

DRAFT



Bruker BioSpin

PH MAS DVT BL4

700.13 MHz

Probe ID: H8780_0002

Inspection Lot: 2023-07-12

NMR TEST SERVICE

Jul 13, 2023

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 5000 Hz)

Line width main [achieved]: [151] <n/a>

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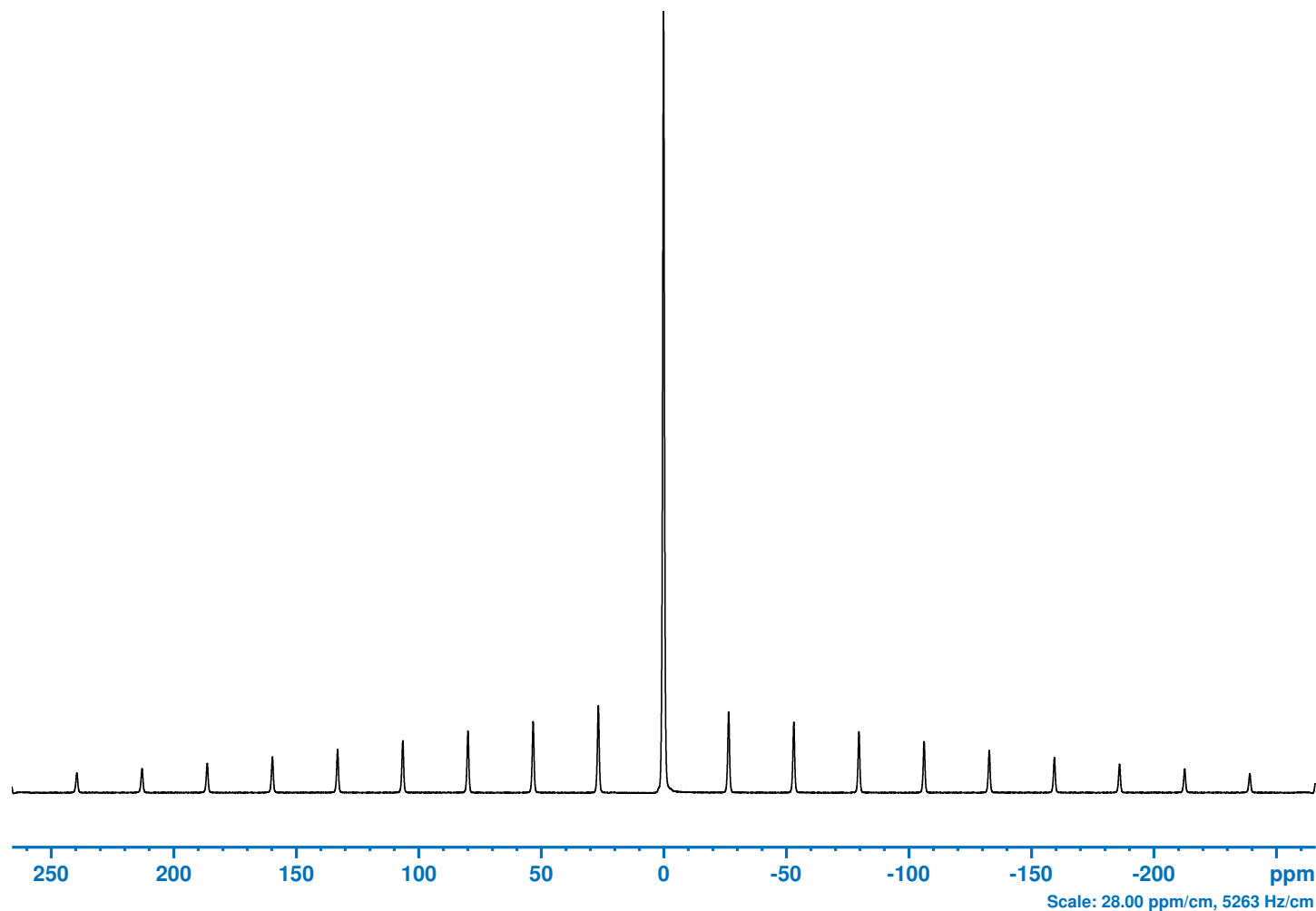
Bruker BioSpin

NPT_79Br_MAS_magicAngle

Current Data Parameters
NAME NPT_79Br_MAS_magicAngle
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230712
Time 13.04 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG onepulse
TD 8192
SOLVENT H2O+D2O
NS 16
DS 0
SWH 100000.000 Hz
FIDRES 24.414062 Hz
AQ 0.0409600 sec
RG 101
DW 5.000 usec
DE 6.50 usec
TE 298.0 K
D1 0.25000000 sec
SFO1 187.9913332 MHz
NUC1 79Br
P1 3.84 usec
PLW1 192.0000000 W

F2 - Processing parameters
SI 131072
SF 187.9913332 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20



SHIM SEQUENCE
skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 15000 Hz)
Determination of spinning stability for 180 s
Pressure values in mbar: DrivePressure=2053/BearingPressure=3169/BearingSensePressure=3167/SupplyPressure=6546/SystemPressure=6176

Spin rate at maximum deviation [measured]: @ MASR 15000 Hz [15002 Hz]
Maximum deviation [achieved]: @ MASR 15000 Hz [2 Hz] <n/a>

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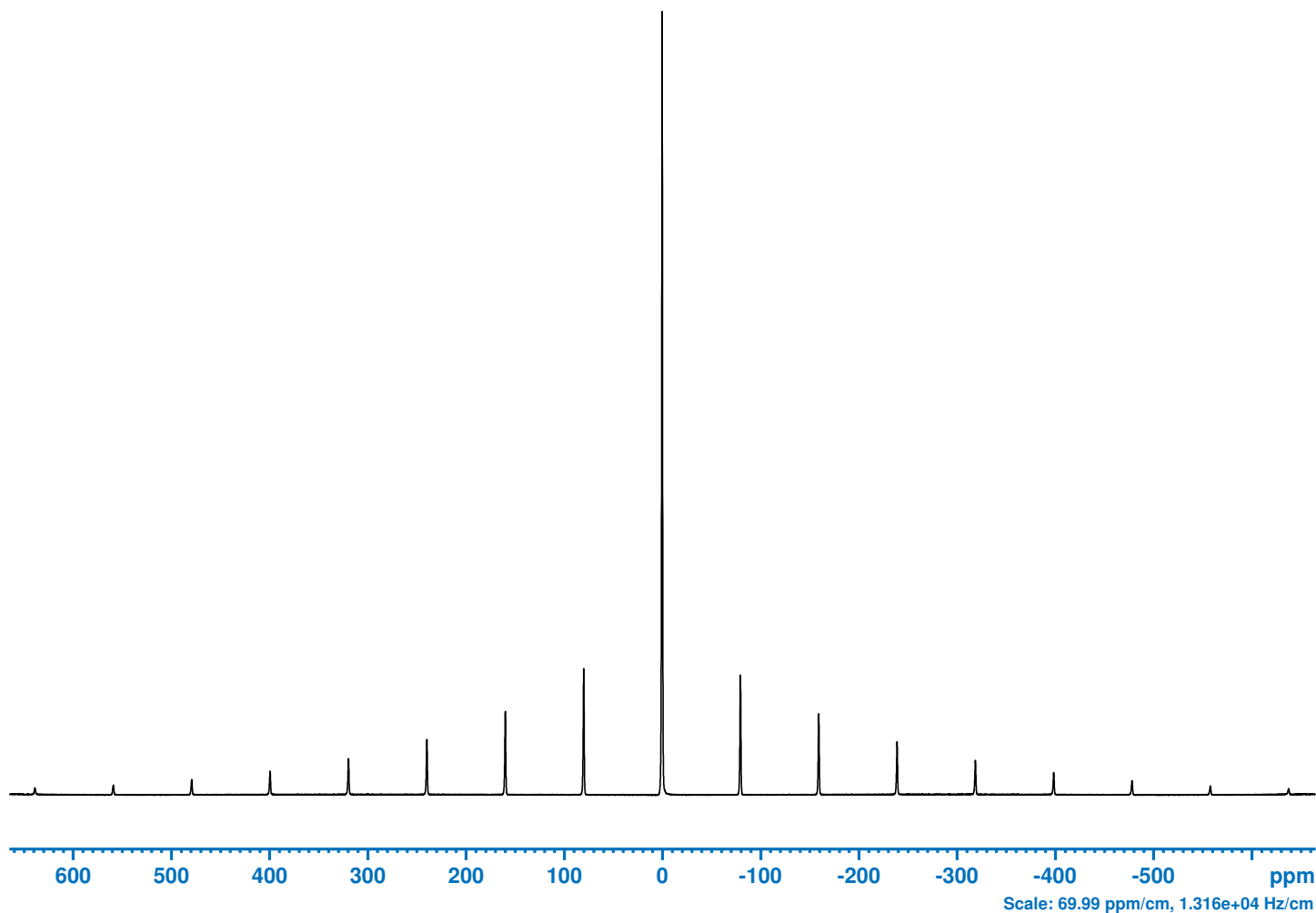
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

Current Data Parameters
NAME NPT_79Br_MAS_maxSpinRate
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230712
Time 13.18 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG onepulse
TD 16384
SOLVENT H2O+D2O
NS 16
DS 0
SWH 250000.000 Hz
FIDRES 30.517578 Hz
AQ 0.0327680 sec
RG 401
DW 2.000 usec
DE 6.50 usec
TE 298.0 K
D1 0.25000000 sec
SFO1 187.9904591 MHz
NUC1 79Br
P1 3.84 usec
PLW1 192.00000000 W

F2 - Processing parameters
SI 32768
SF 187.9904591 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20



SHIM SEQUENCE
skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting, spin rate 5000 Hz)
FIELD was set to 2124.9 for 79Br chemical shift of 59.700 ppm. One field unit corresponds to 0.0064 ppm.

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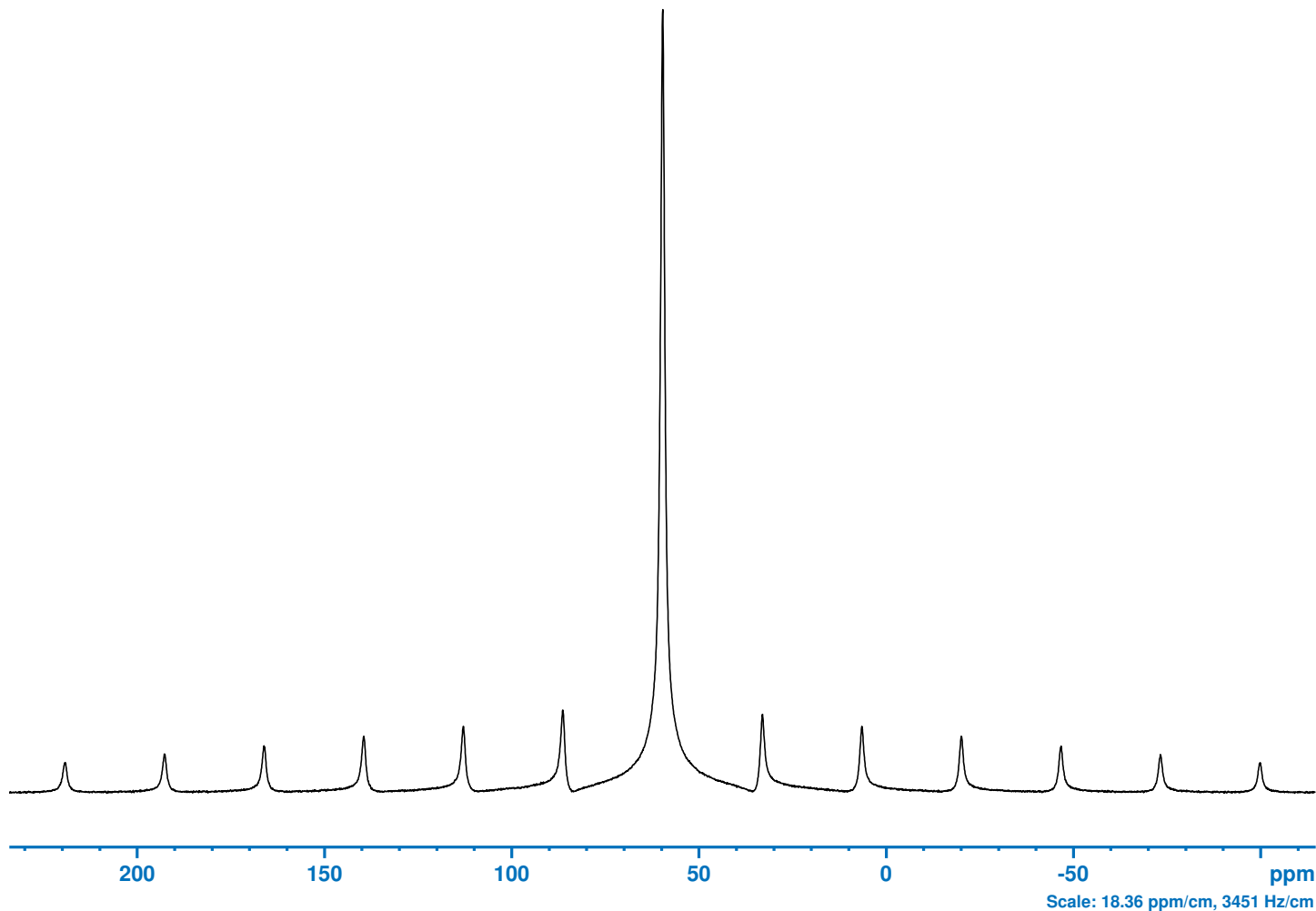
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NPT_79Br_MAS_fieldsetting

Current Data Parameters
NAME NPT_79Br_MAS_fieldsetting
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230712
Time 13.08 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG onepulse
TD 4096
SOLVENT H2O+D2O
NS 1
DS 0
SWH 81967.211 Hz
FIDRES 40.023052 Hz
AQ 0.0249856 sec
RG 101
DW 6.100 usec
DE 6.50 usec
TE 298.0 K
D1 0.50000000 sec
SFO1 187.9912344 MHz
NUC1 79Br
P1 3.84 usec
PLW1 192.0000000 W

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



SHIM SEQUENCE
skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Adamantane (50 ul) (Z151221)
P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 15000 Hz)
ATTENTION: Updated PROSOL Tables with [2.50 us @ 131.3 W]. Calculation based on ==> [2.85 us @ 101.0 W],

P90 MAS 1H pulse [achieved]: @ 101.0 W [2.85 us] <n/a>

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NPT_1H_MAS_p90det_1h

Current Data Parameters
NAME NPT_1H_MAS_p90det_1h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230712
Time 15.17 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG onepulse
TD 2988
SOLVENT H2O+D2O
NS 1
DS 0
SWH 100000.000 Hz
FIDRES 66.934402 Hz
AQ 0.0149400 sec
RG 8
DW 5.000 usec
DE 6.50 usec
TE 298.0 K
D1 5.00000000 sec
SFO1 750.3018457 MHz
NUC1 1H
P1 7.50 usec
PLW1 101.00000000 W

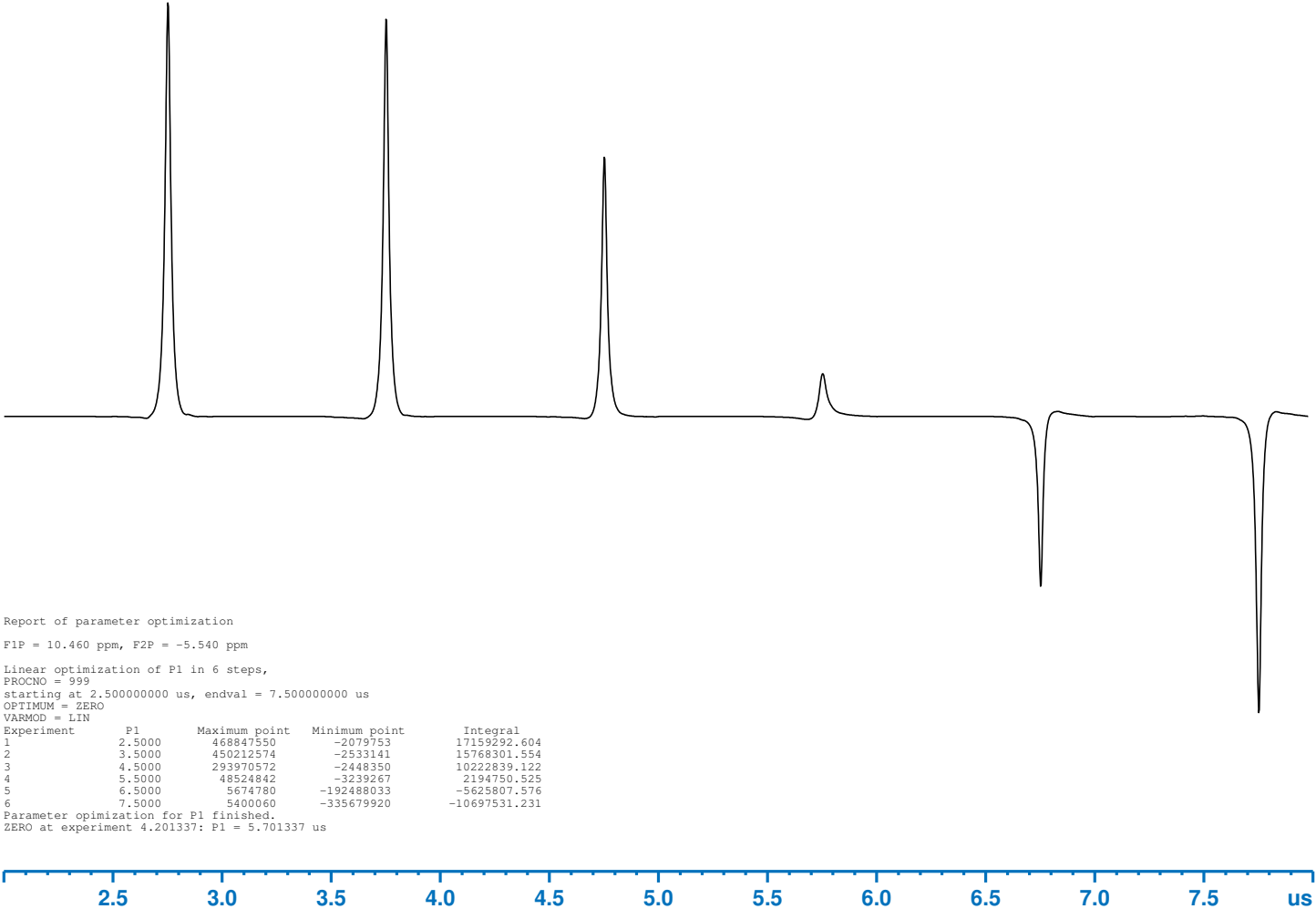
F2 - Processing parameters
SI 4096
SF 750.3000000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20

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

101.0 W 2.50 us
101.0 W 2.50 us 2.85 us 14.0%

SHIM SEQUENCE

skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br, spin rate 5000 Hz)
ATTENTION: Update PROSOL Tables (79Br) failed.

P90 MAS 79Br pulse [achieved]: @ 192.0 W [4.42 us] <n/a>

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NPT_79Br_MAS_p90det_79br

Current Data Parameters
NAME NPT_79Br_MAS_p90det_79br
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230712
Time 13.08 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG onepulse
TD 2048
SOLVENT H2O+D2O
NS 1
DS 0
SWH 100000.000 Hz
FIDRES 97.656250 Hz
AQ 0.0102400 sec
RG 101
DW 5.000 usec
DE 6.50 usec
TE 298.0 K
D1 0.25000000 sec
SFO1 187.9912344 MHz
NUC1 79Br
P1 11.52 usec
PLW1 192.0000000 W

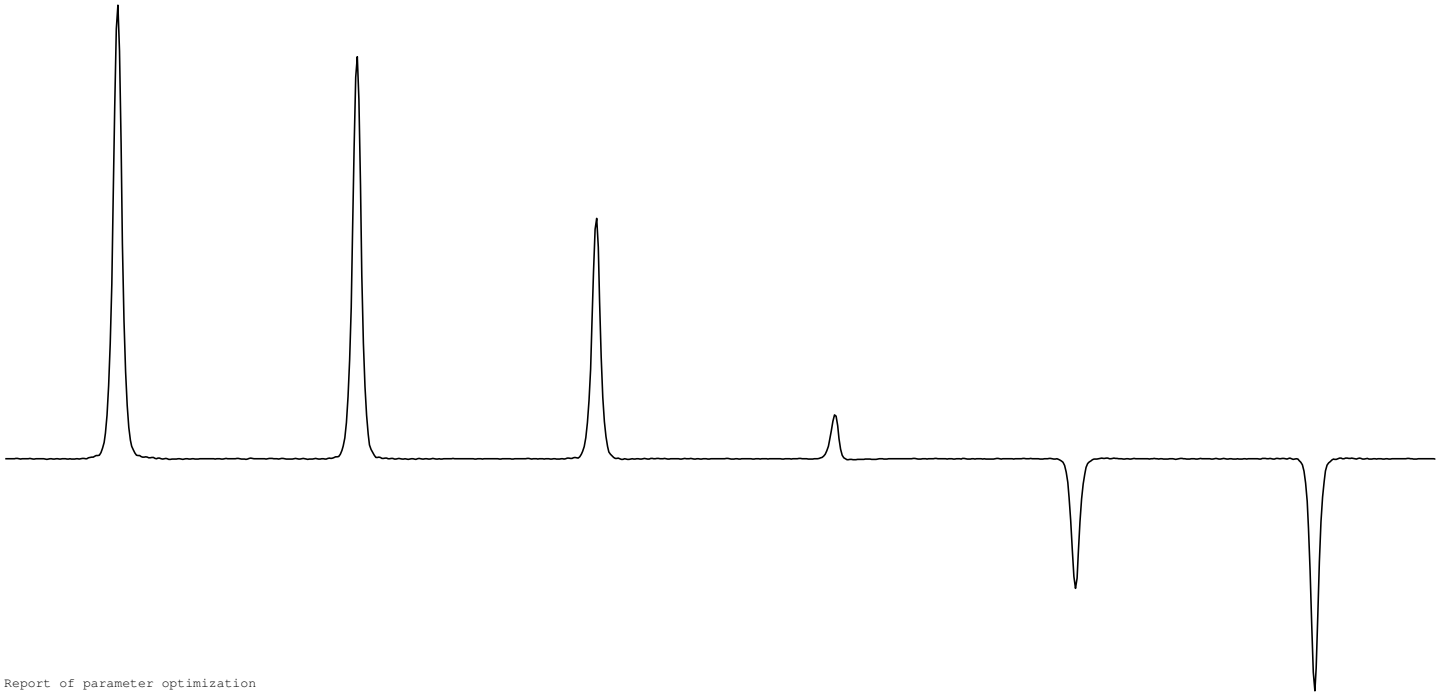
F2 - Processing parameters
SI 4096
SF 187.9800119 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.20

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

192.0 W 3.84 us
192.0 W 3.84 us 4.42 us 15.1%

SHM SEQUENCE

skip shimming



Report of parameter optimization

F1P = 69.700 ppm, F2P = 49.700 ppm

Linear optimization of P1 in 6 steps,
PROCNO = 999
starting at 3.839999914 us, endval = 11.519999504 us
OPTIMUM = ZERO
VARMOD = LIN
Experiment P1 Maximum point Minimum point Integral
1 3.8400 469585148 -652584 21998003.806
2 5.3760 416335811 -507142 18940826.890
3 6.9120 248912621 -703152 10998867.781
4 8.4480 45413564 -992767 1726081.316
5 9.9840 747951 -134197493 -5748495.226
6 11.5200 865670 -240077143 -9999567.665
Parameter optimization for P1 finished.
ZERO at experiment 4.252844: P1 = 8.836368 us



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Alpha-glycine (50 ul) (Z151222)
CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n, spin rate 7500 Hz)

SINO (20.0 ppm) [achieved]: Signal (29.45 ppm), Noise (198.52 to 178.51 ppm) [66.8] <n/a>
Number of scans (NS) [achieved]: [64] <n/a>

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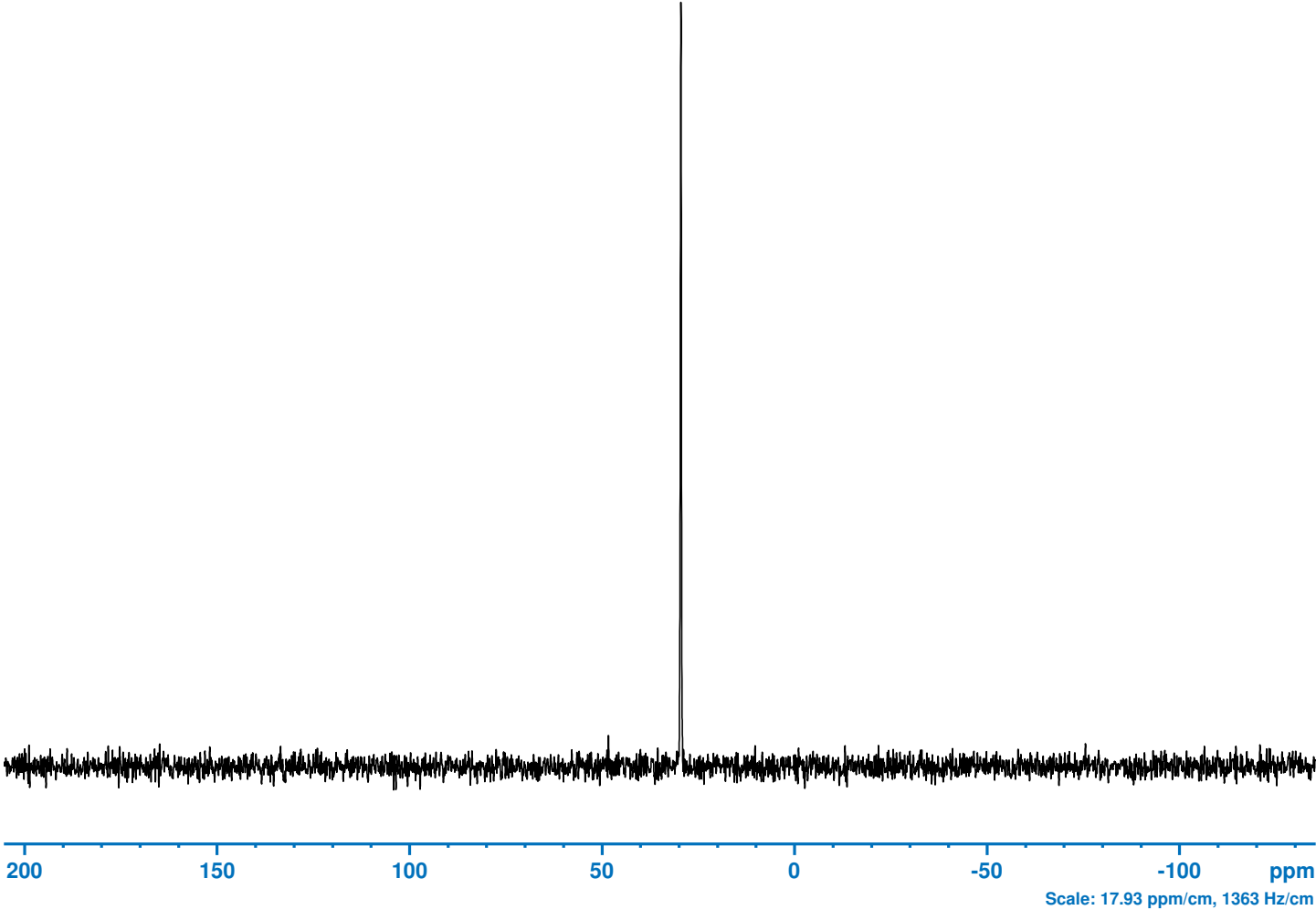
NPT_15N_MAS_sino_cp1h_15n

Current Data Parameters
NAME NPT_15N_MAS_sino_cp1h_15n
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 13.37 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH
PULPROG cp
TD 3012
SOLVENT H2O+D2O
NS 64
DS 0
SWH 30120.482 Hz
FIDRES 20.000320 Hz
AQ 0.0499992 sec
RG 101
DW 16.600 usec
DE 6.50 usec
TE 294.3 K
D1 5.00000000 sec
ZGPGTNS
SFO1 76.0299000 MHz
NUC1 15N
P15 3500.00 usec
PLW1 255.00000000 W
SFO2 750.3046519 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG[2] spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 131.25999451 W
PLW12 142.80000305 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 63.95999908 W

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

SHIM SEQUENCE
skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Ammonium Dihydrogenphosphate (50 ul) (Z151224)
CP 1H-31P sensitivity, MAS (NPT_31P_MAS_sino_cp1h_31p, spin rate 5000 Hz)

SINO (10.0 ppm) [achieved]: Signal (-2.53 ppm), Noise (-105.43 to -115.43 ppm) [10268.3] <n/a>
Number of scans (NS) [achieved]: [4] <n/a>

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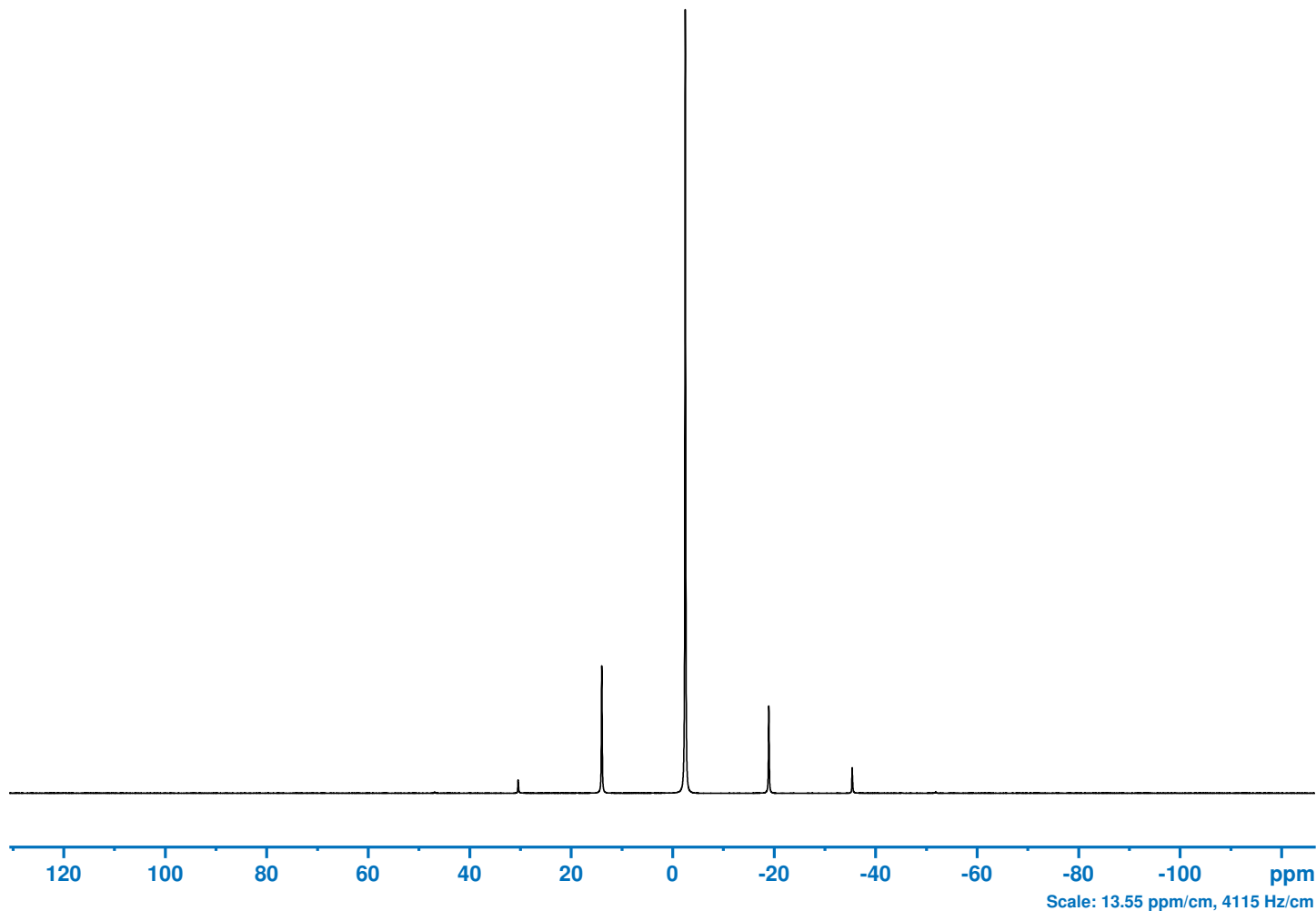
NPT_31P_MAS_sino_cp1h_31p

Current Data Parameters
NAME NPT_31P_MAS_sino_cp1h_31p
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 15.07 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG cp
TD 9090
SOLVENT H2O+D2O
NS 4
DS 0
SWH 90909.094 Hz
FIDRES 20.002001 Hz
AQ 0.0499950 sec
RG 101
DW 5.500 usec
DE 6.50 usec
TE 294.2 K
D1 5.00000000 sec
ZGPGTNS
SFO1 303.7276145 MHz
NUC1 31P
P15 3500.00 usec
PLW1 82.00000000 W
SFO2 750.3054022 MHz
NUC2 1H
CNST21 1.00000000
CPDPRG2 spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 131.25999451 W
PLW12 147.00000000 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 62.40000153 W

F2 - Processing parameters
SI 32768
SF 303.7270070 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

SHIM SEQUENCE
skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Adamantane (50 ul) (Z151221)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 15000 Hz)
ATTENTION: non-standard execution of experiment
SINO (20.0 ppm) [achieved]: Signal (34.48 ppm), Noise (59.26 to 39.26 ppm) [68.9] <n/a>
Linewidth [achieved]: at 50% of signal height [2.3 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>

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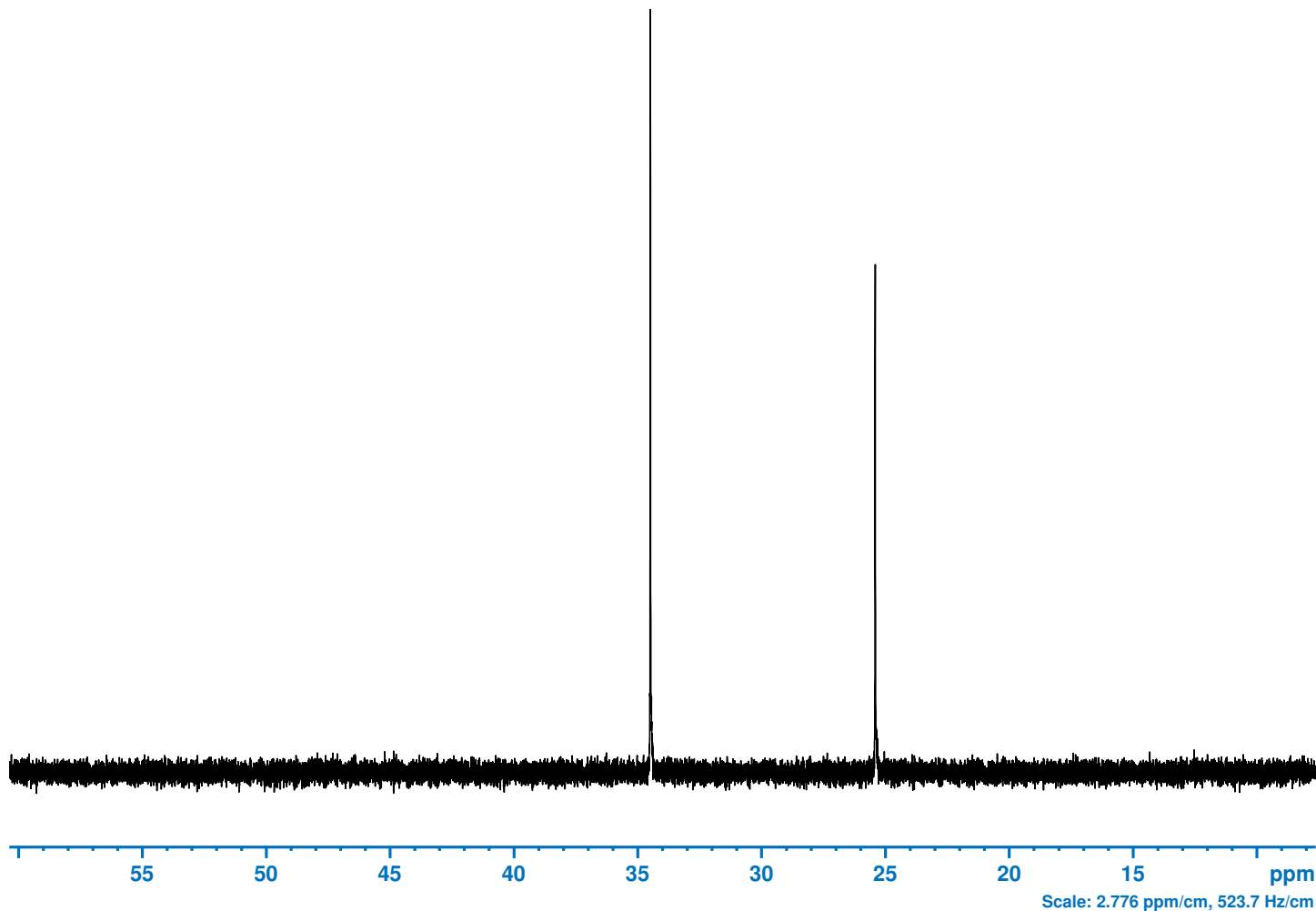
NPT_13C_MAS_sino_13c

Current Data Parameters
NAME NPT_13C_MAS_sino_13c
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230712
Time 15.10 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG hdec
TD 19998
SOLVENT H2O+D2O
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 1.000100 Hz
AQ 0.9999000 sec
RG 101
DW 50.000 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
P15 0 usec
ZGPTNS -Dlacq
SFO1 188.6694995 MHz
NUC1 13C
P1 3.84 usec
PLW1 50.00000000 W
SFO2 750.3018457 MHz
NUC2 1H
CPDPRG2 spinal64
PCPD2 4.80 usec
PLW2 0 W
PLW12 67.00000000 W

F2 - Processing parameters
SI 32768
SF 188.6630850 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 0.20

SHIM SEQUENCE
skip shimming



NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: Adamantane (50 ul) (Z151221)
1H sensitivity, MAS (NPT_1H_MAS_sino_1h, spin rate 15000 Hz)

SINO (20.0 ppm) [achieved]: Signal (-1.59 ppm), Noise (-43.10 to -63.11 ppm) [25504.0] <n/a>
Linewidth [achieved]: at 50% of signal height [357.4 Hz] <n/a>
Number of scans (NS) [achieved]: [1] <n/a>

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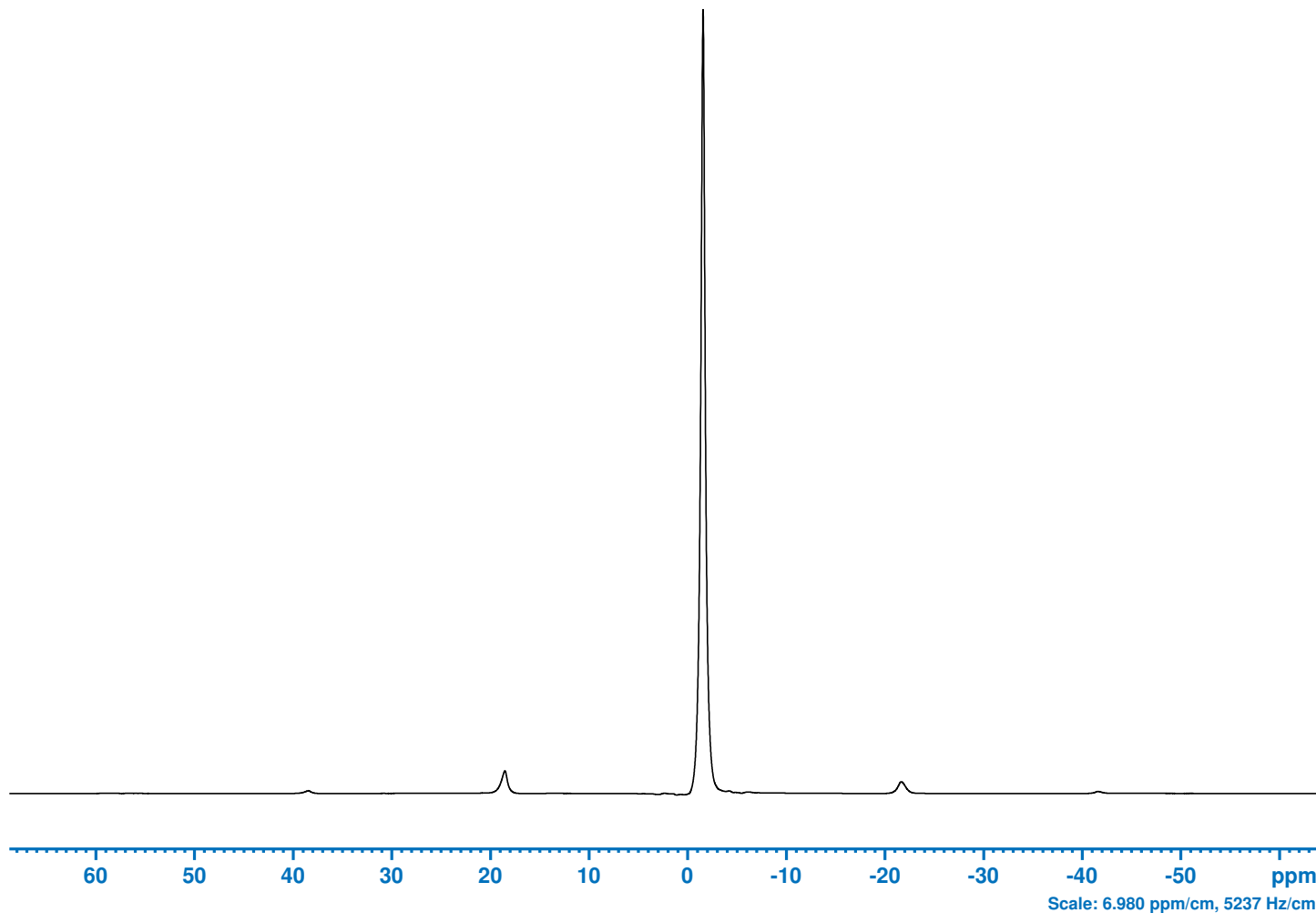
Bruker BioSpin

NPT_1H_MAS_sino_1h

Current Data Parameters
NAME NPT_1H_MAS_sino_1h
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230712
Time 15.26 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG onepulse
TD 2048
SOLVENT H2O+D2O
NS 1
DS 0
SWH 100000.000 Hz
FIDRES 97.656250 Hz
AQ 0.0102400 sec
RG 8
DW 5.000 usec
DE 6.50 usec
TE 298.0 K
D1 5.00000000 sec
SFO1 750.3018457 MHz
NUC1 1H
P1 2.50 usec
PLW1 131.25999451 W

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



SHIM SEQUENCE

skip shimming

NMR TEST SERVICE *** System: AV NEO (750.30 MHz) *** TopSpin 4.1.3
Probe: H8780_0002 PH MAS DVT BL4
Sample: 2-13C, 15N alpha-glycine (50 ul) (Z151223)
CP 1H-15N parameter optimization, MAS (NPT_15N_MAS_paropt_cp1h_15n, spin rate 7500 Hz)

SINO (20.0 ppm): Signal (29.45 ppm), Noise (-103.57 to -123.60 ppm) [3591.6]

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NPT_15N_MAS_paropt_cp1h_15n

Current Data Parameters
NAME NPT_15N_MAS_paropt_cp1h_15n
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20230713
Time 13.11 h
INSTRUM Avance NEO
PROBHD H8780_0002 (PH)
PULPROG cp
TD 5554
SOLVENT H2O+D2O
NS 4
DS 0
SWH 55555.555 Hz
FIDRES 20.005602 Hz
AQ 0.0499860 sec
RG 101
DW 9.000 usec
DE 6.50 usec
TE 294.5 K
D1 5.00000000 sec
ZGPGTNS
SFO1 76.0299000 MHz
NUC1 15N
P15 3500.00 usec
PLW1 255.00000000 W
SFO2 750.3046519 MHz
NUC2 1H
CNST21 1.0000000
CPDPRG2 spinal64
P3 2.50 usec
PCPD2 4.80 usec
PLW2 131.25999451 W
PLW12 142.80000305 W
SPNAM[0] ramp50100.100
SPOAL0 0.500
SPOFFS0 0 Hz
SPW0 63.95999908 W

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

SHIM SEQUENCE
skip shimming

