



ChemFiles

Vol. 2, No. 3

Products for NMR

Aldrich & Isotec

Service

Innovation

Quality

New Products

**Improved NMR
Solvents**

**Products for
Biomolecular NMR**

NMR Tubes

**Aldrich Spectral
Viewer Software**

Custom Synthesis

Contact Information

Bringing Together Quality, Innovation and
Service to Meet All of Your NMR Needs

 **ALDRICH®**

Aldrich & Isotec

Bringing together Quality, Innovation and Service to meet all your NMR needs

Quality

The highest NMR solvent quality is essential for acquiring NMR spectra. Our on-site synthesis, purification, and isotopic enrichment facilities along with an expert Quality Control staff and Quality Assurance department provide you with the highest quality product possible.

Our extensive number of NMR solvents have extremely low residual water, excellent chemical purity, and the highest isotopic enrichment available. All NMR solvents go through rigorous quality control testing throughout the production and packaging process to ensure product specifications are maintained. Every product is analyzed for NMR performance on our High Field NMR system to assure superior quality.

Innovation

We offer many products for use in biomolecular NMR applications such as growth media, labeled nucleotides and labeled amino acids. We continue to focus our resources on further research and development, including refining our processes for the synthesis of new and complex isotopically labeled compounds. We have also added a number of high-purity solvents that offer the highest isotopic enrichment in the industry

We always welcome your request for custom products. For custom requests, please contact Isotec at 800-448-9760(USA) or your local Sigma-Aldrich office if you are in France, Spain, or Portugal. For other international customers, please contact your nearest Isotec agent.

Service

We offer you a wide variety of standard unit sizes and packaging choices. If there is a particular unit size we do not offer or you would rather have the product packaged in something different, please give us a call with your request. We will provide custom packaging on request whenever possible. Ask our expert Technical Service staff about the choice that best suits your needs.

We take pride in the ability to provide you with excellent service. Our state-of-the-art ordering and distribution systems allow us to ship most products the same day they are ordered. It is not just our distribution that wins customers over, but is also our friendly and courteous Customer Service team. Have a technical question? You can feel comfortable knowing our knowledgeable and well-trained technical services specialists can answer your toughest questions.

" We are committed to the success of our Customers, Employees and Shareholders through leadership in **Life Science, High Technology and Service.**"

Visit our Web site at www.sigma-aldrich.com to see the latest products for NMR,
or contact your local Sigma-Aldrich office

Deuterated NMR Solvents

Aldrich and Isotec have shared manufacturing methods to offer a complete line of products for the NMR industry. We continually look for ways to improve our manufacturing process so we can offer you the best NMR solvent quality possible. Take a look at these NMR solvents that now have higher isotopic enrichment.

Chloroform-*d* (previous isotopic purity 99.8 atom % D)

15,182-3	Chloroform- <i>d</i> , 99.9 atom % D	(screw-cap)	50g
		(screw-cap)	100g
		(screw-cap)	10 x 100g
		(Sure/Seal™)	150g
		(screw-cap)	250g
23,689-6	Chloroform- <i>d</i> , 99.9 atom % D	(ampule)	10 x 1.0mL
		(ampule)	5 x 1.0mL
44,133-3	Chloroform- <i>d</i> , 99.9 atom % D	(ampule)	10 x 0.75mL
52,201-5	Chloroform- <i>d</i> , 99.9 atom % D	(ampule)	10 x 0.60mL
30,873-0	Chloroform- <i>d</i> , 99.9 atom % D	(ampule)	5 x 0.5mL
22,578-9	Chloroform- <i>d</i> , 99.9 atom % D (contains 0.03% TMS)	(screw-cap)	100g
		(screw-cap)	10 x 100g
		(Sure/Seal™)	150g
		(screw-cap)	500g
42,366-1	Chloroform- <i>d</i> , 99.9 atom % D (contains 0.03% v/v TMS)	(ampule)	10 x 1.0mL
15,183-1	Chloroform- <i>d</i> , 99.9 atom % D (contains 1% v/v TMS)	(screw-cap)	50g
		(screw-cap)	100g
		(screw-cap)	10 x 100g
		(Sure/Seal™)	150g
		(screw-cap)	250g

Dichloromethane-*d*₂ (previous isotopic purity 99.8 atom % D)

44,432-4	Dichloromethane- <i>d</i> ₂ , 99.9 atom % D	(ampule)	5g
		(ampule)	10g
		(ampule)	25g
52,211-2	Dichloromethane- <i>d</i> ₂ , 99.9 atom % D	(screw-cap)	10g
44,610-6	Dichloromethane- <i>d</i> ₂ , 99.9 atom % D	(ampule)	10 x 0.75mL
52,203-1	Dichloromethane- <i>d</i> ₂ , 99.9 atom % D	(ampule)	10 x 0.6mL
53,050-6	Dichloromethane- <i>d</i> ₂ , 99.9 atom % D (contains 0.1% v/v TMS)	(ampule)	1g
		(ampule)	5g
		(ampule)	10g
		(ampule)	25g

High Purity Solvents

Aldrich now offers high purity NMR solvents that have minimum isotopic purity levels of 99.996 atom % D or better. These solvents offer the highest isotopic enrichment available for NMR applications where purity is absolutely crucial.

EXTRA (minimum 99.996 atom % D)

61,339-8	Deuterium oxide, EXTRA	(ampule)	10 x 0.75mL
61,230-8	(Methyl sulfoxide)- <i>d</i> ₆ , EXTRA	(ampule)	10 x 0.25mL
		(ampule)	10 x 0.50mL
		(ampule)	10 x 0.75mL



ULTRA-D (minimum 99.999 atom % D)

61,340-1	Deuterium oxide, ULTRA-D	(ampule)	10g
57,023-0	Deuterium oxide, ULTRA-D	(ampule)	10 x 0.75mL

Improved DMSO-*d*₆ Now Lower water

We have taken steps to improve the water levels in all of our DMSO listings. Order some today and experience the difference. We have also recently added DMSO-*d*₆ 99.9 atom % D, "Special HOH". D₂O and HOD levels are kept to a minimum to avoid deuterium exchange with easily exchangeable protons in your sample.

61,232-4	(Methyl sulfoxide)- <i>d</i> ₆ , 99.9 atom % D "Special HOH"	(ampule)	25g
		(ampule)	50g

**Aldrich is continually adding new products to its already extensive line of NMR products.
If you would like to suggest a product that we do not currently offer,
please call our Technical Services department at 800-231-8327(USA), or your local Sigma-Aldrich sales office.**

To order: contact your local Sigma-Aldrich office or call 1-800-558-9160 (USA)

Anhydrous NMR solvents

Extra peaks arising from water impurities can mask areas of your NMR spectrum, resulting in valuable structural information that may be hidden from view. The area of the NMR spectrum where water usually appears (from 1-5ppm, depending on the solvent), is also a common area for proton signals arising from important functionalities such as alkanes, alkenes, amines, and alcohols. Aldrich now offers anhydrous NMR solvents that can take the guesswork out of structure determination in this range for you. Aldrich produces every anhydrous deuterated solvent to tight water specifications. Each solvent is produced using the most modern techniques available and are continually monitored to ensure that extremely low water specifications are maintained.

Ampule Packs

			Max ppm of Water
56,955-0	Acetonitrile- d_3 , 99.8 atom % D, anhydrous	10 x 1.0mL	10
56,956-9	Chloroform- d , 99.8 atom % D, anhydrous	5 x 1.0mL 10 x 1.0mL	10
56,953-4	Methyl- d_3 alcohol- d , 99.8+ atom % D, anhydrous	5 x 1.0mL 10 x 1.0mL	100
56,958-5	(Methyl sulfoxide)- d_6 , 99.9 atom % D, anhydrous	5 x 1.0mL 10 x 1.0mL	50

Screw-Cap Bottles

57,070-2	Acetonitrile- d_3 , 99.8 atom % D, anhydrous	50g	10
57,068-0	Benzene- d_6 , 99.6 atom % D, anhydrous	50g	10
57,069-9	Chloroform- d , 99.8 atom % D, anhydrous	50g	10
57,072-9	Methyl- d_3 alcohol- d , 99.8+ atom % D, anhydrous	50g	100
57,067-2	(Methyl sulfoxide)- d_6 , 99.9 atom % D, anhydrous	50g	50
57,071-0	Toluene- d_8 , 99.6 atom % D, anhydrous	50g	10


NMR Reference Standards

We offer an extensive list of NMR reference standards in a variety of tube lengths. If there is a special mix you are interested in that we do not offer, please contact our Technical Services department at 800-231-8327(USA), or your local Sigma-Aldrich sales office.

		Tube Size
61,177-8	1% Chloroform in acetone- d_6 , 99.9 atom % D	3mm x 8in
61,303-7	1% Chloroform in acetone- d_6 , 99.9 atom % D	4mm x 8in
61,174-3	1% Chloroform in acetone- d_6 , 99.9 atom % D	10mm x 8in
61,330-4	2% Chloroform in chloroform- d , 99.9 atom % D	3mm x 8in
61,331-2	2% Chloroform in chloroform- d , 99.9 atom % D	5mm x 8in
61,178-6	5% Chloroform in acetone- d_6 , 99.9 atom % D	3mm x 8in
61,183-2	5% Chloroform in acetone- d_6 , 99.9 atom % D	4mm Nano tube
61,185-9	20% Chloroform in acetone- d_6 , 99.8 atom % D	5mm x 8in
61,251-0	5% 1,2-Dichlorobenzene in acetone- d_6 , 99.9 atom % D	5mm x 8in
61,211-1	40% 1,4-Dioxane in benzene- d_6 , 99.6 atom % D	3mm x 8in
61,179-4	40% 1,4-Dioxane in benzene- d_6 , 99.6 atom % D	4mm Nano tube
61,207-3	40% 1,4-Dioxane and 5mg/mL chromium(III) acetylacetonate in benzene- d_6 , 99.6 atom % D	3mm x 8in
61,190-5	40% 1,4-Dioxane and 5mg/mL chromium(III) acetylacetonate in benzene- d_6 , 99.6 atom % D	5mm x 8in
61,182-4	40% 1,4-Dioxane, and 5mg/mL chromium(III) acetylacetonate in benzene- d_6 , 99.6 atom % D	4mm Nano tube
61,304-5	0.1% Ethylbenzene and 0.01% TMS in chloroform- d , 99.9 atom % D	4mm x 8in
61,026-5	0.1% Ethylbenzene and 0.01% TMS in chloroform- d , 99.9 atom % D	10mm x 8in
61,180-8	0.1% Ethylbenzene and 0.01% TMS in chloroform- d , 99.9 atom % D	4mm Nano tube
61,248-0	0.1% Ethylbenzene, 0.01% TMS and 0.1mg/mL chromium(III) acetylacetonate in chloroform- d , 99.9 atom % D	5mm x 8in
61,293-6	5% Ethylbenzene and 2% TMS in chloroform- d , 99.9 atom % D	5mm x 7in
61,270-7	45% Formamide in (methyl sulfoxide)- d_6 , 99.9 atom % D	3mm x 8in
61,189-1	45% Formamide in (methyl sulfoxide)- d_6 , 99.9 atom % D	5mm x 8in
61,333-9	90% Formamide in (methyl sulfoxide)- d_6 , 99.9 atom % D	3mm x 8in
61,208-1	0.1mg/mL Gadolinium(III) chloride, 0.1% DSS and 1% water in deuterium oxide, 99.9 atom % D	3mm x 8in
61,194-8	0.1mg/mL Gadolinium(III) chloride, 0.1% DSS and 1% water in deuterium oxide, 99.9 atom % D	8mm x 8in
61,181-6	0.1mg/mL Gadolinium(III) chloride in deuterium oxide, 99.9 atom % D	4mm Nano tube
61,192-1	25% Hexamethyldisiloxane in benzene- d_6 , 99.6 atom % D	5mm x 8in
61,329-0	50% Menthol and 0.5% chromium(III) acetylacetonate in chloroform- d , 99.9 atom % D	5mm x 8in
61,216-2	85% Phosphoric acid in deuterium oxide, 99.9 atom % D	5mm x 8in coaxial tube
61,191-3	0.2M Potassium fluoride and 90% water in deuterium oxide, 99.9 atom % D	10mm 8in
61,268-5	0.05% α,α,α -Trifluorotoluene in benzene- d_6 , 99.6 atom % D	3mm x 8in
61,318-5	0.05% α,α,α -Trifluorotoluene in benzene- d_6 , 99.6 atom % D	4mm x 8in
61,117-9	0.0485M Triphenylphosphate in chloroform- d , 99.9 atom % D	8mm x 8in
61,173-5	0.0485M Triphenylphosphate in chloroform- d , 99.9 atom % D	10mm x 8in

Visit our Web site at www.sigma-aldrich.com to see the latest products for NMR, or contact your local Sigma-Aldrich office

LC-NMR Reference Standards

61,244-8	1% Chloroform in acetone- <i>d</i> ₆ , 99.9 atom % D		(screw-cap)	50mL
61,302-9	50mM Sodium acetate and 1% water in deuterium oxide, 99.9 atom % D		(screw-cap)	50mL
61,242-1	1% Water in deuterium oxide, 99.9 atom % D		(screw-cap)	250mL

LC-NMR Solvents

53,089-1	Acetone-<i>d</i>₆ , 99.5 atom % D	(GL-45 bottle)	1L
53,088-3	Acetonitrile-<i>d</i>₃ , 99.8 atom % D	(GL-45 bottle)	1L
56,310-2	Acetonitrile-<i>d</i>₃ , 99.8 atom % D (contains 15-20% D ₂ O)	(GL-45 bottle)	1L
53,086-7	Deuterium oxide , 99.9 atom % D	(GL-45 bottle)	1L
53,087-5	Methyl-<i>d</i>₃ alcohol-<i>d</i> , 99.8+ atom % D	(GL-45 bottle)	1L
34955	Acetonitrile NMR CHROMASOLV®		500mL 6 x 500mL 1L 6 x 1L

Products for Biomolecular NMR

ISOTEC offers an extensive line of stable isotope labeled products for Biomolecular NMR research. ISOTEC's pioneering synthesis knowledge enables us to synthesize compounds that help you reach your goals. For a complete list of unlabeled products for biomolecular applications, please see Fluka's Laboratory Chemicals and Analytical Reagents catalog, or our website at www.sigma-aldrich.com/fluka.

Products for Minimal Media

		Atom %
Sugars		
38,937-4	D-Glucose- ¹³ C ₆ (Dextrose)	99
60,682-0	D-Glucose- ¹³ C ₆ , C- <i>d</i> ₇ (Dextrose)	99 ¹³ C;97-99d
55,200-3	D-Glucose-C- <i>d</i> ₇ (Dextrose)	97-99
60,820-3	D-Glucose- <i>d</i> ₁₂ (Dextrose)	97-99

Selected ¹⁵N Products

29,925-1	Ammonium- ¹⁵ N Chloride	98+
60,946-3	Ammonium- ¹⁵ N Hydroxide (28-30 wt.% aqueous soln)	98+
29,928-6	Ammonium- ¹⁵ N ₂ Sulfate	98+

Labeled Complex Growth Media

60,681-2	ISOGRO™ Powder - Growth Medium (unlabeled)	NA
60,687-1	ISOGRO™ - ¹⁵ N Powder - Growth Medium	98+
60,683-9	ISOGRO™- ¹³ C, ¹⁵ N Powder - Growth Medium	99 ¹³ C;98+ ¹⁵ N
60,829-7	ISOGRO™- ¹³ C, ¹⁵ N,D Powder - Growth Medium	99 ¹³ C;98+ ¹⁵ N;97-99d
60,686-3	ISOGRO™ - ¹³ C Powder - Growth Medium	99
61,672-9	ISOGRO™-D Powder - Growth Medium	97-99

Fully Labeled Nucleic Acids

¹³C,¹⁵N Ribonucleotides (minimum chemical purity 90%)

60,835-1	Adenosine- ¹³ C ₁₀ , ¹⁵ N ₅ 5'-Triphosphate, Sodium Salt	98 ¹³ C;98+ ¹⁵ N
60,837-8	Cytidine- ¹³ C ₉ , ¹⁵ N ₃ 5'-Triphosphate, Sodium Salt	98 ¹³ C;98+ ¹⁵ N
60,838-6	Guanosine- ¹³ C ₁₀ , ¹⁵ N ₅ 5'-Triphosphate, Sodium Salt	98 ¹³ C;98 ¹⁵ N
60,839-4	Uridine- ¹³ C ₉ , ¹⁵ N ₂ 5'-Triphosphate, Sodium Salt	98 ¹³ C;98+ ¹⁵ N

¹³C,¹⁵N Deoxyribonucleotides (Under Development)

60,840-8	Deoxyadenosine- ¹³ C ₁₀ , ¹⁵ N ₅ 5'-Triphosphate, Sodium Salt	98 ¹³ C;98+ ¹⁵ N
60,841-6	Deoxycytidine- ¹³ C ₉ , ¹⁵ N ₃ 5'-Triphosphate, Sodium Salt	98 ¹³ C;98+ ¹⁵ N
60,842-4	Deoxyguanosine- ¹³ C ₁₀ , ¹⁵ N ₅ 5'-Triphosphate, Sodium Salt	98 ¹³ C;98+ ¹⁵ N
60,843-2	Deoxythymidine- ¹³ C ₁₀ , ¹⁵ N ₂ 5'-Triphosphate, Sodium Salt	98 ¹³ C;98+ ¹⁵ N

To order: contact your local Sigma-Aldrich office or call 1-800-558-9160(USA)

Labeled Products for Cell Free Synthesis

Fully labeled ¹⁵N Amino Acids

		Atom %
29,929-4	Glycine- ¹⁵ N	98+
33,215-1	L-4-Hydroxyphenylalanine- ¹⁵ N	98+
33,212-7	L-Alanine- ¹⁵ N	98+
33,212-7	L-Alanine- ¹⁵ N	98+
60,011-3	L-Arginine- ¹⁵ N ₄ HCl	98+
48,591-8	L-Asparagine- ¹⁵ N ₂ •H ₂ O	98+
33,213-5	L-Aspartic- ¹⁵ N Acid	98+
60,912-9	L-Cysteine- ¹⁵ N	98+
33,214-3	L-Glutamic- ¹⁵ N Acid	98+
49,003-2	L-Glutamine- ¹⁵ N ₂	98+
60,901-3	L-Isoleucine- ¹⁵ N	98+
34,096-0	L-Leucine- ¹⁵ N	98+
60,902-1	L-Lysine- ¹⁵ N ₂ HCl	98+
60,924-2	L-Methionine- ¹⁵ N	98+
49,010-5	L-Phenylalanine- ¹⁵ N	98+
60,899-8	L-Proline- ¹⁵ N	98+
60,900-5	L-Serine- ¹⁵ N	98+
60,909-9	L-Threonine- ¹⁵ N	98+
49,017-2	L-Valine- ¹⁵ N	98+

Fully Labeled ¹³C,¹⁵N Amino Acids

48,952-2	Glycine- ¹³ C ₂ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,799-1	L-4-Hydroxyphenylalanine- ¹³ C ₉ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
48,988-3	L-Alanine- ¹³ C ₃ , ¹⁵ N 98+ ¹³ C;98+ ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,803-3	L-Arginine- ¹³ C ₆ , ¹⁵ N ₄ HCL	98+ ¹³ C;98+ ¹⁵ N
60,815-7	L-Asparagine- ¹³ C ₄ , ¹⁵ N ₂ •H ₂ O	98+ ¹³ C;98+ ¹⁵ N
60,783-5	L-Aspartic Acid- ¹³ C ₄ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,785-1	L-Glutamic Acid- ¹³ C ₅ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,798-3	L-Glutamine- ¹³ C ₅ , ¹⁵ N ₂	98+ ¹³ C;98+ ¹⁵ N
60,809-2	L-Isoleucine- ¹³ C ₆ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,806-8	L-Leucine- ¹³ C ₆ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,804-1	L-Lysine- ¹³ C ₈ , ¹⁵ N ₂ HCL	98+ ¹³ C;98+ ¹⁵ N
60,801-7	L-Phenylalanine- ¹³ C ₉ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,811-4	L-Proline- ¹³ C ₅ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,813-0	L-Serine- ¹³ C ₃ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,777-0	L-Threonine- ¹³ C ₄ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N
60,014-8	L-Valine- ¹³ C ₅ , ¹⁵ N	98+ ¹³ C;98+ ¹⁵ N

Products for Peptide Synthesis

Isotec offers an extensive product line of protected amino acids-N-FMOC, N-t-BOC, and CBZ- derivatives fully labeled in the Amino Acid moiety or selectively labeled.

For more information, please contact Isotec at 800-448-9760(USA) or (937)-859-1808. For international customers, please contact your local Sigma-Aldrich office or Isotec agent for pricing & availability on catalog quantities.

Other Products of Interest

		Atom %
44,749-8	Glycerol-d ₈	98
45,452-4	Glycerol-1,1,2,3,3-d ₅	98
48,947-6	Glycerol- ¹³ C ₃	99
49,112-8	Methyl- ¹³ C Alcohol (~12% ¹⁸ O) (Methanol)	99
28,201-4	Acetic Acid- ¹³ C ₂ , Sodium Salt (Sodium Acetate)	99
29,911-1	Acetic-d ₃ Acid- ¹³ C ₂ , Sodium Salt (Sodium Acetate)	99 ¹³ C;99d
17,607-9	Acetic-d ₃ Acid, Sodium Salt (Sodium Acetate)	99

Custom Synthesis

Since 1987, Isotec has been engaged in the custom synthesis of labeled compounds. Isotec's synthesis team is comprised of an impressive group of experienced professionals, who have performed thousands of synthesis projects. Combined with a large inventory of labeled starting materials, Isotec can provide fast turnaround time for custom synthesis, thus allowing customers to perform research and manufacture their products with a short time.

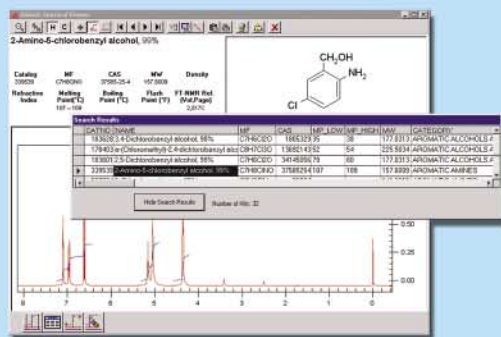
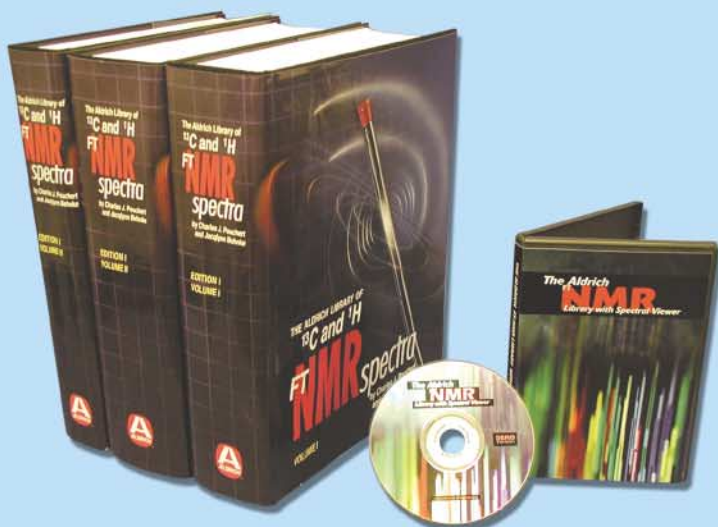
For more information on custom synthesis of labeled isotopes, please contact Isotec at 800-448-9760(USA) or your local Sigma-Aldrich office if you are in France, Spain, or Portugal. For other International customers, please contact your local Isotec agent.

To order: contact your local Sigma-Aldrich office or call 1-800-558-9160(USA)

Introducing...

NEW Electronic FT-NMR Libraries from Aldrich!

The Aldrich FT-NMR Library with Spectral Viewer on CD-ROM is an electronic book that contains high-resolution 300MHz ^1H and 75MHz ^{13}C spectra for the more than 11,800 compounds found in the printed version of The Aldrich Library of ^{13}C and ^1H FT-NMR Spectra. A supplemental library is also available that includes spectra for 3,500 additional compounds not included in the original printed version. Order both the standard and the supplemental library for access to spectra on over 15,000 compounds.



Features:

- Displays ^1H and ^{13}C spectra, integral, chemical structure, and technical data
- Text Searching by Chemical Name, Aldrich Catalog Number, CAS Number, and Molecular Formula
- Advanced data field searching on Chemical Category and physical properties such as Boiling Point, Melting Point, Density, Flash Point, Molecular Weight, and Refractive Index
- Spectra processing using Zoom, Peak Integration, and Peak Labeling
- Print spectra, structure, technical data, integral table and peak listing
- Export spectra to a file (Bitmap, Metafile, or JPEG formats) or to the clipboard (Bitmap or Metafile formats)
- Web link button provides additional technical data from the Sigma-Aldrich Website

Ideal for:

- ✓ Teaching students NMR spectral interpretation
- ✓ Referencing spectra for comparison studies and the identification of unknown compounds
- ✓ Exporting spectra quickly for presentations and papers

Version	Standard library (11,800 compounds) Cat. No.	Supplemental library (3,500 compounds) Cat. No.
Single user, commercial	Z54,126-5	Z53,808-6
Single user, academic	Z54,138-9	Z53,818-3
Network version	Z54,149-4	Z53,797-7
Demo program	Z54,159-1	—

Minimum system requirements:
Pentium® 200MHz, Windows®
95/98/ME/
NT4-SP5/2000, CD-ROM drive,
600MB hard disk space, 64MB RAM.
(PC ONLY)

Aldrich is a registered trademark of Sigma-Aldrich Co. Chemical Abstracts is a registered trademark of the American Chemical Society. Pentium is a registered trademark of Intel Corp. Windows is a registered trademark of Microsoft Corp.

SPECIAL OFFER—Receive a FREE supplemental library if you buy and register the standard product before October 31, 2002!

Aldrich NMR Tubes

Every Aldrich premium-quality NMR tube is inspected and gauged to meet published specifications.

- Aldrich Statement of Conformance stamped on each box of tubes
- Made of ASTM Type I borosilicate glass* for compatibility with ground joints, valves, and vacuum racks
- Precision ground and highly polished for spinning stability and highest resolution
- Thin-wall glass with round-bottoms
- Sandblasted marking spot for labelling samples

*Except disposable grade NMR tubes.



NMR TUBE SELECTION GUIDE

Choose the NMR tube grade that most closely matches the frequency (in MHz) of the spectrometer.

Aldrich Grade	MHz	Applications	Cross Ref. No. (5mm tubes)	
			Wilmad	Kontes
Disposable	30	Student labs, basic studies	WG-Economy	–
Series 30	30	Student labs, basic studies	505-PS	897200
Series 200	60 to 270	Lower field studies	506-PP	897205
Series 300	60 to 360	Routine applications	507-PP	897220
Series 400	200 to 500	High-field, multiple-scan FT-NMR	528-PP	897235
Series 500	500+	Ultra-high resolution	535-PP	897240

Grade	L (in.)	Wall uniformity (in., TIR)	Camber (in.)	Cat. No.
3mm Microsample NMR tubes – 0.012in. wall thickness (Pkg=5 tubes)				
Series 300	7	0.0020	0.0010	Z41,290-2
	8	0.0020	0.0011	Z41,291-0
Series 400	7	0.0010	0.0005	Z41,292-9
	8	0.0010	0.0006	Z41,293-7
Series 500	7	0.0005	0.00025	Z41,294-5
	8	0.0005	0.00035	Z41,295-3
5mm NMR tubes – 0.015in. wall thickness (Pkg=5 tubes)				
Disposable	7	–	–	Z41,277-5
Series 30	7	0.0030	0.002	Z41,278-3
Series 200	7	0.0025	0.002	Z41,279-1
Series 300	7	0.0020	0.0010	Z41,280-5
	8	0.0020	0.0011	Z41,281-3
	9	0.0020	0.0012	Z41,282-1
Series 400	7	0.0010	0.0005	Z41,284-8
	8	0.0010	0.0006	Z41,285-6
Series 500	7	0.0005	0.00025	Z41,286-4
	8	0.0005	0.00035	Z41,287-2
Series 800	7	0.0002	0.00015	Z41,288-0
	8	0.0002	0.00015	Z41,289-9
10mm NMR tubes – 0.018in. wall thickness (Pkg=5 tubes)				
Series 200	7	0.0030	0.0015	Z41,296-1
Series 400	7	0.0015	0.0005	Z41,298-8

TIR-Total Indicator Reading

Wilmad NMR Tubes

Made of Pyrex borosilicate glass (unless otherwise noted) for compatibility with ground joints, valves, and vacuum racks. Precision ground and highly polished for spinning stability and highest resolution. Tubes have round bottoms and include a sandblasted marking spot for labeling samples. Tubes that are 9in. L are for making standards and for use with tip-off manifolds.



SELECTION GUIDE

Grade	Applications
Precision	Frequently used as disposable tubes by students and in rudimentary studies
Imperial	60 to 270MHz, lower field studies
Ultra-Imperial	60 to 360MHz, for routine applications
Royal Imperial	200 to 500MHz, unsurpassed performance in this range
Emperor	500MHz or higher, offers highest precision available

For larger quantities of NMR tubes and glassware, please contact Sigma-Aldrich at 1-800-231-8327(USA) or contact your local Sigma-Aldrich office

3mm Microsample NMR tubes – 0.012in. wall thickness (Pkg=5 tubes)

L (in.)	Concentricity/camber (μm)	Wilmad No.	Cat. No.
300MHz tubes			
7	51/25	307-PP-7	Z27,432-1
8	51/25	307-PP-8	Z27,434-8
9	51/25	307-PP-9	Z27,435-6
360MHz tubes			
7	25/25	327-PP-7	Z27,186-1
8	25/25	327-PP-8	Z27,436-4
9	25/25	327-PP-9	Z27,437-2
400MHz tubes			
7	25/13	328-PP-7	Z27,438-0
8	25/13	328-PP-8	Z27,439-9
9	25/13	328-PP-9	Z27,440-2
500MHz tubes			
7	13/6	335-PP-7	Z27,441-0
8	13/6	335-PP-8	Z27,442-9
9	13/6	335-PP-9	Z27,443-7

5mm amber NMR tubes – 0.015in. wall thickness (Pkg=1 tube)

L (in.)	Concentricity/camber (μm)	Wilmad No.	Cat. No.
100MHz tube			
7	76/51	505-PS-7	Z28,225-1
360MHz tubes			
7	51/25	507-PP-7	Z28,227-8
7	25/25	527-PP-7	Z28,228-6

5mm disposable NMR tubes – 0.015in. wall thickness, N51 glass (Pkg=100 tubes)

L (in.)	Concentricity/camber (μm)	Wilmad No.	Cat. No.
100MHz tubes			
7	76/76	HIP-7	Z51,414-4
8	76/76	HIP-8	Z51,415-2

5mm economy NMR tubes – 0.015in. wall thickness. WG series made of N51 glass. (Pkg=5 tubes)

L (in.)	Concentricity/camber (μm)	Wilmad No.	Cat. No.
100MHz tubes			
7	76/76	WG-5-7	Z27,627-8
8	76/76	WG-5-8	Z27,628-6
9	76/76	WG-5-9	Z27,629-4
7	76/76	512-5-7	Z27,630-8
8	76/76	512-5-8	Z27,631-6
9	76/76	512-5-9	Z27,632-4
7	51/51	506-IM-7	Z51,412-8
8	51/51	506-IM-8	Z51,413-6

To order: contact your local Sigma-Aldrich office or call 1-800-558-9160(USA)

5mm standard NMR tubes – 0.015in. wall thickness (Pkg=5 tubes)

L (in.)	Concentricity/ camber (μm)	Wilmad No.	Cat. No.
100MHz tubes			
7	76/51	505-PS-7	Z27,198-5
8	76/51	505-PS-8	Z27,444-5
9	76/51	505-PS-9	Z27,445-3
7	51/51	506-PP-7	Z28,602-8
8	51/51	506-PP-8	Z28,603-6
9	51/51	506-PP-9	Z28,604-4
200MHz tube			
7	76/51	503-PS-7**	Z41,035-7
360MHz tubes			
7	51/25	507-PP-7	Z27,199-3
8	51/25	507-PP-8	Z27,446-1
9	51/25	507-PP-9	Z27,211-6
7	51/13	526-PP-7	Z27,448-8
8	51/13	526-PP-8	Z27,449-6
9	51/13	526-PP-9	Z27,451-8
7	25/25	527-PP-7	Z27,427-5
8	25/25	527-PP-8	Z27,452-6
9	25/25	527-PP-9	Z27,453-4
400MHz tubes			
7	25/13	528-PP-7	Z27,201-9
8	25/13	528-PP-8	Z27,429-1
9	25/13	528-PP-9	Z27,454-2
500 MHz tubes			
7	13/6	535-PP-7	Z27,202-7
7	13/6	545-PPT-7*	Z40,670-8
8	13/6	535-PP-8	Z27,455-0
9	13/6	535-PP-9	Z27,456-9
800 MHz tubes			
7	3.8/3.8	541-PP-7	Z41,200-7
8	3.8/3.8	541-PP-8	Z41,201-5
900 MHz tubes			
7	2.5/3.8	542-PP-7	Z41,202-3
8	2.5/3.8	542-PP-8	Z41,203-1

* Ultra thin wall (0.09in.)

** Medium wall (0.03in.)

10mm NMR tubes – 0.018in. wall thickness (Pkg=5 tubes)

L (in.)	Concentricity/ camber (μm)	Wilmad No.	Cat. No.
60MHz tubes			
7	NA	513-1PS-7	Z27,477-1
8	NA	513-1PS-8	Z27,479-8
9	NA	513-1PS-9	Z27,480-1
100MHz tubes			
7	254/51	513-1PP-7	Z27,468-2
8	254/51	513-1PP-8	Z27,469-0
9	254/51	513-1PP-9	Z27,470-4
300MHz tubes			
7	76/38	513-3PP-7	Z27,203-5
8	76/38	513-3PP-8	Z27,471-2
9	76/38	513-3PP-9	Z27,204-3

Visit our Web site at www.sigma-aldrich.com to see the latest products for NMR,
or contact your local Sigma-Aldrich office

360MHz tubes			
7	51/25	513-5PP-7	Z27,472-0
8	51/25	513-5PP-8	Z27,473-9
9	51/25	513-5PP-9	Z27,474-7
400MHz tubes			
7	38/13	513-7PP-7	Z27,205-1
8	38/13	513-7PP-8	Z27,475-5
9	38/13	513-7PP-9	Z27,476-3

*Tubes do not have a precision i.d. tolerance.

Wilmad Screw Cap NMR Tubes

NMR tube has an open-top, screw-thread cap with a PTFE/silicone septum that permits addition of reactants or samples via syringe through the cap. Also good for sample storage. Caps and septa are replaceable. Excellent for handling air-sensitive samples and in cell perfusion studies. Tubes are 7in. L.

5mm NMR tubes (Pkg=1 tube)

Concentricity/ camber (μm)	Wilmad No.	Cat. No.
100MHz tube		
76/51	505-TR-7	Z27,191-8
100MHz tube		
51/51	506-TR-7	Z27,192-6
360MHz tube		
51/25	507-TR-7	Z27,193-4
400MHz tube		
25/13	528-TR-7	Z27,194-2
500MHz tube		
13/60	535-TR-7	Z27,195-0

8mm NMR tubes (Pkg=1 tube)

Concentricity/ camber (μm)	Wilmad No.	Cat. No.
400MHz tube		
38/13	513A-7TR	Z27,482-8

10mm NMR tubes (Pkg=1 tube)

Concentricity/ camber (μm)	Wilmad No.	Cat. No.
300MHz tube		
76/38	513-3TRA-7	Z27,196-9
400MHz tube		
38/13	513-7TRA-7	Z27,197-7

Replacement caps and septa for screw-cap NMR tubes

NMR tube size (mm)	Cat. No.	Pkg
Black open-top caps		
5	Z16,253-1	144
10	Z10,645-3	200
Black solid-top caps w/white rubber liner		
5	Z18,880-8	100
10	Z10,641-0	200
Black solid-top caps w/PTFE-faced rubber liner		
10	Z10,643-7	200
PTFE-faced silicone septa		
5	Z16,256-6	120
10	Z10,651-8	100



To order: contact your local Sigma-Aldrich office or call 1-800-558-9160 (USA)

Tell Us About yourself

Name _____
Company _____
Department _____ Mail Stop _____
Address _____ Bldg/Rm # _____
City _____ State _____ Country _____ Postal Code _____
Phone _____ Fax _____
E-mail _____

Place Printed Label Here

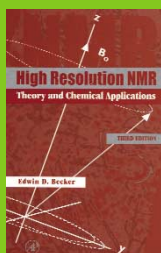
1. Who is your primary supplier of deuterated solvents?
 Aldrich [1AA]
 Other _____
2. Who is your primary supplier of labeled Nucleic Acids?
 Isotec (2AA)
 Other _____
3. Who is your primary supplier of labeled Amino Acids?
 Isotec (3AA)
 Other _____

Please check any of the following free catalog and literature pieces that you would like to receive:

- Aldrich Catalog/Handbook [002]
- Aldrichimica Acta [014]
- Products for NMR [DTW]
- Solvents for Scientific Research [BAO]
- Aldrich Glassware [044]
- Combinatorial Chemistry Catalog [EDZ]
- Polymer Products CD- Catalog & Reference Guide [DGQ]
- SmartBLOCS™ (ERB)
- Reagents for Suzuki Coupling [DTK]

CC3

Reference Books



High Resolution NMR

3rd Ed., E.D. Becker, Academic Press, New York, NY, 1999, 424pp. Hardcover.

This book is intended to allow a graduate student, advanced undergraduate, or researcher to understand NMR at a fundamental level, and to see illustrations of the applications of NMR to the determination of the structure of small organic molecules and macromolecules, including proteins. Emphasis is on the study of NMR in liquids, but the treatment also includes high resolution NMR in the solid state and the principles of NMR imaging and localized spectroscopy.

Z53,982-1

Interpreting Infrared, Raman, and Nuclear Magnetic Resonance Spectra, 2-Volume Set

R.A. Nyquist, Academic Press, New York, NY, 2001, 900pp. Hardcover.

While many useful books cover these techniques, none emphasize the effect of the physical environment of chemical substances upon their molecular vibrations. One goal of this book is to show how changes in the physical environment of a compound aid in the elucidation of molecular structure and in the identification of unknown chemical compositions. This book also gathers key information for the analyst on the nature of solute-solvent interaction, solute concentration, and the effect of temperature.

Z53,961-9

The Aldrich Library of ¹³C and ¹H FT-NMR Spectra

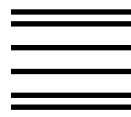
C.J. Pouchert and J. Behne, Aldrich Chemical, Milwaukee, WI, 1992, 4,300pp.

Three volume set of 12,000 high-resolution 300MHz proton and 75MHz ¹³C FT-NMR spectra arranged according to functionality.

Book Z23,103-7

CD-ROM Z54,126-5



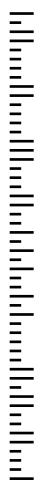
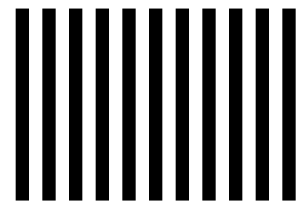


BUSINESS REPLY MAIL
FIRST-CLASS MAIL PERMIT NO. 3038 ST. LOUIS, MO

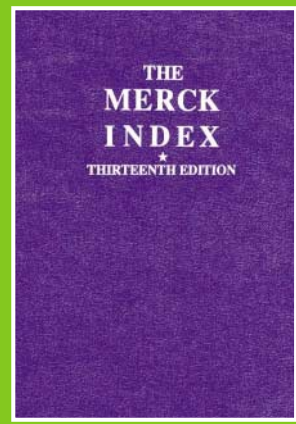
POSTAGE WILL BE PAID BY ADDRESSEE

SIGMA-ALDRICH
P.O. BOX 14508
ST. LOUIS, MO, USA 63178-9916

NO POSTAGE
NECESSARY IF
MAILED IN THE
UNITED STATES



The Merck **INDEX**



*13th ed., Merck & Co.,
Rahway, NJ, 2001,
1,741pp. Hardcover.*

The **NEW** thirteenth edition contains over 10,000 monographs on chemicals, biologicals, and drugs, and provides a variety of information such as CAS registry numbers, molecular weights, physical properties,

toxicity data, descriptions of commercial uses, and references to the scientific and patent literature. Includes an organic name reaction section and a name index with over 50,000 names.

Z52,876-5

Sigma-Aldrich Worldwide Locations

Argentina

Sigma-Aldrich de Argentina, S.A.
Tel: 54 11 4807 0321
Fax: 54 11 4807 0346
E-mail: info@sigma-aldrich.com.ar

Australia

Sigma-Aldrich Pty., Limited
Free Tel: 1-800-800-097
Free Fax: 1-800-800-096
Tel: 61-2-9841-0555
Fax: 61-2-9841-0500
E-mail: ausmail@sial.com

Austria

Sigma-Aldrich Handels GmbH
Tel: 43 1 605 8110
Fax: 43 1 605 8120
E-mail: sigma@sial.co.at

Belgium

Sigma-Aldrich nv/sa
Free Tel: 0800-147 47
Free Fax: 0800-147 45
Tel: 03 899.13.01
Fax: 03 899.13.11
E-mail: sigmaldr@sial.be

Brazil

Sigma-Aldrich Química Brasil Ltda.
Tel: 55-11-231-1866
Fax: 55-11-257-9079
E-mail: sigmabr@ibm.net

Canada

Sigma-Aldrich Canada Ltd.
Free Tel: 800-565-1400
Free Fax: 800-265-3858
Tel: 905-829-9500
Fax: 905-829-9292
E-mail: canada@sial.com

Czech Republic

Sigma-Aldrich s.r.o.
Tel: 00-420-2-2176 1300
Fax: 00-420-2-2176 3300
E-mail:
CZECustSV@eurnotes.sial.com

Denmark

Sigma-Aldrich Denmark A/S
Tel: +45 43 56 59 10
Fax: +45 43 56 59 05
E-mail: denorder@eurnotes.sial.com

Eire

Sigma-Aldrich Ireland Ltd.
Free Tel: 1 800 200 888
Free Fax: 1 800 600 222
Tel: 01 404 1900
Fax: 01 404 1910
E-mail: EICustsv@eurnotes.sial.com

Finland

Sigma-Aldrich Finland
Tel: (09) 350-9250
Fax: (09) 350-92555
E-mail: finorder@eurnotes.sial.com

France

Sigma-Aldrich Chimie S.a.r.l.
Tel Numero Vert: 0800 21 14 08
Fax Numero Vert: 0800 03 10 52
E-mail: fradsv@eurnotes.sial.com

Germany (also SE Europe, the Baltics, Africa and the Middle East)

Sigma-Aldrich Chemie GmbH
FreeCall Tel: 0800-5155 000
FreeCall Fax: 0800-6490 000
Tel: +49(0)89-6513-0
Fax: +49(0)89-6513-1169

E-mail: deorders@eurnotes.sial.com
For Slovakia, Africa, Middle East and other European countries:
Tel: +49(0)89-6513-1807
Fax: +49(0)89-6513-1877

Greece

Sigma-Aldrich (o.m) Ltd.
Tel: 30-1-9948010
Fax: 30-1-9943831
E-mail: sigald@acci.gr

Hungary

Sigma-Aldrich Kft
Tel: 06-1-269-6474
Fax: 06-1-235-9050
E-mail: info@sigma.sial.hu

India

Sigma-Aldrich Corporation
Bangalore, India:
Phone: 91 80 852 4222
Fax: 91 80 852 4214
E-mail: india@sial.com

Israel

Sigma-Aldrich Israel Ltd.
Toll Free Tel: 1-800-70-2222
Tel: 972-8-948-4222
Fax: 972-8-948-4200
E-mail: sigisr@sigma.co.il

Italy

Sigma-Aldrich S.r.l.
Numero Verde: 800-827018
Tel: 02-33417.310
Fax: 02-38010.737
E-mail: itorder@eurnotes.sial.com

Japan

Sigma-Aldrich Japan K.K.
Tel: 81-3-5821-3111
Fax: 81-3-5821-3170

Korea

Sigma-Aldrich Korea
698-84 Maeng-ri
Wonsam-myun
Yong-In City, Kyunggi do
Korea
Tel: 82-31-329-9000
Fax: 82-31-329-9090

Malaysia

Sigma-Aldrich (M) Sdn Bhd
Tel: 03-7824181, 03-7808140
Fax: 03-7824067
E-mail: sigalm@po.jaring.my

Mexico

Sigma-Aldrich Química, S.A. de C.V.
Tel Gratis: 91-800-0075300
Tel: (72) 76 1600
Fax: (72) 76 1601
E-mail: mexico@sial.com

Netherlands

Sigma-Aldrich Chemie BV
Tel Gratis: 0800 022 9088
Fax Gratis: 0800 022 9089
Tel: 31-78-620 54 11
Fax: 31-78-620 54 21
E-mail: nlcustsv@eurnotes.sial.com

Norway

Sigma-Aldrich Norway AS
Tel: 47 23 176 000
Fax: 47 23 176 010
E-mail: nororder@eurnotes.sial.com

Poland

Sigma-Aldrich Sp.zo.o
Tel: (48-61) 823-24-81
Fax: (48-61) 823-27-81
E-mail: plcustsv@eurnotes.sial.com

Portugal

Sigma-Aldrich Quimica S.A.
Free Tel: 800-202180
Free Fax: 800-202178
E-mail, encomendas:
poorders@eurnotes.sial.com

Russia

Sigma-Aldrich Russia
Tel: 7-095-975-3321
Fax: 7-095-975-4792
E-mail: techcare@online.ru

Singapore

Sigma-Aldrich Pte., Ltd.
Tel: (65) 271 1089
Fax: (65) 271 1571
E-mail: sup@sial.com

South Africa

Sigma-Aldrich South Africa (Pty) Ltd.
Tel: +27 11 979 1188
Fax: +27 11 979 1119
E-mail: rsa@sial.com

Spain

Sigma-Aldrich Química S.A.
Free Tel: 900-101376
Free Fax: 900-102028
Tel: 91-6619977
Fax: 91-6619642
E-mail, pedidos:
esorders@eurnotes.sial.com

Sweden

Sigma-Aldrich Sweden AB
Tel: 020-35 05 10
Fax: 020-35 25 22
Outside Sweden Tel: 46-8-742 4200
Outside Sweden Fax: 46-8-742 4243
E-mail: sweorder@eurnotes.sial.com

Switzerland

Fluka Chemie GMBH
Tel: 41-81-755 28 28
Fax: 41-81-755 28 15
Swiss Free Call: 0800 80 00 80
E-mail: fluka@sial.com

United Kingdom

Sigma-Aldrich Company Ltd.
Free Tel: 0800 717181
Free Fax: 0800 378538
Tel: 01202 733114
Fax: 01202 715460
E-mail: ukcustsv@eurnotes.sial.com

United States

Aldrich Chemical Company, Inc.
Toll Free Tel: 1-800-558-9160
Toll Free Fax: 1-800-962-9591
Tel: 414-273-3850
Fax: 414-273-4979
E-mail: aldrich@sial.com
Sigma Chemical Company
Toll Free Tel: 1-800-521-8956
Toll Free Fax: 1-800-325-5052
Tel: 314-771-5765
Fax: 314-771-5757
E-mail: sigma@sial.com



P.O. Box 355
Milwaukee, WI 53201
USA

Return Service Requested

For Development/Manufacturing Quantities
Contact your local Sigma-Aldrich office
and ask for Sigma-Aldrich Fine Chemicals

For Quantity Pricing/Standing Orders
Contact your local Sigma-Aldrich office



World Headquarters • 3050 Spruce St., St. Louis, MO 63103 • (314) 771-5750 • <http://www.sigma-aldrich.com>



The
SIGMA-ALDRICH
Family

SIGMA
Biochemicals and
Reagents for Life
Science Research

ALDRICH
Organics and
Inorganics for
Chemical Synthesis

Fluka
Specialty Chemicals
and Analytical
Reagents for Research

Riedel-deHaën
Laboratory Chemicals
and Reagents for
Research and Analysis

SUPELCO
Chromatography
Products for Analysis
and Purification

Sigma-Aldrich Research is the research sales and marketing division of Sigma-Aldrich, Inc. Sigma-Aldrich Fine Chemicals is the development and manufacturing division of Sigma-Aldrich, Inc.

©2002 Sigma-Aldrich Co. Printed in USA. Aldrich brand products are sold through Sigma-Aldrich, Inc. Sigma-Aldrich, Inc. warrants that its products conform to the information contained in this and other Sigma-Aldrich publications. Purchaser must determine the suitability of the product(s) for their particular use. Additional terms and conditions may apply. Please see reverse side of the invoice or packing slip. SIGMA and are registered trademarks of Sigma-Aldrich Co. Riedel-de Haën®: trademark under license from Riedel-de Haën GmbH.