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.

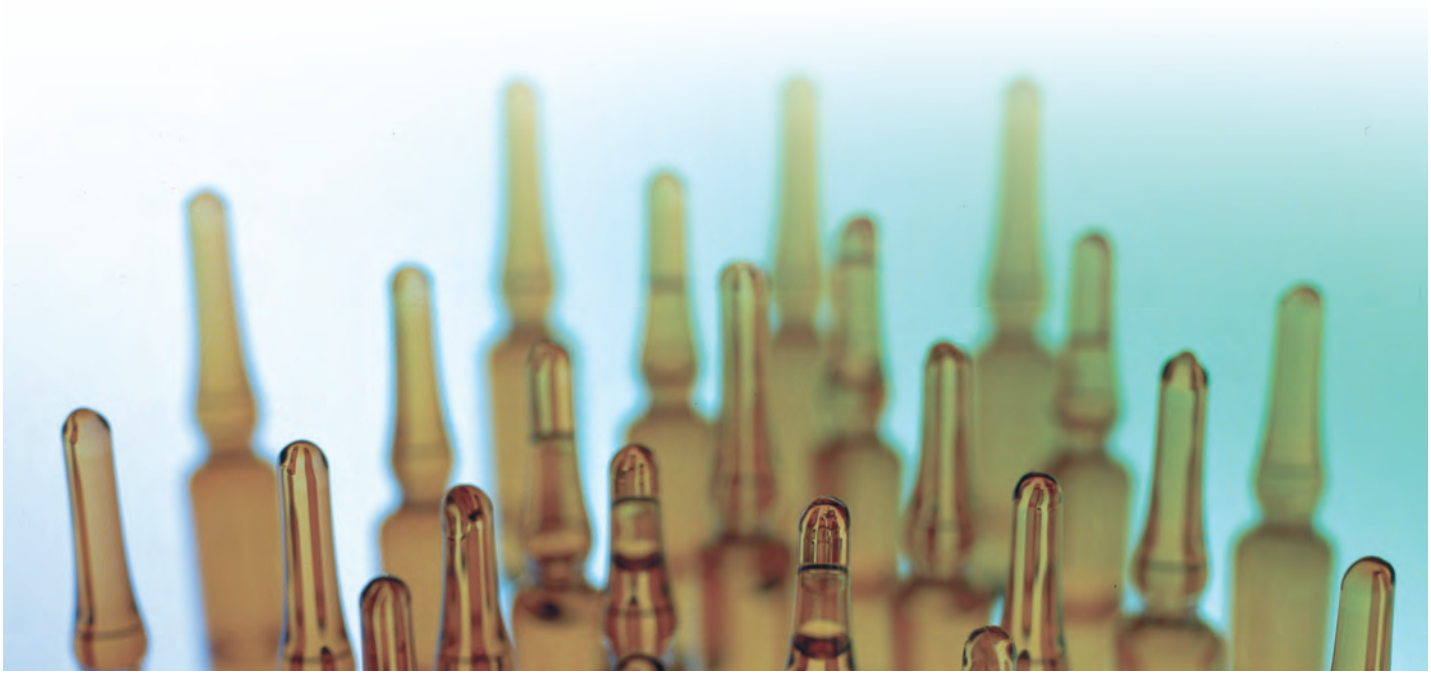
CIL's vision began when it was founded in 1981 by Dr. Joel Bradley, an organic chemist from MIT. Drawing on a commitment to high-quality products, superior customer service, innovative new products and breadth of product lines, CIL quickly emerged as a leader in its field. CIL now produces more than 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, ^{1}H-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

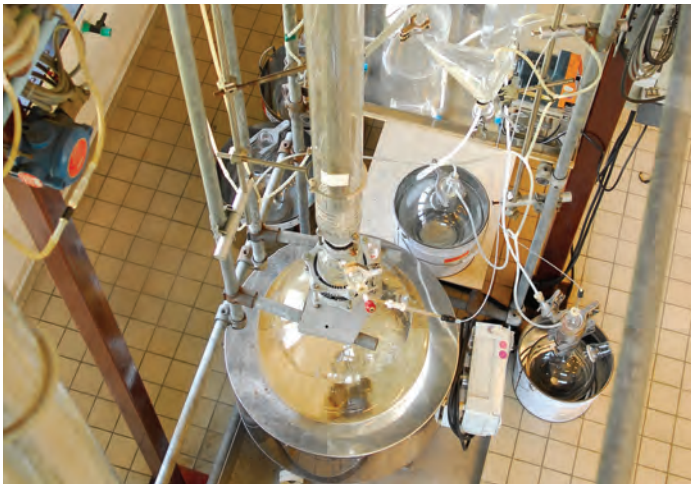
CIL's primary production facility in Andover, Massachusetts, is dedicated to the manufacture of deuterated NMR solvents, stable isotope-labeled chemicals and gases, as well as specific cGMP products. This facility is home to operations staff and production and quality-control teams.

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.

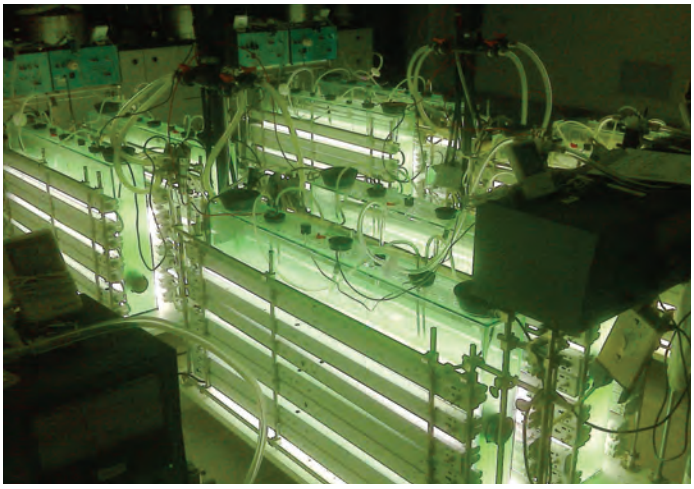
CIL Isotope Separations, LLC (CIS)
Xenia, OH USA

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.



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.



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.

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

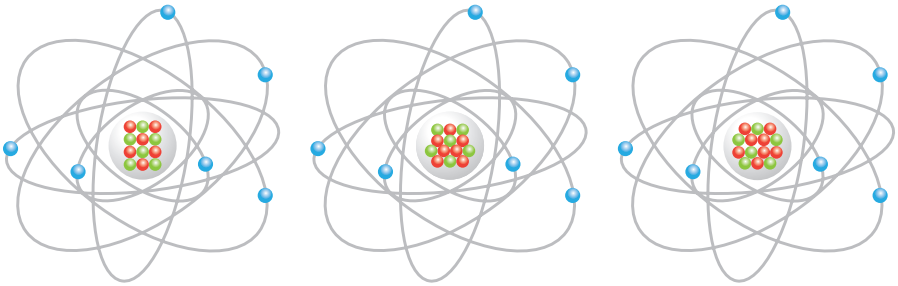
CIL and its direct subsidiary CIL Isotope Separations, LLC, are registered with Emergency Response CHEMTREC®. In the event of a chemical-transportation emergency, CHEMTREC® provides immediate advice for those at the scene of emergencies, then promptly contacts the shipper of the chemicals for more detailed 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.

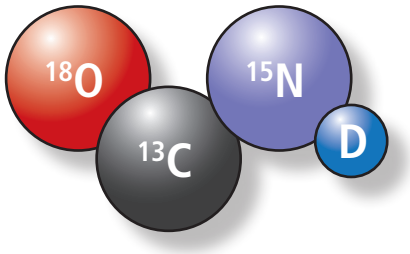


Carbon-12
stable

Carbon-13
stable

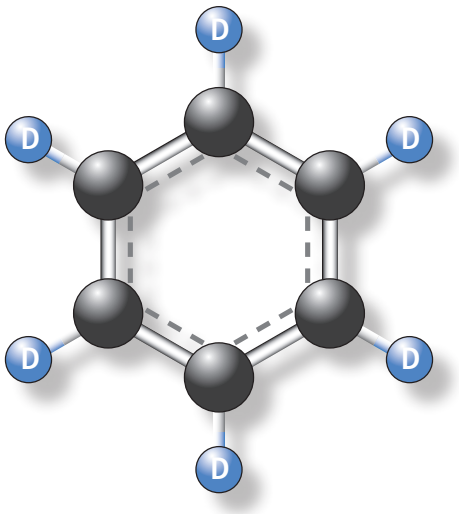
Carbon-14
unstable
(radioactive)

Proton Neutron Electron



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 (^2H = 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

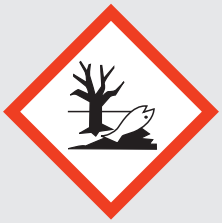
The objective of GHS is to create an internationally recognizable system for HazCom standards, establish a standard format for hazard communication and support the trade of chemicals for international exchange.

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.

GHS Hazard Pictograms and Related Hazards Classes

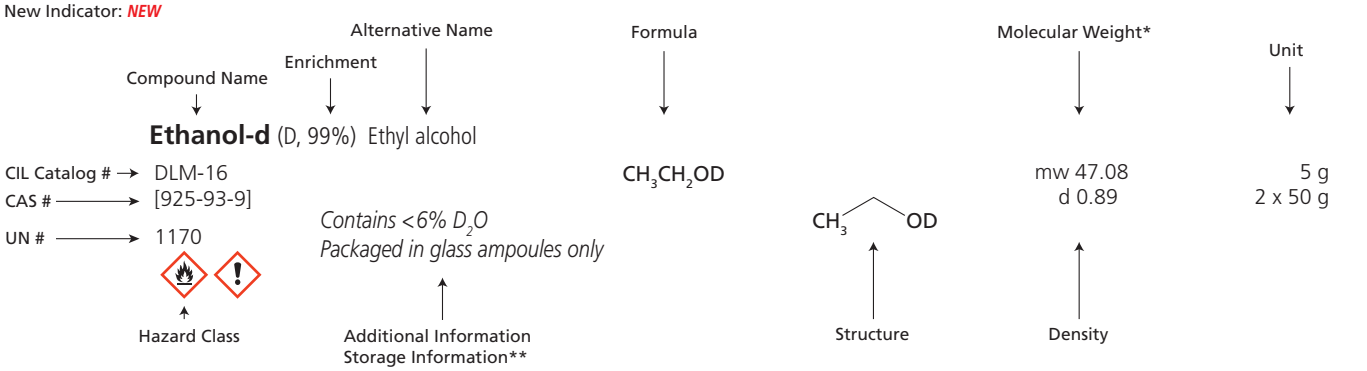
		
Exploding Bomb • Explosives • Self-reactives • Organic peroxides	**Corrosion** • Skin corrosion/burns • Eye damage • Corrosive to metals	**Flame Over Circle** • Oxidizing gases • Oxidizing liquids • Oxidizing solids
		
Gas Cylinder • Gases under pressure	**Environment** • Aquatic toxicity	**Skull and Crossbones** • Acute toxicity (fatal or toxic)
		
Exclamation Point • Irritant (eye and skin) • Skin sensitizer • Acute toxicity • Narcotic effects • Respiratory tract irritant • Hazardous to ozone layer (nonmandatory)	**Health Hazard** • Carcinogen • Mutagenicty • Reproductive toxicity • Respiratory sensitizer • Target organ toxicity • Aspiration toxicity	**Flame** • Flammables • Pyrophorics • Self-heating • Emits flammable gas • Self-reactives • Organic peroxides

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.

Understanding the Product Listings

NMR Solvent Catalog Listings Include:

New Indicator: ***NEW***

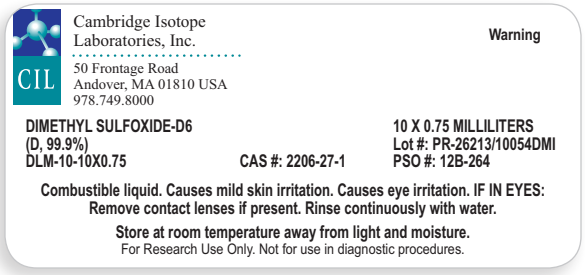


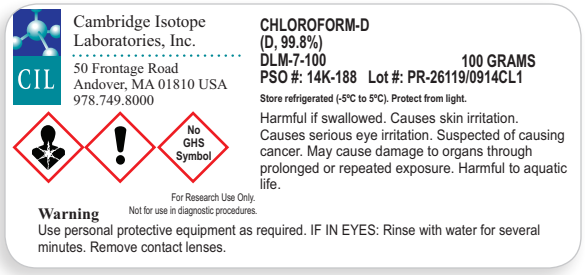
** Molecular weight is based on 100% enrichment* ***Stable if stored under normal conditions, unless otherwise noted*

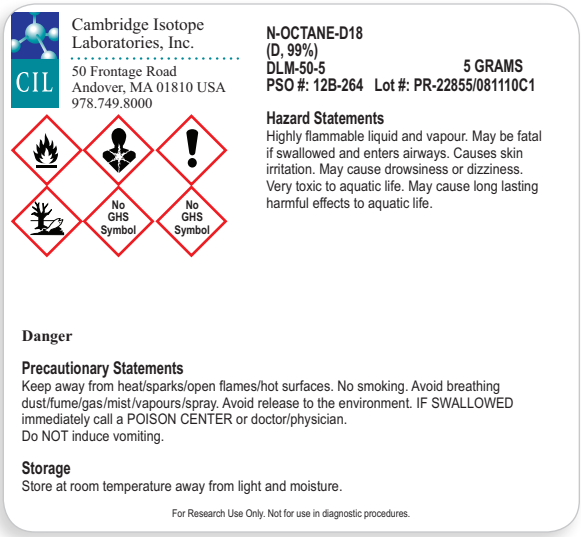
CIL Labels

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







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. ^{1}H-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 ^{1}H-NMR.

CIL's Quality Control Department tests for water content in solvents using the Karl Fischer titration method, and deuterated choloroform 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 [1186-52-3] UN# 2789	CD_3COOD	mw 64.08 d 1.12	10 g 25 g 50 g

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

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

Acetone-d_6 (D, 99.9%)

DLM-9 [666-52-4] UN# 1090	CD_3COCD_3	mw 64.12 d 0.87	10 x 0.5 mL 10 x 0.6 mL 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 [666-52-4] UN# 1090	CD_3COOD_3 *Contains 1% v/v TMS*	mw 64.12 d 0.87	10 x 1 g 3 x (10 x 1 g) 10 g 10 x 10 g 3 x (10 x 10 g) 25 g

Acetone-d_6 (D, 99.9%)

DLM-9tb [666-52-4] UN# 1090	CD_3COCD_3 *Contains 0.05% v/v TMS*	mw 64.12 d 0.87	NEW 10 x 0.5 mL 10 x 1 g 3 x (10 x 1 g) 10 g 10 x 10 g 3 x (10 x 10 g) 25 g

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

DLM-38 [666-52-4] UN# 1090	CD_3COCD_3	mw 64.12 d 0.87	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

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

DLM-38tc [666-52-4] UN# 1090	CD_3COCD_3 *Contains 0.03% v/v TMS*	mw 64.12 d 0.87	10 x 0.75 mL

Acetonitrile-d_3 (D, 96-97%)

DLM-22 [2206-26-0] UN# 1648	$CD_3C{\equiv}N$	mw 44.07 d 0.84	1 L

Acetonitrile-d_3 (D, 99.8%)

DLM-21 [2206-26-0] UN# 1648	$CD_3C{\equiv}N$	mw 44.07 d 0.84	10 x 0.5 mL 10 x 0.6 mL 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 [2206-26-0] UN# 1648	$CD_3C{\equiv}N$ *Contains 0.05% v/v TMS*	mw 44.07 d 0.84	10 x 0.6 mL

Acetonitrile-d_3 "100%" (D, 99.96%)

DLM-53 [2206-26-0]	$CD_3C{\equiv}N$	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-d_6 (D, 99.5%)

DLM-1 [1076-43-3]	C_6D_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-d_6 (D, 99.5%)

DLM-1tb [1076-43-3]	C_6D_6	mw 84.15 d 0.95	10 x 0.6 mL 10 g

UN# 1114

Contains 0.05% v/v TMS

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

DLM-40 [1076-43-3]	C_6D_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-d_6 "100%" (D, 99.96%)

DLM-40tc [1076-43-3]	C_6D_6	mw 84.15 d 0.95	10 x 0.75 mL

UN# 1114

Contains 0.03% v/v TMS

Bromobenzene-d_5 (D, 99.5%)

DLM-9595 [4165-57-5]	C_6D_5Br	mw 162.04 d 1.52	5 g 10 g 25 g

UN# 2514

Chlorobenzene-d_5 (D, 99%)

DLM-263 [3114-55-4]	C_6D_5Cl	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-d_{12} (D, 99.5%)

DLM-17 [1735-17-7]	C_6D_{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-d_{18} (D, 99%) Decahydronaphthalene

DLM-1386 [28788-42-3]	$C_{10}D_{18}$	mw 156.36 d 1.01	1 g 5 g

cis/trans mixture

trans-Decalin-d_{18} (D, 98%)

DLM-1843 [493-02-7] | $C_{10}D_{18}$ | mw 156.36, d 1.01 | 5 g

Deuterium bromide (D, 99%)

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

DBr 48% w/w solution in D_2O
Packaged in clear glass ampoules only

Deuterium chloride (D, 99.5%)

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

DCl 20% w/w solution in D_2O
Packaged in clear glass ampoules only

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

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

DCl 20% w/w solution in D_2O
Packaged in clear glass ampoules only

Deuterium chloride (D, 99.5%)

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

DCl 35% w/w solution in D_2O
Packaged in clear glass ampoules only

Deuterium oxide (D, 70%)

DLM-4-70 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.077 | 1 kg

Deuterium oxide (D, 70%)

DLM-2259-70 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.077 | 1 kg, 1 L

Sterility tested

Deuterium oxide (D, 99%)

DLM-4-99 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 1 kg, 5 kg

Deuterium oxide (D, 99.8%)

DLM-4-99.8 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 1 kg, 10 kg, 20 kg

Deuterium oxide (D, 99.8%)

DLM-2259 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 100 mL, 250 mL, 1 L

Sterility tested

Deuterium oxide (D, 99.9%)

DLM-4 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 x 1 mL, 10 g, 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 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 100 g

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

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

DLM-6 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 x 0.6 mL, 5 x 0.7 mL, 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 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 g

Packaged in serum bottles with Teflon-coated rubber septum tops

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

DLM-6DB [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 x 0.7 mL, 50 g

Contains 0.01 mg/mL DSS

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

DLM-1172 [7789-20-0] UN# 1957 | D_2O | mw 20.03, d 1.11 | 10 g

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

1-2,Dibromoethane-d_4 (D, 99%)

DLM-195 [22581-63-1] UN# 1605 | $Br(CD_2)_2Br$ | mw 191.87, d 2.20 | 10 g, 25 g

1-2,Dichlorobenzene-d_4 (D, 99%)

DLM-158 [2199-69-1] UN# 1591 | $C_6D_4Cl_2$ | mw 151.03, d 1.34 | 1 g, 5 g, 25 g

1-2,Dichloroethane-d_4 (D, 99%)

DLM-18 [17060-07-0] UN# 1184 | $Cl(CD_2)_2Cl$ | mw 102.98, d 1.30 | 1 g, 5 x 1 g, 5 g

Diethyl ether-d_{10} (D, 99%)

DLM-1592 [2679-89-2] UN# 1155 | $(CD_3CD_2)_2O$ | mw 84.10, d 0.80 | 1 g, 5 x 1 g, 5 g

Packaged in ampoules only

Diglyme-d_{14} (D, 98%)

DLM-47 [38086-00-9] — $(CD_3OCD_2CD_2)_2O$ — mw 148.26, d 1.035 — 1 g, 5 g, 5 x 1 g, 10 g

N,N-Dimethylformamide-d_7 (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

Packaged in ampoules only

N,N-Dimethylformamide-d_7 (D, 99.5%) DMF

DLM-25tb [4472-41-7] — $DCON(CD_3)_2$ — mw 80.14, d 1.04 — 10 x 0.6 mL

Contains 0.05% v/v TMS
Packaged in ampoules only

Dimethyl sulfoxide-d_6 (D, 99.9%) DMSO

DLM-10 [2206-27-1] — CD_3SOCD_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

Dimethyl-sulfoxide-d_6 (D, 99.9%) DMSO

DLM-10-s [2206-27-1] — CD_3SOCD_3 — mw 84.17, d 1.18 — NEW 10 mL, 10 g, 25 g

Packaged in serum bottles with Teflon-coated rubber septum tops

Dimethyl-sulfoxide-d_6 (D, 99.9%) DMSO

DLM-10ta [2206-27-1] — CD_3SOCD_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

Contains 1% v/v TMS

Dimethyl-sulfoxide-d_6 (D, 99.9%) DMSO

DLM-10tb [2206-27-1] — CD_3SOCD_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

Contains 0.05% v/v TMS

Dimethyl-sulfoxide-d_6 "100%" (D, 99.96%) DMSO

DLM-34 [2206-27-1] — CD_3SOCD_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

Dimethyl-sulfoxide-d_6 "100%" (D, 99.96%) DMSO

DLM-34tc [2206-27-1] — CD_3SOCD_3 — mw 84.17, d 1.18 — 10 x 0.75 mL

Contains 0.03% v/v TMS

1,4-Dioxane-d_8 (D, 99%) *p*-Dioxane

DLM-28 [17647-74-4] — $C_4D_8O_2$ — 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

UN# 1165

DSS – ^{1}H-NMR chemical shift standard

DLM-8206 [2039-96-5] — $(CH_3)_3Si(CD_2)_3SO_3Na$ — mw 224.4 — 1 g

UN# 1165

Sodium 2,2-dimethyl-2-silapentane-5-sulfonate (D_6 98%)
Chemical purity 97%

DSS – ^{1}H-NMR chemical shift standard

DLM-32 [2039-96-5] — $(CH_3)_3Si(CH_2)_3SO_3Na$ — mw 218.3 — 1 g, 10 g, 50 g

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_3CH_2OD — mw 47.08, d 0.82 — 50 g, 2 x 50 g

UN# 1170

Contains ≤6% D_2O

Ethanol-d_6 (D, 99%) Ethyl alcohol

DLM-31 [1516-08-1] — CD_3CD_2OD — mw 52.11, d 0.89 — 5 x 1 g, 10 x 1 g, 5 g

UN# 1170 3

Anhydrous

Ethanol-d_6 (D, 99%) Ethyl alcohol

DLM-31B [1516-08-1] — CD_3CD_2OD — mw 52.11, d 0.89 — 5 x 1 g, 5 g

UN# 1170 3

Contains ≤6% D_2O

Ethylene glycol-d_6 (D, 98%)

DLM-132 [15054-86-1] — $DOCD_2CD_2OD$ — mw 68.11, d 1.22 — 5 g

Fluorobenzene-d_5 (D, 98%)

DLM-617 [1423-10-5] UN# 2387 — C_6D_5F — mw 101.13, d 1.08 — 1 g

_n_-Heptane-d_{16} (D, 98%)

DLM-423 [33838-52-7] UN# 1206 — $CD_3(CD_2)_5CD_3$ — mw 116.30, d 0.794 — 1 g, 5 g

Hexafluoroacetone trideuterate (D, 99.5%)

DLM-1020 [109640-39-3] — $CF_3COCF_3 \cdot 3\ D_2O$ — mw 226.11, d 1.71 — 10 g

1,1,1,3,3,3-Hexafluoroisopropanol-d_2 (D, 98%)

DLM-143 [38701-74-5] — $(CF_3)_2CDOD$ — mw 170.05, d 1.62 — 1 g, 5 x 1 g, 5 g, 10 g

Hexafluoroisopropyl alcohol, HFIP

_n_-Hexane-d_{14} (D, 98%)

DLM-139 [21666-38-6] UN# 1208 — $CD_3(CD_2)_4CD_3$ — mw 100.26, d 0.767 — 1 g, 5 g

Isopropanol-d_8 (D, 99%) 2-Propyl alcohol

DLM-44 [22739-76-0] UN# 1219 — $(CD_3)_2CDOD$ — mw 68.14, d 0.90 — 5 g, 25 g

Lithium deutoroxide (D, 99.5%)

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

3N in D_2O solution
Packaged in plastic bottles only

Methanol-d (D, 99%) Methyl alcohol

DLM-15 [1455-13-6] UN# 1230 — CH_3OD — mw 33.05, d 0.81 — 50 g, 2 x 50 g

Methanol-d_4 (D, 99.8%) Methyl alcohol

DLM-24 [811-98-3] UN# 1230 — CD_3OD — mw 36.07, d 0.89 — 10 x 0.5 mL, 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-d_4 (D, 99.8%) Methyl alcohol

DLM-24-s [811-98-3] UN# 1230 — CD_3OD — mw 36.07, d 0.89 — 10 g, 25 g, 50 g

Packaged in serum bottles with Teflon-coated rubber septum tops

Methanol-d_4 (D, 99.8%) Methyl alcohol

DLM-24tb [811-98-3] UN# 1230 — CD_3OD — mw 36.07, d 0.89 — NEW 10 x 0.5 mL, 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-d_4 "100%" (D, 99.95%) Methyl alcohol

DLM-51 [811-98-3] UN# 1230 — CD_3OD — mw 36.07, d 0.89 — 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

Methylcyclohexane-d_{14} (D, 99.5%)

DLM-288 [10120-28-2] UN# 2296 — $C_6D_{11}CD_3$ — mw 112.27, d 0.88 — 1 g, 5 g

Methylene chloride-d_2 (D, 99.9%) Dichloromethane

DLM-23 [1665-00-5] UN# 1593 — CD_2Cl_2 — mw 86.95, d 1.30 — NEW 10 x 0.5 mL, 10 x 0.75 mL, 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-d_2 (D, 99.9%) Dichloromethane

DLM-23tb [1665-00-5] UN# 1593 — CD_2Cl_2 — mw 86.95, d 1.35 — 10 x 0.6 mL

Contains 0.05% v/v TMS

Methylene chloride-d_2 "100%" (D, 99.96%) Dichloromethane

DLM-55 [1665-00-5] UN# 1593 — CD_2Cl_2 — mw 86.95, d 1.35 — 10 x 0.5 mL, 10 x 0.6 mL, 5 x 0.75 mL, 10 x 0.75 mL, 5 mL

_N_-Methyl-2-pyrrolidinone-d_9 (D, 97-99%) NMP

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

Nitric acid-d (D, 99%)

DLM-3037 [13587-52-5] — DNO_3 — mw 64.02, d 1.026 — 5 g (of soln.), 25 g (of soln.)

65-70% w/w solution in D_2O
Packaged in clear glass ampoules only

Nitrobenzene-d_5 (D, 99%)

DLM-294 [4165-60-0] UN# 1662 — $C_6D_5NO_2$ — mw 128.14, d 1.25 — 5 g, 10 g, 25 g

Nitromethane-d_3 (D, 99%)

DLM-30 [13031-32-8] UN# 1261 — CD_3NO_2 — mw 64.06, d 1.20 — 10 g, 25 g

***n*-Octane-d_{18}** (D, 99%)

DLM-50 [17252-77-6] UN# 1262 — $CD_3(CD_2)_6CD_3$ — mw 132.34, d 0.815 — 1 g, 5 g

***n*-Pentane-d_{12}** (D, 98%)

DLM-1213 [2031-90-5] UN# 1265 — $CD_3(CD_2)_3CD_3$ — mw 84.22, d 0.73 — 1 g, 5 g

Phosphoric acid-d_3 (D, 99%)

DLM-1132 [14335-33-2] — D_3PO_4 — mw 101.01, d 1.74 — 50 g, 100 g

Approximately 85% w/w solution in D_2O

Pyridine-d_5 (D, 99.5%)

DLM-13 [7291-22-7] UN# 1282 — C_5D_5N — mw 84.13, d 1.05 — 10 x 0.5 mL, 5 x 1 g, 10 x 1 g, 3 x (10 x 1 g), 10 g, 25 g, 50 g

Pyridine-d_5 (D, 99.5%)

DLM-13tb [7291-22-7] UN# 1282 — C_5D_5N — mw 84.13, d 1.05 — NEW 10 x 0.5 mL, 10 x 0.6 mL, 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-d_5 "100%" (D, 99.94%)

DLM-39 [7291-22-7] UN# 1282 — C_5D_5N — mw 84.13, d 1.05 — 5 x 0.5 mL, 10 x 0.5 mL, 5 x 0.75 mL, 10 x 0.75 mL, 5 mL

Sodium deuteroxide (D, 99.5%)

DLM-57 [14014-06-3] UN# 1282 — NaOD — mw 41.00, d 1.46 — 50 g

NaOD 30% w/w solution in D_2O
Packaged in polyethylene bottles

Sodium deuteroxide (D, 99.5%)

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

NaOD 40% w/w solution in D_2O
Packaged in polyethylene bottles

Sulfuric acid-d_2 (D, 99%)

DLM-33 [13813-19-9] UN# 1282 — D_2SO_4 — mw 100.09, d 1.86 — 50 g

96-98% solution in D_2O
Packaged in glass ampoules only

1,1,2,2-Tetrachloroethane-d_2 (D, 99.6%) TCE

DLM-35 [33685-54-0] UN# 1702 — $Cl_2CDCDCl_2$ — mw 169.86, d 1.62 — 5 g, 10 g, 100 g

Tetrahydrofuran-d_8 (D, 99.5%) THF

DLM-36 [1693-74-9] UN# 2056 — mw 80.16, d 0.99 — NEW 10 x 0.5 mL, 10 x 0.75 mL, 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-d_8 "100%" (D, 99.95%) THF

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

Tetramethylsilane TMS

DLM-43 [75-76-3] — $(CH_3)_4Si$ — mw 88.22, d 0.64 — 50 g

NMR grade
Chemical purity 99.9%

TMSP-2,2,3,3-d_4 (D, 98%) Sodium 3-trimethylsilylpropionate

DLM-48 [24493-21-8] — $(CH_3)_3SiCD_2CD_2CO_2Na$ — mw 172.27, d 1.52 — 1 g, 5 x 1 g, 5 g

D_2O reference standard and
^1H-NMR chemical shift standard

Toluene-d_8 (D, 99.5%)

DLM-5 [2037-26-5] UN# 1294 — $C_6D_5CD_3$ — mw 100.19, d 0.94 — 10 x 1 g, 3 x (10 x 1 g), 5 g, 10 g, 25 g, 100 g, 1000 g

Toluene-d_8 "100%" (D, 99.94%)

DLM-42 [2037-26-5] UN# 1294 — $C_6D_5CD_3$ — mw 100.19, d 0.94 — 5 x 0.5 mL, 10 x 0.5 mL, 5 x 0.75 mL, 10 x 0.75 mL, 5 mL

Trifluoroacetic acid-d (D, 99.5%)

DLM-46 [599-00-8] UN# 2699	CF_3COOD *Packaged in ampoules only*	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

2,2,2-Trifluoroethanol-d$_2$ (D, 98%) Trifluoroethyl alcohol

DLM-2318 [77253-67-9]	CF_3CD_2OH	mw 102.05 d 1.37	1 g 5 g

2,2,2-Trifluoroethanol-d$_3$ (D, 99%) Trifluoroethyl alcohol

DLM-27 [77253-67-9]	CF_3CD_2OD	mw 103.06 d 1.42	1 g 5 x 1 g

2,2,2-Trifluoroethanol-d$_3$ "100%" (D, 99.85%) Trifluoroethyl alcohol

DLM-58 [77253-67-9]	CF_3CD_2OD	mw 103.06 d 1.42	1 g 5 g

1,3,5-Trimethyl benzene (D_{12}, 98%) Mesitylene

DLM-3105 [69441-16-3] UN# 2325	$C_3D_3(CD_3)_3$	mw 132.26	5 g

Water, deuterium depleted

DLM-52 [7732-18-5]	H_2O *2-3 ppm deuterium*	mw 18.02 d 1.00	25 g 100 g

o-Xylene-d$_{10}$ (D, 98%)

DLM-808 [56004-61-6] UN# 1307	$C_6D_4(CD_3)_2$	mw 116.23 d 0.953	5 g

p-Xylene-d$_{10}$ (D, 98%)

DLM-313 [41051-88-1] UN# 1307	$C_6D_4(CD_3)_2$	mw 116.23 d 0.948	5 g

^{12}C and ^{12}C/Deuterium-Labeled Solvents (^{13}C Depleted)

Benzene ($^{12}C_6$, 99.95%)

CLM-867 [71-43-2]	$*C_6H_6$ *^{13}C depleted*	mw 78.05 d 0.874	0.8 mL

Chloroform (^{12}C, 99.95%; D, 99%)

CDLM-844 [865-49-6]	$*CDCl_3$ *^{13}C depleted*	mw 120.38 d 1.500	Inquire

Glycerol ($^{12}C_3$, 99.95%; D_8, 98%)

CDLM-8660 [56-81-5]	$DO*CD_2*CD(OD)*CD_2OD$ *^{13}C depleted*	mw 100.11 d 1.250	1g 5g 10g

Methanol (^{12}C, 99.95%) Methyl alcohol

CLM-2472 [67-56-1]	$*CH_3OH$ *^{13}C depleted*	mw 32.04 d .0791	1 g

Methanol (^{12}C, 99.95%; D_4, 99.5%) Methyl alcohol

CDLM-01 [811-98-3]	$*CD_3OD$ *^{13}C depleted*	mw 36.07 d 0.888	0.8 mL 5g

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 $GdCl_3 \cdot 6H_2O$ in D_2O (D, 99.96%)	^{1}H-Homogeneity	5 mm x 8"
DLM-72	40% *p*-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_2O + 01% H_2O	Auto Test Sample	5 mm x 8"
DLM-88	0.1 mg/mL $GdCl_3$ + 0.1% DSS in 20% H_2O in D_2O	Gradient Shimming	5 mm x 8"
CDLM-96	1% $^{13}CH_3I$, 0.2% $Cr(acac)_3$ + 1% $(CH_3O_3)P$ 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_2O + 1% H_2O	Auto Test Sample	5 mm x 8"
DLM-7049	5% Ethyl *trans*-crotonate + 1% TMS in $CDCl_3$ in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
U LM-7047	98% *N*-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.

NORELL® Tubes *(Sold only in North America)*

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NORELL®

www.nmrtubes.com

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

Wilmad-LabGlass NMR Sample Tubes

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

Wilmad LabGlass

www.wilmad-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 dessicator prior to use.
- Precondition an NMR tube by rinsing it with D_2O. Remove residual D_2O by rinsing first with methanol-d_4 or acetone-d_6 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%" D_2O

To avoid loss of enrichment due to exchange with ambient moisture, "100%" D_2O 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 D_2O being removed should be injected into the serum bottle prior to withdrawing D_2O.

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 recommend 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 H_2O + D_2O. In all cases where both H_2O and D_2O 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 D_2O present in the solvents. Thus, a neglible 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 H_2O peak, may be observed in the DMSO-d_6 or acetronitrile-d_3 (for example), due to the slower equilibrium that exists between H_2O and D_2O and these solvents.
- CIL also specializes in ^{13}C-depleted and deuterium-depleted compounds. Please contact us if you do not see the ^{13}C-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 ^{1}H 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°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**
N,N-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 ^{1}H spectra of the residual protons and ^{13}C 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 D_2O). 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 H_20 in addition to the residual solvent peak. When the exchange rate between H_20 and HOD is slow on the NMR timescale the water peak appears as two peaks, a singlet corresponding to H_20 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-d_4 / Acetone-d_6 / Benzene-d_6 / Cyclohexane-d_{12} / Deuterium Oxide / *N,N*-Dimethylformamide-d_7 / Dimethyl Sulfoxide-d_6 / 1,4-Dioxane-d_8 (*p*-Dioxane) / Ethanol-d_6 / Methanol-d_4 / Methylene Chloride-d_2 / Pyridine-d_5 / 1,1,2,2-Tetrachloroethane-d_2 / Toluene-d_8 / Trifluoroacetic Acid-d / 2,2,2-Trifluoroethanol-d_3

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

Acetonitrile-d_3

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-d_8

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 D_2O

Some deuterated solvents are prepared by catalytic exchange of protonated solvent with deuterium oxide and are carefully purified by distillation. Residual water (H_2O in equilibrium exchange with D_2O) 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 D_2O 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-d_6 containing 100 ppm D_2O. The problem becomes worse as the molecular weight of the analyte increases.

Solution

Water (as H_2O, HOD or D_2O) 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*

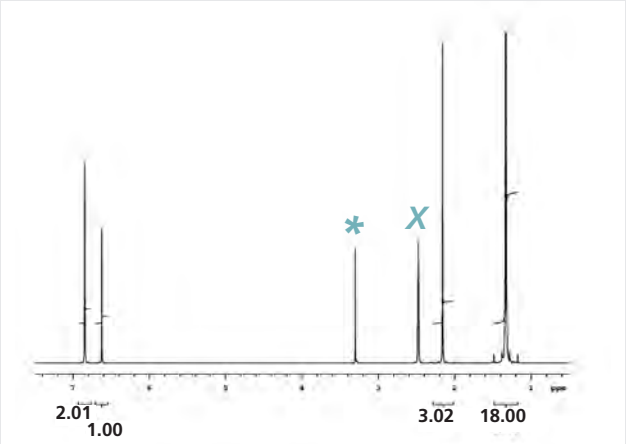


Figure 1. ^{1}H-NMR spectrum of 5.0 mg 2,6-di-*tert*-butyl-4-methylphenol (MW 220.36g / mole) in dry DMSO-d_6. *Note the proper integral ratios of 18:3:1:2 (t-butyl: methyl: ring-H: -OH). Note the single H_2O peak at 3.3 ppm.*

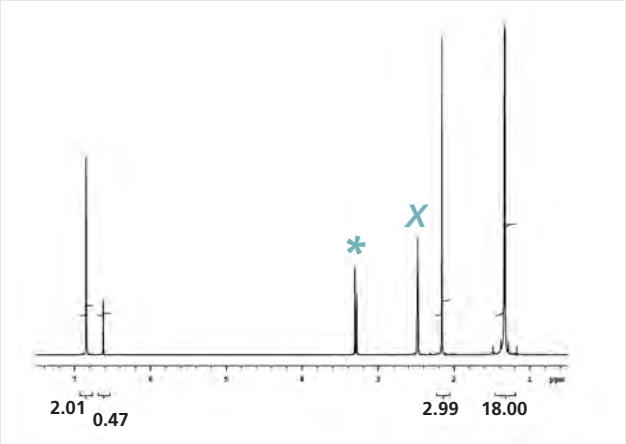


Figure 2. ^{1}H-NMR spectrum of 5.3 mg of 2,6-di-*tert*-butyl-4-methylphenol in DMSO-d_6 with 100 ppm D_2O added. *Note the reduced ratio of the phenolic proton 18:3:2:0.47 (t-butyl: methyl: ring-H: -OH). Note that the HOH and HOD peaks are separated in the spectrum.*

NMR Solvents Chemical Shifts of Selected Compounds in Different Solvents

Compounds	$CDCl_3$	$(CD_3)_2CO$	$(CD_3)_2SO$	C_6D_6	CD_3CN	CD_3OD	D_2O
Solvent residual peak	7.26	2.05	2.50	7.16	1.94	3.31	4.79
H_2O	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	
tert-butyl alcohol	1.28	1.18	1.11 4.19	1.05 1.55	1.16 2.18	1.40	1.24
tert-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-tert-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	
Dicholoromethane	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	
n-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
n-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.; Nvdelman, A. **1997**. NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities. *J Org Chem, 62,* 75-12-7515.

qNMR

Standards for qNMR

Quantitative ^{1}H-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.

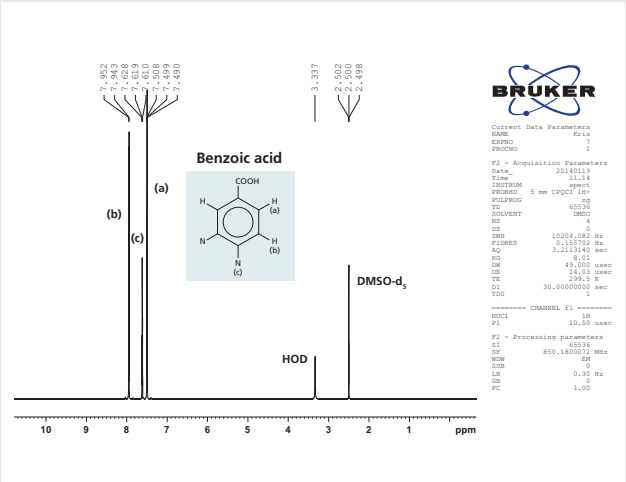


Figure 1. 850 MHz ^{1}H-NMR spectrum of benzoic acid in DMSO-d_6. Resonances from the aromatic protons of benzoic acid, HOD and DMSO-d_5 are assigned. The acid proton resonance from benzoic acid (~12-13 ppm) is not shown. (Courtesy Joe Ray, Baxter Healthcare Corporation, Round Lake, IL)

External Calibration Standards

CIL is pleased to offer external calibration standards for qNMR. The standards are formulated using CIL's high-quality 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 ^{1}H-NMR spectrum of benzoic acid in 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.

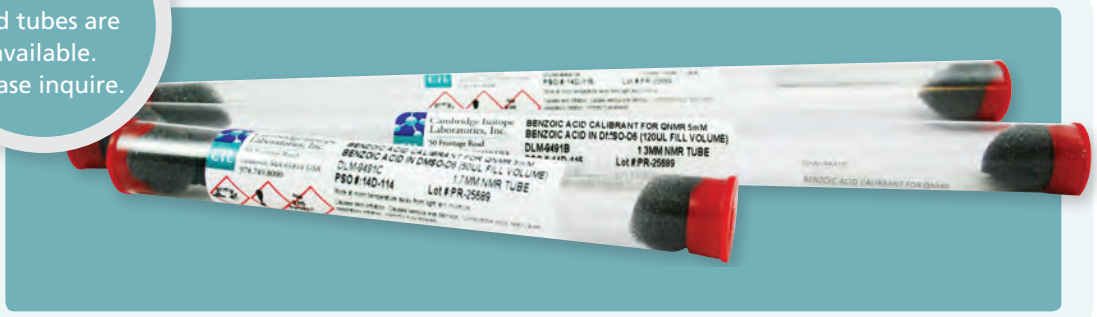
qNMR Standard for External Referencing

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

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 ^{1}H-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.

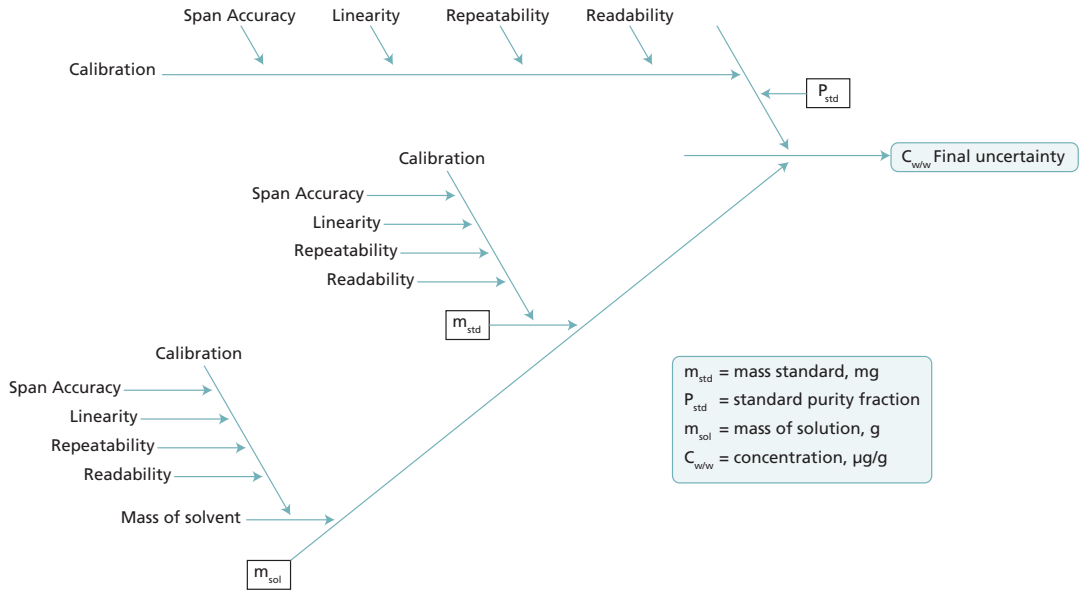
CIL is pleased to offer a ready-to-use DMSO-d_6 solution containing a known amount of benzoic acid for internal referencing. Because this solution is preformulated, the user does not need to weigh a standard material. The elimination of this step will reduce effort and time in sample preparation and 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-d6	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 concentration[1] 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_6, 98%)	Please inquire
DLM-805	Formaldehyde (D_2, 98%) (~20% w/w in D_2O)	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

Find a complete listing of synthetic intermediates here...

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 D_2O on living tissue. It includes a review of potential clinical effects of D_2O 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 ll 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 acohol.

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-d_4 and reveals C=C coupling at the boron center.

Pal, S.; Zavalij, P.Y.; Vedernikov, A.N. **2014**. Oxidative C (sp^3)-H bond cleavage, C-C and C=C coupling at a boron center with O_2 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 H_3PO_4 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.

Reference our complete Environmental product offerings here...

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.

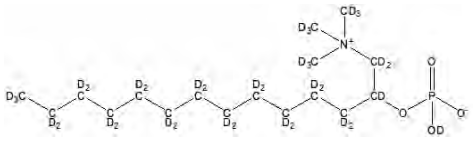
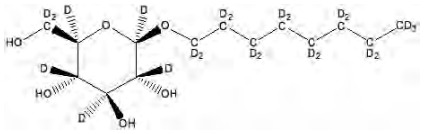
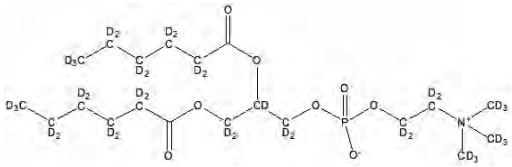
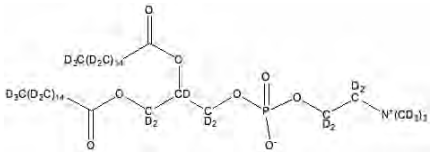
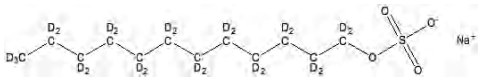
Reference

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 Biochemisty
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 (DPPC) (D_{80}, 98%) CP 95%+ 
DLM-197	Sodium dodecyl sulfate (D_{25}, 98%) 

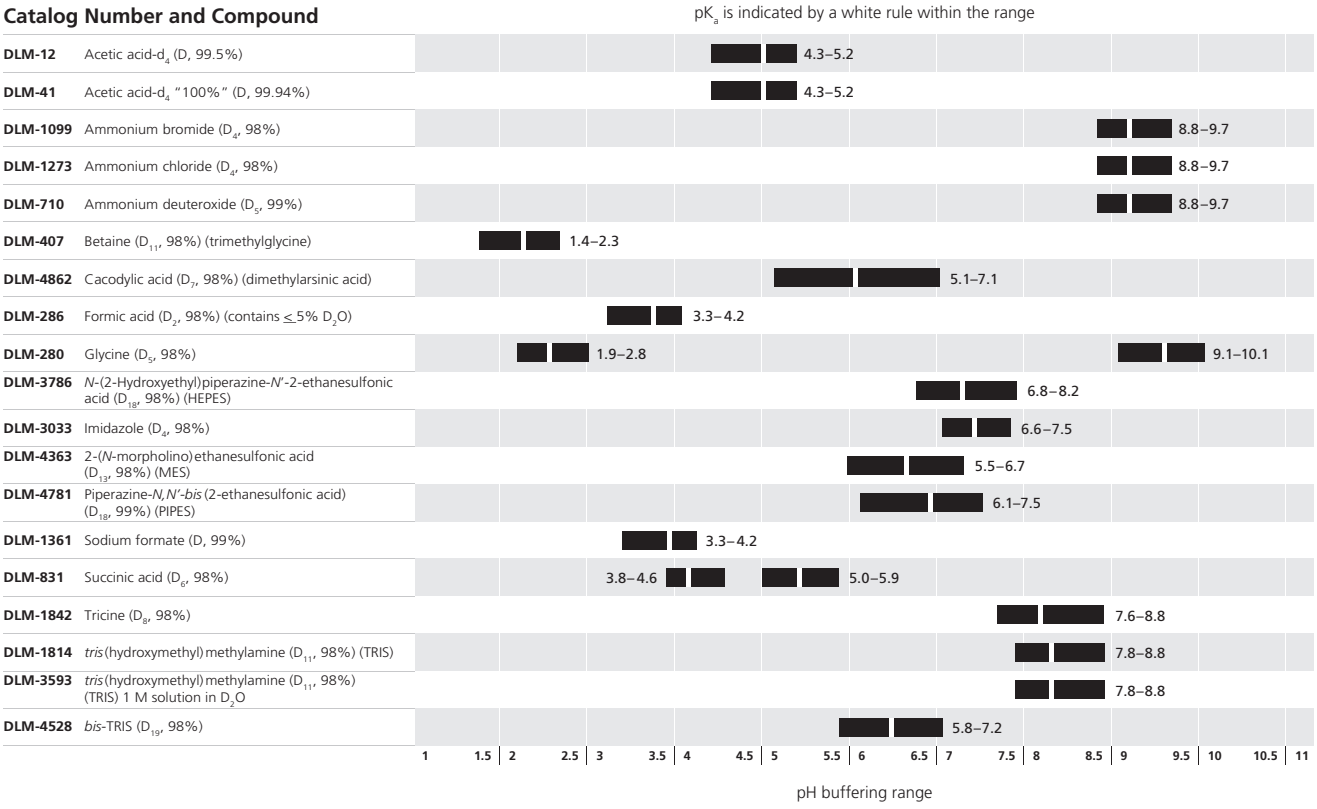
Deuterated Buffers

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 deuteroxide (D_5, 99%) (~25% in soln D_2O)
DLM-407	Betaine (D_{11}, 98%)
DLM-4862	Cacodylic acid (D_7, 98%)
DLM-286	Formic acid (D_2, 98%) (<5% D_2O)
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_2O
DLM-4528	*bis*-TRIS (D_{19}, 98%)

pH Buffering Range Chart



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:

- ^{1}H-^{15}N HSQC (^{15}N-labeled proteins)
- ^{1}H-^{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 ^{1}H-^{15}N-HSQC spectrum.

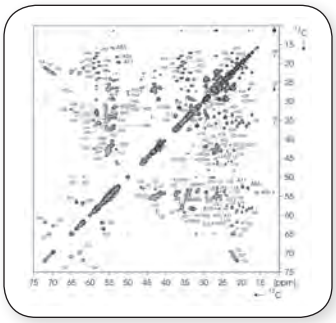
GB1 is offered as a *N*-terminal, tobacco etch virus (TEV)-cleavable 6xHis-tag as a 1.5 mM solution in 137 mM NaCl, 2.7 mM KCl, 8.1 mM Na_2HPO_4, 1.8 mM KH_2PO_4, 0.02% NaN_3, 0.1 mM TSP in 10% D_2O/90% H_2O, pH 6.5. GB1 is noted for its excellent stability at elevated temperatures.

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

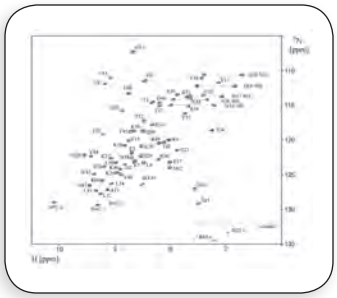
CIL His-Tagged Protein Standards

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

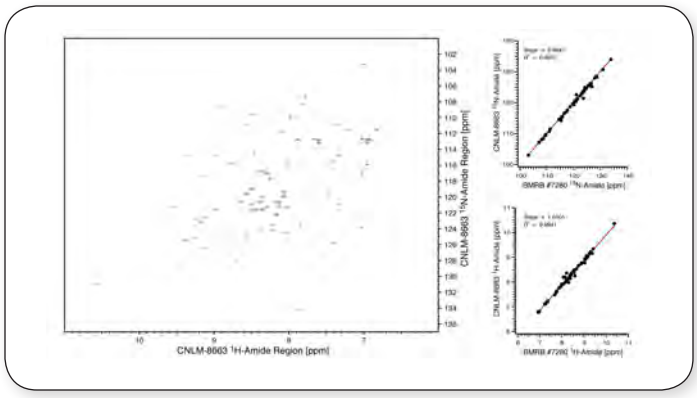
Product	Amino Acid Length
Chicken α-Spectrin SH3 Domain	62 residues
MDETGKELVL ALYDYQEKSP REVTMKKGDI LTLLNSTNKD WWKVEVNDRQ GFVPAAYVKK LD	
His6x-GB1 (β-1 immunoglobulin domain of protein G)	71 residues
MHHHHHHGEN LYFQSMQYKL ILNGKTLKGE TTTEAVDAAT AEKVFKQYAN DNGVDGEWTY DDATKTFTVT E	
GFL Peptide	8 residues
YG**GFL**RRI (bold indicates labeled residues)	



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



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



^{1}H,^{15}N-HSQC of 1.5 mM Immunoglobulin-Binding Domain B1 of Streptococcal Protein G (U-^{13}C, 99%; U-^{15}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 ^{1}H-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-δ1, 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 ^{1}H,^{13}C MBP in 10% D_2O, 0.02% NaN_3, 20 mM sodium phosphate @ pH 7.2

NEX-MBP2: Closed Conformation

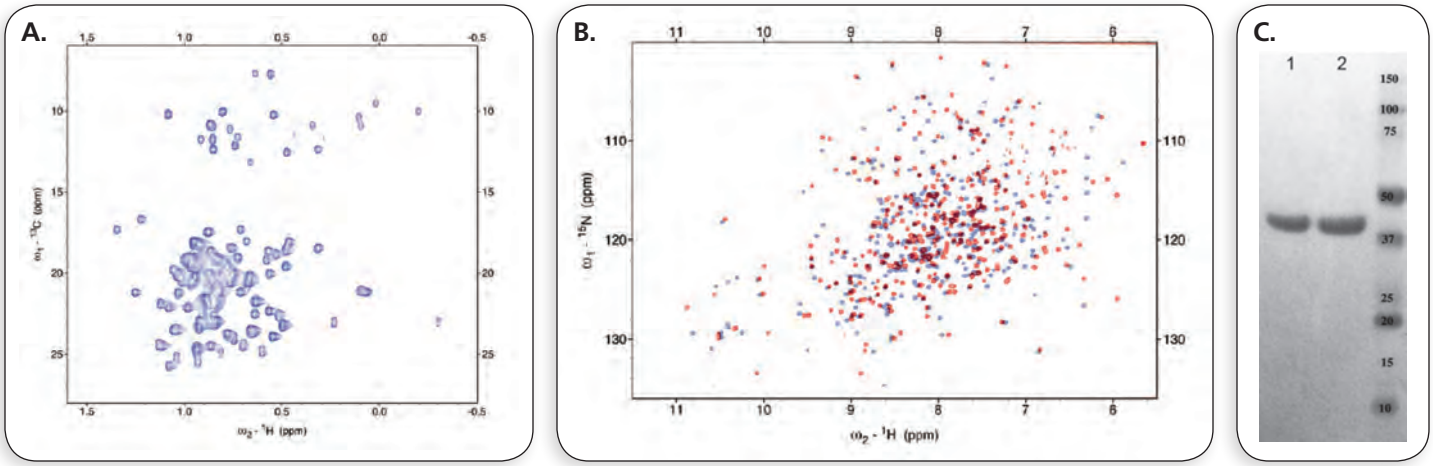
0.5 mM D,^{15}N,^{13}C and ILV methyl ^{1}H,^{13}C MBP with 3 mM maltotriose, 10% D_2O, 0.02% NaN_3, 20 mM sodium phosphate @ pH 7.2

NEX-MBP3: Open Conformation

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

Available in a sealed NMR tube upon request

Contact CIL for different packaging configurations



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

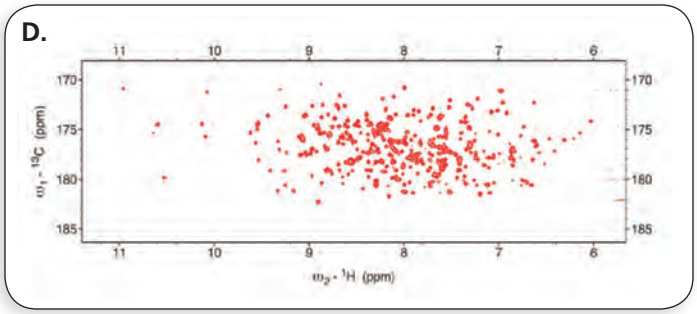
Catalog No.	Label
NEX-MBP1-U-0	unlabeled
NEX-MBP1-N-0	(^{15}N, 95%)
NEX-MBP1-CN-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-MBP1-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-MBP1-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-MBP1-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-MBP1-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

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%; $^{13}CH_3$-ILV)
NEX-MBP2-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

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%; $^{13}CH_3$-ILV)
NEX-MBP3-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)



A. **^{13}C,^{1}H 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 HNCO triple-resonance experiment of NEX-MBP2 "closed" sample**

Protein Sequence

MKIEEGKLVIWINGDKGYNGLAEVGKKFEKDTGIKVTVEHPDKLEEKFPQVAATGDGPDIIFWAH
DRFGGYAQSGLLAEITPDKAFQDKLYPFTWDAVRYNGKLIAYPIAVEALSLIYNKDLLPNPPKTWEE
IPALDKELKAKGKSALMFNLQEPYFTWPLIAADGGYAFKYENGKYDIKDVGVDNAGAKAGLTFL
VDLIKNKHMNADTDYSIAEAAFNKGETAMTINGPWAWSNIDTSKVNYGVTVLPTFKGQPSKP
FVGVLSAGINAASPNKELAKEFLENYLLTDEGLEAVNKDKPLGAVALKSYEEELAKDPRIAATMEN
AQKGEIMPNIPQMSAFWYAVRTAVINAASGRQTVDEALKDAQTRITK

(continued)

X-Filtered NOESY NMR Standard (NEX-XF1)

In an X-filtered experiment, only NOEs between $^{15}N/^{13}C$-^{1}H and $^{14}N/^{12}C$-^{1}H (e.g. interchain NOEs) protons are observed. NOEs between protons connected to $^{15}N,^{13}C$ 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 $^{15}N,^{13}C$-enriched protein (25% homodimer unlabeled; 50% heterodimer unlabeled/labeled; 25% homodimer labeled) and is perfect to set up X-filtered NOESY experiments.

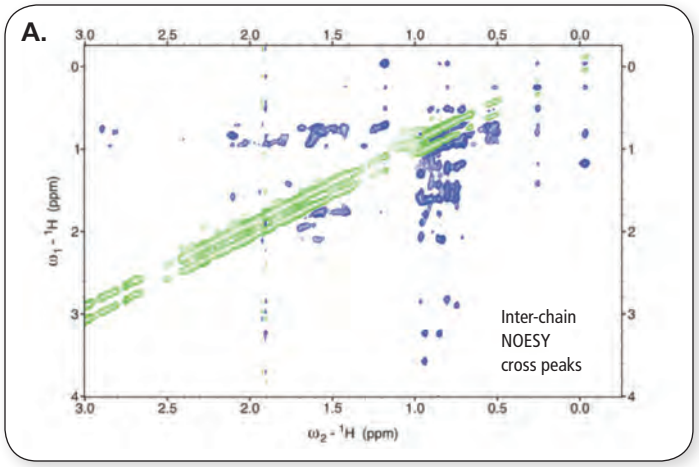
Available in a sealed NMR tube upon request

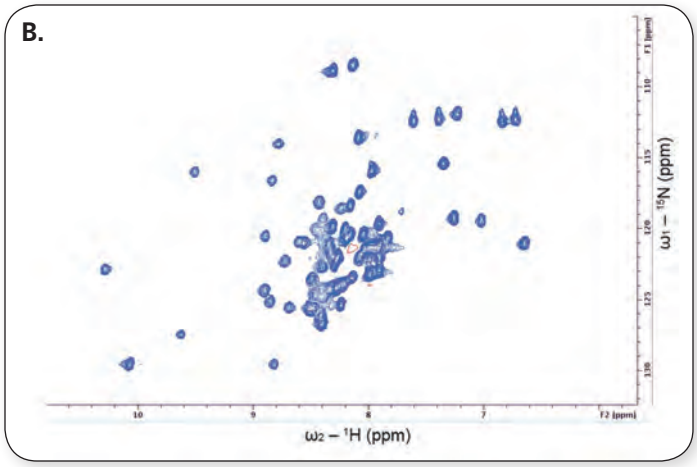
Contact CIL for different packaging configurations

NEX-XF1 homodimer sample formulation:

NEX-XF1: $^{13}C,^{15}N$-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

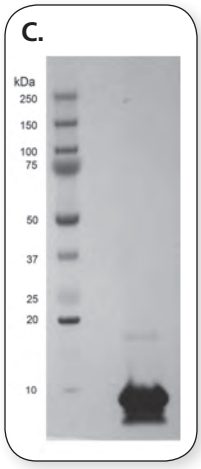




A. **2D ^{1}H-^{1}H plane of $^{1}H,^{13}C$ edited $^{1}H,^{12}C$ X-filtered NOESY**

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

C. **SDS-PAGE GEL NEX-XF1**



Protein Sequence

PKIIEAVYENGVFKPLQKVDLKEGERVKIKLELKVEPIDLGEPVS
VEEIKKIRDGTWMSSLEHHHHHH

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%; $^{13}CH_3$-ILV)
NEX-XF1-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

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%; $^{13}CH_3$-ILV)
NEX-XF1-HIS-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

Ubiquitin (NEX-UB1)

Powder form available

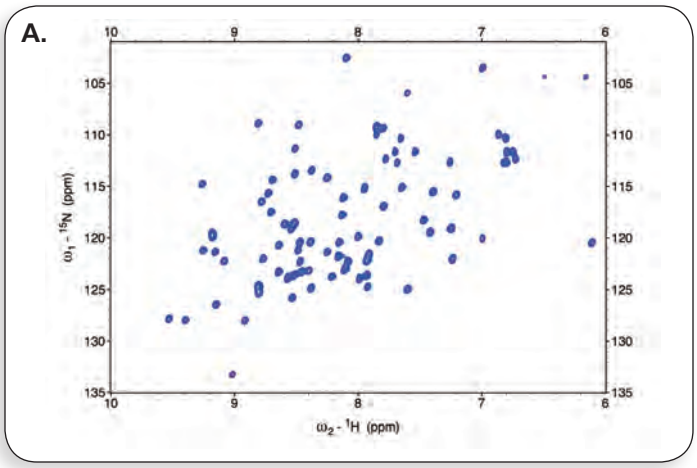
Available in a sealed NMR tube upon request

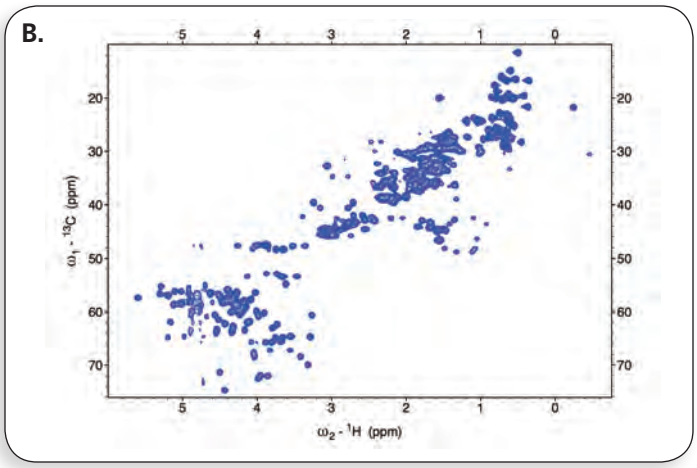
Contact CIL for different packaging configurations

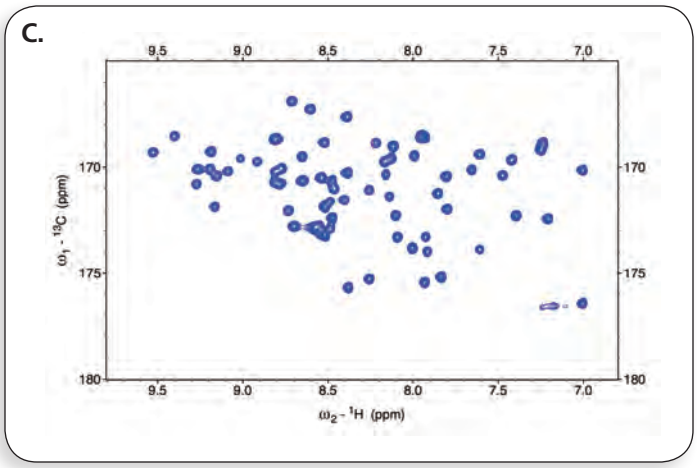
NEX-UB1 is a small 8.8 kDa monomeric protein for which multiple sets of resonance assignments (BMRB database) and 3D structures (PDB database) are publicly available. This protein standard is uniformly ^{15}N,^{13}C enriched. Ubiquitin has been used as an industry-wide standard in the protein NMR field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







A. ^{1}H,^{15}N **HSQC of NEX-UB1**
B. ^{13}C-^{1}H **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%; $^{13}CH_3$-ILV)
NEX-UB1-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

His-Ubiquitin (Human)

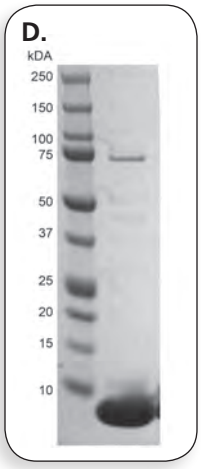
NEX-UBI-HIS-U-0	unlabeled
NEX-UBI-HIS-N-0	(^{15}N, 95%)
NEX-UBI-HIS-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-UBI-HIS-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-UBI-HIS-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-UBI-HIS-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-UBI-HIS-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

Protein Sequence after TEV Cleavage

SHMQIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQR LIFAGKQLEDGRTLSDYNIQKESTLHLVLRLRGG

Protein Sequence before TEV Cleavage

*MGHHHHHHENLYFQ*SHMQIFVKTLTGKTITLEVEPSDTIEN VKAKIQDKEGIPPDQQRLIFAGKQLEDGRTLSDYNIQKESTL HLVLRLRGG



Notes

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