

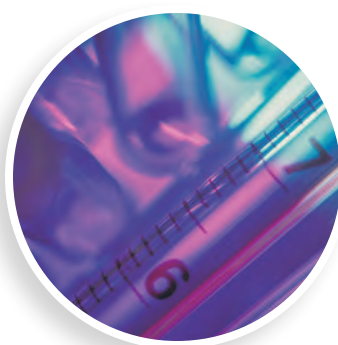


Cambridge Isotope
Laboratories, Inc.

Deuterated Solvents, Reagents & Accessories

for NMR and Synthetic Applications

- NMR Solvents • NMR Reference Standards • NMR Tubes
- qNMR • NMR Protein Standards • Deuterated Detergents
- Deuterated Buffers • Synthetic Intermediates



Enriching Scientific Discovery

Ordering Information

The CIL Customer Service Department is open from 8:00 a.m. to 5:30 p.m. Eastern Standard Time. Orders may be placed by fax, email or via our website 24 hours a day.

Phone: **1.800.322.1174** (North America)
1.978.749.8000

Fax: **1.978.749.2768**

Email: **cilsales@isotope.com**
intlsales@isotope.com (International)

Website: **isotope.com**

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Corporate Overview

Cambridge Isotope Laboratories, Inc. (CIL) is the world leader in the separation and manufacture of stable (nonradioactive) isotopes and isotope-labeled compounds.

With over 400 employees and laboratories in four countries, CIL specializes in the process of labeling biochemical and organic compounds with highly enriched stable isotopes of carbon, hydrogen, nitrogen and oxygen. Our chemists substitute a common atom for a rare, highly valued isotopic component so that the final product can be readily measured or traced using mass spectrometry (MS) or nuclear magnetic resonance (NMR). CIL's products are utilized in laboratories, health care facilities, and medical, government and academic research centers worldwide. We are proud that CIL products have contributed to medical advancements in cancer research, new drug development, environmental analysis, genomics and proteomics, and medical diagnostic research.

CIL's vision began when it was founded in 1981 by Dr. Joel Bradley, an organic chemist from MIT. Drawing on a commitment to high-quality products, superior customer service, innovative new products and breadth of product lines, CIL quickly emerged as a leader in its field. CIL now produces more than 15,000 products and has ISO 13485, ISO/IEC 17025 and ISO Guide 34 quality systems, as well as cGMP production capabilities. The CIL group is comprised of five companies: Cambridge Isotope Laboratories, Inc. (CIL) and CIL Isotope Separations (CIS) in the United States; CIL Canada, Inc. in Montreal, Canada; Euriso-Top in Saclay, France; and ABX GmbH in Dresden, Germany.

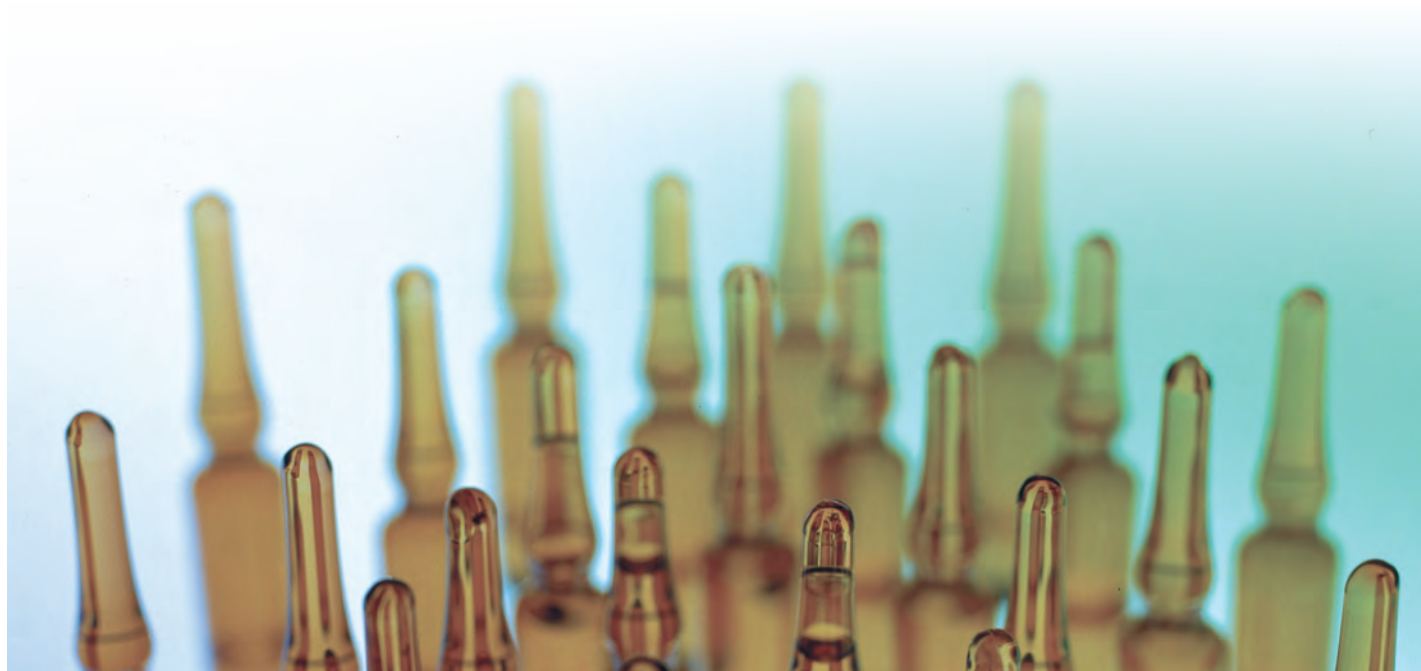
CIL has worked closely with industry leaders and researchers to provide stable isotope-labeled tools needed for improved quantitation of complex systems. This has been particularly true in the last decade, when many innovative techniques

for determining biomarkers for the presence, progression and monitoring of therapeutic response have emerged from the fields of MS-based proteomics and metabolomics.

CIL takes great pride in being able to offer a wide range of NMR solvents with the highest isotopic enrichment and chemical purity. All NMR solvents undergo thorough quality-control testing during the manufacturing and packaging process to verify that product quality is maintained. Continuous improvement and high-quality standards make CIL the preferred supplier to synthesis groups and CROs/CMOs worldwide.

CIL's state-of-the-art cGMP production and associated QC facilities are located at the company's headquarters in Tewksbury, Massachusetts, and the company's primary production laboratories are in Andover, Massachusetts. CIL's isotope-separation facility, located in Xenia, Ohio, houses the world's largest ^{13}C and ^{18}O isotope-separation facilities and the world's only commercial D_2O enrichment columns, as well as large-scale production of deuterium gas and deuterated reagents.

Dr. Bradley and the CIL executive team all share the same commitment to quality and service. CIL's experts collaborate with all of their customers to aid in pivotal research that is being conducted in laboratories worldwide. Our partnerships not only help to support our global reach, but allow us to bring forward innovative products to aid our customers' pursuit of scientific discovery.





NMR Solvents and Deuterated Reagents

Joel Bradley, PhD
Chief Executive Officer

CIL is the world's leading producer of deuterated NMR solvents for analysis and deuterated reagents for synthesis. For more than 30 years, CIL has continually expanded its capabilities to produce deuterated solvents and reagents on a larger scale and at even higher purities. During this time, the chemical synthesis group in Andover, Massachusetts, and the chemical engineering and isotope-separation group in Xenia, Ohio, have worked together

to develop newer and better ways to produce deuterated solvents and reagents for the growing analytical field and for new industrial applications.

CIL is pleased to discuss your needs for any deuterated solvents or reagents.



Quality Control Spotlight

Tim Eckersley, PhD
Director of Analytical Chemistry

The CIL Quality Control laboratory staff specialize in the analysis and characterization of stable isotope-labeled compounds. Their expertise in this area makes the laboratory a world leader in this field. The majority of the staff has been with CIL for ten years or more.

There is a comprehensive quality system in place for analysis of both nonregulated and regulated materials. The quality system covers all aspects of testing, including training of personnel, control of documents, compliance with regulatory requirements, maintenance of equipment, generation of analytical records, general test methods, recording of test results, and handling of out-of-specification results and materials.

CIL is compliant with ICH Q7, ISO 13485, ISO/IEC 17025, and ISO Guide 34 requirements. As such, CIL is routinely audited internally by its QA Department and externally by customers, notified bodies and regulatory agencies (e.g. FDA).

The laboratory handles testing for all of CIL's products and incoming raw materials, as well as in-process work for the production laboratories, shelf life and stability studies. The materials range in complexity and physical form, from simple gases (e.g. labeled oxygen) to complex organic molecules like erythromycin. The laboratory is equipped to test and characterize the 15,000 different materials that constitute the CIL inventory and associated intermediates. Tests range in complexity from simple physical and spectroscopic characterization to chromatographic tests for purity, chirality and mass spectrometric testing for isotopic enrichment.

The in-house testing capabilities cover GC/MS, GC/FID, GC/ECD, HPLC/UV, HPLC/RI, HPLC/ELSD, HPLC/DA, HPLC/Pickering, ^1H -NMR, ^{13}C -NMR, multi-nuclear NMR, wet chem, FTIR, TOC, polarimetry and KF testing. If the instrumentation required for a test is not available in-house, then the testing is subcontracted to a qualified vendor.

The laboratory has the personnel and systems in place to develop and validate new analytical methods, as well as to conduct testing according to all major standards. USP/NF and EP compendia methods are regularly used, and other compendia (BP and JP) are used as required.



Cambridge Isotope Laboratories, Inc. Facilities

CIL has state-of-the-art production facilities for cGMP and non-cGMP manufacturing at its locations in Andover and Tewksbury, Massachusetts.

CIL World Headquarters and cGMP Production Laboratories Tewksbury, MA USA

CIL moved into its new Tewksbury, Massachusetts, facility in the spring of 2013. As the new corporate headquarters, this facility houses the executive team, as well as sales, marketing, finance, regulatory affairs and cGMP production staff. In addition to corporate office space, the facility has a state-of-the-art cGMP suite, which includes production laboratories, dedicated isolation rooms, a dedicated analytical laboratory, a packaging laboratory and a development laboratory.



CIL Production Laboratories Andover, MA USA

CIL's primary production facility in Andover, Massachusetts, is dedicated to the manufacture of deuterated NMR solvents, stable isotope-labeled chemicals and gases, as well as specific cGMP products. This facility is home to operations staff and production and quality-control teams.

The formulations group has over 30 years' experience formulating highly purified labeled materials into high-quality quantitative solutions as analytical standards, either as single-component products or multi-component mixes and calibration solutions.

The quality-control lab is equipped with a wide array of instrumentation, including gas chromatograph/mass spectrometers (GC/MS), high-field NMRs, HPLCs and an FT-IR. CIL's chemistry laboratories are equipped with apparatus for both large-scale (50+ liters) and microscale chemistry, which includes equipment for high-pressure gas reactions, pH and temperature-controlled enzyme chemistry, high-resolution distillation processes, and catalytic reduction with both hydrogen and deuterium. The production laboratories are also equipped with analytical equipment for in-process testing, including GC-FID, GC-ECD and HPLC with UV, RI, ELSD and MS detectors. All of these resources allow CIL to consistently produce products with high chemical and isotopic purity.





CIL Isotope Separations, LLC (CIS) **Xenia, OH USA**

CIL is the world leader in the separation of ^{13}C and ^{18}O . CIL separates both ^{13}C and ^{18}O at its Xenia, OH, facility and has the world's largest production capacity for both ^{13}C and ^{18}O . CIL also has the only nongovernmental D_2O enrichment columns in the world located at its CIS facility.



CIL Canada, Inc. **Montreal, Canada**

CIL Canada, Inc. is CIL's biotech laboratory facility, which produces carbohydrates, enriched media and amino acids for drug-discovery applications. CIL Canada specializes in algal biosynthesis, including spirulina, chlorella and a variety of other algal strains for NMR and proteomics applications.



Euriso-Top **Saclay, France**

Euriso-Top (ET) was founded in January 1991 by a group of researchers from the Commissariat à l'Energie Atomique (CEA). Euriso-Top is Europe's leading producer of deuterated NMR solvents, cGMP urea and stable isotope-labeled compounds. Its quality control and production laboratories are equipped with NMR, MS, HPLC, GC, IR and UV instruments.



ABX GMBH **Dresden, Germany**

ABX is the world's leading supplier of ^{18}F positron emission tomography (PET) precursors, reagent kits and cassettes, including, but not limited to, kits for FDG, FLT, F-choline, NaF, F-Miso and FET. ABX specializes in the manufacture and development of chemicals for nuclear medicine, and its cGMP-approved laboratories, class 100 clean rooms and cGMP radiochemistry development hot lab uniquely position ABX to provide complete PET and SPECT chemistry solutions to radiochemists and radiopharmacists worldwide. ABX's radiochemistry hot lab is equipped with most of the leading commercial PET tracer synthesis boxes and allows ABX to assist customers with the optimization and development of new tracers.

Ordering and Contact Information

Placing an Order

Phone: 1-800-322-1174 (North America) or
1-978-749-8000 (International)
Office hours are 8:00 a.m. to 5:30 p.m.
Eastern Standard Time (EST)

Fax: 1-978-749-2768

Email: cilsales@isotope.com (North America)
intlsales@isotope.com (International)

E-commerce: Visit <http://shop.isotope.com> to request a quote,
place orders, obtain product information or submit
technical questions.

CIL products are constantly updated on the website so be sure
to visit <http://shop.isotope.com> for current information.

Please help us to expedite the shipment of your order by including
the following information:

- Shipping address, including street
- Billing address
- Purchase order number or credit card information
- CIL catalog number and product name
- Quantity: mg (milligrams), g (grams), kg (kilograms),
mL (milliliters), L (liters), etc., as applicable, including
number of units
- Catalog price or CIL quotation number with date given
- Special instructions for packaging or shipping
- Your name, phone number and email address
- End user name, phone number and email address
(if different)
- Preferred mode of shipping (e.g. FedEx or UPS)
- \$50 minimum order

We do not require written confirmation of phone orders for
established customers.

First-Time Orders

If ordering for the first time, please email or fax the following
information on company letterhead to establish a line of credit
with a copy of your order:

- A federal tax identification number
- Three credit/banking references

Also include your shipping address, billing address, phone, fax,
email and URL address.

*To expedite delivery of your first order, prepayment should be
made by credit card or wire transfer in US funds.*

**Please call 1-800-ISOTOPE (1-800-476-8673) to contact your
Regional Sales Manager with any inquiries or to request
a quotation.**

Pricing Information and Terms of Sale

North American Orders

- All prices are in US dollars. Any importation costs for
international orders are not included. Please consult our
Customer Service Department for pricing information or
packaging options.
- When stock is available and subdivision is possible, we will
accept orders for smaller than catalog amounts. Please request
a quotation as a quantity discount may apply.
- Please note that prices are subject to change without notice.
Occasionally the inventory of some products listed may become
depleted. Replacement of stock may be subject to a minimum
order quantity.
- You may check stock and confirm prices by contacting the
CIL Customer Service Department at 1-800-322-1174
(North America only) or cilsales@isotope.com.
- CIL will be pleased to assist customers with firm written
quotations. Most quotes are valid for 30-60 days. Longer
terms may be granted by CIL upon request.
- Net 30 days from invoice date with prior credit approval.
Past-due invoices will be subject to a 1.5% per month service
charge; 18% per annum. We reserve the right to request
payment in advance or COD terms on initial orders with CIL.
- We also accept VISA, MasterCard, American Express and
university purchasing card orders.
- Shipping terms are FCA Andover, MA USA. Any damage to
the package or product in transit is the buyer's responsibility
to adjust with the carrier.
- Domestic shipping charges will be added to invoices (unless
collect shipment is requested).

International Orders

- CIL has an extensive international sales network of over
33 representatives in 27 different countries.
- For international orders or quotations, please contact
CIL International Sales at intlsales@isotope.com or
+1-978-749-8000.
- For a complete distributor listing, please visit www.isotope.com.
- Our representatives and agents are available to assist you with
your requirements for our products. Please consult your local
CIL representative for appropriate pricing and payment terms.
Shipping charges and any applicable import duties and taxes
will be added to orders placed with distributors.
- For direct orders, CIL generally requires prepayment in US
dollars by an international bank check or bank wire transfer.
We will be pleased to provide *pro forma* invoices upon request.
Shipping charges will be added to direct orders. Any applicable
import duties and taxes will be charged to the purchaser by the
shipping company or customs agent.
- Shipping terms are FCA Andover, MA USA. Any damage to
the package or product in transit is the buyer's responsibility
to adjust with the carrier.

Shipping Information

USA

- Shipments within the United States will be sent via UPS, FedEx, or truck.
- Orders within the United States for in-stock items placed before 2 p.m. EST can ship the same day via FedEx or on the next working day via UPS.

Canada

- Canadian shipments will be sent via FedEx or truck.
- Please include the name of your customs broker.
- Orders to Canada for in-stock items will ship one to two working days after receipt of purchase order.

International

- International shipments will be sent via FedEx or best method.
- CIL tries to be as cost effective as possible, but the carrier may assess additional charges.

We will accommodate your shipping instructions whenever it is feasible to do so. CIL reserves the right to change the method of transportation, if required, to comply with transportation regulations. Such a change would not alter your responsibility for payment of shipping charges. Additional shipping charges may apply.

Return Shipment Policy

Returns may be made within 30 days of shipment with prior approval from CIL. We reserve the right to impose restocking charges when a return is at the sole option of the buyer. The buyer is responsible for approving the quality and quantity of any product within the 30-day period stated above. If an error by CIL results in an incorrect or duplicate shipment, a replacement will be sent or the appropriate credit allowed. We typically request return of the original product. Product returns must reference the original purchase order number, CIL order number (e.g. DB-A1000), Returned Goods Authorization (RGA) number, and the date CIL authorized the return. Under no circumstances will credit or replacement be given for products without prior authorization by CIL.

Product Information

Documentation

A Certificate of Analysis (COA) and a Material Safety Data Sheet (MSDS) are supplied with every shipment. Additional product information may be available upon request.

The chemical purity (CP) of CIL products is 98% unless otherwise indicated.

Limited Warranty

CIL represents that the products are, as of the date of shipment, as described in CIL's applicable product literature. CIL makes no other warranty, express or implied, with respect to its products, including any warranty of merchantability or fitness for any particular purpose. CIL's maximum liability for any reason shall be to replace any nonconforming product or refund the applicable purchase price.

Research Use Statement

CIL research products are labeled "For research use only. Not for use in diagnostic procedures." Persons intending to use CIL products in applications involving humans are responsible for complying with all applicable laws and regulations, including, but not limited to, the US FDA, other local regulatory authorities and institutional review boards concerning their specific application or desired use.

It may be necessary to obtain approval for using these research products in humans from the US FDA or the comparable governmental agency in the country of use. CIL will provide supporting information, such as lot-specific analytical data and test method protocols, to assist medical research groups in obtaining approval for the desired use.

Additional Information

24-Hour Emergency Response

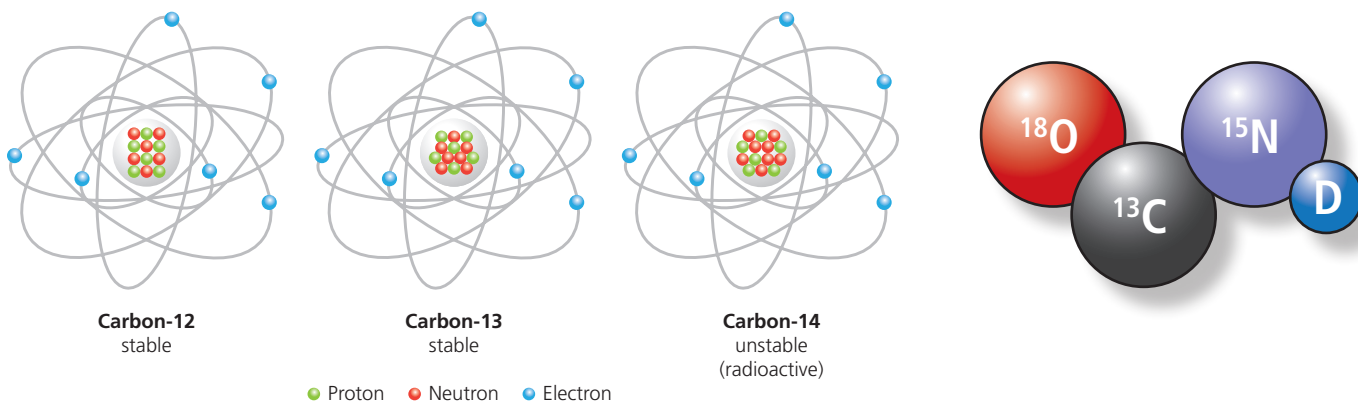
CIL and its direct subsidiary CIL Isotope Separations, LLC, are registered with Emergency Response CHEMTREC®. In the event of a chemical-transportation emergency, CHEMTREC® provides immediate advice for those at the scene of emergencies, then promptly contacts the shipper of the chemicals for more detailed assistance and appropriate follow-up. CHEMTREC® operates 24 hours a day, seven days a week to receive emergency calls. In the case of chemical-transportation emergencies, call one of the following numbers:

Continental United States:	Outside of Continental USA:
1-800-424-9300	1-703-527-3887
	(this number may be called collect)

CHEMTREC is a registered trademark of American Chemistry Council, Inc.

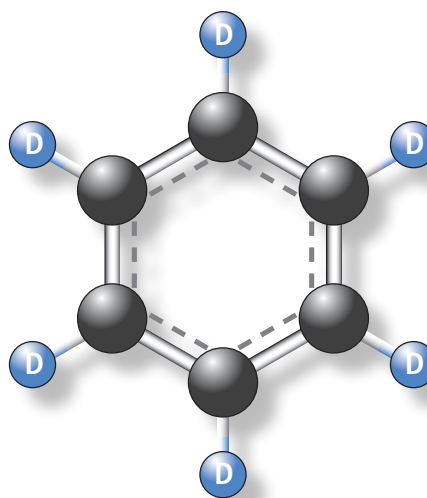
What Is an Isotope?

An isotope is any of two or more forms of a chemical element that has a different number of neutrons in the nucleus. There are 275 stable isotopes of the 81 nonradioactive elements, in addition to over 800 radioactive isotopes. Every element has known isotopic forms. Isotopes of a single element possess almost identical chemical properties.



Isotopic Enrichment

Isotopic enrichment is the average enrichment for each labeled atom in the molecule. It is not the percentage of molecules that are completely isotopically labeled. For instance, benzene (D_6 , 99%) is not 99% C_6D_6 and 1% C_6H_6 . Each of the six hydrogen atoms has a 99% chance of being a deuterium atom ($^2\text{H} = \text{D}$), and a 1% chance of being protium (^1H). Thus, $(99\%)^6$, or about 94% of the benzene molecules, will have a molecular mass that is six atomic mass units (amu) higher than native (unlabeled) benzene. About 6% will have a molecular mass that is 5 amu higher than native benzene. Theoretically, only $(1\%)^6$, or about $10^{-10}\%$, will have the molecular mass of native benzene.



Benzene (D_6 , 99%)

Globally Harmonized System (GHS) of Classification and Labeling of Chemicals

GHS Objectives

The objective of GHS is to create an internationally recognizable system for HazCom standards, establish a standard format for hazard communication and support the trade of chemicals for international exchange.










Material Safety Data Sheets (MSDS) are now referred to as Safety Data Sheets (SDS). The SDS functions as an MSDS for ISO, EU and ANSI requirements:

- Most comprehensive information source
- More hazards, including environmental hazards, are now included
- Provides advice and safety precautions
- Product focused; not workplace or task specific
- Written and supplied by manufacturer

Chemical manufacturers/importers/exporters are still responsible for providing information about the identities and hazards of chemicals. All employers using chemicals within their operations are still required to have a hazard communication program.

Below: World map showing nonstandard pictograms used to depict "toxicity." Below right: GHS pictograms are the new standard, and the map shows that the same icon for "toxicity" is now used worldwide.




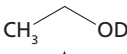
GHS Hazard Pictograms and Related Hazards Classes		
		
Expanding Bomb <ul style="list-style-type: none"> • Explosives • Self-reactives • Organic peroxides 	Corrosion <ul style="list-style-type: none"> • Skin corrosion/burns • Eye damage • Corrosive to metals 	Flame Over Circle <ul style="list-style-type: none"> • Oxidizing gases • Oxidizing liquids • Oxidizing solids
		
Gas Cylinder <ul style="list-style-type: none"> • Gases under pressure 	Environment <ul style="list-style-type: none"> • Aquatic toxicity 	Skull and Crossbones <ul style="list-style-type: none"> • Acute toxicity (fatal or toxic)
		
Exclamation Point <ul style="list-style-type: none"> • Irritant (eye and skin) • Skin sensitizer • Acute toxicity • Narcotic effects • Respiratory tract irritant • Hazardous to ozone layer (nonmandatory) 	Health Hazard <ul style="list-style-type: none"> • Carcinogen • Mutagenicity • Reproductive toxicity • Respiratory sensitizer • Target organ toxicity • Aspiration toxicity 	Flame <ul style="list-style-type: none"> • Flammables • Pyrophorics • Self-heating • Emits flammable gas • Self-reactives • Organic peroxides



Understanding the Product Listings

NMR Solvent Catalog Listings Include:

New Indicator: **NEW**

Compound Name	Enrichment	Alternative Name	Formula	Molecular Weight*	Unit
Ethanol-d (D, 99%)		Ethyl alcohol	$\text{CH}_3\text{CH}_2\text{OD}$	mw 47.08 d 0.89	5 g 2 x 50 g
CIL Catalog # → DLM-16					
CAS # → [925-93-9]					
UN # → 1170					
					
Hazard Class			Structure	Density	

Contains <6% D_2O
Packaged in glass ampoules only

Additional Information
Storage Information**


* Molecular weight is based on 100% enrichment

**Stable if stored under normal conditions, unless otherwise noted

CIL Labels

Our labels include:

- Product name and description
- Health and safety information
- Lot-specific number
- Package size
- Pictograms for hazard recognition
- CAS numbers
- Storage information
- Packaging number
- Catalog number



Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810 USA
978.749.8000


Warning

DIMETHYL SULFOXIDE-D6
(D, 99.9%)
DLM-10-10X0.75

10 X 0.75 MILLILITERS
Lot #: PR-26213/10054DMI
PSO #: 12B-264

Combustible liquid. Causes mild skin irritation. Causes eye irritation. IF IN EYES: Remove contact lenses if present. Rinse continuously with water.

Store at room temperature away from light and moisture.
For Research Use Only. Not for use in diagnostic procedures.




Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810 USA
978.749.8000

N-OCTANE-D18
(D, 99%)
DLM-50-5
PSO #: 12B-264 Lot #: PR-22855/081110C1

5 GRAMS

Hazard Statements
Highly flammable liquid and vapour. May be fatal if swallowed and enters airways. Causes skin irritation. May cause drowsiness or dizziness. Very toxic to aquatic life. May cause long lasting harmful effects to aquatic life.



Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810 USA
978.749.8000

CHLOROFORM-D
(D, 99.8%)
DLM-7-100
PSO #: 14K-188 Lot #: PR-26119/0914CL1

100 GRAMS

Store refrigerated (-5°C to 5°C). Protect from light.
Harmful if swallowed. Causes skin irritation. Causes serious eye irritation. Suspected of causing cancer. May cause damage to organs through prolonged or repeated exposure. Harmful to aquatic life.

Warning
Use personal protective equipment as required. IF IN EYES: Rinse with water for several minutes. Remove contact lenses.

Danger

Precautionary Statements
Keep away from heat/sparks/open flames/hot surfaces. No smoking. Avoid breathing dust/fume/gas/mist/vapours/spray. Avoid release to the environment. IF SWALLOWED immediately call a POISON CENTER or doctor/physician. Do NOT induce vomiting.

Storage
Store at room temperature away from light and moisture.

For Research Use Only. Not for use in diagnostic procedures.

Compounds listed in this catalog are considered nonhazardous unless otherwise noted.

NMR Analysis



About Our Solvents

CIL's NMR solvents are the preferred solvents worldwide for academic, pharmaceutical, industrial and government researchers.

CIL has two dedicated NMR spectrometers for in-process testing, as well as three additional NMR spectrometers in its Quality Control department. Every lot of CIL solvent is routinely tested for both chemical and isotopic purity prior to release to inventory. ^1H -NMR data is acquired for each solvent produced, and some solvents are tested for purity by GC/MS for contaminants that would not be observed by ^1H -NMR.

CIL's Quality Control Department tests for water content in solvents using the Karl Fischer titration method, and deuterated chloroform is tested for presence of phosgene. All chlorinated solvents are tested for acidity.

CIL's solvents are packaged under an argon or nitrogen atmosphere to ensure the purity is not compromised during packaging. CIL uses amber ampoules and bottles to protect photosensitive solvents from degradation. Every bottle or box of ampoules is clearly marked with a lot number for proper identification.



Acetic acid- d_4 (D, 99.5%)

DLM-12	CD_3COOD	mw 64.08	10 g
[1186-52-3]		d 1.12	25 g
UN# 2789			50 g



Acetic acid- d_4 "100%" (D, 99.93%)

DLM-41	CD_3COOD	mw 64.08	10 x 0.75 mL
[1186-52-3]		d 1.12	5 mL
UN# 2789			



Acetone- d_6 (D, 99.9%)

DLM-9	CD_3COCD_3	mw 64.12	10 x 0.5 mL
[666-52-4]		d 0.87	10 x 0.6 mL
UN# 1090			10 x 0.75 mL
			5 x 3 mL
			1 L
			10 x 1 g
			3 x (10 x 1 g)
			10 g
			10 x 10 g
			3 x (10 x 10 g)
			25 g
			100 g



Acetone- d_6 (D, 99.9%)

DLM-9ta	CD_3COOD_3	mw 64.12	10 x 1 g
[666-52-4]		d 0.87	3 x (10 x 1 g)
UN# 1090			10 g
			10 x 10 g
			3 x (10 x 10 g)
			25 g

Contains 1% v/v TMS



Acetone- d_6 (D, 99.9%)

DLM-9tb	CD_3COCD_3	mw 64.12	NEW 10 x 0.5 mL
[666-52-4]		d 0.87	10 x 1 g
UN# 1090			3 x (10 x 1 g)
			10 g
			10 x 10 g
			3 x (10 x 10 g)
			25 g

Contains 0.05% v/v TMS



Acetone- d_6 "100%" (D, 99.96%)

DLM-38	CD_3COCD_3	mw 64.12	5 x 0.5 mL
[666-52-4]		d 0.87	10 x 0.5 mL
UN# 1090			10 x 0.6 mL
			5 x 0.75 mL
			10 x 0.75 mL
			5 mL



Acetone- d_6 "100%" (D, 99.96%)

DLM-38tc	CD_3COCD_3	mw 64.12	10 x 0.75 mL
[666-52-4]		d 0.87	
UN# 1090			



Contains 0.03% v/v TMS

Acetonitrile- d_3 (D, 96-97%)

DLM-22	$\text{CD}_3\text{C}\equiv\text{N}$	mw 44.07	1 L
[2206-26-0]		d 0.84	
UN# 1648			



Acetonitrile- d_3 (D, 99.8%)

DLM-21	$\text{CD}_3\text{C}\equiv\text{N}$	mw 44.07	10 x 0.5 mL
[2206-26-0]		d 0.84	10 x 0.6 mL
UN# 1648			10 x 0.75 mL
			1 L
			10 x 1 g
			3 x (10 x 1 g)
			5 g
			10 g
			25 g
			50 g



Acetonitrile- d_3 (D, 99.8%)

DLM-21tb	$\text{CD}_3\text{C}\equiv\text{N}$	mw 44.07	10 x 0.6 mL
[2206-26-0]		d 0.84	
UN# 1648			



Contains 0.05% v/v TMS

Acetonitrile-d₃ "100%" (D, 99.96%)

DLM-53 [2206-26-0]	CD ₃ C≡N	mw 44.07 d 0.84	10 x 0.5 mL 10 x 0.6 mL 5 x 0.75 mL 10 x 0.75 mL 5 mL
UN# 1648			

**Benzene-d₆** (D, 99.5%)

DLM-1 [1076-43-3]	C ₆ D ₆	mw 84.15 d 0.95	10 x 0.5 mL 10 x 0.6 mL 10 x 0.75 mL 10 x 1 g 3 x (10 x 1 g) 5 g 10 g 10 x 10 g 25 g 50 g 100 g 1000 g
UN# 1114			

**Benzene-d₆** (D, 99.5%)

DLM-1tb [1076-43-3]	C ₆ D ₆	mw 84.15 d 0.95	10 x 0.6 mL 10 g
UN# 1114			



Contains 0.05% v/v TMS

Benzene-d₆ "100%" (D, 99.96%)

DLM-40 [1076-43-3]	C ₆ D ₆	mw 84.15 d 0.95	5 x 0.5 mL 10 x 0.5 mL 5 x 0.75 mL 10 x 0.6 mL 10 x 0.75 mL 5 mL
UN# 1114			

**Benzene-d₆ "100%"** (D, 99.96%)

DLM-40tc [1076-43-3]	C ₆ D ₆	mw 84.15 d 0.95	10 x 0.75 mL
UN# 1114			



Contains 0.03% v/v TMS

Bromobenzene-d₅ (D, 99.5%)

DLM-9595 [4165-57-5]	C ₆ D ₅ Br	mw 162.04 d 1.52	5 g 10 g 25 g
UN# 2514			

**Chlorobenzene-d₅** (D, 99%)

DLM-263 [3114-55-4]	C ₆ D ₅ Cl	mw 117.59 d 1.16	1 g 5 g
UN# 1134			

**Chloroform-d** (D, 99.8%)

DLM-7 [865-49-6]	CDCl ₃	mw 120.38 d 1.50	10 x 0.6 mL 10 x 0.75 mL 10 x 1 g 3 x (10 x 1 g) 50 g 100 g 10 x 100 g 3 x (10 x 100 g)
UN# 1888			



No stabilizers are used in this product

Chloroform-d (D, 99.8%)

DLM-7-50S DLM-7-100S [865-49-6]	CDCl ₃	mw 120.38 d 1.50	50 g 100 g NEW 100 mL
UN# 1888			



Stabilized with silver foil

Chloroform-d (D, 99.8%)

DLM-7ta [865-49-6]	CDCl ₃	mw 120.38 d 1.50	10 x 1 g 3 x (10 x 1 g) 50 g 100 g 10 x 100 g 3 x (10 x 100 g)
UN# 1888			



No stabilizers are used in this product

Chloroform-d (D, 99.8%)

DLM-7ta-100S [865-49-6]	CDCl ₃	mw 120.38 d 1.50	100 g
UN# 1888			



Stabilized with silver foil

Chloroform-d "100%" (D, 99.96%)

DLM-7tb [865-49-6]	CDCl ₃	mw 120.38 d 1.50	10 x 1 g 3 x (10 x 1 g) 50 g 100 g 10 x 100 g 3 x (10 x 100 g)
UN# 1888			



No stabilizers are used in this product

Chloroform-d (D, 99.8%)

DLM-7tb-50S DLM-7tb-100S [865-49-6]	CDCl ₃	mw 120.38 d 1.50	50 g 100 g
UN# 1888			



Stabilized with silver foil

Chloroform-d "100%" (D, 99.96%)

DLM-29 [865-49-6]	CDCl ₃	mw 120.38 d 1.50	10 x 0.25 mL 10 x 0.5 mL 10 x 0.6 mL 5 x 0.75 mL 10 x 0.75 mL 10 mL 5 x 10 mL 50 g
UN# 1888			



No stabilizers are used in this product

Chloroform-d "100%" (D, 99.96%)

DLM-29tc [865-49-6]	CDCl ₃	mw 120.38 d 1.50	10 x 0.75 mL
UN# 1888			

Contains 0.03% v/v TMS
No stabilizers are used in the product**Cyclohexane-d₁₂** (D, 99.5%)

DLM-17 [1735-17-7]	C ₆ D ₁₂	mw 96.23 d 0.89	5 x 1 g 10 x 1 g 3 x (10 x 1 g) 5 g 10 g
UN# 1145			

**Decalin-d₁₈** (D, 99%) Decahydronaphthalene

DLM-1386 [28788-42-3]	C ₁₀ D ₁₈	mw 156.36 d 1.01	1 g 5 g
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cis/trans mixture

trans-Decalin-d₁₈ (D, 98%)

DLM-1843 C₁₀D₁₈ mw 156.36 5 g
[493-02-7] d 1.01

**Deuterium bromide** (D, 99%)

DLM-3021 DBr mw 81.92 10 g (of soln.)
[13536-59-9] d 1.537 50 g (of soln.)



DBr 48% w/w solution in D₂O
Packaged in clear glass ampoules only

Deuterium chloride (D, 99.5%)

DLM-2 DCI mw 37.47 50 g (of soln.)
[7698-05-7] d 1.20



DCI 20% w/w solution in D₂O
Packaged in clear glass ampoules only

Deuterium chloride "100%" (D, 99.96%)

DLM-54 DCI mw 37.47 5 g (of soln.)
[7698-05-7] d 1.20 25 g (of soln.)



DCI 20% w/w solution in D₂O
Packaged in clear glass ampoules only

Deuterium chloride (D, 99.5%)

DLM-3 DCI mw 37.47 50 g (of soln.)
[7698-05-7] d 1.20



DCI 35% w/w solution in D₂O
Packaged in clear glass ampoules only

Deuterium oxide (D, 70%)

DLM-4-70 D₂O mw 20.03 1 kg
[7789-20-0] d 1.077
UN# 1957

Deuterium oxide (D, 70%)

DLM-2259-70 D₂O mw 20.03 1 kg
[7789-20-0] d 1.077 1 L
UN# 1957 Sterility tested

Deuterium oxide (D, 99%)

DLM-4-99 D₂O mw 20.03 1 kg
[7789-20-0] d 1.11 5 kg
UN# 1957

Deuterium oxide (D, 99.8%)

DLM-4-99.8 D₂O mw 20.03 1 kg
[7789-20-0] d 1.11 10 kg
UN# 1957 20 kg

Deuterium oxide (D, 99.8%)

DLM-2259 D₂O mw 20.03 100 mL
[7789-20-0] d 1.11 250 mL
UN# 1957 Sterility tested 1 L

Deuterium oxide (D, 99.9%)

DLM-4 D₂O mw 20.03 10 x 1 mL
[7789-20-0] d 1.11 10 g
UN# 1957 25 g
50 g
100 g
5 x 100 g
10 x 100 g
1000 g
1 L (inquire)

Deuterium oxide (D, 99.9%)

DLM-11 D₂O mw 20.03 100 g
[7789-20-0] d 1.11
UN# 1957

Glass distilled, low paramagnetic, low conductivity
Packaged in plastic bottles only

Deuterium oxide "100%" (D, 99.96%)

DLM-6 D₂O mw 20.03 10 x 0.6 mL
[7789-20-0] d 1.11 5 x 0.7 mL
UN# 1957 10 x 0.7 mL
10 x 0.75 mL
5 x (10 x 0.7 mL)
10 x 1 g
1000 g

Deuterium oxide "100%" (D, 99.96%)

DLM-6-s D₂O mw 20.03 10 g
[7789-20-0] d 1.11
UN# 1957

Packaged in serum bottles with Teflon-coated rubber
septum tops

Deuterium oxide "100%" (D, 99.96%)

DLM-6DB D₂O mw 20.03 10 x 0.7 mL
[7789-20-0] d 1.11 50 g
UN# 1957

Contains 0.01 mg/mL DSS

Deuterium oxide "100%" (D, 99.96%)

DLM-1172 D₂O mw 20.03 10 g
[7789-20-0] d 1.11
UN# 1957

Highest purity, glass distilled, low paramagnetic,
low conductivity. Packaged in plastic bottles only.

1,2-Dibromoethane-d₄ (D, 99%)

DLM-195 Br(CD₂)₂Br mw 191.87 10 g
[22581-63-1] d 2.20 25 g
UN# 1605

**1,2-Dichlorobenzene-d₄** (D, 99%)

DLM-158 C₆D₄Cl₂ mw 151.03 1 g
[2199-69-1] d 1.34 5 g
UN# 1591 25 g

**1,2-Dichloroethane-d₄** (D, 99%)

DLM-18 Cl(CD₂)₂Cl mw 102.98 1 g
[17060-07-0] d 1.30 5 x 1 g
UN# 1184 5 g

**Diethyl ether-d₁₀** (D, 99%)

DLM-1592 (CD₃CD₂)₂O mw 84.10 1 g
[2679-89-2] d 0.80 5 x 1 g
UN# 1155 5 g



Packaged in ampoules only

Diglyme-d₁₄ (D, 98%)

DLM-47 [38086-00-9]	(CD ₃ OCD ₂ CD ₂) ₂ O	mw 148.26 d 1.035	1 g 5 g 5 x 1 g 10 g
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**N,N-Dimethylformamide-d₇** (D, 99.5%) DMF

DLM-25 [4472-41-7]	DCON(CD ₃) ₂	mw 80.14 d 1.04	5 x 1 g 10 x 1 g 5 g 10 g
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Packaged in ampoules only

N,N-Dimethylformamide-d₇ (D, 99.5%) DMF

DLM-25tb [4472-41-7]	DCON(CD ₃) ₂	mw 80.14 d 1.04	10 x 0.6 mL
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Contains 0.05% v/v TMS
Packaged in ampoules only**Dimethyl sulfoxide-d₆** (D, 99.9%) DMSO

DLM-10 [2206-27-1]	CD ₃ SOCD ₃	mw 84.17 d 1.18	10 x 0.5 mL 10 x 0.6 mL 10 x 0.75 mL 5 x 3 mL NEW 10 mL NEW 50 mL 5 x 1 g 10 x 1 g 3 x (10 x 1 g) 5 g 10 g 100 g 10 x 10 g 3 x (10 x 10 g) 25 g 50 g 1000 g
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Dimethyl-sulfoxide-d₆ (D, 99.9%) DMSO

DLM-10-s [2206-27-1]	CD ₃ SOCD ₃	mw 84.17 d 1.18	NEW 10 mL 10 g 25 g
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Packaged in serum bottles with Teflon-coated rubber septum tops

Dimethyl-sulfoxide-d₆ (D, 99.9%) DMSO

DLM-10ta [2206-27-1]	CD ₃ SOCD ₃	mw 84.17 d 1.18	10 x 1 g 3 x (10 x 1) g 5 g 10 g 10 x 10 g 3 x (10 x 10) g 25 g 50 g
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Contains 1% v/v TMS

Dimethyl-sulfoxide-d₆ (D, 99.9%) DMSO

DLM-10tb [2206-27-1]	CD ₃ SOCD ₃	mw 84.17 d 1.18	NEW 10 x 0.5 mL 10 x 0.6 mL 10 x 0.7 mL 10 x 0.75 mL 10 x 1 g 3 x (10 x 1 g) 5 g 10 g 10 x 10 g 3 x (10 x 10 g) 25 g 50 g NEW 100 g
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Contains 0.05% v/v TMS

Dimethyl-sulfoxide-d₆ "100%" (D, 99.96%) DMSO

DLM-34 [2206-27-1]	CD ₃ SOCD ₃	mw 84.17 d 1.18	10 x 0.25 mL 5 x 0.5 mL 10 x 0.5 mL 10 x 0.6 mL 5 x 0.75 mL 10 x 0.75 mL 5 mL
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Dimethyl-sulfoxide-d₆ "100%" (D, 99.96%) DMSO

DLM-34tc [2206-27-1]	CD ₃ SOCD ₃	mw 84.17 d 1.18	10 x 0.75 mL
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Contains 0.03% v/v TMS

1,4-Dioxane-d₈ (D, 99.96%) *p*-Dioxane

DLM-28 [17647-74-4]	C ₄ D ₈ O ₂	mw 96.15 d 1.13	5 x 1 g 10 x 1 g 3 x (10 x 1 g) 5 g 10 g 25 g
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**DSS – ¹H-NMR chemical shift standard**

DLM-8206 [2039-96-5]	(CH ₃) ₃ Si(CD ₂) ₃ SO ₃ Na	mw 224.4	1 g
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UN# 1165

Sodium 2,2-dimethyl-2-silapentane-5-sulfonate (D₆, 98%)
Chemical purity 97%**DSS – ¹H-NMR chemical shift standard**

DLM-32 [2039-96-5]	(CH ₃) ₃ Si(CH ₂) ₃ SO ₃ Na	mw 218.3	1 g 10 g 50 g
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UN# 1165

Sodium 2,2-dimethyl-2-silapentane-5-sulfonate
Chemical purity 97%**Ethanol-d** (D, 99%) Ethyl alcohol

DLM-16 [925-93-9]	CH ₃ CH ₂ OD	mw 47.08 d 0.82	50 g 2 x 50 g
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UN# 1170

Contains ≤6% D₂O**Ethanol-d₆** (D, 99%) Ethyl alcohol

DLM-31 [1516-08-1]	CD ₃ CD ₂ OD	mw 52.11 d 0.89	5 x 1 g 10 x 1 g 5 g
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UN# 1170 3



Anhydrous

Ethanol-d₆ (D, 99%) Ethyl alcohol

DLM-31B [1516-08-1]	CD ₃ CD ₂ OD	mw 52.11 d 0.89	5 x 1 g 5 g
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UN# 1170 3

Contains ≤6% D₂O**Ethylene glycol-d₆** (D, 98%)

DLM-132 [15054-86-1]	DOCD ₂ CD ₂ OD	mw 68.11 d 1.22	5 g
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Fluorobenzene-d₅ (D, 98%)

DLM-617 C₆D₅F mw 101.13 1 g
 [1423-10-5] d 1.08
 UN# 2387

**n-Heptane-d₁₆** (D, 98%)

DLM-423 CD₃(CD₂)₅CD₃ mw 116.30 1 g
 [33838-52-7] d 0.794 5 g
 UN# 1206

**Hexafluoroacetone trideuterate** (D, 99.5%)

DLM-1020 CF₃COCF₃·3 D₂O mw 226.11 10 g
 [109640-39-3] d 1.71

**1,1,1,3,3,3-Hexafluoroisopropanol-d₂** (D, 98%)

DLM-143 (CF₃)₂CDOD mw 170.05 1 g
 [38701-74-5] d 1.62 5 x 1 g
 5 g
 10 g
Hexafluoroisopropyl alcohol, HFIP

**n-Hexane-d₁₄** (D, 98%)

DLM-139 CD₃(CD₂)₄CD₃ mw 100.26 1 g
 [21666-38-6] d 0.767 5 g
 UN# 1208

**Isopropanol-d₈** (D, 99%) 2-Propyl alcohol

DLM-44 (CD₃)₂CDOD mw 68.14 5 g
 [22739-76-0] d 0.90 25 g
 UN# 1219

**Lithium deuteroxide** (D, 99.5%)

DLM-2173 LiOD mw 24.96 25 g
 [12159-20-5] d 1.218 100 g



3N in D₂O solution
 Packaged in plastic bottles only

Methanol-d (D, 99%) Methyl alcohol

DLM-15 CH₃OD mw 33.05 50 g
 [1455-13-6] d 0.81 2 x 50 g
 UN# 1230

**Methanol-d₄** (D, 99.8%) Methyl alcohol

DLM-24 CD₃OD mw 36.07 10 x 0.5 mL
 [811-98-3] d 0.89 10 x 0.6 mL
 10 x 0.75 mL
 1 L
 NEW 5 x 1 g
 10 x 1 g
 3 x (10 x 1 g)
 5 g
 10 g
 10 x 10 g
 25 g
 50 g
 1000 g

**Methanol-d₄** (D, 99.8%) Methyl alcohol

DLM-24-s CD₃OD mw 36.07 10 g
 [811-98-3] d 0.89 25 g
 UN# 1230 50 g



Packaged in serum bottles with Teflon-coated rubber septum tops

Methanol-d₄ (D, 99.8%) Methyl alcohol

DLM-24tb CD₃OD mw 36.07 NEW 10 x 0.5 mL
 [811-98-3] d 0.89 10 x 0.6 mL
 10 x 0.75 mL
 10 x 1 g
 10 g
 10 x 10 g
 NEW 50 g



Contains 0.05% v/v TMS

Methanol-d₄ "100%" (D, 99.95%) Methyl alcohol

DLM-51 CD₃OD mw 36.07 10 x 0.25 mL
 [811-98-3] d 0.89 5 x 0.5 mL
 UN# 1230 10 x 0.5 mL
 10 x 0.6 mL
 5 x 0.75 mL
 10 x 0.75 mL

**Methylcyclohexane-d₁₄** (D, 99.5%)

DLM-288 C₆D₁₁CD₃ mw 112.27 1 g
 [10120-28-2] d 0.88 5 g
 UN# 2296

**Methylene chloride-d₂** (D, 99.9%) Dichloromethane

DLM-23 CD₂Cl₂ mw 86.95 NEW 10 x 0.5 mL
 [1665-00-5] d 1.30 10 x 0.75 mL
 UN# 1593 5 x 3 mL
 5 x 1 g
 10 x 1 g
 3 x (10 x 1 g)
 5 g
 10 g
 25 g
 NEW 100 g

**Methylene chloride-d₂** (D, 99.9%) Dichloromethane

DLM-23tb CD₂Cl₂ mw 86.95 10 x 0.6 mL
 [1665-00-5] d 1.35



Contains 0.05% v/v TMS

Methylene chloride-d₂ "100%" (D, 99.96%) Dichloromethane

DLM-55 CD₂Cl₂ mw 86.95 10 x 0.5 mL
 [1665-00-5] d 1.35 10 x 0.6 mL
 UN# 1593 5 x 0.75 mL
 10 x 0.75 mL
 5 mL

**N-Methyl-2-pyrrolidinone-d₉** (D, 97-99%) NMP

DLM-1988-97 mw 108.19 Please Inquire
 [185964-60-7] d 1.13

**Nitric acid-d** (D, 99%)

DLM-3037 DNO₃ mw 64.02 5 g (of soln.)
 [13587-52-5] d 1.026 25 g (of soln.)



65-70% w/w solution in D₂O
 Packaged in clear glass ampoules only

Nitrobenzene-d₅ (D, 99%)

DLM-294 C₆D₅NO₂ mw 128.14 5 g
 [4165-60-0] d 1.25 10 g
 UN# 1662 25 g

**Nitromethane-d₃** (D, 99%)

DLM-30 CD₃NO₂ mw 64.06 10 g
 [13031-32-8] d 1.20 25 g
 UN# 1261

**n-Octane-d₁₈** (D, 99%)

DLM-50 CD₃(CD₂)₆CD₃ mw 132.34 1 g
 [17252-77-6] d 0.815 5 g
 UN# 1262

**n-Pentane-d₁₂** (D, 98%)

DLM-1213 CD₃(CD₂)₃CD₃ mw 84.22 1 g
 [2031-90-5] d 0.73 5 g
 UN# 1265

**Phosphoric acid-d₃** (D, 99%)

DLM-1132 D₃PO₄ mw 101.01 50 g
 [14335-33-2] d 1.74 100 g

Approximately 85% w/w solution in D₂O

Pyridine-d₅ (D, 99.5%)

DLM-13 C₅D₅N mw 84.13 10 x 0.5 mL
 [7291-22-7] d 1.05 5 x 1 g
 UN# 1282 10 x 1 g
 3 x (10 x 1 g)
 10 g
 25 g
 50 g

3 x (10 x 1 g)

Pyridine-d₅ (D, 99.5%)

DLM-13tb C₅D₅N mw 84.13 **NEW** 10 x 0.5 mL
 [7291-22-7] d 1.05 10 x 0.6 mL
 UN# 1282 5 x 1 g
 10 x 1 g
 3 x (10 x 1 g)
 10 g
 25 g
 50 g

Contains 0.05% v/v TMS

Pyridine-d₅ "100%" (D, 99.94%)

DLM-39 C₅D₅N mw 84.13 5 x 0.5 mL
 [7291-22-7] d 1.05 10 x 0.5 mL
 UN# 1282 5 x 0.75 mL
 10 x 0.75 mL
 5 mL

10 x 0.75 mL

Sodium deuteroxide (D, 99.5%)

DLM-57 NaOD mw 41.00 50 g
 [14014-06-3] d 1.46

NaOD 30% w/w solution in D₂O
 Packaged in polyethylene bottles

Sodium deuteroxide (D, 99.5%)

DLM-45 NaOD mw 41.00 50 g
 [14014-06-3] d 1.46 100 g
 UN# 1282



NaOD 40% w/w solution in D₂O
 Packaged in polyethylene bottles

Sulfuric acid-d₂ (D, 99%)

DLM-33 D₂SO₄ mw 100.09 50 g
 [13813-19-9] d 1.86
 UN# 1282




96-98% solution in D₂O
 Packaged in glass ampoules only

1,1,2,2-Tetrachloroethane-d₂ (D, 99.6%) TCE


DLM-35 Cl₂CDCDCl₂ mw 169.86 5 g
 [33685-54-0] d 1.62 10 g
 UN# 1702 100 g

**Tetrahydrofuran-d₈** (D, 99.5%) THF

DLM-36  mw 80.16 **NEW** 10 x 0.5 mL
 [1693-74-9] d 0.99 10 x 0.75 mL
 UN# 2056 5 x 3 mL
 5 x 1 g
 10 x 1 g
 3 x (10 x 1 g)
 5 g
 10 g

Packaged in ampoules only

Tetrahydrofuran-d₈ "100%" (D, 99.95%) THF

DLM-56  mw 80.16 10 x 0.5 mL
 [1693-74-9] d 0.99 10 x 0.75 mL
 UN# 2056 5 mL

Packaged in ampoules only

Tetramethylsilane TMS

DLM-43 (CH₃)₄Si mw 88.22 50 g
 [75-76-3] d 0.64

NMR grade
 Chemical purity 99.9%

TMSP-2,2,3,3-d₄ (D, 98%) Sodium 3-trimethylsilylpropionate

DLM-48 (CH₃)₃SiCD₂CD₂CO₂Na mw 172.27 1 g
 [24493-21-8] d 1.52 5 x 1 g
 5 g

D₂O reference standard and
¹H-NMR chemical shift standard

Toluene-d₈ (D, 99.5%)

DLM-5 C₆D₅CD₃ mw 100.19 10 x 1 g
 [2037-26-5] d 0.94 3 x (10 x 1 g)
 UN# 1294 5 g
 10 g
 25 g
 100 g
 1000 g




1000 g

Toluene-d₈ "100%" (D, 99.94%)

DLM-42 C₆D₅CD₃ mw 100.19 5 x 0.5 mL
 [2037-26-5] d 0.94 10 x 0.5 mL
 UN# 1294 5 x 0.75 mL
 10 x 0.75 mL
 5 mL

5 mL

Trifluoroacetic acid-d (D, 99.5%)

DLM-46 [599-00-8]	CF ₃ COOD	mw 115.03 d 1.50	NEW 10 x 0.5 mL 10 x 0.75 mL 10 x 1 g 10 g 25 g 4 x 25 g
UN# 2699			
  	Packaged in ampoules only		

2,2,2-Trifluoroethanol-d₂ (D, 98%) Trifluoroethyl alcohol

DLM-2318 [77253-67-9]	CF ₃ CD ₂ OH	mw 102.05 d 1.37	1 g 5 g
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**2,2,2-Trifluoroethanol-d₃** (D, 99%) Trifluoroethyl alcohol

DLM-27 [77253-67-9]	CF ₃ CD ₂ OD	mw 103.06 d 1.42	1 g 5 x 1 g
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**2,2,2-Trifluoroethanol-d₃ "100%"** (D, 99.85%) Trifluoroethyl alcohol

DLM-58 [77253-67-9]	CF ₃ CD ₂ OD	mw 103.06 d 1.42	1 g 5 g
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**1,3,5-Trimethyl benzene** (D₁₂, 98%) Mesitylene

DLM-3105 [69441-16-3]	C ₃ D ₃ (CD ₃) ₃	mw 132.26	5 g
UN# 2325			

**Water, deuterium depleted**

DLM-52 [7732-18-5]	H ₂ O	mw 18.02 d 1.00	25 g 100 g
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2-3 ppm deuterium

o-Xylene-d₁₀ (D, 98%)

DLM-808 [56004-61-6]	C ₆ D ₄ (CD ₃) ₂	mw 116.23 d 0.953	5 g
UN# 1307			

**p-Xylene-d₁₀** (D, 98%)

DLM-313 [41051-88-1]	C ₆ D ₄ (CD ₃) ₂	mw 116.23 d 0.948	5 g
UN# 1307			

**¹²C and ¹²C/Deuterium-Labeled Solvents (¹³C Depleted)****Benzene** (¹²C₆, 99.95%)

CLM-867 [71-43-2]	*C ₆ H ₆	mw 78.05 d 0.874	0.8 mL
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¹³C depleted**Chloroform** (¹²C, 99.95%; D, 99%)

CDLM-844 [865-49-6]	*CDCl ₃	mw 120.38 d 1.500	Inquire
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¹³C depleted**Glycerol** (¹²C₃, 99.95%; D₈, 98%)

CDLM-8660 [56-81-5]	DO*CD ₂ *CD(OD)*CD ₂ OD	mw 100.11 d 1.250	1g 5g 10g
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¹³C depleted**Methanol** (¹²C, 99.95%) Methyl alcohol

CLM-2472 [67-56-1]	*CH ₃ OH	mw 32.04 d .0791	1 g
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¹³C depleted**Methanol** (¹²C, 99.95%; D₄, 99.5%) Methyl alcohol

CDLM-01 [811-98-3]	*CD ₃ OD	mw 36.07 d 0.888	0.8 mL 5g
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¹³C depleted

NMR Reference Standards

As the leading supplier of NMR reference standards to the world's largest NMR manufacturers, CIL has an extensive offering of NMR reference standards. These standards help to assure proper spectrometer performance. CIL's total quality-assurance protocols and in-house manufacturing capabilities guarantee the highest

level of quality the first time, and every time. The NMR reference standards have been evaluated and determined to meet or exceed industry requirements. A representative listing of CIL's most popular NMR reference standards is provided below.

***All reference standards are filled to 2±0.12 inch except for ULM-71 and ULM-69, which are filled to 0.79±0.12 inch, unless noted otherwise.**

Catalog No.	Description	Application	Tube Size
DLM-79	1% 1,2-Dichlorobenzene in acetone-d ₆ (D, 99.9%)	¹ H-Resolution	5 mm x 8"
DLM-74	0.1% Ethylbenzene + 0.01% TMS in chloroform-d "100%" (D, 99.96%)	¹ H-Sensitivity	5 mm x 8"
DLM-67	1% 3-Heptanone in chloroform-d (D, 99.8%)	¹ H APT Test	5 mm x 8"
ULM-73	12% TMS in chloroform	¹ H-Reference/Calibration	5 mm x 8"
DLM-84	5% Ethylbenzene + 2% TMS in chloroform-d (D, 99.8%)	¹ H-Sensitivity/Reference	5 mm x 8"
DLM-76	1% Chloroform in acetone-d ₆ (D, 99.9%)	¹ H-Line Shape	5 mm x 8"
DLM-90	0.1 mg/mL GdCl ₃ ·6H ₂ O in D ₂ O (D, 99.96%)	¹ H-Homogeneity	5 mm x 8"
DLM-72	40% <i>p</i> -Dioxane in benzene-d ₆ (D, 99.6%)	¹³ C-Sensitivity/Resolution	5 mm x 8"
DLM-66	30% Menthol (by weight) in chloroform-d (D, 99.8%)	¹³ C App Test	5 mm x 8"
DLM-68	90% Formamide in DMSO-d ₆ (D, 99.9%)	¹⁵ N-Sensitivity	5 mm x 8"
DLM-77	0.0485 M Triphenylphosphate in chloroform-d (D, 99.8%)	³¹ P-Sensitivity	5 mm x 8"
DLM-78	0.05% α,α,α-Trifluorotoluene in benzene-d ₆ (D, 99.6%)	¹⁹ F-Sensitivity	5 mm x 8"
CDLM-100	0.1% Methanol- ¹³ C + 0.3 mg/mL GdCl ₃ in 98.9% D ₂ O + 0.1% H ₂ O	Auto Test Sample	5 mm x 8"
DLM-88	0.1 mg/mL GdCl ₃ + 0.1% DSS in 20% H ₂ O in D ₂ O	Gradient Shimming	5 mm x 8"
CDLM-96	1% ¹³ CH ₃ I, 0.2% Cr(acac) ₃ + 1% (CH ₃ O) ₃ P in CDCl ₃ "100%"	Indirect Detection Test	5 mm x 8"
DNLM-97	0.2% Cr(acac) ₃ + 2% Benzamide (¹⁵ N,98%+) in DMSO-d ₆ "100%" (D, 99.96%)	Indirect Detection Test	5 mm x 8"
ULM-71	100% Ethylene glycol*	High Temperature Calibrant	5 mm x 8"
ULM-69	100% Methanol*	Low Temperature Calibrant	5 mm x 8"
ULM-92	10% TMS in methanol	Low Temperature Measurement	5 mm x 8"
CDNLM-5003	0.1 M Urea- ¹⁵ N + 0.1 M MeOH- ¹³ C in DMSO-d ₆ 100%	Indirect Detection Experiments	5 mm x 8"
DLM-5022	2% 2-Ethyl-1-indanone in chloroform-d	2D Calibration	5 mm x 8"
CDNLM-7011	0.1% Methanol- ¹³ C - 0.1% acetonitrile- ¹⁵ N + 0.3 mg/mL in 98.8% D ₂ O + 1% H ₂ O	Auto Test Sample	5 mm x 8"
DLM-7049	5% Ethyl <i>trans</i> -crotonate + 1% TMS in CDCl ₃ in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
DLM-7047	98% <i>N</i> -Propyl benzoate + 2% TMS in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
DLM-5001	10% Ethylbenzene in chloroform-d (540 pp tube)	¹³ C Sensitivity	5 mm x 8"

CIL's Commitment

CIL is committed to assisting you with your research by providing **customized solvent mixtures, buffers and NMR standards**. We welcome your requests for **custom formulations** or **other reference standards**, as well as **alternative fill heights** of existing **reference standards**. To submit a custom request, please contact your local CIL representative.

Phone: 1.800.322.1174 (North America)
+1.978.749.8000 (International)
Fax: 978.749.2768
Email: cilsales@isotope.com

Requests may be submitted on our website at isotope.com/request.

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Special Purpose High-Throughput NMR Sample Tubes

Part No.	Package Size	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Concentricity (mm)	Camber (mm)
502-7	50	100	4.97 ± 0.050	4.20 ± 0.050	7	0.020	0.070
502-8	50	100	4.97 ± 0.050	4.20 ± 0.050	8	0.020	0.070

Standard Series for Routine NMR

Part No.	Package Size	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Concentricity (μm)	Camber (μm)
507-HP-7	5	400	4.97 ± 0.013	4.20 ± 0.025	7	0.0070	0.019
507-HP-8	5	400	4.97 ± 0.013	4.20 ± 0.025	8	0.0070	0.019
508-UP-7	5	500	4.97 ± 0.013	4.20 ± 0.025	7	0.0050	0.013
508-UP-8	5	500	4.97 ± 0.013	4.20 ± 0.025	8	0.0050	0.013
XR-55-7	25	300	4.97 ± 0.025	4.20 ± 0.025	7	0.010	0.038
XR-55-8	25	300	4.97 ± 0.025	4.20 ± 0.025	8	0.010	0.038

Select Series for High-Resolution NMR

Part No.	Package Size	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Concentricity (μm)	Camber (μm)
S-5-200-7	5	200	4.97 ± 0.030	4.20 ± 0.030	7	0.0090	0.0350
S-5-200-8	5	200	4.97 ± 0.030	4.20 ± 0.030	8	0.0090	0.0350
S-5-300-7	5	300	4.97 ± 0.025	4.20 ± 0.025	7	0.0070	0.0250
S-5-300-8	5	300	4.97 ± 0.025	4.20 ± 0.025	8	0.0070	0.0250
S-5-400-7	5	400	4.97 ± 0.013	4.20 ± 0.025	7	0.0070	0.0190
S-5-400-8	5	400	4.97 ± 0.013	4.20 ± 0.025	8	0.0070	0.0190
S-5-500-7	5	500	4.97 ± 0.013	4.20 ± 0.025	7	0.0050	0.0130
S-5-500-8	5	500	4.97 ± 0.013	4.20 ± 0.025	8	0.0050	0.0130
S-5-600-7	5	600	4.97 ± 0.006	4.20 ± 0.012	7	0.0040	0.0060

CIL provides a wide selection of NMR tubes. Download a complete guide to help you find the right one for your next research project.

isotope.com/nmrtubes



WilmaLabGlass NMR Sample Tubes

WilmaLabGlass is a leading manufacturer of NMR sample tubes and accessories. CIL has partnered with WilmaLabGlass for many years, offering the best possible Pyrex® and quartz precision tubes, as well as glass tubes and other accessories.



www.wilma-labglass.com

Pyrex® Glass Precision Tubes

5 mm O.D. Precision Tubes

Part No.	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Wall Thickness (mm)	Concentricity (μm)	Camber (μm)
535-PP-7	600	4.9635±0.0065	4.2065±0.0065	7	0.38	13	6
528-PP-7	500	4.9635±0.0065	4.2065±0.0065	7	0.38	25	13
528-PP-8	500	4.9635±0.0065	4.2065±0.0065	8	0.38	25	13
527-PP-7	400	4.9635±0.0065	4.2065±0.0065	7	0.38	25	25
527-PP-8	400	4.9635±0.0065	4.2065±0.0065	8	0.38	25	25
507-PP-7	300	4.9635±0.0065	4.2065±0.0065	7	0.38	51	25
505-PS-7	100	4.9635±0.0065	4.2065±0.0065	7	0.38	76	51

10 mm O.D. Precision Tubes

Part No.	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Wall Thickness (mm)	Concentricity (μm)	Camber (μm)
513-7PP-7	500	9.9935±0.0065	9.07±0.013	7	0.46	38	13
513-1PP-7	200	9.9935±0.0065	9.07±0.013	7	0.46	254	51

NMR Quartz Precision Tubes

Part No.	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Wall Thickness (mm)	Concentricity (μm)	Camber (μm)
535-PP-7QTZ	600	4.9635±0.0065	4.2065±0.0065	7	0.38	13	6
528-PP-7QTZ	500	4.9635±0.0065	4.2065±0.0065	7	0.38	25	13

Coaxial Insert for Samples with Limited Volume

Part No.	MHz Rating	Fits Outer Tube	Stem Height (mm)	Stem O.D. (mm)	Sample Capacity (μL)
WGS-5BL	600	Any Precision Tube with 5 mm O.D., 7" length and 0.38 mm wall thickness	50	2.0195±0.0125	530

Gas-tight NMR Tubes for Air-Sensitive Samples

Part No.	MHz Rating	O.D. (mm)	I.D. (mm)	Tube Length (inch)	Wall Thickness (mm)
528-LPV-7	500	4.9635±0.0065	4.2065±0.0065	7	0.38
507-LPV-7	300	4.9635±0.0065	4.2065±0.0065	7	0.38

N51A Glass Economy Tubes

5 mm O.D. Economy Tubes

Part No.	MHz Rating	O.D. (mm)	Wall Thickness (mm)	Length (inch)	Concentricity (μm)	Camber (μm)
WG-1235-7	>400	4.93395±0.03175	0.43	7	13	6
WG-1228-7	400	4.93395±0.03175	0.43	7	25	13
WG-1228-8	400	4.93395±0.03175	0.43	8	25	13
WG-1226-7	300	4.93395±0.03175	0.43	7	51	13
WG-1226-8	300	4.93395±0.03175	0.43	8	51	13
WG-5MM-ECONOMY-7	100	4.93395±0.03175	0.43	7	76	76
WG-5MM-ECONOMY-8	100	4.93395±0.03175	0.43	8	76	76

Bulk Pack 5 mm Economy Tubes (100 tubes, no cap)

Part No.	MHz Rating	O.D.(mm)	Wall Thickness (mm)	Length (inch)
WG-1000-7	100	4.93395±0.03175	0.43	7

The tube length for the above LPV tubes does not include the valve and the top glass adapter.

Use and Handling of NMR Solvents

CIL has implemented extensive quality-control protocols for the evaluation of chemical and isotopic purities of its solvents. CIL understands that the increase in sensitivity and resolution of today's high-field NMR instruments requires solvents with the highest chemical purity as well as high isotopic enrichment. Each lot of NMR solvents receives thorough quality-control testing before being released for shipment. All ampoules and bottles are clearly marked with both a production and a packaging lot number for easy tracking in the unlikely event that a problem should occur.

Water Peaks

Water contamination is a common problem for deuterated NMR solvents. There are several things that can be done to minimize/eliminate water peaks.

- Consider using single-use ampoules. Many of CIL's solvents are available in single-use breakseal ampoules ranging in size from 0.25 mL to 3 mL.
- Handle solvents in a dry atmosphere.
- Dry NMR tubes and pipettes used for sample preparation overnight in an oven and cool them in a desiccator prior to use.
- Precondition an NMR tube by rinsing it with D₂O. Remove residual D₂O by rinsing first with methanol-d₄ or acetone-d₆ and then with the solvent of choice. This process will not remove water, but it will exchange the protons for deuterium and minimize the water peak.

"100%" D₂O

To avoid loss of enrichment due to exchange with ambient moisture, "100%" D₂O stored in a serum bottle should be sampled with a syringe that has been preflushed with dry nitrogen. Additionally, a volume of dry nitrogen equal to the amount of D₂O being removed should be injected into the serum bottle prior to withdrawing D₂O.

TMS Evaporation

When stored at room temperature (unless noted below) and properly capped, solvents containing TMS should not suffer from TMS evaporation. However, upon extended storage of these solutions, some loss of TMS may occur.

Storage

All serum bottles should be stored upright in a refrigerator; freezing is not recommended. It is recommended that chloroform, diethyl ether, diglyme, tetrahydrofuran and TMS be stored in a refrigerator.

NMR Solvent Technical Tips

- Solvent users often require a specific custom mixture of two or more solvents. CIL's expert packaging technicians are uniquely qualified to formulate custom solvent preparations.
- To measure acidity in deuterium oxide solutions: calculate pD by adding 0.4 to the reading taken from the glass electrode pH meter. (Glasoe and Long. 1960. *J Phys Chem*, 64, 188).
- Dimethyl sulfoxide (DMSO) has a melting point of 18°C, freezing close to room temperature. Upon delivery, DMSO will sometimes be in a solid state. To return the material to a liquid state, thaw it in a warm water bath. Care must be taken to prevent water contamination.
- CIL recommends refrigeration of solvents packaged in serum bottles to extend the product shelf life, maintain high purity and ensure product quality. Serum bottles should be tested after six months.
- It is recommended that chloroform, diethyl ether, diglyme, tetrahydrofuran and TMS be stored in a refrigerator.
- In order to avoid isotopic contamination, some products, especially deuterated compounds, should be handled under an inert atmosphere, such as dry nitrogen or argon.
- You may see a split water peak in your solvent because the Karl Fischer technique measures the total of H₂O + D₂O. In all cases where both H₂O and D₂O are present, there will also be HOD present due to the chemical exchange equilibrium. It is not possible to guarantee there will be no HOD present in the solvents under these circumstances. However, CIL takes great care to minimize the amount of D₂O present in the solvents. Thus, a negligible amount of HOD may remain but will not be observable in the NMR spectrum of most solvents. Occasionally, a separate peak from HOD, ~0.02 ppm upfield of the H₂O peak, may be observed in the DMSO-d₆ or acetonitrile-d₃ (for example), due to the slower equilibrium that exists between H₂O and D₂O and these solvents.
- CIL also specializes in ¹³C-depleted and deuterium-depleted compounds. Please contact us if you do not see the ¹³C-depleted/deuterium-depleted compound of interest.
- CIL welcomes your requests for custom formulations of reference standards not listed in this section.
- CIL's NMR solvent data chart is available as a laminated reference document. Please contact your customer account coordinator to request a copy.

Deuterated Chloroform

The deuterated chloroform produced at CIL is of the highest chemical purity. Over time, chloroform will decompose regardless of the storage container or conditions. Over many months of storage at room temperature (for example, in a stockroom), deuterated chloroform can become acidic. However, decomposition is minimized if bottles are stored refrigerated in the dark.

CIL takes several precautions during production and packaging of chloroform-d to further minimize decomposition. Exposure to oxygen is minimized by using an argon atmosphere during production and packaging. Amber bottles are used to protect the product from light. For international orders, silver foil is added to the solvent to act as a radical scavenger, which helps to stabilize the material over time.

Quality Control of Deuterated Chloroform

To ensure the highest quality, CIL routinely tests each batch of solvent for chemical and isotopic purity. The chemical purity is monitored during production and packaged using ^1H NMR, GC, Karl Fischer titration for total water content and other wet chemical methods for acidity and various impurities.

Proper Storage and Use of Deuterated Chloroform

Unopened bottles of chloroform-d should be refrigerated between -5°C to $+5^\circ\text{C}$ to maximize shelf life. Moisture and oxygen will be introduced to the solvent following initial use due to air entering the bottle upon opening. Decomposition can follow, which results in the deuterated chloroform becoming acidic.

The acidity can be easily tested using the following method:

- A 1 mL aliquot of the solvent is added to a test tube containing 1 mL of distilled water (pH 5.0-7.0) and two drops of bromothymol blue (0.04% w/v).
- The color is compared to a 2 mL blank of distilled water (pH 5.0-7.0). If the sample solution is discolored (yellow) relative to the blank (blue-green), then the deuterated chloroform is acidic.

Samples of deuterated chloroform that have become acidic can be easily neutralized using the following procedure:

- Place 3-5 grams of 5Å molecular sieves into a 50 g or 100 g bottle of the solvent.
- Swirl slightly and allow to stand overnight. Excess water and traces of acidity will be removed. This is also the preferred way to store chloroform-d bottles once they have been opened, as it will keep the solvent dry and stable over time.
- Maintain an inert atmosphere (argon or nitrogen) in the bottle.
- Small “dust or powder” particles may break off from the molecular sieves. However, these particles can be removed simply by filtering the quantity of deuterated chloroform needed for an NMR sample through a small plug of glass wool or cotton in a glass pipette.

Special Applications Requiring Ultra-Dry and Acid-Free Deuterated Chloroform

For applications involving highly acid-sensitive or moisture-sensitive compounds, deuterated chloroform can be further purified prior to use. Solvents treated in the following manner will be exceptionally dry and acid free.

- Place a glass wool plug into a disposable glass pipette (~7 mm diameter).
- Add dry alumina powder into the pipette to a height of 3-4 cm.
- Pass the solvent through the small alumina bed into the sample container containing the product to be analyzed.
- Analyze the sample as soon as possible.

This procedure will ensure that the deuterated chloroform is as dry and free of trace amounts of acid as possible prior to contact with the sample. Note that the chloroform will react with basic compounds, such as alkaloids or amines. If the product is to be recovered, this should take place as soon as possible to minimize possible reaction.

NMR Solvent Data Chart

More Solvents, More Sizes, More Solutions

	¹ H Chemical Shift (ppm from TMS) (multiplicity) ✱	JHD (Hz)	¹³ C Chemical Shift (ppm from TMS) (multiplicity) ✱	JCD (Hz)	¹ H Chemical Shift of HOD (ppm from TMS) ●	Density at 20°C ◆	Melting point (°C) ◆	Boiling point (°C) ◆	Dielectric Constant	Molecular Weight ◆
Acetic acid-d ₄	11.65 (1) 2.04 (5)	2.2	178.99 (1) 20.0 (7)	20	11.5	1.12	16.7	118	6.1	64.08
Acetone-d ₆	2.05 (5)	2.2	206.68 (1) 29.92 (7)	0.9 19.4	2.8*	0.87	-94	56.5	20.7	64.12
Acetonitrile-d ₃	1.94 (5)	2.5	118.69 (1) 1.39 (7)	21	2.1*	0.84	-45	81.6	37.5	44.07
Benzene-d ₆	7.16 (1)		128.39 (3)	24.3	0.4	0.95	5.5	80.1	2.3	84.15
Chloroform-d	7.24 (1)		77.23 (3)	32.0	1.5*	1.50	-63.5	61-62	4.8	120.38
Cyclohexane-d ₁₂	1.38 (1)		26.43 (5)	19	0.8	0.89	6.47	80.7	2.0	96.24
Deuterium oxide	4.80 (DSS) 4.81 (TSP)		NA	NA	4.8	1.11	3.81	101.42	78.5	20.03
<i>N,N</i> -Dimethyl-formamide-d ₇	8.03 (1) 2.92 (5) 2.75 (5)	1.9 1.9	163.15 (3) 34.89 (7) 29.76 (7)	29.4 21.0 21.1	3.5	1.03	-61	153	36.7	80.14
Dimethyl sulfoxide-d ₆	2.50 (5)	1.9	39.51 (7)	21.0	3.3*	1.19	18.55	189	46.7	84.17
1,4-Dioxane-d ₈	3.53 (m)		66.66 (5)	21.9	2.4	1.13	11.8	101.1	2.2	96.16
Ethanol-d ₆	5.19 (1) 3.56 (1) 1.11 (m)		56.96 (5) 17.31 (7)	22 19	5.3	0.89	-114.1	78.5	24.5	52.11
Methanol-d ₄	4.87 (1) 3.31 (5)	1.7	49.15 (7)	21.4	4.9	0.89	-97.8	64.7	32.7	36.07
Methylene chloride-d ₂	5.32 (3)	1.1	54.00 (5)	27.2	1.5	1.35	-95	39.75	8.9	86.95
Pyridine-d ₅	8.74 (1) 7.58 (1) 7.22 (1)		150.35 (3) 135.91 (3) 123.87 (3)	27.5 24.5 25	5	1.05	-41.6	115.2-115.3	12.4	84.13
1,1,2,2-Tetrachloroethane-d ₂	6.0		73.78 (3)			1.62	-44	146.5	8.20	169.86
Tetrahydrofuran-d ₈	3.58 (1) 1.73 (1)		67.57 (5) 25.37 (5)	22.2 20.2	2.4-2.5	0.99	-108.5	66	7.6	80.16
Toluene-d ₈	7.09 (m) 7.00 (1) 6.98 (5) 2.09 (5)	2.3	137.86 (1) 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)	23 24 24 19	0.4	0.94	-95	110.6	2.4	100.19
Trifluoroacetic acid-d	11.50 (1)		164.2 (4) 116.6 (4)		11.5	1.49	-15.4	72.4		115.03
Trifluoroethanol-d ₃	5.02 (1) 3.88 (4x3)	2(9)	126.3 (4) 61.5 (4x5)	22	5	1.41	-43.5	74.05		103.06

O'Neil, M.J.; Heckelman, P.E.; Koch, C.B.; Roman, K.J. 2006. *The Merck Index*, an Encyclopedia of Chemicals, Drugs, and Biologicals – Fourteenth Edition, Merck Co., Inc. Whitehouse Station, NJ.

✱ The ¹H spectra of the residual protons and ¹³C spectra were obtained on a Varian Gemini 200 spectrometer at 295°K. The NMR solvents used to acquire these spectra contain a maximum of 0.05% and 1.0% TMS (v/v) respectively. Since deuterium has a spin of 1, triplets arising from coupling to deuterium have the intensity ratio of 1:1:1. "m" denotes a broad peak with some fine structures. It should be noted that chemical shifts can be dependent on solvent, concentration and temperature.

● Approximate values only; may vary with pH, concentration and temperature.
◆ Melting and boiling points are those of the corresponding unlabeled compound (except for D₂O). These temperature limits can be used as a guide to determine the useful liquid range of the solvents. Information gathered from the Merck Index – Fourteenth Edition.

* HOD Peaks – NMR spectra of "neat" deuterated solvent always exhibit a peak due to H₂O in addition to the residual solvent peak. When the exchange rate between H₂O and HOD is slow on the NMR timescale the water peak appears as two peaks, a singlet corresponding to H₂O and a 1:1:1 triplet corresponding to HOD.

NMR Solvent Storage and Handling Information

Please note that some packaging sizes of some solvents may require special handling not provided below. The bottle or ampoule packaging information should be reviewed for further instructions.

Acetic Acid-d₄ / Acetone-d₆ / Benzene-d₆ / Cyclohexane-d₁₂ / Deuterium Oxide / *N,N*-Dimethylformamide-d₇ / Dimethyl Sulfoxide-d₆ / 1,4-Dioxane-d₈ (*p*-Dioxane) / Ethanol-d₆ / Methanol-d₄ / Methylene Chloride-d₂ / Pyridine-d₅ / 1,1,2,2-Tetrachloroethane-d₂ / Toluene-d₈ / Trifluoroacetic Acid-d / 2,2,2-Trifluoroethanol-d₃

Store at room temperature away from light and moisture. The above products are stable if stored under recommended conditions.

Acetonitrile-d₃

Store at room temperature away from light and moisture. This product is stable for one year after receipt of order if stored under these conditions (unopened). After one year, the solvent should be re-analyzed for chemical purity before use.

Chloroform-d / Tetrahydrofuran-d₈

Store refrigerated between -5° to 5°C away from light and moisture. These products are stable for six months after receipt of order if stored under these conditions (unopened). After six months, the solvent should be re-analyzed for chemical purity before use.

Deuterium Exchange of Labile Protons in Deuterated Solvents Containing Residual D₂O

Some deuterated solvents are prepared by catalytic exchange of protonated solvent with deuterium oxide and are carefully purified by distillation. Residual water (H₂O in equilibrium exchange with D₂O) is kept to a minimum of 20-200 ppm; the higher value corresponds to the amount in the more hygroscopic solvents. The labile deuterons (and protons) of water are available to exchange with labile protons in the chemist's sample and can result in inaccurate integration ratios. The figures below show that just 100 ppm of D₂O can cause problems when studying dilute solutions of analytes. A significant decrease in the integral of 1 labile proton may be observed in a sample containing 5 mg organic compound, MW~200, dissolved in 1 g DMSO-d₆ containing 100 ppm D₂O. The problem becomes worse as the molecular weight of the analyte increases.

Solution

Water (as H₂O, HOD or D₂O) can be minimized by adding molecular sieves to the solvent, agitating the mixture and allowing it to stand for a few hours. The water content may be reduced to about 10-20 ppm in this manner. If exchange still causes a problem, it is recommended to use a less hygroscopic solvent, such as chloroform, methylene chloride or acetonitrile.

X – residual solvent * – residual water

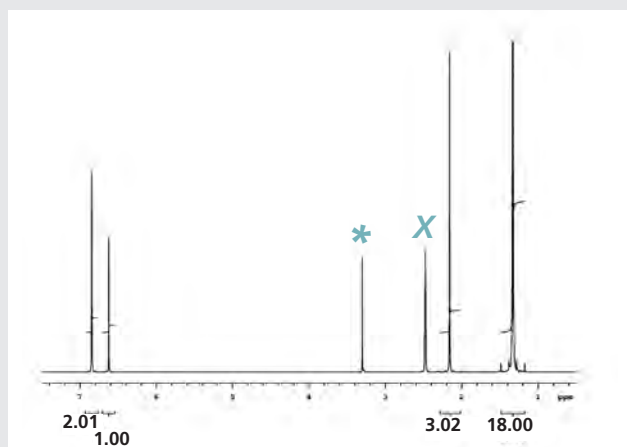


Figure 1. ¹H-NMR spectrum of 5.0 mg 2,6-di-*tert*-butyl-4-methylphenol (MW 220.36g / mole) in dry DMSO-d₆. Note the proper integral ratios of 18:3:1:2 (t-butyl: methyl: ring-H: -OH). Note the single H₂O peak at 3.3 ppm.

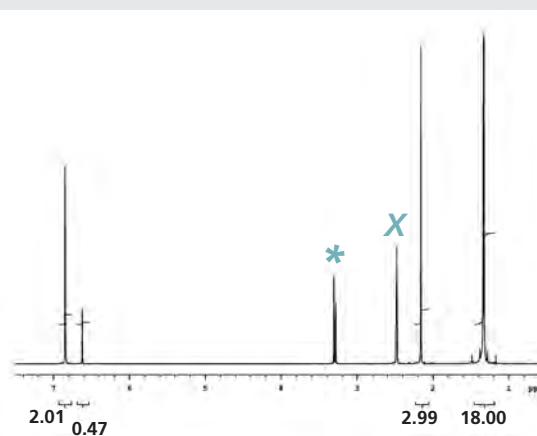


Figure 2. ¹H-NMR spectrum of 5.3 mg of 2,6-di-*tert*-butyl-4-methylphenol in DMSO-d₆ with 100 ppm D₂O added. Note the reduced ratio of the phenolic proton 18:3:2:0.47 (t-butyl: methyl: ring-H: -OH). Note that the HOH and HOD peaks are separated in the spectrum.

NMR Solvents

Chemical Shifts of Selected Compounds in Different Solvents

Compounds	CDCl ₃	(CD ₃) ₂ CO	(CD ₃) ₂ SO	C ₆ D ₆	CD ₃ CN	CD ₃ OD	D ₂ O
Solvent residual peak	7.26	2.05	2.50	7.16	1.94	3.31	4.79
H ₂ O	1.56	2.84	3.33	0.40	2.13	4.87	
Acetic acid	2.10	1.96	1.91	1.55	1.96	1.99	2.08
Acetone	2.17	2.09	2.09	1.55	2.08	2.15	2.22
Acetonitrile	2.10	2.05	2.07	1.55	1.96	2.03	2.06
Benzene	7.36	7.36	7.37	7.15	7.37	7.33	
<i>tert</i> -butyl alcohol	1.28	1.18	1.11 4.19	1.05 1.55	1.16 2.18	1.40	1.24
<i>tert</i> -butyl methyl ether	1.19 3.22	1.13 3.13	1.11 3.08	1.07 3.04	1.14 3.13	1.15 3.20	1.21 3.22
BTH – 2,6-Dimethyl-4- <i>tert</i> -butylphenol	6.98 5.01 2.27 1.43	6.96 2.22 1.41	6.87 6.65 2.18 1.36	7.05 4.79 2.24 1.38	6.97 5.20 2.22 1.39	6.92 2.21 1.40	
Chloroform	7.26	8.02	8.32	6.15	7.58	7.90	
Cyclohexane	1.43	1.43	1.40	1.40	1.44	1.45	
1,2-Dichloroethane	3.73	3.87	3.90	2.90	3.81	3.78	
Dichloromethane	5.30	5.63	5.76	4.27	5.44	5.49	
Diethyl ether	1.21 3.48	1.11 3.41	1.09 3.38	1.11 3.26	1.12 3.42	1.18 3.49	1.17 3.56
Diglyme	3.65 3.57 3.39	3.56 3.47 3.28	3.51 3.38 3.24	3.46 3.34 3.11	3.53 3.45 3.29	3.61 3.58 3.35	3.67 3.61 3.37
1,2-Dimethoxyethane	3.40 3.55	3.28 3.46	3.24 3.43	3.12 3.33	3.28 3.45	3.35 3.52	3.37 3.60
Dimethylacetamide	2.09 3.02 2.94	1.97 3.00 2.83	1.96 2.94 2.78	1.60 2.57 2.05	1.97 2.96 2.83	2.07 3.31 2.92	2.08 3.06 2.90
Dimethylformamide	8.02 2.96 2.88	7.96 2.94 2.78	7.95 2.89 2.73	7.63 2.36 1.86	7.92 2.89 2.77	7.97 2.99 2.86	7.92 3.01 2.85
Dimethyl sulfoxide	2.62	2.52	2.54	1.68	2.50	2.65	2.71
Dioxane	3.71	3.59	3.57	3.35	3.60	3.66	3.75
Ethanol	1.25 3.72 1.32	1.12 3.57 3.39	1.06 3.44 4.63	0.96 3.34	1.12 3.54 2.47	1.19 3.60	1.17 3.65
Ethyl acetate	2.05 4.12 1.26	1.97 4.05 1.20	1.99 4.03 1.17	1.65 3.89 0.92	1.97 4.06 1.20	2.01 4.09 1.24	2.07 4.14 1.24
Ethyl methyl ketone	2.14 2.46 1.06	2.07 2.45 0.96	2.07 2.43 0.91	1.58 1.81 0.85	2.06 2.43 0.96	2.12 2.50 1.01	2.19 3.18 1.26
Ethylene glycol	3.76	3.28	3.34	3.41	3.51	3.59	3.65
“grease”	0.86 1.26	0.87 1.29		0.92 1.36	0.86 1.27	0.88 1.29	
<i>n</i> -Hexane	0.88 1.26	0.88 1.28	0.86 1.25	0.89 1.24	0.89 1.28	0.90 1.29	
HMPA – Hexamethylphosphoramide	2.65	2.59	2.53	2.40	2.57	2.64	2.61
Methanol	3.49 1.09	3.31 3.12	3.16 4.01	3.07	3.28 2.16	3.34	3.34
Nitromethane	4.33	4.43	4.42	2.94	4.31	4.34	4.40
<i>n</i> -Pentane	0.88 1.27	0.88 1.27	0.86 1.27	0.87 1.23	0.89 1.29	0.90 1.29	
2-Propanol	1.22 4.04	1.10 3.90	1.04 3.78	0.95 3.67	1.09 3.87	1.50 3.92	1.17 4.02
Pyridine	8.62 7.29 7.68	8.58 7.35 7.76	8.58 7.39 7.79	8.53 6.66 6.98	8.57 7.33 7.73	8.53 7.44 7.85	8.52 7.45 7.87
Silicone grease – Poly(dimethylsiloxane)	0.07	0.13		0.29	0.08	0.10	
Tetrahydrofuran	1.85 3.76	1.79 3.63	1.76 3.60	1.40 3.57	1.80 3.64	1.87 3.71	1.88 3.74
Toluene	2.36 7.17 7.25	2.32 7.1-7.2 7.1-7.2	2.30 7.18 7.25	2.11 7.02 7.13	2.33 7.1-7.3 7.1-7.3	2.32 7.16 7.16	
Triethylamine	1.03 2.53	0.96 2.45	0.93 2.43	0.96 2.40	0.96 2.45	1.05 2.58	0.99 2.57

Gottlieb, H.; Kotlyar, V.; Nudelman, A. **1997**. NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities. *J Org Chem*, 62, 75-12-7515.

qNMR



Standards for qNMR

Quantitative ^1H -NMR (qNMR) continues to be utilized with much success in the pharmaceutical, chemical and food industries and in many facets of academic research. Regardless of the application, all qNMR methods require a calibration signal whose integrated signal intensity originates or is traceable to a known number of protons. Calibration for qNMR is made using either internal or external referencing methods. External methods rely on the use of a standard solution packaged in a defined NMR tube or capillary to obtain an integral that can be used for sample quantification, whereas internal methods rely on the use of a known amount of standard that is co-dissolved in the sample itself.

External Calibration Standards

CIL is pleased to offer external calibration standards for qNMR. The standards are formulated using CIL's high-quality $\text{DMSO}-d_6$ and benzoic acid from NIST (SRM 350(b)), a standard reference material for acidometry. Both 5 mM and 15 mM benzoic acid concentrations are available. The concentration and associated expanded uncertainty of the benzoic acid has been accurately determined using metrological techniques and verified using qNMR. The ^1H -NMR spectrum of benzoic acid in $\text{DMSO}-d_6$ is presented in Figure 1.

CIL is currently offering these standards in presealed NMR tubes. Please see the information below for details regarding NMR tubes and fill volumes. Other NMR tubes and concentrations may be available upon request.

qNMR Standard for External Referencing

Catalog No.	Description*	NMR Tube**	Part No.	Fill Volume
DLM-9491A	5 mM Benzoic acid in $\text{DMSO}-d_6$	1.7 mm O.D.	Bruker Part No. Z106462	50 μL
DLM-9491B	5 mM Benzoic acid in $\text{DMSO}-d_6$	3 mm O.D.	Wilmad Part No. 335-PP-9	160 μL
DLM-9491C	5 mM Benzoic acid in $\text{DMSO}-d_6$	5 mm O.D.	Wilmad Part No. 528-PP-8	750 μL
DLM-7061A	15 mM Benzoic acid in $\text{DMSO}-d_6$	1.7 mm O.D.	Bruker Part No. Z106462	50 μL
DLM-7061B	15 mM Benzoic acid in $\text{DMSO}-d_6$	3 mm O.D.	Wilmad Part No. 335-PP-9	160 μL
DLM-7061C	15 mM Benzoic acid in $\text{DMSO}-d_6$	5 mm O.D.	Wilmad Part No. 528-PP-8	750 μL

* The benzoic acid concentration and associated uncertainty are reported.

** All tubes are flame-sealed to ensure longevity.

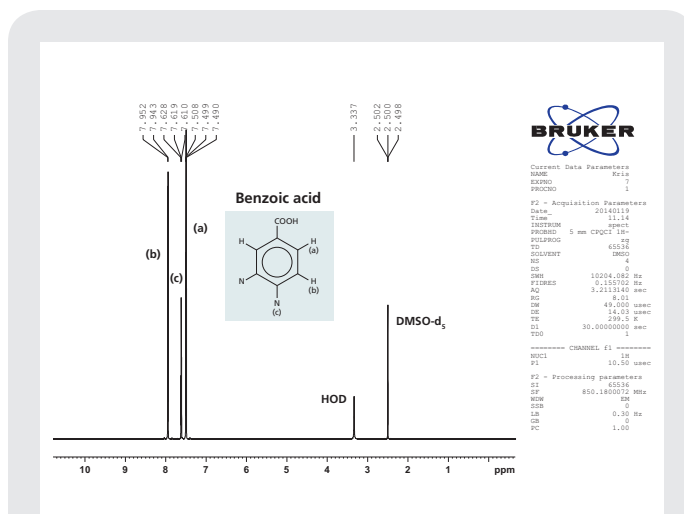


Figure 1. 850 MHz ^1H -NMR spectrum of benzoic acid in $\text{DMSO}-d_6$. Resonances from the aromatic protons of benzoic acid, HOD and $\text{DMSO}-d_6$ are assigned. The acid proton resonance from benzoic acid (~12-13 ppm) is not shown. (Courtesy Joe Ray, Baxter Healthcare Corporation, Round Lake, IL)

Other NMR
fill volumes
and tubes are
available.
Please inquire.



Standards for qNMR *(continued)*

Internal Calibration Standards

The internal reference method commonly gives errors of <1% and is considered to be the most accurate and reproducible method available to obtain quantitative ^1H -NMR spectra. Unfortunately, the reference standard is typically weighed into each sample solution, an action that requires time and effort, and has been reported to the largest source of error with this method.

CIL is pleased to offer a ready-to-use DMSO-d_6 solution containing a known amount of benzoic acid for internal referencing. Because this solution is preformulated, the user does not need to weigh a

standard material. The elimination of this step will reduce effort and time in sample preparation and also may bring about more accurate results than if the user performs this formulation. To use this product, the sample must be soluble in DMSO-d_6 , physically and chemically inert toward benzoic acid and stable in acidic pH. Ideally, there will be no resonances from the sample in the region of benzoic acid aromatic protons (7.4-8.1 ppm), HOD (~3 ppm but is variable) and DMSO-d_5 (2.5 ppm). The benzoic acid concentration with associated uncertainty is presented on the certificate of analysis.

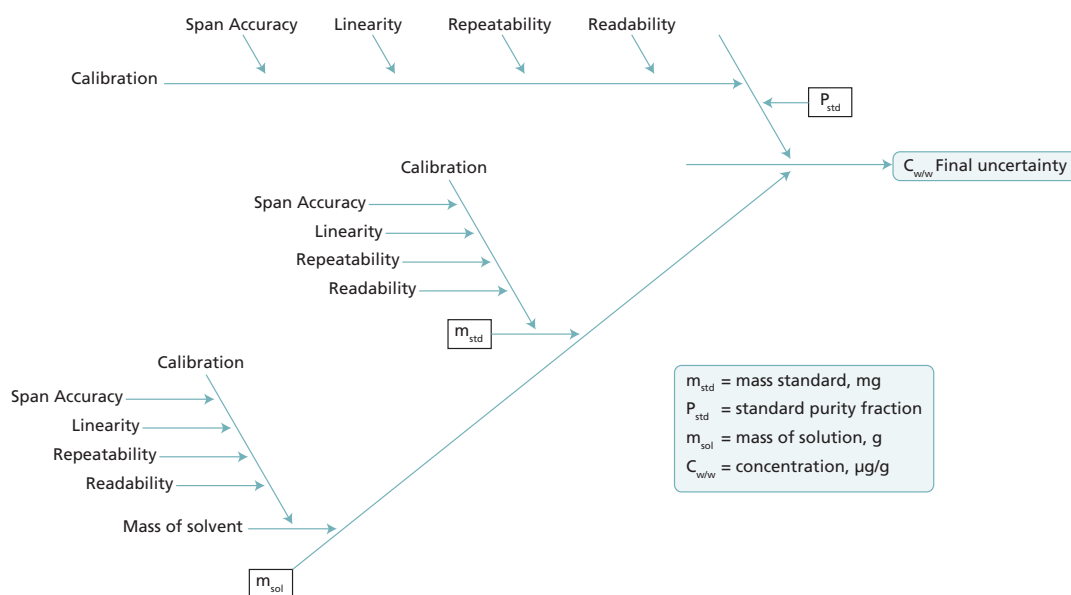
qNMR Standard for Internal Referencing

Catalog No.	Description	Ampoule	Comments
DLM-9491D	5 mM Benzoic acid in DMSO-d_6	1 g	The benzoic acid concentration and associated uncertainty is reported.
DLM-7061D	15 mM Benzoic acid in DMSO-d_6	1 g	The benzoic acid concentration and associated uncertainty is reported.

CIL Formulation Procedure

The procedure that CIL uses to formulate qNMR external calibration reference standard bulk solutions allows for the expanded uncertainty of the concentration of the calibration standard (e.g., benzoic acid) to be determined. Traceability to SI is maintained through the use of weight sets with

calibration traceable to NIST and laboratory balances with NIST-traceable calibration certificates, maintaining an unbroken chain of calibration to the kilogram. The factors contributing to the uncertainty of the benzoic acid concentration¹ is shown in below.



Cause-and-effect diagram of factors contributing to the uncertainty of the benzoic acid concentration in the qNMR standard formulation.

Reference

1. EURACHEM CITAC Guide CG 4, "Quantifying Uncertainty in Analytical Measurement," Third Edition, QUAM:2012

Notes

Synthesis



Stable Isotope-Labeled Synthetic Intermediates

CIL offers over 15,000 stable isotope-labeled products for your synthetic applications. We offer many labeling patterns for common starting materials. For more than 30 years CIL has offered:

- Expertise and quality service from your initial quote request through delivery of your order
- Flexibility of scale for custom and catalog products from milligram to multi-kilogram quantities
- A large selection of labeled compounds, including deuterated reagents and solvents
- cGMP suite for manufacturing clinical trial grade materials (CTM)
- Quantity discounts

Catalog No.	Description	Amount
DLM-9	Acetone-d ₆ (D, 99.9%)	Multiple sizes
DLM-112	Acetaldehyde (D ₄ , 99%)	5 g
DLM-247	Acetyl chloride (D ₃ , 98%)	10 g
DLM-1	Benzene-d ₆ (D, 99.5%)	Multiple sizes
DLM-494	Biphenyl (D ₁₀ , 98%)	1 g
DLM-1945	bis(2-Chloroethoxy) methane (chloroethoxy-D ₈ , 98%)	0.1 g
DLM-1315	Borane (D ₃ , 98%) (1 molar in THF) (+0.005M NABD ₄)	0.25 L
DLM-4747	Borane methylsulfide complex (D ₃ , 99%)	5 g
DLM-398	Bromobenzene (D ₅ , 99%)	25 g
DLM-1116	tert-Butylchloride (D ₉ , 98%)	Multiple sizes
DLM-263	Chlorobenzene-d ₅ (D, 99%)	5 g
CNLM-7289	Cyanamide (¹³ C, 99%; ¹⁵ N ₂ , 98%) (stabilized with < 0.1% acetic acid)	Please inquire
DLM-4	Deuterium oxide (D, 99.9%)	Multiple sizes
DLM-3903	Dimethyl carbonate (D ₆ , 99%)	1 g
DLM-196	Dimethyl sulfate (D ₈ , 98%)	Please inquire
DLM-805	Formaldehyde (D ₂ , 98%) (~20% w/w in D ₂ O)	20 mL of solution

Catalog No.	Description	Amount
DLM-1023	Iodoethane (1,1-D ₂ , 98%) + copper wire	5 g
DLM-1024	Iodoethane (2,2,2-D ₃ , 98%) + copper wire	5 g
DLM-272	Iodoethane (D ₅ , 99%) + copper wire	5 g
DLM-1981	Methanesulfonic acid (D ₄ , 97-98%)	5 g
DLM-24	Methanol-d ₄ (D, 99.8%) methyl alcohol	Multiple sizes
DLM-651	Methyl formate (formyl-D, 99%)	5 g
DLM-362	Methyl iodide + copper wire (D ₃ , 99.5%)	Multiple sizes
DLM-289	Methylamine-HCl (methyl-D ₃ , 98%)	1 g
DLM-3484	Morpholine (2,2,3,3,5,5,6,6-D ₈ , 98%)	1 g
DLM-295	2-Nitrophenol (ring-D ₄ , 98%)	0.1 g
DLM-296	4-Nitrophenol (ring-D ₄ , 98%)	0.1 g
DLM-300	Paraformaldehyde (D ₂ , 99%)	5 g
DLM-370	Phenol (D ₆ , 98%)	5 g
DLM-788	Phthalic anhydride (D ₄ , 98%)	0.5 g
DLM-226	Sodium borodeuteride (D ₄ , 99%) CP 90-95%	Multiple sizes
DLM-1361	Sodium formate (D, 98%)	5 g

CP = chemical purity

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Getting Started with Using Deuterated Products? Or Looking for New Ideas?

A Sampling of Recent and Not-so-Recent Literature Articles, Reviews and Procedures

Comprehensive Tables of Chemical Shifts for the Synthetic Chemist

The following two articles are required reading for every synthetic chemist who uses NMR as an identification method. They provide the necessary information to identify NMR peaks that arise from contaminants in the desired synthetic compound, whether the sample is an in-process or final product.

The first in the list is the original paper and tabulates proton and ^{13}C chemical shifts of over 30 compounds that are routinely used in organic synthesis as reagents, solvents or lubrication materials and how the chemical shift varies depending on the deuterated solvent used in the NMR experiment. Additionally, the authors report the temperature dependence of the chemical shift of residual HOD.

The second article, written by two of the original authors with several others, is more comprehensive. It includes additional potential contaminants, as well as several additional deuterated solvents that are used in organometallics synthesis.

Gottlieb, H.E.; Kotlyar, V.; Nudelman, A. **1997**. NMR chemical shifts of common laboratory solvents as trace impurities. *J Org Chem*, 62.21: 7512-7515.

Fulmer, G.R., et al. **2010**. NMR chemical shifts of trace impurities: common laboratory solvents, organics, and gases in deuterated solvents relevant to the organometallic chemist. *Organometallics*, 29.9: 2176-2179.

H/D Exchange Mass Spectrometry Studies in Protein Structure and Dynamics

The following two articles (one review, one book chapter) describe the coupled use (HDX-MS) of rates of hydrogen/deuterium exchange of amide protons in protein with LC/MS to monitor structure function of protein therapeutics. The first article reviews the current state of the method, and the second article describes in detail a procedure one can follow to use this method in the laboratory.

Wei, H., et al. **2014**. Hydrogen/deuterium exchange mass spectrometry for probing higher order structure of protein therapeutics: methodology and applications. *Drug Discovery Today*, 19.1: 95-102.

Singh, H.; Busenlehner, L.S. **2014**. Probing backbone dynamics with hydrogen/deuterium exchange mass spectrometry. *Protein Dynamics*. Humana Press. 81-99.

Deuteration Aids Mass Spectrometry Imaging in Neuropsychopharmacology Research

The article listed below describes the use of mass spec imaging to study distribution of large (proteins, lipids) and small (drugs, metabolites) molecules in brain tissue *in situ*. The samples are typically prepared with matrix crystals that can interfere with the interpretation of the data. The use of deuterated matrix crystals has improved the analysis by revealing previously unobserved compounds. In addition, deuterated reference standards (cocaine, imipramine) improve the accuracy of quantitation of signal.

Shariatgorji, M.; Svenningsson, P.; Andrén, P.E. **2014**. Mass spectrometry imaging, an emerging technology in neuropsychopharmacology. *Neuropsychopharmacology* 39.1: 34-49.

Effects of Deuteration of Proteins on Proton NMR Parameters

Deuteration of proteins has been successfully used to aid in the study of structure and dynamics. The effect of deuteration on proton and ^{13}C -NMR parameters has been reported in many publications. This review comprehensively describes the quantitative effects of deuteration of proteins specifically on chemical shifts, coupling constants and relaxation parameters. Theoretical treatment is presented along with experimental results that tabulate deuterium isotope shifts.

Tugarinov, V. **2014**. Indirect use of deuterium in solution NMR studies of protein structure and hydrogen bonding. *Prog Nucl Magn Reson Spectrosc*, 77: 49-68.

The Use of Deuterated Solvents and Deuterium Exchange Methods in Metabolite Identification

This book chapter describes a detailed procedure to streamline metabolite identification for drug-discovery studies. The use of fast LC-MS/MS with multiple-stage mass analysis provides a single analysis tool to identify lead candidates in drug development.

Lam, W.W., et al. **2014**. Metabolite Identification in Drug Discovery. *Optim Drug Discovery*, Humana Press. 445-459.

(continued)

Deuterium Isotope Effects in Pharmacology Studies on Living Cells, Organisms and Animals

This article is a comprehensive review on the history, use and effects of D₂O on living tissue. It includes a review of potential clinical effects of D₂O and the potential beneficial use of deuterated drugs, antimicrobials and insecticides. See the following two articles for recent applications.

Kushner, D. J.; Baker, A.; Dunsta II T.G. **1999**. Pharmacological uses and perspectives of heavy water and deuterated compounds. *Can J Physiol Pharmacol*, 77.2: 79-88.

Honeybees Discriminate between Protonated and Deuterated Compounds

Related to the above Review article, this interesting study shows that honeybees can detect differences between isotopomers of the same compound. The authors present data that point to the theory that the honeybees discriminate between compounds based in intramolecular vibration difference, not on structural differences.

Gronenberg, W., et al. **2014**. Honeybees (*Apis mellifera*) learn to discriminate the smell of organic compounds from their respective deuterated isotopomers. *Proc R Soc B*, 281.1778: 20133089.

Deuterated C-Aryl Glycoside as a Potential Drug in the Treatment of Type 2 Diabetes

An emerging field in deuterated pharmaceuticals takes advantage of the kinetic deuterium isotope effect. The effect of deuterium in some compounds can block the formation of potentially harmful metabolites and also improve the effect of the drug on its target. This study describes one such example that may be useful in the treatment of Type 2 diabetes.

Xu, G., et al. **2014**. Design, Synthesis, and Biological Evaluation of Deuterated C-Aryl Glycoside as Potent and Long-Acting Renal Sodium-Dependent Glucose Cotransporter 2 (SGLT2) Inhibitor for the Treatment of Type 2 Diabetes. *J Med Chem*, 57(4), 1236-1251.

Deuterium Aids in Organic Mechanism and Kinetic Studies on Metal Surfaces

Ethanol decomposition on Pd(111) surface was studied using deuterated isotopomers of ethanol to determine the order of bond scission that the O-H bond cleaves prior to the C-H bond.

Williams, R.M.; Pang, S.H.; Medlin, J.W. **2014**. OH versus CH bond scission sequence in ethanol decomposition on Pd (111). *Surf Sci*, 619: 114-118.

Chiral transfer in Pd catalyzed amination of allyl alcohols is reported through the use of kinetic studies using deuterated isotopomers of allyl alcohol.

Sawadjoon, S., et al. **2014**. Mechanistic Insights into the Pd-Catalyzed Direct Amination of Allyl Alcohols: Evidence for an Outer-sphere Mechanism Involving a Palladium Hydride Intermediate. *Chem – Eur J*, 20(6), 1461-1764.

A mechanistic study of gold catalyzed heterocyclization reactions is accomplished through the use of both deuterated solvents and deuterated urea reveals dual σ,π -gold activation in addition to the well-established π -activation.

Gimeno, A., et al. **2014**. Competitive Gold-Activation Modes in Terminal Alkynes: An Experimental and Mechanistic Study. *Chem – Eur J*, 20.3: 683-688.

The mechanism of platinum mediated carbon-carbon bond formation in organoboron compounds using dioxygen is studied using partially deuterated reagents coupled with reaction in methanol-d₄ and reveals C=C coupling at the boron center.

Pal, S.; Zavalij, P.Y.; Vedernikov, A.N. **2014**. Oxidative C (sp³)-H bond cleavage, C-C and C=C coupling at a boron center with O₂ as the oxidant mediated by platinum (ii). *Chem Commun*, 50(40), 5376-5378.

New Methods for Quantitation of Environmental Pollutants

A Sampling of Recent and Not-so-Recent Literature Articles, Reviews and Procedures

Isotope Dilution Mass Spectrometry LC-MS/MS Analysis of Water Pollutants

The authors validated a new IDMS multi-analyte method to quantitate four artificial sweeteners in samples of lake and river waters exposed to wastewater effluent and agricultural run-off. Deuterated analogs were necessary to reduce uncertainty while improving accuracy.

Perkola, N.; Sainio, P. **2014**. Quantification of four artificial sweeteners in Finnish surface waters with isotope dilution mass spectrometry. *Environ Pollut*, 184, 391-396.

GC/MS and NMR Analysis of Atmospheric Pollutants

The authors describe methods for identification of toluene photooxidation products in aerosols. Deuterated toluene aided in the analysis. The MS results include previously unidentified compounds in aerosols. NMR was used to identify several functional groups arising from oligomeric material that cannot be identified using traditional MS methods.

White, S.J.; Jamie, I.M.; Angove, D.E. **2014**. Chemical characterisation of semi-volatile and aerosol compounds from the photooxidation of toluene and NO_x. *Atmos Environ*, 83, 237-244.

Deuterated Conductive Polymers Exhibit Improved Characteristics

This paper describes a comprehensive experimental and theoretical study of the optoelectronic behavior of deuterated conducting polymers. The neutron scattering and Raman results reveal differences in morphology vibrational modes. Distinct changes in device performance and optical properties are also observed.

Shao, M., et al. **2014**. The isotopic effects of deuteration on optoelectronic properties of conducting polymers. *Nat Commun*, 5.

Use of Neutron Imaging to Understand Durability of High Temperature Fuel Cells

The degradation of high T polymer electrolyte fuel cells is accelerated by evaporation of H₃PO₄ along with other processes. Neutron imaging, combined with *in situ* H/D exchange in phosphoric acid, allowed a properly referenced study to determine the distribution of phosphoric acid in fuel cells and its effect on the durability of these cells.

Boillat, P., et al. **2014**. Evaluation of Neutron Imaging for Measuring Phosphoric Acid Distribution in High Temperature PEFCs. *J Electrochem Soc*, 161,3: F192-F198.

Enhancement of Room Temperature Phosphorescence Yield in Deuterated Compounds

Aromatic compounds are useful building blocks for creating new materials with photosensitive applications. One goal is to increase the phosphorescence lifetime and yield at room temperature. This study shows the effect of deuteration position in purely aromatic compounds to phosphorescence yield at room temperature.

Hirata, S., et al. **2014**. Relationship between room temperature phosphorescence and deuteration position in a purely aromatic compound. *Chem Phys Lett*, 591, 119-125.

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Notes

Biomolecular NMR



Deuterated Detergents and Phospholipids for Membrane Proteins

Membrane proteins can be divided into three categories:

1. Integral membrane proteins, which can penetrate the lipid bilayer
2. Peripheral membrane proteins, which are external and bound through noncovalent interactions
3. Lipid-anchored proteins, which are external but bound with covalent bonds.

There is a great interest in determining structure of integral membrane proteins due to the importance of these proteins in participating in cellular processes. Despite the significant, functional importance of membrane proteins, the structural biology has been particularly challenging, which is reflected by the low number of determined membrane protein structures.¹

The determination of the structure and dynamics of membrane proteins using NMR requires samples containing protein that is properly folded. Fortunately, membrane proteins often keep native-like structures in detergent micelles. Deuterated solubilization agents, such as detergents, often make NMR investigations easier compared to using unlabeled agents. In some cases, such as methyl labeling, deuterated reagents of this type are required. CIL is pleased to offer the following deuterated detergents and phospholipid agents for use with membrane proteins.

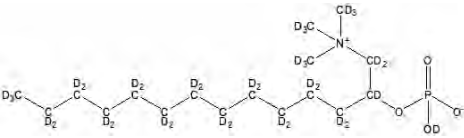
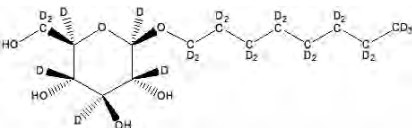
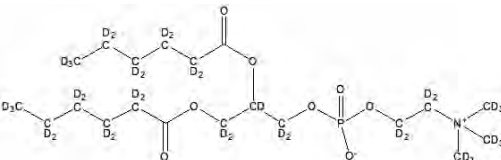
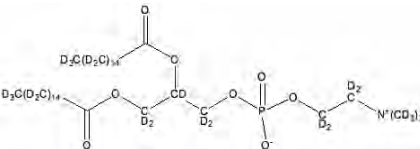
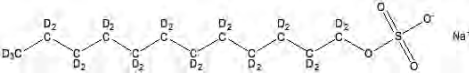
Reference

1. There are 493 unique membrane protein structures as of August 3, 2014. See <http://blanco.biomol.uci.edu/index.shtml> for more information.

"CIL has been a strong supporter of NMR methods of development over the years, providing critical isotope-enriched reagents for research and development, without which many of the recent advances in biomolecular NMR would simply not have been possible. In particular, the broad biological impact and tremendous success of the multidimensional triple-resonance biomolecular NMR would not have been achieved without the high-quality and broadly accessible reagents that CIL has provided to the scientific community over the last 20 years."

Gaetano Montelione, PhD
Professor of Molecular Biology and Biochemistry
Rutgers University Director of the
Northeast Structural Genomics Consortium

Deuterated Detergents and Phospholipids

Catalog No.	Description
DLM-2274	Dodecylphosphocholine (D ₃₈ , 98%)
	
DLM-6726	N-Octyl β-Glucoside (D ₂₄ , 98%)
	
DLM-4341	DL-A-Phosphatidylcholine, dihexanoyl (D ₄₀ , 98%) (DHPC) CP 95%
	
DLM-8256	DL-A-Phosphatidylcholine, dipalmitoyl (D ₈₀ , 98%) (DPPC) CP 95%+
	
DLM-197	Sodium dodecyl sulfate (D ₂₅ , 98%)
	

Deuterated Buffers

CIL offers a wide selection of deuterated buffers for use with aqueous solutions.

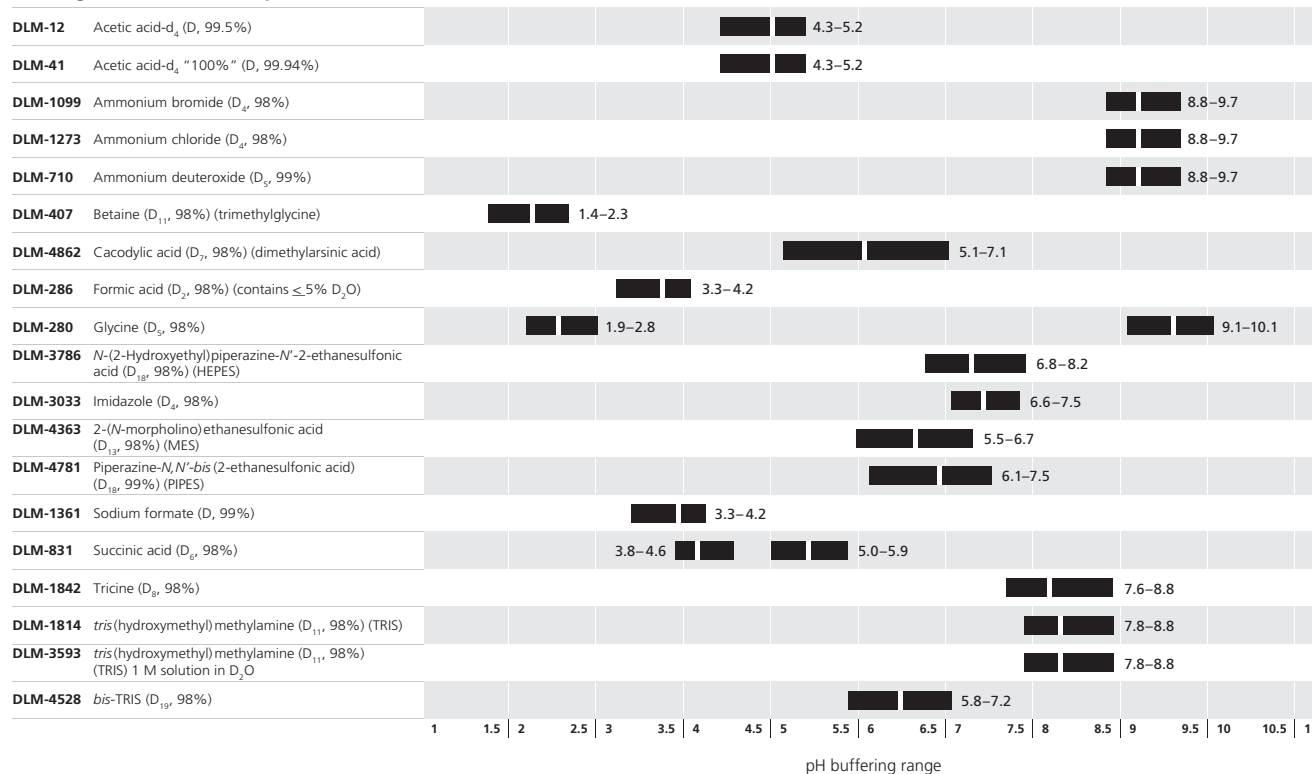
Catalog No.	Description
DLM-12	Acetic acid-d ₄ (D, 99.5%)
DLM-41	Acetic acid-d ₄ "100%" (D, 99.93%)
DLM-1099	Ammonium bromide (D ₄ , 98%)
DLM-1273	Ammonium chloride (D ₄ , 98%)
DLM-710	Ammonium deuterioxide (D ₅ , 99%) (~25% in soln D ₂ O)
DLM-407	Betaine (D ₁₁ , 98%)
DLM-4862	Cacodylic acid (D ₇ , 98%)
DLM-286	Formic acid (D ₂ , 98%) (<5% D ₂ O)
DLM-280	Glycine (D ₅ , 98%)
DLM-3786	HEPES (D ₁₈ , 98%)

Catalog No.	Description
DLM-3033	Imidazole (D ₄ , 98%)
DLM-4363	MES (D ₁₃ , 98%)
DLM-4781	PIPES (D ₁₈ , 98%)
DLM-1361	Sodium formate (D, 98%)
DLM-831	Succinic acid (D ₆ , 98%)
DLM-1842	Tricine (D ₈ , 98%)
DLM-4779	Trimethylamine N-oxide (D ₉ , 98%)
DLM-1814	TRIS (D ₁₁ , 98%)
DLM-3593	TRIS (D ₁₁ , 98%) 1 M in D ₂ O
DLM-4528	bis-TRIS (D ₁₉ , 98%)

pH Buffering Range Chart

Catalog Number and Compound

pK_a is indicated by a white rule within the range



Isotope-Labeled Protein Standards

CIL is pleased to offer isotope-enriched proteins for use as standards in NMR spectroscopy. CIL is also happy to offer new and exciting protein standards manufactured by Nexomics Biosciences, Inc., a New Jersey-based contract research organization that specializes in a broad array of gene-to-structure services for the biopharmaceutical community.

Nexomics provides high-quality, high-purity standards that are invaluable tools for biomolecular NMR research applications.

Each product is accompanied by the following data:

- ^1H - ^{15}N HSQC (^{15}N -labeled proteins)
- ^1H - ^{13}C HSQC (^{13}C -labeled proteins)
- CO-NH projection of 3D HNCO (^{15}N , ^{13}C -labeled proteins)

- SDS PAGE (for all labeled proteins)
- MALDI-TOF (for all labeled proteins)



Isotope-enriched protein standards are ideal for:

- Aiding in the development and testing of new pulse sequences
- Optimizing parameters for a given pulse sequence
- Assessing spectrometer performance
- Training purposes

All protein standards offered by CIL have been chosen for the high-quality spectra they produce and the excellent long-term stability they exhibit.

Protein and Peptide Standards

The Chicken α -Spectrin SH3 Domain is available in microcrystalline form (in an ammonium sulfate emulsion) or as a 9 mg/mL solution (10% D_2O /90% H_2O containing 0.02% NaN_3 , pH 3.5). A full technical data package containing 2D-NMR data and peak assignments accompanies every order for the Chicken α -Spectrin SH3 Domain. Every order for the GB1 is accompanied by a ^1H - ^{15}N -HSQC spectrum.

Catalog No.	Description
CLM-8227	SH3 Domain Protein ($\text{U-}^{13}\text{C}$, 98%)
NLM-6839	SH3 Domain Protein ($\text{U-}^{15}\text{N}$, 98%)
NLM-6839-S	SH3 Domain Protein ($\text{U-}^{15}\text{N}$, 98%) (9 mg/mL solution)
CNLM-6840	SH3 Domain Protein ($\text{U-}^{13}\text{C}$, 98%; $\text{U-}^{15}\text{N}$, 98%) (microcrystalline slurry)
CNLM-6840-S	SH3 Domain Protein (w/ 0.01% sodium azide) ($\text{U-}^{13}\text{C}$, 98%; $\text{U-}^{15}\text{N}$, 98%) (9 mg/mL solution)
CDNLM-6841	SH3 Domain Protein ($\text{U-}^{13}\text{C}$, 98%; U-D , 98%; $\text{U-}^{15}\text{N}$, 98%)
CDNLM-6841-S	SH3 Domain Protein (9 mg/mL solution) ($\text{U-}^{13}\text{C}$, 98%; U-D , 98%; $\text{U-}^{15}\text{N}$, 98%)
CNLM-2408	GFL Peptide Standard (^{13}C , 98%; ^{15}N , 96-99%) 1 mM in DMSO-d_6

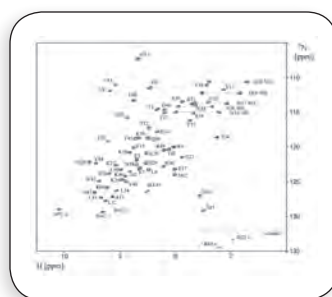
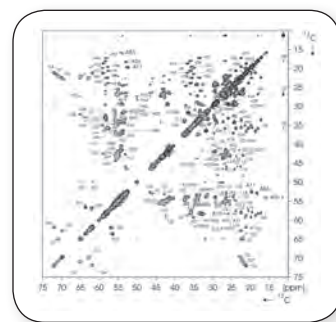
CIL His-Tagged Protein Standards

Catalog No.	Description
CNLM-8663	His-GB1 (^{13}C , 98%+; ^{15}N , 98%+) 1.5 mM in PBS, pH 6.5, 0.02% sodium azide

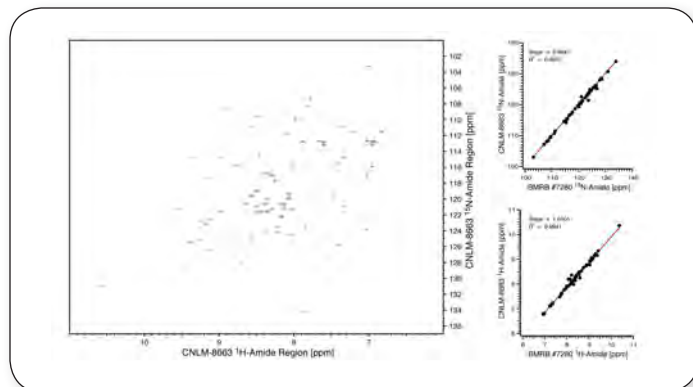
Product	Amino Acid Length
Chicken α -Spectrin SH3 Domain	62 residues
MDETGKELYL ALYDYQEKPQ REVMTKKGDI LTLNSTNKD WWWKEVNDKQ GFVPAAYVKK LD	
His6x-GB1 (β -1 immunoglobulin domain of protein G)	71 residues
MHHHHHHGNG LYFQSMQYKL ILNGKTLKGE TTTEAVDAAT AEKVFKQYAN DNGVDGEWTY DDAKTFTVT E	
GFL Peptide	8 residues
YG GFL RLRI (bold indicates labeled residues)	

GB1 is offered as a *N*-terminal, tobacco etch virus (TEV)-cleavable 6xHis-tag as a 1.5 mM solution in 137 mM NaCl, 2.7 mM KCl, 8.1 mM Na_2HPO_4 , 1.8 mM KH_2PO_4 , 0.02% NaN_3 , 0.1 mM TSP in 10% D_2O /90% H_2O , pH 6.5. GB1 is noted for its excellent stability at elevated temperatures.

(Right) ^{13}C - ^{13}C solid-state NMR spectrum SH3 protein ($\text{U-}^{13}\text{C}$, $\text{U-}^{15}\text{N}$).



(Left) ^1H - ^{15}N -HSQC NMR spectrum of SH3 Domain Protein ($\text{U-}^{13}\text{C}$, $\text{U-}^{15}\text{N}$).



^1H , ^{15}N -HSQC of 1.5 mM Immunoglobulin-Binding Domain B1 of Streptococcal Protein G ($\text{U-}^{13}\text{C}$, 99%; $\text{U-}^{15}\text{N}$, 99%) containing an *N*-terminal His6-tag and TEV protease cleavage site (CNLM-8663-CA, Lot# 20110209). The ^{15}N -amide (top, right) and ^1H -amide (bottom, right) assignments of CNLM-8663-CA show excellent correlation with those previously reported in the Biological Magnetic Resonance Bank for GB1 (BMRB #7280) lacking the His6-TEV leader sequence.

Maltose Binding Protein (NEX-MBP)

NEX-MBP is a 44.9 kDa monomeric protein with multiple sets of resonance assignments (BMRB database) and 3D structures (PDB database) that are publicly available. This product is uniformly D, ^{15}N , ^{13}C -enriched with selective incorporation of protons into methyl groups of Ile- δ 1, Leu- δ and Val- γ side chains. As nonuniform sampling (NUS) and other NMR techniques emerge to push the size limitations of NMR to new boundaries, larger protein standards, such as NEX-MBP, will be required to test data-collection and processing strategies.

NEX-MBP sample formulations:

NEX-MBP1: Apo Conformation

0.5 mM D, ^{15}N , ^{13}C and ILV methyl ^1H , ^{13}C MBP in 10% D_2O , 0.02% NaN_3 , 20 mM sodium phosphate @ pH 7.2

NEX-MBP2: Closed Conformation

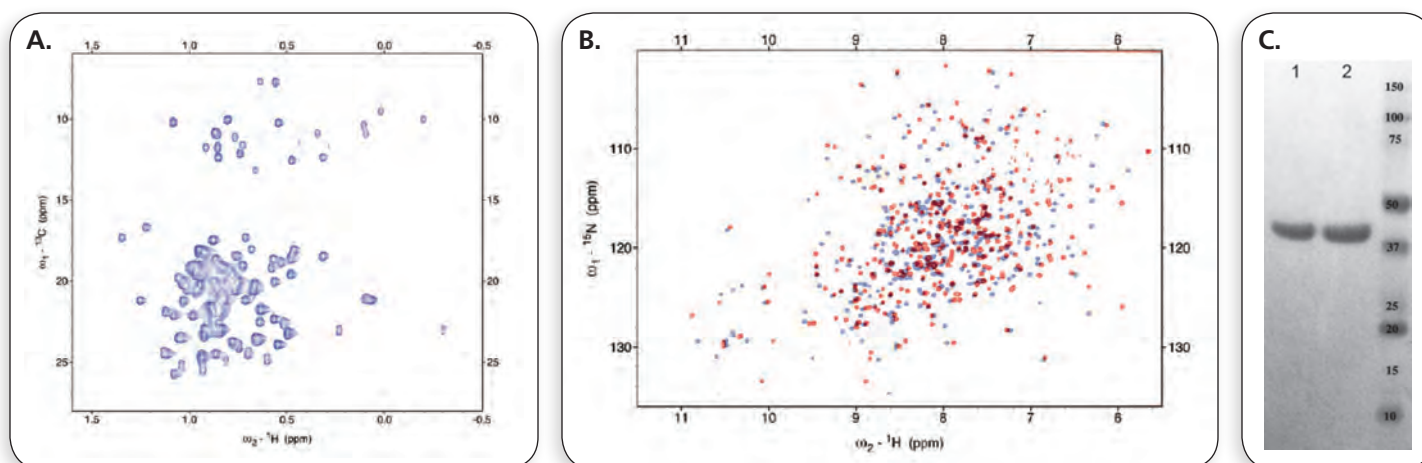
0.5 mM D, ^{15}N , ^{13}C and ILV methyl ^1H , ^{13}C MBP with 3 mM maltotriose, 10% D_2O , 0.02% NaN_3 , 20 mM sodium phosphate @ pH 7.2

NEX-MBP3: Open Conformation

0.5 mM D, ^{15}N , ^{13}C and ILV methyl ^1H , ^{13}C MBP with 2 mM β -cyclodextrin, 10% D_2O , 0.02% NaN_3 , 20 mM sodium phosphate @ pH 7.2

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E. coli Maltose Binding Protein (27-396), Apo Conformation

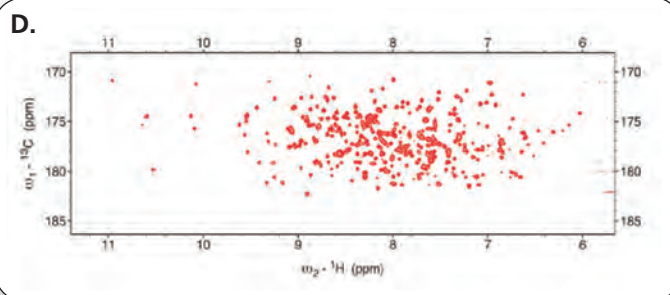
Catalog No.	Label
NEX-MBP1-U-0	unlabeled
NEX-MBP1-N-0	(^{15}N , 95%)
NEX-MBP1-CN-5-0	(^{13}C , 5%; ^{15}N , 95%)
NEX-MBP1-CN-0	(^{13}C , 95%; ^{15}N , 95%)
NEX-MBP1-CDN-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%)
NEX-MBP1-ILV-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-MBP1-ILV-FY-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV-FY)

E. coli Maltose Binding Protein (27-396), Closed Conformation

NEX-MBP2-U-0	unlabeled
NEX-MBP2-N-0	(^{15}N , 95%)
NEX-MBP2-CN-5-0	(^{13}C , 5%; ^{15}N , 95%)
NEX-MBP2-CN-0	(^{13}C , 95%; ^{15}N , 95%)
NEX-MBP2-CDN-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%)
NEX-MBP2-ILV-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-MBP2-ILV-FY-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV-FY)

E. coli Maltose Binding Protein (27-396), Open Conformation

NEX-MBP3-U-0	unlabeled
NEX-MBP3-N-0	(^{15}N , 95%)
NEX-MBP3-CN-5-0	(^{13}C , 5%; ^{15}N , 95%)
NEX-MBP3-CN-0	(^{13}C , 95%; ^{15}N , 95%)
NEX-MBP3-CDN-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%)
NEX-MBP3-ILV-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-MBP3-ILV-FY-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV-FY)



- A. ^{13}C , ^1H HSQC NEX-MBP3 "open" conformation
- B. "Open" (blue) and "closed" (red) superposition
- C. SDS-PAGE GEL NEX-MBP
NEX-MBP3 β -cyclodextrin complexed "open" sample (lane 1)
NEX-MBP2 maltotriose complexed "closed" sample (lane 2)
- D. CO-NH 2D plane of HNC triple-resonance experiment of NEX-MBP2 "closed" sample

Protein Sequence

```

MKIEEGKLIWINGDGKYNGLAEVGGKFEKDTGIKVTVEHPDKLEEFQVAATGDGPDIIWAH
DRFGGYAQSGLLAEITPDKAFQDKLYPFTWDVAVRYNGKLIAYIAVEALSIIYNKDLLPNPKTWEE
IPALDKELKAGKSALMFNLQEPYFTWPLIAADGGYAFKYENGYDIKDVGDVGNAGAKGLTFL
VDLIKNKHMNADTDYSIAEAFNKGGETAMTINGPWAWSNIDTSKVNYGVTVLPTFKGQPSKP
FVGVLGAGINAAASPENKELAKEFLNLYLTDEGLAVNKKPLGAVALKSYEEELAKDPRIAATMEN
AQKGEIMPNIPQMSAFWYAVRTAVINAASGRQTVDEALKDAQTRITK
  
```

(continued)

X-Filtered NOESY NMR Standard (NEX-XF1)

In an X-filtered experiment, only NOEs between $^{15}\text{N}/^{13}\text{C}$ - ^1H and $^{14}\text{N}/^{12}\text{C}$ - ^1H (e.g. interchain NOEs) protons are observed. NOEs between protons connected to $^{15}\text{N}, ^{13}\text{C}$ are filtered (intrachain NOEs). When a uniformly double-labeled protein sample is mixed with a natural-abundance protein sample, the interface will give rise to the only observable NOESY crosspeaks. This powerful strategy enables the spectroscopist to discern intra from inter NOESY crosspeaks, thereby providing essential distance constraints for defining the dimer interface (Lee, et al., 1994, 350:87; Palmer, et al., 1991, 93:151; Schleucher, et al., 1994, 4:301).

NEX-XF1 is a 14 kDa protein (*A. fulgidus* antoxin vapB21 homodimer) for which a set of resonance assignments (bmr7362), 3D structure (2NWT) and other NMR data are available in the public domain. This is a mixture of unlabeled and uniformly $^{15}\text{N}, ^{13}\text{C}$ -enriched protein (25% homodimer unlabeled; 50% heterodimer unlabeled/labeled; 25% homodimer labeled) and is perfect to set up X-filtered NOESY experiments.

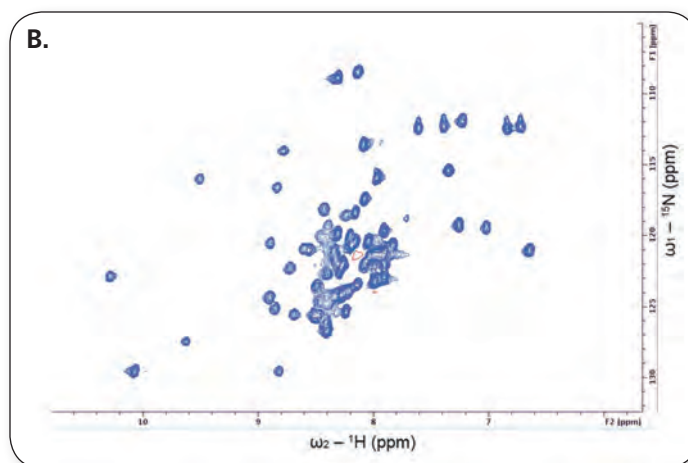
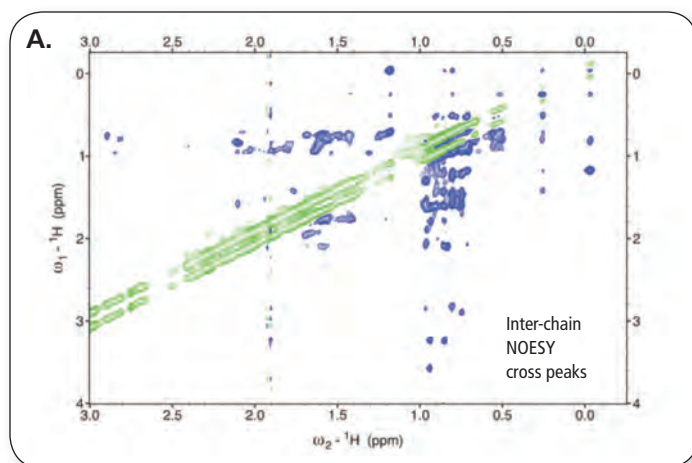
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NEX-XF1 homodimer sample formulation:

NEX-XF1: $^{13}\text{C}, ^{15}\text{N}$ -labeled and unlabeled sample conditions

1 mM protein, 20 mM NH_4OAc pH 5.5, 100 mM NaCl, 5 mM CaCl_2 , 10 mM DTT, 10% D_2O , 0.02 % NaN_3



X-Filtered NOESY NMR Standard

Catalog No.	Label
NEX-XF1-U-0	unlabeled
NEX-XF1-N-0	(^{15}N , 95%)
NEX-XF1-CN-5-0	(^{13}C , 5%; ^{15}N , 95%)
NEX-XF1-CN-0	(^{13}C , 95%; ^{15}N , 95%)
NEX-XF1-CDN-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%)
NEX-XF1-ILV-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-XF1-ILV-FY-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV-FY)

X-Filtered NOESY NMR Standard, His-Tagged

NEX-XF1-HIS-U-0	unlabeled
NEX-XF1-HIS-N-0	(^{15}N , 95%)
NEX-XF1-HIS-CN-5-0	(^{13}C , 5%; ^{15}N , 95%)
NEX-XF1-HIS-CN-0	(^{13}C , 95%; ^{15}N , 95%)
NEX-XF1-HIS-CDN-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%)
NEX-XF1-HIS-ILV-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-XF1-HIS-ILV-FY-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV-FY)

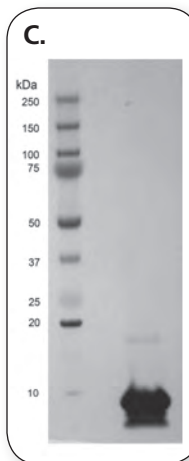
A. 2D ^1H - ^1H plane of $^1\text{H}, ^{13}\text{C}$ edited $^1\text{H}, ^{12}\text{C}$ X-filtered NOESY

B. ^1H - ^{15}N HSQC of NEX-XF1

C. SDS-PAGE GEL NEX-XF1

Protein Sequence

PKIIEAVYENGVFQPLQKVDLKEGERVKIKLELKVPEIDLGEVPS
VEEIKKIRDGTWMSLEHHHHHH



Ubiquitin (NEX-UB1)

NEX-UB1 is a small 8.8 kDa monomeric protein for which multiple sets of resonance assignments (BMRB database) and 3D structures (PDB database) are publicly available. This protein standard is uniformly ^{15}N , ^{13}C enriched. Ubiquitin has been used as an industry-wide standard in the protein NMR field for many years.

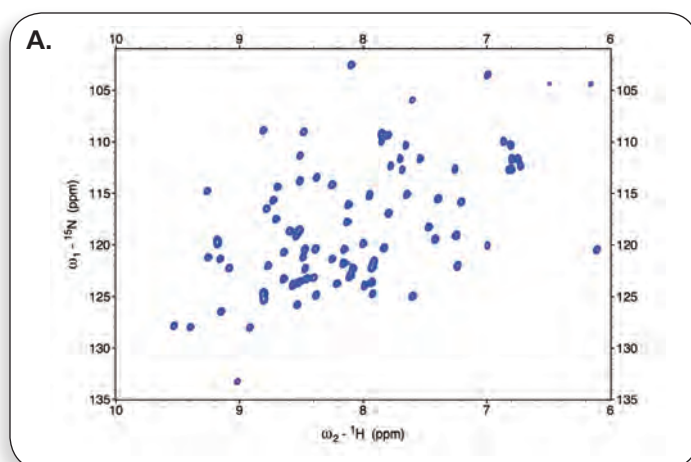
NEX-UB1 sample formulation:

NEX-UB1: Uniformly ^{15}N , ^{13}C -labeled ubiquitin in 90% H_2O ; 10% D_2O
10 mM sodium phosphate buffer, pH 6.5

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A. ^1H , ^{15}N HSQC of NEX-UB1

B. ^{13}C - ^1H HSQC of NEX-UB1

C. CO-NH 2D plane of HNCO triple-resonance experiment of NEX-UB1

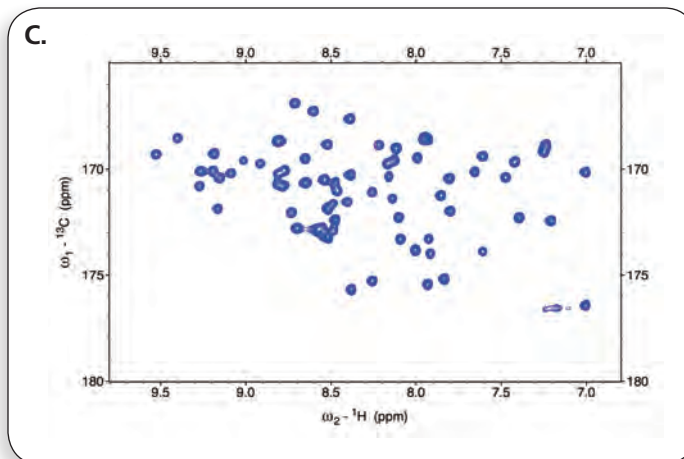
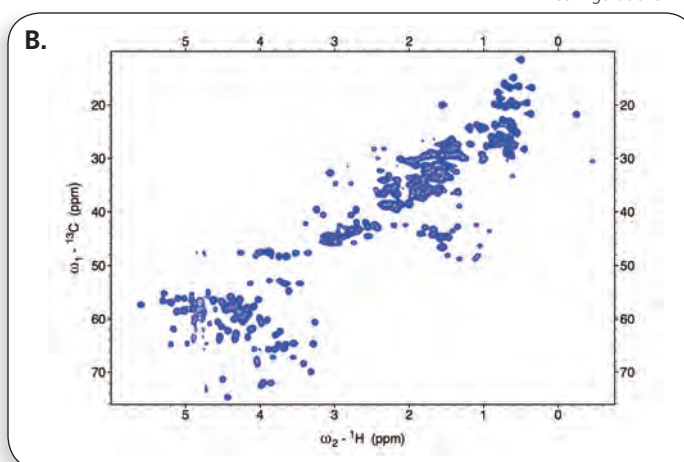
D. SDS-PAGE GEL NEX-UB1

Ubiquitin (Human)

Catalog No.	Label
NEX-UB1-U-0	unlabeled
NEX-UB1-N-0	(^{15}N , 95%)
NEX-UB1-CN-5-0	(^{13}C , 5%; ^{15}N , 95%)
NEX-UB1-CN-0	(^{13}C , 95%; ^{15}N , 95%)
NEX-UB1-CDN-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%)
NEX-UB1-ILV-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-UB1-ILV-FY-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV-FY)

His-Ubiquitin (Human)

Catalog No.	Label
NEX-UBI-HIS-U-0	unlabeled
NEX-UBI-HIS-N-0	(^{15}N , 95%)
NEX-UBI-HIS-5-0	(^{13}C , 5%; ^{15}N , 95%)
NEX-UBI-HIS-CN-0	(^{13}C , 95%; ^{15}N , 95%)
NEX-UBI-HIS-CDN-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%)
NEX-UBI-HIS-ILV-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-UBI-HIS-ILV-FY-0	(^{13}C , 95%; D, 95%; ^{15}N , 95%; $^{13}\text{CH}_3$ -ILV-FY)

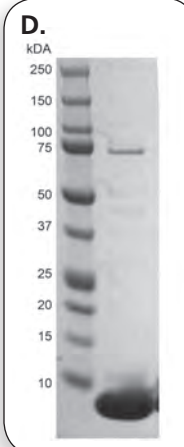


Protein Sequence after TEV Cleavage

SHMQIFVKTLTGKITLEVEPSDTIENVKAKIQDKEGIPPDQQR
LIFAGKQLEDGRTLSDYNIQKESTLHLVLRLLRG

Protein Sequence before TEV Cleavage

MGHHHHHHENLYFQSHMQIFVKTLTGKITLEVEPSDTIEN
VKAKIQDKEGIPPDQQRLLIFAGKQLEDGRTLSDYNIQKESTL
HLVLRLLRG



Notes



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