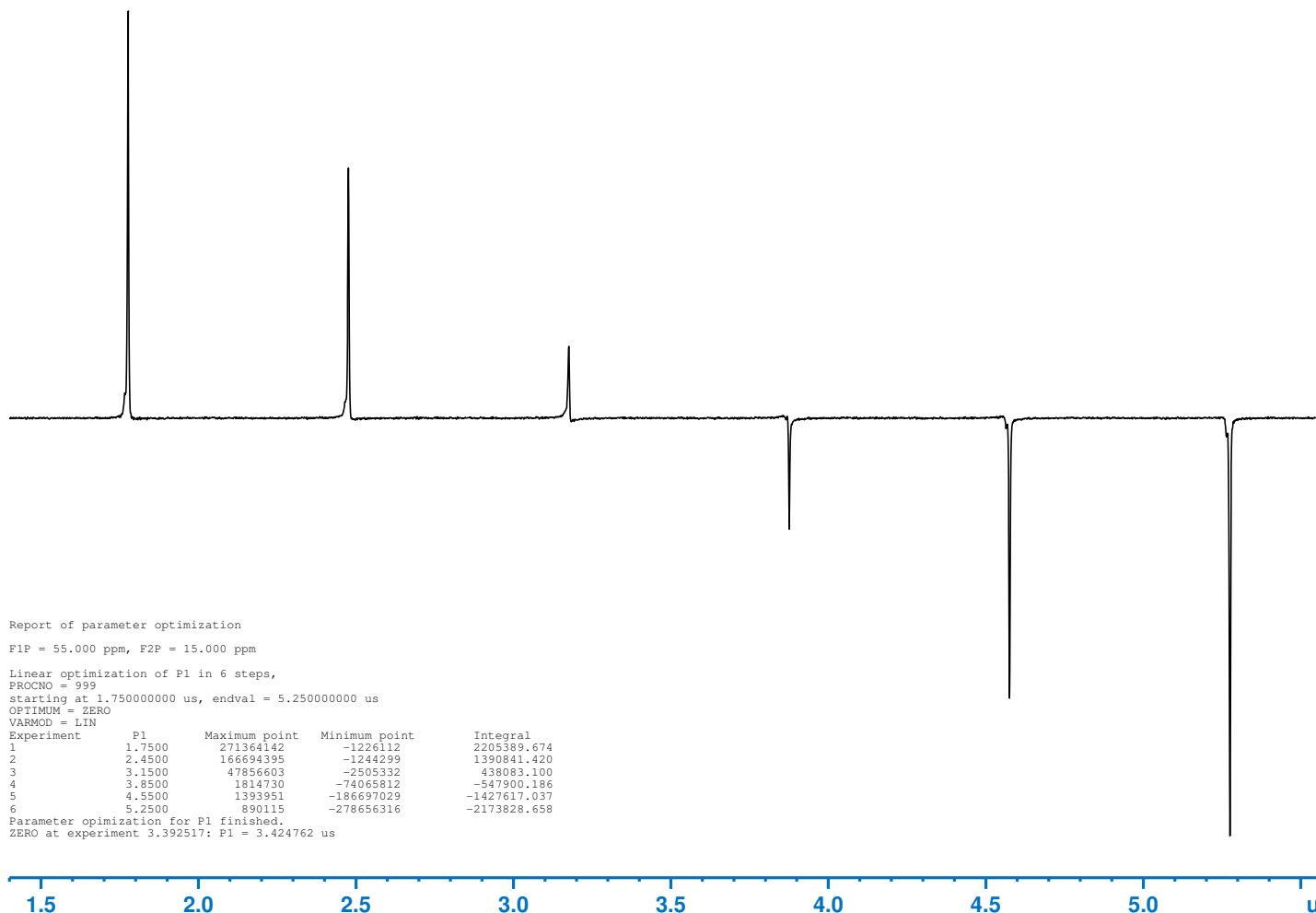
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)
 P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n, spin rate 10000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.50 us @ 78.3 W].

P90_MAS_CP 1H15N power (PLW 11) [achieved]: [82.0 W] <n/a>
 P90_MAS_CP 1H15N pulse (P 1) [achieved/rated]: [3.42 us <= 3.50 us] <pass>



Bruker BioSpin

NPT_15N_MAS_p90det_cp1h_15n



Current Data Parameters
 NAME NPT_15N_MAS_p90det_cp1h_15n
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201201
 Time 8.53 h
 INSTRUM Avance Neo 1GHz
 PROBHD H170062_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
 ZGPGTNS
 SFO1 101.3731996 MHz
 NUC1 15N
 P1 5.25 usec
 P15 3500.00 usec
 PLW1 82.00000000 W
 PLW11 82.00000000 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 1.80 usec
 PCPD2 3.40 usec
 PLW2 44.50099945 W
 PLW12 44.50099945 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 27.19355011 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

 82.0 W 3.50 us
 82.0 W 3.50 us 3.42 us -2.3%

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	271364142	-1226112	2205389.674
2	2.4500	166694395	-1244299	1390841.420
3	3.1500	47856603	-2505332	438083.100
4	3.8500	1814730	-74065812	-547900.186
5	4.5500	1393951	-186697029	-1427617.037
6	5.2500	890115	-278656316	-2173828.658

Parameter optimization for P1 finished.

ZERO at experiment 3.392517: P1 = 3.424762 us

 SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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/rated]: Signal (43.69 ppm), Noise (198.39 to 178.39 ppm) [63.1 >= 60.0] <pass>
Number of scans (NS) [achieved/rated]: [64 <= 64] <pass>
Processed with TDef=2048



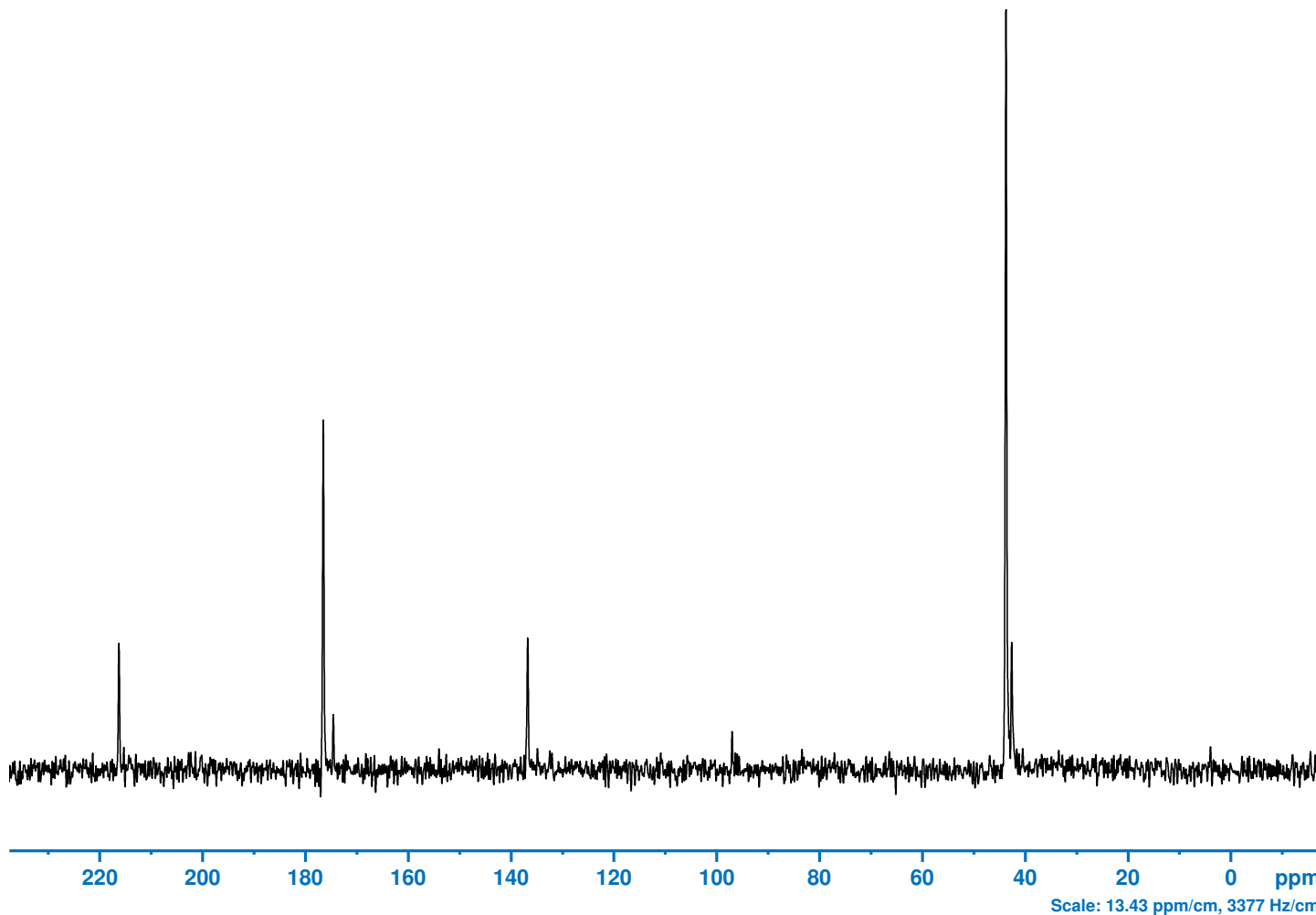
Bruker BioSpin

NPT_13C_MAS_sino_cp1h_13c

Current Data Parameters
NAME NPT_13C_MAS_sino_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201201
Time 9.33 h
INSTRUM Avance Neo 1GHz
PROBHD H170062_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 308.0 K
D1 5.0000000 sec
ZGPTNS
SF01 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 35.14400101 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 1.80 usec
PCPD2 3.40 usec
PLW2 44.50099945 W
PLW12 40.95999908 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 42.77999878 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: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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/rated]: Signal (33.51 ppm), Noise (-22.67 to -42.67 ppm) [7.0 < 8.0] <fail>
Number of scans (NS) [achieved/rated]: [64 <= 64] <pass>



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NPT_15N_MAS_sino_cp1h_15n

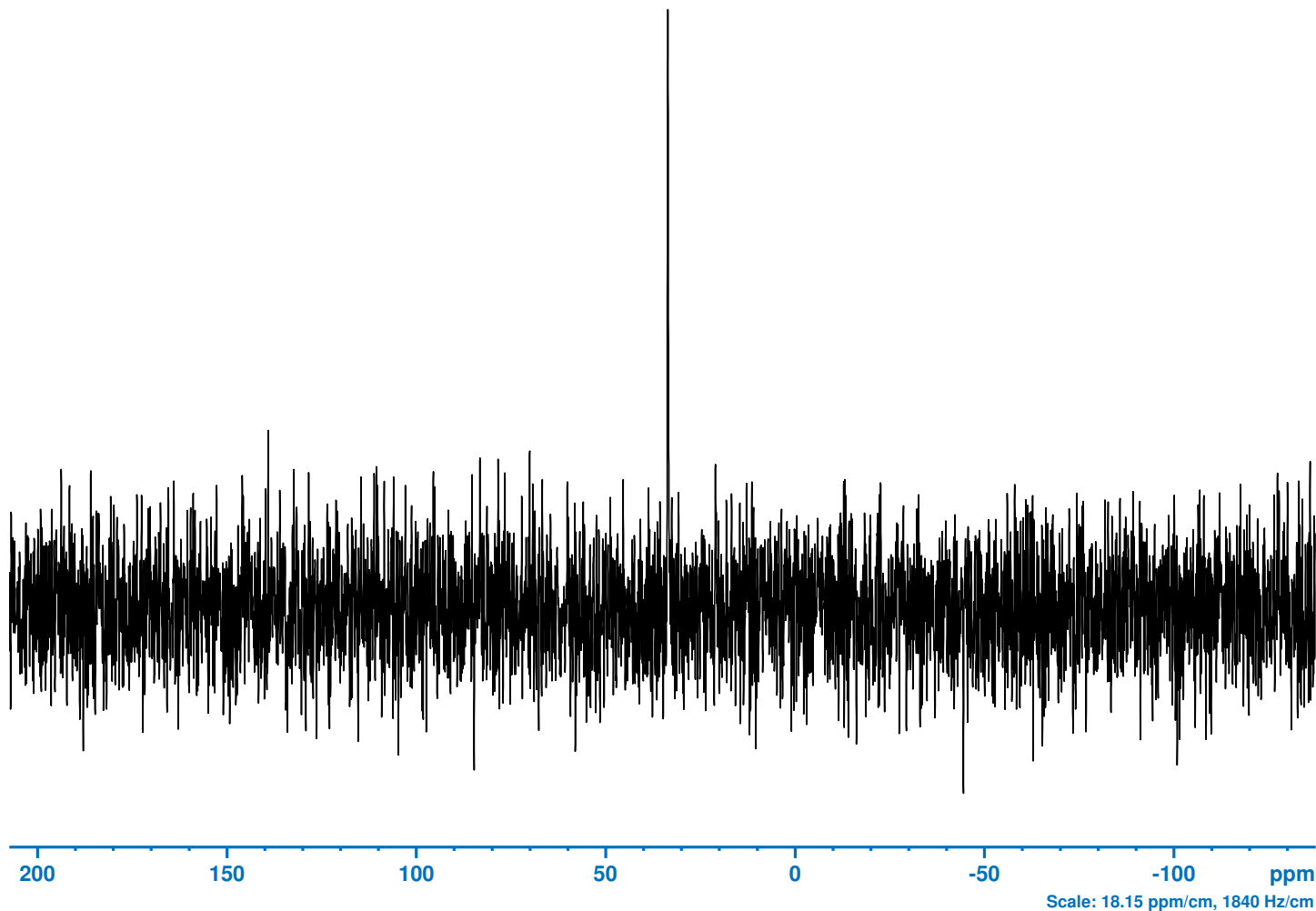
Current Data Parameters
NAME NPT_15N_MAS_sino_cp1h_15n
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201201
Time 10.35 h
INSTRUM Avance Neo 1GHz
PROBHD H170062_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 101.3731996 MHz
NUC1 15N
P15 3500.00 usec
PLW1 78.29399872 W
SFO2 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 1.80 usec
PCPD2 3.40 usec
PLW2 44.50099945 W
PLW12 42.29999924 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 21.76000023 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: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
Sample: Adamantane (3.0 ul) (Z151271)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 40000 Hz)

SINO (20.0 ppm) [achieved]: Signal (38.47 ppm), Noise (34.22 to 14.22 ppm) [29.4] <n/a>
Linewidth [achieved/rated]: at 50% of signal height [3.8 Hz <= 7.0 Hz] <pass>
Number of scans (NS) [achieved/rated]: [16 <= 16] <pass>



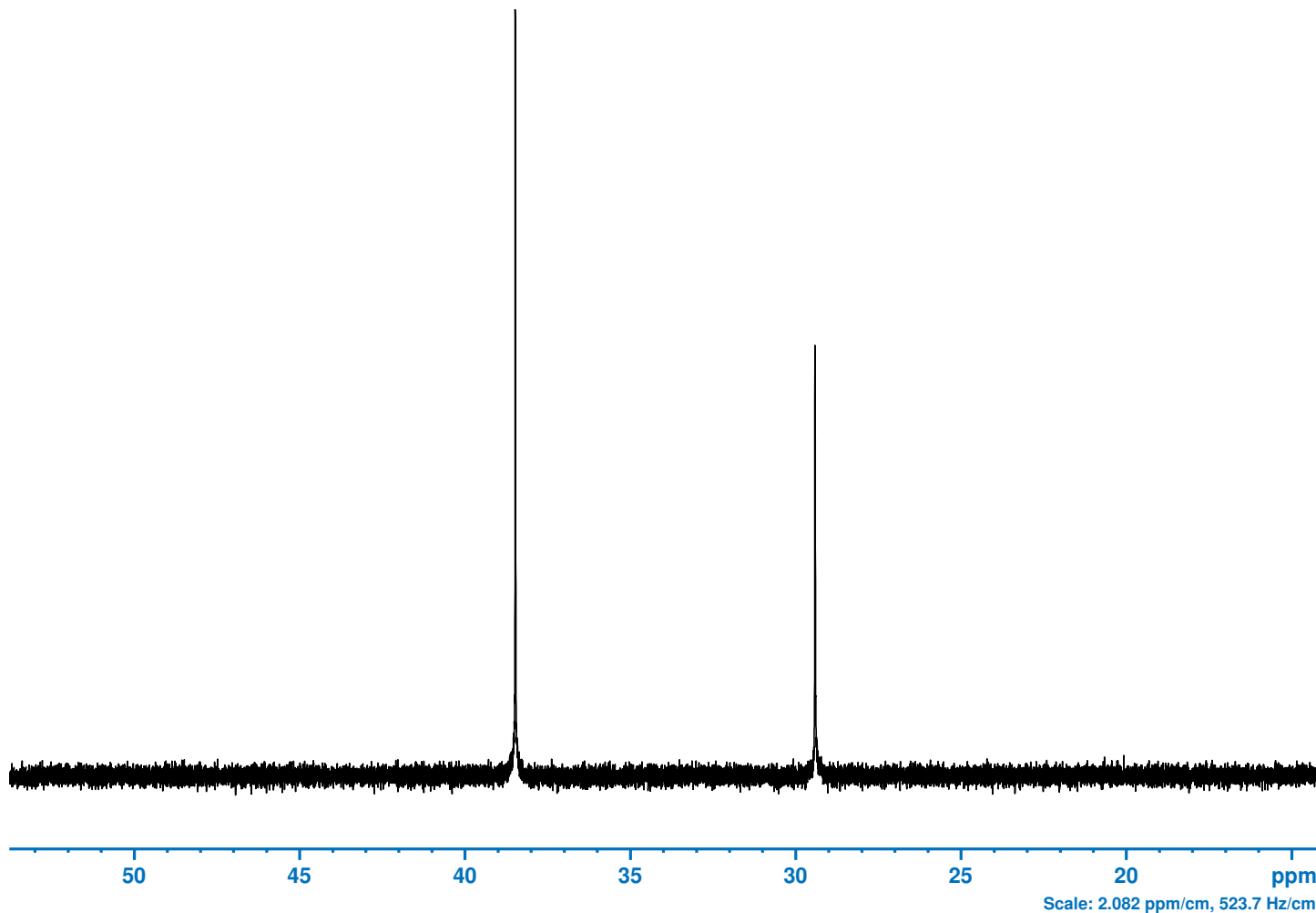
Bruker BioSpin

NPT_13C_MAS_sino_13c

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

F2 - Acquisition Parameters
Date_     20201130
Time      15.38 h
INSTRUM   Avance Neo 1GHz
PROBHD    H170062_0001 (
PULPROG   hpdec
TD         19998
SOLVENT   CDC13
NS         16
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         300.0 K
D1         15.0000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1      251.5593320 MHz
NUC1       13C
P1         3.00 usec
PLW1      36.09999847 W
SFO2      1000.4024610 MHz
NUC2       1H
CPDPRG2   cw
PLW2      44.50099945 W
PLW12     0.23069321 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: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
 Sample: Adamantane (3.0 ul) (Z151271)
 13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 40000 Hz)



Bruker BioSpin

NPT_13C_MAS_sino_13c

```
# Mon Nov 30 15:38:02 2020
##$PROBEIDENTIFIER=H170062_0001
##$PROBENAME=PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
##$SHIMID=292722
#
# Active Shim Gradients
#
Z -58000
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 2201.664
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] -28130.00000504
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] -28187.35206919
SHIM_SETTING [ 4] -0.00000000
SHIM_SETTING [ 5] -10153.35145781
SHIM_SETTING [ 6] 10153.35145781
SHIM_SETTING [ 7] 28187.35206919
SHIM_SETTING [ 8] -28187.35206919
SHIM_SETTING [ 9] -1535.83130352
SHIM_SETTING [10] 1535.83130352
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_ 20201130
Time 15.38 h
INSTRUM Avance Neo 1GHz
PROBHD H170062_0001 (
PULPROG hpdec
TD 19998
SOLVENT CDC13
NS 16
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 300.0 K
D1 15.00000000 sec
P15 0 usec
ZGPTNS -D1acq
SFO1 251.559328 MHz
NUC1 13C
P1 3.00 usec
PLW1 36.09999847 W
SFO2 1000.4024610 MHz
NUC2 1H
CPDPRG2 cw
PLW2 44.50099945 W
PLW12 0.23069321 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: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
Sample: Adamantane (3.0 ul) (Z151271)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 40000 Hz)

SINO (20.0 ppm) [achieved]: Signal (2.38 ppm), Noise (-14.03 to -34.03 ppm) [13164.4] <n/a>
Linewidth [achieved]: at 50% of signal height [187.4 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>



Bruker BioSpin

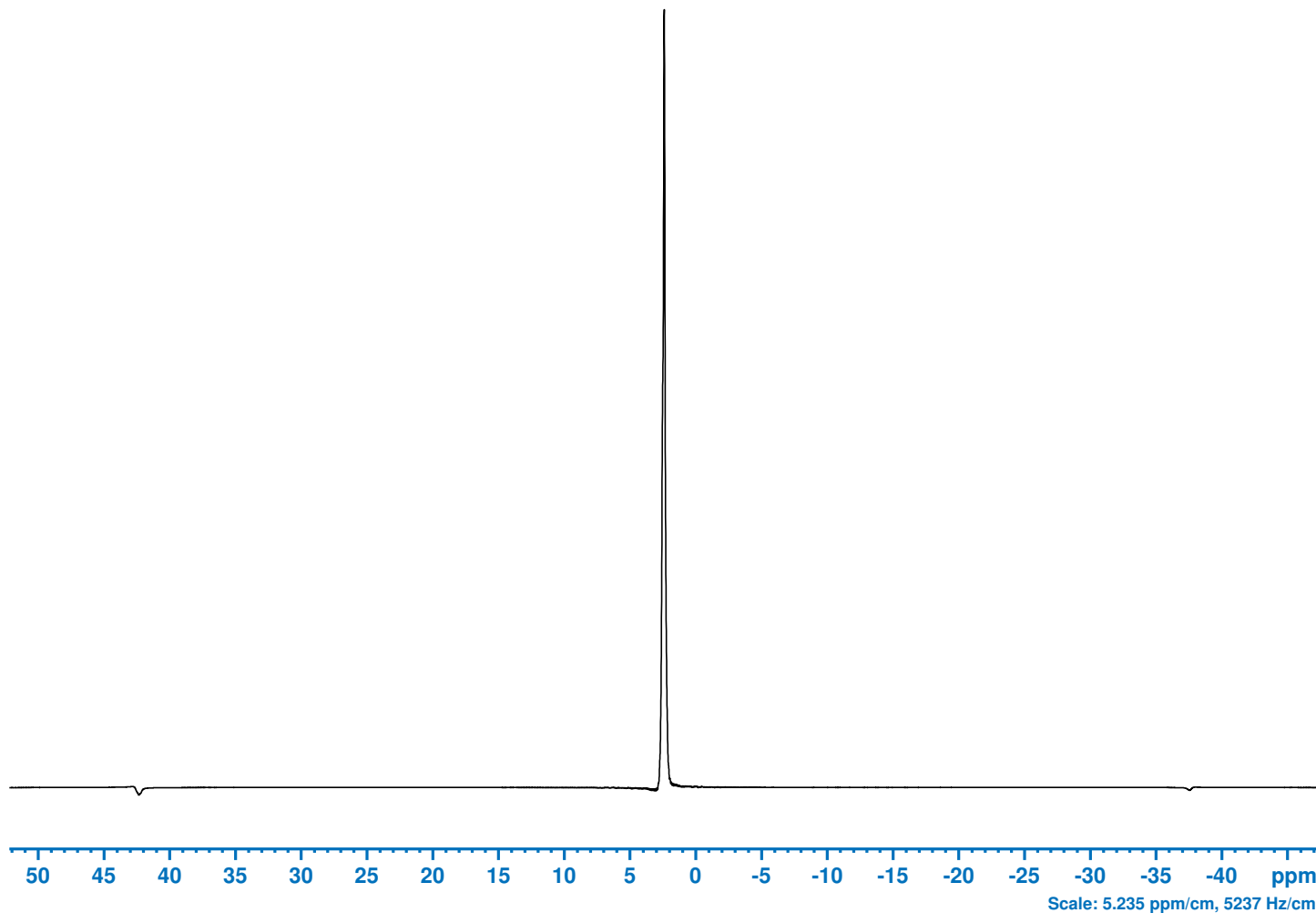
NPT_1H_MAS_sino_1h

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

F2 - Acquisition Parameters
Date_     20201130
Time      15.33 h
INSTRUM   Avance Neo 1GHz
PROBHD    H170062_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         300.0 K
D1         5.00000000 sec
SFO1      1000.4024610 MHz
NUC1       1H
P1         1.80 usec
PLW1       44.50099945 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
-----
```



Scale: 5.235 ppm/cm, 5237 Hz/cm

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)
 Double CP 1H-15N-13C, MAS (NPT_13C_MAS_double_cp1h15n_13c, spin rate 12000 Hz)



Bruker BioSpin

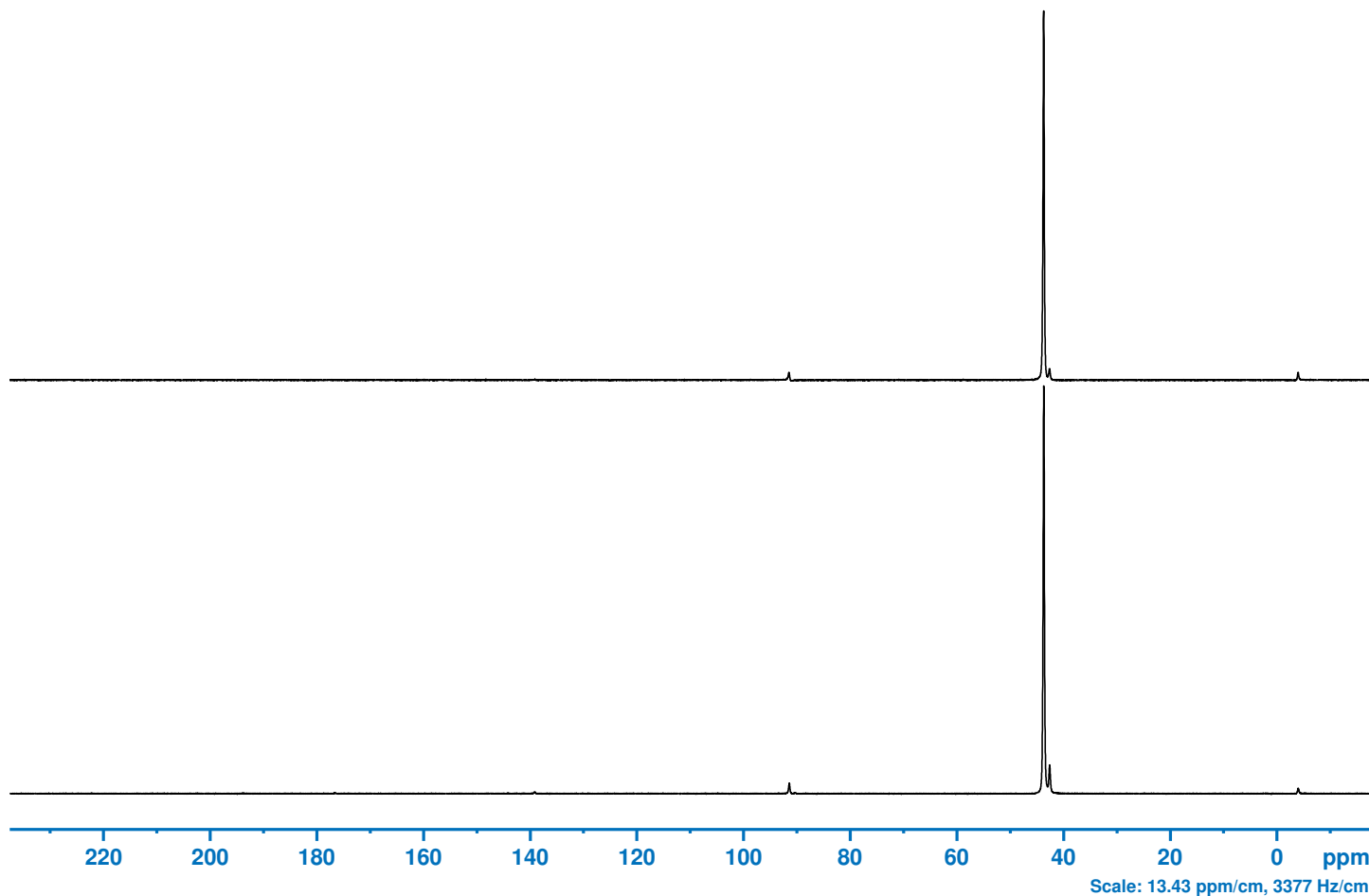
Contact time P15: [8000.0 us]
 Contact time P16: [10000.0 us]
 Transfer efficiency for C-alpha of double CP vs. 1H 13C CP experiment [achieved]: [70.7%] <n/a>
 Double CP C-alpha: SINO (20.0 ppm) = 887.1, Signal (43.67 ppm), Noise (120.02 to 100.02 ppm)
 1H 13 CP C-alpha: SINO (20.0 ppm) = 1254.1, Signal (43.65 ppm), Noise (129.81 to 109.81 ppm)
 Double CP carboxyl: SINO (20.0 ppm) = 1.5, Signal (85 to 65 ppm), Noise (120.02 to 100.02 ppm)
 1H 13 CP carboxyl: SINO (20.0 ppm) = 2.8, Signal (85 to 65 ppm), Noise (129.81 to 109.81 ppm)

NPT_13C_MAS_double_cp1h15n_13c

```
Current Data Parameters
NAME      NPT_13C_MAS_double_cp1h15n_13c
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20201130
Time      17.44 h
INSTRUM   Avance Neo 1GHz
PROBHD    H170062_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     60.0000000
P1         8.33 usec
P2         16.67 usec
P16        10000.00 usec
PLW1       4.55466318 W
PLW11      4.55466318 W
SPNAM[1]   tacn80
SPOAL1     0.500
SPOFFS1    0 Hz
SPW1       7.33333302 W
SFO2       1000.4062025 MHz
NUC2        1H
CNST21     0
CNST24     1.0000000
CPDPRG[2]  spinal64
P3         1.80 usec
P15        8000.00 usec
PCPD2      3.40 usec
PLW2        0 W
PLW12      44.50099945 W
PLW13      40.93999863 W
SPNAM[0]   ramp.100
SPOAL0     0.500
SPOFFS0    0 Hz
SPW0       31.39999962 W
SFO3       101.3731996 MHz
NUC3        15N
PLW3       82.00000000 W
PLW5       28.35100937 W
```

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



NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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 (43.63 ppm), Noise (237.57 to 217.57 ppm) [2114.5]
Processed with TDef=2048



Bruker BioSpin

NPT_13C_MAS_paropt_cp1h_13c

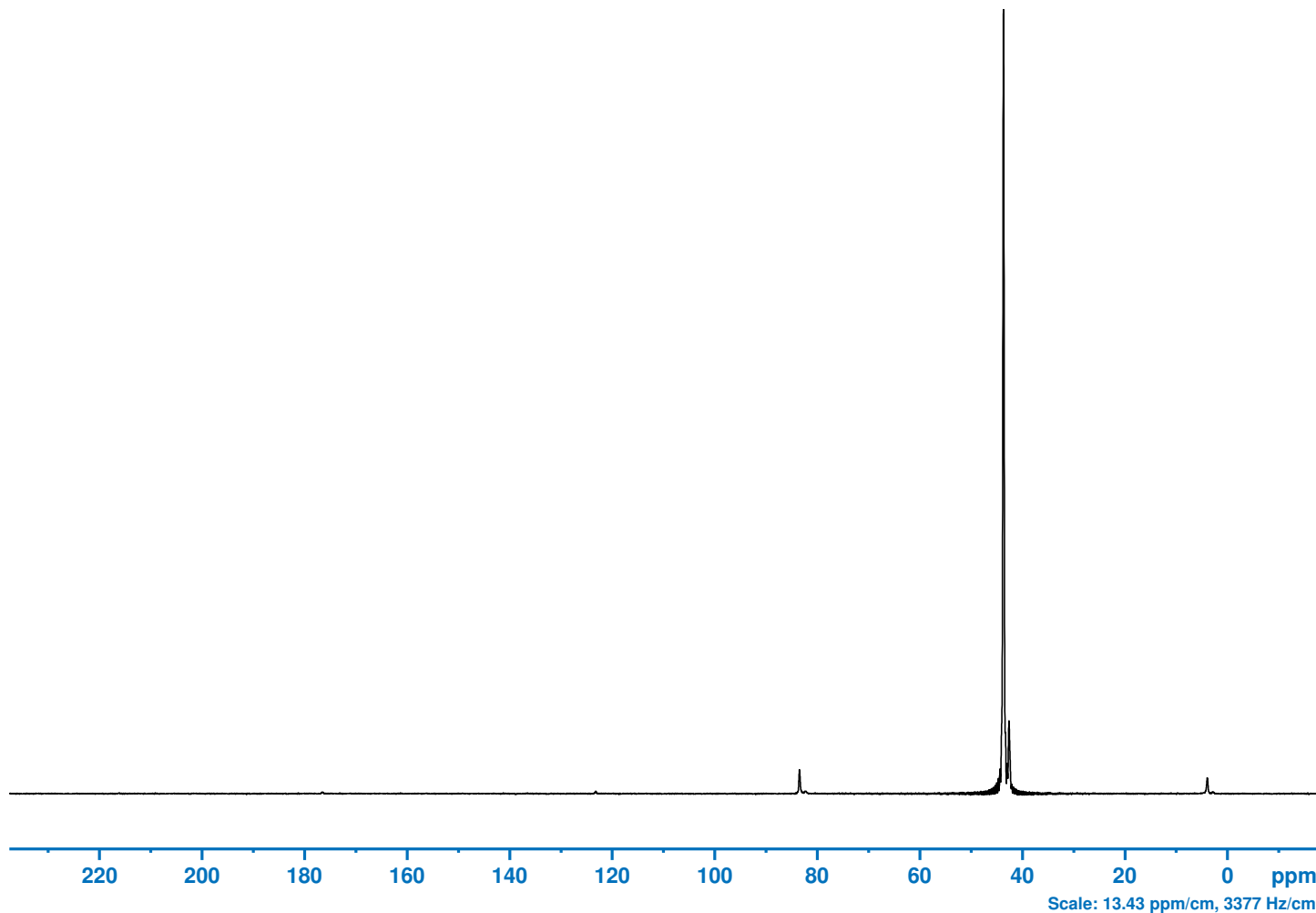
Current Data Parameters
NAME NPT_13C_MAS_paropt_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201130
Time 16.56 h
INSTRUM Avance Neo 1GHz
PROBHD H170062_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 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 35.14400101 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 1.80 usec
PCPD2 3.40 usec
PLW2 44.50099945 W
PLW12 40.95999908 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 42.77999878 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: H170062_0001 PH MAS DVT 1000S6 BL1.3 N/C/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 (33.44 ppm), Noise (326.01 to 306.01 ppm) [708.9]



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_ 20201130
Time 17.11 h
INSTRUM Avance Neo 1GHz
PROBHD H170062_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 101.3731999 MHz
NUC1 15N
P15 3500.00 usec
PLW1 82.0000000 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 1.80 usec
PCPD2 3.40 usec
PLW2 44.50099945 W
PLW12 42.29999924 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 21.76000023 W

F2 - Processing parameters
SI 32768
SF 101.3696520 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

SHIM SEQUENCE

skip shimming

