MilliporeSigma

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One-Stop Shop for NMR Consumables

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Lab & Production Materials

Not just good or great. But gold.

As a leader in life sciences, MilliporeSigma offers a catalog of more than 300,000 products. One of our
core specialties is NMR, for which we produce premium quality solvents, standards, CRMs, and stable isotope reagents, as well as dedicated NMR tubes and accessories.

Our innovative certified reference materials (CRMs) are ideal for a wide range of new applications in quantitative NMR (qNMR), such as metabolomics, biomarker discovery, and physiological pathway research. All our CRMs are traceable to NIST SRM, and produced according to ISO/IEC 17025 and ISO Guide 34 criteria. This double accreditation represents the "gold standard" in reference materials – the highest quality possible.

For more information, please visit
SigmaAldrich.com/NMR

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High Quality NMR Solvents

High quality solvents are essential for the rigorous demands of NMR research and analysis. At MilliporeSigma, we're passionate about quality. That's why we provide the widest range of NMR solvents with excellent chemical purity and the highest isotopic enrichment possible.

To make sure we always offer you the finest quality, we consistently review and improve our methods for solvent purification and water content reduction. And, all our NMR solvents undergo strict quality control testing during production and packaging.

For more specific requirements, we support you with the convenience of customized products and packaging. Our glass bottles, ampules, and septum bottles for NMR solvents are available in the broadest range of configurations and sizes.

Benefits

- Reliable results in NMR spectra
- Excellent chemical purity and highest isotopic enrichment
- Reliable deuteration degrees
- Determination of water content in Karl Fischer and NMR
- Safe, easy handling with septum bottles and glass ampules
- Flexible choice of packaging formats

Cat. No.	Product Description	Isotopic Purity and Internal Standards
Acetic acid-d		
151777-50G	Acetic acid-d	99 atom % D
151777-250G	Acetic acid-d	99 atom % D
151785-50G	Acetic acid-d_4	≥99.5 atom % D
151785-10X1ML	Acetic acid-d_4	≥99.5 atom % D
151785-25G	Acetic acid-d_4	≥99.5 atom % D
151785-10G	Acetic acid-d_4	≥99.5 atom % D
151785-5G	Acetic acid-d_4	≥99.5 atom % D
416886-25G	Acetic acid-d_4	≥99.5 atom % D, contains 0.03 % (v/v) TMS
233315-5G	Acetic acid-d_4	≥99.9 atom % D
233315-10X0.5ML	Acetic acid-d_4	≥99.9 atom % D
Acetone-d_6		
151793-100G	Acetone-d_6	99.9 atom % D
151793-25G	Acetone-d_6	99.9 atom % D
151793-10X1ML	Acetone-d_6	99.9 atom % D
151793-10X0.75ML	Acetone-d_6	99.9 atom % D
151793-10G	Acetone-d_6	99.9 atom % D
151793-50G	Acetone-d_6	99.9 atom % D
444863-1L	Acetone-d_6	99.9 atom % D
444863-10ML-AMP	Acetone-d_6	99.9 atom % D
444863-25ML	Acetone-d_6	99.9 atom % D
444863-100ML	Acetone-d_6	99.9 atom % D
444863-10ML-GL	Acetone-d_6	99.9 atom % D
444863-10X0.6ML	Acetone-d_6	99.9 atom % D
444863-10X0.5ML	Acetone-d_6	99.9 atom % D
444863-50ML	Acetone-d_6	99.9 atom % D
434531-10X1ML	Acetone-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
434531-25G	Acetone-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
434531-10G-GL	Acetone-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
434531-50G	Acetone-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
454133-50G	Acetone-d_6	99.9 atom % D, contains 1 % (v/v) TMS

Cat. No.	Product Description	Isotopic Purity and Internal Standards
454133-25G	Acetone-d_6	99.9 atom % D, contains 1 % (v/v) TMS
175862-10X0.75ML	Acetone-d_6	99.96 atom % D
175862-5G	Acetone-d_6	99.96 atom % D
175862-10X0.5ML	Acetone-d_6	99.96 atom % D
Acetonitrile-d_3		
151807-50G	Acetonitrile-d_3	≥99.8 atom % D
151807-5G	Acetonitrile-d_3	≥99.8 atom % D
151807-10G-GL	Acetonitrile-d_3	≥99.8 atom % D
151807-10X1ML	Acetonitrile-d_3	≥99.8 atom % D
151807-10X0.6ML	Acetonitrile-d_3	≥99.8 atom % D
151807-25G	Acetonitrile-d_3	≥99.8 atom % D
151807-10G-AMP	Acetonitrile-d_3	≥99.8 atom % D
151807-10X0.75ML	Acetonitrile-d_3	≥99.8 atom % D
151807-100G	Acetonitrile-d_3	≥99.8 atom % D
699543-10G	Acetonitrile-d_3	≥99.8 atom % D, Special HOH
699543-50G	Acetonitrile-d_3	≥99.8 atom % D, Special HOH
569550-10X1ML	Acetonitrile-d_3	≥99.8 atom % D, anhydrous
366544-5G	Acetonitrile-d_3	99.8 atom % D, contains 0.03 % (v/v) TMS
366544-10X0.6ML	Acetonitrile-d_3	99.8 atom % D, contains 0.03 % (v/v) TMS
366544-50G	Acetonitrile-d_3	99.8 atom % D, contains 0.03 % (v/v) TMS
366544-25G	Acetonitrile-d_3	99.8 atom % D, contains 0.03 % (v/v) TMS
233331-50G	Acetonitrile-d_3	99.8 atom % D, contains 1 % (v/v) TMS
233323-10X0.5ML	Acetonitrile-d_3	99.96 atom % D
233323-10X0.75ML	Acetonitrile-d_3	99.96 atom % D
233323-5G	Acetonitrile-d_3	99.96 atom % D
233323-25G	Acetonitrile-d_3	99.96 atom % D
Benzene-d_6		
175978-10G	Benzene-d_6	99 atom % D
175978-50G	Benzene-d_6	99 atom % D
151815-10G-AMP	Benzene-d_6	99.6 atom % D
151815-10G-GL	Benzene-d_6	99.6 atom % D

Cat. No.	Product Description	Isotopic Purity and Internal Standards
151815-100G	Benzene-d_6	99.6 atom % D
151815-10X1ML	Benzene-d_6	99.6 atom % D
151815-10X0.75ML	Benzene-d_6	99.6 atom % D
151815-25G	Benzene-d_6	99.6 atom % D
151815-50G	Benzene-d_6	99.6 atom % D
570680-50G	Benzene-d_6	anhydrous, ≥99.6 atom % D
364940-50G	Benzene-d_6	99.6 atom % D, contains 0.03 % (v/v) TMS
364940-10G	Benzene-d_6	99.6 atom % D, contains 0.03 % (v/v) TMS
364940-25G	Benzene-d_6	99.6 atom % D, contains 0.03 % (v/v) TMS
561509-10X.75ML	Benzene-d_6	99.96 atom % D, contains 0.03 % (v/v) TMS
175870-25G	Benzene-d_6	99.96 atom % D
175870-10X0.5ML	Benzene-d_6	99.96 atom % D
175870-10X1ML	Benzene-d_6	99.96 atom % D
Bromobenzene-d_5		
175730-5G	Bromobenzene-d_5	99.5 atom % D
175730-25G	Bromobenzene-d_5	99.5 atom % D
tert-Butanol-d_{10}		
175889-1G	tert-Butanol-d_{10}	99 atom % D
175889-5G	tert-Butanol-d_{10}	99 atom % D
tert-Butyl methyl-d_3 ether		
434132-1G	tert-Butyl methyl-d_3 ether	99 atom % D
Chlorobenzene-d_5		
176605-5G	Chlorobenzene-d_5	99 atom % D
176605-1G	Chlorobenzene-d_5	99 atom % D
Chloroform-d		
151823-10X0.75ML	Chloroform-d	99.8 atom % D
151823-250G	Chloroform-d	99.8 atom % D
151823-1KG	Chloroform-d	99.8 atom % D
151823-100G	Chloroform-d	99.8 atom % D
151823-50G	Chloroform-d	99.8 atom % D
151823-10X0.6ML	Chloroform-d	99.8 atom % D
151823-10X1ML	Chloroform-d	99.8 atom % D
570699-50G	Chloroform-d	≥99.8 atom % D, anhydrous
225789-10X0.6ML	Chloroform-d	99.8 atom % D, contains 0.03 % (v/v) TMS
225789-100G	Chloroform-d	99.8 atom % D, contains 0.03 % (v/v) TMS
225789-500G	Chloroform-d	99.8 atom % D, contains 0.03 % (v/v) TMS
225789-10X1ML	Chloroform-d	99.8 atom % D, contains 0.03 % (v/v) TMS
225789-50G	Chloroform-d	99.8 atom % D, contains 0.03 % (v/v) TMS
612200-100G	Chloroform-d	99.8 atom % D, contains 0.05 % (v/v) TMS
434876-500G	Chloroform-d	99.8 atom % D, contains 0.1 % (v/v) TMS
434876-150G	Chloroform-d	99.8 atom % D, contains 0.1 % (v/v) TMS
434876-100G	Chloroform-d	99.8 atom % D, contains 0.1 % (v/v) TMS

Cat. No.	Product Description	Isotopic Purity and Internal Standards
612200-100G	Chloroform-d	99.8 atom % D, contains 0.05 % (v/v) TMS
151831-50G	Chloroform-d	99.8 atom % D, contains 1 % (v/v) TMS
151831-100G	Chloroform-d	99.8 atom % D, contains 1 % (v/v) TMS
151831-250G	Chloroform-d	99.8 atom % D, contains 1 % (v/v) TMS
416754-250G	Chloroform-d	≥99.8 atom % D, contains 0.5 wt. % silver foil as stabilizer
416754-100G	Chloroform-d	≥99.8 atom % D, contains 0.5 wt. % silver foil as stabilizer
530735-250G	Chloroform-d	≥99.8 atom % D, contains 0.5 wt. % silver foil as stabilizer, 0.03 % (v/v) TMS
530735-100G	Chloroform-d	≥99.8 atom % D, contains 0.5 wt. % silver foil as stabilizer, 0.03 % (v/v) TMS
151858-10X0.75ML	Chloroform-d	99.96 atom % D
151858-50G	Chloroform-d	99.96 atom % D
151858-10X0.5ML	Chloroform-d	99.96 atom % D
151858-10X0.25ML	Chloroform-d	99.96 atom % D
151858-10X1ML	Chloroform-d	99.96 atom % D
151858-10G	Chloroform-d	99.96 atom % D
431915-10ML	Chloroform-d	99.96 atom % D, contains 0.5 wt. % silver wire as stabilizer
431915-50ML	Chloroform-d	99.96 atom % D, contains 0.5 wt. % silver wire as stabilizer
494275-10X0.75ML	Chloroform-d	99.96 atom % D, contains 0.03 % (v/v) TMS
494275-50G	Chloroform-d	99.96 atom % D, contains 0.03 % (v/v) TMS
494275-10G	Chloroform-d	99.96 atom % D, contains 0.03 % (v/v) TMS
Cyclohexane-d_{12}		
151866-10X1ML	Cyclohexane-d_{12}	≥99.6 atom % D
151866-5G	Cyclohexane-d_{12}	≥99.6 atom % D
151866-10G	Cyclohexane-d_{12}	≥99.6 atom % D
151866-1G	Cyclohexane-d_{12}	≥99.6 atom % D
Decahydronaphthalene-d_{18}		
217131-1G	Decahydronaphthalene-d_{18}	98 atom % D
Deuterium oxide		
435767-100G	Deuterium oxide	99 atom % D
435767-25G	Deuterium oxide	99 atom % D
435767-1KG	Deuterium oxide	99 atom % D
617385-1KG	Deuterium oxide	99.8 atom % D
617385-1.107KG	Deuterium oxide	99.8 atom % D
151882-1.107KG	Deuterium oxide	99.9 atom % D
151882-10X1ML	Deuterium oxide	99.9 atom % D
151882-500G	Deuterium oxide	99.9 atom % D
151882-10X0.6ML	Deuterium oxide	99.9 atom % D
151882-100G	Deuterium oxide	99.9 atom % D
151882-250G	Deuterium oxide	99.9 atom % D
151882-1KG	Deuterium oxide	99.9 atom % D

Cat. No.	Product Description	Isotopic Purity and Internal Standards
151882-25G	Deuterium oxide	99.9 atom % D
151882-10X0.75ML	Deuterium oxide	99.9 atom % D
151882-4KG	Deuterium oxide	99.9 atom % D
151882-10G	Deuterium oxide	99.9 atom % D
613444-100G	Deuterium oxide	99.9 atom % D, glass distilled
293040-100G	Deuterium oxide	99.9 atom % D, contains 0.75 wt. % 3-(trimethylsilyl) propionic-2,2,3,3-d_4 acid, sodium salt
293040-25G	Deuterium oxide	99.9 atom % D, contains 0.75 wt. % 3-(trimethylsilyl) propionic-2,2,3,3-d_4 acid, sodium salt
343773-25G	Deuterium oxide	99.9 atom % D, contains 1 % (w/w) 3-(trimethylsilyl)-1-propanesulfonic acid, sodium salt (DSS)
343773-100G	Deuterium oxide	99.9 atom % D, contains 1 % (w/w) 3-(trimethylsilyl)-1-propanesulfonic acid, sodium salt (DSS)
450510-10X0.75ML	Deuterium oxide	99.9 atom % D, contains 0.05 wt. % 3-(trimethylsilyl) propionic-2,2,3,3-d_4 acid, sodium salt
450510-100ML	Deuterium oxide	99.9 atom % D, contains 0.05 wt. % 3-(trimethylsilyl) propionic-2,2,3,3-d_4 acid, sodium salt
450510-25ML	Deuterium oxide	99.9 atom % D, contains 0.05 wt. % 3-(trimethylsilyl) propionic-2,2,3,3-d_4 acid, sodium salt
151890-50G	Deuterium oxide	≥99.96 atom % D
151890-250G	Deuterium oxide	≥99.96 atom % D
151890-10G	Deuterium oxide	≥99.96 atom % D
151890-10X0.75ML	Deuterium oxide	≥99.96 atom % D
151890-10X1ML	Deuterium oxide	≥99.96 atom % D
151890-1KG	Deuterium oxide	≥99.96 atom % D
151890-125G	Deuterium oxide	≥99.96 atom % D
191701-10X0.5ML	Deuterium oxide	99.990 atom % D
191701-10X0.25ML	Deuterium oxide	99.990 atom % D
191701-10G	Deuterium oxide	99.990 atom % D
613398-50G	Deuterium oxide	extra, 99.994 atom % D
613398-10G	Deuterium oxide	extra, 99.994 atom % D
Dibromomethane-d_2		
259020-5G	Dibromomethane-d_2	99 atom % D, contains copper as stabilizer
177865-10X1ML	Dichloromethane-d_2	99.5 atom % D
177865-25G	Dichloromethane-d_2	99.5 atom % D
177865-10G	Dichloromethane-d_2	99.5 atom % D
296163-10G	Dichloromethane-d_2	≥99.5 atom % D, contains 0.03 % (v/v) TMS

Cat. No.	Product Description	Isotopic Purity and Internal Standards
296163-1G	Dichloromethane-d_2	≥99.5 atom % D, contains 0.03 % (v/v) TMS
296163-25G	Dichloromethane-d_2	≥99.5 atom % D, contains 0.03 % (v/v) TMS
444324-25G	Dichloromethane-d_2	99.9 atom % D
444324-10X0.75ML	Dichloromethane-d_2	99.9 atom % D
444324-10X1ML	Dichloromethane-d_2	99.9 atom % D
444324-10X0.6ML	Dichloromethane-d_2	99.9 atom % D
444324-10G	Dichloromethane-d_2	99.9 atom % D
444324-5G	Dichloromethane-d_2	99.9 atom % D
530506-25G	Dichloromethane-d_2	99.9 atom % D, contains 0.1 % (v/v) TMS
530506-1G	Dichloromethane-d_2	99.9 atom % D, contains 0.1 % (v/v) TMS
233366-10X0.5ML	Dichloromethane-d_2	99.96 atom % D
233366-5G	Dichloromethane-d_2	99.96 atom % D
N,N-Dimethylacetamide-d_9		
522414-5G	N,N-Dimethylacetamide-d_9	99 atom % D
522414-1G	N,N-Dimethylacetamide-d_9	99 atom % D
N,N-Dimethylformamide-d_7		
189979-5X0.5ML	N,N-Dimethylformamide-d_7	≥99.5 atom % D
189979-1G	N,N-Dimethylformamide-d_7	≥99.5 atom % D
189979-10G	N,N-Dimethylformamide-d_7	≥99.5 atom % D
189979-5G	N,N-Dimethylformamide-d_7	≥99.5 atom % D
189979-10X0.75ML	N,N-Dimethylformamide-d_7	≥99.5 atom % D
189979-10X1ML	N,N-Dimethylformamide-d_7	≥99.5 atom % D
269905-1G	N,N-Dimethylformamide-d_7	≥99.5 atom % D, contains 1 % (v/v) TMS
269905-10G	N,N-Dimethylformamide-d_7	≥99.5 atom % D, contains 1 % (v/v) TMS
700428-10G	N,N-Dimethylformamide-d_7	≥99.5 atom % D, contains 0.03 % (v/v) TMS
700428-1G	N,N-Dimethylformamide-d_7	≥99.5 atom % D, contains 0.03 % (v/v) TMS

Safe, easy handling with septum bottles and glass ampules

Cat. No.	Product Description	Isotopic Purity and Internal Standards
Dimethyl sulfide-d_6		
416452-1G	Dimethyl sulfide-d_6	99 atom % D
175943-100G	Dimethyl sulfoxide-d_6	99.5 atom % D
175943-50G	Dimethyl sulfoxide-d_6	99.5 atom % D
175943-250G	Dimethyl sulfoxide-d_6	99.5 atom % D
175943-10G	Dimethyl sulfoxide-d_6	99.5 atom % D
151874-25G	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-10G-GL	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-50G-SB	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-10X0.75ML	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-10G-AMP	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-100G	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-5G	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-40KG	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-600G	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-50G-GL	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-10X0.6ML	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-10G-SB	Dimethyl sulfoxide-d_6	99.9 atom % D
151874-10X1ML	Dimethyl sulfoxide-d_6	99.9 atom % D
716731-50ML	Dimethyl sulfoxide-d_6	≥99.9 atom % D, "Special HOH"
716731-10ML	Dimethyl sulfoxide-d_6	≥99.9 atom % D, "Special HOH"
716731-10X0.75ML	Dimethyl sulfoxide-d_6	≥99.9 atom % D, "Special HOH"
570672-10X1ML	Dimethyl sulfoxide-d_6	anhydrous, 99.9 atom % D
570672-50G	Dimethyl sulfoxide-d_6	anhydrous, 99.9 atom % D
296147-10X1ML	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-10X0.75ML	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-10X0.5ML	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-10X0.6ML	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-10G	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-50G	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-25G	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 0.03 % (v/v) TMS
185965-50G	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 1 % (v/v) TMS
185965-25G	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 1 % (v/v) TMS
185965-10G	Dimethyl sulfoxide-d_6	99.9 atom % D, contains 1 % (v/v) TMS
156914-10X0.75ML	Dimethyl sulfoxide-d_6	99.96 atom % D
156914-5G	Dimethyl sulfoxide-d_6	99.96 atom % D
156914-10X0.5ML	Dimethyl sulfoxide-d_6	99.96 atom % D
156914-10X1ML	Dimethyl sulfoxide-d_6	99.96 atom % D
156914-1G	Dimethyl sulfoxide-d_6	99.96 atom % D
156914-25G	Dimethyl sulfoxide-d_6	99.96 atom % D
156914-10X0.25ML	Dimethyl sulfoxide-d_6	99.96 atom % D
417939-5ML	Dimethyl sulfoxide-d_6	99.96 atom % D, contains 0.03 % (v/v) TMS
417939-25ML	Dimethyl sulfoxide-d_6	99.96 atom % D, contains 0.03 % (v/v) TMS
417939-10X0.75ML	Dimethyl sulfoxide-d_6	99.96 atom % D, contains 0.03 % (v/v) TMS
Ethanol		
489336-5G	Ethanol-1,1,2,2,2-d_5	99.5 atom % D
329347-1G	Ethanol-2,2,2-d_3	99 atom % D
186414-1G	Ethanol-d_6	anhydrous, ≥99.5 atom % D
186414-5G	Ethanol-d_6	anhydrous, ≥99.5 atom % D
151904-100G	Ethanol-OD	≥99.5 atom % D
151904-25G	Ethanol-OD	≥99.5 atom % D
452556-100ML	Ethanol-OD	99 atom % D
452556-25ML	Ethanol-OD	99 atom % D
Ether-d_{10}		
613479-1G	Ether-d_{10}	99 atom % D
Ethyl acetate-d_8		
522899-1G	Ethyl acetate-d_8	99.5 atom % D, 99% (CP)
522899-500MG	Ethyl acetate-d_8	99.5 atom % D, 99% (CP)
522899-5G	Ethyl acetate-d_8	99.5 atom % D, 99% (CP)
Ethylbenzene-d_{10}		
437344-10ML	Ethylbenzene-d_{10}	99 atom % D
437344-1ML	Ethylbenzene-d_{10}	99 atom % D
437344-5ML	Ethylbenzene-d_{10}	99 atom % D
Ethylene glycol		
343811-1G	Ethylene glycol-$(OD)_2$	98 atom % D, 99% (CP)
530549-5G	Ethylene glycol-d_6	98 atom % D
347442-1G	Ethylene-d_4 glycol	98 atom % D
Fluorobenzene-d_5		
175803-1G	Fluorobenzene-d_5	98 atom % D
175803-5G	Fluorobenzene-d_5	98 atom % D
Heptane-d_{16}		
303011-1G	Heptane-d_{16}	99 atom % D

Cat. No.	Product Description	Isotopic Purity and Internal Standards
Hexafluoroacetone deuterate		
534773-1G	Hexafluoroacetone deuterate	≥99.5 atom % D
1,1,1,3,3,3-Hexafluoro-2-propanol-OD		
411302-25G	1,1,1,3,3,3-Hexafluoro-2-propanol-OD	98 atom % D
411302-5G	1,1,1,3,3,3-Hexafluoro-2-propanol-OD	98 atom % D
Hexane-d_{14}		
303003-5G	Hexane-d_{14}	99 atom % D
303003-1G	Hexane-d_{14}	99 atom % D
Imidazole-d_4		
437298-1G	Imidazole-d_4	98 atom % D
2-Iodopropane-d_7		
377023-5G	$_2$-Iodopropane-d_7	98 atom % D, contains copper as stabilizer
377023-1G	$_2$-Iodopropane-d_7	98 atom % D, contains copper as stabilizer
Methanol		
343854-10G	Methanol-d_3	99.8 atom % D
343854-5G	Methanol-d_3	99.8 atom % D
343854-1G	Methanol-d_3	99.8 atom % D
422878-10ML	Methanol-d_4	99 atom % D
422878-50ML	Methanol-d_4	99 atom % D
151947-10G-GL	Methanol-d_4	≥99.8 atom % D
151947-1G	Methanol-d_4	≥99.8 atom % D
151947-25G	Methanol-d_4	≥99.8 atom % D
151947-100G	Methanol-d_4	≥99.8 atom % D
151947-5G	Methanol-d_4	≥99.8 atom % D
151947-10G-SB	Methanol-d_4	≥99.8 atom % D
151947-50G-GL	Methanol-d_4	≥99.8 atom % D
151947-50G-SB	Methanol-d_4	≥99.8 atom % D
151947-10G-AMP	Methanol-d_4	≥99.8 atom % D
151947-1KG	Methanol-d_4	≥99.8 atom % D
441384-10X0.6ML	Methanol-d_4	≥99.8 atom % D
441384-10X1ML	Methanol-d_4	≥99.8 atom % D
441384-10X0.75ML	Methanol-d_4	≥99.8 atom % D
441384-10X0.5ML	Methanol-d_4	≥99.8 atom % D
569534-50G	Methanol-d_4	anhydrous, ≥99.8 atom % D
569534-10X1ML	Methanol-d_4	anhydrous, ≥99.8 atom % D
417653-50G	Methanol-d_4	≥99.8 atom % D, contains 1 % (v/v) TMS
417653-10G	Methanol-d_4	≥99.8 atom % D, contains 1 % (v/v) TMS
439029-10G	Methanol-d_4	≥99.8 atom % D, contains 0.1 % (v/v) TMS
439029-50G	Methanol-d_4	≥99.8 atom % D, contains 0.1 % (v/v) TMS
444758-10X0.25ML	Methanol-d_4	99.96 atom % D
444758-10X0.75ML	Methanol-d_4	99.96 atom % D
444758-1G-AMP	Methanol-d_4	99.96 atom % D
444758-10X1ML	Methanol-d_4	99.96 atom % D
444758-10X0.5ML	Methanol-d_4	99.96 atom % D

Cat. No.	Product Description	Isotopic Purity and Internal Standards
444758-10G-AMP	Methanol-d_4	99.96 atom % D
535435-10G	Methanol-d_4	≥99.96 atom % D, contains 0.03 % (v/v) TMS
611646-25G	Methanol-d_4	≥99.8 atom % D, contains 0.05 % (v/v) TMS
611646-10G	Methanol-d_4	≥99.8 atom % D, contains 0.05 % (v/v) TMS
151939-100G	Methanol-OD	99.5 atom % D
151939-25G	Methanol-OD	99.5 atom % D
550574-25G	Methanol-OD	99 atom % D
550574-100G	Methanol-OD	99 atom % D
Methylcyclohexane-d_{14}		
306053-1G	Methylcyclohexane-d_{14}	99.5 atom % D
306053-5G	Methylcyclohexane-d_{14}	99.5 atom % D
Nitrobenzene-d_5		
151955-5G	Nitrobenzene-d_5	99.5 atom % D
151955-25G	Nitrobenzene-d_5	99.5 atom % D
151955-10G	Nitrobenzene-d_5	99.5 atom % D
Nitromethane-d_3		
151963-10X1ML	Nitromethane-d_3	99 atom % D
151963-25G	Nitromethane-d_3	99 atom % D
151963-5G	Nitromethane-d_3	99 atom % D
151963-10G	Nitromethane-d_3	99 atom % D
269867-5G	Nitromethane-d_3	≥99 atom % D, contains 1 % (v/v) TMS
Octane-d_{18}		
151971-5G	Octane-d_{18}	98 atom % D
151971-1G	Octane-d_{18}	98 atom % D
Pentafluorophenol-OD		
411957-5G	Pentafluorophenol-OD	98 atom % D
Pentane-d_{12}		
490482-5G	Pentane-d_{12}	98 atom % D
2-Propanol-1,1,1,3,3,3-d_6		
392898-1G	2-Propanol-1,1,1,3,3,3-d_6	99 atom % D
2-Propanol-d_8		
175897-25G	2-Propanol-d_8	99.5 atom % D
175897-5G	2-Propanol-d_8	99.5 atom % D
Pyridine-d_5		
532975-25G	Pyridine-d_5	≥99.5 atom % D
532975-10G	Pyridine-d_5	≥99.5 atom % D
532975-10X1ML	Pyridine-d_5	≥99.5 atom % D
532975-10X0.6ML	Pyridine-d_5	≥99.5 atom % D
532975-10X0.5ML	Pyridine-d_5	≥99.5 atom % D

Excellent chemical purity and highest isotopic enrichment

Cat. No.	Product Description	Isotopic Purity and Internal Standards
532967-5G	Pyridine-d_5	≥99.5 atom % D, contains 0.03 % (v/v) TMS
532967-10X1ML	Pyridine-d_5	≥99.5 atom % D, contains 0.03 % (v/v) TMS
532967-25G	Pyridine-d_5	≥99.5 atom % D, contains 0.03 % (v/v) TMS
532967-10X0.6ML	Pyridine-d_5	≥99.5 atom % D, contains 0.03 % (v/v) TMS
177970-10X0.75ML	Pyridine-d_5	≥99.96 atom % D
177970-10X0.5ML	Pyridine-d_5	≥99.96 atom % D
1,1,2,2-Tetrachloroethane-d_2		
358703-1G	1,1,2,2-Tetrachloroethane-d_2	≥99.5 atom % D
358703-5G	1,1,2,2-Tetrachloroethane-d_2	≥99.5 atom % D
358703-25G	1,1,2,2-Tetrachloroethane-d_2	≥99.5 atom % D
425362-5G	1,2-Dibromoethane-d_4	99 atom % D
425362-25G	1,2-Dibromoethane-d_4	99 atom % D
331511-1G	1,2-Dichlorobenzene-d_4	98 atom % D
331511-10G	1,2-Dichlorobenzene-d_4	98 atom % D
331511-5G	1,2-Dichlorobenzene-d_4	98 atom % D
396540-5G	1,2-Dichloroethane-d_4	99 atom % D
396540-1G	1,2-Dichloroethane-d_4	99 atom % D
186406-1G	1,4-Dioxane-d_8	≥99 atom % D
302996-1G	1-Butanol-d_{10}	99 atom % D
Tetrahydrofuran-d_8		
184314-5G	Tetrahydrofuran-d_8	≥99.5 atom % D
184314-1G	Tetrahydrofuran-d_8	≥99.5 atom % D
184314-10G	Tetrahydrofuran-d_8	≥99.5 atom % D
441406-10X1.0ML	Tetrahydrofuran-d_8	≥99.5 atom % D
441406-10ML	Tetrahydrofuran-d_8	≥99.5 atom % D
441406-5X.5ML	Tetrahydrofuran-d_8	≥99.5 atom % D
441406-10X.75ML	Tetrahydrofuran-d_8	≥99.5 atom % D
269891-10G	Tetrahydrofuran-d_8	≥99.5 atom % D, contains 1 % (v/v) TMS
269891-1G	Tetrahydrofuran-d_8	≥99.5 atom % D, contains 1 % (v/v) TMS
437727-1G	Tetrahydrofuran-d_8	≥99.5 atom % D, contains 0.03 % (v/v) TMS
437727-10G	Tetrahydrofuran-d_8	≥99.5 atom % D, contains 0.03 % (v/v) TMS
437727-5G	Tetrahydrofuran-d_8	≥99.5 atom % D, contains 0.03 % (v/v) TMS

Cat. No.	Product Description	Isotopic Purity and Internal Standards
Toluene-d_8		
151998-25G	Toluene-d_8	99 atom % D
151998-10G	Toluene-d_8	99 atom % D
151998-50G	Toluene-d_8	99 atom % D
233382-10X1ML	Toluene-d_8	99.96 atom % D
233382-10X0.5ML	Toluene-d_8	99.96 atom % D
233382-1G	Toluene-d_8	99.96 atom % D
269875-25G	Toluene-d_8	99 atom % D, contains 1 % (v/v) TMS
434388-10X1ML	Toluene-d_8	99.6 atom % D
434388-10X0.75ML	Toluene-d_8	99.6 atom % D
434388-5G	Toluene-d_8	99.6 atom % D
434388-10G	Toluene-d_8	99.6 atom % D
434388-25G	Toluene-d_8	99.6 atom % D
471399-5G	Toluene-d_8	99 atom % D, contains 0.03 % (v/v) TMS
471399-25G	Toluene-d_8	99 atom % D, contains 0.03 % (v/v) TMS
570710-50G	Toluene-d_8	anhydrous, 99.6 atom % D
Trifluoroacetic acid-d		
152005-10X0.5ML	Trifluoroacetic acid-d	99.5 atom % D
152005-10G	Trifluoroacetic acid-d	99.5 atom % D
152005-5G	Trifluoroacetic acid-d	99.5 atom % D
152005-10X1ML	Trifluoroacetic acid-d	99.5 atom % D
152005-25G	Trifluoroacetic acid-d	99.5 atom % D
152005-10X0.75ML	Trifluoroacetic acid-d	99.5 atom % D
2,2,2,Trifluoroethanol		
426237-25ML	2,2,2,Trifluoroethanol-OD	99 atom % D
426237-5ML	2,2,2,Trifluoroethanol-OD	99 atom % D
612197-1G	2,2,2-Trifluoroethanol-1,1-d_2	99.5 atom % D
396532-1G	2,2,2-Trifluoroethanol-d_3	≥99.5 atom % D
396532-5G	2,2,2-Trifluoroethanol-d_3	≥99.5 atom % D
m-Xylene-d_{10}		
175919-5G	m-Xylene-d_{10}	98 atom % D
o-Xylene-d_{10}		
175900-5G	o-Xylene-d_{10}	99 atom % D
p-Xylene-d_{10}		
175927-5G	p-Xylene-d_{10}	99 atom % D

TraceCERT® Certified Reference Materials for Quantitative NMR

Quantitative NMR is increasingly used in Pharmaceutical and Chemical Industry as an efficient tool to quantify organic molecules. Most commonly, proton NMR is applied. However, the implementation of qNMR in new fields of application (e.g. metabolomics, biomarker discovery, physiological pathways) brings along more complex molecules and systems, thus making the usage of ^{1}H-qNMR challenging. The use of other NMR active nuclei, namely ^{31}P or ^{19}F can be a better option in such cases. We offer a comprehensive range of more than 20 internal qNMR standards for ^{1}H, ^{31}P and ^{19}F nuclei with different chemical shifts and suitable for a variety of different solvents as described on the following pages. To access the products and to get more detailed technical information about the use of quantitative NMR standards please refer to our website **SigmaAldrich.com/qnmr** where you can also access various publications and articles including our qNMR brochure giving valuable insight and providing tips how to use quantitative NMR.

In 2009, Sigma-Aldrich Switzerland started to apply qNMR under ISO/ IEC 17025 and ISO Guide 34 accreditation to manufacture organic certified reference materials (CRMs). Using a set of internal qNMR standards we built up a considerable portfolio of CRMs for chromatography. So far, more than 200 products are available including pesticides, polyaromatic hydrocarbons (PAH), phenols, plasticizers, cosmetics, antibiotics, air monitoring substances, amino acids, organic pollutants, natural substances and fatty acids. We continuously refined and optimized our qNMR workflows, also taking into account valuable input from CRM users. In the following, we will share some details that will help you to use your NMR instrument for quantitative measurements, achieving maximum accuracy and reproducibility.

Quantification of Organic Compounds

Since most analytical techniques are compound dependent, reliable quantification of organic material is a very challenging task. For example, using HPLC with UV, DAD or fluorescence detection always requires a traceable reference of the very same compound. However, for most organic compounds, no reliable reference material is available. Therefore, the content of an organic material is usually determined by measuring all potential impurities (such as related compounds, water, residual solvents and inorganic impurities) and calculating the content by subtracting the impurity values from a total of 100%.

An alternative to this laborious method is quantitative NMR which, being a relative primary method and having the big advantage, that organic compounds of different chemical structure can be compared quantitatively.

Different referencing techniques have been tested for qNMR, internal as well as external. We usually prefer the internal reference method (**Figure 1**) although the external standard method also certainly has its advantages, e.g., easier recovery of the analyte material, which may be of importance if very expensive material is analyzed. However, with the internal standard method, much higher precision and lower uncertainties can be achieved. Once the materials have been weighed into the same vial, the ratio of analyte and reference stays the same. In contrast to the external standard method, the amount of added solvent, and hence the concentration of the solution, is not critical for the quantification calculation.

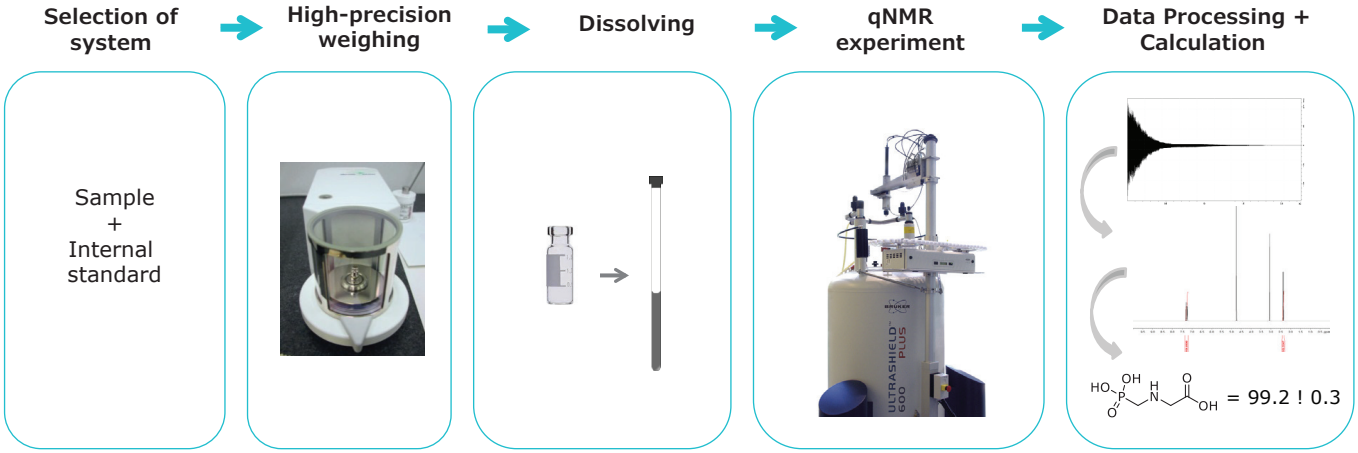

Figure 1: General procedure of a qNMR experiment using an internal standard

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Standards for ^{1}H quantitative NMR, TraceCERT®

		D_2O			$CDCl_3$			DMSO-d_6			CD_3OD			CD_3CN		
PN	Substance	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	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 7.7 7.5	3.7 4.0 3.4	150	8.0 7.6 7.5	3.3 3.7 3.0	>250	8.0 7.6 7.5	4.3 4.4 3.9	>250	8.0 7.7 7.5	4.5 2.5 2.6	80
06856	Duroquinone	-	-	-	2.0	3.3	>250	2.0	3.1	30	2.0	4.0	10	2.0	5.4	20
07038	Dimethyl terephthalate	-	-	-	8.1 4.0	3.6 1.8	160	8.1 3.9	2.9 1.1	20	8.1 4.0	4.4 2.4	4.0	8.1 3.9	4.9 2.6	20
14659	Potassium hydrogen phthalate	7.5	2.5	>250*	-	-	-	-	-	-	7.9	2.5	5.0	-	-	-
40384	1,2,4,5-Tetrachloro-3-nitro-benzene	-	-	-	7.8	10.7	>250	8.5	12.6	>250	8.1	6.4	30	8.0	9.6	10
41867	Dimethyl sulfone	3.0	2.9	>250	3.0	2.7	80	3.0	2.4	>250	3.0	3.3	40	2.9	2.6	>250
42582	Ethyl 4 (dimethyl-amino) benzoate	-	-	-	7.9 6.7 4.3 3.1 1.4	4.1 2.4 2.8 2.3 2.6	>250	7.8 6.7 4.2 3.0 1.3	2.7 1.4 1.8 1.5 2.1	>250	7.9 6.7 4.3 3.0 1.4	4.3 2.4 2.9 2.8 2.7	>250	7.9 6.7 4.3 3.0 1.3	5.6 3.7 4.1 3.6 3.6	50
50409	Thymol	-	-	-	7.1 6.8 6.6 3.2 2.3 1.3	3.8 4.5 4.8 4.3 3.1 1.9	>250	7.0 6.7 6.5 3.1 2.2 1.1	2.0 2.2 2.6 2.3 2.0 0.9	>250	7.0 6.6 6.5 3.2 2.2 1.2	3.7 4.4 5.8 4.0 2.8 1.8	>250	7.1 6.7 6.6 3.2 2.2 1.2	4.9 5.7 5.7 5.2 3.5 2.4	>250
55177	Benzyl benzoate	-	-	-	5.4 8.1	4.3 13.6	>250	5.4 8.0	2.2 8.8	>250	5.4 8.1	2.0 3.9	>250	5.4 8.1	1.0 2.4	>250
74599	1,3,5-Trimethoxy-benzene	-	-	-	6.1 3.8	4.7 2.2	>250	6.1 3.7	3.2 1.4	>250	6.1 3.8	4.8 2.7	>250	6.7 4.3	3.4 2.6	>250
74658	1,2,4,5-Tetramethyl-benzene	-	-	-	7.0 2.2	6.1 4.0	>250	6.9 2.1	4.7 2.6	10	6.9 2.2	5.9 4.3	10	6.9 2.2	7.7 5.0	50
89151	Dimethylmalonic acid	1.3	1.0	100	-	-	-	1.3	0.7	250	1.4	1.0	250	1.4	2.0	30
92816	Maleic acid	6.3	6.1	>250	-	-	-	6.3	3.0	>250	6.3	3.9	20	6.4	6.2	20
93074	Pentachlorobenzene	-	-	-	7.6	5.8	>250	8.2	13.8	15	7.9	8.2	9	7.8	12.2	15
94681	Methyl 3,5-dinitrobenzoate	-	-	-	9.3 9.2 4.1	8.0 6.1 2.6	>250	9.1 8.9 4.0	8.1 8.1 1.6	100	-	-	-	9.1 9.0 4.0	9.0 8.2 3.5	>250

Standards for ^{31}P quantitative NMR, TraceCERT®

		D_2O			$CDCl_3$			DMSO-d_6			CD_3OD			CD_3CN		
PN	Substance	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)
05498	Triphenyl phosphate	-	-	-	-17.7	2.7	>250	-17.3	1.2	>100	-17.5	3.1	>50	-17.0	4.3	>250
92214	Potassium phosphate monobasic	0.08	8.0	>250	-	-	-	-	-	-	-	-	-	-	-	-
96708	Phosphonoacetic acid	15.7	4.6	>250	-	-	-	14.9	1.5	>250	17.7	2.9	>250	-	-	-

Standards for ^{19}F quantitative NMR, TraceCERT®

		D_2O			$CDCl_3$			DMSO-d_6			CD_3OD			CD_3CN		
PN	Substance	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	s (mg/mL)	δ (ppm)	T1 (s)	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

Table 1: This table gives an overview of spectral shifts, solubility and relaxation times in different solvents of 17 ^{1}H-qNMR standards, 3 ^{31}P-qNMR standards and 3 ^{19}F-qNMR standards. They cover the entire spectral range, allowing the quantification of almost any organic molecule by qNMR. Solubility tests were done at room-temperature using commercially available NMR solvents. Tests were performed starting from 1 mg/mL up to 250 mg/mL (mg CRM/ml solvent). $_1$ relaxation times were recorded for the CRM only (c ≈ 5 to 20 mg/mL at 25 °C), but may vary in the mixture. Therefore it is recommended to check the $_1$ delay prior to the qNMR experiment. (*with DCl or NaOD).

Following some basic rules, and with a good balance, it is possible to routinely perform qNMR measurements with 0.5 - 1% measurement uncertainty. Please refer to our website to get more detailed information and tips for a successful qNMR measurement.

In order to minimize the increments by the internal reference, Sigma-Aldrich certified its TraceCERT® CRMs under optimal conditions, so that their uncertainties down to 0.1% would not dominate the overall result, when applying the CRM. Please find a list of the currently available TraceCERT® CRMs for qNMR including some key parameters like typical chemical shifts, relaxation times and solubilities in **Table 1**.

We are currently providing a series of 17 different certified reference materials (CRMs) designed for use in ^{1}H qNMR experiments and each 3 different CRMs for the use in ^{19}F or ^{31}P qNMR experiments. All products are either traceable to primary material from NIST (National Institute of Standards and Technology) or NMIJ (National Metrology Institute of Japan) and are produced under ISO/IEC 17025 and ISO 17034 (formerly ISO Guide 34) double accreditation.

Figure 2 shows the first page of an example certificate, highlighting the most important features such as traceability statement, expiration date, certified value and associated uncertainty. Since the portfolio is continuously expanding, we also recommend viewing the most current product list on **SigmaAldrich.com/qnmr**

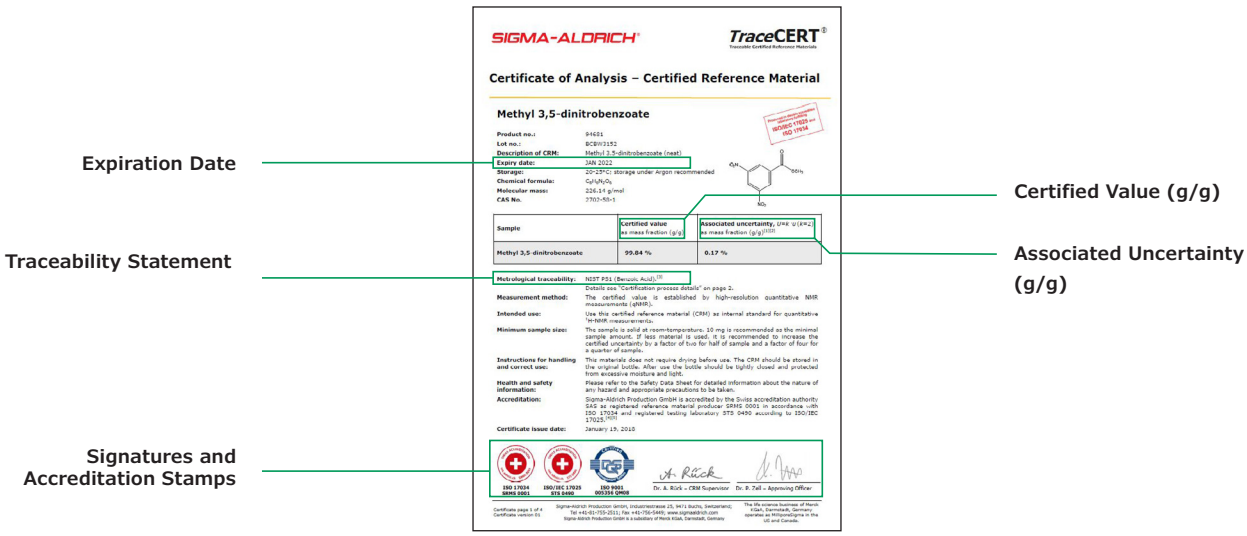

Figure 2: Example of a Certificate 94681 Methyl 3,5-dinitrobenzoate (page 1 of 4)

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Supelco® NMR Reference Standards for Calibration

We also offer a wide range of NMR reference standards needed to verify instrument performance. These standards allow the user to monitor key operational parameters such as pw90, sensitivity, resolution and line shape. We have the combined knowledge and expertise to supply the standards required to ensure proper instrumental qualification and performance verification. MilliporeSigma also provides NMR reference standards for Fluorine Sensitivity and Phosphorus Sensitivity verification and other applications. The NMR Reference Standards are available in several tube sizes from 3 mm x 8" to 10 mm x 8". NMR continues to find new and exciting applications to solve today's analytical challenges.

Cat.No.	Product Description	NMR Tube O.D. x L	Application
611778	1% Chloroform in acetone-d_6 (99.9 atom % D)	3 mm x 8 in.	^{1}H line shape
487163	1% Chloroform in acetone-d_6 (99.9 atom % D)	5 mm x 8 in.	^{1}H line shape
487759	5% Chloroform in acetone-d_6 (99.9 atom % D)	5 mm x 8 in.	^{1}H line shape
551341	5% Ethylbenzene, 2% TMS in chloroform-d (99.8 atom % D)	5 mm x 8 in.	^{1}H sensitivity
487112	0.1% Ethylbenzene, 0.01% TMS in chloroform-d (99.8 atom % D)	3 mm x 8 in.	^{1}H sensitivity
487104	0.1% Ethylbenzene, 0.01% TMS in chloroform-d (99.8 atom % D)	5 mm x 8 in.	^{1}H sensitivity
612065	0.1% Ethylbenzene, 0.01% TMS in chloroform-d (99.8 atom % D)	10 mm x 8 in.	^{1}H sensitivity
487147	1% 1,2-Dichlorobenzene in acetone-d_6 (99.9 atom % D)	5 mm x 8 in.	^{1}H resolution
551333	12% Tetramethylsilane in chloroform-d (99.8 atom % D)	5 mm x 8 in.	^{1}H reference
487139	0.1 mg/mL Gadolinium(III) chloride, 0.1% DSS, 1.0% water in deuterium oxide (99.9 atom % D)	5 mm x 8 in.	Auto test
612073	40% 1,4-Dioxane, 5 mg/mL chromium(III) acetylacetonate in benzene-d_6 (99.6 atom % D)	3 mm x 8 in.	^{13}C PW90, sensitivity
611905	40% 1,4-Dioxane, 5 mg/mL chromium(III) acetylacetonate in benzene-d_6 (99.6 atom % D)	5 mm x 8 in.	^{13}C PW90, sensitivity
551368	40% 1,4-Dioxane in benzene-d_6 (99.6 atom % D)	5 mm x 8 in.	^{13}C PW90, sensitivity
551384	90% Formamide in dimethyl sulfoxide-d_6 (99.9 atom % D)	5 mm x 8 in.	^{15}N sensitivity
487155	1% Iodomethane-13C, 0.2% chromium(III) acetylacetonate, 1% trimethyl phosphite in chloroform-d (99.8 atom % D)	3 mm x 8 in.	Indirect detection test
551406	0.05% α,α,α-Trifl uorotoluene in benzene-d_6 (99.6 atom % D)	5 mm x 8 in.	^{19}F sensitivity
611921	25% Hexamethyldisiloxane in benzene-d_6 (99.6 atom % D)	5 mm x 8 in.	^{29}Si sensitivity
551392	0.0485M Triphenyl phosphate in chloroform-d (99.8 atom % D)	5 mm x 8 in.	^{31}P sensitivity
611735	0.0485M Triphenyl phosphate in chloroform-d (99.8 atom % D)	10 mm x 8 in.	^{31}P sensitivity
612162	85% Phosphoric acid in deuterium oxide (99.9 atom % D)	5 mm x 8 in. (Coaxial)	^{31}P sensitivity

Silylated Products

Cat.No.	Product Description	NMR Tube O.D. x L	Application
87920	Tetramethylsilane, analytical standard, for NMR spectroscopy, ACS reagent	N/A	Internal Standard
T24007	Tetramethylsilane, ACS reagent, NMR grade, ≥99.9%	N/A	Internal Standard
326739	Hexamethyldisiloxane, NMR grade, ≥99.5%	N/A	Internal Standard
269913	3-(Trimethylsilyl)propionic-2,2,3,3-d_4 acid sodium salt, 98 atom % D	N/A	Internal Standard

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NMR Chemical Shifts of Common Synthetic Trace Impurities

This table is to support you in identifying and separating NMR signals of impurities that might originate from residual solvents or from your reaction apparatus. Here we present the NMR shifts of the most commonly used solvents and impurities in organic synthesis - measured in the 7 most frequently used deuterated solvents. With the help of this table you will be able to identify the signals of the impurities and separate them from the signals of your product. Please note that the values given in the tables are temperature- and partly concentration-dependent and therefore represent average values only. The ^{1}H-NMR data were obtained using a 300 MHz spectrometer, the ^{13}C-NMR data using 75 MHz.

^{1}H NMR Data

	proton	mult	$CDCl_3$	$(CD_3)2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
solvent residual peak			7.26	2.05	2.50	7.16	1.94	3.31	4.79
H_2O		s	1.56	2.84	3.33	0.40	2.13	4.87	
acetic acid	CH_3	s	2.10	1.96	1.91	1.55	1.96	1.99	2.08
acetone	CH_3	s	2.17	2.09	2.09	1.55	2.08	2.15	2.22
acetonitrile	CH_3	s	2.10	2.05	2.07	1.55	1.96	2.03	2.06
benzene	CH	s	7.36	7.36	7.37	7.15	7.37	7.33	
tert-butyl alcohol	CH_3	s	1.28	1.18	1.11	1.05	1.16	1.40	1.24
	OH	s			4.19	1.55	2.18		
tert-butyl methyl ether	CCH_3	s	1.19	1.13	1.11	1.07	1.14	1.15	1.21
	OCH_3	s	3.22	3.13	3.08	3.04	3.13	3.20	3.22
BHT[a]	ArH	s	6.98	6.96	6.87	7.05	6.97	6.92	
	OH	s	5.01		6.65	4.79	5.20		
	$ArCH_3$	s	2.27	2.22	2.18	2.24	2.22	2.21	
	$ArC(CH_3)_3$	s	1.43	1.41	1.36	1.38	1.39	1.40	
chloroform	CH	s	7.26	8.02	8.32	6.15	7.58	7.90	
cyclohexane	CH_2	s	1.43	1.43	1.40	1.40	1.44	1.45	
1,2-dichloroethane	CH_2	s	3.73	3.87	3.90	2.90	3.81	3.78	
dichloromethane	CH_2	s	5.30	5.63	5.76	4.27	5.44	5.49	
diethyl ether	CH_3	t,7	1.21	1.11	1.09	1.11	1.12	1.18	1.17
	CH_2	q,7	3.48	3.41	3.38	3.26	3.42	3.49	3.56
diglyme	CH_2	m	3.65	3.56	3.51	3.46	3.53	3.61	3.67
	CH_2	m	3.57	3.47	3.38	3.34	3.45	3.58	3.61
	OCH_3	s	3.39	3.28	3.24	3.11	3.29	3.35	3.37
1,2-dimethox yethane	CH_3	s	3.40	3.28	3.24	3.12	3.28	3.35	3.37
	CH_2	s	3.55	3.46	3.43	3.33	3.45	3.52	3.60
dimethylacetamide	CH_3CO	s	2.09	1.97	1.96	1.6	1.97	2.07	2.08
	NCH_3	s	3.02	3.00	2.94	2.57	2.96	3.31	3.06
	NCH_3	s	2.94	2.83	2.78	2.05	2.83	2.92	2.90
dimethylformamide	CH	s	8.02	7.96	7.95	7.63	7.92	7.97	7.92
	CH_3	s	2.96	2.94	2.89	2.36	2.89	2.99	3.01
	CH_3	s	2.88	2.78	2.73	1.86	2.77	2.86	2.85
dimethyl sulfoxide	CH_3	s	2.62	2.52	2.54	1.68	2.50	2.65	2.71
dioxane	CH_2	s	3.71	3.59	3.57	3.35	3.60	3.66	3.75
ethanol	CH_3	t,7	1.25	1.12	1.06	0.96	1.12	1.19	1.17
	CH_2	q,7	3.72	3.57	3.44	3.34	3.54	3.60	3.65
	OH	s	1.32	3.39	4.63		2.47		
ethyl acetate	CH_3CO	s	2.05	1.97	1.99	1.65	1.97	2.01	2.07
	CH_2CH_3	q,7	4.12	4.05	4.03	3.89	4.06	4.09	4.14
	CH_2CH_3	t,7	1.26	1.20	1.17	0.92	1.20	1.24	1.24
ethyl methyl ketone	CH_3CO	s	2.14	2.07	2.07	1.58	2.06	2.12	2.19
	CH_2CH_3	q,7	2.46	2.45	2.43	1.81	2.43	2.50	3.18
	CH_2CH_3	t,7	1.06	0.96	0.91	0.85	0.96	1.01	1.26
ethylene glycol	CH	s	3.76	3.28	3.34	3.41	3.51	3.59	3.65
"grease"	CH_3	m	0.86	0.87		0.92	0.86	0.88	
	CH_2	br s	1.26	1.29		1.36	1.27	1.29	
n-hexane	CH_3	t	0.88	0.88	0.86	0.89	0.89	0.90	
	CH_2	m	1.26	1.28	1.25	1.24	1.28		
HMPA	CH_3	d, 9.5	2.65	2.59	2.53	2.40	2.57	2.64	2.61
methanol	CH_3	s	3.49	3.31	3.16	3.07	3.28	3.34	3.34
	OH	s	1.09	3.12	4.01		2.16		
nitromethane	CH_3	s	4.33	4.43	4.42	2.94	4.31	4.34	14.40
n-pentane	CH_3	t, 7	0.88	0.88	0.86	0.87	0.89	0.90	
	CH_2	m	1.27	1.27	1.27	1.23	1.29	1.29	
2-propanol	CH_3	d, 6	1.22	1.10	1.04	0.95	1.09	1.50	1.17
	CH	sep, 6	4.04	3.90	3.78	3.67	3.87	3.92	4.02
pyridine	CH(2)	m	8.62	8.58	8.58	8.53	8.57	8.53	8.52
	CH(3)	m	7.29	7.35	7.39	6.66	7.33	7.44	7.45
	CH(4)	m	7.68	7.76	7.79	6.98	7.73	7.85	7.87
Silicone grease	CH_3	s	0.07	0.13		0.29	0.08	0.10	
tetrahydrofuran	CH_2	m	1.85	1.79	1.76	1.40	1.8	1.87	1.88
	CH_2O	m	3.76	3.63	3.60	3.57	3.64	3.71	3.74
toluene	CH_3	s	2.36	2.32	2.30	2.11	2.33	2.32	
	CH*(o/p)*	m	7.17	7.1-7.2	7.18	7.02	7.1-7.3	7.16	
	CH*(m)*	m	7.25	7.1-7.2	7.25	7.13	7.1-7.3		
triethylamine	CH_3	t, 7	1.03	0.96	0.93	0.96	0.96	1.05	0.99
	CH_2	q,7	2.53	2.45	2.43	2.40	2.45	2.58	2.57

[a] 2,6-Dimethyl-4-tert-butylphenol, [b] Hexamethylphosphoramide
Source: H.E. Gottlieb, V. Kotlyar, A. Nudelman, J.Org.Chem. **1997**, 62, 7512.

^{13}C NMR Data

		$CDCl_3$	$(CD_3)2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
solvent signals		77.16±0.06	29.84±0.01 206.26±0.13	39.52±0.06	128.06±0.02	1.32 ±0 .021 118.26±0.02	49.00±0.01	
acetic ocid	CO	175.99	172.31	171.93	175.82	173.21	175.11	177.21
	CH_3	20.81	20.51	20.95	20.37	20.73	20.56	21.03
acetone	CO	207.07	205.87	206.31	204.43	207.43	209.67	215.94
	CH_3	30.92	30.60	30.56	30.14	30.91	30.67	30.89
acetonitrile	CN	116.43	117.60	117.91	116.02	118.26	118.06	119.68
	CH_3	1.89	1.12	1.03	0.20	1.79	0.85	1.47
benzene	CH	128.37	129.15	128.3	128.62	129.32	129.34	
tert-butyl alcohol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH_3	31.25	30.72	30.38	30.47	30.68	30.91	30.29
tert-butyl methyl ether	CCH_3	49.45	49.35	48.70	49.19	49.52	49.66	49.37
	C	72.87	72.81	72.04	72.4	73.17	74.32	75.62
	CCH_3	26.99	27.24	26.79	27.09	27.28	27.22	26.60
BHT	C(1)	151.55	152.51	151.47	152.05	152.42	152.85	
	C(2)	135.87	138.19	139.12	136.08	138.13	139.09	
	CH(3)	125.55	129.05	127.97	128.52	129.61	129.49	
	C(4)	128.27	126.03	124.85	125.83	126.38	126.11	
	CH_3Ar	21.20	21.31	20.97	21.4	21.23	21.38	
	CH_3C	30.33	31.61	31.25	31.34	31.50	31.15	
	C	34.25	35.00	34.33	34.35	35.05	35.36	
chloroform	CH	77.36	79.19	79.16	77.79	79.17	79.44	
cyclohexane	CH_2	26.94	27.51	26.33	27.23	27.63	27.96	
1,2-dimchloroethane	CH_2	43.50	45.25	45.02	43.59	45.54	45.11	
dimchloromethane	CH_2	53.52	54.95	54.84	53.46	55.32	54.78	
diethyl ether	CH_3	15.20	15.78	15.12	15.46	15.63	15.46	14.77
	CH_2	65.91	66.12	62.05	65.94	66.32	66.88	66.42
diglyme	CH_3	59.01	58.77	57.98	58.66	58.9	59.06	58.67
	CH_2	70.51	71.03	69.54	70.87	70.99	71.33	70.05
	CH_2	71.90	72.63	71.25	72.35	72.63	72.92	71.63
1,2-dimethoxyethane	CH_3	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH_2	71.84	72.47	17.07	72.21	72.47	72.72	71.49
dimethylacetamide	CH_3	21.53	21.51	21.29	21.16	21.76	21.32	21.09
	CO	171.07	170.61	169.54	169.95	171.31	173.32	174.57
	NCH_3	35.28	34.89	37.38	34.67	35.17	35.5	35.03
	NCH_3	38.13	37.92	34.42	37.03	38.26	38.43	38.76
dimethylformamide	CH	162.62	162.79	162.29	162.13	163.31	164.73	165.53
	CH_3	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH_3	31.45	31.03	30.73	30.72	31.32	31.61	32.03
dimethyl sulfoxide	CH_3	40.76	41.23	40.45	40.03	41.31	40.45	39.39
dioxane	CH_2	67.14	67.6	66.36	67.16	67.72	68.11	67.19
ethanol	CH_3	18.41	18.89	18.51	18.72	18.8	18.40	17.47
	CH_2	58.28	57.72	56.07	57.86	57.96	58.26	58.05
ethyl acetate	CH_3CO	21.04	20.83	20.68	20.56	21.16	20.88	21.15
	CO	171.36	170.96	170.31	170.44	171.68	172.89	175.26
	CH_2	60.49	60.56	59.74	60.21	60.98	61.5	62.32
	CH_3	14.19	14.50	14.40	14.19	14.54	14.49	13.92
ethyl methyl ketone	CH_3CO	29.49	29.30	29.26	28.56	29.60	29.39	29.49
	CO	209.56	208.30	208.72	206.55	209.88	212.16	218.43
	CH_2CH_3	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH_2CH_3	7.86	8.03	7.61	7.91	8.14	8.09	7.87
ethylene glycol	CH_2	63.79	64.26	62.76	64.34	64.22	64.30	63.17
"grease"	CH_2	29.76	30.73	29.20	30.21	30.86	31.29	
n-hexane	CH_3	14.14	14.34	13.88	14.32	14.43	14.45	
	$CH_2(2)$	22.70	23.28	22.05	23.04	23.40	23.68	
	$CH_2(3)$	31.64	32.30	30.95	31.96	32.36	32.73	
HMPA	CH_3	36.87	37.04	36.42	36.88	37.10	37.00	36.46
methanol	CH_3	50.41	49.77	48.59	49.97	49.90	49.86	49.50
nitromethane	CH_3	62.50	63.21	63.28	61.16	63.66	63.08	63.22
n-pentane	CH_3	14.08	14.29	13.28	14.25	14.37	14.39	
	$CH_2(2)$	22.38	22.98	21.70	22.72	23.08	23.38	
	$CH_2(3)$	34.16	34.83	33.48	34.45	34.89	35.30	
2-propanol	CH_3	25.14	25.67	25.43	25.18	25.55	25.27	24.83
	CH	64.50	63.85	64.92	64.23	64.30	64.71	64.88
pyridine	CH(2)	149.90	150.67	149.58	150.27	150.76	150.07	149.18
	CH(3)	123.75	124.57	123.84	123.58	127.76	125.53	125.12
	CH(4)	135.96	136.56	136.05	135.28	136.89	138.35	138.27
silicone grease	CH_3	1.04	1.40		1.38		2.10	
tetrahydrofuran	CH2	25.62	26.15	25.14	25.72	26.27	26.48	25.67
	CH_20	67.97	68.07	67.03	67.80	68.33	68.83	68.68
toluene	CH_3	21 .46	21.46	20.99	21.10	21.50	21.5	
	C(i)	137 .89	138.48	137.35	137.91	138.90	13 8.85	
	CH(o)	129 .07	129.76	128.88	129.33	129.94	1 29.91	
	CH(m)	12 8.26	129.03	128.18	128.56	129.23	129.2	
	CH(p)	12 5.33	126.12	125.29	125.68	126.28	126.29	
triethylamine	CH_3	11.61	12.49	11.74	12.35	12.38	11.09	9.07
	CH_2	46.25	47.07	45.74	46.77	47.10	46.96	47.19

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