

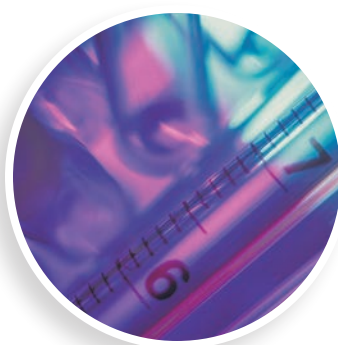


Cambridge Isotope  
Laboratories, Inc.

# 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*

[isotope.com](http://isotope.com)

## Ordering Information

The CIL Customer Service Department is open from 8:00 a.m. to 5:00 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 750 employees and laboratories in five 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; CIL China in Shanghai, China; 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  $^{13}\text{C}$  and  $^{18}\text{O}$  isotope-separation facilities and the world's only commercial  $\text{D}_2\text{O}$  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

CIL is the world's leading producer of deuterated NMR solvents for analysis and deuterated reagents for synthesis. For more than 40 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

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,  $^1\text{H}$ -NMR,  $^{13}\text{C}$ -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.

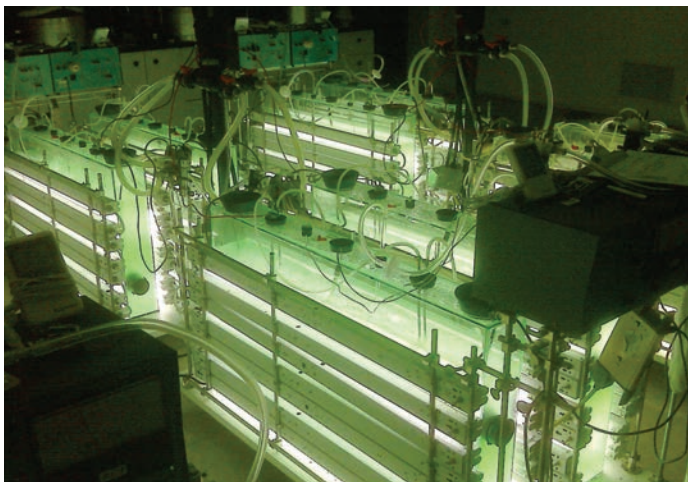






**CIL Isotope Separations, LLC (CIS)**  
**Xenia, OH USA**

CIL is the world leader in the separation of  $^{13}\text{C}$  and  $^{18}\text{O}$ . CIL separates both  $^{13}\text{C}$  and  $^{18}\text{O}$  at its Xenia, OH, facility and has the world's largest production capacity for both  $^{13}\text{C}$  and  $^{18}\text{O}$ . CIL also has the only nongovernmental  $\text{D}_2\text{O}$  enrichment columns in the world located at its CIS facility.



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

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



**Euriso-Top**  
**Saclay, France**

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



**ABX GMBH**  
**Dresden, Germany**

ABX is the world's leading supplier of  $^{18}\text{F}$  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 (ET)

Fax: 1-978-749-2768

Email: [cilsales@isotope.com](mailto:cilsales@isotope.com) (North America)  
[intlsales@isotope.com](mailto: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](mailto: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](mailto:intlsales@isotope.com) or  
+1-978-749-8000.
- For a complete distributor listing, please visit [www.isotope.com](http://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. ET 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.



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

## GHS Objectives

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










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

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

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

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



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


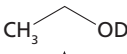




## Understanding the Product Listings

### NMR Solvent Catalog Listings Include:

New Indicator: **NEW**

Compound Name	Enrichment	Alternative Name	Formula	Molecular Weight*	Unit
<b>Ethanol-d</b> (D, 99%)		Ethyl alcohol	$\text{CH}_3\text{CH}_2\text{OD}$	mw 47.08 d 0.89	5 g 2 x 50 g
CIL Catalog # → DLM-16					
CAS # → [925-93-9]					
UN # → 1170					
					
Hazard Class					
		Contains <6% D <sub>2</sub> O Packaged in glass ampoules only			
		Additional Information Storage Information**			
					
			Structure	Density	


\* 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
- Packaging size
- Pictograms for hazard recognition
- CAS numbers
- Storage information
- Packaging number
- Catalog number




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

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

CAS #: 2206-27-1

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

**Warning**  
Combustible liquid. Causes mild skin irritation. Causes eye irritation. IF IN EYES: Remove contact lenses if present. Rinse continuously with water.  
Store at room temperature away from light and moisture.  
For Research Use Only. Not for use in diagnostic procedures.



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

**N-OCTANE-D18**  
(D, 99%)  
DLM-50-5


5 GRAMS  
PSO #: 12B-264 Lot #: PR-22855/081110C1

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

**Danger**

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

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



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

**CHLOROFORM-D**  
(D, 99.8%)  
DLM-7-100

100 GRAMS  
PSO #: 14K-188 Lot #: PR-26119/0914CL1

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

**Warning**  
Use personal protective equipment as required. IF IN EYES: Rinse with water for several minutes. Remove contact lenses.  
For Research Use Only. Not for use in diagnostic procedures.

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

## 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.  $^1\text{H}$ -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  $^1\text{H}$ -NMR.

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

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



### Acetic acid- $\text{d}_4$ (D, 99.5%)

DLM-12	$\text{CD}_3\text{COOD}$	mw 64.08	10 g
[1186-52-3]		d 1.12	25 g
UN# 2789			50 g



### Acetic acid- $\text{d}_4$ "100%" (D, 99.93%)

DLM-41	$\text{CD}_3\text{COOD}$	mw 64.08	10 x 0.75 mL
[1186-52-3]		d 1.12	5 mL
UN# 2789			



### Acetone- $\text{d}_6$ (D, 99.9%)

DLM-9	$\text{CD}_3\text{COCD}_3$	mw 64.12	10 x 0.5 mL
[666-52-4]		d 0.87	10 x 0.6 mL
UN# 1090			10 x 0.75 mL
			5 x 3 mL
			1 L
			10 x 1 g
			3 x (10 x 1 g)
			10 g
			10 x 10 g
			3 x (10 x 10 g)
			25 g
			100 g



### Acetone- $\text{d}_6$ (D, 99.9%)

DLM-9ta	$\text{CD}_3\text{COOD}_3$	mw 64.12	10 x 1 g
[666-52-4]		d 0.87	3 x (10 x 1 g)
UN# 1090			10 g
			10 x 10 g
			3 x (10 x 10 g)
			25 g

Contains 1% v/v TMS



### Acetone- $\text{d}_6$ (D, 99.9%)

DLM-9tb	$\text{CD}_3\text{COCD}_3$	mw 64.12	10 x 0.5 mL
[666-52-4]		d 0.87	10 x 1 g
UN# 1090			3 x (10 x 1 g)
			10 g
			10 x 10 g
			3 x (10 x 10 g)
			25 g

Contains 0.05% v/v TMS



### Acetone- $\text{d}_6$ "100%" (D, 99.96%)

DLM-38	$\text{CD}_3\text{COCD}_3$	mw 64.12	5 x 0.5 mL
[666-52-4]		d 0.87	10 x 0.5 mL
UN# 1090			10 x 0.6 mL
			5 x 0.75 mL
			10 x 0.75 mL
			5 mL



### Acetone- $\text{d}_6$ "100%" (D, 99.96%)

DLM-38tc	$\text{CD}_3\text{COCD}_3$	mw 64.12	10 x 0.75 mL
[666-52-4]		d 0.87	
UN# 1090			



Contains 0.03% v/v TMS

### Acetonitrile- $\text{d}_3$ (D, 96-97%)

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



### Acetonitrile- $\text{d}_3$ (D, 99.8%)

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



### Acetonitrile- $\text{d}_3$ (D, 99.8%)

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






Contains 0.05% v/v TMS



**Acetonitrile-d<sub>3</sub> "100%" (D, 99.96%)**

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

**Benzene-d<sub>6</sub> (D, 99.5%)**

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




**Benzene-d<sub>6</sub> (D, 99.5%)**

DLM-1tb [1076-43-3]	C <sub>6</sub> D <sub>6</sub>	mw 84.15 d 0.95	10 × 0.6 mL 10 g
UN# 1114			
   Contains 0.05% v/v TMS			

**Benzene-d<sub>6</sub> "100%" (D, 99.96%)**

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

**Benzene-d<sub>6</sub> "100%" (D, 99.96%)**

DLM-40tc [1076-43-3]	C <sub>6</sub> D <sub>6</sub>	mw 84.15 d 0.95	10 × 0.75 mL
UN# 1114			
   Contains 0.03% v/v TMS			



**Bromobenzene-d<sub>5</sub> (D, 99.5%)**

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



**Chlorobenzene-d<sub>5</sub> (D, 99%)**

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



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

DLM-7 [865-49-6]	CDCl <sub>3</sub>	mw 120.38 d 1.50	10 × 0.6 mL 10 × 0.75 mL 10 × 1 g 3 × (10 × 1 g) 50 g 100 g 10 × 100 g 3 × (10 × 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 <sub>3</sub>	mw 120.38 d 1.50	50 g 100 g 100 mL
UN# 1888			
  Stabilized with silver foil			



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

DLM-7ta [865-49-6]	CDCl <sub>3</sub>	mw 120.38 d 1.50	10 × 1 g 3 × (10 × 1 g) 50 g 100 g 10 × 100 g 3 × (10 × 100 g)
UN# 1888			
  No stabilizers are used in this product			



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

DLM-7ta-100S [865-49-6]	CDCl <sub>3</sub>	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 <sub>3</sub>	mw 120.38 d 1.50	10 × 1 g 3 × (10 × 1 g) 50 g 100 g 10 × 100 g 3 × (10 × 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 <sub>3</sub>	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 <sub>3</sub>	mw 120.38 d 1.50	10 × 0.25 mL 10 × 0.5 mL 10 × 0.6 mL 5 × 0.75 mL 10 × 0.75 mL 10 mL 5 × 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 <sub>3</sub>	mw 120.38 d 1.50	10 × 0.75 mL
UN# 1888			
  Contains 0.03% v/v TMS No stabilizers are used in the product			

**Cyclohexane-d<sub>12</sub> (D, 99.5%)**

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

**Decalin-d<sub>18</sub> (D, 99%) Decahydronaphthalene**

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

**trans-Decalin-d<sub>18</sub>** (D, 98%)

DLM-1843 C<sub>10</sub>D<sub>18</sub> mw 156.36 5 g  
[493-02-7] d 1.01

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

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



DBr 48% w/w solution in D<sub>2</sub>O  
Packaged in clear glass ampoules only

**Deuterium chloride** (D, 99.5%)

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



DCI 20% w/w solution in D<sub>2</sub>O  
Packaged in clear glass ampoules only

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

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



DCI 20% w/w solution in D<sub>2</sub>O  
Packaged in clear glass ampoules only

**Deuterium chloride** (D, 99.5%)

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



DCI 35% w/w solution in D<sub>2</sub>O  
Packaged in clear glass ampoules only

**Deuterium oxide** (D, 70%)

DLM-4-70 D<sub>2</sub>O mw 20.03 1 kg  
[7789-20-0] d 1.077  
UN# 1957

**Deuterium oxide** (D, 70%)

DLM-2259-70 D<sub>2</sub>O mw 20.03 1 kg  
[7789-20-0] d 1.077 1 L  
UN# 1957 Sterility tested

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

DLM-4-99 D<sub>2</sub>O mw 20.03 1 kg  
[7789-20-0] d 1.11 5 kg  
UN# 1957

**Deuterium oxide** (D, 99.8%)

DLM-4-99.8 D<sub>2</sub>O mw 20.03 1 kg  
[7789-20-0] d 1.11 10 kg  
UN# 1957 20 kg

**Deuterium oxide** (D, 99.8%)

DLM-2259 D<sub>2</sub>O mw 20.03 100 mL  
[7789-20-0] d 1.11 250 mL  
UN# 1957 Sterility tested 1 L

**Deuterium oxide** (D, 99.9%)

DLM-4 D<sub>2</sub>O mw 20.03 10 × 1 mL  
[7789-20-0] d 1.11 10 g  
UN# 1957 25 g  
50 g  
100 g  
5 × 100 g  
10 × 100 g  
1000 g  
1 L (inquire)

**Deuterium oxide** (D, 99.9%)

DLM-11 D<sub>2</sub>O mw 20.03 100 g  
[7789-20-0] d 1.11  
UN# 1957

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

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

DLM-6 D<sub>2</sub>O mw 20.03 10 × 0.6 mL  
[7789-20-0] d 1.11 5 × 0.7 mL  
UN# 1957 10 × 0.7 mL  
10 × 0.75 mL  
5 × (10 × 0.7 mL)  
10 × 1 g  
1000 g

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

DLM-6-s D<sub>2</sub>O mw 20.03 10 g  
[7789-20-0] d 1.11  
UN# 1957

Packaged in serum bottles with Teflon-coated rubber septum tops

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

DLM-6DB D<sub>2</sub>O mw 20.03 10 × 0.7 mL  
[7789-20-0] d 1.11 50 g  
UN# 1957

Contains 0.01 mg/mL DSS

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

DLM-1172 D<sub>2</sub>O mw 20.03 10 g  
[7789-20-0] d 1.11  
UN# 1957

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

**1,2-Dibromoethane-d<sub>4</sub>** (D, 99%)

DLM-195 Br(CD<sub>2</sub>)<sub>2</sub>Br mw 191.87 10 g  
[22581-63-1] d 2.20 25 g  
UN# 1605

**1,2-Dichlorobenzene-d<sub>4</sub>** (D, 99%)

DLM-158 C<sub>6</sub>D<sub>4</sub>Cl<sub>2</sub> mw 151.03 1 g  
[2199-69-1] d 1.34 5 g  
UN# 1591 25 g

**1,2-Dichloroethane-d<sub>4</sub>** (D, 99%)

DLM-18 Cl(CD<sub>2</sub>)<sub>2</sub>Cl mw 102.98 1 g  
[17060-07-0] d 1.30 5 × 1 g  
UN# 1184 5 g

**Diethyl ether-d<sub>10</sub>** (D, 99%)

DLM-1592 (CD<sub>3</sub>CD<sub>2</sub>)<sub>2</sub>O mw 84.10 1 g  
[2679-89-2] d 0.80 5 × 1 g  
UN# 1155 5 g



Packaged in ampoules only

**Diglyme-d<sub>14</sub>** (D, 98%)

DLM-47 [38086-00-9]	(CD <sub>3</sub> OCDCD <sub>2</sub> CD <sub>2</sub> ) <sub>2</sub> O	mw 148.26 d 1.035	1 g 5 g 5 × 1 g 10 g
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**N,N-Dimethylformamide-d<sub>7</sub>** (D, 99.5%) DMF

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

**N,N-Dimethylformamide-d<sub>7</sub>** (D, 99.5%) DMF

DLM-25tb [4472-41-7]	DCON(CD <sub>3</sub> ) <sub>2</sub>	mw 80.14 d 1.04	10 × 0.6 mL
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Contains 0.05% v/v TMS  
Packaged in ampoules only**Dimethyl sulfoxide-d<sub>6</sub>** (D, 99.9%) DMSO

DLM-10 [2206-27-1]	CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17 d 1.18	10 × 0.5 mL 10 × 0.6 mL 10 × 0.75 mL 5 × 3 mL 10 mL 50 mL 5 × 1 g 10 × 1 g 3 × (10 × 1 g) 5 g 10 g 100 g 10 × 10 g 3 × (10 × 10 g) 25 g 50 g 1000 g
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**Dimethyl-sulfoxide-d<sub>6</sub>** (D, 99.9%) DMSO

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

**Dimethyl-sulfoxide-d<sub>6</sub>** (D, 99.9%) DMSO

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

**Dimethyl-sulfoxide-d<sub>6</sub>** (D, 99.9%) DMSO

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

**Dimethyl-sulfoxide-d<sub>6</sub> "100%"** (D, 99.95%) DMSO

DLM-34 [2206-27-1]	CD <sub>3</sub> SOCD <sub>3</sub>	mw 84.17 d 1.18	5 × 0.5 mL 10 × 0.5 mL 10 × 0.75 mL 5 mL
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**Dimethyl-sulfoxide-d<sub>6</sub> "100%"** (D, 99.96%) DMSO

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

**1,4-Dioxane-d<sub>8</sub>** (D, 99%) *p*-Dioxane

DLM-28 [17647-74-4]	C <sub>4</sub> D <sub>8</sub> O <sub>2</sub>	mw 96.15 d 1.13	5 × 1 g 10 × 1 g 3 × (10 × 1 g) 5 g 10 g 25 g
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UN# 1165

**DSS – <sup>1</sup>H-NMR chemical shift standard**

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

Sodium 2,2-dimethyl-2-silapentane-5-sulfonate (D<sub>6</sub> 98%)  
Chemical purity 97%**DSS – <sup>1</sup>H-NMR chemical shift standard**

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

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

DLM-16 [925-93-9]	CH <sub>3</sub> CH <sub>2</sub> OD	mw 47.08 d 0.82	50 g 2 × 50 g
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UN# 1170

Contains ≤6% D<sub>2</sub>O**Ethanol-d<sub>6</sub>** (D, 99%) Ethyl alcohol

DLM-31 [1516-08-1]	CD <sub>3</sub> CD <sub>2</sub> OD	mw 52.11 d 0.89	5 × 1 g 10 × 1 g 5 g
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UN# 1170 3



Anhydrous

**Ethanol-d<sub>6</sub>** (D, 99%) Ethyl alcohol

DLM-31B [1516-08-1]	CD <sub>3</sub> CD <sub>2</sub> OD	mw 52.11 d 0.89	5 × 1 g 5 g
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UN# 1170 3

Contains ≤6% D<sub>2</sub>O**Ethylene glycol-d<sub>6</sub>** (D, 98%)

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

DLM-617 C<sub>6</sub>D<sub>5</sub>F mw 101.13 1 g  
 [1423-10-5] d 1.08  
 UN# 2387

**n-Heptane-d<sub>16</sub>** (D, 98%)

DLM-423 CD<sub>3</sub>(CD<sub>2</sub>)<sub>5</sub>CD<sub>3</sub> mw 116.30 1 g  
 [33838-52-7] d 0.794 5 g  
 UN# 1206

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

DLM-1020 CF<sub>3</sub>COCF<sub>3</sub>·3 D<sub>2</sub>O mw 226.11 10 g  
 [109640-39-3] d 1.71

**1,1,1,3,3,3-Hexafluoroisopropanol-d<sub>2</sub>** (D, 98%)

DLM-143 (CF<sub>3</sub>)<sub>2</sub>CDOD mw 170.05 1 g  
 [38701-74-5] d 1.62 5 x 1 g  
 5 g  
 10 g  
*Hexafluoroisopropyl alcohol, HFIP*

**n-Hexane-d<sub>14</sub>** (D, 98%)

DLM-139 CD<sub>3</sub>(CD<sub>2</sub>)<sub>4</sub>CD<sub>3</sub> mw 100.26 1 g  
 [21666-38-6] d 0.767 5 g  
 UN# 1208

**Isopropanol-d<sub>8</sub>** (D, 99%) 2-Propyl alcohol

DLM-44 (CD<sub>3</sub>)<sub>2</sub>CDOD mw 68.14 5 g  
 [22739-76-0] d 0.90 25 g  
 UN# 1219

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

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



3N in D<sub>2</sub>O solution  
 Packaged in plastic bottles only

**Methanol-OD** (D, 99%) Methyl alcohol

DLM-15 CH<sub>3</sub>OD mw 33.05 50 g  
 [1455-13-6] d 0.81 2 x 50 g  
 UN# 1230

**Methanol-d<sub>4</sub>** (D, 99.8%) Methyl alcohol

DLM-24 CD<sub>3</sub>OD mw 36.07 10 x 0.5 mL  
 [811-98-3] d 0.89 10 x 0.6 mL  
 10 x 0.75 mL  
 1 L  
 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<sub>4</sub>** (D, 99.8%) Methyl alcohol

DLM-24-s CD<sub>3</sub>OD mw 36.07 10 g  
 [811-98-3] d 0.89 25 g  
 UN# 1230 50 g



Packaged in serum bottles with Teflon-coated rubber septum tops

**Methanol-d<sub>4</sub>** (D, 99.8%) Methyl alcohol

DLM-24tb CD<sub>3</sub>OD mw 36.07 10 x 0.5 mL  
 [811-98-3] d 0.89 10 x 0.6 mL  
 10 x 0.75 mL  
 10 x 1 g  
 10 g  
 10 x 10 g  
 50 g



Contains 0.05% v/v TMS

**Methanol-d<sub>4</sub> "100%"** (D, 99.95%) Methyl alcohol

DLM-51 CD<sub>3</sub>OD mw 36.07 10 x 0.25 mL  
 [811-98-3] d 0.89 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<sub>14</sub>** (D, 99.5%)

DLM-288 C<sub>6</sub>D<sub>11</sub>CD<sub>3</sub> mw 112.27 1 g  
 [10120-28-2] d 0.88 5 g  
 UN# 2296

**Methylene chloride-d<sub>2</sub>** (D, 99.9%) Dichloromethane

DLM-23 CD<sub>2</sub>Cl<sub>2</sub> mw 86.95 10 x 0.5 mL  
 [1665-00-5] d 1.30 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  
 100 g

**Methylene chloride-d<sub>2</sub>** (D, 99.9%) Dichloromethane

DLM-23tb CD<sub>2</sub>Cl<sub>2</sub> mw 86.95 10 x 0.6 mL  
 [1665-00-5] d 1.35



Contains 0.05% v/v TMS

**Methylene chloride-d<sub>2</sub> "100%"** (D, 99.96%) Dichloromethane

DLM-55 CD<sub>2</sub>Cl<sub>2</sub> mw 86.95 10 x 0.5 mL  
 [1665-00-5] d 1.35 10 x 0.6 mL  
 5 x 0.75 mL  
 10 x 0.75 mL  
 5 mL

**N-Methyl-2-pyrrolidinone-d<sub>9</sub>** (D, 97-99%) NMP

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

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

DLM-3037 DNO<sub>3</sub> mw 64.02 5 g (of soln.)  
 [13587-52-5] d 1.026 25 g (of soln.)



65-70% w/w solution in D<sub>2</sub>O  
 Packaged in clear glass ampoules only



**Nitrobenzene-d<sub>5</sub>** (D, 99%)

DLM-294 C<sub>6</sub>D<sub>5</sub>NO<sub>2</sub> mw 128.14 5 g  
 [4165-60-0] d 1.25 10 g  
 UN# 1662 25 g

**Nitromethane-d<sub>3</sub>** (D, 99%)

DLM-30 CD<sub>3</sub>NO<sub>2</sub> mw 64.06 10 g  
 [13031-32-8] d 1.20 25 g  
 UN# 1261

**n-Octane-d<sub>18</sub>** (D, 99%)

DLM-50 CD<sub>3</sub>(CD<sub>2</sub>)<sub>6</sub>CD<sub>3</sub> mw 132.34 1 g  
 [17252-77-6] d 0.815 5 g  
 UN# 1262

**n-Pentane-d<sub>12</sub>** (D, 98%)

DLM-1213 CD<sub>3</sub>(CD<sub>2</sub>)<sub>3</sub>CD<sub>3</sub> mw 84.22 1 g  
 [2031-90-5] d 0.73 5 g  
 UN# 1265

**Phosphoric acid-d<sub>3</sub>** (D, 99%)

DLM-1132 D<sub>3</sub>PO<sub>4</sub> mw 101.01 50 g  
 [14335-33-2] d 1.74 100 g

Approximately 85% w/w solution in D<sub>2</sub>O

**Pyridine-d<sub>5</sub>** (D, 99.5%)

DLM-13 C<sub>5</sub>D<sub>5</sub>N mw 84.13 10 × 0.5 mL  
 [7291-22-7] d 1.05 5 × 1 g  
 UN# 1282 10 × 1 g  
 3 × (10 × 1 g)  
 10 g  
 25 g  
 50 g

**Pyridine-d<sub>5</sub>** (D, 99.5%)

DLM-13tb C<sub>5</sub>D<sub>5</sub>N mw 84.13 10 × 0.5 mL  
 [7291-22-7] d 1.05 10 × 0.6 mL  
 UN# 1282 5 × 1 g  
 10 × 1 g  
 3 × (10 × 1 g)  
 10 g  
 25 g  
 50 g



Contains 0.05% v/v TMS

**Pyridine-d<sub>5</sub> "100%"** (D, 99.94%)

DLM-39 C<sub>5</sub>D<sub>5</sub>N mw 84.13 5 × 0.5 mL  
 [7291-22-7] d 1.05 10 × 0.5 mL  
 UN# 1282 10 × 0.75 mL  
 5 mL

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

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

NaOD 30% w/w solution in D<sub>2</sub>O  
Packaged in polyethylene bottles**Sodium deuteroxide** (D, 99.5%)

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


NaOD 40% w/w solution in D<sub>2</sub>O  
Packaged in polyethylene bottles**Sulfuric acid-d<sub>2</sub>** (D, 99%)

DLM-33 D<sub>2</sub>SO<sub>4</sub> mw 100.09 50 g  
 [13813-19-9] d 1.86  
 UN# 1282

96-98% solution in D<sub>2</sub>O  
Packaged in glass ampoules only**1,1,2,2-Tetrachloroethane-d<sub>2</sub>** (D, 99.6%) TCE

DLM-35 Cl<sub>2</sub>CDCDCl<sub>2</sub> mw 169.86 5 g  
 [33685-54-0] d 1.62 10 g  
 UN# 1702 100 g

**Tetrahydrofuran-d<sub>8</sub>** (D, 99.5%) THF

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



Packaged in ampoules only

**Tetrahydrofuran-d<sub>8</sub> "100%"** (D, 99.95%) THF

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

**Tetramethylsilane** TMS

DLM-43 (CH<sub>3</sub>)<sub>4</sub>Si mw 88.22 50 g  
 [75-76-3] d 0.64

NMR grade  
Chemical purity 99.9%

**TMSP-2,2,3,3-d<sub>4</sub>** (D, 98%) Sodium 3-trimethylsilylpropionate

DLM-48 (CH<sub>3</sub>)<sub>3</sub>SiCD<sub>2</sub>CD<sub>2</sub>CO<sub>2</sub>Na mw 172.27 1 g  
 [24493-21-8] d 1.52 5 × 1 g  
 5 g

D<sub>2</sub>O reference standard and  
<sup>1</sup>H-NMR chemical shift standard

**Toluene-d<sub>8</sub>** (D, 99.5%)




DLM-5 C<sub>6</sub>D<sub>5</sub>CD<sub>3</sub> mw 100.19 10 × 1 g  
 [2037-26-5] d 0.94 3 × (10 × 1 g)  
 UN# 1294 5 g  
 10 g  
 25 g  
 100 g  
 1000 g

**Toluene-d<sub>8</sub> "100%"** (D, 99.94%)

DLM-42 C<sub>6</sub>D<sub>5</sub>CD<sub>3</sub> mw 100.19 5 × 0.5 mL  
 [2037-26-5] d 0.94 10 × 0.5 mL  
 UN# 1294 5 × 0.75 mL  
 10 × 0.75 mL  
 5 mL



**Trifluoroacetic acid-d** (D, 99.5%)

DLM-46 [599-00-8]	CF <sub>3</sub> COOD	mw 115.03 d 1.50	10 × 0.5 mL 10 × 0.75 mL
UN# 2699			10 × 1 g 10 g 25 g 4 × 25 g
  	<i>Packaged in ampoules only</i>		

**2,2,2-Trifluoroethanol-d<sub>2</sub>** (D, 98%) Trifluoroethyl alcohol

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

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

DLM-58 [77253-67-9]	CF <sub>3</sub> CD <sub>2</sub> OD	mw 103.06 d 1.42	1 g 5 g
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**1,3,5-Trimethyl benzene** (D<sub>12</sub>, 98%) Mesitylene

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

**Water, deuterium depleted**

DLM-52 [7732-18-5]	H <sub>2</sub> O	mw 18.02 d 1.00	25 g 100 g
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*2-3 ppm deuterium***o-Xylene-d<sub>10</sub>** (D, 98%)

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

**p-Xylene-d<sub>10</sub>** (D, 98%)

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

**<sup>12</sup>C and <sup>12</sup>C/Deuterium-Labeled Solvents (<sup>13</sup>C Depleted)****Benzene** (<sup>12</sup>C<sub>6</sub>, 99.95%)

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

CDLM-844 [865-49-6]	*CDCl <sub>3</sub>	mw 120.38 d 1.500	Inquire
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**Methanol** (<sup>12</sup>C, 99.95%) Methyl alcohol

CLM-2472 [67-56-1]	*CH <sub>3</sub> OH	mw 32.04 d .0791	1 g
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**Methanol** (<sup>12</sup>C, 99.95%; D<sub>4</sub>, 99.5%) Methyl alcohol

CDLM-01 [811-98-3]	*CD <sub>3</sub> OD	mw 36.07 d 0.888	0.8 mL 5g
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## 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 <sub>6</sub> (D, 99.9%)	<sup>1</sup> H-Resolution	5 mm x 8"
DLM-74	0.1% Ethylbenzene + 0.01% TMS in chloroform-d "100%" (D, 99.96%)	<sup>1</sup> H-Sensitivity	5 mm x 8"
DLM-67	1% 3-Heptanone in chloroform-d (D, 99.8%)	<sup>1</sup> H APT Test	5 mm x 8"
ULM-73	12% TMS in chloroform	<sup>1</sup> H-Reference/Calibration	5 mm x 8"
DLM-84	5% Ethylbenzene + 2% TMS in chloroform-d (D, 99.8%)	<sup>1</sup> H-Sensitivity/Reference	5 mm x 8"
DLM-76	1% Chloroform in acetone-d <sub>6</sub> (D, 99.9%)	<sup>1</sup> H-Line Shape	5 mm x 8"
DLM-90	0.1 mg/mL GdCl <sub>3</sub> ·6H <sub>2</sub> O in D <sub>2</sub> O (D, 99.96%)	<sup>1</sup> H-Homogeneity	5 mm x 8"
DLM-72	40% <i>p</i> -Dioxane in benzene-d <sub>6</sub> (D, 99.6%)	<sup>13</sup> C-Sensitivity/Resolution	5 mm x 8"
DLM-66	30% Menthol (by weight) in chloroform-d (D, 99.8%)	<sup>13</sup> C App Test	5 mm x 8"
DLM-68	90% Formamide in DMSO-d <sub>6</sub> (D, 99.9%)	<sup>15</sup> N-Sensitivity	5 mm x 8"
DLM-77	0.0485 M Triphenylphosphate in chloroform-d (D, 99.8%)	<sup>31</sup> P-Sensitivity	5 mm x 8"
DLM-78	0.05% α,α,α,-Trifluorotoluene in benzene-d <sub>6</sub> (D, 99.6%)	<sup>19</sup> F-Sensitivity	5 mm x 8"
CDLM-100	0.1% Methanol- <sup>13</sup> C + 0.3 mg/mL GdCl <sub>3</sub> in 98.9% D <sub>2</sub> O + 01% H <sub>2</sub> O	Auto Test Sample	5 mm x 8"
DLM-88	0.1 mg/mL GdCl <sub>3</sub> + 0.1% DSS in 20% H <sub>2</sub> O in D <sub>2</sub> O	Gradient Shimming	5 mm x 8"
CDLM-96	1% <sup>13</sup> CH <sub>3</sub> I, 0.2% Cr(acac) <sub>3</sub> + 1% (CH <sub>3</sub> O) <sub>3</sub> P in CDCl <sub>3</sub> "100%"	Indirect Detection Test	5 mm x 8"
DNLM-97	0.2% Cr(acac) <sub>3</sub> + 2% Benzamide ( <sup>15</sup> N,98%+) in DMSO-d <sub>6</sub> "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- <sup>15</sup> N + 0.1 M MeOH- <sup>13</sup> C in DMSO-d <sub>6</sub> 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- <sup>13</sup> C - 0.1% acetonitrile- <sup>15</sup> N + 0.3 mg/mL in 98.8% D <sub>2</sub> O + 1% H <sub>2</sub> O	Auto Test Sample	5 mm x 8"
ULM-7049	5% Ethyl <i>trans</i> -crotonate + 1% TMS in CDCl <sub>3</sub> in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
DLM-7047	98% <i>N</i> -Propyl benzoate + 2% TMS in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
DLM-5001	10% Ethylbenzene in chloroform-d (540 pp tube)	<sup>13</sup> 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](mailto:cilsales@isotope.com)

Requests may be submitted on our website at [isotope.com/request](http://isotope.com/request).

## NORELL<sup>®</sup> Tubes *(Sold only in North America)*

Since 2006, CIL has partnered with NORELL<sup>®</sup> to offer our customers the convenience and quality of purchasing our solvents and NORELL<sup>®</sup>'s standard or select series NMR tubes together. CIL offers NORELL<sup>®</sup> NMR tubes in North America only. International customers should contact their local independent distributor.

**NORELL<sup>®</sup>**

[www.nmrtubes.com](http://www.nmrtubes.com)

NORELL<sup>®</sup> is a registered trademark of Norell, Inc.

### 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

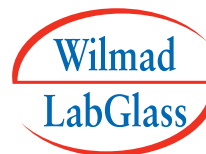
Part No.	Package Size	MHz Rating	O.D. (mm)	I.D. (mm)	Length (inch)	Concentricity (μm)	Camber (μm)
507-HP-7	5	400	4.97 ± 0.013	4.20 ± 0.025	7	0.0070	0.019
507-HP-8	5	400	4.97 ± 0.013	4.20 ± 0.025	8	0.0070	0.019
508-UP-7	5	500	4.97 ± 0.013	4.20 ± 0.025	7	0.0050	0.013
508-UP-8	5	500	4.97 ± 0.013	4.20 ±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

## 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.



[www.wilmad-labglass.com](http://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 desiccator prior to use.
- Precondition an NMR tube by rinsing it with D<sub>2</sub>O. Remove residual D<sub>2</sub>O by rinsing first with methanol-d<sub>4</sub> or acetone-d<sub>6</sub> 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<sub>2</sub>O

To avoid loss of enrichment due to exchange with ambient moisture, "100%" D<sub>2</sub>O 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<sub>2</sub>O being removed should be injected into the serum bottle prior to withdrawing D<sub>2</sub>O.

### TMS Evaporation

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

### Storage

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

## NMR Solvent Technical Tips

- Solvent users often require a specific custom mixture of two or more solvents. CIL's expert packaging technicians are uniquely qualified to formulate custom solvent preparations.
- To measure acidity in deuterium oxide solutions: calculate pD by adding 0.4 to the reading taken from the glass electrode pH meter. (Glasoe and Long. 1960. *J Phys Chem*, 64, 188).
- Dimethyl sulfoxide (DMSO) has a melting point of 18°C, freezing close to room temperature. Upon delivery, DMSO will sometimes be in a solid state. To return the material to a liquid state, thaw it in a warm water bath. Care must be taken to prevent water contamination.
- CIL recommends refrigeration of solvents packaged in serum bottles to extend the product shelf life, maintain high purity and ensure product quality. Serum bottles should be tested after six months.
- It is recommended that chloroform, diethyl ether, diglyme, tetrahydrofuran and TMS be stored in a refrigerator.
- In order to avoid isotopic contamination, some products, especially deuterated compounds, should be handled under an inert atmosphere, such as dry nitrogen or argon.
- You may see a split water peak in your solvent because the Karl Fischer technique measures the total of H<sub>2</sub>O + D<sub>2</sub>O. In all cases where both H<sub>2</sub>O and D<sub>2</sub>O 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<sub>2</sub>O present in the solvents. Thus, a negligible amount of HOD may remain but will not be observable in the NMR spectrum of most solvents. Occasionally, a separate peak from HOD, ~0.02 ppm upfield of the H<sub>2</sub>O peak, may be observed in the DMSO-d<sub>6</sub> or acetonitrile-d<sub>3</sub> (for example), due to the slower equilibrium that exists between H<sub>2</sub>O and D<sub>2</sub>O and these solvents.
- CIL also specializes in <sup>13</sup>C-depleted and deuterium-depleted compounds. Please contact us if you do not see the <sup>13</sup>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  $^1\text{H}$  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  $-5^\circ\text{C}$  to  $+5^\circ\text{C}$  to maximize shelf life. Moisture and oxygen will be introduced to the solvent following initial use due to air entering the bottle upon opening. Decomposition can follow, which results in the deuterated chloroform becoming acidic.

The acidity can be easily tested using the following method:

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

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

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

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

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

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

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

# NMR Solvent Data Chart

More Solvents, More Sizes, More Solutions

	<sup>1</sup> H Chemical Shift (ppm from TMS) (multiplicity) ✱	JHD (Hz)	<sup>13</sup> C Chemical Shift (ppm from TMS) (multiplicity) ✱	JCD (Hz)	<sup>1</sup> 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 <sub>4</sub>	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 <sub>6</sub>	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 <sub>3</sub>	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 <sub>6</sub>	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 <sub>12</sub>	1.38 (1)		26.43 (5)	19	0.8	0.89	6.47	80.7	2.0	96.24
Deuterium oxide	4.80 (DSS) 4.81 (TSP)		NA	NA	4.8	1.11	3.81	101.42	78.5	20.03
<i>N,N</i> -Dimethyl-formamide-d <sub>7</sub>	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 <sub>6</sub>	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 <sub>8</sub>	3.53 (m)		66.66 (5)	21.9	2.4	1.13	11.8	101.1	2.2	96.16
Ethanol-d <sub>6</sub>	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 <sub>4</sub>	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 <sub>2</sub>	5.32 (3)	1.1	54.00 (5)	27.2	1.5	1.35	-95	39.75	8.9	86.95
Pyridine-d <sub>5</sub>	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 <sub>2</sub>	6.0		73.78 (3)			1.62	-44	146.5	8.20	169.86
Tetrahydrofuran-d <sub>8</sub>	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 <sub>8</sub>	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 <sub>3</sub>	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 <sup>1</sup>H spectra of the residual protons and <sup>13</sup>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<sub>2</sub>O). 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<sub>2</sub>O in addition to the residual solvent peak. When the exchange rate between H<sub>2</sub>O and HOD is slow on the NMR timescale the water peak appears as two peaks, a singlet corresponding to H<sub>2</sub>O 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<sub>4</sub> / Acetone-d<sub>6</sub> / Benzene-d<sub>6</sub> / Cyclohexane-d<sub>12</sub> / Deuterium Oxide / *N,N*-Dimethylformamide-d<sub>7</sub> / Dimethyl Sulfoxide-d<sub>6</sub> / 1,4-Dioxane-d<sub>8</sub> (*p*-Dioxane) / Ethanol-d<sub>6</sub> / Methanol-d<sub>4</sub> / Methylene Chloride-d<sub>2</sub> / Pyridine-d<sub>5</sub> / 1,1,2,2-Tetrachloroethane-d<sub>2</sub> / Toluene-d<sub>8</sub> / Trifluoroacetic Acid-d / 2,2,2-Trifluoroethanol-d<sub>3</sub>

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

### Acetonitrile-d<sub>3</sub>

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<sub>8</sub>

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<sub>2</sub>O

Some deuterated solvents are prepared by catalytic exchange of protonated solvent with deuterium oxide and are carefully purified by distillation. Residual water (H<sub>2</sub>O in equilibrium exchange with D<sub>2</sub>O) 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<sub>2</sub>O 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<sub>6</sub> containing 100 ppm D<sub>2</sub>O. The problem becomes worse as the molecular weight of the analyte increases.

### Solution

Water (as H<sub>2</sub>O, HOD or D<sub>2</sub>O) 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

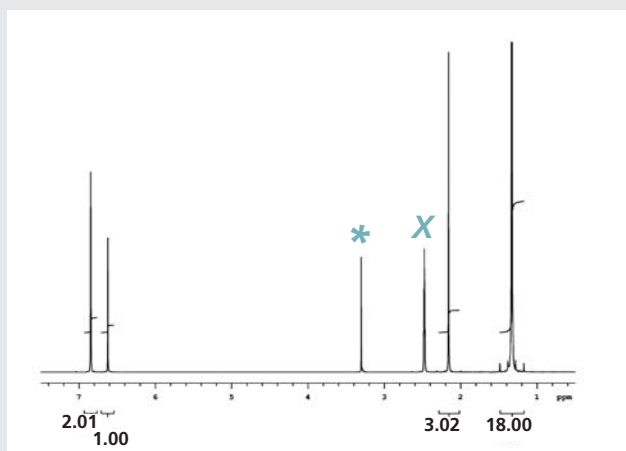


Figure 1. <sup>1</sup>H-NMR spectrum of 5.0 mg 2,6-di-*tert*-butyl-4-methylphenol (MW 220.36g / mole) in dry DMSO-d<sub>6</sub>. Note the proper integral ratios of 18:3:1:2 (t-butyl: methyl: ring-H: -OH). Note the single H<sub>2</sub>O peak at 3.3 ppm.

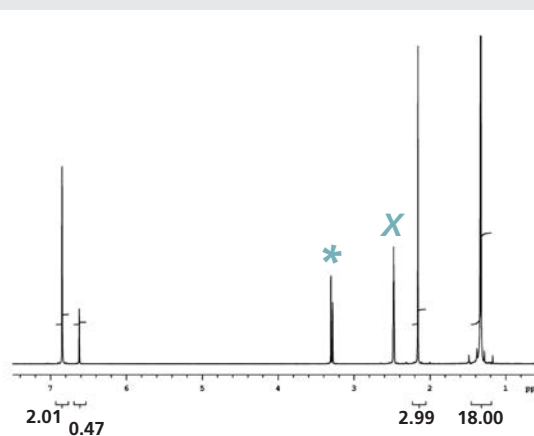


Figure 2. <sup>1</sup>H-NMR spectrum of 5.3 mg of 2,6-di-*tert*-butyl-4-methylphenol in DMSO-d<sub>6</sub> with 100 ppm D<sub>2</sub>O added. Note the reduced ratio of the phenolic proton 18:3:2:0.47 (t-butyl: methyl: ring-H: -OH). Note that the HOH and HOD peaks are separated in the spectrum.

# NMR Solvents

## Chemical Shifts of Selected Compounds in Different Solvents

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

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

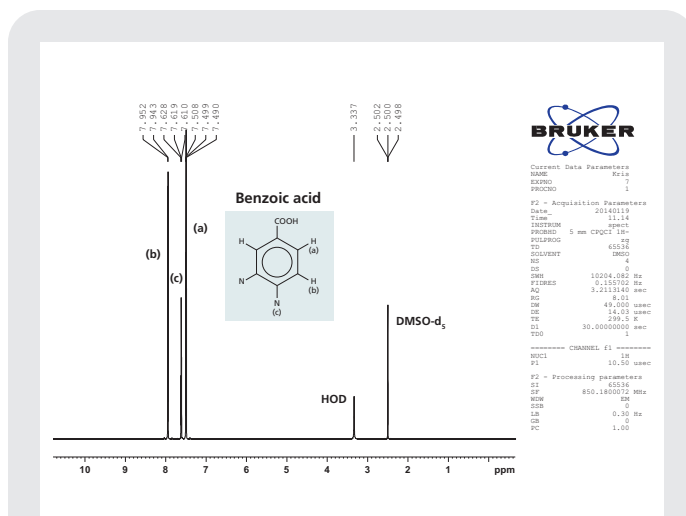
## Standards for qNMR

Quantitative  $^1\text{H}$ -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.

### External Calibration Standards

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

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



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

### qNMR Standard for External Referencing

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

\* 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  $^1\text{H}$ -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.

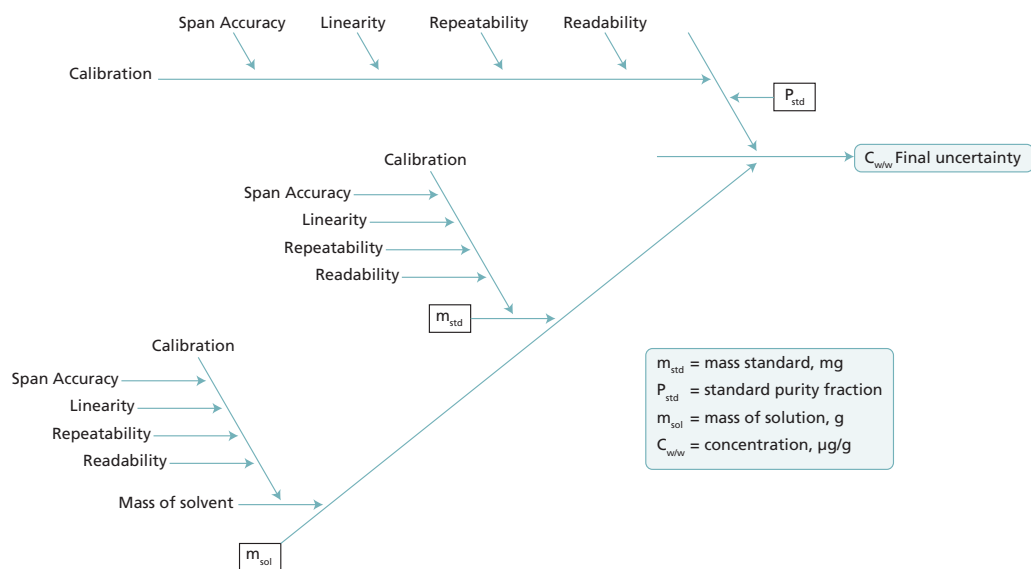
### qNMR Standard for Internal Referencing

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- $d_6$	1 g	The benzoic acid concentration and associated uncertainty is reported.
DLM-7092	2 mM DSS- $d_6$ + 80 mM potassium phosphate buffer in deuterium oxide (D, 99.96%)	5 × 0.5 mL	
DLM-7093	100 mM DSS- $d_6$ in water (D, 98%)	5 × 0.5 mL	
DLM-7095	50 mM DSS- $d_6$ in water (D, 98%)	5 × 0.5 mL	
DLM-7096	20 mM DSS- $d_6$ in water (D, 98%)	5 × 0.5 mL	
DLM-7094	5 mM DSS- $d_6$ in water (D, 98%)	5 × 0.5 mL	

### 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<sup>1</sup> 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



## 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 <sub>6</sub> (D, 99.9%)	Multiple sizes
DLM-112	Acetaldehyde (D <sub>4</sub> , 99%)	5 g
DLM-247	Acetyl chloride (D <sub>3</sub> , 98%)	10 g
DLM-1	Benzene-d <sub>6</sub> (D, 99.5%)	Multiple sizes
DLM-494	Biphenyl (D <sub>10</sub> , 98%)	1 g
DLM-1945	bis(2-Chloroethoxy) methane (chloroethoxy-D <sub>8</sub> , 98%)	0.1 g
DLM-1315	Borane (D <sub>3</sub> , 98%) (1 molar in THF) (+0.005M NABD <sub>4</sub> )	0.25 L
DLM-4747	Borane methylsulfide complex (D <sub>3</sub> , 99%)	5 g
DLM-398	Bromobenzene (D <sub>5</sub> , 99%)	25 g
DLM-1116	<i>tert</i> -Butylchloride (D <sub>9</sub> , 98%)	Multiple sizes
DLM-263	Chlorobenzene-d <sub>5</sub> (D, 99%)	5 g
CNLM-7289	Cyanamide ( <sup>13</sup> C, 99%; <sup>15</sup> N <sub>2</sub> , 98%) (stabilized with < 0.1% acetic acid)	Please inquire
DLM-4	Deuterium oxide (D, 99.9%)	Multiple sizes
DLM-3903	Dimethyl carbonate (D <sub>6</sub> , 99%)	1 g
DLM-196	Dimethyl sulfate (D <sub>6</sub> , 98%)	Please inquire
DLM-805	Formaldehyde (D <sub>2</sub> , 98%) (~20% w/w in D <sub>2</sub> O)	20 mL of solution

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

CP = chemical purity

## 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.<sup>1</sup>

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

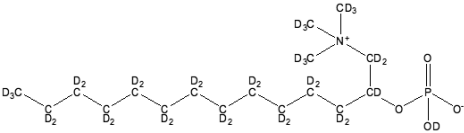
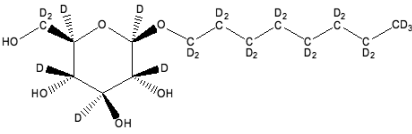
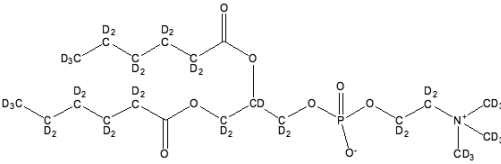
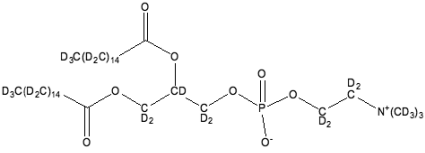
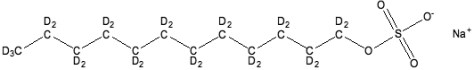
### Reference

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

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

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

### Deuterated Detergents and Phospholipids

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

## Deuterated Buffers

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

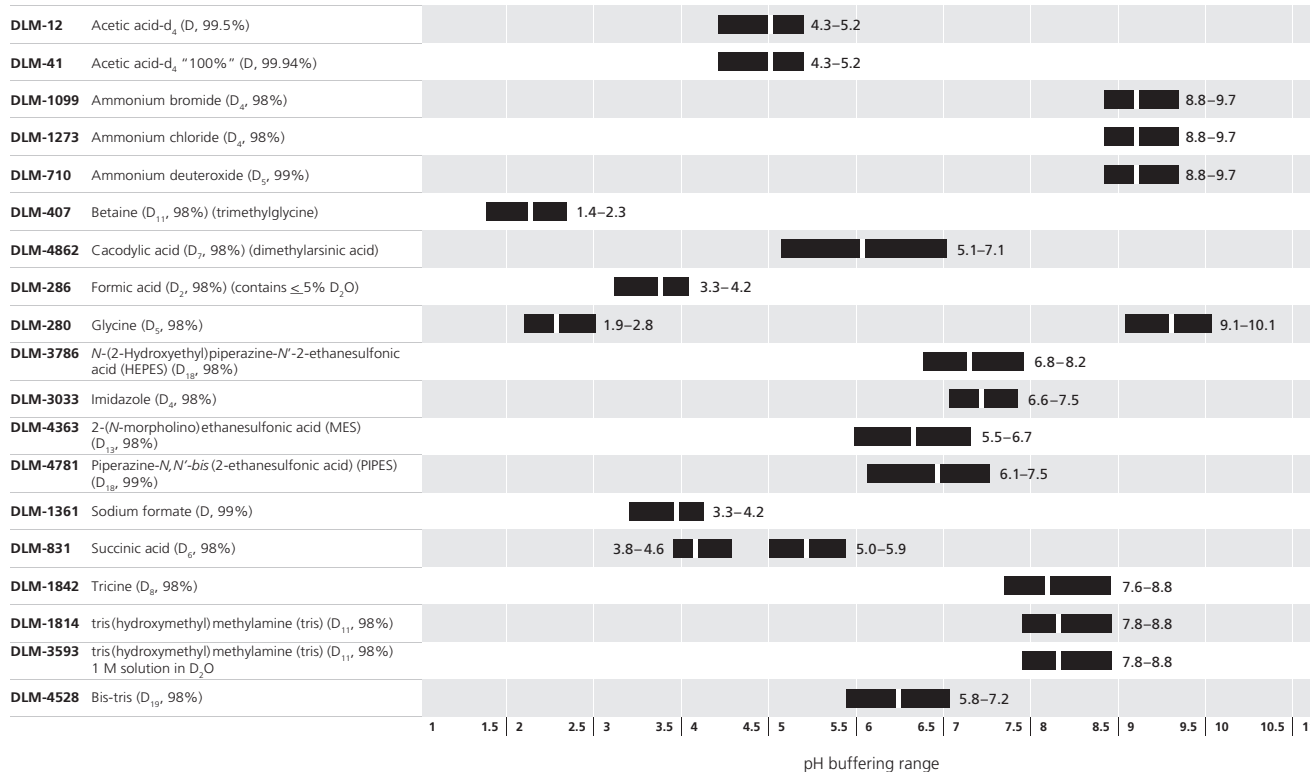
Catalog No.	Description
DLM-12	Acetic acid-d <sub>4</sub> (D, 99.5%)
DLM-41	Acetic acid-d <sub>4</sub> "100%" (D, 99.93%)
DLM-1099	Ammonium bromide (D <sub>4</sub> , 98%)
DLM-1273	Ammonium chloride (D <sub>4</sub> , 98%)
DLM-710	Ammonium deuterioxide (D <sub>5</sub> , 99%) (~25% in soln D <sub>2</sub>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

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

### pH Buffering Range Chart

#### Catalog Number and Compound

pK<sub>a</sub> is indicated by a white rule within the range



## Isotope-Labeled Protein Standards

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

Nexomics provides high-quality, high-purity standards that are invaluable tools for biomolecular NMR research applications. Each product is accompanied by the following data:

- $^1\text{H}$ - $^{15}\text{N}$  HSQC ( $^{15}\text{N}$ -labeled proteins)
- $^1\text{H}$ - $^{13}\text{C}$  HSQC ( $^{13}\text{C}$ -labeled proteins)
- CO-NH projection of 3D HNCO ( $^{15}\text{N}$ ,  $^{13}\text{C}$ -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  $\alpha$ -Spectrin SH3 Domain is available in microcrystalline form (in an ammonium sulfate emulsion) or as a 9 mg/mL solution (10%  $\text{D}_2\text{O}$ /90%  $\text{H}_2\text{O}$  containing 0.02%  $\text{NaN}_3$ , pH 3.5). A full technical data package containing 2D-NMR data and peak assignments accompanies every order for the Chicken  $\alpha$ -Spectrin SH3 Domain. Every order for the GB1 is accompanied by a  $^1\text{H}$ - $^{15}\text{N}$ -HSQC spectrum.

Catalog No.	Description
CLM-8227	SH3 Domain Protein ( $\text{U-}^{13}\text{C}$ , 98%)
NLM-6839	SH3 Domain Protein ( $\text{U-}^{15}\text{N}$ , 98%)
NLM-6839-S	SH3 Domain Protein ( $\text{U-}^{15}\text{N}$ , 98%) (9 mg/mL solution)
CNLM-6840	SH3 Domain Protein ( $\text{U-}^{13}\text{C}$ , 98%; $\text{U-}^{15}\text{N}$ , 98%) (microcrystalline slurry)
CNLM-6840-S	SH3 Domain Protein (w/ 0.01% sodium azide) ( $\text{U-}^{13}\text{C}$ , 98%; $\text{U-}^{15}\text{N}$ , 98%) (9 mg/mL solution)
CDNLM-6841	SH3 Domain Protein ( $\text{U-}^{13}\text{C}$ , 98%; $\text{U-D}$ , 98%; $\text{U-}^{15}\text{N}$ , 98%)
CDNLM-6841-S	SH3 Domain Protein (9 mg/mL solution) ( $\text{U-}^{13}\text{C}$ , 98%; $\text{U-D}$ , 98%; $\text{U-}^{15}\text{N}$ , 98%)
CNLM-2408	GFL Peptide Standard ( $^{13}\text{C}$ , 98%; $^{15}\text{N}$ , 96-99%) 1 mM in $\text{DMSO-d}_6$

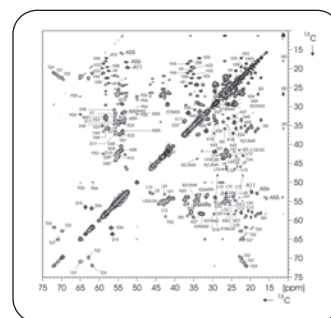
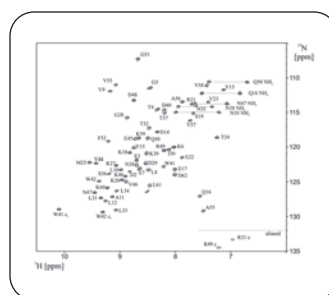
## CIL His-Tagged Protein Standards

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

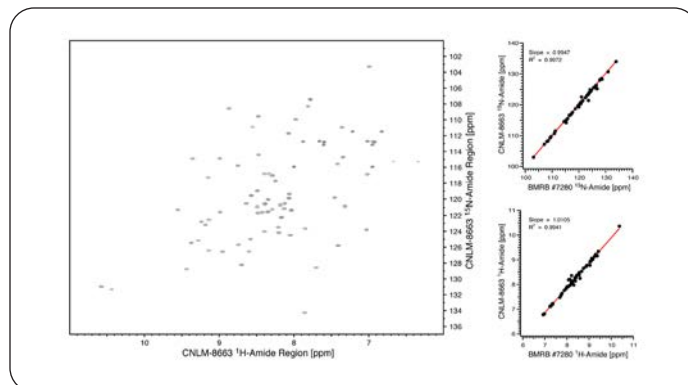
Product	Amino Acid Length
Chicken $\alpha$ -Spectrin SH3 Domain	62 residues
MDETGKELYL ALYDYQEKPQ REVMTKKGDI LTLNSTNKD WWWKEVNDKQ GFVPAAYVKK LD	
His6x-GB1 ( $\beta$ -1 immunoglobulin domain of protein G)	71 residues
MHHHHHHGNG LYFQSMQYKL ILNGKTLKGE TTTEAVDAAT AEKVFKQYAN DNGVDGEWTV DDAKTFTVT E	
GFL Peptide	8 residues
YG <b>GFL</b> RR (bold indicates labeled residues)	

GB1 is offered as a *N*-terminal, tobacco etch virus (TEV)-cleavable 6xHis-tag as a 1.5 mM solution in 137 mM NaCl, 2.7 mM KCl, 8.1 mM  $\text{Na}_2\text{HPO}_4$ , 1.8 mM  $\text{KH}_2\text{PO}_4$ , 0.02%  $\text{NaN}_3$ , 0.1 mM TSP in 10%  $\text{D}_2\text{O}$ /90%  $\text{H}_2\text{O}$ , pH 6.5. GB1 is noted for its excellent stability at elevated temperatures.

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



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



$^1\text{H}$ ,  $^{15}\text{N}$ -HSQC of 1.5 mM Immunoglobulin-Binding Domain B1 of Streptococcal Protein G ( $\text{U-}^{13}\text{C}$ , 99%;  $\text{U-}^{15}\text{N}$ , 99%) containing an *N*-terminal His6-tag and TEV protease cleavage site (CNLM-8663-CA, Lot# 20110209). The  $^{15}\text{N}$ -amide (top, right) and  $^1\text{H}$ -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,  $^{15}\text{N}$ ,  $^{13}\text{C}$ -enriched with selective incorporation of protons into methyl groups of Ile- $\delta$ 1, Leu- $\delta$  and Val- $\gamma$  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,  $^{15}\text{N}$ ,  $^{13}\text{C}$  and ILV methyl  $^1\text{H}$ ,  $^{13}\text{C}$  MBP in 10%  $\text{D}_2\text{O}$ , 0.02%  $\text{NaN}_3$ , 20 mM sodium phosphate @ pH 7.2

#### NEX-MBP2: Closed Conformation

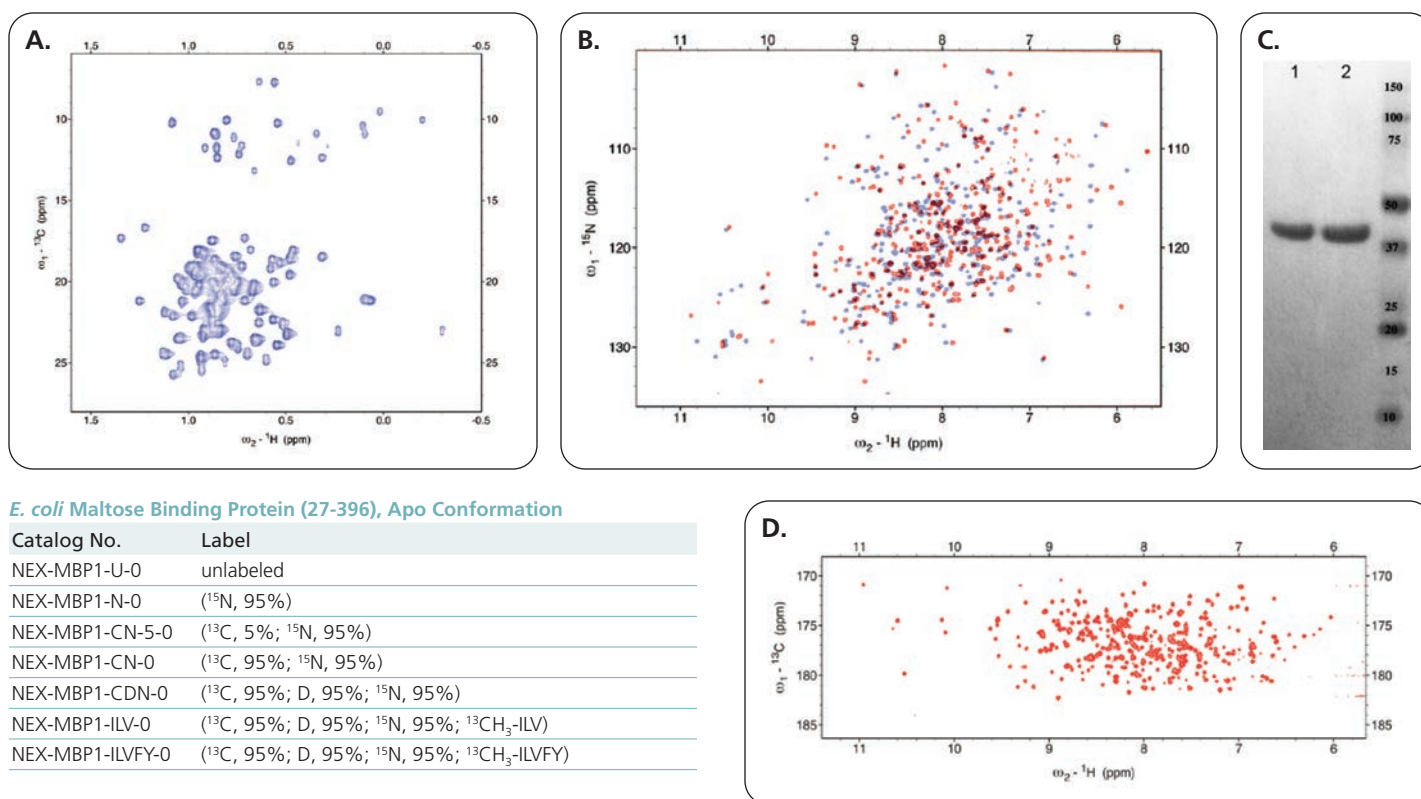
0.5 mM D,  $^{15}\text{N}$ ,  $^{13}\text{C}$  and ILV methyl  $^1\text{H}$ ,  $^{13}\text{C}$  MBP with 3 mM maltotriose, 10%  $\text{D}_2\text{O}$ , 0.02%  $\text{NaN}_3$ , 20 mM sodium phosphate @ pH 7.2

#### NEX-MBP3: Open Conformation

0.5 mM D,  $^{15}\text{N}$ ,  $^{13}\text{C}$  and ILV methyl  $^1\text{H}$ ,  $^{13}\text{C}$  MBP with 2 mM  $\beta$ -cyclodextrin, 10%  $\text{D}_2\text{O}$ , 0.02%  $\text{NaN}_3$ , 20 mM sodium phosphate @ pH 7.2

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

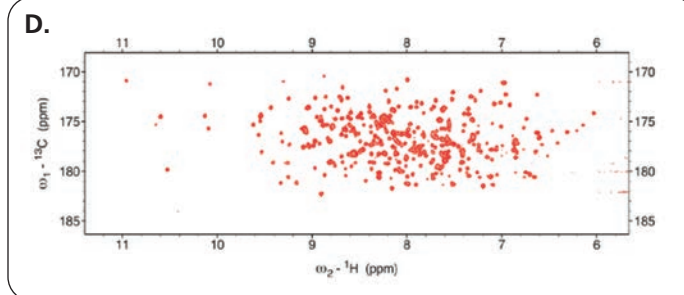
Catalog No.	Label
NEX-MBP1-U-0	unlabeled
NEX-MBP1-N-0	( $^{15}\text{N}$ , 95%)
NEX-MBP1-CN-5-0	( $^{13}\text{C}$ , 5%; $^{15}\text{N}$ , 95%)
NEX-MBP1-CN-0	( $^{13}\text{C}$ , 95%; $^{15}\text{N}$ , 95%)
NEX-MBP1-CDN-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%)
NEX-MBP1-ILV-0	( $^{13}\text{C}$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

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

Catalog No.	Label
NEX-MBP2-U-0	unlabeled
NEX-MBP2-N-0	( $^{15}\text{N}$ , 95%)
NEX-MBP2-CN-5-0	( $^{13}\text{C}$ , 5%; $^{15}\text{N}$ , 95%)
NEX-MBP2-CN-0	( $^{13}\text{C}$ , 95%; $^{15}\text{N}$ , 95%)
NEX-MBP2-CDN-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%)
NEX-MBP2-ILV-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-MBP2-ILV-FY-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%; $^{13}\text{CH}_3$ -ILV-FY)

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

Catalog No.	Label
NEX-MBP3-U-0	unlabeled
NEX-MBP3-N-0	( $^{15}\text{N}$ , 95%)
NEX-MBP3-CN-5-0	( $^{13}\text{C}$ , 5%; $^{15}\text{N}$ , 95%)
NEX-MBP3-CN-0	( $^{13}\text{C}$ , 95%; $^{15}\text{N}$ , 95%)
NEX-MBP3-CDN-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%)
NEX-MBP3-ILV-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-MBP3-ILV-FY-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%; $^{13}\text{CH}_3$ -ILV-FY)



#### A. $^{13}\text{C}$ , $^1\text{H}$ HSQC NEX-MBP3 "open" conformation

#### B. "Open" (blue) and "closed" (red) superposition

#### C. SDS-PAGE GEL NEX-MBP

NEX-MBP3  $\beta$ -cyclodextrin complexed "open" sample (lane 1)

NEX-MBP2 maltotriose complexed "closed" sample (lane 2)

#### D. CO-NH 2D plane of HNCQ triple-resonance experiment of NEX-MBP2 "closed" sample

### Protein Sequence

```

MKIEEGKLIWINGDKGYNGLAIEVGKKFEKDTGIKVTVEHPDKLEEFQVAATGDGPDIIFWAH
DRFGGYAQSGLLAEITPDKAFQDKLYPFTWDVARYNGKLIAYIAVEALSILYNKDLLPNPKTWEE
IPALDKELKAKGKSALMFNLQEPYFTWPLIADGGYAFKYENGYDIKDVGDVNAGAKAGLTL
VDLIKNKHMNADTDYSIAEAFNKGKETAMTINGPWAWNSIDTSKVNYGVTVLPTFKGQSPK FV
GVLSAGINAASPNKELAKEFLENLLTDEGLEAVNKDKPLGAVALKSYEEELAKDPRIATMEN AQ
KGEIMPNIQPMASFYAVRTAVINAASGRQTVDEALKDAQTRITK
  
```



## X-Filtered NOESY NMR Standard (NEX-XF1)

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

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

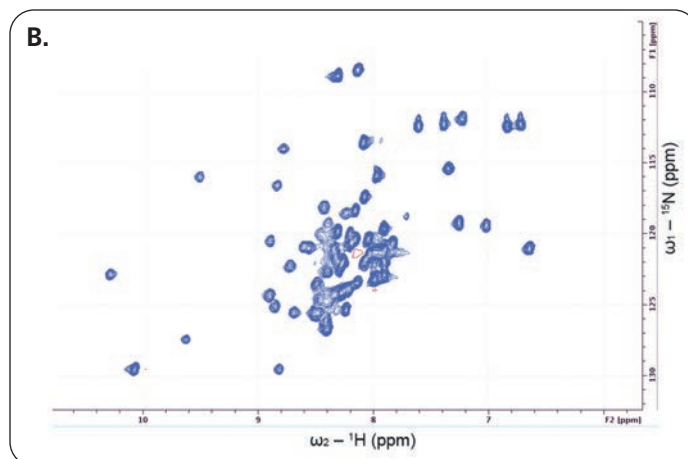
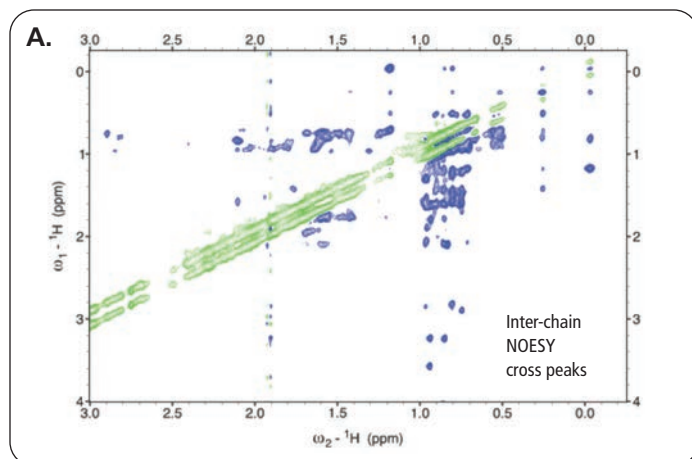
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### NEX-XF1 homodimer sample formulation:

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

1 mM protein, 20 mM  $\text{NH}_4\text{OAc}$  pH 5.5, 100 mM NaCl, 5 mM  $\text{CaCl}_2$ , 10 mM DTT, 10%  $\text{D}_2\text{O}$ , 0.02 %  $\text{NaN}_3$



### X-Filtered NOESY NMR Standard

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

### X-Filtered NOESY NMR Standard, His-Tagged

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

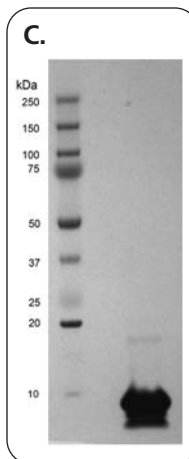
**A.** 2D  $^1\text{H}$ - $^1\text{H}$  plane of  $^1\text{H}, ^{13}\text{C}$  edited  $^1\text{H}, ^{12}\text{C}$  X-filtered NOESY

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

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

### Protein Sequence

PKIIEAVYENG VFKPLQKVDLKEGERVKIKLKVLPIDLGEPVS  
VEEIKKIRDGTWMSLEHHHHHH



## Ubiquitin (NEX-UB1)

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

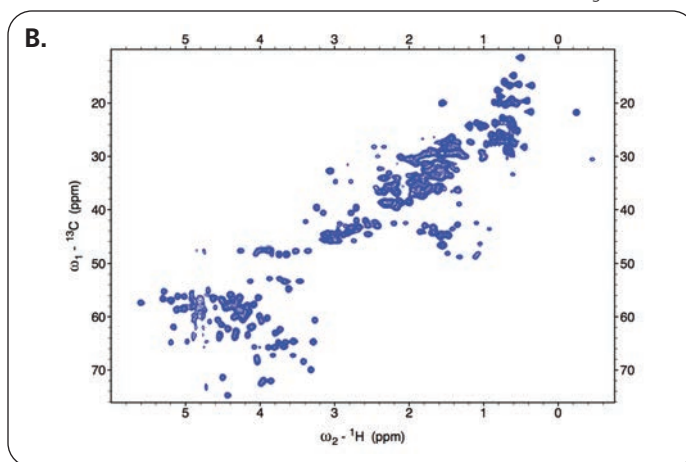
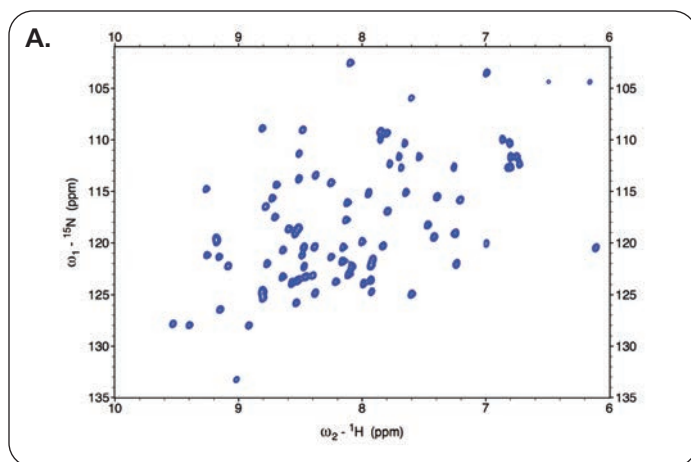
### NEX-UB1 sample formulation:

**NEX-UB1:** Uniformly  $^{15}\text{N}$ ,  $^{13}\text{C}$ -labeled ubiquitin in 90%  $\text{H}_2\text{O}$ ; 10%  $\text{D}_2\text{O}$   
10 mM sodium phosphate buffer, pH 6.5

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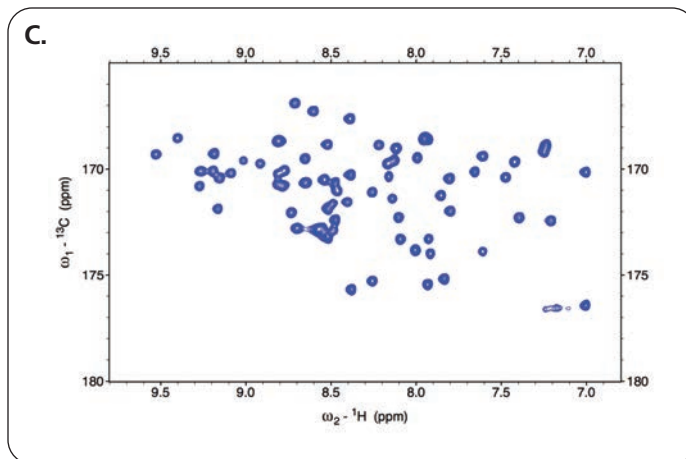


A.  $^1\text{H}$ ,  $^{15}\text{N}$  HSQC of NEX-UB1

B.  $^{13}\text{C}$ - $^1\text{H}$  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	( $^{15}\text{N}$ , 95%)
NEX-UB1-CN-5-0	( $^{13}\text{C}$ , 5%; $^{15}\text{N}$ , 95%)
NEX-UB1-CN-0	( $^{13}\text{C}$ , 95%; $^{15}\text{N}$ , 95%)
NEX-UB1-CDN-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%)
NEX-UB1-ILV-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%; $^{13}\text{CH}_3$ -ILV)
NEX-UB1-ILV-FY-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%; $^{13}\text{CH}_3$ -ILV-FY)

### His-Ubiquitin (Human)

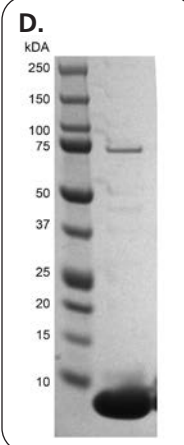
NEX-UBI-HIS-U-0	unlabeled
NEX-UBI-HIS-N-0	( $^{15}\text{N}$ , 95%)
NEX-UBI-HIS-5-0	( $^{13}\text{C}$ , 5%; $^{15}\text{N}$ , 95%)
NEX-UBI-HIS-CN-0	( $^{13}\text{C}$ , 95%; $^{15}\text{N}$ , 95%)
NEX-UBI-HIS-CDN-0	( $^{13}\text{C}$ , 95%; D, 95%; $^{15}\text{N}$ , 95%)
NEX-UBI-HIS-ILV-0	( $^{13}\text{C}$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

### Protein Sequence after TEV Cleavage

SHMQIFVKTLTGKITLEVEPSDTIENVKAKIQDKEGIPPDQQR  
LIFAGKQLEDGRTLSDYNIQKESTLHLVLRLLRG

### Protein Sequence before TEV Cleavage

MGHHHHHHENLYFQSHMQIFVKTLTGKITLEVEPSDTIEN VK  
AKIQDKEGIPPDQQR LIFAGKQLEDGRTLSDYNIQKESTL  
HLVLRLLRG



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