

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

750 MHz

Probe ID: Z180004_0001

Report Name: 2024-09-04

● 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 4.4.0
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, 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 ₃ in 90% H ₂ O + 10% D ₂ 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 ₆ H ₅] ₃ PO ₄) in Acetone-D6 (50 ul)
Z142231	0.1 mg/ml Gadolinium Chloride, 0.1% Methanol-13C, 1% H ₂ O in D ₂ O (50 ul)
Z151220	Potassium Bromide (KBr, 80 ul)

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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)

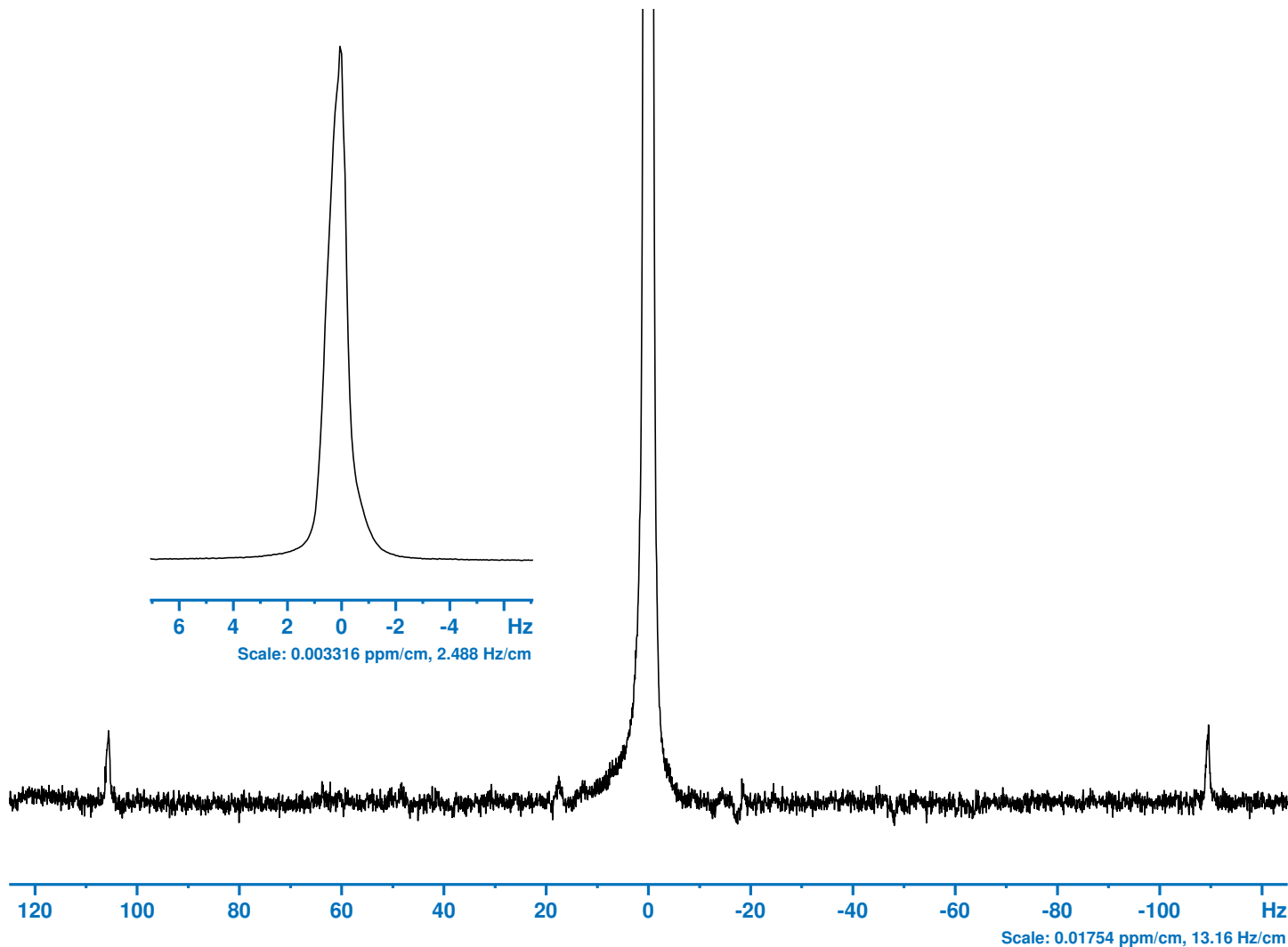
Line width [achieved/rated]: at 0.11% of signal height [15.3 Hz <= 18.0 Hz] <pass>
 Line width [achieved/rated]: at 0.55% of signal height [6.2 Hz <= 12.0 Hz] <pass>
 Line width [achieved/rated]: at 50% of signal height [0.74 Hz <= 1.00 Hz] <pass>



Bruker BioSpin

NPT_1H_HRMAS_lineshape

Current Data Parameters			
NAME	NPT_1H_HRMAS_lineshape		
EXPNO	2		
PROCNO	1		
F2 - Acquisition Parameters		Additional Parameters	
Date_	20240903	Field	996.163
Time	14.56 h	Lock Phase	326.958
INSTRUM	Avance NEO	Lock Power	-34.000
PROBHD	Z180004_0001 (Lock Gain	95.930
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	20.00 usec		
TE	298.0 K		
D1	9.11600113 sec		
TD0	1		
SFO1	750.3057695 MHz		
NUC1	1H		
P0	2.67 usec		
P1	8.00 usec		
PLW1	13.02900028 W		
F2 - Processing parameters			
SI	8192		
SF	750.3060194 MHz		
WDW	no		
SSB	0		
LB	0 Hz		
GB	0		
PC	4.00		



SHIM SEQUENCE
 skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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

```
# Tue Sep 3 12:56:35 2024
$$$PROBEIDENTIFIER=Z180004_0001
$$$PROBENAME=PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
$$$MAGNETID=BR.091075110
$$$CRYOSTATID=BD228972
$$$SHIMID=292721
```

Active Shim Gradients

```
#
Z -8841
Z2 0
Z3 5140
Z4 0
Z5 0
Z6 0
Z7 0
Z8 0
X 20
XZ 552
XZ2 -92
XZ3 0
XZ4 0
XZ5 0
Y 10458
YZ -65221
YZ2 10988
YZ3 0
YZ4 0
YZ5 0
XY -1529
XYZ 448
XYZ2 0
XYZ3 0
XYZ4 0
XYZ5 0
(X2-Y2) -45710
(X2-Y2) Z 19835
(X2-Y2) Z2 0
(X2-Y2) Z3 0
(X2-Y2) Z4 0
(X2-Y2) Z5 0
X3 560
X3Z 0
Y3 -10959
Y3Z 0
```

Lock Parameter

```
#
FIELD 996.163
LOCKPHASE 326.958
LOCKPOWER -34.000
LOCKGAIN 95.930
```

```
LOCKDC -70.000
LOCKSHIFT 2.040
LOOPGAIN 15.133
LOOPTIME 0.047
LOOPFILTER 1468.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1] -3854.79351007
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] 4626.79396195
SHIM_SETTING [ 4] -0.00000000
SHIM_SETTING [ 5] -82.20679818
SHIM_SETTING [ 6] 82.20679818
SHIM_SETTING [ 7] 2668.07515676
SHIM_SETTING [ 8] -2668.07515676
SHIM_SETTING [ 9] 1720.97431136
SHIM_SETTING [10] -1720.97431136
SHIM_SETTING [11] 0.00000000
SHIM_SETTING [12] -10958.78862549
SHIM_SETTING [13] -10958.78862549
SHIM_SETTING [14] 271.55187859
SHIM_SETTING [15] 477.99903528
SHIM_SETTING [16] -626.00132870
SHIM_SETTING [17] 343.85017216
SHIM_SETTING [18] -184.94888678
SHIM_SETTING [19] 135.22677438
SHIM_SETTING [20] -60.33390916
SHIM_SETTING [21] -9736.75793508
SHIM_SETTING [22] -49406.75793574
SHIM_SETTING [23] -31728.00125595
SHIM_SETTING [24] -59691.99866106
SHIM_SETTING [25] -13447.80020552
SHIM_SETTING [26] -22313.29244361
SHIM_SETTING [27] 271.55187859
SHIM_SETTING [28] -44788.84855814
SHIM_SETTING [29] -498.03763830
SHIM_SETTING [30] -698.17145333
SHIM_SETTING [31] -27877.36660368
SHIM_SETTING [32] 85653.15086023
SHIM_SETTING [33] -541.41066403
SHIM_SETTING [34] -1436.94000738
SHIM_SETTING [35] -1213.36395949
SHIM_SETTING [36] -1844.63646349
SHIM_SETTING [37] 13163.06699113
SHIM_SETTING [38] -9943.17310912
SHIM_SETTING [39] 34602.39794789
SHIM_SETTING [40] 0.00000000
```

NPT_1H_HRMAS_lineshape

```
Current Data Parameters
NAME NPT_1H_HRMAS_lineshape
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240903
Time 14.56 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 20.00 usec
TE 298.0 K
D1 9.11600113 sec
TDO 1
SF01 750.3057695 MHz
NUC1 1H
P0 2.67 usec
P1 8.00 usec
PLW1 13.02900028 W

F2 - Processing parameters
SI 8192
SF 750.3060194 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 4.00
```

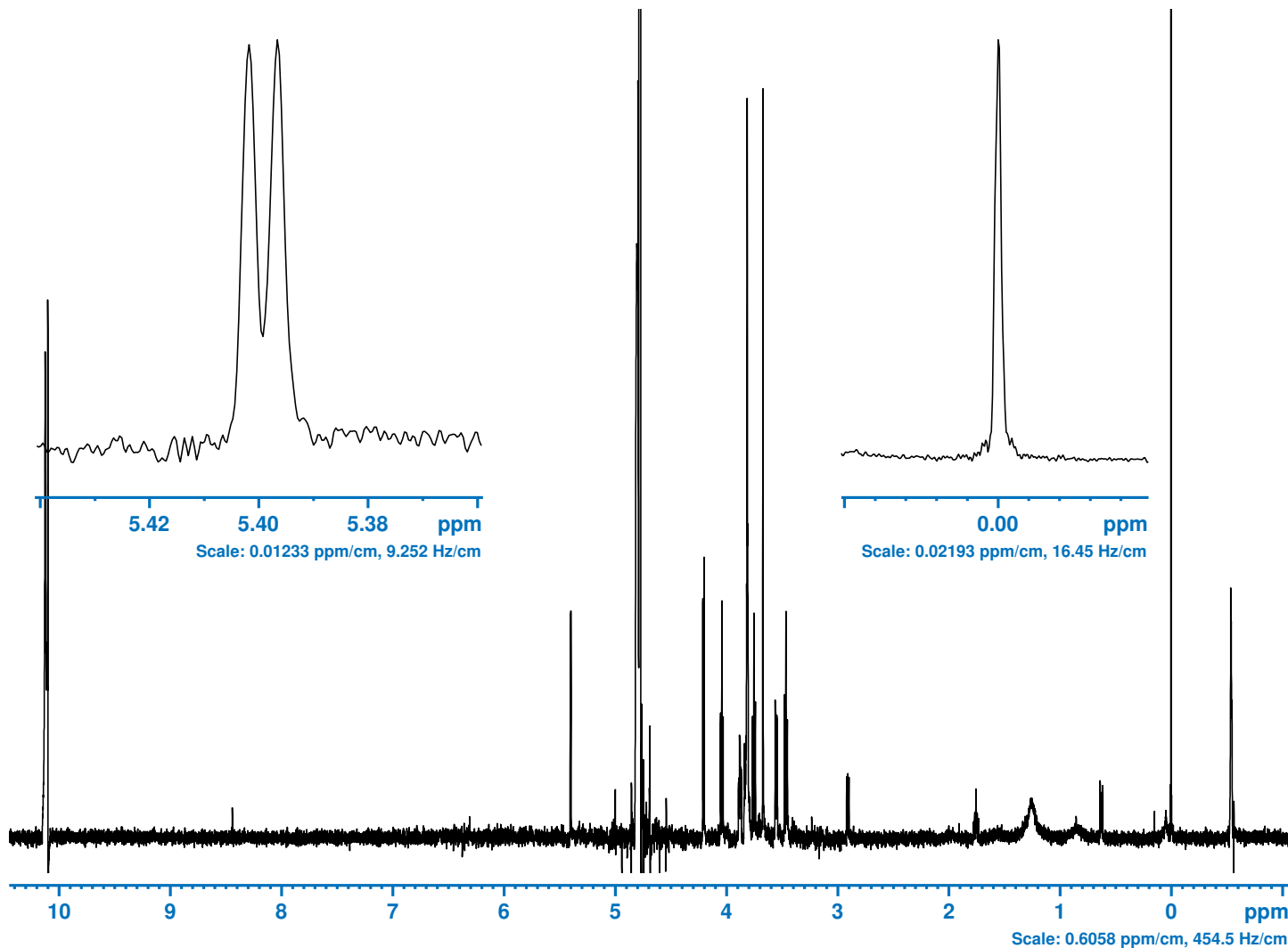
NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: 2 mM Sucrose, 0.5 mM DSS, 2 mM NaN₃ in 90% H₂O + 10% D₂O (50 ul) (Z142222)
 Watersuppression (NPT_1H_HRMAS_watersuppression, spin rate 4000 Hz)
 PULPROG = zgpr, Input_L23 = 1, O1 = 3521.92 Hz (optimized), OvFl = 0

Linewidth [achieved]: at 50 % of DSS signal [29.4 Hz] <n/a>
 Linewidth [achieved]: at 10 % of DSS signal [41.6 Hz] <n/a>
 Splitting anomeric proton [achieved]: [27%] <n/a>
 SINO (1.5 ppm) [achieved/rated]: Signal (6.00 to 5.20 ppm), Noise (9.96 to 8.46 ppm) [37.0 >= 22.0] <pass>



Bruker BioSpin

NPT_1H_HRMAS_watersuppression



Current Data Parameters
 NAME NPT_1H_HRMAS_watersuppression
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240903
 Time 13.04 h
 INSTRUM Avance NEO
 PROBHD Z180004_0001 ()
 PULPROG zgpr
 TD 19090
 SOLVENT H2O+D2O
 NS 8
 DS 4
 SWH 9090.909 Hz
 FIDRES 0.952426 Hz
 AQ 1.0499500 sec
 RG 101
 DW 55.000 usec
 DE 20.00 usec
 TE 298.0 K
 D1 5.00000000 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 750.3035219 MHz
 NUC1 1H
 P1 8.00 usec
 PLW1 13.02900028 W
 PLW9 0.00003335 W

Additional Parameters
 Field 1016.136
 Lock Phase 289.750
 Lock Power -18.000
 Lock Gain 111.869
 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 32768
 SF 750.2999427 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.10

SHIM SEQUENCE
 - topshim hrmas <pass>

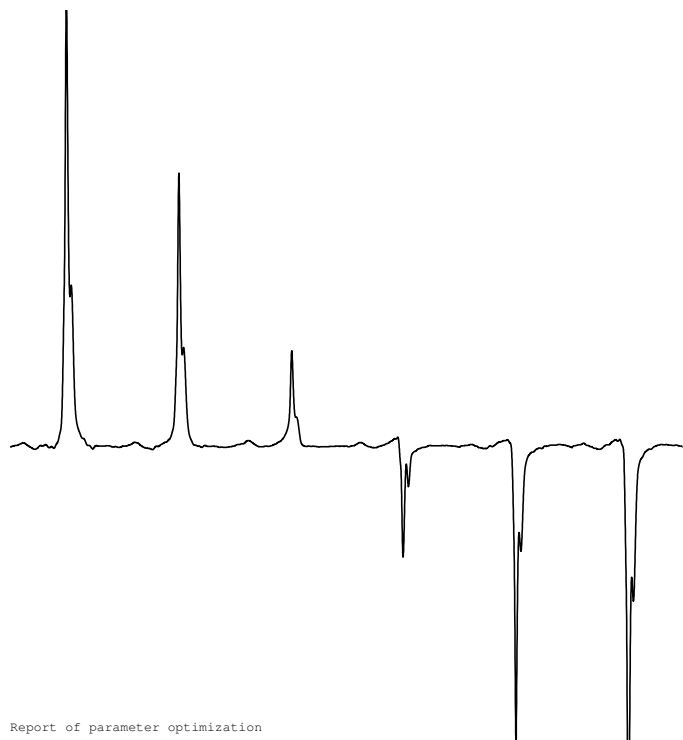
NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (50 ul) (Z142223)
 P90 1H pulse calibration (NPT_1H_p90determinationf1_1h, spin rate 4000 Hz)
 Result: [180/2] = 10.0 us @ 11.5 W [360] = 39.3 us ==> [PDelay = 2*180 - 360] = 0.6 us
 ATTENTION: Updated PROSOL Tables with [10.0 us @ 11.4 W]
 Deviation from pulse target value (= 10.0 us): -0.4%



Bruker BioSpin

P90 1H pulse [achieved/rated]: @ 11.5 W [10.0 us <= 10.0 us] <pass>

NPT_1H_p90determinationf1_1h



Report of parameter optimization

F1P = 5.524863 ppm, F2P = 5.418240 ppm.

Linear Optimization of P 1 in 6 steps,
 PROCNO = 999
 Starting at 15.000000us ending at 25.000000us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	15.00	210834918.0	-1335348.5	11158342.5
2	17.00	126995500.5	-1490910.0	6997650.5
3	19.00	44449492.0	-234523.8	2829277.8
4	21.00	4276622.2	-51410526.2	-1757926.2
5	23.00	3069664.0	-138453152.0	-6179552.3
6	25.00	3249913.5	-205765749.0	-9478967.4

Zero found at P 1 = 19.927383 us



Report of parameter optimization

F1P = 5.524863 ppm, F2P = 5.418240 ppm.

Linear Optimization of P 1 in 6 steps,
 PROCNO = 999
 Starting at 29.891075us ending at 49.818459us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	29.89	3396570.0	-268237952.5	-12468936.2
2	33.88	1792445.5	-191752388.5	-9492350.1
3	37.86	1221870.6	-56857314.1	-2430201.5
4	41.85	104667419.0	-2833724.2	4876058.5
5	45.83	202545525.5	-2243075.0	9695958.4
6	49.82	205205651.5	-1944947.5	9724129.8

Zero found at P 1 = 39.264931 us



Current Data Parameters
 NAME NPT_1H_p90determinationf1_1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240904
 Time 10.59 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 20.00 usec
 TE 298.0 K
 DI 1.45500004 sec
 TDO 1
 SF01 750.3041053 MHz
 NUC1 1H
 P1 49.82 usec
 PLW1 11.46170044 W

Additional Parameters
 Field 1018.831
 Lock Phase 9.081
 Lock Power -19.000
 Lock Gain 90.009
 Lock DC -70.000
 Lock Shift 2.490
 Loop Gain 8.796
 Loop Time 0.087
 Loop Filter 515.676
 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
 8.34 W 10.0 us 11.7 us 17.2%
 8.34 W 10.0 us 10.0 us -0.4%
 11.5 W 10.0 us 10.0 us -0.4%

 SHIM SEQUENCE
 - topshim hrmas <pass>

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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 (200.0 Hz) [achieved/rated]: Signal (3.00 to 2.00 ppm), Noise (3.34 to 3.07 ppm) [168.3 >= 110.0] <pass>



Bruker BioSpin

NPT_1H_sensitivity

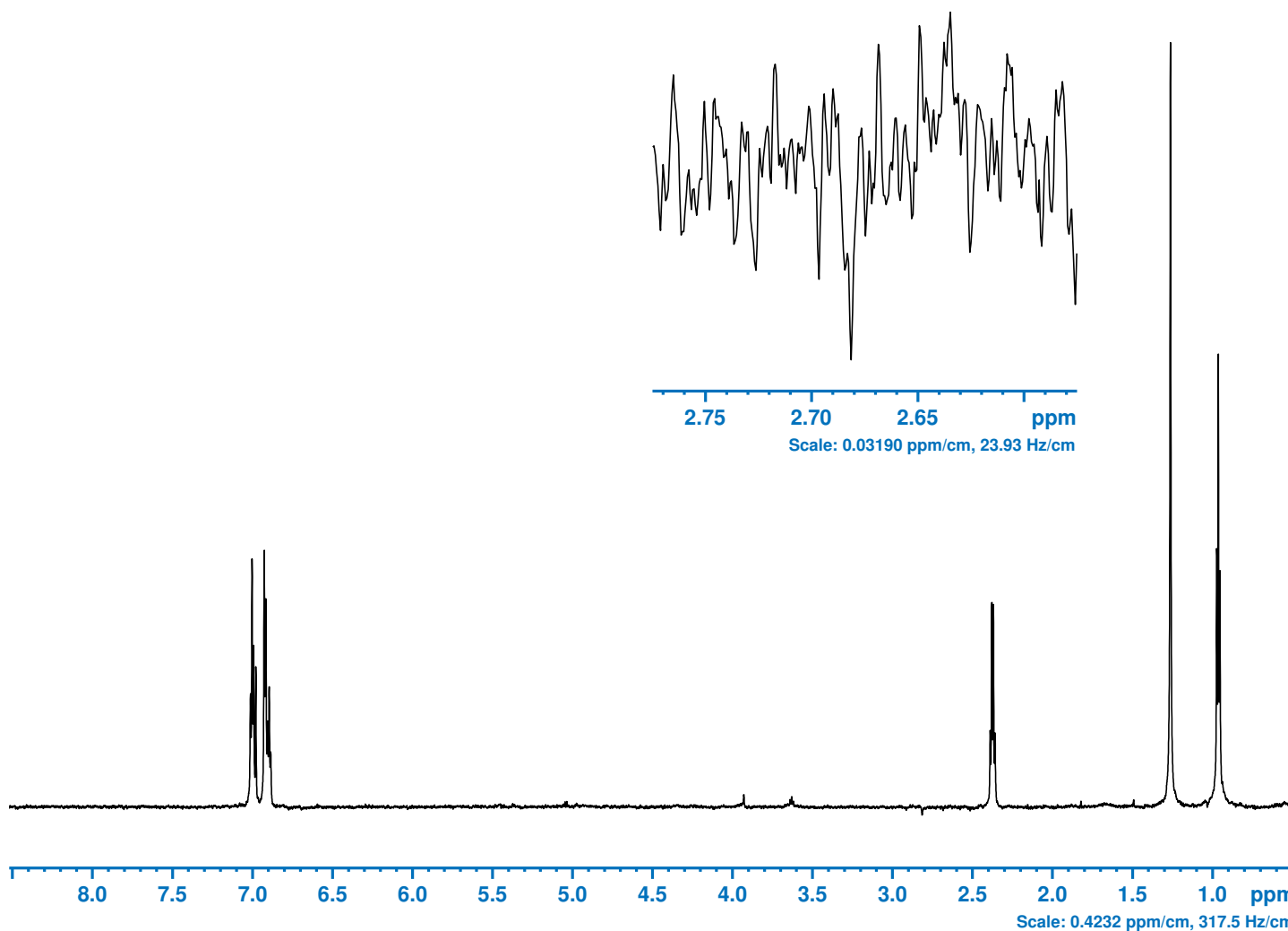
Current Data Parameters
 NAME NPT_1H_sensitivity
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240904
 Time 13.30 h
 INSTRUM Avance NEO
 PROBHD Z180004_0001 (
 PULPROG zg
 TD 32768
 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 20.00 usec
 TE 298.0 K
 D1 113.57360077 sec
 TD0 1
 SF01 750.3030012 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 11.37899971 W

Additional Parameters
 Field 1008.357
 Lock Phase 51.078
 Lock Power -27.000
 Lock Gain 117.588
 Lock DC -70.000
 Lock Shift 7.240
 Loop Gain -9.400
 Loop Time 0.464
 Loop Filter 50.000
 Gas Flow external

F2 - Processing parameters
 SI 16384
 SF 750.3002294 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

SHIM SEQUENCE
 skip shimming



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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)



Bruker BioSpin

```
# Wed Sep 4 11:30:29 2024
$$$PROBEIDENTIFIER=Z180004_0001
$$$PROBENAME=PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
$$$MAGNETID=BR.091075110
$$$CRYOSTATID=BD228972
$$$SHIMID=292721
```

Active Shim Gradients

```
#
Z -8721
Z2 0
Z3 5140
Z4 0
Z5 0
Z6 0
Z7 0
Z8 0
X 20
XZ 552
XZ2 -92
XZ3 0
XZ4 0
XZ5 0
Y 10458
YZ -65221
YZ2 10988
YZ3 0
YZ4 0
YZ5 0
XY -1529
XYZ 448
XYZ2 0
XYZ3 0
XYZ4 0
XYZ5 0
(X2-Y2) -45710
(X2-Y2) Z 19835
(X2-Y2) Z2 0
(X2-Y2) Z3 0
(X2-Y2) Z4 0
(X2-Y2) Z5 0
X3 560
X3Z 0
Y3 -10959
Y3Z 0
```

Lock Parameter

```
#
FIELD 1008.357
LOCKPHASE 51.078
LOCKPOWER -27.000
LOCKGAIN 117.588
```

```
LOCKDC -70.000
LOCKSHIFT 7.240
LOOPGAIN -9.400
LOOPTIME 0.464
LOOPFILTER 50.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1] -3796.59351007
SHIM_SETTING [ 2] 0.00000000
SHIM_SETTING [ 3] 4633.75977177
SHIM_SETTING [ 4] -0.00000000
SHIM_SETTING [ 5] -74.08738379
SHIM_SETTING [ 6] 74.08738379
SHIM_SETTING [ 7] 2665.37118311
SHIM_SETTING [ 8] -2665.37118311
SHIM_SETTING [ 9] 1716.45873298
SHIM_SETTING [10] -1716.45873298
SHIM_SETTING [11] 0.00000000
SHIM_SETTING [12] -10958.78862549
SHIM_SETTING [13] -10958.78862549
SHIM_SETTING [14] 271.55187859
SHIM_SETTING [15] 477.99903528
SHIM_SETTING [16] -626.00132870
SHIM_SETTING [17] 343.85017216
SHIM_SETTING [18] -184.94888678
SHIM_SETTING [19] 135.22677438
SHIM_SETTING [20] -60.33390916
SHIM_SETTING [21] -9736.75793508
SHIM_SETTING [22] -49406.75793574
SHIM_SETTING [23] -31728.00125595
SHIM_SETTING [24] -59691.99866106
SHIM_SETTING [25] -13447.80020552
SHIM_SETTING [26] -22313.29244361
SHIM_SETTING [27] 271.55187859
SHIM_SETTING [28] -44788.84855814
SHIM_SETTING [29] -498.03763830
SHIM_SETTING [30] -698.17145333
SHIM_SETTING [31] -27877.36660368
SHIM_SETTING [32] 85653.15086023
SHIM_SETTING [33] -541.41066403
SHIM_SETTING [34] -1436.94000738
SHIM_SETTING [35] -1213.36395949
SHIM_SETTING [36] -1844.63646349
SHIM_SETTING [37] 13163.06699113
SHIM_SETTING [38] -9943.17310912
SHIM_SETTING [39] 34602.39794789
SHIM_SETTING [40] 0.00000000
```

NPT_1H_sensitivity

```
Current Data Parameters
NAME NPT_1H_sensitivity
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20240904
Time 13.30 h
INSTRUM Avance NEO
PROBHD Z180004_0001 (
PULPROG zg
TD 32768
SOLVENT CDC13
NS 1
DS 0
SWH 7462.687 Hz
FIDRES 0.455486 Hz
AQ 2.1954560 sec
RG 101
DW 67.000 usec
DE 20.00 usec
TE 298.0 K
D1 113.57360077 sec
TDO 1
SF01 750.3030012 MHz
NUC1 1H
P1 10.00 usec
PLW1 11.37899971 W

F2 - Processing parameters
SI 16384
SF 750.3002294 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
```

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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 integral sensitivity (NPT_1H_inno, spin rate 4000 Hz)

SINO (2.0 ppm) [achieved]: Signal (3.00 to 2.00 ppm), Noise (11.00 to 9.00 ppm) [27] <n/a>
 INNO (2.0 ppm) [achieved]: Signal (3.00 to 2.00 ppm), Noise (11.00 to 9.00 ppm) [778] <n/a>



Bruker BioSpin

NPT_1H_inno

Current Data Parameters

NAME NPT_1H_inno
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20240904
 Time 13.35 h
 INSTRUM Avance NEO
 PROBHD Z180004_0001 (
 PULPROG zg
 TD 258288
 SOLVENT CDC13
 NS 1
 DS 0
 SWH 14705.882 Hz
 FIDRES 0.113872 Hz
 AQ 8.7817917 sec
 RG 101
 DW 34.000 usec
 DE 20.00 usec
 TE 298.0 K
 D1 113.57360077 sec
 DI 1
 SFO1 750.3030012 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 11.37899971 W

Additional Parameters

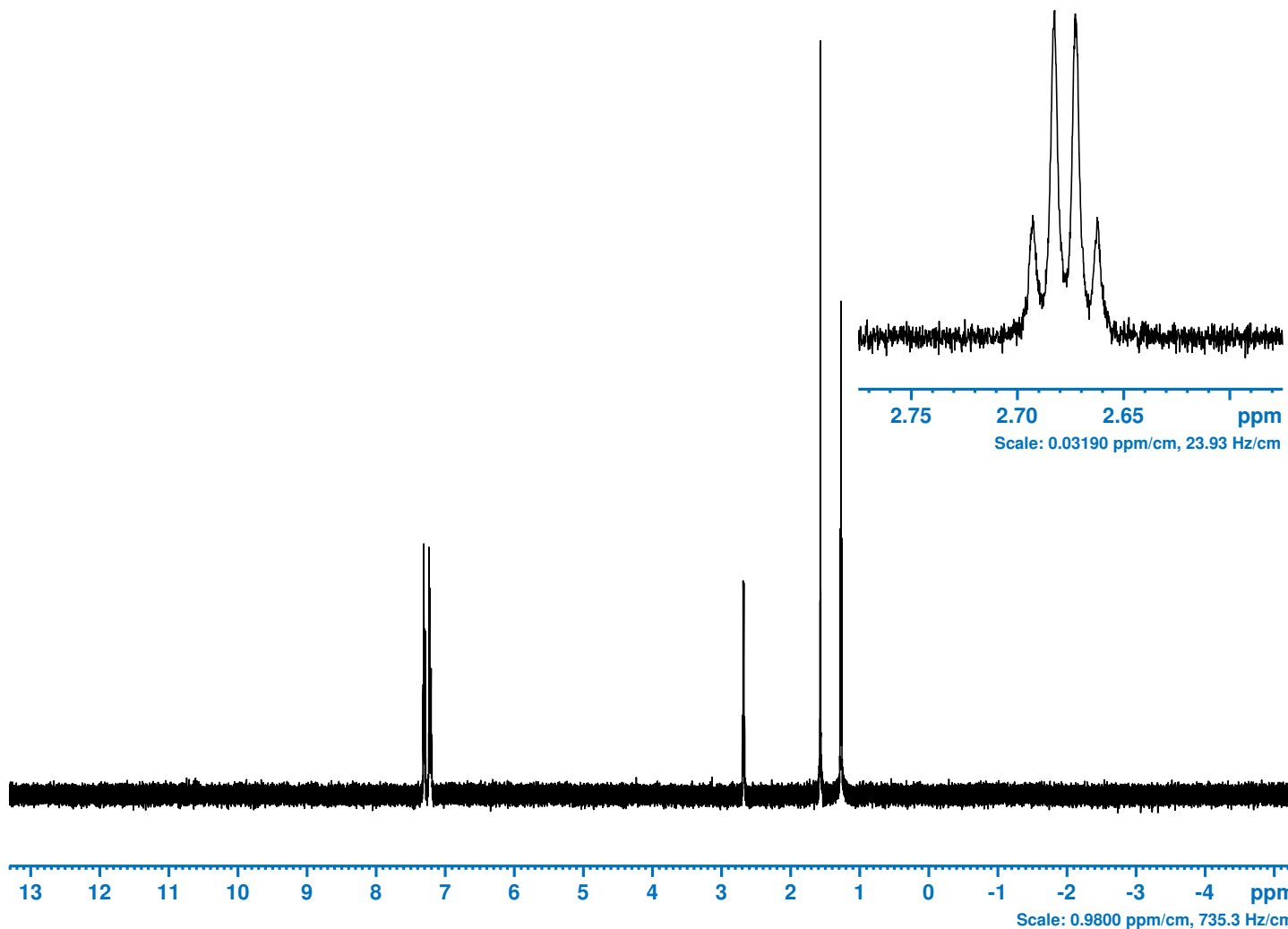
Field 1008.167
 Lock Phase 51.078
 Lock Power -27.000
 Lock Gain 117.588
 Lock DC -70.000
 Lock Shift 7.240
 Loop Gain -9.400
 Loop Time 0.464
 Loop Filter 50.000
 Gas Flow external

F2 - Processing parameters

SI 131072
 SF 750.3000000 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

SHIM SEQUENCE

skip shimming



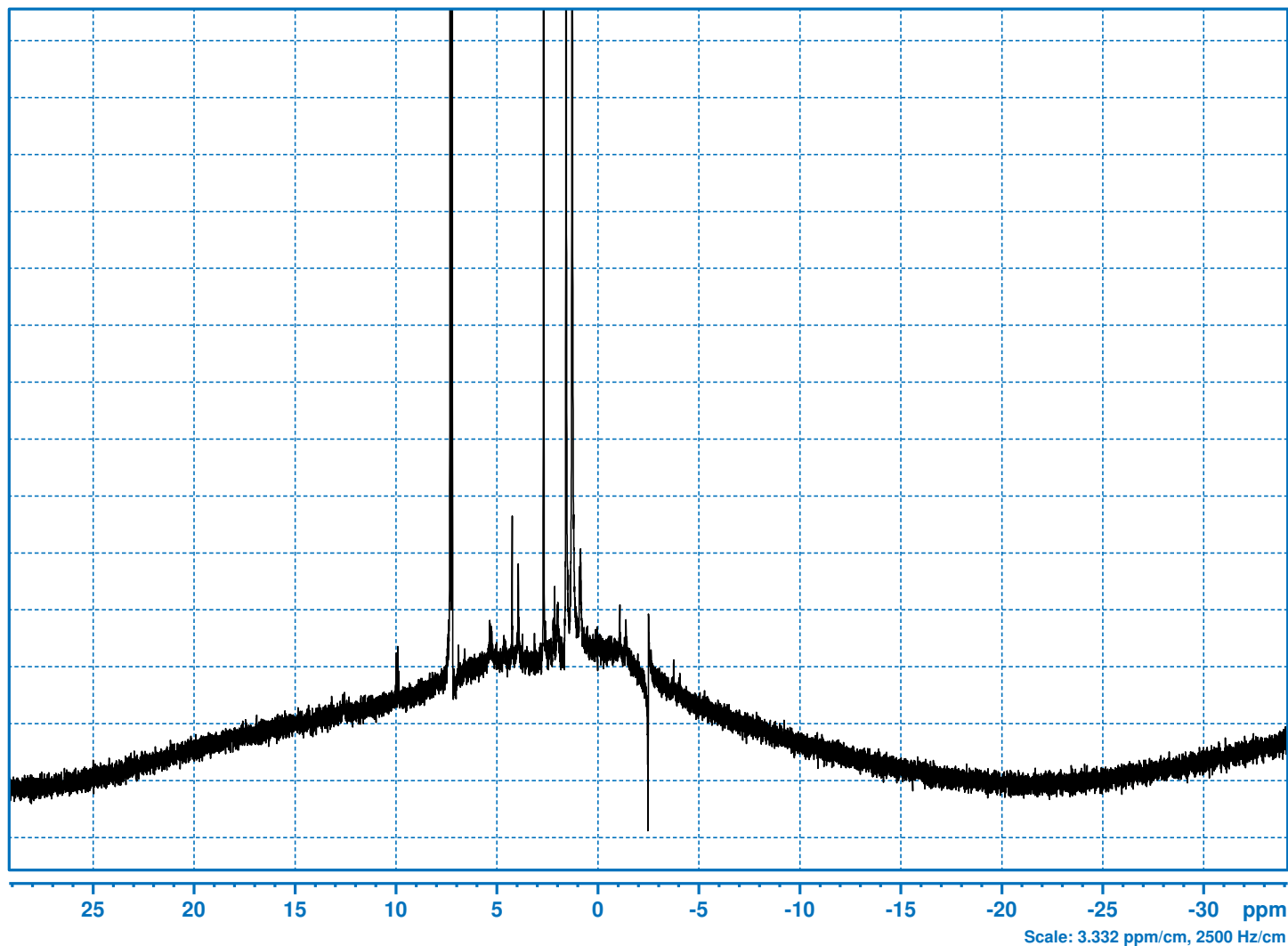
NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: 0.1% Ethylbenzene (EB) in Chloroform-D (50 ul) (Z142221)
 1H background with sample (NPT_1H_backgr_withsample, spin rate 4000 Hz)
 Flipangle = 45 degree

Background measurement (CY-scaling = 200.0 cm)



Bruker BioSpin

NPT_1H_backgr_withsample



Current Data Parameters
 NAME NPT_1H_backgr_withsample
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240904
 Time 13.33 h
 INSTRUM Avance NEO
 PROBHD Z180004_0001 ()
 PULPROG npt_zg30
 TD 32768
 SOLVENT CDC13
 NS 10
 DS 4
 SWH 50000.000 Hz
 FIDRES 3.051758 Hz
 AQ 0.3276800 sec
 RG 101
 DW 10.000 usec
 DE 20.00 usec
 TE 298.0 K
 DI 3.83732009 sec
 TDO 1
 SFO1 750.2981243 MHz
 NUC1 1H
 CNST10 45.0000000
 P0 5.00 usec
 P1 10.00 usec
 PLW1 11.37899971 W

Additional Parameters
 Field 1008.249
 Lock Phase 51.078
 Lock Power -27.000
 Lock Gain 117.588
 Lock DC -70.000
 Lock Shift 7.240
 Loop Gain -9.400
 Loop Time 0.464
 Loop Filter 50.000
 Gas Flow external

F2 - Processing parameters
 SI 32768
 SF 750.3000000 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

SHIM SEQUENCE
 skip shimming

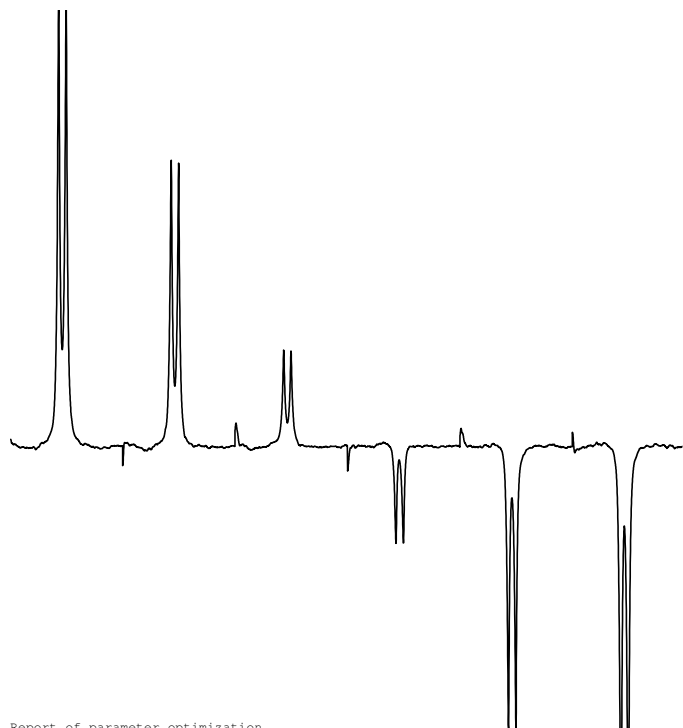
NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (50 ul) (Z142223)
 Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c, spin rate 4000 Hz)
 Result: [90] = 10.0 us @ 70.2 W [270] = 29.8 us ==> [PDelay = 3*90 - 270] = 0.2 us
 ATTENTION: Updated PROSOL Tables with [10.0 us @ 70.2 W]
 Deviation from pulse target value (= 10.0 us): -0.0%



Bruker BioSpin

P90 13C pulse [achieved/rated]: @ 70.2 W [10.0 us <= 10.0 us] <pass>

NPT_1H_p90determinationf2_13c



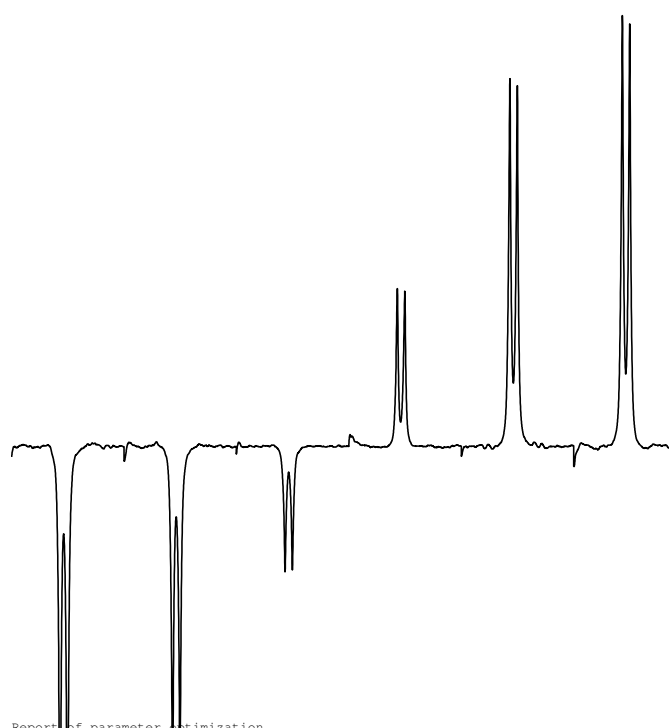
Report of parameter optimization

F1P = 3.120246 ppm, F2P = 3.013623 ppm.

Linear Optimization of P 3 in 6 steps,
 PROCNO = 999
 Starting at 5.000000us ending at 15.000000us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P 3	Maximum point	Minimum point	Integral
1	5.00	4796968.1	-33587.0	316627.1
2	7.00	3027950.1	-203569.5	194854.1
3	9.00	1018903.6	-41354.3	74481.5
4	11.00	42716.3	-1023987.3	-58027.0
5	13.00	190919.8	-2982176.0	-176927.5
6	15.00	150760.2	-4628344.6	-282128.1

Zero found at P 3 = 9.997512 us



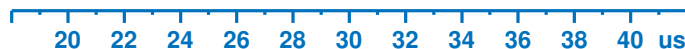
Report of parameter optimization

F1P = 3.120246 ppm, F2P = 3.013623 ppm.

Linear Optimization of P 3 in 6 steps,
 PROCNO = 999
 Starting at 19.995024us ending at 39.990047us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P 3	Maximum point	Minimum point	Integral
1	20.00	49246.3	-6408007.6	-397057.7
2	23.99	64732.3	-4974469.2	-307290.0
3	27.99	58753.0	-1773561.6	-110702.5
4	31.99	2228066.2	-23978.0	138648.1
5	35.99	5195861.5	-138112.0	315719.5
6	39.99	6087232.1	-286889.4	352816.8

Zero found at P 3 = 29.765432 us



Current Data Parameters
 NAME NPT_1H_p90determinationf2_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240904
 Time 11.12 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 2.56
 DW 2166.700 usec
 DE 20.00 usec
 TE 298.0 K
 CNST2 139.0000000
 D1 2.56970811 sec
 D2 0.00359712 sec
 TD0 1
 SFO1 750.3023011 MHz
 NUC1 1H
 P1 5.00 usec
 PLW1 11.37899971 W
 SFO2 188.6724116 MHz
 NUC2 13C
 P3 39.99 usec
 PLW2 70.21485901 W

Additional Parameters
 Field 1019.024
 Lock Phase 9.081
 Lock Power -19.000
 Lock Gain 90.009
 Lock DC -70.000
 Lock Shift 2.490
 Loop Gain 8.796
 Loop Time 0.087
 Loop Filter 515.676
 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 *****

FLW90	P90	P90[det]	Deviation
74.2 W	10.0 us		
74.2 W	10.0 us	9.7 us	-2.7%
70.2 W	10.0 us	10.0 us	-0.0%

SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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 (127.62 ppm), Noise (120.09 to 80.09 ppm) [92.8 >= 35.0] <pass>



Bruker BioSpin

NPT_13C_sensitivity

Current Data Parameters
 NAME NPT_13C_sensitivity
 EXPNO 1
 PROCNO 1

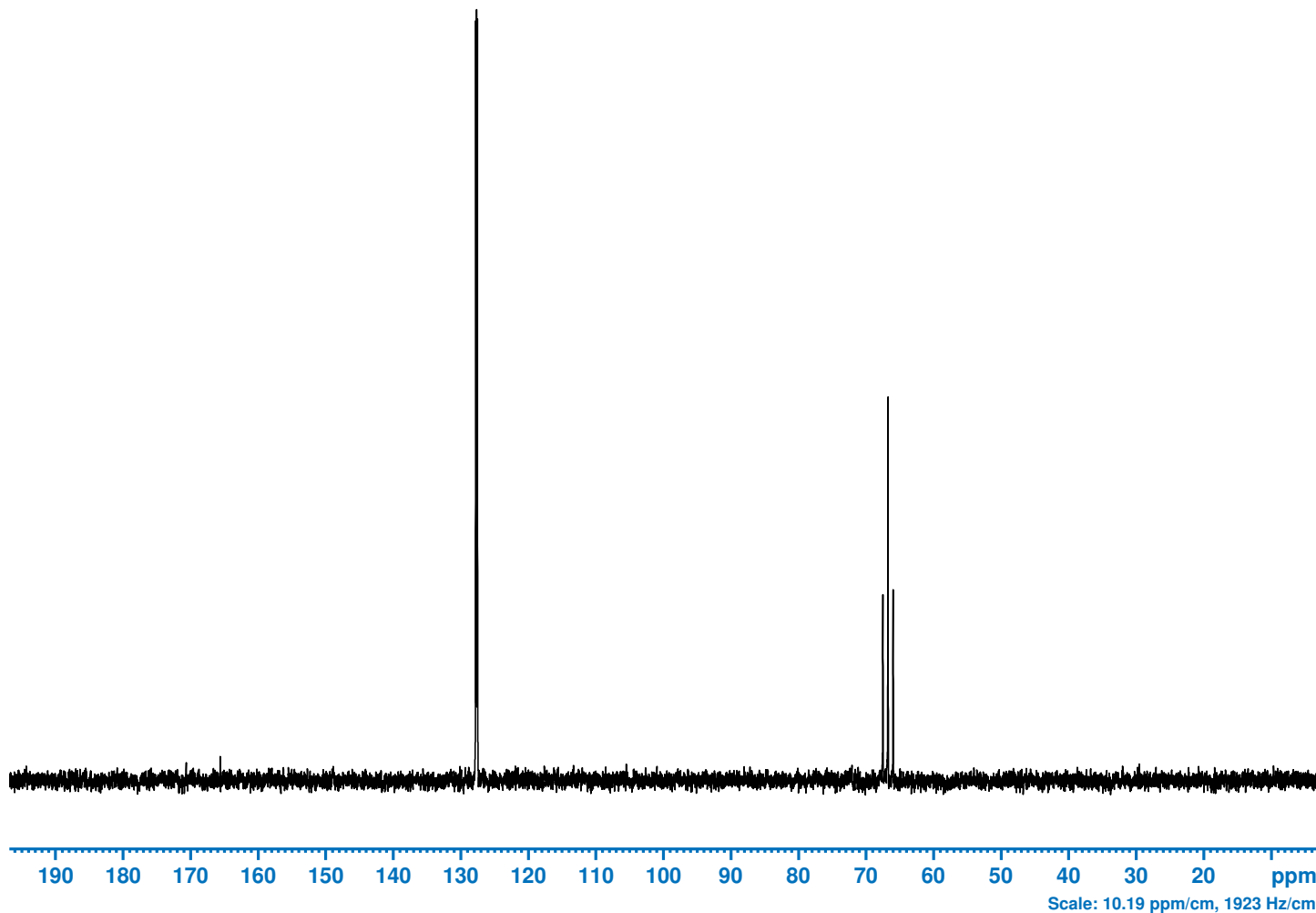
F2 - Acquisition Parameters
 Date_ 20240904
 Time 12.33 h
 INSTRUM Avance NEO
 PROBHD Z180004_0001 (
 PULPROG zg
 TD 65536
 SOLVENT C6D6
 NS 1
 DS 0
 SWH 38461.538 Hz
 FIDRES 1.173753 Hz
 AQ 0.8519680 sec
 RG 101
 DW 13.000 usec
 DE 6.63 usec
 TE 298.0 K
 D1 829.14801025 sec
 TD0 1
 SFO1 188.6819490 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 70.18000031 W

Additional Parameters
 Field 991.568
 Lock Phase 54.124
 Lock Power -24.000
 Lock Gain 104.321
 Lock DC -70.000
 Lock Shift 7.160
 Loop Gain 15.133
 Loop Time 0.047
 Loop Filter 1467.800
 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 4.4.0
 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 2000 Hz)
 Result: [180/2] = 12.0 us @ 35.2 W [360] = 47.2 us ==> [PDelay = 2*180 - 360] = 0.8 us
 ATTENTION: Updated PROSOL Tables with [12.0 us @ 35.2 W]
 Deviation from pulse target value (= 12.0 us): 0.0%



Bruker BioSpin

P90 31P pulse [achieved/rated]: @ 35.2 W [12.0 us <= 12.0 us] <pass>

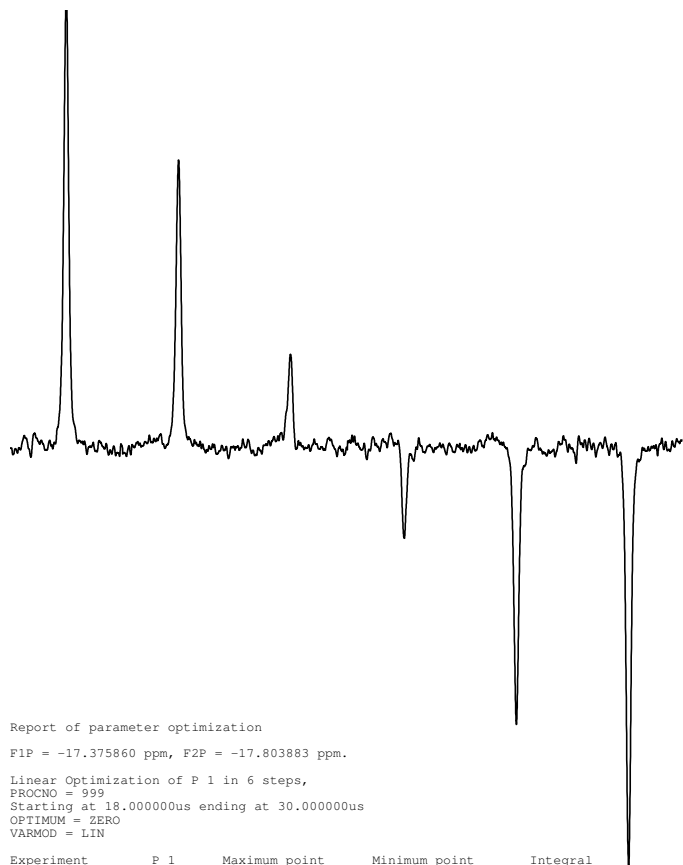
NPT_31P_p90determinationf1_31p

Current Data Parameters
 NAME NPT_31P_p90determinationf1_31p
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240904
 Time 16.03 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
 DI 17.64999962 sec
 TD0 1
 SF01 303.7216647 MHz
 NUC1 31P
 P1 60.00 usec
 PLW1 35.19387817 W

Additional Parameters
 Field 995.212
 Lock Phase 75.059
 Lock Power -34.000
 Lock Gain 99.206
 Lock DC -70.000
 Lock Shift 2.040
 Loop Gain 15.133
 Loop Time 0.047
 Loop Filter 1467.800
 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



Zero found at P 1 = 24.001677 us



Zero found at P 1 = 47.160836 us



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

 35.2 W 12.0 us
 35.2 W 12.0 us 12.0 us 0.0%

SHIM SEQUENCE

- topshim hrmas <pass>

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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)
 31P sensitivity (NPT_31P_sensitivity, spin rate 2000 Hz)

SINO (5.0 ppm) [achieved/rated]: Signal (-17.59 ppm), Noise (-1.78 to -6.79 ppm) [78.0 >= 30.0] <pass>



Bruker BioSpin

NPT_31P_sensitivity

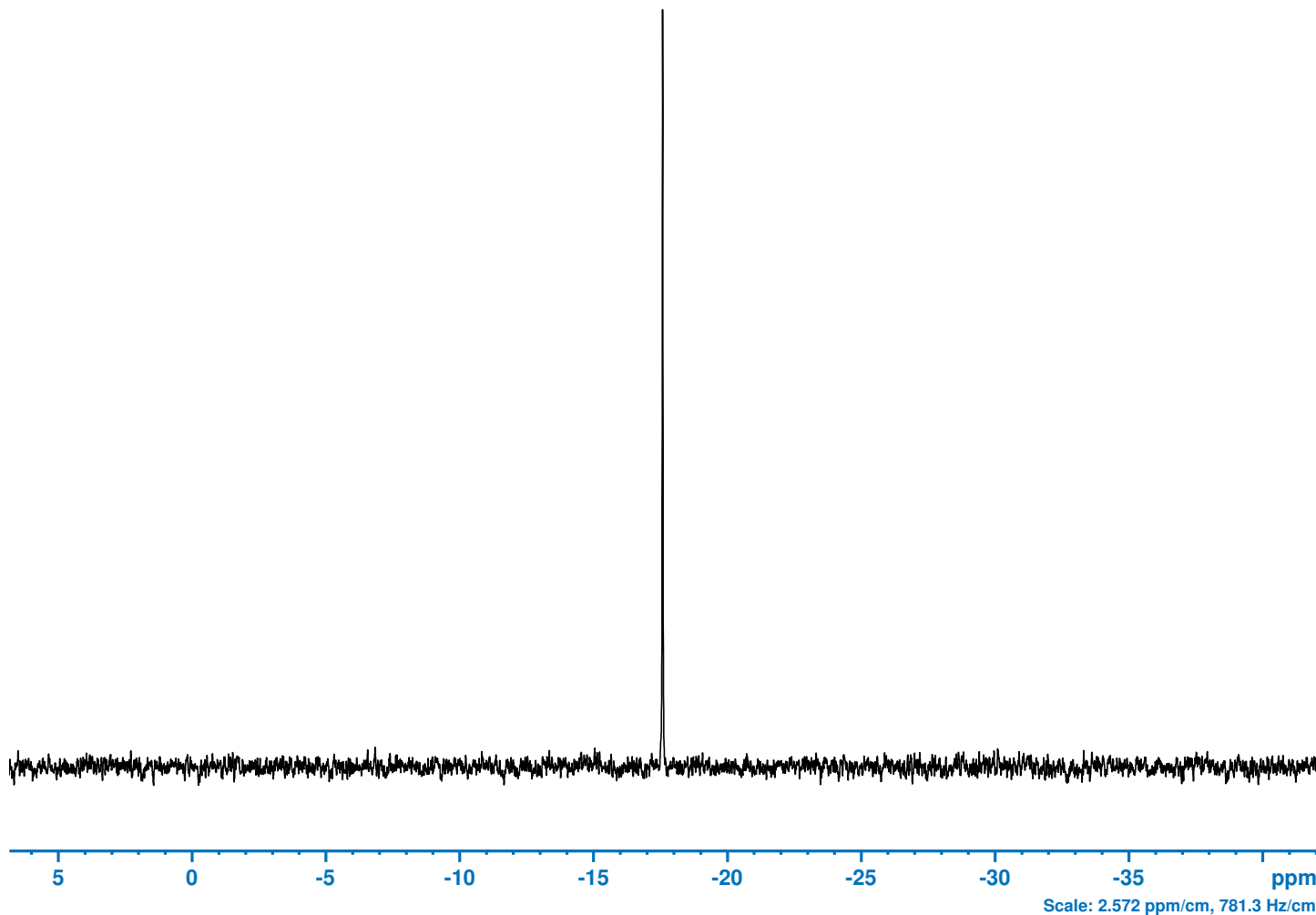
Current Data Parameters
 NAME NPT_31P_sensitivity
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240904
 Time 16.06 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
 SFO1 303.7216590 MHz
 NUC1 31P
 P1 12.00 usec
 PLW1 35.19900131 W

Additional Parameters
 Field 995.230
 Lock Phase 75.059
 Lock Power -34.000
 Lock Gain 99.206
 Lock DC -70.000
 Lock Shift 2.040
 Loop Gain 15.133
 Loop Time 0.047
 Loop Filter 1467.800
 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
 skip shimming



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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] = 499.8 us @ 104 mW [360] = 1946.9 us ==> [PDelay = 2*180 - 360] = 52.5 us
 ATTENTION: Updated PROSOL Tables with [500.0 us @ 104 mW]
 Deviation from pulse target value (= 500.0 us): -0.0%

P90 2H pulse [achieved/rated]: @ 104 mW [499.8 us <= 500.0 us] <pass>



Bruker BioSpin

NPT_prep_p90det_d

Current Data Parameters

NAME NPT_prep_p90det_d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20240904
 Time 10.36 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 45.2
 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 115.1759046 MHz
 NUC1 2H
 P1 2499.22 usec
 PLW1 0.10383580 W

Additional Parameters

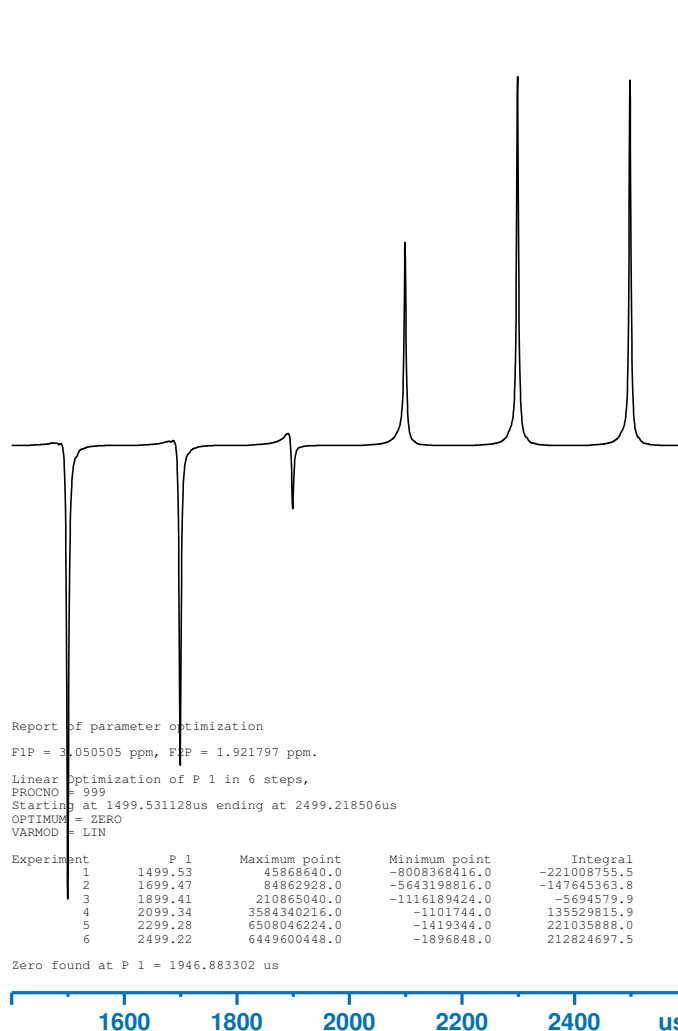
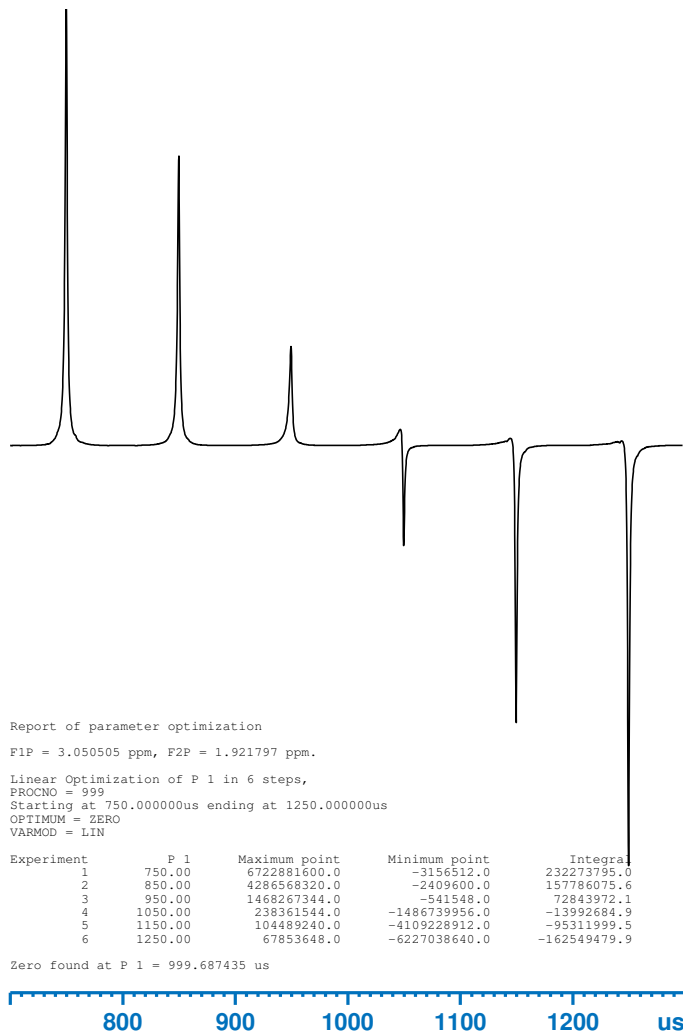
Field 1018.494
 Lock Phase 339.900
 Lock Power -9.000
 Lock Gain 90.683
 Lock DC -70.000
 Lock Shift 2.490
 Loop Gain 8.796
 Loop Time 0.087
 Loop Filter 515.676
 Gas Flow external

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
104 mW	500.0 us		
104 mW	500.0 us	499.8 us	-0.0%



SHIM SEQUENCE

- topshim hrmas lockoff solvent=DMSO O1P=2.49 <pass>

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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

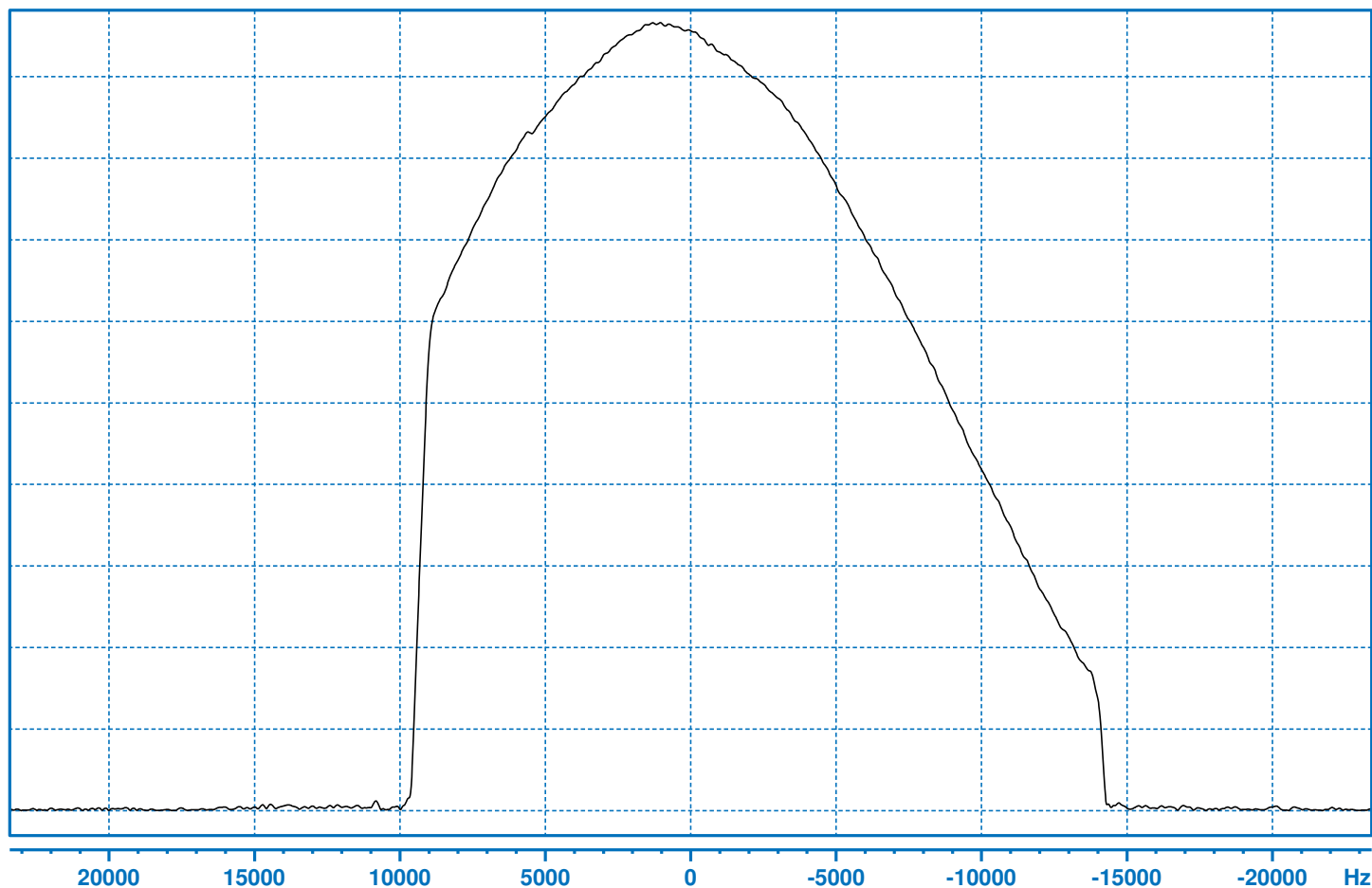


Bruker BioSpin

Z-Profile (-): Deviation [achieved]: of measured strength (5.7 G/cm*A) from PICS value (6.1 G/cm*A) [6.3%] <n/a>

NPT_1H_gradientprofile_neg

Current Data Parameters			
NAME	NPT_1H_gradientprofile_neg		
EXPNO	1		
PROCNO	1		
F2 - Acquisition Parameters		Additional Parameters	
Date_	20240903	Field	1018.262
Time	13.09 h	Lock Phase	325.420
INSTRUM	Avance NEO	Lock Power	-18.000
PROBHD	Z180004_0001 (Lock Gain	110.004
PULPROG	npt_imgcpld	Lock DC	-70.000
TD	1024	Lock Shift	4.700
SOLVENT	H2O+D2O	Loop Gain	-9.189
NS	1	Loop Time	0.456
DS	0	Loop Filter	49.120
SWH	81967.213 Hz	Gas Flow	external
FIDRES	160.092209 Hz		
AQ	0.0062464 sec		
RG	50.8		
DW	6.100 usec		
DE	20.00 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 %		
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 4.4.0
 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

Z-Profile (+): Deviation [achieved]: of measured strength (5.7 G/cm*A) from PICS value (6.1 G/cm*A) [6.7%] <n/a>



Bruker BioSpin

NPT_1H_gradientprofile_pos

Current Data Parameters

NAME NPT_1H_gradientprofile_pos
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20240903
 Time 13.12 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 57
 DW 6.100 usec
 DE 20.00 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

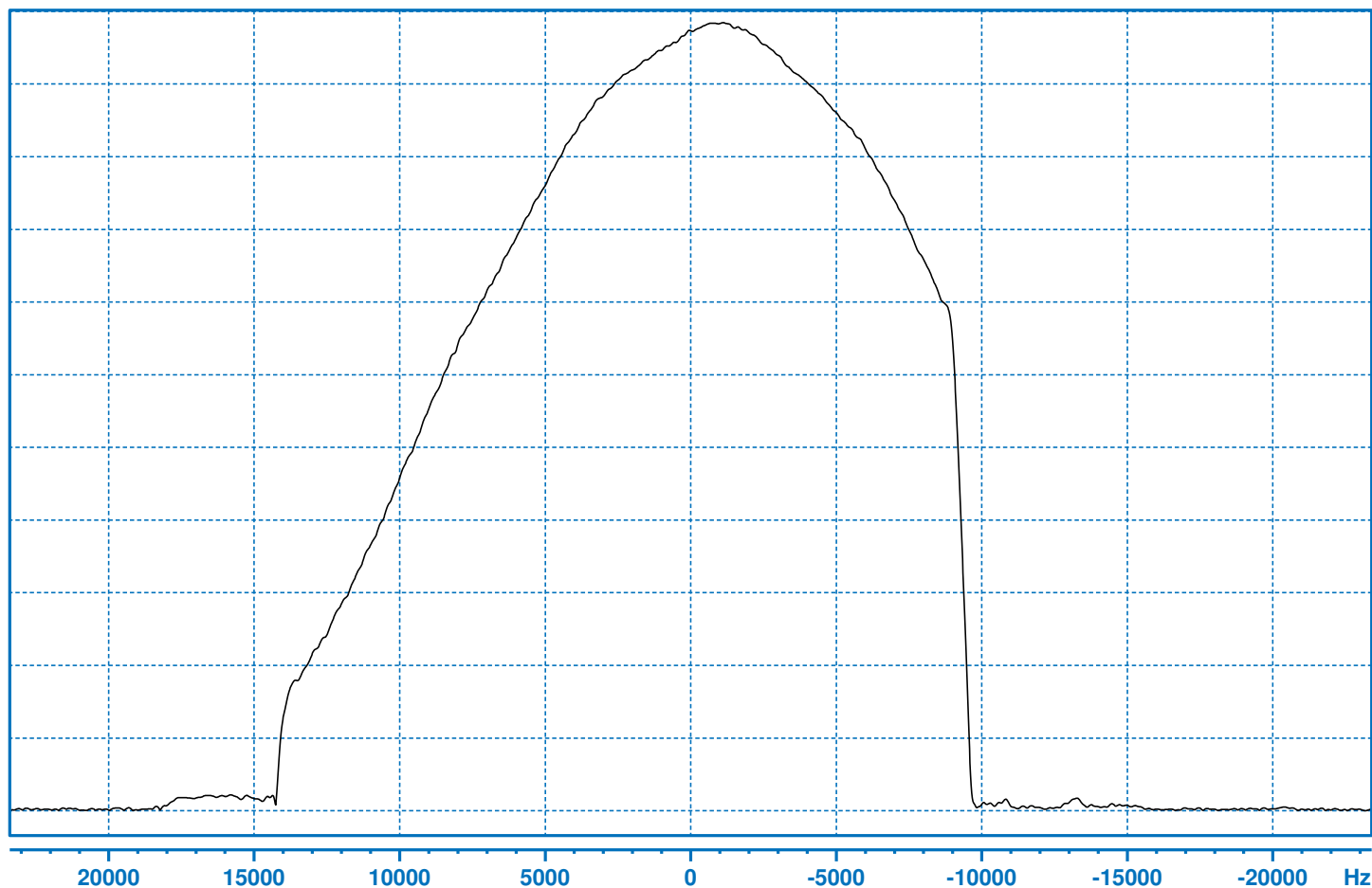
Field 1018.503
 Lock Phase 325.420
 Lock Power -18.000
 Lock Gain 110.004
 Lock DC -70.000
 Lock Shift 4.700
 Loop Gain -9.189
 Loop Time 0.456
 Loop Filter 49.120
 Gas Flow external

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 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: 0.1 mg/ml Gadolinium Chloride, 0.1% Methanol-13C, 1% H2O in D2O (50 ul) (Z142231)
 Gradient recovery stability test (NPT_1H_gradrec_stest_1h, spin rate 4000 Hz)
 Shape: RECT.1, amplitude: 0.0 A (0.0 % of probe maximum)



Bruker BioSpin

HDO line width value at 50% [achieved/rated]: [3.8 Hz <= 4.5 Hz] <pass>
 Max deviation of peak intensity (%) from mean (= 99.77%) of peaks 1 (10.00 us) to 26 (1.000 s) [achieved/rated]: [0.82% <= 1.00%] <pass>
 Max phase deviation (deg) of peaks 1 (10.00 us) to 26 (1.000 s) [achieved/rated]: [1.70 deg <= 3.00 deg] <pass>

NPT_1H_gradrec_stest_1h

```
Current Data Parameters
NAME      NPT_1H_gradrec_stest_1h
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20240904
Time      14.35 h
INSTRUM   Avance NEO
PROBHD    Z180004_0001 (
PULPROG   npt_gradrecvd
TD         30444
SOLVENT   D2O
NS         1
DS         2
SWH        5555.556 Hz
FIDRES     0.364969 Hz
AQ         2.7399600 sec
RG         101
DW          90.000 usec
DE         20.00 usec
TE         298.0 K
D0          0 sec
D1         5.00000000 sec
D11        0.03000000 sec
D12        0.00005000 sec
VDLIST     npt_gradrec
vd_list    0.00001000 sec
SF01       750.3035262 MHz
NUC1       1H
P1         10.00 usec
PLW1       11.37899971 W
GPNAM[1]   RECT.1
GPZ1       0 %
P16        5000.00 usec

Additional Parameters
Field      1012.132
Lock Phase 48.358
Lock Power -18.000
Lock Gain  88.732
Lock DC    -70.000
Lock Shift 4.700
Loop Gain  11.126
Loop Time  0.064
Loop Filter 745.449
Gas Flow   external

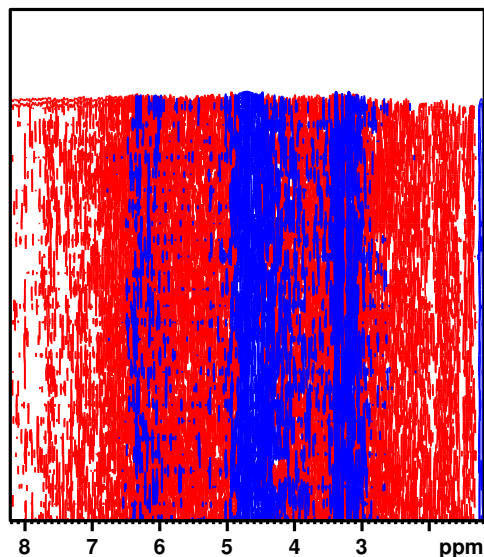
===== F1 INDIRECT DIMENSION =====
td1      26
sw_F1    9.946224

F1 - Acquisition parameters
TD        26
SF01      750.3035 MHz
FIDRES    574.052795 Hz
SW        9.946 ppm
FnMODE    QF (no-frequency)

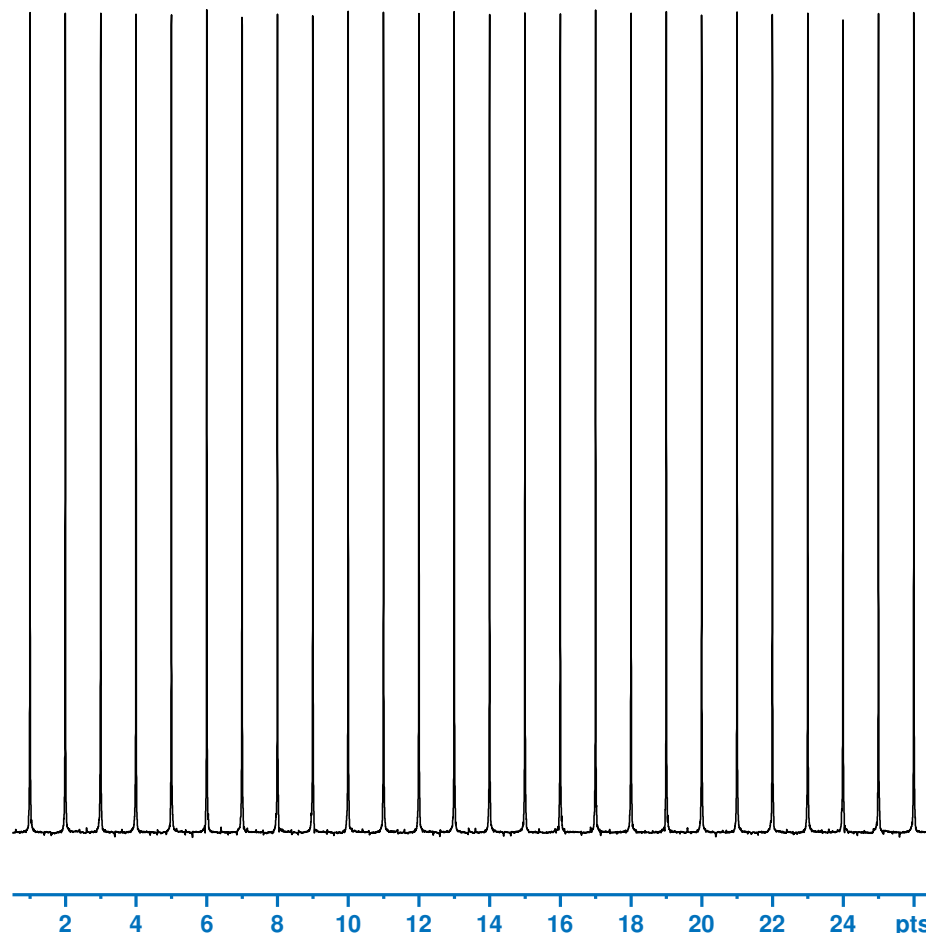
F2 - Processing parameters
SI        32768
SF        750.3000000 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        0.40

F1 - Processing parameters
SI        32
MC2       QF (no-frequency)
SF        750.3000000 MHz
WDW       no
SSB       0
LB        0 Hz
GB        0

SHIM SEQUENCE
skip shimming
```



NO	Rec. Delay	Scaled Int.	B0-Shift [Hz]	+APK0	Scaled Sino
1	10.00 us	99.87	1.33	-0.80	102.60
2	15.85 us	99.79	1.32	-1.60	113.98
3	25.12 us	99.73	1.25	0.00	108.09
4	39.81 us	99.62	1.28	0.60	112.08
5	63.10 us	99.59	1.12	-1.40	98.81
6	100.0 us	100.20	1.07	-0.20	108.12
7	158.5 us	99.23	0.96	-0.20	108.70
8	251.2 us	99.61	0.91	-1.10	98.85
9	398.1 us	99.53	0.96	-0.30	103.94
10	630.9 us	100.00	0.89	-1.70	93.31
11	1.000 ms	99.85	0.83	-1.00	104.48
12	1.585 ms	99.84	0.73	-1.20	111.47
13	2.512 ms	100.07	0.76	-0.10	92.63
14	3.981 ms	99.75	0.63	-1.00	115.84
15	6.310 ms	99.78	0.71	0.30	113.48
16	10.00 ms	99.73	0.54	-0.30	100.56
17	15.85 ms	100.15	0.60	-0.40	117.80
18	25.12 ms	99.92	0.42	-0.60	116.62
19	39.81 ms	99.96	0.39	-0.80	115.54
20	63.10 ms	99.66	0.48	-0.70	98.87
21	0.100 s	99.91	0.29	-1.20	103.93
22	0.158 s	99.64	0.19	-0.40	91.96
23	0.251 s	99.91	0.24	-1.40	92.66
24	0.398 s	98.95	0.17	-0.30	113.35
25	0.631 s	99.73	0.11	-0.20	111.12
26	1.000 s	100.00	0.00	0.00	100.00



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: 0.1 mg/ml Gadolinium Chloride, 0.1% Methanol-13C, 1% H2O in D2O (50 ul) (Z142231)
 Gradient recovery test for Z-direction [-] (NPT_1H_gradrecZ_sqn_1h, spin rate 4000 Hz)
 Gradient amplifier: Internal Gradient Amplifier, shape: RECT.1, amplitude: -3.9 A (39.0 % of probe maximum)



Bruker BioSpin

NPT_1H_gradrecZ_sqn_1h

```
Current Data Parameters
NAME      NPT_1H_gradrecZ_sqn_1h
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20240904
Time      15.06 h
INSTRUM   Avance NEO
PROBHD    Z180004_0001 (
PULPROG   npt_gradrecvd
TD         30444
SOLVENT   D2O
NS         1
DS         2
SWH        5555.556 Hz
FIDRES     0.364969 Hz
AQ         2.7399600 sec
RG         101
DW         90.000 usec
DE         20.00 usec
TE         298.0 K
D0         0 sec
D1         5.00000000 sec
D11        0.03000000 sec
D12        0.00005000 sec
VDLIST     npt_gradrec
vd_list    0.00001000 sec
SF01       750.3035264 MHz
NUC1       1H
P1         10.00 usec
PLW1       11.37899971 W
GPNAM[1]   RECT.1
GPZ1       -39.00 %
P16        1000.00 usec

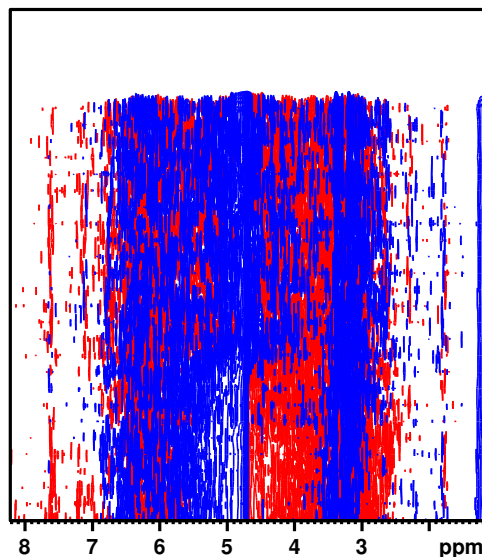
===== F1 INDIRECT DIMENSION =====
td1        26
sw_F1      9.946224

F1 - Acquisition parameters
TD         26
SF01       750.3035 MHz
FIDRES     574.052795 Hz
SW         9.946 ppm
FnMODE     QF (no-frequency)

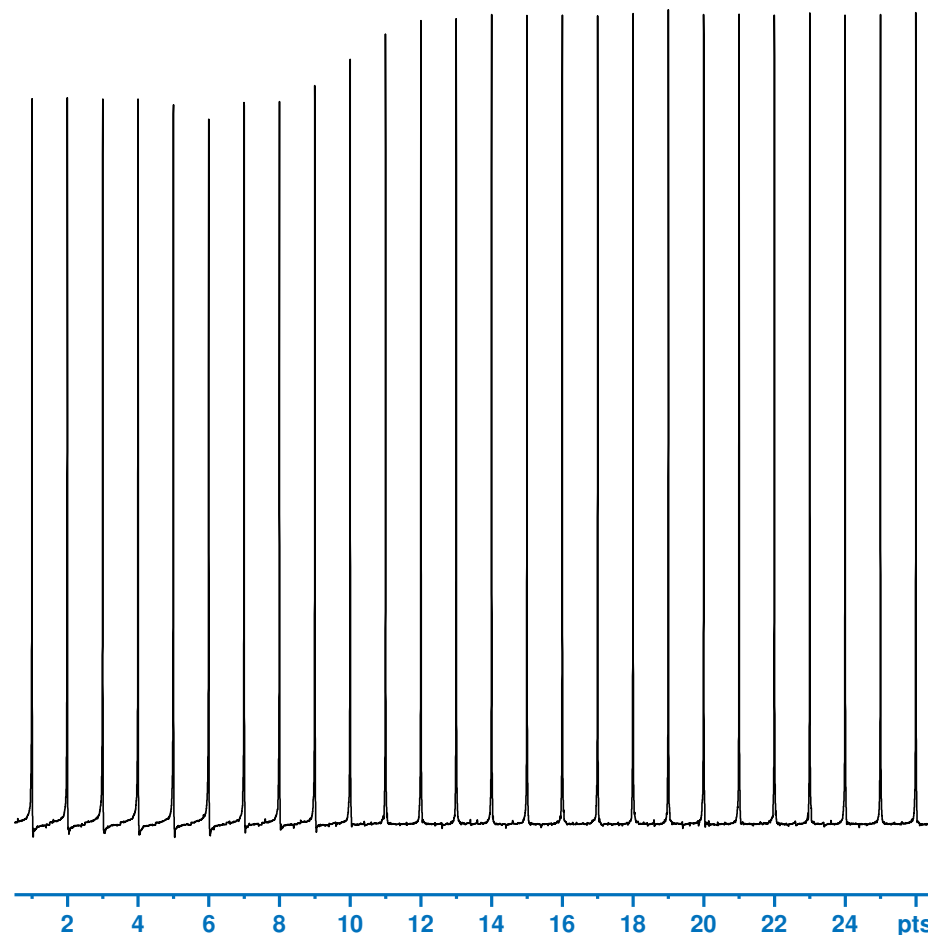
F2 - Processing parameters
SI         32768
SF         750.3000000 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         0.40

F1 - Processing parameters
SI         32
MC2        QF (no-frequency)
SF         750.3000000 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0

SHIM SEQUENCE
skip shimming
```



NO	Rec. Delay	Scaled Int.	B0-Shift [Hz]	+APK0	Scaled Sino
1	10.00 us	89.32	1.36	10.10	82.12
2	15.85 us	89.55	1.34	9.20	77.84
3	25.12 us	89.41	1.21	9.80	77.78
4	39.81 us	89.42	1.16	10.20	93.84
5	63.10 us	88.68	1.11	7.80	83.55
6	100.0 us	86.90	1.14	9.70	80.19
7	158.5 us	88.88	0.94	5.30	77.07
8	251.2 us	89.02	0.96	6.10	79.84
9	398.1 us	90.91	0.95	4.50	88.33
10	630.9 us	94.23	0.86	1.70	79.30
11	1.000 ms	97.28	0.74	-0.40	87.69
12	1.585 ms	98.98	0.68	-1.40	77.01
13	2.512 ms	99.30	0.60	-2.30	76.98
14	3.981 ms	99.77	0.54	0.10	76.75
15	6.310 ms	99.67	0.49	0.00	89.63
16	10.00 ms	99.61	0.48	-1.60	75.47
17	15.85 ms	99.51	0.34	0.20	85.92
18	25.12 ms	99.91	0.34	-2.80	76.16
19	39.81 ms	100.28	0.26	-1.70	85.69
20	63.10 ms	99.66	0.36	0.00	86.59
21	0.100 s	99.80	0.17	-0.50	85.23
22	0.158 s	99.68	0.15	-0.30	90.17
23	0.251 s	99.85	0.12	-1.20	87.58
24	0.398 s	99.72	0.04	-0.60	87.27
25	0.631 s	99.69	-0.06	-1.20	87.34
26	1.000 s	100.00	0.00	0.00	100.00



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
Sample: 0.1 mg/ml Gadolinium Chloride, 0.1% Methanol-13C, 1% H2O in D2O (50 ul) (Z142231)
Gradient recovery test for Z-direction [+] (NPT_1H_gradrecZ_sq_1h, spin rate 4000 Hz)
Gradient amplifier: Internal Gradient Amplifier, shape: RECT.1, amplitude: 3.9 A (39.0 % of probe maximum)



Bruker BioSpin

NPT_1H_gradrecZ_sq_1h

```
Current Data Parameters
NAME      NPT_1H_gradrecZ_sq_1h
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20240904
Time      15.00 h
INSTRUM   Avance NEO
PROBHD    Z180004_0001 (
PULPROG   npt_gradrecv
TD         30444
SOLVENT   D2O
NS         1
DS         2
SWH        5555.556 Hz
FIDRES     0.364969 Hz
AQ         2.7399600 sec
RG         101
DW         90.000 usec
DE         20.00 usec
TE         298.0 K
D0         0 sec
D1         5.00000000 sec
D11        0.03000000 sec
D12        0.00005000 sec
VDLIST     npt_gradrec
vd_list    0.00001000 sec
SF01       750.3035261 MHz
NUC1       1H
P1         10.00 usec
PLW1       11.37899971 W
GPNAM[1]   RECT.1
GPZ1       39.00 %
P16        1000.00 usec

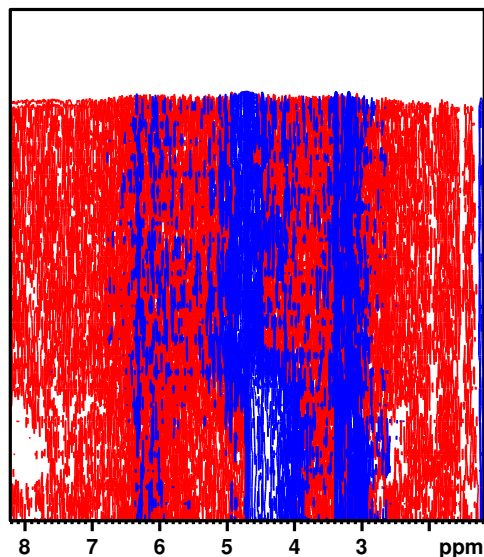
===== F1 INDIRECT DIMENSION =====
td1        26
sw_F1      9.946224

F1 - Acquisition parameters
TD         26
SF01       750.3035 MHz
FIDRES     574.052795 Hz
SW         9.946 ppm
FnMODE     QF (no-frequency)

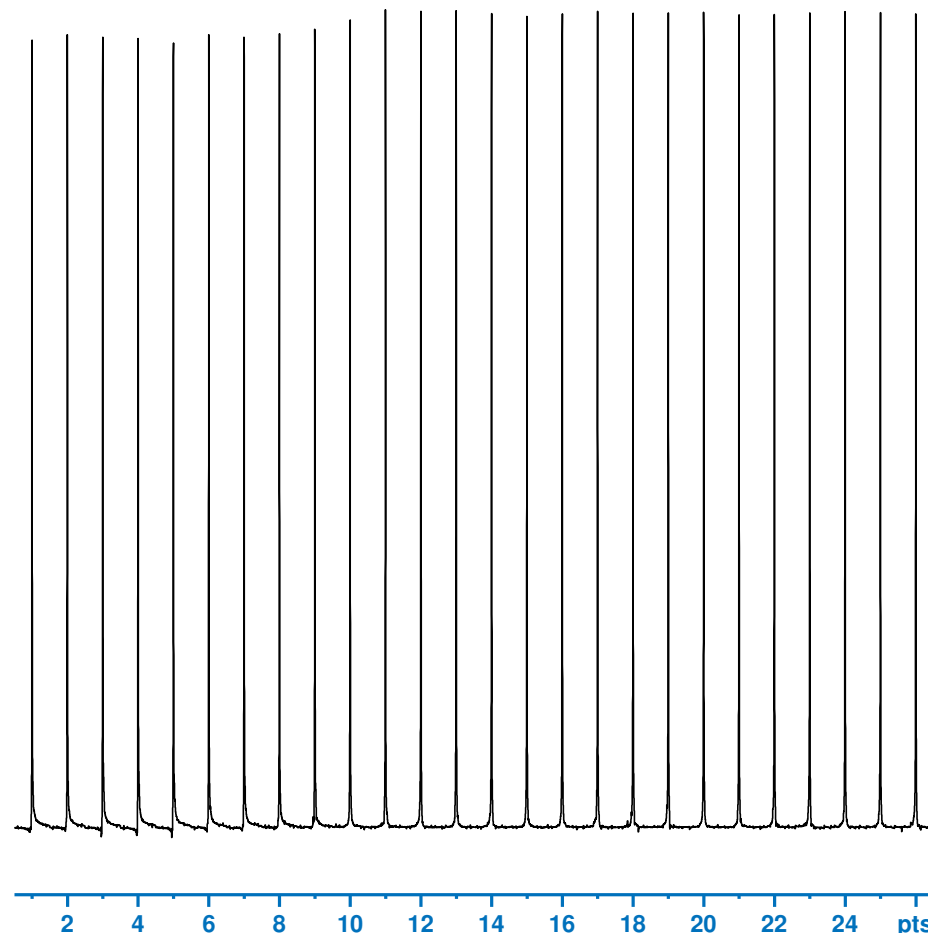
F2 - Processing parameters
SI         32768
SF         750.3000000 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         0.40

F1 - Processing parameters
SI         32
MC2        QF (no-frequency)
SF         750.3000000 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0

SHIM SEQUENCE
skip shimming
```



EVALUATION RESULTS OF GRADIENT RECOVERY MEASUREMENT					
NO	Rec. Delay	Scaled Int.	B0-Shift [Hz]	+APK0	Scaled Sino
1	10.00 us	96.75	1.07	-12.00	86.99
2	15.85 us	97.44	1.12	-9.60	79.26
3	25.12 us	97.10	1.06	-11.03	81.03
4	39.81 us	96.94	0.92	-12.00	78.07
5	63.10 us	96.57	0.91	-11.50	84.18
6	100.0 us	97.42	0.83	-9.70	83.68
7	158.5 us	97.12	0.82	-9.30	77.48
8	251.2 us	97.61	0.77	-7.60	91.27
9	398.1 us	98.07	0.64	-6.00	91.42
10	630.9 us	99.28	0.80	-2.30	73.72
11	1.000 ms	100.47	0.73	-1.80	84.91
12	1.585 ms	100.40	0.55	0.30	79.87
13	2.512 ms	100.37	0.61	-1.60	83.73
14	3.981 ms	100.02	0.46	-0.50	90.25
15	6.310 ms	99.66	0.44	-1.80	91.89
16	10.00 ms	99.98	0.44	-1.80	77.45
17	15.85 ms	100.28	0.42	0.40	89.89
18	25.12 ms	100.07	0.21	-1.40	77.31
19	39.81 ms	100.23	0.18	-0.10	95.73
20	63.10 ms	100.22	0.20	-1.00	101.73
21	0.100 s	99.87	0.18	-1.80	87.82
22	0.158 s	99.86	0.06	-1.00	97.68
23	0.251 s	100.05	0.10	0.40	82.48
24	0.398 s	100.24	0.04	-0.30	95.81
25	0.631 s	100.11	-0.08	-1.20	90.64
26	1.000 s	100.00	0.00	0.00	100.00



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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)
 1H B1 homogeneity integral (NPT_1H_b1homogeneityInt_1h, spin rate 4000 Hz)
 P0 = 10.00 us (PDelay = 0.60 us), PLW1 = 11.4 W
 Number of Steps: [3x13] Stepsize: [10 deg] VP List Increment: [1.11 us] 90deg Range: [30 deg to 150 deg, 3.3 us to 16.7 us]
 450deg Range: [390 deg to 510 deg, 40.9 us to 54.3 us] 810deg Range: [750 deg to 870 deg, 82.7 us to 96.1 us]



Bruker BioSpin

NPT_1H_b1homogeneityInt_1h

1H B1 homogeneity amplitude [achieved]: at 450 deg [68.8%] <n/a>
 1H B1 homogeneity amplitude [achieved]: at 810 deg [50.4%] <n/a>
 1H B1 homogeneity integral [achieved]: at 450 deg [60.8%] <n/a>
 1H B1 homogeneity integral [achieved]: at 810 deg [44.7%] <n/a>

```
Current Data Parameters
NAME      NPT_1H_b1homogeneityInt_1h
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20240904
Time      11.08 h
INSTRUM   Avance NEO
PROBHD    Z180004_0001 (
PULPROG   npt_plb1hom2d
TD         1024
SOLVENT    DMSO
NS         1
DS         4
SWH        230.766 Hz
FIDRES     0.450714 Hz
AQ         2.2187009 sec
RG         45.2
DW         2166.700 usec
DE         20.00 usec
TE         298.0 K
D1         7.31640005 sec
D12        0.00002000 sec
Plist      20.00 usec
TDav       1

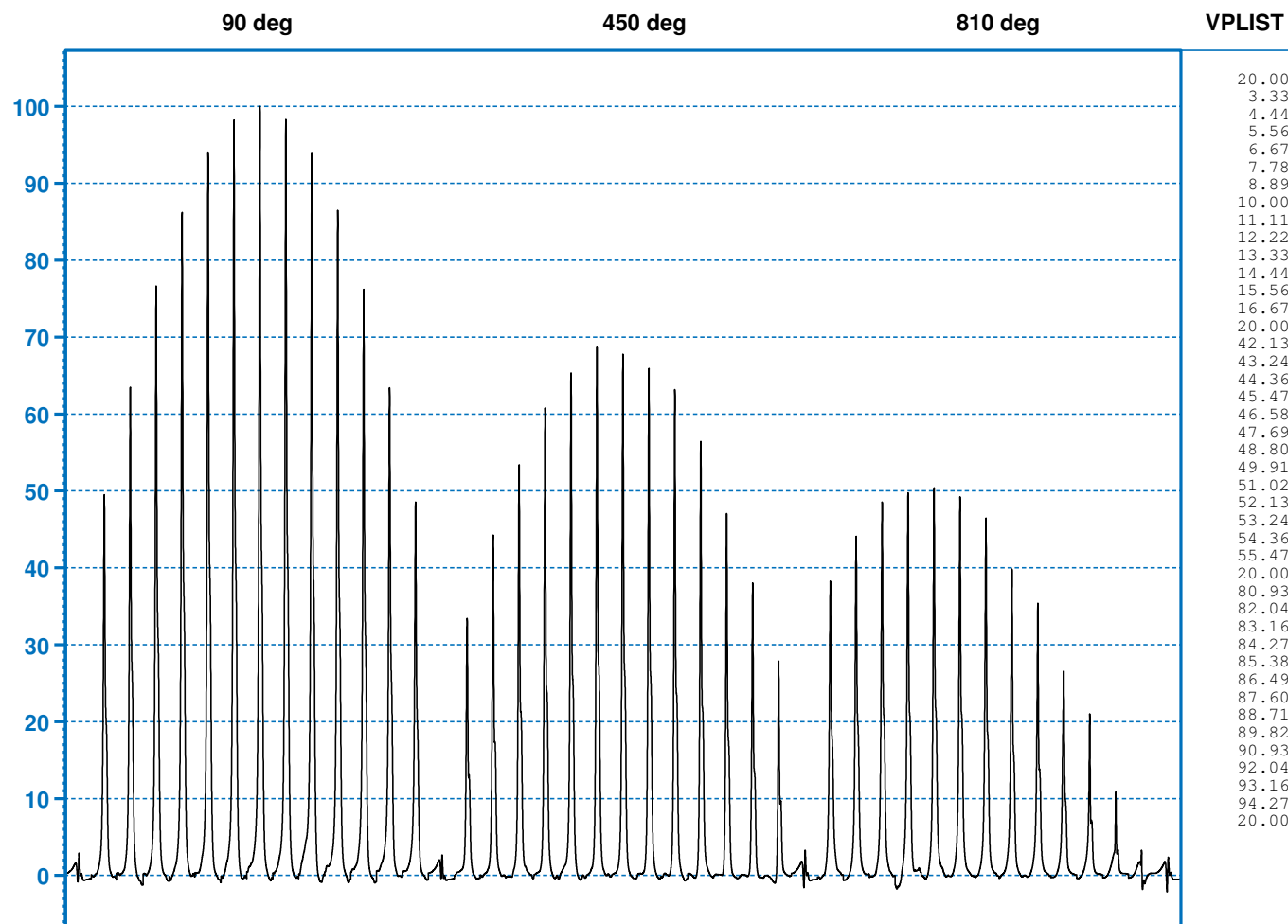
===== F1 INDIRECT DIMENSION =====
td1        43
sw_F1      1110.623779

F1 - Acquisition parameters
TD         43
SF01       750.3041 MHz
FIDRES     38758.398438 Hz
SW         1110.624 ppm
FMODE      QF(no-frequency)

F2 - Processing parameters
SI         4096
SF         750.3000000 MHz
WDW         EM
SSB         0
LB         1.00 Hz
GB         0
PC         0.40

F1 - Processing parameters
SI         64
MC2         QF(no-frequency)
SF         750.3000000 MHz
WDW         no
SSB         0
LB         0 Hz
GB         0

SHIM SEQUENCE
skip shimming
```



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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)
 13C B1 homogeneity integral (NPT_1H_b1homogeneityInt_13c, spin rate 4000 Hz)
 P3=10.00 us (PDelay=0.20 us), PLW2=70.2 W
 Number of Steps: [3x13] Stepsize: [10 deg] VPListIncrement: [1.11us] 0deg_Range: [60 deg to 0 deg to 60 deg, 6.7 us to 0 us to 6.7 us]
 360deg_Range: [300 deg to 420 deg, 33.0us to 46.4us] 720deg_Range: [660 deg to 780 deg, 52.8 us to 66.2 us]

13C B1 homogeneity amplitude [achieved]: at 360 deg [90.5%] <n/a>
 13C B1 homogeneity amplitude [achieved]: at 720 deg [76.8%] <n/a>
 13C B1 homogeneity integral [achieved]: at 360 deg [81.8%] <n/a>
 13C B1 homogeneity integral [achieved]: at 720 deg [71.2%] <n/a>



Bruker BioSpin

NPT_1H_b1homogeneityInt_13c

```
Current Data Parameters
NAME      NPT_1H_b1homogeneityInt_13c
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20240904
Time      11.23 h
INSTRUM   Avance NEO
PROBHD    Z180004_0001 (
PULPROG   npt_p3b1hom2d
TD         1024
SOLVENT    DMSO
NS         1
DS         4
SWH        230.766 Hz
FIDRES     0.450714 Hz
AQ         2.2187009 sec
RG         45.2
DW         2166.700 usec
DE         20.00 usec
TE         298.0 K
CNST2     139.0000000
D1         9.68512535 sec
D2         0.00359712 sec
D12        0.00002000 sec
Plist      10.00 usec
TDav       1
SF01       750.3023011 MHz
NUC1       1H
P1         3.33 usec
PLW1       11.37899971 W

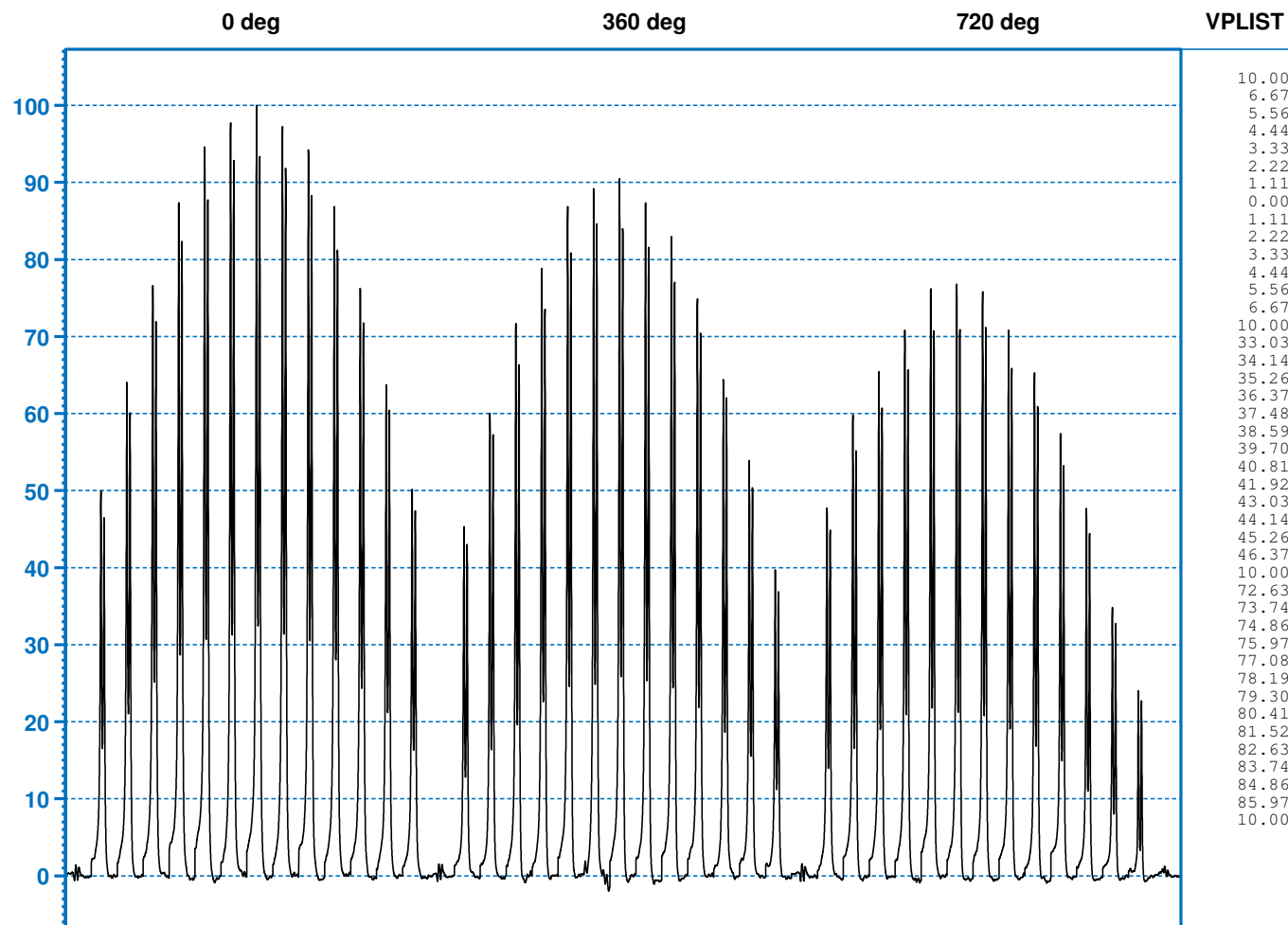
===== F1 INDIRECT DIMENSION =====
td1        43
sw_F1      1110.623779

F1 - Acquisition parameters
TD          43
SF01        750.3023 MHz
FIDRES      38758.304688 Hz
SW          1110.624 ppm
FnMODE      QF(no-frequency)

F2 - Processing parameters
SI          4096
SF          750.3000000 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          0.50

F1 - Processing parameters
SI          64
MC2         QF(no-frequency)
SF          750.3000000 MHz
WDW         no
SSB         0
LB          0 Hz
GB          0

-----
SHIM SEQUENCE
-----
skip shimming
-----
```



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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)
 2H B1 homogeneity integral (NPT_prep_b1homogeneityInt_d, spin rate 4000 Hz)
 P0 = 500.00 us (PDelay = 52.50 us), PLW1 = 104 mW
 Number of Steps: [3x13] Stepsize: [10 deg] VP List Increment: [55.56 us] 90deg Range: [30 deg to 150 deg, 166.7 us to 833.3 us]
 450deg Range: [390 deg to 510 deg, 1956.7 us to 2623.3 us] 810deg Range: [750 deg to 870 deg, 4114.2 us to 4780.8 us]

2H B1 homogeneity amplitude [achieved]: at 450 deg [72.4%] <n/a>
 2H B1 homogeneity amplitude [achieved]: at 810 deg [63.9%] <n/a>
 2H B1 homogeneity integral [achieved]: at 450 deg [71.3%] <n/a>
 2H B1 homogeneity integral [achieved]: at 810 deg [59.8%] <n/a>



Bruker BioSpin

NPT_prep_b1homogeneityInt_d

```
Current Data Parameters
NAME      NPT_prep_b1homogeneityInt_d
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20240904
Time      10.50 h
INSTRUM   Avance NEO
PROBHD    Z180004_0001 (
PULPROG   npt_p1blhom2hd
TD         1024
SOLVENT    DMSO
NS         1
DS         4
SWH        230.766 Hz
FIDRES     0.450714 Hz
AQ         2.2187009 sec
RG         45.2
DW         2166.700 usec
DE         6.50 usec
TE         298.0 K
D1         4.43079996 sec
D11        0.03000000 sec
D12        0.00002000 sec
D20        0.50000000 sec
Plist      1000.00 usec
TDav       1

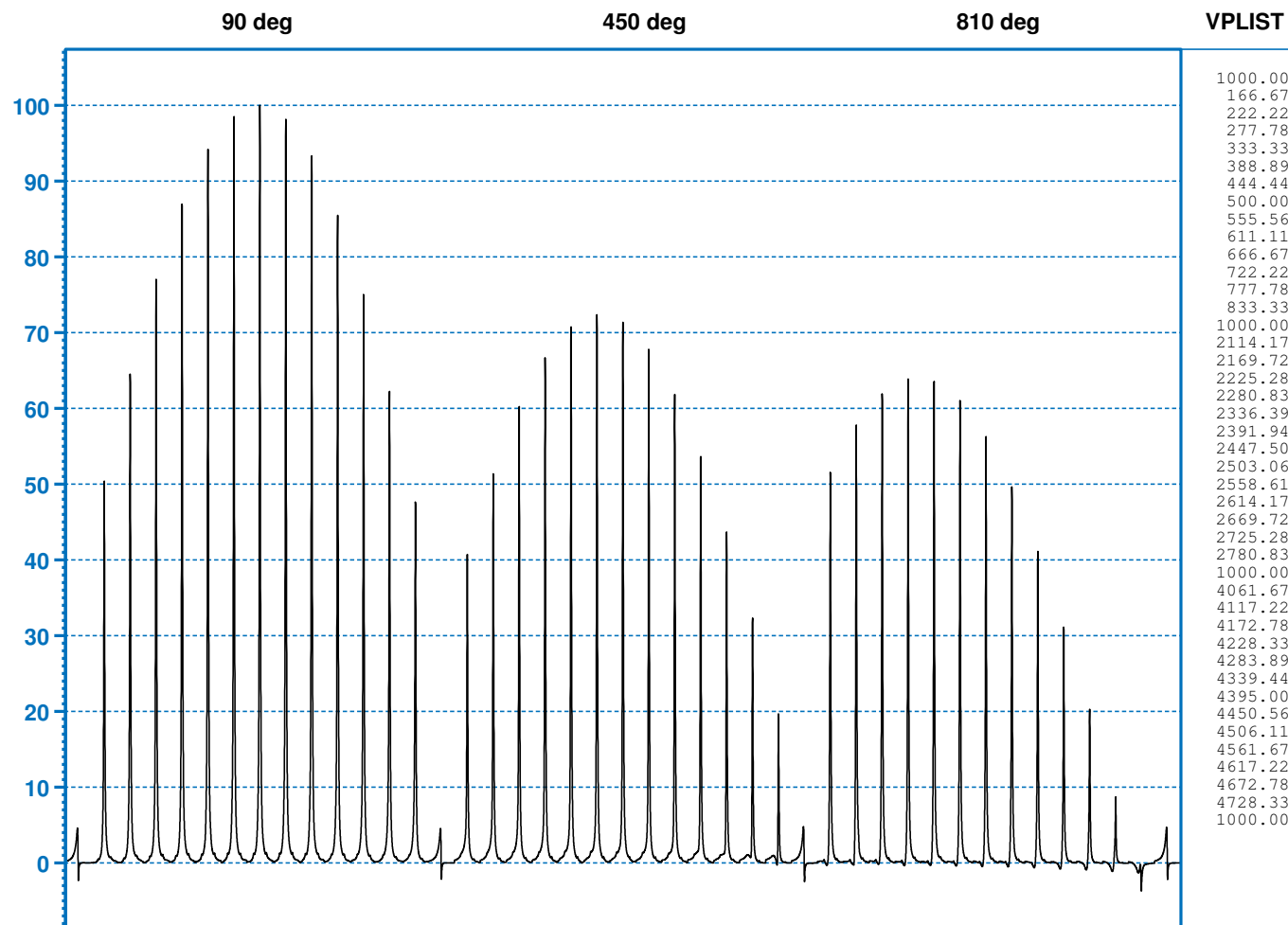
===== F1 INDIRECT DIMENSION =====
td1        43
sw_F1      542.630371

F1 - Acquisition parameters
TD         43
SF01       115.1759 MHz
FIDRES     2906.879883 Hz
SW         542.630 ppm
FnMODE     QF (no-frequency)

F2 - Processing parameters
SI         4096
SF         115.1756183 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         0.40

F1 - Processing parameters
SI         64
MC2        QF (no-frequency)
SF         115.1756183 MHz
WDW        no
SSB        0
LB         0 Hz
GB         0

SHIM SEQUENCE
- topshim hrmas lockoff solvent=DMSO O1P=2.49 <pass>
```



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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)
 Optimization of 2H locksetting (NPT_prep_locksettings_d, spin rate 4000 Hz)
 Update of edlock [active] for SOLVENT: H2O+D2O
 Modification: [LOCKPHASE = 334.5, LOCKGAIN = 110.00, LOOPGAIN = -9.19, LOOPTIME = 0.456, LOOPFILTER = 49.1]



Bruker BioSpin

NPT_prep_locksettings_d

Current LOCK Settings (according to 2Hlock)						
Solvent	FIELD	LOCKPOWER	LOOPGAIN	LOOPTIME	LOOPFILTER	LOCKPHASE
H2O+D2O	1012.1	-18.0	-9.2	0.4557	49.1	334.5

Current Data Parameters
 NAME NPT_prep_locksettings_d
 EXPNO 1
 PROCNO 1
 Date 20240903 13.07 h

SHIM SEQUENCE
 skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: 0.1 mg/ml Gadolinium Chloride, 0.1% Methanol-13C, 1% H2O in D2O (50 ul) (Z142231)
 Vibration Test using Doped Water Sample (NPT_1H_vibration_doped_water, spin rate 4000 Hz)

Linewidth at 50% of signal height [achieved/rated]: [3.4 Hz <= 4.5 Hz] <pass>
 SINO (4000 Hz) [achieved]: Noise (11.0 to 5.7 ppm) [1842.0] <n/a>
 Maximum of STD found at 171.2 Hz [achieved]: over the range 30.0 Hz to 250.0 Hz [2654.6] <n/a>
 Maximum of STD found at 1214.3 Hz [achieved]: over the range 250.0 Hz to 2000.0 Hz [418.3] <n/a>
 Maximum of STD found at 2191.8 Hz [achieved]: over the range 2000.0 Hz to 4800.0 Hz [74.5] <n/a>



Bruker BioSpin

NPT_1H_vibration_doped_water

Current Data Parameters
 NAME NPT_1H_vibration_doped_water
 EXPNO 1
 PROCNO 1
 Date 20240904 14.44 h

Additional Parameters

Field 1011.988
 Lock Phase 48.358
 Lock Power -18.000
 Lock Gain 88.732
 Lock DC -70.000
 Lock Shift 4.700
 Loop Gain -17.900
 Loop Time 0.681
 Loop Filter 20.000
 Gas Flow external

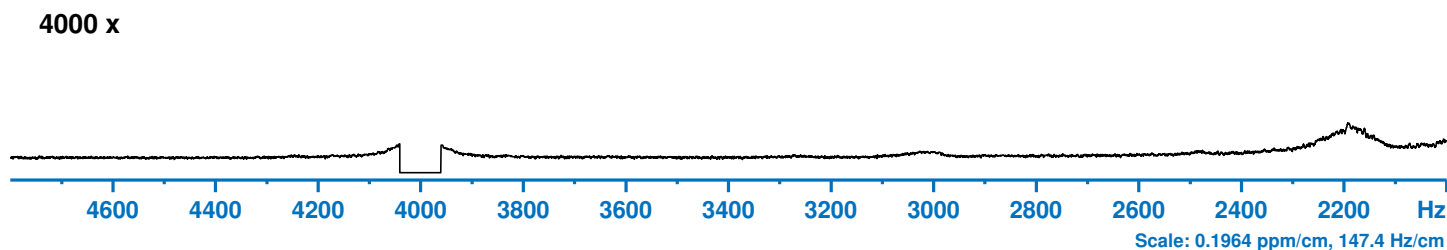
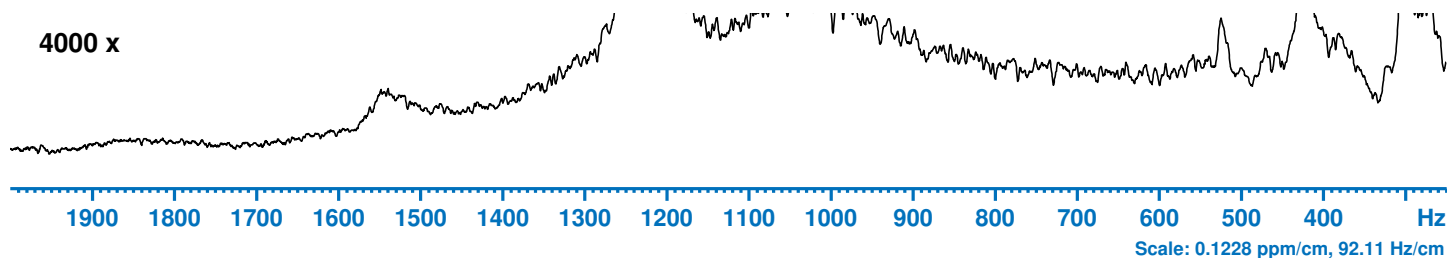
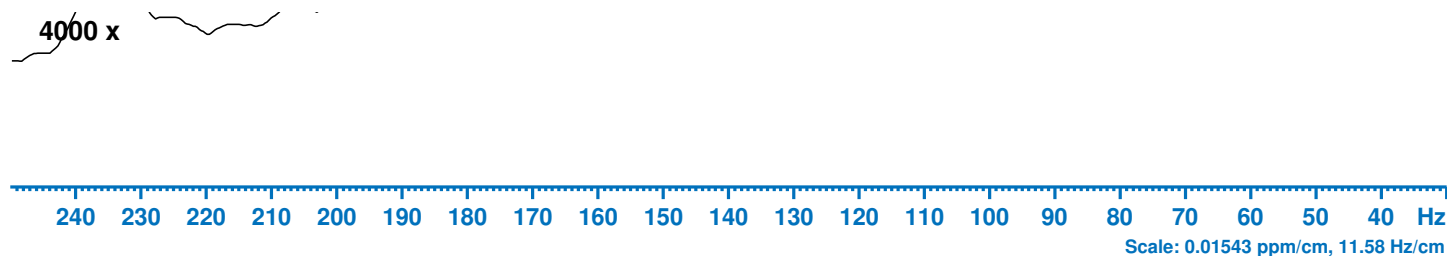
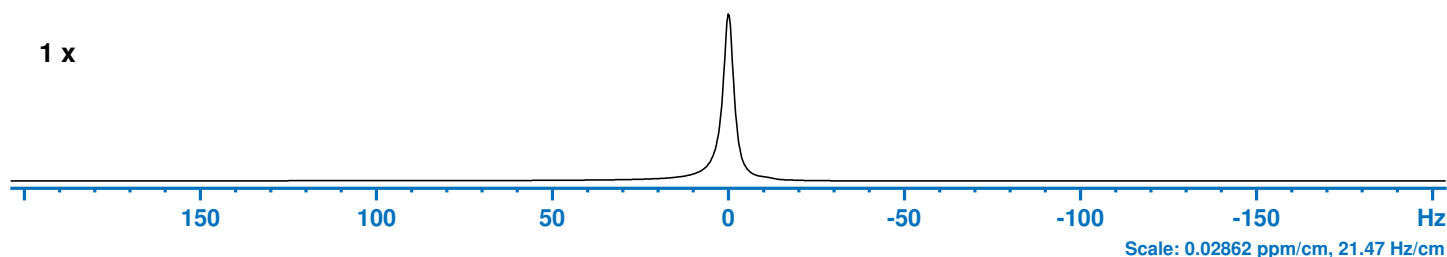
Range	30 Hz to	250 Hz
Peak	Freq [Hz]	STD [ppm]
1	171.2	2654.6
2	62.5	1376.2
3	44.8	1260.3
4	47.9	1236.0
5	128.1	1221.5
6	34.4	916.6
7	86.7	497.5
8	98.4	460.8

Range	250 Hz to	2000 Hz
Peak	Freq [Hz]	STD [ppm]
1	1214.3	418.3
2	1220.7	396.5
3	1204.2	393.8
4	1207.5	392.0
5	1228.6	367.8
6	1196.3	363.6
7	1237.8	336.7
8	1190.0	325.3

Range	2000 Hz to	4800 Hz
Excluded	3960 Hz to	4040 Hz
Peak	Freq [Hz]	STD [ppm]
1	2191.8	74.5
2	2181.6	70.0
3	2175.3	68.1
4	2159.4	66.6
5	2171.2	66.8
6	2205.0	64.6
7	2201.5	64.1
8	2213.1	62.0

SHIM SEQUENCE

skip shimming



NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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 [9.0 us @ 128.7 W].

P90 HRMAS 79Br pulse [achieved/rated]: @ 130.7 W [8.9 us <= 9.0 us] <pass>



Bruker BioSpin

NPT_79Br_HRMAS_p90det_79br

Current Data Parameters
 NAME NPT_79Br_HRMAS_p90det_79br
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240903
 Time 12.02 h
 INSTRUM Avance NEO
 PROBHD Z180004_0001 (Z151220)
 PULPROG zgpg30
 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
 SF01 187.9912343 MHz
 NUC1 79Br
 P1 27.00 usec
 PLW1 130.67900085 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
105.8 W	10.0 us		
130.7 W	9.0 us	8.9 us	-0.8%

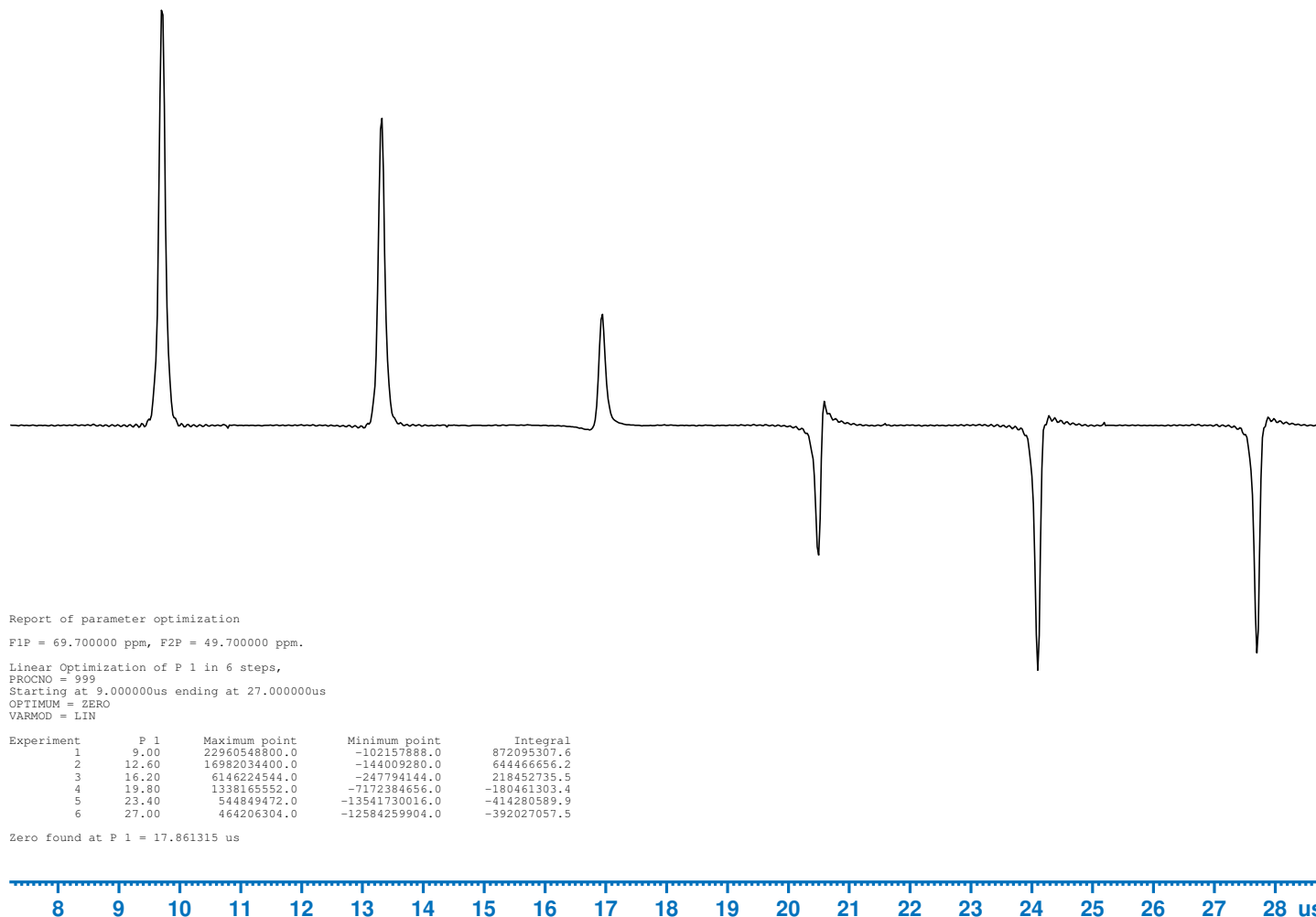
Report of parameter optimization

F1P = 69.700000 ppm, F2P = 49.700000 ppm.

Linear Optimization of P 1 in 6 steps,
 PROCNO = 999
 Starting at 9.000000us ending at 27.000000us
 OPTIMUM = ZERO
 VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	9.00	22960548800.0	-102157888.0	872095307.6
2	12.60	16982034400.0	-144009280.0	644466656.2
3	16.20	6146224544.0	-247794144.0	218452735.5
4	19.80	1338165552.0	-7172384656.0	-180461303.4
5	23.40	544849472.0	-13541730016.0	-414280589.9
6	27.00	464206304.0	-12584259904.0	-392027057.5

Zero found at P 1 = 17.861315 us



SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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]: [126 <= 130] <pass>
 Line width of side band number 4 (@ -15984 Hz) [achieved/rated]: [126 <= 130] <pass>
 Line width of side band number 7 (@ -27972 Hz) [achieved/rated]: [127 <= 140] <pass>
 Line width of side band number 10 (@ -39960 Hz) [achieved/rated]: [128 <= 150] <pass>



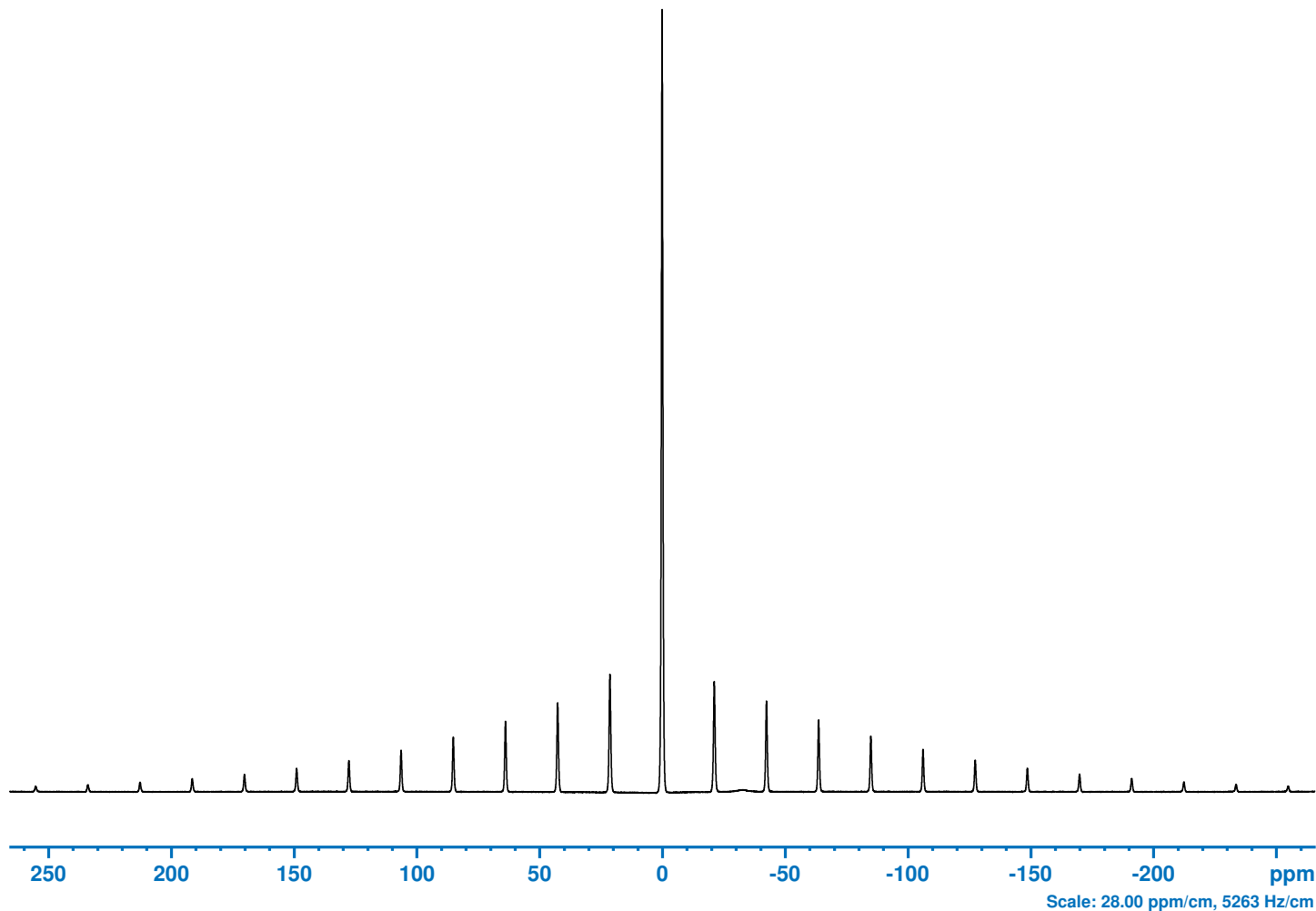
Bruker BioSpin

NPT_79Br_HRMAS_magicAngle

Current Data Parameters
 NAME NPT_79Br_HRMAS_magicAngle
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240903
 Time 12.43 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 187.9904764 MHz
 NUC1 79Br
 P1 9.00 usec
 PLW1 128.66999817 W

F2 - Processing parameters
 SI 131072
 SF 187.9904764 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.20



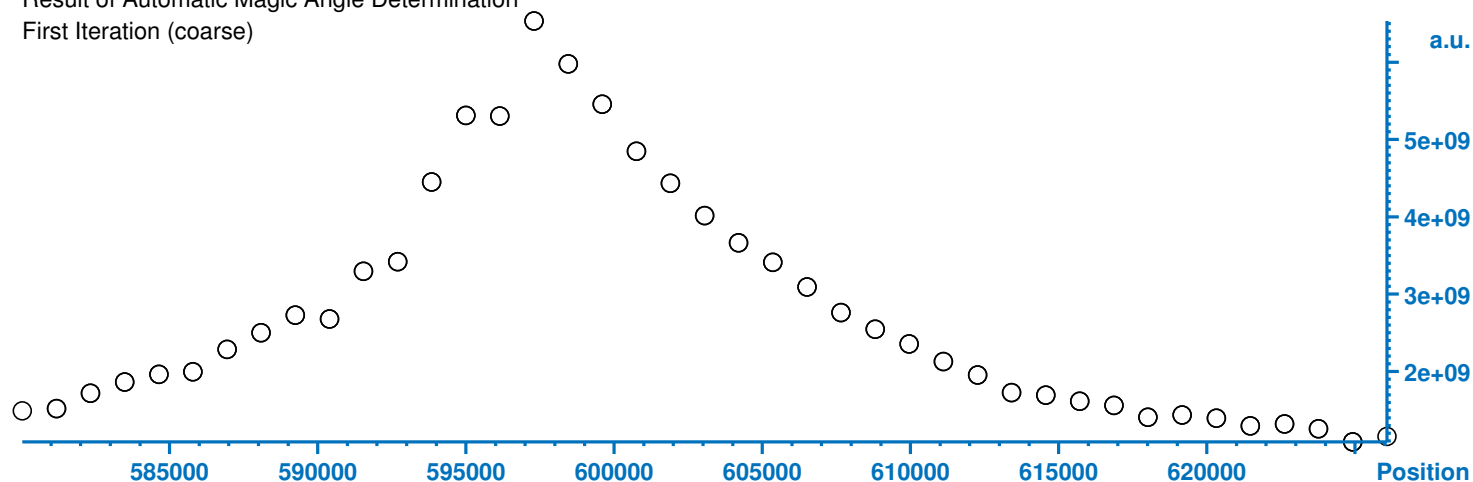
NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
 Magic Angle setting, HRMAS (NPT_79Br_HRMAS_magicAngle, spin rate 4000 Hz)



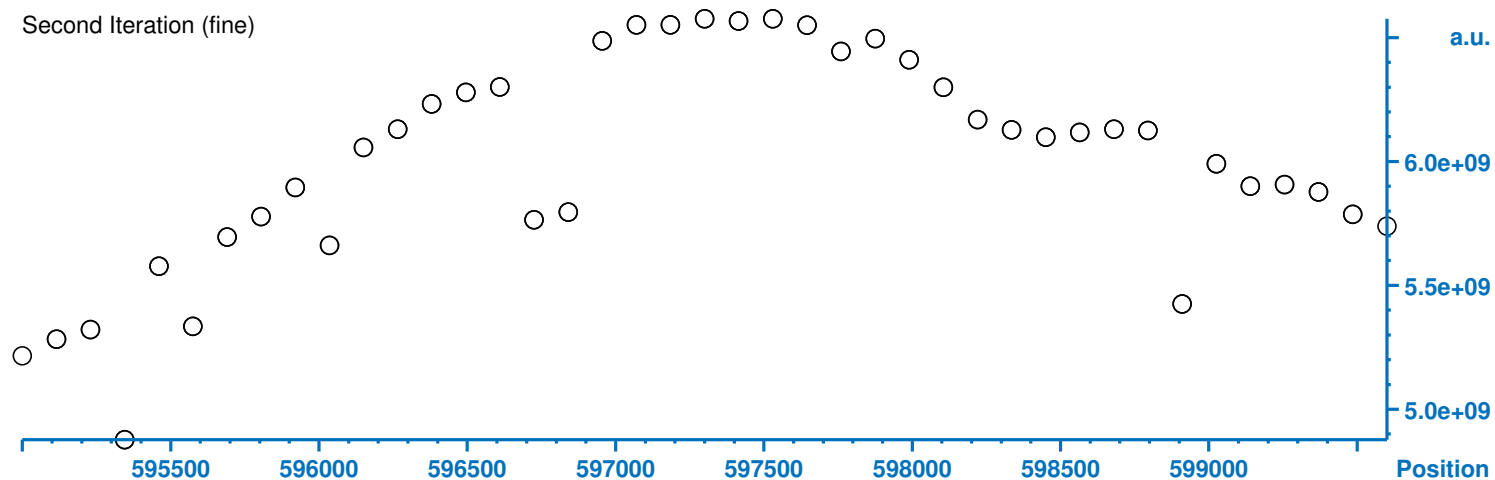
Bruker BioSpin

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 4.4.0
 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=2013/BearingPressure=2787/BearingSensePressure=2738/SupplyPressure=7486/SystemPressure=7342

Spin rate at maximum deviation [measured]: @ MASR 15000 Hz [14998 Hz]
 Maximum deviation [achieved/rated]: @ MASR 15000 Hz [2.000 Hz <= 5.000 Hz] <pass>



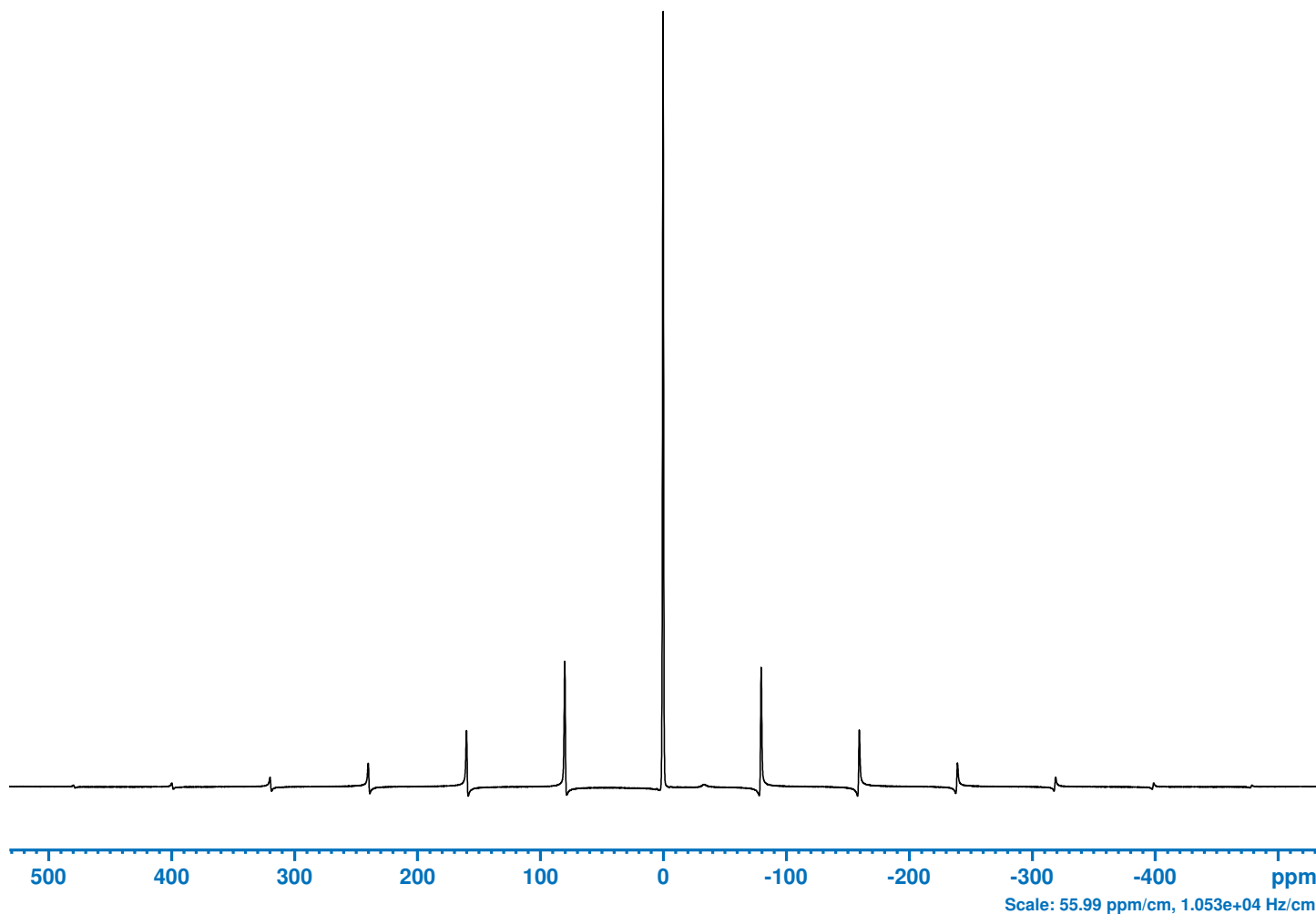
Bruker BioSpin

NPT_79Br_HRMAS_maxSpinRate

Current Data Parameters
 NAME NPT_79Br_HRMAS_maxSpinRate
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240903
 Time 12.33 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
 SFO1 187.9904007 MHz
 NUC1 79Br
 P1 9.00 usec
 PLW1 128.66999817 W

F2 - Processing parameters
 SI 16384
 SF 187.9904007 MHz
 WDW no
 SSB 0
 LB 0 Hz
 GB 0
 PC 0.20



● Additional PDFs of Report

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

750 MHz

Probe ID: Z180004_0001

Report Name: 2024-09-04

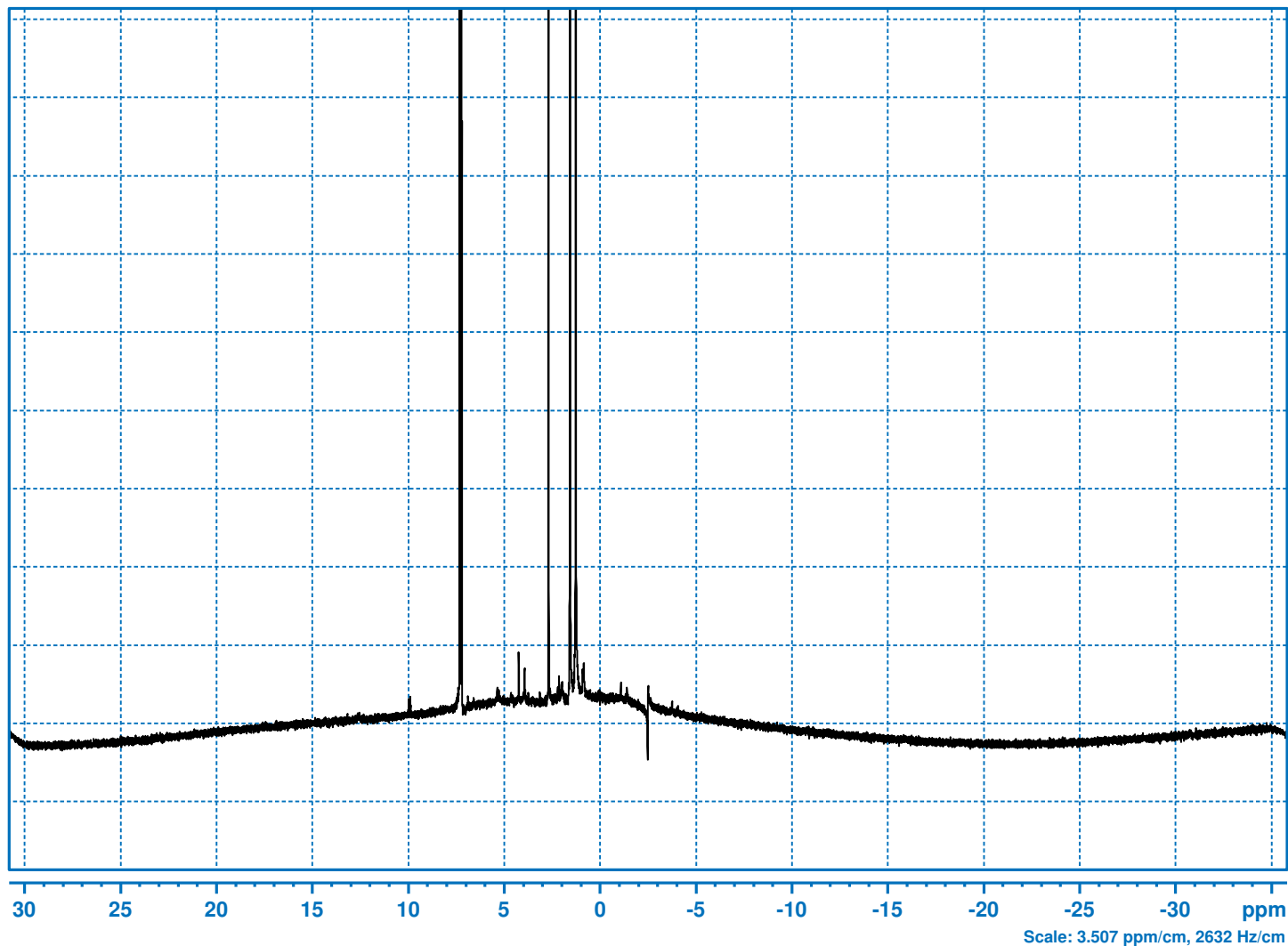
NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 Probe: Z180004_0001 PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
 Sample: 0.1% Ethylbenzene (EB) in Chloroform-D (50 ul) (Z142221)
 1H background with sample (NPT_1H_backgr_withsample, spin rate 4000 Hz)
 Flipangle = 45 degree

Background measurement (CY-scaling = 200.0 cm)



Bruker BioSpin

NPT_1H_backgr_withsample



Current Data Parameters
 NAME NPT_1H_backgr_withsample
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240904
 Time 13.33 h
 INSTRUM Avance NEO
 PROBHD z180004_0001 ()
 PULPROG npt_zg0
 TD 32768
 SOLVENT CDCl3
 NS 10
 DS 4
 SWH 50000.000 Hz
 FIDRES 3.051758 Hz
 AQ 0.3276800 sec
 RG 101
 DW 10.000 usec
 DE 20.00 usec
 TE 298.0 K
 D1 3.83732009 sec
 TD0 1
 SFO1 750.2981243 MHz
 NUC1 1H
 CNST10 45.0000000
 P0 5.00 usec
 P1 10.00 usec
 PLW1 11.37899971 W

Additional Parameters
 Field 1008.249
 Lock Phase 51.078
 Lock Power -27.000
 Lock Gain 117.588
 Lock DC -70.000
 Lock Shift 7.240
 Loop Gain -9.400
 Loop Time 0.464
 Loop Filter 50.000
 Gas Flow external

F2 - Processing parameters
 SI 32768
 SF 750.3000000 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

SHIM SEQUENCE
 skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (750.30 MHz) *** TopSpin 4.4.0
 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 (200.0 Hz) [achieved/rated]: Signal (3.00 to 2.00 ppm), Noise (3.34 to 3.07 ppm) [168.3 >= 110.0] <pass>



Bruker BioSpin

NPT_1H_sensitivity

Current Data Parameters
 NAME NPT_1H_sensitivity
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20240904
 Time 13.30 h
 INSTRUM Avance NEO
 PROBHD z180004_0001 (
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 1
 DS 0
 SWH 7462.687 Hz
 FIDRES 0.455486 Hz
 AQ 2.1954560 sec
 RG 101
 DW 67.000 usec
 DE 20.00 usec
 TE 298.0 K
 D1 113.57360077 sec
 TD0 1
 SF01 750.3030012 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 11.37899971 W

Additional Parameters
 Field 1008.357
 Lock Phase 51.078
 Lock Power -27.000
 Lock Gain 117.588
 Lock DC -70.000
 Lock Shift 7.240
 Loop Gain -9.400
 Loop Time 0.464
 Loop Filter 50.000
 Gas Flow external

F2 - Processing parameters
 SI 16384
 SF 750.3000175 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

 SHIM SEQUENCE
 skip shimming

