DRAFT

CP2.1 TXO 1200SA N/C-H-D-05 Z XT

1200 MHz

Probe ID: Z175498_0004

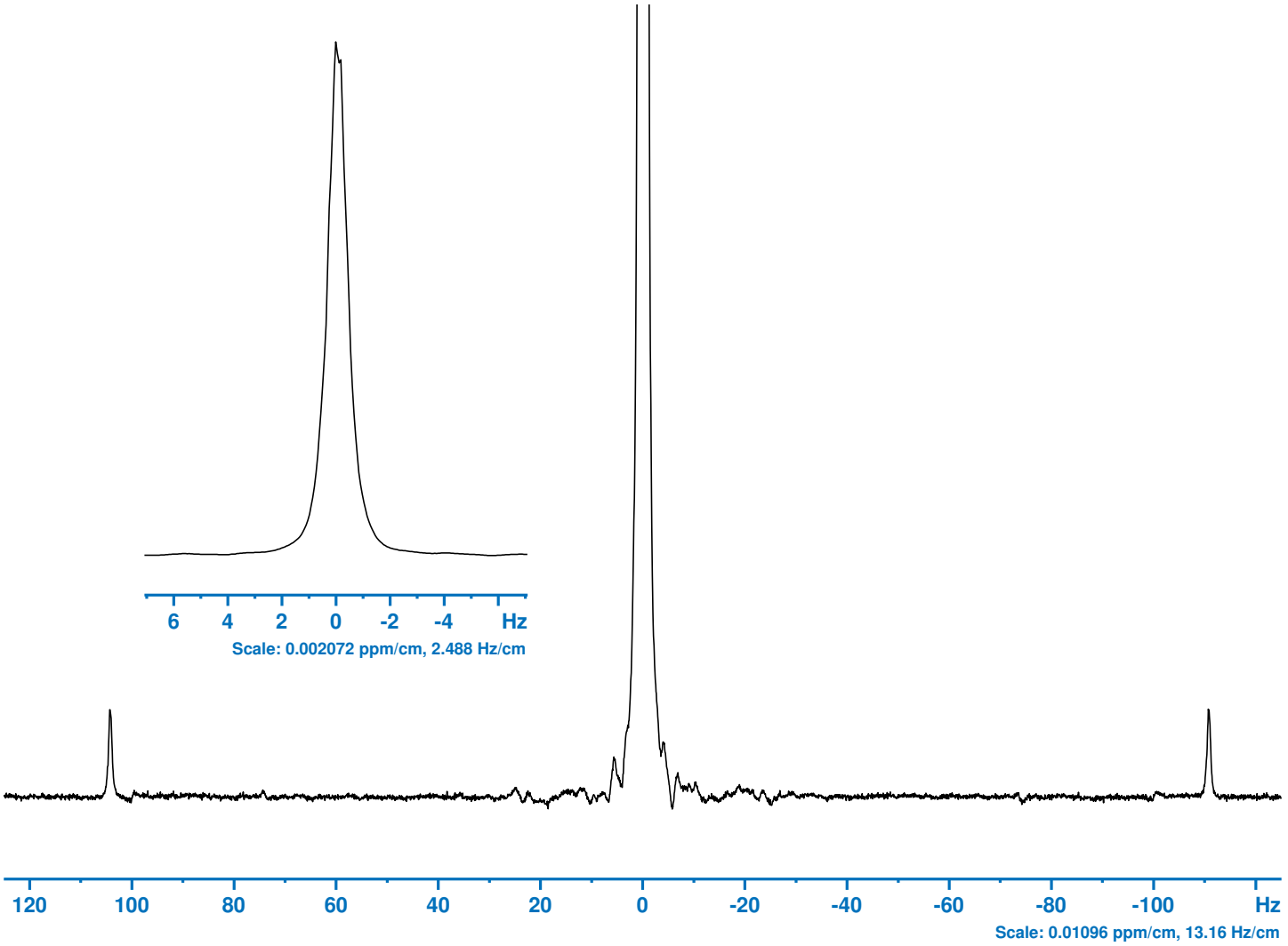
Inspection Lot: 2025-04-02

NMR TEST ACCEPTANCE

Apr 3, 2025

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)

Line width [achieved/rated]: at 0.11% of signal height [11.2 Hz <= 30.0 Hz] <pass>
Line width [achieved/rated]: at 0.55% of signal height [5.9 Hz <= 15.0 Hz] <pass>
Line width [achieved/rated]: at 50% of signal height [0.80 Hz <= 1.50 Hz] <pass>



Bruker BioSpin

NPT_1H_lineshape_nrot

```
Current Data Parameters
NAME       NPT_1H_lineshape_nrot
EXPNO                          4
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20250403
Time                      7.17 h
INSTRUM                  Avance
PROBHD     Z175498_0004 (CP2.1 TXO 1200SA N/C-H-
PULPROG                   zg30
TD                       32768
SOLVENT                Acetone
NS                             1
DS                             0
SWH                 1000.000 Hz
FIDRES                 0.061035 Hz
AQ                 16.3840000 sec
RG                           101
DW                     500.000 usec
DE                      10.00 usec
TE                      298.0 K
D1                  9.11600000 sec
TD0                            1
SFO1            1200.4093874 MHz
NUC1                        1H
P0                      3.33 usec
P1                      10.00 usec
PLW1                30.88200000 W

F2 - Processing parameters
SI                          8192
SF              1200.4096374 MHz
WDW                           no
SSB                            0
LB                          0 Hz
GB                             0
PC                          4.00

Additional Parameters

Field              -5680.034
Lock Phase           231.300
Lock Power           -34.000
Lock Gain             96.811
Lock DC              -61.000
Lock Shift             2.040
Loop Gain             15.133
Loop Time              0.047
Loop Filter         1468.000
Gas Flow             535 l/h
Atma Unit       Z147150_3250

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

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 0.3% Chloroform in Acetone-D6 (Z10701)
1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)

Bruker BioSpin

NPT_1H_lineshape_nrot

```
# Thu Apr  3 06:17:35 2025
#$$PROBEIDENTIFIER=Z175498_0004
#$$PROBENAME=CP2.1 TXO 1200SA N/C-H-D-05 Z XT
#$$MAGNETID=BZH 16'1200'78A
#$$CRYOSTATID=S'394'54-12394
#$$SHIMID=292722
#
# Active Shim Gradients
#
Z                       14172
Z2                      37783
Z3                       -505
Z4                       6322
Z5                       -565
Z6                       3136
Z7                     -21881
Z8                     -16145
X                       -7574
XZ                     -10221
XZ2                      4753
XZ3                      6250
XZ4                      4398
XZ5                      -5499
Y                       -1577
YZ                       7895
YZ2                      -5067
YZ3                      4320
YZ4                      4806
YZ5                     -14038
XY                      -2229
XYZ                     -7289
XYZ2                     2946
XYZ3                     595
XYZ4                     -7438
XYZ5                     -1442
(X2-Y2)                  396
(X2-Y2)Z                 6036
(X2-Y2)Z2                -4690
(X2-Y2)Z3                -14160
(X2-Y2)Z4                -2664
(X2-Y2)Z5                -776
X3                       -7107
X3Z                      -8167
Y3                       149
Y3Z                      -5536
#
# Lock Parameter
#
FIELD           -5680.034
LOCKPHASE         231.300
LOCKPOWER         -34.000
LOCKGAIN           96.811
LOCKDC           -61.000
LOCKSHIFT          2.040
LOOPGAIN          15.133
LOOPTIME           0.047
LOOPFILTER      1468.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1]     6990.96353313
SHIM_SETTING [ 2]    45788.84254245
SHIM_SETTING [ 3]     7024.39563122
SHIM_SETTING [ 4]   -24126.76162284
SHIM_SETTING [ 5]    12047.28581404
SHIM_SETTING [ 6]     8292.12653194
SHIM_SETTING [ 7]   -17176.84975968
SHIM_SETTING [ 8]    38540.60993519
SHIM_SETTING [ 9]    34326.82363527
SHIM_SETTING [10]   -12326.15972887
SHIM_SETTING [11]        0.00000000
SHIM_SETTING [12]     5685.54541028
SHIM_SETTING [13]    -5386.67083824
SHIM_SETTING [14]      514.11811976
SHIM_SETTING [15]    -5891.50304024
SHIM_SETTING [16]     7064.76030039
SHIM_SETTING [17]   -27415.23508835
SHIM_SETTING [18]    -2667.02252831
SHIM_SETTING [19]    -4536.23686268
SHIM_SETTING [20]     1248.60084142
SHIM_SETTING [21]   -10321.72924314
SHIM_SETTING [22]    -1018.14893303
SHIM_SETTING [23]    19442.27786272
SHIM_SETTING [24]    -6454.93062149
SHIM_SETTING [25]   -14129.13813184
SHIM_SETTING [26]    13044.30414090
SHIM_SETTING [27]    -7408.29085064
SHIM_SETTING [28]     3359.78626504
SHIM_SETTING [29]    -9468.57218463
SHIM_SETTING [30]    -4518.36855166
SHIM_SETTING [31]    -6784.38305730
SHIM_SETTING [32]   -10497.26098903
SHIM_SETTING [33]    -9222.50397807
SHIM_SETTING [34]     5325.14514117
SHIM_SETTING [35]    -2945.02768802
SHIM_SETTING [36]     9048.79622353
SHIM_SETTING [37]    14080.14879958
SHIM_SETTING [38]    -5093.68806529
SHIM_SETTING [39]      563.84338712
SHIM_SETTING [40]        0.00000000
```

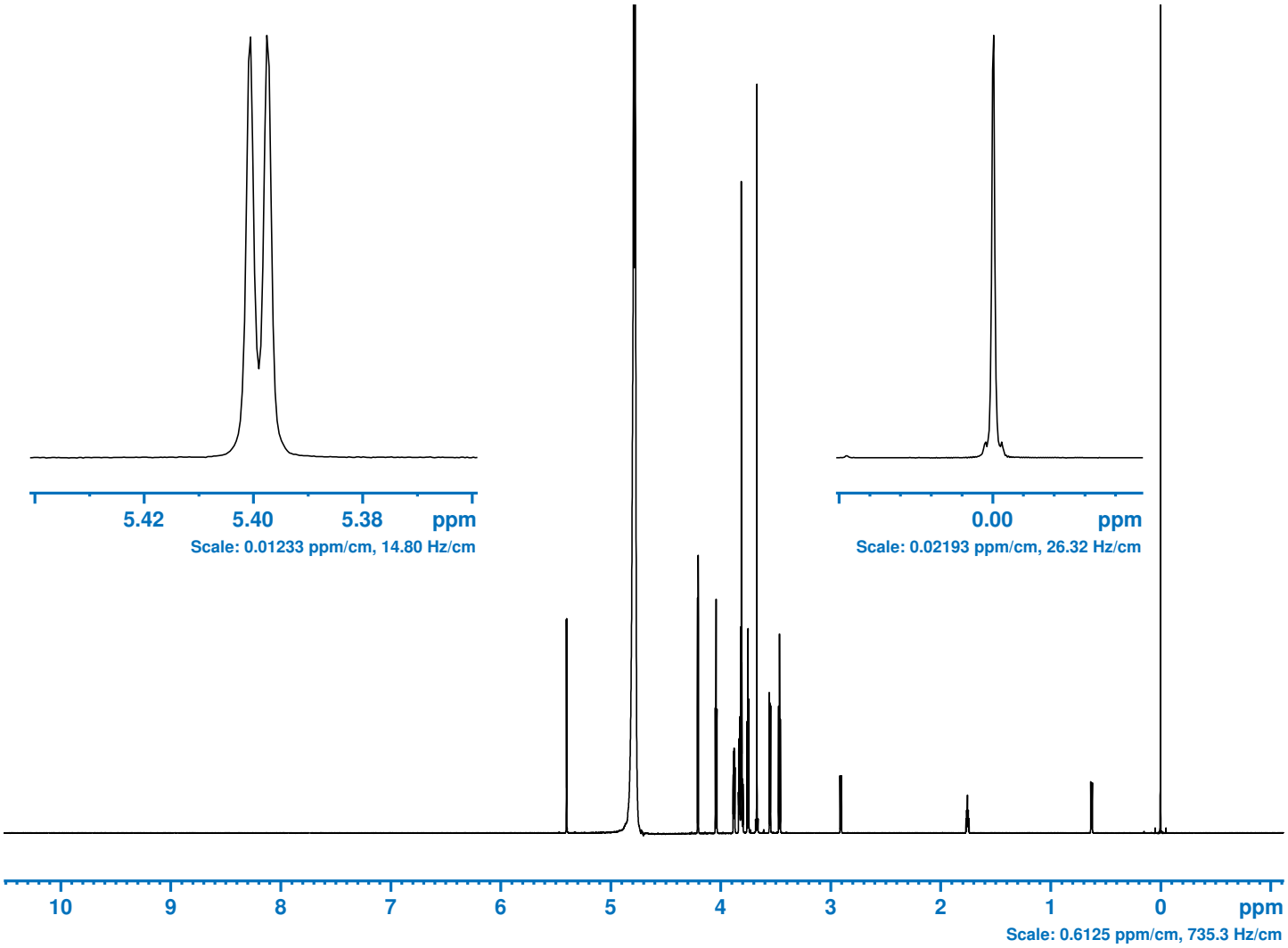
```
Current Data Parameters
NAME       NPT_1H_lineshape_nrot
EXPNO                          4
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20250403
Time                       7.17 h
INSTRUM                  Avance
PROBHD     Z175498_0004 (CP2.1 TXO 1200SA N/C-H-
PULPROG                    zg30
TD                        32768
SOLVENT                 Acetone
NS                             1
DS                             0
SWH                     1000.000 Hz
FIDRES                  0.061035 Hz
AQ                    16.3840000 sec
RG                           101
DW                      500.000 usec
DE                       10.00 usec
TE                       298.0 K
D1                    9.11600000 sec
TD0                            1
SFO1                1200.4093874 MHz
NUC1                         1H
P0                         3.33 usec
P1                        10.00 usec
PLW1                 30.88200000 W

F2 - Processing parameters
SI                          8192
SF                  1200.4096374 MHz
WDW                           no
SSB                            0
LB                             0 Hz
GB                             0
PC                          4.00
```

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 2 mM Sucrose, 0.5 mM DSS, 2 mM NaN3 in 90% H2O + 10% D2O (40 mm filling height) (Z10902)
Watersuppression with 535 l/h gas flow (NPT_1H_watersuppression_535l, spin rate 0 Hz)
PULPROG = zgpr, Input_L23 = 1, O1 = 5639.67 Hz (optimized), OvFl = 1

Linewidth [achieved/rated]: at 50 % of DSS signal [31.9 Hz <= 100.0 Hz] <pass>
Linewidth [achieved/rated]: at 10 % of DSS signal [67.3 Hz <= 200.0 Hz] <pass>
Splitting anomeric proton [achieved/rated]: [21% <= 25%] <pass>
SINO (1.5 ppm) [achieved/rated]: Signal (6.00 to 5.20 ppm), Noise (9.17 to 7.67 ppm) [1188.1 >= 850.0] <pass>



Bruker BioSpin

NPT_1H_watersuppression_535l

```
Current Data Parameters
NAME       NPT_1H_watersuppression_5351
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20250402
Time                         16.24 h
INSTRUM                      Avance
PROBHD     Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG                       zgpr
TD                           30882
SOLVENT                    H2O+D2O
NS                               8
DS                               4
SWH                    14705.882 Hz
FIDRES                     0.952392 Hz
AQ                     1.0499880 sec
RG                             101
DW                        34.000 usec
DE                        10.00 usec
TE                          298.0 K
D1                     5.00000000 sec
D12                    0.00002000 sec
TD0                              1
SFO1                1200.4056397 MHz
NUC1                           1H
P1                        10.00 usec
PLW1                30.88200000 W
PLW9                 0.00012353 W

F2 - Processing parameters
SI                           32768
SF                  1200.3998985 MHz
WDW                             no
SSB                              0
LB                            0 Hz
GB                               0
PC                            0.10

Additional Parameters

Field                -6887.951
Lock Phase             237.122
Lock Power             -18.000
Lock Gain              110.916
Lock DC                -61.000
Lock Shift               4.700
Loop Gain               -5.000
Loop Time                0.350
Loop Filter            100.000
Gas Flow             535 l/h
Atma Unit    Z147150_3250
```

```
------------------------------------------------------------------------
SHIM SEQUENCE
------------------------------------------------------------------------
- ro off wait <pass>
- topshim fine ws30 seriousws tunea ordmax=8 <pass>
------------------------------------------------------------------------
```

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
P90 1H pulse calibration (NPT_1H_p90determinationf1_1h, spin rate 0 Hz)
Result: [180/2] = 9.9 us @ 31.7 W [360] = 38.5 us ==> [PDelay = 2*180 - 360] = 1.1 us
ATTENTION: Updated PROSOL Tables with [10.0 us @ 30.9 W]
Deviation from pulse target value (= 10.0 us): -1.2%

P90 1H pulse [achieved/rated]: @ 31.7 W [9.9 us <= 10.0 us] <pass>

Bruker BioSpin

NPT_1H_p90determinationf1_1h

Current Data Parameters

NAME	NPT_1H_p90determinationf1_1h
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

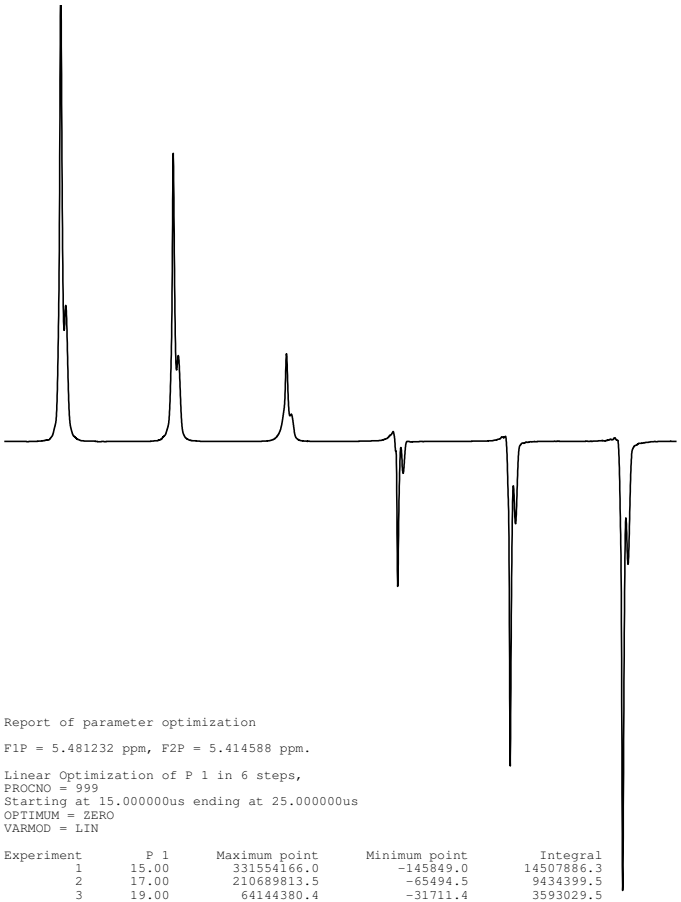
Date_	20250402
Time	16.06 h
INSTRUM	Avance
PROBHD	Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG	zg
TD	300
SOLVENT	DMSO
NS	1
DS	0
SWH	230.766 Hz
FIDRES	1.538438 Hz
AQ	0.6500100 sec
RG	10
DW	2166.700 usec
DE	10.00 usec
TE	298.0 K
D1	1.60500000 sec
TD0	1
SFO1	1200.4065397 MHz
NUC1	1H
P1	49.39 usec
PLW1	31.65424675 W

F2 - Processing parameters

SI	2048
SF	1200.4000000 MHz
WDW	SINE
SSB	2
LB	0 Hz
GB	0
PC	1.00

Additional Parameters

Field	-6834.501
Lock Phase	237.122
Lock Power	-19.000
Lock Gain	93.964
Lock DC	-61.000
Lock Shift	2.490
Loop Gain	5.000
Loop Time	0.250
Loop Filter	500.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250



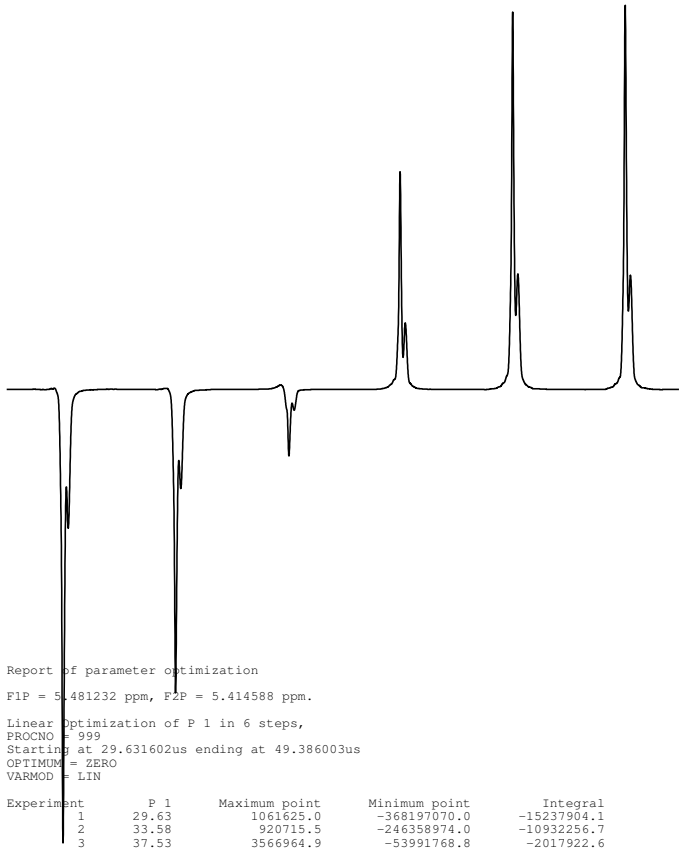
Report of parameter optimization

F1P = 5.481232 ppm, F2P = 5.414588 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	331554166.0	-145849.0	14507886.3
2	17.00	210689813.5	-65494.5	9434399.5
3	19.00	64144380.4	-31711.4	3593029.5
4	21.00	7217311.0	-105909375.5	-2171281.4
5	23.00	3738461.0	-237258376.0	-7446325.5
6	25.00	2507703.0	-328283715.0	-11694145.8

Zero found at P 1 = 19.754401 us



Report of parameter optimization

F1P = 5.481232 ppm, F2P = 5.414588 ppm.

Linear Optimization of P 1 in 6 steps,
PROCNO = 999
Starting at 29.631602us ending at 49.386003us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	29.63	1061625.0	-368197070.0	-15237904.1
2	33.58	920715.5	-246358974.0	-10932256.7
3	37.53	3566964.9	-53991768.8	-2017922.6
4	41.48	176776619.0	-72981.5	7244268.5
5	45.44	306432062.0	-149668.0	13066915.0
6	49.39	311733529.0	-173082.0	13029197.8

Zero found at P 1 = 38.457731 us

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

PLW90	P90	P90[det]	Deviation
23.0 W	10.0 us		
23.0 W	10.0 us	11.7 us	17.3%
31.7 W	10.0 us	9.9 us	-1.2%

SHIM SEQUENCE

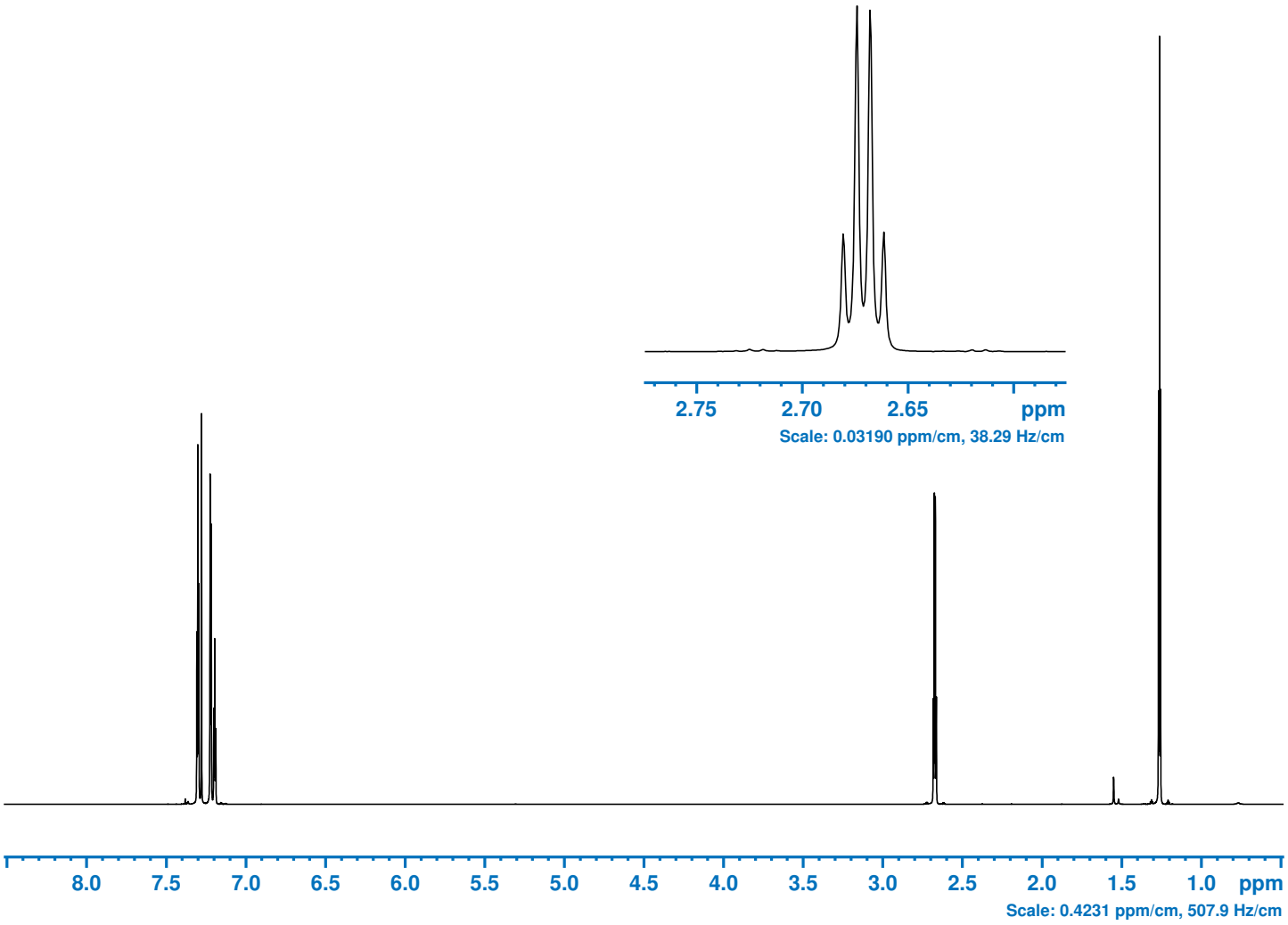
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 0.1% Ethylbenzene (EB) in Chloroform-D (Z10120)
1H sensitivity (NPT_1H_sensitivity, spin rate 0 Hz)

SINO (2.0 ppm) [achieved]: Signal (3.00 to 2.00 ppm), Noise (5.04 to 3.04 ppm) [5803.3] <n/a>
SINO (200.0 Hz) [achieved/rated]: Signal (3.00 to 2.00 ppm), Noise (3.92 to 3.75 ppm) [7010.2 >= 4800.0] <pass>

Bruker BioSpin

NPT_1H_sensitivity



Current Data Parameters

NAME	NPT_1H_sensitivity
EXPNO	5
PROCNO	1

F2 - Acquisition Parameters

Date_	20250402
Time	18.43 h
INSTRUM	Avance
PROBHD	Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG	zg
TD	32768
SOLVENT	CDCl3
NS	1
DS	0
SWH	11904.762 Hz
FIDRES	0.726609 Hz
AQ	1.3762560 sec
RG	101
DW	42.000 usec
DE	10.00 usec
TE	298.0 K
D1	113.57360000 sec
TD0	1
SFO1	1200.4048016 MHz
NUC1	1H
P1	10.00 usec
PLW1	30.88200000 W

F2 - Processing parameters

SI	16384
SF	1200.4000058 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

Additional Parameters

Field	-6723.961
Lock Phase	239.700
Lock Power	-27.000
Lock Gain	122.388
Lock DC	-61.000
Lock Shift	7.240
Loop Gain	-9.400
Loop Time	0.464
Loop Filter	50.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250

SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c, spin rate 0 Hz)
Result: [90] = 10.0 us @ 116.1 W [270] = 29.5 us ==> [PDelay = 3*90 - 270] = 0.5 us
ATTENTION: Updated PROSOL Tables with [10.0 us @ 116.2 W]
Deviation from pulse target value (= 10.0 us): 0.1%

P90 13C pulse [achieved/rated]: @ 116.1 W [10.0 us <= 10.0 us] <pass>

Bruker BioSpin

NPT_1H_p90determinationf2_13c

Current Data Parameters

NAME	NPT_1H_p90determinationf2_13c
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

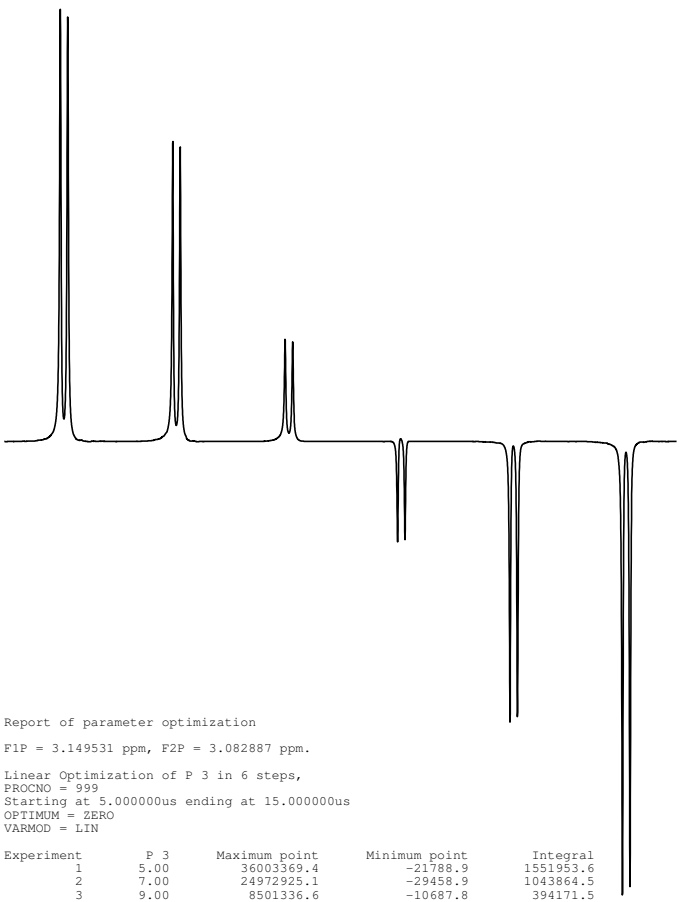
Date_	20250402
Time	16.12 h
INSTRUM	Avance
PROBHD	Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG	decp90
TD	1000
SOLVENT	DMSO
NS	1
DS	0
SWH	230.766 Hz
FIDRES	0.461531 Hz
AQ	2.1667000 sec
RG	2.56
DW	2166.700 usec
DE	10.00 usec
TE	298.0 K
CNST2	139.0000000
D1	2.95970798 sec
D2	0.00359713 sec
TD0	1
SFO1	1200.4037407 MHz
NUC1	1H
P1	5.00 usec
PLW1	30.88200000 W
SFO2	301.8557416 MHz
NUC2	13C
P3	40.03 usec
PLW2	116.06969707 W

F2 - Processing parameters

SI	2048
SF	1200.4000000 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	0.10

Additional Parameters

Field	-6828.941
Lock Phase	237.122
Lock Power	-19.000
Lock Gain	93.964
Lock DC	-61.000
Lock Shift	2.490
Loop Gain	5.000
Loop Time	0.250
Loop Filter	500.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250



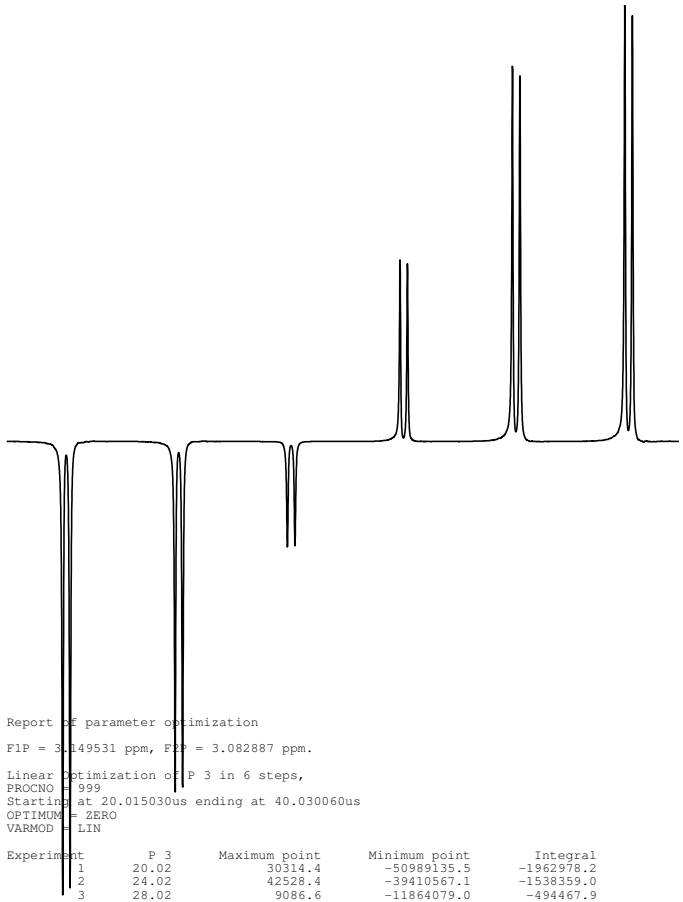
Report of parameter optimization

F1P = 3.149531 ppm, F2P = 3.082887 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	36003369.4	-21788.9	1551953.6
2	7.00	24972925.1	-29458.9	1043864.5
3	9.00	8501336.6	-10687.8	394171.5
4	11.00	203379.1	-8374513.2	-245398.7
5	13.00	21125.6	-23383427.1	-858345.2
6	15.00	23708.2	-37780495.4	-1389365.2

Zero found at P 3 = 10.007515 us



Report of parameter optimization

F1P = 3.149531 ppm, F2P = 3.082887 ppm.

Linear Optimization of P 3 in 6 steps,
PROCNO = 999
Starting at 20.015030us ending at 40.030060us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 3	Maximum point	Minimum point	Integral
1	20.02	30314.4	-50989135.5	-1962978.2
2	24.02	42528.4	-39410567.1	-1538359.0
3	28.02	9086.6	-11864079.0	-494467.9
4	32.02	20404422.8	-23324.0	690839.2
5	36.03	42154997.0	-36812.5	1552275.4
6	40.03	49056490.2	-56412.0	1787922.5

Zero found at P 3 = 29.492817 us

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

PLW90	P90	P90[det]	Deviation
132.4 W	10.0 us		
132.4 W	10.0 us	9.4 us	-6.4%
116.1 W	10.0 us	10.0 us	0.1%

SHIM SEQUENCE

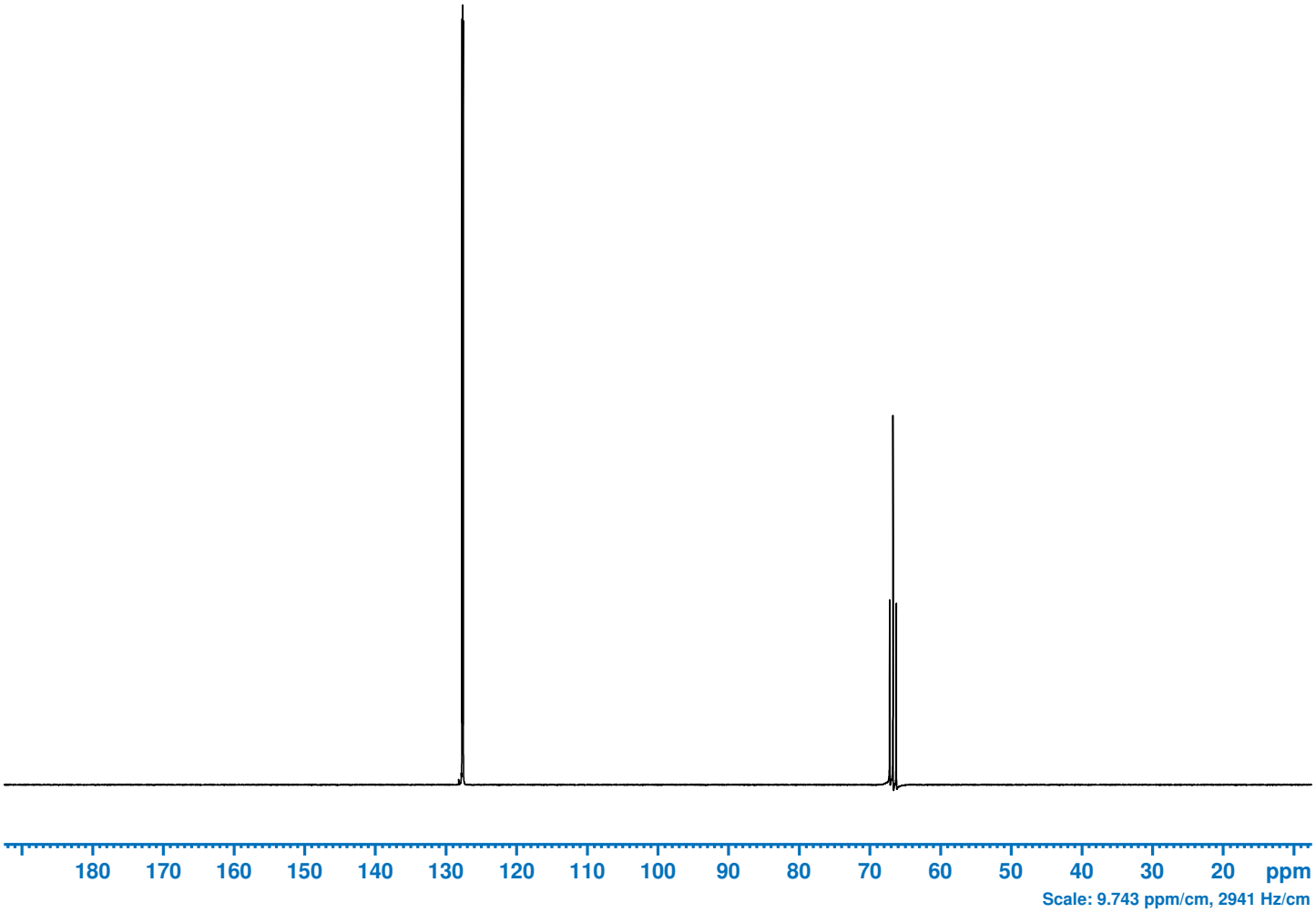
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 40% Dioxane in Benzene-D6 (ASTM) (Z10163)
13C sensitivity (NPT_13C_sensitivity, spin rate 0 Hz)

SINO (40.0 ppm) [achieved/rated]: Signal (127.61 ppm), Noise (120.72 to 80.72 ppm) [4093.1 >= 2600.0] <pass>

Bruker BioSpin

NPT_13C_sensitivity



Scale: 9.743 ppm/cm, 2941 Hz/cm

Current Data Parameters

NAME	NPT_13C_sensitivity
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20250402
Time	17.54 h
INSTRUM	Avance
PROBHD	Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG	zg
TD	65536
SOLVENT	C6D6
NS	1
DS	0
SWH	58823.529 Hz
FIDRES	1.795152 Hz
AQ	0.5570560 sec
RG	101
DW	8.500 usec
DE	18.07 usec
TE	298.0 K
D1	829.44294400 sec
TD0	1
SFO1	301.8710004 MHz
NUC1	13C
P1	10.00 usec
PLW1	116.24000000 W

F2 - Processing parameters

SI	131072
SF	301.8408201 MHz
WDW	EM
SSB	0
LB	3.50 Hz
GB	0
PC	1.40

Additional Parameters

Field	-6733.361
Lock Phase	278.300
Lock Power	-24.000
Lock Gain	109.386
Lock DC	-61.000
Lock Shift	7.160
Loop Gain	15.133
Loop Time	0.047
Loop Filter	1467.800
Gas Flow	535 l/h
Atma Unit	Z147150_3250

SHIM SEQUENCE

- topshim fine ws5 tunea ordmax=8 <pass>

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
Indirect P90 15N pulse calibration (NPT_1H_p90determinationf2_15n, spin rate 0 Hz)
Result: [90] = 32.0 us @ 71.2 W [270] = 96.0 us ==> [PDelay = 3*90 - 270] = -0.1 us
ATTENTION: Updated PROSOL Tables with [32.0 us @ 71.1 W]
Deviation from pulse target value (= 32.0 us): -0.0%

P90 15N pulse [achieved/rated]: @ 71.2 W [32.0 us <= 32.0 us] <pass>

Bruker BioSpin

NPT_1H_p90determinationf2_15n

Current Data Parameters

NAME	NPT_1H_p90determinationf2_15n
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

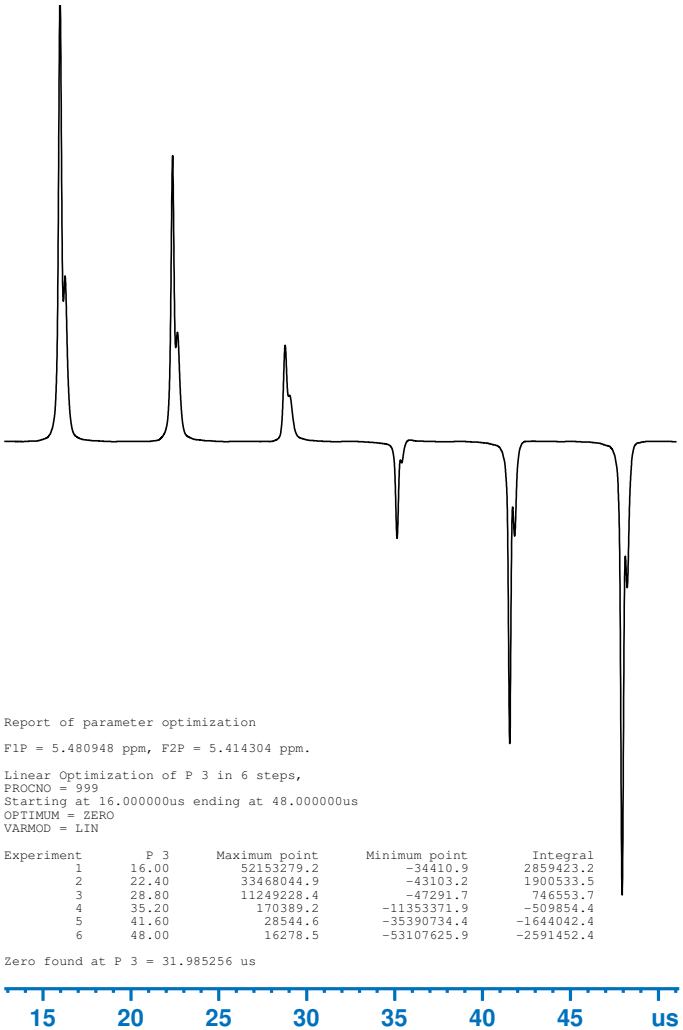
Date_	20250402
Time	16.02 h
INSTRUM	Avance
PROBHD	Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG	decp90
TD	200
SOLVENT	DMSO
NS	1
DS	0
SWH	230.766 Hz
FIDRES	2.307657 Hz
AQ	0.4333400 sec
RG	2.56
DW	2166.700 usec
DE	10.00 usec
TE	298.0 K
CNST2	88.5000000
D1	0.68643398 sec
D2	0.00564971 sec
TD0	1
SFO1	1200.4065393 MHz
NUC1	1H
P1	6.67 usec
PLW1	23.00000000 W
SFO2	121.6447104 MHz
NUC2	15N
P3	127.94 usec
PLW2	71.19518910 W

F2 - Processing parameters

SI	2048
SF	1200.4000000 MHz
WDW	SINE
SSB	2
LB	0 Hz
GB	0
PC	1.00

Additional Parameters

Field	-6837.979
Lock Phase	237.122
Lock Power	-19.000
Lock Gain	93.964
Lock DC	-61.000
Lock Shift	2.490
Loop Gain	5.000
Loop Time	0.250
Loop Filter	500.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250



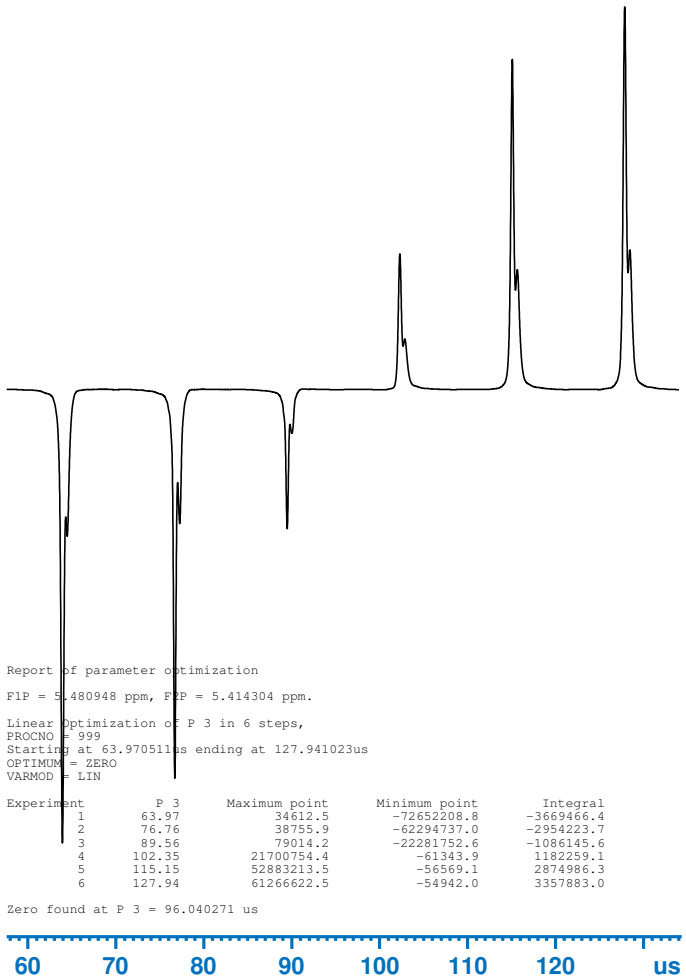
Report of parameter optimization

F1P = 5.480948 ppm, F2P = 5.414304 ppm.

Linear Optimization of P 3 in 6 steps,
PROCNO = 999
Starting at 16.000000us ending at 48.000000us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 3	Maximum point	Minimum point	Integral
1	16.00	52153279.2	-34410.9	2859423.2
2	22.40	33468044.9	-43103.2	1900533.5
3	28.80	11249228.4	-47291.7	746553.7
4	35.20	170389.2	-11353371.9	-509854.4
5	41.60	28544.6	-35390734.4	-1644042.4
6	48.00	16278.5	-53107625.9	-2591452.4

Zero found at P 3 = 31.985256 us



Report of parameter optimization

F1P = 5.480948 ppm, F2P = 5.414304 ppm.

Linear Optimization of P 3 in 6 steps,
PROCNO = 999
Starting at 63.970511us ending at 127.941023us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 3	Maximum point	Minimum point	Integral
1	63.97	34612.5	-72652208.8	-3669466.4
2	76.76	38755.9	-62294737.0	-2954223.7
3	89.56	79014.2	-22281752.6	-1086145.6
4	102.35	21700754.4	-61343.9	1182259.1
5	115.15	52883213.5	-56569.1	2874986.3
6	127.94	61266622.5	-54942.0	3357883.0

Zero found at P 3 = 96.040271 us

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

PLW90	P90	P90[det]	Deviation
73.8 W	32.0 us		
73.8 W	32.0 us	31.3 us	-2.3%
70.4 W	32.0 us	32.1 us	0.3%
70.9 W	32.0 us	32.1 us	0.2%
71.2 W	32.0 us	32.0 us	-0.0%

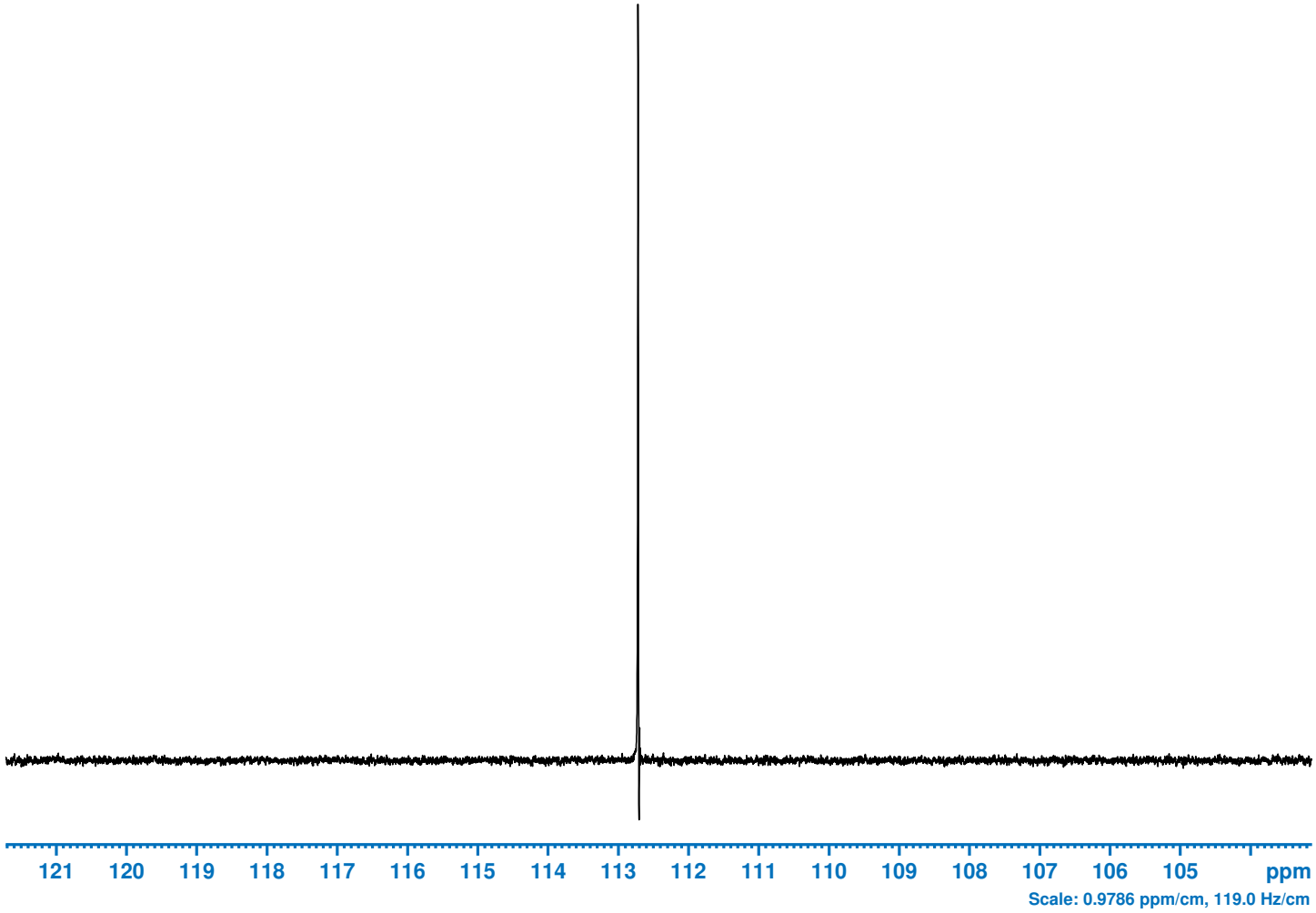
SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 90% Formamide in Dimethyl Sulfoxide-D6 (Z10187)
15N sensitivity with 1H decoupling (NPT_15N_sensitivity_dec1h, spin rate 0 Hz)
PCPD2 1H pulse determined using pulsecal: 68.13 us @ 1.02 W

SINO (2.0 ppm) [achieved/rated]: Signal (112.71 ppm), Noise (119.58 to 117.57 ppm) [217.9 >= 200.0] <pass>

Bruker BioSpin



Scale: 0.9786 ppm/cm, 119.0 Hz/cm

NPT_15N_sensitivity_dec1h

Current Data Parameters

NAME	NPT_15N_sensitivity_dec1h
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20250403
Time	11.26 h
INSTRUM	Avance
PROBHD	Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG	zgig
TD	32768
SOLVENT	DMSO
NS	1
DS	0
SWH	2380.952 Hz
FIDRES	0.145322 Hz
AQ	6.8812800 sec
RG	101
DW	210.000 usec
DE	18.00 usec
TE	298.0 K
D1	123.11872000 sec
D11	0.03000000 sec
TD0	1
SFO1	121.6491501 MHz
NUC1	15N
P1	32.00 usec
PLW1	71.13000000 W
SFO2	1200.4087629 MHz
NUC2	1H
CPDPRG2	waltz64
PCPD2	68.13 usec
PLW2	30.88200000 W
PLW12	1.02090000 W

F2 - Processing parameters

SI	16384
SF	121.6354756 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Additional Parameters

Field	-5456.622
Lock Phase	247.300
Lock Power	-19.000
Lock Gain	114.556
Lock DC	-61.000
Lock Shift	2.490
Loop Gain	-9.400
Loop Time	0.464
Loop Filter	50.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250

SHIM SEQUENCE

- topshim fine ws5 tunea ordmax=8 <pass>

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
P90 2H pulse calibration (NPT_prep_p90det_d, spin rate 0 Hz)
Result: [180/2] = 149.5 us @ 17.4 W [360] = 565.5 us ==> [PDelay = 2*180 - 360] = 32.4 us
ATTENTION: Updated PROSOL Tables with [150.0 us @ 17.3 W]
Deviation from pulse target value (= 150.0 us): -0.3%

P90 2H pulse [achieved/rated]: @ 17.4 W [149.5 us <= 150.0 us] <pass>

Bruker BioSpin

NPT_prep_p90det_d

Current Data Parameters

NAME	NPT_prep_p90det_d
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

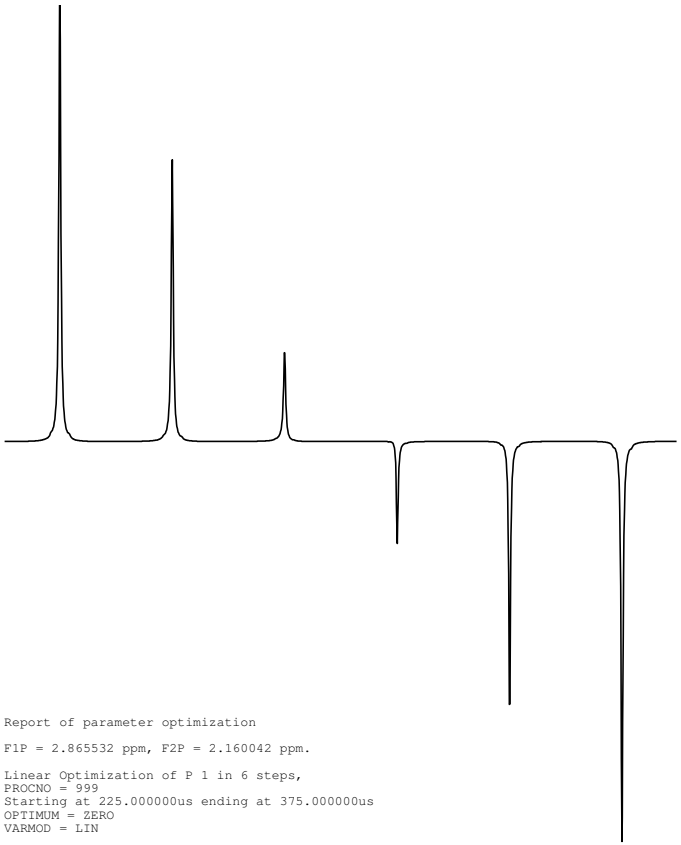
Date_	20250402
Time	15.35 h
INSTRUM	Avance
PROBHD	Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG	npt_zg2h
TD	1024
SOLVENT	DMSO
NS	1
DS	0
SWH	1000.000 Hz
FIDRES	1.953125 Hz
AQ	0.5120000 sec
RG	28.5
DW	500.000 usec
DE	18.00 usec
TE	298.0 K
D1	0.35000000 sec
D11	0.03000000 sec
D12	0.00010000 sec
TD0	1
SFO1	184.2691718 MHz
NUC1	2H
P1	747.38 usec
PLW1	17.37210828 W

F2 - Processing parameters

SI	2048
SF	184.2687088 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00

Additional Parameters

Field	-6862.959
Lock Phase	237.122
Lock Power	-9.000
Lock Gain	93.991
Lock DC	-61.000
Lock Shift	2.490
Loop Gain	5.000
Loop Time	0.250
Loop Filter	500.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250



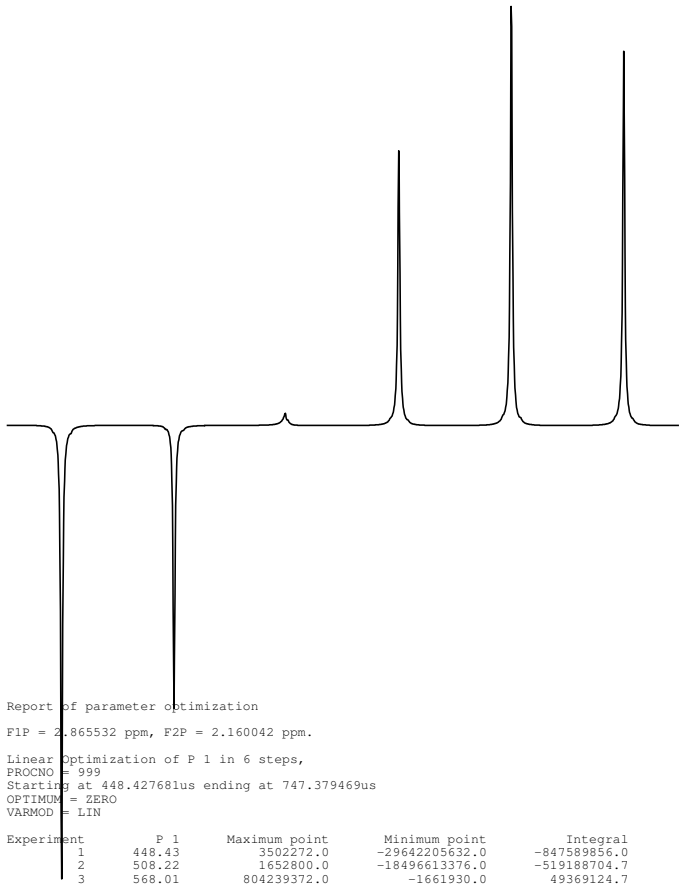
Report of parameter optimization

F1P = 2.865532 ppm, F2P = 2.160042 ppm.

Linear Optimization of P 1 in 6 steps,
PROCNO = 999
Starting at 225.000000us ending at 375.000000us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	225.00	27634890752.0	-3095680.0	839648360.6
2	255.00	17168089728.0	-2252896.0	533066292.1
3	285.00	5409612720.0	-1340816.0	191132268.9
4	315.00	6535008.0	-6222472464.0	-155325758.6
5	345.00	1682944.0	-16034989536.0	-461329611.5
6	375.00	2423680.0	-24366658880.0	-698942405.0

Zero found at P 1 = 298.951788 us



Report of parameter optimization

F1P = 2.865532 ppm, F2P = 2.160042 ppm.

Linear Optimization of P 1 in 6 steps,
PROCNO = 999
Starting at 448.427681us ending at 747.379469us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	448.43	3502272.0	-29642205632.0	-847589856.0
2	508.22	1652800.0	-18496613376.0	-519188704.7
3	568.01	804239372.0	-1661930.0	49369124.7
4	627.80	17955906304.0	-2108288.0	587511243.2
5	687.59	27375992640.0	-2939264.0	857587383.9
6	747.38	24443239552.0	-2810304.0	751782571.7

Zero found at P 1 = 565.517016 us

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

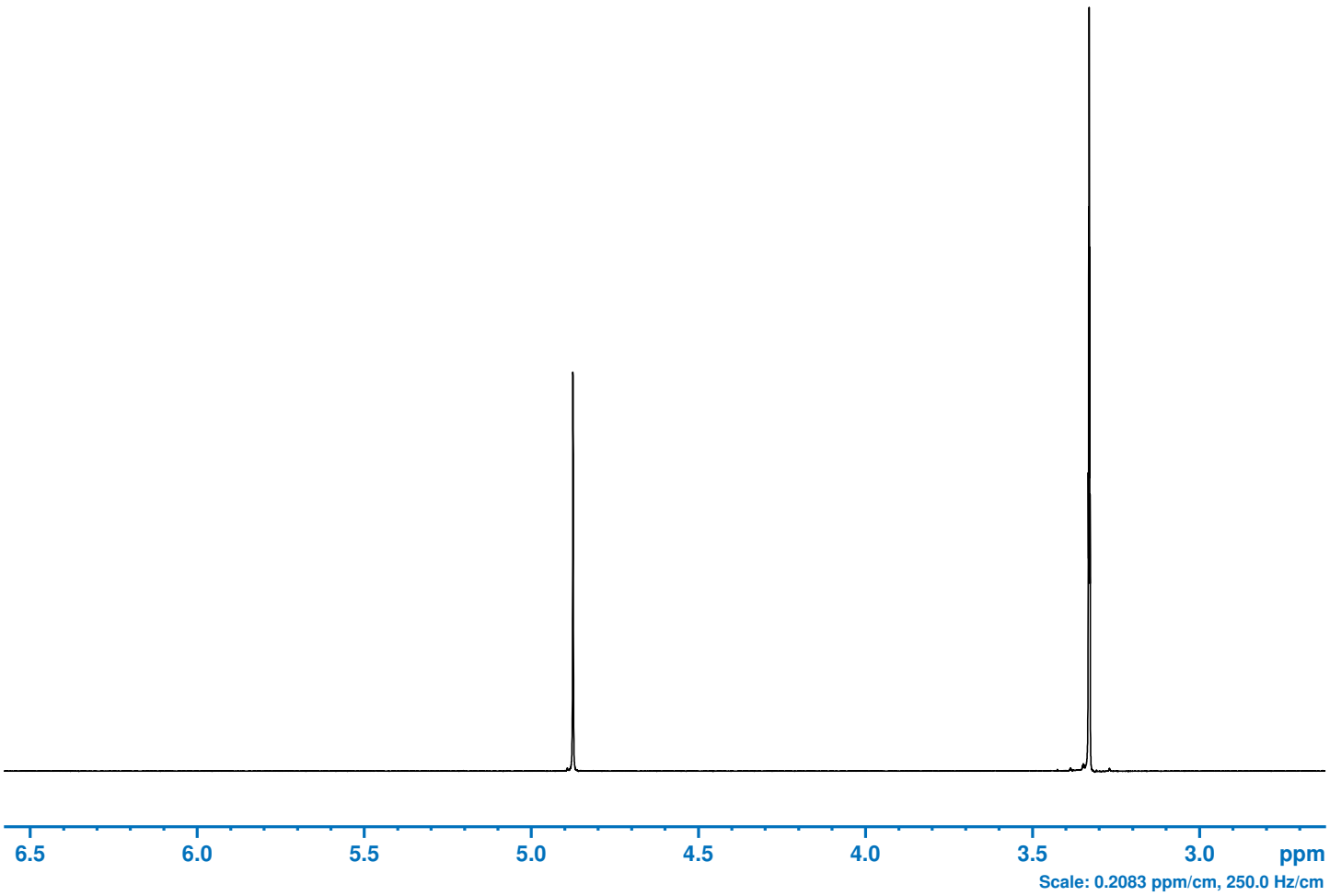
PLW90	P90	P90[det]	Deviation
17.4 W	150.0 us		
17.4 W	150.0 us	149.5 us	-0.3%

SHIM SEQUENCE

- ro off wait <pass>
- topshim fine ws5 tunea ordmax=8 <pass>

NMR TEST ACCEPTANCE *** System: AV NEO (1200.40 MHz) *** TopSpin 4.4.1
Probe: Z175498_0004 CP2.1 TXO 1200SA N/C-H-D-05 Z XT *** Sample Depth: 21 mm
Sample: Temperature Calibration - 99.8% Methanol-D4 (Z10627)
1H temperature calibration with 99.8% MeOD (NPT_1H_tempcalib_998meod, spin rate 20 Hz)
Temperature is calibrated for a range of 298.0 to 308.0 K
Temperature Correction: y = 1.028 * x + (-5.156)

Standard air flow: [535.0 l/h]
Standard temperature: [298.0 K]
Apparent temperature without correction: [294.9 K]
T_target = 298.0 K, T_measured (with correction) = 298.0 K, Signal 1 = 4.8748 ppm, Signal 2 = 3.3292 ppm
Version = BSVT, setPoint = 298.000 K, AirFlow = 535.000 l/h, XP = 2.481, TI = 61.612, TD = 10.269



Bruker BioSpin

NPT_1H_tempcalib_998meod

Current Data Parameters

NAME	NPT_1H_tempcalib_998meod
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20250402
Time	15.24 h
INSTRUM	Avance
PROBHD	Z175498_0004 (CP2.1 TXO 1200SA N/C-H-D
PULPROG	zg30
TD	8192
SOLVENT	MeOD
NS	1
DS	0
SWH	5000.000 Hz
FIDRES	1.220703 Hz
AQ	0.8192000 sec
RG	8
DW	100.000 usec
DE	10.00 usec
TE	298.0 K
D1	2.00000000 sec
TD0	1
SFO1	1200.4055218 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
PLW1	16.00000000 W

F2 - Processing parameters

SI	16384
SF	1200.4000000 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	0.10

Additional Parameters

Field	-6849.435
Lock Phase	237.122
Lock Power	-34.000
Lock Gain	98.219
Lock DC	-61.000
Lock Shift	3.300
Loop Gain	-5.000
Loop Time	0.100
Loop Filter	100.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250

SHIM SEQUENCE

- topshim fine ws5 tunea ordmax=8 <pass>