

**PH MASDVT750W4 BL1.3 X/Y/H**

**750 MHz**

**Probe ID: H170225\_0001**

**Report Name: 2023-04-13**

● Probe NMR Test Data: PH MASDVT750W4 BL1.3 X/Y/H

Probe Related Information

EC-Level	0
Gas Compensation	nitrogen
Gradient System	unknown
ATM Accessory	false
Temperature Sensor Type	TypeT
Proton Frequency [MHz]	750
Diameter [mm]	1.3

Spectrometer Related Information

Type	AV NEO
CF Frequency [MHz]	750.30
Shim System	BOSS-WB
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
System Number	442759

● PICS Data

H170225\_0001.ph

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H170225_0001.ph
=====
$Bis,1,20220504,2048,PICS,5#
$Production,H170225,0001,00,00,,BNMRDE,20220504#
$Name,PH MASDVT750W4 BL1.3 X/Y/H#
$ProbeCompatibility,1.0,WB,4,750#
$ProbeType,1.1,MAS,0,0#
$ProbeSample,1.0,1.3,0#
$ProbeTemperature,1.0,TypeT,-30,70#
$ProbeHeaterTemperature,1.0,TypeK,-274,600#
$ProbeGasFlow,1.0,,,600,50,2000,,,#
$ProbeAllCoils,1.1,,1#
$ProbeCoil,1.0,1,2,5,3,BB,BB,1H#
$ProbeChannel,1.1,1H,,,60,,,FALSE,,,#
$ProbeBB,2.0,2,31P-15N,,,,,,#
$ProbeBBSets,1.0,31P,,,80,,,#
$ProbeBBSets,1.0,79Br/13C,,,120,,,#
$ProbeBBSets,1.0,15N,,,220,,,#
$ProbeMas,1.0,8000,67000,0,1,0,0,0,0,0#
$EndBis,FC,84#
```

● Required Samples **PH MASDVT750W4 BL1.3 X/Y/H**

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)
Z151274	Ammonium Dihydrogenphosphate (3.0 ul)

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
Sample: Potassium Bromide (KBr, 3.0 ul) (Z151270)  
Magic Angle setting, MAS (NPT\_79Br\_MAS\_magicAngle, spin rate 20000 Hz)

Line width main [achieved/rated]: [148 <= 168] <pass>  
Line width of side band number 2 (@ -40004 Hz) [achieved/rated]: [211 <= 220] <pass>



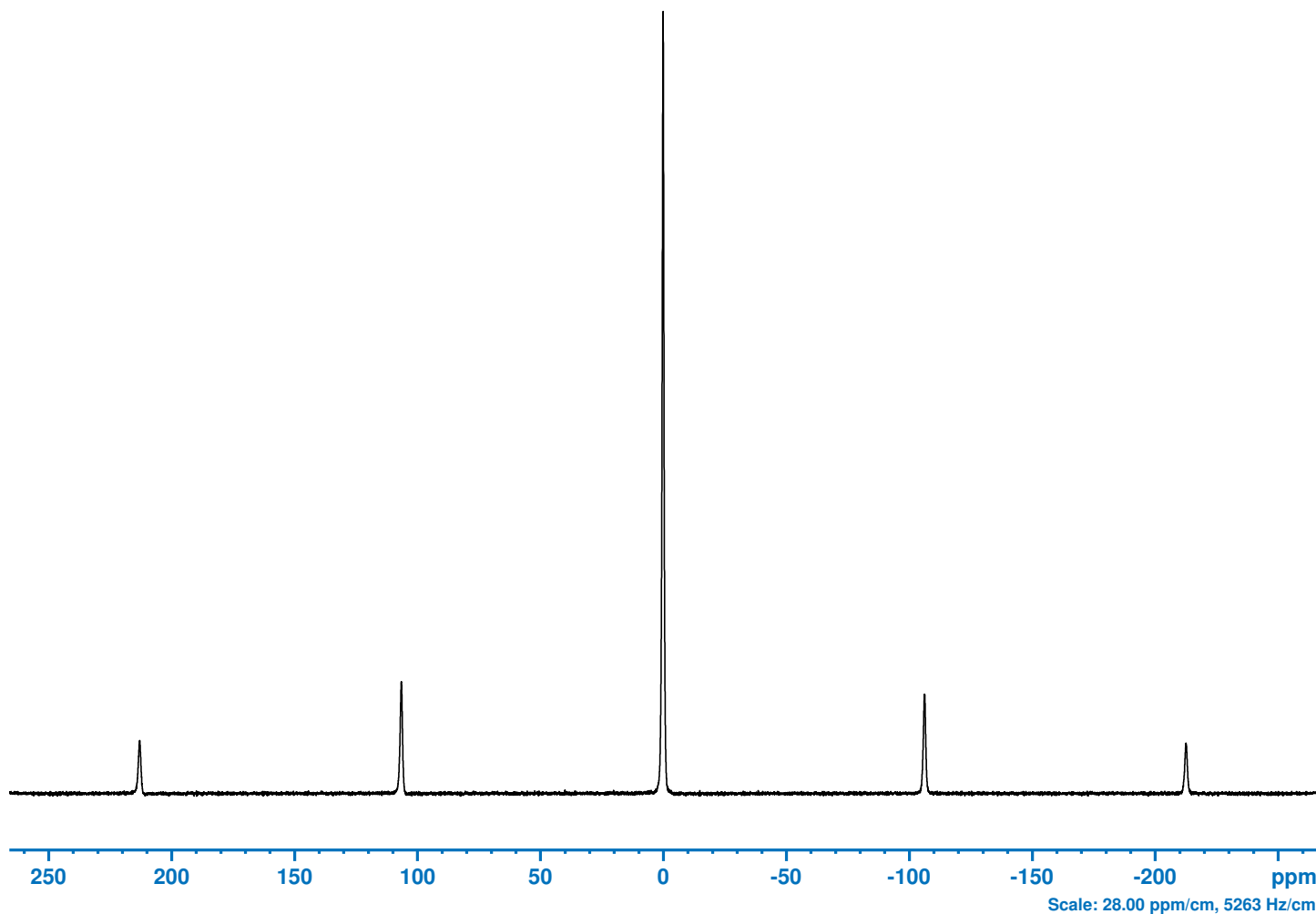
Bruker BioSpin

### NPT\_79Br\_MAS\_magicAngle

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

F2 - Acquisition Parameters  
Date\_ 20230414  
Time 8.27 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (   
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 298.2 K  
D1 0.25000000 sec  
SFO1 187.9912306 MHz  
NUC1 79Br  
P1 3.00 usec  
PLW1 20.58600044 W

F2 - Processing parameters  
SI 131072  
SF 187.9912306 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 0.20



SHIM SEQUENCE  
skip shimming

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 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=3736/BearingPressure=3180/BearingSensePressure=3189/SupplyPressure=5691/SystemPressure=4838

Spin rate at maximum deviation [measured]: @ MASR 67000 Hz [67005 Hz]  
 Maximum deviation [achieved]: @ MASR 67000 Hz [5 Hz] <n/a>



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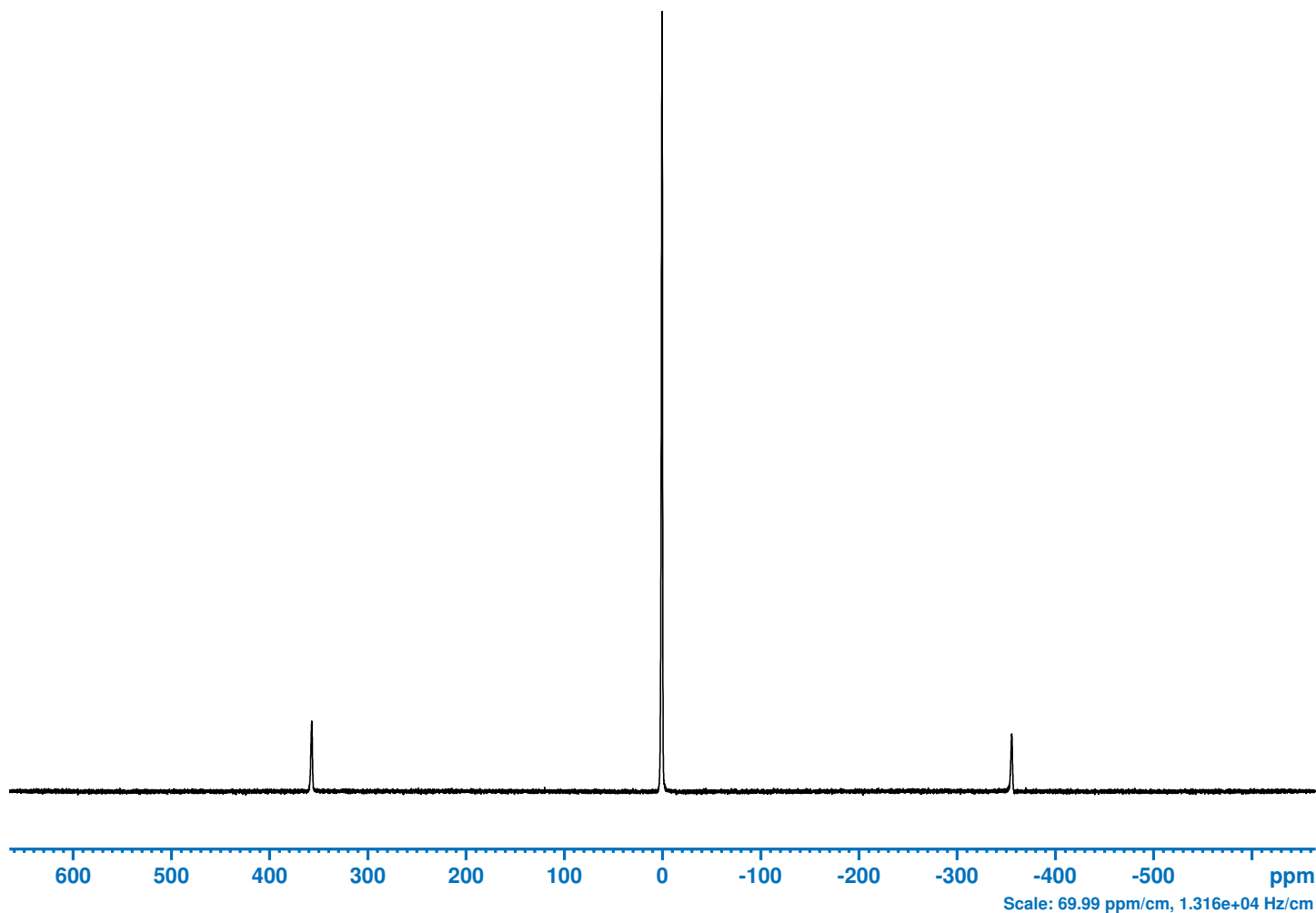
# NPT\_79Br\_MAS\_maxSpinRate

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

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 13.56 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 (   
 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 187.9910155 MHz  
 NUC1 79Br  
 P1 3.00 usec  
 PLW1 20.58600044 W

F2 - Processing parameters  
 SI 32768  
 SF 187.9910155 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20

SHIM SEQUENCE  
 skip shimming



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
Sample: Potassium Bromide (KBr, 3.0 ul) (Z151270)  
Optimization of 79Br frequency (NPT\_79Br\_MAS\_fieldsetting, spin rate 8000 Hz)  
FIELD was set to 2162.7 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0064 ppm.



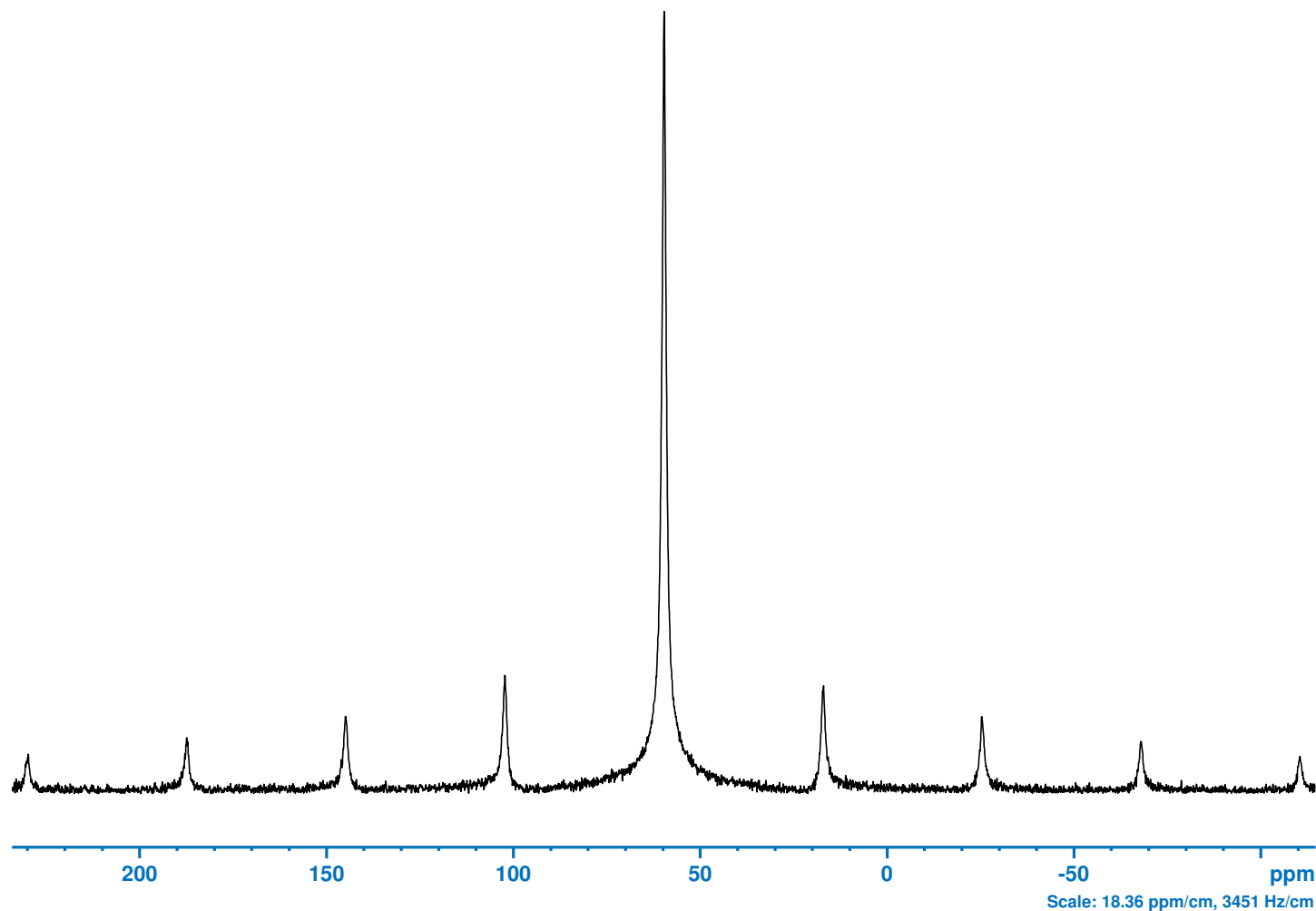
Bruker BioSpin

### NPT\_79Br\_MAS\_fieldsetting

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

F2 - Acquisition Parameters  
Date\_ 20230413  
Time 13.45 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (   
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 3.00 usec  
PLW1 20.58600044 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 ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Adamantane (3.0 ul) (Z151271)  
 Optimization of 13C frequency (NPT\_13C\_MAS\_fieldsetting\_dec1h, spin rate 67000 Hz)  
 FIELD was set to 2104.9 for 13C chemical shift of 38.460 ppm. One field unit corresponds to 0.0071 ppm.



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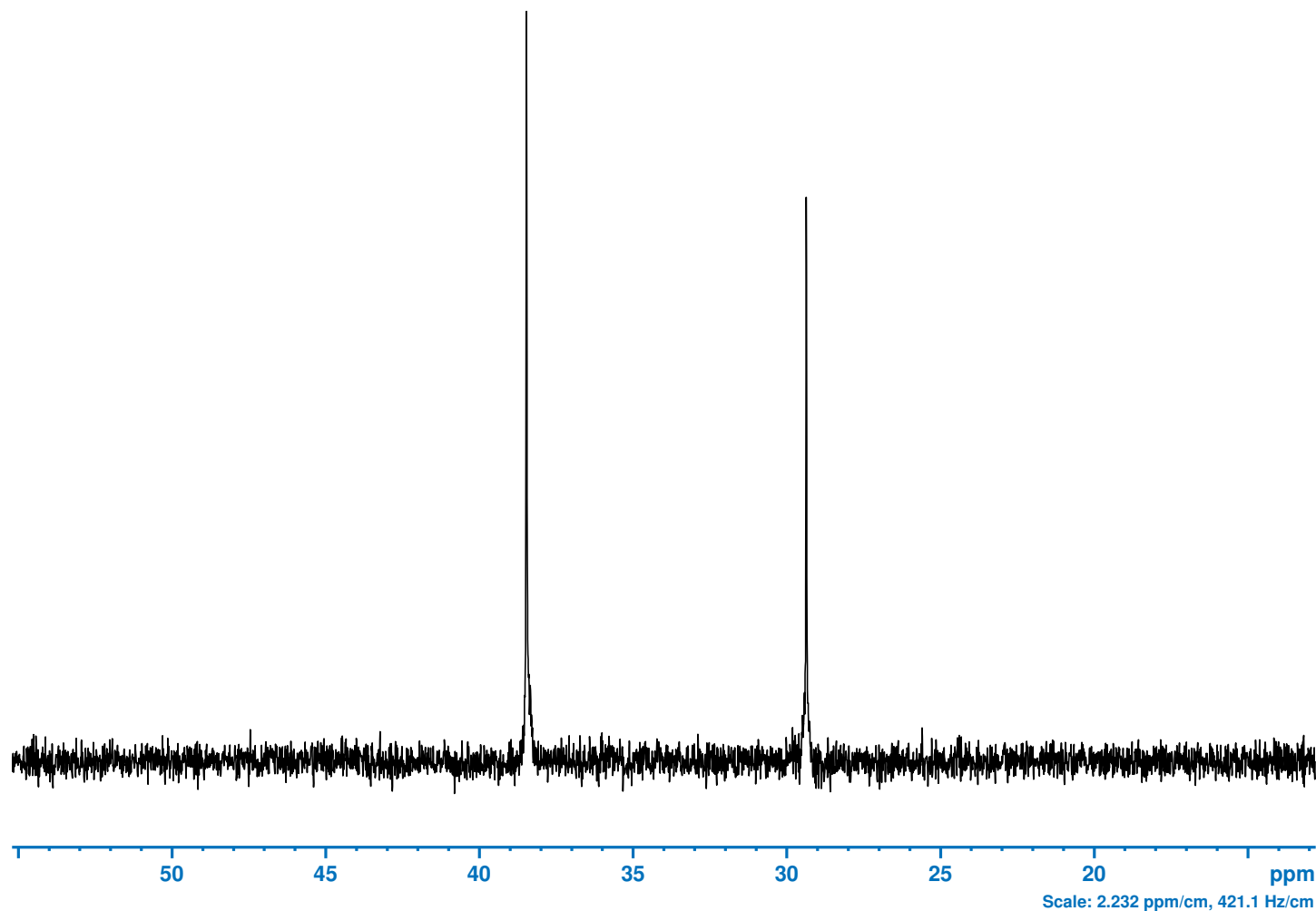
# NPT\_13C\_MAS\_fieldsetting\_dec1h

Current Data Parameters  
 NAME NPT\_13C\_MAS\_fieldsetting\_dec1h  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 11.43 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001  
 PULPROG hpdec  
 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 188.6694995 MHz  
 NUC1 13C  
 P1 2.80 usec  
 PLW1 24.20000076 W  
 SFO2 750.3017067 MHz  
 NUC2 1H  
 CPDPRG2 cw  
 PLW2 55.01699829 W  
 PLW12 0.55568552 W

F2 - Processing parameters  
 SI 8192  
 SF 188.6630850 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 FC 0.50

SHIM SEQUENCE  
 skip shimming





NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Adamantane (3.0 ul) (Z151271)  
 P90 1H pulse calibration, MAS (NPT\_1H\_MAS\_p90det\_1h, spin rate 67000 Hz)  
 ATTENTION: Updated PROSOL Tables with [1.50 us @ 55.0 W].

P90 MAS 1H pulse [achieved/rated]: @ 56.5 W [1.48 us <= 1.50 us] <pass>



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## NPT\_1H\_MAS\_p90det\_1h

Current Data Parameters  
 NAME NPT\_1H\_MAS\_p90det\_1h  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230412  
 Time 17.36 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 ( )  
 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 4.50 usec  
 PLW1 56.51359940 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
50.0 W	1.50 us		
50.0 W	1.50 us	1.56 us	4.0%
56.5 W	1.50 us	1.48 us	-1.3%

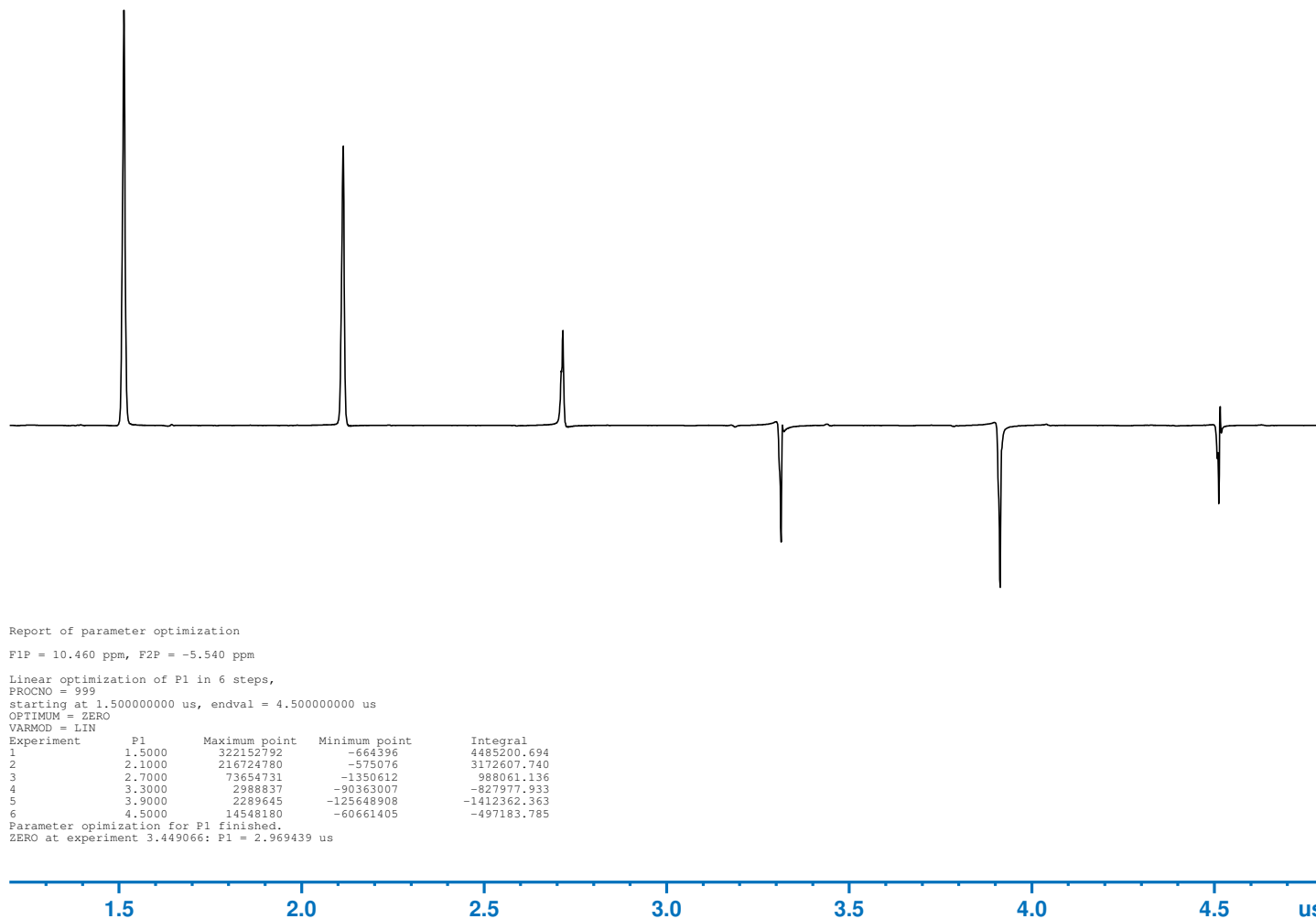
Report of parameter optimization

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	322152792	-664396	4485200.694
2	2.1000	216724780	-575076	3172607.740
3	2.7000	73654731	-1350612	988061.136
4	3.3000	2988837	-90363007	-827977.933
5	3.9000	2289645	-125648908	-1412362.363
6	4.5000	14548180	-60661405	-497183.785

Parameter optimization for P1 finished.  
 ZERO at experiment 3.449066: P1 = 2.969439 us



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 SHIM SEQUENCE

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 skip shimming  
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NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 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 [3.00 us @ 20.6 W].

P90 MAS 79Br pulse [achieved/rated]: @ 22.3 W [2.88 us <= 3.00 us] <pass>



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## NPT\_79Br\_MAS\_p90det\_79br

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

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 13.07 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 ( )  
 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 9.00 usec  
 PLW1 22.33687019 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
38.0 W	3.00 us	2.25 us	-25.0%
38.0 W	3.00 us	2.88 us	-4.0%
22.3 W	3.00 us	2.88 us	-4.0%

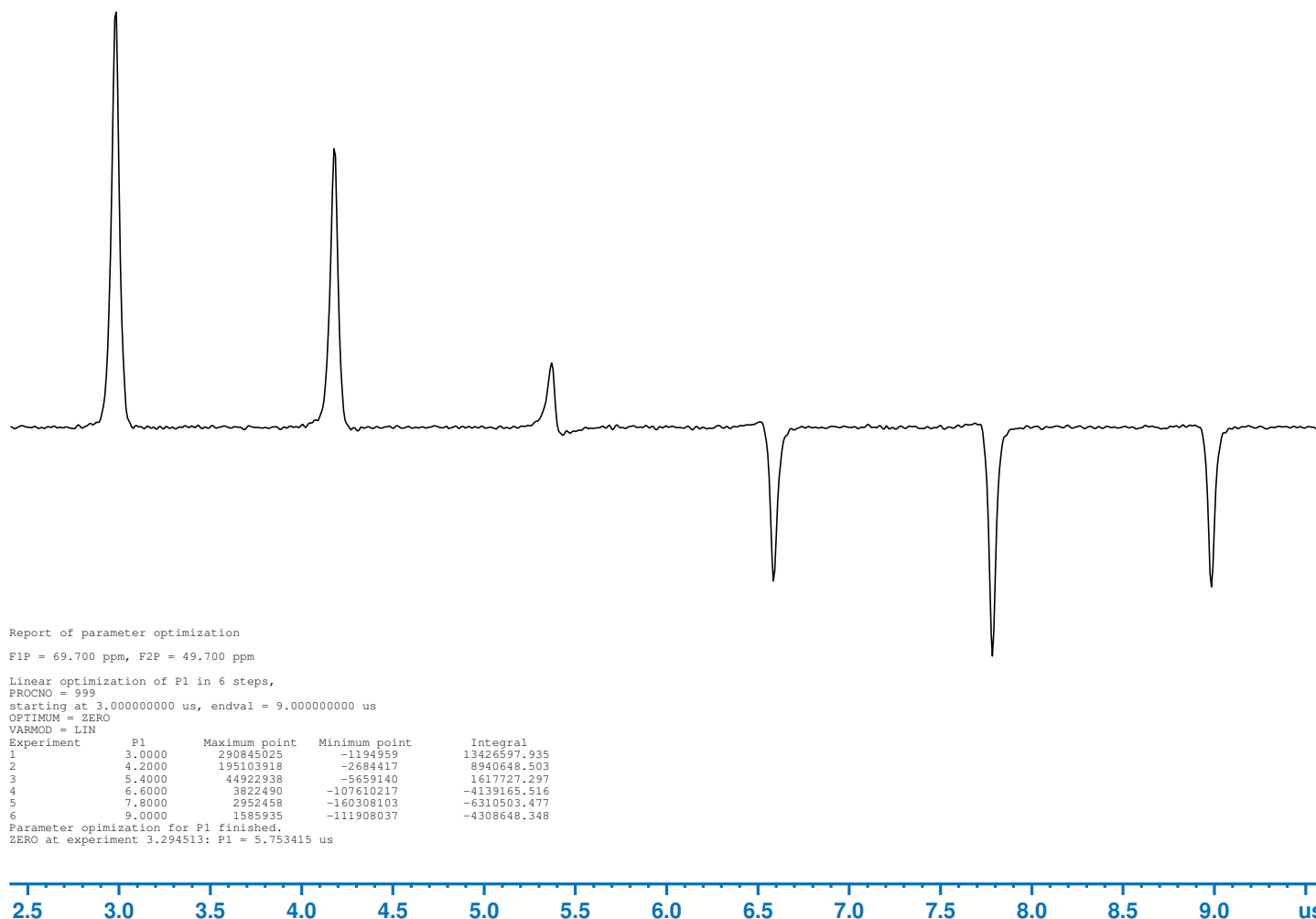
Report of parameter optimization

F1P = 69.700 ppm, F2P = 49.700 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	290845025	-1194959	13426597.935
2	4.2000	195103918	-2684417	8940648.503
3	5.4000	44922938	-5659140	1617727.297
4	6.6000	3822490	-107610217	-4139165.516
5	7.8000	2952458	-160308103	-6310503.477
6	9.0000	1585935	-111908037	-4308648.348

Parameter optimization for P1 finished.  
 ZERO at experiment 3.294513: P1 = 5.753415 us



SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
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 8000 Hz)  
ATTENTION: Updated PROSOL Tables with [2.80 us @ 21.4 W].

P90\_MAS\_CP 1H13C power (PLW 11) [achieved/rated]: [24.2 W <= 25.0 W] <pass>  
P90\_MAS\_CP 1H13C pulse (P 1) [achieved/rated]: [2.63 us <= 2.80 us] <pass>



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## NPT\_13C\_MAS\_p90det\_cp1h\_13c

Current Data Parameters  
NAME NPT\_13C\_MAS\_p90det\_cp1h\_13c  
EXPNO 2  
PROCNO 1

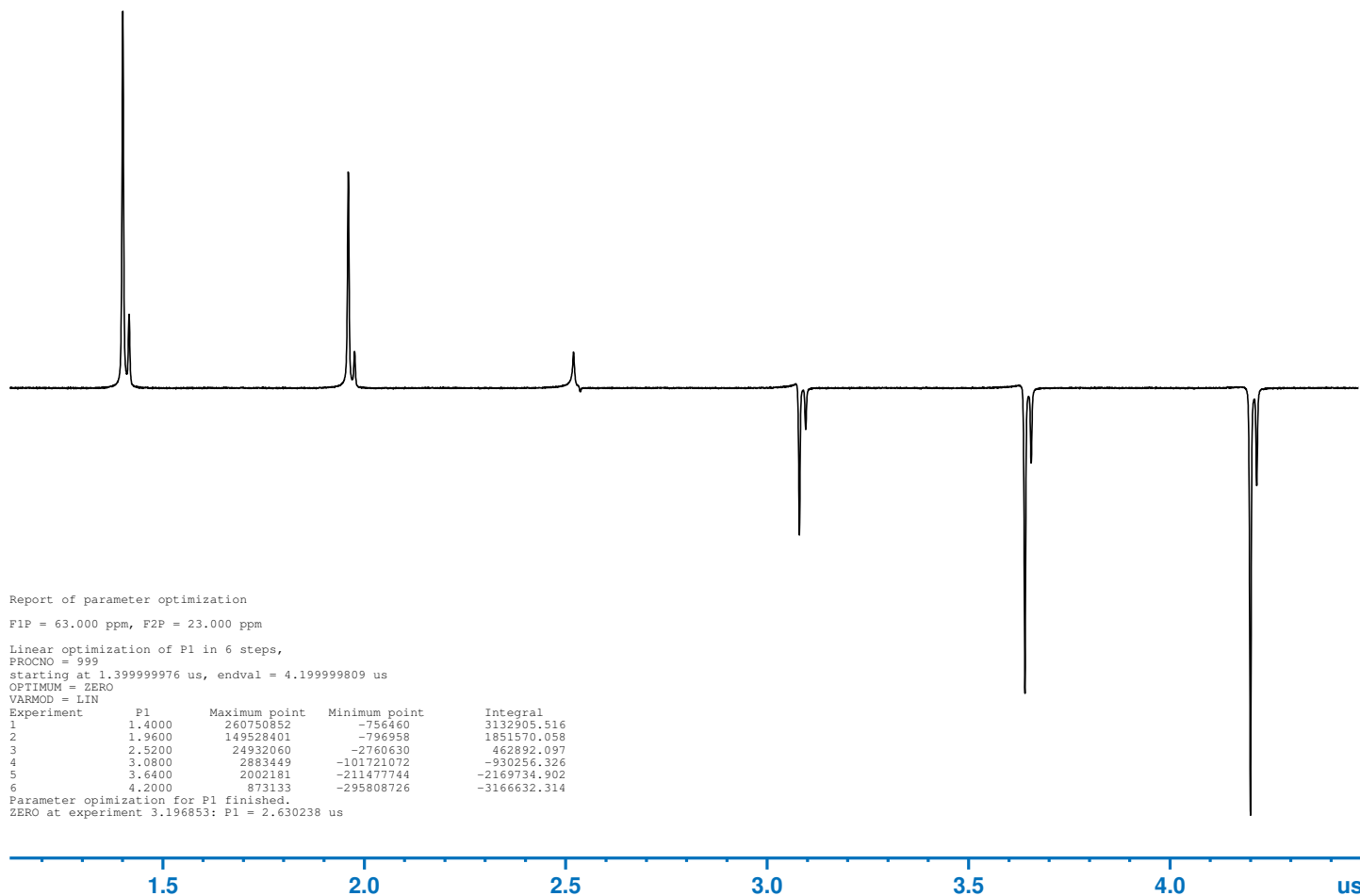
F2 - Acquisition Parameters  
Date\_ 20230413  
Time 14.24 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001  
PULPROG cp90  
TD 5554  
SOLVENT H2O+D2O  
NS 4  
DS 0  
SWH 55555.555 Hz  
FIDRES 20.005602 Hz  
AQ 0.0499860 sec  
RG 101  
DW 9.000 usec  
DE 6.50 usec  
TE 298.1 K  
D1 5.00000000 sec  
ZGPTNS  
SFO1 188.6711975 MHz  
NUC1 13C  
P1 4.20 usec  
P15 2000.00 usec  
PLW1 24.20000076 W  
PLW11 24.20000076 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.0000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 55.01699829 W  
PLW12 55.01699829 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 39.03153992 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  
-----  
24.2 W 2.80 us  
24.2 W 2.80 us 2.63 us -6.1%

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 1.399999976 us, endval = 4.1999999809 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	1.4000	260750852	-756460	3132905.516
2	1.9600	149528401	-796958	1851570.058
3	2.5200	24932060	-2760630	462892.097
4	3.0800	2883449	-101721072	-930256.326
5	3.6400	2002181	-211477744	-2169734.902
6	4.2000	873133	-295808726	-3166632.314

Parameter optimization for P1 finished.

ZERO at experiment 3.196853: P1 = 2.630238 us

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)  
P90 13C 1H-13C CP shortest pulse calibration, MAS (NPT\_13C\_MAS\_shortestPulse\_cp1h\_13c, spin rate 8000 Hz)

P90\_MAS\_CP 1H13C power (PLW 11) [achieved/rated]: [50.0 W <= 50.0 W] <pass>  
P90\_MAS\_CP 1H13C pulse (P 1) [achieved/rated]: [1.85 us <= 2.00 us] <pass>



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## NPT\_13C\_MAS\_shortestPulse\_cp1h\_13c

Current Data Parameters  
NAME NPT\_13C\_MAS\_shortestPulse\_cp1h\_13c  
EXPNO 1  
PROCNO 1

### F2 - Acquisition Parameters

Date\_ 20230413  
Time 14.36 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (PULPROG cp90  
TD 5554  
SOLVENT H2O+D2O  
NS 4  
DS 0  
SWH 55555.555 Hz  
FIDRES 20.005502 Hz  
AQ 0.0499860 sec  
RG 101  
DW 9.000 usec  
DE 6.50 usec  
TE 298.2 K  
D1 5.00000000 sec  
ZGPGTNS  
SFO1 188.6711975 MHz  
NUC1 13C  
P1 3.00 usec  
P15 2000.00 usec  
PLW1 21.35099983 W  
PLW11 50.00000000 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.0000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 55.01699829 W  
PLW12 55.01699829 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 39.03153992 W

### F2 - Processing parameters

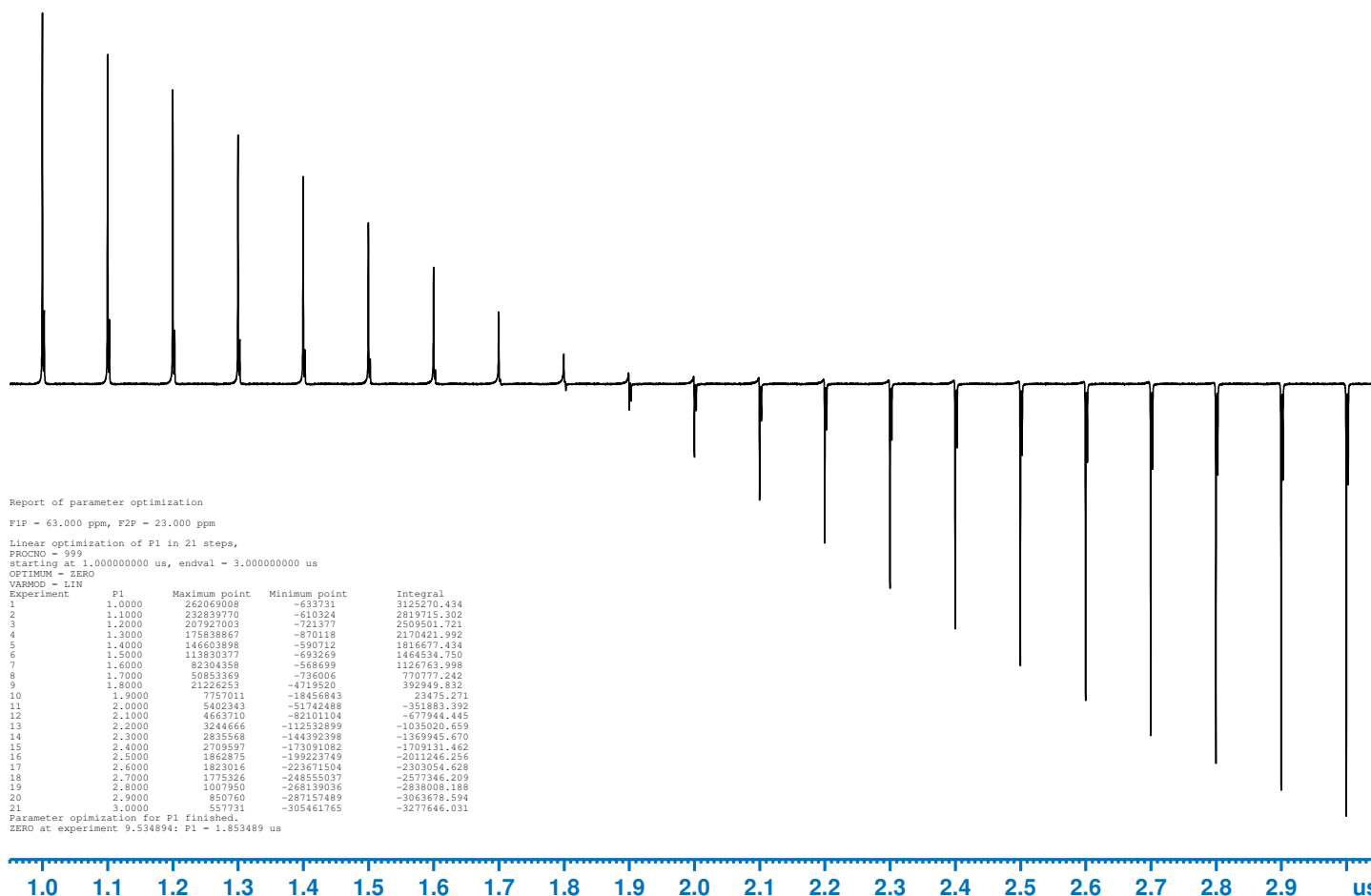
SI 8192  
SF 188.6630851 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 0.20

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

PLW90	P90	P90[det]	Deviation
21.4 W	2.80 us		
50.0 W	2.00 us	1.85 us	-7.5%

### SHIM SEQUENCE

skip shimming



### Report of parameter optimization

F1P = 63.000 ppm, F2P = 23.000 ppm

Linear optimization of P1 in 21 steps,

PROCNO = 999

starting at 1.000000000 us, endval = 3.000000000 us

OPTIMUM = ZERO

VARIABLE = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	1.0000	262069008	-633731	3125270.434
2	1.1000	232839770	-610324	2819715.302
3	1.2000	207927003	-721377	2509501.721
4	1.3000	175838867	-870118	2170421.992
5	1.4000	146603898	-590712	1816677.434
6	1.5000	113830377	-693269	1464534.750
7	1.6000	82304358	-568699	1126763.998
8	1.7000	50853369	-736006	770777.242
9	1.8000	21226253	-471520	392949.832
10	1.9000	7757011	-18456843	23475.271
11	2.0000	5402343	-51742488	-351883.392
12	2.1000	4663710	-82111104	-677944.445
13	2.2000	3244666	-112532899	-1035020.659
14	2.3000	2835568	-144392398	-1369945.670
15	2.4000	2709897	-173091082	-1709131.462
16	2.5000	1862875	-199223749	-2011246.256
17	2.6000	1823016	-223671504	-2303054.628
18	2.7000	1775326	-248555037	-2577346.209
19	2.8000	1007950	-268139036	-2838008.188
20	2.9000	850760	-287157489	-3063678.594
21	3.0000	557751	-305461765	-3277646.031

Parameter optimization for P1 finished.

ZERO at experiment 9.534894: P1 = 1.853489 us

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Adamantane (3.0 ul) (Z151271)  
 P90 13C pulse calibration, MAS (NPT\_13C\_MAS\_p90det\_13c, spin rate 67000 Hz)  
 ATTENTION: Updated PROSOL Tables with [2.80 us @ 24.2 W].

P90 MAS 13C pulse [achieved/rated]: @ 25.1 W [2.75 us <= 2.80 us] <pass>



Bruker BioSpin

## NPT\_13C\_MAS\_p90det\_13c

Current Data Parameters  
 NAME NPT\_13C\_MAS\_p90det\_13c  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 11.35 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 (   
 PULPROG hpdec  
 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 188.6694995 MHz  
 NUC1 13C  
 P1 8.40 usec  
 PLW1 25.06419945 W  
 SFO2 750.3018457 MHz  
 NUC2 1H  
 CPDPRG[2] cw  
 PLW2 55.01699829 W  
 PLW12 0.55568552 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
50.0 W	3.00 us		
57.4 W	2.80 us	1.81 us	-35.4%
25.1 W	2.80 us	2.75 us	-1.8%

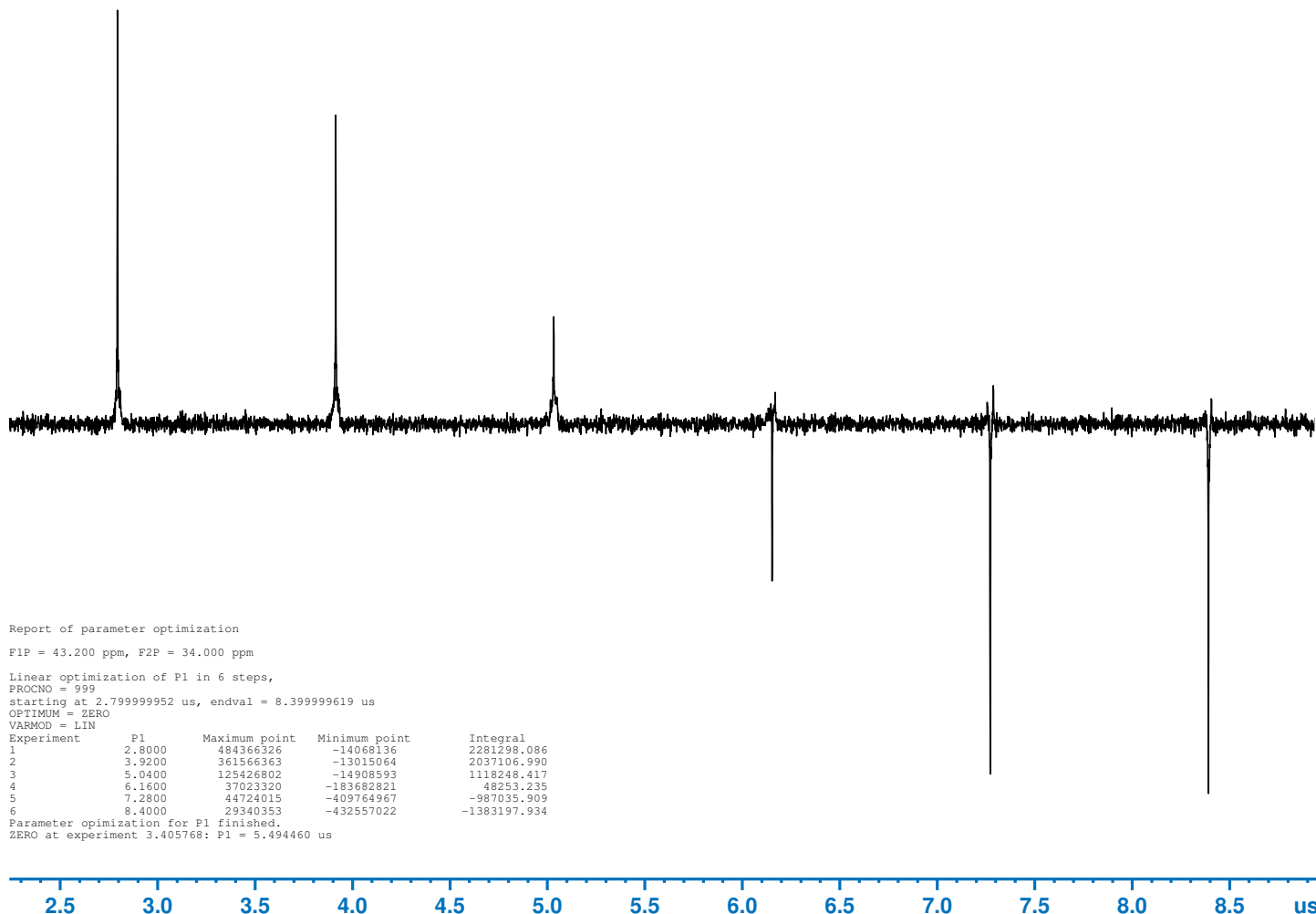
Report of parameter optimization

F1P = 43.200 ppm, F2P = 34.000 ppm

Linear optimization of P1 in 6 steps,  
 PROCNO = 999  
 starting at 2.799999952 us, endval = 8.3999999619 us  
 OPTIMUM = ZERO  
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.8000	484366326	-14068136	2281298.086
2	3.9200	361566363	-13015064	2037106.990
3	5.0400	125426802	-14908593	1118248.417
4	6.1600	37023320	-183682821	48253.235
5	7.2800	44724015	-409764967	-987035.909
6	8.4000	29340353	-432557022	-1383197.934

Parameter optimization for P1 finished.  
 ZERO at experiment 3.405768: P1 = 5.494460 us



SHM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
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 8000 Hz)  
ATTENTION: Updated PROSOL Tables with [5.00 us @ 28.0 W].

P90\_MAS\_CP 1H15N power (PLW 11) [achieved/rated]: [34.9 W <= 75.0 W] <pass>  
P90\_MAS\_CP 1H15N pulse (P 1) [achieved/rated]: [4.48 us <= 5.00 us] <pass>



Bruker BioSpin

## NPT\_15N\_MAS\_p90det\_cp1h\_15n

Current Data Parameters  
NAME NPT\_15N\_MAS\_p90det\_cp1h\_15n  
EXPNO 1  
PROCNO 1

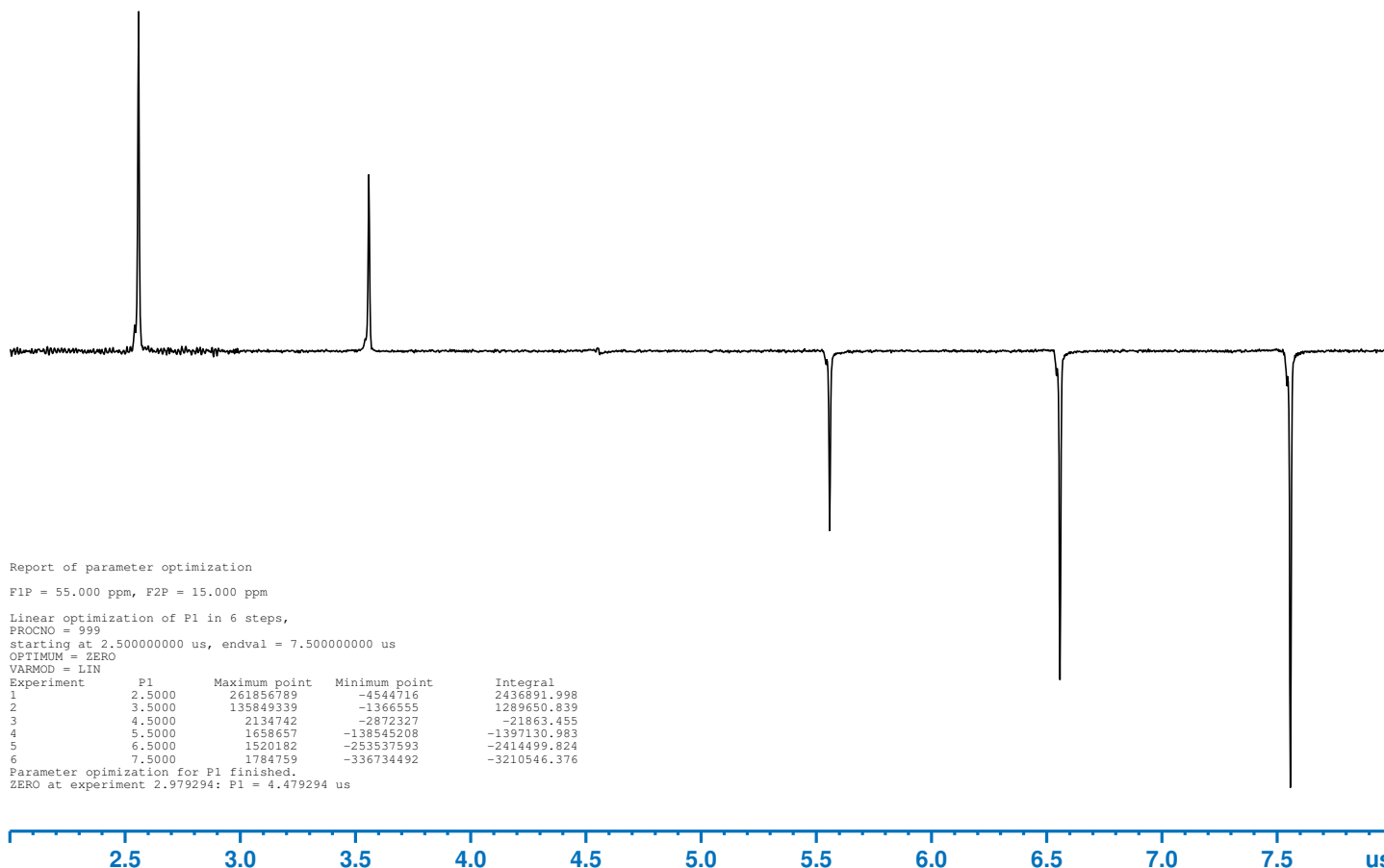
F2 - Acquisition Parameters  
Date\_ 20230413  
Time 16.28 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (cp90)  
PULPROG cp90  
TD 3012  
SOLVENT H2O+D2O  
NS 4  
DS 0  
SWH 30120.482 Hz  
FIDRES 20.000320 Hz  
AQ 0.0499992 sec  
RG 101  
DW 16.600 usec  
DE 6.50 usec  
TE 298.1 K  
D1 5.00000000 sec  
ZGPTNS  
SFO1 76.0299000 MHz  
NUC1 15N  
P1 7.50 usec  
P15 3500.00 usec  
PLW1 34.86899948 W  
PLW11 34.86899948 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.0000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 55.01699829 W  
PLW12 55.01699829 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 11.84494019 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  
-----  
34.9 W 5.00 us  
34.9 W 5.00 us 4.48 us -10.4%

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 2.500000000 us, endval = 7.500000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.5000	261856789	-4544716	2436891.998
2	3.5000	135849339	-1366555	1289650.839
3	4.5000	2134742	-2872327	-21863.455
4	5.5000	1658657	-138545208	-1397130.983
5	6.5000	1520182	-253537593	-2414499.824
6	7.5000	1784759	-336734492	-3210546.376

Parameter optimization for P1 finished.

ZERO at experiment 2.979294: P1 = 4.479294 us

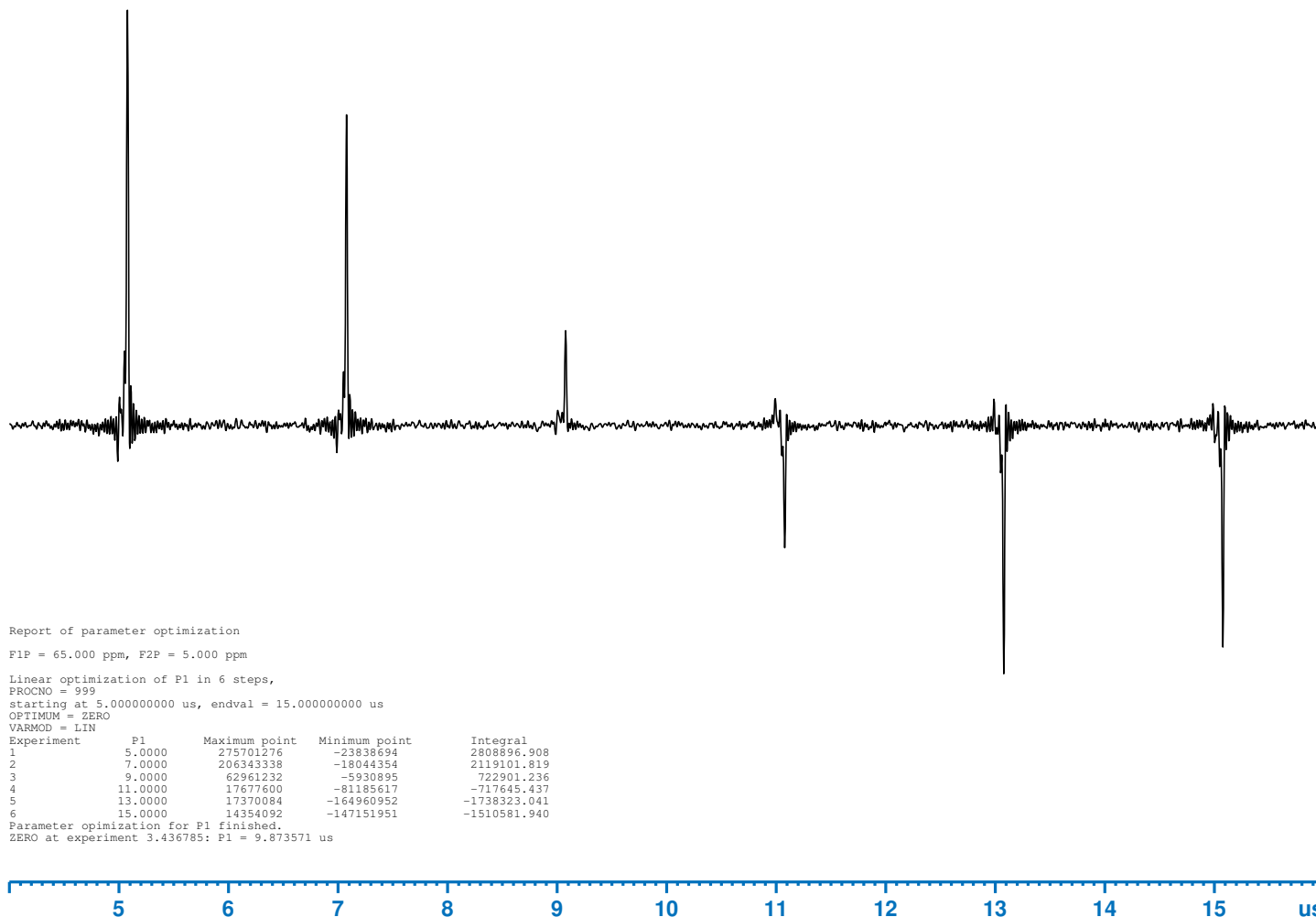
NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: 2-13C, 15N alpha-glycine (2 mg, 3.0 ul) (Z151273)  
 P90 15N pulse calibration, MAS (NPT\_15N\_MAS\_p90det\_15n, spin rate 8000 Hz)  
 ATTENTION: Updated PROSOL Tables with [5.00 us @ 34.9 W].

P90 MAS 15N pulse [achieved/rated]: @ 35.7 W [4.94 us <= 5.00 us] <pass>



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## NPT\_15N\_MAS\_p90det\_15n



Current Data Parameters  
 NAME NPT\_15N\_MAS\_p90det\_15n  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 16.21 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 ( )  
 PULPROG hspec  
 TD 1510  
 SOLVENT H2O+D2O  
 NS 4  
 DS 0  
 SWH 38461.539 Hz  
 FIDRES 50.942436 Hz  
 AQ 0.0196300 sec  
 RG 101  
 DW 13.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 15.00000000 sec  
 P15 0 usec  
 ZGPTNS -Dlacq  
 SFO1 76.0299000 MHz  
 NUC1 15N  
 P1 15.00 usec  
 PLW1 35.72100067 W  
 SFO2 750.3046519 MHz  
 NUC2 1H  
 CPDPRG[2] spinal64  
 PCPD2 2.80 usec  
 PLW2 55.01699829 W  
 PLW12 55.01699829 W

F2 - Processing parameters  
 SI 4096  
 SF 76.0272387 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.50

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

PLW90	P90	P90[det]	Deviation
90.0 W	3.15 us		
35.7 W	5.00 us	4.94 us	-1.2%

SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
Sample: Ammonium Dihydrogenphosphate (3.0 ul) (Z151274)  
P90 31P 1H-31P CP pulse calibration, MAS (NPT\_31P\_MAS\_p90det\_cp1h\_31p, spin rate 15000 Hz)  
ATTENTION: Updated PROSOL Tables with [4.00 us @ 21.4 W].

P90\_MAS\_CP 1H31P power (PLW 11) [achieved/rated]: [22.2 W <= 33.0 W] <pass>  
P90\_MAS\_CP 1H31P pulse (P 1) [achieved/rated]: [3.93 us <= 4.00 us] <pass>



Bruker BioSpin

## NPT\_31P\_MAS\_p90det\_cp1h\_31p

Current Data Parameters  
NAME NPT\_31P\_MAS\_p90det\_cp1h\_31p  
EXPNO 1  
PROCNO 1

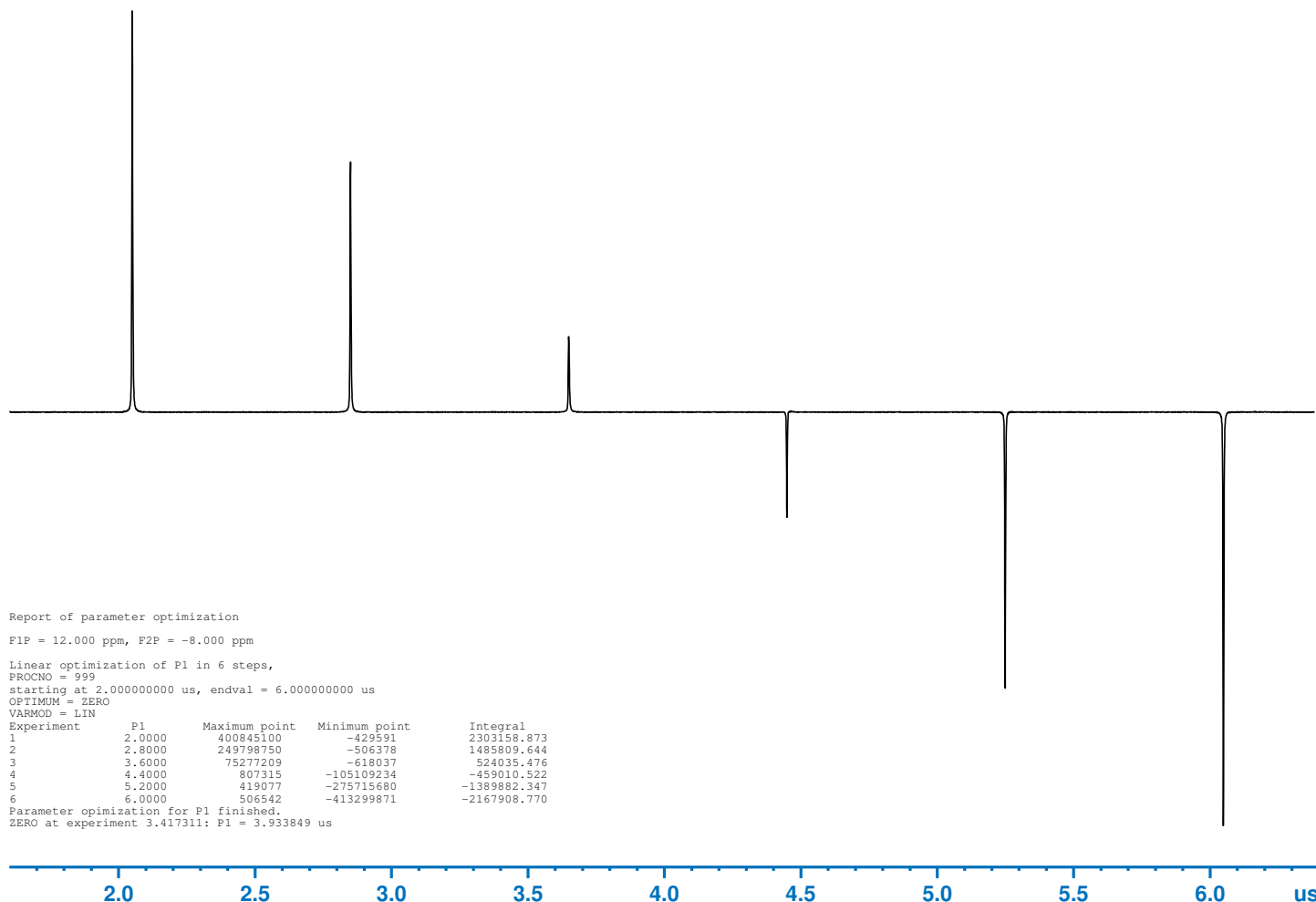
F2 - Acquisition Parameters  
Date\_ 20230413  
Time 18.46 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (cp90)  
PULPROG cp90  
TD 9090  
SOLVENT H2O+D2O  
NS 4  
DS 0  
SWH 90909.094 Hz  
FIDRES 20.002001 Hz  
AQ 0.0499950 sec  
RG 101  
DW 5.500 usec  
DE 6.50 usec  
TE 298.1 K  
D1 5.00000000 sec  
ZGPGTNS  
SFO1 303.7276145 MHz  
NUC1 31P  
P1 6.00 usec  
P15 3500.00 usec  
PLW1 22.18899918 W  
PLW11 22.18899918 W  
SFO2 750.3054022 MHz  
NUC2 1H  
CNST21 1.00000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 55.01699829 W  
PLW12 55.01699829 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 21.14854050 W

F2 - Processing parameters  
SI 16384  
SF 303.7270072 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

\*\*\*\*\* P90 Pulse Determination History \*\*\*\*\*  
PLW90 P90 P90[det] Deviation  
22.2 W 4.00 us 3.93 us -1.7%

SHIM SEQUENCE

skip shimming



Report of parameter optimization

F1P = 12.000 ppm, F2P = -8.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

Starting at 2.000000000 us, endval = 6.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	2.0000	400845100	-429591	2303158.873
2	2.8000	249798750	-506378	1485809.644
3	3.6000	75277209	-618037	524035.476
4	4.4000	807315	-105109234	-459010.522
5	5.2000	419077	-275715680	-1389882.347
6	6.0000	506542	-413299871	-2167908.770

Parameter optimization for P1 finished.

ZERO at experiment 3.417311: P1 = 3.933849 us



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
Sample: Ammonium Dihydrogenphosphate (3.0 ul) (Z151274)  
P90 31P 1H-31P CP shortest pulse calibration, MAS (NPT\_31P\_MAS\_shortestPulse\_cp1h\_31p, spin rate 15000 Hz)

P90\_MAS\_CP 1H31P power (PLW 11) [achieved/rated]: [50.0 W <= 50.0 W] <pass>  
P90\_MAS\_CP 1H31P pulse (P 1) [achieved/rated]: [2.65 us <= 3.00 us] <pass>



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## NPT\_31P\_MAS\_shortestPulse\_cp1h\_31p

Current Data Parameters  
NAME NPT\_31P\_MAS\_shortestPulse\_cp1h\_31p  
EXPNO 1  
PROCNO 1

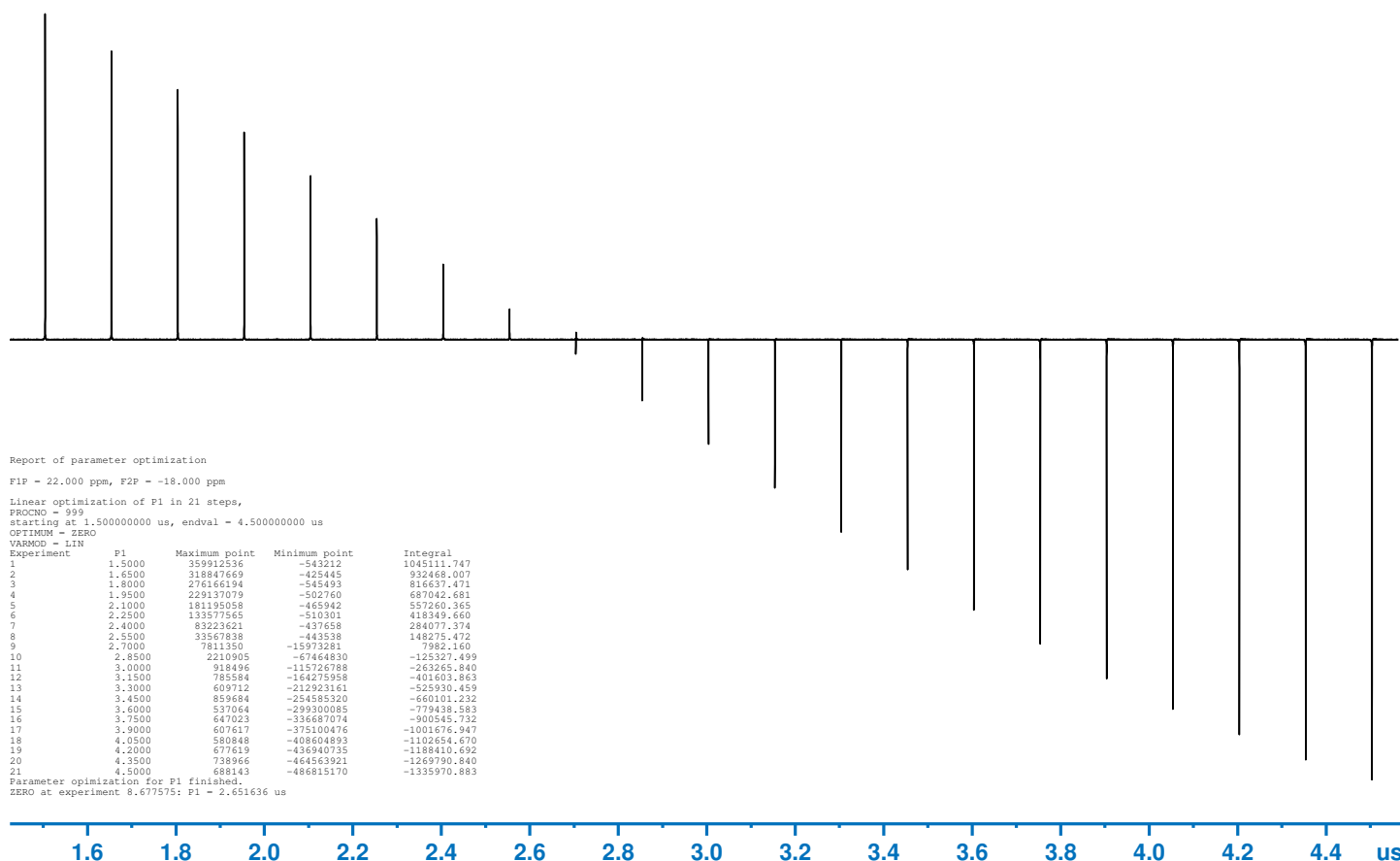
F2 - Acquisition Parameters  
Date\_ 20230413  
Time 18.57 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (PULPROG cp90  
TD 9090  
SOLVENT H2O+D2O  
NS 4  
DS 0  
SWH 90909.094 Hz  
FIDRES 20.002001 Hz  
AQ 0.0499950 sec  
RG 101  
DW 5.500 usec  
DE 6.50 usec  
TE 298.0 K  
D1 5.00000000 sec  
ZGPGTNS  
SF01 303.7276145 MHz  
NUC1 31P  
P1 4.50 usec  
P15 3500.00 usec  
PLW1 21.41900063 W  
PLW11 50.00000000 W  
SF02 750.3054022 MHz  
NUC2 1H  
CNST21 1.00000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 55.01699829 W  
PLW12 55.01699829 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 21.14854050 W

F2 - Processing parameters  
SI 16384  
SF 303.7270072 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

\*\*\*\*\* P90 Pulse Determination History \*\*\*\*\*  
PLW90 P90 P90[det] Deviation  
-----  
21.4 W 4.00 us  
50.0 W 3.00 us 2.65 us -11.7%

SHIM SEQUENCE

skip shimming



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Ammonium Dihydrogenphosphate (3.0 ul) (Z151274)  
 P90 31P pulse calibration, MAS (NPT\_31P\_MAS\_p90det\_31p, spin rate 15000 Hz)  
 ATTENTION: Updated PROSOL Tables with [4.00 us @ 22.2 W]. Calculation based on ==> [3.28 us @ 33.0 W]

P90 MAS 31P pulse [achieved/rated]: @ 33.0 W [3.28 us <= 4.00 us] <pass>



Bruker BioSpin

## NPT\_31P\_MAS\_p90det\_31p

Current Data Parameters  
 NAME NPT\_31P\_MAS\_p90det\_31p  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 18.42 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 ( hpdec  
 PULPROG 3256  
 TD  
 SOLVENT H2O+D2O  
 NS 1  
 DS 2  
 SWH 40650.406 Hz  
 FIDRES 24.969538 Hz  
 AQ 0.0400488 sec  
 RG 101  
 DW 12.300 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 10.00000000 sec  
 P15 0 usec  
 ZGPTNS -Dlacq  
 SFO1 303.7276145 MHz  
 NUC1 31P  
 P1 12.00 usec  
 PLW1 33.00000000 W  
 SFO2 750.3054022 MHz  
 NUC2 1H  
 CPDPRG[2] spinal64  
 PCPD2 2.80 usec  
 PLW2 55.01699829 W  
 PLW12 55.01699829 W

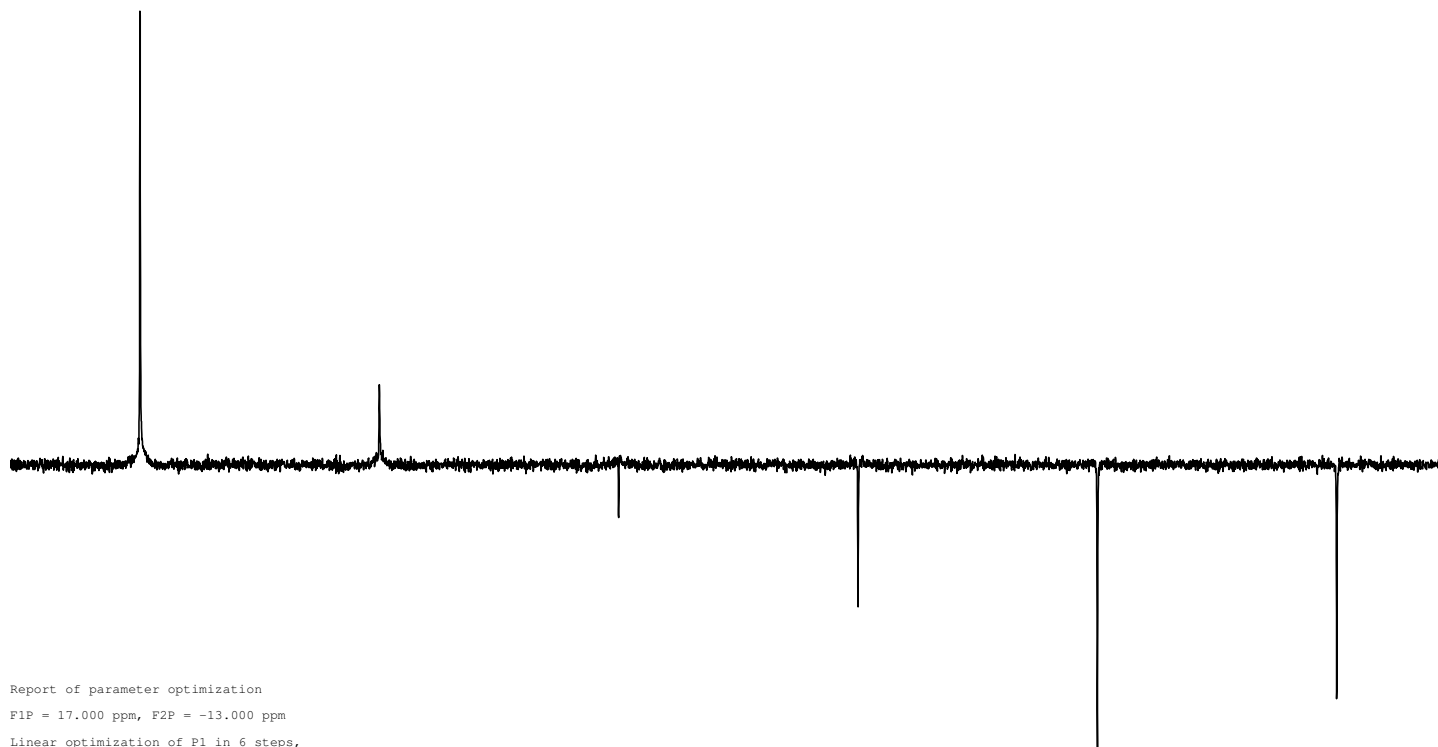
F2 - Processing parameters  
 SI 8192  
 SF 303.7270072 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.50

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

PLW90	P90	P90[det]	Deviation
33.0 W	4.00 us		
33.0 W	4.00 us	3.28 us	-18.0%

SHIM SEQUENCE

skip shimming



Report of parameter optimization

F1P = 17.000 ppm, F2P = -13.000 ppm

Linear optimization of P1 in 6 steps,

PROCNO = 999

starting at 4.000000000 us, endval = 12.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	4.0000	286352551	-5860971	1615698.194
2	5.6000	50540385	-5541218	381681.530
3	7.2000	6085349	-33326292	23948.020
4	8.8000	6142492	-89681499	-255214.892
5	10.4000	6472117	-179678035	-577733.809
6	12.0000	5803747	-147644624	-528532.625

Parameter optimization for P1 finished.

ZERO at experiment 2.602628: P1 = 6.564204 us

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 11.0 11.5 12.0 us

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Alpha-glycine (2 mg, 3.0 ul) (Z151272)  
 CP 1H-13C sensitivity, MAS (NPT\_13C\_MAS\_sino\_cp1h\_13c, spin rate 8000 Hz)

SINO (20.0 ppm) [achieved/rated]: Signal (42.93 ppm), Noise (199.75 to 179.74 ppm) [130.0 >= 76.0] <pass>  
 Number of scans (NS) [achieved/rated]: [64 <= 64] <pass>  
 Processed with TDef=2048



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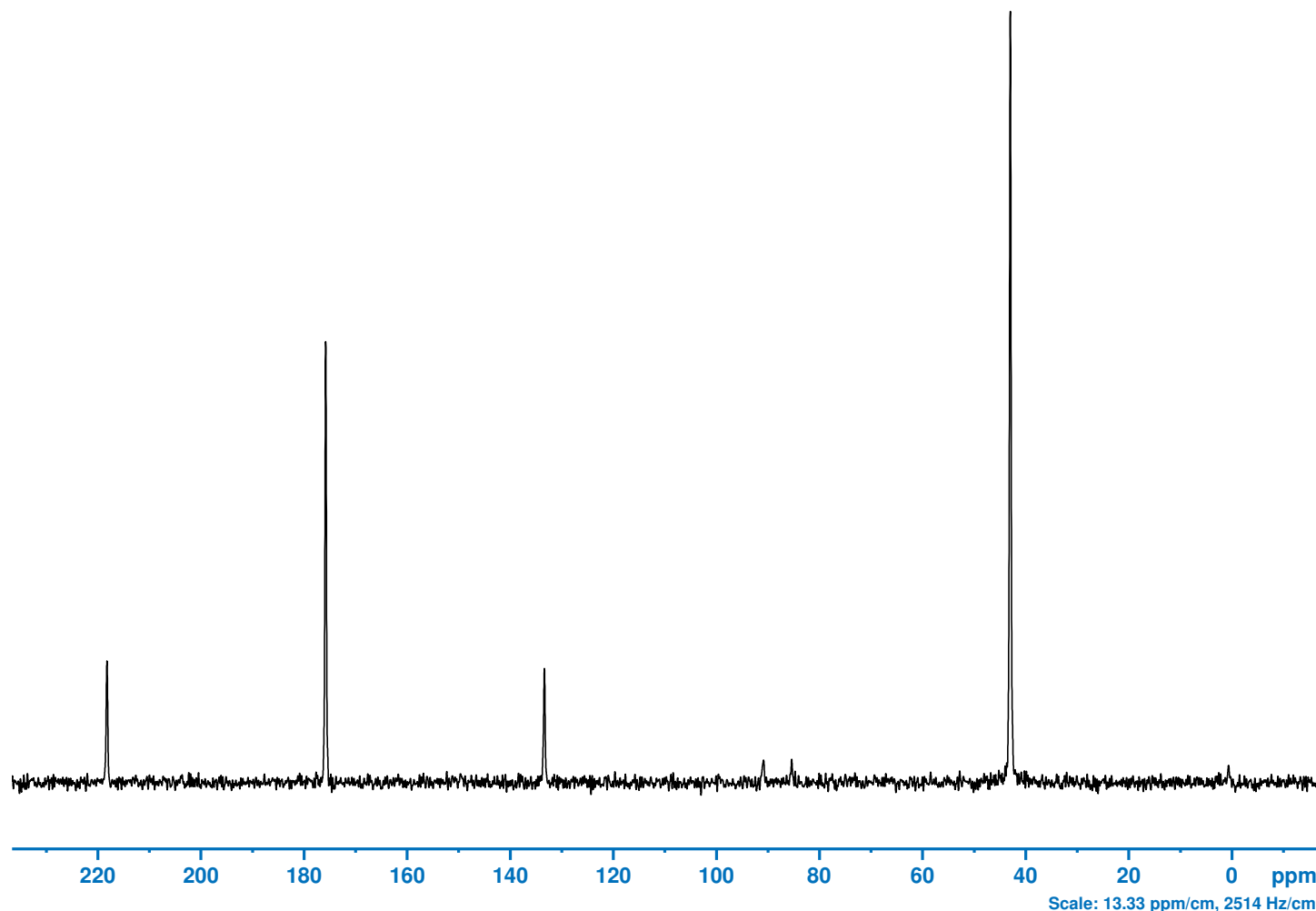
# NPT\_13C\_MAS\_sino\_cp1h\_13c

Current Data Parameters  
 NAME NPT\_13C\_MAS\_sino\_cp1h\_13c  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 15.30 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 (cp  
 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 298.1 K  
 D1 5.00000000 sec  
 ZGPGTNS  
 SFO1 188.6838379 MHz  
 NUC1 13C  
 P15 2000.00 usec  
 PLW1 21.35099983 W  
 SFO2 750.3046519 MHz  
 NUC2 1H  
 CNST21 1.00000000  
 CPDPRG2 spinal64  
 P3 1.50 usec  
 PCPD2 2.80 usec  
 PLW2 55.01699829 W  
 PLW12 45.47999954 W  
 SPNAM[0] ramp50100.100  
 SPOAL0 0.500  
 SPOFFS0 0 Hz  
 SPW0 33.34999847 W

F2 - Processing parameters  
 SI 32768  
 SF 188.6630850 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 FC 0.20

SHIM SEQUENCE  
 skip shimming



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Alpha-glycine (2 mg, 3.0 ul) (Z151272)  
 CP 1H-15N sensitivity, MAS (NPT\_15N\_MAS\_sino\_cp1h\_15n, spin rate 12000 Hz)

SINO (20.0 ppm) [achieved]: Signal (32.68 ppm), Noise (66.94 to 46.93 ppm) [22.4] <n/a>  
 Number of scans (NS) [achieved/rated]: [256 <= 256] <pass>



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

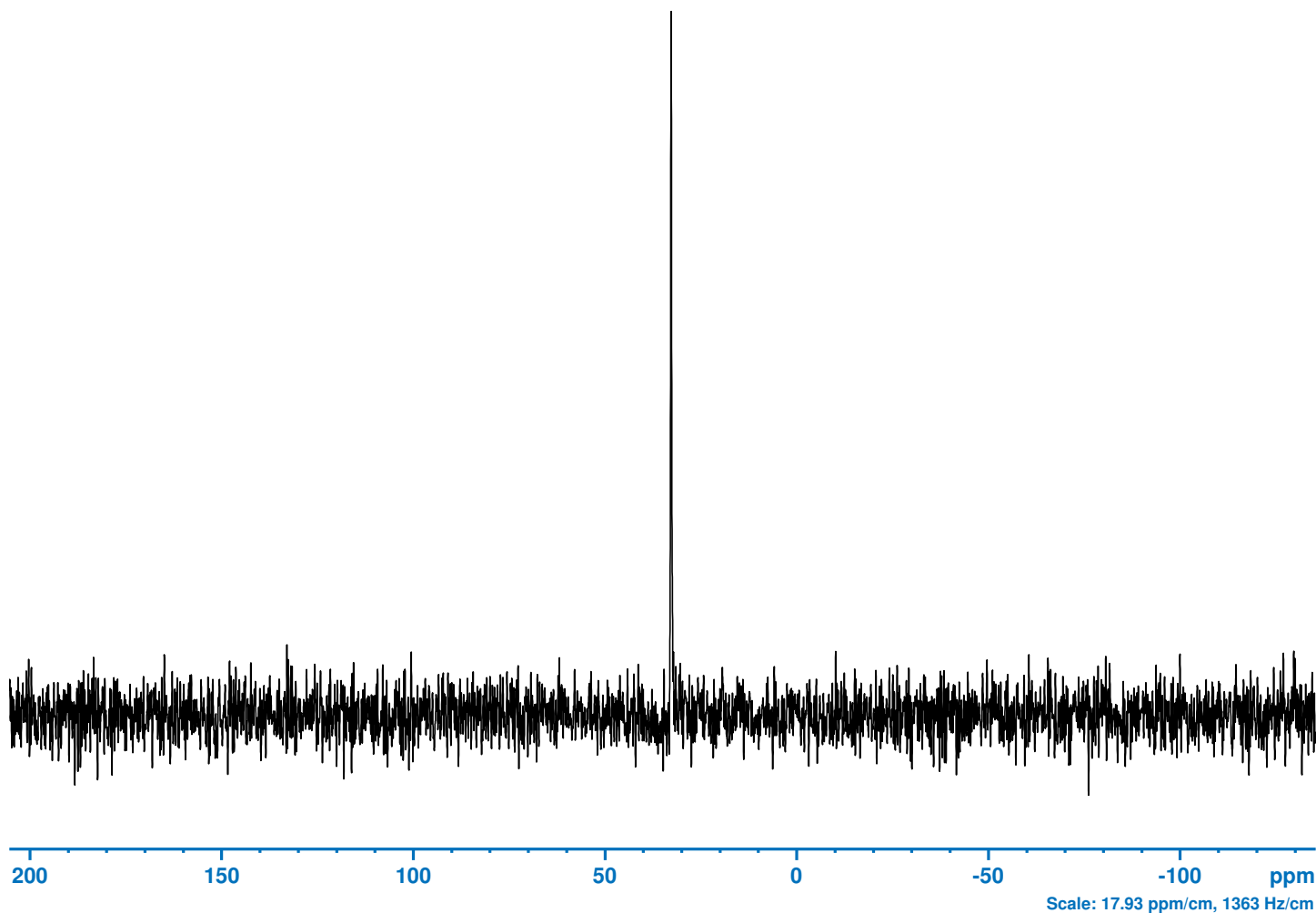
Current Data Parameters  
 NAME NPT\_15N\_MAS\_sino\_cp1h\_15n  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 17.40 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 (cp  
 PULPROG cp  
 TD 3012  
 SOLVENT H2O+D2O  
 NS 256  
 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 76.0299000 MHz  
 NUC1 15N  
 P15 3500.00 usec  
 PLW1 27.99300003 W  
 SFO2 750.3046519 MHz  
 NUC2 1H  
 CNST21 1.0000000  
 CPDPRG2 spinal64  
 P3 1.50 usec  
 PCPD2 2.80 usec  
 PLW2 55.01699829 W  
 PLW12 57.31999969 W  
 SPNAM[0] ramp50100.100  
 SPOAL0 0.500  
 SPOFFS0 0 Hz  
 SPW0 16.25000000 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 ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Ammonium Dihydrogenphosphate (3.0 ul) (Z151274)  
 CP 1H-31P sensitivity, MAS (NPT\_31P\_MAS\_sino\_cp1h\_31p, spin rate 15000 Hz)

SINO (10.0 ppm) [achieved]: Signal (0.73 ppm), Noise (-74.55 to -84.55 ppm) [2490.2] <n/a>  
 Number of scans (NS) [achieved/rated]: [4 <= 4] <pass>



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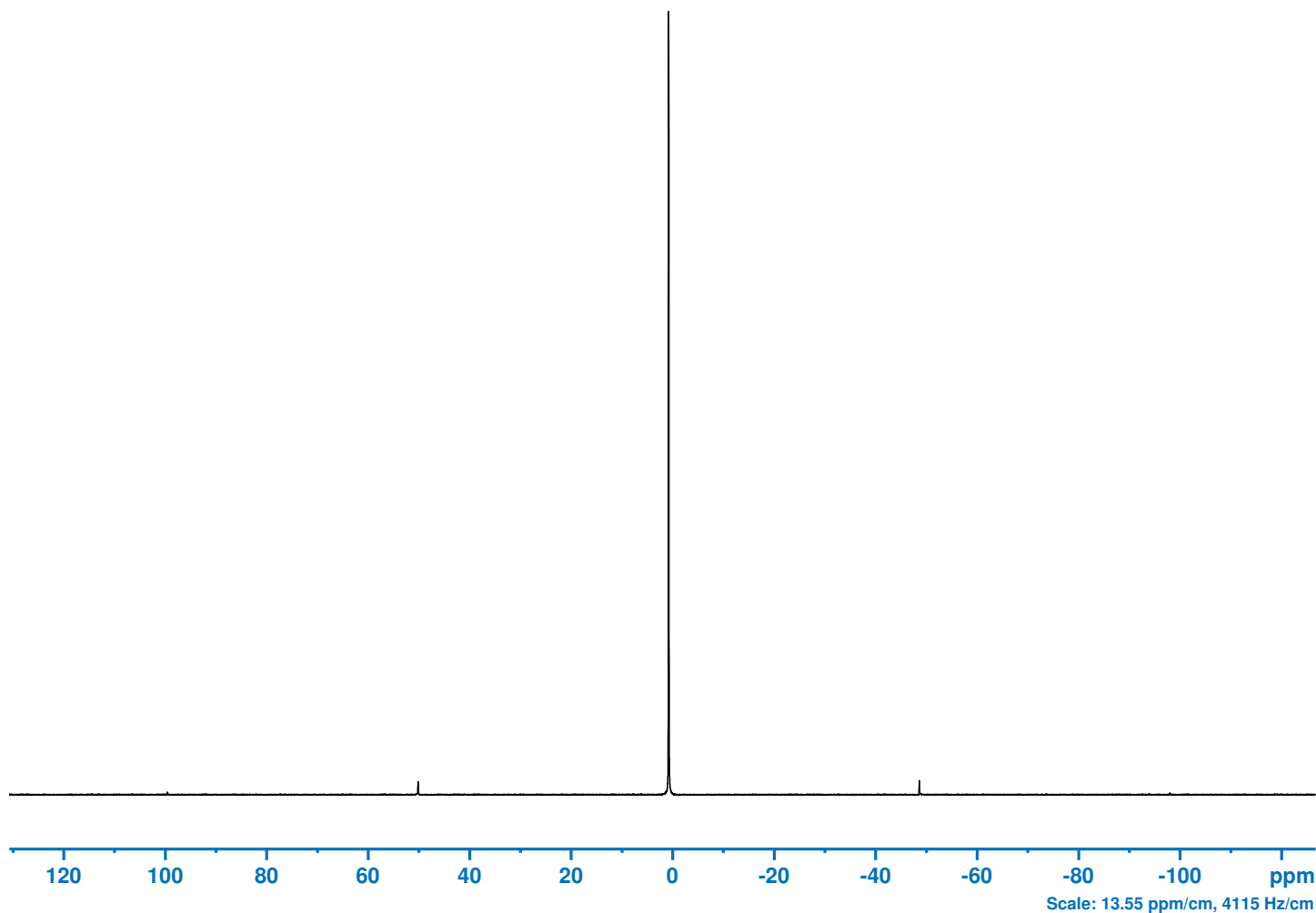
## NPT\_31P\_MAS\_sino\_cp1h\_31p

Current Data Parameters  
 NAME NPT\_31P\_MAS\_sino\_cp1h\_31p  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 19.12 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 (cp  
 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 298.0 K  
 D1 5.00000000 sec  
 ZGPGTNS  
 SFO1 303.7276145 MHz  
 NUC1 31P  
 P15 3500.00 usec  
 PLW1 21.41900063 W  
 SFO2 750.3054022 MHz  
 NUC2 1H  
 CNST21 1.0000000  
 CPDPRG2 spinal64  
 P3 1.50 usec  
 PCPD2 2.80 usec  
 PLW2 55.01699829 W  
 PLW12 51.40000153 W  
 SPNAM[0] ramp50100.100  
 SPOAL0 0.500  
 SPOFFS0 0 Hz  
 SPW0 29.59000015 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 ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
Sample: Adamantane (3.0 ul) (Z151271)  
13C sensitivity, MAS (NPT\_13C\_MAS\_sino\_13c, spin rate 67000 Hz)

SINO (20.0 ppm) [achieved]: Signal (38.20 ppm), Noise (27.75 to 7.75 ppm) [49.0] <n/a>  
Linewidth [achieved/rated]: at 50% of signal height [4.2 Hz <= 12.0 Hz] <pass>  
Number of scans (NS) [achieved/rated]: [16 <= 16] <pass>



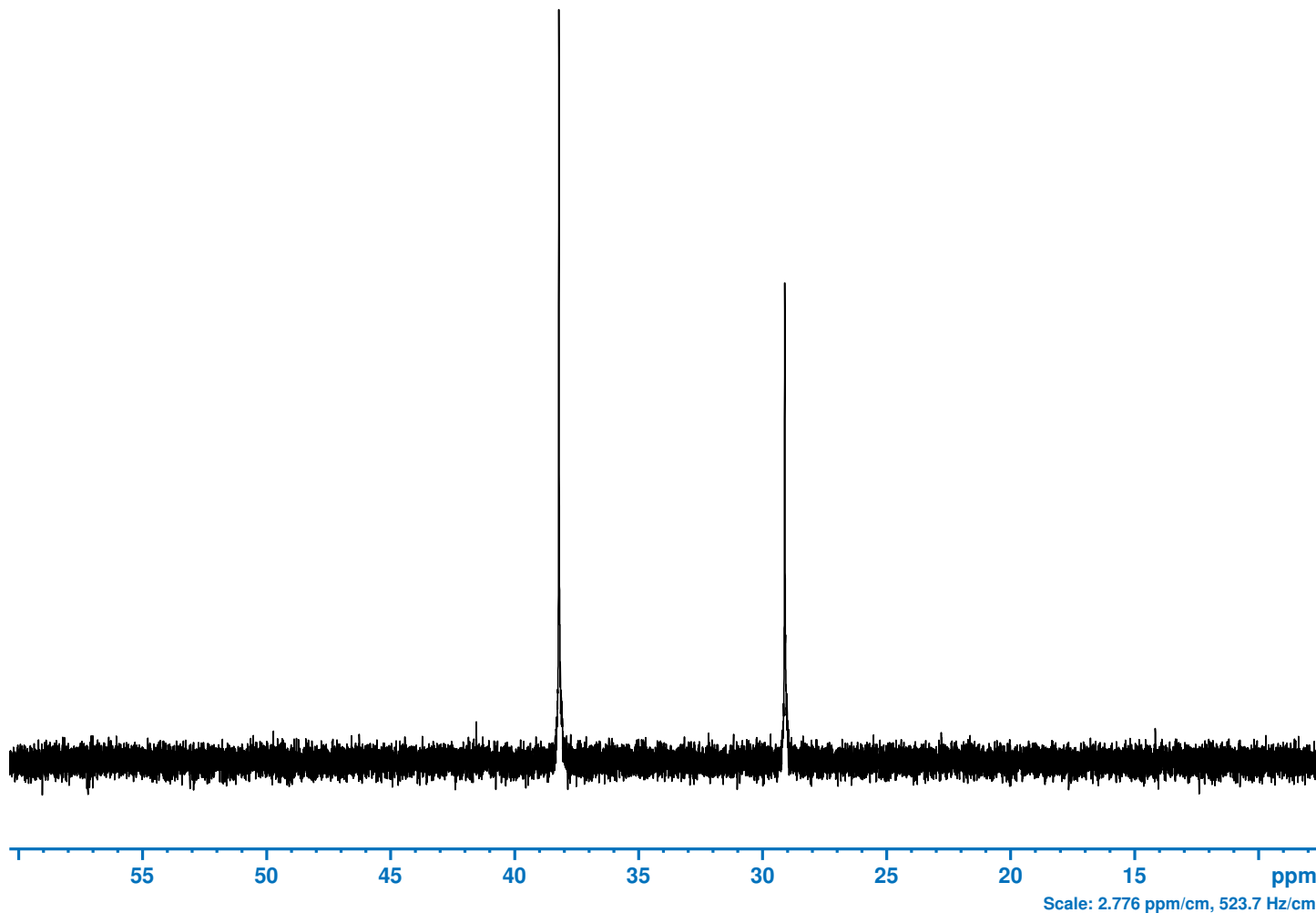
Bruker BioSpin

### NPT\_13C\_MAS\_sino\_13c

Current Data Parameters  
NAME NPT\_13C\_MAS\_sino\_13c  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230413  
Time 12.55 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 ( )  
PULPROG hpdec  
TD 19998  
SOLVENT H2O+D2O  
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 298.0 K  
D1 15.00000000 sec  
P15 0 usec  
ZGPGTNS -Dlacq  
SFO1 188.6694995 MHz  
NUC1 13C  
P1 2.80 usec  
PLW1 24.20000076 W  
SFO2 750.3018457 MHz  
NUC2 1H  
CPDPRG2 cw  
PLW2 55.01699829 W  
PLW12 0.55568552 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 ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Adamantane (3.0 ul) (Z151271)  
 13C sensitivity, MAS (NPT\_13C\_MAS\_sino\_13c, spin rate 67000 Hz)



Bruker BioSpin

# NPT\_13C\_MAS\_sino\_13c

```
# Thu Apr 13 10:55:53 2023
##$PROBEIDENTIFIER=H170225_0001
##$PROBENAME=PH MASDVT750W4 BL1.3 X/Y/H
##$SHIMID=272623
#
# Active Shim Gradients
#
Z -55800
Z2 0
Z3 0
Z4 0
Z5 0
Z6 0
X 0
XZ 0
XZ2 0
XZ3 0
XZ4 0
Y 11000
YZ 30000
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 2124.400
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] -13949.99936363
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] -0.00000000
SHIM_SETTING [ 4] 1942.99829632
SHIM_SETTING [ 5] -1942.78582752
SHIM_SETTING [ 6] -428.47653826
SHIM_SETTING [ 7] 428.26501116
SHIM_SETTING [ 8] 32.98209682
SHIM_SETTING [ 9] -33.80593128
SHIM_SETTING [10] 4525.36522175
SHIM_SETTING [11] -4524.93558660
SHIM_SETTING [12] -0.00000000
SHIM_SETTING [13] -0.00000000
SHIM_SETTING [14] 0.00000000
SHIM_SETTING [15] -0.00005820
SHIM_SETTING [16] 0.00034115
SHIM_SETTING [17] -0.00006102
SHIM_SETTING [18] -0.00025230
SHIM_SETTING [19] -0.00096123
SHIM_SETTING [20] 0.00010951
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] 9983.46420304
SHIM_SETTING [29] 0.00000000
SHIM_SETTING [30] 0.00000000
SHIM_SETTING [31] -6342.38801822
SHIM_SETTING [32] -5016.53530447
SHIM_SETTING [33] 0.00000000
SHIM_SETTING [34] 0.00000000
SHIM_SETTING [35] 0.00000000
SHIM_SETTING [36] 0.00000000
SHIM_SETTING [37] -27.03223990
SHIM_SETTING [38] 2630.03826937
SHIM_SETTING [39] 842.38801822
SHIM_SETTING [40] 0.00000000
```

```
Current Data Parameters
NAME NPT_13C_MAS_sino_13c
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230413
Time 12.55 h
INSTRUM Avance NEO
PROBHD H170225_0001 (
PULPROG hpdec
TD 19998
SOLVENT H2O+D2O
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 298.0 K
D1 15.00000000 sec
P15 0 usec
ZGPGTNS -Dlacq
SFO1 188.6694995 MHz
NUC1 13C
P1 2.80 usec
PLW1 24.20000076 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG2 cw
PLW2 55.01699829 W
PLW12 0.55568552 W

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

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
Sample: Adamantane (3.0 ul) (Z151271)  
1H sensitivity, MAS (NPT\_1H\_MAS\_sino\_1h, spin rate 67000 Hz)

SINO (20.0 ppm) [achieved]: Signal (2.35 ppm), Noise (-43.83 to -63.84 ppm) [5156.7] <n/a>  
Linewidth [achieved]: at 50% of signal height [134.6 Hz] <n/a>  
Number of scans (NS) [achieved/rated]: [16 <= 16] <pass>



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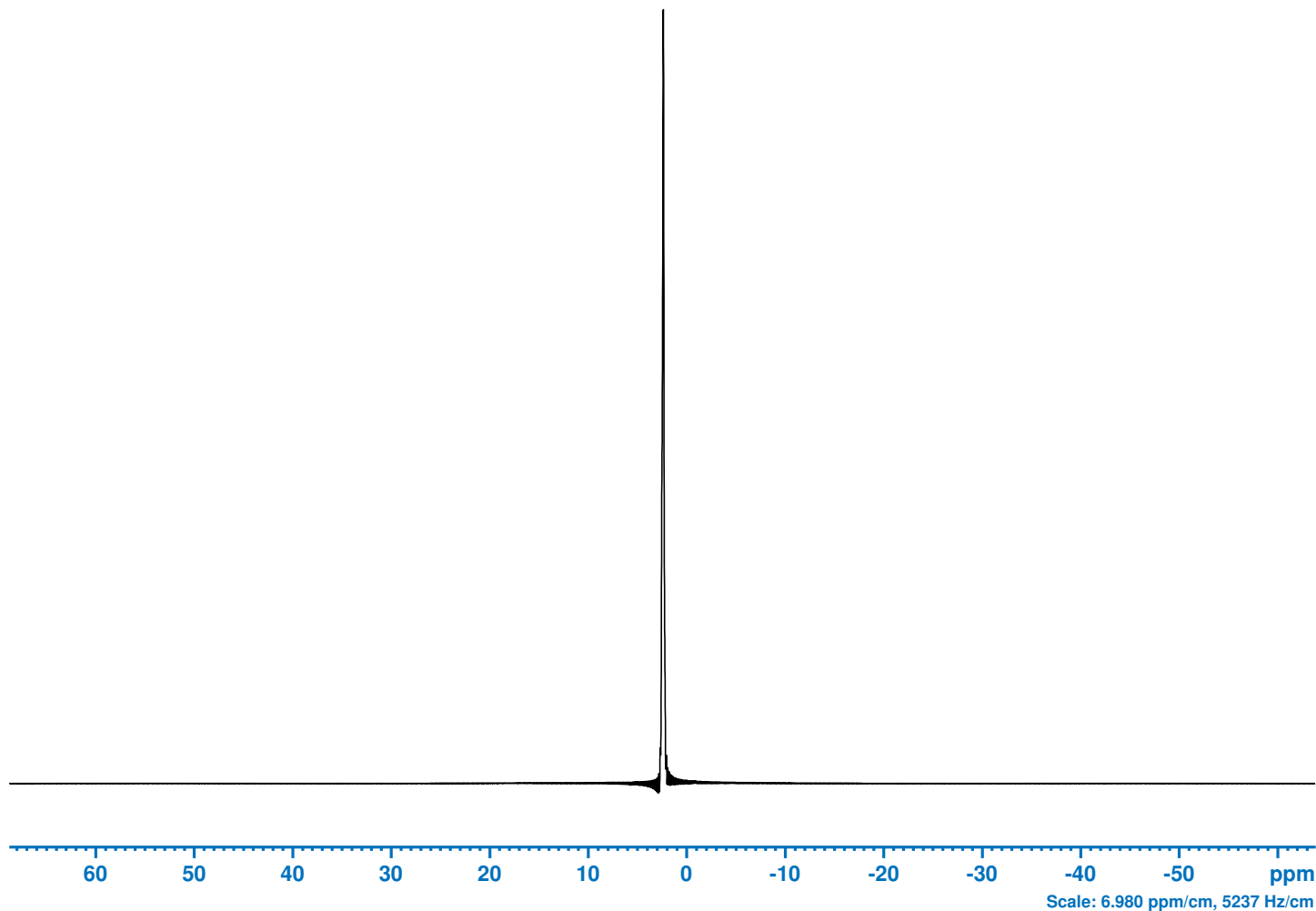
### NPT\_1H\_MAS\_sino\_1h

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

F2 - Acquisition Parameters  
Date\_ 20230413  
Time 11.46 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (  
PULPROG onepulse  
TD 2048  
SOLVENT H2O+D2O  
NS 16  
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 1.50 usec  
PLW1 55.01699829 W

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

-----  
SHIM SEQUENCE  
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skip shimming  
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NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
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 8000 Hz)

SINO (20.0 ppm): Signal (42.91 ppm), Noise (172.44 to 152.43 ppm) [1992.0]  
Processed with TDef=2048



Bruker BioSpin

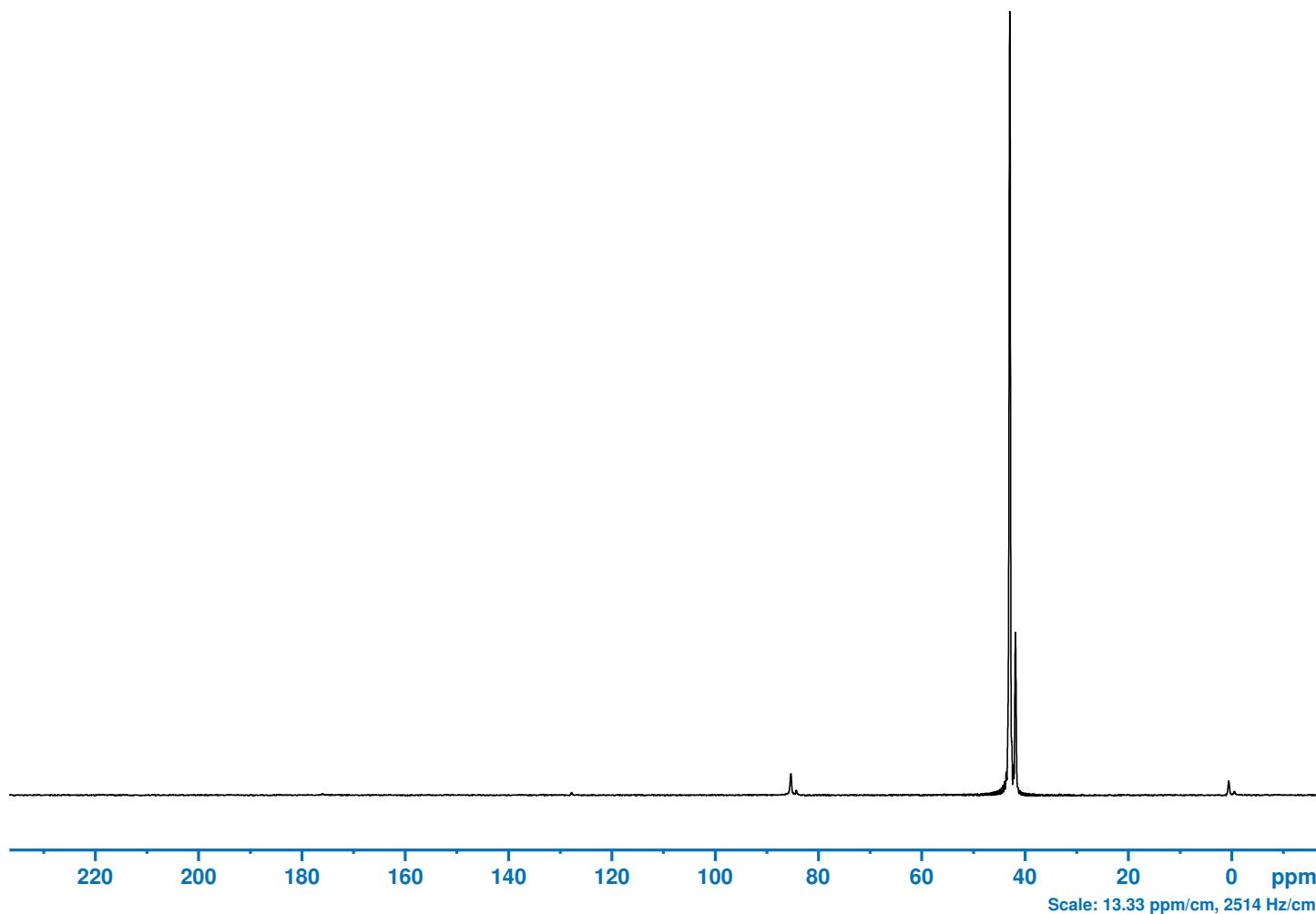
### NPT\_13C\_MAS\_paropt\_cp1h\_13c

Current Data Parameters  
NAME NPT\_13C\_MAS\_paropt\_cp1h\_13c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230413  
Time 14.50 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (cp  
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 298.1 K  
D1 5.00000000 sec  
ZGPGTNS  
SFO1 188.6838379 MHz  
NUC1 13C  
P15 2000.00 usec  
PLW1 21.35099983 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.0000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 55.01699829 W  
PLW12 45.47999954 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 33.34999847 W

F2 - Processing parameters  
SI 32768  
SF 188.6630850 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 0.20

SHIM SEQUENCE  
skip shimming



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
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 12000 Hz)

SINO (20.0 ppm): Signal (32.68 ppm), Noise (-43.27 to -63.30 ppm) [510.4]



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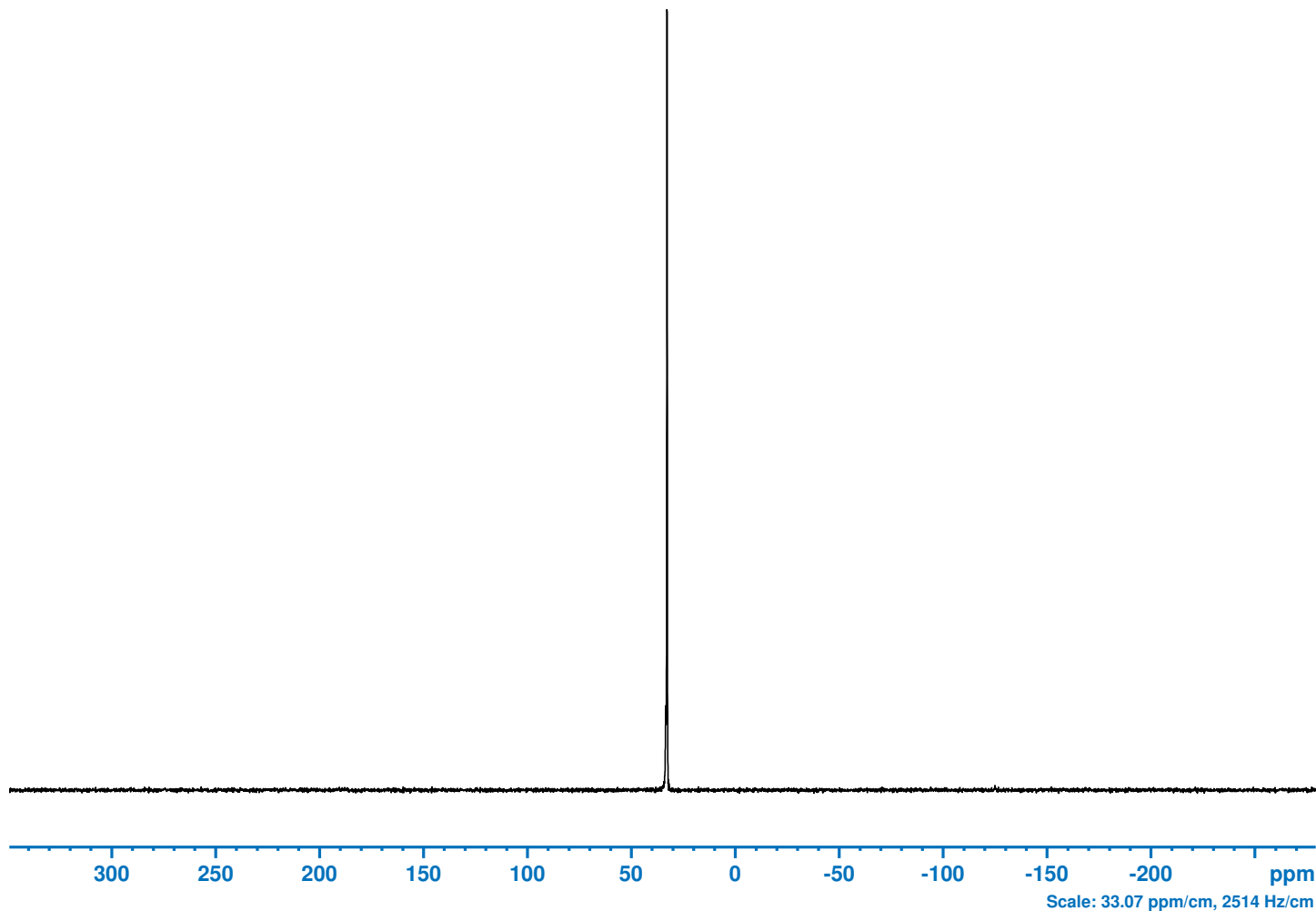
### NPT\_15N\_MAS\_paropt\_cp1h\_15n

Current Data Parameters  
NAME NPT\_15N\_MAS\_paropt\_cp1h\_15n  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230413  
Time 18.02 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (cp  
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 298.0 K  
D1 5.00000000 sec  
ZGPGTNS  
SFO1 76.0299000 MHz  
NUC1 15N  
P15 3500.00 usec  
PLW1 27.99300003 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.00000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 55.01699829 W  
PLW12 49.91999817 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 18.95000076 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 MASDVT750W4 BL1.3 X/Y/H**

**750 MHz**

**Probe ID: H170225\_0001**

**Report Name: 2023-04-13**

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.1.3  
 Probe: H170225\_0001 PH MASDVT750W4 BL1.3 X/Y/H  
 Sample: Potassium Bromide (KBr, 3.0 ul) (Z151270)  
 Magic Angle setting, MAS (NPT\_79Br\_MAS\_magicAngle, spin rate 20000 Hz)  
 ATTENTION: non-standard execution of experiment  
 Line width main [achieved/rated]: [115 <= 168] <pass>  
 Line width of side band number 2 (@ -40019 Hz) [achieved/rated]: [196 <= 220] <pass>



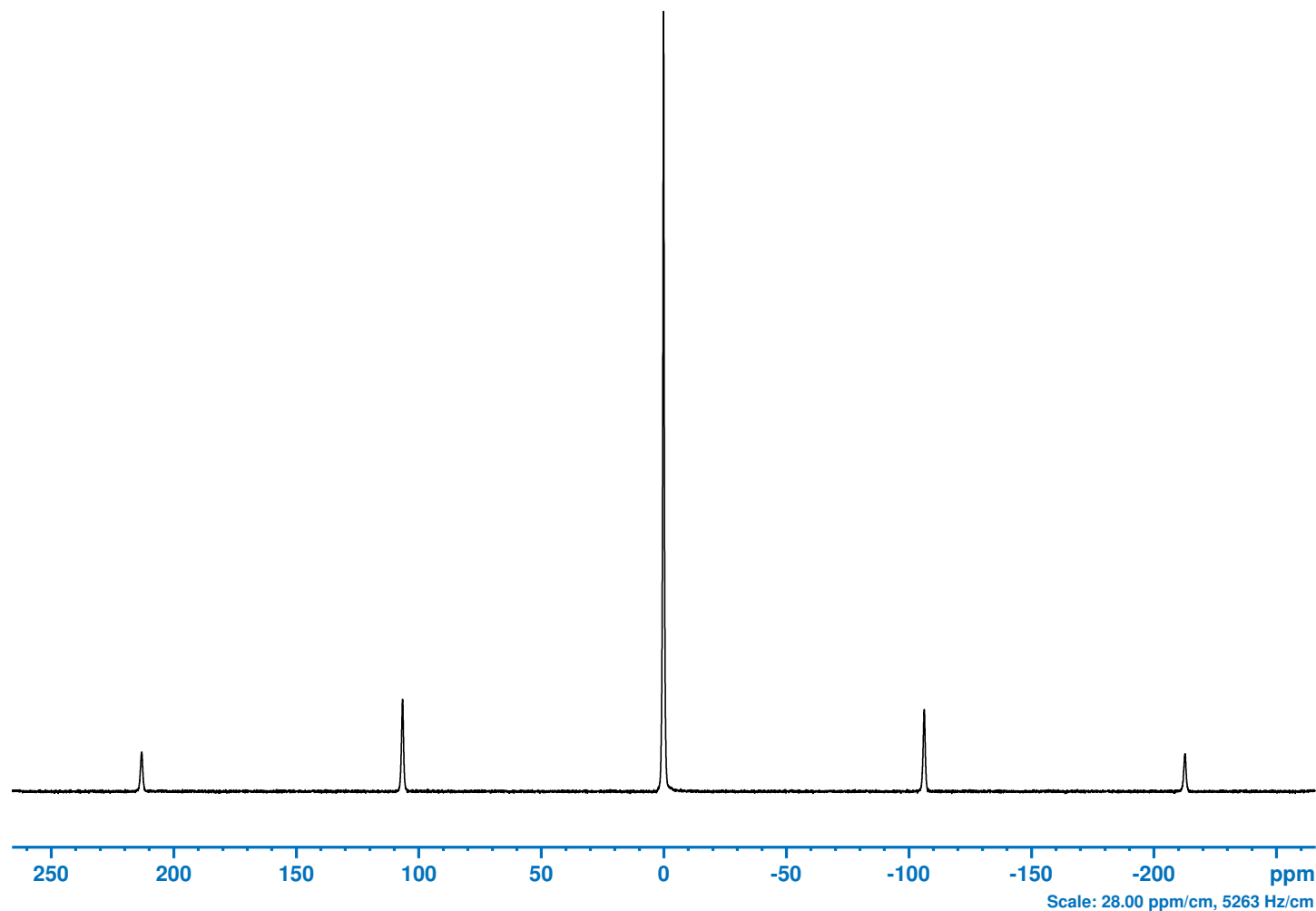
Bruker BioSpin

# NPT\_79Br\_MAS\_magicAngle

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

F2 - Acquisition Parameters  
 Date\_ 20230413  
 Time 13.35 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 (   
 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 187.9912750 MHz  
 NUC1 79Br  
 P1 2.27 usec  
 PLW1 35.97494125 W

F2 - Processing parameters  
 SI 131072  
 SF 187.9912750 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20



SHIM SEQUENCE  
 skip shimming