

# **NMR Test Spectrometer**

## **Report Name: 2023-07-13**

### **AV NEO (750 MHz) 442759**

**Content:**

- Configuration Information ([uxnmr.info](http://uxnmr.info))
- IP Config Information
- Probe: H8780\_0002 / 2023-07-12

**Jul 13, 2023**

**NMR TEST SERVICE**



## ● Configuration Information [uxnmr.info](http://uxnmr.info)

### CONFIGURATION INFORMATION

=====

```
Path      : /opt/topspin/conf/instr/spect/uxnmr.info
Date      : Wed Jun 28 12:20:24 2023
Release   : TopSpin 4.1.3
Installed in : /opt/topspin
Host      : BladeEpu
OS        : CentOS Linux release 7.2.1511 (Core)
SPECTR-OS : Version 4.1.166.20220113
CPU       : Intel(R) Core(TM) i5-8400H CPU @ 2.50GHz (8 cores at 900 MHz with Hyperthreading)
User      : root (root)
System    : Avance Neo 750 NMR spectrometer
1H-frequency : 750.3 MHz
Description : Avance NEO
Bruker Order : 442759
Configured in: BladeEpu:/opt/topspin/conf/instr/spect
```

#### AQ-Rack:

```
- SCU: AV4I SCU SYSTEM CONTROL UNIT Z162978/00387 ECL 02.00
- {EPU}: AV4I SCU SYSTEM CONTROL UNIT Z162978/00387 ECL 02.00
- {GTU}: AV4I SCU SYSTEM CONTROL UNIT Z162978/00387 ECL 02.00
Location: slot 7 in rack 1
Connection: at IP 192.168.180.18 via PCIe #4
Firmware Version: 20210312125813
- Gradient resolution: 1.0 us
Devices: MTD at /dev/mtd2, RTD at /dev/bbu/rtdd4.4, GPROC at /dev/bbu/gproc4.7
Sequencer: GCube, TCube
- GCube1
- TCube1
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/06699 ECL 02.05
Location: slot 3 in rack 1
Connection: at IP 192.168.180.38 via PCIe #9
Firmware Version: 20210312121750
Devices: MTD at /dev/mtdd1, DRX at /dev/bbu/drx9.5, RTD at /dev/bbu/rtdd4.4
Sequencer: FCube
- FCube1
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/06698 ECL 02.05
Location: slot 4 in rack 1
Connection: at IP 192.168.180.46 via PCIe #11
Firmware Version: 20210312121750
Devices: MTD at /dev/mtdd2, DRX at /dev/bbu/drx11.5, RTD at /dev/bbu/rtdd1.4
Sequencer: FCube
- FCube2
- TRX 1200: AV4 TRANSCEIVER 1200 Z148391/06700 ECL 02.05
Location: slot 5 in rack 1
Connection: at IP 192.168.180.54 via PCIe #13
Firmware Version: 20210312121750
Devices: MTD at /dev/mtdd2, DRX at /dev/bbu/drx13.5, RTD at /dev/bbu/rtdd1.4
Sequencer: FCube
- FCube3
- PSM-A: AV4 PSM-A Z149510/02732 ECL 03.01
- HPPR/2 COVER2: HPPR/2 Cover2N Z178831/00167 ECL 00.00
HPPR2: - HPPR/2 preamplifier connected via AqRack
Type : HPPR/2
Controller: Cover/2
no LED display for tuning and matching
Module 1 : HPLNA 1H19F (reflection meter with CRP-Bias capability)
PN=Z103207, SN=00209 from 20210618
Module 2 : 2H
PN=Z003475, SN=00210 from 20190312
Module 3 : HPLNA BB31P (reflection meter without CRP-Bias capability)
PN=Z111095, SN=00223 from 20190705
Module 4 : 13C/79Br
PN=Z003526, SN=00207 from 20180612
```

```
Module 5 : HPLNA BB31P (reflection meter without CRP-Bias capability)
PN=Z111095, SN=00221 from 20190315
Module 6 : 31P
PN=Z102451, SN=00200 from 20210622
```

```
- HPLNA 1H19F: HPLNA 1H MODULE 750 Z103207/00209 ECL 06.05
- 2H: HPPR/2 2H MODULE 750 Z003475/00210 ECL 07.00
- HPLNA BB31P: HPLNA XBB 31P MODULE 750 Z111095/00223 ECL 04.04
- 13C/79Br: HPPR/2 13C MODULE 750 Z003526/00207 ECL 08.00
- HPLNA BB31P: HPLNA XBB 31P MODULE 750 Z111095/00221 ECL 04.04
- 31P: HPPR/2 31P MODULE 750 Z102451/00200 ECL 07.01
- RACK: AV4I AQS CHASSIS Z175600/00370 ECL 00.00
- PSM-48V: AV4 PSM-48V Z149850/04474 ECL 01.02
- PSM-D: AV4 PSM-D Z149520/02583 ECL 01.01
- FANTRAY: AV4I AQS FAN TRAY Z175900/00312 ECL 00.00
- REF 1200: AV4 REFERENCE 1200 Z148270/02367 ECL 02.02
```

#### Transmitters at the spectrometer subnet:

```
BLA-W144060-000236 W144060/000236 ECL 41:
- TCP/IP address = 192.168.99.13
- Firmware VS = 20210223
- Amplifier = AV4 BLABB1000 15-600: W144060/000236 ECL 41
- Controller = BLA CONTROL BOARD 7: W133936/025326 ECL 40
BLA-W144060-000235 W144060/000235 ECL 41:
- TCP/IP address = 192.168.99.12
- Firmware VS = 20210223
- Amplifier = AV4 BLABB1000 15-600: W144060/000235 ECL 41
- Controller = BLA CONTROL BOARD 7: W133936/025302 ECL 40
BLA-W144058-000036 W144058/000036 ECL 02:
- TCP/IP address = 192.168.99.11
- Firmware VS = 20210223
- Amplifier = AV4 BLAH1000 700-900: W144058/000036 ECL 02
- Controller = BLA CONTROL BOARD 7: W133936/023492 ECL 40
LTX Z109892/00208 ECL 02.02:
- TCP/IP address = 192.168.99.10
- Amplifier = BSM/2 LOCK TRANSCEIVER 750: Z109892/00208 ECL 02.02
```

#### Gradient amplifiers at the spectrometer subnet:

```
BGA1: BGAU_W154248_0136
- TCP/IP address = 192.168.99.16
- Firmware version = 20210916
- Web version = 8.10
- Current limits = 0.0/X, 0.0/Y, 0.0/Z (in A)
BGA2: BGAU_W154248_0137
- TCP/IP address = 192.168.99.15
- Firmware version = 20210916
- Web version = 8.10
- Current limits = 0.0/X, 0.0/Y, 0.0/Z (in A)
BGA3: BGAU_W154248_0139
- TCP/IP address = 192.168.99.14
- Firmware version = 20210916
- Web version = 8.10
- Current limits = 0.0/X, 0.0/Y, 0.0/Z (in A)
```

```
BSMS: BSM/2 connected to ethernet
- TCP/IP address = 192.168.99.10
- ELCB firmware version = 20210921
- ELCB = BSM/2 ELCB: Z100818/09250 ECL 07.03
- GAB current limits = 0.0/X, 0.0/Y, 10.0/Z (in A)
- Shim System = BOSS-WB
- SCB channels = 40
- Shim matrix file: 272623fa.dat
```

## ● Configuration Information [uxnmr.info](http://uxnmr.info)

```
- Active shims: Z Z2 Z3 Z4 Z5 X XZ XZ2 (X2-Y2) XY Y Y2 YZ2 (X2-Y2)Z2 XZ4 XZ3 Z6 (X2-Y2)Z YZ4 YZ3 XYZ2 XYZ X3Z X3
- Magnet polarity: SN (Bruker), uses standard H0 polarity
- L-TRX = BSMS/2 LOCK TRANSCEIVER 750: Z109892/00208 ECL 02.02
- Lock: on L-TRX board, supports 2H
- VTU_SFB = BSMS/2 SFB-E SENSOR & PNEUMATIC BD: Z115192/00870 ECL 05.05
- VTU_VPSB1 = AV4 VARIABLE POWER SUPPLY BD DC-E: Z140144/00301 ECL 01.02

VTU: in BSMS/2 connected to ethernet
- TCP/IP address = 192.168.99.10

- Firmware version = 20220315_1040
MAS Control Unit: MAS_H139288_0479
- TCP/IP address = 192.168.98.5

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
Line Distribution Unit 3: PDU3
- TCP/IP address = 192.168.99.102

RF cable connections (detected)
-----
TRX1 NORM output -> input 1 of transmitter 3 (AV4 BLAH1000 700-900 W144058/000036 at TCP/IP 192.168.99.11)
TRX1 AUX output -> input 1 of transmitter 4 (BSMS/2 LOCK TRANSCEIVER 750 Z109892/00208 at TCP/IP 192.168.99.10)
TRX2 NORM output -> input 1 of transmitter 2 (AV4 BLABB1000 15-600 W144060/000235 at TCP/IP 192.168.99.12)
TRX2 AUX output -> open
TRX3 NORM output -> input 1 of transmitter 1 (AV4 BLABB1000 15-600 W144060/000236 at TCP/IP 192.168.99.13)
TRX3 AUX output -> open

Blanking cable connections (detected)
-----
transmitter 1 = AV4 BLABB1000 15-600 W144060/000236 at TCP/IP 192.168.99.13:
- amplifier B-100W uses blanking 3
- amplifier B-100W uses blanking 3

transmitter 2 = AV4 BLABB1000 15-600 W144060/000235 at TCP/IP 192.168.99.12:
- amplifier B-100W uses blanking 2
- amplifier B-100W uses blanking 2

transmitter 3 = AV4 BLAH1000 700-900 W144058/000036 at TCP/IP 192.168.99.11:
- amplifier 1H-1000W uses blanking 1
- amplifier 1H-100W uses blanking 1

transmitter 4 = BSMS/2 LOCK TRANSCEIVER 750 Z109892/00208 at TCP/IP 192.168.99.10:
- amplifier 2H-5W uses blanking 9

Preamplifier connections (detected)
-----
Tune-TRX1 -> HPLNA 1H19F -> REC1
Tune-TRX1 -> 2H -> REC1
Tune-TRX2 -> HPLNA BB31P -> REC2
Tune-TRX2 -> 13C/79Br -> REC2
Tune-TRX3 -> HPLNA BB31P -> REC3
Tune-TRX3 -> 31P -> REC3
```

## ● 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::bee9:2fff:fea0:537c prefixlen 64 scopeid 0x20<link>
ether bc:e9:2f:a0:53:7c txqueuelen 1000 (Ethernet)
RX packets 17818916 bytes 9829517277 (9.1 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 17956789 bytes 2956245504 (2.7 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 132.229.125.41 netmask 255.255.255.0 broadcast 132.229.125.255
inet6 fe80::88d8:b392:8bfa:f470 prefixlen 64 scopeid 0x20<link>
ether bc:e9:2f:a0:53:7d txqueuelen 1000 (Ethernet)
RX packets 1031909 bytes 222154028 (211.8 MiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 759406 bytes 442532649 (422.0 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 5805518 bytes 2555691505 (2.3 GiB)
RX errors 0 dropped 0 overruns 0 frame 0
TX packets 5805518 bytes 2555691505 (2.3 GiB)
TX errors 0 dropped 0 overruns 0 carrier 0 collisions 0
```

**PH MAS DVT BL4**

**700.13 MHz**

**Probe ID: H8780\_0002**

**Inspection Lot: 2023-07-12**

**Jul 13, 2023**

**NMR TEST SERVICE**

● Probe NMR Test Data: PH MAS DVT BL4

### Probe Related Information

EC-Level	0
Gas Compensation	nitrogen
Gradient System	none
ATM Accessory	false
Temperature Sensor Type	TypeT
Proton Frequency [MHz]	700.13
Diameter [mm]	4.0

### Spectrometer Related Information

Type	AV NEO
CF Frequency [MHz]	750.30
Shim System	BOSS-WB
Shim System Offset	Standard
Software	TopSpin 4.1.3
OS	CentOS Linux release 7.9.2009 (Core)
Host Name	avance750
Magnet System	WB
Magnet Coil No	BR.091075110
Dewar No	BD228972
Helium Level	93%
System Number	442759

● Required Samples PH MAS DVT BL4

Z151220	Potassium Bromide (KBr, 80 ul)
Z151221	Adamantane (50 ul)
Z151222	Alpha-glycine (50 ul)
Z151223	2-13C, 15N alpha-glycine (50 ul)
Z151224	Ammonium Dihydrogenphosphate (50 ul)

NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H8780\_0002 PH MAS DVT BL4  
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)  
Magic Angle setting, MAS (NPT\_79Br\_MAS\_magicAngle, spin rate 5000 Hz)

Line width main [achieved]: [151] <n/a>



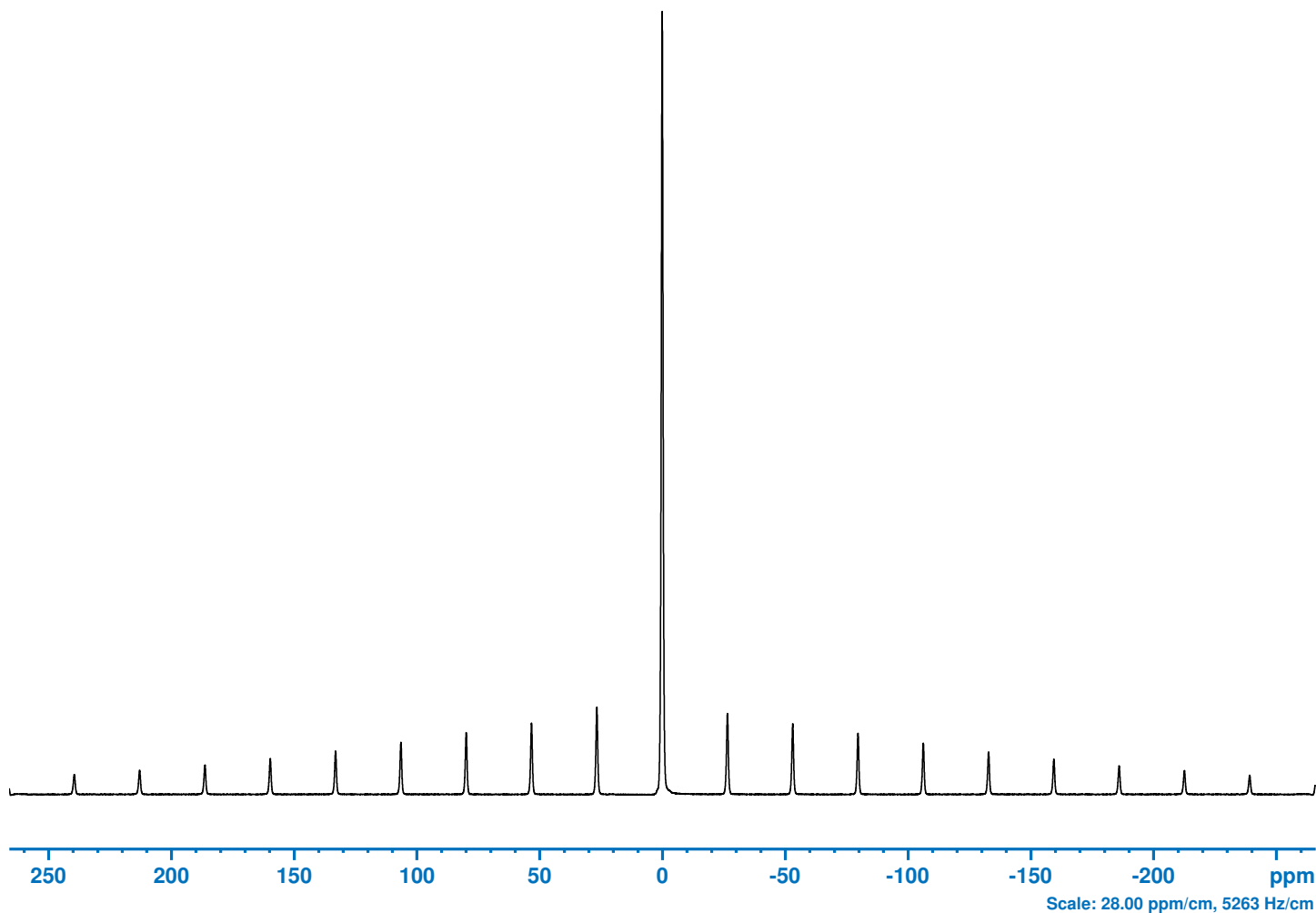
Bruker BioSpin

### NPT\_79Br\_MAS\_magicAngle

Current Data Parameters  
NAME NPT\_79Br\_MAS\_magicAngle  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230712  
Time 13.04 h  
INSTRUM Avance NEO  
PROBHD H8780\_0002 (PH)  
PULPROG onepulse  
TD 8192  
SOLVENT H2O+D2O  
NS 16  
DS 0  
SWH 100000.000 Hz  
FIDRES 24.414062 Hz  
AQ 0.0409600 sec  
RG 101  
DW 5.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 0.25000000 sec  
SFO1 187.9913332 MHz  
NUC1 79Br  
P1 3.84 usec  
PLW1 192.00000000 W

F2 - Processing parameters  
SI 131072  
SF 187.9913332 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 0.20



SHIM SEQUENCE  
skip shimming



NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3

Probe: H8780\_0002 PH MAS DVT BL4

Sample: Potassium Bromide (KBr, 80 ul) (Z151220)

Maximum spin rate testing, MAS (NPT\_79Br\_MAS\_maxSpinRate, spin rate 15000 Hz)

Determination of spinning stability for 180 s

Pressure values in mbar: DrivePressure=2053/BearingPressure=3169/BearingSensePressure=3167/SupplyPressure=6546/SystemPressure=6176

Spin rate at maximum deviation [measured]: @ MASR 15000 Hz [15002 Hz]

Maximum deviation [achieved]: @ MASR 15000 Hz [2 Hz] <n/a>



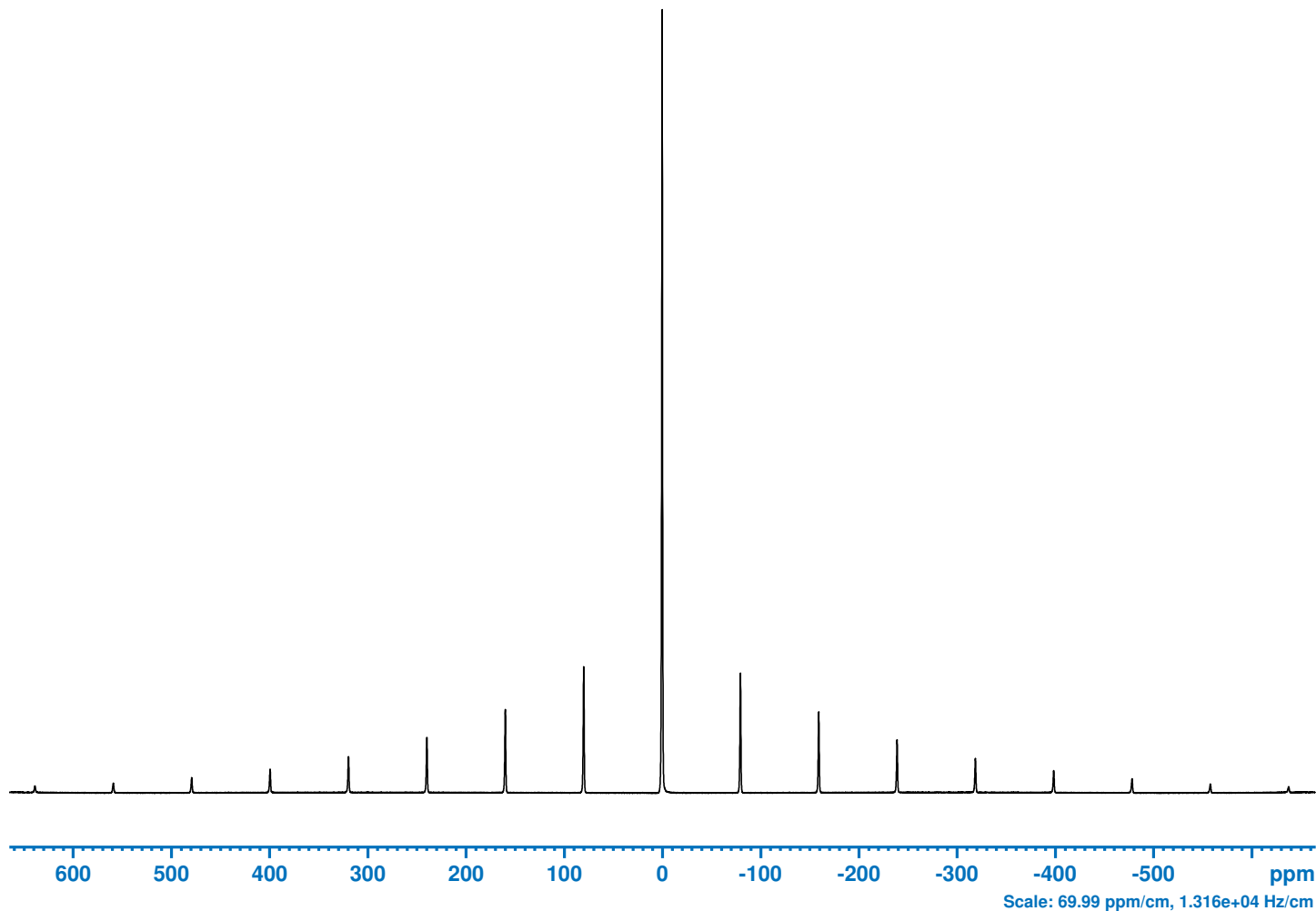
Bruker BioSpin

### NPT\_79Br\_MAS\_maxSpinRate

Current Data Parameters  
NAME NPT\_79Br\_MAS\_maxSpinRate  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230712  
Time 13.18 h  
INSTRUM Avance NEO  
PROBHD H8780\_0002 (PH)  
PULPROG onepulse  
TD 16384  
SOLVENT H2O+D2O  
NS 16  
DS 0  
SWH 250000.000 Hz  
FIDRES 30.517578 Hz  
AQ 0.0327680 sec  
RG 101  
DW 2.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 0.25000000 sec  
SFO1 187.9904591 MHz  
NUC1 79Br  
P1 3.84 usec  
PLW1 192.00000000 W

F2 - Processing parameters  
SI 32768  
SF 187.9904591 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 0.20



SHIM SEQUENCE  
skip shimming

NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H8780\_0002 PH MAS DVT BL4  
 Sample: Potassium Bromide (KBr, 80 ul) (Z151220)  
 Optimization of 79Br frequency (NPT\_79Br\_MAS\_fieldsetting, spin rate 5000 Hz)  
 FIELD was set to 2124.9 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0064 ppm.



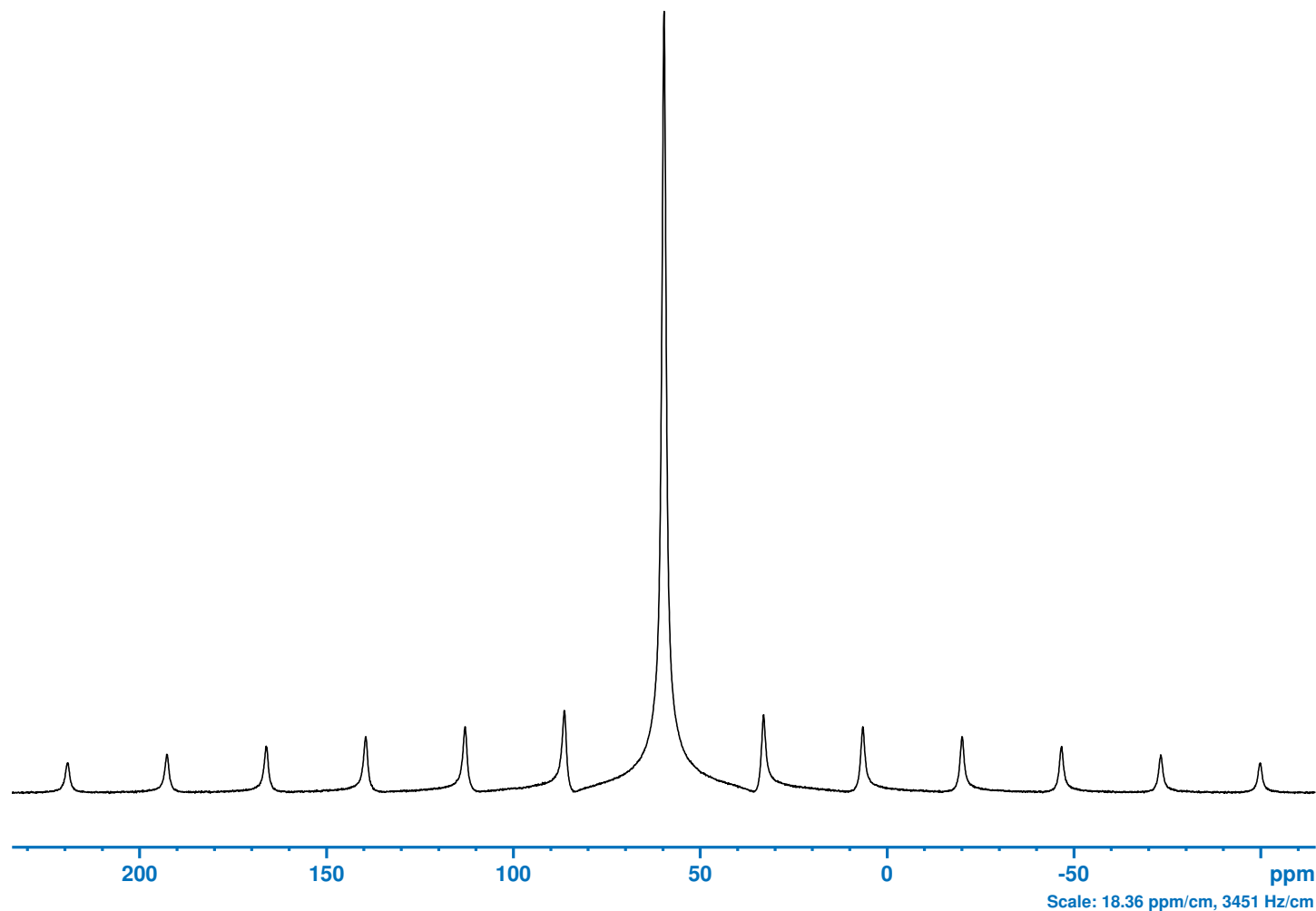
Bruker BioSpin

# NPT\_79Br\_MAS\_fieldsetting

Current Data Parameters  
 NAME NPT\_79Br\_MAS\_fieldsetting  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230712  
 Time 13.08 h  
 INSTRUM Avance NEO  
 PROBHD H8780\_0002 (PH)  
 PULPROG onepulse  
 TD 4096  
 SOLVENT H2O+D2O  
 NS 1  
 DS 0  
 SWH 81967.211 Hz  
 FIDRES 40.023052 Hz  
 AQ 0.0249856 sec  
 RG 101  
 DW 6.100 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 0.50000000 sec  
 SFO1 187.9912344 MHz  
 NUC1 79Br  
 P1 3.84 usec  
 PLW1 192.00000000 W

F2 - Processing parameters  
 SI 8192  
 SF 187.9800120 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.50



SHIM SEQUENCE  
 skip shimming

NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H8780\_0002 PH MAS DVT BL4  
 Sample: Adamantane (50 ul) (Z151221)  
 P90 1H pulse calibration, MAS (NPT\_1H\_MAS\_p90det\_1h, spin rate 15000 Hz)  
 ATTENTION: Updated PROSOL Tables with [2.50 us @ 131.3 W]. Calculation based on ==> [2.85 us @ 101.0 W]

P90 MAS 1H pulse [achieved]: @ 101.0 W [2.85 us] <n/a>



Bruker BioSpin

## NPT\_1H\_MAS\_p90det\_1h

Current Data Parameters  
 NAME NPT\_1H\_MAS\_p90det\_1h  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230712  
 Time 15.17 h  
 INSTRUM Avance NEO  
 PROBHD H8780\_0002 (PH)  
 PULPROG onepulse  
 TD 2988  
 SOLVENT H2O+D2O  
 NS 1  
 DS 0  
 SWH 100000.000 Hz  
 FIDRES 66.934402 Hz  
 AQ 0.0149400 sec  
 RG 8  
 DW 5.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 5.00000000 sec  
 SFO1 750.3018457 MHz  
 NUC1 1H  
 P1 7.50 usec  
 PLW1 101.00000000 W

F2 - Processing parameters  
 SI 4096  
 SF 750.3000000 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20

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

PLW90	P90	P90[det]	Deviation
101.0 W	2.50 us		
101.0 W	2.50 us	2.85 us	14.0%

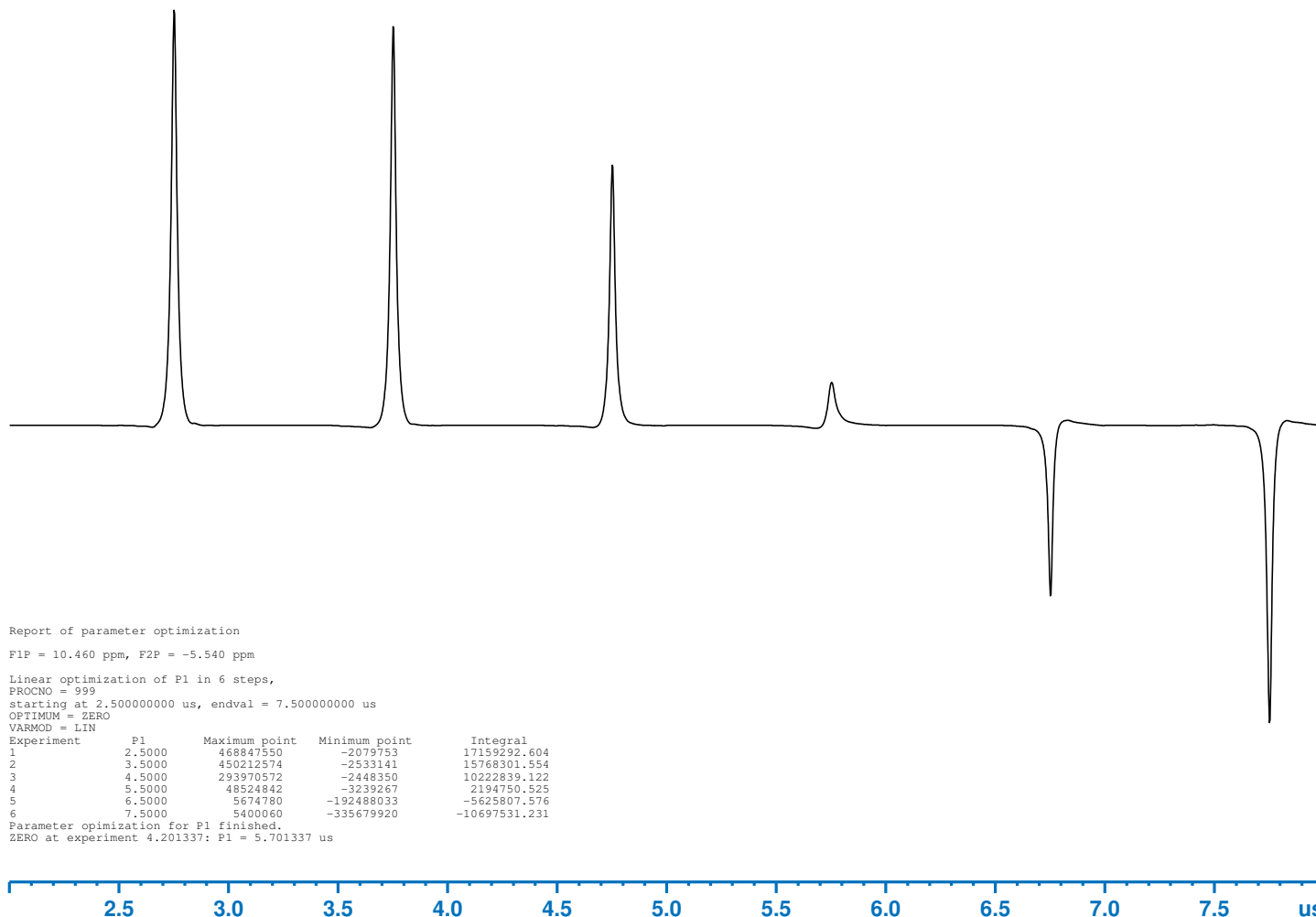
Report of parameter optimization

F1P = 10.460 ppm, F2P = -5.540 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	468847550	-2079753	17159292.604
2	3.5000	450212574	-2533141	15768301.554
3	4.5000	293970572	-2448350	10222839.122
4	5.5000	48524842	-3239267	2194750.525
5	6.5000	5674780	-192488033	-5625807.576
6	7.5000	5400060	-335679920	-10697531.231

Parameter optimization for P1 finished.  
 ZERO at experiment 4.201337: P1 = 5.701337 us



-----  
 SHIM SEQUENCE

-----  
 skip shimming

NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H8780\_0002 PH MAS DVT BL4  
 Sample: Potassium Bromide (KBr, 80 ul) (Z151220)  
 P90 79Br pulse calibration, MAS (NPT\_79Br\_MAS\_p90det\_79br, spin rate 5000 Hz)  
 ATTENTION: Update PROSOL Tables (79Br) failed.

P90 MAS 79Br pulse [achieved]: @ 192.0 W [4.42 us] <n/a>



Bruker BioSpin

## NPT\_79Br\_MAS\_p90det\_79br

Current Data Parameters  
 NAME NPT\_79Br\_MAS\_p90det\_79br  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230712  
 Time 13.08 h  
 INSTRUM Avance NEO  
 PROBHD H8780\_0002 (PH)  
 PULPROG onepulse  
 TD 2048  
 SOLVENT H2O+D2O  
 NS 1  
 DS 0  
 SWH 100000.000 Hz  
 FIDRES 97.656250 Hz  
 AQ 0.0102400 sec  
 RG 101  
 DW 5.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 0.25000000 sec  
 SFO1 187.9912344 MHz  
 NUC1 79Br  
 P1 11.52 usec  
 PLW1 192.0000000 W

F2 - Processing parameters  
 SI 4096  
 SF 187.9800119 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20

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

PLW90	P90	P90[det]	Deviation
192.0 W	3.84 us		
192.0 W	3.84 us	4.42 us	15.1%

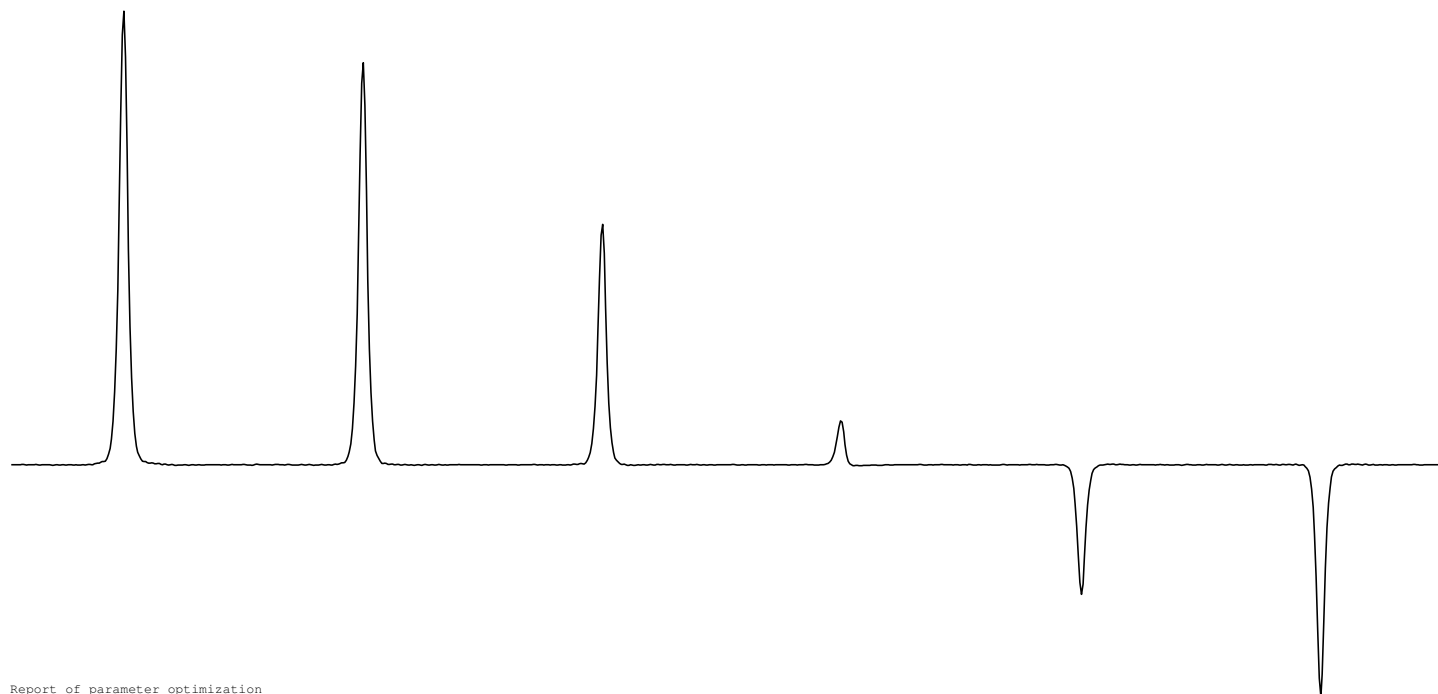
Report of parameter optimization

F1P = 69.700 ppm, F2P = 49.700 ppm

Linear optimization of P1 in 6 steps,  
 PROCNO = 999  
 starting at 3.839999914 us, endval = 11.519999504 us  
 OPTIMUM = ZERO  
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	3.8400	469585148	-652584	21998003.806
2	5.3760	416335811	-507142	18940826.890
3	6.9120	248912621	-703152	10998867.781
4	8.4480	45413564	-992767	1726081.316
5	9.9840	747951	-134197493	-5748495.226
6	11.5200	865670	-240077143	-9999567.665

Parameter optimization for P1 finished.  
 ZERO at experiment 4.252844: P1 = 8.836368 us



SHIM SEQUENCE

skip shimming

NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H8780\_0002 PH MAS DVT BL4  
Sample: Alpha-glycine (50 ul) (Z151222)  
CP 1H-15N sensitivity, MAS (NPT\_15N\_MAS\_sino\_cp1h\_15n, spin rate 7500 Hz)

SINO (20.0 ppm) [achieved]: Signal (29.45 ppm), Noise (198.52 to 178.51 ppm) [66.8] <n/a>  
Number of scans (NS) [achieved]: [64] <n/a>



Bruker BioSpin

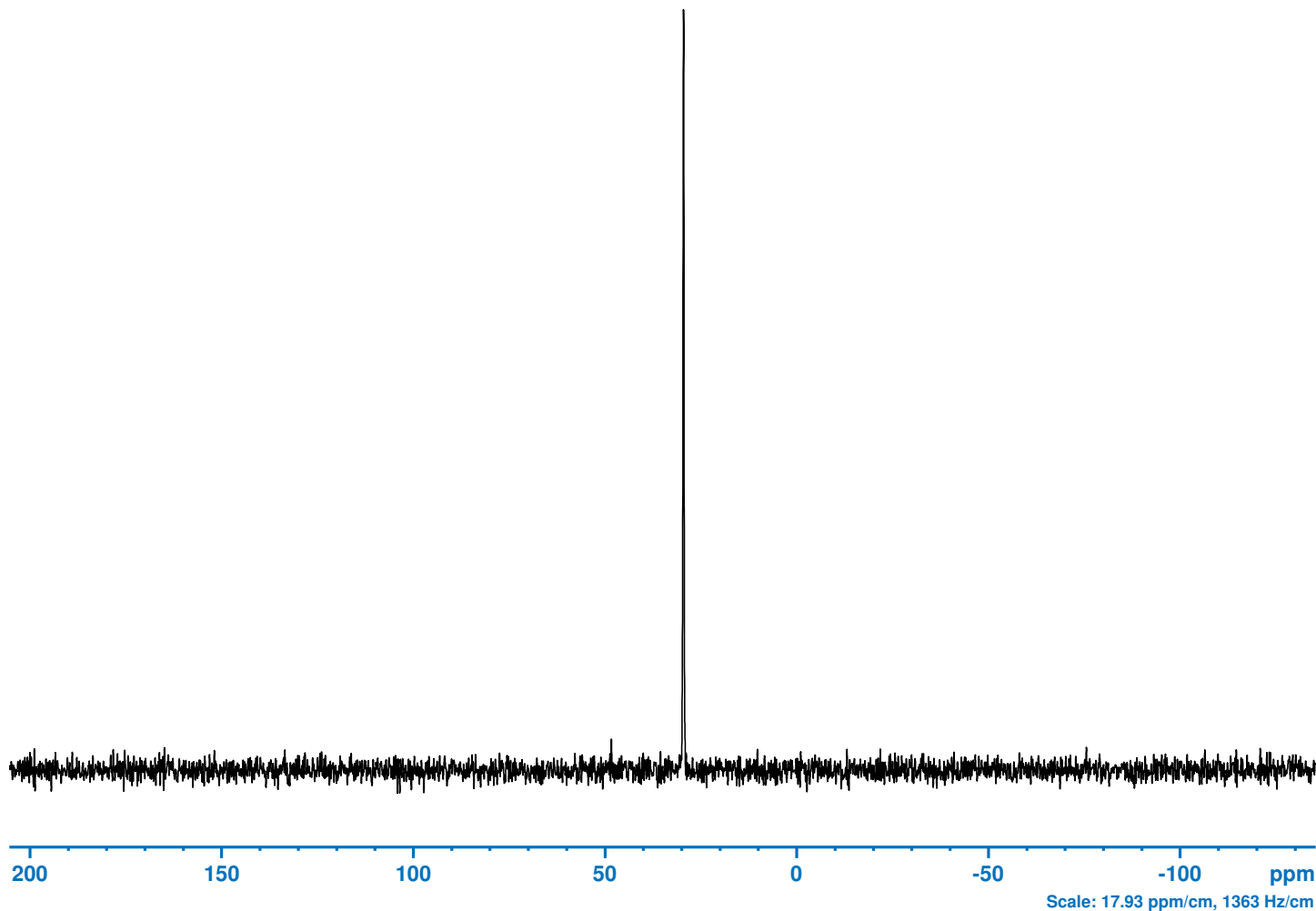
### NPT\_15N\_MAS\_sino\_cp1h\_15n

Current Data Parameters  
NAME NPT\_15N\_MAS\_sino\_cp1h\_15n  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230713  
Time 13.37 h  
INSTRUM Avance NEO  
PROBHD H8780\_0002 (PH)  
PULPROG cp  
TD 3012  
SOLVENT H2O+D2O  
NS 64  
DS 0  
SWH 30120.482 Hz  
FIDRES 20.000320 Hz  
AQ 0.0499992 sec  
RG 101  
DW 16.600 usec  
DE 6.50 usec  
TE 294.3 K  
D1 5.0000000 sec  
ZGPGTNS  
SFO1 76.0299000 MHz  
NUC1 15N  
P15 3500.00 usec  
PLW1 255.00000000 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.0000000  
CPDPRG2 spinal64  
P3 2.50 usec  
PCPD2 4.80 usec  
PLW2 131.25999451 W  
PLW12 142.80000305 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 63.95999908 W

F2 - Processing parameters  
SI 32768  
SF 76.0272390 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

SHIM SEQUENCE  
skip shimming



NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H8780\_0002 PH MAS DVT BL4  
Sample: Ammonium Dihydrogenphosphate (50 ul) (Z151224)  
CP 1H-31P sensitivity, MAS (NPT\_31P\_MAS\_sino\_cp1h\_31p, spin rate 5000 Hz)

SINO (10.0 ppm) [achieved]: Signal (-2.53 ppm), Noise (-105.43 to -115.43 ppm) [10268.3] <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 2  
PROCNO 1

#### F2 - Acquisition Parameters

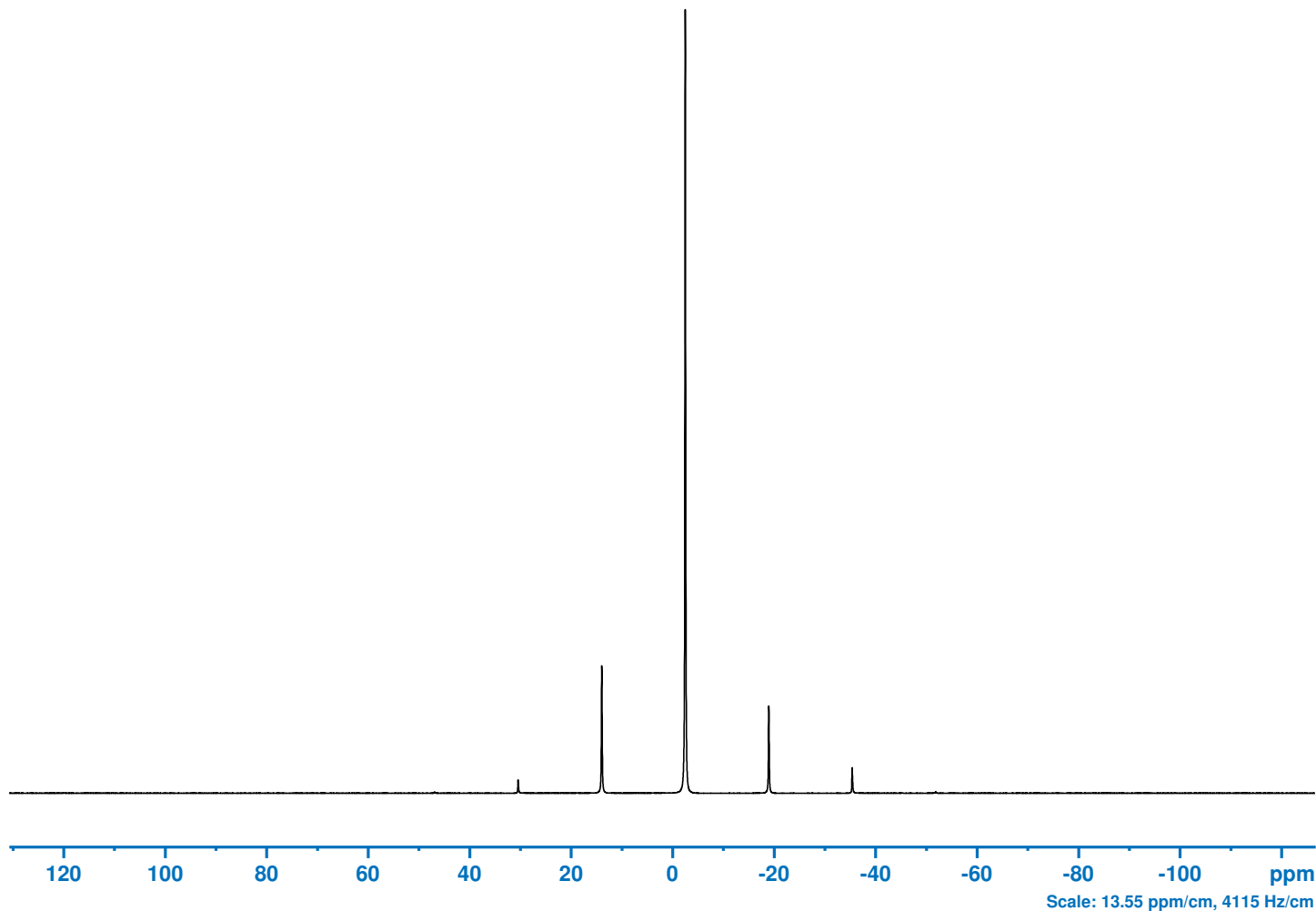
Date\_ 20230713  
Time 15.07 h  
INSTRUM Avance NEO  
PROBHD H8780\_0002 (PH)  
PULPROG cp  
TD 9090  
SOLVENT H2O+D2O  
NS 4  
DS 0  
SWH 90909.094 Hz  
FIDRES 20.002001 Hz  
AQ 0.0499950 sec  
RG 101  
DW 5.500 usec  
DE 6.50 usec  
TE 294.2 K  
D1 5.00000000 sec  
ZGPGTNS  
SFO1 303.7276145 MHz  
NUC1 31P  
P15 3500.00 usec  
PLW1 82.00000000 W  
SFO2 750.3054022 MHz  
NUC2 1H  
CNST21 1.00000000  
CPDPRG2 spinal64  
P3 2.50 usec  
PCPD2 4.80 usec  
PLW2 131.25999451 W  
PLW12 147.00000000 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 62.40000153 W

#### F2 - Processing parameters

SI 32768  
SF 303.7270070 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

SHIM SEQUENCE

skip shimming



NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H8780\_0002 PH MAS DVT BL4  
 Sample: Adamantane (50 ul) (Z151221)  
 13C sensitivity, MAS (NPT\_13C\_MAS\_sino\_13c, spin rate 15000 Hz)  
 ATTENTION: non-standard execution of experiment  
 SINO (20.0 ppm) [achieved]: Signal (34.48 ppm), Noise (59.26 to 39.26 ppm) [68.9] <n/a>  
 Linewidth [achieved]: at 50% of signal height [2.3 Hz] <n/a>  
 Number of scans (NS) [achieved]: [1] <n/a>



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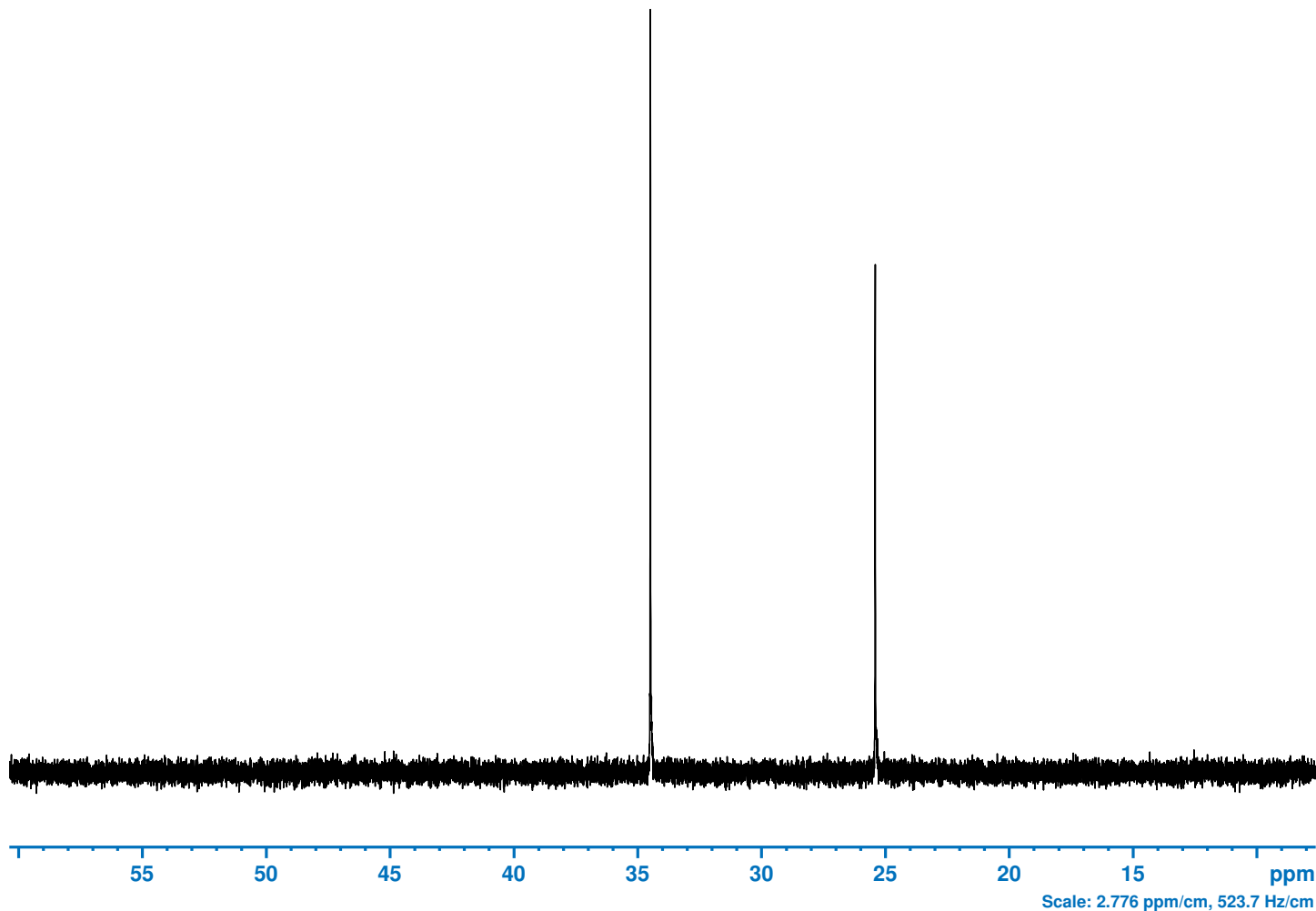
# NPT\_13C\_MAS\_sino\_13c

Current Data Parameters  
 NAME NPT\_13C\_MAS\_sino\_13c  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230712  
 Time 15.10 h  
 INSTRUM Avance NEO  
 PROBHD H8780\_0002 (PH)  
 PULPROG hdec  
 TD 19998  
 SOLVENT H2O+D2O  
 NS 1  
 DS 0  
 SWH 10000.000 Hz  
 FIDRES 1.000100 Hz  
 AQ 0.9999000 sec  
 RG 101  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 F15 0 usec  
 ZGPTNS -Dlacq  
 SFO1 188.6694995 MHz  
 NUC1 13C  
 P1 3.84 usec  
 PLW1 50.00000000 W  
 SFO2 750.3018457 MHz  
 NUC2 1H  
 CPDPRG[2] spinal64  
 PCPD2 4.80 usec  
 PLW2 0 W  
 PLW12 67.00000000 W

F2 - Processing parameters  
 SI 32768  
 SF 188.6630850 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20

SHIM SEQUENCE  
 skip shimming



NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H8780\_0002 PH MAS DVT BL4  
Sample: Adamantane (50 ul) (Z151221)  
1H sensitivity, MAS (NPT\_1H\_MAS\_sino\_1h, spin rate 15000 Hz)

SINO (20.0 ppm) [achieved]: Signal (-1.59 ppm), Noise (-43.10 to -63.11 ppm) [25504.0] <n/a>  
Linewidth [achieved]: at 50% of signal height [357.4 Hz] <n/a>  
Number of scans (NS) [achieved]: [1] <n/a>



Bruker BioSpin

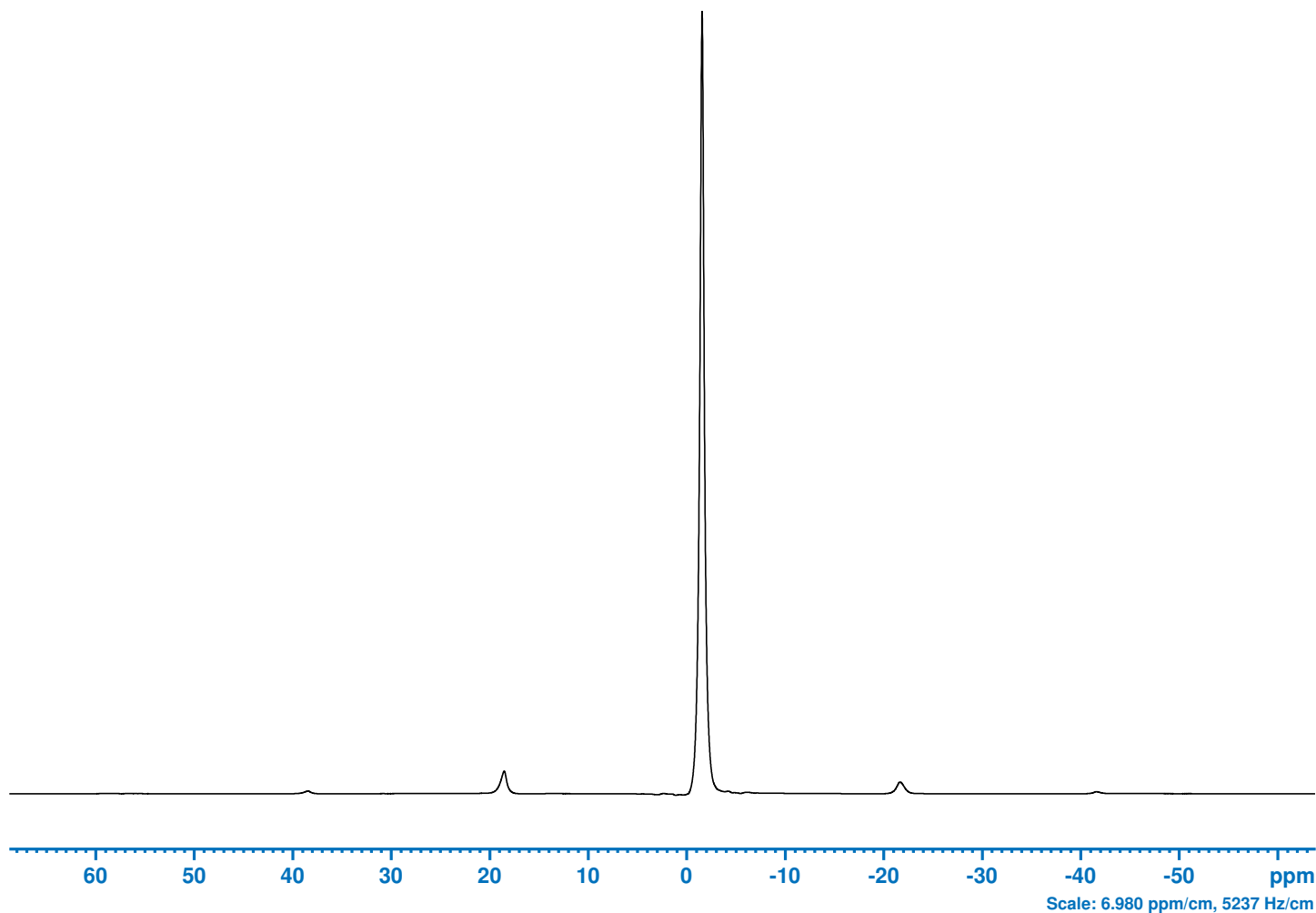
### NPT\_1H\_MAS\_sino\_1h

Current Data Parameters  
NAME NPT\_1H\_MAS\_sino\_1h  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230712  
Time 15.26 h  
INSTRUM Avance NEO  
PROBHD H8780\_0002 (PH)  
PULPROG onepulse  
TD 2048  
SOLVENT H2O+D2O  
NS 1  
DS 0  
SWH 100000.000 Hz  
FIDRES 97.656250 Hz  
AQ 0.0102400 sec  
RG 8  
DW 5.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 5.00000000 sec  
SFO1 750.3018457 MHz  
NUC1 1H  
P1 2.50 usec  
PLW1 131.25999451 W

F2 - Processing parameters  
SI 16384  
SF 750.3000000 MHz  
WDW EM  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

SHIM SEQUENCE  
skip shimming





NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H8780\_0002 PH MAS DVT BL4  
Sample: 2-13C, 15N alpha-glycine (50 ul) (Z151223)  
CP 1H-15N parameter optimization, MAS (NPT\_15N\_MAS\_paropt\_cp1h\_15n, spin rate 7500 Hz)

SINO (20.0 ppm): Signal (29.45 ppm), Noise (-103.57 to -123.60 ppm) [3591.6]



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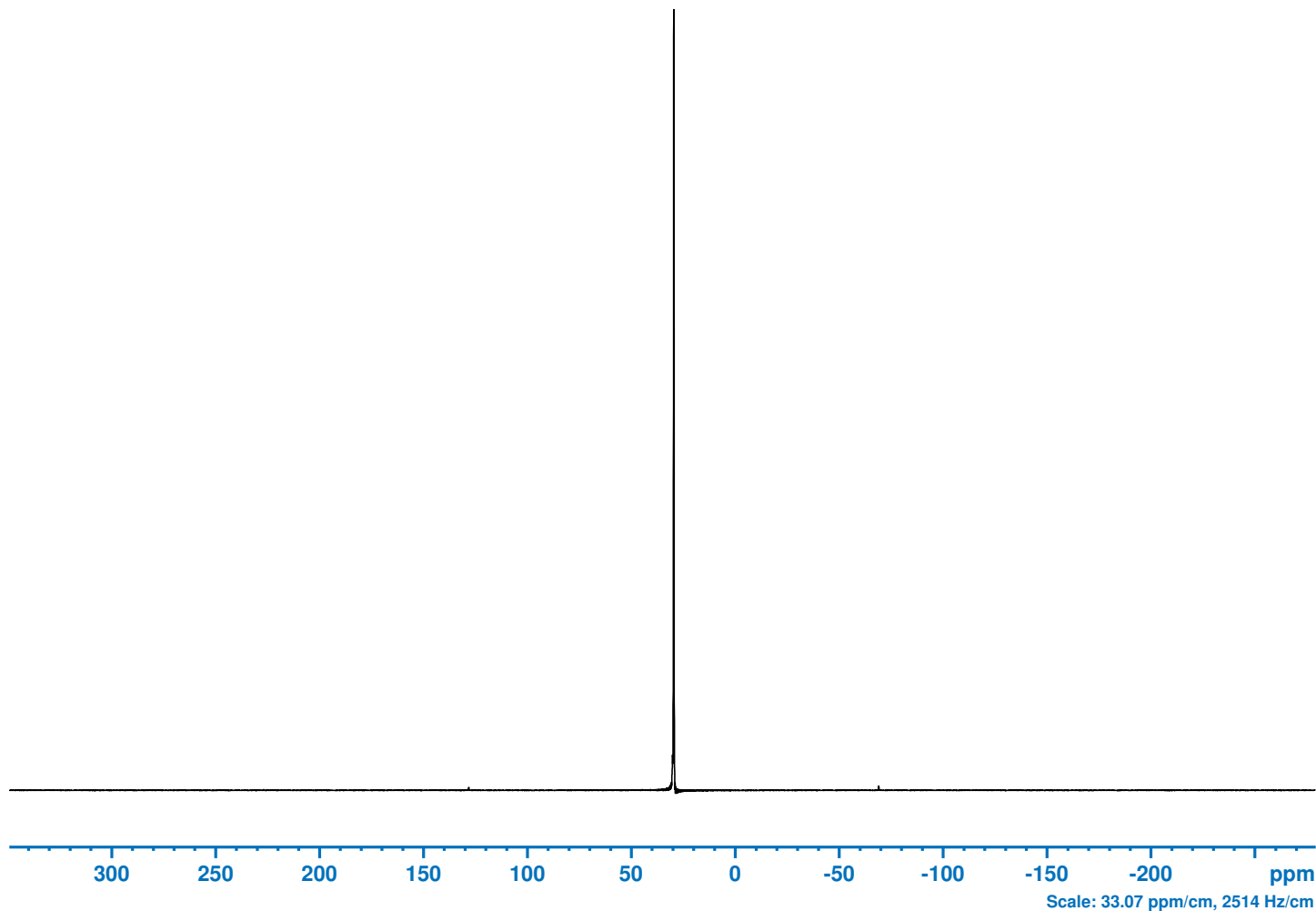
### NPT\_15N\_MAS\_paropt\_cp1h\_15n

Current Data Parameters  
NAME NPT\_15N\_MAS\_paropt\_cp1h\_15n  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230713  
Time 13.11 h  
INSTRUM Avance NEO  
PROBHD H8780\_0002 (PH)  
PULPROG cp  
TD 5554  
SOLVENT H2O+D2O  
NS 4  
DS 0  
SWH 55555.555 Hz  
FIDRES 20.005602 Hz  
AQ 0.0499860 sec  
RG 101  
DW 9.000 usec  
DE 6.50 usec  
TE 294.5 K  
D1 5.00000000 sec  
ZGPGTNS  
SFO1 76.0299000 MHz  
NUC1 15N  
P15 3500.00 usec  
PLW1 255.00000000 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.0000000  
CPDPRG2 spinal64  
P3 2.50 usec  
PCPD2 4.80 usec  
PLW2 131.25999451 W  
PLW12 142.80000305 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 63.95999908 W

F2 - Processing parameters  
SI 32768  
SF 76.0272390 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

SHIM SEQUENCE  
skip shimming



- Additional Report of Inspection Lot

**PH MAS DVT BL4**

**700.13 MHz**

**Probe ID: H8780\_0002**

**Inspection Lot: 2023-07-12**

NMR TEST SERVICE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H8780\_0002 PH MAS DVT BL4  
 Sample: Adamantane (50 ul) (Z151221)  
 13C sensitivity, MAS (NPT\_13C\_MAS\_sino\_13c, spin rate 15000 Hz)  
 ATTENTION: non-standard execution of experiment  
 SINO (20.0 ppm) [achieved]: Signal (34.48 ppm), Noise (59.26 to 39.26 ppm) [68.9] <n/a>  
 Linewidth [achieved]: at 50% of signal height [2.3 Hz] <n/a>  
 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 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230712  
 Time 15.10 h  
 INSTRUM Avance NEO  
 PROBHD H8780\_0002 (PH)  
 PULPROG hpdcc  
 TD 19998  
 SOLVENT H2O+D2O  
 NS 1  
 DS 0  
 SWH 10000.000 Hz  
 FIDRES 1.000100 Hz  
 AQ 0.9999000 sec  
 RG 101  
 DW 50.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 P15 0 usec  
 ZGPTNS -Dlacc  
 SFO1 188.6694995 MHz  
 NUC1 13C  
 P1 3.84 usec  
 PLW1 50.00000000 W  
 SFO2 750.3018457 MHz  
 NUC2 1H  
 CPDPRG2 spinal64  
 PCPD2 4.80 usec  
 PLW2 0 W  
 PLW12 67.00000000 W

F2 - Processing parameters  
 SI 32768  
 SF 188.6630850 MHz  
 WDW EM  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20

SHIM SEQUENCE  
 skip shimming

