

PH MAS DVT 750W4 BL4 X/Y/H

750.3 MHz

Probe ID: H8780_0007

Report Name: 2023-07-13

● Probe NMR Test Data: **PH MAS DVT 750W4 BL4 X/Y/H**

Probe Related Information

EC-Level	0
Gas Compensation	nitrogen
Gradient System	none
ATM Accessory	false
Temperature Sensor Type	TypeT
Proton Frequency [MHz]	750.3
Diameter [mm]	4.0

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

● **Required Samples** PH MAS DVT 750W4 BL4 X/Y/H

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

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 5000 Hz)

Line width main [achieved]: [142] <n/a>



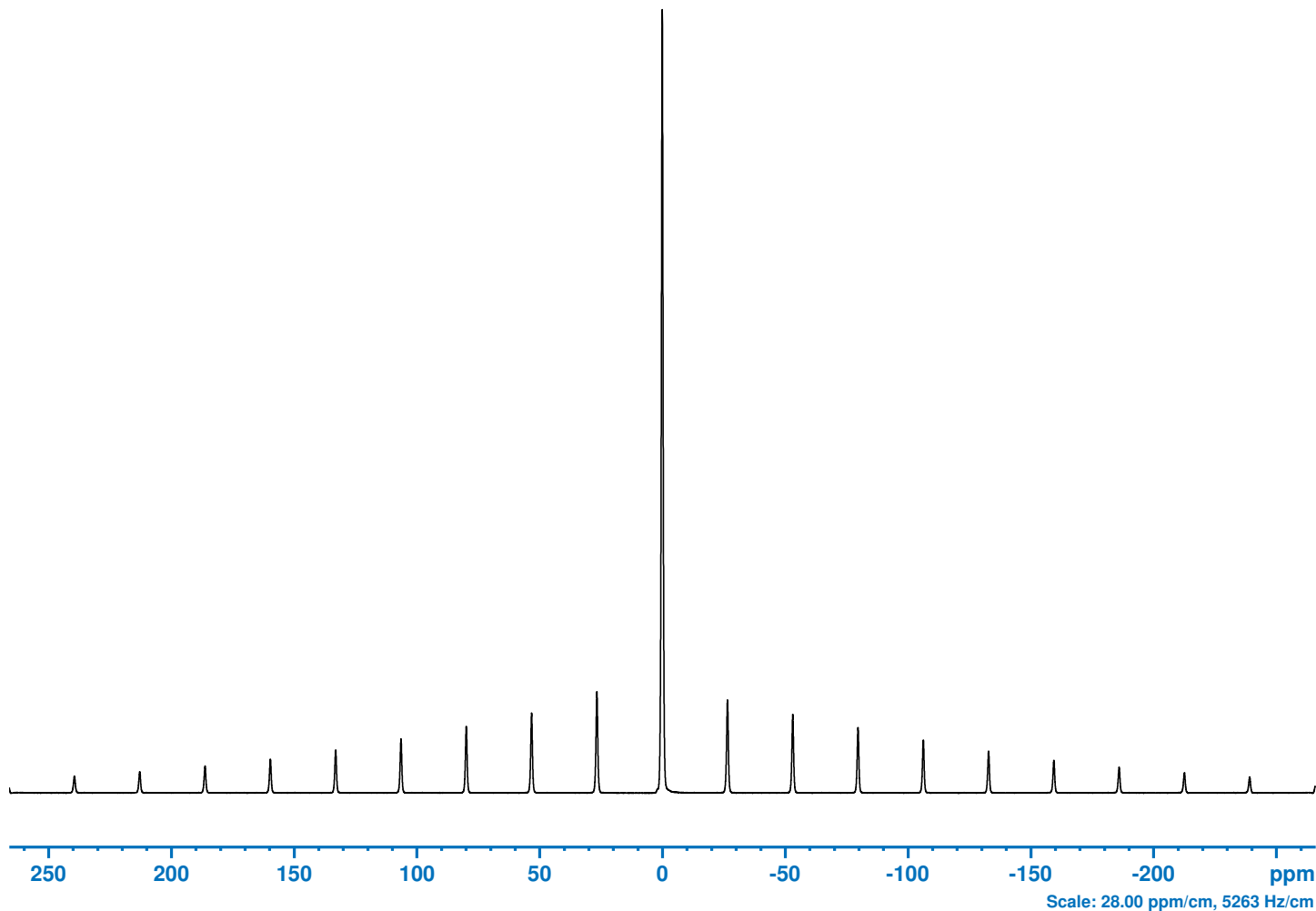
Bruker BioSpin

NPT_79Br_MAS_magicAngle

Current Data Parameters
NAME NPT_79Br_MAS_magicAngle
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 16.26 h
INSTRUM Avance NEO
PROBHD H8780_0007 (PH)
PULPROG onepulse
TD 8192
SOLVENT H2O+D2O
NS 16
DS 0
SWH 100000.000 Hz
FIDRES 24.414062 Hz
AQ 0.0409600 sec
RG 101
DW 5.000 usec
DE 6.50 usec
TE 294.4 K
D1 0.25000000 sec
SFO1 187.9904818 MHz
NUC1 79Br
P1 3.84 usec
PLW1 189.75000000 W

F2 - Processing parameters
SI 131072
SF 187.9904818 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20



SHIM SEQUENCE
skip shimming

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

Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H

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

Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 15000 Hz)

Determination of spinning stability for 180 s

Pressure values in mbar: DrivePressure=1960/BearingPressure=3180/BearingSensePressure=3187/SupplyPressure=6802/SystemPressure=6162

Spin rate at maximum deviation [measured]: @ MASR 15000 Hz [14978 Hz]

Maximum deviation [achieved]: @ MASR 15000 Hz [22 Hz] <n/a>



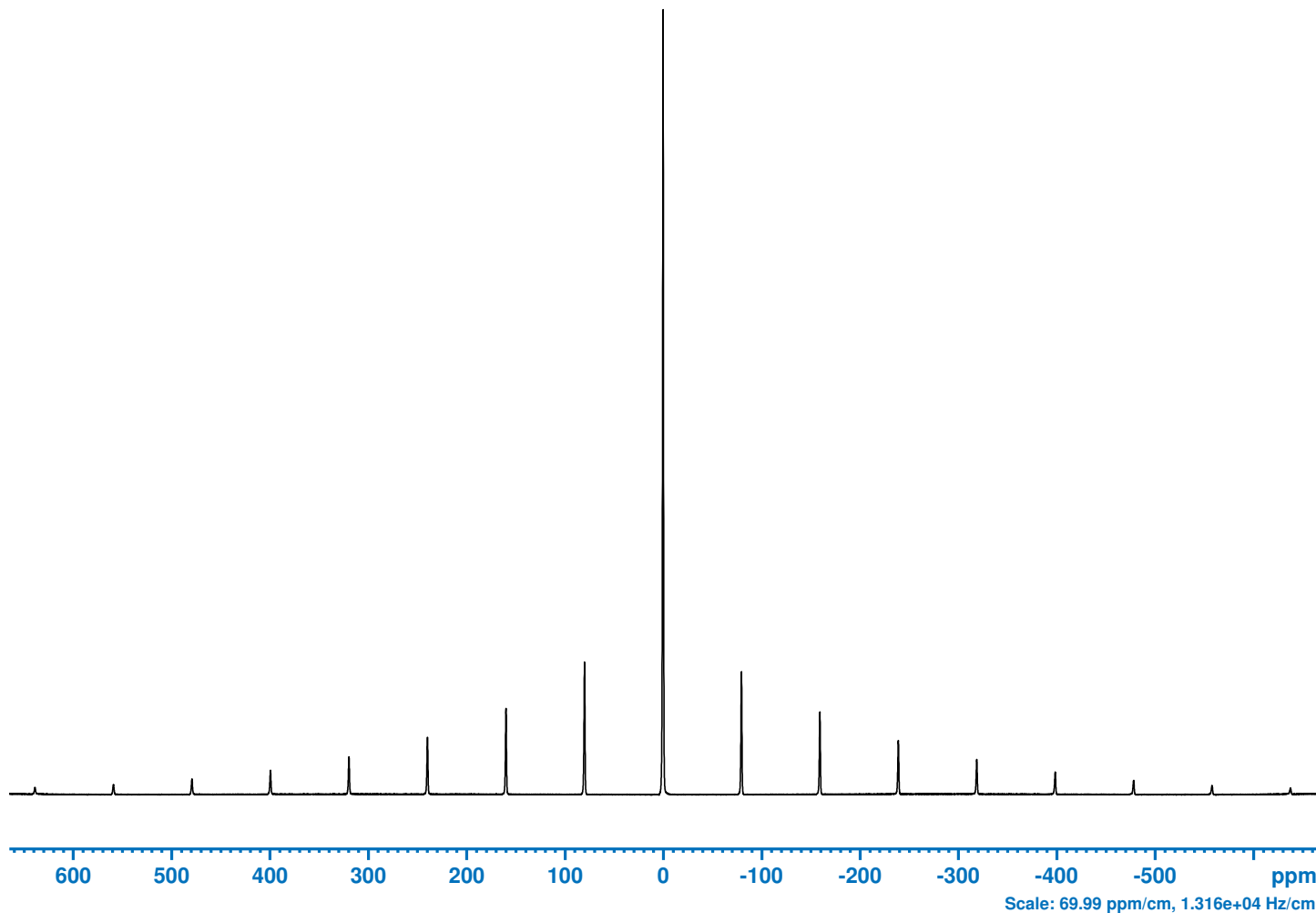
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

Current Data Parameters
NAME NPT_79Br_MAS_maxSpinRate
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 16.34 h
INSTRUM Avance NEO
PROBHD H8780_0007 (PH)
PULPROG onepulse
TD 16384
SOLVENT H2O+D2O
NS 16
DS 0
SWH 250000.000 Hz
FIDRES 30.517578 Hz
AQ 0.0327680 sec
RG 401
DW 2.000 usec
DE 6.50 usec
TE 301.2 K
D1 0.25000000 sec
SFO1 187.9911949 MHz
NUC1 79Br
P1 3.84 usec
PLW1 189.75000000 W

F2 - Processing parameters
SI 32768
SF 187.9911949 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20



SHIM SEQUENCE
skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
 Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
 Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting, spin rate 5000 Hz)
 FIELD was set to 1989.7 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0064 ppm.



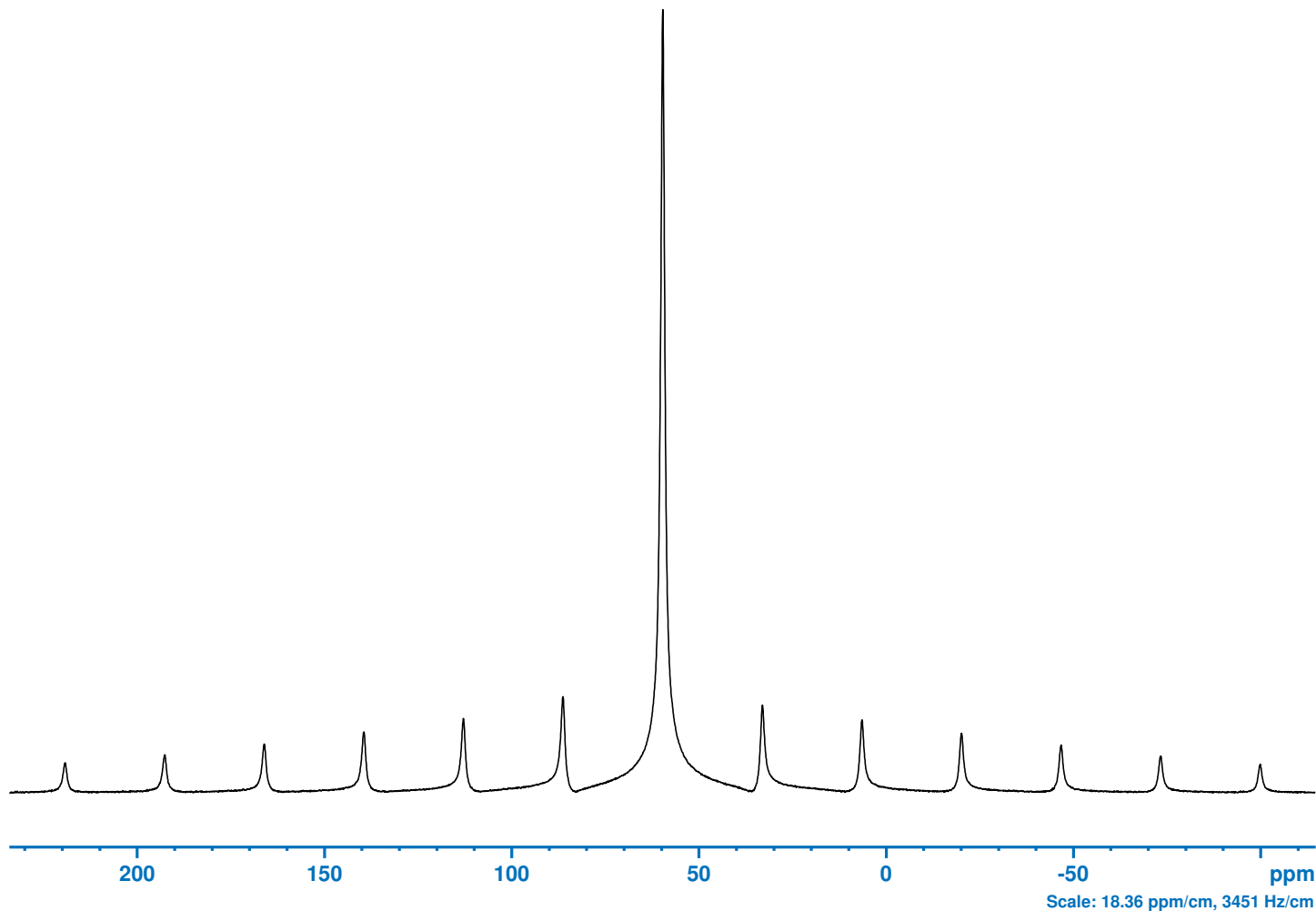
Bruker BioSpin

NPT_79Br_MAS_fieldsetting

Current Data Parameters
 NAME NPT_79Br_MAS_fieldsetting
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230713
 Time 16.26 h
 INSTRUM Avance NEO
 PROBHD H8780_0007 (PH)
 PULPROG onepulse
 TD 4096
 SOLVENT H2O+D2O
 NS 1
 DS 0
 SWH 81967.211 Hz
 FIDRES 40.023052 Hz
 AQ 0.0249856 sec
 RG 101
 DW 6.100 usec
 DE 6.50 usec
 TE 294.4 K
 D1 0.50000000 sec
 SFO1 187.9912344 MHz
 NUC1 79Br
 P1 3.84 usec
 PLW1 189.7500000 W

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



 SHIM SEQUENCE
 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br, spin rate 5000 Hz)
ATTENTION: Updated PROSOL Tables with [3.84 us @ 189.7 W].

P90 MAS 79Br pulse [achieved]: @ 174.0 W [4.01 us] <n/a>



Bruker BioSpin

NPT_79Br_MAS_p90det_79br

Current Data Parameters
NAME NPT_79Br_MAS_p90det_79br
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 16.22 h
INSTRUM Avance NEO
PROBHD H8780_0007 (PH)
PULPROG onepulse
TD 2048
SOLVENT H2O+D2O
NS 1
DS 0
SWH 100000.000 Hz
FIDRES 97.656250 Hz
AQ 0.0102400 sec
RG 101
DW 5.000 usec
DE 6.50 usec
TE 294.5 K
D1 0.25000000 sec
SFO1 187.9912344 MHz
NUC1 79Br
P1 11.52 usec
PLW1 174.0000000 W

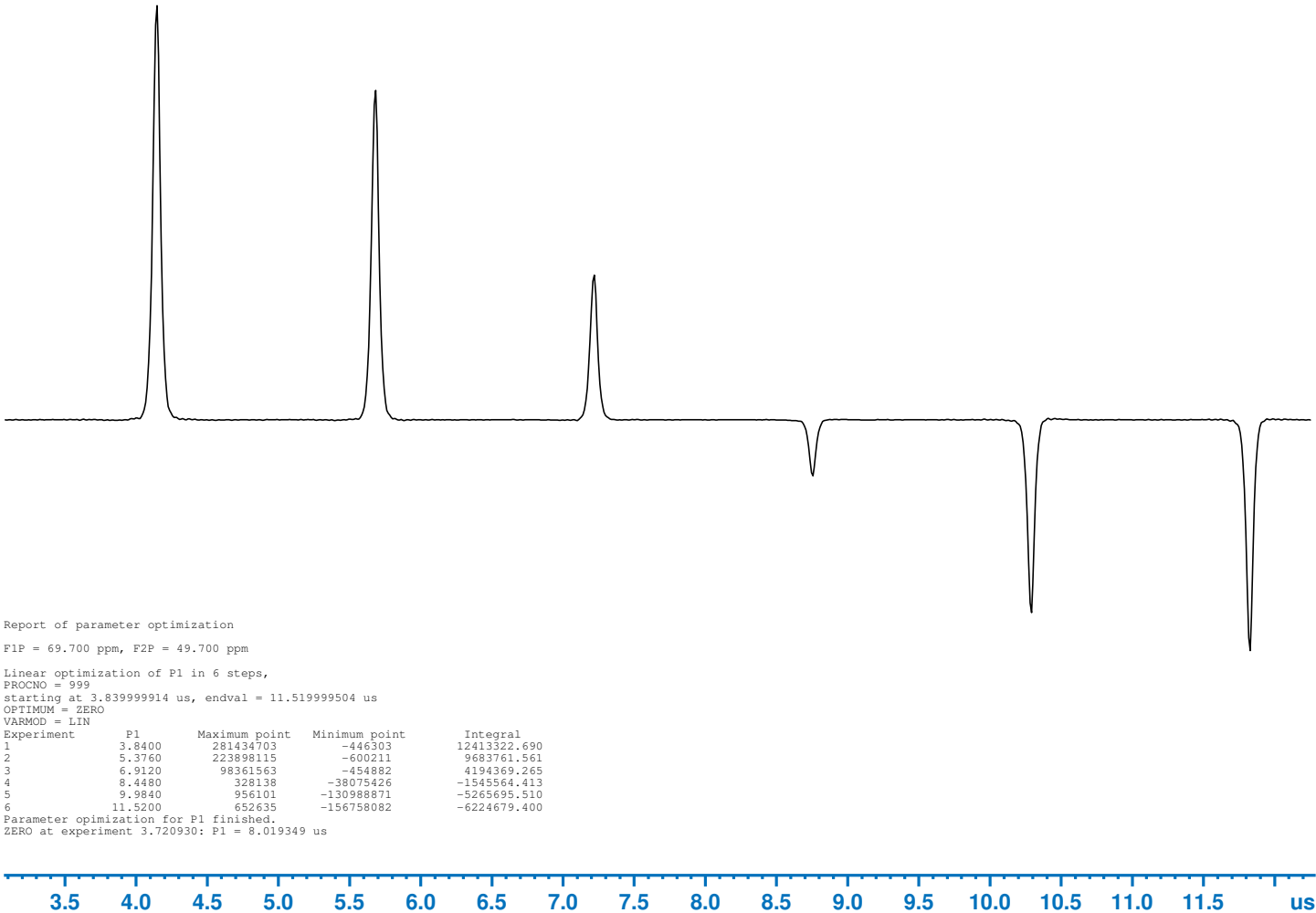
F2 - Processing parameters
SI 4096
SF 187.9800119 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20

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

PLW90	P90	P90[det]	Deviation
174.0 W	3.84 us		
174.0 W	3.84 us	4.01 us	4.4%

SHM SEQUENCE

skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
 Sample: Adamantane (50 ul) (Z151221)
 P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c, spin rate 15000 Hz)
 ATTENTION: Updated PROSOL Tables with [3.84 us @ 171.8 W].

P90 MAS 13C pulse [achieved]: @ 186.1 W [3.69 us] <n/a>



Bruker BioSpin

NPT_13C_MAS_p90det_13c

Current Data Parameters
 NAME NPT_13C_MAS_p90det_13c
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230713
 Time 17.10 h
 INSTRUM Avance NEO
 PROBHD H8780_0007 (PH)
 PULPROG hpdcc
 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 300.2 K
 D1 15.00000000 sec
 P15 0 usec
 ZGPTNS -Dlacc
 SFO1 188.6694995 MHz
 NUC1 13C
 P1 11.52 usec
 PLW1 186.05000305 W
 SFO2 750.3018457 MHz
 NUC2 1H
 CPDPRG[2] cw
 PLW2 141.00000000 W
 PLW12 0.19828130 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
186.1 W	3.84 us		
186.1 W	3.84 us	3.69 us	-3.9%

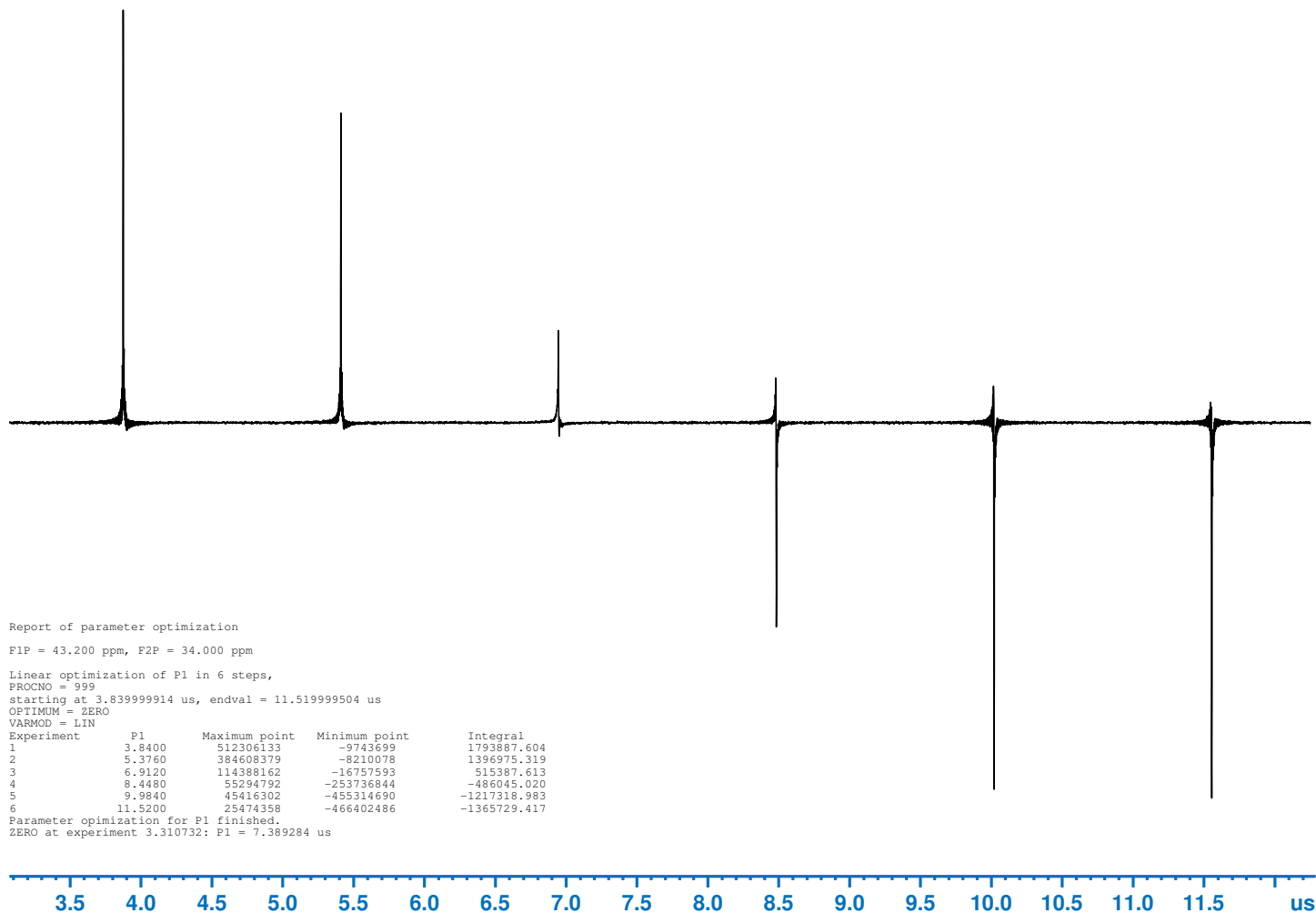
Report of parameter optimization

F1P = 43.200 ppm, F2P = 34.000 ppm

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

Experiment	P1	Maximum point	Minimum point	Integral
1	3.8400	512306133	-9743699	1793887.604
2	5.3760	384608379	-8210078	1396975.319
3	6.9120	114388162	-16757593	515387.613
4	8.4480	55294792	-253736844	-486045.020
5	9.9840	45416302	-455314690	-1217318.983
6	11.5200	25474358	-466402486	-1365729.417

Parameter optimization for P1 finished.
 ZERO at experiment 3.310732: P1 = 7.389284 us



 SHM SEQUENCE

 skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
Sample: Alpha-glycine (50 ul) (Z151222)
CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c, spin rate 7500 Hz)

SINO (20.0 ppm) [achieved]: Signal (43.48 ppm), Noise (77.53 to 57.53 ppm) [601.2] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>
Processed with TDef=2048



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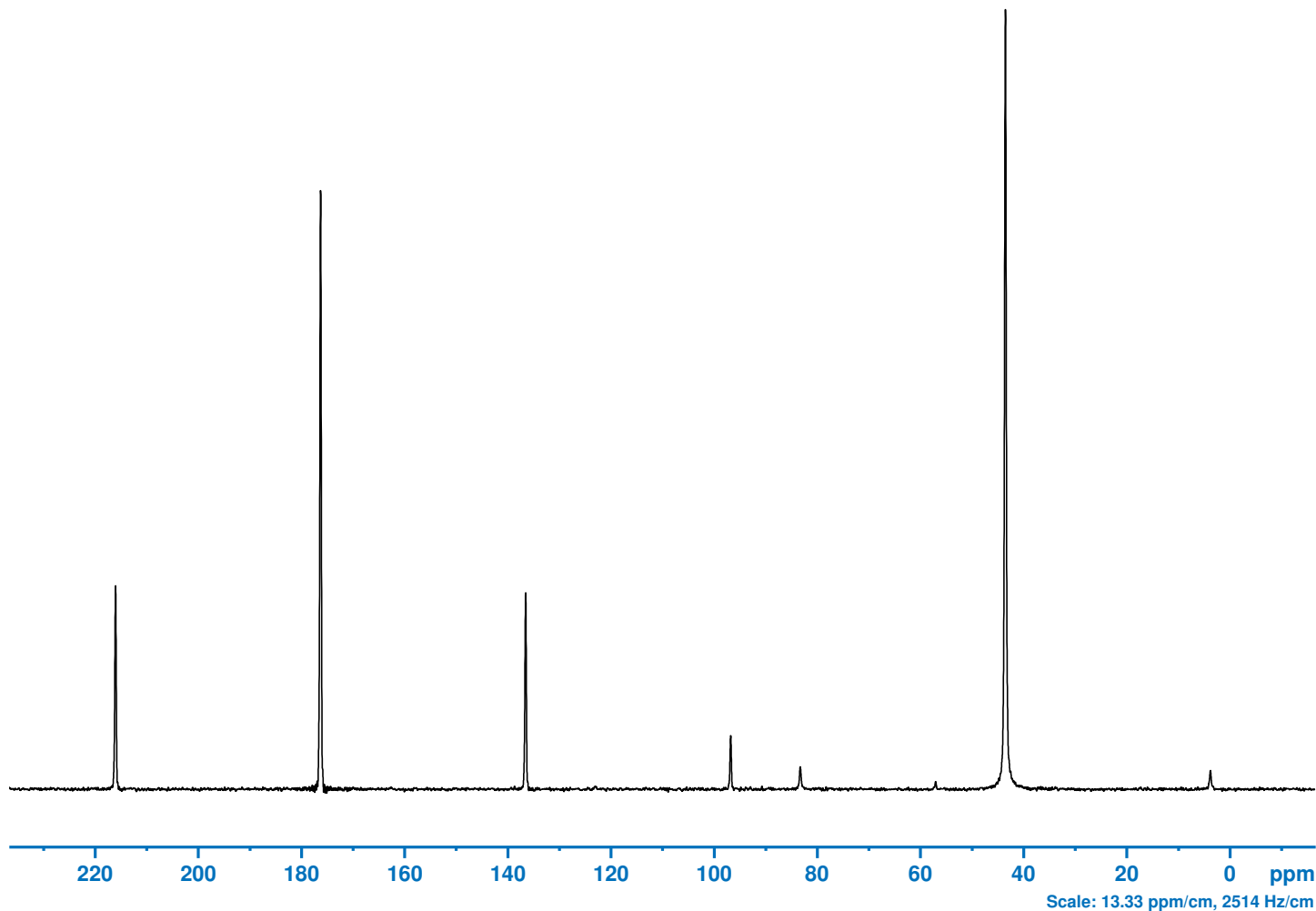
NPT_13C_MAS_sino_cp1h_13c

Current Data Parameters
NAME NPT_13C_MAS_sino_cp1h_13c
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 17.52 h
INSTRUM Avance NEO
PROBHD H8780_0007 (PH)
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 296.1 K
D1 5.00000000 sec
ZGPTNS
SFO1 188.6838379 MHz
NUC1 13C
P15 2000.00 usec
PLW1 171.80000305 W
SFO2 750.3046519 MHz
NUC2 1H
CNST21 1.00000000
CPDPRG[2] spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 141.00000000 W
PLW12 147.00000000 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 147.00000000 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 SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
Sample: Alpha-glycine (50 ul) (Z151222)
CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n, spin rate 7500 Hz)

SINO (20.0 ppm) [achieved]: Signal (33.33 ppm), Noise (175.59 to 155.58 ppm) [61.7] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>



Bruker BioSpin

NPT_15N_MAS_sino_cp1h_15n

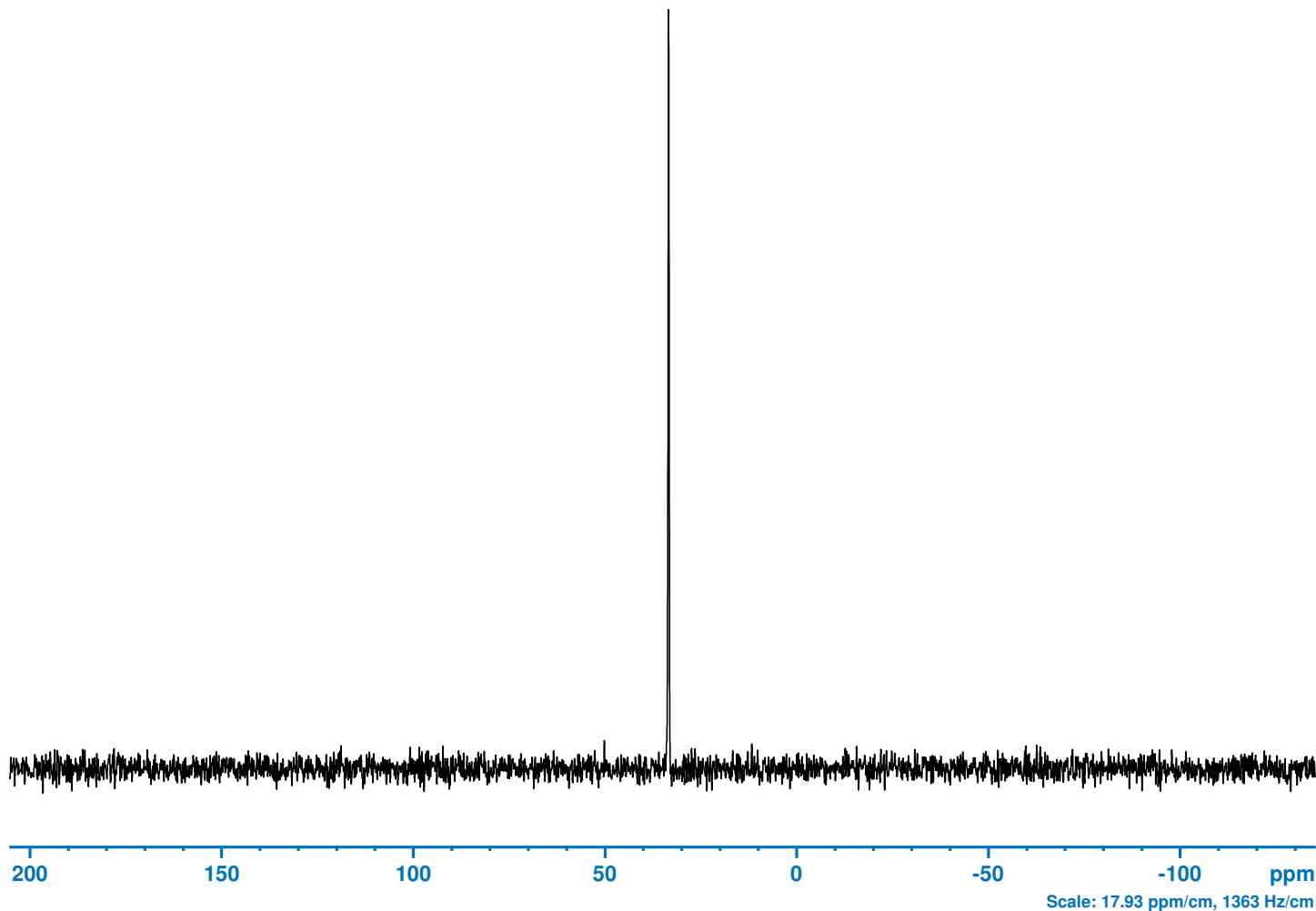
Current Data Parameters
NAME NPT_15N_MAS_sino_cp1h_15n
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 18.26 h
INSTRUM Avance NEO
PROBHD H8780_0007 (PH
PULPROG cp
TD 3012
SOLVENT H2O+D2O
NS 64
DS 0
SWH 30120.482 Hz
FIDRES 20.000320 Hz
AQ 0.0499992 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 297.4 K
D1 5.0000000 sec
ZGPGTNS
SFO1 76.0299000 MHz
NUC1 15N
P15 3500.00 usec
PLW1 229.00000000 W
SFO2 750.3046519 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 141.00000000 W
PLW12 143.58000183 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 57.97999954 W

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

SHIM SEQUENCE

skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
 Sample: Adamantane (50 ul) (Z151221)
 13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 15000 Hz)

SINO (20.0 ppm) [achieved]: Signal (38.37 ppm), Noise (27.66 to 7.66 ppm) [172.4] <n/a>
 Linewidth [achieved]: at 50% of signal height [1.4 Hz] <n/a>
 Number of scans (NS) [achieved]: [1] <n/a>



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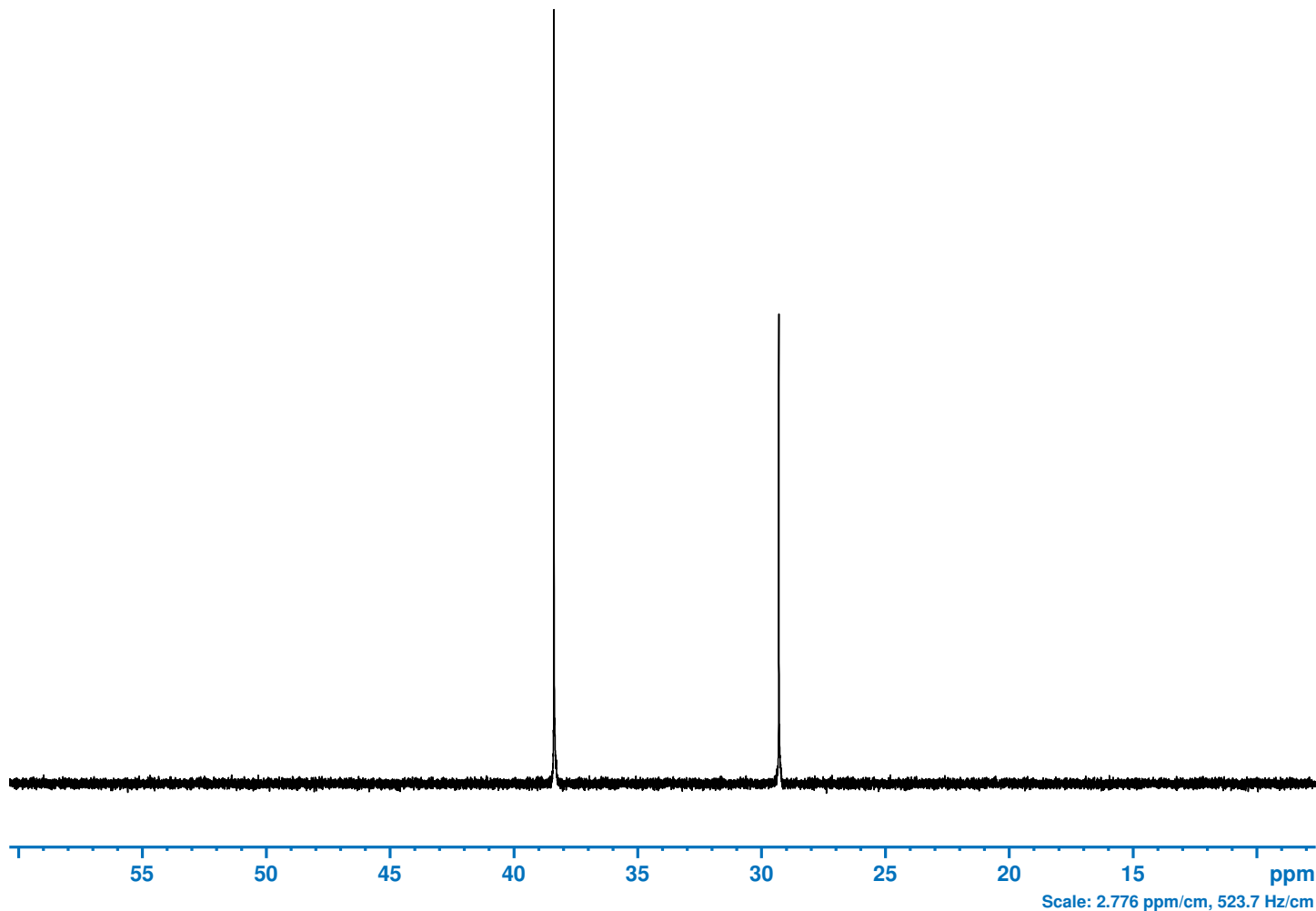
NPT_13C_MAS_sino_13c

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

F2 - Acquisition Parameters
Date_     20230713
Time      17.11 h
INSTRUM   Avance NEO
PROBHD    H8780_0007 (PH)
PULPROG   hpdec
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         300.2 K
D1         15.00000000 sec
P15        0 usec
ZGPGTNS   -Dlacq
SFO1      188.6694995 MHz
NUC1       13C
P1         3.84 usec
PLW1       171.80000305 W
SFO2       750.3018457 MHz
NUC2       1H
CPDPRG2    cw
PLW2       141.00000000 W
PLW12      0.19828130 W

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



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
 Sample: Adamantane (50 ul) (Z151221)
 13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 15000 Hz)



Bruker BioSpin

NPT_13C_MAS_sino_13c

```
# Thu Jul 13 15:11:26 2023
##$PROBEIDENTIFIER=H8780_0007
##$PROBENAME=PH MAS DVT 750W4 BL4 X/Y/H
##$SHIMID=272623
#
# Active Shim Gradients
#
Z -73605
Z2 5304
Z3 0
Z4 0
Z5 0
Z6 0
X 23254
XZ -3296
XZ2 0
XZ3 0
XZ4 0
Y 26000
YZ 0
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 1989.669
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] -18401.25100000
SHIM_SETTING [ 2] -415.67300000
SHIM_SETTING [ 3] -115.34900000
SHIM_SETTING [ 4] 2202.02200000
SHIM_SETTING [ 5] -2923.71200000
SHIM_SETTING [ 6] 399.04800000
SHIM_SETTING [ 7] 1529.16200000
SHIM_SETTING [ 8] -1282.49400000
SHIM_SETTING [ 9] -1370.59300000
SHIM_SETTING [10] 6794.14300000
SHIM_SETTING [11] -5143.97200000
SHIM_SETTING [12] 0.00000000
SHIM_SETTING [13] 0.00000000
SHIM_SETTING [14] 0.00000000
SHIM_SETTING [15] 4426.04300000
SHIM_SETTING [16] 6074.04300000
SHIM_SETTING [17] -5418.81600000
SHIM_SETTING [18] -6208.18400000
SHIM_SETTING [19] 2605.41600000
SHIM_SETTING [20] 2897.34000000
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] 5870.00700000
SHIM_SETTING [29] 0.00000000
SHIM_SETTING [30] 0.00000000
SHIM_SETTING [31] -6500.00000000
SHIM_SETTING [32] 5870.00700000
SHIM_SETTING [33] 0.00000000
SHIM_SETTING [34] 0.00000000
SHIM_SETTING [35] -0.00000000
SHIM_SETTING [36] -0.00000000
SHIM_SETTING [37] 3076.28000000
SHIM_SETTING [38] 3076.28000000
SHIM_SETTING [39] -6500.00000000
SHIM_SETTING [40] 0.00000000
```

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

F2 - Acquisition Parameters
Date_ 20230713
Time 17.11 h
INSTRUM Avance NEO
PROBHD H8780_0007 (PH
PULPROG hpdcc
TD 19998
SOLVENT H2O+D2O
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 1.000100 Hz
AQ 0.9999000 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 300.9 K
D1 15.00000000 sec
P15 0 usec
ZGPGTNS -D1acq
SFO1 188.6694995 MHz
NUC1 13C
P1 3.84 usec
PLW1 171.80000305 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG2 cw
PLW2 141.00000000 W
PLW12 0.19828130 W

F2 - Processing parameters
SI 32768
SF 188.6630850 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: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
Sample: Adamantane (50 ul) (Z151221)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 15000 Hz)

SINO (20.0 ppm) [achieved]: Signal (2.32 ppm), Noise (-39.33 to -59.34 ppm) [21605.3] <n/a>
Linewidth [achieved]: at 50% of signal height [354.3 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>



Bruker BioSpin

NPT_1H_MAS_sino_1h

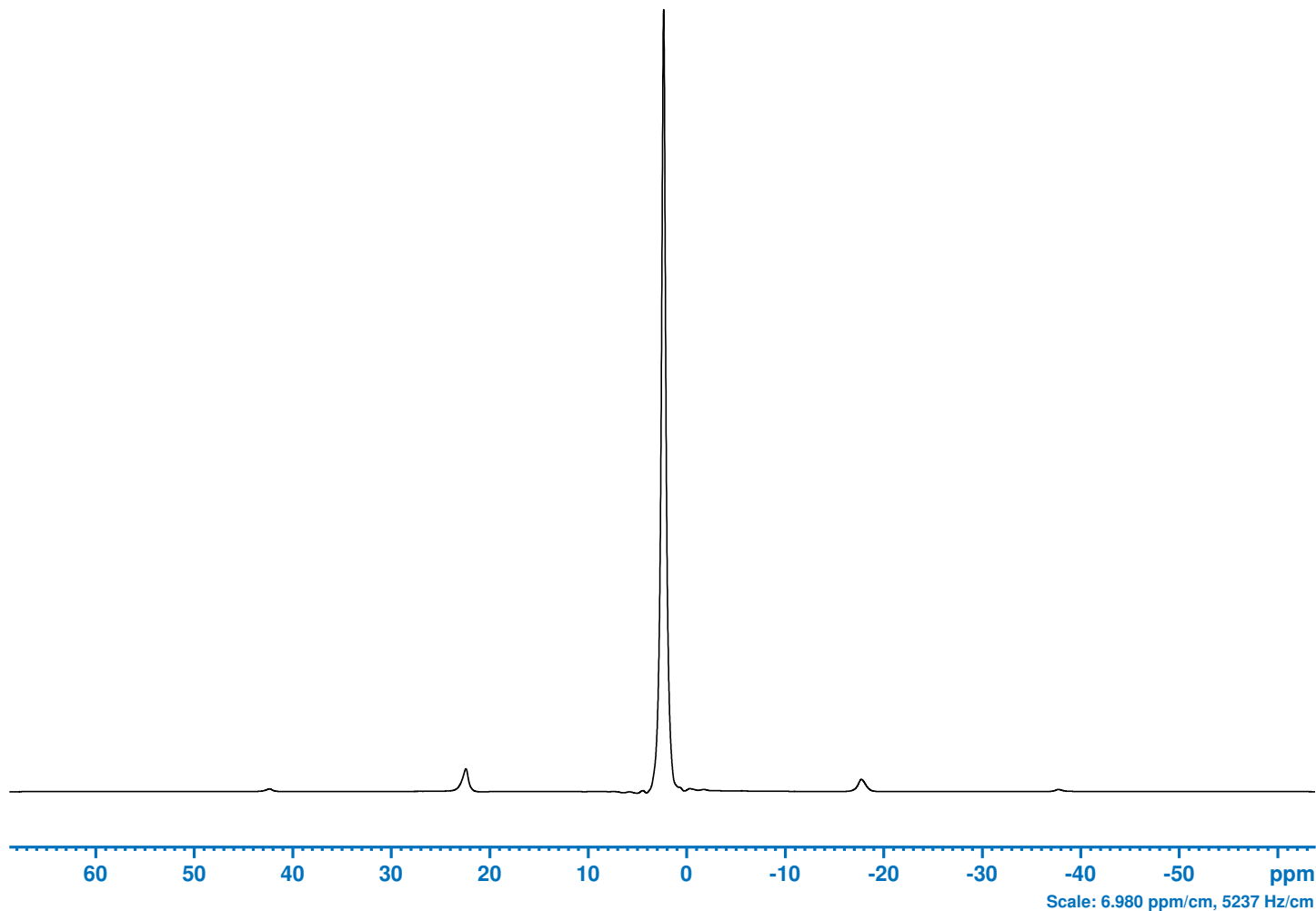
Current Data Parameters
NAME NPT_1H_MAS_sino_1h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 16.55 h
INSTRUM Avance NEO
PROBHD H8780_0007 (PH)
PULPROG onepulse
TD 2048
SOLVENT H2O+D2O
NS 1
DS 0
SWH 100000.000 Hz
FIDRES 97.656250 Hz
AQ 0.0102400 sec
RG 8
DW 5.000 usec
DE 6.50 usec
TE 300.2 K
D1 5.00000000 sec
SFO1 750.3018457 MHz
NUC1 1H
P1 2.50 usec
PLW1 141.00000000 W

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

SHIM SEQUENCE

skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
 Probe: H8780_0007 PH MAS DVT 750W4 BL4 X/Y/H
 Sample: 2-13C, 15N alpha-glycine (50 ul) (Z151223)
 CP 1H-13C parameter optimization, MAS (NPT_13C_MAS_paropt_cp1h_13c, spin rate 7500 Hz)

SINO (20.0 ppm): Signal (43.46 ppm), Noise (205.64 to 185.64 ppm) [7519.3]
 Processed with TDef=2048



Bruker BioSpin

NPT_13C_MAS_paropt_cp1h_13c

Current Data Parameters
 NAME NPT_13C_MAS_paropt_cp1h_13c
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20230713
 Time 17.33 h
 INSTRUM Avance NEO
 PROBHD H8780_0007 (PH)
 PULPROG cp
 TD 5554
 SOLVENT H2O+D2O
 NS 4
 DS 0
 SWH 55555.555 Hz
 FIDRES 20.005602 Hz
 AQ 0.0499860 sec
 RG 101
 DW 9.000 usec
 DE 6.50 usec
 TE 296.0 K
 D1 5.00000000 sec
 ZGPTNS
 SFO1 188.6838379 MHz
 NUC1 13C
 P15 2000.00 usec
 PLW1 171.80000305 W
 SFO2 750.3046519 MHz
 NUC2 1H
 CNST21 1.0000000
 CPDPRG[2] spinal64
 P3 2.50 usec
 PCPD2 4.80 usec
 PLW2 141.00000000 W
 PLW12 147.00000000 W
 SPNAM[0] ramp50100.100
 SPOAL0 0.500
 SPOFFS0 0 Hz
 SPW0 147.00000000 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

