

# Attractive.

MagniSolv™, deuterated solvents.





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# MagniSolv™, deuterated solvents for NMR (Nuclear Magnetic Resonance spectroscopy)

MagniSolv™ deuterated solvents are required wherever chemical research is carried out and are indispensable for the most important method in the structural analysis of organic molecules – the NMR spectroscopy. NMR is a non-destructive, information-rich analytical technique helping researchers to understand molecular structure and dynamics. A NMR experiment provides connectivity information – which atoms are attached to each other in a molecule, the spatial orientation and the motions of the molecule in its natural environment. Such structural information is especially critical in proteomics/genomics and drug discovery applications where scientists desire a deeper understanding of protein target molecules and their spatial relationships with synthetic drug candidates.

A wide range of MagniSolv™ deuterated solvents with extremely low residual water, excellent chemical purity, and the highest isotopic enrichment available can satisfy the most demanding requirements of researchers. Depending on application and sensitivity of the NMR spectrometer EMD Millipore offers MagniSolv™ solvents with deuteration degrees between 98% and 99.96%. In case of all the water soluble deuterated standard products, water content is specified according to both Karl Fischer and NMR. This is a unique benefit for our customers and underpins the position of EMD Millipore as a supplier of chemicals of the highest quality and reliability.

EMD Millipore provides a wide range of different packaging types (bottles, practical ampoules and septum bottles) and packaging sizes. Concerning the septum bottles we have the broadest range of deuterated products in this customer friendly packaging material. Here EMD Millipore's vast experience in the optimization of packaging is a unique benefit that we can fully utilize. We are also prepared to offer bulk quantities of MagniSolv™ deuterated compounds. This also applies to special package sizes and other grades.



### The history of NMR spectroscopy

The first successful nuclear magnetic resonance (NMR) experiment was made in 1946 independently by two scientists in the United States. Felix Bloch, working at Stanford University, and Edward Purcell, from Harvard University, found that when certain nuclei were placed in a magnetic field they absorbed energy in the radio frequency range of the electromagnetic spectrum, and re-emitted this energy when the nuclei transferred to their original state. The strength of the magnetic field and the radio frequency matched each other as earlier demonstrated by Sir Joseph Larmor (Irish physicist 1857–1942) and is known as the Larmor relationship (i.e., the angular frequency of precession of the nuclear spins being proportional to the strength of the magnetic field).

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This phenomenon was termed NMR as follows:
"Nuclear"as only the nuclei of certain atoms reacted in
that way; "Magnetic" as a magnetic field was required;
"Resonance" because of the direct frequency dependence
of the magnetic and radio frequency fields.
With this discovery NMR spectroscopy was born and
soon became an important analytical method in the
study of the composition of chemical compounds.
For this discovery Bloch and Purcell were awarded
the Nobel Prize for Physics in 1952.

Interestingly, Dr. Isidor Rabi, an American physicist who was awarded the Nobel Prize for Physics in 1944 for his invention of the atomic and molecular beam magnetic resonance method of observing atomic spectra, came across the NMR experiment in the late 1930's but considered it to be an artifact of his apparatus and disregarded its importance.

### Your Benefits

- Reliable results in the NMR-spectra by
  - excellent chemical purity and highest isotopic enrichment
  - reliable deuteration degrees
  - determination of water content in two ways (Karl Fischer and NMR)
- Easy and safe handling with septum bottles and glass ampoules
- Flexibility: broad packaging variety

Further Information please find in our lab tool "NMR chemical shifts" (W. 284109)

# Ordering information MagniSolv™ deuterated solvents A-D

	Product	Deuteration degree [%]	H <sub>2</sub> O+D <sub>2</sub> O (KF) [%]	H <sub>2</sub> O (NMR) [%]	Density at 20 °C [g/ml]	* *	Content [g]	Catalogue No
Α	Acetic acid-D1 99.5 % D	> 99.5	-	-	1.06	25 ml GL	26.50	M150350025
	Acetic acid-D4 99.5 %	> 99.5	< 0.05	_	1.12	10 x 0.75 ml GA	8.40	M150360009
					1.12	10 ml GA	11.20	M150360010
	Acetone-D6 99.9 % D	> 99.9	< 0.03	< 0.02	0.87	10 x 0.5 ml GA	4.35	M000210005
						10 x 0.75 ml GA	6.53	M000210009
						10 ml SB	8.70	M000210010
						25 ml GL	21.75	M000210025
						100 ml GL	87.00	M000210100
	Acetone-D6 99.96 % D	> 99.96	< 0.03	< 0.02	0.87	10 x 0.75 ml GA	6.53	M119690009
	Acetonitrile-D3 99 % D	> 99	< 0.10	< 0.05	0.84	10 ml SB	8.40	M029040010
	Acetonitrile-D3 99.8 % D	> 99.8	< 0.10	< 0.05	0.84	10 ml SB	8.40	M002200010
	Acetonitrile-D3 99.96 % D	> 99.96	< 0.02	< 0.01	0.84	1 ml GA	0.84	M137530001
						10 x 0.75 ml GA	6.30	M137530009
	Ammonia-D3 26 wt % in D <sub>2</sub> 0	> 99.5	_	_	1.06	10 ml GA	10.60	M150080010
						25 ml GL	26.50	M150080025
	tert-Butanol (ol-D) 99 % D	> 99	-	-	0.80	25 ml GL	20.00	M150140025
С	Chloroform 99.5 % D; 1 vol. % TMS stabilized with silver	> 99.5	-	< 0.02	1.50	25 ml GL	37.50	M133590025
						100 ml GL	150.00	M133590100
	Chloroform-D1 99.8 % D not stabilized	> 99.8	-	< 0.01	1.50	25 ml GL	37.50	M024500025
						100 ml GL	150.00	M024500100
						500 ml GL	750.00	M024500500
	Chloroform-D1 99.8 % D stabilized with silver	> 99.8	-	< 0.01	1.50	25 ml GL	37.50	M034200025
						100 ml GL	150.00	M034200100
						500 ml GL	750.00	M034200500
	Chloroform 99.8 % D;	> 99.8	-	< 0.01	1.50	25 ml GL	37.50	M032960025
	0.03 % TMS stabilized with					100 ml GL	150.00	M032960100
	silver					500 ml GL	750.00	M032960500
	Chloroform-D1 99.96 % D	> 99.96	-	< 0.005	1.50	10 x 0.75 ml GA	11.25	M024460009
						10 ml GA	15.00	M024460010
	25ml stabilized with silver					25 ml GL	37.50	M024460025
	100ml stabilized with silver					100 ml GL	150.00	M024460100
	Cumene (Isopropylbenzene)-D12 99 % D	> 99	-	_	0.95	1 ml GA	0.87	M150230001
	Cyclohexane-D12 99.5 % D	> 99.5	< 0.05	< 0.03	0.89	10 x 0.5 ml GA	4.45	M150240005
						10 x 0.75 ml GA	6.68	M150240009
						5 ml GA	4.45	M150240006
	n-Decane-D22 99 % D	> 99	-	_	0.85	1 ml GA	0.85	M150270001
	Deuterium chloride 20 wt % in D <sub>2</sub> O 99.5 % D	> 99.5	-	-	1.19	25 ml GL	29.75	M150160025
	Deuterium chloride 20 wt % in D <sub>2</sub> O 99.95 % D	> 99.95	-	-	1.19	10 ml GA	11.90	M150170010

 $\mathsf{GA} = \mathsf{glass} \; \mathsf{ampoule} \; | \; \mathsf{SB} = \mathsf{septum} \; \mathsf{bottle} \; | \; \mathsf{GL} = \mathsf{glass} \; \mathsf{bottle} \; |$ 

## Ordering information MagniSolv™ deuterated solvents D-L

F	Product	Deuteration degree [%]	H <sub>2</sub> 0+D <sub>2</sub> 0 (KF) [%]	H <sub>2</sub> O (NMR) [%]	Density at 20 °C [g/ml]	* * *	Content [g]	Catalogue N
	Deuterium chloride 38 wt %	> 99.5	-	-	1.26	10 ml GA	12.60	M15018001
	in D <sub>2</sub> O 99.5 % D					50 ml GL	63.00	M15018005
	Deuterium oxide 99.9 % D	> 99.9			1.11	10 x 0.75 ml GA	8.33	M13366000
ľ						10 ml SB	11.10	M1336600
						25 ml GL	27.75	M13366002
						100 ml GL	111.00	M13366010
						500 ml GL	555.00	M13366050
	Deuterium oxide 99.96 % D	> 99.96	_	_	1.11	10 x 0.5 ml GA	5.55	M0342800
						10 x 0.75 ml GA	8.33	M03428000
						10 ml SB	11.10	M0342800
						100 ml GL	111.00	M03428010
	1.2-Dichlorobenzene-D4 99 % D	> 99		< 0.03	1.34	5 ml GA	6.70	M1502900
	Dichloromethane-D2 99.8 % D	> 99.8		< 0.01	1.36	10 x 0.75 ml GA	10.20	M13720000
						10 ml GA	13.60	M1372000
_	Dichloromethane-D2 99.96 % D	> 99.96	-	< 0.005	1.36	10 x 0.5 ml GA	6.80	M0420000
						10 x 0.75 ml GA	10.20	M0420000
						10 ml GA	13.60	M0420000
-	Diethylether-D10 99 % D	> 99			0.78	1 ml GA	1.00	M15031000
-	Dimethylacetamide-D9 99 % D	> 99			1.03	1 ml GA	1.03	M1503200
-	Dimethylformamide-D7 99.5 % D	> 99.5	< 0.05	< 0.03	1.05	1 ml GA	1.05	M1165600
	,					10 x 0.75 ml GA	7.88	M1165600
-	Dimethylsulfate-D6 99.5 % D	> 99.5			1.40	5 ml GA	7.00	M1503400
-	Dimethylsulfoxide-D6 99.8 % D	> 99.8	< 0.03	< 0.02	1.19	10 x 0.5 ml GA	5.95	M0342400
Di	Jillieti ji Sanokate Bo oolo 10 B			(3.02		10 x 0.75 ml GA	8.93	M0342400
						10 ml SB	11.90	M0342400
						10 ml GA	11.90	M0342400
						25 ml GL	29.75	M0342400
						50 ml SB	59.5	M0342400
						100 ml GL	119.00	M0342401
-	Dimethylsulfoxide-D6 99.9 % D; 0.1 vol. % TMS	> 99.9	< 0.03	< 0.02	1.19	10 x 0.6 ml GA	7.14	M0358700
						25 ml SB	29.75	M0358700
						25 ml SB	29.75	M0358700
						100 ml GL	119.00	M0385701
-	Dimethylsulfoxide-D6 99.8 % D;	> 99.8		-	1.19	50 ml SB	59.5	M0359100
	0.03 vol. % TMS					100 ml GL	119.00	M0359101
-	Dimethylsulfoxide-D6 99.96 % D	) D > 99.96	< 0.02	< 0.01	1.19	10 x 0.5 ml GA	5.95	M0356200
	TELITY ISUITONIUC - DO 33.30 - 70 D					10 x 0.75 ml GA	8.93	M0356200
						10 ml GA	11.90	M0356.00
						25 ml GL	29.75	M0356200
-	Dimethylsulfoxide-D6 99.96 % D;	> 99.96	< 0.02	< 0.01	1.19	5 ml GA	5.95	M0359200
	0.03 vol. % TMS	> 55.50	< 0.02	< 0.01	1.15	25 ml GL	29.75	M0359200
-	Ethanol-D6 99 % D	> 99	< 0.10	< 0.05	0.90	1 ml GA	0.90	M0345000
-	Ethanol (ol-D) abs. 99.5 % D	> 99.5			0.80	50 ml GL	40.00	M1503700
-	Formic acid-D2 97 wt % in D <sub>2</sub> 0	> 99.5			1.27	10 ml GA	12.70	M1336500
_	Havefluore 2 present D2	- 00 F						
_	Hexafluoro-2-propanol-D2 99.5 % D	> 99.5	-	-	1.65	1 ml GA	1.65	M1504100
_		> 99.5			0.77	5 ml GA 1 ml GA	8.25 0.77	M1504100 M1504100 M1504300

GA = glass ampoule | SB = septum bottle | GL = glass bottle Note: \* Catalog Number is not available in Canada.

# Ordering information MagniSolv™ deuterated solvents M-X

	Product	Deuteration degree [%]	H <sub>2</sub> 0+D <sub>2</sub> 0 (KF) [%]	H <sub>2</sub> O (NMR) [%]	Density at 20 °C [g/ml]	* *	Content [g]	Catalogue No.
М	Methylcyclohexane-D14 99.5 % D	> 99.5	-	-	0.88	5 ml GA	4.40	M150530005
	Methanol (ol-D) 99.5 % D	> 99.5	_	_	0.81	50 ml GL	40.50	M150510050
						100 ml GL	81.00	M150510100
	Methanol-D4 99.8 % D	> 99.8	< 0.03	_	0.89	1 ml GA	0.89	M060280001
						10 x 0.5 ml GA	4.45	M060280005
						10 x 0.75 ml GA	6.68	M060280009
						10 ml SB	8.90	M060280010
						25 ml GL	22.25	M060280025
						25 ml SB	22.25	M060280026
						100 ml GL	89.00	M060280100
	Methanol-D4 99.95 % D	> 99.95	< 0.02	_	0.89	10 x 0.5 ml GA	4.45	M060250005
						10 x 0.75 ml GA	6.68	M060250009
	Methanol-D3 99.5 % D	> 99.5	-	-	0.87	1 ml GA	0.87	M150520001
						5 ml GA	4.35	M150520005
	Naphthalene-D8 98 % D	> 98	_	_		1 g GL	1.00	M150000001
	Nitrobenzene-D5 99.5 % D	> 99.5	_	_	1.25	10 ml GA	12.53	M150010010
	Nitromethane-D3 99 % D	> 99	< 0.10	< 0.05	1.18	2 x 0.75 ml GA	1.77	M029140002*
0	n-Octane-D18 99 % D	> 99	_	_	0.82	1 g GA	0.82	M150020001
	Phenol-D6 98 % D	> 98	_	_	-	5 g GL	5.00	M150030005
	Phosphoric acid-D3 85 wt % in D <sub>2</sub> O 99 % D	> 99	_	_	1.74	10 ml GA	17.40	M150580010
	2-Propanol (ol-D) 98 % D	> 98	-	-	0.79	25 ml GL	19.75	M150440025
	2-Propanol-D8 99.5 % D	> 99.5	-	-	0.89	5 ml GA	4.45	M150450005
	Pyridine-D5 99.8 % D	> 99.8	< 0.03	< 0.02	1.05	10 x 0.75 ml GA	7.88	M074750009
						10 ml SB	10.50	M074750010
	Sodium deuterium oxide $30 \text{ wt } \%$ in $D_2 O 99.5 \% D$	> 99.5	-	-	1.46	25 ml GL	36.50	M150550025
	Sulfuric acid-D2 96-98 wt % in D <sub>2</sub> 0	> 99.5	-	-	1.88	25 ml GL	47.00	M150600025
						50 ml GL	94.00	M150600050
	Styrene-D8 98 % D	> 99	-	-	0.98	1 ml GA	0.98	M150610001
						10 ml GA	9.80	M150610010
	Tetrachloroethane-D2 99.5 % D	> 99.5	-	< 0.02	1.62	10 x 0.75 ml GA	12.15	M034950009
						25 ml GL	40.50	M034950025
	Tetramethylsilane	> 99.7	_		0.64	100 ml GL	64.00	M081830100
	TMS-Propionic acid-D4-Na 98 % D	> 98	-	_	_	1 g GL	1.00	M086520001
	Tetrahydrofuran-D8 99.5 % D	> 99.5	< 0.05	< 0.03	0.99	1 ml GA	0.99	M133640001
						10 x 0.75 ml GA	7.43	M133640009
						10 ml SB	9.90	M133640010
	Toluene-D8 99.5 % D	> 99.5	-	< 0.02	0.94	10 ml SB	9.40	M133680010
	Trifluoroacetic acid-D1 99.5 % D	> 99.5	< 0.05	< 0.03	1.50	10 ml GA	15.00	M133630010
	p-Xylene-D10 99.5 % D	> 99.5	_	_	0.95	10 ml GA	9.50	M150050010

 $GA = glass\ ampoule\ |\ SB = septum\ bottle\ |\ GL = glass\ bottle\ Note:\ ^*$  Catalog Number is not available in Canada.

# NMR Nuclear magnetic resonance MagniSolv™ deuterated solvents

Whatever you require! EMD Millipore provides a wide range of products in different packaging types and -sizes.







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