

CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT

600 MHz

Probe ID: Z168568_0015

Report Name: 2025-03-11

● Probe NMR Test Data: **CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT**

Probe Related Information

EC-Level	0.03
Sample Depth (standard) [mm]	21
Sample Depth (water-based Solvents) [mm]	21
Gas Compensation	nitrogen
Gradient System	Z
ATM Accessory	true
Temperature Sensor Type	PT100
Proton Frequency [MHz]	600
Diameter [mm]	5.0

Spectrometer Related Information

Type	AV III
CF Frequency [MHz]	600.13
Shim System	BOSS3-SB
Software	TopSpin 3.7.0
Operating System	CentOS Linux release 7.9.2009 (Core)
Host Name	av600
Magnet System	SB
Magnet	
Cryostat	
System Number	10017285

● PICS Data

Z168568_0015.ph

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Z168568_0015.ph
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$Production, Z168568, 0015, 00.03, , BCH, 20210108#
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$ProbeTemperature, 1.0, PT100, -42, 171#
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● **Required Samples** CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT

Z10263 100 mM Urea- ^{15}N , 100 mM Methanol- ^{13}C in Dimethyl Sulfoxide- D_6

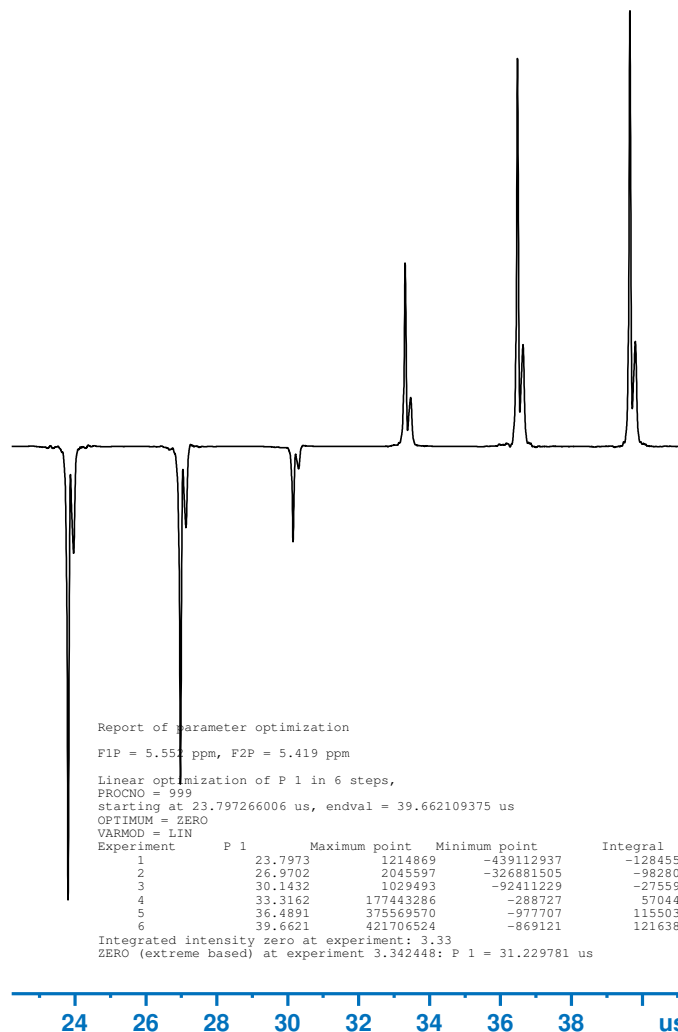
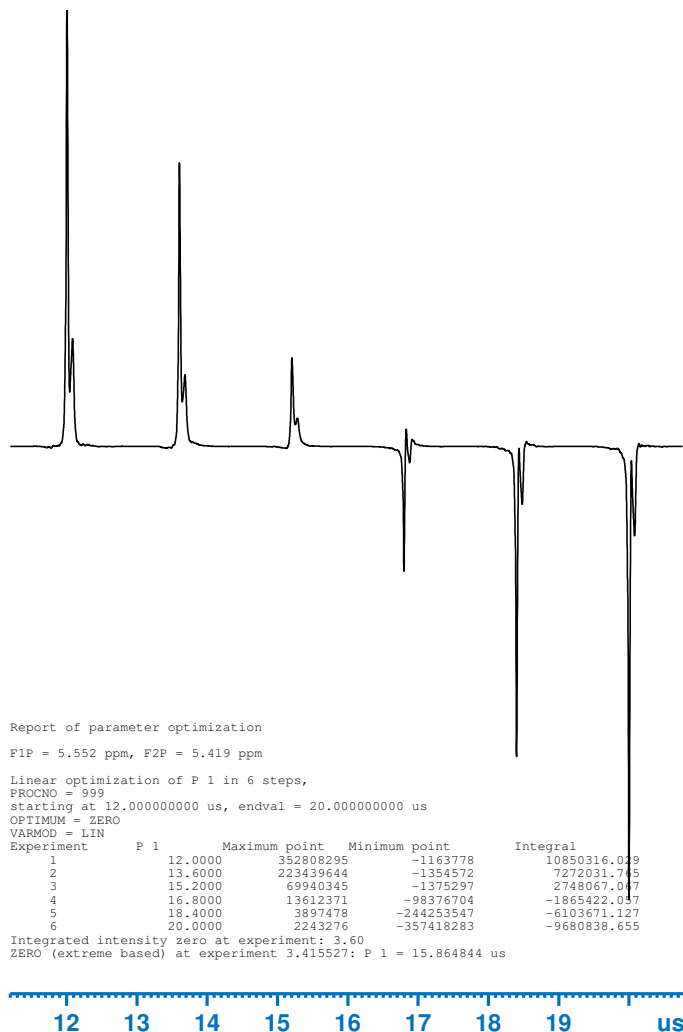
NMR TEST SERVICE *** System: AV III (600.13 MHz) *** TopSpin 3.7.0
 Probe: Z168568_0015 CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT *** Sample Depth: 21 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 P90 1H pulse calibration (NPT_1H_p90determinationf1_1h, spin rate 0 Hz)
 Result: [180/2] = 7.9 us @ 5.65 W [360] = 31.2 us ==> [PDelay = 2*180 - 360] = 0.5 us
 ATTENTION: Updated PROSOL Tables with [8.0 us @ 5.55 W]
 Deviation from pulse target value (= 8.0 us): -0.8%

P90 1H pulse [achieved/rated]: @ 5.65 W [7.9 us <= 8.0 us] <pass>



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NPT_1H_p90determinationf1_1h



Current Data Parameters
 NAME NPT_1H_p90determinationf1_1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250311
 Time 15.06 h
 INSTRUM AVANCEIII600
 PROBHD Z168568_0015
 PULPROG zg
 TD 300
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 142.045 Hz
 FIDRES 0.946970 Hz
 AQ 1.0560000 sec
 RG 22.6
 DW 3520.000 usec
 DE 29.00 usec
 TE 298.0 K
 DI 1.34508002 sec
 TD0 1
 SF01 600.1332922 MHz
 NUC1 1H
 P1 39.66 usec
 PLW1 5.64838696 W

Additional Parameters
 Field 4974.491
 Lock Phase 199.273
 Lock Power -10.000
 Lock Gain 96.571
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 535 l/h
 Atma Unit Z147150_0414

F2 - Processing parameters
 SI 2048
 SF 600.1300000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 5.65 W 8.0 us
 5.65 W 8.0 us 7.9 us -0.8%

 SHIM SEQUENCE

 skip shimming

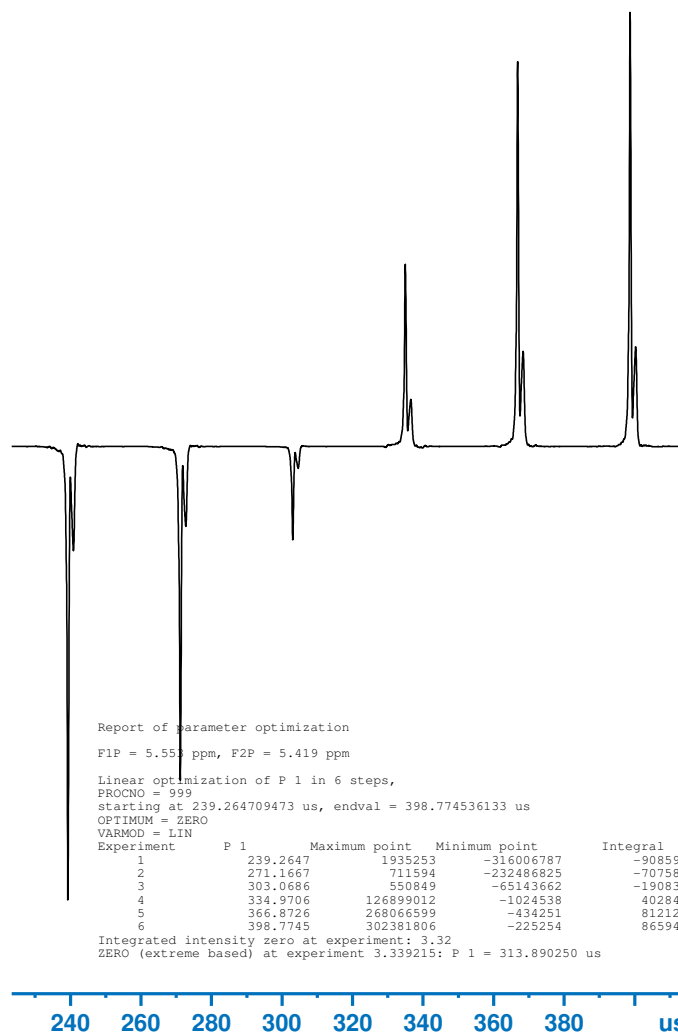
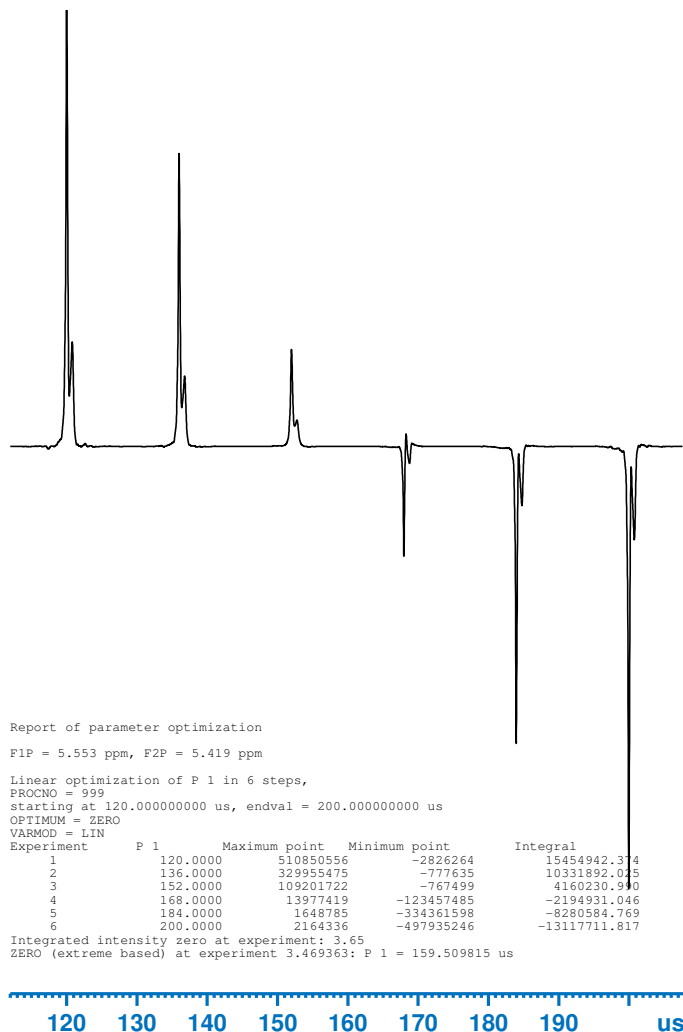
NMR TEST SERVICE *** System: AV III (600.13 MHz) *** TopSpin 3.7.0
 Probe: Z168568_0015 CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT *** Sample Depth: 21 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 CPD 1H pulse calibration (NPT_1H_cpddeterminationf1_1h, spin rate 0 Hz)
 Error while reading -> popt.protocol! Evaluation line missing!!ATTENTION: Updated CPD-Pulse in PROSOL Tables with [80.0 us @ 52.7 mW]
 Deviation between determined power and power calculated from hardpulse was -5.3%

CPD 1H pulse [achieved/rated]: @ 53.1 mW [79.8 us <= 80.0 us] <pass>



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NPT_1H_cpddeterminationf1_1h



Current Data Parameters
 NAME NPT_1H_cpddeterminationf1_1h
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250311
 Time 15.09 h
 INSTRUM AVANCEIII600
 PROBHD Z168568_0015 ()
 PULPROG zg
 TD 300
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 142.045 Hz
 FIDRES 0.946970 Hz
 AQ 1.0560000 sec
 RG 32
 DW 3520.000 usec
 DE 29.00 usec
 TE 298.0 K
 D1 1.34508002 sec
 TD0 1
 SFO1 600.1332924 MHz
 NUC1 1H
 P1 398.77 usec
 PLW1 0.05305400 W

Additional Parameters
 Field 4974.491
 Lock Phase 199.273
 Lock Power -10.000
 Lock Gain 96.571
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 535 l/h
 Atma Unit Z147150_0414

F2 - Processing parameters
 SI 2048
 SF 600.1300000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 53.1 mW 80.0 us
 53.1 mW 80.0 us 79.8 us -0.3%

 SHIM SEQUENCE
 skip shimming

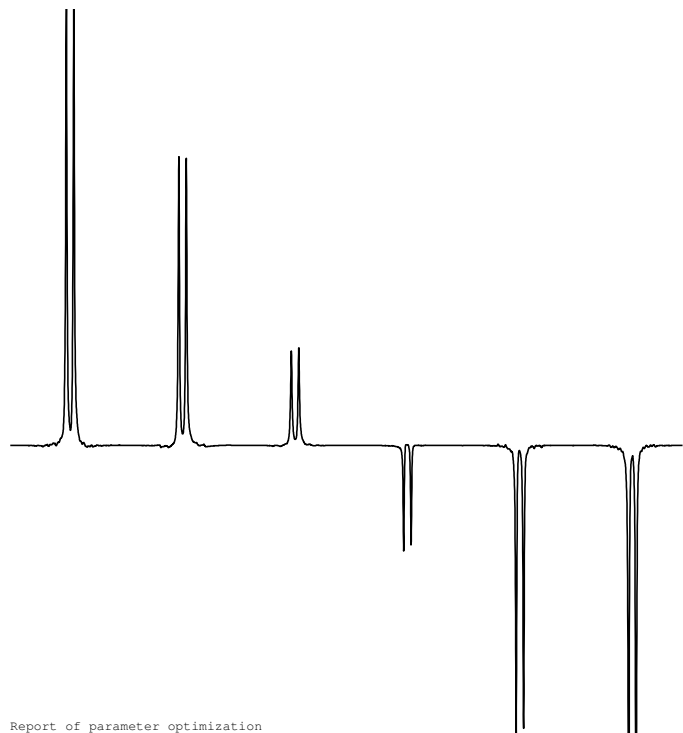
NMR TEST SERVICE *** System: AV III (600.13 MHz) *** TopSpin 3.7.0
 Probe: Z168568_0015 CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT *** Sample Depth: 21 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c, spin rate 0 Hz)
 Result: [90] = 12.0 us @ 91.7 W [270] = 34.7 us ==> [PDelay = 3*90 - 270] = 1.2 us
 ATTENTION: Updated PROSOL Tables with [12.0 us @ 91.0 W]
 Deviation from pulse target value (= 12.0 us): -0.4%

P90 13C pulse [achieved/rated]: @ 91.7 W [12.0 us <= 12.0 us] <pass>



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NPT_1H_p90determinationf2_13c



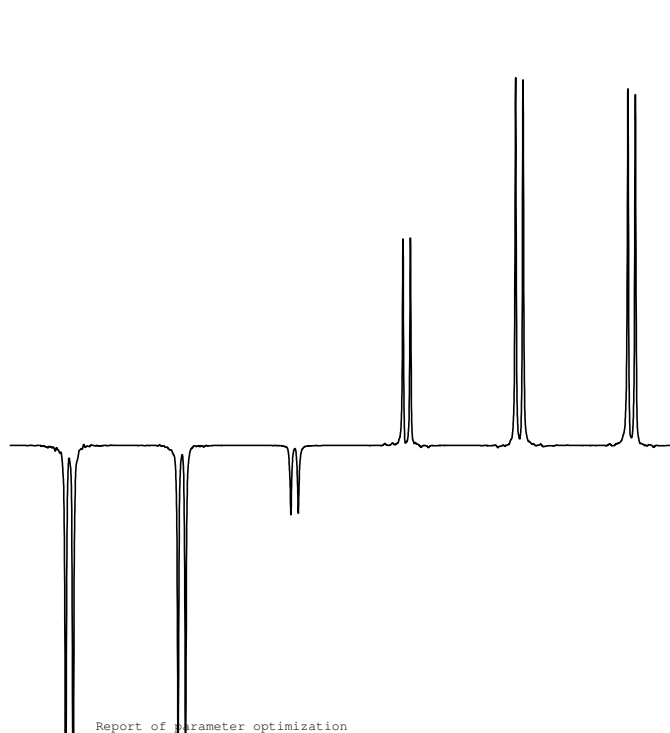
Report of parameter optimization

F1P = 3.127 ppm, F2P = 2.993 ppm

Linear optimization of P 3 in 6 steps,
 PROCNO = 999
 starting at 6.000000000 us, endval = 18.000000000 us

Experiment	P 3	Maximum point	Minimum point	Integral
1	6.0000	423559932	-1511995	15292151.5
2	8.4000	269643565	-2053427	9826327.0
3	10.8000	91091570	-893504	3791750.2
4	13.2000	787882	-98526377	-2603132.122
5	15.6000	1185078	-270274702	-8840241.573
6	18.0000	641719	-413419230	-13950749.504

Integrated intensity zero at experiment: 3.59
 ZERO (extreme based) at experiment 3.480395: P 3 = 11.952949 us



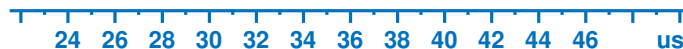
Report of parameter optimization

F1P = 3.127 ppm, F2P = 2.993 ppm

Linear optimization of P 3 in 6 steps,
 PROCNO = 999
 starting at 23.905897141 us, endval = 47.811794281 us

Experiment	P 3	Maximum point	Minimum point	Integral
1	23.9059	655606	-272531782	-96436
2	28.6871	417476	-195483000	-71189
3	33.4683	36253	-41618469	-18307
4	38.2494	124586489	-1362346	36619
5	43.0306	220917769	-1402499	69424
6	47.8118	214349720	-1055994	70546

Integrated intensity zero at experiment: 3.33
 ZERO (extreme based) at experiment 3.250404: P 3 = 34.665485 us



Current Data Parameters
 NAME NPT_1H_p90determinationf2_13c
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250311
 Time 15.13 h
 INSTRUM AVANCEIII600
 PROBHD Z168568_0015 ()
 PULPROG decp90
 TD 1000
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 205.052 Hz
 FIDRES 0.410105 Hz
 AQ 2.4384000 sec
 RG 18
 DW 2438.400 usec
 DE 29.00 usec
 TE 298.0 K
 CNST2 139.0000000
 D1 2.34730792 sec
 D2 0.00359712 sec
 TD0 1
 SFO1 600.1318364 MHz
 NUC1 1H
 P1 4.00 usec
 PLW1 5.55340004 W
 SFO2 150.9102684 MHz
 NUC2 13C
 P3 47.81 usec
 PLW2 91.69313812 W

Additional Parameters
 Field 4974.491
 Lock Phase 199.273
 Lock Power -10.000
 Lock Gain 96.571
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 535 l/h
 Atma Unit Z147150_0414

F2 - Processing parameters
 SI 2048
 SF 600.1300000 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 FC 0.10

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 93.8 W 12.0 us 11.9 us -1.2%
 93.8 W 12.0 us 12.0 us -0.4%
 91.7 W 12.0 us 12.0 us -0.4%

SHIM SEQUENCE

skip shimming

NMR TEST SERVICE *** System: AV III (600.13 MHz) *** TopSpin 3.7.0
 Probe: Z168568_0015 CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT *** Sample Depth: 21 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 Indirect CPD 13C pulse calibration (NPT_1H_cpddeterminationf2_13c, spin rate 0 Hz)
 Error while reading -> popt.protocol! Evaluation line missing!!ATTENTION: Updated CPD-Pulse in PROSOL Tables with [55.0 us @ 4.11 W]
 Deviation between determined power and power calculated from hardpulse was -5.3%

CPD 13C pulse [achieved/rated]: @ 4.15 W [54.8 us <= 55.0 us] <pass>



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NPT_1H_cpddeterminationf2_13c

Current Data Parameters
 NAME NPT_1H_cpddeterminationf2_13c
 EXPNO 1
 PROCNO 1

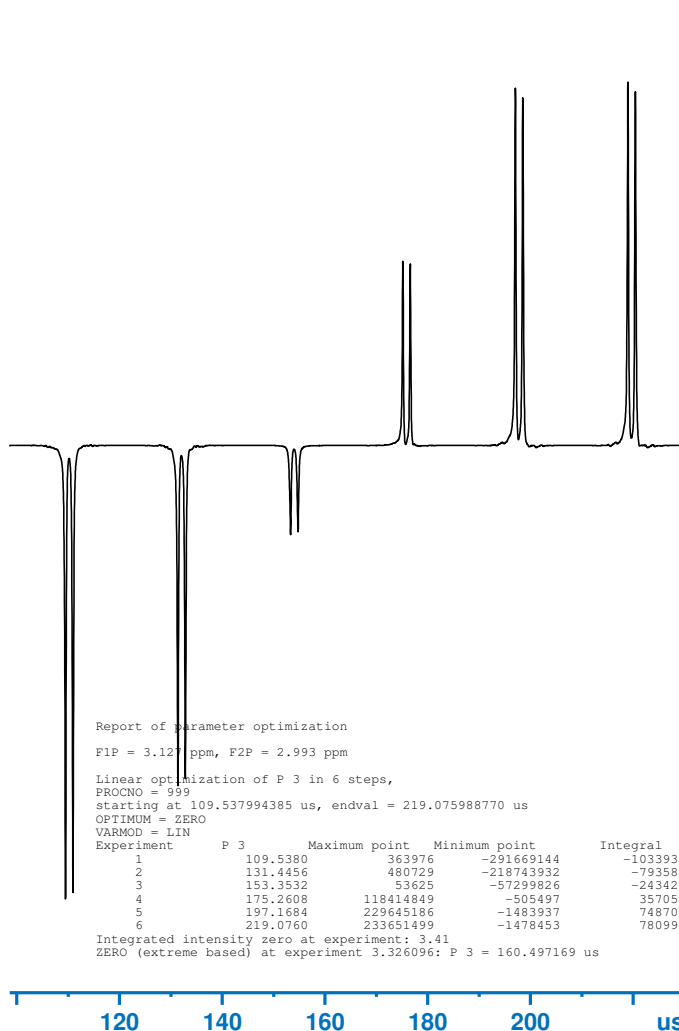
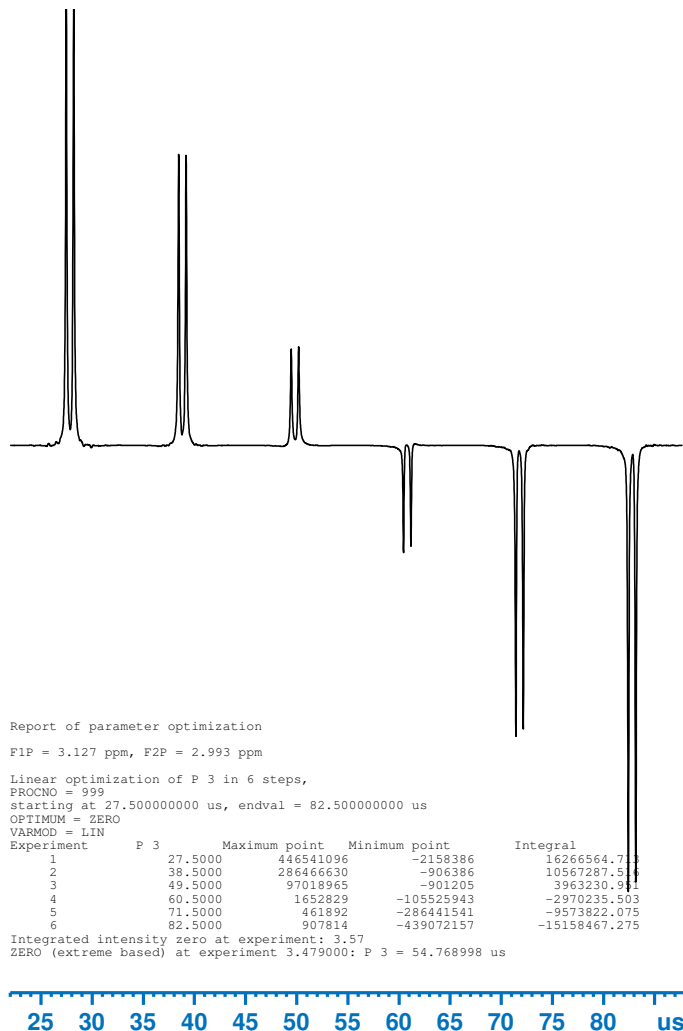
F2 - Acquisition Parameters
 Date_ 20250311
 Time 15.17 h
 INSTRUM AVANCEIII600
 PROBHD Z168568_0015 ()
 PULPROG decp90
 TD 1000
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 205.052 Hz
 FIDRES 0.410105 Hz
 AQ 2.4384000 sec
 RG 20.2
 DW 2438.400 usec
 DE 29.00 usec
 TE 298.0 K
 CNST2 139.0000000
 D1 2.34730792 sec
 D2 0.00359712 sec
 TD0 1
 SFO1 600.1318363 MHz
 NUC1 1H
 P1 4.00 usec
 PLW1 5.55340004 W
 SFO2 150.9102684 MHz
 NUC2 13C
 P3 219.08 usec
 PLW2 4.14767408 W

Additional Parameters
 Field 4974.491
 Lock Phase 199.273
 Lock Power -10.000
 Lock Gain 96.571
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 535 l/h
 Atma Unit Z147150_0414

F2 - Processing parameters
 SI 2048
 SF 600.1300000 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 0.10

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 4.15 W 55.0 us
 4.15 W 55.0 us 54.8 us -0.4%

SHIM SEQUENCE
 skip shimming



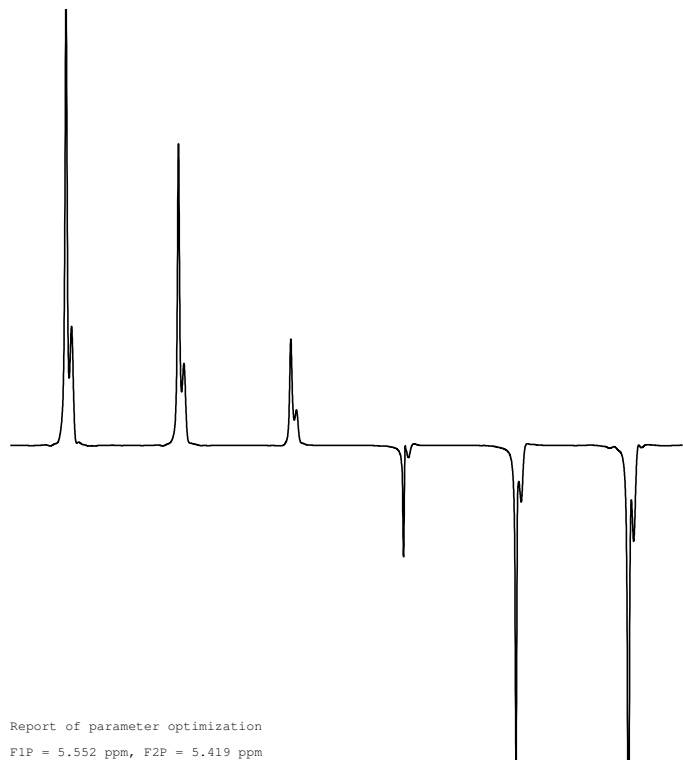
NMR TEST SERVICE *** System: AV III (600.13 MHz) *** TopSpin 3.7.0
 Probe: Z168568_0015 CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT *** Sample Depth: 21 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 Indirect P90 15N pulse calibration (NPT_1H_p90determinationf2_15n, spin rate 0 Hz)
 Result: [90] = 24.9 us @ 208.2 W [270] = 73.5 us ==> [PDelay = 3*90 - 270] = 1.3 us
 ATTENTION: Updated PROSOL Tables with [25.0 us @ 207.3 W]
 Deviation from pulse target value (= 25.0 us): -0.2%



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P90 15N pulse [achieved/rated]: @ 208.2 W [24.9 us <= 25.0 us] <pass>

NPT_1H_p90determinationf2_15n



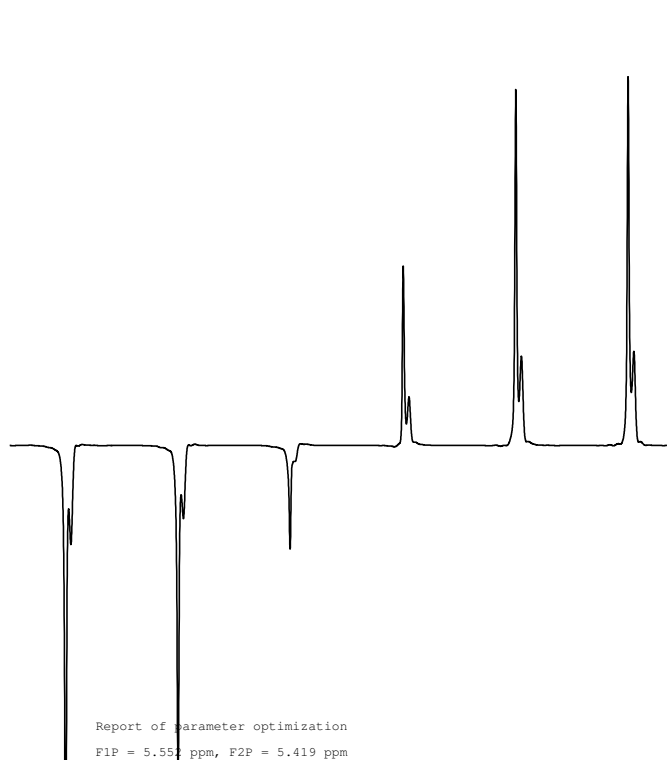
Report of parameter optimization

F1P = 5.552 ppm, F2P = 5.419 ppm

Linear optimization of P 3 in 6 steps,
 PROCNO = 999
 starting at 12.500000000 us, endval = 37.500000000 us

Experiment	P 3	Maximum point	Minimum point	Integral
1	12.5000	295889212	-419938	10876734.27
2	17.5000	196690432	-284300	7337174.742
3	22.5000	69352485	-171401	3001979.331
4	27.5000	1124044	-72662395	-1696417.213
5	32.5000	1163512	-207006710	-6072606.826
6	37.5000	483632	-290712326	-9777879.011

Integrated intensity zero at experiment: 3.64
 ZERO (extreme based) at experiment 3.488347: P 3 = 24.941733 us



Report of parameter optimization

F1P = 5.552 ppm, F2P = 5.419 ppm

Linear optimization of P 3 in 6 steps,
 PROCNO = 999
 starting at 49.883464813 us, endval = 99.766929626 us

Experiment	P 3	Maximum point	Minimum point	Integral
1	49.8835	876782	-400691850	-135869
2	59.8602	1103980	-307173007	-104261
3	69.8369	1575359	-91508719	-31373
4	79.8135	158322155	-1239025	49613
5	89.7902	314532435	-692969	102698
6	99.7669	325746518	-325049	106978

Integrated intensity zero at experiment: 3.39
 ZERO (extreme based) at experiment 3.366283: P 3 = 73.491140 us



Current Data Parameters
 NAME NPT_1H_p90determinationf2_15n
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250311
 Time 15.24 h
 INSTRUM AVANCEIII600
 PROBHD Z168568_0015
 PULPROG decp90
 TD 200
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 142.045 Hz
 FIDRES 1.420455 Hz
 AQ 0.7040000 sec
 RG 28.5
 DW 3520.000 usec
 DE 29.00 usec
 TE 298.0 K
 CNST2 88.5000000
 D1 0.51315397 sec
 D2 0.00564972 sec
 TD0 1
 SFO1 600.1332922 MHz
 NUC1 1H
 P1 5.33 usec
 PLW1 5.55340004 W
 SFO2 60.8152616 MHz
 NUC2 15N
 P3 99.77 usec
 PLW2 208.23170471 W

Additional Parameters
 Field 4975.231
 Lock Phase 200.465
 Lock Power -10.000
 Lock Gain 101.899
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 535 l/h
 Atma Unit Z147150_0414

F2 - Processing parameters
 SI 2048
 SF 600.1300000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 FC 1.00

***** P90 Pulse Determination History *****				
PLW90	P90	P90[det]	Deviation	
213.8 W	25.0 us			
213.8 W	25.0 us	24.6 us	-1.8%	
206.6 W	25.0 us	25.1 us	0.3%	
208.2 W	25.0 us	24.9 us	-0.2%	

SHIM SEQUENCE

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

NMR TEST SERVICE *** System: AV III (600.13 MHz) *** TopSpin 3.7.0
 Probe: Z168568_0015 CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT *** Sample Depth: 21 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 Indirect CPD 15N pulse calibration (NPT_1H_cpddeterminationf2_15n, spin rate 0 Hz)
 Error while reading -> popt.protocol! Evaluation line missing!!ATTENTION: Updated CPD-Pulse in PROSOL Tables with [170.0 us @ 4.40 W]
 Deviation between determined power and power calculated from hardpulse was -1.9%

CPD 15N pulse [achieved/rated]: @ 4.44 W [169.3 us <= 170.0 us] <pass>



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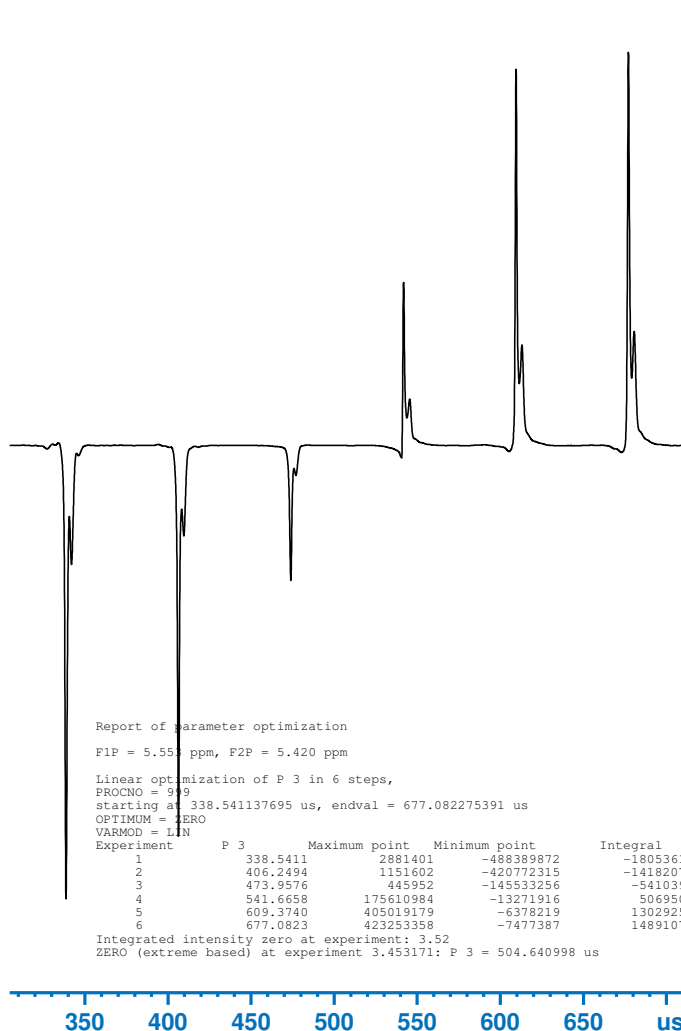
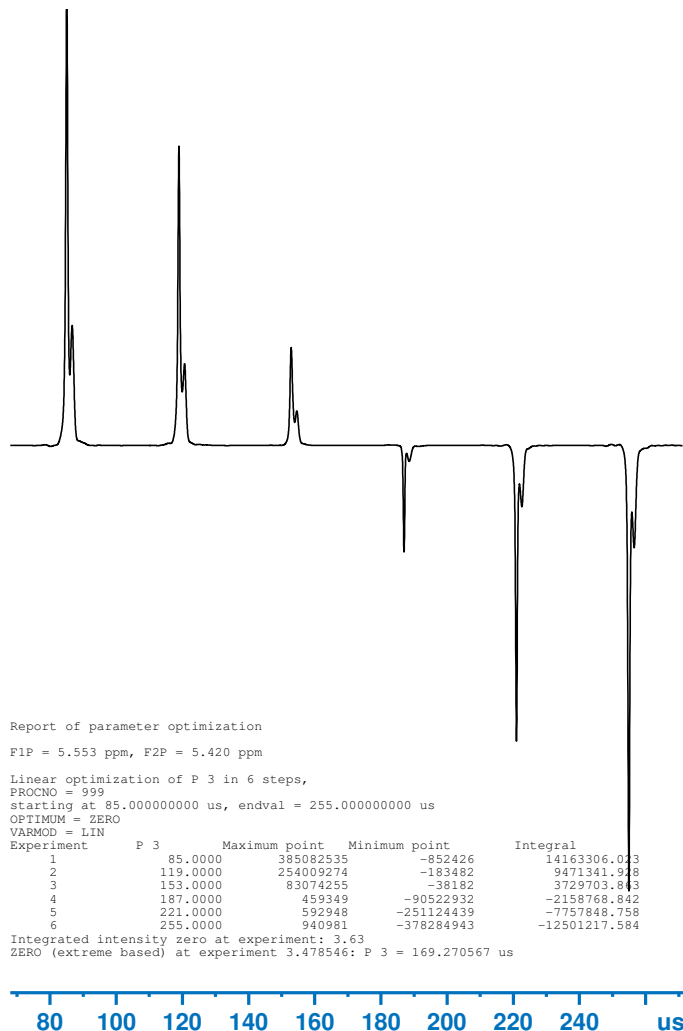
NPT_1H_cpddeterminationf2_15n

Current Data Parameters
 NAME NPT_1H_cpddeterminationf2_15n
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250311
 Time 15.26 h
 INSTRUM AVANCEIII600
 PROBHD Z168568_0015 ()
 PULPROG decp90
 TD 200
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 142.045 Hz
 FIDRES 1.420455 Hz
 AQ 0.7040000 sec
 RG 36
 DW 3520.000 usec
 DE 29.00 usec
 TE 298.0 K
 CNST2 88.5000000
 D1 0.51315397 sec
 D2 0.00564972 sec
 TD0 1
 SFO1 600.1332924 MHz
 NUC1 1H
 P1 5.33 usec
 PLW1 5.55340004 W
 SFO2 60.8152616 MHz
 NUC2 15N
 P3 677.08 usec
 PLW2 4.43612099 W

Additional Parameters
 Field 4975.231
 Lock Phase 200.465
 Lock Power -10.000
 Lock Gain 101.889
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 535 l/h
 Atma Unit Z147150_0414

F2 - Processing parameters
 SI 2048
 SF 600.1300000 MHz
 WDW SINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00



***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 4.63 W 170.0 us 166.2 us -2.2%
 4.63 W 170.0 us 169.3 us -0.4%
 4.44 W 170.0 us 169.3 us -0.4%

SHIM SEQUENCE
 skip shimming

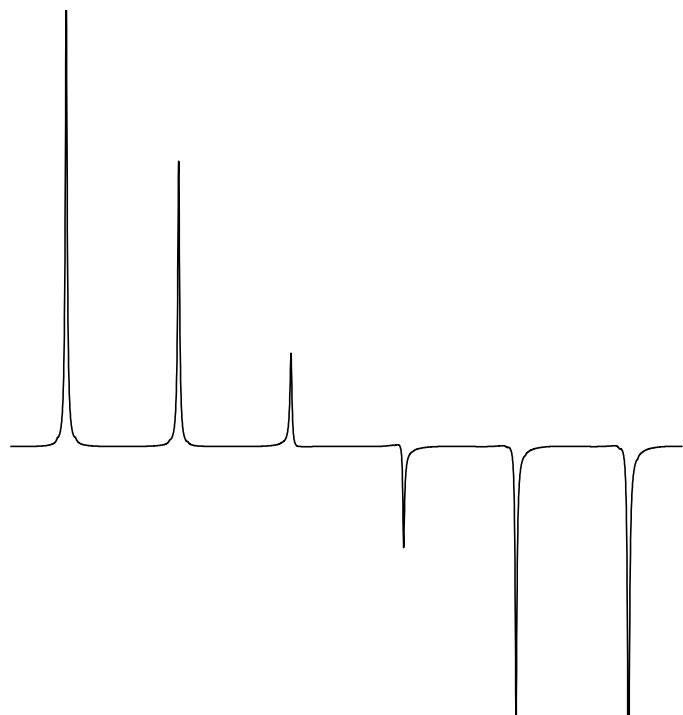
NMR TEST SERVICE *** System: AV III (600.13 MHz) *** TopSpin 3.7.0
 Probe: Z168568_0015 CP2.1 TCI 600S3 H&F/C/N-D-05 Z XT *** Sample Depth: 21 mm
 Sample: 100 mM Urea-15N, 100 mM Methanol-13C in Dimethyl Sulfoxide-D6 (Z10263)
 P90 2H pulse calibration (NPT_prep_p90det_d, spin rate 0 Hz)
 Result: [180/2] = 67.9 us @ 41.4 W [360] = 251.7 us ==> [PDelay = 2*180 - 360] = 19.8 us
 ATTENTION: Updated PROSOL Tables with [68.0 us @ 41.2 W]
 Deviation from pulse target value (= 68.0 us): -0.2%

P90 2H pulse [achieved/rated]: @ 41.4 W [67.9 us <= 68.0 us] <pass>



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NPT_prep_p90det_d



Report of parameter optimization

F1P = 3.190 ppm, F2P = 1.779 ppm

Linear optimization of P 1 in 6 steps,
 PROCNO = 999
 starting at 102.000000000 us, endval = 170.000000000 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	102.0000	390010468	-45454	11983217.075
2	115.6000	245372096	-15108	7615613.570
3	129.2000	80034366	-282451	2650193.820
4	142.8000	1521698	-86823416	-2545001.818
5	156.4000	674711	-231509480	-6922162.422
6	170.0000	562526	-339952488	-10267469.084

Integrated intensity zero at experiment: 3.51
 ZERO (extreme based) at experiment 3.479656: P 1 = 135.723324 us



Report of parameter optimization

F1P = 3.190 ppm, F2P = 1.779 ppm

Linear optimization of P 1 in 6 steps,
 PROCNO = 999
 starting at 203.584991455 us, endval = 339.308319092 us

OPTIMUM = ZERO

VARMOD = LIN

Experiment	P 1	Maximum point	Minimum point	Integral
1	203.5850	540162	-394892916	-119672
2	230.7297	775385	-218514022	-65922
3	257.8743	64766895	-569398	22687
4	285.0190	307123874	-45320	95776
5	312.1637	398225485	-16033	123558
6	339.3083	295901602	-12850	92382

Integrated intensity zero at experiment: 2.74
 ZERO (extreme based) at experiment 2.771369: P 1 = 251.668201 us

Current Data Parameters
 NAME NPT_prep_p90det_d
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20250311
 Time 15.04 h
 INSTRUM AVANCEIII600
 PROBHD Z168568_0015 ()
 PULPROG npt_2g2h
 TD 1024
 SOLVENT DMSO
 NS 1
 DS 0
 SWH 500.601 Hz
 FIDRES 0.977735 Hz
 AQ 1.0227712 sec
 RG 18
 DW 998.800 usec
 DE 18.00 usec
 TE 298.0 K
 D1 0.34999999 sec
 D11 0.03000000 sec
 D12 0.00010000 sec
 TD0 1
 SFO1 92.1238378 MHz
 NUC1 2H
 P1 339.31 usec
 PLW1 41.35681915 W

Additional Parameters
 Field 4974.491
 Lock Phase 199.273
 Lock Power -10.000
 Lock Gain 96.571
 Lock DC -75.000
 Lock Shift 2.490
 Loop Gain 5.000
 Loop Time 0.250
 Loop Filter 500.000
 Gas Flow 535 l/h
 Atma Unit

F2 - Processing parameters
 SI 2048
 SF 92.1236090 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

***** P90 Pulse Determination History *****
 PLW90 P90 P90[det] Deviation
 41.4 W 68.0 us
 41.4 W 68.0 us 67.9 us -0.2%

SHIM SEQUENCE

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