

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

**750 MHz**

**Probe ID: H170225\_0001**

**Report Name: 2023-08-08\_13\_TRmode**

● 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,,1,1#
$ProbeCoil,1.0,1,2.5,3,BB,BB,1H#
$ProbeChannel,1.1,1H,,,60,,,FALSE,,,#
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$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#
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● **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)

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 8000 Hz)

Line width main [achieved/rated]: [146 <= 146] <pass>  
 Line width of side band number 5 (@ -40004 Hz) [achieved/rated]: [157 <= 160] <pass>



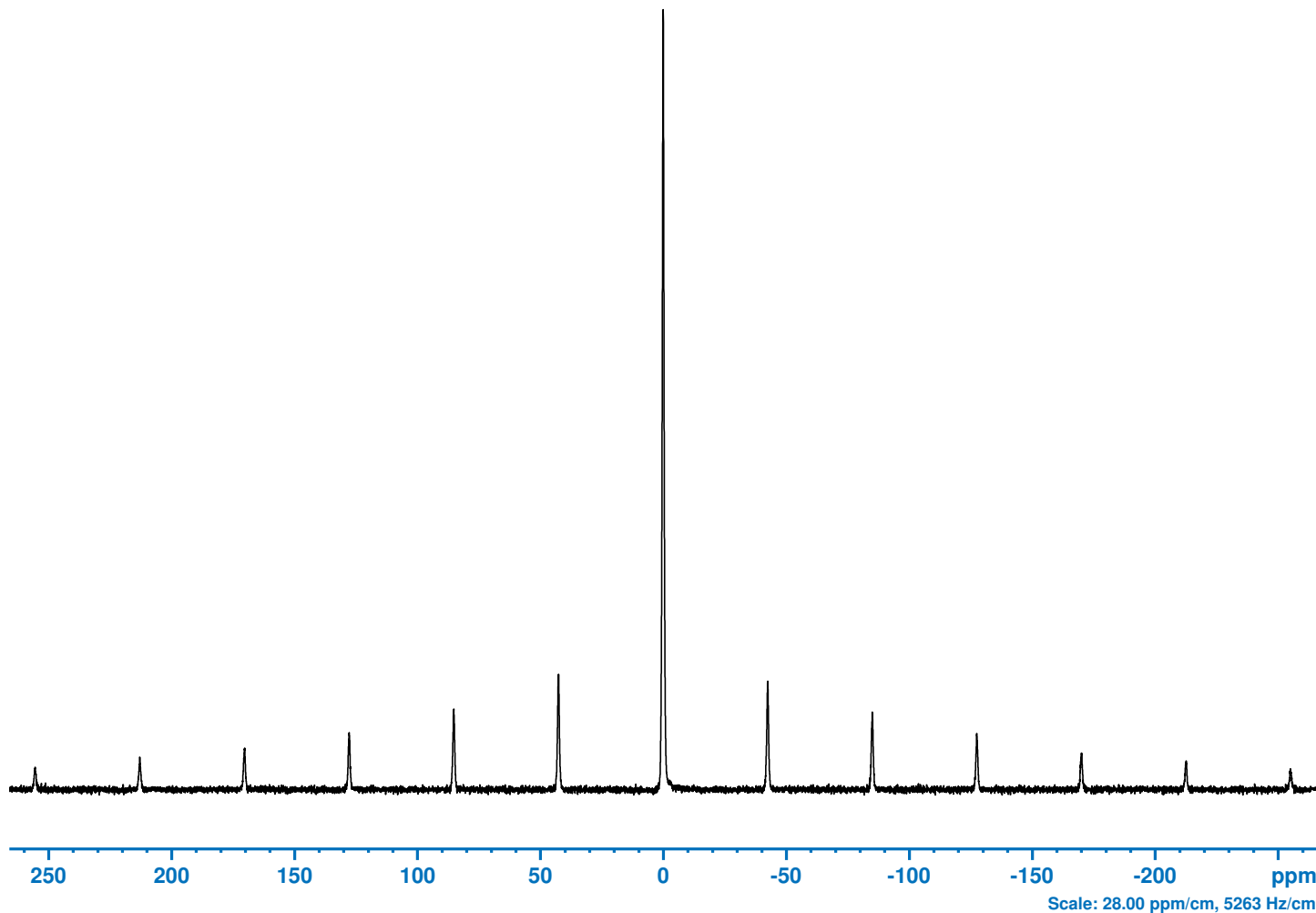
Bruker BioSpin

# NPT\_79Br\_MAS\_magicAngle

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

F2 - Acquisition Parameters  
 Date\_ 20230807  
 Time 13.15 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 (1H/13C)  
 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 187.9912542 MHz  
 NUC1 79Br  
 P1 3.00 usec  
 PLW1 66.56700134 W

F2 - Processing parameters  
 SI 131072  
 SF 187.9912542 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20



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 SHIM SEQUENCE  
 skip shimming  
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NMR TEST ACCEPTANCE \*\*\* System: AV NEO (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 2015.9 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0064 ppm.



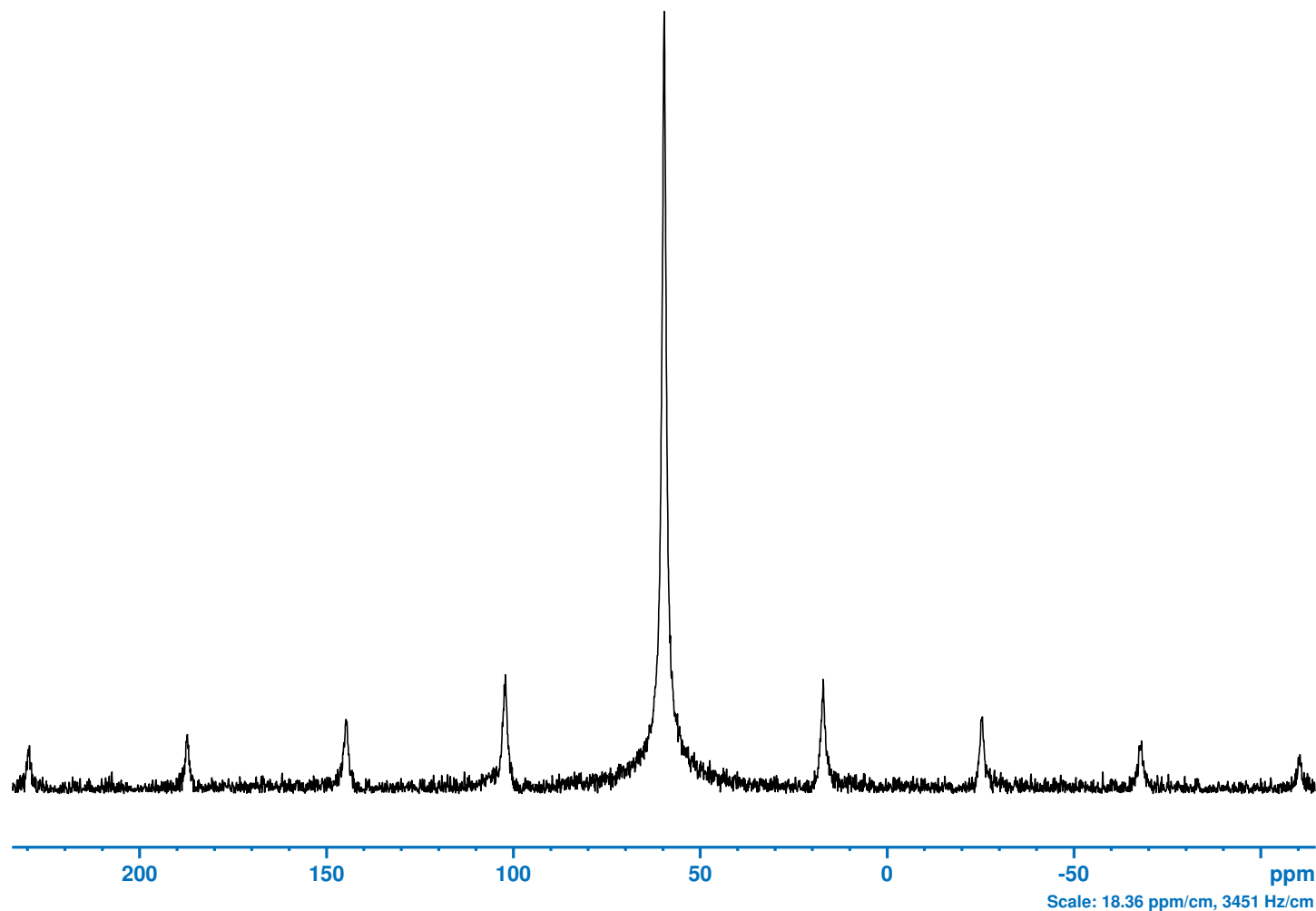
Bruker BioSpin

# NPT\_79Br\_MAS\_fieldsetting

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

F2 - Acquisition Parameters  
 Date\_ 20230807  
 Time 12.12 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 66.56700134 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 <sup>13</sup>C frequency (NPT\_13C\_MAS\_fieldsetting\_dec1h, spin rate 67000 Hz)  
 FIELD was set to 1975.6 for <sup>13</sup>C chemical shift of 38.460 ppm. One field unit corresponds to 0.0071 ppm.



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# NPT\_13C\_MAS\_fieldsetting\_dec1h

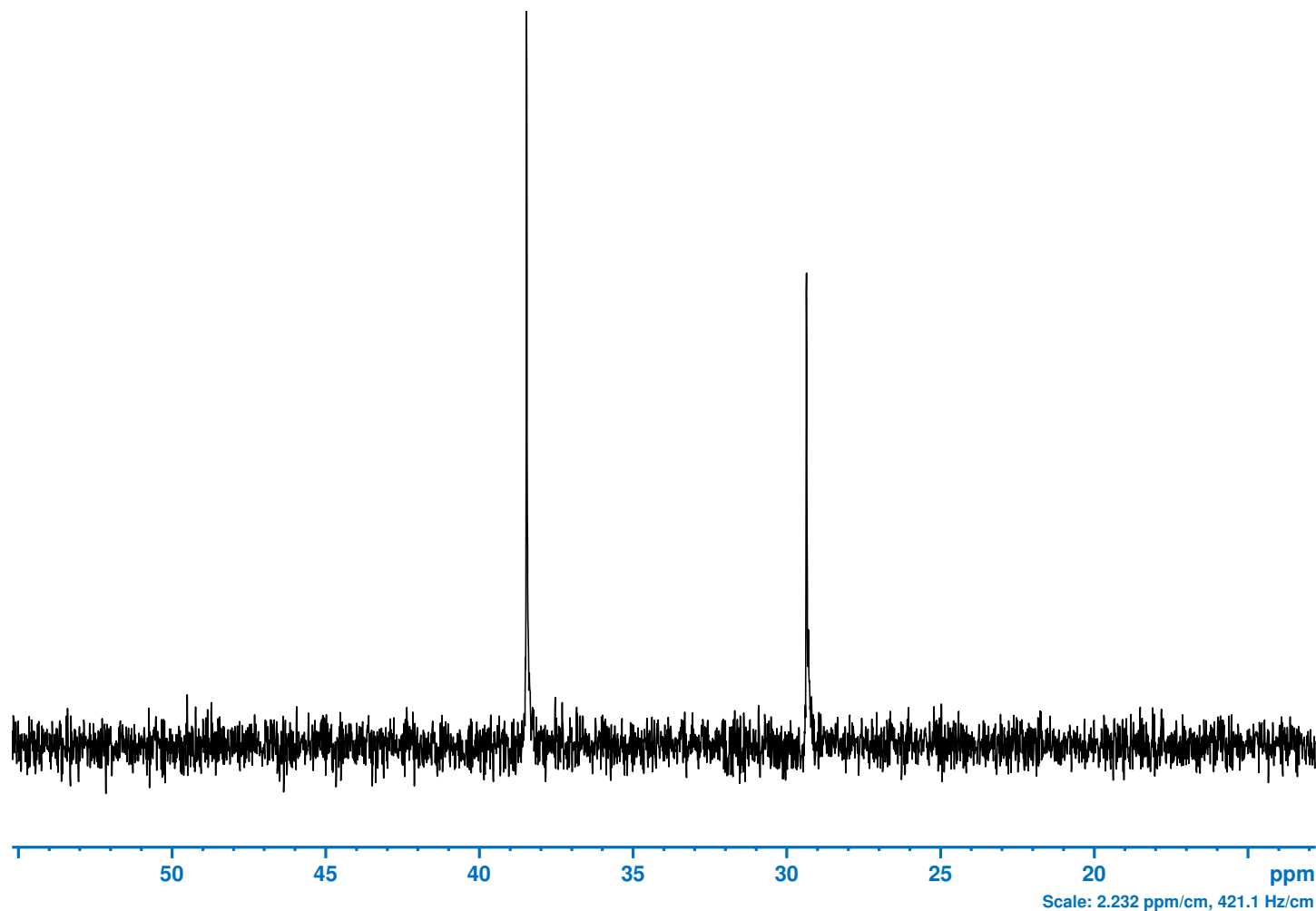
Current Data Parameters  
 NAME NPT\_13C\_MAS\_fieldsetting\_dec1h  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230807  
 Time 15.36 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 63.29399872 W  
 SFO2 750.3017031 MHz  
 NUC2 1H  
 CPDPRG2 cw  
 PLW2 49.30500031 W  
 PLW12 0.49799281 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 @ 49.3 W].

P90 MAS 1H pulse [achieved/rated]: @ 55.0 W [1.42 us <= 1.50 us] <pass>



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## NPT\_1H\_MAS\_p90det\_1h

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

F2 - Acquisition Parameters  
 Date\_ 20230807  
 Time 15.03 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 55.01699829 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
55.0 W	1.50 us		
55.0 W	1.50 us	1.42 us	-5.3%

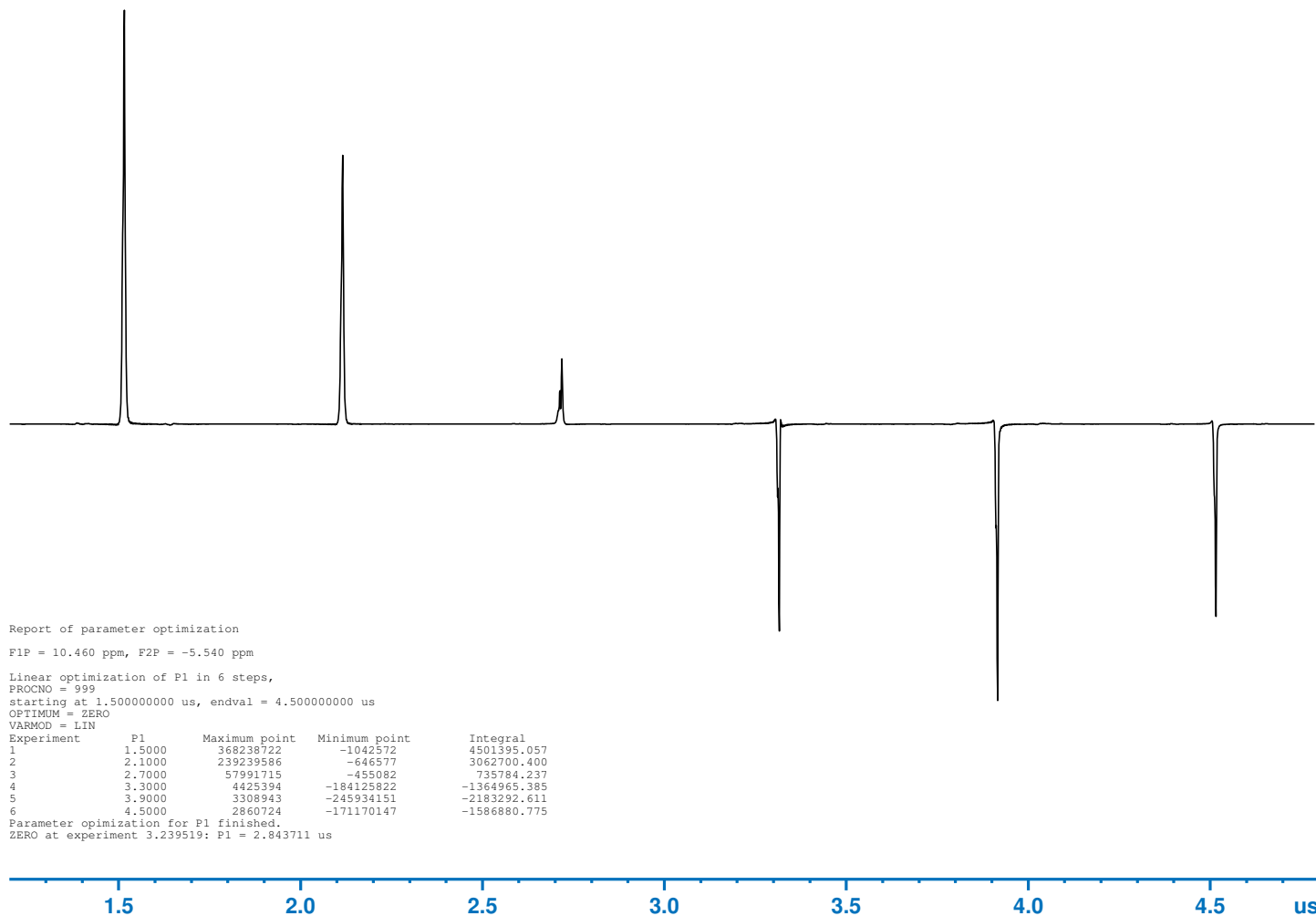
Report of parameter optimization

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	368238722	-1042572	4501395.057
2	2.1000	239239586	-646577	3062700.400
3	2.7000	57991715	-455082	735784.237
4	3.3000	4425394	-184125822	-1364965.385
5	3.9000	3308943	-245934151	-2183292.611
6	4.5000	2860724	-171170147	-1586880.775

Parameter optimization for P1 finished.  
 ZERO at experiment 3.239519: P1 = 2.843711 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 @ 66.6 W].

P90 MAS 79Br pulse [achieved/rated]: @ 68.4 W [2.96 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\_ 20230807  
 Time 12.05 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 68.37859344 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
65.0 W	3.00 us	3.01 us	0.3%
65.0 W	3.00 us	3.01 us	0.3%
68.4 W	3.00 us	2.96 us	-1.3%

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	316468498	-5240733	14839655.574
2	4.2000	226066264	-4355363	10791958.019
3	5.4000	73232962	-7957147	2934386.387
4	6.6000	7655742	-94768788	-3744317.832
5	7.8000	3344340	-164819173	-6839473.684
6	9.0000	4163309	-140405756	-5473563.871

Parameter optimization for P1 finished.  
 ZERO at experiment 3.435906: P1 = 5.923087 us



2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0 8.5 9.0 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 @ 67.5 W].

P90\_MAS\_CP 1H13C power (PLW 11) [achieved/rated]: [69.5 W <= 70.0 W] <pass>  
 P90\_MAS\_CP 1H13C pulse (P 1) [achieved/rated]: [2.76 us <= 2.80 us] <pass>  
 RF Field = 89KHz



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

Current Data Parameters  
 NAME NPT\_13C\_MAS\_p90det\_cp1h\_13c  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230807  
 Time 16.18 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  
 ZGPGTNS  
 SFO1 188.6711975 MHz  
 NUC1 13C  
 P1 4.20 usec  
 P15 2000.00 usec  
 PLW1 63.29399872 W  
 PLW11 69.49067688 W  
 SFO2 750.3046519 MHz  
 NUC2 1H  
 CNST21 1.0000000  
 CPDPRG2 spinal64  
 P3 1.50 usec  
 PCPD2 2.80 usec  
 PLW2 49.30500031 W  
 PLW12 49.30500031 W  
 SPNAM[0] ramp50100.100  
 SPOAL0 0.500  
 SPOFFS0 0 Hz  
 SPW0 34.97919083 W

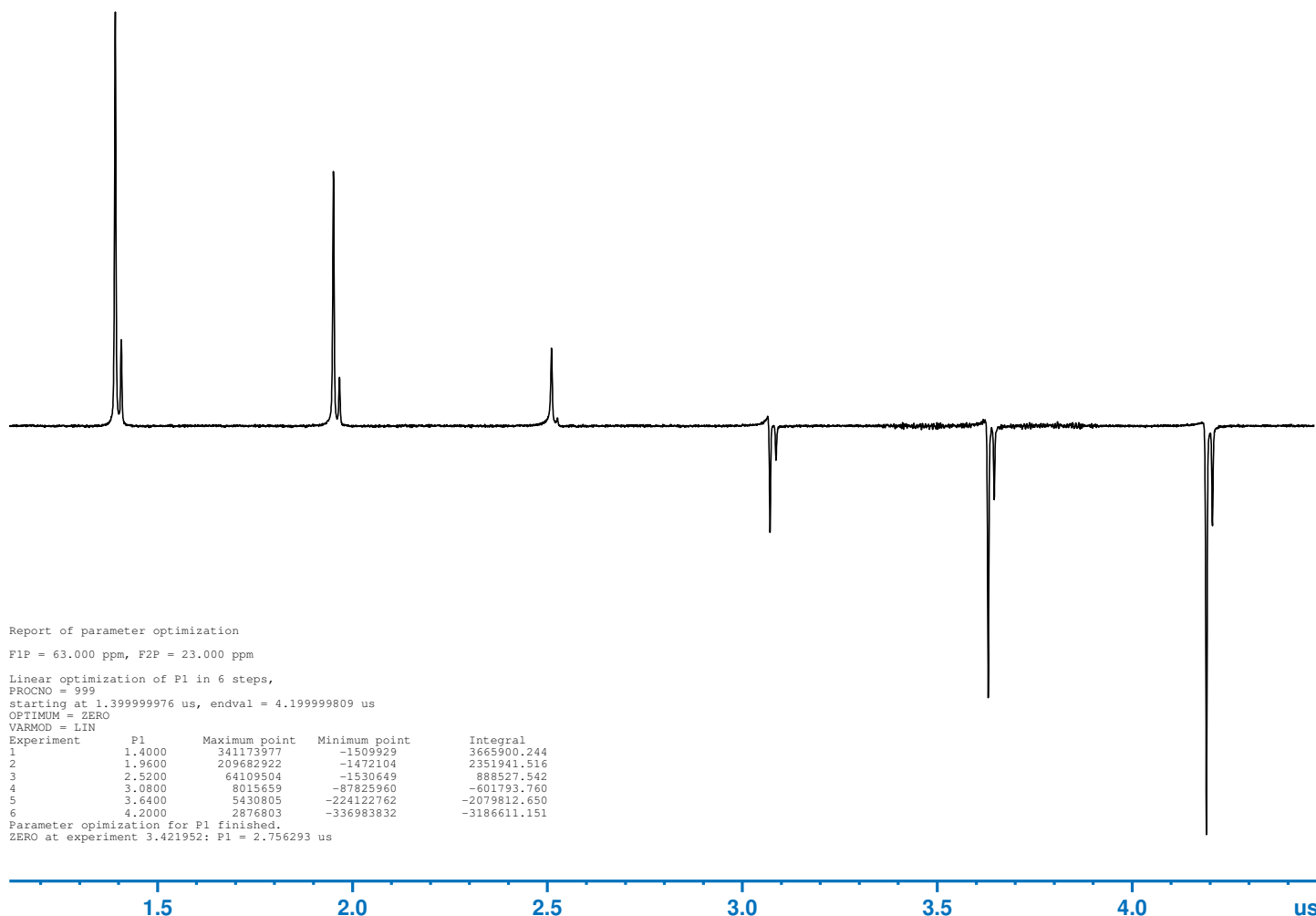
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 SI 8192  
 SF 188.6630851 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20

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

PLW90	P90	P90[det]	Deviation
63.3 W	2.80 us		
63.3 W	2.80 us	2.87 us	2.5%
69.5 W	2.80 us	2.76 us	-1.4%

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 13C pulse calibration, MAS (NPT\_13C\_MAS\_p90det\_13c, spin rate 67000 Hz)  
 ATTENTION: Updated PROSOL Tables with [2.80 us @ 63.3 W].

P90 MAS 13C pulse [achieved/rated]: @ 66.6 W [2.73 us <= 2.80 us] <pass>



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## NPT\_13C\_MAS\_p90det\_13c

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

F2 - Acquisition Parameters  
 Date\_ 20230807  
 Time 15.28 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 66.58162689 W  
 SFO2 750.3018457 MHz  
 NUC2 1H  
 CPDPRG[2] cw  
 PLW2 49.30500031 W  
 PLW12 0.49799281 W

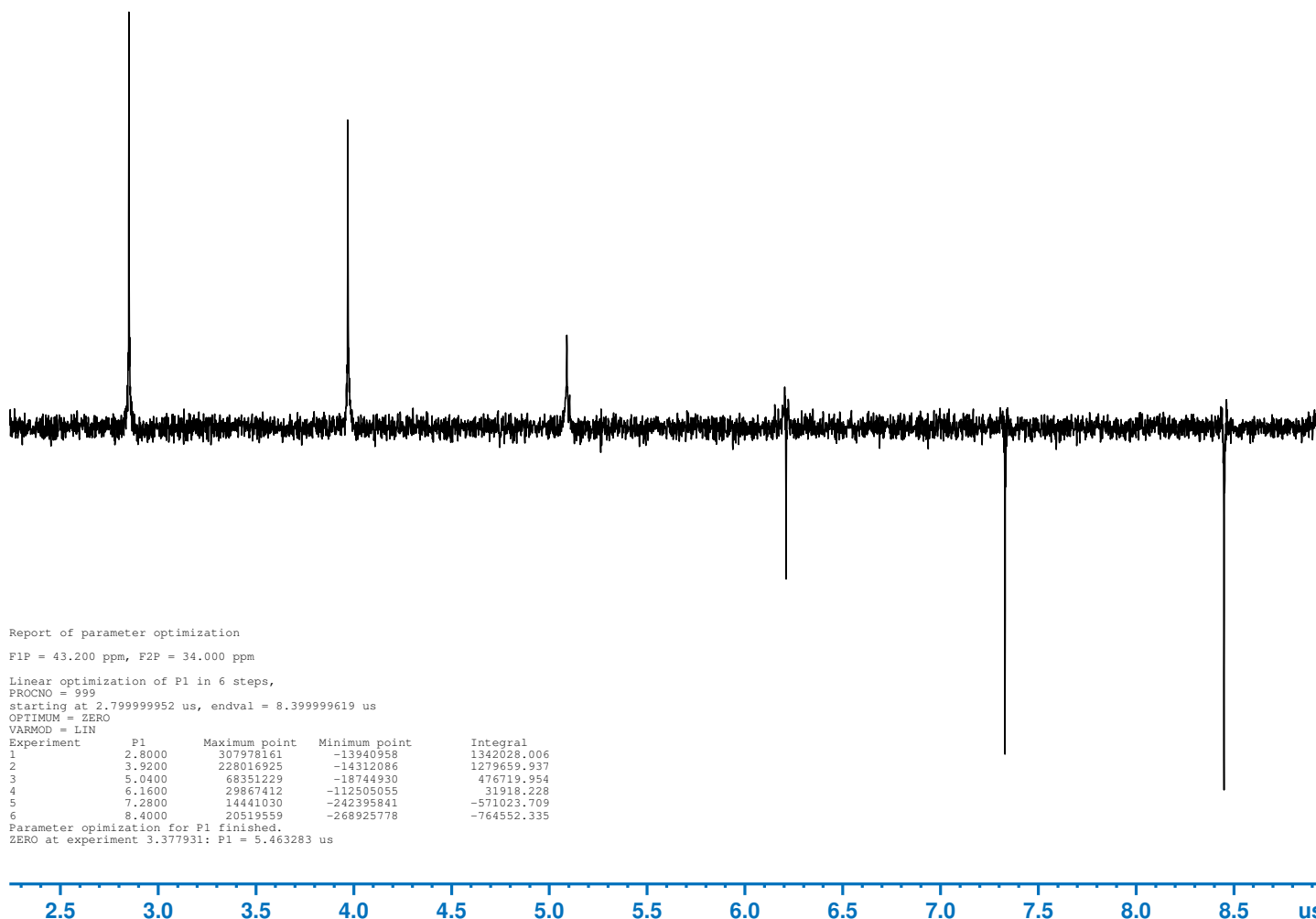
F2 - Processing parameters  
 SI 8192  
 SF 188.6630851 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 FC 0.50

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

PLW90	P90	P90[det]	Deviation
58.0 W	3.00 us		
66.6 W	2.80 us	2.73 us	-2.5%

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 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 @ 30.0 W].

P90\_MAS\_CP 1H15N power (PLW 11) [achieved/rated]: [38.3 W <= 75.0 W] <pass>  
P90\_MAS\_CP 1H15N pulse (P 1) [achieved/rated]: [4.43 us <= 5.00 us] <pass>



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

Current Data Parameters  
NAME NPT\_15N\_MAS\_p90det\_cp1h\_15n  
EXPNO 2  
PROCNO 1

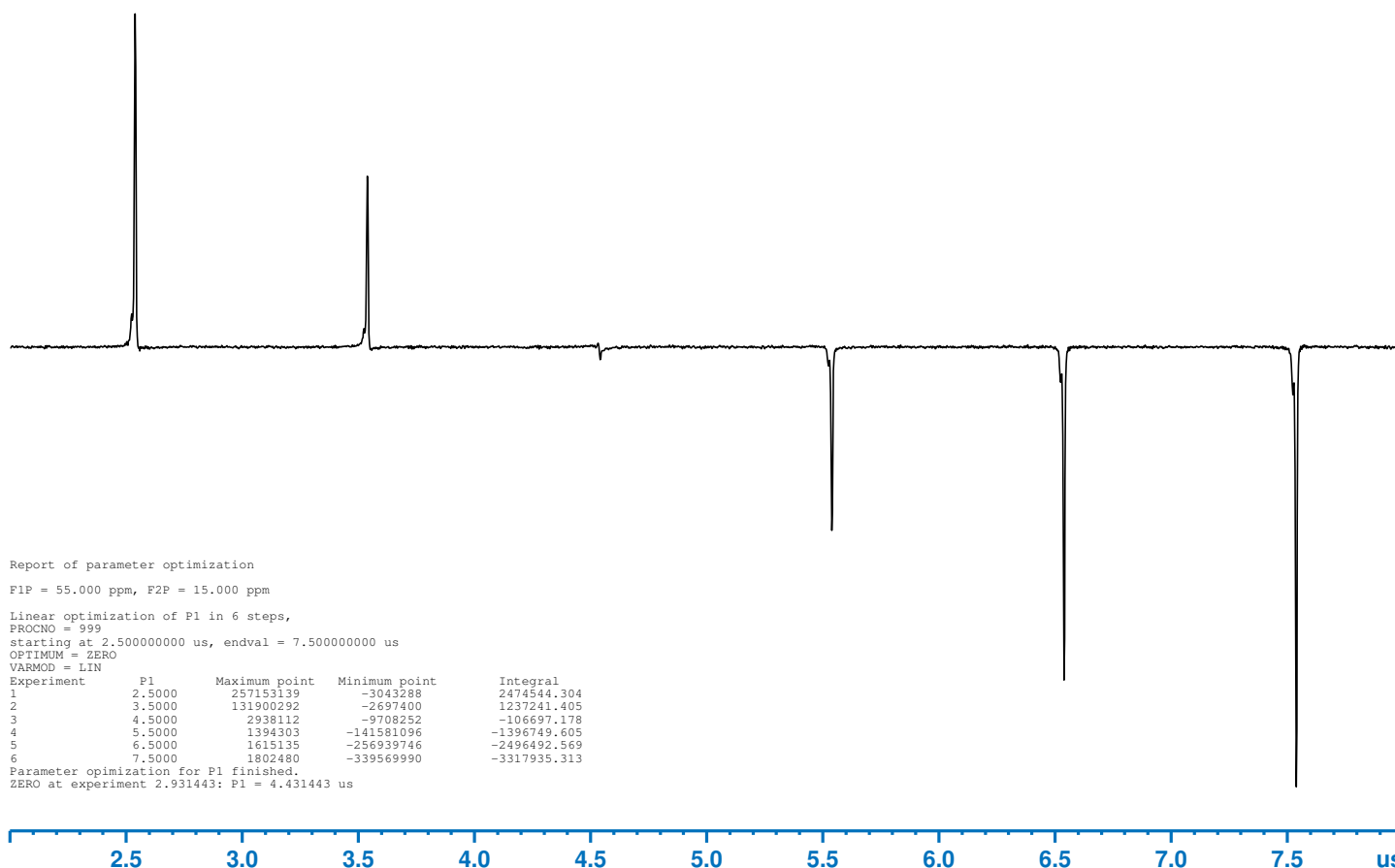
F2 - Acquisition Parameters  
Date\_ 20230808  
Time 10.31 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (cp90)  
PULPROG cp90  
TD 3012  
SOLVENT H2O+D2O  
NS 4  
DS 0  
SWH 30120.482 Hz  
FIDRES 20.000320 Hz  
AQ 0.0499992 sec  
RG 101  
DW 16.600 usec  
DE 6.50 usec  
TE 298.1 K  
D1 5.00000000 sec  
ZGPGTNS  
SFO1 76.0299000 MHz  
NUC1 15N  
P1 7.50 usec  
P15 3500.00 usec  
PLW1 38.25899887 W  
PLW11 38.25899887 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.0000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 49.30500031 W  
PLW12 49.30500031 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 10.61516953 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  
-----  
38.3 W 5.00 us  
38.3 W 5.00 us 4.43 us -11.4%

-----  
SHIM SEQUENCE  
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skip shimming  
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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

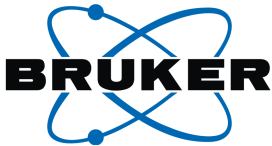
Experiment	P1	Maximum point	Minimum point	Integral
1	2.5000	257153139	-3043288	2474544.304
2	3.5000	131900292	-2697400	1237241.405
3	4.5000	2938112	-106697.178	-1396749.605
4	5.5000	1394303	-141581096	-2496492.569
5	6.5000	1615135	-339569990	-3317935.313
6	7.5000	1802480		

Parameter optimization for P1 finished.

ZERO at experiment 2.931443: P1 = 4.431443 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 @ 38.3 W].

P90 MAS 15N pulse [achieved/rated]: @ 40.0 W [4.89 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\_ 20230808  
Time 10.23 h  
INSTRUM Avance NEO  
PROBHD H170225\_0001 (   
PULPROG hpdec  
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 40.00000000 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CPDPRG[2] spinal64  
PCPD2 2.80 usec  
PLW2 49.30500031 W  
PLW12 49.30500031 W

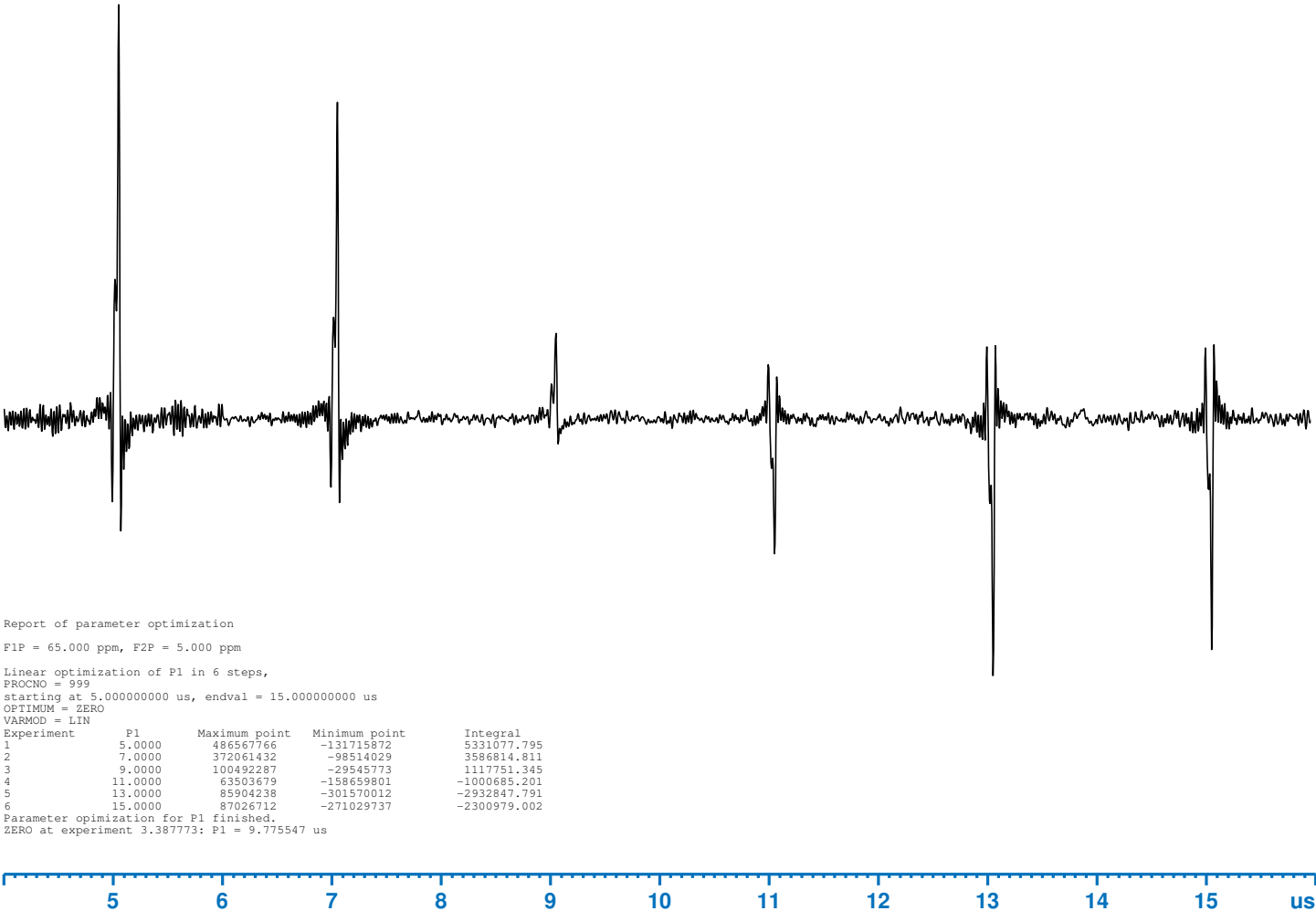
F2 - Processing parameters  
SI 4096  
SF 76.0272387 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 0.50

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

PLW90	P90	P90[det]	Deviation
40.0 W	5.00 us		
40.0 W	5.00 us	4.89 us	-2.2%

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: 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]: Signal (43.66 ppm), Noise (198.42 to 178.41 ppm) [76.0] <n/a>  
Number of scans (NS) [achieved/rated]: [64 <= 64] <pass>  
Processed with TDef=2048



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

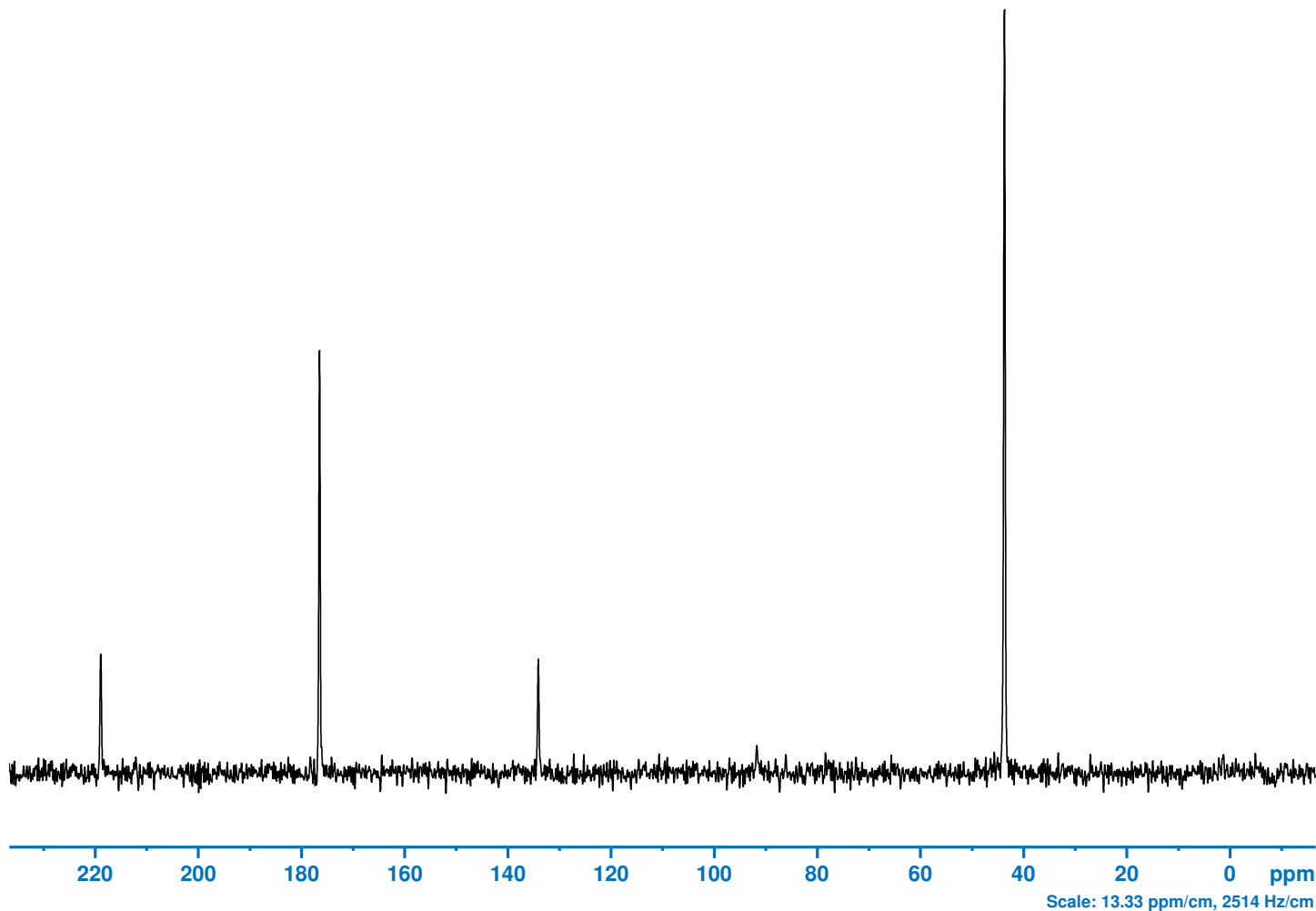
Current Data Parameters  
NAME NPT\_13C\_MAS\_sino\_cp1h\_13c  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230808  
Time 10.06 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 67.51899719 W  
SFO2 750.3046519 MHz  
NUC2 1H  
CNST21 1.0000000  
CPDPRG2 spinal64  
P3 1.50 usec  
PCPD2 2.80 usec  
PLW2 49.30500031 W  
PLW12 47.15999985 W  
SPNAM[0] ramp50100.100  
SPOAL0 0.500  
SPOFFS0 0 Hz  
SPW0 35.83000183 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: Alpha-glycine (2 mg, 3.0 ul) (Z151272)  
 CP 1H-15N sensitivity, MAS (NPT\_15N\_MAS\_sino\_cp1h\_15n, spin rate 8000 Hz)

SINO (20.0 ppm) [achieved]: Signal (33.42 ppm), Noise (-86.92 to -106.93 ppm) [23.9] <n/a>  
 Number of scans (NS) [achieved/rated]: [256 <= 256] <pass>



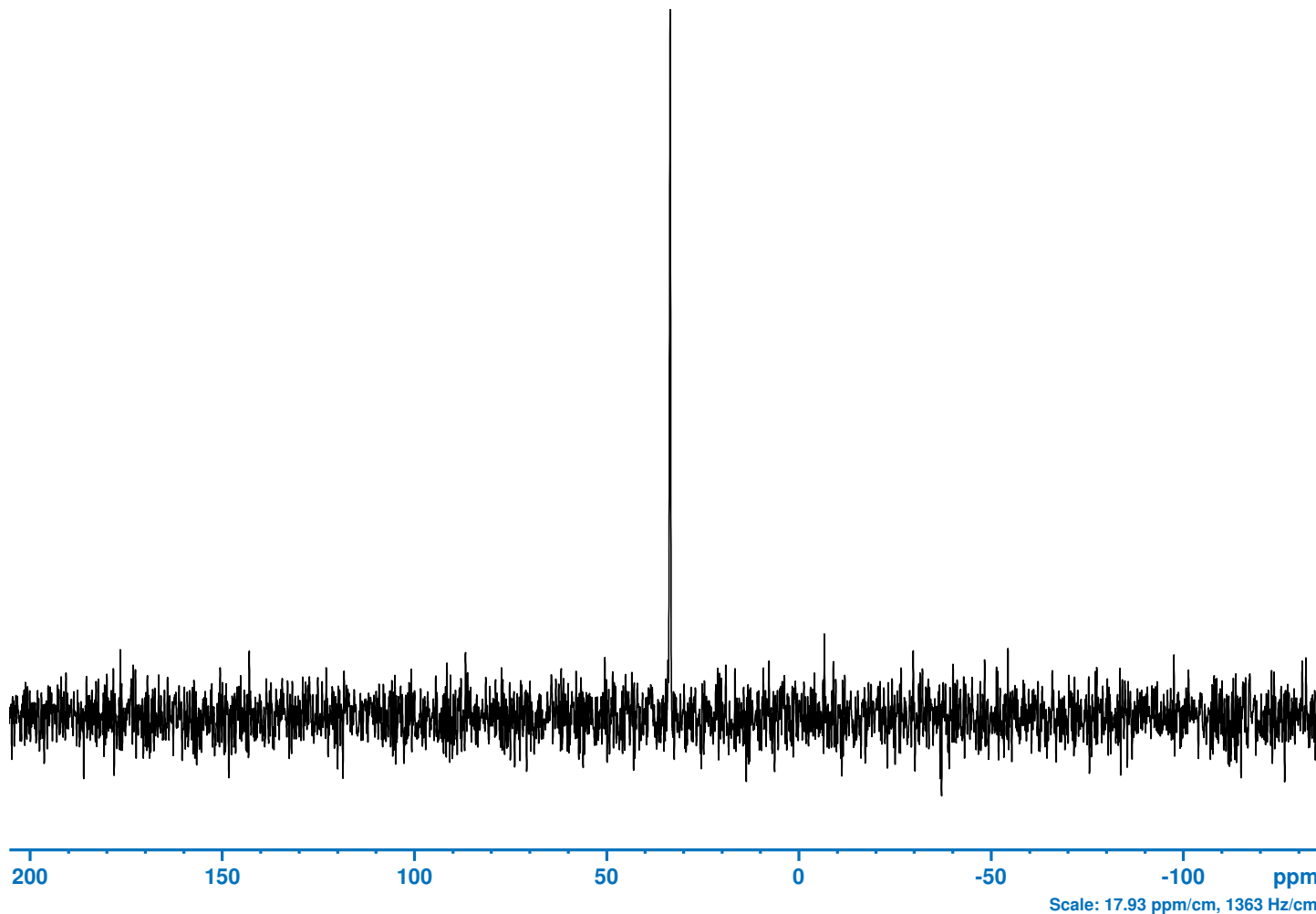
Bruker BioSpin

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

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

F2 - Acquisition Parameters  
 Date\_ 20230808  
 Time 11.20 h  
 INSTRUM Avance NEO  
 PROBHD H170225\_0001 (cp  
 PULPROG 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 298.1 K  
 D1 5.00000000 sec  
 ZGPGTNS  
 SFO1 76.0299000 MHz  
 NUC1 15N  
 P15 3500.00 usec  
 PLW1 30.03300095 W  
 SFO2 750.3046519 MHz  
 NUC2 1H  
 CNST21 1.0000000  
 CPDPRG2 spinal64  
 P3 1.50 usec  
 PCPD2 2.80 usec  
 PLW2 49.30500031 W  
 PLW12 47.15999985 W  
 SPNAM[0] ramp50100.100  
 SPOAL0 0.500  
 SPOFFS0 0 Hz  
 SPW0 15.89999962 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: Adamantane (3.0 ul) (Z151271)  
 13C sensitivity, MAS (NPT\_13C\_MAS\_sino\_13c, spin rate 67000 Hz)

SINO (20.0 ppm) [achieved]: Signal (38.47 ppm), Noise (27.64 to 7.63 ppm) [43.1] <n/a>  
 Linewidth [achieved/rated]: at 50% of signal height [2.3 Hz <= 12.0 Hz] <pass>  
 Number of scans (NS) [achieved/rated]: [16 <= 16] <pass>



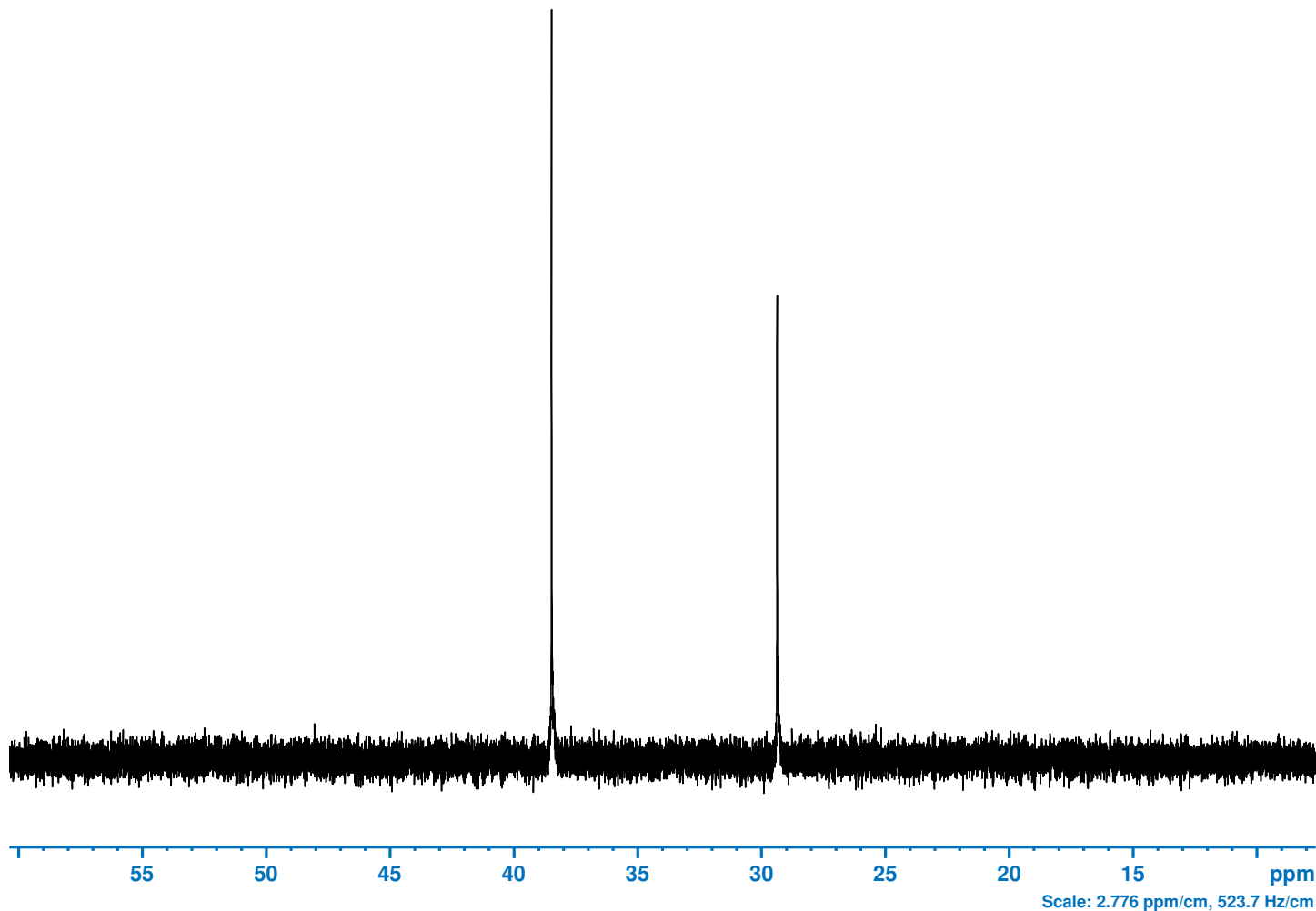
Bruker BioSpin

## NPT\_13C\_MAS\_sino\_13c

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

F2 - Acquisition Parameters
Date_     20230807
Time      15.43 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       63.29399872 W
SFO2       750.3018457 MHz
NUC2       1H
CPDPRG2    cw
PLW2       49.30500031 W
PLW12      0.49799281 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

```
# Mon Aug 7 13:43:39 2023
$$$PROBEIDENTIFIER=H170225_0001
$$$PROBENAME=PH MASDVT750W4 BL1.3 X/Y/H
$$$SHIMID=272623
#
# Active Shim Gradients
#
Z -71800
Z2 0
Z3 0
Z4 0
Z5 0
Z6 0
X 0
XZ 0
XZ2 0
XZ3 0
XZ4 0
Y 0
YZ -345000
YZ2 0
YZ3 0
YZ4 0
XY 0
XYZ 0
XYZ2 0
XYZ3 0
(X2-Y2) 0
(X2-Y2) Z 160000
(X2-Y2) Z2 0
(X2-Y2) Z3 0
X3 0
X3Z 0
Y3 0
Y3Z 0
#
# Lock Parameter
#
FIELD 1975.629
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] -17949.99900000
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] -0.00000000
SHIM_SETTING [ 4] 2500.13000000
SHIM_SETTING [ 5] -2499.85800000
SHIM_SETTING [ 6] -551.33800000
SHIM_SETTING [ 7] 551.06500000
SHIM_SETTING [ 8] 42.43900000
SHIM_SETTING [ 9] -43.49900000
SHIM_SETTING [10] 5822.96100000
SHIM_SETTING [11] -5822.40900000
SHIM_SETTING [12] -0.00000000
SHIM_SETTING [13] 0.00000000
SHIM_SETTING [14] 0.00000000
SHIM_SETTING [15] -0.00000000
SHIM_SETTING [16] 0.00000000
SHIM_SETTING [17] -0.00000000
SHIM_SETTING [18] -0.00000000
SHIM_SETTING [19] -0.00100000
SHIM_SETTING [20] 0.00000000
SHIM_SETTING [21] 40000.00000000
SHIM_SETTING [22] -40000.00000000
SHIM_SETTING [23] -28196.62000000
SHIM_SETTING [24] 28196.62000000
SHIM_SETTING [25] 8939.24100000
SHIM_SETTING [26] -8939.24100000
SHIM_SETTING [27] 0.00000000
SHIM_SETTING [28] -86250.00000000
SHIM_SETTING [29] 0.00000000
SHIM_SETTING [30] 0.00000000
SHIM_SETTING [31] 41312.45800000
SHIM_SETTING [32] 86250.00000000
SHIM_SETTING [33] 0.00000000
SHIM_SETTING [34] 0.00000000
SHIM_SETTING [35] -0.00000000
SHIM_SETTING [36] -0.00000000
SHIM_SETTING [37] 15278.15600000
SHIM_SETTING [38] -15278.15600000
SHIM_SETTING [39] -41312.45800000
SHIM_SETTING [40] 0.00000000
```

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

F2 - Acquisition Parameters
Date_ 20230807
Time 15.43 h
INSTRUM Avance NEO
PROBHD H170225_0001 (
PULPROG hpdac
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 63.29399872 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG2 cw
PLW2 49.30500031 W
PLW12 0.49799281 W

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

SINO (20.0 ppm) [achieved]: Signal (2.34 ppm), Noise (-43.83 to -63.84 ppm) [5927.1] <n/a>  
 Linewidth [achieved]: at 50% of signal height [132.1 Hz] <n/a>  
 Number of scans (NS) [achieved/rated]: [16 <= 16] <pass>



**Bruker BioSpin**

***NPT\_1H\_MAS\_sino\_1h***

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

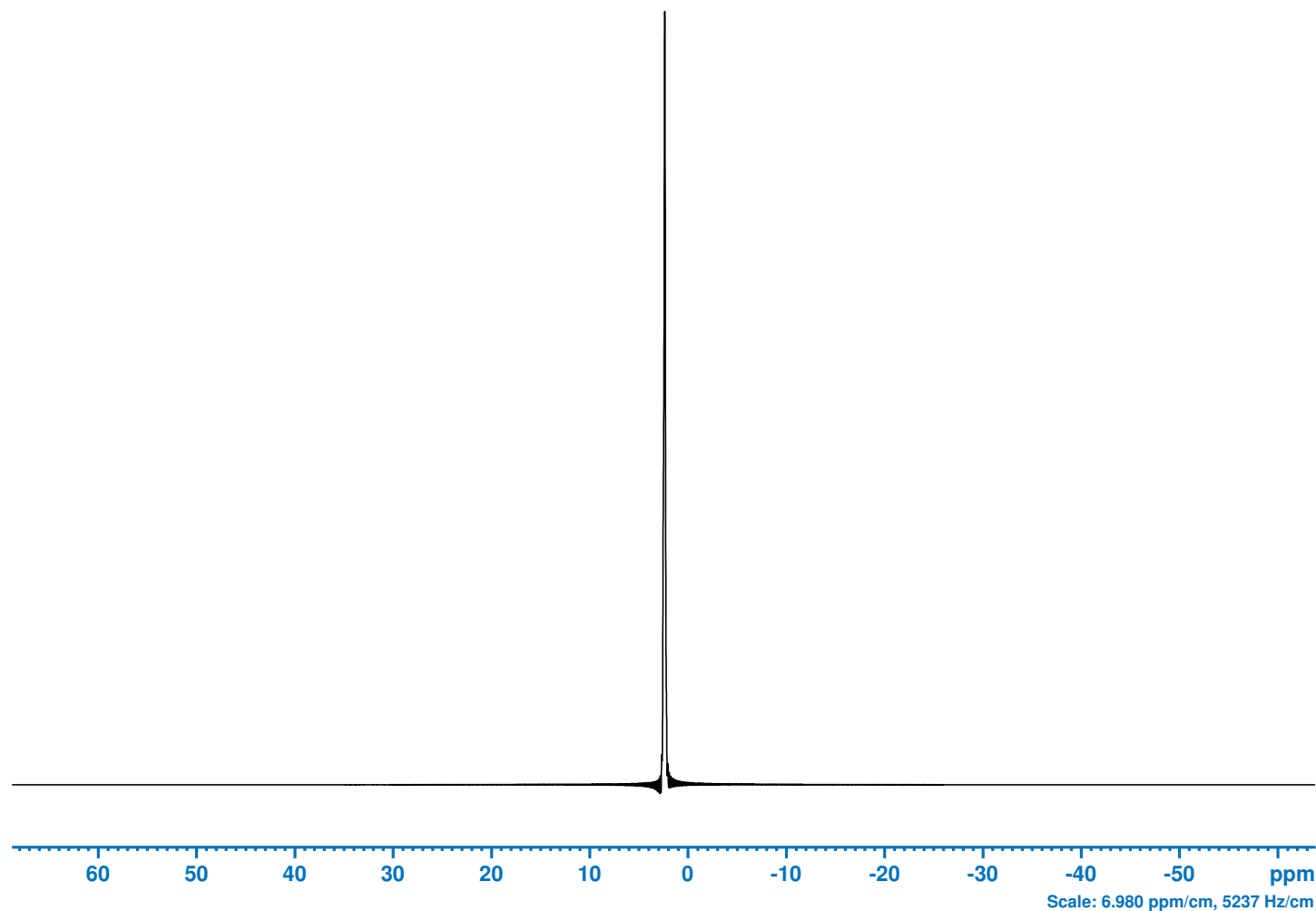
```

F2 - Acquisition Parameters
Date_                20230807
Time                 15.38 h
INSTRUM              Avance NEO
PROBHD              H170225_000 (
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                   5.0000000 sec
SP01                 750.3018457 MHz
NUC1                 1H
P1                   1.50 usec
PLW1                 49.30500031 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 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 (43.57 ppm), Noise (121.81 to 101.80 ppm) [1086.6]  
 Processed with TDef=2048



Bruker BioSpin

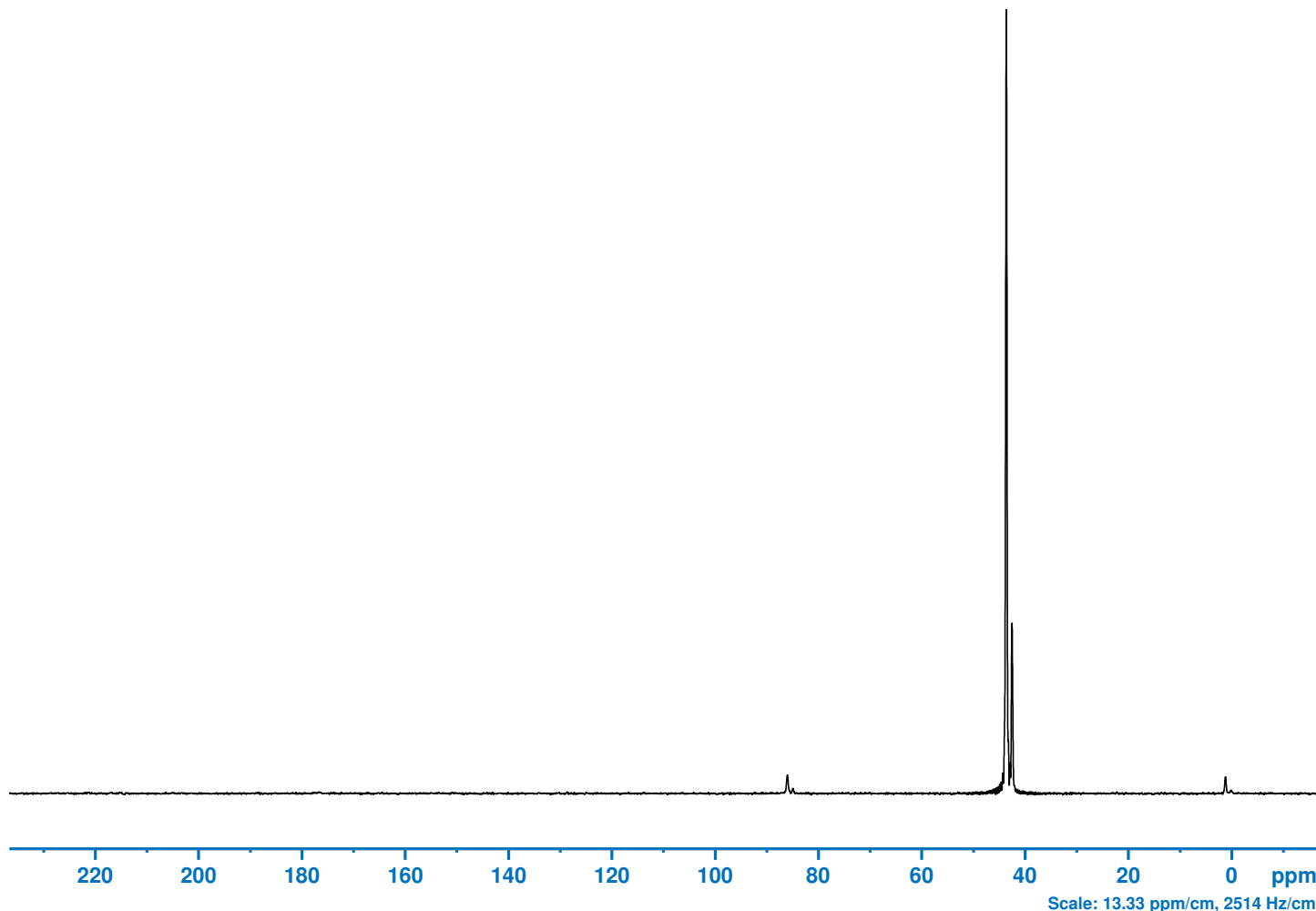
# NPT\_13C\_MAS\_paropt\_cp1h\_13c

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

F2 - Acquisition Parameters  
 Date\_ 20230807  
 Time 16.35 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 67.51899719 W  
 SFO2 750.3046519 MHz  
 NUC2 1H  
 CNST21 1.0000000  
 CPDPRG2 spinal64  
 P3 1.50 usec  
 PCPD2 2.80 usec  
 PLW2 49.30500031 W  
 PLW12 47.15999985 W  
 SPNAM[0] ramp50100.100  
 SPOAL0 0.500  
 SPOFFS0 0 Hz  
 SPW0 35.83000183 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 8000 Hz)

SINO (20.0 ppm): Signal (33.41 ppm), Noise (283.04 to 263.02 ppm) [503.7]



Bruker BioSpin

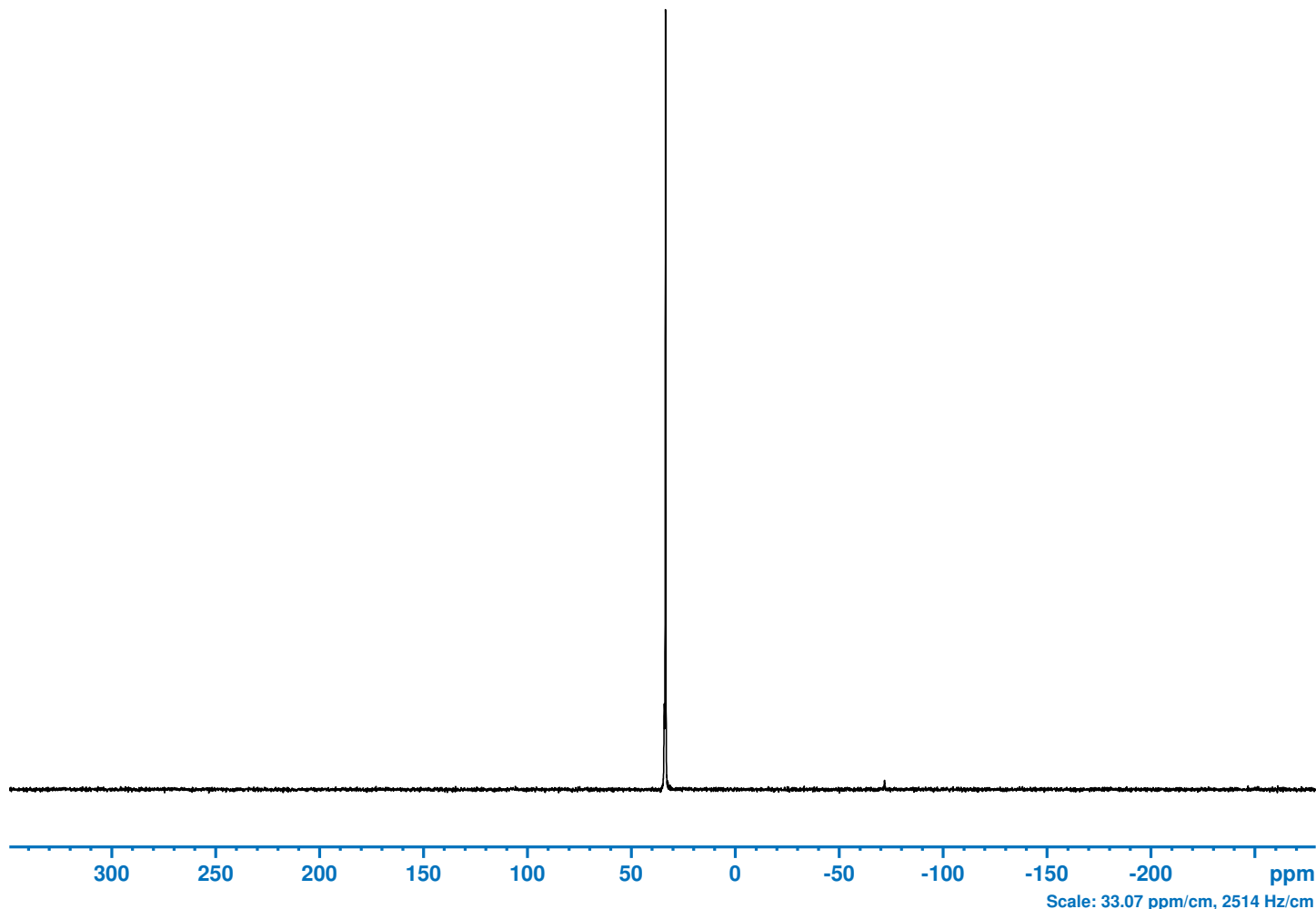
# NPT\_15N\_MAS\_paropt\_cp1h\_15n

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

F2 - Acquisition Parameters  
 Date\_ 20230808  
 Time 10.43 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 76.0299000 MHz  
 NUC1 15N  
 P15 3500.00 usec  
 PLW1 30.03300095 W  
 SFO2 750.3046519 MHz  
 NUC2 1H  
 CNST21 1.0000000  
 CPDPRG2 spinal64  
 P3 1.50 usec  
 PCPD2 2.80 usec  
 PLW2 49.30500031 W  
 PLW12 47.15999985 W  
 SPNAM[0] ramp50100.100  
 SPOAL0 0.500  
 SPOFFS0 0 Hz  
 SPW0 15.89999962 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 PDFs of Report

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

**750 MHz**

**Probe ID: H170225\_0001**

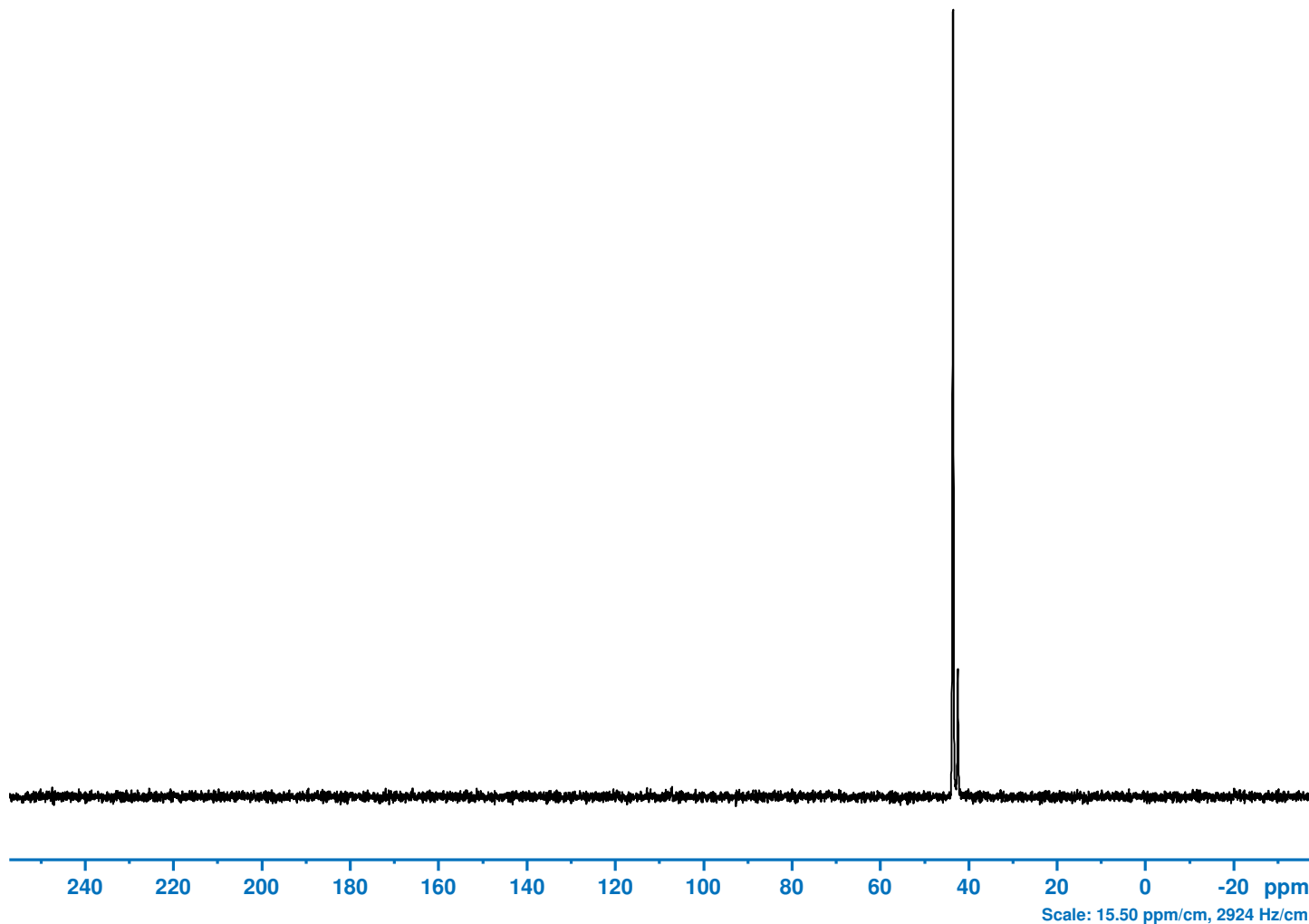
**Report Name: 2023-08-08\_13\_TRmode**

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)  
 Double CP made manualy  
 ns = 16



Bruker BioSpin

+/NPT\_ExpName.txt



```
Current Data Parameters
NAME      NPT_13C_MAS_double_cp1h15n_13c_ALG
EXPNO      4
PROCNO     1

F2 - Acquisition Parameters
Date_      20230808
Time       12.06 h
INSTRUM    Avance NEO
PROBHD     H170225_0001 (
PULPROG    doubcp
TD         554
SOLVENT    H2O+D2O
NS         16
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
CNST11     1.0000000
DO         0.00000300 sec
D1         5.00000000 sec
IN0        0 sec
L0         0
SFO1       188.6838379 MHz
NUC1       13C
CNST9      110.0000000
CNST10     20.0000000
P1         8.33 usec
P2         16.67 usec
P16        10000.00 usec
PLW1       7.62262392 W
PLW11      7.62262392 W
SPNAM[1]   tacn80
SPOAL1     0.500
SPOFFS1    0 Hz
SPW1       11.91034985 W
SFO2       750.3046519 MHz
NUC2       1H
CNST21     0
CNST24     1.0000000
CPDPRG[2]  spinal64
P3         1.50 usec
P15        4000.00 usec
PCPD2      2.80 usec
PLW2       0 W
PLW12      49.30500031 W
PLW13      49.30500031 W
SPNAM[0]   ramp.100
SPOAL0     0.500
SPOFFS0    0 Hz
SPW0       12.12981987 W
SFO3       76.0299000 MHz
NUC3       15N
PLW3       30.03300095 W
PLW5       21.19128036 W

F2 - Processing parameters
SI         32768
SF         188.6630851 MHz
WDW        EM
SSB        NPT_ShimSQColumn.txt
GB         0
PC         0.20
```