

# Attractive.

## MagniSolv<sup>™</sup>, deuterated solvents.





## MagniSolv<sup>™</sup>, deuterated solvents for NMR (Nuclear Magnetic Resonance spectroscopy)

MagniSolv<sup>™</sup> 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, informationrich 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 Merck 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 Merck Millipore as a supplier of chemicals of highest quality and reliability.

Merck 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 Merck 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).

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)
- Innovative packaging for long-term storage without quality loss
- Easy, save and accident-free handling with septum bottles and glass ampoules
- Flexibility through broad packaging variety for less chemical and packaging waste

### Ordering information MagniSolv<sup>™</sup> 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
Acetic acid-D1 99.5 % D	>99.5	-	-	1.06	25 ml GL	26.50	8.15035.0025
Acetic acid-D4 99.5 %	>99.5	<0.05	-	1.12	10 x 0.75 ml GA	8.40	8.15036.0009
				1.12	10 ml GA	11.20	8.15036.0010
Acetone-D6 99.9 % D	>99.9	< 0.03	< 0.02	0.87	10 x 0.5 ml GA	4.35	1.00021.0005
					10 x 0.75 ml GA	6.53	1.00021.0009
					10 ml SB	8.70	1.00021.0010
					25 ml GL	21.75	1.00021.0025
					100 ml GL	87.00	1.00021.0100
Acetone-D6 99.96 % D	>99.96	< 0.03	<0.02	0.87	10 x 0.75 ml GA	6.53	1.11969.0009
Acetonitrile-D3 99 % D	>99	<0.10	<0.05	0.84	10 ml SB	8.40	1.02904.0010
Acetonitrile-D3 99.8 % D	>99.8	<0.10	<0.05	0.84	10 ml SB	8.40	1.00220.0010
Acetonitrile-D3 99.96 % D	>99.96	< 0.02	<0.01	0.84	1 ml GA	0.84	1.13753.0001
					10 x 0.75 ml GA	6.30	1.13753.0009
Ammonia-D3 26 wt % in D <sub>2</sub> 0	>99.5	_	_	1.06	10 ml GA	10.60	8.15008.0010
					25 ml GL	26.50	8.15008.0025
Benzene-D6 99.6 % D	>99.6	-	<0.02	0.95	10 x 0.75 ml GA	7.13	1.01789.0009
					10 ml SB	9.50	1.01789.0010
					100 ml GL	95.00	1.01789.0100
Benzene-D6 99.96 % D	>99.96			0.95	10 x 0.75 ml GA	7.13	1.01766.0009
					10 ml GA	9.50	1.01766.0010
tert-Butanol (ol-D) 99 % D	>99	_		0.80	25 ml GL	20.00	8.15014.0025
Chloroform 99.5 % D;	>99.5	_	<0.02	1.50	25 ml GL	37.50	1.13359.0025
1 vol. % TMS stabilized with silver					100 ml GL	150.00	1.13359.0100
Chloroform-D1 99.8 % D not stabilized	>99.8	-	<0.01	1.50	25 ml GL	37.50	1.02450.0025
					100 ml GL	150.00	1.02450.0100
					500 ml GL	750.00	1.02450.0500
Chloroform-D1 99.8 % D stabilized with silver	>99.8	-	<0.01	1.50	25 ml GL	37.50	1.03420.0025
					100 ml GL	150.00	1.03420.0100
					500 ml GL	750.00	1.03420.0500
Chloroform 99.8 % D; 0.03 % TMS stabilized with silver	>99.8	-	<0.01	1.50	25 ml GL	37.50	1.03296.0025
					100 ml GL	150.00	1.03296.0100
					500 ml GL	750.00	1.03296.0500
Chloroform-D1 99.96 % D	>99.96	_	< 0.005	1.50	10 x 0.75 ml GA	11.25	1.02446.0009
					10 ml GA	15.00	1.02446.0010
25 ml stabilized with silver					25 ml GL	37.50	1.02446.0025
100 ml stabilized with silver					100 ml GL	150.00	1.02446.0100
Cumene (Isopropylbenzene)-D12 99 % D	>99	-		0.95	1 ml GA	0.87	8.15023.0001
Cyclohexane-D12 99.5 % D	>99.5	< 0.05	< 0.03	0.89	10 x 0.5 ml GA	4.45	8.15024.0005
					10 x 0.75 ml GA	6.68	8.15024.0009
					5 ml GA	4.45	8.15024.0006
n-Decane-D22 99 % D	>99	-	_	0.85	1 ml GA	0.85	8.15027.0001
Deuterium chloride 20 wt % in D <sub>2</sub> O 99.5 % D	>99.5	-		1.19	25 ml GL	29.75	8.15016.0025
Deuterium chloride 20 wt % in D <sub>2</sub> O 99.95 % D	>99.95	_	-	1.19	10 ml GA	11.90	8.15017.0010

GA = glass ampoule | SB = septum bottle | GL = glass bottle

### Ordering information MagniSolv<sup>™</sup> deuterated solvents D – E

	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 N
	Deuterium chloride 38 wt %	>99.5	-	-	1.26	10 ml GA	12.60	8.15018.001
ľ	in D <sub>2</sub> 0 99.5 % D					50 ml GL	63.00	8.15018.005
ľ	Deuterium oxide 99.9 % D	>99.9	-	_	1.11	10 x 0.75 ml GA	8.33	1.13366.000
						10 ml SB	11.10	1.13366.001
						25 ml GL	27.75	1.13366.002
						100 ml GL	111.00	1.13366.010
						500 ml GL	555.00	1.13366.050
	Deuterium oxide 99.96 % D	>99.96	_	_	1.11	10 x 0.5 ml GA	5.55	1.03428.000
						10 x 0.75 ml GA	8.33	1.03428.000
						10 ml SB	11.10	1.03428.00
						100 ml GL	111.00	1.03428.010
	1.2-Dichlorobenzene-D4 99 % D	>99	-	<0.03	1.34	5 ml GA	6.70	8.15029.000
	Dichloromethane-D2 99.8 % D	>99.8	-	<0.01	1.36	10 x 0.75 ml GA	10.20	1.13720.00
						10 ml GA	13.60	1.13720.00
	Dichloromethane-D2 99.96 % D	>99.96	-	< 0.005	1.36	10 x 0.5 ml GA	6.80	1.04200.00
						10 x 0.75 ml GA	10.20	1.04200.00
						10 ml GA	13.60	1.04200.00
	Diethylether-D10 99 % D	>99	-	-	0.78	1 ml GA	1.00	8.15031.00
	Dimethylacetamide-D9 99 % D	>99	-	-	1.03	1 ml GA	1.03	8.15032.00
	Dimethylformamide-D7 99.5 % D	>99.5	< 0.05	< 0.03	1.05	1 ml GA	1.05	1.11656.00
						10 x 0.75 ml GA	7.88	1.11656.00
1	Dimethylsulfate-D6 99.5 % D	>99.5		_	1.40	5 ml GA	7.00	8.15034.00
1	Dimethylsulfoxide-D6 99.8 % D	>99.8	< 0.03	< 0.02	1.19	10 x 0.5 ml GA	5.95	1.03424.00
						10 x 0.75 ml GA	8.93	1.03424.00
						10 ml SB	11.90	1.03424.00
						10 ml GA	11.90	1.03424.00
						25 ml GL	29.75	1.03424.00
						50 ml SB	59.5	1.03424.00
						100 ml GL	119.00	1.03424.01
	Dimethylsulfoxide-D6 99.9 % D;	>99.9	< 0.03	< 0.02	1.19	10 x 0.6 ml GA	7.14	1.03587.00
	0.1 vol. % TMS					25 ml SB	29.75	1.03587.00
						25 ml SB	29.75	1.03587.00
						100 ml GL	119.00	1.03857.01
	Dimethylsulfoxide-D6 99.8 % D; 0.03 vol. % TMS	>99.8	-	-	1.19	50 ml SB	59.5	1.03591.00
	0.03 001. %0 11015					100 ml GL	119.00	1.03591.01
	Dimethylsulfoxide-D6 99.96 % D	>99.96	< 0.02	<0.01	1.19	10 x 0.5 ml GA	5.95	1.03562.00
						10 x 0.75 ml GA	8.93	1.03562.00
1						10 ml GA	11.90	1.03562.00
1						25 ml GL	29.75	1.03562.00
ľ	Dimethylsulfoxide-D6 99.96 % D;	>99.96	<0.02	<0.01	1.19	5 ml GA	5.95	1.03592.00
	0.03 vol. % TMS					25 ml GL	29.75	1.03592.00
ŀ	Ethanol-D6 99 % D	>99	<0.10	< 0.05	0.90	1 ml GA	0.90	1.03450.00
ŀ	Ethanol (ol-D) abs. 99.5 % D	>99.5			0.80	50 ml GL	40.00	8.15037.00

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### Ordering information MagniSolv<sup>™</sup> deuterated solvents F – X

	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]	1 C C C C C C C C C C C C C C C C C C C	Content [g]	Catalogue No.
	Formic acid-D2 97 wt $\%$ in D <sub>2</sub> O	>99.5	-	-	1.27	10 ml GA	12.70	1.13365.0010
Н	Hexafluoro-2-propanol-D2 99.5 % D	>99.5		-		5 ml GA	8.25	8.15041.0005
	n-Hexane-D14 99 % D	>99		_	0.77	1 ml GA	0.77	8.15043.0001
L	Lithiumaluminiumdeuterid 98 %	>98	_	_	_	5 g GL	5.00	8.15048.0005
Μ	Methylcyclohexane-D14 99.5 % D	>99.5	-	-	0.88	5 ml GA	4.40	8.15053.0005
	Methanol (ol-D) 99.5 % D	>99.5	-	_	0.81	50 ml GL	40.50	8.15051.0050
		_				100 ml GL	81.00	8.15051.0100
	Methanol-D4 99.8 % D	>99.8	< 0.03	-	0.89	1 ml GA	0.89	1.06028.0001
						10 x 0.5 ml GA	4.45	1.06028.0005
						10 x 0.75 ml GA	6.68	1.06028.0009
						10 ml SB	8.90	1.06028.0010
						25 ml GL	22.25	1.06028.0025
						25 ml SB	22.25	106028.0026
						100 ml GL	89.00	1.06028.0100
	Methanol-D4 99.95 % D	>99.95	< 0.02	-	0.89	10 x 0.5 ml GA	4.45	1.06025.0005
						10 x 0.75 ml GA	6.68	1.06025.0009
	Methanol-D3 99.5 % D	>99.5	_	_	0.87	1 ml GA	0.87	8.15052.0001
						5 ml GA	4.35	8.15052.0005
	Naphthalene-D8 98 % D	>98	_	_		1 g GL	1.00	8.15000.0001
	Nitrobenzene-D5 99.5 % D	>99.5	-	_	1.25	10 ml GA	12.53	8.15001.0010
	Nitromethane-D3 99 % D	>99	<0.10	<0.05	1.18	2 x 0.75 ml GA	1.77	1.02914.0002
0	n-Octane-D18 99 % D	>99	_	_	0.82	1 g GA	0.82	8.15002.0001
	Phenol-D6 98 % D	>98	-	-	-	5 g GL	5.00	8.15003.0005
	Phosphoric acid-D3 85 wt % in D <sub>2</sub> O 99 % D	>99	-	-	1.74	10 ml GA	17.40	8.15058.0010
	2-Propanol (ol-D) 98 % D	>98	-	-	0.79	25 ml GL	19.75	8.15044.0025
	2-Propanol-D8 99.5 % D	>99.5	-	-	0.89	5 ml GA	4.45	8.15045.0005
	Pyridine-D5 99.8 % D	>99.8	< 0.03	<0.02	1.05	10 x 0.75 ml GA	7.88	1.07475.0009
						10 ml SB	10.50	1.07475.0010
	Sodium deuterium oxide 30 wt % in D <sub>2</sub> O 99.5 % D	>99.5	-	-	1.46	25 ml GL	36.50	8.15055.0025
	Sulfuric acid-D2 96 – 98 wt % in D <sub>2</sub> 0	>99.5	-	-	1.88	25 ml GL	47.00	8.15060.0025
	-					50 ml GL	94.00	8.15060.0050
	Styrene-D8 98 % D	>99	-	-	0.98	1 ml GA	0.98	8.15061.0001
						10 ml GA	9.80	8.15061.0010
	Tetrachloroethane-D2 99.5 % D	>99.5	-	< 0.02	1.62	10 x 0.75 ml GA	12.15	1.03495.0009
						25 ml GL	40.50	1.03495.0025
	Tetramethylsilane	>99.7	-		0.64	100 ml GL	64.00	1.08183.0100
	TMS-Propionic acid-D4-Na 98 % D	>98	-	-	-	1 g GL	1.00	1.08652.0001
	Tetrahydrofuran-D8 99.5 % D	>99.5	< 0.05	<0.03	0.99	1 ml GA	0.99	1.13364.0001
						10 x 0.75 ml GA	7.43	1.13364.0009
						10 ml SB	9.90	1.13364.0010
	Toluene-D8 99.5 % D	>99.5	_	<0.02	0.94	10 ml SB	9.40	1.13368.0010
	Trifluoroacetic acid-D1 99.5 % D	>99.5	< 0.05	<0.03	1.50	10 ml GA	15.00	1.13363.0010
Х	p-Xylene-D10 99.5 % D	>99.5	_	_	0.95	10 ml GA	9.50	8.15005.0010

 $GA = glass ampoule \mid SB = septum bottle \mid GL = glass bottle$ 

# NMR Nuclear magnetic resonance MagniSolv<sup>™</sup> deuterated solvents

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



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





For further information on Merck Millipore and our products contact: Merck KGaA 64271 Darmstadt, Germany www.merckmillipore.com

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