DRAFT

CP2.1 TCI 1200SA H/C/N-D-03 Z

1200 MHz

Probe ID: Z161014_0006

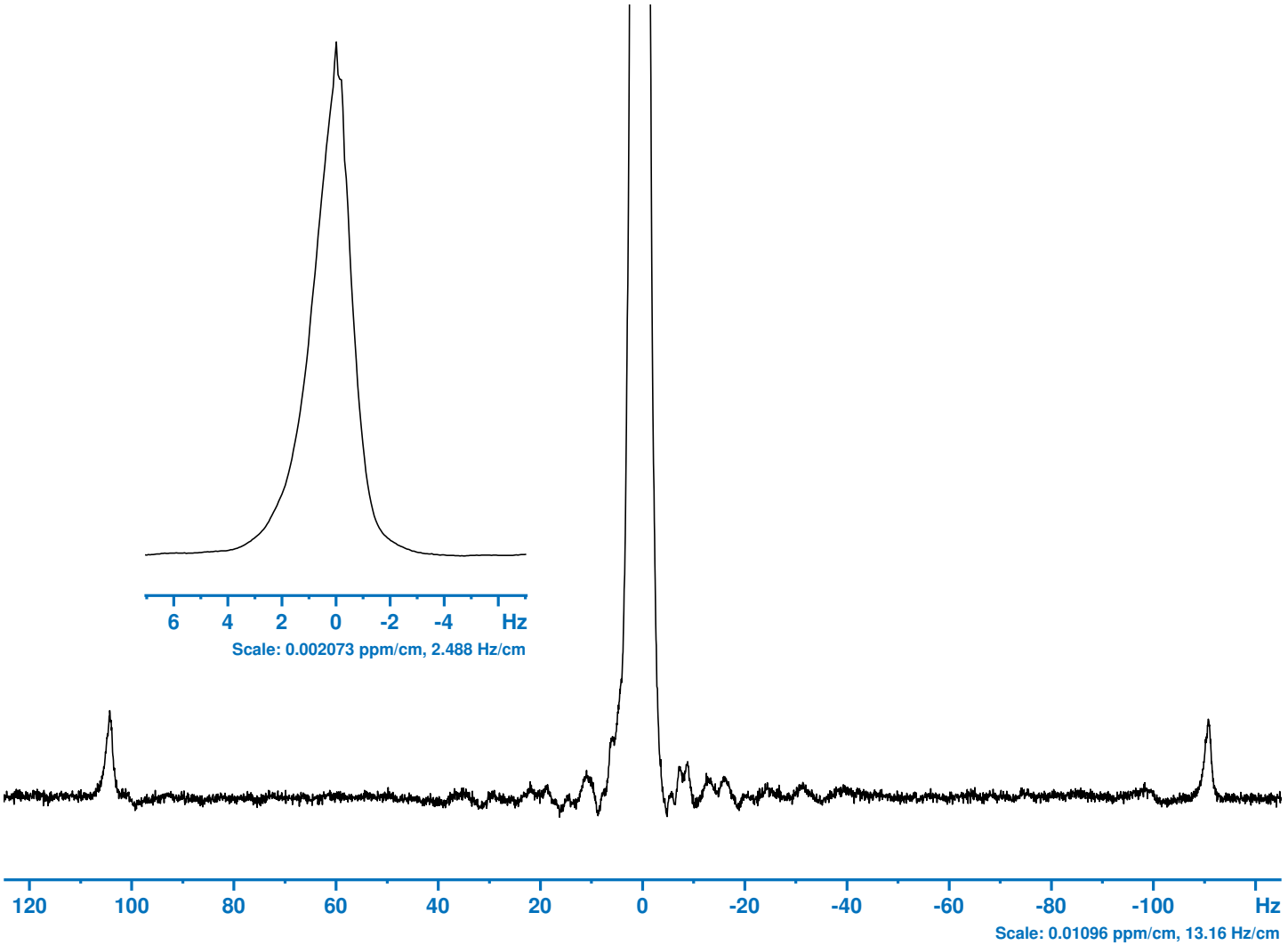
Inspection Lot: 2025-03-29

NMR TEST ACCEPTANCE

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 0.3% Chloroform in Acetone-D6 (Z10029)
1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)

Line width [achieved/rated]: at 0.11% of signal height [11.4 Hz <= 30.0 Hz] <pass>
Line width [achieved/rated]: at 0.55% of signal height [8.1 Hz <= 15.0 Hz] <pass>
Line width [achieved/rated]: at 50% of signal height [1.43 Hz <= 1.50 Hz] <pass>

Bruker BioSpin



NPT_1H_lineshape_nrot

Current Data Parameters

NAME	NPT_1H_lineshape_nrot
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20250331
Time	8.16 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-D
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	1200.2893863 MHz
NUC1	1H
P0	2.33 usec
P1	7.00 usec
PLW1	11.31600000 W

F2 - Processing parameters

SI	8192
SF	1200.2896363 MHz
WDW	no
SSB	0
LB	0 Hz
GB	0
PC	4.00

Additional Parameters

Field	5668.163
Lock Phase	131.098
Lock Power	-34.000
Lock Gain	106.332
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

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

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 0.3% Chloroform in Acetone-D6 (Z10029)
1H lineshape without sample rotation (NPT_1H_lineshape_nrot, spin rate 0 Hz)

Bruker BioSpin

NPT_1H_lineshape_nrot

```
# Mon Mar 31 07:16:11 2025
#$$PROBEIDENTIFIER=Z161014_0006
#$$PROBENAME=CP2.1 TCI 1200SA H/C/N-D-03 Z
#$$MAGNETID=BZH 16'1200'78A
#$$CRYOSTATID=S'394'54-12394
#$$SHIMID=292722
#
# Active Shim Gradients
#
Z                       14964
Z2                      42470
Z3                       -595
Z4                       -915
Z5                      -4152
Z6                       6360
Z7                     -11460
Z8                         39
X                       -5929
XZ                      -9208
XZ2                      6148
XZ3                      3085
XZ4                      4495
XZ5                      1671
Y                        3184
YZ                       8698
YZ2                     -4958
YZ3                     -1508
YZ4                      8283
YZ5                      6250
XY                      -3476
XYZ                     -7872
XYZ2                      269
XYZ3                     3885
XYZ4                     2172
XYZ5                      699
(X2-Y2)                  -279
(X2-Y2)Z                 5556
(X2-Y2)Z2               -4277
(X2-Y2)Z3              -11865
(X2-Y2)Z4                -986
(X2-Y2)Z5               -3102
X3                      -8802
X3Z                     -2862
Y3                       1718
Y3Z                     -3939
#
# Lock Parameter
#
FIELD           5668.163
LOCKPHASE                131.098
LOCKPOWER                -34.000
LOCKGAIN                 106.332
LOCKDC          -61.000
LOCKSHIFT                  2.040
LOOPGAIN                  15.133
LOOPTIME                   0.047
LOOPFILTER              1468.000
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1]     7679.53040698
SHIM_SETTING [ 2]    41059.59297247
SHIM_SETTING [ 3]     4091.32798850
SHIM_SETTING [ 4]    -5926.46023710
SHIM_SETTING [ 5]     2024.22880187
SHIM_SETTING [ 6]      428.29202190
SHIM_SETTING [ 7]     3834.35323508
SHIM_SETTING [ 8]    43801.65833506
SHIM_SETTING [ 9]    28155.11981759
SHIM_SETTING [10]    -5050.65506756
SHIM_SETTING [11]        0.00000000
SHIM_SETTING [12]     5657.58074580
SHIM_SETTING [13]    -2220.60048588
SHIM_SETTING [14]    -2880.66495462
SHIM_SETTING [15]    -2311.53714557
SHIM_SETTING [16]     9365.35603481
SHIM_SETTING [17]   -21515.13691276
SHIM_SETTING [18]    -7271.28149016
SHIM_SETTING [19]     1006.27684295
SHIM_SETTING [20]    -3434.76493182
SHIM_SETTING [21]    -9037.67829083
SHIM_SETTING [22]     -792.31083640
SHIM_SETTING [23]    14219.23190281
SHIM_SETTING [24]    -6541.49420061
SHIM_SETTING [25]   -13431.22840099
SHIM_SETTING [26]    14020.15738173
SHIM_SETTING [27]    -5657.12221847
SHIM_SETTING [28]    12459.06316605
SHIM_SETTING [29]     2959.14962035
SHIM_SETTING [30]    -2690.92025124
SHIM_SETTING [31]     5173.25135575
SHIM_SETTING [32]    -6548.83894690
SHIM_SETTING [33]    -5767.31401101
SHIM_SETTING [34]     3824.91529166
SHIM_SETTING [35]   -13616.31737709
SHIM_SETTING [36]     1927.22639970
SHIM_SETTING [37]     2665.36605107
SHIM_SETTING [38]    16115.32194860
SHIM_SETTING [39]    -8968.03597011
SHIM_SETTING [40]        0.00000000
```

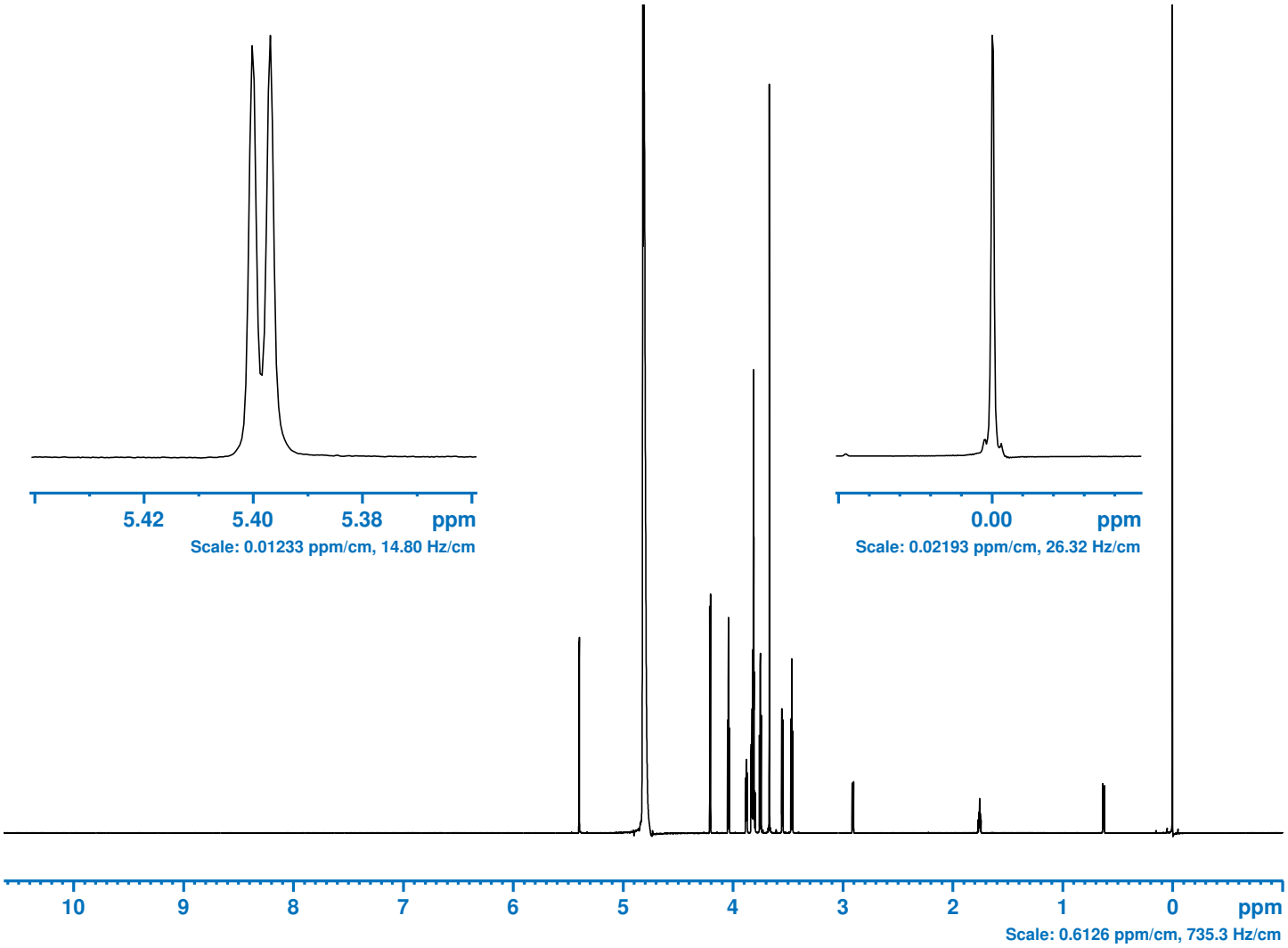
```
Current Data Parameters
NAME       NPT_1H_lineshape_nrot
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20250331
Time                        8.16 h
INSTRUM                   Avance
PROBHD     Z161014_0006 (CP2.1 TCI 1200SA H/C/N-
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                1200.2893863 MHz
NUC1                          1H
P0                         2.33 usec
P1                         7.00 usec
PLW1                  11.31600000 W

F2 - Processing parameters
SI                          8192
SF                  1200.2896363 MHz
WDW                           no
SSB                            0
LB                             0 Hz
GB                             0
PC                          4.00
```

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 2 mM Sucrose, 0.5 mM DSS, 2 mM NaN3 in 90% H2O + 10% D2O (Z10036)
Watersuppression with 535 l/h gas flow (NPT_1H_watersuppression_535l, spin rate 0 Hz)
PULPROG = zgpr, Input_L23 = 1, O1 = 5638.60 Hz (optimized), OvFl = 1

Linewidth [achieved/rated]: at 50 % of DSS signal [29.2 Hz <= 75.0 Hz] <pass>
Linewidth [achieved/rated]: at 10 % of DSS signal [51.2 Hz <= 150.0 Hz] <pass>
Splitting anomeric proton [achieved/rated]: [19% <= 25%] <pass>
SINO (1.5 ppm) [achieved/rated]: Signal (6.00 to 5.20 ppm), Noise (8.77 to 7.27 ppm) [1180.0 >= 800.0] <pass>



Bruker BioSpin

NPT_1H_watersuppression_535l

Current Data Parameters

NAME	NPT_1H_watersuppression_5351
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20250330
Time	7.51 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-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	1200.2856386 MHz
NUC1	1H
P1	7.00 usec
PLW1	14.00000000 W
PLW9	0.00002744 W

F2 - Processing parameters

SI	32768
SF	1200.2798594 MHz
WDW	no
SSB	0
LB	0 Hz
GB	0
PC	0.10

Additional Parameters

Field	3068.593
Lock Phase	131.098
Lock Power	-18.000
Lock Gain	117.475
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

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10037)
P90 1H pulse calibration (NPT_1H_p90determinationf1_1h, spin rate 0 Hz)
Result: [180/2] = 7.0 us @ 11.3 W [360] = 27.5 us ==> [PDelay = 2*180 - 360] = 0.5 us
ATTENTION: Updated PROSOL Tables with [7.0 us @ 11.3 W]
Deviation from pulse target value (= 7.0 us): 0.1%

P90 1H pulse [achieved/rated]: @ 11.3 W [7.0 us <= 7.0 us] <pass>

Bruker BioSpin

NPT_1H_p90determinationf1_1h

Current Data Parameters

NAME	NPT_1H_p90determinationf1_1h
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

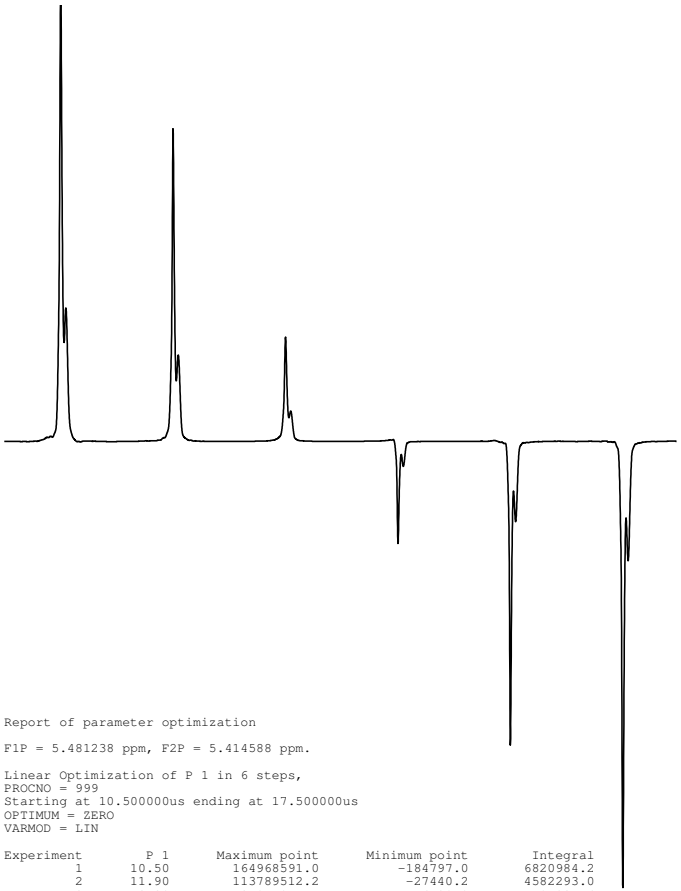
Date_	20250331
Time	8.05 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-D
PULPROG	zg
TD	300
SOLVENT	DMSO
NS	1
DS	0
SWH	230.766 Hz
FIDRES	1.538438 Hz
AQ	0.6500100 sec
RG	5
DW	2166.700 usec
DE	10.00 usec
TE	298.0 K
D1	1.60500000 sec
TD0	1
SFO1	1200.2865390 MHz
NUC1	1H
P1	35.02 usec
PLW1	11.30412409 W

F2 - Processing parameters

SI	2048
SF	1200.2800000 MHz
WDW	SINE
SSB	2
LB	0 Hz
GB	0
PC	1.00

Additional Parameters

Field	5567.822
Lock Phase	131.098
Lock Power	-19.000
Lock Gain	101.056
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



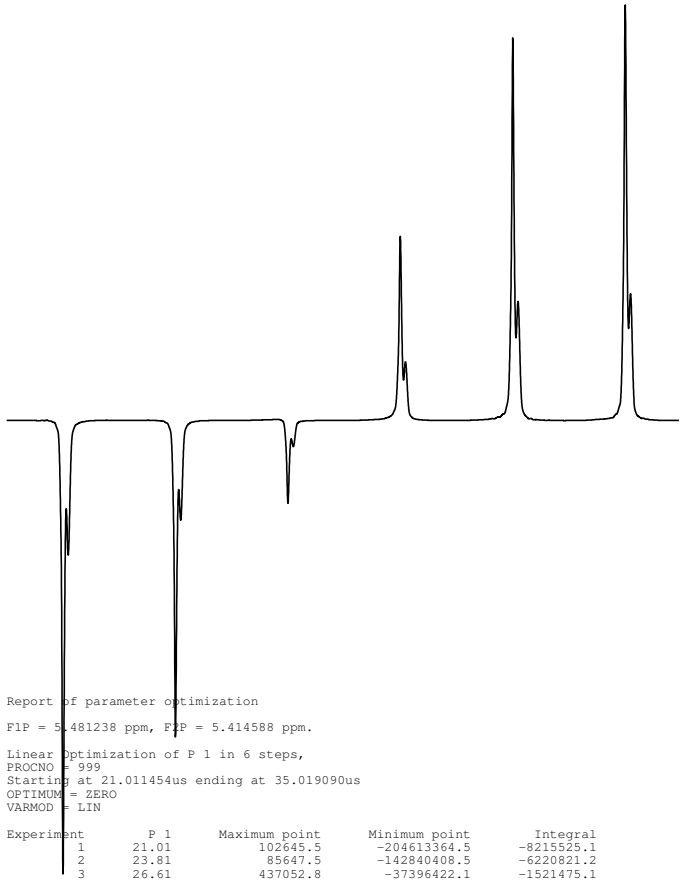
Report of parameter optimization

F1P = 5.481238 ppm, F2P = 5.414588 ppm.

Linear Optimization of P 1 in 6 steps,
PROCNO = 999
Starting at 10.500000us ending at 17.500000us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	10.50	164968591.0	-184797.0	6820984.2
2	11.90	113789512.2	-27440.2	4582293.0
3	13.30	37941041.5	-16420.0	1707234.6
4	14.70	694336.5	-37122193.5	-1106237.3
5	16.10	335443.5	-110444548.8	-3856831.2
6	17.50	156844.0	-162311993.5	-5904216.2

Zero found at P 1 = 14.007636 us



Report of parameter optimization

F1P = 5.481238 ppm, F2P = 5.414588 ppm.

Linear Optimization of P 1 in 6 steps,
PROCNO = 999
Starting at 21.011454us ending at 35.019090us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	21.01	102645.5	-204613364.5	-8215525.1
2	23.81	85647.5	-142840408.5	-6220821.2
3	26.61	437052.8	-37396422.1	-1521475.1
4	29.42	83047234.5	-24432.8	3977922.2
5	32.22	172506829.5	-81504.5	7854036.5
6	35.02	187392526.0	-57539.5	8430590.9

Zero found at P 1 = 27.484352 us

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

PLW90	P90	P90[det]	Deviation
11.3 W	7.0 us		
11.3 W	7.0 us	7.0 us	0.1%

SHIM SEQUENCE

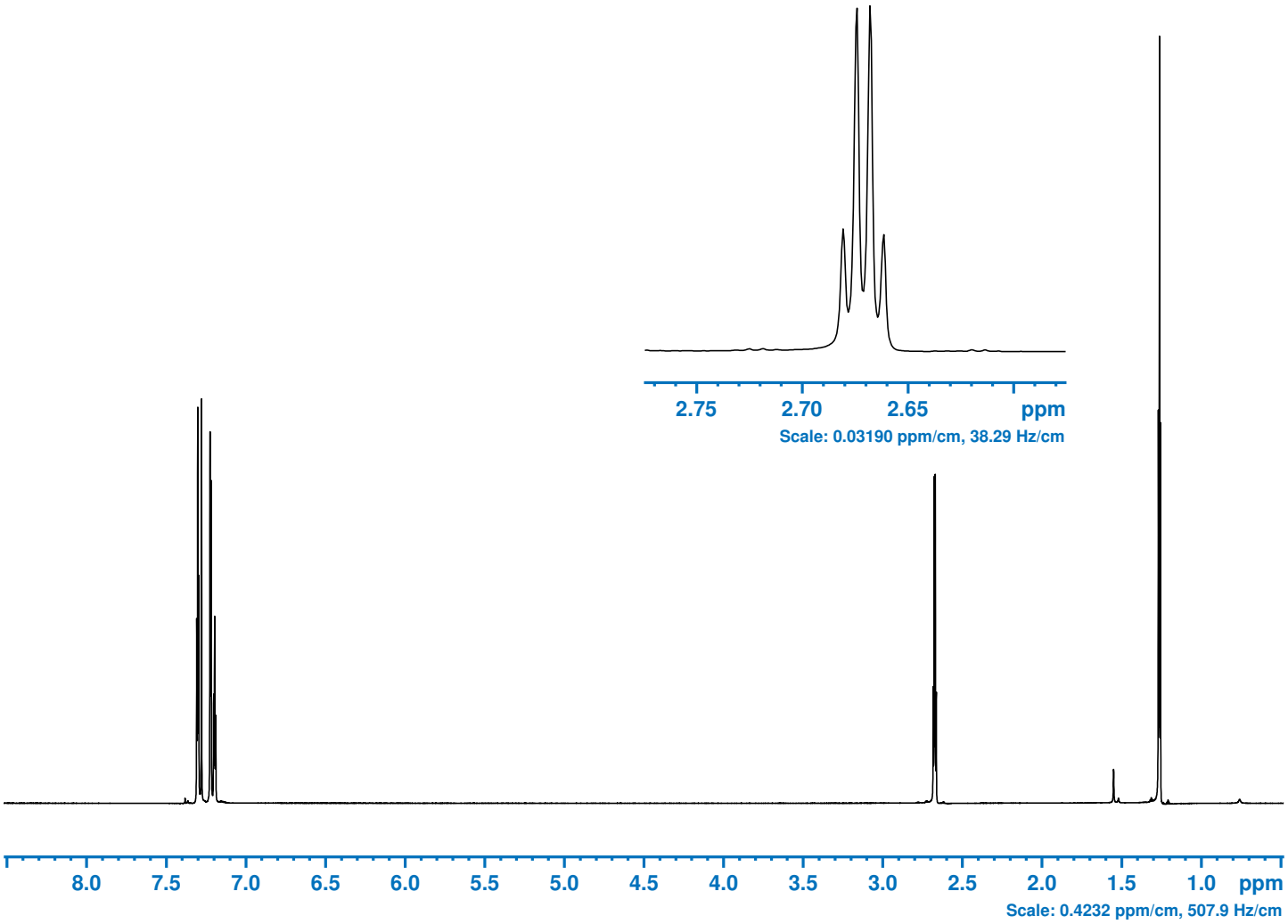
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 0.1% Ethylbenzene (EB) in Chloroform-D (Z10033)
1H sensitivity (NPT_1H_sensitivity, spin rate 0 Hz)

SINO (2.0 ppm) [achieved]: Signal (3.00 to 2.00 ppm), Noise (5.30 to 3.30 ppm) [4283.9] <n/a>
SINO (200.0 Hz) [achieved/rated]: Signal (3.00 to 2.00 ppm), Noise (5.30 to 5.13 ppm) [4948.1 >= 4000.0] <pass>

Bruker BioSpin

NPT_1H_sensitivity



Current Data Parameters

NAME	NPT_1H_sensitivity
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20250331
Time	9.17 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-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	1200.2848011 MHz
NUC1	1H
P1	7.00 usec
PLW1	11.31600000 W

F2 - Processing parameters

SI	16384
SF	1200.2800064 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

Additional Parameters

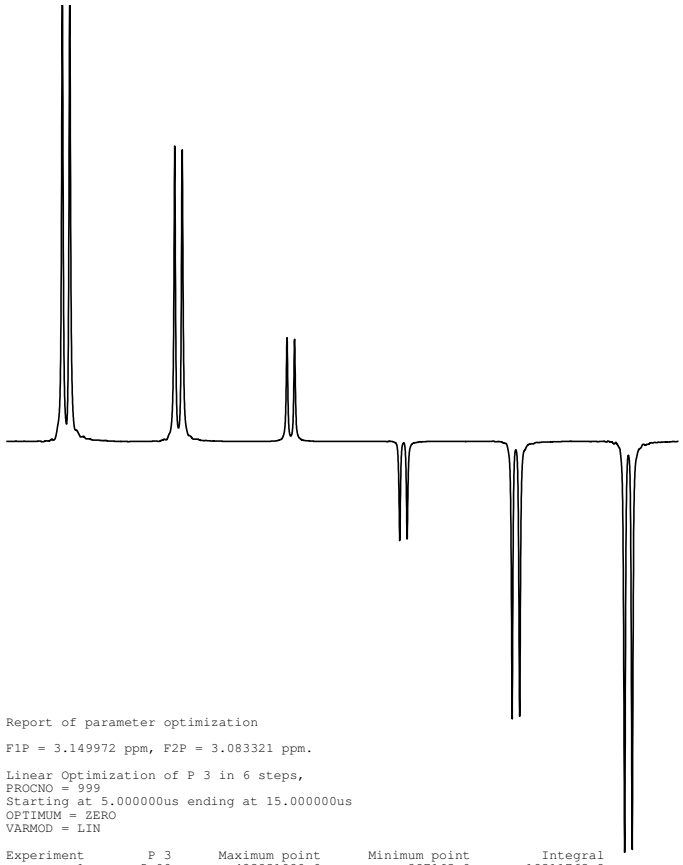
Field	5593.428
Lock Phase	131.098
Lock Power	-27.000
Lock Gain	127.685
Lock DC	-61.000
Lock Shift	7.240
Loop Gain	-12.000
Loop Time	0.400
Loop Filter	100.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250

SHIM SEQUENCE

- topshim fine ws5 tunea ordmax=8 <pass>

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10037)
Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c, spin rate 0 Hz)
Result: [90] = 10.0 us @ 261.5 W [270] = 29.7 us ==> [PDelay = 3*90 - 270] = 0.3 us
ATTENTION: Updated PROSOL Tables with [10.0 us @ 262.7 W]
Deviation from pulse target value (= 10.0 us): 0.2%

P90 13C pulse [achieved/rated]: @ 261.5 W [10.0 us <= 10.0 us] <pass>



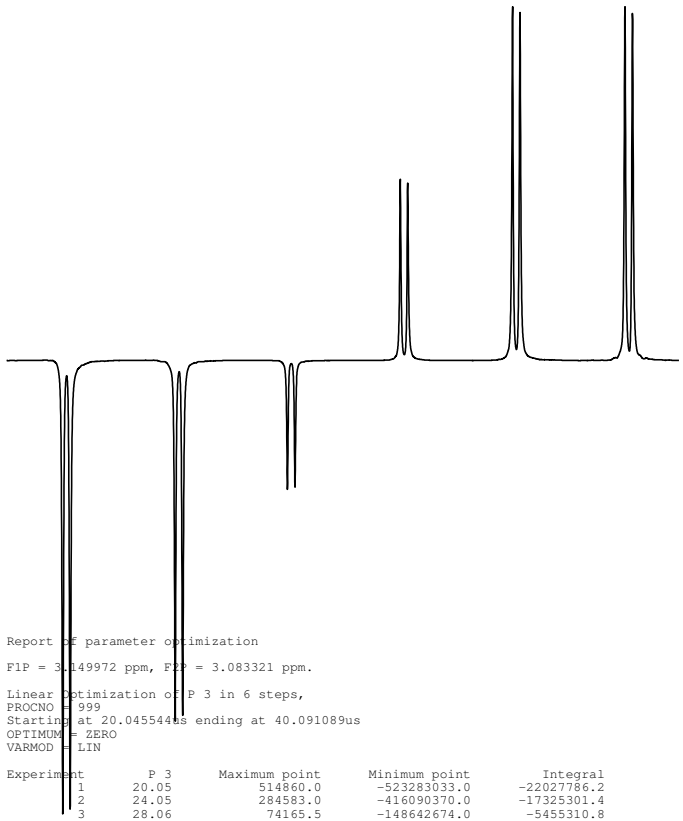
Report of parameter optimization

F1P = 3.149972 ppm, F2P = 3.083321 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	423831920.0	-287163.0	18311763.8
2	7.00	275999565.0	-206421.0	12249934.2
3	9.00	96943890.5	-55557.8	4145347.5
4	11.00	177491.8	-92626938.8	-3460691.7
5	13.00	272993.0	-259154872.0	-10890562.5
6	15.00	342383.0	-384041397.0	-16518600.8

Zero found at P 3 = 10.022772 us



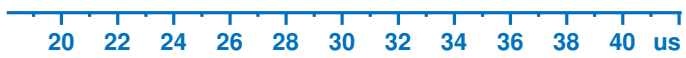
Report of parameter optimization

F1P = 3.149972 ppm, F2P = 3.083321 ppm.

Linear Optimization of P 3 in 6 steps,
PROCNO = 999
Starting at 20.045544us ending at 40.091089us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 3	Maximum point	Minimum point	Integral
1	20.05	514860.0	-523283033.0	-22027786.2
2	24.05	284583.0	-416090370.0	-17325301.4
3	28.06	74165.5	-148642674.0	-5455310.8
4	32.07	209029893.0	-80438.0	7682632.7
5	36.08	408201530.0	-176776.0	16153813.1
6	40.09	408160203.0	-194397.0	16307315.0

Zero found at P 3 = 29.729880 us



Bruker BioSpin

NPT_1H_p90determinationf2_13c

Current Data Parameters

NAME	NPT_1H_p90determinationf2_13c
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20250331
Time	7.57 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-D
PULPROG	decp90
TD	1000
SOLVENT	DMSO
NS	1
DS	0
SWH	230.766 Hz
FIDRES	0.461531 Hz
AQ	2.1667000 sec
RG	32
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	1200.2837408 MHz
NUC1	1H
P1	3.50 usec
PLW1	11.19100000 W
SFO2	301.8255661 MHz
NUC2	13C
P3	40.09 usec
PLW2	261.53515671 W

F2 - Processing parameters

SI	2048
SF	1200.2800000 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	0.10

Additional Parameters

Field	5561.173
Lock Phase	131.098
Lock Power	-19.000
Lock Gain	101.056
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

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

PLW90	P90	P90[det]	Deviation
150.0 W	10.0 us		
150.0 W	10.0 us	13.2 us	32.0%
261.5 W	10.0 us	10.0 us	0.2%

SHIM SEQUENCE

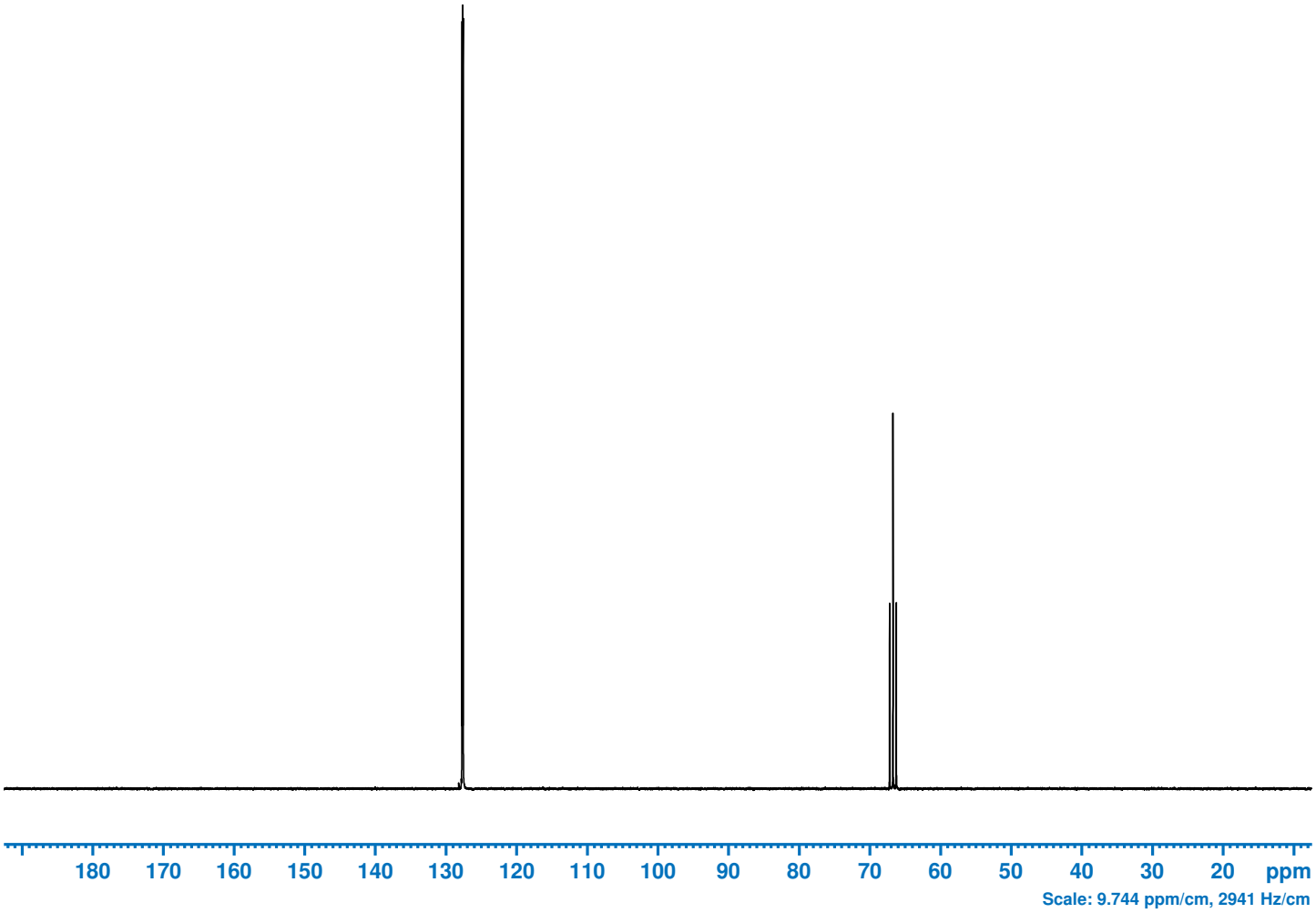
skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 40% Dioxane in Benzene-D6 (ASTM) (Z10035)
13C sensitivity (NPT_13C_sensitivity, spin rate 20 Hz)

SINO (40.0 ppm) [achieved/rated]: Signal (127.62 ppm), Noise (120.41 to 80.41 ppm) [914.7 >= 650.0] <pass>

Bruker BioSpin

NPT_13C_sensitivity



Current Data Parameters

NAME	NPT_13C_sensitivity
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20250331
Time	9.29 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-D
PULPROG	zg
TD	65340
SOLVENT	C6D6
NS	1
DS	0
SWH	58823.529 Hz
FIDRES	1.800537 Hz
AQ	0.5553900 sec
RG	101
DW	8.500 usec
DE	18.07 usec
TE	298.0 K
D1	120.00000000 sec
TD0	1
SFO1	301.8408233 MHz
NUC1	13C
P1	10.00 usec
PLW1	262.73000000 W

F2 - Processing parameters

SI	131072
SF	301.8106461 MHz
WDW	EM
SSB	0
LB	3.50 Hz
GB	0
PC	1.40

Additional Parameters

Field	5666.343
Lock Phase	131.098
Lock Power	-24.000
Lock Gain	119.826
Lock DC	-61.000
Lock Shift	7.160
Loop Gain	-0.000
Loop Time	0.200
Loop Filter	300.000
Gas Flow	535 l/h
Atma Unit	Z147150_3250

SHIM SEQUENCE

- topshim fine ws5 tunea ordmax=8 <pass>

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10037)
Indirect P90 15N pulse calibration (NPT_1H_p90determinationf2_15n, spin rate 0 Hz)
Result: [90] = 32.0 us @ 219.1 W [270] = 85.4 us ==> [PDelay = 3*90 - 270] = 10.7 us
ATTENTION: Updated PROSOL Tables with [32.0 us @ 219.7 W]
Deviation from pulse target value (= 32.0 us): 0.1%

P90 15N pulse [achieved/rated]: @ 219.1 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

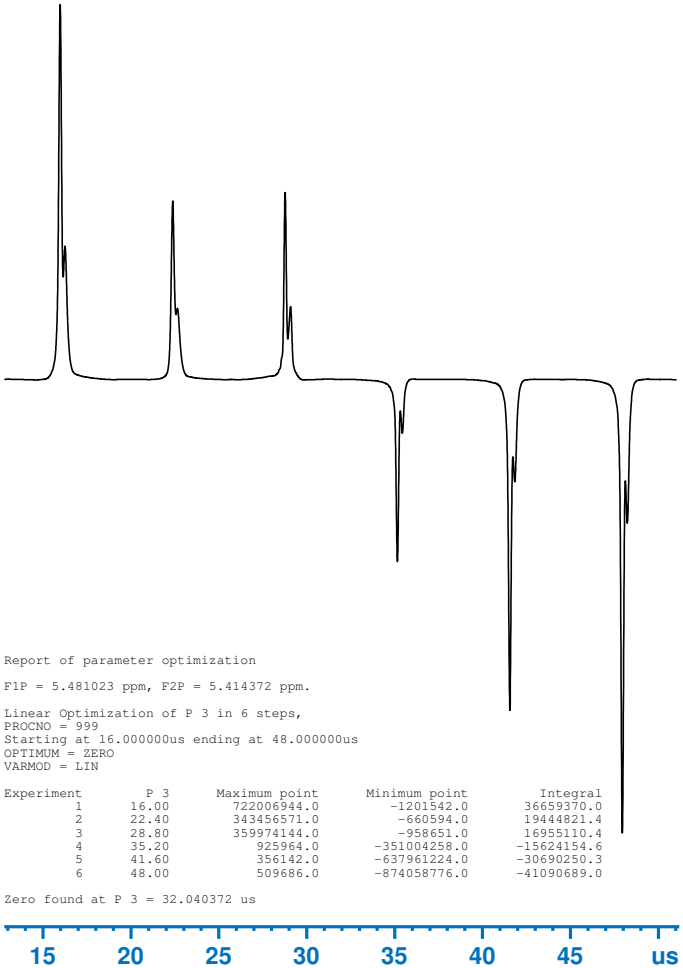
Date_	20250331
Time	8.02 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-D
PULPROG	decp90
TD	200
SOLVENT	DMSO
NS	1
DS	0
SWH	230.766 Hz
FIDRES	2.307657 Hz
AQ	0.4333400 sec
RG	32
DW	2166.700 usec
DE	10.00 usec
TE	298.0 K
CNST2	88.5000000
D1	0.68643398 sec
D2	0.00564971 sec
TD0	1
SFO1	1200.2865388 MHz
NUC1	1H
P1	4.67 usec
PLW1	11.19100000 W
SFO2	121.6325499 MHz
NUC2	15N
P3	128.16 usec
PLW2	219.14948379 W

F2 - Processing parameters

SI	2048
SF	1200.2800000 MHz
WDW	SINE
SSB	2
LB	0 Hz
GB	0
PC	1.00

Additional Parameters

Field	5564.942
Lock Phase	131.098
Lock Power	-19.000
Lock Gain	101.056
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



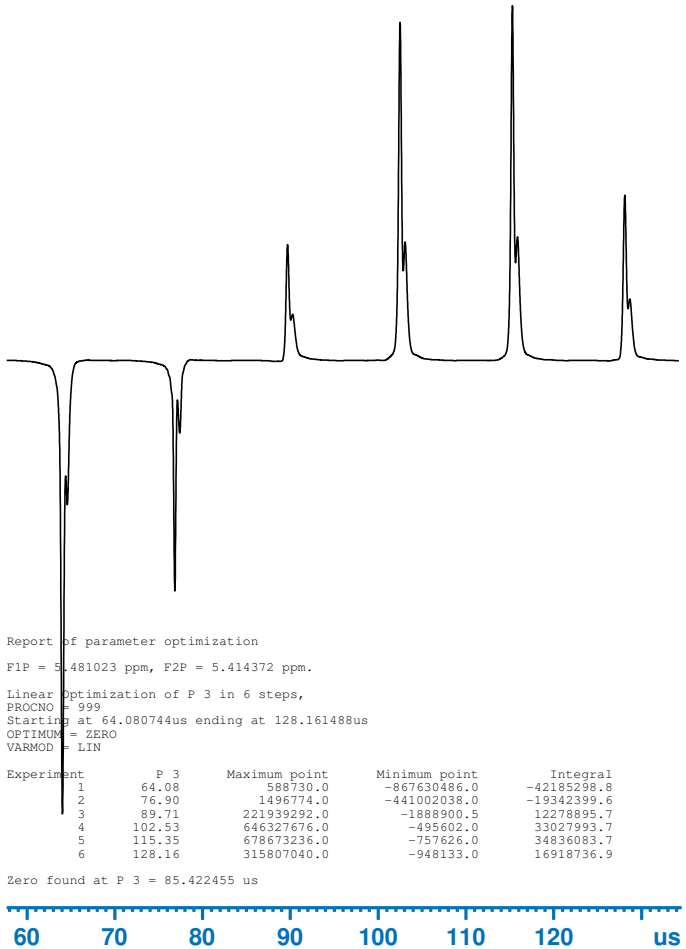
Report of parameter optimization

F1P = 5.481023 ppm, F2P = 5.414372 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	722006944.0	-1201542.0	36659370.0
2	22.40	343456571.0	-660594.0	19444821.4
3	28.80	359974144.0	-958651.0	16955110.4
4	35.20	925964.0	-351004258.0	-15624154.6
5	41.60	356142.0	-637961224.0	-30690250.3
6	48.00	509686.0	-874058776.0	-41090689.0

Zero found at P 3 = 32.040372 us



Report of parameter optimization

F1P = 5.481023 ppm, F2P = 5.414372 ppm.

Linear Optimization of P 3 in 6 steps,
PROCNO = 999
Starting at 64.080744us ending at 128.161488us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 3	Maximum point	Minimum point	Integral
1	64.08	588730.0	-867630486.0	-42185298.8
2	76.90	1496774.0	-441002038.0	-19342399.6
3	89.71	221939292.0	-1888900.5	12278895.7
4	102.53	646327676.0	-495602.0	33027993.7
5	115.35	678673236.0	-757626.0	34836083.7
6	128.16	315807040.0	-948133.0	16918736.9

Zero found at P 3 = 85.422455 us

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

PLW90	P90	P90[det]	Deviation
120.0 W	32.0 us		
120.0 W	32.0 us	38.8 us	21.2%
176.3 W	32.0 us	36.9 us	15.3%
234.3 W	32.0 us	30.9 us	-3.3%
219.1 W	32.0 us	32.0 us	0.1%

SHIM SEQUENCE

skip shimming

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10037)
P90 2H pulse calibration (NPT_prep_p90det_d, spin rate 0 Hz)
Result: [180/2] = 100.0 us @ 28.0 W [360] = 378.7 us ==> [PDelay = 2*180 - 360] = 21.5 us
ATTENTION: Updated PROSOL Tables with [100.0 us @ 28.0 W]
Deviation from pulse target value (= 100.0 us): 0.0%

P90 2H pulse [achieved/rated]: @ 28.0 W [100.0 us <= 100.0 us] <pass>

Bruker BioSpin

NPT_prep_p90det_d

Current Data Parameters

NAME	NPT_prep_p90det_d
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

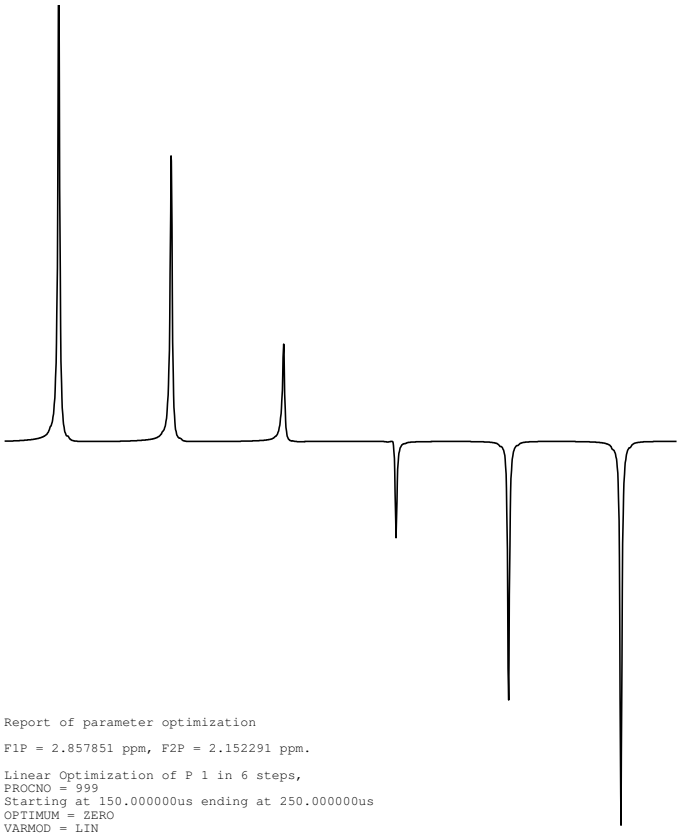
Date_	20250331
Time	7.46 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-D
PULPROG	npt_zg2h
TD	1024
SOLVENT	DMSO
NS	1
DS	0
SWH	1000.000 Hz
FIDRES	1.953125 Hz
AQ	0.5120000 sec
RG	45.2
DW	500.000 usec
DE	18.00 usec
TE	298.0 K
D1	0.35000000 sec
D11	0.03000000 sec
D12	0.00010000 sec
TD0	1
SFO1	184.2507496 MHz
NUC1	2H
P1	500.14 usec
PLW1	28.02392765 W

F2 - Processing parameters

SI	2048
SF	184.2502880 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.00

Additional Parameters

Field	5549.623
Lock Phase	131.098
Lock Power	-9.000
Lock Gain	99.892
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



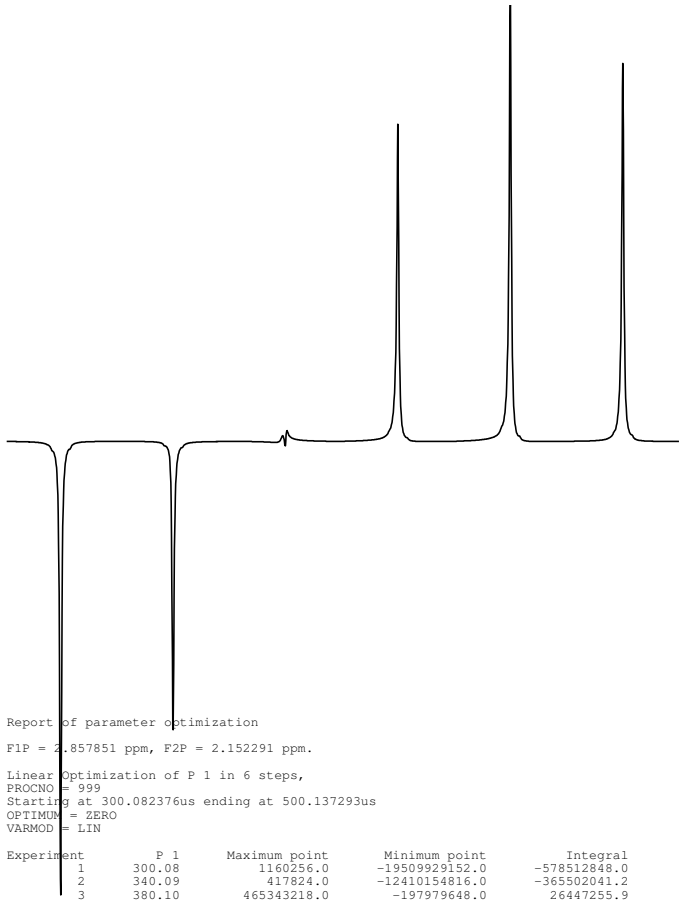
Report of parameter optimization

F1P = 2.857851 ppm, F2P = 2.152291 ppm.

Linear Optimization of P 1 in 6 steps,
PROCNO = 999
Starting at 150.000000us ending at 250.000000us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	150.00	18766106368.0	-3388160.0	601350859.9
2	170.00	11812166848.0	-4902144.0	390396523.7
3	190.00	4030762184.0	-8444568.0	146061379.6
4	210.00	3963440.0	-3986732416.0	-100547275.4
5	230.00	514496.0	-10697720544.0	-299422962.1
6	250.00	131936.0	-15873827296.0	-458840216.8

Zero found at P 1 = 200.054917 us



Report of parameter optimization

F1P = 2.857851 ppm, F2P = 2.152291 ppm.

Linear Optimization of P 1 in 6 steps,
PROCNO = 999
Starting at 300.082376us ending at 500.137293us
OPTIMUM = ZERO
VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	300.08	1160256.0	-19509929152.0	-578512848.0
2	340.09	417824.0	-12410154816.0	-365502041.2
3	380.10	465343218.0	-197979648.0	26447255.9
4	420.12	13648310688.0	-2745568.0	452148692.4
5	460.13	19304480192.0	-3821632.0	625491071.8
6	500.14	16260823424.0	-795520.0	520733137.8

Zero found at P 1 = 378.658275 us

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

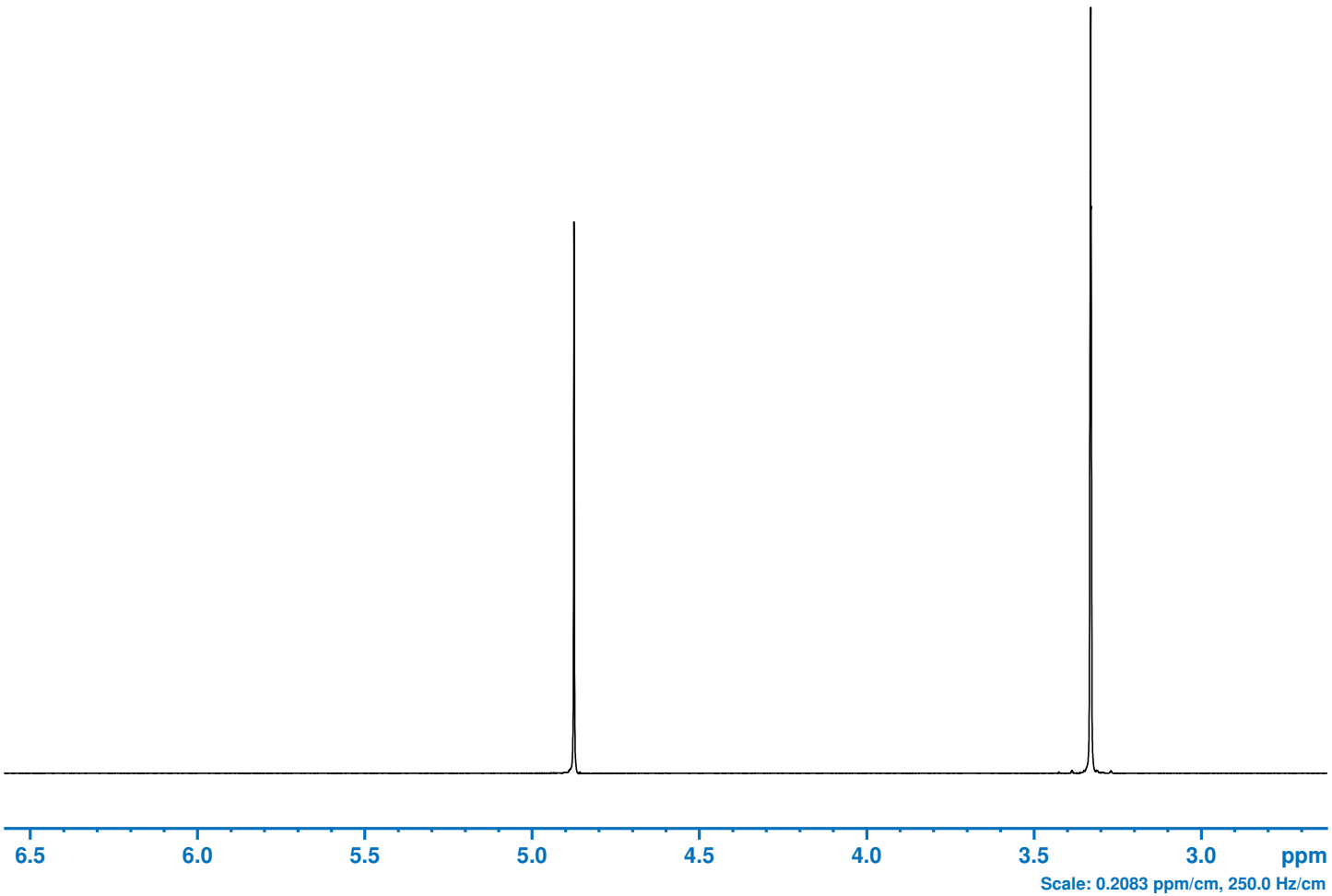
PLW90	P90	P90[det]	Deviation
20.0 W	100.0 us		
20.0 W	100.0 us	117.2 us	17.2%
27.4 W	100.0 us	101.0 us	1.0%
28.0 W	100.0 us	100.0 us	0.0%

SHIM SEQUENCE

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

NMR TEST ACCEPTANCE *** System: AV NEO (1200.28 MHz) *** TopSpin 4.4.1
Probe: Z161014_0006 CP2.1 TCI 1200SA H/C/N-D-03 Z *** Sample Depth: 21 mm
Sample: Temperature Calibration - 99.8% Methanol-D4 (Z10053)
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 = 1.040 * x + (-8.653)

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) = 298.1 K, Signal 1 = 4.8741 ppm, Signal 2 = 3.3294 ppm
Version = BSVT, setPoint = 298.000 K, AirFlow = 535.000 l/h, XP = 1.663, TI = 86.962, TD = 14.494



Bruker BioSpin

NPT_1H_tempcalib_998meod

Current Data Parameters

NAME	NPT_1H_tempcalib_998meod
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20250331
Time	7.32 h
INSTRUM	Avance
PROBHD	Z161014_0006 (CP2.1 TCI 1200SA H/C/N-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	1200.2855213 MHz
NUC1	1H
P0	2.33 usec
P1	7.00 usec
PLW1	14.00000000 W

F2 - Processing parameters

SI	16384
SF	1200.2800000 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	0.10

Additional Parameters

Field	5545.062
Lock Phase	131.098
Lock Power	-34.000
Lock Gain	106.638
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

skip shimming