

## 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	
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## Bruker Information

Office	BRUKER Netherlands
Engineer	Narendra/Keylla
Central Hotline Phone	+31 (0) 88 11 22 700
Central Hotline E-Mail	Service.bbio.benelux@bruker.com

## Probe Information

Order No.	443419
Contract No.	
Description	PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z
P/N	Z180004
S/N	0001

## Installation Summary

I, an authorized customer representative, acknowledge that the above referenced probe was installed and demonstrated to operate in accordance with the specifications mutually agreed upon by both parties. We accept the delivery and installation of this probe as specified in the purchase order and release Bruker from any further obligation, other than those obligations as specified during the warranty period. If the contract requires a formal acceptance protocol this document serves as such.

## Warranty

The warranty period commences according to the contractual agreement.

Place	2333 AL Leiden, Netherlands	Place	2333 AL Leiden, Netherlands
Date	September 4, 2024	Date	September 4, 2024

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Sai Sankar Gupta, K.B.  
Customer representative signature

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Narendra/Keylla  
Bruker representative signature

Spectrometer Information

Order No.	442759
System	Avance Neo 750
Location	FW.0.01
TopSpin Version	TopSpin 4.4.0 - Build local

NMR Probe

Description	Probe ID	Inspection Lot	Status
PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z	Z180004_0001	PL030000051056	pass

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

Installation Checklist

<b>Installation</b>	<b>pass</b>	<b>fail</b>	<b>n/a</b>	<b>Optional Components</b>	<b>pass</b>	<b>fail</b>	<b>n/a</b>
All firmware	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Sample Changer	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Cortab for required nuclei	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	MAS controller	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Lift / spin calibration	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	High power equipment	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
<b>Customer Training</b>	<b>pass</b>	<b>fail</b>	<b>n/a</b>	LC-NMR	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Basic safety	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Liquid Handler SamplePro Tube	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Handling of cryogenic liquids	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Micro-Imaging	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Troubleshooting	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	Diffusion	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Backup (nmr_save, Images)	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	CryoProbe / Cryoplatfrom	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Introduction to IconNMR	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	BNL / BSNL	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Assure-SST / Performance check	<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"/>
CryoProbe	<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"/>
Handling / cleaning of probe	<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"/>
He cylinder exchange	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
He compressor cooling	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
RF heating / power limits	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
RF routing	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
<b>Acceptance and Warranty</b>	<b>pass</b>	<b>fail</b>	<b>n/a</b>				
Explanation of warranty	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>				
Customer support hotlines	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>				

General Test Information

Summary of Inspection Lot

Description	Probe ID	Inspection Lot
PI HRMAS-750-W4/S7-H/P/C/D-4.0-Z	Z180004_0001	PL030000051056

Experiments Measured

Sample	Experiment	Status
Z142220	1H lineshape with magic angle spinning (NPT_1H_HRMAS_lineshape)	pass
Z142222	Watersuppression (NPT_1H_HRMAS_watersuppression)	pass
Z142223	P90 1H pulse calibration (NPT_1H_p90determinationf1_1h)	pass
Z142221	1H sensitivity (NPT_1H_sensitivity)	pass
Z142221	1H integral sensitivity (NPT_1H_inno)	pass
Z142221	1H background with sample (NPT_1H_backgr_withsample)	pass
Z142223	Indirect P90 13C pulse calibration (NPT_1H_p90determinationf2_13c)	pass
Z142224	13C sensitivity (NPT_13C_sensitivity)	pass
Z142226	P90 31P pulse calibration (NPT_31P_p90determinationf1_31p)	pass
Z142226	31P sensitivity (NPT_31P_sensitivity)	pass
Z142223	P90 2H pulse calibration (NPT_prep_p90det_d)	pass
Z142222	1H Z-gradient profile [-] (NPT_1H_gradientprofile_neg)	pass
Z142222	1H Z-gradient profile [+] (NPT_1H_gradientprofile_pos)	pass
Z142231	Gradient recovery stability test (NPT_1H_gradrec_stest_1h)	pass
Z142231	Gradient recovery test for Z-direction [-] (NPT_1H_gradrecZ_sqn_1h)	pass
Z142231	Gradient recovery test for Z-direction [+] (NPT_1H_gradrecZ_sqp_1h)	pass
Z142223	1H B1 homogeneity integral (NPT_1H_b1homogeneityInt_1h)	pass
Z142223	13C B1 homogeneity integral (NPT_1H_b1homogeneityInt_13c)	pass
Z142223	2H B1 homogeneity integral (NPT_prep_b1homogeneityInt_d)	pass
Z142222	Optimization of 2H locksetting (NPT_prep_locksettings_d)	pass
Z142231	Vibration Test using Doped Water Sample (NPT_1H_vibration_doped_water)	pass
Z151220	P90 79Br pulse calibration, HRMAS (NPT_79Br_HRMAS_p90det_79br)	pass
Z151220	Magic Angle setting, HRMAS (NPT_79Br_HRMAS_magicAngle)	pass
Z151220	Maximum spin rate testing, HRMAS (NPT_79Br_HRMAS_maxSpinRate)	pass

Achieved Specifications

Pulse Width

Nucleus	Sample		90° Pulse		Power Limit [W]	Method	Status
			Duration [µs]	Power [W]			
1H	Z142223	spec.	10.0	-	100	direct	pass
		ach.	10.0	11.462			
13C	Z142223	spec.	10.0	-	200	indirect	pass
		ach.	10.0	70.2			
2H	Z142223	spec.	500.0	-	27	direct	pass
		ach.	499.8	0.1			
31P	Z142226	spec.	12.0	-	300	direct	pass
		ach.	12.0	35			
79Br	Z151220	spec.	9.0	-	200	direct	pass
		ach.	8.9	130.7			

**Sensitivity**

Nucleus	Sample		S/N	Remarks	Status
<sup>1</sup> H	Z142221	spec.	110.0	noise: 200 Hz variable, method: sino best	pass
		ach.	168.3		
<sup>13</sup> C	Z142224	spec.	35.0	noise: 40 ppm variable, method: sino best	pass
		ach.	92.8		
<sup>31</sup> P	Z142226	spec.	30.0	noise: 5 ppm variable, method: sino best	pass
		ach.	78.0		

**Lineshape without Rotation**

Nucleus	Sample		50% [Hz]	0.55% [Hz]	0.11% [Hz]	Status
<sup>1</sup> H	Z142220	spec.	1.00	12.0	18.0	pass
		ach.	0.74	6.2	15.3	

**Water Suppression**

Nucleus	Sample		Splitting [%]	10% [Hz]	50% [Hz]	S/N	Flow [l/h]	Status
<sup>1</sup> H	Z142222	spec.	-	-	-	22.0	n/a	pass
		ach.	27	41.6	29.4	37.0		

**Gradient Recovery**

Nucleus	Sample		Signal Recovery [%]	Recovery Time [μs]	Gradient Time [ms]	Gradient Strength [T/m]	Gradient	Status
<sup>1</sup> H	Z142231	spec.	70.00	100.0	1.0	0.24	+Z	pass
		ach.	96.75	10.0				
<sup>1</sup> H	Z142231	spec.	70.00	100.0	1.0	-0.24	-Z	pass
		ach.	89.32	10.0				

**Samples used for Inspection Lot**

Sample	Description
Z142220	1% Chloroform (CHCl <sub>3</sub> ) in Acetone-D <sub>6</sub> (50 μl)
Z142221	0.1% Ethylbenzene (EB) in Chloroform-D (50 μl)
Z142222	2 mM Sucrose, 0.5 mM DSS, 2 mM NaN <sub>3</sub> in 90% H <sub>2</sub> O + 10% D <sub>2</sub> O (50 μl)
Z142223	100 mM Urea- <sup>15</sup> N ([ <sup>15</sup> NH <sub>2</sub> ] <sub>2</sub> CO), 100 mM Methanol- <sup>13</sup> C ( <sup>13</sup> CH <sub>3</sub> OH) in Dimethyl Sulfoxide-D <sub>6</sub> (50 μl)
Z142224	40% Dioxane in Benzene-D <sub>6</sub> (ASTM, 50 μl)
Z142226	0.0485 M Triphenyl Phosphate (TPP, [C <sub>6</sub> H <sub>5</sub> ] <sub>3</sub> PO <sub>4</sub> ) in Acetone-D <sub>6</sub> (50 μl)
Z142231	0.1 mg/ml Gadolinium Chloride (GdCl <sub>3</sub> ), 0.1% Methanol- <sup>13</sup> C ( <sup>13</sup> CH <sub>3</sub> OH), 1% H <sub>2</sub> O in D <sub>2</sub> O (50 μl)
Z151220	Potassium Bromide (KBr, 80 ul)

## Remarks / Exclusions

Only  $^{31}\text{P}$  sample was done at 2KHz spinning

All the NMRPT experiments performed while magnet legs "OFF" since old elastic bumpers are not working properly, its prototype magnet 750MHz. We didnt observe the vibrations in the spectra.

The samples prepared onsite with customer 4mm rotors (H6283)

0.1% EB in  $\text{cdcl}_3$

Labeled Urea in DMSO

ASTM in  $\text{C}_6\text{D}_6$

Doped water

TPP in acetone

The HRMAS standard samples used from Bruker france (Hz07213 (79.2/50ul)

Kbr with silicon grease

Sucrose in  $\text{H}_2\text{O}+\text{D}_2\text{O}$  ( prepared onsite 09.08.2023)

1%  $\text{CHCl}_3$  in Acetone ( prepared onsite 09.08.2023)