BRUKER LABSCAPE CONSUMABLES, TOOLS AND REFERENCE STANDARDS

Liquid-State NMR

We’ve got you covered

Innovation with Integrity

BRUKER LABSCAPE CONSUMABLES, TOOLS AND REFERENCE STANDARDS

Get the Best Results from Your NMR System

Why Bruker Liquid-State NMR Consumables?

Bruker liquid-state NMR consumables are designed to ensure reliable results, protect sensitive hardware, and deliver consistent performance across routine and advanced NMR experiments. Developed in close alignment with Bruker NMR systems, they combine NMR grade materials with precise mechanical specifications to support data quality, reproducibility, and long instrument lifetime.

Benefits

- Compatibility with Bruker systems for reliable measurement results
- Increased productivity
- Probe safety and sample changer reliability
- Cost-saving and sustainable consumables solutions

Bruker liquid-state NMR consumables are engineered to meet the mechanical and material requirements of high-resolution NMR spectroscopy. They are developed in alignment with Bruker spectrometer and probe specifications to ensure compatibility, reproducibility, and protection of critical hardware components. Tight control of geometry, materials, and manufacturing tolerances supports stable experimental conditions and long instrument lifetime.

Bruker NMR tubes are manufactured for optimal shimmability, i.e. with precisely controlled outer diameter, wall thickness and straightness. These parameters are critical for maintaining homogeneous sample positioning within the RF coil and minimizing susceptibility-induced distortions. The delivered geometric consistency reduces spinning sidebands and contributes to high spectral resolution and line shape stability across both routine and advanced experiments. Compatibility is ensured across all high-resolution systems without frequency limitations.

Bruker spinners are designed for well-controlled gas dynamics at the interface of probe, sample and spinner, to ensure stable thermal coupling behavior within the probe for optimal VT control and sample rotation. The spinner–tube interface enables a precise, reproducible and stable fit, supporting a smooth and controlled insert and eject process via the lift gas system. During operation, optimized mass distribution and material properties ensure vibration-free spinning, even under elevated VT gas flow conditions required for efficient temperature regulation. Stable spinning is essential, as fluctuations in gas flow and mechanical imbalance can directly impact temperature homogeneity and spectral quality. The result is reliable performance across standard and variable-temperature experiments, including high-flow VT conditions.

Bruker caps are produced from chemically resistant polymers selected for compatibility with a wide range of organic solvents and demanding sample environments. Their sealing performance minimizes solvent evaporation and concentration changes during measurements, which is particularly critical in VT experiments where a gas flow interacts with the sample environment. Integrated 2D barcode labeling supports unambiguous sample identification and traceability in automated workflows.

Bruker reference samples are certified for dimensional accuracy, concentricity, and high chemical purity, ensuring reliable positioning within the sensitive volume of the probe and well-defined spectral properties. Their precisely controlled chemical composition provides consistent and traceable reference signals. Widely established and trusted across the NMR community, they serve as a stable standard for calibration, validation, and benchmarking of spectrometer performance, supporting reproducible quality control and system verification procedures.

Together, the Bruker liquid-state NMR consumables portfolio enables stable sample handling, precise temperature control under defined VT gas flow conditions, and consistent spinning performance - ensuring high spectral fidelity, reproducibility, and operational robustness across manual and automated NMR workflows.

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Tubes & Caps

Bruker offers both unracked as well as single (1 x 96 tubes) and multiple rack (5 x 96 tubes) products.

As standard, each of the products includes patented shape caps with narrow angular tolerances, ECC200 coded to allow tracking of samples and experiments.

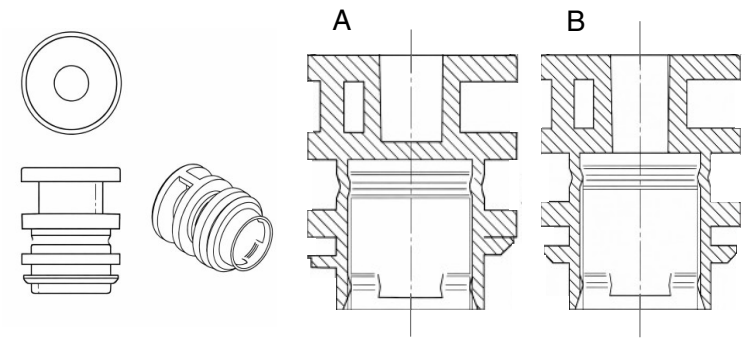
The caps are labeled with a 10-digit unique code, written both in machine-readable form and in human-readable numbers. The first 2 digits identify the tube diameters, the next 8 digits are a unique serial number.

Bruker caps are crafted from high-quality Orgalloy® plastic, offering excellent resistance to a variety of chemicals and NMR solvents such as $CdCl_3$, MeOD, and DMSO. It is nonetheless advisable to avoid direct contact between the sample solution and the cap. While the caps are designed to securely seal the tubes, it is best to limit long-term storage to prevent evaporation of the solvent. The mechanical strength of the product has been tested and validated from 4 °C to 60 °C.

Overall, using Bruker coded caps offers several benefits:

- Unique identification of samples
- Possibility to use the 2D-code-based IconNMR workflow
- Ensuring compatibility when mixing different diameters in the SampleJet
- Certified to ensure quality and traceability to the raw material level

Bruker offers both open and closed caps for tubes and SampleJet systems to provide flexibility across different workflows and sample handling requirements. Open caps are ideal for applications requiring rapid access, easy pipetting, or frequent sample manipulation, while closed caps help minimize evaporation, reduce contamination risk, and support safer handling during storage or automated processing. Both cap types are fully compatible with POM balls, ensuring reliable sample positioning and consistent performance across applications.



Cross-sections of NMR Spare Caps to illustrate the difference between closed (A) and open (B) caps

Unracked NMR Tubes with Closed Coded Caps

100 x Tubes and Closed Coded Caps, 4" Length (SampleJet Operations), Suitable for all Frequencies

Material Number	Outer Diameter	Wall Thickness	Camber	Concentricity
Z172599	5 mm	0.38 mm	60 µm	30 µm
Z172597	3 mm	0.38 mm	60 µm	30 µm

5 mm 4" tubes and closed coded caps **(Z172599)**

100 x Tubes and Closed Coded Caps, 7" Length (Manual, SampleCase and SampleJet Open-Shop Operations), Suitable for all Frequencies

Material Number	Outer Diameter	Wall Thickness	Camber	Concentricity
Z172600	5 mm	0.38 mm	60 µm	30 µm
Z172598	3 mm	0.29 mm	60 µm	30 µm

3 mm 7" tubes and closed coded caps **(Z172598)**

Unracked NMR Tubes with Open Coded Caps

100 x Tubes and Open Coded Caps, 4" Length (SampleJet Operations), Suitable for all Frequencies

Material Number	Outer Diameter	Wall Thickness	Camber	Concentricity
34100277	5 mm	0.38 mm	60 µm	30 µm
34105721	3 mm	0.30 mm	60 µm	30 µm

5 mm 4" tubes and open coded caps **(34100277)**

100 x Tubes and Open Coded Caps, 7" Length (Manual, SampleCase and SampleJet Open-Shop Operations), Suitable for all Frequencies

Material Number	Outer Diameter	Wall Thickness	Camber	Concentricity
34105722	5 mm	0.38 mm	60 µm	30 µm
34105723	3 mm	0.30 mm	60 µm	30 µm

5 mm 7" tubes and open coded caps **(34105723)**

Racked NMR Tubes with Open Coded Caps

Bruker racked tubes & caps products are specifically created and produced to match the storage capacity and strict specifications of the SampleJet autosampler.

1 Rack x 96 Tubes, 4" Length, Suitable for all Frequencies

Material Number	Outer Diameter	Wall Thickness	Camber	Concentricity
Z112273	5 mm	0.38 mm	60 µm	30 µm
Z112272	3 mm	0.38 mm	60 µm	30 µm
Z106462	1.7 mm	0.2 mm	20 µm	No spinning
Z107504	1 mm	0.1 mm	20 µm	No spinning

Single rack **(Z112272)**

5 Racks x 96 Tubes, 4" Length, Suitable for all Frequencies

Material Number	Outer Diameter	Wall Thickness	Camber	Concentricity
Z168405	5 mm	0.38 mm	60 µm	30 µm
Z168406	3 mm	0.38 mm	60 µm	30 µm
Z168407	1.7 mm	0.2 mm	20 µm	No spinning
Z168408	1 mm	0.1 mm	20 µm	No spinning

Five racks **(Z168405)**

Spare Caps

For simple refilling of the racks and for open access shop, caps are available for 3 mm and 5 mm diameters. Spare coded and uncoded caps for 3 mm and 5 mm tubes complete the SampleJet consumables portfolio.

100 x Closed Coded Caps

Material Number	Diameter	Color
Z106779	5 mm (4.97 mm ± 0.05 mm)	Purple
Z107163	3 mm (3 mm ± 0.05 mm)	Green

3 mm caps **(Z107163)**

100 x Closed Uncoded Caps

Material Number	Diameter	Color
Z105683	5 mm (4.97 mm ± 0.05 mm)	Purple
Z107474	3 mm (3 mm ± 0.05 mm)	Green

5 mm caps **(Z105683)**

100 x Open Uncoded Caps

Material Number	Diameter	Color
Z105912	5 mm (4.97 mm ± 0.05 mm)	Purple
Z107376	3 mm (3 mm ± 0.05 mm)	Green

3 mm caps **(Z107376)**

Cap Sealing & Color Coding

Bruker colored POM balls are designed to tightly seal the holes of open caps and simplify sample recognition. They are perfect for environments where multiple users work with automation units but also to color-code tubes in any laboratory setting.

The balls can be either used to color-mark one or a few selected tubes or to mark a whole rack of tubes and they can be used to mark both open and closed caps alike. Dedicated pinch tools are available to help locking the POM balls in place.

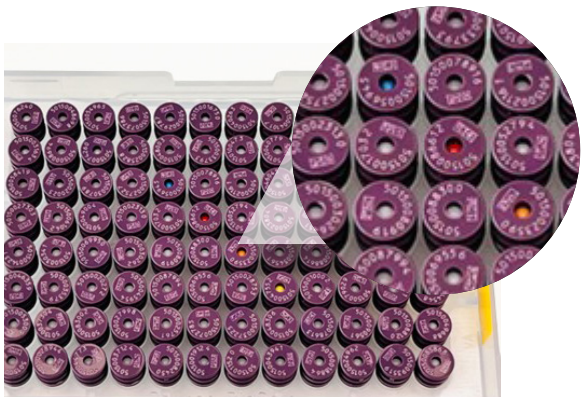
Sealing the caps with a ball has several benefits compared to other sealing methods:

- Sealed caps are as tight as Bruker caps without holes
- The sealing process is fast, easy, reliable and repeatable
- There is no remaining gap or hole as with a pierced membrane
- The balls are made from a single solid structure with no bounding or surface coating or painting
- The tubes remain clean, as they remain in the rack
- The balls do not interfere with sample transport or matrix code label reading
- The balls allow easy marking of different tubes with various colors

POM balls

Set of 100 POM Balls to Tightly Close SampleJet Caps

Material Number	Color
Z147554	Traffic red
Z72497	Opaque white
Z147553	Azure blue
Z147552	Pastel orange
Z147555	Zinc yellow



Marked caps with colored POM balls

Tools

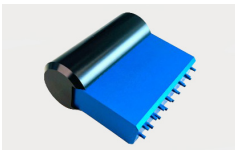
Pinch Tool

Material Number	Description
Z72498	POM balls pinch tool for closing SampleJet tubes

POM balls pinch tool
(Z72498)

Multi Pinch Tool

Material Number	Description
H177028	Multi POM balls pinch tool for closing SampleJet tubes supports simultaneously closing to 16 caps with balls



Multi pinch tool
(H177028)

NMR Septum Caps 5 mm

Bruker package of 100 PTFE septum caps for 5 mm standard NMR tubes (1811642) are ideal for sample filling with piercing needle in liquid handlers or for air-sensitive samples.

NMR septum caps
(1811642)

Specialty Tubes

Bruker specialty NMR tubes are designed to optimize spectral quality under specific experimental constraints:

- **Valved (J. Young-type) tubes:** Airtight sealing for air- or moisture-sensitive samples; suitable for experiments under controlled atmosphere or pressure.
- **MATCH™ tubes:** Minimize magnetic susceptibility mismatches between sample, solvent, and glass, improving field homogeneity and reducing line broadening. Preferred when sample volume is limited but sufficient concentration is possible; the reduced diameter maximizes filling of the active coil region and signal-to-noise ratio without dilution.
- **Shigemi tubes:** Feature a susceptibility-matched adjustable plunger to confine the sample to the RF coil region and precisely control filling height. Enhance sensitivity while minimizing susceptibility interface artefacts; particularly suitable for limited-volume samples, method development, and sensitive experiments (e.g., multi-pulse sequences, decoupling, water suppression).
- **Shaped tubes (non-cylindrical):** Designed for samples with high electrical conductivity or dielectric losses, they are compatible only with inverse CryoProbes and TXO CryoProbes. By reducing effective sample diameter and controlling orientation within the RF coil, they minimize RF field attenuation and dielectric losses, resulting in shorter pulse widths, and higher signal-to-noise ratio. They are recommended for lossy samples (e.g., buffered aqueous or saline solutions).

Key distinction: While MATCH™ tubes reduce effective sample diameter, they do not control sample orientation; shaped tubes are specifically designed to orient lossy samples with respect to RF field distribution.

Bruker application teams will gladly support optimal sample geometry choice.

Bruker Valved Tubes

Bruker NMR valved tubes are expertly designed to prevent samples from coming into contact with atmospheric oxygen or moisture, ensuring the integrity of your samples. These tubes allow for effortless management of air-sensitive NMR samples without the need for flame sealing, making them ideal for applications requiring an inert atmosphere.

The tubes are available in two lengths, optimized and validated in Bruker application labs for your NMR configuration:

Material Number	Description
34101319	Standard: Suitable for Fourier 80 and floor-standing NMR systems with manual sample loading
34101320	Short: Suitable for floor-standing NMR systems with and without a SampleCase or SampleXpress

Bruker valved tubes **(34101319** and **34101320)**

Technical Specifications:

- 5 mm outer diameter
- Completely greaseless Teflon assembly which ensures ease of use and simple disassembly for cleaning
- Achieves a vacuum level of 1 x 10^{-6} mbar with the valve
- Internal positive pressure rating: 1 bar (14.7 PSI)
- Equipped with a Teflon-covered O-ring that eliminates material incompatibilities
- Recommended working temperature range -15 °C to +130 °C

MATCH™ Tubes

The Bruker BioSpin MATCH™ system provides a simple and cost-efficient way to optimize signal-to-noise ratio (S/N) by matching the NMR tube diameter to the available sample amount or desired sample volume. By reducing the tube diameter, dilution that would otherwise be required in a standard 5 mm tube is avoided, and a larger fraction of the sample can be detected.

Provided as set of 10 tubes, they have a length of 100 mm and must be used with a MATCH device.

MATCH™ tubes **(86553)**

Material Number	MATCH Insert Assembly	Inner Diameter	Sample Volume (Based on Height of 40 mm)
86553	1.0 mm	0.7 mm	15 ul
29138	1.7 mm	1.3 mm	50 ul
67539	2.0 mm	1.6 mm	80 ul
16545	2.5 mm	2.1 mm	140 ul
86464	3.0 mm	2.4 mm	190 ul
86463	4.0 mm	3.7 mm	360 ul
HZ12654	4.25 mm	3.45 mm	375 ul
86462	5.0 mm	4.2 mm	560 ul

Note: Compatible with 5 mm and 3 mm probes only.

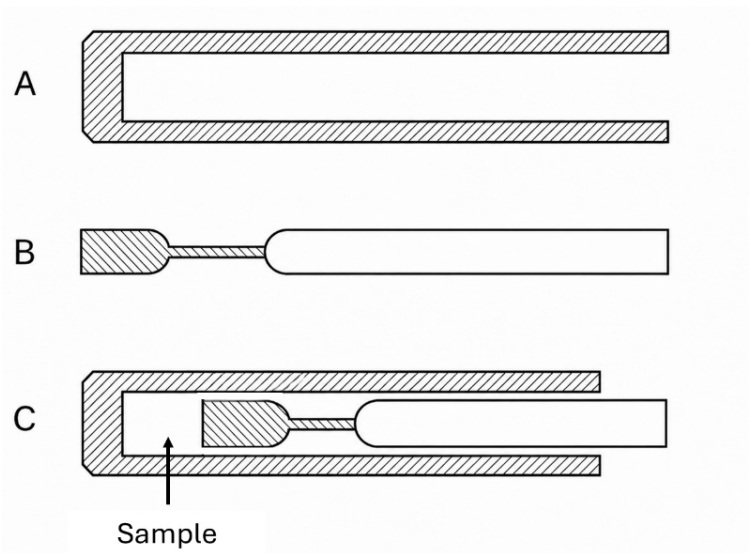
Bruker Optimized Shigemi Tubes

Shigemi tubes are designed to optimize NMR sensitivity and spectral quality when only limited sample volumes are available. By using a susceptibility-matched glass insert and plunger, the sample volume can be reduced while keeping the liquid sample precisely positioned within the region of the RF detection coil. This ensures that essentially the entire sample contributes to the detected signal rather than extending outside the active coil region, improving signal-to-noise ratio and experimental efficiency. In addition, the susceptibility-matched design reduces field distortions and maintains high spectral resolution even with small sample volumes. Bruker-optimized Shigemi tubes further feature geometry specifically matched to Bruker probes, ensuring correct positioning of the sample relative to the RF coil and reliable performance across Bruker NMR systems.

Bruker Shigemi tubes are optimized to high-precision tolerances and recommended for 5 mm CryoProbes.

Bruker optimized Shigemi tubes **(Z10685A)**

Material Number	Solvent
Z10684A	Cd_3OD
Z10682A	$CdCl_3$
Z10681A	D_2O
Z10685A	DMSO-d_6



Cross-section of the outer tube (A), inner tube (B) and Shigemi tube assembly (C).

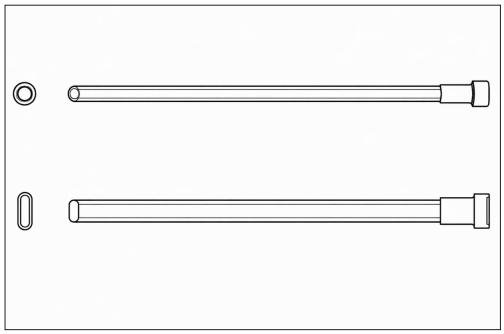
Technical Specifications:

- Insert length 190.0 mm
- Insert OD-A 4.1 mm
- Insert OD-B 4.17 +/-0.01 mm
- Outer tube length 180.0 mm
- Outer tube ID 4.2 mm
- Outer tube OD 4.965 +/-0.01 mm
- Bottom length 8.0 mm
- Supplied as single tube

Shaped Tubes

Shaped NMR tubes are designed to improve experimental performance for samples with high electrical conductivity or dielectric losses. They are compatible with inverse CryoProbes and TXO CryoProbes. For samples with losses exceeding approximately the equivalent of 60 mM NaCl in water, conventional cylindrical tubes lead to enhanced sample noise contribution resulting in RF field attenuation and inefficient excitation, resulting in reduced signal-to-noise ratio (SNR) and longer pulse widths. Shaped tubes address this by modifying the geometry of the sample volume, reducing the effective sample diameter within the RF coil. This design lowers dielectric losses, enabling shorter pulse widths and higher SNR. As a result, shaped tubes are particularly beneficial for buffered aqueous, saline, or other conductive samples where optimal RF performance is critical for achieving high quality, high signal-to-noise NMR data.

Shaped tubes **(Z106898)**



Cross-sections of standard round tubes and of shaped tubes

Technical Specifications:

- Length 203 mm (8")
- Wall thickness 0.25 mm
- Delivered with cap
- Selected quality with guaranteed shimmability warranty
- Supplied as single tube

Please note that a CryoProbe with sample positioning unit (i.e. TCI, QCI, TXO) and a Shaped Sample Tube Shuttle (Z75327) are required.

InsightMR Flow Tubes

Bruker offers packages of 5 NMR spare tubes (H184581) designed and tested by Bruker for the InSightMR Flow Unit.

This flow tube enables online monitoring of chemical reactions in real-time under real conditions. This is achieved by fast and continuous transfer of reaction mixtures from a reaction vessel into the flow tube, located in the NMR probe, with temperature control from the vessel to the probe.

InsightMR flow tubes **(H184581)**

Accessories

Bruker shuttles and spinners are precision-engineered components that ensure accurate and reliable sample transfer, positioning and stable rotation within the NMR probe. The spinner directly holds the NMR tube, with tight tolerances on geometry and mass distribution to enable smooth, vibration-free spinning under defined rotation and VT gas conditions. The SampleJet shuttle, in contrast, is used for sample handling and transfer, particularly in automated or high-throughput environments, enabling safe and reproducible transport of the tube between the sample changer and the magnet.

Spinners

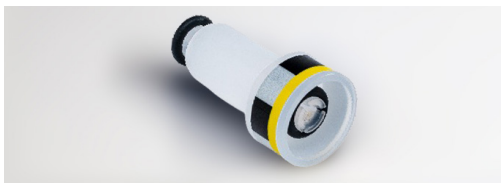
Spinners for Standard-Bore Systems

NMR spinners are designed for 3 mm, 5 mm, and 10 mm NMR tubes, and are compatible with standard-bore NMR systems. Our spinners are available in different materials (POM, Kel-F, Ceramic) to suit a wide range of experimental temperatures. These spinners ensure stable rotation, precise tube positioning, and reliable performance across a wide range of NMR applications.

Material Number	Size	Material	Temperature Range
Z192388	10 mm	Ceramics	-150 °C to +150 °C
Z169633	5 mm		
Z49727	3 mm		
H00306	10 mm	Kel-F	-40 °C to +120 °C
H00177	5 mm		
Z45666	3 mm		
Z5293	10 mm	POM	0 °C to +80 °C
Z42516	5 mm		
Z42516A (Type A Spinner Plastic (POM) - selected quality for use at 500 MHz and higher)	5 mm		
Z45665	3 mm		

5 mm POM spinner for standard-bore shim systems **(Z42516)**

5 mm ceramic spinner for standard-bore shim systems **(Z169633)**



5 mm KelF spinner for standard-bore shim systems **(H100177)**

ATTENTION: FASTM Type 1 Class A Borosilicate Glass Tubes are required for analysis above or below room temperature. All suitable tubes provided by Bruker are ASTM Type 1 Class A Borosilicate Glass Tubes.

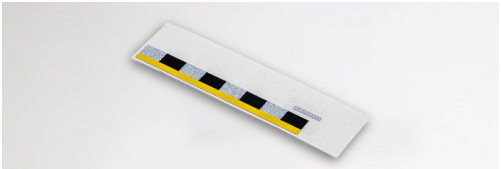
UHF Spinners

Note that ultra-high field NMR systems generate very strong magnetic fields and field gradients along the bore of the magnet, which can exert significant magnetic forces on samples, spinners and shuttles during insertion into the magnet bore. Magnetically compensated shuttles or spinners are designed to mitigate these forces by incorporating materials with different magnetic susceptibilities arranged to balance the magnetic forces. This design enables stable and controlled transport of the sample through regions with high magnetic field gradients and facilitates reliable positioning in the homogeneous measurement region. As a result, patented UHF versions of Bruker Spinners improve handling, alignment, and measurement stability in high-field NMR experiments.

Material Number	Size	Material	Temperature Range
Z179024	5 mm	PCTFE / Titanium	-40 °C to +120 °C
Z179026	3 mm	PCTFE / Titanium	-40 °C to +120 °C

Labels for Standard-Bore Spinners

Set of 20 self-adhesive labels for standard-bore spinners. These are required for detecting the sample upon insertion to the probe and spin-up.



Labels for standard-bore spinners **(Z42852)**

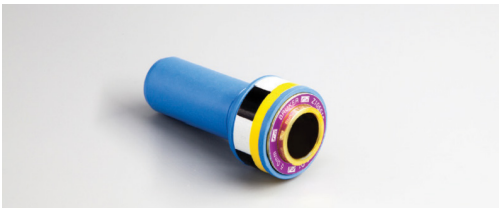
Shuttles

Shuttles for SampleJet Automated Sample Loader System

Material Number	Diameter	Max. Temperature	Label Color	Comment
Z105515	5 mm	150 °C	Purple	
Z179270	5 mm	150 °C	Purple	UHF Version*
Z105909	3 mm	150 °C	Green	
Z179269	3 mm	150 °C	Green	UHF Version*
Z106558	1.7 mm	150 °C	Gray	
Z117078	1.7 mm	150°C	Gray	UHF Version*.**
Z107648	1 mm	150 °C	Black	

** UHF= Ultra-High Field (≥ 1 GHz)*

*** Note that the 1.7 mm shuttles are NOT compatible with a 1.7 mm probe. They are used when measurements with a 1.7 mm tube are conducted in a 3 or 5 mm probe.*



5 mm shuttle **(Z105515)**

Shaped Sample Tube Shuttle

Shuttle for shaped sample tubes, standard-bore, T_{max} = 80 °C. Note that a CryoProbe with a sample positioning unit is required.

Shaped sample tube shuttle **(Z186848)**

Shaped Shigemi Tube Shuttle

Shuttle for 5 mm salt tolerant susceptibility matched slot tube from Shigemi Inc.

Standard-bore, T_{max} = 80 °C. Note that a CryoProbe with a sample positioning unit is required.

Shaped Shigemi tube shuttle **(Z137538)**

POM Shuttle to Hold 1 - 1.7 mm Sample Tubes in 1 - 1.7 mm Probes

Compatible with the SampleCase family of sample changers

Shuttle POM **(Z106492)**

Match Tube Insert Assemblies

MATCH™ Insert assemblies are to be inserted in a 10 mm spinner (Spinner standard-bore shimsystems). It is recommended to use MATCH insert assemblies with corresponding size MATCH™ tubes only, for standard-bore shimsystems. Compatible with the SampleCase family of sample changers.

Technical Specifications:

- The MATCH™ device is a holder for 100 mm long NMR sample tubes with outer diameter range from 1.0 to 5.0 mm
- The MATCH™ device fits into a standard 10 mm Bruker spinner
- The MATCH™ insert assembly is suited for all non-spinning applications
- The grippers are color-coded based on the NMR tube diameter
- NMR tubes can be easily exchanged while the MATCH™ device is still mounted in the spinner
- The MATCH™ grippers have a chemically inert seal to minimize the evaporation of solvent

MATCH™ insert assembly **(H12198)**

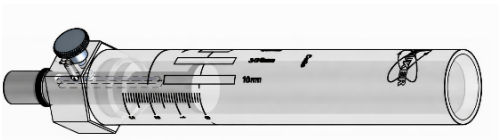
Material Number	Diameter
H9870	5 mm
H9869	4 mm
H9868	3 mm
H12183	2.5 mm
H12182	2 mm
H12181	1.7 mm*
H12198	1 mm*

** 1 and 1.7mm match tube assemblies are not compatible with the 1 and 1.7mm probes. They are intended for use with 1 and 1.7mm tubes in a 3 or 5 mm probe.*

Other Accessories

Sample Tube Depth Adjustment Device

The sample tube depth adjustment device is designed to adjust the relative position of an NMR sample tube and the spinner. It ensures placing the samples at the correct height/depth with respect to the RF coils in Bruker's NMR probes.



Sample tube depth adjustment device **(Z119229)**

CryoProbe Sample Cavity Cleaner

Cleaning device for sample cavity of 5 mm CryoProbes (Z119123).

CryoProbe sample cavity cleaning device **(Z119123)**

Dummy Sample

The dummy sample (H177861) is used to teach the Fourier 80 PAL sample changer its position relative to the Fourier 80 and to verify its calibration.

Standard Reference Samples & Accessories

Bruker reference samples are certified and optimized for ideal concentricity and standardized filling heights of either 40 or 60 mm, ensuring reliable calibration, validation, and benchmarking of NMR systems. This defined geometry supports consistent RF excitation and detection conditions, providing confidence in system performance and enabling users to achieve reproducible, comparable experimental results across instruments and over time.

SDS Webpage

Certificate Webpage

5 mm NMR reference sample

Certified NMR Standard Reference Samples for 10 mm Probes

Material Number	Test	Composition
Z10250	^{1}H lineshape	1% chloroform ($CHCl_3$) in acetone-d_6
Z10121	^{1}H sensitivity	0.1% ethylbenzene (EB) in chloroform-d
Z10268	Water suppression	2 mM sucrose, 0.5 mM DSS, 2 mM NaN_3 in H_2O/D_2O (90:10)
Z10265	^{15}N & ^{13}C pulse calibration	100 mM ^{15}N-enriched urea, 100 mM ^{13}C-enriched methanol in DMSO-d_6
Z10164	^{13}C sensitivity & resolution (ASTM)	40% dioxane in benzene-d_6
Z10154	^{13}C sensitivity & ^{1}H decoupling	10% ethylbenzene (EB) in chloroform-d
Z10202	^{31}P sensitivity	0.0485 M triphenyl phosphate (TPP) in acetone-d_6
Z10188	^{13}N sensitivity	90% formamide in DMSO-d_6
Z10235	^{13}F sensitivity	0.05% α,α,α-trifluorotoluene (TFT) in chloroform-d
Z10210	^{29}Si sensitivity	85% hexamethyldisiloxane (HMDSO) in benzene-d_6
Z10628	Temperature calibration (282–330 K) – NMR thermometer	99.8% methanol-d_4
Z10130	High-temperature calibration (300–380 K)	80% ethylene glycol in DMSO-d_6
Z10128	Low-temperature calibration (180–300 K)	4% methanol (CH_3OH) in methanol-d_4
Z10085	Gradient recovery test	0.1 mg $GdCl_3$/ml in D_2O with 1% H_2O and 0.1% CH_3OH (^{13}C)

Certified NMR Standard Reference Samples for 10 mm CryoProbes

Material Number	Test	Composition
Z10702	^{1}H lineshape	0.3% chloroform ($CHCl_3$) in acetone-d_6

Certified NMR Standard Reference Samples for 5 mm Probes

Material Number	Test	Composition
Z10248	^{1}H lineshape	1% chloroform ($CHCl_3$) in acetone-d_6
Z10120	^{1}H sensitivity	0.1% ethylbenzene (EB) in chloroform-d
Z10246	Water suppression	2 mM sucrose, 0.5 mM DSS, 2 mM NaN_3 in H_2O/D_2O (90:10)
Z10263	^{15}N & ^{13}C pulse calibration	100 mM ^{15}N-enriched urea, 100 mM ^{13}C-enriched methanol in DMSO-d_6
Z10163	^{13}C sensitivity & resolution (ASTM)	40% dioxane in benzene-d_6
Z10153	^{13}C sensitivity & ^{1}H decoupling	10% ethylbenzene (EB) in chloroform-d
Z10201	^{31}P sensitivity	0.0485 M triphenyl phosphate (TPP) in acetone-d_6
Z10187	^{15}N sensitivity	90% formamide in DMSO-d_6
Z10234	^{19}F sensitivity	0.05% α,α,α-trifluorotoluene (TFT) in chloroform-d
Z10209	^{29}Si sensitivity	85% hexamethyldisiloxane (HMDSO) in benzene-d_6
Z10627	Temperature calibration (282–330 K) – NMR thermometer	99.8% methanol-d_4
Z10129	High-temperature calibration (300–380 K)	80% ethylene glycol in DMSO-d_6
Z10127	Low-temperature calibration (180–300 K)	4% methanol (CH_3OH) in methanol-d_4
Z10083	Gradient recovery test	0.1 mg $GdCl_3$/ml in D_2O with 1% H_2O and 0.1% CH_3OH (^{13}C)
Z10093	2D experiments	25 mM cyclosporine in benzene-d_6
Z10298	1D NOE difference	100 mg/mL pamoic acid in DMSO-d_6 with 1% tetramethylsilane (TMS)

Certified NMR Standard Reference Samples for 5 mm RT Probes at 200-300 MHz

Material Number	Test	Composition
Z10230	^{1}H lineshape	3% chloroform ($CHCl_3$), 0.2% tetramethylsilane (TMS) in acetone-d_6

Certified NMR Standard Reference Samples for 5 mm CryoProbes and RT Inverse Probes at 700 MHz or Higher

Material Number	Test	Composition
Z10701	^{1}H lineshape	0.3% chloroform ($CHCl_3$) in acetone-d_6
Z10902	Water suppression	2 mM sucrose, 0.5 mM DSS, 2 mM NaN_3 in H_2O/D_2O (90:10)

Certified NMR Standard Reference Samples for 3 mm Probes

Material Number	Test	Composition
Z10030	^{1}H lineshape	1% chloroform ($CHCl_3$) in acetone-d_6
Z10033	^{1}H sensitivity	0.1% ethylbenzene (EB) in chloroform-d
Z10036	Water suppression	2 mM sucrose, 0.5 mM DSS, 2 mM NaN_3 in H_2O/D_2O (90:10)
Z10037	^{13}N & ^{13}C pulse calibration	100 mM 15N-enriched urea, 100 mM ^{13}C-enriched methanol in DMSO-d_6
Z10035	^{13}C sensitivity & resolution (ASTM)	40% dioxane in benzene-d_6
Z10034	^{13}C sensitivity & ^{1}H decoupling	10% ethylbenzene (EB) in chloroform-d
Z10038	^{31}P sensitivity	0.0485 M triphenyl phosphate (TPP) in acetone-d_6
Z10039	^{15}N sensitivity	90% formamide in DMSO-d_6
Z10040	^{19}F sensitivity	0.05% α,α,α-trifluorotoluene (TFT) in chloroform-d
Z10053	Temperature calibration (282–330 K) – NMR thermometer	99.8% methanol-d_4
Z10044	High-temperature calibration (300–380 K)	80% ethylene glycol in DMSO-d_6
Z10043	Low-temperature calibration (180–300 K)	4% methanol (CH3OH) in methanol-d_4
Z10046	Gradient recovery test	0.1 mg $GdCl_3$/ml in D_2O with 1% H_2O and 0.1% CH_3OH (^{13}C)
Z10051	2D experiments	25 mM cyclosporine in benzene-d_6

Certified NMR Standard Reference Samples for 3 mm CryoProbes and RT Inverse Probes at 700 MHz or Higher

Material Number	Test	Composition
Z10029	^{1}H lineshape	0.3% chloroform ($CHCl_3$) in acetone-d_6

Certified NMR Standard Reference Samples for 1.7 mm Probes

Material Number	Test	Composition
Z10717	^{1}H lineshape	1% chloroform ($CHCl_3$) in acetone-d_6
Z10718	^{1}H sensitivity	0.1% ethylbenzene (EB) in chloroform-d
Z10720	Water suppression	10 mM sucrose, 0.5 mM DSS, 2 mM NaN_3 in H_2O/D_2O (90:10)
Z10721	^{15}N & ^{13}C pulse calibration	100 mM ^{15}N-enriched urea, 100 mM ^{13}C-enriched methanol in DMSO-d_6
Z10724	^{13}C sensitivity & resolution (ASTM)	40% dioxane in benzene-d_6
Z10723	^{13}C sensitivity & ^{1}H decoupling	10% ethylbenzene (EB) in chloroform-d
Z10722	^{31}P sensitivity	0.0485 M triphenyl phosphate (TPP) in acetone-d_6
Z10728	^{19}F sensitivity	0.05% α,α,α-trifluorotoluene (TFT) in chloroform-d
Z10734	Temperature calibration (282–330 K) – NMR thermometer	99.8% methanol-d_4
Z10727	Gradient recovery test	0.1 mg $GdCl_3$/ml in D_2O with 1% H_2O and 0.1% CH_3OH (^{13}C)

Certified NMR Standard Reference Samples for 1,7 mm CryoProbes and RT inverse probes at 700 MHz or higher

Material Number	Test	Composition
Z10230	^{1}H lineshape	3% chloroform ($CHCl_3$), 0.2% tetramethylsilane (TMS) in acetone-d_6

Certified NMR Standard Reference Samples for 1 mm Probes

Material Number	Test	Composition
Z100926	^{1}H lineshape	1% chloroform ($CHCl_3$) in acetone-d_6
Z100927	^{1}H sensitivity	0.1% ethylbenzene (EB) in chloroform-d
Z100930	Water suppression	10 mM sucrose, 0.5 mM DSS, 2 mM NaN_3 in H_2O/D_2O (90:10)
Z100932	^{15}N & ^{13}C pulse calibration	100 mM ^{15}N-enriched urea, 100 mM ^{13}C-enriched methanol in DMSO-d_6
Z100933	Gradient recovery test	0.1 mg $GdCl_3$/ml in D_2O with 1% H_2O and 0.1% CH_3OH (^{13}C)

Accessories for Standard Reference Samples

Storage Box for NMR Tubes

Light weight and secure storage box for storage and transport of NMR tubes or reference samples.

Material Number	Diameter	Number of Positions
47677	1 mm - 1.7 mm	8
1812105	3 mm - 5 mm	20
47675	10 mm	5

Storage box for NMR tubes
(1812105)

Coded Caps for Standard Reference Samples

Material Number	Diameter	Color
Z163895	5 mm (4.97 mm ± 0.05 mm)	Purple
Z163894	3 mm (3 mm ± 0.05 mm)	Green

5 mm caps for standard reference samples
(Z163895)

Fourier 80 Standard Reference Samples

Material Number	Test	Composition
Z10690	^{1}H sensitivity	1% ethylbenzene (EB) in chloroform-d
Z10694	^{13}C sensitivity	100% ethylbenzene (EB)
1807022	^{31}P sensitivity	0.485 M triphenyl phosphate (TPP) in acetone-d_6
1814255	^{19}F sensitivity	0.5% α,α,α-trifluorotoluene (TFT) in chloroform-d
1811573	^{29}Si sensitivity	100% hexamethyldisiloxane (HMDSO)
1900589	Temperature calibration (282–330 K) – NMR thermometer	99.8% methanol-d_4
1900592	High-temperature calibration (300–380 K)	80% ethylene glycol in DMSO-d_6
Z10692	^{1}H and ^{13}C pulse calibration	1 M ^{13}C-methanol in D_2O
Z10688	Shim sample	5% H_2O, 0.6 mM $CuSO_4$
Z10689	Lineshape sample	20% chloroform ($CHCl_3$) in acetone-d_6
Z187876	AT shim sample	100 mg/ml pamoic acid in DMSO-d_6 with 1% tetramethylsilane (TMS)
1807009	^{7}Li sensitivity	1 M lithium bromide (LiBr) in D_2O
1811571	^{11}B sensitivity	0.75 M boric acid in D_2O
1902712	^{23}Na sensitivity	0.5 M sodium chloride (NaCl) in D_2O

Fourier 80 Sample Accessories

Cap for Flame-Sealed Samples

Special holder (H182310) for flame-sealed samples, designed to accommodate the geometric variability introduced during flame sealing, enabling the use of flame-sealed tubes in a Fourier 80.

Fourier 80 cap for flame-sealed samples
(H182310)

Flame-Sealed Tube Cap Guide

The flame-sealed tube cap guide (H182387) is an alignment tool for use with flame-sealed tubes. It ensures precise positioning when mounting the required holder (H182310), enabling use in the Fourier 80.

Flame-sealed tube cap guide
(H182387)

Sample Holder

The Fourier 80 sample holder (Z186193) ensures precise tube depth and accurate sample positioning in the Fourier 80. It is compatible with Bruker NMR tubes (Z172600, 7” length, 5 mm outer diameter).

Sample holder **(Z186193)**

Cap for Reference Samples

These caps are mounted on the corresponding Fourier 80 standard reference samples to ensure unambiguous identification.

Material Number	Reference Sample	Reference Sample Material Number	POM Ball Color
W182501	Lineshape	Z10689	White
W182500	Shim	Z10688	Blue

Cap for reference Fourier reference samples **(W182501)**

Documentation such as safety data sheets for the sample substances and dedicated Bruker certificates of conformity are available for all standard samples and reagents.

Z10083 NMR-SAMPLE 0,1 mg GdCl3/ml D2O + 1% H2O + 0,1% CH3OH 13C (DOPED WATER)

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Version: 2022.9
SDS No: ZAD12832

SECTION 1: Identification

1.1. Identification

Product form : Mixture
Product name : Z10683 NMR-SAMPLE 0,1 mg GdCl3/ml D2O + 1% H2O + 0,1% CH3OH 13C (DOPED WATER)
Other means of identification : Z186693/1 mm
Z187727/1.7 mm
Z186840/3 mm
Z186835 mm
Z10685/10 mm
Further information : CPID - 288929.33

1.2. Recommended use and restrictions on use

Use of the substance/mixture : Industrial
Scientific research and development
Restrictions on use : All other uses are not recommended

1.3. Supplier

Manufacturer:
Bruker Biospin Corporation
15 Fortune Dr
Billerica, MA 01821,
T +1 978-667-9580
sds.bbio@bruker.com - www.bruker.com
E-mail address of competent person responsible for the SDS: sds@gbk-ingelheim.de

1.4. Emergency telephone number

Emergency number : Emergency CONTACT (24-Hour-Number)
GBK/Infotrac ID: 84135: (USA domestic) 1 800 535 5053 or international (001) 352 323 3500

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification
Not classified

2.2. GHS Label elements, including precautionary statements

GHS US labeling
No labeling applicable

2.3. Other hazards which do not result in classification

No additional information available

2.4. Unknown acute toxicity (GHS US)

No additional information available

US - en 1/8

Certificate of Conformity

NMR STANDARD SAMPLE

TEST	'DOPED WATER'		
COMPOSITION	**0.1mg GdCl3 / ml D2O + 1% H2O + 0.1% CH3OH 13C** (Gadolinium(III) chloride)		
DESCRIPTION	Solution in a sealed 10mm NMR tube, 60mm filling height		
USE	'DOPED WATER' Gradient Recovery Test and Console Test		
NMR-TUBE TYPE	Precision Tube, Ø 10mm, wall thickness 0.46mm		
REF NMR-SAMPLE	Z10085	BATCH NMR-SAMPLE	0000528934
REF MIXTURE	Z187092	BATCH MIXTURE	0000528931
DATE OF CERTIFICATION	28.08.2025	VALIDITY	28.08.2029
NMR-SPECTRUM	Refer to the respective spectrum on: Certificates for Standard Reference Samples | Bruker www.bruker.com/content/bruker/int/en/resources/certificates-data-sheets/coc.html		
NOTE	The certificate is valid for 4 years from the date of certification, provided storage conditions are met.		
STORAGE CONDITION	Store in the original container at ambient temperature, under dry conditions and protected from direct sunlight. Under adverse conditions (especially exposure to direct sunlight and temperatures > 40 °C) the Standard Sample may degrade.		
HAZARDS	Refer to the corresponding Safety Data Sheet (SDS) on: SDS Sheets Magnetic Resonance | Bruker www.bruker.com/en/resources/certificates-data-sheets/msds.html		
GUIDELINES	This certificate attests that the above-mentioned Standard Sample has been produced in accordance with standard operating procedures (SOPs) based on the ISO 9001 management system and fully meets the stated product specifications. All source materials are fully traceable.		
MANUFACTURER	Bruker Switzerland AG, Industriestrasse 26, CH-8117 Faellanden / Switzerland for Bruker BioSpin Group		
PLACE AND DATE OF ISSUE	Faellanden, 28.08.2025	SIGNATURE - preparer	Worakul Tubniyom, Laboratory Assistant
		SIGNATURE - reviewer	Samuel Gut, Production Manager

Innovation with Integrity

NMR

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