Eurisotop

A CAMBRIDGE ISOTOPE LABORATORIES COMPANY

NMR

PRODUCT LINE

Euriso-Top makes excellence a reality.

For over 25 years, Euriso-Top has been manufacturing and distributing the widest range of labeled compounds. We have been committed to providing the highest quality products to our customers and our technical expertise has enabled us to support the researchers in their scientific applications.

Since we belong to Cambridge Isotope Laboratories, our portfolio has been boosted to a worldwide dimension.
Our brand has been reinforced and our reputation strengthened. Our product range keeps on expanding bringing to more than 8,000 references to better adapt to your needs. Our growth is the result of our dedication to build a strong relationship with our customers that include collaboration, innovation and technical support. Our sales managers are always an available resource for questions regarding our products.

It is with great pride that we present our dedicated product line for NMR. In this, you will find a comprehensive listing of our products and all the information you need for your research. We hope that this catalogue will satisfy you.

Thank you for giving us the opportunity to partner with you since 1991, we will continue on the path to excellence.

Jean-Louis Schaffar
President

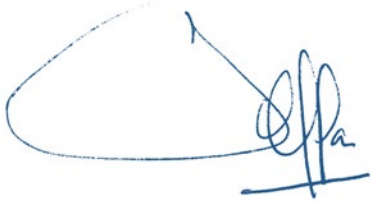


Table of Contents

05 NMR Solvents

11 *NMR Reference Standards*

12 *Data Chart Solvents*

14 *^{1}H Chemical Shifts*

15 *^{13}C Chemical Shifts*

16 *^{15}N Chemical Shifts*

17 *NMR Chemical Shifts of Trace Impurities*

19 NMR Tubes from Norell®

20 *Norell® Secure Series™*

21 *Norell® Select Series™*

22 *Norell® Standard Series™*

23 qNMR

24 *Standards for qNMR*

26 Synthesis

29 Biomolecular NMR

30 *Deuterated Detergents*

31 *Deuterated Buffers*

32 *Cell-Free Synthesis of Labeled Proteins*

33 *Isotope-Labeled Protein Standards*

34 *Maltose Binding Protein*

35 *X-Filtered NOESY NMR Standard*

36 *Ubiquitin*

37 *^{13}C Enriched Substrates for Hyperpolarization*

38 *Pyruvic Acid (1-^{13}C)*

39 Technical Information

40 *What is an Isotope ?*

41 *Quality Control*

44 *Security Concept*

46 *Ordering Information*

EURISO-TOP has been helping to carry out your day to day projects since 1991.

Quality

We are proud to offer the best quality manufacture of labeled compounds, from the supply of raw materials right up until delivery to your laboratory. Our production plant is in the center of the French Atomic Energy Commission (CEA) in Saclay. Our continually updating methods of production can be attributed to the expertise of the CEA scientists, who are among the pioneers of such techniques, and who have contributed significantly to theoretical advances in spectroscopy. Our experience and skills allow us to guarantee top quality products with the highest level of chemical purity and isotopic enrichment. Rigorous controls are made at all stages of the process in our laboratories, allowing us to ensure the consistently highest quality of our solvents to meet your requirements.

Production

Supply of raw materials
Solvents and reagents with a high chemical purity are selected from audited suppliers and tested before acceptance.
Quality control and in-process control
Our production and distillation units are automated and function under an inert nitrogen atmosphere. During the production and distillation processes and at the time of batch release, chemical and isotopic purity are carefully assessed with our 400 MHz NMR spectrometer. Traces of water are quantified by the Karl Fischer method and any non-protonated impurities by gas chromatography. Tests are routinely carried out for acidity and lack of phosgene in our chlorinated solvents.

Packaging

Supply of packaging materials
We select the best containers, vials or ampoules from the suppliers to the pharmaceutical industry and test them to ensure adequate protection against deterioration or contamination of our solvents.
Process line clearance
Our laboratory is filled with automated bottle and ampoule conditioners which are cleaned according to strict internal procedures and are validated so as not to compromise on quality. The containers are then carefully dried to prevent pollution of the solvent through remaining traces of water.
In process-control and batch release of finished products
Euriso-top uses amber ampoules and bottles to protect photosensitive solvents from degradation. Every bottle and box of ampoules are clearly labeled with a lot number for a perfect identification. A Certificate of Analysis (CoA) and a Safety Data Sheet (SDS) are supplied with every shipment.

Sample Bank

Each package is given a batch number for constant traceability, allowing us to process your queries quickly and accurately.

NMR Solvents

NMR Solvents

Each batch of production is routinely tested for chemical and isotopic purity after initial purification, before packaging, and after packaging.

In order to avoid isotopic contamination, all our deuterated solvents are handled under an inert atmosphere, such as dry nitrogen or argon.

Some of our solvents are packaged in septum vials to avoid moisture contaminations.
To get more information about your usual solvent, please refer to the data charts.

Solvent	Water %	I.E.	Code	Qty
Acetic Acid-d4 CD_3COOD d = 1,12 **CAS N° : 1186-52-3** H314 H226 P280 P310 P305+P351+P338 DANGER	max. 0,05%	min. 99,50% D	D012BB	2 x 0,75 mL
			D012EA	1 x 10 mL
		min. 99,91% D	D041BB	2 x 0,75 mL
Acetone-d6 CD_3COCD_3 D = 0,87 **CAS N° : 666-52-4** H225 H319 H336 P210 P261 P305+P351+P338 store at +4°C DANGER	max. 0,02%	min. 99,80% D	D009T	10 x 0,6 mL
			D009B	10 x 0,75 mL
			D009FE	10 mL
			D009ES*	5 x 10 mL
			D009F	25 mL
			D009H	100 mL
	max. 0,01%	min. 99,96% D	D038B	10 x 0,75 mL
Acetone-d6 + 0,03% v/v	max. 0,01%	min. 99,96% D	D338B	10 x 0,75 mL
Acetonitrile-d3 CD_3CN d = 0,84 **CAS N° : 2206-26-0** H225 H302 H312 H332 H319 P210 P280 P305+P351+P338 DANGER	max. 0,05%	min. 99,80% D	D021B	10 x 0,75 mL
			D021FD	5 mL
			D021FE	10 mL
			D021EAS*	10 mL
			D021Z	100 g
	max. 0,02%	min. 99,96% D	D044BB	2 x 0,75 mL
Acetonitrile-d3 + 0,03% TMS	max. 0,02%	min. 99,96% D	D344BB	2 x 0,75 mL
Benzene-d6 C_6D_6 d = 0,95 **CAS N° : 1076-43-3** H225 H372 H319 H304 H340 H350 H315 P301+P310 P305+P351+P338 P308+P313 P331 DANGER	max. 0,02%	min. 99,50% D	D001B	10 x 0,75 mL
			D001ES*	5 x 10 mL
			D001F	25 mL
			D001FE	10 mL
			D001H	10 mL
			D001T	10 x 0,6 mL
	max. 0,01%	min. 99,96% D	D040B	10 x 0,75 mL
n-Butanol-d10 $C_4D_{10}O$ d = 0,92 **CAS N° : 34193-38-9** H315 H226 H 302 H318 H335 H336 P280 P261 P305+P351+P338 DANGER	max. 0,05%	min. 98,00% D	D081FD	1 x 5 mL

S* = Vials «Penicillin» Type

Solvent	Water %	I.E.	Code	Qty
Chloroform-d $CDCl_3$ d = 1,5 **CAS N° : 865-49-6** H302 H315 H351 H373 P305+P351+P338 store at +4°C	max. 0,01%	min. 99,50% D	D006H	100 mL
			D006K	500 mL
	max. 0,01%	min. 99,80% D	D007T	10 x 0,6 mL
			D007B	10 x 0,75 mL
			D007FE	10 mL
			D007F	25 mL
			D007H	100 mL
			D007J	250 mL
			D007K	500 mL
			D007KAG[1]	500 mL
			D007L	1 x 1 L
			D007Z	100 g
	max. 0,01%	min. 99,96% D	D029T	10 x 0,6 mL
			D029B	10 x 0,75 mL
			D029F	25 mL
Chloroform-d + 1% TMS	max. 0,01%	min. 99,80% D	D213H	100 mL
Chloroform-d + 0,03% TMS	max. 0,01%	min. 99,80% D	D307F	25 mL
			D307H	100 mL
			D307HAG[1]	100 mL
			D307K	500 mL
			D307KAG[1]	500 mL
			D307Z	100 g
	max. 0,01%	min. 99,96% D	D329T	10 x 0,6 mL
			D329B	10 x 0,75 mL
			D329F	25 mL
Cyclohexane-d12 C_6D_{12} d = 0,89 **CAS N° : 1735-17-7** H225 H304 H315 H336 H410 P210 P261 P301+P310 P331	max. 0,02%	min. 99,50% D	D017BB	2 x 0,75 mL
			D017FD	5 mL
Deuterium Oxide D_2O d = 1,11 **CAS N° : 7789-20-0** H331 H314 P280 P301+P310 P305+P351+P338		min. 99,90% D	D214B	10 x 0,75 mL
			D214FE	10 mL
			D214F	25 mL
			D214FS*	25 mL
			D214H	100 mL
			D214K	500 mL
			D214L	1 x 1 L
		min. 99,96% D	D215T	10 x 0,6 mL
			D215B	10 x 0,75 mL
			D215ES*	5 x 10 mL
			D215F	25 mL
			D215H	100 mL
			D215K	500 mL

S* = Vials «Penicillin» Type
G[1] = With silver foil

Solvent	Water %	I.E.	Code	Qty
1.2-Dichlorobenzene d4 $C_6D_4Cl_2$ d = 1,34 **CAS N° : 2199-69-1** H319 H315 H302 H335 H410 P261 P305+P351+P338 	max. 0,05%	min. 99,00% D	**D220FD**	5 mL
1.4-Dichlorobenzene d4 $C_6D_4Cl_2$ d = 1,34 **CAS N° : 3855-82-1** H319 H351 H400 H410 P280 P301+P310 	max. 0,01%	min. 98,00% D	**D222PH**	1 x 5 g
Dimethylformamide-d7 $DCON(CD_3)_2$ d = 1,03 **CAS N° : 4472-41-7** H360d H332 H312 H319 P280 P305+P351+P338 	max. 0,05%	min. 99,50% D	**D110BB** **D110FD**	2 x 0,75 mL 5 mL
Dioxane-d8 $C_4D_8O_2$ d = 1,13 H225 H319 H335 H351 P210 P261 P305+P351+P338 	max. 0,1%	min. 99,00% D	**D112BB** **D112CB**	2 x 0,75 mL 2 x 1 mL
DMSO-d6 (Dimethylsulfoxide) CD_3SOCD_3 d = 1,19 **CAS N° : 2206-27-1** H335 P305+P351+P338  	max. 0,02% max. 0,02% max. 0,02% 	min. 99,80% D min. 99,90% D min. 99,96% D 	**D010B** **D010T** **D010FD** **D010FE** **D010F** **D010ES*** **D010H** **D031T** **D031F** **D031H** **D034T** **D034B** **D034FD** **D034EAS*** **D034H**	10 x 0,75 mL 10 x 0,6 mL 5 mL 10 mL 25 mL 5 x 10 mL 100 mL 10 x 0,6 mL 25 mL 100 mL 10 x 0,6 mL 10 x 0,75 mL 5 mL 10 mL 100 mL
DMSO-d6 + 0.03% v/v TMS	max. 0,02% max. 0,02% 	min. 99,80% D min. 99,96% D 	**D310B** **D310ES*** **D310F** **D310H** **D334T** **D334B**	10 x 0,75 mL 5 x 10 mL 25 mL 100 mL 10 x 0,6 mL 10 x 0,75 mL
DMSO-d6 + 0.06% v/v TMS	max. 0,02%	min. 99,80% D	**D610B** **D610F**	10 x 0,75 mL 25 mL
Ethanol-d6 C_2D_5OD d = 0.89 **CAS N° : 1516-08-1** H229 P210  	max. 0,3%	min. 99,00% D	**D114CB** **D114FD**	2 X 1 mL 5 mL
Ethanol-OD C_2H_5OD d = 0,81 **CAS N° : 925-93-9** H225 P210  	max. 6%	min. 99,00% D	**D043F** **D043H**	1 x 25 mL 1 x 100 mL

S* = Vials «Penicillin» Type

Solvent	Water %	I.E.	Code	Qty
Hexafluoroisopropanol-d2 	max. 0,3%	min. 99,00% D	**D052CB**	2 x 1 mL
$(CF_3)_2CDOD$			**D052FD**	5 mL
d = 1,62 **CAS N° : 38701-74-5**			**D052FE**	10 mL
H314 H302 H312 H332 P280 P305+P351+P338				
Isopropanol-d8 	max. 0,1%	min. 99,00% D	**D072V**	1 x 10 g
$(CD_3)_2CDOD$				
d = 0,90 **CAS N° : 22739-76-0**				
H225 H319 H336 P210 P261 P305+P351+P338				
Methanol-d3  	max. 1,0%	min. 99,50% D	**D047B**	10 x 0,75 mL
CD_3OH			**D047FD**	5 mL
d = 0,86 **CAS N° : 1849-29-2**				
H225 H301 H311 H331 H370 P210 P260 P280 P301+P310 P307+P311				
Methanol-d4	max. 0,03%	min. 99,80% D	**D024T**	10 x 0,6 mL
CD_3OD			**D024B**	10 x 0,75 mL
d = 0,89 **CAS N° : 811-98-3**			**D024FE**	10 mL
H225 H301 H311 H331 H370 P210 P260 P280 P301+P310 P307+P311			**D024ES***	5 x 10 mL
			**D024F**	25 mL
			D024FS*	25 mL
			D024H	100 mL
	max. 0,02%	min. 99,95% D	**D048T**	10 x 0,75 mL
			D048B	5 mL
			D048FD	10 x 0,6 mL
Methanol-d4 + 0,03%TMS 	max. 0,03%	min. 99,80% D	**D324B**	10 x 0,75 mL
			D324FE	10 mL
	max. 0,02%	min. 99,95% D	**D348BB**	2 x 0,75 mL
Methanol-OD 	max. 0,1%	min. 99,00% D	**D015F**	25 mL
CH_3OD				
d=0,79 **CAS N° : 1455-13-6**				
H225 H301 H311 H331 H370 P210 P260 P280 P301+P310 P307+P311				
Methylene Chloride-d2 	max. 0,01%	min. 99,80% D	**D023T**	10 x 0,6 mL
CD_2Cl_2			**D023B**	10 x 0,75 mL
d = 1,35 **CAS N° : 1665-00-5**			**D023F**	25 mL
H351 P281			**D023FE**	10 mL
	max. 0,01%	min. 99,96% D	**D049BB**	2 x 0,75 mL
Pyridine-d5 	max. 0,05%	min. 99,50% D	**D013T**	10 x 0,6 mL
C_5D_5N			**D013B**	10 x 0,75 mL
d = 1,05 **CAS N° : 7291-22-7**			**D013FE**	10 mL
H225 H302 H312 H332 P305+P351+P338			**D013F**	25 mL
	max. 0,05%	min. 99,94% D	**D039BB**	2 x 0,75 mL
Tetrachloroethane-d2 	max. 0,02%	min. 99,60% D	**D218FE**	10 mL
$Cl_2DCCDCl_2$			**D218F**	25 mL
d = 1,62 **CAS N° : 33685-54-0** 				
H330 H310 H411 P260				

S* = Vials «Penicillin» Type

Solvent	Water %	I.E.	Code	Qty
Tetrahydrofuran-d8   C_4D_8O d = 0,99 **CAS N° : 1693-74-9** H225 H319 H335 P210 P261 P305+P351+P338	max. 0,05%	min. 99,50% D	**D149BB**	2 x 0,75 mL
			D149CB	2 x 1 mL
			D149F	25 mL
			D149FE	10 mL
Toluene-d8  $C_6D_5CD_3$ d = 0,94 **CAS N° : 2037-26-5**	max. 0,02%	min. 99,50% D	**D005BB**	2 x 0,75 mL
			D005FE	10 mL
			D005F	25 mL
			D042BB	2 x 0,75 mL
Trifluoroacetic Acid-d1  $COODCF_3$ d = 1,5 **CAS N° : 599-00-8** H332 H314 H412 P280 P305+P351+P338	max. 0,02%	min. 99,94% D	**D022BB**	2 x 0,75 mL
			D022EA	1 x 10 mL
Trifluoroethanol-d2, OH  $CF_3(COOD)$ d = 1,37 **CAS N° : 132248-58-9** H319 H226 H302 H312 H332 H335 H315 P280 P305+P351+P338	max. 0,1%	min. 98,00% D	**D208BB**	2 x 0,75 mL
Trifluoroethanol-d3  CF_3CD_2OD d = 1,42 **CAS N° : 77253-67-9** H319 H226 H302 H312 H332 H335 H315 P280 P305+P351+P338	max. 0,1%	min. 99,00% D	**D027BB**	2 x 0,75 mL

Other NMR Deuterated Compounds

Deuterium Chloride (7,6N in D20 solution)  DCl d = 1,25 **CAS N° : 7698-05-7** H314 H335 P280 P301+P310 P305+P351+P338		min. 99,00% D	**D070Z**	1 x 100 g
Sodium Deuteroxide (40% w/w solution in D20)  NaOD d = 1,5 **CAS N° : 14014-06-3** H314 P280 P301+P310 P305+P351+P338		min. 99,50% D	**D076Y**	1 x 50 g
Sulfuric Acid-d2 (96-98% w/w solution in D20)  D_2SO_4 d = 1,86 **CAS N° : 13813-19-9** H314 P280 P301+P310 P305+P351+P338		min. 99,00% D	**D077Z**	1 x 100 g

S* = Vials «Penicillin» Type

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.

Reference	Description	Application	Tube Size
DLM-79	1% 1,2-Dichlorobenzene in acetone-d_6 (D, 99.9%)	^{1}H-Resolution	5 mm x 8"
DLM-74	0.1% Ethylbenzene + 0.01% TMS in chloroform-d "100%" (D, 99.96%)	^{1}H-Sensitivity	5 mm x 8"
DLM-67	1% 3-Heptanone in chloroform-d (D, 99.8%)	^{1}H APT Test	5 mm x 8 "
ULM-73	12% TMS in chloroform	^{1}H-Reference/Calibration	5 mm x 8"
DLM-84	5% Ethylbenzene + 2% TMS in chloroform-d (D, 99.8%)	^{1}H-Sensitivity/Reference	5 mm x 8"
DLM-76	1% Chloroform in acetone-d_6 (D, 99.9%)	^{1}H-Line Shape	5 mm x 8"
DLM-90	0.1 mg/mL GdCl3·6H_2O in D_2O (D, 99.96%)	^{1}H-Homogeneity	5 mm x 8"
DLM-72	40% *p*-Dioxane in benzene-d_6 (D, 99.6%)	^{13}C-Sensitivity/Resolution	5 mm x 8"
DLM-66	30% Menthol (by weight) in chloroform-d (D, 99.8%)	^{13}C App Test	5 mm x 8"
DLM-68	90% Formamide in DMSO-d_6 (D, 99.9%)	^{15}N-Sensitivity	5 mm x 8"
DLM-77	0.0485 M Triphenylphosphate in chloroform-d (D, 99.8%)	^{31}P-Sensitivity	5 mm x 8"
DLM-78	0.05% α,α,α,-Trifluorotoluene in benzene-d_6 (D, 99.6%)	^{19}F-Sensitivity	5 mm x 8"
CDLM-100	0.1% Methanol-^{13}C + 0.3 mg/mL $GdCl_3$ in 98.9% D_2O + 01% H_2O	Auto Test Sample	5 mm x 8"
DLM-88	0.1 mg/mL $GdCl_3$ + 0.1% DSS in 20% H_2O in D_2O	Gradient Shimming	5 mm x 8"
CDLM-96	1% $^{13}CH_3I$, 0.2% $Cr(acac)_3$ + 1% $(CH_3O_3)P$ in $CDCl_3$ "100%"	Indirect Detection Test	5 mm x 8"
DNLM-97	0.2% $Cr(acac)_3$ + 2% Benzamide (^{15}N,98%+) in DMSO-d_6 "100%" (D, 99.96%)	Indirect Detection Test	5 mm x 8"
ULM-71	100% Ethylene glycol*	High Temperature Calibrant	5 mm x 8"
ULM-69	100% Methanol*	Low Temperature Calibrant	5 mm x 8"
ULM-92	10% TMS in methanol	Low Temperature Measurement	5 mm x 8"
CDNLM-5003	0.1 M Urea-^{15}N + 0.1 M MeOH-^{13}C in DMSO-d_6 100%	Indirect Detection Experiments	5 mm x 8"
DLM-5022	2% 2-Ethyl-1-indanone in chloroform-d	2D Calibration	5 mm x 8"
CDNLM-7011	0.1% Methanol-^{13}C - 0.1% acetonitrile-^{15}N + 0.3 mg/mL in 98.8% D_2O + 1% H_2O	Auto Test Sample	5 mm x 8"
ULM-7049	5% Ethyl *trans*-crotonate + 1% TMS in $CDCl_3$ in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
DLM-7047	98% N-Propyl benzoate + 2% TMS in a 7" sealed NMR tube/fill height 50 mm	General Test Sample	5 mm x 7"
DLM-5001	10% Ethylbenzene in chloroform-d (540 pp tube)	^{13}C Sensitivity	5 mm x 8"
DLM-5000	3% Chloroform + 0.2% Tms In Acetone-D_6	^{1}H line shape	5 mm x 8"
DLM-5030	0.3% Chloroform In Acetone-D_6	^{1}H line shape	5 mm x 8"
DLM-5004	100 mg/mL Cholesteryl Acetate In Chloroform-D	^{1}H line shape	5 mm x 8"
DLM-7005	99% D_2O 1%H_2O		100 G
DLM-64	1% Ethylbenzene + 2% TMS In Chloroform-D	^{1}H sensitivity	5 mm x 8"
DLM-5001	10% Ethylbenzene in chloroform-d (540 pp tube)	^{1}H sensitivity	5 mm x 8"
DLM-5008	0.1% Ethylbenzene In Chloroform-D (540 pp Tube)	^{1}H sensitivity	5 mm x 8"
DLM-5006	80% Ethylene Glycol + 20% DMSO-d_6	High temperature calibration	5 mm x 8"
DLM-68	90% Formamide in DMSO-d_6 (D, 99.9%)	^{15}N sensitivity	5 mm x 8"
DLM-5007	4% Methanol + 96% Methanol-D_4	Low temperature callibration	5 mm x 8"
DLM-7003	NMR Reference Standard/50 Millimolar Acetic Acid	Sodium Salt In 99% D_2O	50 mL
DLM-7027C	2 mm Sucrose + 0.25 mm Dss + 0.25 mm Nan_3 In 90% H_2O/10% D_2O (V/V)		3 mm x 8"
DLM-91	2 mm Sucrose + 0.5 mm Dss + 2 mm Nan_3 In 90% H_2O/10% D_2O H2O:D2O=V/V		5 mm x 8"
U001FS	Tetramethylsilane		25 mL
D219PF	TMSP-D_4		1 g

We are 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 representative.

Data chart

Solvent	^{1}H Chemical Shift* (ppm from TMS) (multiplicity)	JHD (Hz)	Carbon-13 Chemical Shift* (ppm from TMS) (multiplicity)	JCD (Hz)	^{1}H Chemical Shift of HOD** (ppm from TMS)
Acetic acid-d_4	11.65 (1) 2.04 (5)	2.2	178.99 (1) 20.0 (7)	20	11.5
Acetone-d_6	2.05 (5)	2.2	206.68 (1) 29.92 (7)	0.9 19.4	2.8
Acetonitrile-d_3	1.94 (5)	2.5	118.69 (1) 1.39 (7)	21	2.1
Benzene-d_6	7.16 (1)		128.39 (3)	24.3	0.4
Chloroform-d	7.24 (1)		77.23 (3)	32.0	1.5
Cyclohexane-d_{12}	1.38 (1)		26.43 (5)	19	0.8
Deuterium oxide	4.80 (DSS) 4.81 (TSP)		NA	NA	4.8
N,N-Dimethyl-formamide-d_7	8.03 (1) 2.92 (5) 2.75 (5)	 1.9 1.9	163.15 (3) 34.89 (7) 29.76 (7)	29.4 21.0 21.1	3.5
1,2 Dichlorobenzene-d_4	6.93 (1) 7.19 (1)		127.19 (3) 130.04 (3) 132.39		0.8
Dimethyl sulfoxide-d_6	2.50 (5)	1.9	39.51 (7)	21.0	3.3
1,4-Dioxane-d_8	3.53 (m)		66.66 (5)	21.9	2.4
Ethanol-d_6	5.19 (1) 3.56 (1) 1.11 (m)		 56.96 (5) 17.31 (7)	 22 19	5.3
Hexafluoroisopropanol-d_2	4.41 (m) 4.86 (1)		68.07 (m) 120.66 (4)		
Isopropanol-d_8	1.1 (1) 3.89 (1) 5.27 (1)		25.8 (7) 64.5 (3)		
Methanol-d_4	4.78 (1) 3.31 (5)	 1.7	 49.15 (7)	 21.4	4.9
Methylene chloride-d_2	5.32 (3)	1.1	54.00 (5)	27.2	1.5
Pyridine-d_5	8.74 (1) 7.58 (1) 7.22 (1)		150.35 (3) 135.91 (3) 123.87 (3)	27.5 24.5 25	5
Tetrachloroethane-d_2	6.0 (1)		73.78 (3)		
Tetrahydrofuran-d_8	3.58 (1) 1.73 (1)		67.57 (5) 25.37 (5)	22.2 20.2	2.4-2.5
Toluene-d_8	 7.09 (m) 7.00 (1) 6.98 (5) 2.09 (5)	 2.3	137.86 (1) 129.24 (3) 128.33 (3) 125.49 (3) 20.4 (7)	 23 24 24 19	0.4
Trifluoroacetic Acid-d	11.50 (1)		164.2 (4) 116.6 (4)		11.5
Trifluoroethanol-d_3	5.02 (1) 3.88 (4x3)	 2(9)	126.3 (4) 61.5 (4x5)	 22	5

* The ^{1}H spectra of the residual protons and ^{13}C spectra were obtained on a Varian Gemini 200 spectro-meter 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.

Solvent	Density at 20°C***	Melting point (°C)***	Boiling point (°C)***	Dielectric Constant	Molecular Weight***
Acetic acid-d_4	1.12	16.7	118	6.1	64.08
Acetone-d_6	0.87	-94	56.5	20.7	64.12
Acetonitrile-d_3	0.84	-45	81.6	37.5	44.07
Benzene-d_6	0.95	5.5	80.1	2.3	84.15
Chloroform-d	1.50	-63.5	61-62	4.8	120.38
Cyclohexane-d_{12}	0.89	6.47	80.7	2.0	96.24
Deuterium oxide	1.11	3.81	101.42	78.5	20.03
N,N-Dimethyl-formamide-d_7	1.03	-61	153	36.7	80.14
1,2 Dichlorobenzene-d_4	1.3	-17	181	9.8	151.03
Dimethyl sulfoxide-d_6	1.19	18.45	189	46.7	84.17
1,4-Dioxane-d_8	1.13	11.8	101.1	2.2	96.16
Ethanol-d_6	0.89	-114.1	78.5	24.5	52.11
1,1,1,3,3,3-Hexafluoroisopropanol-d_2	1.6	-4	59		170.05
Isopropanol-d_8	0.9	-89	83	18.3	68.4
Methanol-d_4	0.89	-97.8	64.7	32.7	36.07
Methylene chloride-d_2	1.35	-95	39.75	8.9	86.95
Pyridine-d_5	1.05	-42	115-116	12.4	84.13
1,1,2,2-Tetrachloroethane-d_2	1.62	-44	147	8.2	169.86
Tetrahydrofuran-d_8	0.99	-108.5	66	7.6	80.16
Toluene-d_8	0.94	-95	110.6	2.4	100.19
Trifluoroacetic Acid-d	1.41	-15.4	72.4		115.03
Trifluoroethanol-d_3	1.41	-43.3	75		103.06

** Approximate values only, may vary with pH,concentration and temperature.
*** Melting and boiling points are those of the corresponding unlabeled compound (except for D_2O).These temperature limits can be used as a guide to determine the useful liquid range of the solvents. Information gathered from the Merck Index - Eleventh Edition.

S. Budavari, MJ. O'Neil, A. Smith, P.E. Heckelman, The Merck Index, an Encyclopedia of Chemicals, Drugs and Biologicals - Eleventh Edition, Merck Co., Inc. Rahway, NJ, 1989.

^{1}H Chemical Shifts

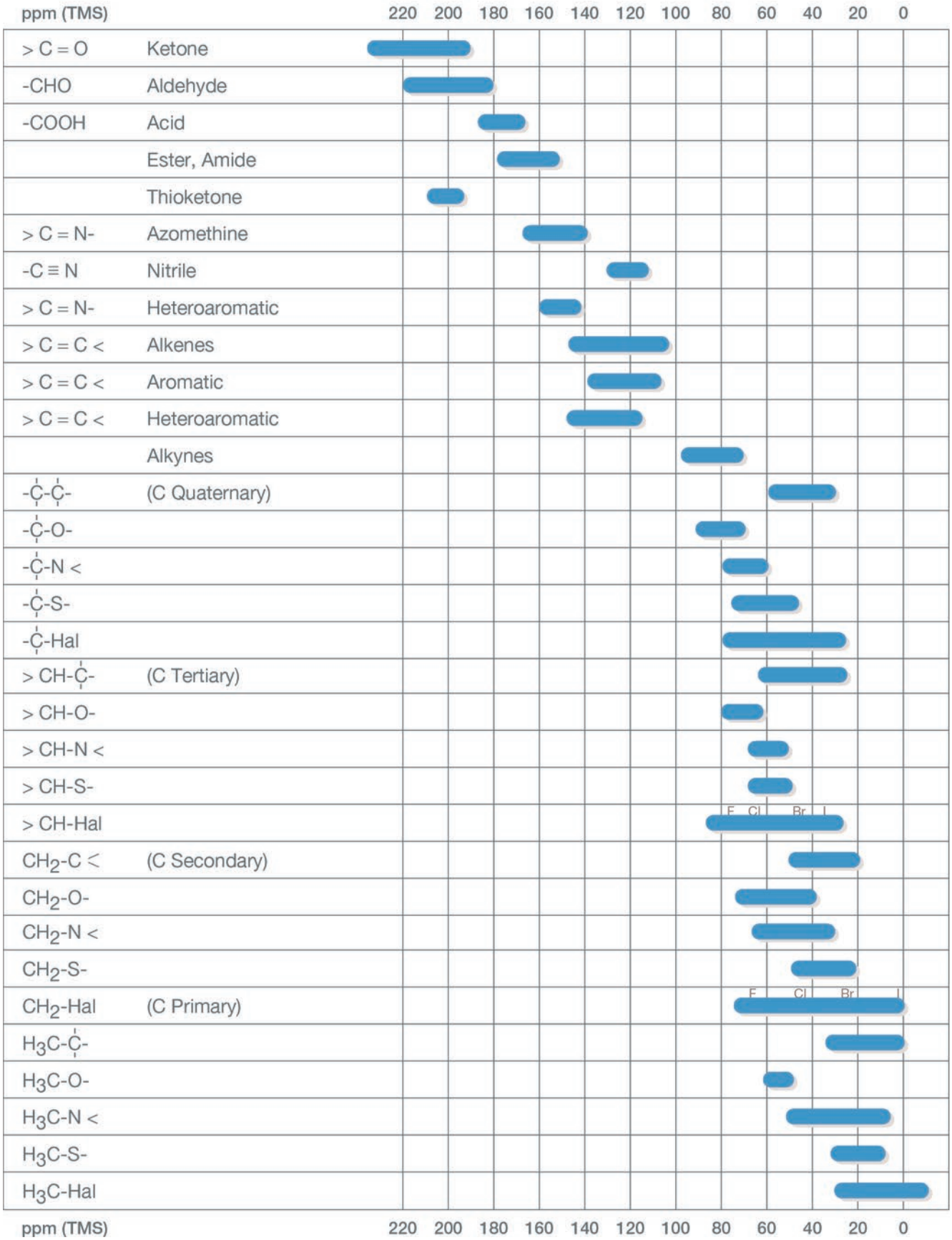
^{1}H Nuclear Spin : 1/2
TMS = 0 ppm

δ ^{1}H (ppm)

^{13}C Chemical Shifts

^{13}C Nuclear Spin : 1/2
TMS = 0 ppm

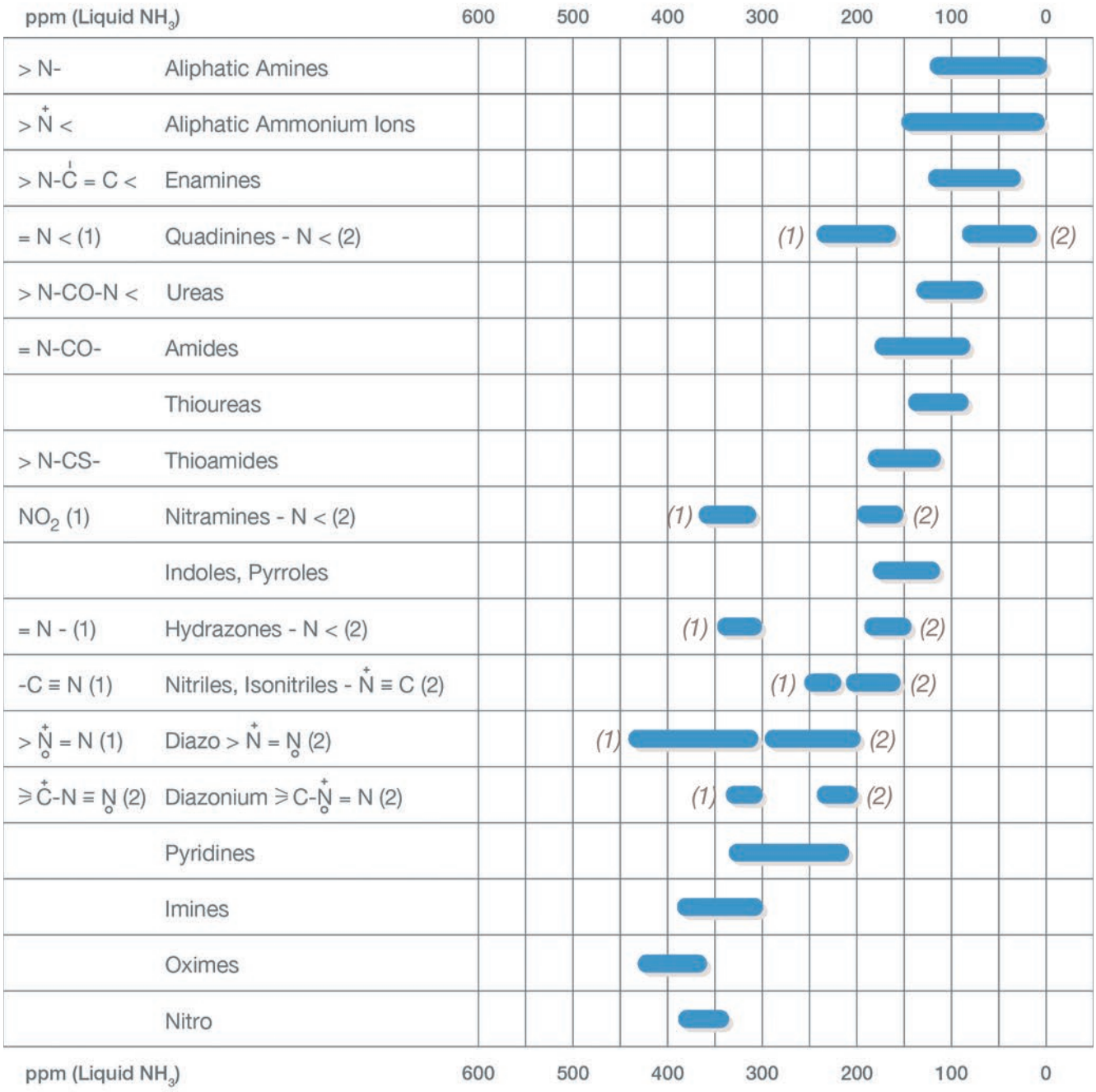
$\delta\ ^{13}C$ (ppm)



^{15}N Chemical Shifts

^{15}N Nuclear Spin : 1/2
Liquid NH_3 = 0 ppm

$\delta\ ^{15}N$ (ppm)



NMR Chemical Shifts of Trace Impurities

Common Laboratory Solvents, Organics, and Gases in Deuterated Solvents Relevant to the Organometallic Chemist

Table 1. ^{1}H NMR Data[a]

	proton	mult	THF-d_8	CD_2Cl_2	$CDCl_3$	toluene-d_8	C_6D_6	C_6D_5Cl	$(CD_3)_2CO$	$(CD_3)_2SO$	CD_3CN	TFE-d_3	CD_3OD	D_2O
solvent residual signals			1.72 3.58	5.32	7.26	2.08 6.97 7.01 7.09	7.16	6.96 6.99 7.14	2.05	2.50	1.94	5.02 3.88	3.31	4.79
water	OH	s	2.46	1.52	1.56	0.43	0.40	1.03	2.84[b]	3.33[b]	2.13	3.66	4.87	
acetic acid	CH_3	s	1.89	2.06	2.10	1.57	1.52	1.76	1.96	1.91	1.96	2.06	1.99	2.08
acetone	CH_3	s	2.05	2.12	2.17	1.57	1.55	1.77	2.09	2.09	2.08	2.19	2.15	2.22
acetonitrile	CH_3	s	1.95	1.97	2.10	0.69	0.58	1.21	2.05	2.07	1.96	1.95	2.03	2.06
benzene	CH	s	7.31	7.35	7.36	7.12	7.15	7.20	7.36	7.37	7.37	7.36	7.33	
tert -butyl alcohol	CH_3	s	1.15	1.24	1.28	1.03	1.05	1.12	1.18	1.11	1.16	1.28	1.40	1.24
	OH	s[c]	3.16			0.58	0.63	1.30		4.19	2.18	2.20		
chloroform	CH	s	7.89	7.32	7.26	6.10	6.15	6.74	8.02	8.32	7.58	7.33	7.90	
18-crown-6	CH_2	s	3.57	3.59	3.67	3.36	3.39	3.41	3.59	3.51	3.51	3.64	3.64	3.80
cyclohexane	CH_2	s	1.44	1.44	1.43	1.40	1.40	1.37	1.43	1.40	1.44	1.47	1.45	
1,2-dichloroethane	CH_2	s	3.77	3.76	3.73	2.91	2.90	3.26	3.87	3.90	3.81	3.71	3.78	
dichloromethane	CH_2	s	5.51	5.33	5.30	4.32	4.27	4.77	5.63	5.76	5.44	5.24	5.49	
diethyl ether	CH_3	t, 7	1.12	1.15	1.21	1.10	1.11	1.10	1.11	1.09	1.12	1.20	1.18	1.17
	CH_2	q, 7	3.38	3.43	3.48	3.25	3.26	3.31	3.41	3.38	3.42	3.58	3.49	3.56
diglyme	CH_2	m	3.43	3.57	3.65	3.43	3.46	3.49	3.56	3.51	3.53	3.67	3.61	3.67
	CH_2	m	3.53	3.50	3.57	3.31	3.34	3.37	3.47	3.38	3.45	3.62	3.58	3.61
	OCH_3	s	3.28	3.33	3.39	3.12	3.11	3.16	3.28	3.24	3.29	3.41	3.35	3.37
dimethylformamide	CH	s	7.91	7.96	8.02	7.57	7.63	7.73	7.96	7.95	7.92	7.86	7.97	7.92
	CH_3	s	2.88	2.91	2.96	2.37	2.36	2.51	2.94	2.89	2.89	2.98	2.99	3.01
	CH_3	s	2.76	2.82	2.88	1.96	1.86	2.30	2.78	2.73	2.77	2.88	2.86	2.85
1,4-dioxane	CH_2	s	3.56	3.65	3.71	3.33	3.35	3.45	3.59	3.57	3.60	3.76	3.66	3.75
DME	CH_3	s	3.28	3.34	3.40	3.12	3.12	3.17	3.28	3.24	3.28	3.40	3.35	3.37
	CH_2	s	3.43	3.49	3.55	3.31	3.33	3.37	3.46	3.43	3.45	3.61	3.52	3.60
ethane	CH_3	s	0.85	0.85	0.87	0.81	0.80	0.79	0.83	0.82	0.85	0.85	0.85	0.82
ethanol	CH_3	t, 7	1.10	1.19	1.25	0.97	0.96	1.06	1.12	1.06	1.12	1.22	1.19	1.17
	CH_2	q, 7[d]	3.51	3.66	3.72	3.36	3.34	3.51	3.57	3.44	3.54	3.71	3.60	3.65
	OH	s[c,d]	3.30	1.33	1.32	0.83	0.50	1.39	3.39	4.63	2.47			
ethyl acetate	CH_3CO	s	1.94	2.00	2.05	1.69	1.65	1.78	1.97	1.99	1.97	2.03	2.01	2.07
	CH_2CH_3	q, 7	4.04	4.08	4.12	3.87	3.89	3.96	4.05	4.03	4.06	4.14	4.09	4.14
	CH_2CH_3	t, 7	1.19	1.23	1.26	0.94	0.92	1.04	1.20	1.17	1.20	1.26	1.24	1.24
ethylene	CH_2	s	5.36	5.40	5.40	5.25	5.25	5.29	5.38	5.41	5.41	5.40	5.39	5.44
ethylene glycol	CH_2	s[e]	3.48	3.66	3.76	3.36	3.41	3.58	3.28	3.34	3.51	3.72	3.59	3.65
H grease[f]	CH_3	m	0.85–0.91	0.84–0.90	0.84–0.87	0.89–0.96	0.90–0.98	0.86–0.92	0.90	0.82–0.88		0.88–0.94	0.86–0.93	
	CH_2	br s	1.29	1.27	1.25	1.33	1.32	1.30	1.29	1.24		1.33	1.29	
hexamethylbenzene	CH_3	s	2.18	2.20	2.24	2.10	2.13	2.10	2.17	2.14	2.19	2.24	2.19	
n-hexane	CH_3	t, 7	0.89	0.89	0.88	0.88	0.89	0.85	0.88	0.86	0.89	0.91	0.90	
	CH_2	m	1.29	1.27	1.26	1.22	1.24	1.19	1.28	1.25	1.28	1.31	1.29	
HMDSO	CH_3	s	0.07	0.07	0.07	0.10	0.12	0.10	0.07	0.06	0.07	0.08	0.07	0.28
HMPA	CH_3	d,9.5	2.58	2.60	2.65	2.42	2.40	2.47	2.59	2.53	2.57	2.63	2.64	2.61
hydrogen	H_2	s	4.55	4.59	4.62	4.50	4.47	4.49	4.54	4.61	4.57	4.53	4.56	
imidazole	CH(2)	s	7.48	7.63	7.67	7.30	7.33	7.53	7.62	7.63	7.57	7.61	7.67	7.78
	CH(4,5)	s	6.94	7.07	7.10	6.86	6.90	7.01	7.04	7.01	7.01	7.03	7.05	7.14
methane	CH_4	s	0.19	0.21	0.22	0.17	0.16	0.15	0.17	0.20	0.20	0.18	0.20	0.18
methanol	CH_3	s[g]	3.27	3.42	3.49	3.03	3.07	3.25	3.31	3.16	3.28	3.44	3.34	3.34
	OH	s[c,g]	3.02	1.09	1.09			1.30	3.12	4.01	2.16			
nitromethane	CH_3	s	4.31	4.31	4.33	3.01	2.94	3.59	4.43	4.42	4.31	4.28	4.34	4.40
n-pentane	CH_3	t, 7	0.89	0.89	0.88	0.87	0.87	0.84	0.88	0.86	0.89	0.90	0.90	
	CH_2	m	1.31	1.30	1.27	1.25	1.23	1.23	1.27	1.27	1.29	1.33	1.29	
propane	CH_3	t, 7.3	0.90	0.90	0.90	0.89	0.86	0.84	0.88	0.87	0.90	0.90	0.91	0.88
	CH_2	sept, 7.3	1.33	1.32	1.32	1.32	1.26	1.26	1.31	1.29	1.33	1.33	1.34	1.30
2-propanol	CH_3	d, 6	1.08	1.17	1.22	0.95	0.95	1.04	1.10	1.04	1.09	1.20	1.50	1.17
	CH	sept, 6	3.82	3.97	4.04	3.65	3.67	3.82	3.90	3.78	3.87	4.05	3.92	4.02
propylene	CH_3	dt, 6.4, 1.5	1.69	1.71	1.73	1.55	1.55	1.58	1.68	1.68	1.70	1.70	1.70	1.70
	$CH_2(1)$	dm, 10	4.89	4.93	4.94	4.92	4.95	4.91	4.90	4.94	4.93	4.93	4.91	4.95
	$CH_2(2)$	dm, 17	4.99	5.03	5.03	4.98	5.01	4.98	5.00	5.03	5.04	5.03	5.01	5.06
	CH	m	5.79	5.84	5.83	5.70	5.72	5.72	5.81	5.80	5.85	5.87	5.82	5.90
pyridine	CH(2,6)	m	8.54	8.59	8.62	8.47	8.53	8.51	8.58	8.58	8.57	8.45	8.53	8.52
	CH(3,5)	m	7.25	7.28	7.29	6.67	6.66	6.90	7.35	7.39	7.33	7.40	7.44	7.45
	CH(4)	m	7.65	7.68	7.68	6.99	6.98	7.25	7.76	7.79	7.73	7.82	7.85	7.87
pyrrole	NH	br t	9.96	8.69	8.40	7.71	7.80	8.61	10.02	10.75	9.27			
	CH(2,5)	m	6.66	6.79	6.83	6.43	6.48	6.62	6.77	6.73	6.75	6.84	6.72	6.93
	CH(3,4)	m	6.02	6.19	6.26	6.27	6.37	6.27	6.07	6.01	6.10	6.24	6.08	6.26
pyrrolidine[h]	$CH_2(2,5)$	m	2.75	2.82	2.87	2.54	2.54	2.64		2.67	2.75	3.11	2.80	3.07
	$CH_2(3,4)$	m	1.59	1.67	1.68	1.36	1.33	1.43		1.55	1.61	1.93	1.72	1.87
silicone grease	CH_3	s	0.11	0.09	0.07	0.26	0.29	0.14	0.13	−0.06	0.08	0.16	0.10	
tetrahydrofuran	$CH_2(2,5)$	m	3.62	3.69	3.76	3.54	3.57	3.59	3.63	3.60	3.64	3.78	3.71	3.74
	$CH_2(3,4)$	m	1.79	1.82	1.85	1.43	1.40	1.55	1.79	1.76	1.80	1.91	1.87	1.88
toluene	CH_3	s	2.31	2.34	2.36	2.11	2.11	2.16	2.32	2.30	2.33	2.33	2.32	
	CH(2,4,6)	m	7.10	7.15	7.17	6.96–7.01	7.02	7.01–7.08	7.10–7.20	7.18	7.10–7.30	7.10–7.30	7.16	
	CH(3,5)	m	7.19	7.24	7.25	7.09	7.13	7.10–7.17	7.10–7.20	7.25	7.10–7.30	7.10–7.30	7.16	
triethylamine	CH_3	t, 7	0.97	0.99	1.03	0.95	0.96	0.93	0.96	0.93	0.96	1.31	1.05	0.99
	CH_2	q,7	2.46	2.48	2.53	2.39	2.40	2.39	2.45	2.43	2.45	3.12	2.58	2.57

[a] Except for the compounds in solutions 8–10, as well as the gas samples, hexamethylbenzene, and the corrected values mentioned in the Supporting Information, all data for the solvents $CDCl_3$, C_6D_6, $(CD_3)_2CO$, $(CD_3)_2SO$, CD_3CN, CD_3OD, and D_2O were previously reported in ref 2. [b] A signal for HDO is also observed in $(CD_3)_2SO$ (3.30 ppm) and $(CD_3)_2CO$ (2.81 ppm), often seen as a 1:1:1 triplet ($^2J_{H,D}$ = 1 Hz). [c] Not all OH signals were observable. [d] In some solvents, the coupling interaction between the CH_2 and the OH protons may be observed (J = 5 Hz). [e] In CD_3CN, the OH proton was seen as a multiplet at 2.69 ppm, as well as extra coupling to the CH_2 resonance. [f] Apiezon brand H grease. [g] In some solvents, a coupling interaction between the CH_3 and the OH protons may be observed (J = 5.5 Hz). [h] Pyrrolidine was observed to react with $(CD_3)_2CO$.

Table 2. $^{13}C\{^1H\}$ NMR Data[a]

	carbon	THF-d_8	CD_2Cl_2	$CDCl_3$	toluene-d_8	C_6D_6	C_6D_5Cl	$(CD_3)_2CO$	$(CD_3)_2SO$	CD_3CN	TFE-d_3	CD_3OD	D_2O
solvent signals		67.21 25.31	53.84	77.16	137.48 128.87 127.96 125.13 20.43	128.06	134.19 129.26 128.25 125.96	29.84 206.26	39.52	1.32 118.26	61.50 126.28	49.00	
acetic acid	CO	171.69	175.85	175.99	175.30	175.82	175.67	172.31	171.93	173.21	177.96	175.11	177.21
	CH_3	20.13	20.91	20.81	20.27	20.37	20.40	20.51	20.95	20.73	20.91	20.56	21.03
acetone	CO	204.19	206.78	207.07	204.00	204.43	204.83	205.87	206.31	207.43	32.35	209.67	215.94
	CH_3	30.17	31.00	30.92	30.03	30.14	30.12	30.60	30.56	30.91	214.98	30.67	30.89
acetonitrile	CN	116.79	116.92	116.43	115.76	116.02	115.93	117.60	117.91	118.26	118.95	118.06	119.68
	CH_3	0.45	2.03	1.89	0.03	0.20	0.63	1.12	1.03	1.79	1.00	0.85	1.47
benzene	CH	128.84	128.68	128.37	128.57	128.62	128.38	129.15	128.30	129.32	129.84	129.34	
tert -butyl alcohol	$(CH_3)_3C$	67.50	69.11	69.15	68.12	68.19	68.19	68.13	66.88	68.74	72.35	69.40	70.36
	$(CH_3)_3C$	30.57	31.46	31.25	30.49	30.47	31.13	30.72	30.38	30.68	31.07	30.91	30.29
carbon dioxide	CO_2	125.69	125.26	124.99	124.86	124.76	126.08	125.81	124.21	125.89	126.92	126.31	
carbon disulfide	CS_2	193.37	192.95	192.83	192.71	192.69	192.49	193.58	192.63	193.60	196.26	193.82	197.25
carbon tetrachloride	CCl_4	96.89	96.52	96.34	96.57	96.44	96.38	96.65	95.44	96.68	97.74	97.21	96.73
chloroform	CH	79.24	77.99	77.36	77.89	77.79	77.67	79.19	79.16	79.17	78.83	79.44	
18-crown-6	CH_2	71.34	70.47	70.55	70.86	70.59	70.55	71.25	69.85	71.22	70.80	71.47	70.14
cyclohexane	CH_2	27.58	27.38	26.94	27.31	27.23	26.99	27.51	26.33	27.63	28.34	27.96	
1,2-dichloroethane	CH_2	44.64	44.35	43.50	43.40	43.59	43.60	45.25	45.02	45.54	45.28	45.11	
dichloromethane	CH_2	54.67	54.24	53.52	53.47	53.46	53.54	54.95	54.84	55.32	54.46	54.78	
diethyl ether	CH_3	15.49	15.44	15.20	15.47	15.46	15.35	15.78	15.12	15.63	15.33	15.46	14.77
	CH_2	66.14	66.11	65.91	65.94	65.94	65.79	66.12	62.05	66.32	67.55	66.88	66.42
diglyme	CH_3	58.72	58.95	59.01	58.62	58.66	58.42	58.77	57.98	58.90	59.40	59.06	58.67
	CH_2	71.17	70.70	70.51	70.92	70.87	70.56	71.03	69.54	70.99	73.05	71.33	70.05
	CH_2	72.72	72.25	71.90	72.39	72.35	72.07	72.63	71.25	72.63	71.33	72.92	71.63
dimethylformamide	CH	161.96	162.57	162.62	161.93	162.13	162.01	162.79	162.29	163.31	166.01	164.73	165.53
	CH_3	35.65	36.56	36.50	35.22	35.25	35.45	36.15	35.73	36.57	37.76	36.89	37.54
	CH_3	30.70	31.39	31.45	30.64	30.72	30.71	31.03	30.73	31.32	30.96	31.61	32.03
1,4-dioxane	CH_2	67.65	67.47	67.14	67.17	67.16	66.95	67.60	66.36	67.72	68.52	68.11	67.19
DME	CH_3	58.72	59.02	59.08	58.63	58.68	58.31	58.45	58.03	58.89	59.52	59.06	58.67
	CH_2	72.58	72.24	71.84	72.25	72.21	71.81	72.47	71.17	72.47	72.87	72.72	71.49
ethane	CH_3	6.79	6.91	6.89	6.94	6.96	6.91	6.88	6.61	6.99	7.01	6.98	
ethanol	CH_3	18.90	18.69	18.41	18.78	18.72	18.55	18.89	18.51	18.80	18.11	18.40	17.47
	CH_2	57.60	58.57	58.28	57.81	57.86	57.63	57.72	56.07	57.96	59.68	58.26	58.05
ethyl acetate	CH_3CO	20.45	21.15	21.04	20.46	20.56	20.50	20.83	20.68	21.16	21.18	20.88	21.15
	CO	170.32	171.24	171.36	170.02	170.44	170.20	170.96	170.31	171.68	175.55	172.89	175.26
	CH_2	60.30	60.63	60.49	60.08	60.21	60.06	60.56	59.74	60.98	62.70	61.50	62.32
	CH_3	14.37	14.37	14.19	14.23	14.19	14.07	14.50	14.40	14.54	14.36	14.49	13.92
ethylene	CH_2	123.09	123.20	123.13	122.92	122.96	122.95	123.47	123.52	123.69	124.08	123.46	
ethylene glycol	CH_2	64.35	64.08	63.79	64.29	64.34	64.03	64.26	62.76	64.22	64.87	64.30	63.17
H grease[b]	CH_2	30.45	30.14	29.71	30.31	30.22	30.11						
hexamethylbenzene	C	131.88	132.09	132.21	131.72	131.79	131.54	132.22	131.10	132.61	134.04	132.53	
	CH_3	16.71	16.93	16.98	16.84	16.95	16.68	16.86	16.60	16.94	17.04	16.90	
n-hexane	CH_3	14.22	14.28	14.14	14.34	14.32	14.18	14.34	13.88	14.43	14.63	14.45	
	CH_2(2,5)	23.33	23.07	22.70	23.12	23.04	22.86	23.28	22.05	23.40	24.06	23.68	
	CH_2(3,4)	32.34	32.01	31.64	32.06	31.96	31.77	32.30	30.95	32.36	33.17	32.73	
HMDSO	CH_3	1.83	1.96	1.97	1.99	2.05	1.92	2.01	1.96	2.07	2.09	1.99	2.31
HMPA[c]	CH_3	36.89	36.99	36.87	36.80	36.88	36.64	37.04	36.42	37.10	37.21	37.00	36.46
imidazole	CH(2)	135.72	135.76	135.38	135.57	135.76	135.50	135.89	135.15	136.33	136.58	136.31	136.65
	CH(4,5)	122.20	122.16	122.00	122.13	122.16	121.96	122.31	121.55	122.78	122.93	122.60	122.43
methane	CH_4	−4.90	−4.33	−4.63	−4.34	−4.29	−4.33	−5.33	−4.01	−4.61	−5.88	−4.90	
methanol	CH_3	49.64	50.45	50.41	49.90	49.97	49.66	49.77	48.59	49.90	50.67	49.86	49.50[d]
nitromethane	CH_3	62.49	63.03	62.50	61.14	61.16	61.68	63.21	63.28	63.66	63.17	63.08	63.22
n-pentane	CH_3	14.18	14.24	14.08	14.27	14.25	14.10	14.29	13.28	14.37	14.54	14.39	
	CH_2(2,4)	23.00	22.77	22.38	22.79	22.72	22.54	22.98	21.70	23.08	23.75	23.38	
	CH_2(3)	34.87	34.57	34.16	34.54	34.45	34.26	34.83	33.48	34.89	35.76	35.30	
propane	CH_3	16.60	16.63	16.63	16.65	16.66	16.56	16.68	16.34	16.73	16.93	16.80	
	CH_2	16.82	16.63	16.37	16.63	16.60	16.48	16.78	15.67	16.91	17.46	17.19	
2-propanol	CH_3	25.70	25.43	25.14	25.24	25.18	25.14	25.67	25.43	25.55	25.21	25.27	24.38
	CH	66.14	64.67	64.50	64.12	64.23	64.18	63.85	64.92	64.30	66.69	64.71	64.88
propylene	CH_3	19.27	19.47	19.50	19.32	19.38	19.32	19.42	19.20	19.48	19.63	19.50	
	CH_2	115.74	115.70	115.74	115.89	115.92	115.86	116.03	116.07	116.12	116.38	116.04	
	CH	134.02	134.21	133.91	133.61	133.69	133.57	134.34	133.55	134.78	136.00	134.61	
pyridine	CH(2,6)	150.57	150.27	149.90	150.25	150.27	149.93	150.67	149.58	150.76	149.76	150.07	149.18
	CH(3,5)	124.08	124.06	123.75	123.46	123.58	123.49	124.57	123.84	127.76	126.27	125.53	125.12
	CH(4)	135.99	136.16	135.96	135.17	135.28	135.32	136.56	136.05	136.89	139.62	138.35	138.27
pyrrole	CH(2,5)	118.03	117.93	117.77	117.61	117.78	117.65	117.98	117.32	118.47	119.61	118.28	119.06
	CH(3,4)	107.74	108.02	107.98	108.15	108.21	108.03	108.04	107.07	108.31	108.85	108.11	107.83
pyrrolidine[e]	CH_2(2,5)	45.82	47.02	46.93	47.12	46.86	46.75		46.51	47.57	47.43	47.23	46.83
	CH_2(3,4)	26.17	25.83	25.56	25.75	25.65	25.59		25.26	26.34	25.73	26.29	25.86
silicone grease	CH_3	1.20	1.22	1.19	1.37	1.38	1.09	1.40			2.87	2.10	
tetrahydrofuran	CH_2(2,5)	68.03	68.16	67.97	67.75	67.80	67.64	68.07	67.03	68.33	69.53	68.83	68.68
	CH_2(3,4)	26.19	25.98	25.62	25.79	25.72	25.68	26.15	25.14	26.27	26.69	26.48	25.67
toluene	CH_3	21.29	21.53	21.46	21.37	21.10	21.23	21.46	20.99	21.50	21.62	21.50	
	C(1)	138.24	138.36	137.89	137.84	137.91	137.65	138.48	137.35	138.90	139.92	138.85	
	CH(2,6)	129.47	129.35	129.07	129.33	129.33	129.12	129.76	128.88	129.94	130.58	129.91	
	CH(3,5)	128.71	128.54	128.26	128.51	128.56	128.31	129.03	128.18	129.23	129.79	129.20	
	CH(4)	125.84	125.62	125.33	125.66	125.68	125.43	126.12	125.29	126.28	126.82	126.29	
triethylamine	CH_3	12.51	12.12	11.61	12.39	12.35	11.87	12.49	11.74	12.38	9.51	11.09	9.07
	CH_2	47.18	46.75	46.25	46.82	46.77	46.36	47.07	45.74	47.10	48.45	46.96	47.19

[a] Except for the compounds in solutions 8−10, as well as the gas samples, hexamethylbenzene, and the corrected values mentioned in the Supporting Information, all data for the solvents $CDCl_3$, C_6D_6, $(CD_3)_2CO$, $(CD_3)_2SO$, CD_3CN, CD_3OD, and D_2O were previously reported in ref 2. [b] Apiezon brand H grease. [c] Phosphorus coupling was observed ($^2J_{PC}$ = 3 Hz). [d] Internal reference; see text. [e] Pyrrolidine was observed to react with $(CD_3)_2CO$.

NMR Tubes from Norell®

Norell® Tubes for NMR

Eurisotop has partnered with Norell® for many years, offering the best possible Pyrex® and quartz precision tubes, as well as glass tubes and other accessories.

Secure 55 Series™ (5mm) and High Throughput NMR Tubes

The Secure 55 Series™ NMR tubes are made from ASTM Type I Class B borosilicate glass ("high expansion" borosilicate glass) and parallel the properties of the Standard Series™ NMR tubes from Norell. These tubes are ideal for near room temperature analyses of routine samples exposed to slight thermal gradients.

Reference	Spinner Turbine	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
S55-1000-050-1780	Bruker	1000	5	4.97 ± 0.004	4.20 ± 0.006	0,003	0,004	178
S55-1000-050-2030	Agilent/Varian	1000	5	4.97 ± 0.004	4.20 ± 0.006	0,003	0,004	203
S55-0800-050-1780	Bruker	800	5	4.97 ± 0.005	4.20 ± 0.012	0,004	0,005	178
S55-0800-050-2030	Agilent/Varian	800	5	4.97 ± 0.005	4.20 ± 0.012	0,004	0,005	203
S55-0600-050-1780	Bruker	600	5	4.97 ± 0.006	4.20 ± 0.012	0,004	0,006	178
S55-0600-050-2030	Agilent/Varian	600	5	4.97 ± 0.006	4.20 ± 0.012	0,004	0,006	203
S55-0500-050-1780	Bruker	500	5	4.97 ± 0.013	4.20 ± 0.025	0,005	0,013	178
S55-0500-050-2030	Agilent/Varian	500	5	4.97 ± 0.013	4.20 ± 0.025	0,005	0,013	203
S55-0400-050-1780	Bruker	400	5	4.97 ± 0.013	4.20 ± 0.025	0,007	0,019	178
S55-0400-050-2030	Agilent/Varian	400	5	4.97 ± 0.013	4.20 ± 0.025	0,007	0,019	203
S55-0HTP-050-1780	Bruker	HTPLUS	50	4.97 ± 0.050	4.20 ± 0.050	0,02	0,07	178
S55-0HTP-050-2030	Agilent/Varian	HTPLUS	50	4.97 ± 0.050	4.20 ± 0.050	0,02	0,07	203
S55-00HT-050-1780	Bruker	HT	100	4.97 ± 0.050	4.20 ± 0.050	0,02	0,07	178
S55-00HT-050-2030	Agilent/Varian	HT	100	4.97 ± 0.050	4.20 ± 0.050	0,02	0,07	203

Secure 33 Series™ NMR Tubes

The Secure 33 Series™ NMR tubes are made from ASTM Type I Class A borosilicate glass ("low expansion" borosilicate glass such as Corning Pyrex® 7740) and match the properties of the Select Series™ NMR tubes from Norell. Because of the low coeficient of thermal expansion, Secure 33 Series™ NMR tubes show a high degree of thermal shock resistance, a necessary attribute to prevent breakage when large temperature variations are expected in variable temperature studies, degassing samples through freeze-pump-thaw cycles, etc

5mm / Reference	Spinner Turbine	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
S33-1000-050-1780	Bruker	1000	5	4.97 ± 0.003	4.20 ± 0.006	0,0018	0,0027	178
S33-1000-050-2030	Agilent/Varian	1000	5	4.97 ± 0.003	4.20 ± 0.006	0,0018	0,0027	203
S33-0900-050-1780	Bruker	900	5	4.97 ± 0.004	4.20 ± 0.006	0,002	0,003	178
S33-0900-050-2030	Agilent/Varian	900	5	4.97 ± 0.004	4.20 ± 0.006	0,002	0,003	203
S33-0800-050-1780	Bruker	800	5	4.97 ± 0.005	4.20 ± 0.012	0,0025	0,0038	178
S33-0800-050-2030	Agilent/Varian	800	5	4.97 ± 0.005	4.20 ± 0.012	0,0025	0,0038	203
S33-0600-050-1780	Bruker	600	5	4.97 ± 0.006	4.20 ± 0.012	0,004	0,006	178
S33-0600-050-2030	Agilent/Varian	600	5	4.97 ± 0.006	4.20 ± 0.012	0,004	0,006	203
S33-0500-050-1780	Bruker	500	5	4.97 ± 0.013	4.20 ± 0.025	0,005	0,013	178
S33-0500-050-2030	Agilent/Varian	500	5	4.97 ± 0.013	4.20 ± 0.025	0,005	0,013	203
S33-0400-050-1780	Bruker	400	5	4.97 ± 0.013	4.20 ± 0.025	0,007	0,019	178
S33-0400-050-2030	Agilent/Varian	400	5	4.97 ± 0.013	4.20 ± 0.025	0,007	0,019	203

3mm / Reference	Spinner Turbine	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
S33-1000-030-1780	Bruker	1000	5	2.99 ± 0.003	2.41 ± 0.006	0,0018	0,0027	178
S33-1000-030-2030	Agilent/Varian	1000	5	2.99 ± 0.003	2.41 ± 0.006	0,0018	0,0027	203
S33-0900-030-1780	Bruker	900	5	2.99 ± 0.004	2.41 ± 0.006	0,002	0,003	178
S33-0900-030-2030	Agilent/Varian	900	5	2.99 ± 0.004	2.41 ± 0.006	0,002	0,003	203
S33-0800-030-1780	Bruker	800	5	2.99 ± 0.005	2.41 ± 0.010	0,0025	0,0038	178
S33-0800-030-2030	Agilent/Varian	800	5	2.99 ± 0.005	2.41 ± 0.010	0,0025	0,0038	203
S33-0600-030-1780	Bruker	600	5	2.99 ± 0.006	2.41 ± 0.012	0,004	0,006	178
S33-0600-030-2030	Agilent/Varian	600	5	2.99 ± 0.006	2.41 ± 0.012	0,004	0,006	203
S33-0500-030-1780	Bruker	500	5	2.99 ± 0.010	2.41 ± 0.015	0,005	0,013	178
S33-0500-030-2030	Agilent/Varian	500	5	2.99 ± 0.010	2.41 ± 0.015	0,005	0,013	203
S33-0400-030-1780	Bruker	400	5	2.99 ± 0.013	2.41 ± 0.020	0,007	0,019	178
S33-0400-030-2030	Agilent/Varian	400	5	2.99 ± 0.013	2.41 ± 0.020	0,007	0,019	203

Norell® Select Series™

Manufactured from ASTM Type 1 Class A Glass, Commonly Referred to as Pyrex®

Norell ® "Select Series" NMR tubes are manufactured out of ASTM Type 1 Class A glass, commonly referred to as Pyrex® 7740 (Corning), Duran® (Schott Glass), or Kimax® KG-33 (Kimble) glass. Key properties that make this glass type desirable for NMR are its high degree of thermal shock resistance and low expansion coefficient. This allows for a greater margin of safety from breakage when used in variable temperature applications and freeze/thaw cycling, or under any other application where large temperature variations are required in the experiment. Each NMR tube is checked for concentricity and camber

- Engineered for a new generation of high-throughput lab automation systems.
- Superior NorLoc™ cap (U.S. Patent No. 8,054,080) attaches semi-permanently for multiple use and for critical applications.
- Safe for cold refrigeration storage, works with cryo-probes and variable temperature studies.

Select Series (10mm)

Reference	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
S-10-600-7	600	5	10.00 ± 0.006	8.76 ± 0.012	0,004	0,006	178
S-10-600-8	600	5	10.00 ± 0.006	8.76 ± 0.012	0,004	0,006	203
S-10-500-7	500	5	10.00 ± 0.013	8.76 ± 0.025	0,005	0,007	178
S-10-500-8	500	5	10.00 ± 0.013	8.76 ± 0.025	0,005	0,007	203

Select Series (5mm)

Reference	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
S-5-1000-7	1000	5	4.97 ± 0.003	4.20 ± 0.006	0,0018	0,0027	178
S-5-1000-8	1000	5	4.97 ± 0.003	4.20 ± 0.006	0,0018	0,0027	203
S-5-900-7	900	5	4.97 ± 0.004	4.20 ± 0.006	0,002	0,003	178
S-5-900-8	900	5	4.97 ± 0.004	4.20 ± 0.006	0,002	0,003	203
S-5-800-7	800	5	4.97 ± 0.005	4.20 ± 0.012	0,0025	0,0038	178
S-5-800-8	800	5	4.97 ± 0.005	4.20 ± 0.012	0,0025	0,0038	203
S-5-600-7	600	5	4.97 ± 0.006	4.20 ± 0.012	0,004	0,006	178
S-5-600-8	600	5	4.97 ± 0.006	4.20 ± 0.012	0,004	0,006	203
S-5-500-7	500	5	4.97 ± 0.013	4.20 ± 0.025	0,005	0,013	178
S-5-500-8	500	5	4.97 ± 0.013	4.20 ± 0.025	0,005	0,013	203
S-5-400-7	400	5	4.97 ± 0.013	4.20 ± 0.025	0,007	0,019	178
S-5-400-8	400	5	4.97 ± 0.013	4.20 ± 0.025	0,007	0,019	203

Select Series (3mm)

Reference	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
S-3-1000-7	1000	5	2.99 ± 0.003	2.41 ± 0.006	0,0018	0,0027	178
S-3-1000-8	1000	5	2.99 ± 0.003	2.41 ± 0.006	0,0018	0,0027	203
S-3-900-7	900	5	2.99 ± 0.004	2.41 ± 0.006	0,002	0,003	178
S-3-900-8	900	5	2.99 ± 0.004	2.41 ± 0.006	0,002	0,003	203
S-3-800-7	800	5	2.99 ± 0.005	2.41 ± 0.010	0,0025	0,0038	178
S-3-800-8	800	5	2.99 ± 0.005	2.41 ± 0.010	0,0025	0,0038	203
S-3-600-7	600	5	2.99 ± 0.006	2.41 ± 0.012	0,004	0,006	178
S-3-600-8	600	5	2.99 ± 0.006	2.41 ± 0.012	0,004	0,006	203
S-3-500-7	500	5	2.99 ± 0.010	2.41 ± 0.015	0,005	0,013	178
S-3-500-8	500	5	2.99 ± 0.010	2.41 ± 0.015	0,005	0,013	203
S-3-400-7	400	5	2.99 ± 0.013	2.41 ± 0.020	0,007	0,019	178
S-3-400-8	400	5	2.99 ± 0.013	2.41 ± 0.020	0,007	0,019	203
S-3-HT-7	HT	25	2.99 ± 0.030	2.41 ± 0.030	0,011	0,04	178
S-3-HT-8	HT	25	2.99 ± 0.030	2.41 ± 0.030	0,011	0,04	203

Norell® Standard Series™

Manufactured from ASTM Type 1 Class B Glass, Commonly Referred to as N-51A

Norell® "Standard Series" NMR tubes are manufactured out of ASTM Type 1 Class B glass, commonly referred to as N-51A. Applications that are suited for using this type of glass are routine NMR where samples are run under room temperatures with no thermal gradients. It is therefore not recommended to fuse this glass with standard vacuum manifolds and the like, since these are generally made out of Type 1 Class A glass. Each NMR tube is checked for concentricity and camber specifications.

Through our advanced manufacturing process, the NMR tube bottoms are uniformly hemispherical and consistent, thereby minimizing shimming and susceptibility differences among samples. This uniformity extends throughout the wall thickness of the tubes, maximizing the concentricity among tubes and lots. This translates to more consistent placement of the contained sample volumes in today's advanced, highly homogeneous, high field NMR magnets. NMR tubes are manufactured with round bottoms and are available with flat bottoms upon request.

Standard Series Ultra Precision (5mm)

Reference	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
5020-USP-7	1000	5	4.97 ± 0.004	4.20 ± 0.006	0,003	0,004	178
5020-USP-8	1000	5	4.97 ± 0.004	4.20 ± 0.006	0,003	0,004	203
5010-USP-7	750	5	4.97 ± 0.005	4.20 ± 0.012	0,004	0,005	178
5010-USP-8	750	5	4.97 ± 0.005	4.20 ± 0.012	0,004	0,005	203
509-UP-7	600	5	4.97 ± 0.006	4.20 ± 0.012	0,004	0,006	178
509-UP-8	600	5	4.97 ± 0.006	4.20 ± 0.012	0,004	0,006	203
508-UP-7	500	5	4.97 ± 0.013	4.20 ± 0.025	0,005	0,013	178
508-UP-8	500	5	4.97 ± 0.013	4.20 ± 0.025	0,005	0,013	203
507-HP-7	400	5	4.97 ± 0.013	4.20 ± 0.025	0,007	0,019	178
507-HP-8	400	5	4.97 ± 0.013	4.20 ± 0.025	0,007	0,019	203
506-P-7	300	25	4.97 ± 0.025	4.20 ± 0.025	0,007	0,025	178
506-P-8	300	25	4.97 ± 0.025	4.20 ± 0.025	0,007	0,025	203
XR-55-7	300	25	4.97 ± 0.025	4.20 ± 0.025	0,01	0,038	178
XR-55-8	300	25	4.97 ± 0.025	4.20 ± 0.025	0,01	0,038	203
505-P-7	200	25	4.97 ± 0.030	4.20 ± 0.030	0,01	0,04	178
505-P-8	200	25	4.97 ± 0.030	4.20 ± 0.030	0,01	0,04	203

Standard Series Economy (5mm)

Reference	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
502-7	HTPLUS	50	4.97 ± 0.050	4.20 ± 0.050	0,02	0,07	178
502-8	HTPLUS	50	4.97 ± 0.050	4.20 ± 0.050	0,02	0,07	203
552-7	HTPLUS	5	4.97 ± 0.050	4.20 ± 0.050	0,02	0,07	178
552-8	HTPLUS	5	4.97 ± 0.050	4.20 ± 0.050	0,02	0,07	203
ST500-7	HT	100	4.97 ± 0.070	4.20 ± 0.070	0,025	0,075	178
ST500-8	HT	100	4.97 ± 0.070	4.20 ± 0.070	0,025	0,075	203
ST550-7	HT	5	4.97 ± 0.070	4.20 ± 0.070	0,025	0,075	178
ST550-8	HT	5	4.97 ± 0.070	4.20 ± 0.070	0,025	0,075	203

Standard Series Ultra Precision (10mm)

Reference	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
1008-UP-7	400	5	10.00 ± 0.013	8.76 ± 0.025	0,005	0,07	178
1008-UP-8	400	5	10.00 ± 0.013	8.76 ± 0.025	0,005	0,07	203
1005-P-7	300	5	10.00 ± 0.013	8.76 ± 0.025	0,02	0,013	178
1005-P-8	300	5	10.00 ± 0.013	8.76 ± 0.025	0,02	0,013	203

Standard Series Ultra Economy (10mm)

Reference	MHz	Packs of	O.D. (mm)	I.D. (mm)	Concentricity (mm)	Camber ±(mm)	Length (mm)
1001-7	200	100	10.00 ± 0.013	8.76 ± 0.025	nominal	nominal	178
1001-8	200	100	10.00 ± 0.013	8.76 ± 0.025	nominal	nominal	203

qNMR

Standards for qNMR

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

External Calibration Standards

We are pleased to offer external calibration standards for qNMR. The standards are formulated using Euriso-Top's high-quality DMSO-d and benzoic acid from NIST (SRM 350(b)), a standard reference material for acidometry. Both 5 mM and 15 mM benzoic acid concentrations are available. The concentration and associated expanded uncertainty of the benzoic acid has been accurately determined using metrological techniques and verified using qNMR. The 1H-NMR spectrum of benzoic acid in 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.

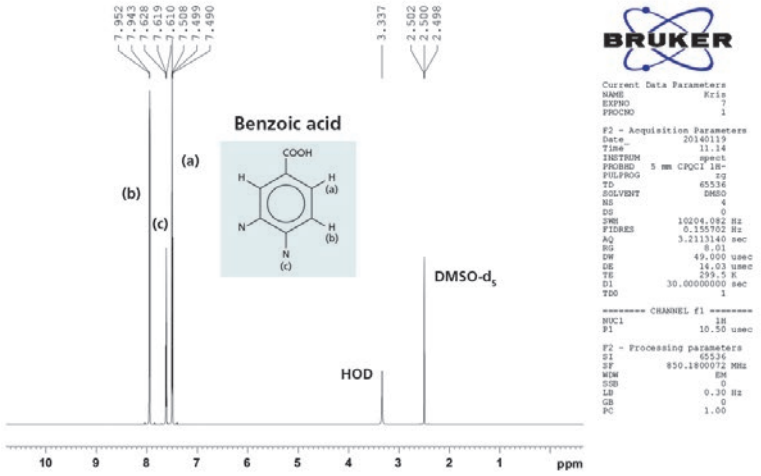


Figure 1. 850 MHz 1H-NMR spectrum of benzoic acid in DMSO-d6. Resonances from the aromatic protons of benzoic acid, HOD and DMSO-d5 are assigned. The acid proton resonance from benzoic acid (~12-13 ppm) is not shown. (Courtesy Joe Ray, Baxter Healthcare Corporation, Round Lake, IL)

qNMR Standard for External Referencing

Reference	Description*	NMR Tube**	Fill Volume
DLM-9491A	5 mM Benzoic acid in DMSO-d6	1 .7 mm O .D .	50 µL
DLM-9491B	5 mM Benzoic acid in DMSO-d6	3 mm O .D .	160 µL
DLM-9491C	5 mM Benzoic acid in DMSO-d6	5 mm O .D .	750 µL
DLM-7061A	15 mM Benzoic acid in DMSO-d6	1 .7 mm O .D .	50 µL
DLM-7061B	15 mM Benzoic acid in DMSO-d6	3 mm O .D .	160 µL
DLM-7061C	15 mM Benzoic acid in DMSO-d6	5 mm O .D .	750 µL

* The benzoic acid concentration and associated uncertainty are reported.
** All tubes are flame-sealed to ensure longevity.

Standards for qNMR

Internal Calibration Standards

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

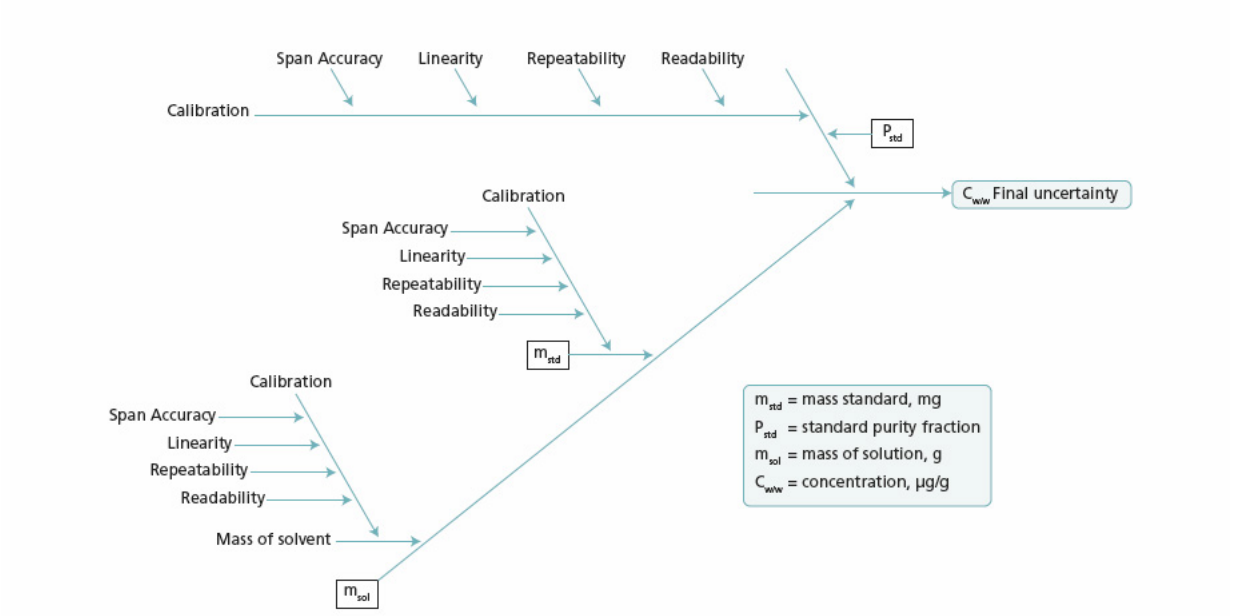
We are pleased to offer a ready-to-use DMSO-d6 solution containing a known amount of benzoic acid for internal referencing. Because this solution is preformulated, the user does not need to weigh a standard material. The elimination of this step will reduce effort and time in sample preparation and also may bring about more accurate results than if the user performs this formulation. To use this product, the sample must be soluble in DMSO-d6, 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-d5 (2.5 ppm). The benzoic acid concentration with associated uncertainty is presented on the certificate of analysis.

qNMR Standard for Internal Referencing

Reference	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.

Formulation Procedure

The procedure that CIL uses to formulate qNMR external calibration reference standard bulk solutions allows for the expanded uncertainty of the concentration of the calibration standard (e.g., benzoic acid) to be determined. Traceability to SI is maintained through the use of weight sets with calibration traceable to NIST and laboratory balances with NIST-traceable calibration certificates, maintaining an unbroken chain of calibration to the kilogram. The factors contributing to the uncertainty of the benzoic acid concentration1 is shown in below.



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

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

Synthesis

Cambridge Isotope Laboratories Inc. offers over 15,000 stable isotope-labeled products for your synthetic applications, including the manufacturing of APIs. Many labeling patterns are available for common starting materials. For more than 35 years, CIL has offered :

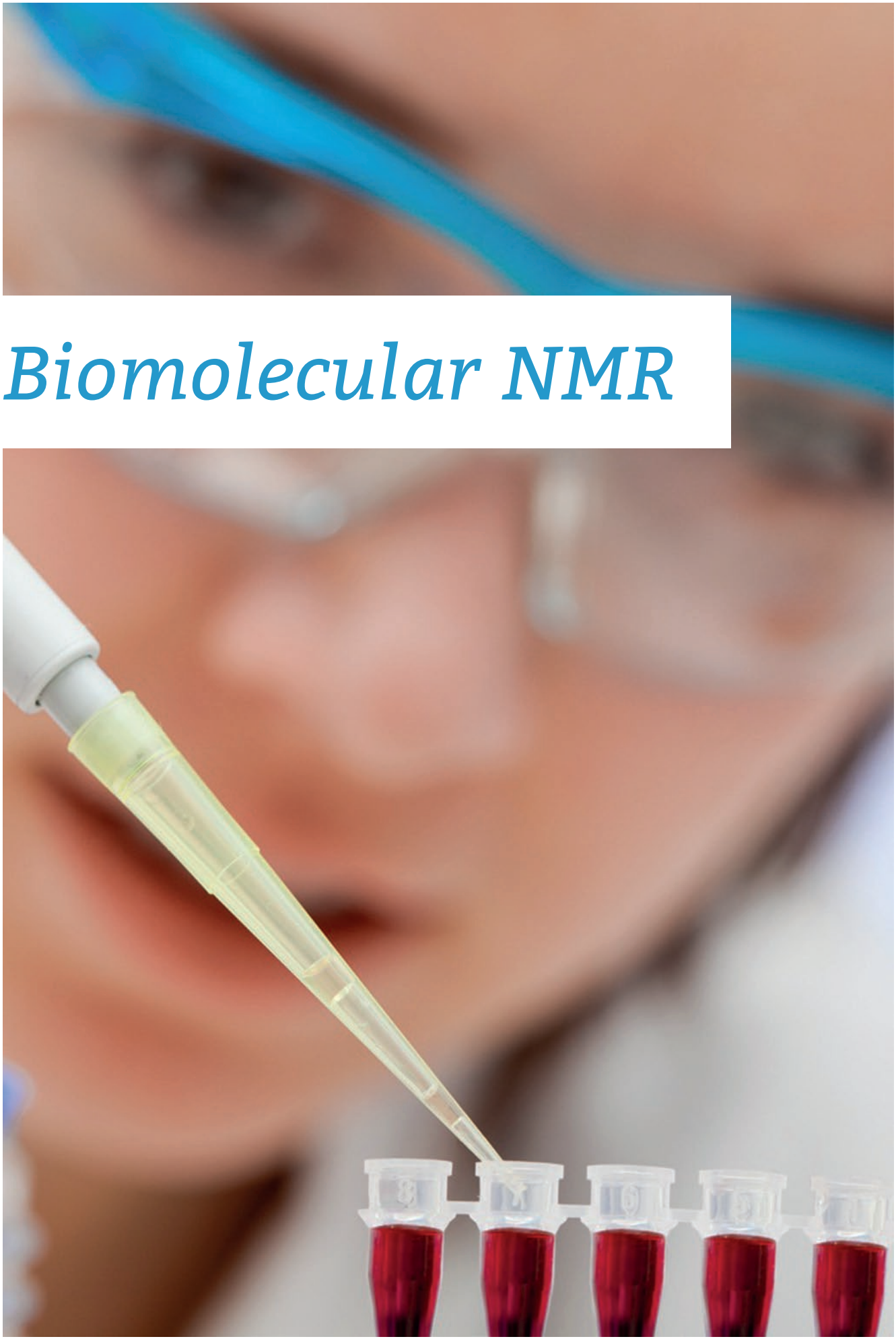
• Expertise and quality service from initial quote request through delivery
• Flexibility of scale for custom and catalog products from milligram to multi-kilogram quantities
• cGMP suite for manufacturing clinical trial grade materials (CTM)

Reference	Description
CLM-173	Acetaldehyde (1,2-$^{13}C_2$, 99%)
DLM-112	Acetaldehyde-d_4 (D, 99%)
CLM-2483	Acetanilide (ring-$^{13}C_6$, 99%)
CLM-105	Acetic acid (1,2-$^{12}C_2$, 99.95%)
D012*	Acetic acid-d_4
DLM-1556	Acetic acid-d (D, 98%)
CLM-1160	Acetic anhydride (2,2'-$^{13}C_2$, 99%)
CLM-1161	Acetic anhydride (1,1',2,2'-$^{13}C_4$, 99%)
DLM-1162	Acetic anhydride-d_6 (D, 98%)
CLM-1334	Acetone ($^{13}C_3$, 99%)
CLM-1306	Acetone (1,3-$^{13}C_2$, 99%)
CLM-245	Acetone (2-^{13}C, 99%)
D009*	Acetone-d_6
CLM-1242	Acetonitrile (1,2-$^{13}C_2$, 99%)
CLM-1260	Acetonitrile (1-^{13}C, 99%)
CLM-1588	Acetonitrile (2-^{13}C, 99%)
NLM-175	Acetonitrile (^{15}N, 98%+)
CDLM-6208	Acetyl chloride ($^{13}C_2$, 99%; D_3, 98%)
CLM-246	Acetyl chloride (1-^{13}C, 99%)
CLM-703	Acetyl chloride (2-^{13}C, 99%)
CLM-704	Acetyl chloride (1,2-$^{13}C_2$, 99%)
DLM-247	Acetyl chloride-d_3 (D, 98%)
DLM-855	Acrylic-2,3,3-d_3 acid (D, 98%) (+ 0.1% 4-methoxyphenol) <5% H_2O
NLM-177	Ammonium acetate (^{15}N, 98%+)
NLM-1320	Ammonium hydroxide (^{15}N, 98%+) 3.3 N in H_2O
NLM-3929	Ammonium hydroxide (^{15}N, 98%+) 6 N in H_2O
CLM-714	Aniline ($^{13}C_6$, 99%)
CNLM-4805	Aniline ($^{13}C_6$, 98%+;^{15}N, 98%+)
DLM-862	Aniline-ring-d_5 (D, 98%)
NLM-1314	Aniline (^{15}N, 98%+)
CLM-1337	Anisole (ring-$^{13}C_6$, 99%)
CLM-466	Barium carbonate (^{13}C, 98%+)
CLM-180	Benzaldehyde (ring-$^{13}C_6$, 99%) + 0.1% hydroquinone
CLM-182	Benzene ($^{13}C_6$, 99%)
D001*	Benzene-d_6
CLM-1813	Benzoic acid (ring-$^{13}C_6$, 99%)
CLM-657	Benzoic acid (carboxyl-^{13}C, 99%)
CLM-2298	Benzyl alcohol (ring-$^{13}C_6$, 99%)

* Different grades are available with varying specifications. Please inquire for details.

Reference	Description
DLM-494	Biphenyl-d_{10} (D, 98%)
DLM-1945	Bis(2-Chloroethoxy)-d8 methane (D, 98%)
DLM-1315	Borane-d3 (D, 98%) (1 molar in THF) + 0.005M $NaBD_4$
DLM-4747	Borane-d3 methylsulfide complex (D, 99%)
CLM-1339	Bromoacetic acid (1,2-$^{13}C_2$, 99%)
CLM-723	Bromoacetic acid (1-^{13}C, 99%)
CLM-724	Bromoacetic acid (2-^{13}C, 99%)
CLM-871	Bromobenzene ($^{13}C_6$, 99%)
DLM-398	Bromobenzene-d_5 (D, 99%)
DLM-874	Bromoethane-d_5 (D, 98%)
DLM-181	1,4-Butanediol-2,2,3,3-d4 (D, 98%)
DLM-1664	t-Butanol-d_{10} (D, 98%)
DM-1116	t-Butyl chloride-d_9 (D, 98%)
CLM-730	Carbon disulfide (^{13}C, 97-99%)
CLM-185*	Carbon dioxide (^{13}C)
CLM-189*	Carbon monoxide (^{13}C)
HPG-040	Carbon monoxide (high purity) CP 99.99%
HPG-045	Carbon monoxide (high purity) CP 99.995%
CLM-1829	Chlorobenzene ($^{13}C_6$, 99%)
DLM-263	Chlorobenzene-d_5 (D, 99%)
D007*	Chloroform-d
DLM-337	Chloromethane-d_3 (D, 99%)
CNLM-7289	Cyanamide (^{13}C, 99%; $^{15}N_2$, 98%) stabilized with < 0.1% acetic acid
DLM-1560	Cyclohexanone-d_{10} (D, 98%)
DLM-2781	Cyclopentyl bromide-d_9 (D, 98%)
DLM-1003*	Deuterium (D, 99.96%) <400 ppm HD
DLM-408*	Deuterium
DLM-458*	Deuterium chloride (D, 99%)
DLM-3*	Deuterium chloride (D, 99.5%) DCl 35% w/w solution in D_2O
DLM-54	Deuterium chloride (D, 99.5%) DCl 20% w/w solution in D_2O
D214*	Deuterium oxide
CLM-1340	1,4-Dibromobenzene ($^{13}C_6$, 99%)
DLM-195	1,2-Dibromoethane-d_4 (D, 99%)
D220FD	1,2-Dichlorobenzene-d_4 (D, 99%)
CLM-1585	Diethyl acetamidomalonate (2-^{13}C, 99%)
CNLM-6677	Diethyl acetamidomalonate (1,2,3-$^{13}C_3$, 99%; ^{15}N, 98%)
NLM-3421	Diethyl acetamidomalonate (^{15}N, 98%)
CLM-4324	Diethyl acetylenedicarboxylate (1,2,3,4-$^{13}C_4$, 99%)
CLM-3603	Diethyl malonate (1,2,3-$^{13}C_3$, 99%)
CLM-495	Diethyl malonate (2-^{13}C, 99%)
CLM-521	Diethyl malonate (1,3-$^{13}C_2$, 99%)
CDLM-7163	Diethyl succinate (1,2,3,4-$^{13}C_4$, 99%; 2,2,3,3-D_4, 98%)
CLM-1620	Diethyl succinate (1,2,3,4-$^{13}C_4$, 99%)
DLM-265	Dimethyl-d_6-amine·HCl (D, 98%)
DLM-3903	Dimethyl carbonate-d_6 (D, 99%)
CLM-266	Dimethyl sulfate ($^{13}C_2$, 99%)

Reference	Description
DLM-196	Dimethyl sulfate-d_6 (D, 98%)
DLM-10*	Dimethyl sulfoxide-d_6
DLM-25	N,N-Dimethylformamide-d_7 (D, 99.5%)
DLM-1670	N,N-Dimethylformamide (formyl-D, 98-99%)
D043*	Ethanol-OD (D, 99%)
D114*	Ethanol-d_6 (D, 99%)
DLM-9660	N-Ethylaniline-d_{10} (D, 98%)
DLM-9626	N-Ethyl-d_5-aniline (D, 98%)
DLM-347	Ethylene-d_4 (D, 98%)
CLM-1121	Ethyl acetate (2-^{13}C, 99%)
CLM-1122	Ethyl acetate (1,2-$^{13}C_2$, 99%)
CLM-131	Ethyl acetate (1-^{13}C, 99%)
CLM-3297	Ethyl acetoacetate (1,2,3,4-$^{13}C_4$, 99%)
CLM-1009	Ethyl bromoacetate (1-^{13}C, 99%)
CLM-1010	Ethyl bromoacetate (2-^{13}C, 99%)
CLM-1011	Ethyl bromoacetate (1,2-$^{13}C_2$, 99%)
CLM-4326	Fluorobenzene ($^{13}C_6$, 99%)
CLM-806	Formaldehyde (^{13}C, 99%) ~20% w/w in H_2O
DLM-805	Formaldehyde-d_2 (D, 98%) ~20% w/w in D_2O
CDLM-4599	Formaldehyde (^{13}C, 99%; D_2, 98%) 20% w/w in D_2O
CLM-2032	Formamide (^{13}C, 99%)
DLM-743	Formic acid (formyl-D, 98%) <5% H_2O
DLM-286	Formic acid-d_2 (D, 98%) <5% D_2O
CDLM-6062	Fumaric acid (1-^{13}C, 99%; 2,3-D_2, 99%)
CLM-4454	Fumaric acid (1,4-$^{13}C_2$, 99%)
DLM-423	n-Heptane-d_{16} (D, 98%)
NLM-352	Hydrazine sulfate ($^{15}N_2$, 98%+)
NLM-426	Hydroxylamine·HCl (^{15}N, 98%+)
CLM-1892	Iodoethane (2-^{13}C, 99%) + copper wire
CLM-741	Iodoethane (1,2-$^{13}C_2$, 99%) + copper wire
DLM-272	Iodoethane-d_5 (D, 99%) + copper wire
DLM-1023	Iodoethane-1,1-d_2 (D, 98%) + copper wire
DLM-1024	Iodoethane-2,2,2-d_3 (D, 98%) + copper wire
CLM-4714	Isopropanol (2-^{13}C, 99%)
D072*	Isopropanol-d_8 (D, 99%)
DLM-6201	a-Ketoglutaric acid-3,3,4,4-d_4 (D, 98%) CP 90%
DLM-356	Lithium aluminum deuteride (D_4, 98%)
DLM-1945	bis(2-Chloroethoxy)-d_8 methane (D, 98%)
DLM-1981	Methanesulfonic acid-d_4 (D, 97-98%)
CLM-359	Methanol (^{13}C, 99%)
D015*	Methanol-OD (D, 99%)
D024*	Methanol-d_4
CDLM-688	Methanol (^{13}C, 99%; D_4, 99%)
CLM-360	Methylamine·HCl (^{13}C, 99%)
DLM-1500*	Methyl-d_3-amine (D, 98%)
DLM-289	Methyl-d_3-amine·HCl (D, 98%)
D023*	Methylene chloride-d_2 (D, 99.8%)
DLM-9707	Methyl-d_3-methanesulfonate (D, 98%)
DLM-651	Methyl formate (formyl-D, 99%)
CDLM-1037	Methyl iodide (^{12}C, 99.95%; D_3, 99.5%) + copper wire
CDLM-1537	Methyl iodide (^{13}C, 99%; D_3, 99%) + copper wire
CDLM-6015	Methyl iodide (^{13}C, 99%; D_2, 98%) + copper wire
DLM-362	Methyl iodide (D_3, 99.5%) + copper wire
CLM-287	Methyl iodide (^{13}C, 99%) + copper wire
DLM-3484	Morpholine-2,2,3,3,5,5,6,6-d_8 (D, 98%)
CLM-675	Nitrobenzene ($^{13}C_6$, 99%)
NLM-1042	Nitrobenzene (^{15}N, 98%+)
CLM-1043	Nitromethane (^{13}C, 99%)
NLM-600	Nitromethane (^{15}N, 98%+)
DLM-295	2-Nitrophenol-ring-d_4 (D, 98%)
DLM-296	4-Nitrophenol-ring-d_4 (D, 98%)
DLM-619	Octanoic acid-d_{15} (D, 98%)
CLM-2002	Oxalic acid (1,2-$^{13}C_2$, 99%)
CDLM-2702	Paraformaldehyde (^{13}C, 99%; D_2, 98%)
CLM-229	Paraformaldehyde (^{13}C, 99%)
DLM-300	Paraformaldehyde-d_2 (D, 99%)
CLM-216	Phenol ($^{13}C_6$, 99%)
DLM-370	Phenol-d_6 (D, 98%)
OLM-1057	Phosphoric acid ($^{18}O_4$, 96%) 80-85% in ^{18}O water
DLM-788	Phthalic anhydride-d_4 (D, 98%)
NLM-6081	Phthalimide (^{15}N, 98%+)
DLM-9813	Pivalic acid-trimethyl-d_9 (D, 98%)
CLM-297	Potassium cyanide (^{13}C, 99%)
CNLM-1961	Potassium cyanide (^{13}C, 99%; ^{15}N, 98%+)
NLM-111	Potassium cyanide (^{15}N, 98%+)
NLM-367	Potassium phthalimide (^{15}N, 98%+)
DLM-3078*	N-Propanol-d_7 (D, 98%)
DLM-9662	Pyrrolidine-2,2,3,3,4,4,5,5-d_8 (D, 98%)
DLM-226	Sodium borodeuteride-d_4 (D, 99%) CP 95%
CLM-378	Sodium cyanide (^{13}C, 99%) CP 96%
NLM-3005	Sodium cyanide (^{15}N, 98%+) CP 96%
D076*	Sodium deuteroxide (D, 99.5%) 40% in D_2O
CDLM-6203	Sodium formate (^{13}C, 99%; D, 98%)
CLM-583	Sodium formate (^{13}C, 99%)
DLM-1361	Sodium formate (D, 98%)
NLM-658	Sodium nitrite (^{15}N, 98%+)
CLM-2440	Sodium pyruvate ($^{13}C_3$, 99%)
DLM-8206	Sodium 2,2-dimethyl-2-silapentane-5-sulfo-nate-d_6 (DSS) (D, 98%)
CLM-1084	Succinic acid (1,4-$^{13}C_2$, 99%)
CLM-1199	Succinic acid (2,3-$^{13}C_2$, 99%)
CLM-2473	Succinic anhydride (1,2,3,4-$^{13}C_4$, 99%)
D077*	Sulfuric acid-d_2 (D, 99%) 96-98% in
D2OD149	Tetrahydrofuran-d_8 (D, 99.5%)
DLM-2729	Tetramethylsilane-d_{12} (D, 98%)
CLM-6069	Toluene (ring-$^{13}C_6$, 99%)
D005*	Toluene-d_8 (D, 99.5%)
CLM-4833	Triethyl orthoacetate (1,2-$^{13}C_2$, 99%)
CLM-3742	Triethyl orthoformate (formyl-^{13}C, 99%)
D022*	Trifluoroacetic acid-d
NLM-1697	Uric acid (1,3-$^{15}N_2$, 98%+)



Biomolecular NMR

Deuterated Detergents and Phospholipids for Membrane Proteins

Membrane proteins can be divided into three categories :

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

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

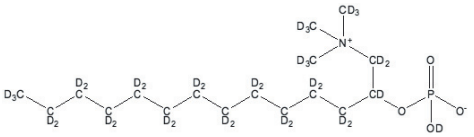
The determination of the structure and dynamics of membrane proteins using NMR requires samples containing protein that is properly folded. Fortunately, membrane proteins often keep native-like structures in detergent micelles. Deuterated solubilization agents, such as detergents, often make NMR investigations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

Reference

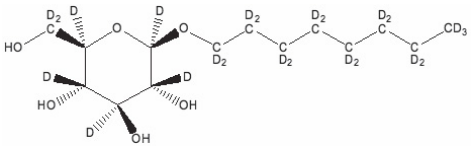
[1] There are 493 unique membrane protein structures as of August 3, 2014. See http: // blanco.biomol.uci.edu / index.shtml for more information.

Deuterated Detergents and Phospholipids

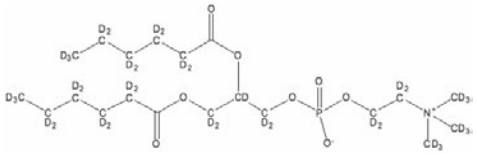
Reference	Description
DLM-2274	Dodecylphosphocholine (D38, 98%)



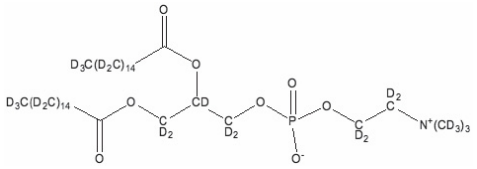
DLM-6726	N-Octyl β-Glucoside (D24, 98%)



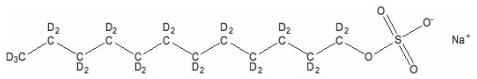
DLM-4341	DL-A-Phosphatidylcholine, dihexanoyl (D40, 98%) (DHPC) CP 95%



DLM-8256	DL-A-Phosphatidylcholine, dipalmitoyl (DPPC) (U-D80, 98%) CP 95%+



DLM-197	Sodium dodecyl sulfate (D25, 98%)



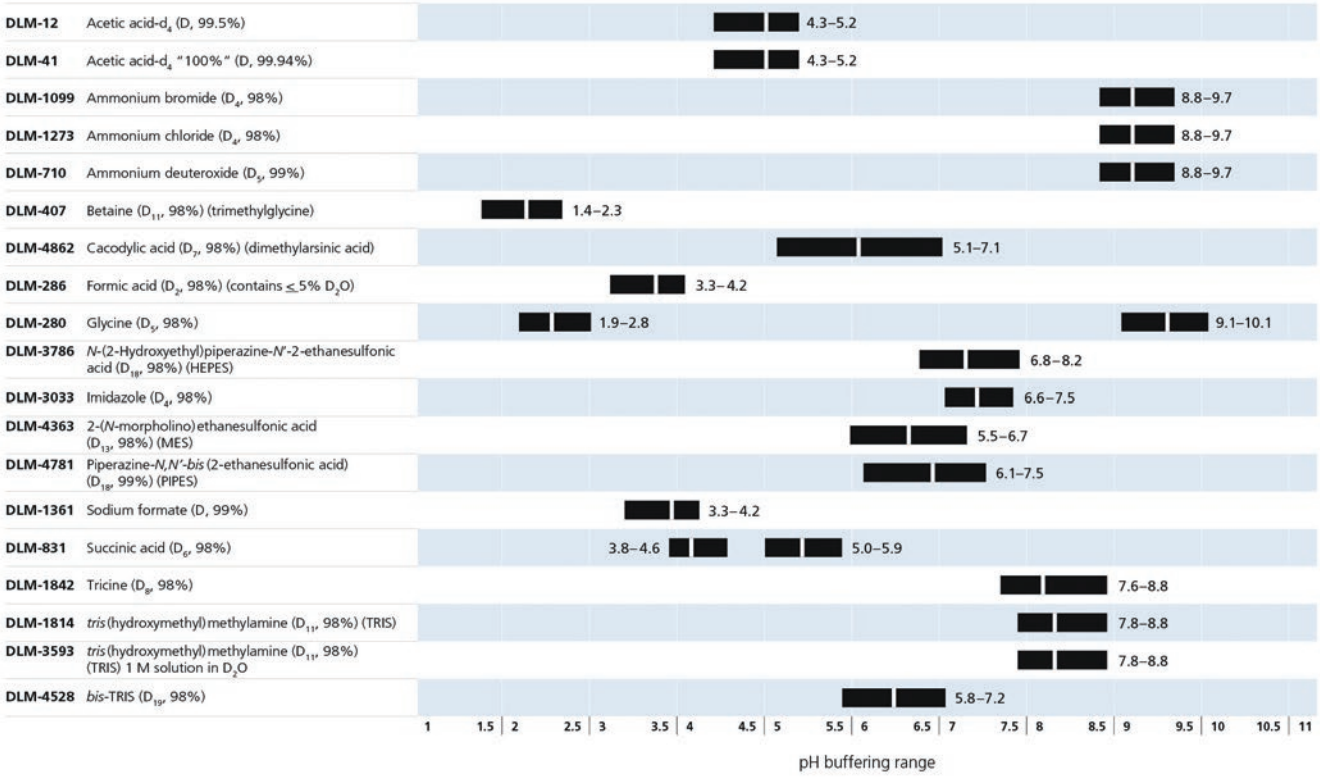
Deuterated Buffers

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

Reference	Description
D012	Acetic acid D_4 (D, 99.5%)
D041	Acetic acid D_4 "100%" (D, 99.91%)
DLM-1099	Ammonium bromide (D_4, 98%)
DLM-1273	Ammonium chloride (D_4, 98%)
DLM-710	Ammonium deuteroxide (D_5, 99%) (~25% in soln D_2O)
DLM-407	Betaine (D_{11}, 98%)
DLM-4862	Cacodylic acid (D_7, 98%)
DLM-286	Formic acid (D_2, 98%) (<5% D_2O)
DLM-280	Glycine (D_5, 98%)
DLM-3786	HEPES (D_{18}, 98%)
DLM-3033	Imidazole (D_4, 98%)

Reference	Description
DLM-4363	MES (D_{13}, 98%
DLM-4781	PIPES (D_{18}, 98%)
DLM-197	Sodium Dodecyl sulfate (D_{25}, 98%)
DLM-1361	Sodium formate (D, 98%)
DLM-831	Succinic acid (D_6, 98%)
DLM-1842	Tricine (D_8, 98%)
DLM-4779	Trimethylamine N-oxide (D_9, 98%)
DLM-1817	TRIMETHYLAMINE:DCL (D_{10}, 98%)
DLM-1814	TRIS (D_{11}, 98%)
DLM-3593	TRIS (D_{11}, 98%) 1 M in D_2O
DLM-4528	bis-TRIS (D_{19}, 98%)

pH Buffering Range Chart



Cell-Free Synthesis of Labeled Proteins for NMR Studies

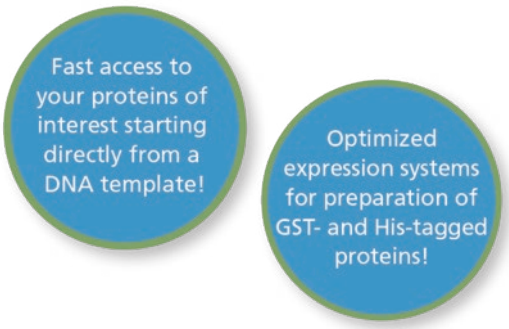
Euriso-Top is pleased to offer kits and reagents manufactured by CellFree Sciences Co., Ltd. (CFS) for cell-free protein synthesis. The CellFree Sciences' ENDEXT® wheat germ cell-free system permits both high-throughput protein screening and overnight microgram- to milligram-scale protein production. Protein-synthesis protocols for the ENDEXT® system have been optimized for a wide range of proteins, and when used with Euriso-Top amino acids, offer an ideal platform for producing uniform or selective labeled protein for NMR applications.

Cell-free protein synthesis uses an open reaction format that allows for easy manipulation of reaction conditions to:

- add labeled amino acids for NMR studies
- add cofactors for protein(s) complexes
- add liposomes for expression of membrane proteins
- add detergents for increased solubility
- adjust redox conditions for formation of disulfide bridges

Cell-free synthesis using CFS and Euriso-Top reagents are ideal for expressing labeled:

- toxic proteins
- membrane proteins
- protein with selective incorporation of labeled amino acids
- proteins having very high incorporation rates for labeled amino acids
- proteins containing unnatural amino acids
- protein complexes composed of multiple proteins in a single reaction



Easy Three-step Process to Produce your Proteins of Interest

1. Prepare expression template by PCR or cloning into expression vector
2. Cell-free protein synthesis and affinity tag-based purification
3. Protein characterization

Try cell-free protein synthesis for your next NMR sample!

How to Proceed

Step 1: Test and optimize protein expression

- Use the Premium Plus Expression Kit or a Protein Research Kit to produce unlabeled protein on a small scale.
- If desired, contact CFS for more information on cell-free protein-expression services for testing your proteins of interest.

Step 2: Express labeled proteins using cell-free protein-synthesis expression kits and reagents

- Several ready-to-use WEPRO® Protein Expression Kits are available for uniform ^{15}N and ^{13}C, ^{15}N labeling containing enough reagents for up to 6 × 6 mL bilayer reactions.
- WEPRO8240 Protein Expression Kits are available for producing selective or uniform labeled protein using Euriso-Top amino acids (sold separately).

Step 3: Production of bulk quantities (mg -> g) (optional)

- Cell-free protein synthesis allows rapid testing of expression conditions that can directly be used in large-scale protein production.
- Bulk program for reagent sales to large-scale user using feeding methods for protein synthesis.
- Fully automated solutions to protein synthesis on Protemist® protein synthesizers.

Contact Euriso-Top or CFS for more information on large-scale cell-free protein-expression services for your proteins of interest.

Stable Isotope-Labeled Standards and XF-1 Protein Pairs for X-Filtered NOESY

In parternship with Nexomics Biosciences and CIL, Euriso-top is pleased to offer new and exciting isotope-enriched proteins for use as standards in NMR spectroscopy. Isotope-enriched protein standards are ideal for:

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

Nexomics Biosciences, Inc. is a New Jersey-based contract research organization that specializes in a broad array of gene-to-structure services to the biopharmaceutical community.

Gaetano Montelione, CEO of Nexomics Biosciences, Inc., is an expert in the determination of protein structures using NMR. He is a Distinguished Professor of Molecular Biology and Biochemistry at the Center for Advanced Biotechnology and Medicine, Rutgers University, and has over 300 publications.

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

- ^{1}H-^{15}N HSQC (^{15}N-labeled proteins)
- ^{1}H-^{13}C HSQC (^{13}C-labeled proteins)
- CO-NH projection of 3D HNCO (^{15}N,^{13}C-labeled proteins)
- SDS PAGE (for all labeled proteins)
- MALDI-TOF (for all labeled proteins)
- ^{15}N-edited X-filtered 2D NOESY (NEX-XF1)

Maltose Binding Protein (NEX-MBP)

NEX-MBP is a 44.9 kDa monomeric protein for which multiple sets of resonance assignments (BMRB database) and 3D structures (PDB database) are publicly available. This product is uniformly ^{2}H,^{15}N,^{13}C-enriched with selective incorporation of protons into methyl groups of Ile-δ1, Leu-δ and Val-γ side chains. As nonuniform sampling (NUS) and other NMR techniques emerge to push the size limitations of NMR to new boundaries, large 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 ^{2}H,^{15}N,^{13}C and ILV methyl ^{1}H,^{13}C MBP in 10% D2O, 0.02% NaN_3, 20 mM sodium phosphate @ pH 7.2
NEX-MBP2: Closed Conformation
0.5 mM ^{2}H,^{15}N,^{13}C and ILV methyl ^{1}H,^{13}C MBP with 3 mM maltotriose, 10% D2O, 0.02% NaN_3, 20 mM sodium phosphate @ pH 7.2
NEX-MBP3: Open Conformation
0.5 mM ^{2}H,^{15}N,^{13}C and ILV methyl ^{1}H,^{13}C MBP with 2 mM β-cyclodextrin, 10% D2O, 0.02% NaN_3, 20 mM sodium phosphate @ pH 7.2

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

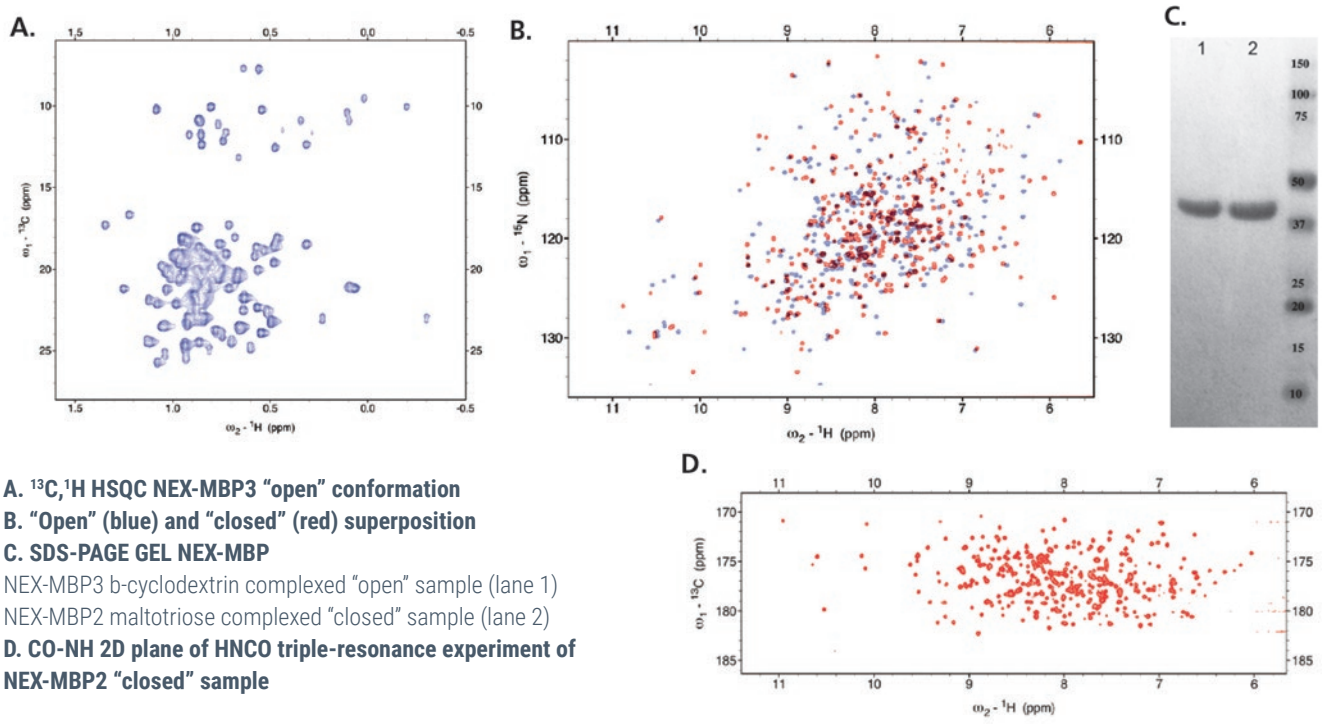
Reference	Label
NEX-MBP1-U-0	unlabeled
NEX-MBP1-N-0	(^{15}N, 95%)
NEX-MBP1-CN-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-MBP1-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-MBP1-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-MBP1-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-MBP1-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

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

Reference	Label
NEX-MBP2-U-0	unlabeled
NEX-MBP2-N-0	(^{15}N, 95%)
NEX-MBP2-CN-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-MBP2-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-MBP2-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-MBP2-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-MBP2-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

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

Reference	Label
NEX-MBP3-U-0	unlabeled
NEX-MBP3-N-0	(^{15}N, 95%)
NEX-MBP3-CN-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-MBP3-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-MBP3-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-MBP3-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-MBP3-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)



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

Protein Sequence MKIEEGKLVIWINGDKGYNGLAEVGKKFEKDTGIKVTVEHPDKLEEKFPQVAATGDGPDIIFWAHDRFGGYAQSGLLAEIT-PDKAFQDKLYPFTWDAVRYNGKLIAYPIAVEALSLIYNKDLLPNPPKTWEEIPALDKELKAKGKSALMFNLQEPYFTWPLIAADGGYAFKYENGKYDIKDVGVD-NAGAKAGLTFLVDLIKNKHMNADTDYSIAEAAFNKGETAMTINGPWAWSNIDTSKVNYGVTVLPTFKGQPSKPFVGVLSAGINAASPNKELAKEFLENYLLT-DEGLEAVNKDKPLGAVALKSYEEELAKDPRIAATMENAQKGEIMPNIPQMSAFWYAVRTAVINAASGRQTVDEALKDAQTRITK

X-Filtered NOESY NMR Standard (NEX-XF1)

In an X-filtered experiment, only NOEs between $^{15}N/^{13}C$-1H and $^{14}N/^{12}C$-1H (e.g. interchain NOEs) protons are observed. NOEs between protons connected to $^{15}N,^{13}C$ are filtered (intrachain NOEs). When uniformly double-labeled protein sample is mixed with a naturalabundance protein sample, the interface will give rise to the only observable NOESY cross peaks. This powerful strategy enables the spectroscopist to discern intra from inter NOESY cross peaks, 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 16 kDa protein (A. fulgidus antitoxin vapB21 homodimer) for which a set of resonance assignments (bmr7362), 3D structure (^{2}NWT) and other NMR data are available in the public domain. This is a mixture of unlabeled and uniformly $^{15}N,^{13}C$-enriched protein (25% homodimer unlabeled; 50% heterodimer unlabeled/labeled; 25% homodimer labeled) and is perfect to set up X-filtered NOESY experiments.

NEX-XF1 Homodimer Sample Formulation:

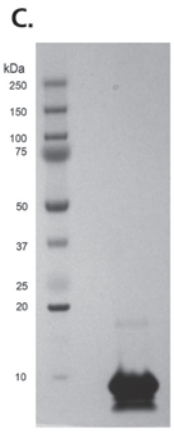
NEX-XF1: $^{13}C,^{15}N$-labeled and unlabeled sample conditions. 1 mM protein, 20 mM NH4OAc pH 5.5, 100 mM NaCl, 5 mM CaCl2, 10% D2O, 0.02 % NaN_3

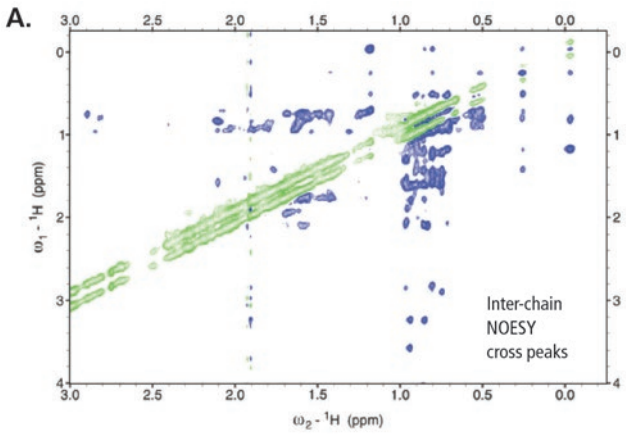
X-Filtered NOESY NMR Standard

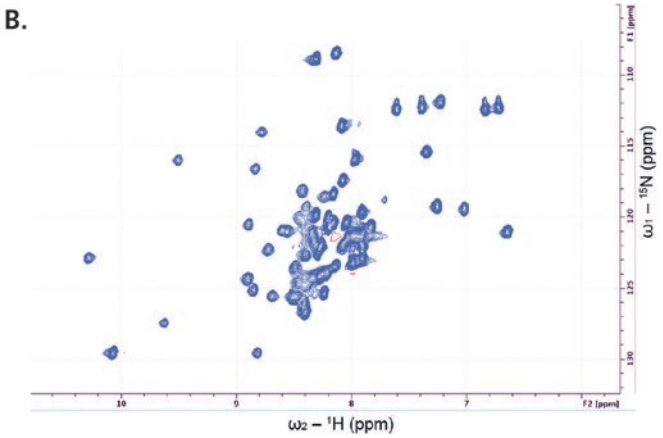
Reference	Label
NEX-XF1-U-0	unlabeled
NEX-XF1-N-0	(^{15}N, 95%)
NEX-XF1-CN-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-XF1-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-XF1-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-XF1-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-XF1-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

X-Filtered NOESY NMR Standard, His-Tagged

Reference	Label
NEX-XF1-HIS-U-0	unlabeled
NEX-XF1-HIS-N-0	(^{15}N, 95%)
NEX-XF1-HIS-CN-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-XF1-HIS-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-XF1-HIS-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-XF1-HIS-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-XF1-HIS-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-IL-VFY)







A. 2D ^{1}H-1H plane of $^{1}H,^{13}C$ edited $^{1}H,^{12}C$ X-filtered NOESY
B. ^{1}H-15N HSQC of NEX-XF1
C. SDS-PAGE GEL NEX-XF1

Protein Sequence PKIIEAVYENGVFKPLQKVDLKEGERVKIKLELKVEPIDLGEPVSVEEIKKIRDGTWMSSLEHHHHHH

Ubiquitin (NEX-UB1)

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

NEX-UB1 Sample Formulations:

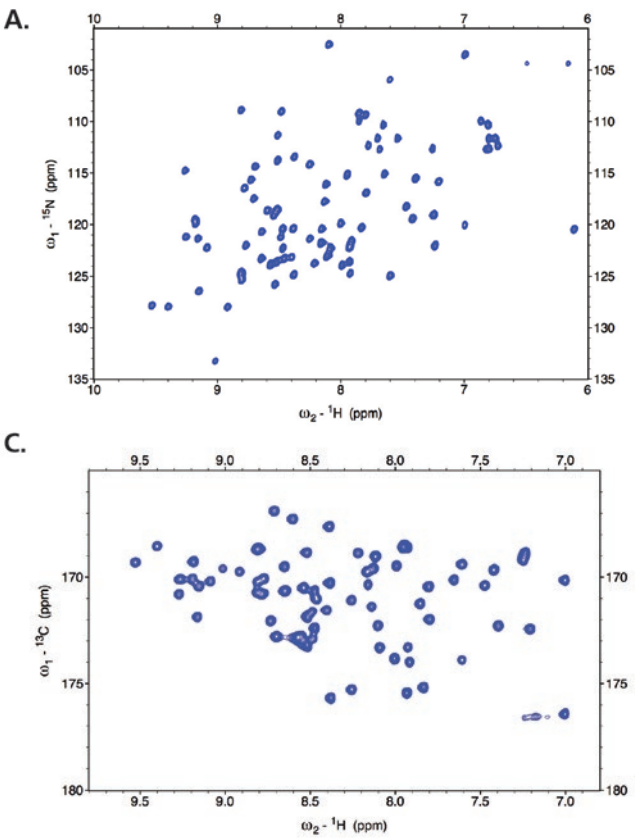
NEX-UB1: Uniformly ^{15}N,^{13}C-labeled ubiquitin in 90% H_2O; 10% D_2O
10 mM sodium phosphate buffer, pH 6.5

Ubiquitin (Human)

Reference	Label
NEX-UB1-U-0	unlabeled
NEX-UB1-N-0	(^{15}N, 95%)
NEX-UB1-CN-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-UB1-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-UB1-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-UB1-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-UB1-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)

His-Ubiquitin (Human)

Reference	Label
NEX-UB1-HIS-U-0	unlabeled
NEX-UB1-HIS-N-0	(^{15}N, 95%)
NEX-UB1-HIS-CN-5-0	(^{13}C, 5%; ^{15}N, 95%)
NEX-UB1-HIS-CN-0	(^{13}C, 95%; ^{15}N, 95%)
NEX-UB1-HIS-CDN-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%)
NEX-UB1-HIS-ILV-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILV)
NEX-UB1-HIS-ILVFY-0	(^{13}C, 95%; D, 95%; ^{15}N, 95%; $^{13}CH_3$-ILVFY)



A. ^{1}H,^{15}N HSQC of NEX-UB1
B. ^{13}C-1H HSQC of NEX-UB1
C. CO-NH 2D plane of HNCO triple-resonance experiment of NEX-UB1
D. SDS-PAGE GEL NEX-UB1

Protein Sequence after TEV Cleavage SHMQIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQRLIFAGKQLEDGRTLSDYNIQKESTLHLVLRLRGG
Protein Sequence before TEV Cleavage MGHHHHHHHENLYFQSHMQIFVKTLTGKTITLEVEPSDTIENVKAKIQDKEGIPPDQQRLIFAGKQLEDGRTLS-DYNIQKESTLHLVLRLRGG

^{13}C Enriched Substrates for Hyperpolarization

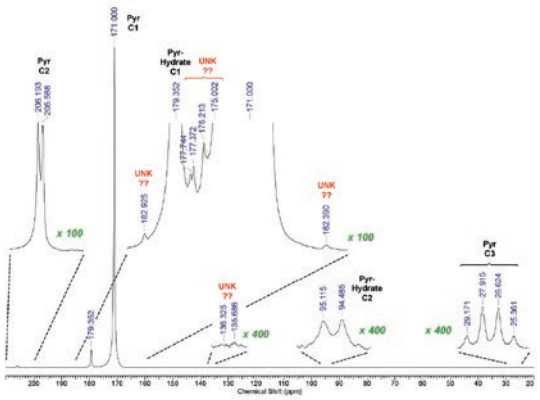
Reference	Label
CLM-245	Acetone (2-^{13}C, 99%)
CLM-116	L-Alanine (1-^{13}C, 99%)
CLM-113	Acetic acid (1,2-$^{13}C_2$, 99%)
CLM-317	Acetic acid (1-^{13}C, 99%)
CLM-318	Acetic acid (2-^{13}C, 99%)
CLM-1189*	D-Mannitol (1-^{13}C, 98%)
CLM-4761	DMSO ($^{13}C_2$, 99%)
CLM-7350	Ethyl pyruvate (1-^{13}C, 99%)
CLM-1527	Fructose (2-^{13}C, 99%)
CLM-4454	Fumaric acid (1,4-$^{13}C_2$, 99%)
CDLM-8473	Fumaric acid (1,4-$^{13}C_2$, 99%; 2,3-D2, 98%)
CDLM-6062	Fumaric acid (1-^{13}C, 99%; 2,3-D2, 98%)
CLM-420	D-Glucose (1-^{13}C, 98-99%)
CDLM-3813*	D-Glucose ($^{13}C_6$, 99%; D7, 97%+)
CLM-2717	D-Glucose (1-^{13}C, 99%; 6-^{13}C, 97%+)
CLM-674*	L-Glutamic acid (1-^{13}C, 99%)
CLM-1166	L-Glutamine (5-^{13}C, 99%)
CLM-2093	α–Ketoisocaproate, sodium salt (1-^{13}C, 99%)
CLM-646	Propionic acid (1-^{13}C, 99%)
CLM-647	Propionic acid ($^{13}C_3$, 99%)
CLM-8077	Pyruvic acid (1-^{13}C, 99%)

Reference	Label
CLM-8849	Pyruvic acid (2-^{13}C, 99%)
CLM-156*	Sodium acetate (1-^{13}C, 99%)
CLM-381*	Sodium acetate (2-^{13}C, 99%)
CLM-440*	Sodium acetate (1,2-$^{13}C_2$, 99%)
CLM-441*	Sodium bicarbonate (^{13}C, 99%)
CLM-1256*	Sodium butyrate (1-^{13}C, 99%)
CLM-1577*	Sodium L-lactate (1-^{13}C, 99%)
CLM-1578*	Sodium L-lactate (3-^{13}C, 98%)
CLM-1579	Sodium L-lactate ($^{13}C_3$, 98%)
CLM-1506	Sodium propionate (2-^{13}C, 99%)
CLM-1865*	Sodium propionate ($^{13}C_3$, 99%)
CLM-3042	Sodium propionate (2,3-$^{13}C_2$, 99%)
CLM-771*	Sodium propionate (1-^{13}C, 99%)
CLM-1082*	Sodium pyruvate (1-^{13}C, 99%)
CLM-1575*	Sodium pyruvate (3-^{13}C, 99%)
CLM-1580	Sodium pyruvate (2-^{13}C, 99%)
CLM-3507	Sodium pyruvate (1,2-$^{13}C_2$, 99%)
CLM-1084	Succinic acid (1,4-$^{13}C_2$, 99%)
CLM-8493	Succinic acid (1-^{13}C, 99%)
CLM-311	Urea (^{13}C, 99%)
CLM-8077	Pyruvic acid (1-^{13}C, 99%)

* Microbiological and pyrogen tested (MPT) grade available. MPT-grade products are research-grade products that are tested in the bulk form for S. aureas, P. aeruginosa, E. coli, Salmonella, aerobic bacteria, yeast and mold and for bacterial endotoxins. Package sizes typically include 1.0 and 2.0 g.

Pyruvic Acid (1-^{13}C)

We supplies pyruvic acid (1-^{13}C) to research groups world-wide that are either developing and/or applying dissolution DNP techniques to study metabolism. To satisfy the need for the ever-increasing amounts of pyruvic acid (1-^{13}C) being used in investigations, CIL has developed a robust, synthetic process that is readily scalable. This process has recently been optimized so that CIL is now able to offer product with high chemical purity and exceptional lot-to-lot consistency.



^{13}C DNP spectrum of pyruvic acid (1-^{13}C). First scan of CIL's pyruvic acid (1-^{13}C) was provided by Karlos Moreno and Matthew Merritt from the UTSW Medical Center in Dallas, TX.

Research Grade

Catalog No. CLM-8077

QC Testing for Research-Grade Pyruvic Acid (1-^{13}C)*

QC Test	Result*
^{13}C NMR for Identification	Conforms
^{1}H NMR for Chemical Purity	Pass
GC/MS for Isotopic Enrichment	99.1%
HPLC for Chemical Purity	98.0%
Karl Fischer Titration for Total Water Content	3383 ppm
Titration for Chemical Purity	99.8%

cGMP Grade

Catalog No. CLM-8077-CTM

Product Specifications for CTM-Grade Material**

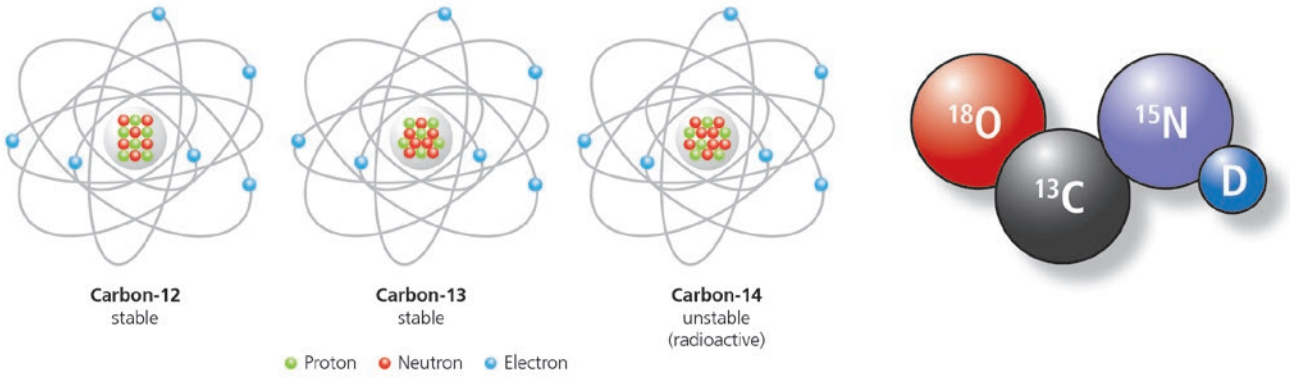
tests	Method	Acceptance Criteria
Identification	^{13}C NMR	Conforms
Identification	1H NMR	Conforms
Identification	IR	Conforms
Appearance	Visual inspec-tion	Colorless to yellow, clear, viscous liquid
Isotopic Enrichment	GC/MS	>98%
Residual Solvents	HS-GC	Acetone:< 5000 µg/g Acetonitrile: < 200 µg/g
HPLC for Related Impurities	HPLC	AH113462/E: < 3.00% Area
HPLC for Related Impurities Total Unidentified Impurities	HPLC	< 2.00% area
Water Content	IR	< 4.5% (w/w)
Assay	HPLC	89.0-103.5%
Bacterial endotoxin	USP <85>	<25 EU/mL
Total Aerobic Microbial Count (TAMC)	USP <61>	<10 CFU/mL

*Results for Lot PR-24550 are shown. Actual results may vary.
** Products prepared under the CTM classification may conform to materials suitable for Phase 1 Clinical Trials as described in Section 19 of the ICH Guidance Q7A, "cGMP Guidance for Active Pharmaceutical Ingredients (APIs)."

Technical informations

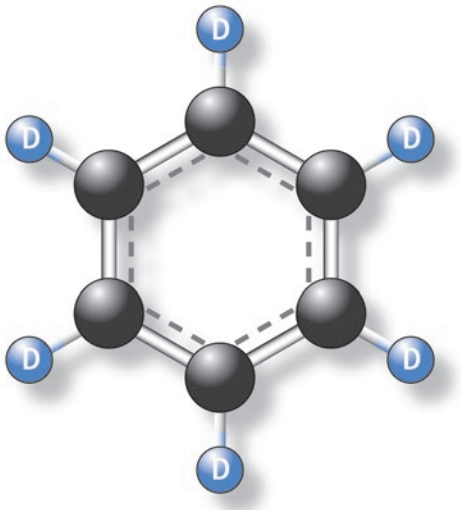
What Is an Isotope?

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



Isotopic Enrichment

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



Benzene (D_6, 99%)

Quality Control

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 . 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 us to consistently produce products with high chemical and isotopic purity .
All our production is evaluated before and after packaging.

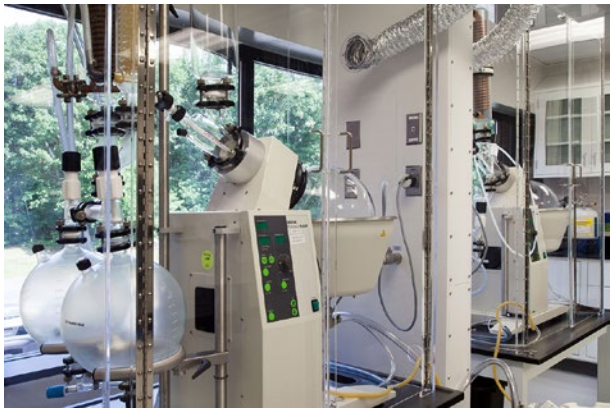
Our experience and skill allow us to obtain a chemical purity of NMR Deuterated Solvents higher or equal to 99,9% ; for other NMR labeled Compounds chemical purity is higher than 98%.

Water contamination is a common problem for deuterated NMR solvents. The water content of our solvents is tested via the KF titration method by our Quality Control Department.

Advices and tips on how to minimize/eliminate water peaks :

- Consider using single-use ampoules. Many of our solvents are available in single-use break seal ampoules ranging in size from 0,25 mL to 3 mL.
- Handle solvents in a dry atmosphere.
- Dry NMR tubes and pipettes used for sample preparation overnight in an oven and cool them in a dessicator prior to use.
- Precondition an NMR tube by rinsing it with D_2O

Remove residual D_2O by rinsing with methanol-d4 or acetone-d6 and then with the solvent of choice. This process will not remove water, but it will exchange the protons for deuterium and minimize the water peak.



Stability Study

Our stability studies have allowed us to establish optimal storage conditions for the majority of our products, details of which are made available.

Packing and Shipping

Our shipping department makes every effort to ensure prompt delivery of our products to your laboratory in the most secure manner possible. Certificates of Analysis (COA) and Material Safety Data Sheets (MSDS) are supplied with every shipment

Environment and Security

EURISO-TOP has been committed to reducing its liquid, solid and gaseous emissions for several years. Risk analyses and working environment checks allow us to carefully pinpoint the presence of VOCs and to ensure maximum safety of our teams at work.
Our chemical waste is taken care of by leaders in the field of treatment and the collection is carefully organised.
EURISO-TOP is actively involved in recycling metals, wood, plastic, glass and cardboard every day. The use of recyclable packaging (cardboard boxes, standardised use of cushioning materials …) helps to extend our involvement in the environmental chain with the assistance of our service carriers.

Storage

Chloroform-d, Methylene Chloride-d_2, Tetramethylsilane (TMS), Tetrahydrofuran-d_8 and Tetrachloro ethane-d are not stabilised and are thus very sensitive to ultra-violet light and oxidation. Their storage under refrigeration at less than +4°C guarantees a longer shelf life. Before use, the vial should be left at room temperature to warm up before opening under an anhydrous, inert atmosphere. Tetramethylsilane (TMS) is a very volatile compound (bp = 26°C). To minimise its loss, it is packaged in a "penicillin" type vial sealed with a Teflon faced septum. It is necessary to keep it in a refrigerator.

Melting Point

Dimethyl Sulfoxide (DMSO) has a melting point of 18°C, freezing close to room temperature. It may be at a solid state when delivered, but to turn it to a liquid state just thaw it in a warm water bath. Care must be taken to prevent water contamination.

The products offered by EURISO-TOP, as shown in this catalogue or otherwise, are for laboratory research use only. Use in any other way than laboratory applications is the sole responsibility of the researcher.

Choice of Solvent

Depending on several criteria :
- Solubility of the sample,
- Position of the peak of residual proton,
- Consequence on the chemical shift of the solute due to interactions with solvent molecules,
- Temperature of experiment,
- Polarity of solvent.

Handling of NMR Solvents

All deuterated solvents must be handled in a strict anhydrous and inert atmosphere (dry nitrogen or argon) in order to minimise the absorption of moisture. This absorption leads not only to an increase in the HDO concentration and the resultant signal in ^{1}H NMR spectrum, but also to an exchange of the easily labile protons (especially heteroatom-linked protons). Solvent vials must be immediately re-closed after use and the solvent removed from an ampoule transferred into a dry vial.

Very hygroscopic solvents packed in "penicillin" type vials are withdrawn with a syringe. It is recommended to flush into the vial an amount of dry nitrogen equivalent to the amount of solvent to be collected.

Sample Concentration

The signal of the protons of the dissolved substance should be greater than the signal of the residual proton of the solvent used. So the quantity of the product depends on the isotopic enrichment of the solvent and on the field applied in the NMR spectrometer.

Tube Preparation

In order to ensume optimum measurements, we would advise the user to work with unused NMR tubes. Otherwise, before use the NMR tube must be perfectly cleaned and dried. To avoid contamination with residual water absorbed into the inner wall of the NMR tube, we recommend keeping 1 mL or more of Deuterium Oxide in the tube over night, to decant and wash it with Acetone -d6 or Methyl Alcohol-d4 and to store it in a "dessicator" saturated with Deuterium Oxide. To clean the outer wall of the NMR tube use a soft piece of cloth.

Reference Material

The position of the peak of the solvents can change with the temperature and the pH of the solution. In certain cases, it is not recommended to use it for calibration. The reference material for the ^{1}H and ^{13}C NMR is Tetramethylsilane (TMS). TMS is not soluble in heavy water, so the internal reference for this solvent is : (2,2,3,3) Trimethylsilyl-3 Propionic Acid, Sodium salt (TMSP).

Packaging Information

The products are packaged according to their physical and chemical properties.
We use the best available packaging materials to enable a simple and safe utilisation while preserving the quality of the products. Quality is carefully monitored during production and packaging, using instrumental analysis.
EURISO-TOP offers a large range of packaging options. We will try to accommodate special packaging request for a modest additional fee.

Solid and Liquid Packaging

1. **Flame-sealed glass ampoules under inert atmosphere.**
2. **Screw-cap glass vials.**
3. **Vials "penicillin" type with Teflon** sealed under inert atmosphere, for Acetone, Acetonitrile, Benzene, DMSO, Methanol and also for Deuterium oxide®.

Security Concept

The United Nations have adopted the Globally Harmonised System (GHS) on a worldwide scale, strengthened by the European application for the REACH regulation (Registration, Evaluation, Authorisation and restriction of Chemicals), which finds its practical application in the CLP regulation (Classifying, Labelling and Packaging) to standardise the classification of hazards. New hazard pictograms, warning labels and precautionary hazard statements have been created in order to keep you better protected and informed of the risks associated with the use of chemicals.

Labels are regularly updated in good faith to meet advances in knowledge and regulations. On some containers, as required by regulations, labelling is reduced due to restrictions on available space. All information is available on our website www.eurisotop.com

GHS 01 Heating may cause an explosion

GHS 02 Heating may cause a fire

GHS 03 May intensify fire ; oxidizer

GHS 04 Contains gas under pressure ; may explode when heated

GHS 05 Causes serious eye damage

GHS 06 Toxic if swallowed

GHS 07 May cause an allergie skin reaction

GHS 08 May cause allergy or asthma symptoms or breathing difficulties if inhaled

GHS 09 Toxic to the aquatic life with long lasting effects

Signal words : DANGER or WARNING

EUH001	Explosive when dry.
EUH006	Explosive with or without contact with air.
EUH014	Reacts violently with water.
EUH018	In use, may form flammable/explosive vapour-air mixture.
EUH019	May form explosive peroxides.
EUH029	Contact with water liberates toxic gas.
EUH031	Contact with acids liberates toxic gas.
EUH032	Contact with acids liberates very toxic gas.
EUH044	Risk of explosion if heated under confinement.
EUH059	Hazardous to the ozone layer.
EUH066	Repeated exposure may cause skin dryness or cracking.
EUH070	Toxic by eye contact.
EUH071	Corrosive to the respiratory tract.
EUH201	Contains lead. Should not be used on surfaces liable to be chewed or sucked by children.
EUH201A	Warning! Contains lead.
EUH202	Cyanoacrylate. Danger. Bonds skin and eyes in seconds. Keep out of the reach of children.
EUH203	Contains chromium (VI). May produce an allergic reaction.
EUH204	Contains isocyanates. May produce an allergic reaction.
EUH205	Contains epoxy constituents. May produce an allergic reaction.
EUH206	Warning! Do not use together with other products. May release dangerous gases (chlorine)
EUH207	Warning! Contains cadmium. Dangerous fumes are formed during use. See information supplied by the manufacturer. Comply with the safety instructions.
EUH208	Contains (name of sensitising substance). May produce an allergic reaction.
EUH209	Can become highly flammable in use.
EUH209A	Can become flammable in use.
EUH210	Safety data sheet available on request.
EUH401	To avoid risks to human health and the environment, comply with the instructions for use.

Phrases H

H200	Unstable explosives.
H201	Explosive; mass explosion hazard.
H202	Explosive, severe projection hazard.
H203	Explosive; fire, blast or projection hazard.
H204	Fire or projection hazard.
H205	May mass explode in fire.
H220	Extremely flammable gas.
H221	Flammable gas.
H222	Extremely flammable aerosol.
H223	Flammable aerosol.
H224	Extremely flammable liquid and vapour.
H225	Highly flammable liquid and vapour.
H226	Flammable liquid and vapour.
H227	Combustible liquid
H228	Flammable solid.
H240	Heating may cause an explosion.
H241	Heating may cause a fire or explosion.
H242	Heating may cause a fire.
H250	Catches fire spontaneously if exposed to air.
H251	Self-heating: may catch fire.
H252	Self-heating in large quantities; may catch fire.
H260	In contact with water releases flammable gases which may ignite spontaneously.
H261	In contact with water releases flammable gases.
H270	May cause or intensify fire; oxidiser.
H271	May cause fire or explosion; strong oxidiser.
H272	May intensify fire; oxidiser.
H280	Contains gas under pressure; may explode if heated.
H281	Contains refrigerated gas; may cause cryogenic burns or injury.
H290	May be corrosive to metals.
H300	Fatal if swallowed.
H301	Toxic if swallowed.
H302	Harmful if swallowed.
H303	May be harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H305	May be harmful if swallowed and enters airways
H310	Fatal in contact with skin.
H311	Toxic in contact with skin.
H312	Harmful in contact with skin.
H313	May be harmful in contact with skin.
H314	Causes severe skin burns and eye damage.
H315	Causes skin irritation.
H316	Causes mild skin irritation.
H317	May cause an allergic skin reaction.
H318	Causes serious eye damage.
H319	Causes serious eye irritation.
H320	Causes eye irritation
H330	Fatal if inhaled.
H331	Toxic if inhaled.
H332	Harmful if inhaled.
H333	May be harmful if inhaled.
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H340	Very toxic to aquatic life.
H341	Suspected of causing genetic defects.
H350	May cause cancer.
H351	Suspected of causing cancer.
H360	May damage fertility or the unborn child.
H360d	May damage unborn child.
H361	Suspected of damaging fertility or the unborn child.
H361d	Suspected of damaging the unborn child
H362	May cause harm to breast-fed children.
H370	Causes damage to organs.
H371	May cause damage to organs.
H372	Causes damage to organs through prolonged or repeated exposure.
H373	May cause damage to organs through prolonged or repeated exposure.
H400	Very toxic to aquatic life.
H401	Toxic to aquatic life.
H402	Harmful to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.
H411	Toxic to aquatic life with long lasting effects.
H412	Harmful to aquatic life with long lasting effects.
H413	May cause long lasting harmful effects to aquatic life.

Phrases P

P101 ..... If medical advice is needed, have product container or label at hand.
P102 ..... Keep out of reach of children.
P103 ..... Read label before use.
P201 ..... Obtain special instructions before use.
P202 ..... Do not handle until all safety precautions have been read and understood.
P210 ..... Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P211 ..... Do not spray on an open flame or other ignition source.
P220 ..... Keep/Store away from clothing/…/combustible materials.
P221 ..... Take any precaution to avoid mixing with combustibles…
P222 ..... Do not allow contact with air.
P223 ..... Keep away from any possible contact with water, because of violent reaction and possible flash fire.
P230 ..... Keep wetted with…
P231 ..... Handle under inert gas.
P232 ..... Protect from moisture.
P233 ..... Keep container tightly closed.
P234 ..... Keep only in original container.
P235 ..... Keep cool.
P240 ..... Ground/bond container and receiving equipment.
P241 ..... Use explosion-proof electrical/ventilating/lighting/…/equipment.
P242 ..... Use only non-sparking tools.
P243 ..... Take precautionary measures against static discharge.
P244 ..... Keep reduction valves free from grease and oil.
P250 ..... Do not subject to grinding/shock/…/friction.
P251 ..... Pressurized container: Do not pierce or burn, even after use.
P260 ..... Do not breathe dust/fume/gas/mist/vapours/spray.
P261 ..... Avoid breathing dust/fume/gas/mist/vapours/spray.
P262 ..... Do not get in eyes, on skin, or on clothing.
P263 ..... Avoid contact during pregnancy/while nursing.
P264 ..... Wash … thoroughly after handling.
P270 ..... Do no eat, drink or smoke when using this product.
P271 ..... Use only outdoors or in a well-ventilated area.
P272 ..... Contaminated work clothing should not be allowed out of the workplace.
P273 ..... Avoid release to the environment.
P280 ..... Wear protective gloves/protective clothing/eye protection/face protection.
P281 ..... Use personal protective equipment as required.
P282 ..... Wear cold insulating gloves/face shield/eye protection.
P283 ..... Wear fire/flame resistant/retardant clothing.
P284 ..... Wear respiratory protection.
P285 ..... In case of inadequate ventilation wear respiratory protection.
P301 ..... IF SWALLOWED:
P302 ..... IF ON SKIN:
P303 ..... IF ON SKIN (or hair):
P304 ..... IF INHALED:
P305 ..... IF IN EYES:
P306 ..... IF ON CLOTHING:
P307 ..... IF exposed:
P308 ..... IF exposed or concerned:
P309 ..... IF exposed or if you feel unwell:
P310 ..... Immediately call a POISON CENTER or doctor/physician.
P311 ..... Call a POISON CENTER or doctor/physician.
P312 ..... Call a POISON CENTER or doctor/physician if you feel unwell.
P313 ..... Get medical advice/attention.
P314 ..... Get medical advice/attention if you feel unwell.
P315 ..... Get immediate medical advice/attention.
P320 ..... Specific treatment is urgent (see … on this label).
P321 ..... Specific treatment (see … on this label).
P322 ..... Specific measures (see … on this label).
P330 ..... Rinse mouth.
P331 ..... Do NOT induce vomiting.
P332 ..... If skin irritation occurs:
P333 ..... If skin irritation or rash occurs:
P334 ..... Immerse in cool water/wrap in wet bandages.
P335 ..... Brush off loose particles from skin.
P336 ..... Thaw frosted parts with lukewarm water. Do no rub affected area.
P337 ..... If eye irritation persists:
P338 ..... Remove contact lenses, if present and easy to do. Continue rinsing.
P340 ..... Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P341 ..... If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing.
P342 ..... If experiencing respiratory symptoms:
P350 ..... Gently wash with plenty of soap and water.
P351 ..... Rinse cautiously with water for several minutes.
P352 ..... Wash with plenty of soap and water.
P353 ..... Rinse skin with water/shower.
P360 ..... Rinse immediately contaminated clothing and skin with plenty of water before removing clothes.
P361 ..... Remove/Take off immediately all contaminated clothing.
P362 ..... Take off contaminated clothing and wash before reuse.
P363 ..... Wash contaminated clothing before reuse.
P370 ..... In case of fire:
P371 ..... In case of major fire and large quantities:
P372 ..... Explosion risk in case of fire.
P373 ..... DO NOT fight fire when fire reaches explosives.
P374 ..... Fight fire with normal precautions from a reasonable distance.
P375 ..... Fight fire remotely due to the risk of explosion.
P376 ..... Stop leak if safe to do so.
P377 ..... Leaking gas fire: Do not extinguish, unless leak can be stopped safely.
P378 ..... Use … for extinction.
P380 ..... Evacuate area.
P381 ..... Eliminate all ignition sources if safe to do so.
P390 ..... Absorb spillage to prevent material damage.
P391 ..... Collect spillage.
P401 ..... Store …
P402 ..... Store in a dry place.
P403 ..... Store in a well-ventilated place.
P404 ..... Store in a closed container.
P405 ..... Store locked up.
P406 ..... Store in corrosive resistant/… container with a resistant inner liner.
P407 ..... Maintain air gap between stacks/pallets.
P410 ..... Protect from sunlight.
P411 ..... Store at temperatures not exceeding … oC/…oF.
P412 ..... Do not expose to temperatures exceeding 50 oC/122oF.
P413 ..... Store bulk masses greater than … kg/… lbs at temperatures not exceeding … oC/…oF.
P420 ..... Store away from other materials.
P422 ..... Store contents under …
P501 ..... Dispose of contents/container to …
P231 + P232 ..... Handle under inert gas. Protect from moisture.
P235 + P410 ..... Keep cool. Protect from sunlight.
P301+P310 ..... IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P301+P312 ..... IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
P302+P334 ..... IF ON SKIN: Immerse in cool water/wrap in wet bandages.
P302+P350 ..... IF ON SKIN: Gently wash with plenty of soap and water.
P302+P352 ..... IF ON SKIN: Wash with plenty of soap and water.
P304+P312 ..... IF INHALED: Call a POISON CENTER or doctor/physician if you feel unwell.
P304+P340 ..... IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P304+P341 ..... IF INHALED: If breathing is difficult, remove victim to fresh air and keep at rest in a position comfortable for breathing.
P306+P360 ..... IF ON CLOTHING: rinse immediately contaminated clothing and skin with plenty of water before removing clothes.
P307+P311 ..... IF exposed: Call a POISON CENTER or doctor/physician.
P308+P313 ..... IF exposed or concerned: Get medical advice/attention.
P309+P310 ..... IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.
P309+P311 ..... IF exposed or if you feel unwell: Call a POISON CENTER or doctor/physician.
P332+P313 ..... If skin irritation occurs: Get medical advice/attention.
P333+P313 ..... If skin irritation or rash occurs: Get medical advice/attention.
P335+P334 ..... Brush off loose particles from skin. Immerse in cool water/wrap in wet bandages.
P337+P313 ..... If eye irritation persists: Get medical advice/attention.
P342+P311 ..... If experiencing respiratory symptoms: Call a POISON CENTER or doctor/physician.
P370+P376 ..... In case of fire: Stop leak if safe to do so.
P370+P378 ..... In case of fire: Use … for extinction.
P370+P380 ..... In case of fire: Evacuate area.
P402+P404 ..... Store in a dry place. Store in a closed container.
P403+P233 ..... Store in a well-ventilated place. Keep container tightly closed.
P403+P235 ..... Store in a well-ventilated place. Keep cool.
P410+P403 ..... Protect from sunlight. Store in a well-ventilated place.
P410+P412 ..... Protect from sunlight. Do no expose to temperatures exceeding 50 oC/122oF.
P411+P235 ..... Store at temperatures not exceeding … oC/…oF. Keep cool.
P301+P330+P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off immediately all contaminated clothing. Rinse skin with water/shower.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P370+P380+P375 In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.
P371+P380+P375 In case of major fire and large quantities: Evacuate area. Fight fire remotely due to the risk of explosion.

Ordering Information

Conditions of sales

Our prices are usually in Euros (mainly DAP) and are exclusive of state or local taxes.

All written quotations will be honoured for 30 days unless specified.

For Transport, see your EURISO-TOP representative for appropriate pricing. Freight and/or shipping charges could also be added depending on the amount of the order.

Payment terms are net 30 days from date of invoice unless otherwise stated. Overdue invoices will be subject to late-payment penalties. From the due date, late payment interest will be applied as of right at the legal interest rate multiplied by 3 (three).

Shipping and Delivery

Our goal is to ship your order out to you as fast as we possibly can. Depending on the product purchased, the availability of the products and size of the order placed, your order may be split into multiple shipments to expedite the shipment of your entire order.

European Legislation

All shipments containing Deuterated solvents outside the E.U. are considered as dual-used materials by the European authorities. Pursuant to the regulation, export of dual-use items outside the EU customs territory generally requires an export autorisation. Your sales representative would let you have the appropriate documents to enable Euriso-Top to obtain the mandatory and applicable export license.

Returns

If your order is missing a product, contains a damaged item or other concern, please contact your sales representative at Euriso-Top or email us at sales@eurisotop.com We accept returns of unopened, unused items in their original packaging within 30 days of delivery, prior to Euris-Top approval. The buyer is responsible for approving the quality and quantity of any product within the 30 days period stated above. Product returns must reference the original purchase order number. If an error by Euriso-Top results in an incorrect or duplicate shipment, a replacement will be sent, or the appropriate credit allowed. Under no circumstances will credit or replacement be given for products without prior authorization by Euriso-Top.

Eurisotop
A CAMBRIDGE ISOTOPE LABORATORIES COMPANY

To request a quotation or place an order, please contact us

France & International

Tel : +33 (0)1 69 41 97 98
Fax : +33 (0)1 69 41 93 52
E-mail : sales@eurisotop.com

Euriso-Top Headquarter
Parc des Algorithmes, Bâtiment Homère
Route de l'Orme
F-91194 Saint-Aubin Cedex

Euriso-Top Production Plant
Bat 547-E / CEA Saclay
Route de Chateaufort
F-91191 Gif sur Yvette Cedex

Germany & Austria

Tel : +49 (0) 681 99 63 338
Fax : +49 (0) 681 99 63 438
E-mail : sales@eurisotop.de

Euriso-Top GmbH
Lebacher Str. 4
D - 66005 Saarbrücken

CIL Cambridge Isotope Laboratories

Headquarter

Cambridge Isotope Laboratories, Inc.
3 Highwood Drive
Tewksbury, MA 01876