

**PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z**

**750 MHz**

**Probe ID: Z180004\_0001**

**Report Name: 2023-08-10\_HRMAS\_TXI**

**Aug 10, 2023**

**NMR TEST ACCEPTANCE**

● Probe NMR Test Data: **PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z**

### Probe Related Information

EC-Level	0
Gas Compensation	air
Gradient System	Z
ATM Accessory	true
Temperature Sensor Type	TypeT
Proton Frequency [MHz]	750
Diameter [mm]	4.0

### Spectrometer Related Information

Type	AV NEO
CF Frequency [MHz]	750.30
Shim System	BOSS3-SB
Software	TopSpin 4.3.0
OS	CentOS Linux release 7.9.2009 (Core)
Host Name	avance750
Magnet System	SB
Magnet	BR.091075110
Cryostat	BD228972
System Number	442759



● PICS Data

Z180004\_0001.ph

```
Z180004_0001.ph
=====
$Bis, 1, 20220107, 8192, PICS, 6#
$Production, Z180004, 0001, 00.00, , BCH, 20211213#
$Name, PT HRMAS-750-W4/S7-H/P/C/D-4.0-Z#
$ProbeCompatibility, 1.0, WB, 4, 750#
$ProbeType, 1.2, HRMAS, 0, 0, 0#
$ProbeSample, 2.0, 4.0, 0, 0, 0, 0#
$ProbeTemperature, 1.0, TypeI, -30, 80#
$ProbeHeaterTemperature, 1.0, TypeI, , 400#
$ProbeGasFlow, 1.1, , , , , , , , A#
$ProbeAllCoils, 2.0, 1#
$ProbeCoil, 3.0, 1, 4, 1H, 8.0, 31P, 8.0, 13C[13C-79Br], 8.0, 2H, 8.0#
$ProbeChannel, 3.0, 1H, T/R/W, 1H, T.0, 8/-, T.0, 1/+#
$ProbeChannel, 3.0, 13C, T/R/W, 13C-79Br, T.0, 2/-, T.0, 7/+#
$ProbeChannel, 3.0, 31P, T/R/W, 31P, T.0, 4/-, T.0, 6/+#
$ProbeChannel, 3.0, 2H, T/R/W, 2H, T.0, 3/-, 0, F#
$ProbeZ-Grad, 2.0, System, , 6.1, 10, #
$ProbeGradInfo, 1.1, Z156573, , , , 25, , , , , #
$ProbeMas, 1.2, 0, 15000, 0, 0, 2, 20000, 620000, 1, 11000, 5, 626073, 580000#
$ProbeChannelNucleusATMA, 1.0, 1H, 1H, 750.130, None, 711502, 167435#
$ProbeChannelNucleusATMA, 1.0, 13C, 13C, 188.620, None, 205561, 262511#
$ProbeChannelNucleusATMA, 1.0, 31P, 31P, 303.658, None, 290944, 715733#
$ProbeChannelNucleusATMA, 1.0, 2H, 2H, 115.150, None, 283674, 715733#
$ProbeChannelNucleusATMA, 1.0, 13C, 79Br, 187.937, None, 160247, 265965#
$ProbeChannelNucleusWob, 1.0, 1H, 1H, 10.0#
$ProbeChannelNucleusWob, 1.0, 13C, 13C, 3.0#
$ProbeChannelNucleusWob, 1.0, 31P, 31P, 4#
$ProbeChannelNucleusWob, 1.0, 2H, 2H, 2.0#
$ProbeChannelNucleusWob, 1.0, 13C, 79Br, 3.0#
$ProbeATMAOrder, 1.0, 5, 2H, 13C, 31P, 2H, 1H#
$ProbeATMA DriveRange, 2.1, 1, 101000-305000, 100000, 1953, MECH#
$ProbeATMA DriveRange, 2.1, 2, 101000-613000, 100000, 994, MECH#
$ProbeATMA DriveRange, 2.1, 3, 101000-613000, 100000, 500, MECH#
$ProbeATMA DriveRange, 2.1, 4, 150000-1183000, 100000, 3246, MECH#
$ProbeATMA DriveRange, 2.1, 5, 100000-726073, 728073, -15000, MECH#
$ProbeATMA DriveRange, 2.1, 6, 150000-1183000, 100000, 1740, MECH#
$ProbeATMA DriveRange, 2.1, 7, 101000-613000, 100000, 1020, MECH#
$ProbeATMA DriveRange, 2.1, 8, 150000-1159000, 100000, 4934, MECH#
$AtmaOpticalInterface, 1.0, 3, R, 0, 0#
$ProbePowerNucleus, 1.0, 1H[1H], 100, #
$ProbePowerNucleus, 1.0, 13C[13C-79Br], 200, #
$ProbePowerNucleus, 1.0, 31P[31P], 300, #
$ProbePowerNucleus, 1.0, 2H[2H], 27, #
$EndBis, 33, 45#
```

● **Required Samples** **PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z**

Z142220	1% Chloroform in Acetone-D6 (50 ul)
Z142221	0.1% Ethylbenzene (EB) in Chloroform-D (50 ul)
Z142222	2 mM Sucrose, 0.5 mM DSS, 2 mM NaN <sub>3</sub> in 90% H <sub>2</sub> O + 10% D <sub>2</sub> O (50 ul)
Z142223	100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (50 ul)
Z142224	40% Dioxane in Benzene-D6 (ASTM, 50 ul)
Z142226	0.0485 M Triphenyl Phosphate (TPP, [C <sub>6</sub> H <sub>5</sub> ] <sub>3</sub> PO <sub>4</sub> ) in Acetone-D6 (50 ul)
Z151220	Potassium Bromide (KBr, 80 ul)

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 1% Chloroform in Acetone-D6 (50 ul) (Z142220)  
 1H lineshape with magic angle spinning (NPT\_1H\_HRMAS\_lineshape, spin rate 4000 Hz)

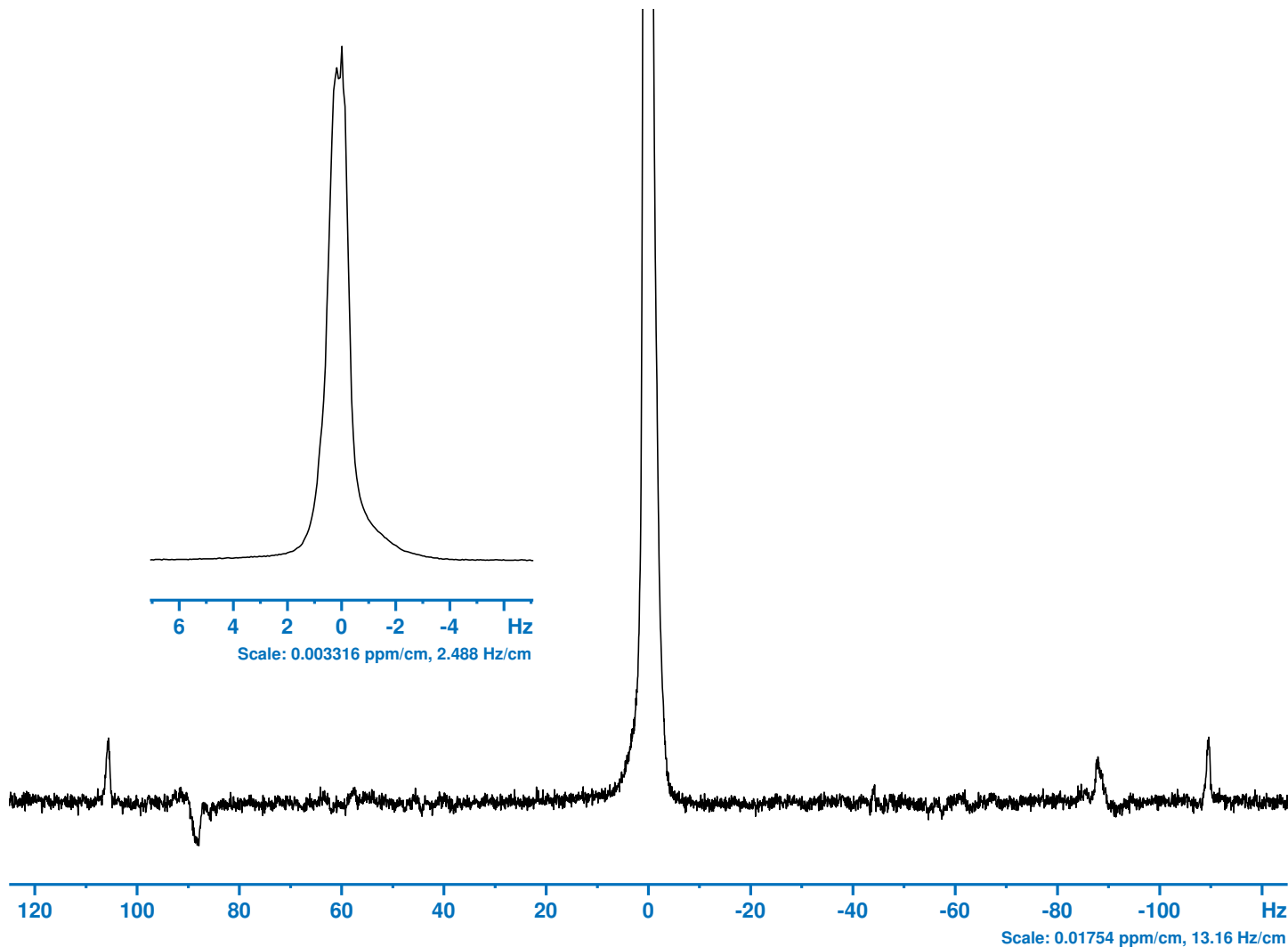
Line width [achieved/rated]: at 0.11% of signal height [11.6 Hz <= 18.0 Hz] <pass>  
 Line width [achieved/rated]: at 0.55% of signal height [6.8 Hz <= 12.0 Hz] <pass>  
 Line width [achieved/rated]: at 50% of signal height [0.79 Hz <= 1.00 Hz] <pass>



Bruker BioSpin

## NPT\_1H\_HRMAS\_lineshape

Current Data Parameters			
NAME	NPT_1H_HRMAS_lineshape		
EXPNO	9		
PROCNO	1		
F2 - Acquisition Parameters		Additional Parameters	
Date_	20230810	Field	1357.763
Time	18.48 h	Lock Phase	349.000
INSTRUM	Avance NEO	Lock Power	-34.000
PROBHD	Z180004_0001 (	Lock Gain	93.860
PULPROG	zg30	Lock DC	-70.000
TD	32768	Lock Shift	2.040
SOLVENT	Acetone	Loop Gain	15.133
NS	4	Loop Time	0.047
DS	0	Loop Filter	1468.000
SWH	1000.000 Hz	Gas Flow	external
FIDRES	0.061035 Hz		
AQ	16.3840008 sec		
RG	101		
DW	500.000 usec		
DE	6.50 usec		
TE	298.0 K		
D1	9.11600113 sec		
TD0	1		
SFO1	750.3057701 MHz		
NUC1	1H		
P0	2.67 usec		
P1	8.00 usec		
PLW1	13.02900028 W		
F2 - Processing parameters			
SI	8192		
SF	750.3060202 MHz		
WDW	no		
SSB	0		
LB	0 Hz		
GB	0		
PC	4.00		



SHIM SEQUENCE  
 - topshim hrmas <pass>

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 1% Chloroform in Acetone-D6 (50 ul) (Z142220)  
 1H lineshape with magic angle spinning (NPT\_1H\_HRMAS\_lineshape, spin rate 4000 Hz)



Bruker BioSpin

# NPT\_1H\_HRMAS\_lineshape

```
# Thu Aug 10 16:48:24 2023
$$$PROBEIDENTIFIER=Z180004_0001
$$$PROBENAME=PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
$$$SHIMID=292721
#
# Active Shim Gradients
#
Z          -4518
Z2         0
Z3        1523
Z4         0
Z5         0
Z6         0
Z7         0
Z8         0
X          -46
XZ         334
XZ2        -36
XZ3         0
XZ4         0
XZ5         0
Y          5402
YZ        -39304
YZ2        4247
YZ3         0
YZ4         0
YZ5         0
XY        -501
XYZ        173
XYZ2        0
XYZ3        0
XYZ4        0
XYZ5        0
(X2-Y2)    -27661
(X2-Y2) Z   9521
(X2-Y2) Z2  0
(X2-Y2) Z3  0
(X2-Y2) Z4  0
(X2-Y2) Z5  0
X3         216
X3Z         0
Y3        -4235
Y3Z         0
#
# Lock Parameter
#
FIELD      1357.763
LOCKPHASE   349.000
LOCKPOWER  -34.000
LOCKGAIN    93.860
```

```
LOCKDC      -70.000
LOCKSHIFT    2.040
LOOPGAIN     15.133
LOOPTIME     0.047
LOOPFILTER   1468.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1] -2062.84169371
SHIM_SETTING [ 2]  0.00000000
SHIM_SETTING [ 3] 1260.31301011
SHIM_SETTING [ 4] -0.00000000
SHIM_SETTING [ 5] -152.83602314
SHIM_SETTING [ 6] 152.83602314
SHIM_SETTING [ 7]  833.12242322
SHIM_SETTING [ 8] -833.12242322
SHIM_SETTING [ 9]  581.24102344
SHIM_SETTING [10] -581.24102344
SHIM_SETTING [11]  0.00000000
SHIM_SETTING [12] -4235.31063044
SHIM_SETTING [13] -4235.31063044
SHIM_SETTING [14]  104.94832937
SHIM_SETTING [15]  256.54044471
SHIM_SETTING [16] -410.94780176
SHIM_SETTING [17]  136.74354812
SHIM_SETTING [18] -182.97274565
SHIM_SETTING [19]  48.11926812
SHIM_SETTING [20] -70.11851338
SHIM_SETTING [21] -8374.35871966
SHIM_SETTING [22] -27415.84416824
SHIM_SETTING [23] -20949.70429216
SHIM_SETTING [24] -34372.34229749
SHIM_SETTING [25] -8692.55738175
SHIM_SETTING [26] -12947.96805590
SHIM_SETTING [27]  104.94832937
SHIM_SETTING [28] -30178.89748823
SHIM_SETTING [29] -157.45213408
SHIM_SETTING [30] -234.79908394
SHIM_SETTING [31] -16166.11103774
SHIM_SETTING [32] 48428.99750934
SHIM_SETTING [33] -151.31172982
SHIM_SETTING [34] -497.41247848
SHIM_SETTING [35] -379.39151650
SHIM_SETTING [36] -623.36329461
SHIM_SETTING [37]  8228.25272673
SHIM_SETTING [38] -5696.19557886
SHIM_SETTING [39] 21485.89399085
SHIM_SETTING [40]  0.00000000
```

```
Current Data Parameters
NAME      NPT_1H_HRMAS_lineshape
EXPNO     9
PROCNO    1

F2 - Acquisition Parameters
Date_     20230810
Time      18.48 h
INSTRUM   Avance NEO
PROBHD    Z180004_0001 (
PULPROG   zg30
TD         32768
SOLVENT    Acetone
NS         4
DS         0
SWH        1000.000 Hz
FIDRES     0.061035 Hz
AQ         16.3840008 sec
RG         101
DW         500.000 usec
DE         6.50 usec
TE         298.0 K
D1         9.11600113 sec
TD0        1
SF01       750.3057701 MHz
NUC1       1H
P0         2.67 usec
P1         8.00 usec
PLW1       13.02900028 W

F2 - Processing parameters
SI         8192
SF         750.3060202 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0
PC         4.00
```

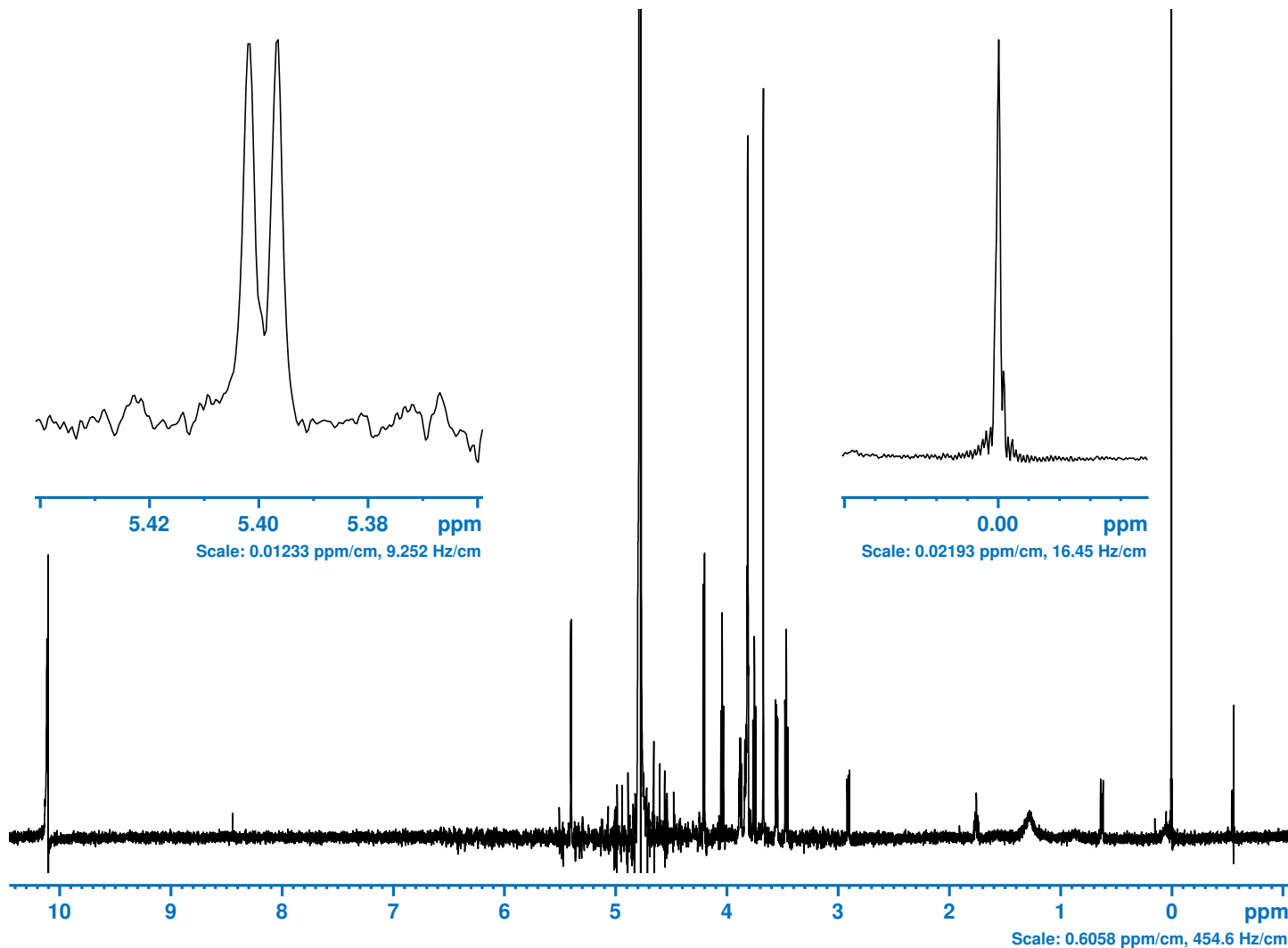
NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 2 mM Sucrose, 0.5 mM DSS, 2 mM NaN3 in 90% H2O + 10% D2O (50 ul) (Z142222)  
 Watersuppression (NPT\_1H\_HRMAS\_watersuppression, spin rate 4000 Hz)  
 PULPROG = zgpr, Input\_L23 = 1, O1 = 3524.73 Hz (optimized), OvFl = 0

Linewidth [achieved]: at 50 % of DSS signal [16.4 Hz] <n/a>  
 Linewidth [achieved]: at 10 % of DSS signal [29.1 Hz] <n/a>  
 Splitting anomeric proton [achieved]: [22%] <n/a>  
 SINO (1.5 ppm) [achieved]: Signal (6.00 to 5.20 ppm), Noise (10.00 to 8.50 ppm) [45.1] <n/a>



Bruker BioSpin

## NPT\_1H\_HRMAS\_watersuppression



Current Data Parameters  
 NAME NPT\_1H\_HRMAS\_watersuppression  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters		Additional Parameters	
Date_	20230810	Field	1377.359
Time	19.23 h	Lock Phase	350.500
INSTRUM	Avance NEO	Lock Power	-18.000
PROBHD	Z180004_0001 (	Lock Gain	109.671
PULPROG	zgpr	Lock DC	-70.000
TD	19090	Lock Shift	4.700
SOLVENT	H2O+D2O	Loop Gain	-5.000
NS	8	Loop Time	0.350
DS	4	Loop Filter	100.000
SWH	9090.909 Hz	Gas Flow	external
FIDRES	0.952426 Hz		
AQ	1.0499500 sec		
RG	101		
DW	55.000 usec		
DE	6.50 usec		
TE	298.0 K		
D1	5.00000000 sec		
D12	0.00002000 sec		
TD0	1		
SFO1	750.3035247 MHz		
NUC1	1H		
P1	8.00 usec		
PLW1	13.02900028 W		
PLW9	0.00003335 W		

F2 - Processing parameters  
 SI 32768  
 SF 750.2999442 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.10

SHIM SEQUENCE  
 - topshim hrmas <pass>

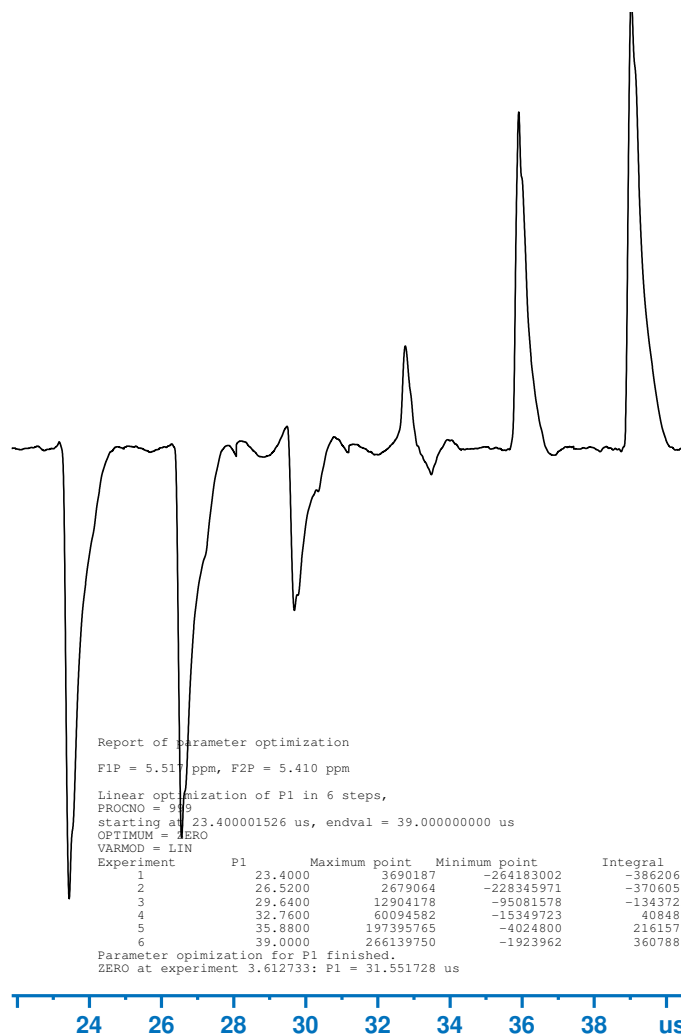
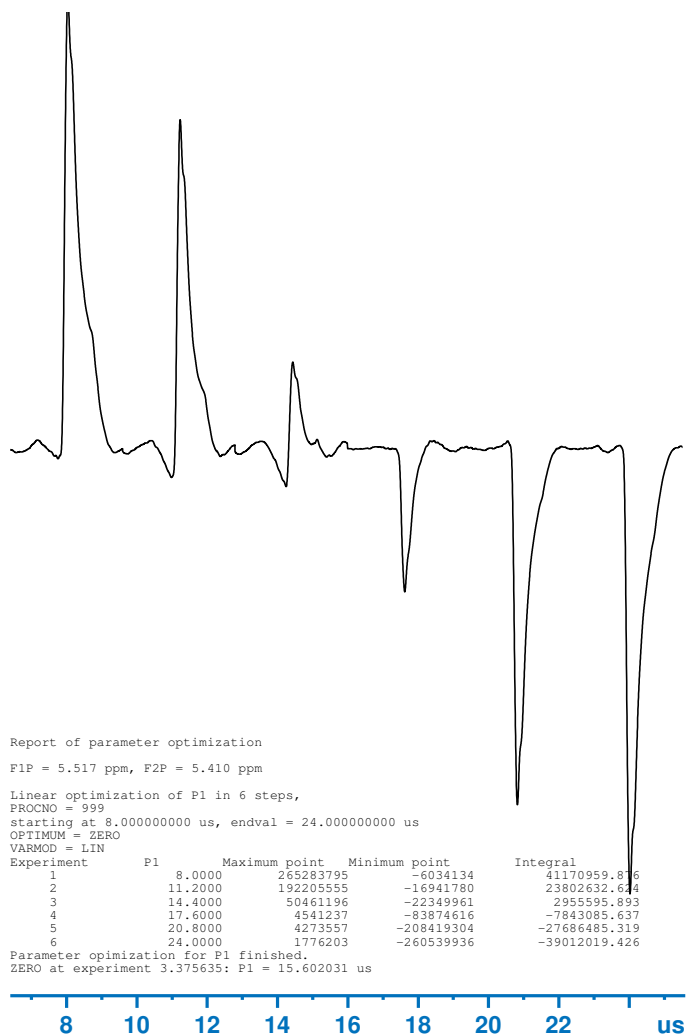
NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (50 ul) (Z142223)  
 P90 1H pulse calibration (NPT\_1H\_p90determinationf1\_1h, spin rate 4000 Hz)  
 Result: [180/2] = 7.8 us @ 13.7 W [360] = 31.6 us ==> [PDelay = 2\*180 - 360] = -0.4 us  
 ATTENTION: Updated PROSOL Tables with [8.0 us @ 13.0 W]  
 Deviation from pulse target value (= 8.0 us): -2.5%



Bruker BioSpin

P90 1H pulse [achieved/rated]: @ 13.7 W [7.8 us <= 8.0 us] <pass>

## NPT\_1H\_p90determinationf1\_1h



Current Data Parameters  
 NAME NPT\_1H\_p90determinationf1\_1h  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230809  
 Time 17.35 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 ( )  
 PULPROG zg  
 TD 300  
 SOLVENT DMSO  
 NS 1  
 DS 0  
 SWH 230.766 Hz  
 FIDRES 1.538438 Hz  
 AQ 0.6500100 sec  
 RG 45.2  
 DW 2166.700 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.45500004 sec  
 TD0 1  
 SF01 750.3040994 MHz  
 NUC1 1H  
 P1 39.00 usec  
 PLW1 13.70538998 W

Additional Parameters  
 Field 1914.539  
 Lock Phase 333.500  
 Lock Power -19.000  
 Lock Gain 98.000  
 Lock DC -70.000  
 Lock Shift 2.490  
 Loop Gain 5.000  
 Loop Time 0.250  
 Loop Filter 500.000  
 Gas Flow external

F2 - Processing parameters  
 SI 2048  
 SF 750.3000000 MHz  
 WDW SINE  
 SSB 2  
 LB 0 Hz  
 GB 0  
 PC 1.00

\*\*\*\*\* P90 Pulse Determination History \*\*\*\*\*  
 PLW90 P90 P90[det] Deviation  
 -----  
 8.81 W 10.0 us 7.6 us -5.0%  
 14.4 W 8.0 us 7.8 us -2.5%  
 13.7 W 8.0 us 7.8 us -2.5%

-----  
 SHIM SEQUENCE  
 - topshim hrmas <pass>  
 -----



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 0.1% Ethylbenzene (EB) in Chloroform-D (50 ul) (Z142221)  
 1H sensitivity (NPT\_1H\_sensitivity, spin rate 4000 Hz)

SINO (2.0 ppm) [achieved]: Signal (3.00 to 2.00 ppm), Noise (5.34 to 3.34 ppm) [260.4] <n/a>  
 SINO (200.0 Hz) [achieved/rated]: Signal (3.00 to 2.00 ppm), Noise (6.47 to 6.20 ppm) [309.8 >= 110.0] <pass>



Bruker BioSpin

# NPT\_1H\_sensitivity

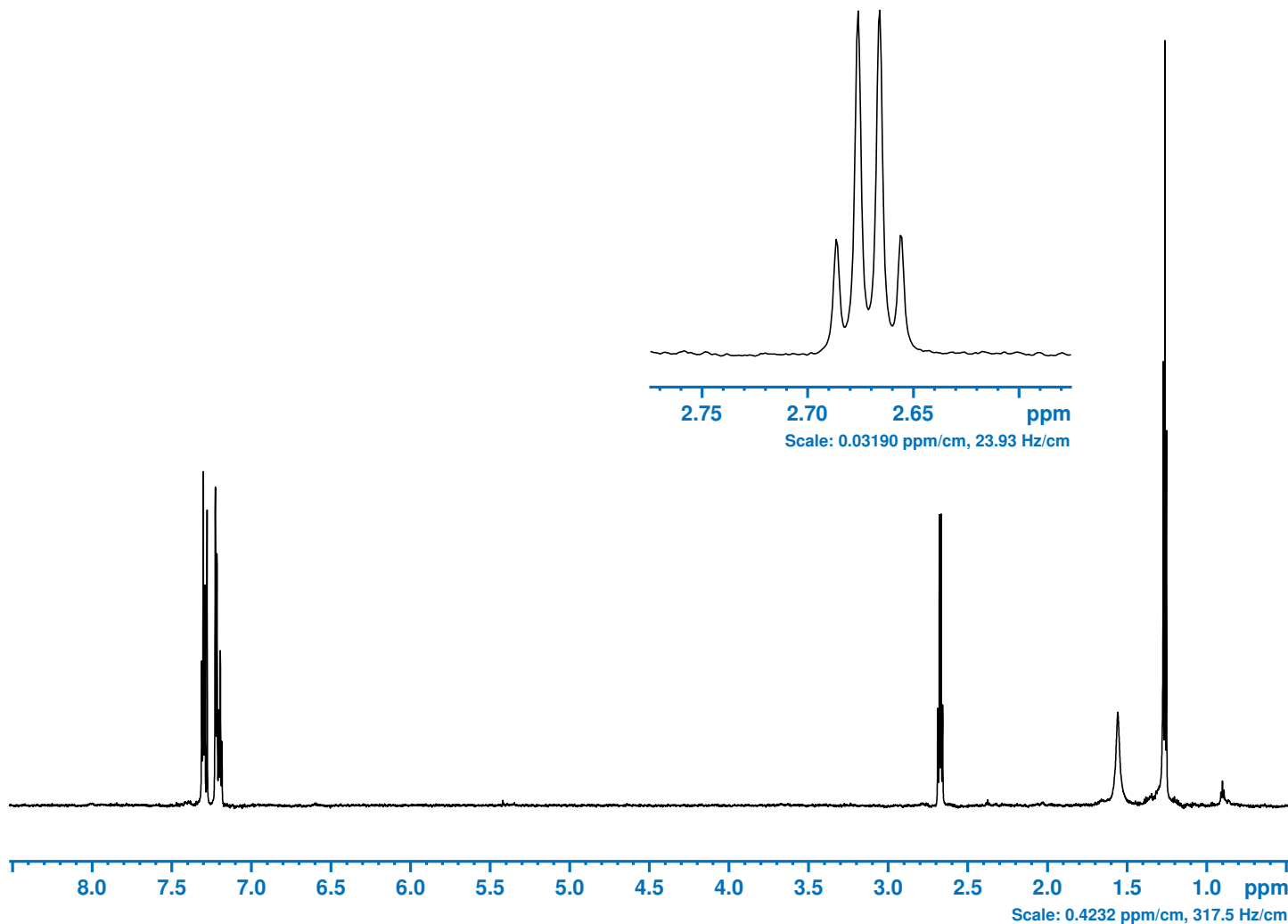
Current Data Parameters  
 NAME NPT\_1H\_sensitivity  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230810  
 Time 17.05 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 ( 2g  
 PULPROG 32768  
 TD 1  
 SOLVENT CDC13  
 NS 1  
 DS 0  
 SWH 7462.687 Hz  
 FIDRES 0.455496 Hz  
 AQ 2.1954560 sec  
 RG 101  
 DW 67.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 113.57360077 sec  
 D10 1  
 SFO1 750.3030012 MHz  
 NUC1 1H  
 P1 8.00 usec  
 PLW1 13.02900028 W

Additional Parameters  
 Field 1373.990  
 Lock Phase 349.000  
 Lock Power -27.000  
 Lock Gain 111.057  
 Lock DC -70.000  
 Lock Shift 7.240  
 Loop Gain -12.000  
 Loop Time 0.400  
 Loop Filter 100.000  
 Gas Flow external

F2 - Processing parameters  
 SI 16384  
 SF 750.3000060 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

SHIM SEQUENCE  
 - topshim hrmas <pass>



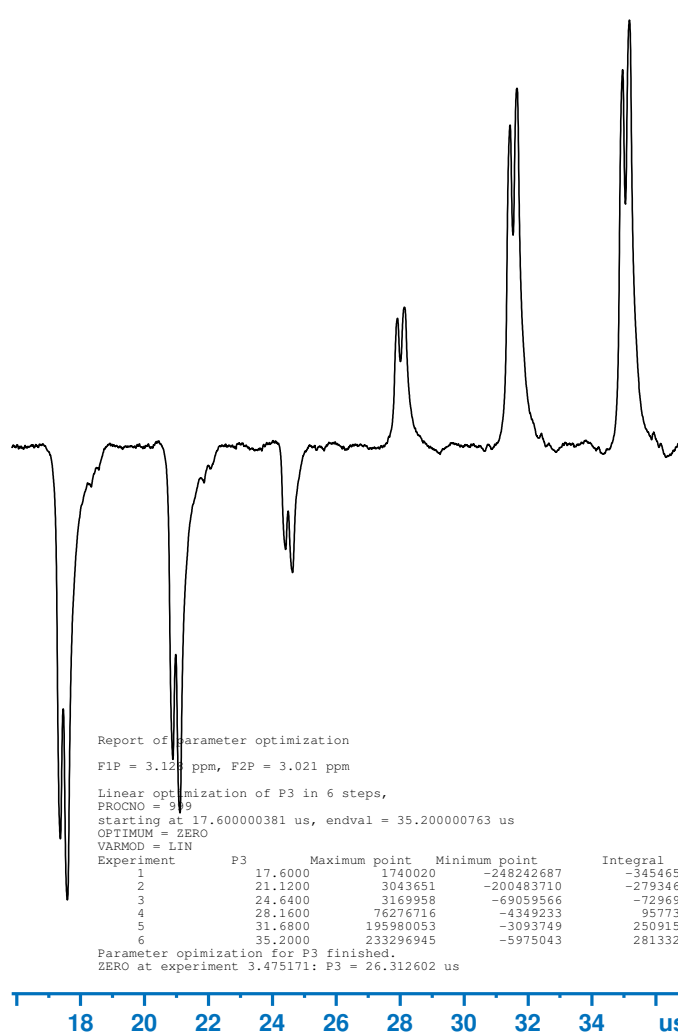
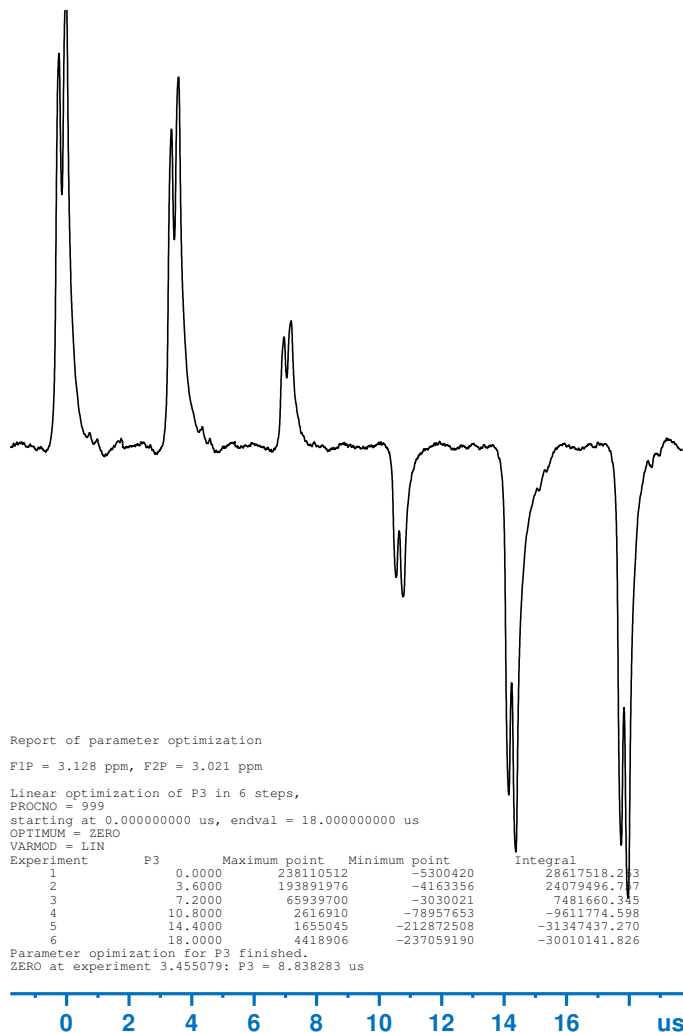
NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (50 ul) (Z142223)  
 Indirect P90 13C pulse calibration (NPT\_1H\_p90determinationf2\_13c, spin rate 4000 Hz)  
 Result: [90] = 8.8 us @ 81.4 W [270] = 26.3 us ==> [PDelay = 3\*90 - 270] = 0.1 us  
 ATTENTION: Updated PROSOL Tables with [9.0 us @ 77.8 W]  
 Deviation from pulse target value (= 9.0 us): -2.2%



Bruker BioSpin

P90 13C pulse [achieved/rated]: @ 81.4 W [8.8 us <= 9.0 us] <pass>

## NPT\_1H\_p90determinationf2\_13c



Current Data Parameters  
 NAME NPT\_1H\_p90determinationf2\_13c  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230809  
 Time 18.07 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 ( )  
 PULPROG decp90  
 TD 1000  
 SOLVENT DMSO  
 NS 1  
 DS 0  
 SWH 230.766 Hz  
 FIDRES 0.461531 Hz  
 AQ 2.1666999 sec  
 RG 32  
 DW 2166.700 usec  
 DE 6.50 usec  
 TE 298.0 K  
 CNST2 139.0000000  
 D1 2.56970811 sec  
 D2 0.00359712 sec  
 TD0 1  
 SFO1 750.3023069 MHz  
 NUC1 1H  
 P1 4.00 usec  
 PLW1 13.02900028 W  
 SFO2 188.6724116 MHz  
 NUC2 13C  
 P3 35.20 usec  
 PLW2 81.3718380 W

Additional Parameters  
 Field 1915.368  
 Lock Phase 16.500  
 Lock Power -19.000  
 Lock Gain 98.524  
 Lock DC -70.000  
 Lock Shift 2.490  
 Loop Gain 5.000  
 Loop Time 0.250  
 Loop Filter 500.000  
 Gas Flow external

F2 - Processing parameters  
 SI 2048  
 SF 750.3000000 MHz  
 WDW EM  
 SSB 0  
 LB 0.50 Hz  
 GB 0  
 FC 0.10

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

PLW90	P90	P90[det]	Deviation
80.0 W	9.0 us		
83.6 W	9.0 us	8.7 us	-3.3%
81.4 W	9.0 us	8.8 us	-2.2%

-----  
 SHIM SEQUENCE  
 -----  
 - topshim hrmas <pass>  
 -----

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 40% Dioxane in Benzene-D6 (ASTM, 50 ul) (Z142224)  
 13C sensitivity (NPT\_13C\_sensitivity, spin rate 4000 Hz)

SINO (40.0 ppm) [achieved/rated]: Signal (127.61 ppm), Noise (121.89 to 81.89 ppm) [76.4 >= 35.0] <pass>



Bruker BioSpin

### NPT\_13C\_sensitivity

Current Data Parameters  
 NAME NPT\_13C\_sensitivity  
 EXPNO 1  
 PROCNO 1

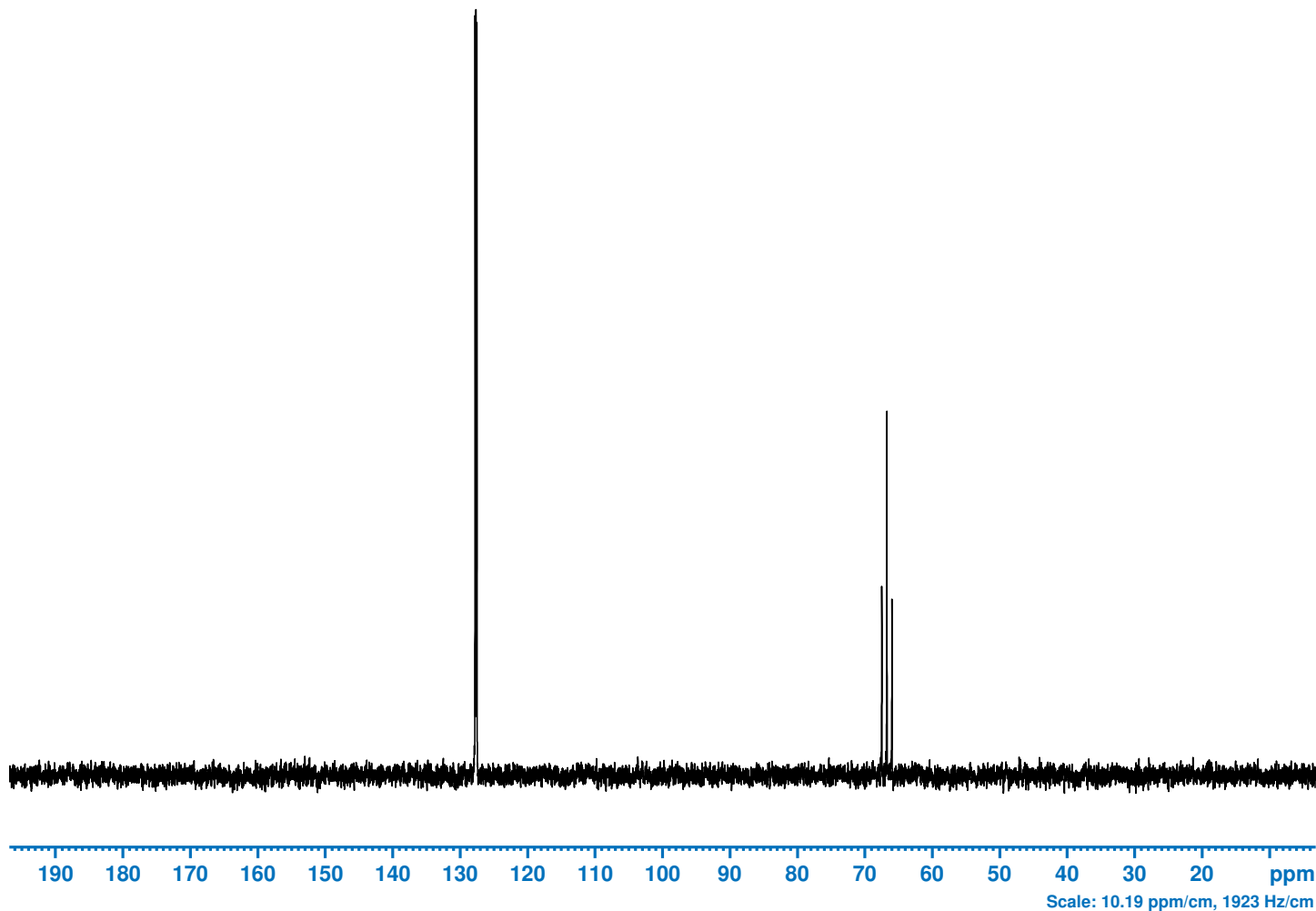
F2 - Acquisition Parameters  
 Date\_ 20230810  
 Time 17.32 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 (   
 PULPROG zg  
 TD 65536  
 SOLVENT C6D6  
 NS 1  
 DS 0  
 SWH 38461.538 Hz  
 FIDRES 1.173753 Hz  
 AQ 0.8519680 sec  
 RG 101  
 DW 13.000 usec  
 DE 7.27 usec  
 TE 298.0 K  
 D1 829.14801025 sec  
 TD0 1  
 SFO1 188.6819490 MHz  
 NUC1 13C  
 P1 9.00 usec  
 PLW1 77.79499817 W

Additional Parameters  
 Field 1354.501  
 Lock Phase 349.000  
 Lock Power -24.000  
 Lock Gain 102.288  
 Lock DC -70.000  
 Lock Shift 7.160  
 Loop Gain -0.000  
 Loop Time 0.200  
 Loop Filter 300.000  
 Gas Flow external

F2 - Processing parameters  
 SI 131072  
 SF 188.6630851 MHz  
 WDW EM  
 SSB 0  
 LB 3.50 Hz  
 GB 0  
 PC 1.40

-----  
 SHIM SEQUENCE

-----  
 - topshim hrmas <pass>  
 -----



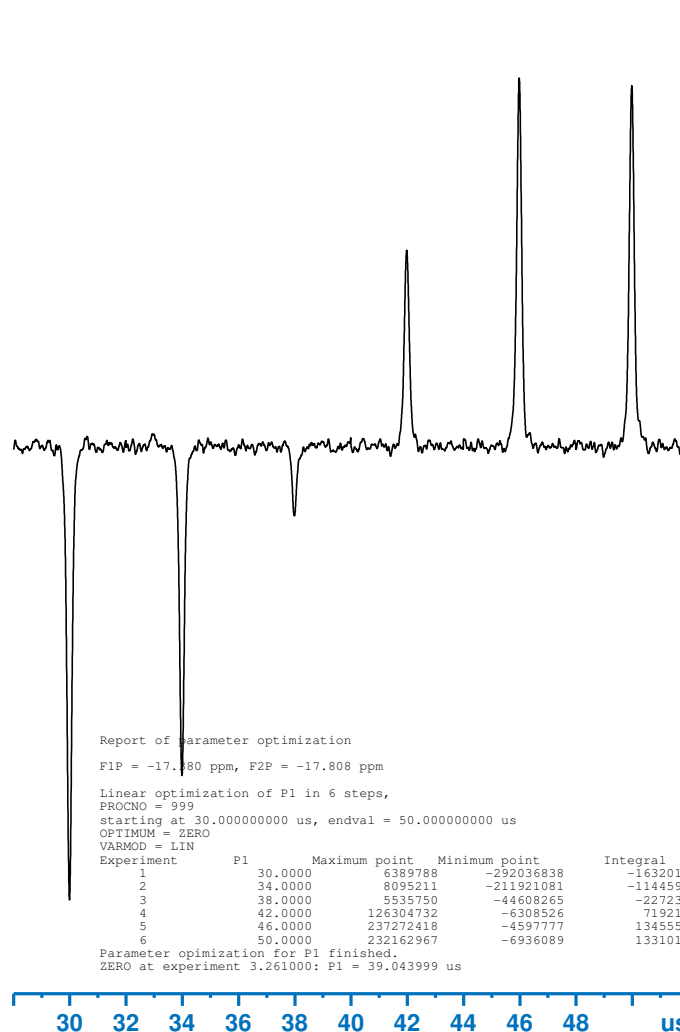
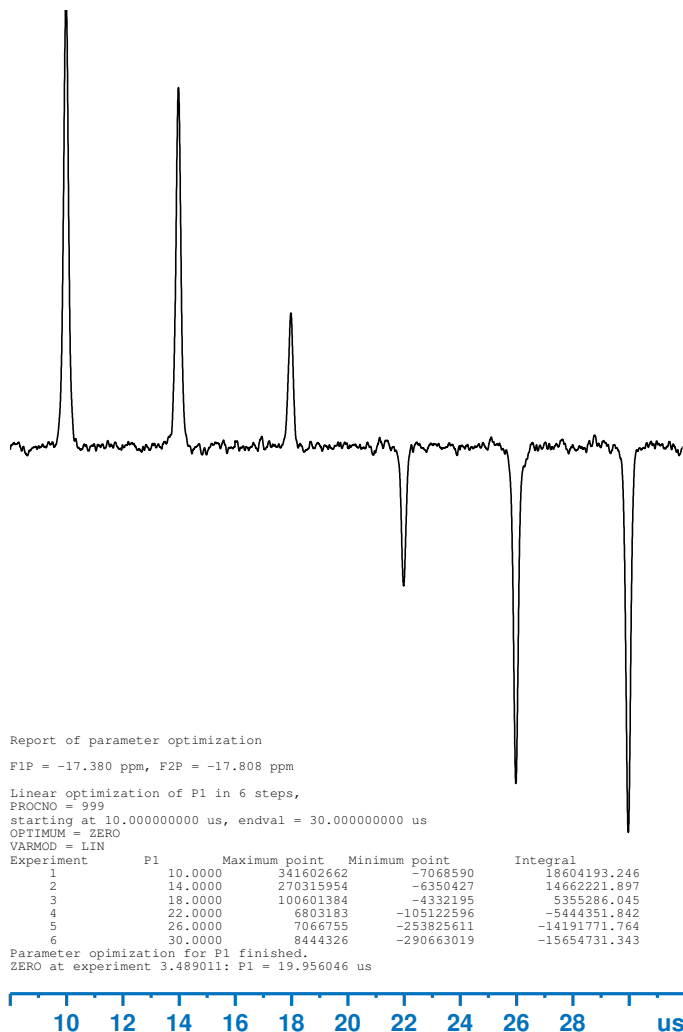
NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 0.0485 M Triphenyl Phosphate (TPP, [C6H5]3PO4) in Acetone-D6 (50 ul) (Z142226)  
 P90 31P pulse calibration (NPT\_31P\_p90determinationf1\_31p, spin rate 4000 Hz)  
 Result: [180/2] = 10.0 us @ 52.2 W [360] = 39.0 us ==> [PDelay = 2\*180 - 360] = 1.0 us  
 ATTENTION: Updated PROSOL Tables with [10.0 us @ 52.2 W]  
 Deviation from pulse target value (= 10.0 us): 0.0%



Bruker BioSpin

P90 31P pulse [achieved/rated]: @ 52.2 W [10.0 us <= 10.0 us] <pass>

## NPT\_31P\_p90determinationf1\_31p



Current Data Parameters  
 NAME NPT\_31P\_p90determinationf1\_31p  
 EXPNO 3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230810  
 Time 18.09 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 ( )  
 PULPROG zg  
 TD 1000  
 SOLVENT Acetone  
 NS 1  
 DS 0  
 SWH 396.825 Hz  
 FIDRES 0.793651 Hz  
 AQ 1.2600000 sec  
 RG 101  
 DW 1260.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 17.64999962 sec  
 TD0 1  
 SFO1 303.7216633 MHz  
 NUC1 31P  
 P1 50.00 usec  
 PLW1 52.25000000 W

Additional Parameters  
 Field 1357.895  
 Lock Phase 349.000  
 Lock Power -34.000  
 Lock Gain 97.891  
 Lock DC -70.000  
 Lock Shift 2.040  
 Loop Gain -2.000  
 Loop Time 0.100  
 Loop Filter 200.000  
 Gas Flow external

F2 - Processing parameters  
 SI 4096  
 SF 303.7270072 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 1.00

\*\*\*\*\* P90 Pulse Determination History \*\*\*\*\*  
 PLW90 P90 P90[det] Deviation  
 50.0 W 10.0 us  
 52.2 W 10.0 us 10.0 us 0.0%

-----  
 SHIM SEQUENCE  
 - topshim hrmas <pass>  
 -----

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 0.0485 M Triphenyl Phosphate (TPP, [C<sub>6</sub>H<sub>5</sub>]<sub>3</sub>PO<sub>4</sub>) in Acetone-D<sub>6</sub> (50 ul) (Z142226)  
 31P sensitivity (NPT\_31P\_sensitivity, spin rate 4000 Hz)

SINO (5.0 ppm) [achieved/rated]: Signal (-17.59 ppm), Noise (1.69 to -3.32 ppm) [74.2 >= 30.0] <pass>



Bruker BioSpin

### NPT\_31P\_sensitivity

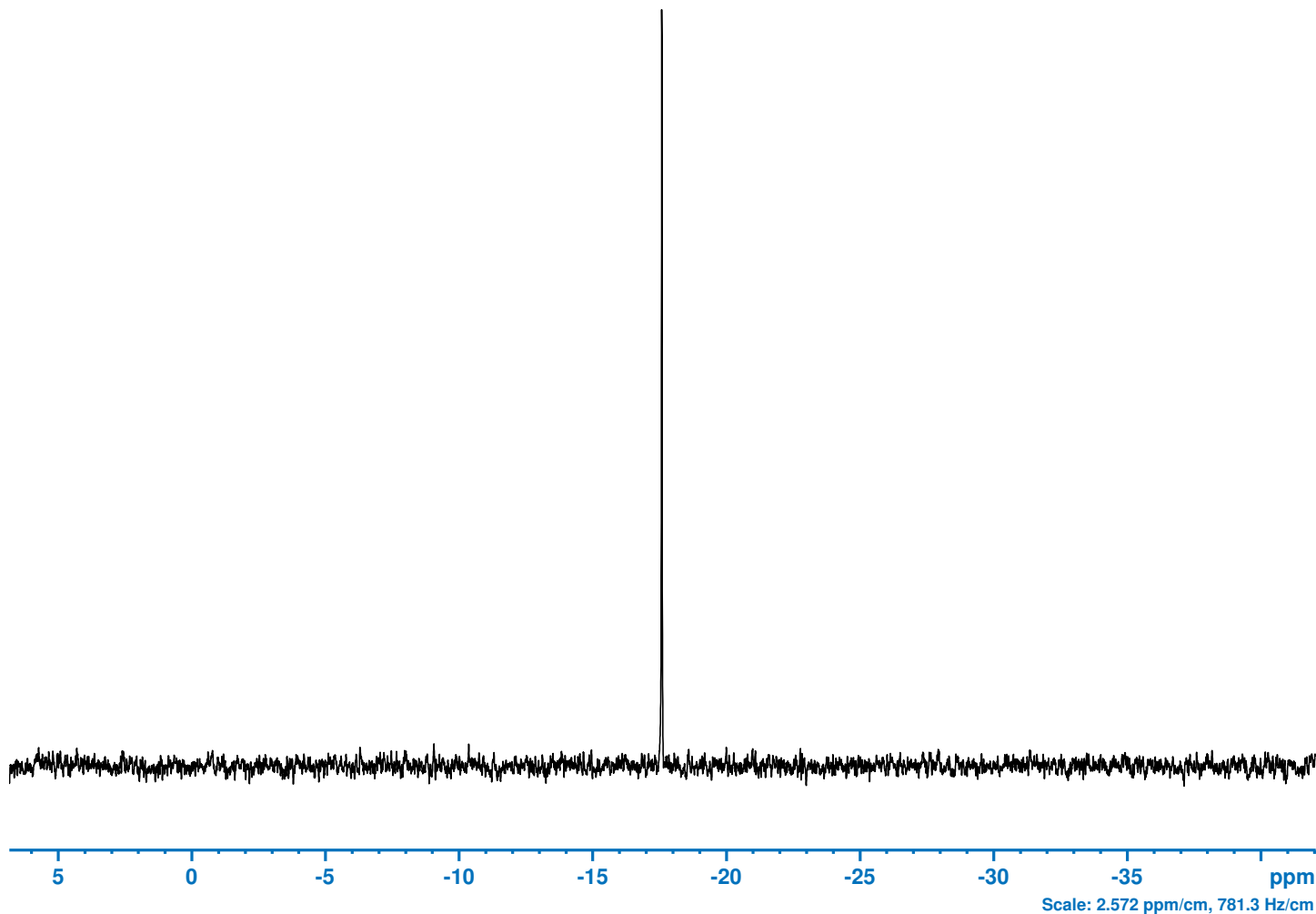
Current Data Parameters  
 NAME NPT\_31P\_sensitivity  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230810  
 Time 18.30 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 (   
 PULPROG zg  
 TD 32768  
 SOLVENT Acetone  
 NS 1  
 DS 0  
 SWH 15625.000 Hz  
 FIDRES 0.953674 Hz  
 AQ 1.0485760 sec  
 RG 101  
 DW 32.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 119.95140076 sec  
 TD0 1  
 SF01 303.7216590 MHz  
 NUC1 31P  
 P1 10.00 usec  
 PLW1 52.25000000 W

Additional Parameters  
 Field 1356.703  
 Lock Phase 349.000  
 Lock Power -34.000  
 Lock Gain 96.782  
 Lock DC -70.000  
 Lock Shift 2.040  
 Loop Gain -2.000  
 Loop Time 0.100  
 Loop Filter 200.000  
 Gas Flow external

F2 - Processing parameters  
 SI 16384  
 SF 303.7270072 MHz  
 WDW EM  
 SSB 0  
 LB 5.00 Hz  
 GB 0  
 PC 1.40

SHIM SEQUENCE  
 - topshim hrmas <pass>



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 0.0485 M Triphenyl Phosphate (TPP, [C<sub>6</sub>H<sub>5</sub>]<sub>3</sub>PO<sub>4</sub>) in Acetone-D<sub>6</sub> (50 µl) (Z142226)  
 31P sensitivity with 1H decoupling (NPT\_31P\_sensitivity\_dec1h, spin rate 4000 Hz)

SINO (5.0 ppm) [achieved]: Signal (-17.59 ppm), Noise (-0.50 to -5.50 ppm) [94.1] <n/a>

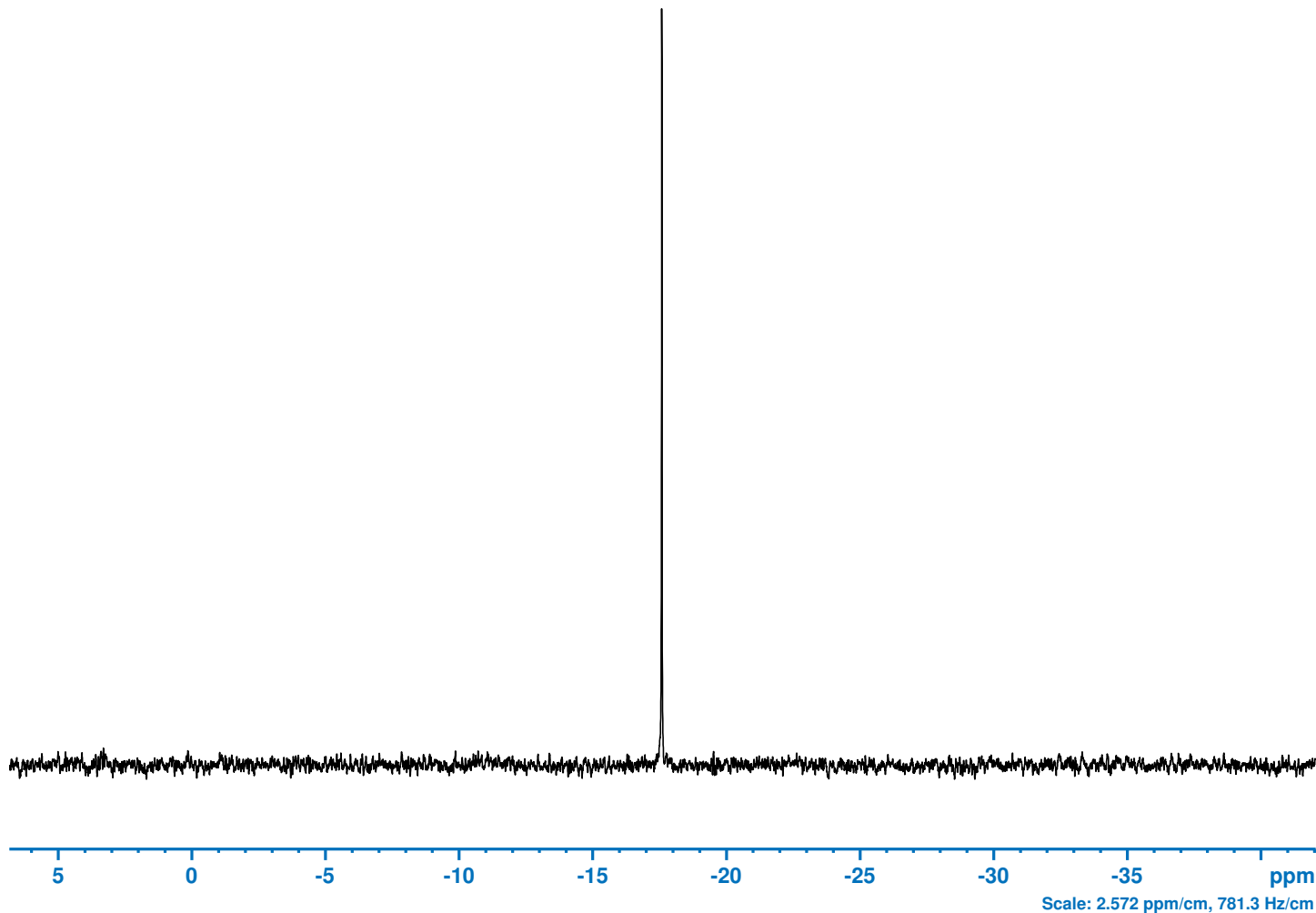


Bruker BioSpin

# NPT\_31P\_sensitivity\_dec1h

Current Data Parameters		Additional Parameters	
NAME	NPT_31P_sensitivity_dec1h	Field	1357.003
EXPNO	1	Lock Phase	349.000
PROCNO	1	Lock Power	-34.000
F2 - Acquisition Parameters		Lock Gain	97.846
Date_	20230810	Lock DC	-70.000
Time	18.19 h	Lock Shift	2.040
INSTRUM	Avance NEO	Loop Gain	-2.000
PROBHD	Z180004_0001 (	Loop Time	0.100
PULPROG	zgig	Loop Filter	200.000
TD	32768	Gas Flow	external
SOLVENT	Acetone		
NS	1		
DS	0		
SWH	15625.000 Hz		
FIDRES	0.953674 Hz		
AQ	1.0485760 sec		
RG	101		
DW	32.000 usec		
DE	6.50 usec		
TE	298.0 K		
D1	119.95140076 sec		
D11	0.03000000 sec		
TD0	1		
SFO1	303.7216590 MHz		
NUC1	31P		
P1	10.00 usec		
PLW1	52.25000000 W		
SFO2	750.3037515 MHz		
NUC2	1H		
CPDPRG2	waltz64		
PCPD2	60.00 usec		
PLW2	13.02900028 W		
PLW12	0.23162000 W		
F2 - Processing parameters			
SI	16384		
SF	303.7270072 MHz		
WDW	EM		
SSB	0		
LB	5.00 Hz		
GB	0		
PC	1.40		

SHIM SEQUENCE  
 - topshim hrmas <pass>



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (50 ul) (Z142223)  
 P90 2H pulse calibration (NPT\_prep\_p90det\_d, spin rate 4000 Hz)  
 Result: [180/2] = 87.9 us @ 2.77 W [360] = 350.8 us ==> [PDelay = 2\*180 - 360] = 0.8 us  
 ATTENTION: Updated PROSOL Tables with [90.0 us @ 2.64 W]  
 Deviation from pulse target value (= 90.0 us): -2.3%

P90 2H pulse [achieved/rated]: @ 2.77 W [87.9 us <= 90.0 us] <pass>



Bruker BioSpin

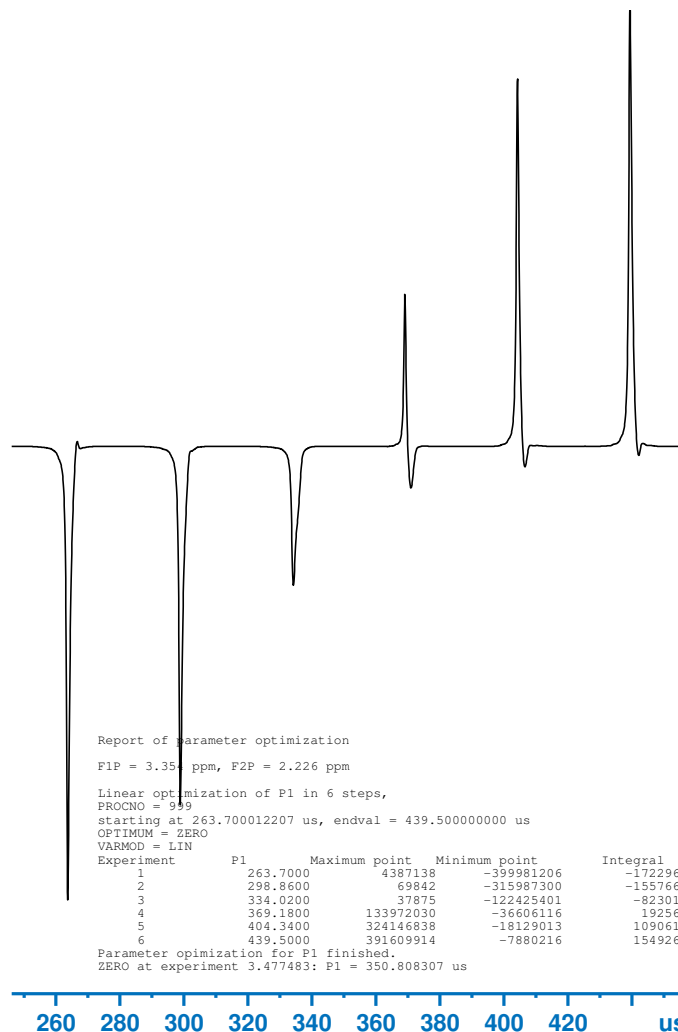
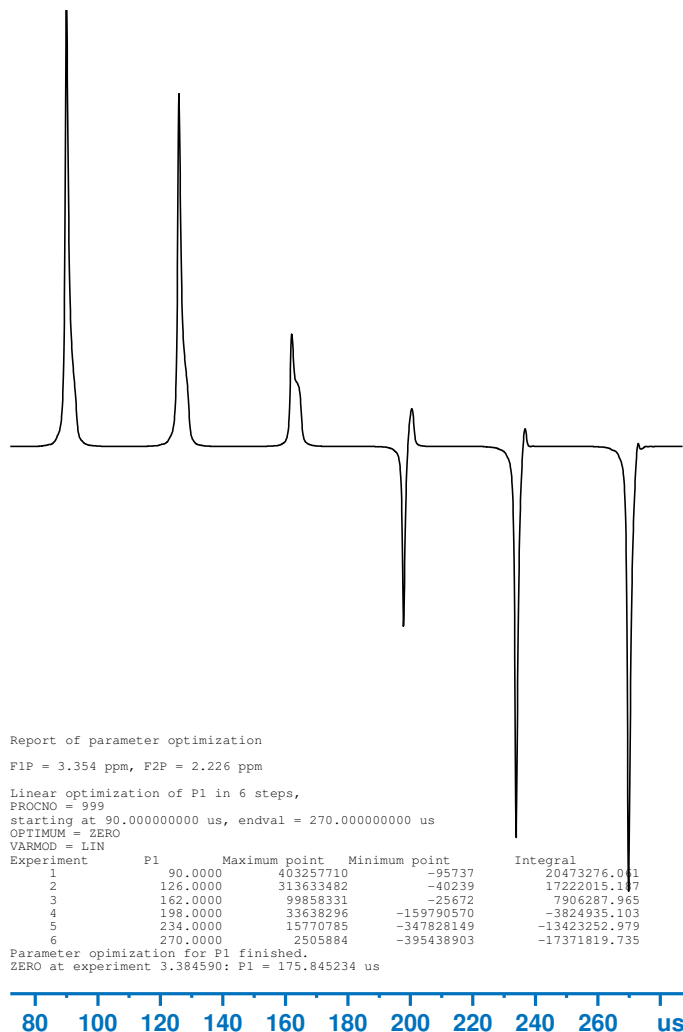
## NPT\_prep\_p90det\_d

Current Data Parameters  
 NAME NPT\_prep\_p90det\_d  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230809  
 Time 17.11 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 ( )  
 PULPROG npt\_zg2h  
 TD 1024  
 SOLVENT DMSO  
 NS 1  
 DS 0  
 SWH 625.000 Hz  
 FIDRES 1.220703 Hz  
 AQ 0.8192000 sec  
 RG 4  
 DW 800.000 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 0.34999999 sec  
 D11 0.03000000 sec  
 D12 0.00010000 sec  
 TD0 1  
 SFO1 115.1759396 MHz  
 NUC1 2H  
 P1 439.50 usec  
 PLW1 2.77141809 W

Additional Parameters  
 Field 1869.083  
 Lock Phase 333.500  
 Lock Power -9.000  
 Lock Gain 119.900  
 Lock DC -70.000  
 Lock Shift 2.490  
 Loop Gain 5.000  
 Loop Time 0.250  
 Loop Filter 500.000  
 Gas Flow external

F2 - Processing parameters  
 SI 2048  
 SF 115.1756183 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 1.00



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

PLW90	P90	P90[det]	Deviation
3.00 W	90.0 us		
3.13 W	90.0 us	83.8 us	-6.9%
2.84 W	90.0 us	86.9 us	-3.4%
2.77 W	90.0 us	87.9 us	-2.3%

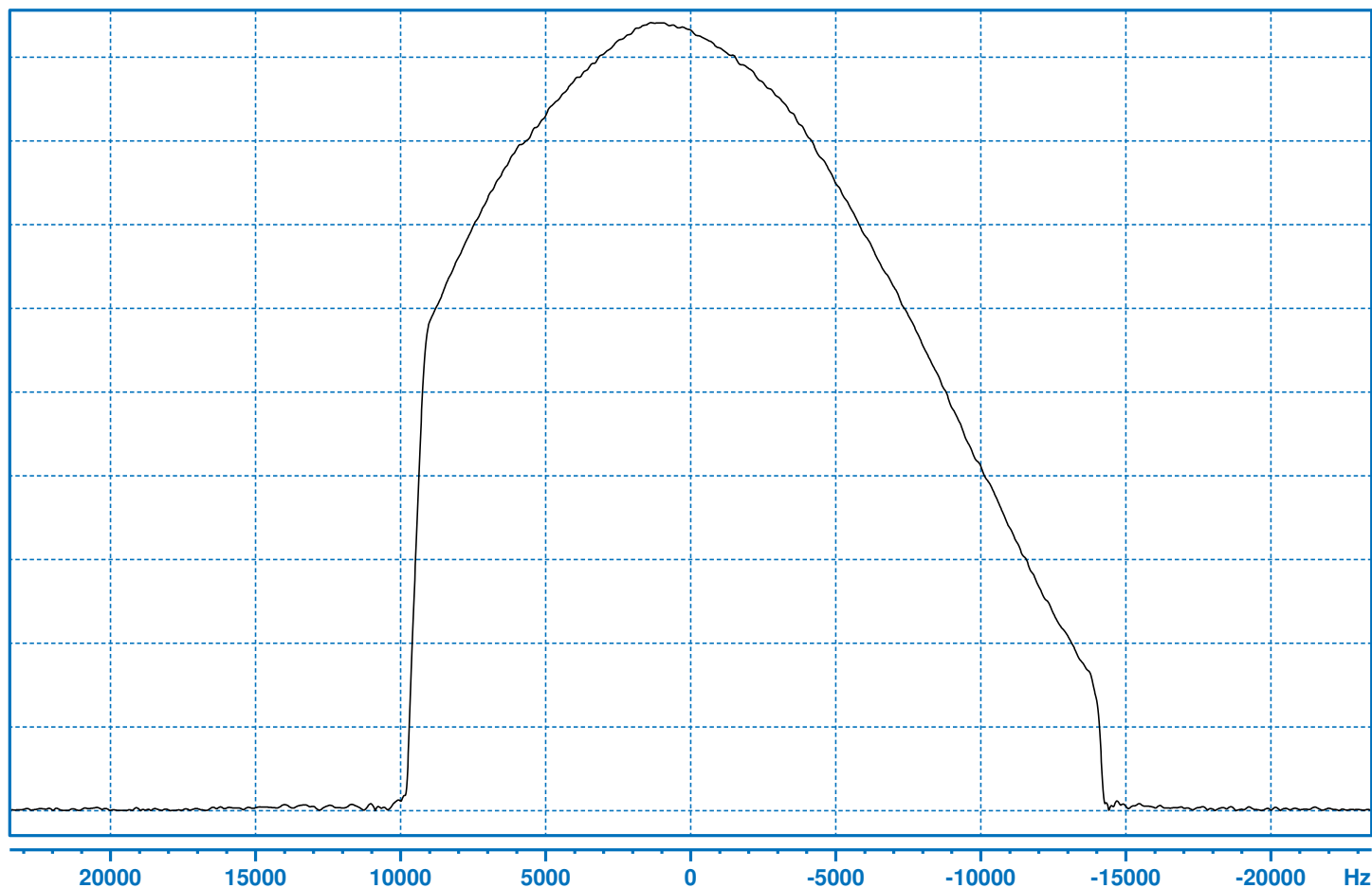
SHIM SEQUENCE  
 skip shimming

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 2 mM Sucrose, 0.5 mM DSS, 2 mM NaN3 in 90% H2O + 10% D2O (50 ul) (Z142222)  
 1H Z-gradient profile [-] (NPT\_1H\_gradientprofile\_neg, spin rate 4000 Hz)  
 Gradient amplifier: Internal gradient amplifier



Bruker BioSpin

## NPT\_1H\_gradientprofile\_neg



```
Current Data Parameters
NAME      NPT_1H_gradientprofile_neg
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20230810
Time      19.11 h
INSTRUM   Avance NEO
PROBHD    Z180004_0001 (
PULPROG   npt_imgcgpld
TD        1024
SOLVENT   H2O+D2O
NS        1
DS        0
SWH        81967.213 Hz
FIDRES     160.092209 Hz
AQ         0.0062464 sec
RG         45.2
DW         6.100 usec
DE         6.50 usec
TE         298.0 K
D1         0.50000000 sec
D11        0.03000000 sec
D15        0.00500000 sec
D21        0.00025000 sec
D27        0.00200000 sec
SFO1       750.3035264 MHz
NUC1       1H
FO         2.00 usec
PLW0       0.64340752 W
PLW1       13.02900028 W
GPZ1       -11.00 %
GPZ2       13.75 %

Additional Parameters
Field      1377.531
Lock Phase 350.500
Lock Power -18.000
Lock Gain  109.871
Lock DC    -70.000
Lock Shift 4.700
Loop Gain  -5.000
Loop Time  0.350
Loop Filter 100.000
Gas Flow   external

F2 - Processing parameters
SI         4096
SF         750.3035264 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0
PC         1.00
```

```
SHIM SEQUENCE
- topshim hrmas <pass>
```



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: 2 mM Sucrose, 0.5 mM DSS, 2 mM NaN3 in 90% H2O + 10% D2O (50 ul) (Z142222)  
 1H Z-gradient profile [+] (NPT\_1H\_gradientprofile\_pos, spin rate 4000 Hz)  
 Gradient amplifier: Internal gradient amplifier



Bruker BioSpin

## NPT\_1H\_gradientprofile\_pos

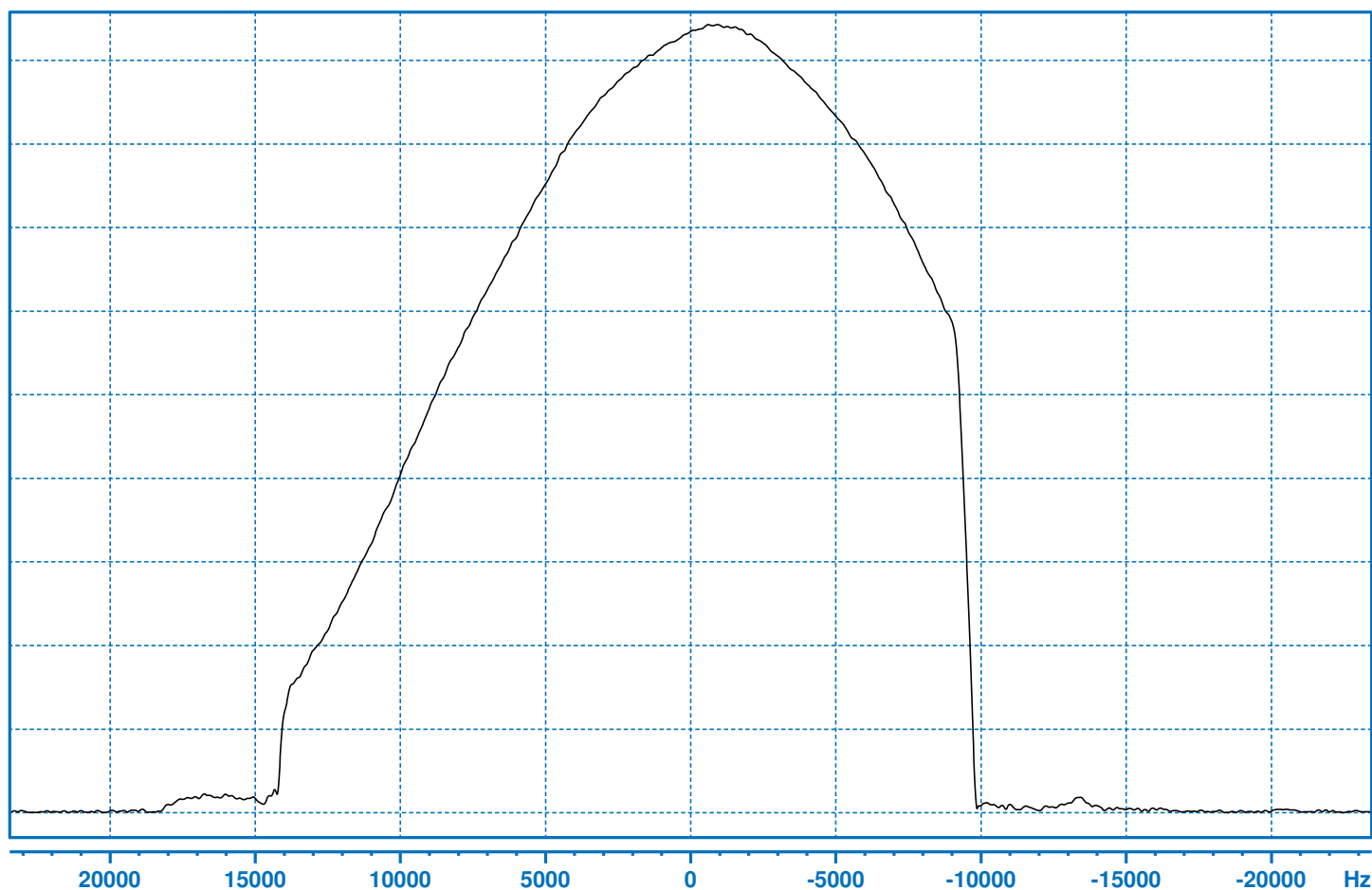
Current Data Parameters  
 NAME NPT\_1H\_gradientprofile\_pos  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230810  
 Time 19.16 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 ( )  
 PULPROG npt\_imgcgld  
 TD 1024  
 SOLVENT H2O+D2O  
 NS 1  
 DS 0  
 SWH 81967.213 Hz  
 FIDRES 160.092209 Hz  
 AQ 0.0062464 sec  
 RG 45.2  
 DW 6.100 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 0.50000000 sec  
 D11 0.03000000 sec  
 D15 0.00500000 sec  
 D21 0.00025000 sec  
 D27 0.00200000 sec  
 SFO1 750.3035264 MHz  
 NUC1 1H  
 P0 2.00 usec  
 PLW0 0.64340752 W  
 PLW1 13.02900028 W  
 GPZ1 11.00 %  
 GPZ2 -13.75 %

Additional Parameters  
 Field 1377.442  
 Lock Phase 350.500  
 Lock Power -18.000  
 Lock Gain 109.671  
 Lock DC -70.000  
 Lock Shift 4.700  
 Loop Gain -5.000  
 Loop Time 0.350  
 Loop Filter 100.000  
 Gas Flow external

F2 - Processing parameters  
 SI 4096  
 SF 750.3035264 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 FC 1.00

SHIM SEQUENCE  
 - topshim hrmas <pass>



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: Potassium Bromide (KBr, 80 ul) (Z151220)  
 P90 79Br pulse calibration, HRMAS (NPT\_79Br\_HRMAS\_p90det\_79br, spin rate 4000 Hz)  
 ATTENTION: Updated PROSOL Tables with [10.0 us @ 108.0 W].

P90 HRMAS 79Br pulse [achieved]: @ 108.0 W [10.0 us] <n/a>



Bruker BioSpin

## NPT\_79Br\_HRMAS\_p90det\_79br

Current Data Parameters  
 NAME NPT\_79Br\_HRMAS\_p90det\_79br  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20230809  
 Time 16.37 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001  
 PULPROG zg  
 TD 2048  
 SOLVENT None  
 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  
 TD0 1  
 SFO1 187.9912343 MHz  
 NUC1 79Br  
 P1 30.00 usec  
 PLW1 108.00000000 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
108.0 W	10.0 us		
108.0 W	10.0 us	10.0 us	0.0%

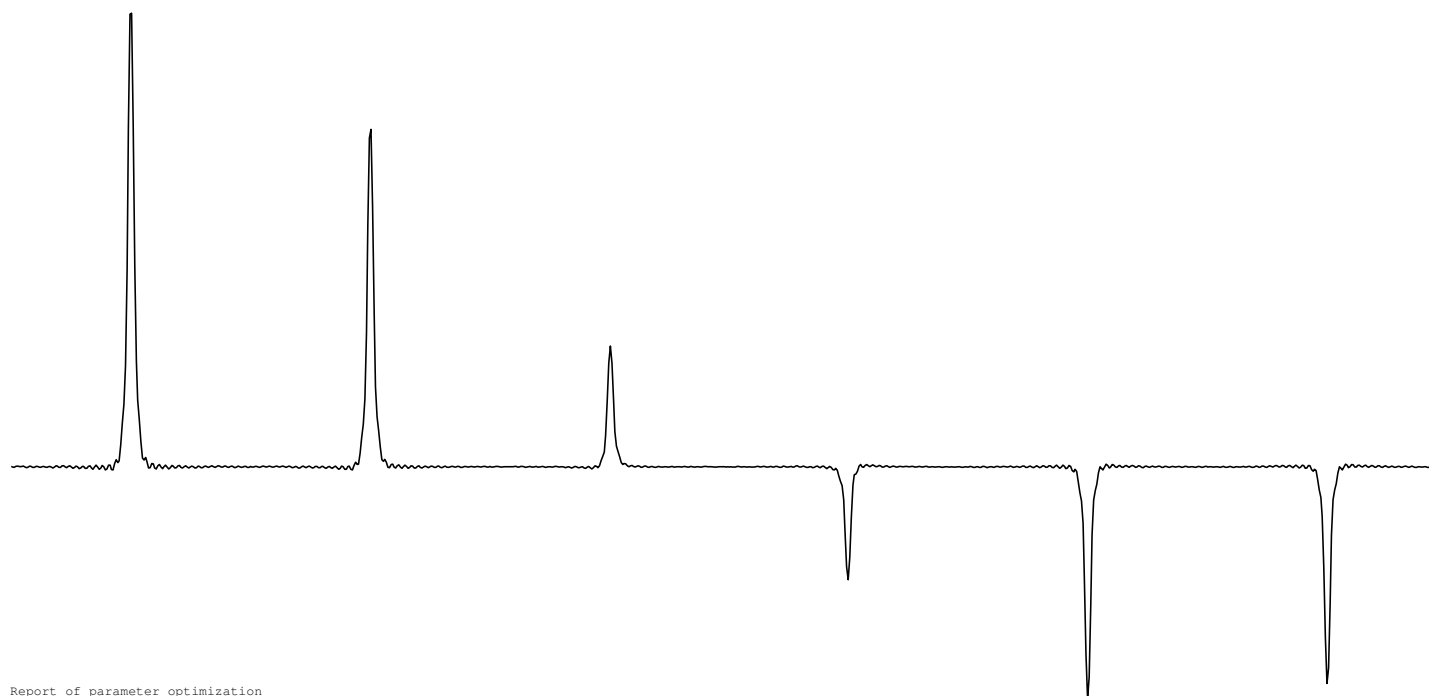
Report of parameter optimization

F1P = 69.700 ppm, F2P = 49.700 ppm

Linear optimization of P1 in 6 steps,  
 PROCNO = 999  
 Starting at 10.000000000 us, endval = 30.000000000 us  
 OPTIMUM = ZERO  
 VARMOD = LIN

Experiment	P1	Maximum point	Minimum point	Integral
1	10.0000	362155040	-2382118	12847406.890
2	14.0000	269352228	-2478240	9327234.813
3	18.0000	96433147	-1716709	3140714.013
4	22.0000	1800955	-90033554	-2717220.387
5	26.0000	2184246	-185408979	-6015542.774
6	30.0000	2083109	-172989409	-5576393.265

Parameter optimization for P1 finished.  
 ZERO at experiment 3.517160: P1 = 20.068641 us



SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)  
Magic Angle setting, HRMAS (NPT\_79Br\_HRMAS\_magicAngle, spin rate 4000 Hz)

Line width main [achieved/rated]: [101 <= 110] <pass>  
Line width of side band number 10 (@ -39999 Hz) [achieved/rated]: [115 <= 126] <pass>



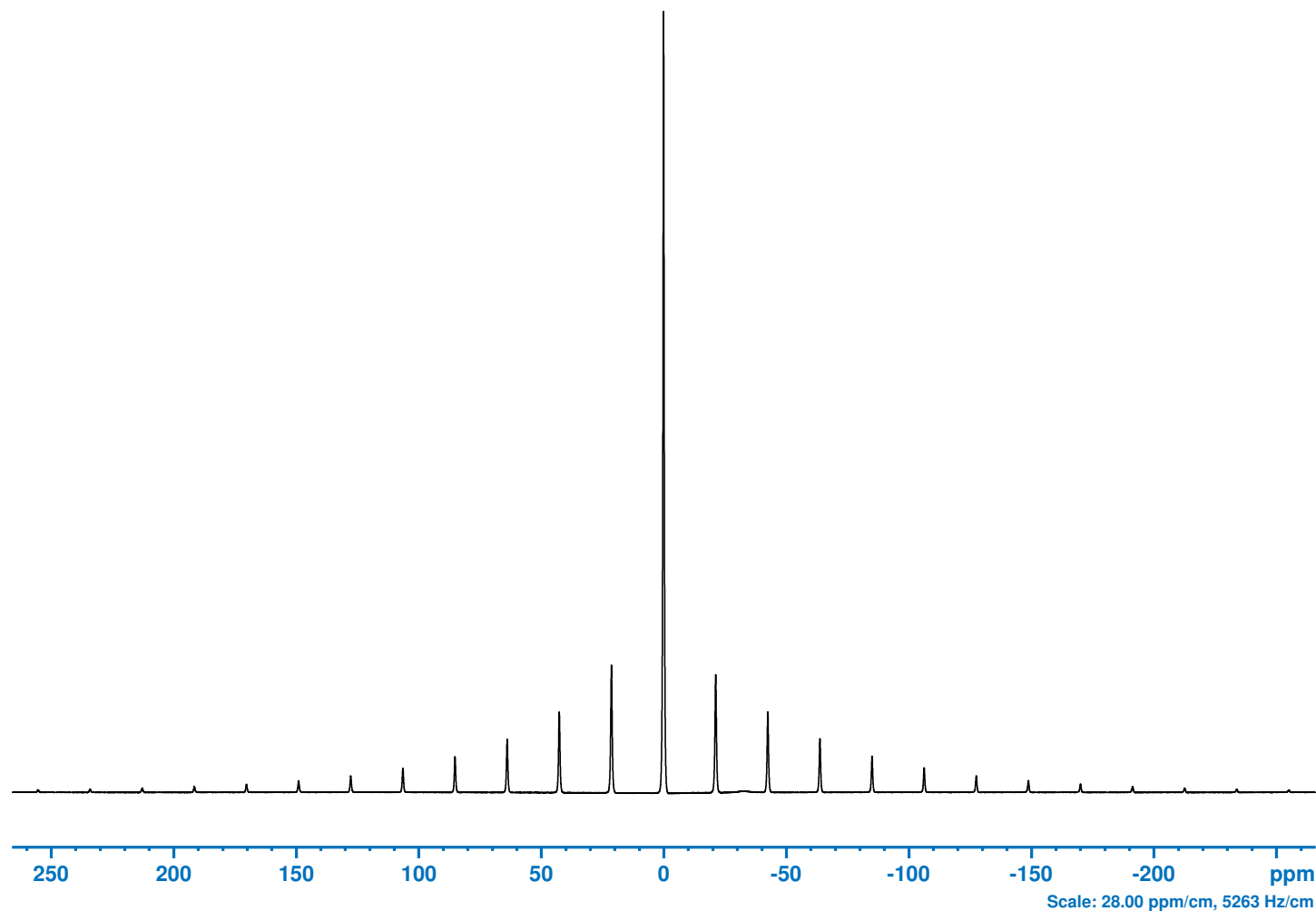
Bruker BioSpin

### NPT\_79Br\_HRMAS\_magicAngle

Current Data Parameters  
NAME NPT\_79Br\_HRMAS\_magicAngle  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20230809  
Time 16.44 h  
INSTRUM Avance NEO  
PROBHD Z180004\_0001 (   
PULPROG zg  
TD 8192  
SOLVENT None  
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  
TD0 1  
SFO1 187.9912229 MHz  
NUC1 79Br  
P1 10.00 usec  
PLW1 108.00000000 W

F2 - Processing parameters  
SI 131072  
SF 187.9912229 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 0.20



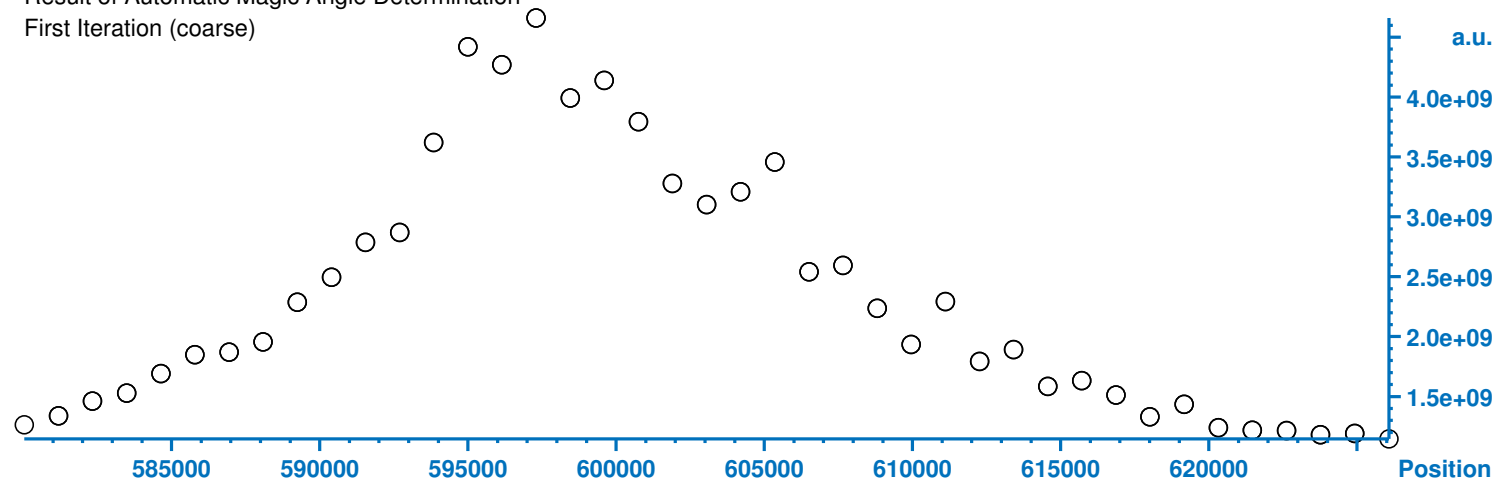
NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: Potassium Bromide (KBr, 80 ul) (Z151220)  
 Magic Angle setting, HRMAS (NPT\_79Br\_HRMAS\_magicAngle, spin rate 4000 Hz)



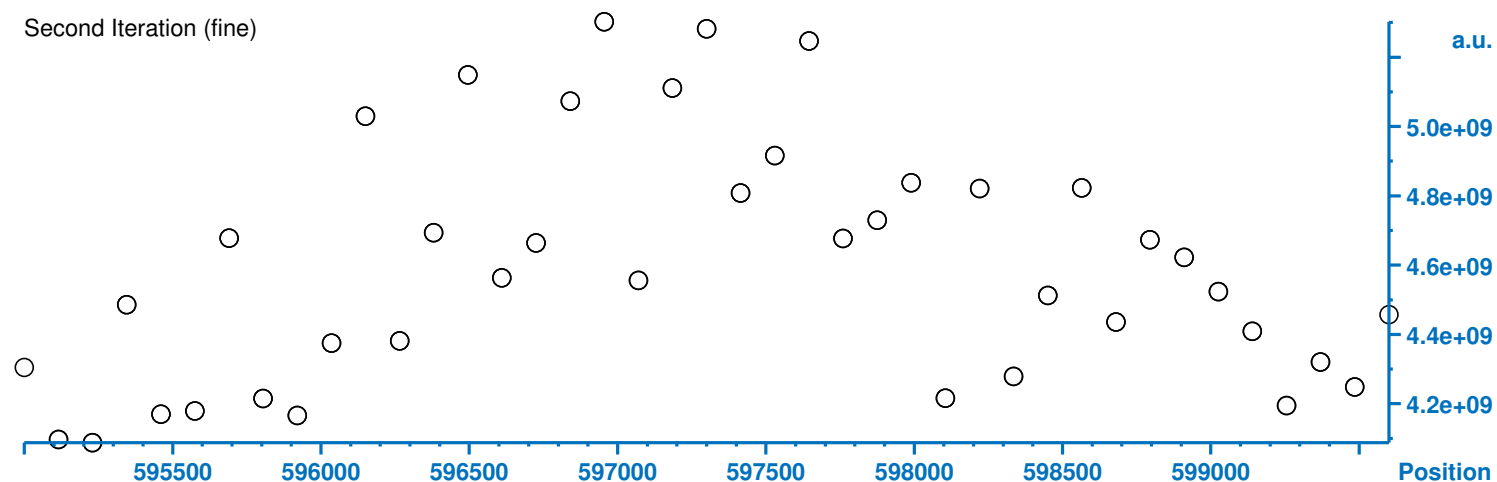
Bruker BioSpin

# NPT\_79Br\_HRMAS\_magicAngle

## Result of Automatic Magic Angle Determination First Iteration (coarse)



## Second Iteration (fine)



NMR TEST ACCEPTANCE \*\*\* System: AV NEO (750.30 MHz) \*\*\* TopSpin 4.3.0  
 Probe: Z180004\_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z  
 Sample: Potassium Bromide (KBr, 80 ul) (Z151220)  
 Maximum spin rate testing, HRMAS (NPT\_79Br\_HRMAS\_maxSpinRate, spin rate 15000 Hz)  
 Determination of spinning stability for 180 s  
 Pressure values in mbar: DrivePressure=2680/BearingPressure=3107/BearingSensePressure=3093/SupplyPressure=6790/SystemPressure=6051

Spin rate at maximum deviation [measured]: @ MASR 15000 Hz [14997 Hz]  
 Maximum deviation [achieved]: @ MASR 15000 Hz [3 Hz] <n/a>



Bruker BioSpin

# NPT\_79Br\_HRMAS\_maxSpinRate

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

F2 - Acquisition Parameters  
 Date\_ 20230809  
 Time 16.58 h  
 INSTRUM Avance NEO  
 PROBHD Z180004\_0001 (   
 PULPROG zg  
 TD 8192  
 SOLVENT None  
 NS 16  
 DS 0  
 SWH 200000.000 Hz  
 FIDRES 48.828125 Hz  
 AQ 0.0204800 sec  
 RG 101  
 DW 2.500 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 0.25000000 sec  
 TD0 1  
 SF01 187.9911488 MHz  
 NUC1 79Br  
 P1 10.00 usec  
 PLW1 108.00000000 W

F2 - Processing parameters  
 SI 16384  
 SF 187.9911488 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 0.20

