

Customer Information

Customer Name	Sai Sankar Gupta, K.B.
Operator Name	Sai Sankar Gupta, K.B.
Company	University of Leiden
Address	Wassenaarseweg 76
Postal Code / City / Country	2333 AL Leiden, Netherlands
Phone Contact Customer	0031715274638
Fax	
E-Mail	k.b.sai.sankar.gupta@lic.leidenuniv.nl

Bruker Information

Office	GSEC
Engineer	HM Smith
Service Contract No.	
SAP Service Ticket No.	

Spectrometer Information

Order No.	HCAB-76_00003
System	Avance Neo 750
Console Part and Serial No	HCAB-76 / 3
Coil	BR.091075110
Dewar	BD228972
Location	
TopSpin Version	TopSpin 4.1.3 - Build 17

Installation Summary

Approval

Place 2333 AL Leiden, Netherlands
Date September 30, 2021

Place 2333 AL Leiden, Netherlands
Date September 30, 2021

Sai Sankar Gupta, K.B.
Customer representative signature

HM Smith
Bruker representative signature

NMR Probes

Description	Probe ID	Inspection Lot	Status
BBI 750WB H-BB-D-05 Z	Z5663_0001	2021-09-22	fail
PATXI	Z5661_0001	2021-09-29	pass

Copies of all spectra (default and additional) are included in customer's PDF report.

Service Checklist

General Components	pass	fail	n/a
All firmware	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Software updated	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Cortab	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Lift / spin calibration	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
He / N2 log files	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
MICS	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
BSMS	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
AQS chassis	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Shim system turbine cleaned	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Door filter(s) replaced	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Optional Components	pass	fail	n/a
Sample Changer	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
MAS controller	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
High power equipment	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
LC-NMR	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Liquid Handler SamplePro Tube	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Micro-Imaging	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Diffusion	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
CryoProbe / Cryoplatfom	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
BNL / BSNL	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Additional cooling/heating units (like BCU1 / BCU2)	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
LT-MAS (Low Temperature MAS equipment)	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Gyrotron magnet and DNP console	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>

General Test Information

Summary of Inspection Lot

Description	Probe ID	Inspection Lot
BBI 750WB H-BB-D-05 Z	Z5663_0001	2021-09-22

Experiments Measured

Sample	Experiment	Status
Z10701	1H lineshape without sample rotation (NPT_1H_lineshape_nrot)	pass
Z10263	P90 1H pulse calibration (NPT_1H_p90determinationf1_1h)	pass
Z10120	1H sensitivity (NPT_1H_sensitivity)	pass
Z10263	Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c)	fail
Z10263	Indirect P90 15N pulse calibration (NPT_1H_p90determinationf2_15n)	pass
Z10201	P90 31P pulse calibration (NPT_31P_p90determinationf1_31p)	pass
Z10201	31P sensitivity (NPT_31P_sensitivity)	pass
Z10701	Inverse spin echo difference (NPT_1H_hmqc1df2_13c)	pass
Z10701	B0 magnet drift experiment (NPT_1H_b0drifftest)	pass

Experiments not Measured

Sample	Experiment
Z10902	Watersuppression with 670 l/h gas flow (NPT_1H_watersuppression_670l)
Z10163	13C sensitivity (NPT_13C_sensitivity)
Z10163	P90 13C pulse calibration (NPT_13C_p90det_astm_13c)

Achieved Specifications

Pulse Width

Nucleus	Sample		90° Pulse		Power Limit [W]	Method	Status
			Duration [μs]	Power [W]			
¹ H	Z10263	spec.	-	-	30	direct	pass
		ach.	10.4	14.9			
¹³ C	Z10263	spec.	-	-	300	indirect	fail
		ach.	-10.0	300.0			
¹⁵ N	Z10263	spec.	-	-	600	indirect	pass
		ach.	23.2	300.0			
³¹ P	Z10201	spec.	-	-	210	direct	pass
		ach.	18.3	200.0			

Sensitivity

Nucleus	Sample		S/N	Remarks	Status
¹ H	Z10120	spec.	-	noise: 2 ppm variable, method: sino best	pass
		ach.	1161.7		
¹ H	Z10120	spec.	-	noise: 200 Hz variable, method: sino best	pass
		ach.	1324.4		
³¹ P	Z10201	spec.	-	noise: 5 ppm variable, method: sino best	pass
		ach.	156.9		

Lineshape without Rotation

Nucleus	Sample		50% [Hz]	0.55% [Hz]	0.11% [Hz]	Status
¹ H	Z10701	spec.	-	-	-	pass
		ach.	0.48	5.0	11.2	

Samples used for Inspection Lot

Sample	Description
Z10120	0.1% Ethylbenzene (EB) in Chloroform-D
Z10163	40% Dioxane in Benzene-D ₆ (ASTM)
Z10201	0.0485 M Triphenyl Phosphate (TPP, [C ₆ H ₅] ₃ PO ₄) in Acetone-D ₆
Z10263	100 mM Urea- ¹⁵ N ([¹⁵ NH ₂] ₂ CO), 100 mM Methanol- ¹³ C (¹³ CH ₃ OH) in Dimethyl Sulfoxide-D ₆
Z10701	0.3% Chloroform (CHCl ₃) in Acetone-D ₆
Z10902	2 mM Sucrose, 0.5 mM DSS, 2 mM NaN ₃ in 90% H ₂ O + 10% D ₂ O (40 mm filling height)

Summary of Inspection Lot

Description
PATXI

Probe ID
Z5661_0001

Inspection Lot
2021-09-29

Experiments Measured

Sample	Experiment	Status
Z10701	1H lineshape without sample rotation (NPT_1H_lineshape_nrot)	pass
Z10263	P90 1H pulse calibration (NPT_1H_p90determinationf1_1h)	pass
Z10120	1H sensitivity (NPT_1H_sensitivity)	pass
Z10263	Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c)	pass
Z10263	Indirect P90 15N pulse calibration (NPT_1H_p90determinationf2_15n)	pass
Z10902	2H sensitivity, 10% D2O (NPT_prep_sensitivity_10_d)	pass
Z10701	Inverse spin echo difference (NPT_1H_hmqc1df2_13c)	pass
Z10701	B0 magnet drift experiment (NPT_1H_b0drifttest)	pass
Z10701	1H lineshape stability test (NPT_1H_lineshapeStability)	pass

Experiments not Measured

Sample	Experiment
Z10902	Watersuppression with 670 l/h gas flow (NPT_1H_watersuppression_670l)
Z10163	13C sensitivity (NPT_13C_sensitivity)

Achieved Specifications

Pulse Width

Nucleus	Sample		90° Pulse		Power Limit [W]	Method	Status
			Duration [μs]	Power [W]			
¹ H	Z10263	spec.	-	-	30	direct	pass
		ach.	8.4	20.0			
¹³ C	Z10263	spec.	-	-	500	indirect	pass
		ach.	10.4	300.0			
¹⁵ N	Z10263	spec.	-	-	500	indirect	pass
		ach.	36.9	300.0			

Sensitivity

Nucleus	Sample		S/N	Remarks	Status
¹ H	Z10120	spec.	-	noise: 2 ppm variable, method: sino best	pass
		ach.	1304.3		
¹ H	Z10120	spec.	-	noise: 200 Hz variable, method: sino best	pass
		ach.	1535.9		
² H	Z10902	spec.	-	noise: 50 ppm, method: sino, 10% D2O	pass
		ach.	3018.9		

Lineshape without Rotation

Nucleus	Sample		50% [Hz]	0.55% [Hz]	0.11% [Hz]	Status
¹ H	Z10701	spec.	-	-	-	pass
		ach.	0.71	6.4	12.2	

Samples used for Inspection Lot

Sample	Description
Z10120	0.1% Ethylbenzene (EB) in Chloroform-D
Z10163	40% Dioxane in Benzene-D ₆ (ASTM)
Z10263	100 mM Urea- ¹⁵ N ([¹⁵ NH ₂] ₂ CO), 100 mM Methanol- ¹³ C (¹³ CH ₃ OH) in Dimethyl Sulfoxide-D ₆
Z10701	0.3% Chloroform (CHCl ₃) in Acetone-D ₆
Z10902	2 mM Sucrose, 0.5 mM DSS, 2 mM NaN ₃ in 90% H ₂ O + 10% D ₂ O (40 mm filling height)

Remarks / Exclusions