

DRAFT



Bruker BioSpin

PH MASDVT 750W4 EFREE2 BL3.2 C/N/H

750 MHz

Probe ID: H11833_0001

Inspection Lot: 2021-10-19

NMR TEST SERVICE

Oct 20, 2021

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 5000 Hz)

Line width main [achieved]: [135] <n/a>

DRAFT



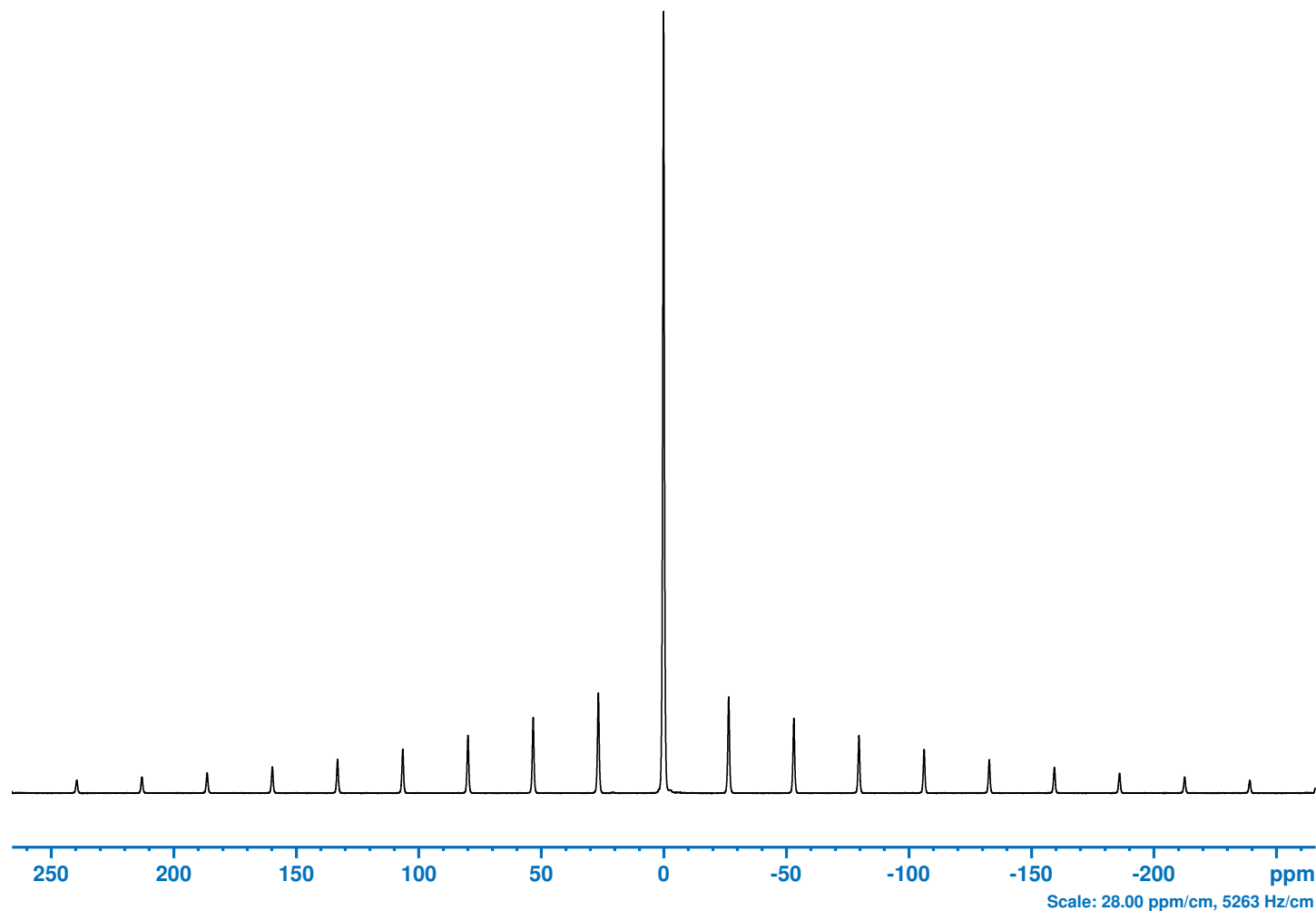
Bruker BioSpin

NPT_79Br_MAS_magicAngle

Current Data Parameters
NAME NPT_79Br_MAS_magicAngle
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 12.31 h
INSTRUM Avance
PROBHD H11833_0001 (P)
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 187.9912362 MHz
NUC1 79Br
P1 2.60 usec
PLW1 187.50000000 W

F2 - Processing parameters
SI 131072
SF 187.9912362 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: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 23000 Hz)
Determination of spinning stability for 180 s
Pressure values in mbar: DrivePressure=2396/BearingPressure=3164/BearingSensePressure=3164/SupplyPressure=6521/SystemPressure=6625

Spin rate at maximum deviation [measured]: @ MASR 23000 Hz [23003 Hz]
Maximum deviation [achieved]: @ MASR 23000 Hz [3 Hz] <n/a>

DRAFT



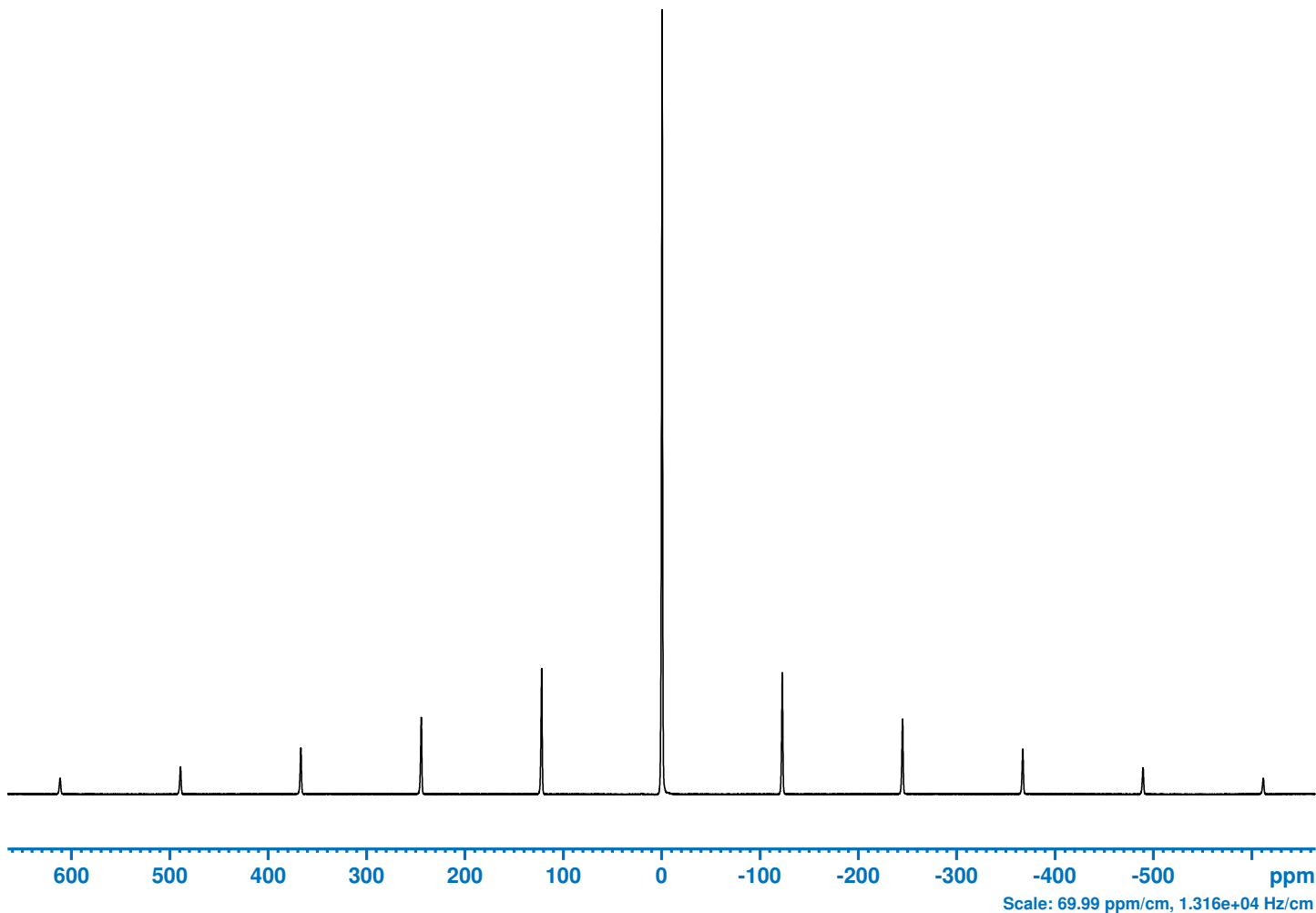
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

Current Data Parameters
NAME NPT_79Br_MAS_maxSpinRate
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 12.49 h
INSTRUM Avance
PROBHD H11833_0001 (P)
PULPROG onepulse
TD 16384
SOLVENT H2O+D2O
NS 16
DS 0
SWH 250000.000 Hz
FIDRES 30.517578 Hz
AQ 0.0327680 sec
RG 401
DW 2.000 usec
DE 6.50 usec
TE 297.8 K
D1 0.25000000 sec
SFO1 187.9912201 MHz
NUC1 79Br
P1 2.60 usec
PLW1 187.5000000 W

F2 - Processing parameters
SI 32768
SF 187.9912201 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: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting, spin rate 5000 Hz)
FIELD was set to 3172.9 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0065 ppm.

DRAFT



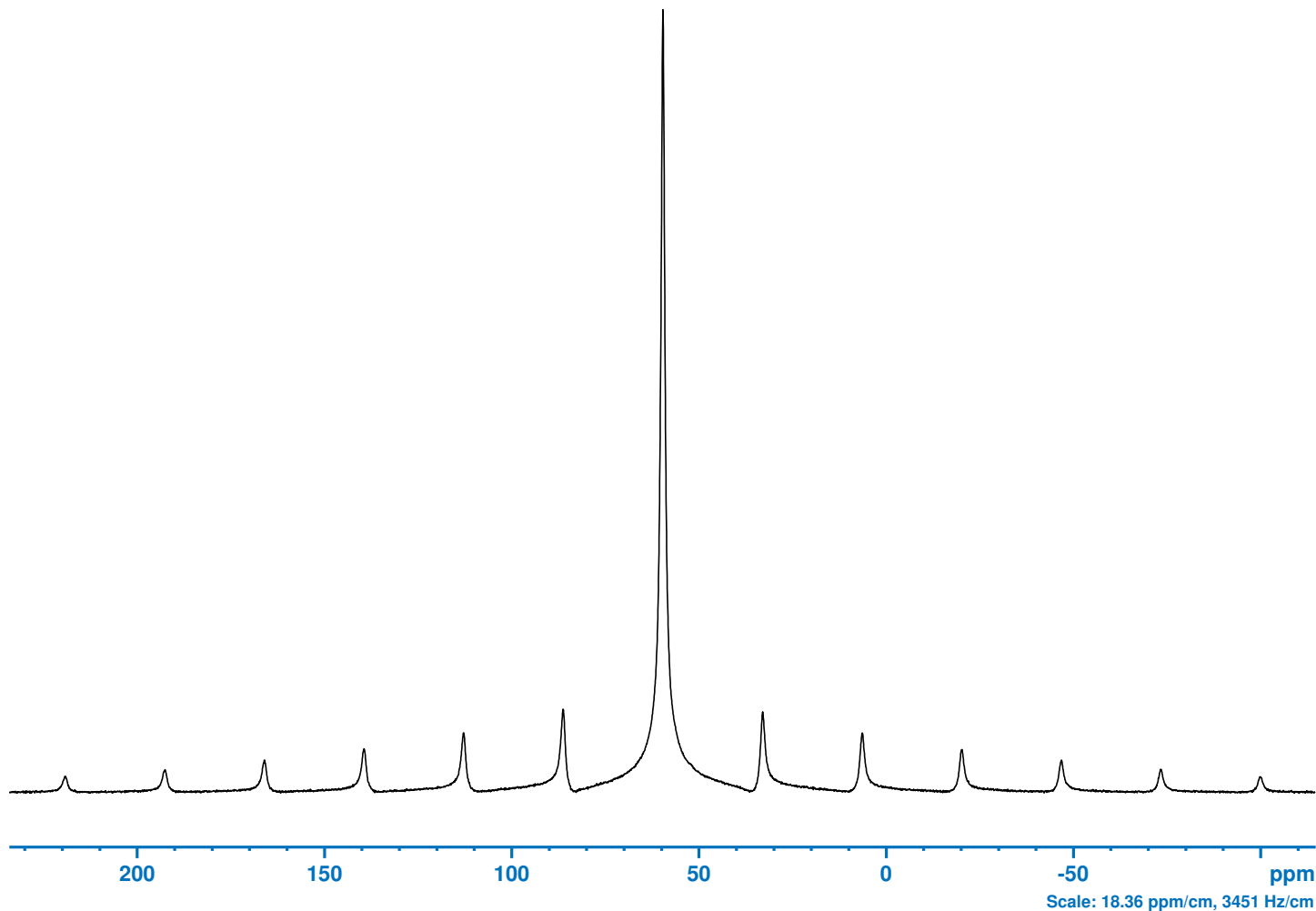
Bruker BioSpin

NPT_79Br_MAS_fieldsetting

Current Data Parameters
NAME NPT_79Br_MAS_fieldsetting
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 12.16 h
INSTRUM Avance
PROBHD H11833_0001 (P)
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 296.3 K
D1 0.50000000 sec
SFO1 187.9912343 MHz
NUC1 79Br
P1 2.60 usec
PLW1 120.0000000 W

F2 - Processing parameters
SI 8192
SF 187.9800119 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: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Adamantane (34 ul) (Z151231)
P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 24000 Hz)
ATTENTION: Updated PROSOL Tables with [2.50 us @ 175.3 W]. Calculation based on ==> [3.59 us @ 85.0 W],

DRAFT

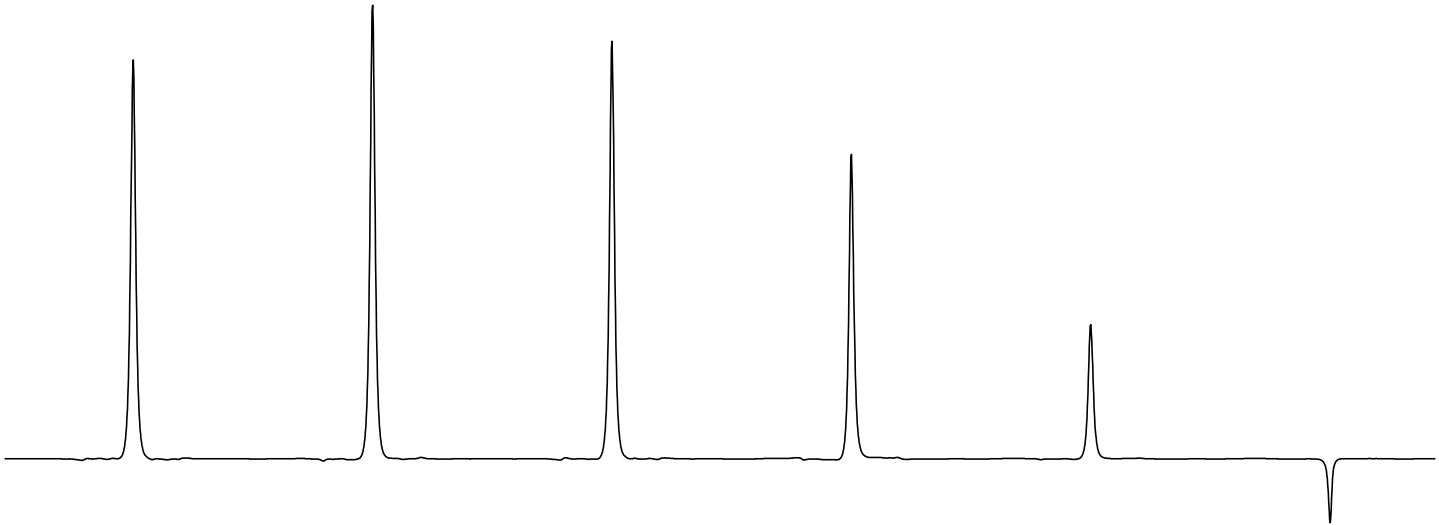


Bruker BioSpin

P90 MAS 1H pulse [achieved]: @ 85.0 W [3.59 us] <n/a>

NPT_1H_MAS_p90det_1h

Current Data Parameters
NAME NPT_1H_MAS_p90det_1h
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211019
Time 13.31 h
INSTRUM Avance
PROBHD H11833_0001 (P
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 85.00000000 W
F2 - Processing parameters
SI 4096
SF 750.3000000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20



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 413149279 -1652166 11230451.245
2 3.5000 469913065 -2343122 12525297.513
3 4.5000 432533622 -1269690 11458210.282
4 5.5000 315261941 -1143553 8376457.217
5 6.5000 138858756 -904335 3810999.152
6 7.5000 403318 -66116779 -1310916.797
Parameter optimization for P1 finished.
ZERO at experiment 5.677441: P1 = 7.177441 us

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

PLW90	P90	P90[det]	Deviation
85.0 W	2.50 us		
85.0 W	2.50 us	3.59 us	43.6%

SHIM SEQUENCE
skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Potassium Bromide (KBr, 34 ul) (Z151230)
P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br, spin rate 5000 Hz)
ATTENTION: Updated PROSOL Tables with [2.60 us @ 187.5 W]. Calculation based on ==> [3.25 us @ 120.0 W]

P90 MAS 79Br pulse [achieved]: @ 120.0 W [3.25 us] <n/a>

DRAFT



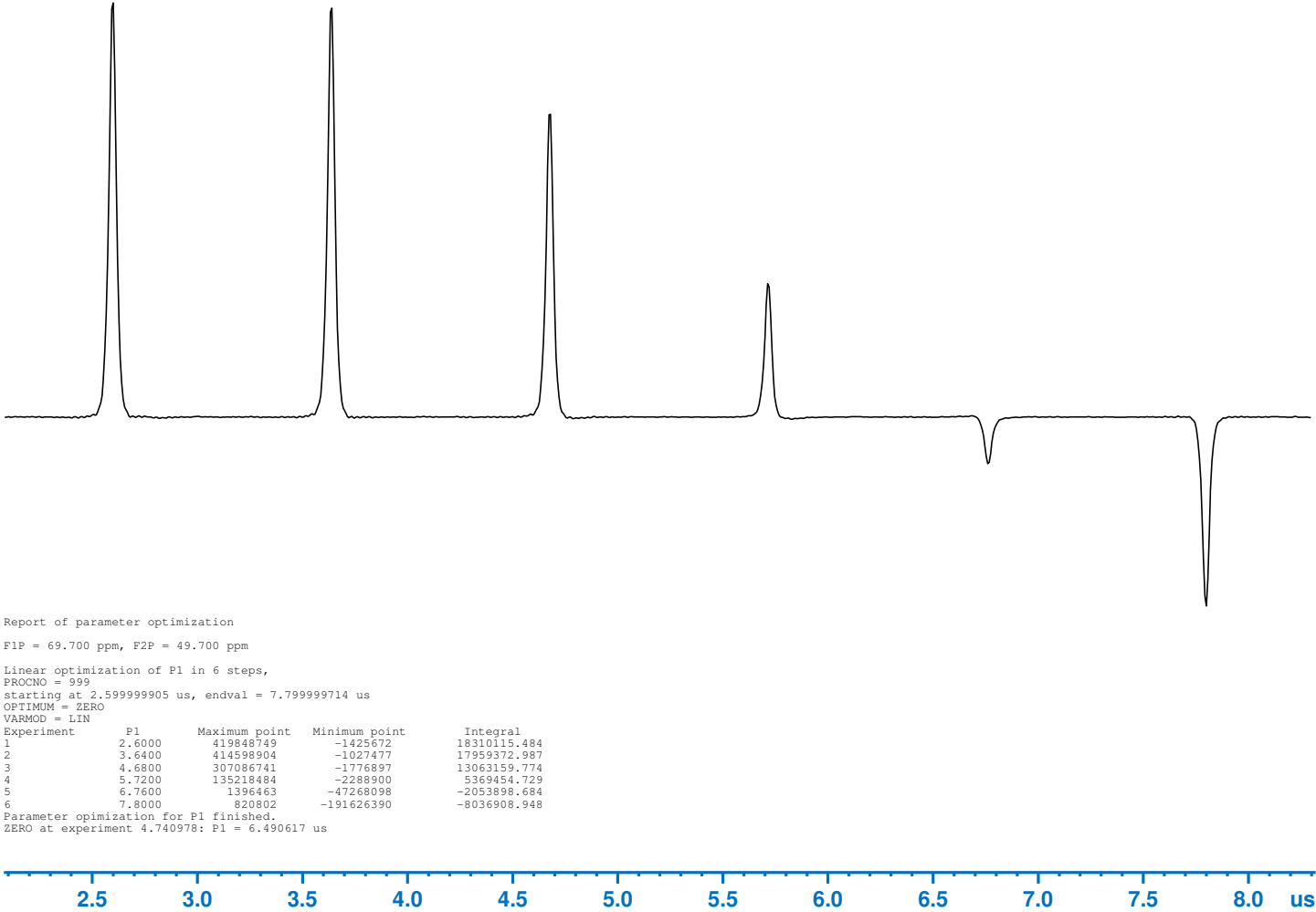
Bruker BioSpin

NPT_79Br_MAS_p90det_79br

Current Data Parameters
NAME NPT_79Br_MAS_p90det_79br
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 12.18 h
INSTRUM Avance
PROBHD H11833_0001 (P)
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 297.2 K
D1 0.25000000 sec
SFO1 187.9912343 MHz
NUC1 79Br
P1 7.80 usec
PLW1 120.00000000 W

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



Report of parameter optimization
F1P = 69.700 ppm, F2P = 49.700 ppm

Linear optimization of P1 in 6 steps,
PROCNO = 999
Starting at 2.599999905 us, endval = 7.799999714 us
OPTIMUM = ZERO
VARMOD = LIN
Experiment P1 Maximum point Minimum point Integral
1 2.6000 419848749 -1425672 18310115.484
2 3.6400 414598904 -1027477 17959372.987
3 4.6800 307086741 -1776897 13063159.774
4 5.7200 135218484 -2288900 5369454.729
5 6.7600 1396463 -47268098 -2053898.684
6 7.8000 820802 -191626390 -8036908.948
Parameter optimization for P1 finished.
ZERO at experiment 4.740978: P1 = 6.490617 us

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

120.0 W 2.60 us
120.0 W 2.60 us 3.25 us 25.0%

SHIM SEQUENCE

skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Alpha-glycine (34 ul) (Z151232)
P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c, spin rate 7500 Hz)
ATTENTION: Updated PROSOL Tables with [3.50 us @ 99.8 W].

P90_MAS_CP 1H13C power (PLW 11) [achieved]: [91.7 W] <n/a>
P90_MAS_CP 1H13C pulse (P 1) [achieved]: [3.65 us] <n/a>

DRAFT



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_ 20211019
Time 14.40 h
INSTRUM Avance
PROBHD H11833_0001 (P)
PULPROG cp90
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 298.1 K
D1 5.00000000 sec
ZGPTNS
SFO1 188.6711976 MHz
NUC1 13C
P1 5.25 usec
P15 2000.00 usec
PLW1 91.72799683 W
PLW11 91.72799683 W
SFO2 750.3046519 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 175.27999878 W
PLW12 175.27999878 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 232.76870728 W

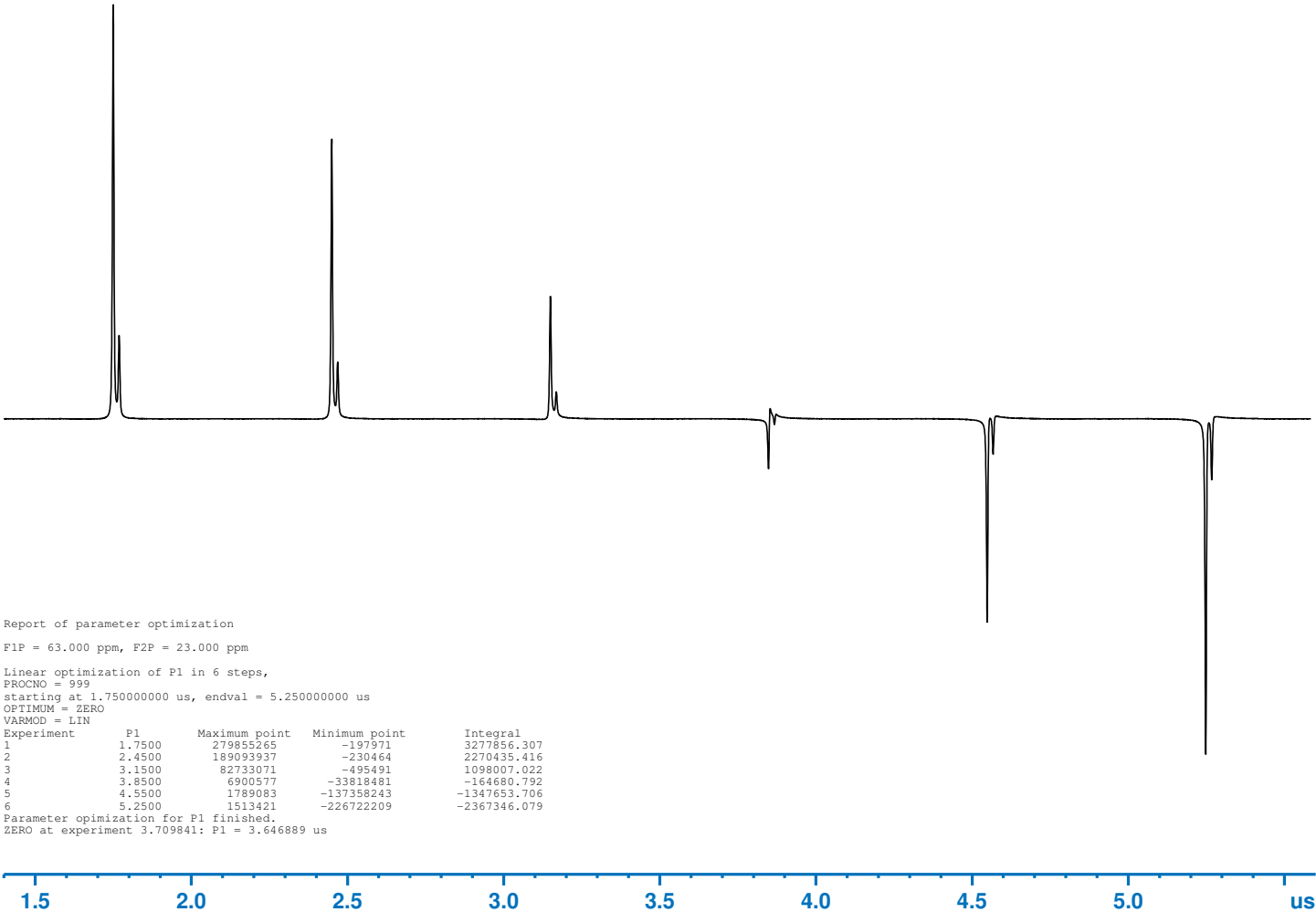
F2 - Processing parameters
SI 8192
SF 188.6630851 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20

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

91.7 W 3.50 us 3.65 us 4.3%

SHIM SEQUENCE

skip shimming



Report of parameter optimization

F1P = 63.000 ppm, F2P = 23.000 ppm

Linear optimization of P1 in 6 steps,
PROCNO = 999
Starting at 1.750000000 us, endval = 5.250000000 us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	1.7500	279855265	-197971	3277856.307
2	2.4500	189093937	-230464	2270435.416
3	3.1500	82733071	-495491	1098007.022
4	3.8500	6900577	-33818481	-164680.792
5	4.5500	1789083	-137358243	-1347653.706
6	5.2500	1513421	-226722209	-2367346.079

Parameter optimization for P1 finished.
ZERO at experiment 3.709841: P1 = 3.646889 us

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Adamantane (34 ul) (Z151231)
P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c, spin rate 24000 Hz)
ATTENTION: Updated PROSOL Tables with [3.50 us @ 91.7 W]. Calculation based on ==> [2.94 us @ 130.0 W],

P90 MAS 13C pulse [achieved]: @ 130.0 W [2.94 us] <n/a>

DRAFT



Bruker BioSpin

NPT_13C_MAS_p90det_13c

Current Data Parameters
NAME NPT_13C_MAS_p90det_13c
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 14.09 h
INSTRUM Avance
PROBHD H11833_0001 (P
PULPROG hdec
TD 4000
SOLVENT H2O+D2O
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 5.000000 Hz
AQ 0.2000000 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 15.00000000 sec
P15 0 usec
ZGPTNS -Dlacq
SFO1 188.6694996 MHz
NUC1 13C
P1 10.50 usec
PLW1 130.00000000 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG[2] cw
PLW2 175.27999878 W
PLW12 0.63100803 W

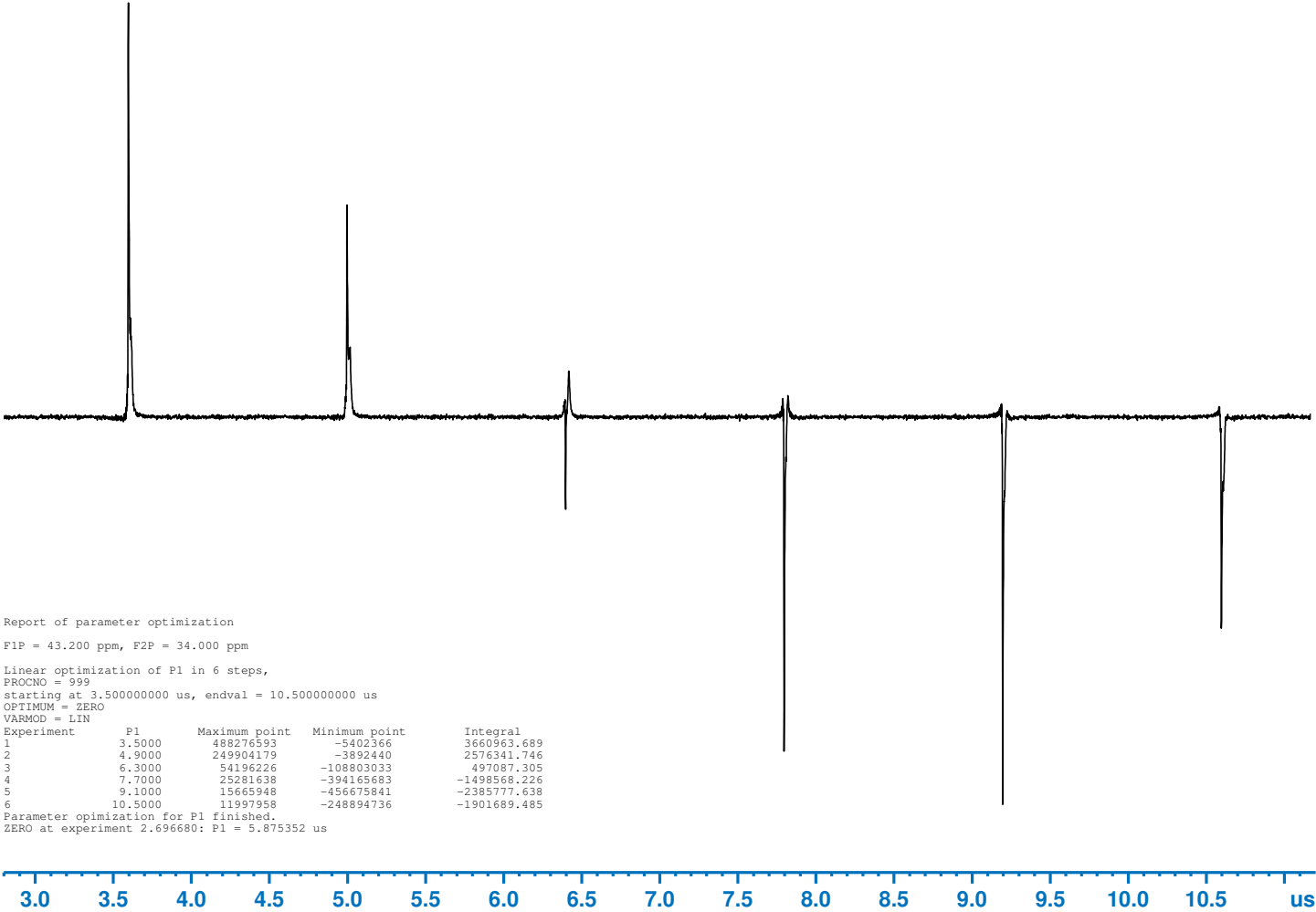
F2 - Processing parameters
SI 8192
SF 188.6630851 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
FC 0.50

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

130.0 W 3.50 us
130.0 W 3.50 us 2.94 us -16.0%

SHM SEQUENCE

skip shimming



Report of parameter optimization

F1P = 43.200 ppm, F2P = 34.000 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 488276593 -5402366 3660963.689
2 4.9000 249904179 -3892440 2576341.746
3 6.3000 54196226 -108803033 497087.305
4 7.7000 25281638 -394165683 -1498568.226
5 9.1000 15665948 -456675841 -2385777.638
6 10.5000 11997958 -248894736 -1901689.485
Parameter optimization for P1 finished.
ZERO at experiment 2.696680: P1 = 5.875352 us

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Alpha-glycine (34 ul) (Z151232)
P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n, spin rate 7500 Hz)
ATTENTION: Updated PROSOL Tables with [4.50 us @ 318.9 W].

P90_MAS_CP 1H15N power (PLW 11) [achieved]: [180.0 W] <n/a>
P90_MAS_CP 1H15N pulse (P 1) [achieved]: [5.99 us] <n/a>

DRAFT



Bruker BioSpin

NPT_15N_MAS_p90det_cp1h_15n

Current Data Parameters
NAME NPT_15N_MAS_p90det_cp1h_15n
EXPNO 1
PROCNO 1

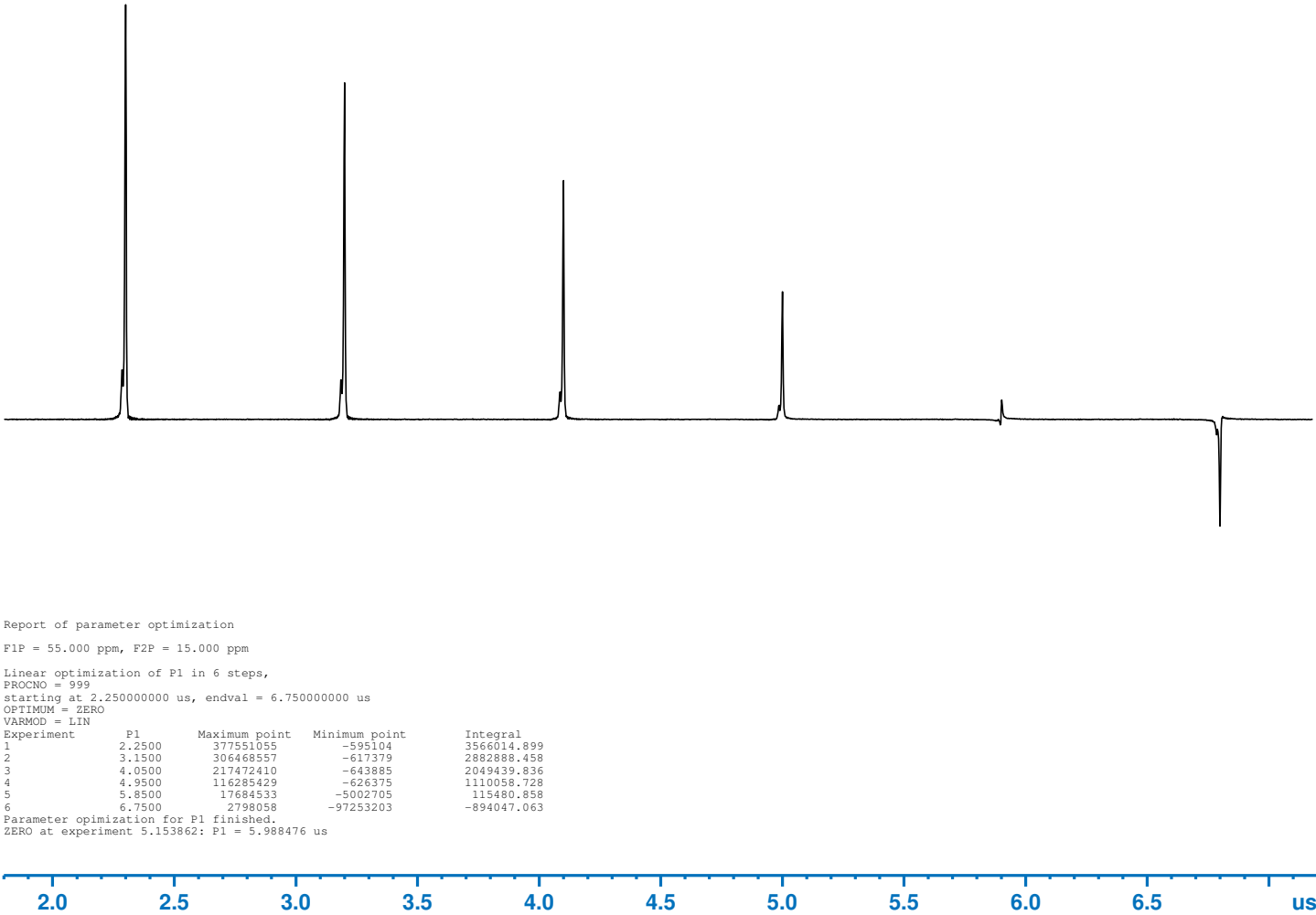
F2 - Acquisition Parameters
Date_ 20211019
Time 15.08 h
INSTRUM Avance
PROBHD H11833_0001 (P)
PULPROG cp90
TD 3012
SOLVENT H2O+D2O
NS 4
DS 0
SWH 30120.482 Hz
FIDRES 20.000320 Hz
AQ 0.0499992 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 298.2 K
D1 5.00000000 sec
ZGPTNS
SFO1 76.0298997 MHz
NUC1 15N
P1 6.75 usec
P15 3500.00 usec
PLW1 180.00000000 W
PLW11 180.00000000 W
SFO2 750.3046519 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 175.27999878 W
PLW12 175.27999878 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 123.89579773 W

F2 - Processing parameters
SI 4096
SF 76.0272387 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

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

PLW90	P90	P90[det]	Deviation
180.0 W	4.50 us		
180.0 W	4.50 us	5.99 us	33.1%

SHM 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 2.250000000 us, endval = 6.750000000 us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.2500	377551055	-595104	3566014.899
2	3.1500	306468557	-617379	2882888.458
3	4.0500	217472410	-643885	2049439.836
4	4.9500	116285429	-626375	1110058.728
5	5.8500	17684533	-5002705	115480.858
6	6.7500	2798058	-97253203	-894047.063

Parameter optimization for P1 finished.
ZERO at experiment 5.153862: P1 = 5.988476 us

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Alpha-glycine (34 ul) (Z151232)
CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c, spin rate 7500 Hz)

SINO (20.0 ppm) [achieved]: Signal (42.79 ppm), Noise (118.79 to 98.78 ppm) [673.2] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>
Processed with TDef=2048

DRAFT



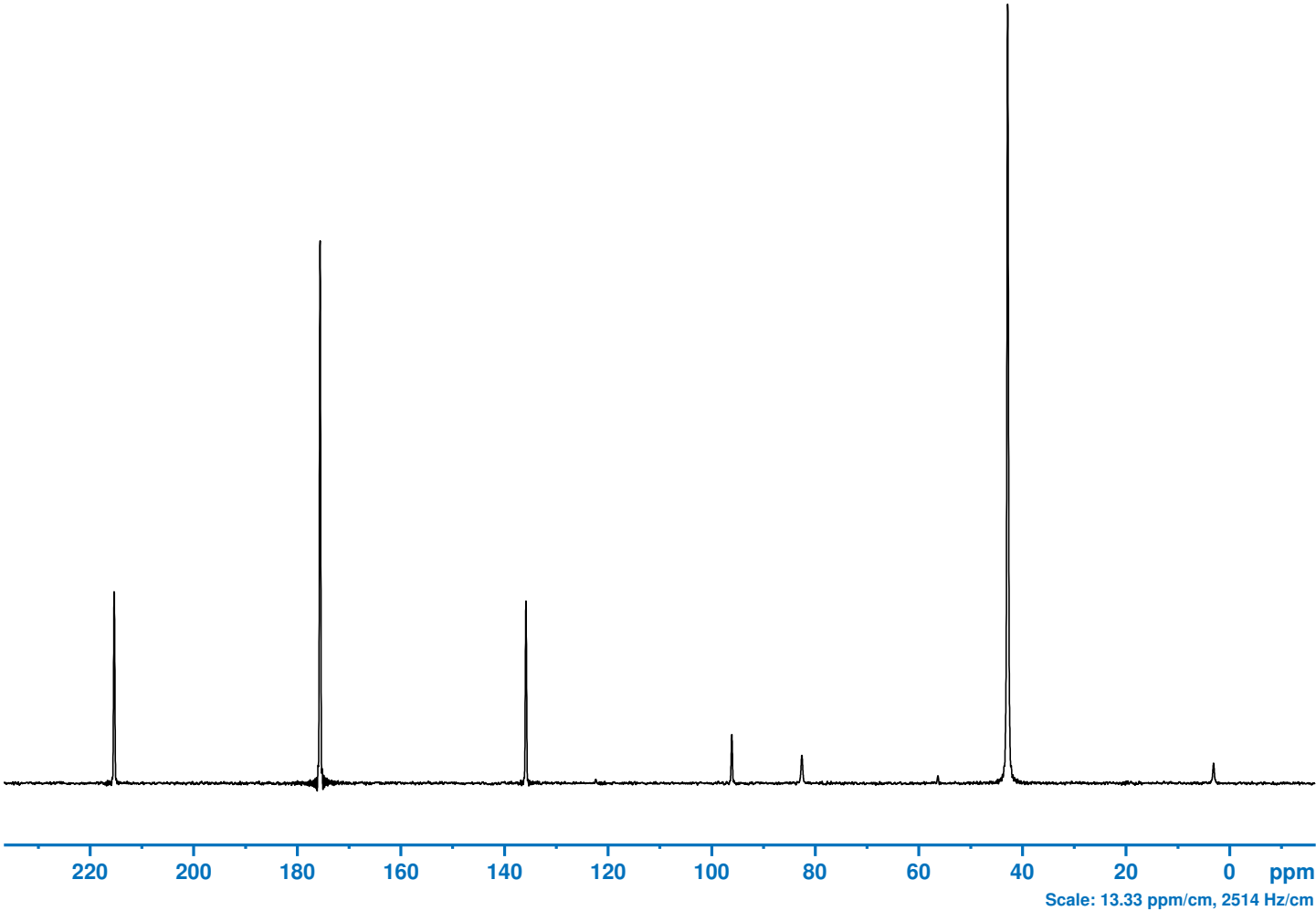
Bruker BioSpin

NPT_13C_MAS_sino_cp1h_13c

Current Data Parameters
NAME NPT_13C_MAS_sino_cp1h_13c
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211020
Time 10.43 h
INSTRUM Avance
PROBHD H11833_0001 (P
PULPROG cp
TD 5554
SOLVENT H2O+D2O
NS 64
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 298.0 K
D1 5.00000000 sec
ZGPGTNS
SFO1 188.6838380 MHz
NUC1 13C
P15 2000.00 usec
PLW1 99.75900269 W
SFO2 750.3046519 MHz
NUC2 1H
CNST21 1.00000000
CPDPRG2 spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 175.27999878 W
PLW12 182.25999451 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 194.14999390 W

F2 - Processing parameters
SI 32768
SF 188.6630851 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: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Alpha-glycine (34 ul) (Z151232)
CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n, spin rate 7500 Hz)

SINO (20.0 ppm) [achieved]: Signal (32.61 ppm), Noise (25.64 to 5.63 ppm) [84.4] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>

DRAFT



Bruker BioSpin

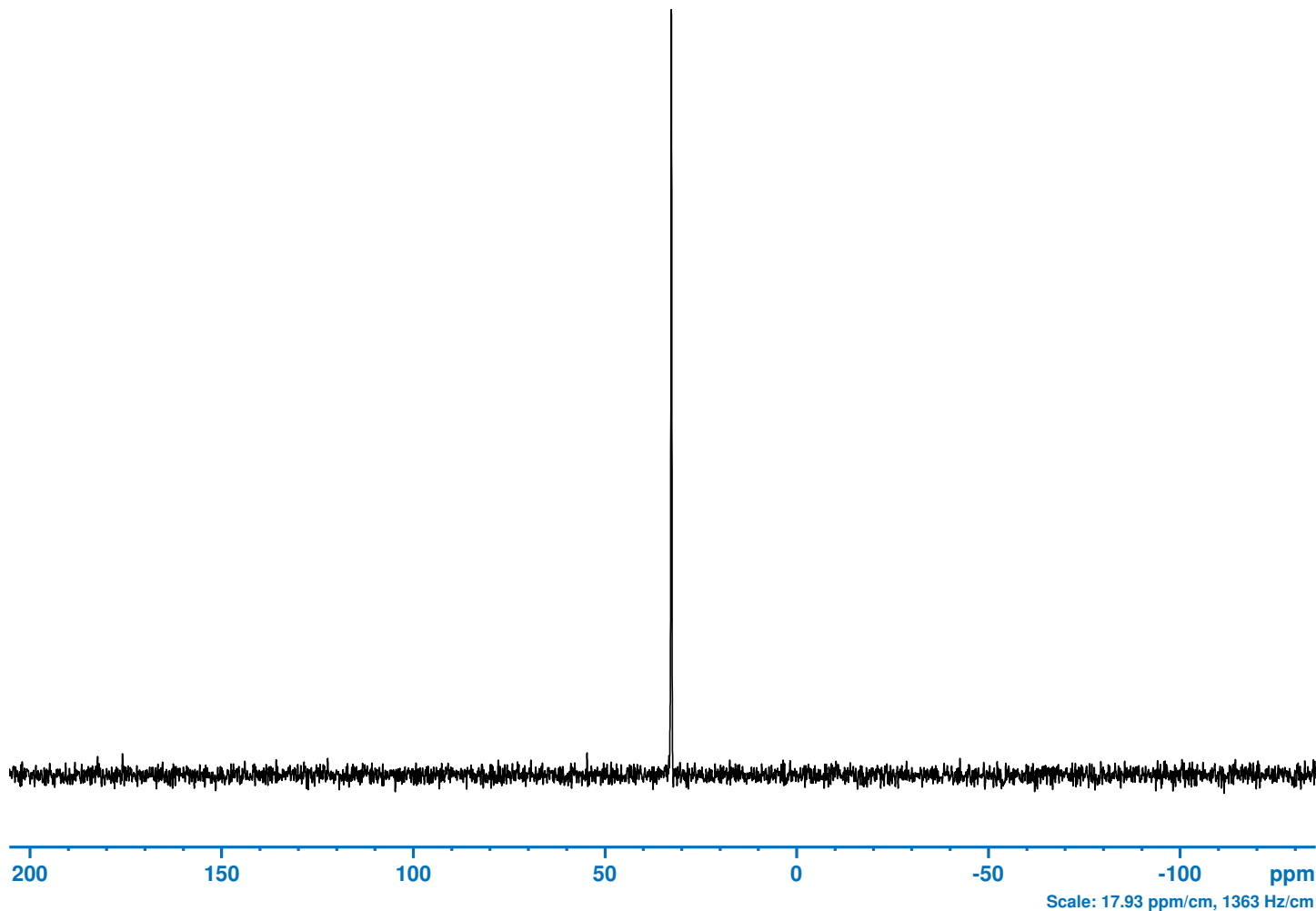
NPT_15N_MAS_sino_cp1h_15n

Current Data Parameters
NAME NPT_15N_MAS_sino_cp1h_15n
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211020
Time 11.20 h
INSTRUM Avance
PROBHD H11833_0001 (P
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 298.0 K
D1 5.0000000 sec
ZGPGTNS
SFO1 76.0298997 MHz
NUC1 15N
P15 3500.00 usec
PLW1 318.92999268 W
SFO2 750.3046519 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 175.27999878 W
PLW12 161.22999573 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 111.45999908 W

F2 - Processing parameters
SI 32768
SF 76.0272387 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: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Adamantane (34 ul) (Z151231)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 23980 Hz)

SINO (20.0 ppm) [achieved]: Signal (37.93 ppm), Noise (60.36 to 40.36 ppm) [52.4] <n/a>
Linewidth [achieved]: at 50% of signal height [5.3 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>

DRAFT



Bruker BioSpin

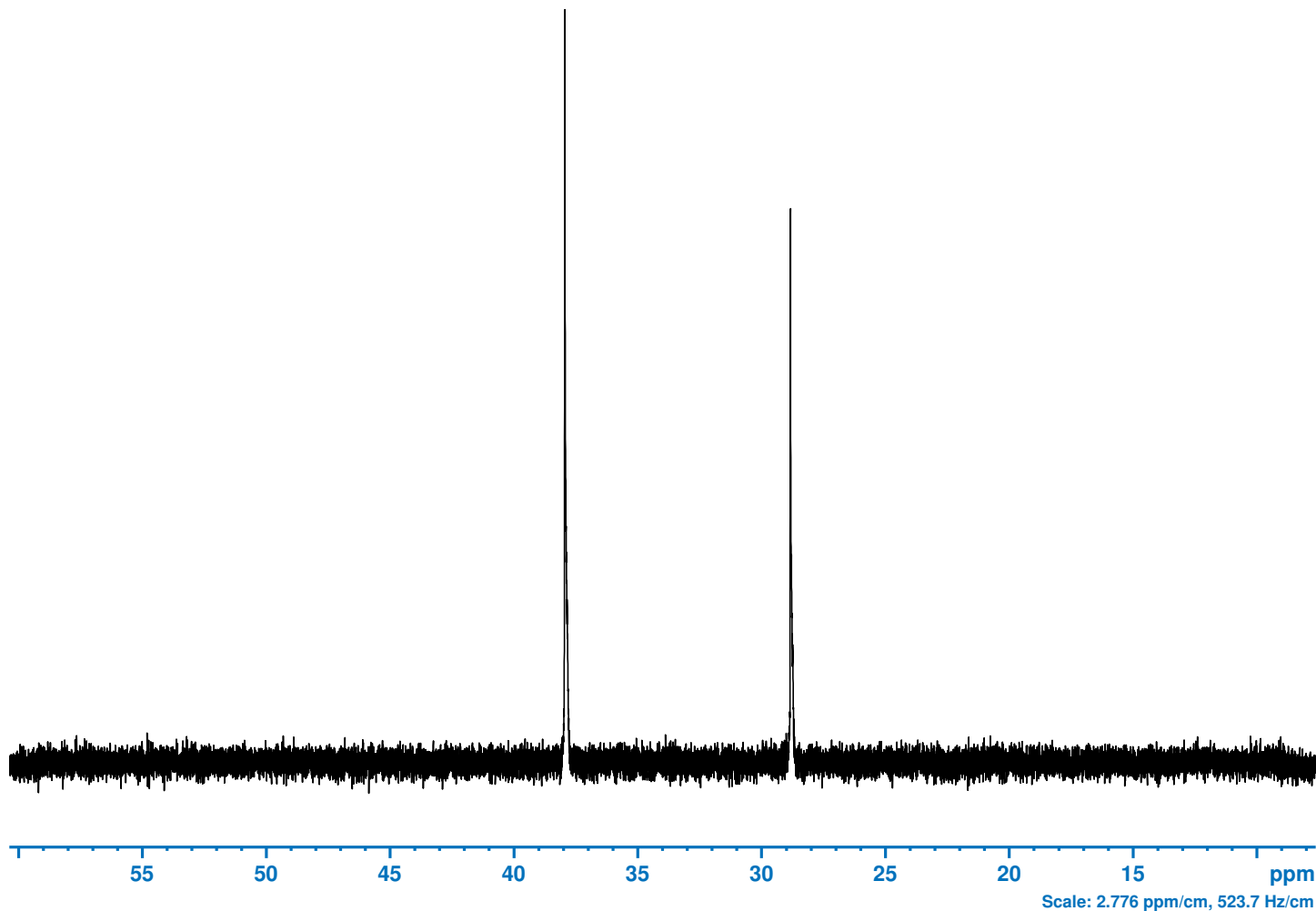
NPT_13C_MAS_sino_13c

Current Data Parameters
NAME NPT_13C_MAS_sino_13c
EXPNO 501
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 14.24 h
INSTRUM Avance
PROBHD H11833_0001 (P)
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 15.00000000 sec
P15 0 usec
ZGPGTNS -Dlacc
SFO1 188.6694996 MHz
NUC1 13C
P1 3.50 usec
PLW1 91.72799683 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG2 cw
PLW2 175.27999878 W
PLW12 0.62995678 W

F2 - Processing parameters
SI 32768
SF 188.6630851 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: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Adamantane (34 ul) (Z151231)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 23980 Hz)

DRAFT



Bruker BioSpin

NPT_13C_MAS_sino_13c

```
# Tue Oct 19 12:24:28 2021
##$PROBEIDENTIFIER=H11833_0001
##$PROBENAME=PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
##$SHIMID=272623
#
# Active Shim Gradients
#
Z -32510
Z2 0
Z3 0
Z4 0
Z5 0
Z6 0
X -350
XZ 0
XZ2 0
XZ3 0
XZ4 0
Y 2300
YZ -2800
YZ2 0
YZ3 0
YZ4 0
XY 0
XYZ 0
XYZ2 0
XYZ3 0
(X2-Y2) 0
(X2-Y2) Z 0
(X2-Y2) Z2 0
(X2-Y2) Z3 0
X3 0
X3Z 0
Y3 0
Y3Z 0
#
# Lock Parameter
#
FIELD 3172.873
LOCKPHASE 30.000
LOCKPOWER -8.000
LOCKGAIN 109.219
LOCKDC -70.000
LOCKSHIFT 4.700
LOOPGAIN -5.000
LOOPTIME 0.350
LOOPFILTER 100.000
#
IEEE64_VERSION_CODE 1
#
```

```
# Shim currents
#
SHIM_SETTING [ 1] -8127.49987255
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] 0.00000000
SHIM_SETTING [ 4] 1132.02262374
SHIM_SETTING [ 5] -1131.89943035
SHIM_SETTING [ 6] -249.63718606
SHIM_SETTING [ 7] 249.51399609
SHIM_SETTING [ 8] 19.21606552
SHIM_SETTING [ 9] -19.69548428
SHIM_SETTING [10] 2636.55242012
SHIM_SETTING [11] -2636.30130789
SHIM_SETTING [12] 0.00000000
SHIM_SETTING [13] 0.00000000
SHIM_SETTING [14] 0.00000000
SHIM_SETTING [15] -79.01924802
SHIM_SETTING [16] -79.01924802
SHIM_SETTING [17] 87.50027464
SHIM_SETTING [18] 87.50027464
SHIM_SETTING [19] -41.41112998
SHIM_SETTING [20] -41.41112998
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] -180.72969409
SHIM_SETTING [29] 0.00000000
SHIM_SETTING [30] 0.00000000
SHIM_SETTING [31] -239.71010748
SHIM_SETTING [32] 1219.26973051
SHIM_SETTING [33] 0.00000000
SHIM_SETTING [34] 0.00000000
SHIM_SETTING [35] 0.00000000
SHIM_SETTING [36] 0.00000000
SHIM_SETTING [37] 396.12871413
SHIM_SETTING [38] 148.13581605
SHIM_SETTING [39] -910.28983188
SHIM_SETTING [40] 0.00000000
```

```
Current Data Parameters
NAME NPT_13C_MAS_sino_13c
EXPNO 501
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 14.24 h
INSTRUM Avance
PROBHD H11833_0001 (P
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 15.00000000 sec
P15 0 usec
ZGPGTNS -D1acq
SFO1 188.6694996 MHz
NUC1 13C
P1 3.50 usec
PLW1 91.72799683 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG2 cw
PLW2 175.27999878 W
PLW12 0.62995678 W

F2 - Processing parameters
SI 32768
SF 188.6630851 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
FC 0.20
```

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H11833_0001 PH MASDVT 750W4 EFREE2 BL3.2 C/N/H
Sample: Adamantane (34 ul) (Z151231)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 23990 Hz)

SINO (20.0 ppm) [achieved]: Signal (1.81 ppm), Noise (63.99 to 43.98 ppm) [29517.0] <n/a>
Linewidth [achieved]: at 50% of signal height [264.3 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>

DRAFT



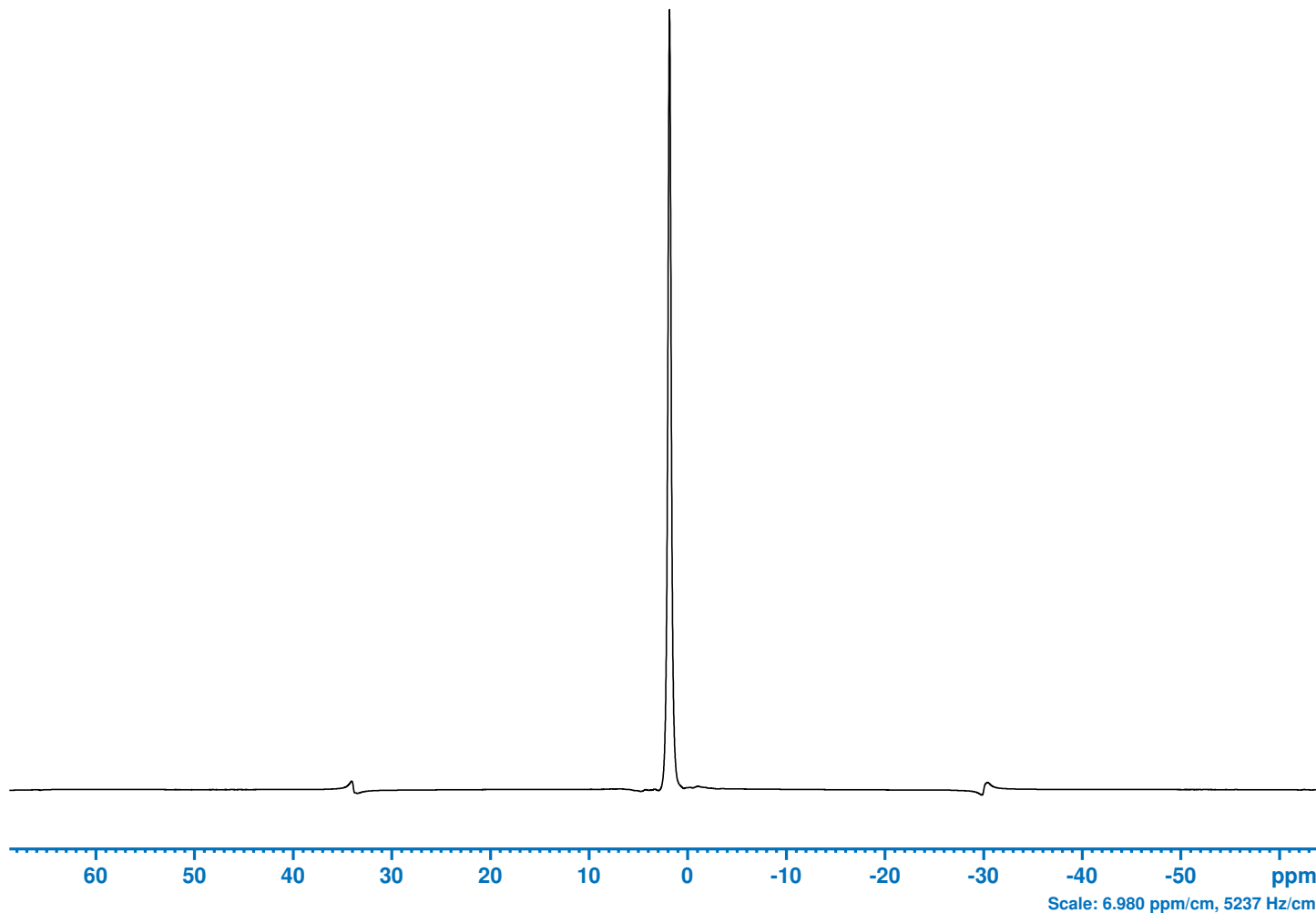
Bruker BioSpin

NPT_1H_MAS_sino_1h

Current Data Parameters
NAME NPT_1H_MAS_sino_1h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211019
Time 14.12 h
INSTRUM Avance
PROBHD H11833_0001 (P)
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 175.27999878 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
