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# High Quality NMR Solvents

High quality solvents are essential for the rigorous demands of NMR research and analysis. At Merck, 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
<b>Acetic acid-d</b>		
151777-50G	Acetic acid-d	99 atom % D
151777-250G	Acetic acid-d	99 atom % D
151785-50G	Acetic acid-d <sub>4</sub>	≥99.5 atom % D
151785-10X1ML	Acetic acid-d <sub>4</sub>	≥99.5 atom % D
151785-25G	Acetic acid-d <sub>4</sub>	≥99.5 atom % D
151785-10G	Acetic acid-d <sub>4</sub>	≥99.5 atom % D
151785-5G	Acetic acid-d <sub>4</sub>	≥99.5 atom % D
416886-25G	Acetic acid-d <sub>4</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
233315-5G	Acetic acid-d <sub>4</sub>	≥99.9 atom % D
233315-10X0.5ML	Acetic acid-d <sub>4</sub>	≥99.9 atom % D
<b>Acetone-d<sub>6</sub></b>		
151793-100G	Acetone-d <sub>6</sub>	99.9 atom % D
151793-25G	Acetone-d <sub>6</sub>	99.9 atom % D
151793-10X1ML	Acetone-d <sub>6</sub>	99.9 atom % D
151793-10X0.75ML	Acetone-d <sub>6</sub>	99.9 atom % D
151793-10G	Acetone-d <sub>6</sub>	99.9 atom % D
151793-50G	Acetone-d <sub>6</sub>	99.9 atom % D
444863-1L	Acetone-d <sub>6</sub>	99.9 atom % D
444863-10ML-AMP	Acetone-d <sub>6</sub>	99.9 atom % D
444863-25ML	Acetone-d <sub>6</sub>	99.9 atom % D
444863-100ML	Acetone-d <sub>6</sub>	99.9 atom % D
444863-10ML-GL	Acetone-d <sub>6</sub>	99.9 atom % D
444863-10X0.6ML	Acetone-d <sub>6</sub>	99.9 atom % D
444863-10X0.5ML	Acetone-d <sub>6</sub>	99.9 atom % D
444863-50ML	Acetone-d <sub>6</sub>	99.9 atom % D
434531-10X1ML	Acetone-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
434531-25G	Acetone-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
434531-10G-GL	Acetone-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
434531-50G	Acetone-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
454133-50G	Acetone-d <sub>6</sub>	99.9 atom % D, contains 1 % (v/v) TMS

Cat. No.	Product Description	Isotopic Purity and Internal Standards
454133-25G	Acetone-d <sub>6</sub>	99.9 atom % D, contains 1 % (v/v) TMS
175862-10X0.75ML	Acetone-d <sub>6</sub>	99.96 atom % D
175862-5G	Acetone-d <sub>6</sub>	99.96 atom % D
175862-10X0.5ML	Acetone-d <sub>6</sub>	99.96 atom % D
<b>Acetonitrile-d<sub>3</sub></b>		
151807-50G	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
151807-5G	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
151807-10G-GL	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
151807-10X1ML	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
151807-10X0.6ML	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
151807-25G	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
151807-10G-AMP	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
151807-10X0.75ML	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
151807-100G	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D
699543-10G	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D, Special HOH
699543-50G	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D, Special HOH
569550-10X1ML	Acetonitrile-d <sub>3</sub>	≥99.8 atom % D, anhydrous
366544-5G	Acetonitrile-d <sub>3</sub>	99.8 atom % D, contains 0.03 % (v/v) TMS
366544-10X0.6ML	Acetonitrile-d <sub>3</sub>	99.8 atom % D, contains 0.03 % (v/v) TMS
366544-50G	Acetonitrile-d <sub>3</sub>	99.8 atom % D, contains 0.03 % (v/v) TMS
366544-25G	Acetonitrile-d <sub>3</sub>	99.8 atom % D, contains 0.03 % (v/v) TMS
233331-50G	Acetonitrile-d <sub>3</sub>	99.8 atom % D, contains 1 % (v/v) TMS
233323-10X0.5ML	Acetonitrile-d <sub>3</sub>	99.96 atom % D
233323-10X0.75ML	Acetonitrile-d <sub>3</sub>	99.96 atom % D
233323-5G	Acetonitrile-d <sub>3</sub>	99.96 atom % D
233323-25G	Acetonitrile-d <sub>3</sub>	99.96 atom % D
<b>Benzene-d<sub>6</sub></b>		
175978-10G	Benzene-d <sub>6</sub>	99 atom % D
175978-50G	Benzene-d <sub>6</sub>	99 atom % D
151815-10G-AMP	Benzene-d <sub>6</sub>	99.6 atom % D
151815-10G-GL	Benzene-d <sub>6</sub>	99.6 atom % D



Cat. No.	Product Description	Isotopic Purity and Internal Standards
151815-100G	Benzene-d <sub>6</sub>	99.6 atom % D
151815-10X1ML	Benzene-d <sub>6</sub>	99.6 atom % D
151815-10X0.75ML	Benzene-d <sub>6</sub>	99.6 atom % D
151815-25G	Benzene-d <sub>6</sub>	99.6 atom % D
151815-50G	Benzene-d <sub>6</sub>	99.6 atom % D
570680-50G	Benzene-d <sub>6</sub>	anhydrous, ≥99.6 atom % D
364940-50G	Benzene-d <sub>6</sub>	99.6 atom % D, contains 0.03 % (v/v) TMS
364940-10G	Benzene-d <sub>6</sub>	99.6 atom % D, contains 0.03 % (v/v) TMS
364940-25G	Benzene-d <sub>6</sub>	99.6 atom % D, contains 0.03 % (v/v) TMS
561509-10X.75ML	Benzene-d <sub>6</sub>	99.96 atom % D, contains 0.03 % (v/v) TMS
175870-25G	Benzene-d <sub>6</sub>	99.96 atom % D
175870-10X0.5ML	Benzene-d <sub>6</sub>	99.96 atom % D
175870-10X1ML	Benzene-d <sub>6</sub>	99.96 atom % D
<b>Bromobenzene-d<sub>5</sub></b>		
175730-5G	Bromobenzene-d <sub>5</sub>	99.5 atom % D
175730-25G	Bromobenzene-d <sub>5</sub>	99.5 atom % D
<b>tert-Butanol-d<sub>10</sub></b>		
175889-1G	tert-Butanol-d <sub>10</sub>	99 atom % D
175889-5G	tert-Butanol-d <sub>10</sub>	99 atom % D
<b>tert-Butyl methyl-d<sub>3</sub> ether</b>		
434132-1G	tert-Butyl methyl-d <sub>3</sub> ether	99 atom % D
<b>Chlorobenzene-d<sub>5</sub></b>		
176605-5G	Chlorobenzene-d <sub>5</sub>	99 atom % D
176605-1G	Chlorobenzene-d <sub>5</sub>	99 atom % D
<b>Chloroform-d</b>		
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
<b>Cyclohexane-d<sub>12</sub></b>		
151866-10X1ML	Cyclohexane-d <sub>12</sub>	≥99.6 atom % D
151866-5G	Cyclohexane-d <sub>12</sub>	≥99.6 atom % D
151866-10G	Cyclohexane-d <sub>12</sub>	≥99.6 atom % D
151866-1G	Cyclohexane-d <sub>12</sub>	≥99.6 atom % D
<b>Decahydronaphthalene-d<sub>18</sub></b>		
217131-1G	Decahydronaphthalene-d <sub>18</sub>	98 atom % D
<b>Deuterium oxide</b>		
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 <sub>4</sub> acid, sodium salt
293040-25G	Deuterium oxide	99.9 atom % D, contains 0.75 wt. % 3-(trimethylsilyl) propionic-2,2,3,3-d <sub>4</sub> 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 <sub>4</sub> acid, sodium salt
450510-100ML	Deuterium oxide	99.9 atom % D, contains 0.05 wt. % 3-(trimethylsilyl) propionic-2,2,3,3-d <sub>4</sub> acid, sodium salt
450510-25ML	Deuterium oxide	99.9 atom % D, contains 0.05 wt. % 3-(trimethylsilyl) propionic-2,2,3,3-d <sub>4</sub> 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
<b>Dibromomethane-d<sub>2</sub></b>		
259020-5G	Dibromomethane-d <sub>2</sub>	99 atom % D, contains copper as stabilizer
177865-10X1ML	Dichloromethane-d <sub>2</sub>	99.5 atom % D
177865-25G	Dichloromethane-d <sub>2</sub>	99.5 atom % D
177865-10G	Dichloromethane-d <sub>2</sub>	99.5 atom % D
296163-10G	Dichloromethane-d <sub>2</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS

Cat. No.	Product Description	Isotopic Purity and Internal Standards
296163-1G	Dichloromethane-d <sub>2</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
296163-25G	Dichloromethane-d <sub>2</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
444324-25G	Dichloromethane-d <sub>2</sub>	99.9 atom % D
444324-10X0.75ML	Dichloromethane-d <sub>2</sub>	99.9 atom % D
444324-10X1ML	Dichloromethane-d <sub>2</sub>	99.9 atom % D
444324-10X0.6ML	Dichloromethane-d <sub>2</sub>	99.9 atom % D
444324-10G	Dichloromethane-d <sub>2</sub>	99.9 atom % D
444324-5G	Dichloromethane-d <sub>2</sub>	99.9 atom % D
530506-25G	Dichloromethane-d <sub>2</sub>	99.9 atom % D, contains 0.1 % (v/v) TMS
530506-1G	Dichloromethane-d <sub>2</sub>	99.9 atom % D, contains 0.1 % (v/v) TMS
233366-10X0.5ML	Dichloromethane-d <sub>2</sub>	99.96 atom % D
233366-5G	Dichloromethane-d <sub>2</sub>	99.96 atom % D
<b>N,N-Dimethylacetamide-d<sub>9</sub></b>		
522414-5G	N,N-Dimethylacetamide-d <sub>9</sub>	99 atom % D
522414-1G	N,N-Dimethylacetamide-d <sub>9</sub>	99 atom % D
<b>N,N-Dimethylformamide-d<sub>7</sub></b>		
189979-5X0.5ML	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D
189979-1G	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D
189979-10G	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D
189979-5G	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D
189979-10X0.75ML	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D
189979-10X1ML	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D
269905-1G	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D, contains 1 % (v/v) TMS
269905-10G	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D, contains 1 % (v/v) TMS
700428-10G	N,N-Dimethylformamide-d <sub>7</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
700428-1G	N,N-Dimethylformamide-d <sub>7</sub>	≥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
<b>Dimethyl sulfide-d<sub>6</sub></b>		
416452-1G	Dimethyl sulfide-d <sub>6</sub>	99 atom % D
175943-100G	Dimethyl sulfoxide-d <sub>6</sub>	99.5 atom % D
175943-50G	Dimethyl sulfoxide-d <sub>6</sub>	99.5 atom % D
175943-250G	Dimethyl sulfoxide-d <sub>6</sub>	99.5 atom % D
175943-10G	Dimethyl sulfoxide-d <sub>6</sub>	99.5 atom % D
151874-25G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-10G-GL	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-50G-SB	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-10X0.75ML	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-10G-AMP	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-100G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-5G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-40KG	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-600G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-50G-GL	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-10X0.6ML	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-10G-SB	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
151874-10X1ML	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D
716731-50ML	Dimethyl sulfoxide-d <sub>6</sub>	≥99.9 atom % D, "Special HOH"
716731-10ML	Dimethyl sulfoxide-d <sub>6</sub>	≥99.9 atom % D, "Special HOH"
716731-10X0.75ML	Dimethyl sulfoxide-d <sub>6</sub>	≥99.9 atom % D, "Special HOH"
570672-10X1ML	Dimethyl sulfoxide-d <sub>6</sub>	anhydrous, 99.9 atom % D
570672-50G	Dimethyl sulfoxide-d <sub>6</sub>	anhydrous, 99.9 atom % D
296147-10X1ML	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-10X0.75ML	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-10X0.5ML	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-10X0.6ML	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-10G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-50G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
296147-25G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 0.03 % (v/v) TMS
185965-50G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 1 % (v/v) TMS
185965-25G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 1 % (v/v) TMS

Cat. No.	Product Description	Isotopic Purity and Internal Standards
185965-10G	Dimethyl sulfoxide-d <sub>6</sub>	99.9 atom % D, contains 1 % (v/v) TMS
156914-10X0.75ML	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D
156914-5G	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D
156914-10X0.5ML	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D
156914-10X1ML	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D
156914-1G	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D
156914-25G	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D
156914-10X0.25ML	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D
417939-5ML	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D, contains 0.03 % (v/v) TMS
417939-25ML	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D, contains 0.03 % (v/v) TMS
417939-10X0.75ML	Dimethyl sulfoxide-d <sub>6</sub>	99.96 atom % D, contains 0.03 % (v/v) TMS
<b>Ethanol</b>		
489336-5G	Ethanol-1,1,2,2,2-d <sub>5</sub>	99.5 atom % D
329347-1G	Ethanol-2,2,2-d <sub>3</sub>	99 atom % D
186414-1G	Ethanol-d <sub>6</sub>	anhydrous, ≥99.5 atom % D
186414-5G	Ethanol-d <sub>6</sub>	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
<b>Ether-d<sub>10</sub></b>		
613479-1G	Ether-d <sub>10</sub>	99 atom % D
<b>Ethyl acetate-d<sub>8</sub></b>		
522899-1G	Ethyl acetate-d <sub>8</sub>	99.5 atom % D, 99% (CP)
522899-500MG	Ethyl acetate-d <sub>8</sub>	99.5 atom % D, 99% (CP)
522899-5G	Ethyl acetate-d <sub>8</sub>	99.5 atom % D, 99% (CP)
<b>Ethylbenzene-d<sub>10</sub></b>		
437344-10ML	Ethylbenzene-d <sub>10</sub>	99 atom % D
437344-1ML	Ethylbenzene-d <sub>10</sub>	99 atom % D
437344-5ML	Ethylbenzene-d <sub>10</sub>	99 atom % D
<b>Ethylene glycol</b>		
343811-1G	Ethylene glycol-(OD) <sub>2</sub>	98 atom % D, 99% (CP)
530549-5G	Ethylene glycol-d <sub>6</sub>	98 atom % D
347442-1G	Ethylene-d <sub>4</sub> glycol	98 atom % D
<b>Fluorobenzene-d<sub>5</sub></b>		
175803-1G	Fluorobenzene-d <sub>5</sub>	98 atom % D
175803-5G	Fluorobenzene-d <sub>5</sub>	98 atom % D
<b>Heptane-d<sub>16</sub></b>		
303011-1G	Heptane-d <sub>16</sub>	99 atom % D

Cat. No.	Product Description	Isotopic Purity and Internal Standards
<b>Hexafluoroacetone deuterate</b>		
534773-1G	Hexafluoroacetone deuterate	≥99.5 atom % D
<b>1,1,1,3,3,3-Hexafluoro-2-propanol-OD</b>		
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
<b>Hexane-d<sub>14</sub></b>		
303003-5G	Hexane-d <sub>14</sub>	99 atom % D
303003-1G	Hexane-d <sub>14</sub>	99 atom % D
<b>Imidazole-d<sub>4</sub></b>		
437298-1G	Imidazole-d <sub>4</sub>	98 atom % D
<b>2-Iodopropane-d<sub>7</sub></b>		
377023-5G	<sub>2</sub> -Iodopropane-d <sub>7</sub>	98 atom % D, contains copper as stabilizer
377023-1G	<sub>2</sub> -Iodopropane-d <sub>7</sub>	98 atom % D, contains copper as stabilizer
<b>Methanol</b>		
343854-10G	Methanol-d <sub>3</sub>	99.8 atom % D
343854-5G	Methanol-d <sub>3</sub>	99.8 atom % D
343854-1G	Methanol-d <sub>3</sub>	99.8 atom % D
422878-10ML	Methanol-d <sub>4</sub>	99 atom % D
422878-50ML	Methanol-d <sub>4</sub>	99 atom % D
151947-10G-GL	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-1G	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-25G	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-100G	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-5G	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-10G-SB	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-50G-GL	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-50G-SB	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-10G-AMP	Methanol-d <sub>4</sub>	≥99.8 atom % D
151947-1KG	Methanol-d <sub>4</sub>	≥99.8 atom % D
441384-10X0.6ML	Methanol-d <sub>4</sub>	≥99.8 atom % D
441384-10X1ML	Methanol-d <sub>4</sub>	≥99.8 atom % D
441384-10X0.75ML	Methanol-d <sub>4</sub>	≥99.8 atom % D
441384-10X0.5ML	Methanol-d <sub>4</sub>	≥99.8 atom % D
569534-50G	Methanol-d <sub>4</sub>	anhydrous, ≥99.8 atom % D
569534-10X1ML	Methanol-d <sub>4</sub>	anhydrous, ≥99.8 atom % D
417653-50G	Methanol-d <sub>4</sub>	≥99.8 atom % D, contains 1 % (v/v) TMS
417653-10G	Methanol-d <sub>4</sub>	≥99.8 atom % D, contains 1 % (v/v) TMS
439029-10G	Methanol-d <sub>4</sub>	≥99.8 atom % D, contains 0.1 % (v/v) TMS
439029-50G	Methanol-d <sub>4</sub>	≥99.8 atom % D, contains 0.1 % (v/v) TMS
444758-10X0.25ML	Methanol-d <sub>4</sub>	99.96 atom % D
444758-10X0.75ML	Methanol-d <sub>4</sub>	99.96 atom % D
444758-1G-AMP	Methanol-d <sub>4</sub>	99.96 atom % D
444758-10X1ML	Methanol-d <sub>4</sub>	99.96 atom % D
444758-10X0.5ML	Methanol-d <sub>4</sub>	99.96 atom % D

Cat. No.	Product Description	Isotopic Purity and Internal Standards
444758-10G-AMP	Methanol-d <sub>4</sub>	99.96 atom % D
535435-10G	Methanol-d <sub>4</sub>	≥99.96 atom % D, contains 0.03 % (v/v) TMS
611646-25G	Methanol-d <sub>4</sub>	≥99.8 atom % D, contains 0.05 % (v/v) TMS
611646-10G	Methanol-d <sub>4</sub>	≥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
<b>Methylcyclohexane-d<sub>14</sub></b>		
306053-1G	Methylcyclohexane-d <sub>14</sub>	99.5 atom % D
306053-5G	Methylcyclohexane-d <sub>14</sub>	99.5 atom % D
<b>Nitrobenzene-d<sub>5</sub></b>		
151955-5G	Nitrobenzene-d <sub>5</sub>	99.5 atom % D
151955-25G	Nitrobenzene-d <sub>5</sub>	99.5 atom % D
151955-10G	Nitrobenzene-d <sub>5</sub>	99.5 atom % D
<b>Nitromethane-d<sub>3</sub></b>		
151963-10X1ML	Nitromethane-d <sub>3</sub>	99 atom % D
151963-25G	Nitromethane-d <sub>3</sub>	99 atom % D
151963-5G	Nitromethane-d <sub>3</sub>	99 atom % D
151963-10G	Nitromethane-d <sub>3</sub>	99 atom % D
269867-5G	Nitromethane-d <sub>3</sub>	≥99 atom % D, contains 1 % (v/v) TMS
<b>Octane-d<sub>18</sub></b>		
151971-5G	Octane-d <sub>18</sub>	98 atom % D
151971-1G	Octane-d <sub>18</sub>	98 atom % D
<b>Pentafluorophenol-OD</b>		
411957-5G	Pentafluorophenol-OD	98 atom % D
<b>Pentane-d<sub>12</sub></b>		
490482-5G	Pentane-d <sub>12</sub>	98 atom % D
<b>2-Propanol-1,1,1,3,3,3-d<sub>6</sub></b>		
392898-1G	2-Propanol-1,1,1,3,3,3-d <sub>6</sub>	99 atom % D
<b>2-Propanol-d<sub>8</sub></b>		
175897-25G	2-Propanol-d <sub>8</sub>	99.5 atom % D
175897-5G	2-Propanol-d <sub>8</sub>	99.5 atom % D
<b>Pyridine-d<sub>5</sub></b>		
532975-25G	Pyridine-d <sub>5</sub>	≥99.5 atom % D
532975-10G	Pyridine-d <sub>5</sub>	≥99.5 atom % D
532975-10X1ML	Pyridine-d <sub>5</sub>	≥99.5 atom % D
532975-10X0.6ML	Pyridine-d <sub>5</sub>	≥99.5 atom % D
532975-10X0.5ML	Pyridine-d <sub>5</sub>	≥99.5 atom % D

**Excellent chemical purity and highest isotopic enrichment**

Cat. No.	Product Description	Isotopic Purity and Internal Standards
532967-5G	Pyridine-d <sub>5</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
532967-10X1ML	Pyridine-d <sub>5</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
532967-25G	Pyridine-d <sub>5</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
532967-10X0.6ML	Pyridine-d <sub>5</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
177970-10X0.75ML	Pyridine-d <sub>5</sub>	≥99.96 atom % D
177970-10X0.5ML	Pyridine-d <sub>5</sub>	≥99.96 atom % D
<b>1,1,2,2-Tetrachloroethane-d<sub>2</sub></b>		
358703-1G	1,1,2,2-Tetrachloroethane-d <sub>2</sub>	≥99.5 atom % D
358703-5G	1,1,2,2-Tetrachloroethane-d <sub>2</sub>	≥99.5 atom % D
358703-25G	1,1,2,2-Tetrachloroethane-d <sub>2</sub>	≥99.5 atom % D
425362-5G	1,2-Dibromoethane-d <sub>4</sub>	99 atom % D
425362-25G	1,2-Dibromoethane-d <sub>4</sub>	99 atom % D
331511-1G	1,2-Dichlorobenzene-d <sub>4</sub>	98 atom % D
331511-10G	1,2-Dichlorobenzene-d <sub>4</sub>	98 atom % D
331511-5G	1,2-Dichlorobenzene-d <sub>4</sub>	98 atom % D
396540-5G	1,2-Dichloroethane-d <sub>4</sub>	99 atom % D
396540-1G	1,2-Dichloroethane-d <sub>4</sub>	99 atom % D
186406-1G	1,4-Dioxane-d <sub>8</sub>	≥99 atom % D
302996-1G	1-Butanol-d <sub>10</sub>	99 atom % D
<b>Tetrahydrofuran-d<sub>8</sub></b>		
184314-5G	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D
184314-1G	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D
184314-10G	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D
441406-10X1.0ML	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D
441406-10ML	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D
441406-5X.5ML	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D
441406-10X.75ML	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D
269891-10G	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D, contains 1 % (v/v) TMS
269891-1G	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D, contains 1 % (v/v) TMS
437727-1G	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
437727-10G	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS
437727-5G	Tetrahydrofuran-d <sub>8</sub>	≥99.5 atom % D, contains 0.03 % (v/v) TMS

Cat. No.	Product Description	Isotopic Purity and Internal Standards
<b>Toluene-d<sub>8</sub></b>		
151998-25G	Toluene-d <sub>8</sub>	99 atom % D
151998-10G	Toluene-d <sub>8</sub>	99 atom % D
151998-50G	Toluene-d <sub>8</sub>	99 atom % D
233382-10X1ML	Toluene-d <sub>8</sub>	99.96 atom % D
233382-10X0.5ML	Toluene-d <sub>8</sub>	99.96 atom % D
233382-1G	Toluene-d <sub>8</sub>	99.96 atom % D
269875-25G	Toluene-d <sub>8</sub>	99 atom % D, contains 1 % (v/v) TMS
434388-10X1ML	Toluene-d <sub>8</sub>	99.6 atom % D
434388-10X0.75ML	Toluene-d <sub>8</sub>	99.6 atom % D
434388-5G	Toluene-d <sub>8</sub>	99.6 atom % D
434388-10G	Toluene-d <sub>8</sub>	99.6 atom % D
434388-25G	Toluene-d <sub>8</sub>	99.6 atom % D
471399-5G	Toluene-d <sub>8</sub>	99 atom % D, contains 0.03 % (v/v) TMS
471399-25G	Toluene-d <sub>8</sub>	99 atom % D, contains 0.03 % (v/v) TMS
570710-50G	Toluene-d <sub>8</sub>	anhydrous, 99.6 atom % D
<b>Trifluoroacetic acid-d</b>		
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
<b>2,2,2-Trifluoroethanol</b>		
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 <sub>2</sub>	99.5 atom % D
396532-1G	2,2,2-Trifluoroethanol-d <sub>3</sub>	≥99.5 atom % D
396532-5G	2,2,2-Trifluoroethanol-d <sub>3</sub>	≥99.5 atom % D
<b>m-Xylene-d<sub>10</sub></b>		
175919-5G	m-Xylene-d <sub>10</sub>	98 atom % D
<b>o-Xylene-d<sub>10</sub></b>		
175900-5G	o-Xylene-d <sub>10</sub>	99 atom % D
<b>p-Xylene-d<sub>10</sub></b>		
175927-5G	p-Xylene-d <sub>10</sub>	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  $^1\text{H}$ -qNMR challenging. The use of other NMR active nuclei, namely  $^{31}\text{P}$  or  $^{19}\text{F}$  can be a better option in such cases. We offer a comprehensive range of more than 20 internal qNMR standards for  $^1\text{H}$ ,  $^{31}\text{P}$  and  $^{19}\text{F}$  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](http://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.

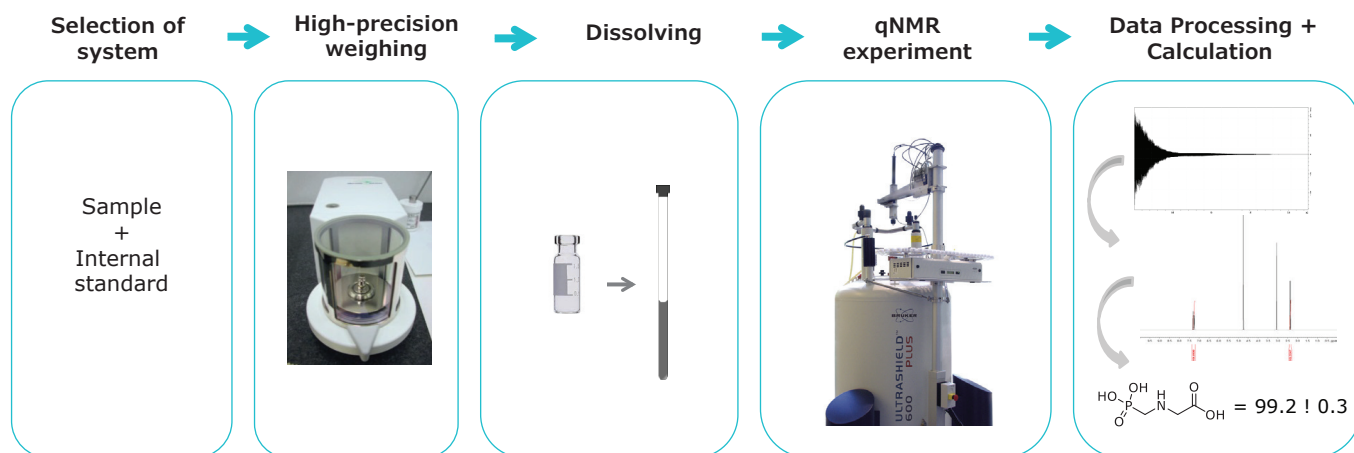


Figure 1: General procedure of a qNMR experiment using an internal standard

## Standards for <sup>1</sup>H quantitative NMR, TraceCERT®

PN	Substance	D <sub>2</sub> O			CDCl <sub>3</sub>			DMSO-d <sub>6</sub>			CD <sub>3</sub> OD			CD <sub>3</sub> CN		
		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-Trimethoxybenzene	-	-	-	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 <sup>31</sup>P quantitative NMR, TraceCERT®

PN	Substance	D <sub>2</sub> O			CDCl <sub>3</sub>			DMSO-d <sub>6</sub>			CD <sub>3</sub> OD			CD <sub>3</sub> CN		
		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 <sup>19</sup>F quantitative NMR, TraceCERT®

PN	Substance	D <sub>2</sub> O			CDCl <sub>3</sub>			DMSO-d <sub>6</sub>			CD <sub>3</sub> OD			CD <sub>3</sub> CN		
		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'-Difluorobenzophenone	-	-	-	-105.8	2.4	>250	-106.5	1.4	150	-108.1	2.8	30	-108.3	2.3	140
53396	2,4-Dichlorobenzotrifluoride	-	-	-	-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 <sup>1</sup>H-qNMR standards, 3 <sup>31</sup>P-qNMR standards and 3 <sup>19</sup>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). <sub>1</sub> 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 <sub>1</sub> 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 <sup>1</sup>H qNMR experiments and each 3 different CRMs for the use in <sup>19</sup>F or <sup>31</sup>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](http://SigmaAldrich.com/qnmr)

**Expiration Date** → 2018-02-28

**Traceability Statement** → Metrological traceability: NIST F21 (through Au), [1]

**Signatures and Accreditation Stamps** → [Accreditation logos and signatures]

**Certified Value (g/g)** → 99.84 %

**Associated Uncertainty (g/g)** → 0.17 %

**Chemical Structure:** COC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1

**Table 1: Certified Value and Associated Uncertainty**

Sample	Certified value wt mass fraction (g/g)	Associated uncertainty, 1σ wt mass fraction (g/g) <sup>[1]</sup>
Methyl 3,5-dinitrobenzoate	99.84 %	0.17 %

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

# 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. Merck 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 <sub>6</sub> (99.9 atom % D)	3 mm x 8 in.	<sup>1</sup> H line shape
487163	1% Chloroform in acetone-d <sub>6</sub> (99.9 atom % D)	5 mm x 8 in.	<sup>1</sup> H line shape
487759	5% Chloroform in acetone-d <sub>6</sub> (99.9 atom % D)	5 mm x 8 in.	<sup>1</sup> H line shape
551341	5% Ethylbenzene, 2% TMS in chloroform-d (99.8 atom % D)	5 mm x 8 in.	<sup>1</sup> H sensitivity
487112	0.1% Ethylbenzene, 0.01% TMS in chloroform-d (99.8 atom % D)	3 mm x 8 in.	<sup>1</sup> H sensitivity
487104	0.1% Ethylbenzene, 0.01% TMS in chloroform-d (99.8 atom % D)	5 mm x 8 in.	<sup>1</sup> H sensitivity
612065	0.1% Ethylbenzene, 0.01% TMS in chloroform-d (99.8 atom % D)	10 mm x 8 in.	<sup>1</sup> H sensitivity
487147	1% 1,2-Dichlorobenzene in acetone-d <sub>6</sub> (99.9 atom % D)	5 mm x 8 in.	<sup>1</sup> H resolution
551333	12% Tetramethylsilane in chloroform-d (99.8 atom % D)	5 mm x 8 in.	<sup>1</sup> 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 <sub>6</sub> (99.6 atom % D)	3 mm x 8 in.	<sup>13</sup> C PW90, sensitivity
611905	40% 1,4-Dioxane, 5 mg/mL chromium(III) acetylacetonate in benzene-d <sub>6</sub> (99.6 atom % D)	5 mm x 8 in.	<sup>13</sup> C PW90, sensitivity
551368	40% 1,4-Dioxane in benzene-d <sub>6</sub> (99.6 atom % D)	5 mm x 8 in.	<sup>13</sup> C PW90, sensitivity
551384	90% Formamide in dimethyl sulfoxide-d <sub>6</sub> (99.9 atom % D)	5 mm x 8 in.	<sup>15</sup> N sensitivity
487155	1% Iodomethane- <sup>13</sup> C, 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 <sub>6</sub> (99.6 atom % D)	5 mm x 8 in.	<sup>19</sup> F sensitivity
611921	25% Hexamethyldisiloxane in benzene-d <sub>6</sub> (99.6 atom % D)	5 mm x 8 in.	<sup>29</sup> Si sensitivity
551392	0.0485M Triphenyl phosphate in chloroform-d (99.8 atom % D)	5 mm x 8 in.	<sup>31</sup> P sensitivity
611735	0.0485M Triphenyl phosphate in chloroform-d (99.8 atom % D)	10 mm x 8 in.	<sup>31</sup> P sensitivity
612162	85% Phosphoric acid in deuterium oxide (99.9 atom % D)	5 mm x 8 in. (Coaxial)	<sup>31</sup> 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 <sub>4</sub> acid sodium salt, 98 atom % D	N/A	Internal Standard

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- Tube caps
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These tubes have the tightest specifications for concentricity and camber, ensuring a well-balanced spin rate and the highest shimming quality.

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Magnetic susceptibility matched to CDCl<sub>3</sub>, CD<sub>3</sub>OD, DMSO-d<sub>6</sub>, or D<sub>2</sub>O for best resolution.
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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  $^1\text{H}$ -NMR data were obtained using a 300 MHz spectrometer, the  $^{13}\text{C}$ -NMR data using 75 MHz.

## $^1\text{H}$ NMR Data

	proton	mult	$\text{CDCl}_3$	$(\text{CD}_3)_2\text{CO}$	$(\text{CD}_3)_2\text{SO}$	$\text{C}_6\text{D}_6$	$\text{CD}_3\text{CN}$	$\text{CD}_3\text{OD}$	$\text{D}_2\text{O}$
solvent residual peak									
$\text{H}_2\text{O}$		s	7.26	2.05	2.50	7.16	1.94	3.31	4.79
acetic acid	$\text{CH}_3$	s	2.10	1.96	1.91	1.55	1.96	1.99	2.08
acetone	$\text{CH}_3$	s	2.17	2.09	2.09	1.55	2.08	2.15	2.22
acetonitrile	$\text{CH}_3$	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	
<i>tert</i> -butyl alcohol	$\text{CH}_3$	s	1.28	1.18	1.11	1.05	1.16	1.40	1.24
	OH	s			4.19	1.55	2.18		
<i>tert</i> -butyl methyl ether	$\text{CCH}_3$	s	1.19	1.13	1.11	1.07	1.14	1.15	1.21
	$\text{OCH}_3$	s	3.22	3.13	3.08	3.04	3.13	3.20	3.22
BHT <sup>a</sup>	ArH	s	6.98	6.96	6.87	7.05	6.97	6.92	
	OH	s	5.01		6.65	4.79	5.20		
	$\text{ArCH}_3$	s	2.27	2.22	2.18	2.24	2.22	2.21	
	$\text{ArC}(\text{CH}_3)_3$	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	$\text{CH}_2$	s	1.43	1.43	1.40	1.40	1.44	1.45	
1,2-dichloroethane	$\text{CH}_2$	s	3.73	3.87	3.90	2.90	3.81	3.78	
dichloromethane	$\text{CH}_2$	s	5.30	5.63	5.76	4.27	5.44	5.49	
diethyl ether	$\text{CH}_3$	t,7	1.21	1.11	1.09	1.11	1.12	1.18	1.17
	$\text{CH}_2$	q,7	3.48	3.41	3.38	3.26	3.42	3.49	3.56
diglyme	$\text{CH}_2$	m	3.65	3.56	3.51	3.46	3.53	3.61	3.67
	$\text{CH}_2$	m	3.57	3.47	3.38	3.34	3.45	3.58	3.61
	$\text{OCH}_3$	s	3.39	3.28	3.24	3.11	3.29	3.35	3.37
1,2-dimethoxyethane	$\text{CH}_3$	s	3.40	3.28	3.24	3.12	3.28	3.35	3.37
	$\text{CH}_2$	s	3.55	3.46	3.43	3.33	3.45	3.52	3.60
dimethylacetamide	$\text{CH}_3\text{CO}$	s	2.09	1.97	1.96	1.6	1.97	2.07	2.08
	$\text{NCH}_3$	s	3.02	3.00	2.94	2.57	2.96	3.31	3.06
	$\text{NCH}_3$	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
	$\text{CH}_3$	s	2.96	2.94	2.89	2.36	2.89	2.99	3.01
	$\text{CH}_3$	s	2.88	2.78	2.73	1.86	2.77	2.86	2.85
dimethyl sulfoxide	$\text{CH}_3$	s	2.62	2.52	2.54	1.68	2.50	2.65	2.71
dioxane	$\text{CH}_2$	s	3.71	3.59	3.57	3.35	3.60	3.66	3.75
ethanol	$\text{CH}_3$	t,7	1.25	1.12	1.06	0.96	1.12	1.19	1.17
	$\text{CH}_2$	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	$\text{CH}_3\text{CO}$	s	2.05	1.97	1.99	1.65	1.97	2.01	2.07
	$\text{CH}_2\text{CH}_3$	q,7	4.12	4.05	4.03	3.89	4.06	4.09	4.14
	$\text{CH}_2\text{CH}_3$	t,7	1.26	1.20	1.17	0.92	1.20	1.24	1.24
ethyl methyl ketone	$\text{CH}_3\text{CO}$	s	2.14	2.07	2.07	1.58	2.06	2.12	2.19
	$\text{CH}_2\text{CH}_3$	q,7	2.46	2.45	2.43	1.81	2.43	2.50	3.18
	$\text{CH}_2\text{CH}_3$	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"	$\text{CH}_3$	m	0.86	0.87		0.92	0.86	0.88	
	$\text{CH}_2$	br s	1.26	1.29		1.36	1.27	1.29	
n-hexane	$\text{CH}_3$	t	0.88	0.88	0.86	0.89	0.89	0.90	
	$\text{CH}_2$	m	1.26	1.28	1.25	1.24	1.28		
HMPA	$\text{CH}_3$	d, 9.5	2.65	2.59	2.53	2.40	2.57	2.64	2.61
methanol	$\text{CH}_3$	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	$\text{CH}_3$	s	4.33	4.43	4.42	2.94	4.31	4.34	14.40
n-pentane	$\text{CH}_3$	t, 7	0.88	0.88	0.86	0.87	0.89	0.90	
	$\text{CH}_2$	m	1.27	1.27	1.27	1.23	1.29	1.29	
2-propanol	$\text{CH}_3$	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	$\text{CH}_3$	s	0.07	0.13		0.29	0.08	0.10	
tetrahydrofuran	$\text{CH}_2$	m	1.85	1.79	1.76	1.40	1.8	1.87	1.88
	$\text{CH}_2\text{O}$	m	3.76	3.63	3.60	3.57	3.64	3.71	3.74
toluene	$\text{CH}_3$	s	2.36	2.32	2.30	2.11	2.33	2.32	
	CH( <i>o/p</i> )	m	7.17	7.1-7.2	7.18	7.02	7.1-7.3	7.16	
	CH( <i>m</i> )	m	7.25	7.1-7.2	7.25	7.13	7.1-7.3		
triethylamine	$\text{CH}_3$	t, 7	1.03	0.96	0.93	0.96	0.96	1.05	0.99
	$\text{CH}_2$	q,7	2.53	2.45	2.43	2.40	2.45	2.58	2.57

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

### <sup>13</sup>C NMR Data

		CDCl <sub>3</sub>	(CD <sub>3</sub> ) <sub>2</sub> CO	(CD <sub>3</sub> ) <sub>2</sub> SO	C <sub>6</sub> D <sub>6</sub>	CD <sub>3</sub> CN	CD <sub>3</sub> OD	D <sub>2</sub> O
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 acid	CO	175.99	172.31	171.93	175.82	173.21	175.11	177.21
	CH <sub>3</sub>	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 <sub>3</sub>	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 <sub>3</sub>	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	
<i>tert</i> -butyl alcohol	C	69.15	68.13	66.88	68.19	68.74	69.40	70.36
	CH <sub>3</sub>	31.25	30.72	30.38	30.47	30.68	30.91	30.29
<i>tert</i> -butyl methyl ether	CCH <sub>3</sub>	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
BHT	CCH <sub>3</sub>	26.99	27.24	26.79	27.09	27.28	27.22	26.60
	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 <sub>3</sub> Ar	21.20	21.31	20.97	21.4	21.23	21.38	
	CH <sub>3</sub> C	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 <sub>2</sub>	26.94	27.51	26.33	27.23	27.63	27.96	
1,2-dimchloroethane	CH <sub>2</sub>	43.50	45.25	45.02	43.59	45.54	45.11	
dimchloromethane	CH <sub>2</sub>	53.52	54.95	54.84	53.46	55.32	54.78	
diethyl ether	CH <sub>3</sub>	15.20	15.78	15.12	15.46	15.63	15.46	14.77
	CH <sub>2</sub>	65.91	66.12	62.05	65.94	66.32	66.88	66.42
diglyme	CH <sub>3</sub>	59.01	58.77	57.98	58.66	58.9	59.06	58.67
	CH <sub>2</sub>	70.51	71.03	69.54	70.87	70.99	71.33	70.05
	CH <sub>2</sub>	71.90	72.63	71.25	72.35	72.63	72.92	71.63
1,2-dimethoxyethane	CH <sub>3</sub>	59.08	58.45	58.01	58.68	58.89	59.06	58.67
	CH <sub>2</sub>	71.84	72.47	17.07	72.21	72.47	72.72	71.49
dimethylacetamide	CH <sub>3</sub>	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 <sub>3</sub>	35.28	34.89	37.38	34.67	35.17	35.5	35.03
	NCH <sub>3</sub>	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 <sub>3</sub>	36.50	36.15	35.73	35.25	36.57	36.89	37.54
	CH <sub>3</sub>	31.45	31.03	30.73	30.72	31.32	31.61	32.03
dimethyl sulfoxide	CH <sub>3</sub>	40.76	41.23	40.45	40.03	41.31	40.45	39.39
dioxane	CH <sub>2</sub>	67.14	67.6	66.36	67.16	67.72	68.11	67.19
ethanol	CH <sub>3</sub>	18.41	18.89	18.51	18.72	18.8	18.40	17.47
	CH <sub>2</sub>	58.28	57.72	56.07	57.86	57.96	58.26	58.05
ethyl acetate	CH <sub>3</sub> CO	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 <sub>2</sub>	60.49	60.56	59.74	60.21	60.98	61.5	62.32
	CH <sub>3</sub>	14.19	14.50	14.40	14.19	14.54	14.49	13.92
ethyl methyl ketone	CH <sub>3</sub> CO	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 <sub>2</sub> CH <sub>3</sub>	36.89	36.75	35.83	36.36	37.09	37.34	37.27
	CH <sub>2</sub> CH <sub>3</sub>	7.86	8.03	7.61	7.91	8.14	8.09	7.87
ethylene glycol	CH <sub>2</sub>	63.79	64.26	62.76	64.34	64.22	64.30	63.17
"grease"	CH <sub>2</sub>	29.76	30.73	29.20	30.21	30.86	31.29	
<i>n</i> -hexane	CH <sub>3</sub>	14.14	14.34	13.88	14.32	14.43	14.45	
	CH <sub>2</sub> (2)	22.70	23.28	22.05	23.04	23.40	23.68	
	CH <sub>2</sub> (3)	31.64	32.30	30.95	31.96	32.36	32.73	
HMPA	CH <sub>3</sub>	36.87	37.04	36.42	36.88	37.10	37.00	36.46
methanol	CH <sub>3</sub>	50.41	49.77	48.59	49.97	49.90	49.86	49.50
nitromethane	CH <sub>3</sub>	62.50	63.21	63.28	61.16	63.66	63.08	63.22
<i>n</i> -pentane	CH <sub>3</sub>	14.08	14.29	13.28	14.25	14.37	14.39	
	CH <sub>2</sub> (2)	22.38	22.98	21.70	22.72	23.08	23.38	
	CH <sub>2</sub> (3)	34.16	34.83	33.48	34.45	34.89	35.30	
2-propanol	CH <sub>3</sub>	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 <sub>3</sub>	1.04	1.40		1.38		2.10	
tetrahydrofuran	CH <sub>2</sub>	25.62	26.15	25.14	25.72	26.27	26.48	25.67
	CH <sub>2</sub> O	67.97	68.07	67.03	67.80	68.33	68.83	68.68
toluene	CH <sub>3</sub>	21.46	21.46	20.99	21.10	21.50	21.5	
	C(i)	137.89	138.48	137.35	137.91	138.90	138.85	
	CH(o)	129.07	129.76	128.88	129.33	129.94	129.91	
	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 <sub>3</sub>	11.61	12.49	11.74	12.35	12.38	11.09	9.07
	CH <sub>2</sub>	46.25	47.07	45.74	46.77	47.10	46.96	47.19

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