

NMR Test Spectrometer

Report Name: 0.7mm_Install

AV NEO (1000 MHz) 408457

Content:

- Configuration Information ([uxnmr.info](#))
- IP Config Information
- Probe: H171374_0001 / 0.7mm_Install



● Configuration Information uxnmr.info

CONFIGURATION INFORMATION

=====

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

AQ-Rack:
- EPU/2: AV4 EPU/2 Embedded Processing Unit H153448F1/01415 ECL 01.04
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/04540 ECL 02.03
Location: slot 1 in rack 1
Connection: at IP 192.168.180.14 via PCIe #3
Firmware Version: 20190906112554
Devices: MTD at /dev/mtd2, DRX at /dev/bbu/drx3.5, RTD at /dev/bbu/rttd3.4
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/rttd4.4
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/rttd5.4
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/rttd6.4
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/rttd9.4, 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 17783935 bytes 5237485657 (4.8 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 21903954 bytes 3896344675 (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 1044849 bytes 193596947 (184.6 MiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 511671 bytes 93545450 (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 30176182 bytes 5107273481 (4.7 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 30176182 bytes 5107273481 (4.7 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
```

PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E

1000 MHz

Probe ID: H171374_0001

Inspection Lot: 0.7mm_Install

● Probe NMR Test Data: PH MASDVT1000S6 BL0.7 N/D/C/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] _____ 0.7

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

H171374_0001.ph

```
H171374_0001.ph
=====
$Bis,1,20200820,2048,PICS,5#
$Production,H171374,0001,00,00,,BNMRDE,20200818#
$Name,PH MASDVT1000S6 BLO-7 N/D/C/H NO_I/E#
$ProbeCompatibility,1.0,SB,6,1000#
$ProbeType,1.1,MAS,0,0#
$ProbeSample,1.0,0.7,0#
$ProbeTemperature,1.0,TypeT,-50,80#
$ProbeHeaterTemperature,1.0,TypeK,-274,600#
$ProbeGasFlow,1.0,,,,600,50,2000,,,#
$ProbeAllCoils,1.1,1,1#
$ProbeCoil,1.0,1,1.8,4,1H,13C/79Br,2H,15N#
$ProbeChannel,1.1,1H,,,,25,,,FALSE,,,,#
$ProbeChannel,1.1,13C/79Br,,,,30,,,,0,,,,#
$ProbeChannel,1.1,2H,,,,30,,,,0,,,,#
$ProbeChannel,1.1,15N,,,,60,,,,0,,,,#
$ProbeMas,1.0,40000,111000,0,0,0,0,0,0,0#
$EndBis,BE,F5#
```

● **Required Samples** PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E

Z163271	Potassium Bromide (KBr, 0.5 ul)
Z163274	Adamantane (0.5 ul)
Z163275	Alpha-glycine (0.5 ul)
Z163276	2-13C, 15N alpha-glycine (0.5 ul)

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_/E
Sample: Potassium Bromide (KBr, 0.5 ul) (Z163271)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 40000 Hz)

Line width main [achieved]: [147] <n/a>



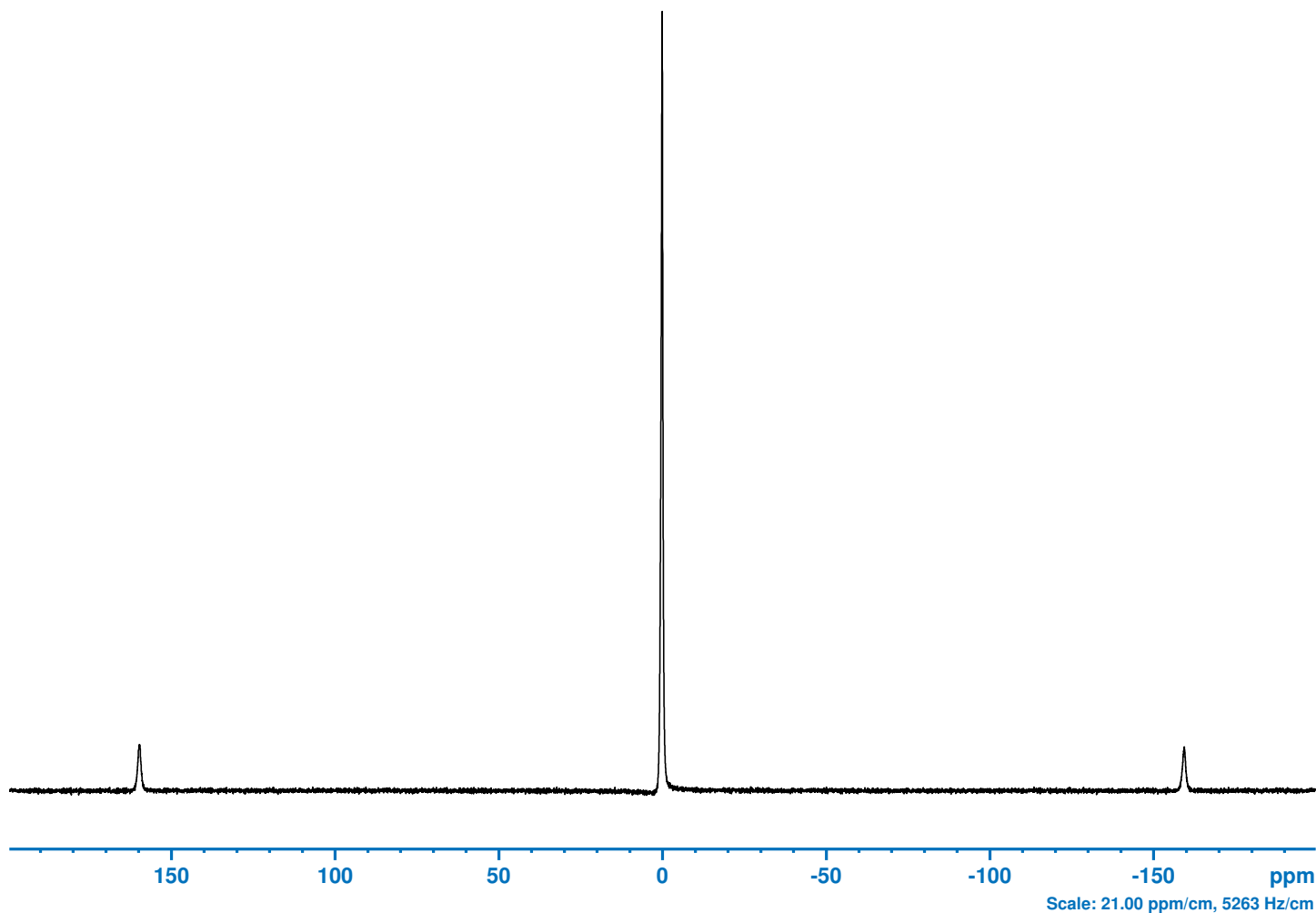
Bruker BioSpin

NPT_79Br_MAS_magicAngle

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

F2 - Acquisition Parameters
Date_     20201203
Time      12.59 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171374_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         311.0 K
D1         0.2500000 sec
SFO1       250.6551474 MHz
NUC1       79Br
P1         3.50 usec
PLW1       12.97900009 W

F2 - Processing parameters
SI         131072
SF         250.6551474 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: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
Sample: Potassium Bromide (KBr, 0.5 ul) (Z163271)
Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 111000 Hz)
Determination of spinning stability for 180 s
Pressure values in mbar: DrivePressure=3749/BearingPressure=2598/BearingSensePressure=2600/SupplyPressure=7070/SystemPressure=7291

Spin rate at maximum deviation [measured]: @ MASR 111000 Hz [111010 Hz]
Maximum deviation [achieved/rated]: @ MASR 111000 Hz [10 Hz <= 111 Hz] <pass>



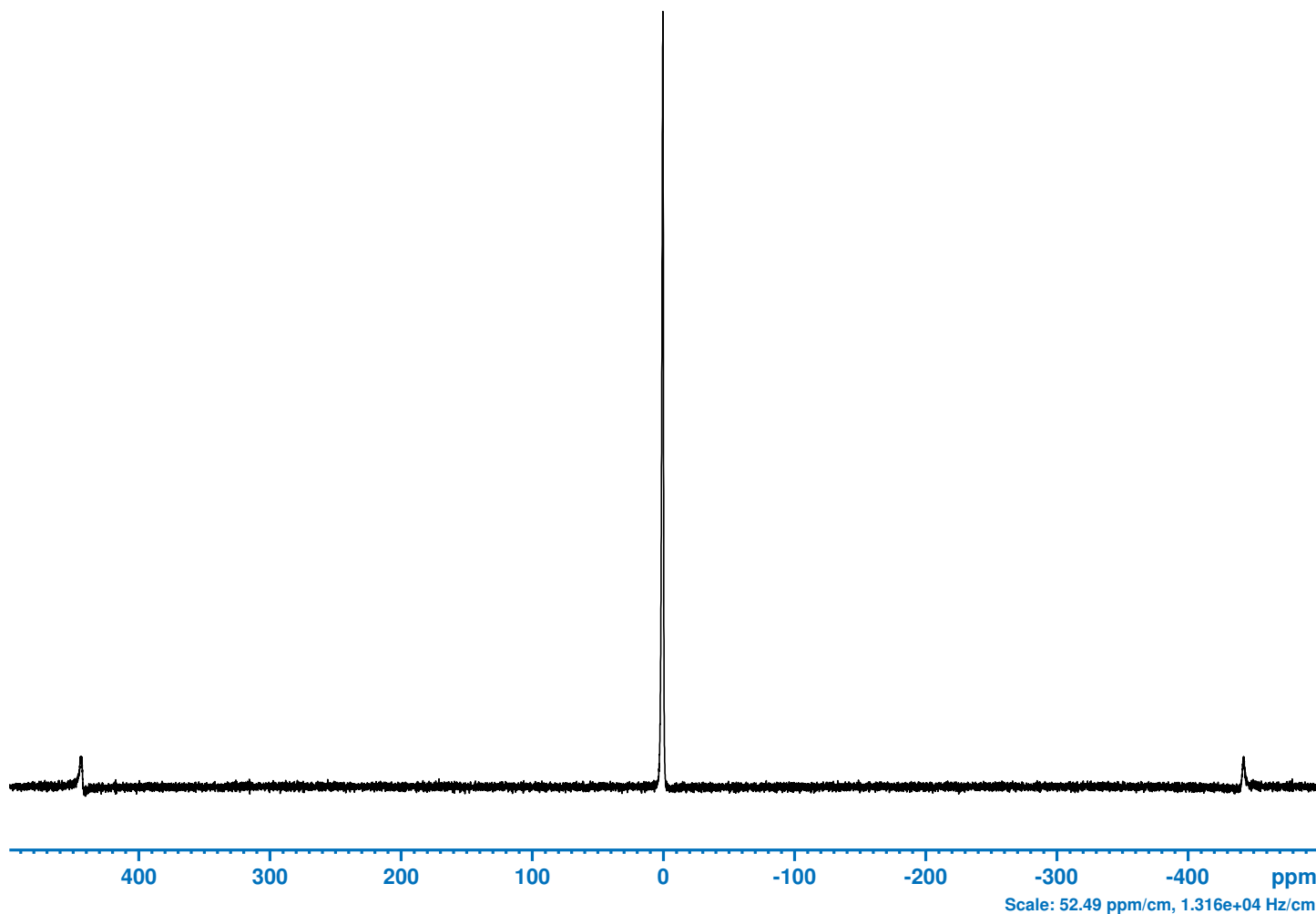
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

Current Data Parameters
NAME NPT_79Br_MAS_maxSpinRate
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201203
Time 13.23 h
INSTRUM Avance Neo 1GHz
PROBHD H171374_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 311.0 K
D1 0.25000000 sec
SFO1 250.6548162 MHz
NUC1 79Br
P1 3.50 usec
PLW1 12.97900009 W

F2 - Processing parameters
SI 32768
SF 250.6548162 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: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_1/E
Sample: Potassium Bromide (KBr, 0.5 ul) (Z163271)
Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting, spin rate 40000 Hz)
FIELD was set to 2093.9 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0070 ppm.



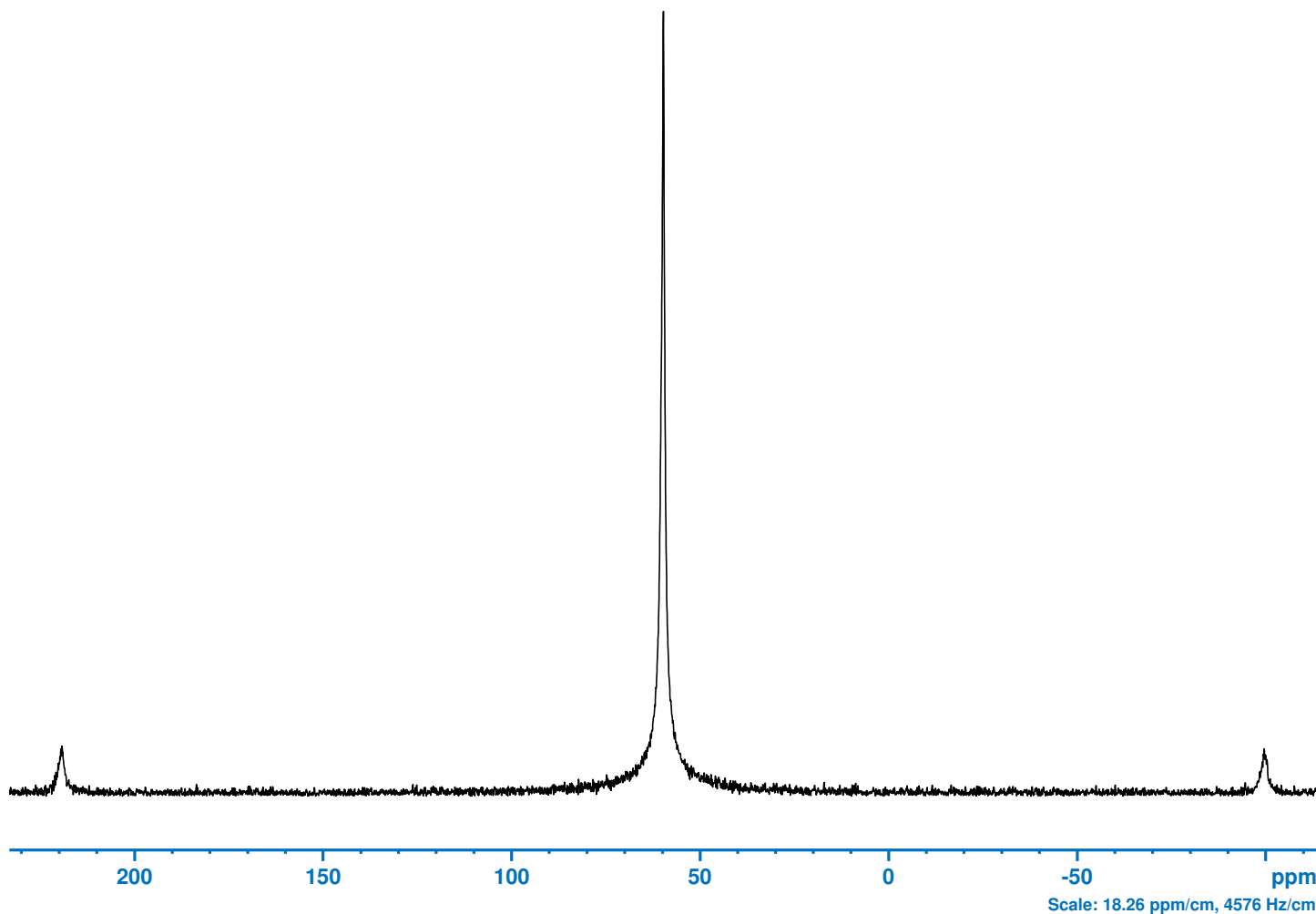
Bruker BioSpin

NPT_79Br_MAS_fieldsetting

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

F2 - Acquisition Parameters
Date_     20201203
Time      13.00 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171374_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         311.0 K
D1         0.5000000 sec
SFO1      250.6549791 MHz
NUC1       79Br
P1         3.50 usec
PLW1      12.97900009 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: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
Sample: Adamantane (0.5 ul) (Z163274)
Optimization of 13C frequency (NPT_13C_MAS_fieldsetting_dec1h, spin rate 80000 Hz)
FIELD was set to 1982.4 for 13C chemical shift of 38.460 ppm. One field unit corresponds to 0.0071 ppm.



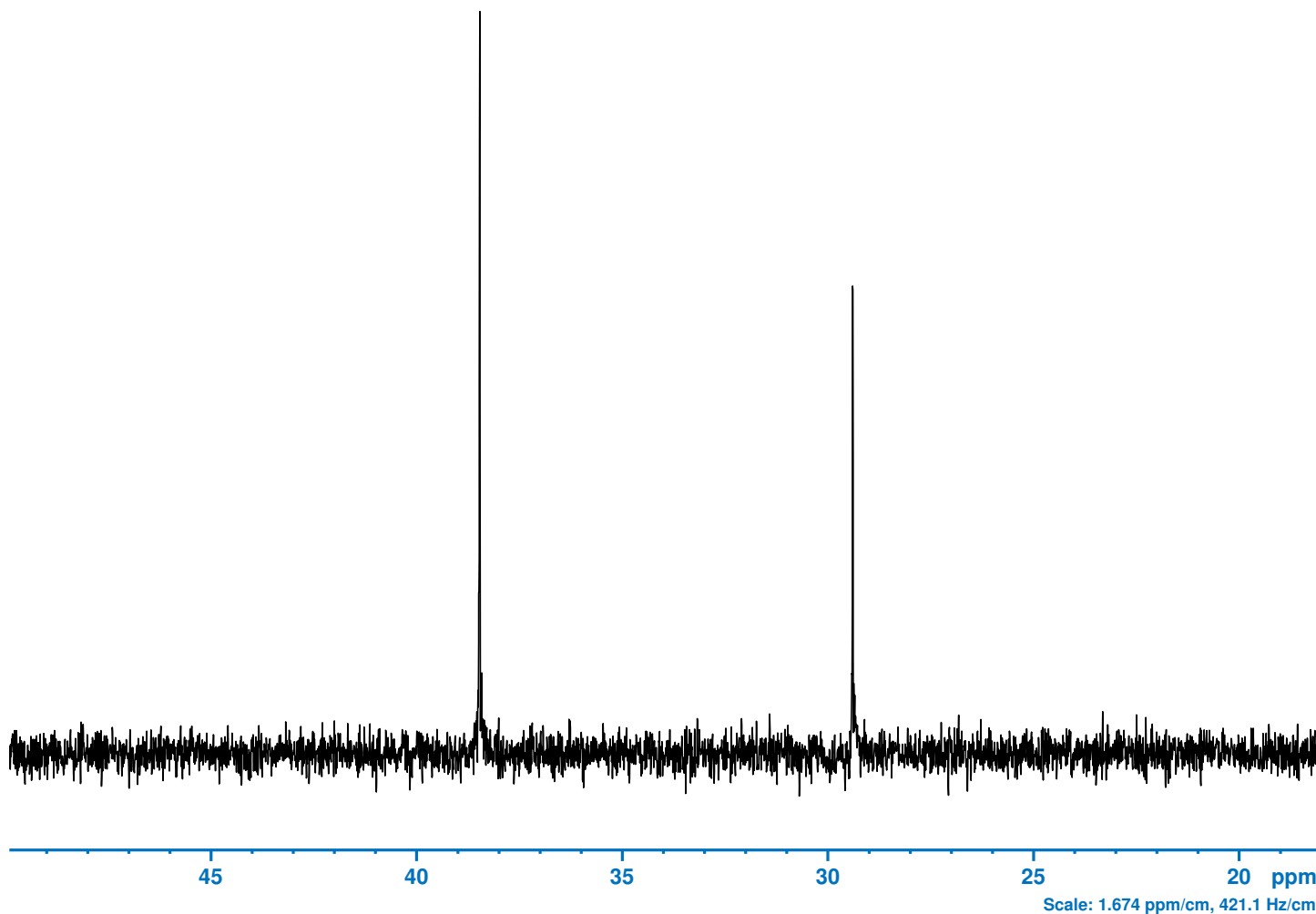
Bruker BioSpin

NPT_13C_MAS_fieldsetting_dec1h

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

F2 - Acquisition Parameters
Date_     20201203
Time      14.31 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171374_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         311.0 K
D1         15.0000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1      251.5593320 MHz
NUC1       13C
P1         3.00 usec
PLW1       17.11700058 W
SFO2      1000.4023669 MHz
NUC2       1H
CPDPRG2    cw
PLW2       14.00800037 W
PLW12      0.20171520 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

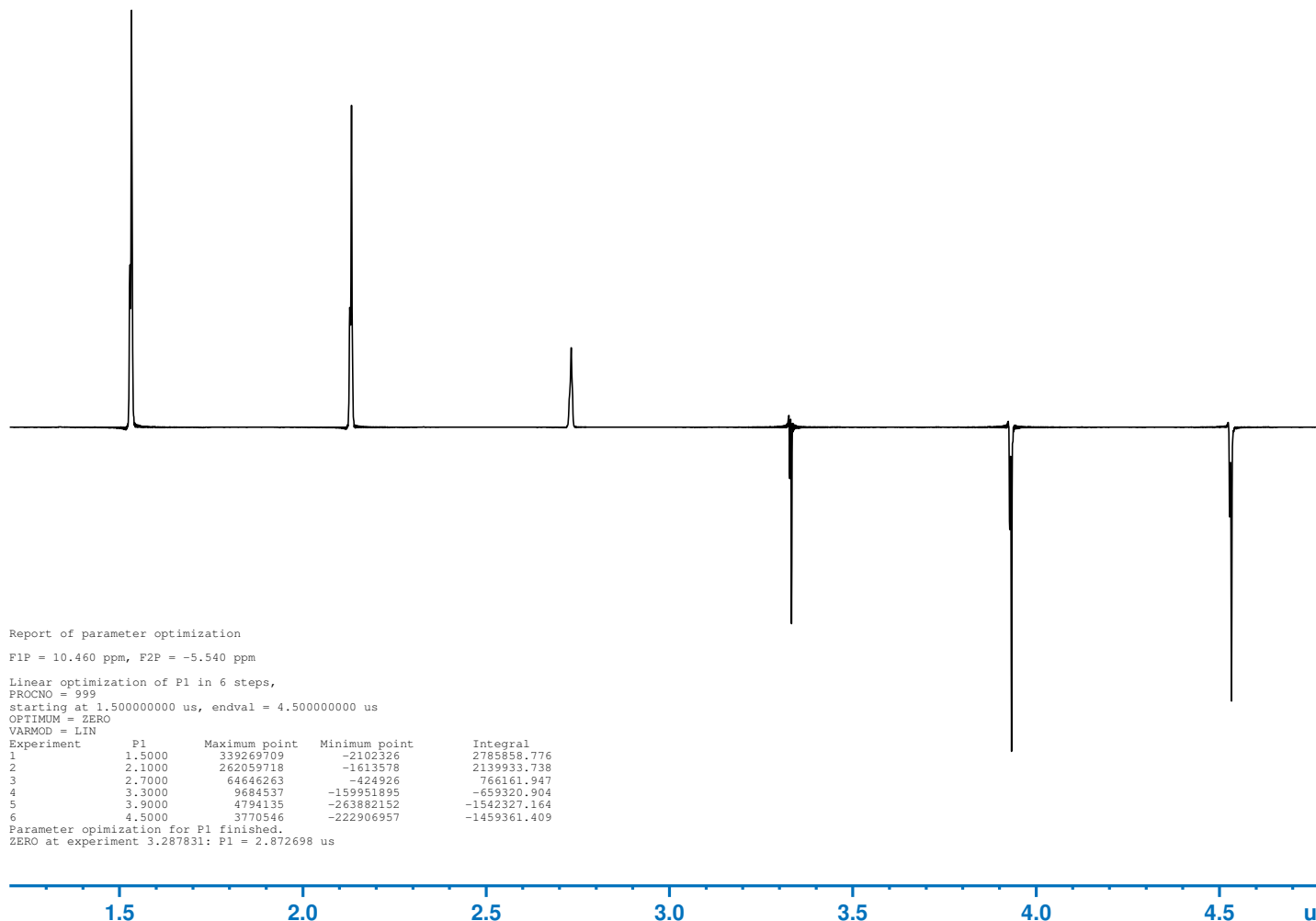
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
 Sample: Adamantane (0.5 ul) (Z163274)
 P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 80000 Hz)
 ATTENTION: Updated PROSOL Tables with [1.50 us @ 14.0 W].



Bruker BioSpin

P90 MAS 1H pulse [achieved/rated]: @ 15.2 W [1.44 us <= 1.50 us] <pass>

NPT_1H_MAS_p90det_1h



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

F2 - Acquisition Parameters
Date_     20201203
Time      14.18 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171374_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         311.0 K
D1         5.00000000 sec
SFO1      1000.4024610 MHz
NUC1       1H
P1         4.50 usec
PLW1      15.19999981 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
-----
15.2 W     1.50 us     1.44 us     -4.0%
```

Report of parameter optimization

F1P = 10.460 ppm, F2P = -5.540 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	339269709	-2102326	2785858.776
2	2.1000	262059718	-1613578	2139933.738
3	2.7000	64646263	-424926	766161.947
4	3.3000	9684537	-159951895	-659320.904
5	3.9000	4794135	-263882152	-1542327.164
6	4.5000	3770546	-222906957	-1459361.409

Parameter optimization for P1 finished.

ZERO at experiment 3.287831: P1 = 2.872698 us

 SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_1/E
 Sample: Potassium Bromide (KBr, 0.5 ul) (Z163271)
 P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br, spin rate 40000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.50 us @ 13.0 W].

P90 MAS 79Br pulse [achieved/rated]: @ 14.0 W [3.37 us <= 3.50 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 3.500000000 us, endval = 10.500000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	3.5000	407091330	-2717995	15659752.243
2	4.9000	281782347	-3271586	11461125.466
3	6.3000	81445987	-3685336	3516568.932
4	7.7000	25238132	-172080257	-4880682.854
5	9.1000	7044007	-278703772	-8625851.903
6	10.5000	3279331	-226008128	-7278395.068

Parameter optimization for P1 finished.

ZERO at experiment 3.321253: P1 = 6.749754 us

Current Data Parameters
 NAME NPT_79Br_MAS_p90det_79br
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20201203
 Time 12.58 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171374_0001 ()
 PULPROG onepulse
 TD 4000
 SOLVENT CDC13
 NS 1
 DS 0
 SWH 200000.000 Hz
 FIDRES 100.000000 Hz
 AQ 0.0100000 sec
 RG 101
 DW 2.500 usec
 DE 6.500 usec
 TE 311.0 K
 D1 0.25000000 sec
 SFO1 250.6549791 MHz
 NUC1 79Br
 P1 10.50 usec
 PLW1 14.00000000 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
14.0 W	3.50 us		
14.0 W	3.50 us	3.37 us	-3.7%

 SHIM SEQUENCE

 skip shimming



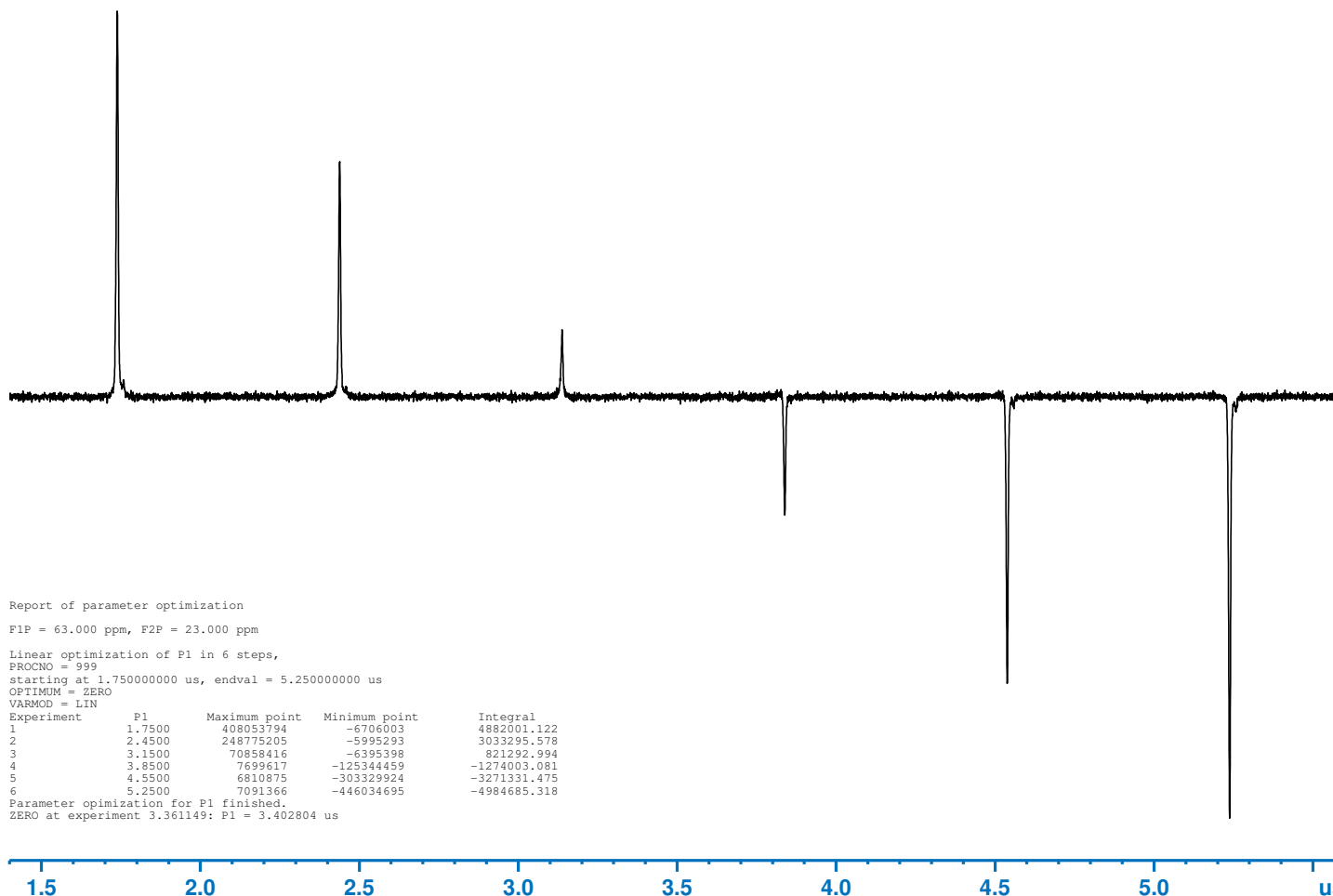
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (0.5 ul) (Z163276)
 P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c, spin rate 40000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.50 us @ 11.9 W].



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P90_MAS_CP 1H13C power (PLW 11) [achieved]: [12.6 W] <n/a>
 P90_MAS_CP 1H13C pulse (P 1) [achieved/rated]: [3.40 us <= 3.50 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_ 20201203
 Time 14.54 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171374_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 311.0 K
 D1 5.00000000 sec
 ZGPTNS
 SFO1 251.5615968 MHz
 NUC1 13C
 P1 5.25 usec
 P15 2000.00 usec
 PLW1 12.57575989 W
 PLW11 12.57575989 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 1.50 usec
 PCPD2 2.80 usec
 PLW2 14.00800037 W
 PLW12 14.00800037 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 23.91695023 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

 17.1 W 3.00 us
 12.6 W 3.50 us 3.40 us -2.9%

Report of parameter optimization

F1P = 63.000 ppm, F2P = 23.000 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	408053794	-6706003	4882001.122
2	2.4500	248775205	-5995293	3033295.578
3	3.1500	70858416	-6395398	821292.994
4	3.8500	7699617	-125344459	-1274003.081
5	4.5500	6810875	-303329924	-3271331.475
6	5.2500	7091366	-446034695	-4984685.318

Parameter optimization for P1 finished.

ZERO at experiment 3.361149: P1 = 3.402804 us

 SHIM SEQUENCE

 skip shimming

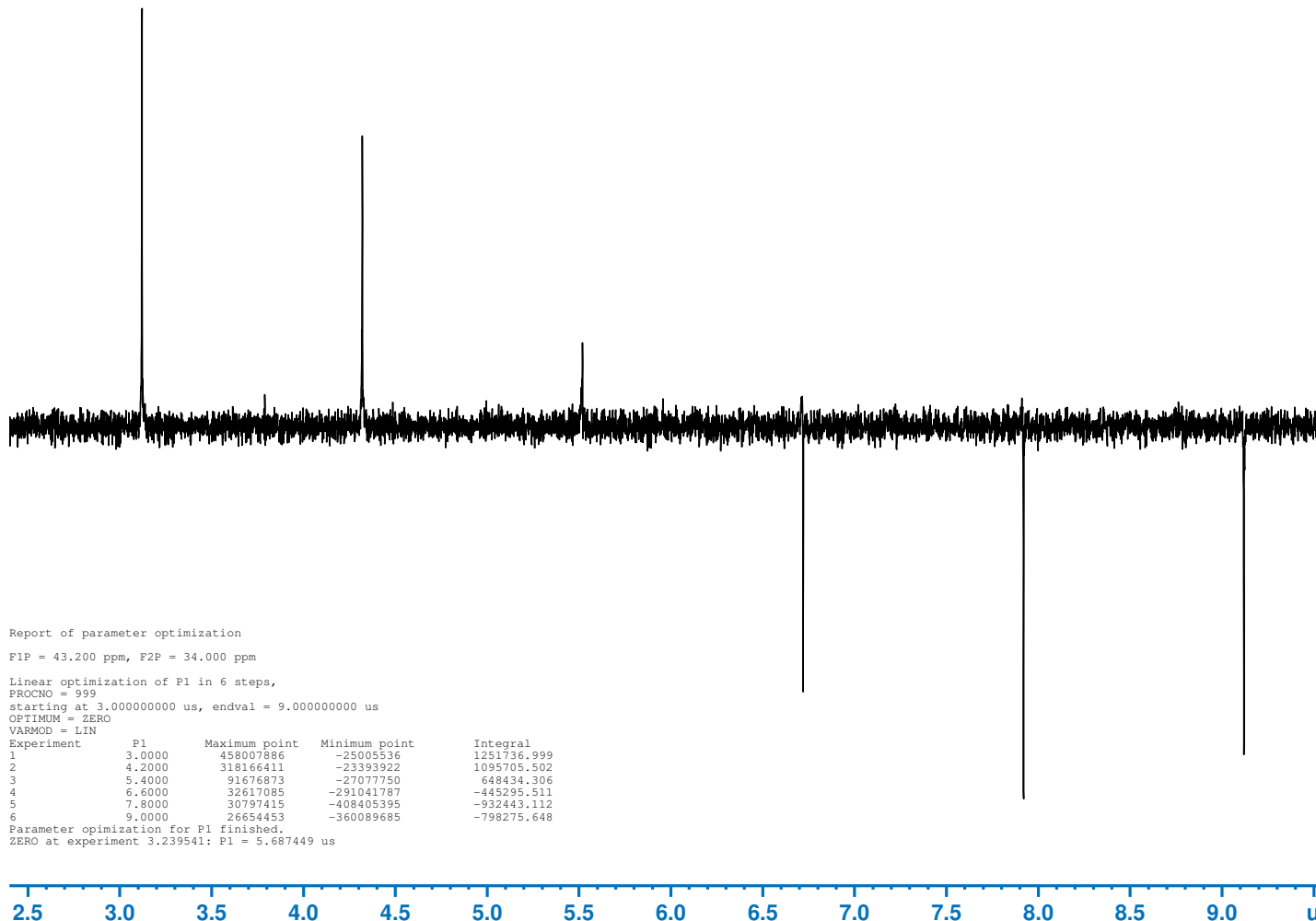
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
 Sample: Adamantane (0.5 ul) (Z163274)
 P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c, spin rate 80000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.00 us @ 17.1 W].



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P90 MAS 13C pulse [achieved/rated]: @ 19.1 W [2.84 us <= 3.00 us] <pass>

NPT_13C_MAS_p90det_13c



Current Data Parameters
 NAME NPT_13C_MAS_p90det_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201203
 Time 14.26 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171374_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 311.0 K
 D1 15.00000000 sec
 P15 0 usec
 ZGPTNS -D1acq
 SFO1 251.5593328 MHz
 NUC1 13C
 P1 9.00 usec
 PLW1 19.10000038 W
 SFO2 1000.4024610 MHz
 NUC2 1H
 CPDPRG2 cw
 PLW2 14.00800037 W
 PLW12 0.20171520 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

 19.1 W 3.00 us
 19.1 W 3.00 us 2.84 us -5.3%

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	458007886	-25005536	1251736.999
2	4.2000	318166411	-23393922	1095705.502
3	5.4000	91676873	-27077750	648434.306
4	6.6000	32617085	-291041787	-445295.511
5	7.8000	30797415	-408405395	-932443.112
6	9.0000	26654453	-360089685	-798275.648

Parameter optimization for P1 finished.

ZERO at experiment 3.239541: P1 = 5.687449 us

 SHIM SEQUENCE

 skip shimming

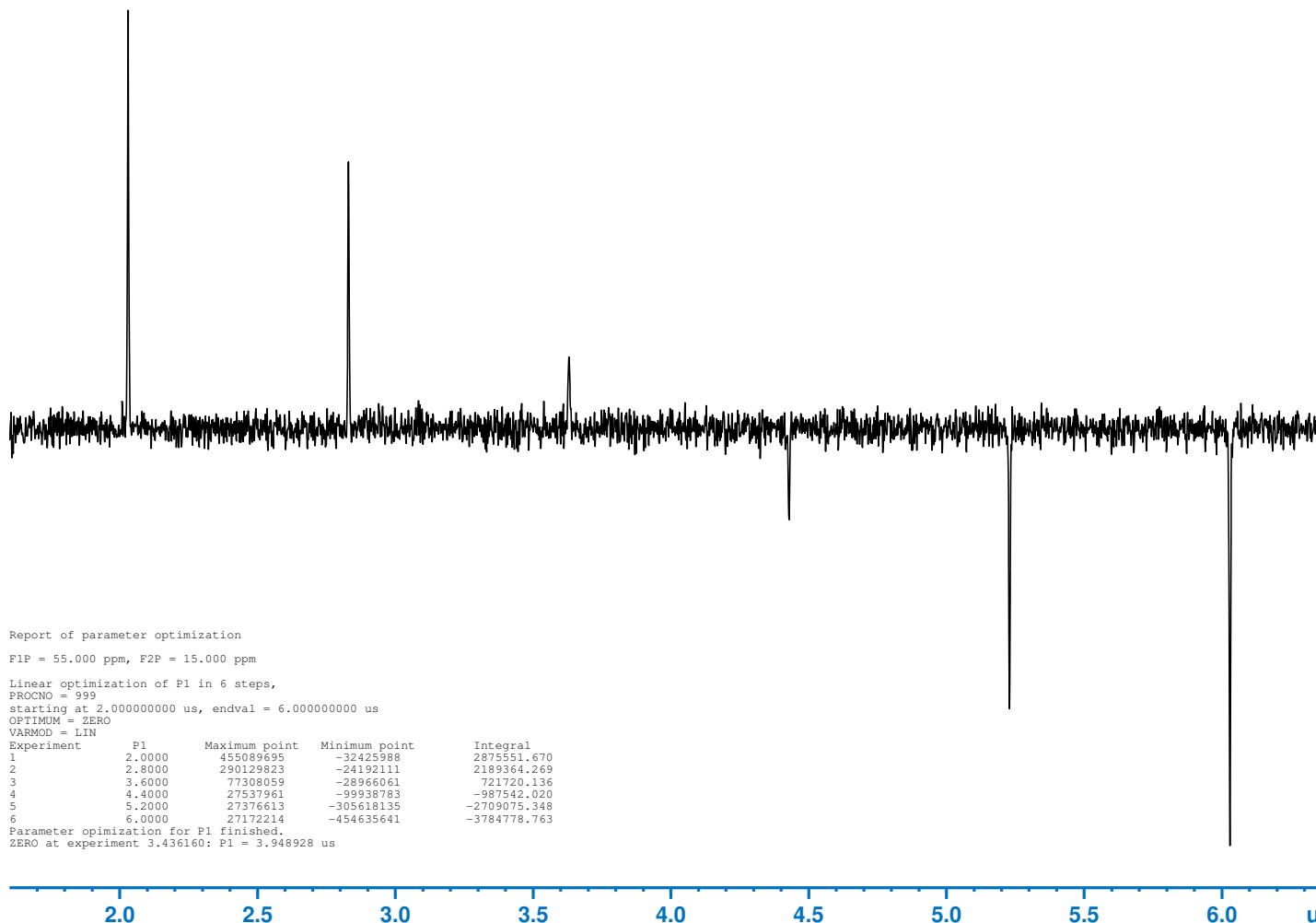
NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
 Probe: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (0.5 ul) (Z163276)
 P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n, spin rate 40000 Hz)
 ATTENTION: Updated PROSOL Tables with [4.00 us @ 49.9 W].



P90_MAS_CP 1H15N power (PLW 11) [achieved]: [51.2 W] <n/a>
 P90_MAS_CP 1H15N pulse (P 1) [achieved/rated]: [3.95 us <= 4.00 us] <pass>

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NPT_15N_MAS_p90det_cp1h_15n



Current Data Parameters
 NAME NPT_15N_MAS_p90det_cp1h_15n
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201203
 Time 15.16 h
 INSTRUM Avance Neo 1GHz
 PROBHD H171374_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 311.0 K
 D1 5.00000000 sec
 ZGPGTNS
 SFO1 101.3731996 MHz
 NUC1 15N
 P1 6.00 usec
 P15 3500.00 usec
 PLW1 24.20000076 W
 PLW11 51.17245102 W
 SFO2 1000.4062025 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal164
 P3 1.50 usec
 PCPD2 2.80 usec
 PLW2 14.00800037 W
 PLW12 14.00800037 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 8.40368843 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

 20.0 W 4.40 us
 24.2 W 4.00 us 5.69 us 42.2%
 51.2 W 4.00 us 3.95 us -1.2%

 SHIM SEQUENCE

skip shimming

Report of parameter optimization

F1P = 55.000 ppm, F2P = 15.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 2.000000000 us, endval = 6.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.0000	455089695	-32425988	2875551.670
2	2.8000	290129823	-24192111	2189364.269
3	3.6000	77308059	-28966061	721720.136
4	4.4000	27537961	-99938783	-987542.020
5	5.2000	27376613	-305618135	-2709075.348
6	6.0000	27172214	-454635641	-3784778.763

Parameter optimization for P1 finished.

ZERO at experiment 3.436160: P1 = 3.948928 us

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
Sample: Alpha-glycine (0.5 ul) (Z163275)
CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c, spin rate 40000 Hz)

SINO (20.0 ppm) [achieved]: Signal (42.49 ppm), Noise (16.19 to -3.81 ppm) [7.0] <n/a>
Number of scans (NS) [achieved/rated]: [64 <= 64] <pass>
Processed with TDef=2048



Bruker BioSpin

NPT_13C_MAS_sino_cp1h_13c

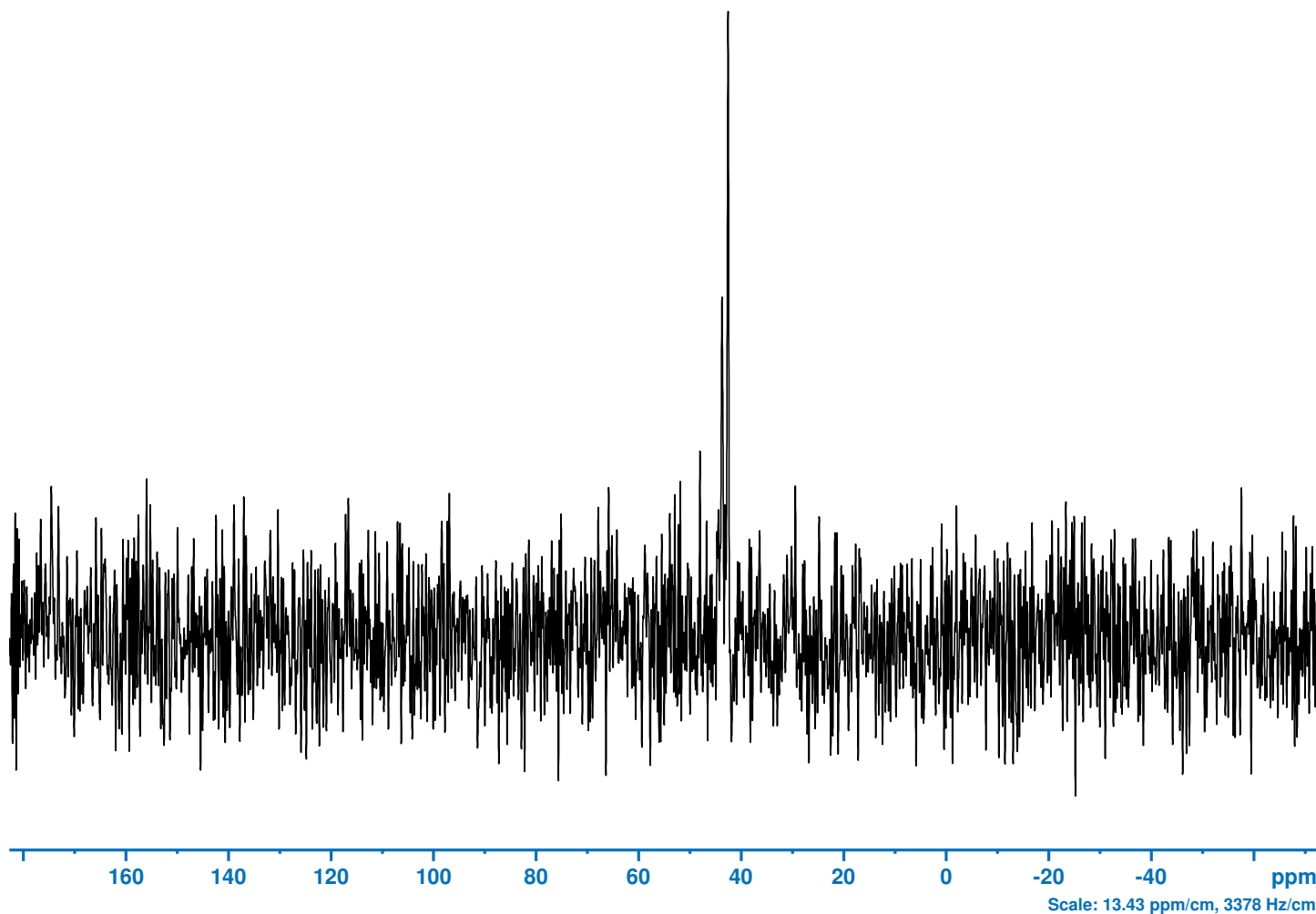
Current Data Parameters
NAME NPT_13C_MAS_sino_cp1h_13c
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201203
Time 17.24 h
INSTRUM Avance Neo 1GHz
PROBHD H171374_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 311.0 K
D1 5.0000000 sec
ZGPTNS
SF01 251.5646560 MHz
NUC1 13C
P15 2000.00 usec
PLW1 11.86699963 W
SF02 1000.4022832 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 1.50 usec
PCPD2 2.80 usec
PLW2 14.00800037 W
PLW12 14.00000000 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 16.70000076 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: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
Sample: Adamantane (0.5 ul) (Z163274)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 80000 Hz)



Bruker BioSpin

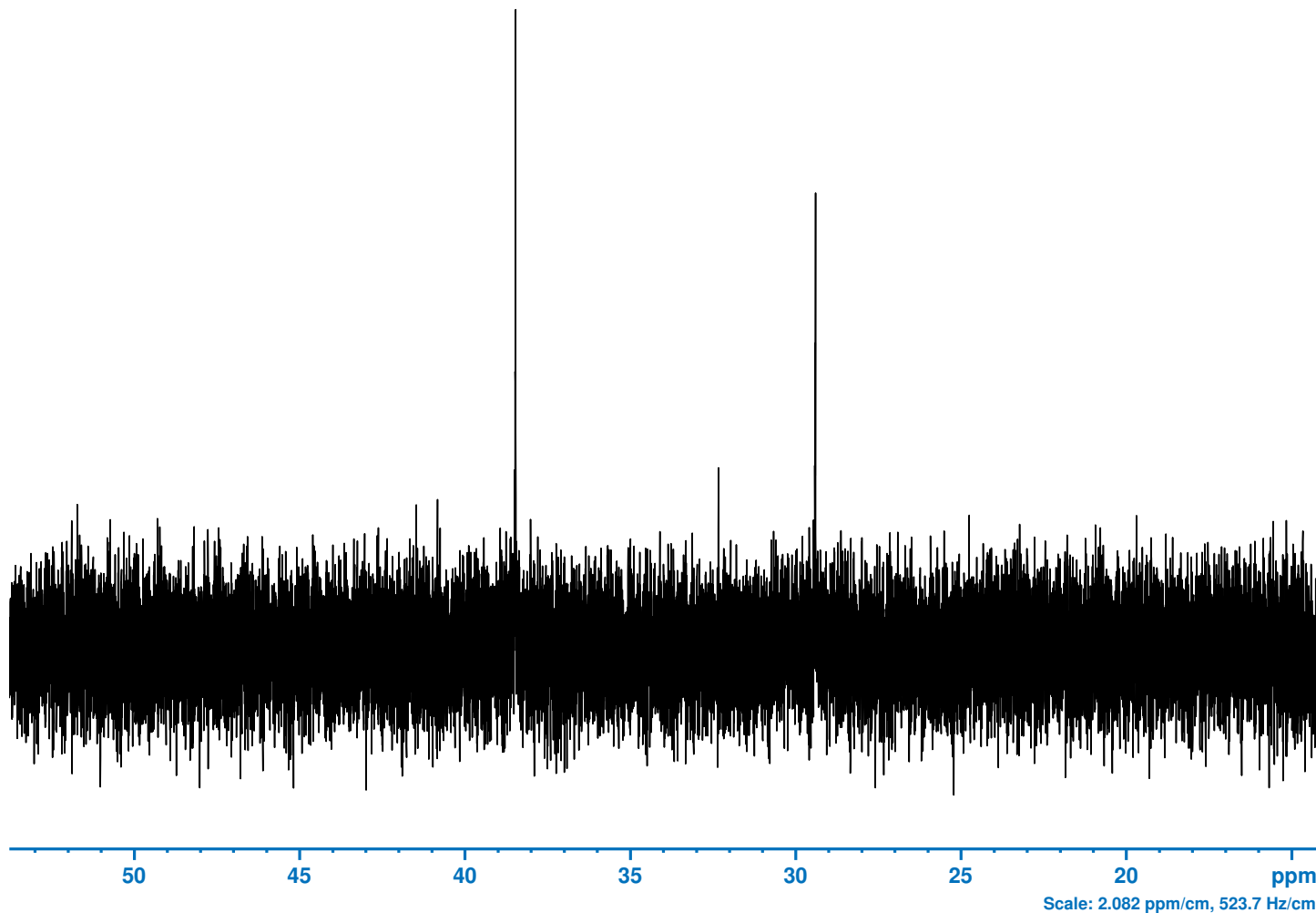
SINO (20.0 ppm) [achieved]: Signal (38.46 ppm), Noise (35.85 to 15.85 ppm) [8.2] <n/a>
Linewidth [achieved/rated]: at 50% of signal height [3.5 Hz <= 7.0 Hz] <pass>
Number of scans (NS) [achieved]: [1] <n/a>

NPT_13C_MAS_sino_13c

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

F2 - Acquisition Parameters
Date_     20201203
Time      14.31 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171374_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         311.0 K
D1         15.0000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1      251.5593320 MHz
NUC1       13C
P1         3.00 usec
PLW1      17.11700058 W
SFO2      1000.4024610 MHz
NUC2       1H
CPDPRG2   cw
PLW2      14.00800037 W
PLW12     0.20171520 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: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
 Sample: Adamantane (0.5 ul) (Z163274)
 13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 80000 Hz)



Bruker BioSpin

NPT_13C_MAS_sino_13c

```
# Thu Dec 3 14:31:57 2020
##$PROBEIDENTIFIER=H171374_0001
##$PROBENAME=PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
##$SHIMID=292722
#
# Active Shim Gradients
#
Z          14000
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)    10000
(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      1982.430
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] 6789.99999496
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] 6803.84359663
SHIM_SETTING [ 4] -0.00000000
SHIM_SETTING [ 5] 2450.80897032
SHIM_SETTING [ 6] -2450.80897032
SHIM_SETTING [ 7] -6803.84359663
SHIM_SETTING [ 8] 6803.84359663
SHIM_SETTING [ 9] 370.71790051
SHIM_SETTING [10] -370.71790051
SHIM_SETTING [11] 0.00000000
SHIM_SETTING [12] 0.00000000
SHIM_SETTING [13] -0.00000000
SHIM_SETTING [14] -0.00000000
SHIM_SETTING [15] -0.00001596
SHIM_SETTING [16] -0.00000142
SHIM_SETTING [17] -0.00001311
SHIM_SETTING [18] -0.00000614
SHIM_SETTING [19] -0.00000584
SHIM_SETTING [20] -0.00000327
SHIM_SETTING [21] 6469.42854435
SHIM_SETTING [22] 6469.42854435
SHIM_SETTING [23] 9999.99999928
SHIM_SETTING [24] 9999.99999928
SHIM_SETTING [25] 3911.73623683
SHIM_SETTING [26] 3911.73623683
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_     20201203
Time      14.31 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171374_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         311.0 K
D1         15.0000000 sec
P15        0 usec
ZGPTNS    -D1acq
SFO1       251.559328 MHz
NUC1       13C
P1         3.00 usec
PLW1       17.11700058 W
SFO2       1000.4024610 MHz
NUC2       1H
CPDPRG2    cw
PLW2       14.00800037 W
PLW12      0.20171520 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: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
Sample: Adamantane (0.5 ul) (Z163274)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 80000 Hz)

SINO (20.0 ppm) [achieved]: Signal (2.38 ppm), Noise (-27.27 to -47.27 ppm) [4812.8] <n/a>
Linewidth [achieved]: at 50% of signal height [93.1 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>



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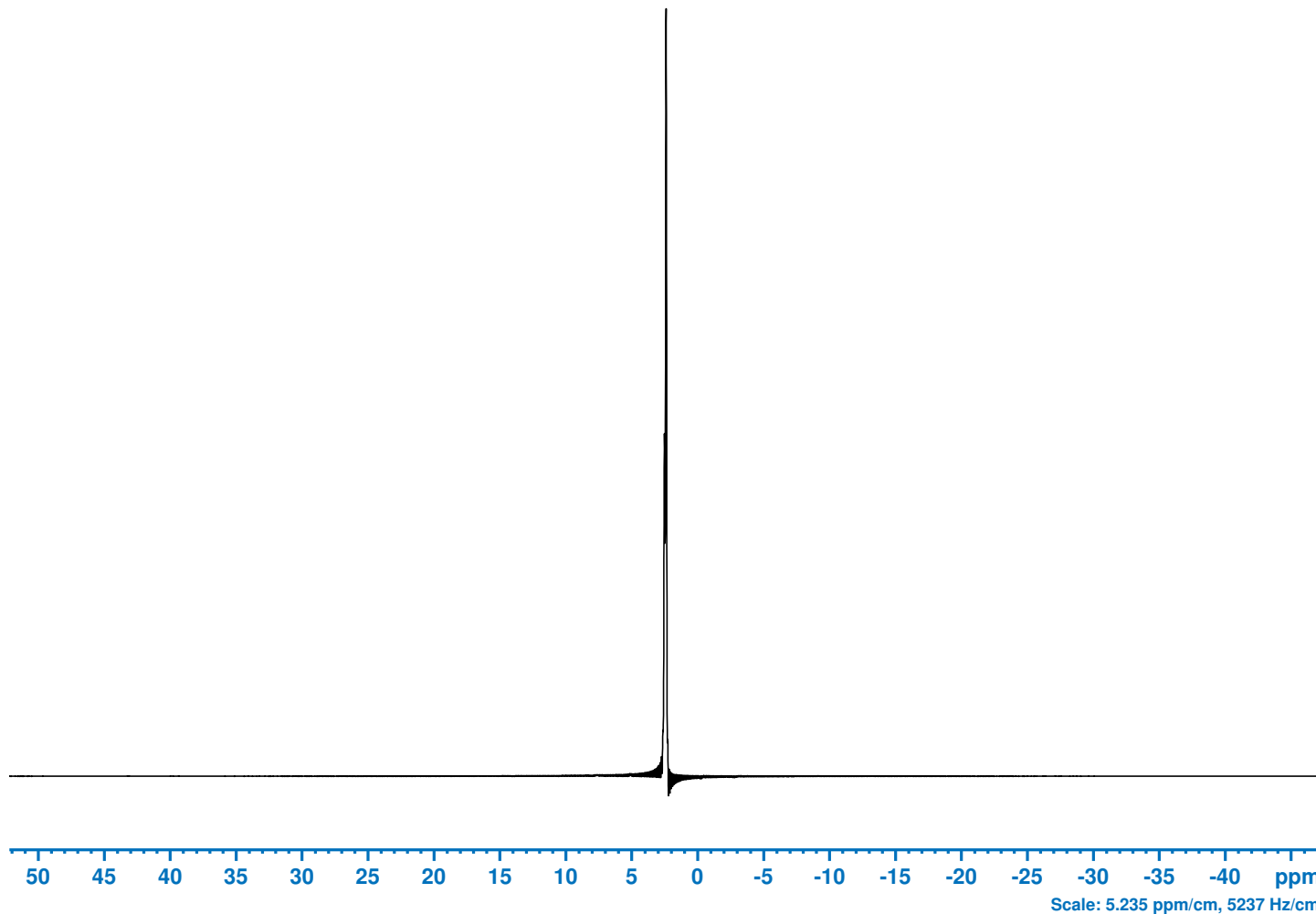
NPT_1H_MAS_sino_1h

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

F2 - Acquisition Parameters
Date_     20201203
Time      14.31 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171374_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         311.0 K
D1         5.0000000 sec
SFO1      1000.4024610 MHz
NUC1       1H
P1         1.50 usec
PLW1      14.00800037 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: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
 Sample: 2-13C, 15N alpha-glycine (0.5 ul) (Z163276)
 Double CP 1H-15N-13C, MAS (NPT_13C_MAS_double_cp1h15n_13c, spin rate 40000 Hz)



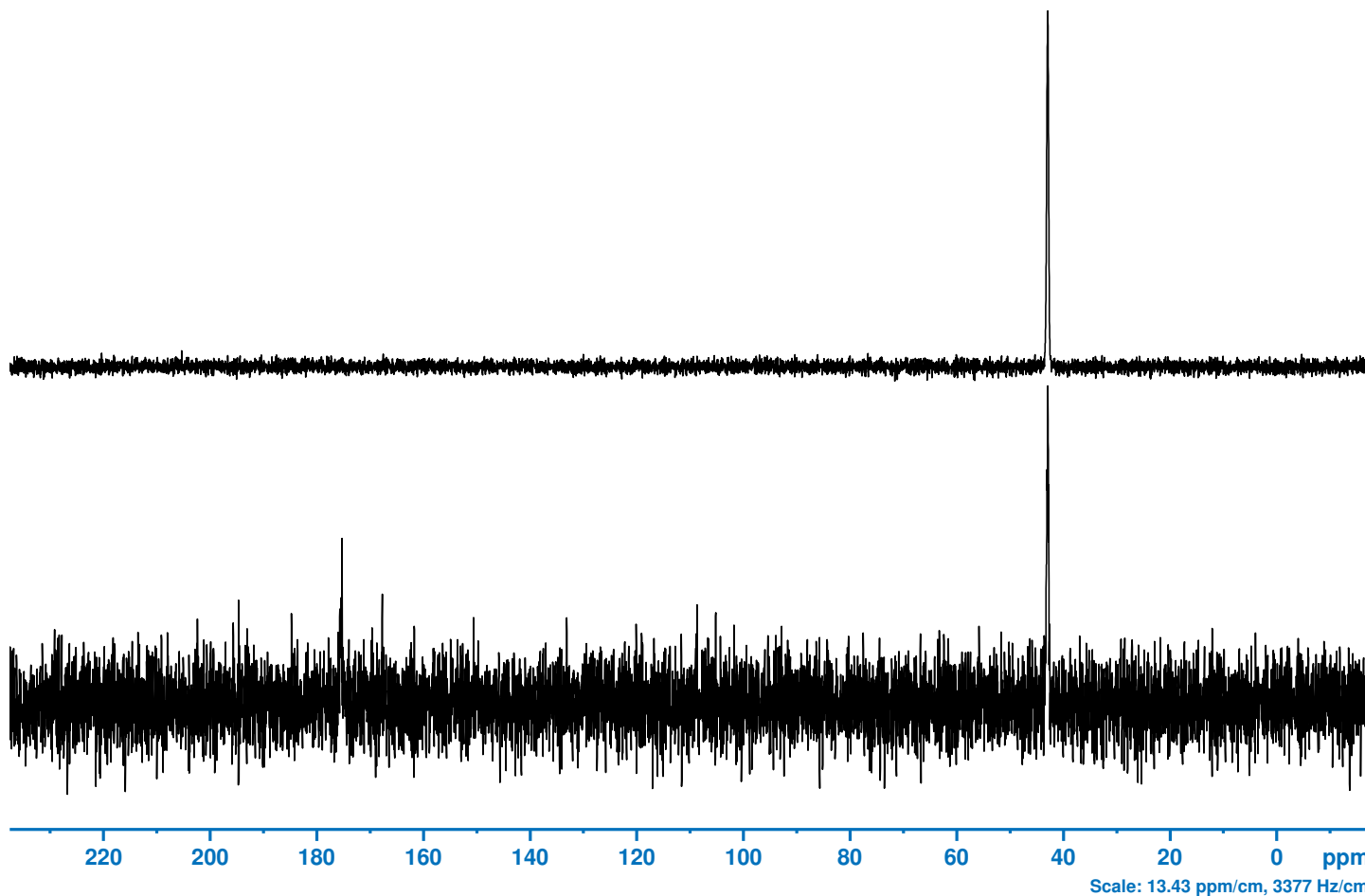
Bruker BioSpin

Contact time P15: [9000.0 us]
 Contact time P16: [10000.0 us]
 Transfer efficiency for C-alpha of double CP vs. 1H 13C CP experiment [achieved]: [715.5%] <n/a>
 Double CP C-alpha: SINO (20.0 ppm) = 50.8, Signal (42.88 ppm), Noise (159.20 to 139.20 ppm)
 1H 13 CP C-alpha: SINO (20.0 ppm) = 7.1, Signal (42.87 ppm), Noise (149.40 to 129.40 ppm)
 Double CP carboxyl: SINO (20.0 ppm) = 1.8, Signal (85 to 65 ppm), Noise (159.20 to 139.20 ppm)
 1H 13 CP carboxyl: SINO (20.0 ppm) = 3.7, Signal (85 to 65 ppm), Noise (149.40 to 129.40 ppm)

NPT_13C_MAS_double_cp1h15n_13c

```
Current Data Parameters
NAME      NPT_13C_MAS_double_cp1h15n_13c
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20201215
Time      10.05 h
INSTRUM   Avance Neo 1GHz
PROBHD    H171374_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         311.0 K
CNST11    1.0000000
DQ         0.00000300 sec
D1         5.00000000 sec
IN0        0 sec
LO         0
SFO1      251.5784507 MHz
NUC1       13C
CNST9     110.0000000
CNST10    40.0000000
P1         18.75 usec
P2         37.50 usec
P16        10000.00 usec
PLW1       0.41349900 W
PLW11      0.41349900 W
SPNAM[1]   tacn80
SPOAL1     0.500
SPOFFS1    0 Hz
SPW1       0.50000000 W
SFO2       1000.4062025 MHz
NUC2        1H
CNST21     0
CNST24     1.0000000
CPDPRG[2]  spinal64
P3         1.50 usec
P15        9000.00 usec
PCPD2      2.80 usec
PLW2        0 W
PLW12      14.00800037 W
PLW13      12.31999969 W
SPNAM[0]   ramp.100
SPOAL0     0.500
SPOFFS0    0 Hz
SPW0       14.00000000 W
SFO3       101.3731996 MHz
NUC3        15N
PLW3       49.90100098 W
PLW5       9.08419991 W
```



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

NMR TEST ACCEPTANCE *** System: AV NEO (1000.40 MHz) *** TopSpin 4.0.9
Probe: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
Sample: 2-13C, 15N alpha-glycine (0.5 ul) (Z163276)
CP 1H-13C parameter optimization, MAS (NPT_13C_MAS_paropt_cp1h_13c, spin rate 40000 Hz)

SINO (20.0 ppm): Signal (43.62 ppm), Noise (120.02 to 100.02 ppm) [378.4]
Processed with TDef=2048



Bruker BioSpin

NPT_13C_MAS_paropt_cp1h_13c

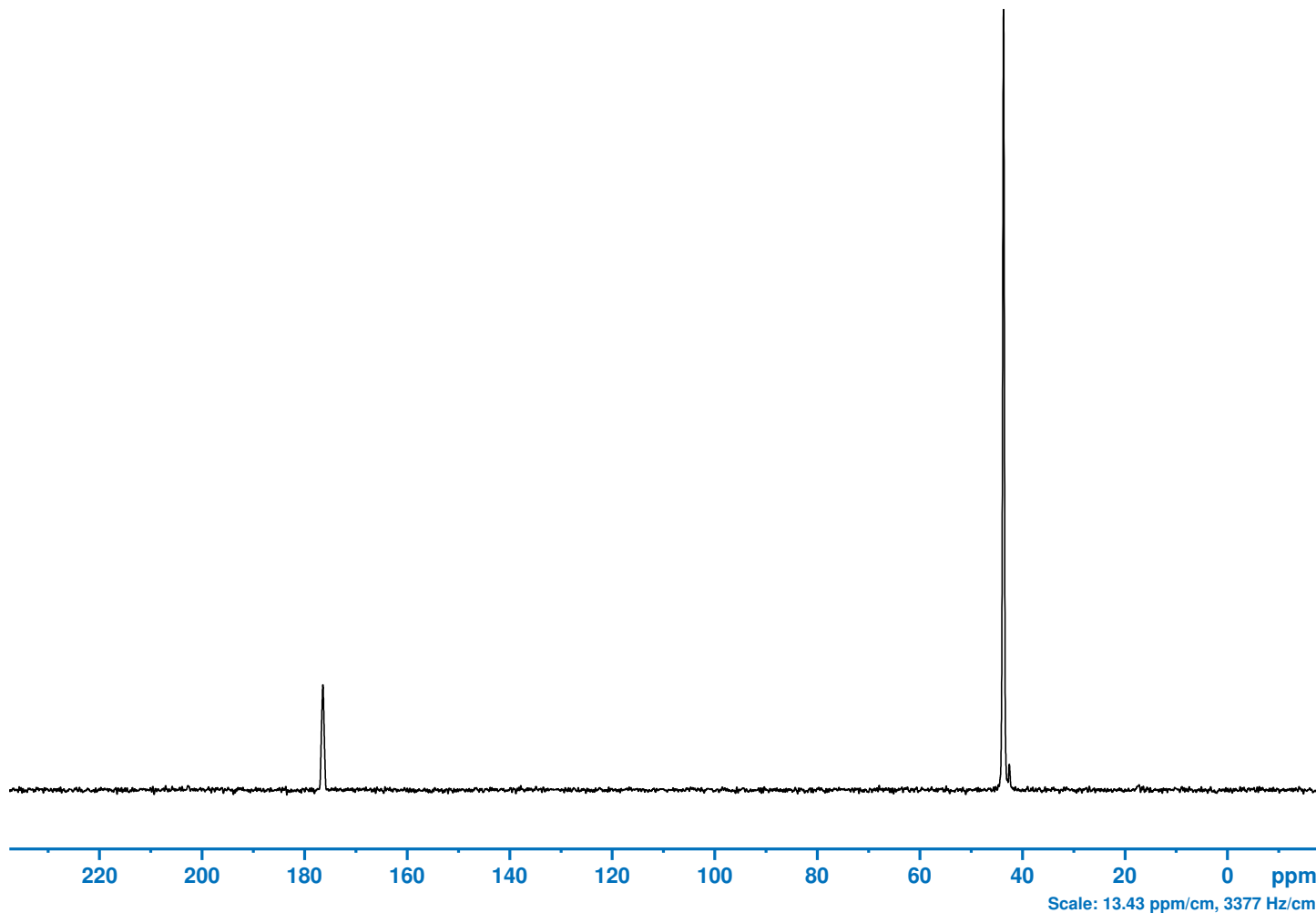
Current Data Parameters
NAME NPT_13C_MAS_paropt_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201203
Time 15.04 h
INSTRUM Avance Neo 1GHz
PROBHD H171374_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 311.0 K
D1 5.0000000 sec
ZGPTNS
SF01 251.5784507 MHz
NUC1 13C
P15 2000.00 usec
PLW1 11.86699963 W
SF02 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 1.50 usec
PCPD2 2.80 usec
PLW2 14.00800037 W
PLW12 15.11999989 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 16.70000076 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: H171374_0001 PH MASDVT1000S6 BL0.7 N/D/C/H NO_I/E
Sample: 2-13C, 15N alpha-glycine (0.5 ul) (Z163276)
CP 1H-15N parameter optimization, MAS (NPT_15N_MAS_paropt_cp1h_15n, spin rate 40000 Hz)

SINO (20.0 ppm): Signal (33.42 ppm), Noise (-261.54 to -281.54 ppm) [119.1]



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_ 20201203
Time 15.27 h
INSTRUM Avance Neo 1GHz
PROBHD H171374_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 311.0 K
D1 5.0000000 sec
ZGPTNS
SFO1 101.3731996 MHz
NUC1 15N
P15 3500.00 usec
PLW1 49.90100098 W
SFO2 1000.4062025 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 1.50 usec
PCPD2 2.80 usec
PLW2 14.00800037 W
PLW12 12.88000011 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 14.10000038 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

