Quantitative NMR Excellence

Trust *Trace***CERT**® Certified Reference Materials for Reliable Results

Supelco®
Analytical Products

Our Quality Grades

*Trace*CERT® Certified Reference Materials (CRMs)

What makes *Trace*CERT® CRMs stand above others?

Many different standards are available covering a wide range of quality, service, and price. As the world's number one supplier of research chemicals and standards, we introduced *Trace*CERT® reference materials to underpin our leading position in terms of quality and customer convenience.

What makes *Trace*CERT® standards higher in quality?

The *Trace*CERT® line of products, produced and certified under ISO 17034 in accordance with metrological guidelines, ensures the highest accuracy, low uncertainties, and in-depth documentation, making these CRMs completely reliable and traceable to primary material from National Metrology Institutes (NMIs), such as NIST or NMIJ. Moreover, our robust packaging strategy ensures the integrity of certified values during transit and delivery.

Our *Trace*CERT® line of qNMR certified reference materials are analyzed by our ISO/IEC 17025 accredited laboratories in Buchs, Switzerland.

Laboratories accredited under ISO/IEC 17025, along with those in regulated settings, maintain consistent practices, rigorous controls, and thorough documentation—equipping them to face routine authority audits with confidence. ISO/IEC 17025 is a recognized international accreditation for laboratories and is accepted worldwide through the International Laboratory Accreditation Organization (ILAC), and every country has its own accreditation bodies that are members of the ILAC. Our *Trace*CERT® line of qNMR certified reference materials are produced from the highest purity starting material.

SRMS 0001 STS 0490

The Certificate of Analysis for our certified reference material grade *Trace*CERT® line of qNMR standards includes:

- Certified content tested by high-resolution quantitative NMR measurements (qNMR)
- Produced and certified under ISO 17034, which includes accredited measurements under ISO/IEC 17025. The lab is accredited by the Swiss Accreditation Service SAS.
- Maximum accuracy with calculated uncertainties, lot-specific values, and traceable to primary material from an NMI, e.g. NIST or NMIJ.
- Detailed Certificate of Analysis in accordance with ISO 33401

Our Certificates of Analysis for Certified Reference Materials meet all requirements as indicated by ISO 33401.

1. Title of the document
2. Unique identifier of the RM
3. Name of the RM
4. Name and contact details of the RM producer
5. Intended use
6. Minimum sample size
7. Period of validity
8. Storage information
9. Instructions for handling and use
10. Document components (Page number and the total number of pages)
11. Document version
12. Property of interest
13. Description of the material
14. Property value and associated uncertainty
15. Metrological traceability
16. Name and function of the RM producer's approving officer

Certificate of a Certified Reference Material Grade *Trace*CERT® qNMR Standard

Supelco®

www.sigmaaldrich.com

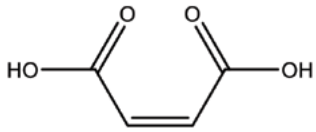
1 Certified Reference Material

Reference material certificate

Maleic acid 3

TraceCERT®

Product no.:	92816 2
Lot no.:	BCCN5306
Description of CRM:	solid neat material 13
7 **Expiry date:**	AUG 2029
Storage:	15-25°C; storage under Argon
8 **Chemical formula:**	$C_4H_4O_4$
Molecular mass:	116.07 g/mol
CAS No.:	110-16-7



Sample 12	Certified value ± Expanded uncertainty, $U_{CRM}=k \cdot u_{CRM}$ (k=2)[1][2] as mass fraction
Maleic acid	**0.9982 g/g ± 0.0019 g/g** (99.82 % ± 0.19 %) 14

15 **Metrological traceability:**	Traceable to the SI through an unbroken chain of comparisons via NIST PS1 (Benzoic acid)[3] Details see "Certification process details" on page 2.
Measurement method:	The certified value is established by high-resolution quantitative NMR measurements (qNMR) in accordance with ISO/IEC 17025.[4]
Intended use: 5	Use this certified reference material (CRM) as standard for quantitative ^{1}H-NMR measurements.
Minimum sample size: 6	The sample is solid at room-temperature. 10 mg is recommended as the minimum sample size. If less material is used, it is recommended to increase the certified uncertainty by a factor of two for half of sample and a factor of four for a quarter of sample.
9 **Instructions for handling and correct use:**	This material does not require drying before use. The CRM should be stored in the original bottle. After use the bottle should be tightly closed and protected from excessive moisture and light. Test stability of the CRM in mixture and/or in solution for the desired duration of the experiment.
Accreditation:	Sigma-Aldrich Production GmbH is accredited by the Swiss Accreditation Service SAS as reference material producer under no. SRMS 0001 in accordance with international standard ISO 17034.[5]
Certificate issue date:	28 AUG 2025

ilac-MRA

SWISS ACCREDITATION sas.admin.ch SRMS 0001

ISO 17034
SRMS 0001

Dr. P. Zell – Approving Officer
(Quality Assurance)

16

4 Sigma-Aldrich Production GmbH, Industriestrasse 25, 9471 Buchs, Switzerland;
Tel +41-81-755-2511; Fax +41-81-756-5449; www.sigmaaldrich.com
Sigma-Aldrich Production GmbH is a subsidiary of Merck KGaA, Darmstadt, Germany.

Unlocking the Power of Quantitative NMR in the Pharmaceutical and Chemical Industries

Quantitative Nuclear Magnetic Resonance (qNMR) has rapidly become one of the most important tools in the pharmaceutical and chemical industries for accurately quantifying organic molecules. While proton NMR is the most used method, the expansion of qNMR into various other areas such as metabolomics, biomarker discovery, and physiological pathways introduces more complex molecules and systems. This complexity can make using ^{1}H-qNMR challenging. Exploring other NMR-active nuclei such as ^{31}P or ^{19}F can offer better options in such cases.[1,2]

This brochure invites you to explore the exciting world of qNMR. Since 2009, we have been applying qNMR under ISO/IEC 17025 for the development of organic certified reference materials (CRMs). All our CRMs are produced under ISO 17034 at our facility in Switzerland. With a robust set of over 20 different qNMR standards for ^{1}H, ^{31}P, and ^{19}F nuclei, we have developed an extensive portfolio of additional CRMs for use in chromatography. Currently, we offer more than 1500 products across various categories, including:

- Environmental: pesticides, polyaromatic hydrocarbons (PAHs), phenols, air monitoring substances, and PFAS.
- Food & Beverages: extractables and leachables, food contact materials, cosmetics, amino acids and IFRA allergenic compounds.
- Pharma: pharmaceutical secondary standards and impurities.

Our diverse range of CRMs ensures that you have the reliable references necessary for accurate analysis in your field. We continuously refine our qNMR expertise, incorporating valuable feedback from CRM users.

In the following sections, we will share essential tips to help you optimize your NMR instrument for quantitative measurements, ensuring maximum accuracy and reproducibility. Additionally, we will introduce you to our *Trace***CERT®** CRMs, which are used to certify organic CRMs, providing you with reliable results that are traceable to a primary standard from a National Metrology Institute (NMI) such as NIST or NMIJ, and ultimately traceable to the International System of Units (SI).[3]

The Challenge of Quantifying Organic Compounds

Reliable quantification of organic materials can be quite challenging, especially since most analytical techniques are dependent on the specific compound being analyzed. For instance, using HPLC with UV, DAD, or fluorescence detection necessitates a traceable reference for the exact same compound. Unfortunately, reliable reference materials are often not available for many organic compounds.

Determining the content of an organic material typically involves measuring all potential impurities—including related compounds, water, residual solvents, and inorganic impurities—and calculating the content by subtracting these impurity values from a total of 100%. However, this method assumes that no potential impurities have been overlooked and that the related impurities measured by a chromatographic method respond in the same way as the target analyte, which is often not the case. An alternative to this labor-intensive approach is the use of a relative primary method, such as qNMR.[4] While NMR has been a crucial qualitative method for the structure elucidation of organic compounds for the past 50 years, its quantitative applications have gained significant importance over the last decades.

Using Internal or External Calibration

Various referencing techniques have been explored for qNMR, including both internal and external calibration methods. Bharti and Roy provided a comprehensive overview of these methods, highlighting their advantages and drawbacks.[5] External referencing approaches involve using NMR tubes with coaxial inserts to separate the analyte and the standard. Additionally, electronic reference methods, such as ERETIC (Electronic Reference To access In vivo Concentration), utilize an electronically generated signal as the internal reference. PULCON (Pulse Length Based Concentration Determination) is an NMR technique that determines analyte concentration by comparing its signal intensity to that of an external reference.[6]

Achieving low measurement uncertainties is critical for the development of Certified Reference Materials (CRMs). Several authors have discussed the advantages of using the internal reference method.[7, 8, 9] While we generally prefer this method (as shown in **Figure 1**), the external standard method also has its benefits, such as easier recovery of analyte material, which can be important when analyzing very expensive substances.

However, the internal standard method typically offers much higher precision and lower uncertainties. Once the materials are weighed into the same vial, the ratio of the analyte to the reference remains constant.

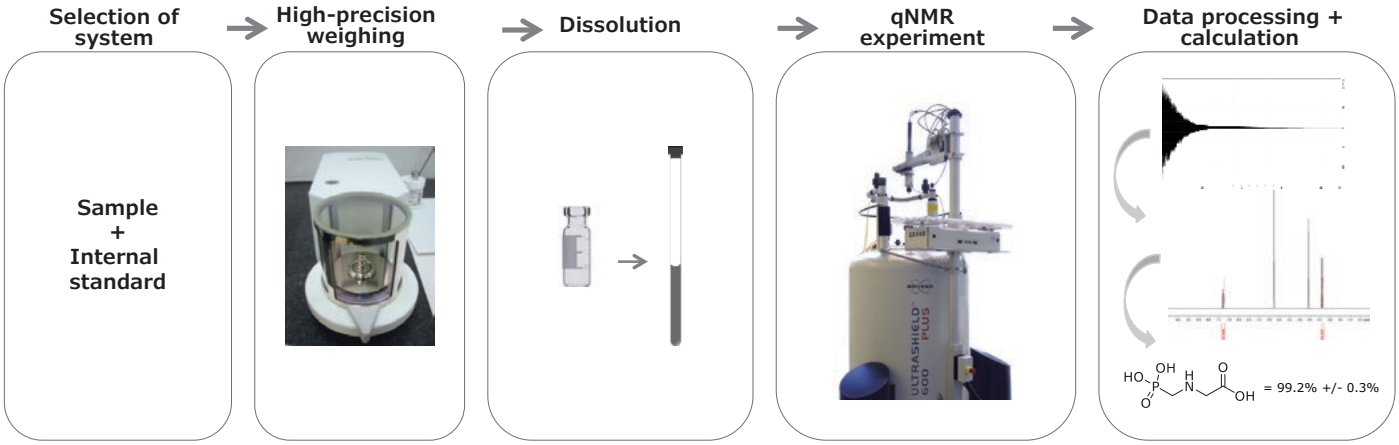


Figure 1: General procedure of a qNMR experiment using an internal standard

Things to Consider: Step-by-Step

The following recommendations focus on the internal standard method, although many are equally applicable to the external standard method.

1. Selection of a Suitable Reference Material

When choosing qNMR reference materials, ensure they possess the following characteristics:

- **High Purity:** This minimizes signal overlap, leading to clearer results.
- **Non-Hygroscopic and Non-Volatile:** These properties ensure stability and facilitate accurate weighing.
- **Free of Residual Water:** This reduces baseline effects that can interfere with measurements.
- **Highly Soluble:** The reference material should dissolve well in common deuterated NMR solvents to ensure effective analysis.
- **Unique and Stable Signals:** It should provide distinct and consistent signals with clear chemical shifts.
- **Limited Number of Signals:** Preferably, the reference should have only a few signals to minimize overlap with analyte signals.

Different samples may require different reference materials, but it is sufficient to have one well-separated signal from each compound in the spectrum. For accurate and precise qNMR measurements, a signal intensity ratio of 1:1 is recommended, though it is not mandatory. All commercially available **qNMR** *Trace***CERT**® materials meet the mentioned criteria, are traceable to primary material from NIST (e.g. PS1) or NMIJ and can be directly used as CRMs in qNMR analyses.

2. Compatibility Checks

Before conducting compatibility checks between the analyte and the internal standard, it is essential to first test the stability of the analyte in the selected deuterated solvent. Begin by performing measurements at t=0, and then repeat the measurements at later intervals, such as t=5, 12, or 24 hours, to evaluate stability over time.

Once you have selected a suitable reference standard, particularly for internal calibration, it is crucial to assess the mixture's chemical stability and inertness. This evaluation helps prevent any unwanted reactions between the sample, reference, or solvent. We recommend conducting compatibility checks through NMR experiments. By measuring the tolerance between the sample and the standard at the initial time and at a subsequent interval, you can account for the expected duration of all planned repetitions, ensuring that the mixture remains stable throughout the analysis.

Additionally, verify that the relevant signals for quantification do not overlap or interfere with potential impurities. It may be necessary to experiment with different combinations of solvents and internal standards to determine the most favorable analytical setup.

3. Metrological Weighing

Reliable weighing values are essential, as they have a direct impact on the results, and it is recommended that they are performed in a metrological manner. Utilizing a microbalance or a similar high-precision balance is crucial for success. Using a less sensitive balance can lead to increased uncertainty contributions from the weighing procedure, which raises the question of the level of precision that should ultimately be achieved.

We use XPR6U Ultra-microbalances from METTLER TOLEDO, with a readability of 100 ng, certified by DKD, and calibrated with OIML Class E2 weights. The balance is placed on a 400 kg stone table inside a safety weighing cabinet, and an antistatic device is installed to eliminate potential static charge. This setup also minimizes air fluctuations caused by air conditioning, or heating.

Climate conditions are monitored in parallel with each weighing step, allowing for subsequent air buoyancy correction. Samples and references are not weighed directly into the NMR tube; instead, they are weighed into an HPLC vial, which can be resealed for complete solvation after adding the deuterated solvent. It is important to avoid common weighing errors, such as eccentric loading, and it is recommended to use glass vials and metal spatulas rather than plastic, due to the risk of static charge.

4. Instrument Settings

We utilize Bruker and Jeol 600 MHz spectrometers equipped with 5 mm CPP TCI cryo and room temperature probe heads, respectively. Instruments with either higher or lower magnetic fields are also suitable for quantification purposes. To achieve high precision, and if time permits, it is advisable to apply a 90° pulse instead of a 30° pulse. This adjustment enhances the signal-to-noise ratio (S/N) and reduces artifacts. No spinning is employed to avoid the formation of spinning sidebands, which could complicate the spectrum. Before commencing the actual qNMR experiment, it is essential to determine the T1 relaxation time in the mixture. This is one of the most critical factors for obtaining consistent results. The T1 relaxation time can be measured using the inversion recovery experiment, which operates based on a 180° pulse followed by a 90° pulse after a variable delay. Tables below lists the T1 relaxation times for *Trace***CERT**® CRMs in various deuterated solvents. Since T1 relaxation times vary with concentration, the mixture, and the solvent, we recommend evaluating the relaxation time within the mixture, for example, simultaneously with the compatibility check. To calculate D1, it is recommended that the longest resulting T1 (relaxation delay) in a mixture be multiplied by a minimum factor of 5–10.

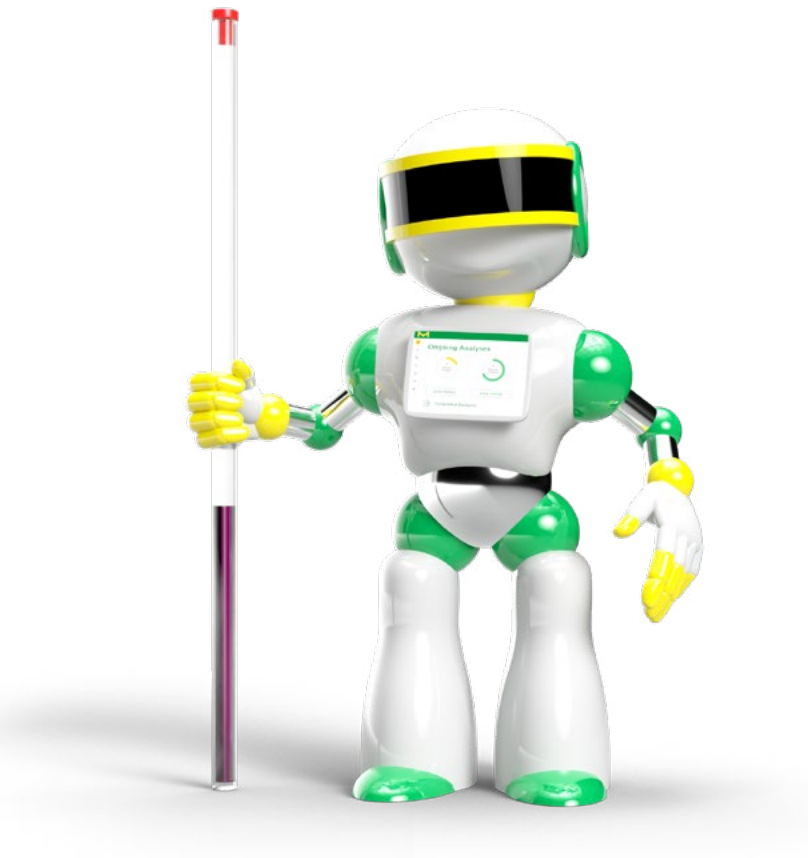
5. Spectra Evaluation

After zero filling and exponential weighing of the FID, the Fourier Transformation is applied. Phase correction and baseline correction are two critical steps in processing spectra. For more accurate integrals, it is generally preferable to perform the integration process manually, as this approach can lead to greater precision and lower uncertainty contributions. However, there are various software solutions available that offer automated processing and integration. Ultimately, the decision rests with the customer to choose between achieving more accurate and precise results through manual integration or opting for less time-consuming automated processing, which may be less accurate. It is essential to consistently perform the integration step for both signals (analyte and reference), and you should either include or exclude the ^{13}C satellites for each signal. The choice depends significantly on the signal shape and any potential impurities near the signals of interest.

6. Content Calculation

We recommend conducting sufficient measurements (e.g. 5–10) to ensure a statistically relevant contribution to the overall measurement uncertainty. The quantification of the sample content is directly calculated from the NMR peak integrals, along with the initial weights of the sample and reference substance, their molecular masses, the number of nuclei contributing to the respective signals, and the certified purity of the reference standard. Please note that a sample may contain both the analyte and potential impurities, which has to be taken into account in the calculation formula. To achieve even more precise results, weighing values can be corrected for air buoyancy if the climate conditions in the lab and the densities of the materials are known.

ChemisTwin®: The online portal ChemisTwin®[10] can be used for automated content determination. It automates spectral integration and performs content calculations directly from the acquired spectra, without requiring manual post-processing. Also, the certified content of the *Trace***CERT**® CRMs are directly accessible in **ChemisTwin**® portal for the current lots. All weights, integration traces and calculation steps are recorded in exportable reports to save analyst time and reduce operator-dependent variability. Please contact us for a demo or a free trial of **ChemisTwin® portal**.



7. Uncertainty Budget

In addition to the statistical contribution (Type A), there are several other contributions (Type B) to consider. All parameters in the equation contribute to the overall measurement uncertainty budget, but with varying magnitudes.[11] The contribution is zero for the number of nuclei in small molecules, very small for molecular masses and weighing values (depending on the balance used), and medium for the individual contribution of the operator. The largest contributions often arise from the repeatability of the measurements or the purity of the reference standard. Merck provides qNMR Standards with the highest purity and remarkably low extended measurement uncertainty to minimize impacts to the measurement uncertainty for the customer. In addition to these uncertainty contributions for the qNMR measurement, the homogeneity and stability of the material must be assessed, although this is primarily relevant for a CRM producer. This assessment results in analysis of variance (ANOVA) data that may be included in the calculation of uncertainty. The recommended minimal sample size is stated in the certificate, along with a hard expiry date. In most cases, the measurement uncertainty is enhanced by a coverage factor of k=2.

$$P_{Sample} = \frac{I_{Analyte}}{I_{CRM}} \bullet \frac{N_{CRM}}{N_{Analyte}} \bullet \frac{M_{Analyte}}{M_{CRM}} \bullet \frac{m_{CRM}}{m_{Sample}} \bullet P_{CRM}$$

P_{Sample} = *Purity of the sample as mass fraction [g/g]*
P_{CRM} = *Purity of the CRM as mass fraction [g/g]*
$I_{Analyte}$ = *Integral of the analyte signal*
I_{CRM} = *Integral of the CRM signal*
$N_{Analyte}$ = *Number of nuclei (analyte)*
N_{CRM} = *Number of nuclei (CRM)*
$M_{Analyte}$ = *Molecular mass of the analyte [g/mol]*
M_{CRM} = *Molecular mass of the CRM [g/mol]*
M_{CRM} = *Mass of reference*
M_{sample} = *Mass of sample*

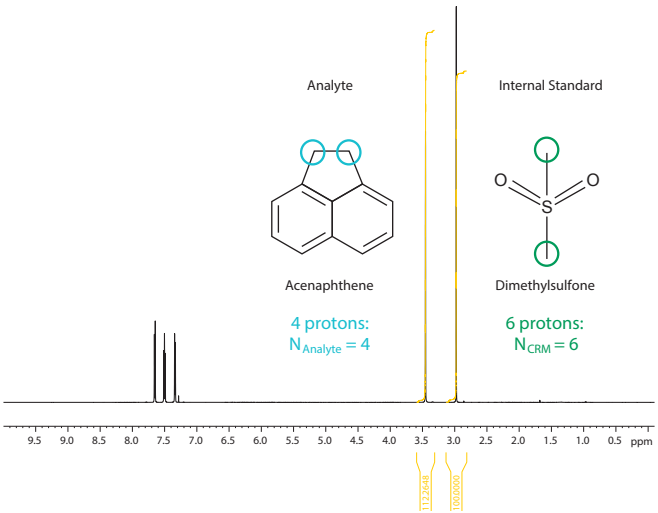


Figure 2: Example of a ^{1}H qNMR Spectrum with internal standard calibration.

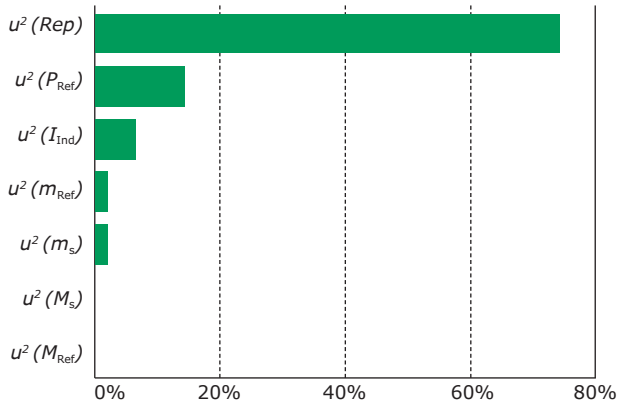


Figure 3: Overview on typical contributions to the relative standard uncertainty (relative squared contributions are given)

To minimize increments from the internal reference for the user, we have certified our *Trace***CERT®** CRMs under optimal conditions, ensuring that the uncertainty contributions are as low as possible and do not dominate the overall result.[12] By following some basic rules and utilizing a good balance, it is possible to routinely perform qNMR measurements with a measurement uncertainty of 0.5–1%.

*Trace*CERT® Certified Reference Materials for qNMR

Cat. No.	Substance	D_2O			$CDCl_3$			DMSO-d_6			CD_3OD			CD_3CN		
		δ	T1	s	δ	T1	s	δ	T1	s	δ	T1	s	δ	T1	s
		ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL
01380	Ethylene carbonate	4.5	5.5	>250	4.5	7.0	>250	4.5	2.7	>250	4.5	5.3	>250	4.5	2.0	>250
03826	Calcium formate	8.4	3.4	>250**	-	-	-	-	-	-	-	-	-	-	-	-
06185	Benzoic acid	-	-	-	8.1	3.7	150	8	3.3	>250	8	4.3	>250	8.0	4.5	80
					7.7	4.0		7.6	3.7		7.6	4.4		7.7	2.5	
					7.5	3.4		7.5	3.0		7.5	3.9		7.5	2.6	
07038	Dimethyl terephthalate	-	-	-	8.1	3.6	160	8.1	2.9	20	8.1	4.4	4	8.1	4.9	20
					4.0	1.8		3.9	1.1		4	2.4		3.9	2.6	
14659	Potassium hydrogen phthalate	7.5	2.5	>250*	-	-	-	-	-	-	7.9	2.5	5	-	-	-
40384	1,2,4,5-Tetra-chloro-3-nitro-benzene	-	-	-	7.8	10.7	>250	8.5	12.6	>250	8.1	6.4	50	8.0	9.6	10
41867	Dimethyl sulfone	3.0	2.9	>250	3	2.7	80	3	2.4	>250	3	3.3	40	2.9	2.6	>250
42582	Ethyl 4(dimethyl-amino) benzoate	-	-	-	7.9	3.8	>250	7.8	2.5	>250	7.9	3.4	>250	7.9	5.6	50
					6.7	2.4		6.7	1.4		6.7	2.5		6.7	3.7	
					4.3	2.8		4.2	1.9		4.3	3.3		4.3	4.1	
					3.1	2.0		3	1.5		3	2.2		3.0	3.6	
					1.4	2.5		1.3	2.1		1.4	2.7		1.3	3.6	
50409	Thymol	-	-	-	7.1	3.8	>250	7	2.0	>250	7	3.7	>250	7.1	4.9	>250
					6.8	4.5		6.7	2.2		6.6	4.4		6.7	5.7	
					6.6	4.8		6.5	2.6		6.5	5.8		6.6	5.7	
					3.2	4.3		3.1	2.3		3.2	4		3.2	5.2	
					2.3	3.1		2.2	2.0		2.2	2.8		2.2	3.5	
					1.3	1.9		1.1	0.9		1.2	1.8		1.2	2.4	
74599	1,3,5-Trimethoxy benzene	-	-	-	6.1	4.7	>250	6.1	3.2	>250	6.1	4.8	>250	6.7	3.4	>250
					3.8	2.2		3.7	1.4		3.8	2.7		4.3	2.6	
74658	1,2,4,5-Tetra-methylbenzene	-	-	-	7.0	6.1	>250	6.9	4.7	10	6.9	5.9	20	6.9	7.7	50
					2.2	4.0		2.1	2.6		2.2	4.3		2.2	5.0	
89151	Dimethyl malonic acid	1.3	1.0	100	-	-	-	1.3	0.7	250	1.4	1	250	1.4	2.0	30
92816	Maleic acid	6.3	6.1	>250	-	-	-	6.3	3.0	>250	6.3	3.9	10	6.4	6.2	20
94681	Methyl 3,5-dinitrobenzoate	-	-	-	9.3	8.0	>250	9.1	9.4	100	-	-	-	9.1	9.0	>250
					9.2	6.1		8.9	7.6					9.0	8.2	
					4.1	2.6		4.0	1.5					4.0	3.5	
93074	Pentachlorobenzene	-	-	-	7.6	5.8	>250	8.2	13.8	15	7.9	8.2	9	7.8	12.2	15
53396	2,4-Dichlorobenzotrifluoride	-	-	-	7.6	4.8		8.0	9.5	>250	7.8	5.2		7.8	6.3	
					7.5	6.7		7.9	3.6		7.7	7.2		7.7	8.7	
					7.4	6	>250	7.7	5.1		7.5	6.1	>250	7.5	7.3	>250
80730	2-Chloro-4-Fluorotoluene	-	-	-	7.2	6		7.4	6.5		7.3	6.7		7.3	7.6	
					7.1	7		7.1	6.4		7.1	7		7.2	8.7	
					6.9	6.3		2.3	3.1	>250	7	6.9		7	8	
					2.3	4.3	>250				2.3	4.8	>250	2.3	5.3	>250

All Relaxation times (T1) are measured at a concentration of around 10 mg/ml
* with NaOD
**dissolves with DCl

Standards for ^{19}F quantitative NMR, *Trace*CERT®

Cat. No.	Substance	D_2O			$CDCl_3$			DMSO-d_6			CD_3OD			CD_3CN		
		δ	T1	s	δ	T1	s	δ	T1	s	δ	T1	s	δ	T1	s
		ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL
07563	4,4'-Difluoro-benzophenone	-	-	-	-105.8	2.4	>250	-106.5	1.4	150	-108.1	2.8	30	-108.3	2.3	140
53396	2,4-Dichloro-benzotrifluoride	-	-	-	-62.5	2.3	>250	-61.2	1.2	>250	-65.4	3.3	>250	-63.0	2.9	>250
80730	2-Chloro-4-Fluorotoluene	-	-	-	-115.8	4.4	>250	-115.3	3.3	>250	-117.7	4.8	>250	-117.3	4.7	>250

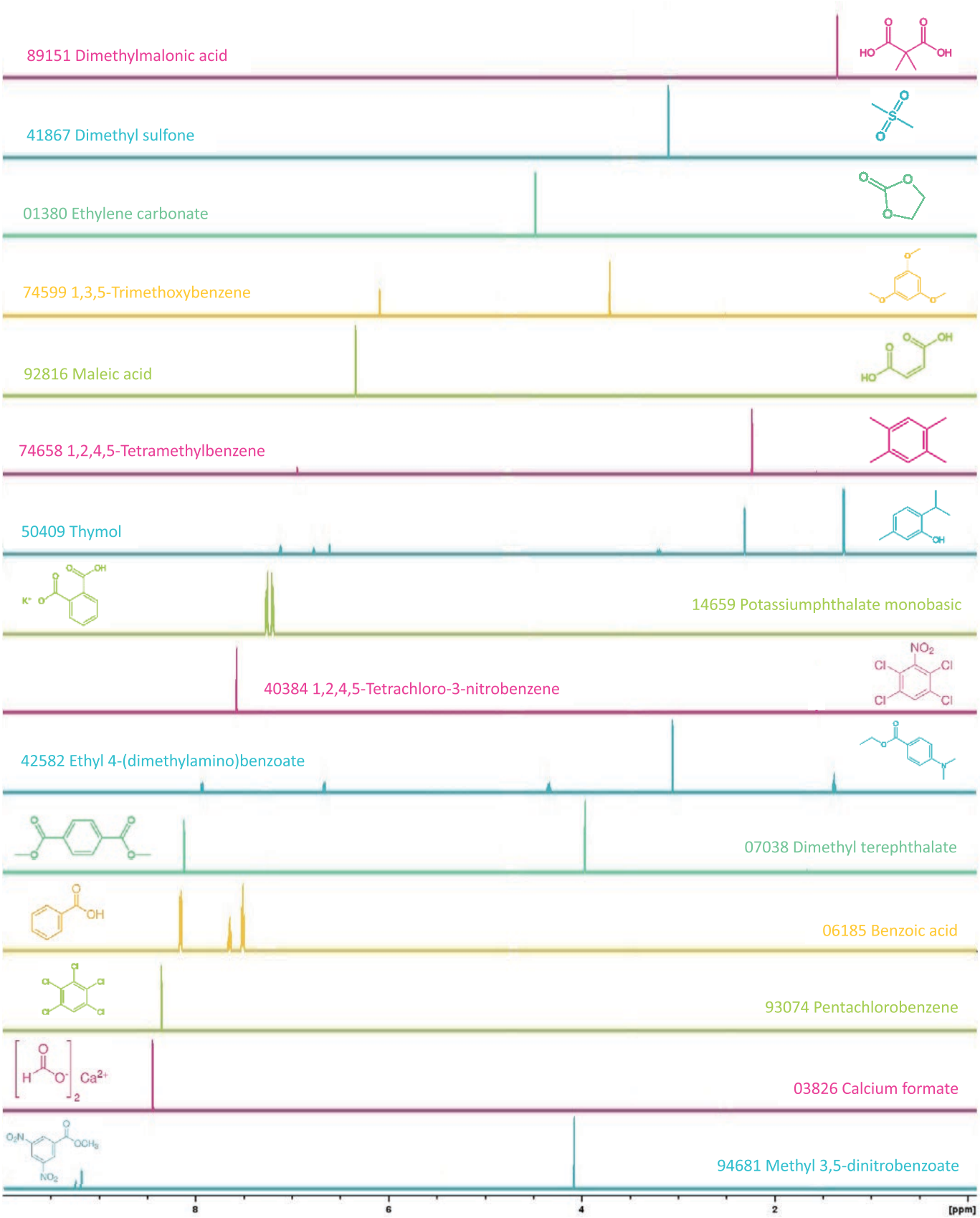
All Relaxation times (T1) are measured at concentration around 10 mg/ml

Standards for ^{31}P quantitative NMR, *Trace*CERT®

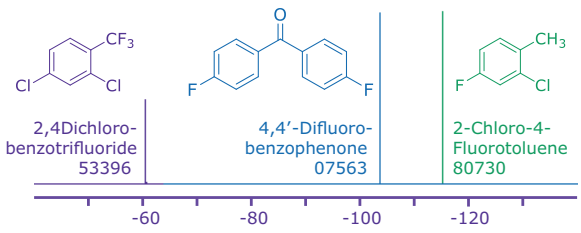
Cat. No.	Substance	D_2O			$CDCl_3$			DMSO-d_6			CD_3OD			CD_3CN		
		δ	T1	s	δ	T1	s	δ	T1	s	δ	T1	s	δ	T1	s
		ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL	ppm	s	mg/mL
05498	Triphenyl phosphate	-	-	-	-17.7	2.7	>250	-17.3	1.2	>100	-17.5	3.1	>10	-17	4.3	>250
92214	Potassium phosphate monobasic	0.08	8	>250	-	-	-	-	-	-	-	-	-	-	-	-
96708	Phosphono acetic acid	15.70	4.6	>250	-	-	-	14.9	1.5	>250	17.7	2.9	>250	-	-	-

All Relaxation times (T1) are measured at concentration around 10 mg/ml

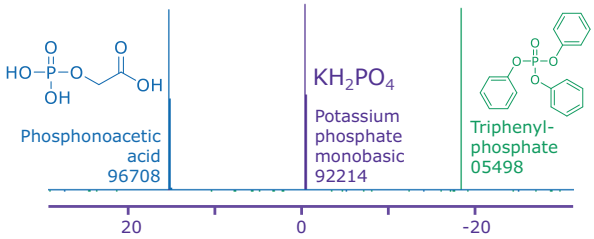
NMR Spectra for ^{1}H qNMR Standards, *Trace*CERT®



NMR Spectra for ^{19}F qNMR Standards, *Trace*CERT®



NMR Spectra for ^{31}P qNMR Standards, *Trace*CERT®



We currently offer a series of 17 different Certified Reference Materials (CRMs) designed specifically for use in ^{1}H qNMR experiments, along with 3 additional CRMs for ^{19}F qNMR and 3 CRMs designed for ^{31}P qNMR experiments. For some time now, we have offered the option to employ the ^{19}F qNMR standards simultaneously as ^{1}H qNMR standards too and plan to do so as well for ^{31}P standards. This significant advancement enables the use of a single standard for two different nuclei, greatly enhancing efficiency and simplifying the analytical process. All products are either traceable to NIST (National Institute of Standards and Technology) and/or NMIJ (National Metrology Institute of Japan) primary material and are produced under ISO 17034 accreditation, which signifies the highest achievable quality level in the industry. The currently available CRMs are listed, including chemical shifts of the signals, solubility values, and concentration-dependent relaxation times. This information will assist you in identifying the most suitable reference material for your qNMR tasks.

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