AcroSeal Packaging

An Application Guide



Solvents and Reagents

Drier For Longer





Introduction

Organic reagents have a wide series of applications in drug discovery, agrochemical research, flavours and fragrances, diagnostics and NMR analysis. Reactions often involve the use of air and moisture sensitive solvents, pyrophoric and hazardous reagents. Our AcroSeal™ packaging is an industry leading packaging solution for safe handling of these types of materials.

This brochure provides an overview of the key advantages of AcroSeal packaging for your research and outlines some important reactions that could benefit.

AcroSeal Packaging Provides...



PERFORMANCE

The specially designed multi-layer septum ensures a better re-seal thus minimizing atmospheric exposure and protecting the quality of your air and moisture sensitive solvents and reagents.



CONVENIENCE

A wide range of pre-prepared reagents in solution are available, reducing the risks and saving the time and effort of making your own.



SAFETY

Our AcroSeal cap system ensures you can transfer the contents of the bottle safely into your reaction vessel minimizing your exposure to potentially hazardous chemicals.





Contents

	Page no.
Introduction	2
Performance	3
Grignard Reagents	4
Convenience	5-6
Organolithium Reagents	7
Safety	8
Hydride Reducing Reagents	9
Other AcroSeal Packaged Products	
Top Tips for Using AcroSeal Packaging	



When carrying out synthetic organic chemistry, exposing many solvents and reagents to air and moisture inhibits their ability to perform properly and can cause some, if not all, of the following issues:

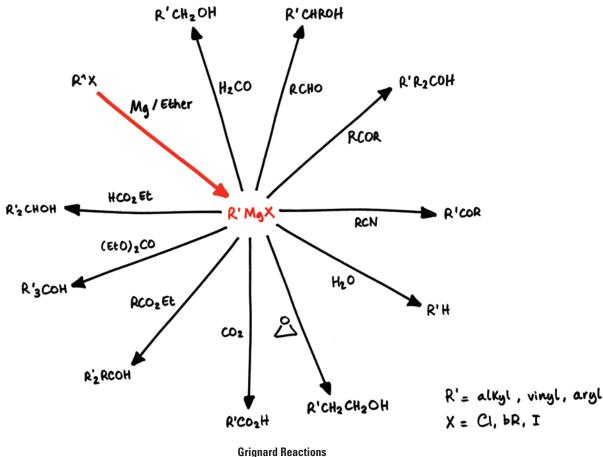
- · A failed synthesis
- · Poor yield
- · Greater number of by-products/impurities
- More challenging purification

Our AcroSeal packaging solution is innovative and simple as we endeavour to:-

- · Pack the product when it is as dry as possible
- · Make it easy to keep it dry when transferring from the packaging into your dry system
- · Ensure products stay dry between repeated use

Grignard Reaction

The Grignard reaction is an essential method in the formation of carbon-carbon bonds. In reactions involving Grignard Reagents it is essential to exclude water and air, which rapidly destroy the reagent. Therefore, we provide these sensitive reagents in the industry-leading AcroSeal packaging, preventing the degradation of the reagents. An example of a reaction that can be severely affected by the presence of water is the grignard reaction.



Grignard Reagents

A selection of our grignard reagents can be found in the table below.

Product Code	Product Name	CAS no.
20953	Allylmagnesium bromide, 1M solution in diethyl ether, AcroSeal	1730-25-2
20967	Allylmagnesium chloride, 1.7M solution in THF, AcroSeal	2622-05-1
38955	Benzylmagnesium chloride, 1.4M solution in THF, AcroSeal	6921-34-2
42746	3-Butenylmagnesium bromide, 0.5M solution in THF, AcroSeal	7103-09-5
33167	tert-Butylmagnesium chloride, 1.7M solution in THF, AcroSeal	677-22-5
39749	3-Chlorophenylmagnesium bromide, 0.5M solution in THF, AcroSeal	36229-42-2
44595	Cyclopropylmagnesium bromide, 0.5M solution in 2-MeTHF, AcroSeal	23719-80-4
39761	Cyclopropylmagnesium bromide, 0.5M solution in THF, AcroSeal	23719-80-4
43190	(1,3-Dioxan-2-ylethyl)magnesium bromide, 0.5M solution in THF, AcroSeal	480438-44-6
34729	Ethylmagnesium bromide, 3M in diethyl ether, AcroSeal	925-90-6
21047	Ethylmagnesium bromide, 0.9M solution in THF, AcroSeal	925-90-6
25257	Ethylmagnesium chloride, 2.7M (25 wt.%) solution in THF, AcroSeal	2386-64-3
43912	Ethynylmagnesium bromide, 0.5M solution in THF, AcroSeal	4301-14-8
38895	Ethynylmagnesium chloride, 0.6M solution in THF/Toluene, AcroSeal	65032-27-1
43303	Heptylmagnesium bromide, 1M solution in diethyl ether, AcroSeal	13125-66-1
42775	Isopropenylmagnesium bromide, 0.5M solution in THF, AcroSeal	13291-18-4
42678	Isopropylmagnesium bromide, 3M solution in 2-MeTHF, AcroSeal	920-39-8
21285	Isopropylmagnesium chloride, 2.0M solution in THF, AcroSeal	1068-55-9
38628	Isopropylmagnesium chloride - Lithium chloride complex, 1.3M solution in THF, AcroSeal	745038-86-2
21073	2-Mesitylmagnesium bromide, 1M solution in THF, AcroSeal	2633-66-1
37742	4-Methoxyphenylmagnesium bromide, 1M solution in THF, AcroSeal	13139-86-1
42741	2-Methylallylmagnesium chloride, 0.5M solution in THF, AcroSeal	5674-01-1
18354	Methylmagnesium bromide, 3M solution in diethyl ether, AcroSeal	75-16-1
39112	Methylmagnesium bromide, 3.2M solution in 2-MeTHF, AcroSeal	75-16-1
37738	Methylmagnesium bromide, 1M solution in THF, AcroSeal	75-16-1
25256	Methylmagnesium chloride, 3M (22 wt.%) solution in THF, AcroSeal	676-58-4
42740	Methylmagnesium iodide, 3M solution in diethyl ether, AcroSeal	917-64-6
43556	2-Methyl-1-propenylmagnesium bromide, 0.5M solution in THF, AcroSeal	38614-36-7
43874	Pentafluorophenylmagnesium bromide, 0.5M solution in diethyl ether, AcroSeal	879-05-0
43467	1-Propenylmagnesium bromide, 0.5M solution in THF, AcroSeal	14092-04-7
42607	1-Propynylmagnesium bromide, 0.5M solution in THF, AcroSeal	16466-97-0
37746	(Trimethylsilyl)methylmagnesium chloride, 1.3M solution in THF, AcroSeal	13170-43-9
44597	Vinylmagnesium bromide, 1M solution in 2-MeTHF, AcroSeal	1826-67-1
20939	Vinylmagnesium bromide, 0.7M solution in THF, AcroSeal	1826-67-1
25259	Vinylmagnesium chloride, 1.9M (16.5 wt.%) solution in THF, AcroSeal	3536-96-7



Freshly preparing anhydrous solvents and reagents for use in chemical synthesis is not a trivial exercise and takes time, specialized equipment and handling practices. For example, preparing gaseous solutions can involve handling cylinders and distillation.



Glove box to handle air and moisture sensitive reagents

Alkyllithium Reagents

The most common members of the alkyllithium family are n-Butyllithium, Methyllithium and tert-Butyllithium and these are widely used in organic synthesis. Fresh solutions can be created in the lab, requiring complex, potentially hazardous and time consuming steps, including movement and use of gas cylinders and distillation steps.

Alternatively, AcroSeal packaging provides a wide range of anhydrous solvents and reagents for immediate use, saving you both time and money.

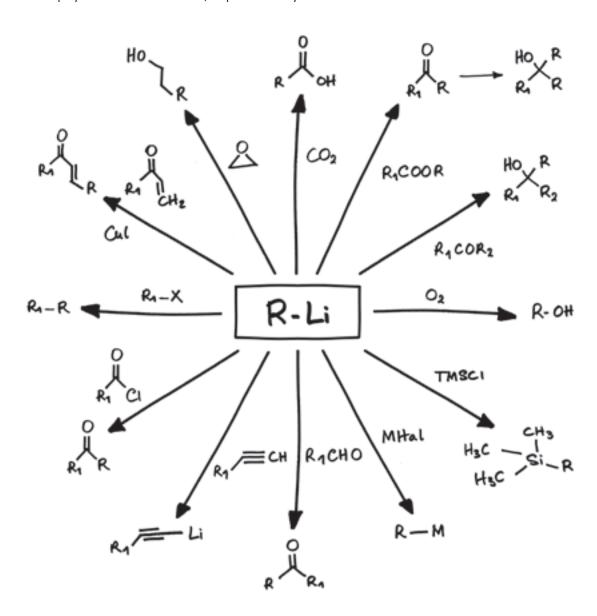
Some examples of their applications are given below:

- **Metallation** Many hundreds of functionalised organolithium compounds have been prepared by the metallation reaction with n-Butyllithium or other alkyllithium compounds.
- Ortho-metallation Metallation of an aromatic ring near a substituent, which acts as a "directed metalation group", is called ortho-metallation.
- Nucleophilic Addition and Substitution Stabilized organolithium compounds like enolates and sulfonyl carbanions can react as nucleophiles with alkyl-halogenides and carbonylcompounds in a wide range of reactions:
 - Alkylation of Alkyl-halogenides
 - Addition to Carbonyl-compounds
 - Alkylation of Allyl-halogenides
 - Epoxide-Ring Opening
 - Conjugate Addition
 - Addition to Carbon dioxide

5



- Halogen-Metal Exchange The Halogen-metal exchange reaction was discovered in the late 1930s by Gilman and Wittig. The reaction is often used to prepare vinyl and aryllithium compounds from the more reactive alkyllithium species.
- **Transmetallation** The organolithium compounds are very often used to prepare other metallorganic compounds through the transmetallation reaction.
- Anionic Polymerisation A major industrial use of alkyllithium compounds, specifically n-Butyllithium, is the catalysis of the anionic polymerization of butadiene, isoprene and styrene.



Organolithium Reactions

Organolithium Reagents

A selection of our organolithium reagents can be found in the table below.

Product Code	Product Name	CAS no.
37749	n-Butyllithium, 2.2M solution in cyclohexane, AcroSeal	109-72-8
21335	n-Butyllithium, 2.5M solution in hexanes, AcroSeal	109-72-8
18127	n-Butyllithium, 1.6M solution in hexanes, AcroSeal	109-72-8
37893	n-Butyllithium, 2.7M solution in toluene, AcroSeal	109-72-8
18754	sec-Butyllithium, 1.3M sol. in cyclohexane/hexane (92/8), AcroSeal	598-30-1
39654	tert-Butyllithium, 1.9M solution in pentane, AcroSeal	594-19-4
44592	tert-Butyllithium, 2M (18%) solution in heptane, AcroSeal	594-19-4
30165	n-Hexyllithium, 33 wt.% solution in n-hexane, AcroSeal	21369-64-2
37759	Isobutyllithium, 1.6M solution in heptane, AcroSeal	920-36-5
43988	Lithium acetylide ethylenediamine complex, 25 wt.% slurry in toluene, AcroSeal	6867-30-7
43455	Lithium aluminium hydride bis(tetrahydrofuran), 1M solution in toluene, AcroSeal	123439-81-6
38023	Lithium bis(trimethylsilyl)amide, 0.9M solution in methylcyclohexane, AcroSeal	4039-32-1
34567	Lithium bis(trimethylsilyl)amide, 1.0M sol. in methyl tert-butyl ether, AcroSeal	4039-32-1
44611	Lithium bis(trimethylsilyl)amide, 15% in 2-MeTHF/Ethylbenzene, AcroSeal	4039-32-1
20955	Lithium bis(trimethylsilyl)amide, 1M solution in THF, AcroSeal	4039-32-1
34770	Lithium bis(trimethylsilyl)amide, 1M solution in THF/Ethylbenzene, AcroSeal	4039-32-1
44684	Lithium tert-butoxide, 0.9M (8 wt.%) solution in 2-MeTHF, AcroSeal	1907-33-1
37931	Lithium tert-butoxide, 2.2M solution in THF, AcroSeal	1907-33-1
26883	Lithium diisopropylamide, 2M sol. in THF/n-heptane/ethylbenzene, AcroSeal	4111-54-0
43287	Lithium diisopropylamide mono(tetrahydrofuran), 1.5M solution in cyclohexane, AcroSeal	123333-84-6
43362	Lithium diphenylphosphide, 0.5M solution in THF, AcroSeal	65567-06-8
38017	Lithium ethoxide, 1M solution in ethanol, AcroSeal	2388-07-0
39650	Lithium isopropoxide, 3M solution in THF, AcroSeal	2388-10-5
33675	Lithium methoxide, pure, 2.2M (10 wt%) solution in methanol, AcroSeal	865-34-9
38861	Lithium phenoxide, 0.6M solution in THF, AcroSeal	555-24-8
43350	Lithium thiophenolate, 0.6M solution in THF, AcroSeal	2973-86-6
17645	Lithium tri-sec-butylborohydride, 1M solution in THF, AcroSeal	38721-52-7
37758	Lithium tri-tert-butoxyaluminohydride, 1.1M solution in THF, AcroSeal	17476-04-9
45069	Lithium triethylborohydride, 1.7M solution in THF, AcroSeal	22560-16-3
38065	Lithium (trimethylsilyl)acetylide, 0.5M solution in THF/hexanes, AcroSeal	54655-07-1
43911	Lithium tris[(3-ethyl-3-pentyl)oxy]aluminohydride, 0.5M solution in THF, AcroSeal	79172-99-9
18875	Methyllithium, 1.6 M sol. in diethyl ether (± 5% w/v), AcroSeal	917-54-4
18129	Methyllithium, 2.2M (6wt%) in diethyl ether with LiBr, AcroSeal	332360-06-2
44584	Methyllithium, 3% solution in 2-MeTHF/cumene, AcroSeal	917-54-4
37745	(Trimethylsilyl)methyllithium, 0.7M (10 wt%) solution in hexanes, AcroSeal	1822-00-0



The highly reactive reagents often required in organic synthesis may be hazardous to use, including compounds that can be pyrophoric, toxic, carcinogenic, mutagenic, corrosive and odourous e.g. thiols.

AcroSeal packaging provides a safer solution for handling these reagents by allowing removal of the reagent from the bottle under an inert atmosphere and without exposure to the contents.

Lithium Aluminium Hydride

Lithium aluminium hydride is an example of an extremely pyrophoric reducing agent, used in organic synthesis, especially for the reduction of esters, carboxylic acids and amides.

Lithium Aluminium Hydride Reactions

Hydride Reducing Reagents

A selection of our hydride reducing reagents can be found in the table below.

Product code	Product name	CAS no.
20105	Diisobutylaluminium hydride, 1.0M solution in heptane, AcroSeal	1191-15-7
18379	Diisobutylaluminium hydride, 1M solution in hexanes, AcroSeal	1191-15-7
20103	Diisobutylaluminium hydride, 1.1M solution in cyclohexane, AcroSeal	1191-15-7
20108	Diisobutylaluminium hydride, 1.2M (20 wt.%) solution in toluene, AcroSeal	1191-15-7
19949	Lithium aluminium hydride, 1M solution in THF, AcroSeal	16853-85-3
37732	Lithium aluminium hydride, 2.4M solution in THF, AcroSeal	16853-85-3
38557	Lithium aluminium hydride, 3.5M (15 wt.%) solution in toluene/THF, AcroSeal	16853-85-3
19951	Lithium aluminium hydride, 4.0M solution in diethyl ether, AcroSeal	16853-85-3
43455	Lithium aluminium hydride bis(tetrahydrofuran), 1M solution in toluene, AcroSeal	123439-81-6
42888	Lithium borohydride, 4M (10 wt.%) solution in THF, AcroSeal	16949-15-8
37758	Lithium tri-tert-butoxyaluminohydride, 1.1M solution in THF, AcroSeal	17476-04-9
17645	Lithium tri-sec-butylborohydride, 1M solution in THF, AcroSeal	38721-52-7
43911	Lithium tris[(3-ethyl-3-pentyl)oxy]aluminohydride, 0.5M solution in THF, AcroSeal	79172-99-9
20968	Lithium trisiamylborohydride, 1M solution in THF, AcroSeal	60217-34-7
20547	Potassium tri-sec-butylborohydride, 1M solution in THF, AcroSeal	54575-49-4
18918	Potassium triisopropoxyborohydride, 1M solution in THF, AcroSeal	42278-67-1
43091	Sodium bis(2-methoxyethoxy)aluminium hydride, 70 wt.% solution in toluene (approx. 3.5M) , AcroSeal	22722-98-1
19113	Sodium borohydride, 0.5M solution in diglyme, AcroSeal	16940-66-2
42913	Sodium borohydride, 12% solution in 40% aq. NaOH solution, AcroSeal	16940-66-2
37245	Sodium cyanoborohydride, 1M solution in THF, AcroSeal	25895-60-7
20003	Sodium triethylborohydride, 1M solution in THF, AcroSeal	17979-81-6
42914	Sodium tri-sec-butylborohydride, 1M solution in THF, AcroSeal	67276-04-4

Other AcroSeal Packaged Products

Alongside the aforementioned categories of reagents, a broad range of other products are available packaged in AcroSeal, including:

- Deuterated solvents
- · Extra dry solvents
- Organics
- Organometallics
- Reagents in solution

A selection of these reagents can be found in the tables below.

Product code	Product name	CAS no.
Deuterated Solv	ents	
21742	Acetonitrile-d3, for NMR, 99.8 atom% D, AcroSeal	2206-26-0
42677	Chloroform-d, for NMR, 99.8 atom % D, AcroSeal	865-49-6
42693	Deuterium oxide, for NMR, 99.8 atom % D, AcroSeal	7789-20-0
43399	Dichloromethane-d2, for NMR, 99.5 atom % D, AcroSeal	1665-00-5
42694	Methyl sulfoxide-d6, for NMR, 99.9 atom% D, AcroSeal	2206-27-1
Extra Dry Solver	nts	
36431	Acetonitrile, 99.9%, Extra Dry over Molecular Sieve, AcroSeal	75-05-8
34846	Dichloromethane, 99.8%, Extra Dry over Molecular Sieve, Stabilized, AcroSeal	75-09-2
34843	N,N-Dimethylformamide, 99.8%, Extra Dry over Molecular Sieve, AcroSeal	68-12-2
34845	Tetrahydrofuran, 99.5%, Extra Dry over Molecular Sieve, Stabilized, AcroSeal	109-99-9
32697	Tetrahydrofuran, 99.85%, Extra Dry, stabilized, AcroSeal	109-99-9
Organics		
42727	Chlorodiisopropylphosphine, 96%, AcroSeal	40244-90-4
44618	N,N'-Diisopropylcarbodiimide, 99%, AcroSeal	693-13-0
42720	Pivaldehyde, 97%, AcroSeal	630-19-3
43646	Trioctylphosphine, 90%, technical grade, AcroSeal	4731-53-7
44724	Xylenes, 99%, for biochemistry and histology, mixed isomers with ethylbenzene, AcroSeal	1330-20-7
Organometallics	S	
30176	Bis(cyclopentadienyl)dimethyltitanium, 5 wt% in toluene, AcroSeal	1271-66-5
37756	Diisobutylaluminium chloride, 0.8M solution in heptane, AcroSeal	1779-25-5
18379	Diisobutylaluminium hydride, 1M solution in hexane, AcroSeal	1191-15-7
37724	Dimethylzinc, 1.2M solution in toluene, AcroSeal	544-97-8
18927	Trimethylaluminium, 1.0M solution in heptane, AcroSeal	75-24-1
Reagents in Sol	ution	
17706	Borane-methyl sulfide complex, 94%, AcroSeal	13292-87-0
17508	Borane-tetrahydrofuran complex, 1M solution in THF, Stabilized, AcroSeal	14044-65-6
17668	Boron trichloride, 1M solution in methylene chloride, AcroSeal	10294-34-5
38836	Hydrogen chloride, 4N solution in 1,4-dioxane, AcroSeal	7647-01-0
42879	Potassium tert-butoxide, pure, 1.6-1.7M (20 wt.%) solution in THF, AcroSeal	865-47-4

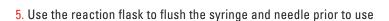
Top Tips for Using AcroSeal Packaging

To get the best results using AcroSeal packaging, we recommend the following process:

- 1. Puncture the septum
- 2. Withdraw the required amount
- 3. Replace the nitrogen blanket
- 4. Store upright to prevent prolonged product contact with the seal

Advanced tips:

- Prepare the nitrogen balloon in advance and use two balloons, one inside the other
- 2. Purge the doubled balloons with nitrogen three times before use
- 3. Bend the needle as it makes it easier to use and control
- 4. Flush each needle and syringe with nitrogen three times before use



To get the best results from the septum, we recommend you use 18 to 21 gauge needles and puncture in a clock face pattern to avoid piercing the septum in the same place.

If you require a large amount of solvent remove the whole cap under an inert atmosphere and decant the desired amount of product from the bottle.

For further tips on how to use AcroSeal packaged products, view our demonstration video at wwr.com.

In conclusion, AcroSeal packaging offers a superior advantage for your organic synthesis by providing quality products, saving you time and keeping you safer!



To view the full list of AcroSeal packaged products visit vwr.com.



Austria

VWR International GmbH Graumanngasse 7 1150 Vienna Tel.: +43 1 97 002 0

Fax: +43 1 97 002 600 Email: info.at@vwr.com

Belgium

VWR International bvba Researchpark Haasrode 2020 Geldenaaksebaan 464 3001 Leuven

Tel.: 016 385 011 Fax: 016 385 385

Email: vwr.be@vwr.com

Czech Republic

VWR International s. r. o. Veetee Business Park Pražská 442

CZ - 281 67 St říbrná Skalice

Tel.: +420 321 570 321 Fax: +420 321 570 320 Email: info.cz@vwr.com

Denmark

VWR International A/S Tobaksvejen 21 2860 Søborg Tel.: 43 86 87 88

Fax: 43 86 87 90 Email: info.dk@vwr.com

Finland

VWR International Oy Valimotie 9 00380 Helsinki Tel.: 09 80 45 51 Fax: 09 80 45 52 00

Email: info.fi@vwr.com

France

VWR International S.A.S. Le Périgares – Bâtiment B 201, rue Carnot 94126 Fontenay-sous-Bois cedex

Tel.: 0 825 02 30 30

Fax: 0 825 02 30 35 Email: info.fr@vwr.com

Germany

VWR International GmbH Hilpertstraße 20a D - 64295 Darmstadt Freecall: 0800 702 00 07 Fax: 0180 570 22 22 Email: info.de@vwr.com

Hungary

VWR International Kft. Simon László u. 4. 4034 Debrecen Tel.: (52) 521-130 Fax: (52) 470-069 Email: info.hu@vwr.com

India

VWR Lab Products Private Limited No.139. BDA Industrial Suburb, 6th Main, Tumkur Road, Peenya Post,

Bangalore, India – 560058 Tel.: +91-80-28078400 Fax: +91-80-28078410 Email: vwr_india@vwr.com

Ireland / Northern Ireland

VWR International Ltd / VWR International (Northern Ireland) Ltd Orion Business Campus Northwest Business Park Ballycoolin Dublin 15

Tel.: 01 88 22 222 Fax: 01 88 22 333 Email: sales.ie@vwr.com VWR International S.r.l. Via San Giusto 85 20153 Milano (MI) Tel.: 02-3320311

Fax: 800 152999/02-40090010 Email: info.it@vwr.com

The Netherlands

Italy

VWR International B.V.
Postbus 8198
1005 AD Amsterdam
Tel.: 020 4808 400
Fax: 020 4808 480
Email: info.nl@vwr.com

Norway

VWR International AS
Haavard Martinsens vei 30
0978 Oslo
Tel.: 22 90 00 00

Fax: 815 00 940

Email: info.no@vwr.com

Poland

VWR International Sp. z o.o. Limbowa 5 80-175 Gdansk Tel.: 058 32 38 200 Fax. 058 32 38 205 Email: info.pl@vwr.com

Portugal

VWR International -Material de Laboratório, Lda Centro Empresarial de Alfragide Rua da Indústria, nº 6 2610-088 Alfragide Tel.: 21 3600 770 Fax: 21 3600 798/9

Email: info.pt@vwr.com

Spain

VWR International Eurolab S.L. C/ Tecnología 5-17 A-7 Llinars Park 08450 - Llinars del Vallès Barcelona

Tel.: 902 222 897 Fax: 902 430 657 Email: info.es@vwr.com

Sweden

VWR International AB Fagerstagatan 18a 163 94 Stockholm Tel.: 08 621 34 00 Fax: 08 621 34 66

Email: kundservice.se@vwr.com

Switzerland

VWR International GmbH Lerzenstrasse 16/18 8953 Dietikon Tel.: 044 745 13 13 Fax: 044 745 13 10 Email: info.ch@vwr.com

Turkey

VWR International Laboratuar Teknolojileri Ltd. Şti. Orta Mah. Cemal Gürsel Caddesi Ördekcioglu Is merkezi No.32/1 34896 Pendik - Istanbul

Tel.: +90216 598 2900 Fax: +90216 598 2907

UK

VWR International Ltd Customer Service Centre Hunter Boulevard - Magna Park Lutterworth Leicestershire I F17 4XN

Tel.: 0800 22 33 44 Fax: 01455 55 85 86 Email: uksales@vwr.com

