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**ACR̄OS**  
**ORGANICS**

# Organics Handbook

We are pleased to introduce the

# Organics Handbook



## Featuring Acros Organics and Maybridge products

*It offers a comprehensive portfolio of essential chemicals, functional reagents, and organic building blocks to meet the evolving needs of organic and medicinal chemists in the fields of research and development and drug discovery. Our heritage of quality, packaging innovation and new product development has made us the brands scientists trust for their organics and fine chemicals needs.*

### THIS ORGANICS HANDBOOK FEATURES:

- Combined Acros Organics products and Maybridge building blocks
- Over 20,000 chemicals with 40,000 listings
- More than 2,000 new products and 6,000 new pack sizes
- Easy-to-use square-style pages
- AcroSeal Packaging: the industry leading packaging for air and moisture sensitive reagents
- Fisher Chemical industry leading Optima LC-MS grade solvents
- Application guides and literature citations
- Enhanced SKU and packaging information

### THE BROAD RANGING PRODUCT PORTFOLIO OFFERS THE ORGANIC CHEMIST GREATER CONVENIENCE

PRODUCT RANGE AND SERVICE	ORGANICS PORTFOLIO (INCLUDING ACROS ORGANICS BRAND AND MAYBRIDGE BRAND)
<b>Preparation, Purification and Analysis</b>	More than 1,500 basics such as acids, bases, inorganic salts, and chromatography products for daily use.
<b>Building Blocks</b>	Over 10,000 building blocks for synthetic organic chemistry as well as over 5,000 pharmacophorically relevant building blocks for drug discovery.
<b>Functional Reagents</b>	Over 1,500 reagents for functional group transformation.
<b>Biochemicals and Reagents</b>	About 1,000 organic compounds for use in biology and or biochemistry applications.
<b>Screening Library</b>	A highly diverse set of over 55,000 compounds with either hit-like and lead-like properties.
<b>Customer Weighing</b>	Building blocks and screening compounds weighed to customers specific requirements in a wide variety of formats.
<b>Custom Synthesis and Medicinal Chemistry Service</b>	Custom synthesis of building blocks and small to medium screening library design and synthesis.

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### Contact your local distributor.

For a complete and up-to-date list of distributors, please go to our website [www.acros.com](http://www.acros.com)

## How to order

### ORDERING

There is no minimum order size at Acros Organics. All orders are welcome. Written confirmation of a telephone order is not required. However, if you need to send a confirmation order, please mark clearly with "confirmation".

### PRICES

All prices in our catalogue are mentioned in local currency, ex-works and are exclusive of VAT.

For the latest price information contact our customer service.

### SHIPMENT INFORMATION

Orders are shipped in principle on the day that we receive them. If you have special requirements, please mention this clearly on your order.

### RETURNED GOODS PROCEDURE

Please contact your sales office before sending goods back to us. Acros Organics will not accept returned goods without prior approval of our sales department.

Please ask our customer service for a 'Return Goods Authorisation'. A 'Return Goods Authorisation' form will be sent to you, together with the relevant documentation. This form needs to be added to the shipment.

If you placed a wrong order or want to return products, we have to ask for a "restocking fee". Transport costs are also at your expense in that case. Under no circumstance must chemicals be posted.

### COLD PACK

We are able to pack products that need to be kept at a low temperature in a so-called "cold pack"; If you want your products sent to you in a cold pack, please mention this on your order. Please contact your customer service for additional charges.

## AcroSeal®

### ACROSEAL® PACKAGING: THE SOLUTION FOR AIR AND MOISTURE SENSITIVE REAGENTS

AcroSeal packaging is the industry-leading packaging for air and moisture sensitive reagents. The AcroSeal packaging is designed to deliver the best performance among the comparable packagings in the marketplace.

The innovative quadrant style screw cap with the specially designed septum provides:

- **Convenience:** large surface area with easy access to large amount of products.
- **Quality:** the specially designed multi-layer septum ensures better re-seal.
- **Performance:** reduces the rate of moisture uptake by up to 50% compared to the competitive packaging.
- **Safety:** minimizes the potential needle puncture-related incidents

**The key features and benefits of AcroSeal Packaging can be most demonstrated for the extra dry solvents:**

**RELIABILITY:** AcroSeal packaging uses a specially designed, multi-layer septum consisting of a sandwich of three layers of engineering polymer material - an inner silicone layer surrounded by PTFE resin layers. The thickness of AcroSeal septum is twice as much as that of the septum used in the competitive brand packaging. The thick inner silicone layer allows for better resealing around needle punctures. The outer PTFE layers ensure the chemical compatibility of the septum material with the reagents.

**INTEGRITY:** AcroSeal closure system features a quadrant-style cap design that holds the septum in place, reducing the risk of bulging or deformation mechanically or through use over time. AcroSeal

packaging has a tamper evident seal to assure that the bottle is visibly unopened and the quality has not been compromised.

**CONVENIENCE:** AcroSeal packaging is designed to provide a larger surface area available for syringe punctures, providing more than 15 times the surface area than the septum of the competing brand. The larger surface area makes it possible to avoid repeated puncture in the same spot over time, therefore reducing the risk of deformation and providing better resealing.

The AcroSeal packaging screw closure allows not only syringe withdrawal of a reagent through the septum but also permits ready access to a larger volume of the solvent with the option to reseal the closure by hand. By contrast, the competing brand has a crimp cap design, meaning that the reagent within is only accessible with a syringe unless a special tool is used. Once de-crimped, the cap cannot be replaced.

**SAFETY:** Because the use of the products involve syringe and needles, it is important that the packaging is designed in such away that the potential risk of needle puncture can be minimized. AcroSeal packaging requires 40% less force to puncture through the septum than the competitive brand packaging. The greater the force required to puncture through the septum, the more likely for needle puncture-related accidents to occur.

**PERFORMANCE:** Moisture uptake studies have shown that overall the AcroSeal packaging with its particular closure design appears to allow a slower rate of moisture uptake than the familiar competing brand's closure design.

## AcroSeal® Product Range

- **EXTRA DRY SOLVENTS:** a wide range of solvents in three different grades with moisture content of less than 50ppm at the time of packing
  - Standard Grade: Suitable for most of the applications.
  - Molecular Sieves Grade: Stored over molecular sieves for prolonged shelf life.
  - Supreme Grade: Filtered through 0.2 micro filters for dust-free applications.
- **ORGANOMETALLIC COMPOUNDS:** Broad selection including Grignard reagents, organolithium, and organotin, organozinc, and organoaluminium compounds.
- **REAGENTS IN SOLUTION:** Commonly used reactive reagents and corrosive gaseous reagents in the ready to use solutions. Key products include boranes, hydrides, organic bases and Lewis acids. AcroSeal Packaging reduces the hazard of handling and improves the safety of using the products.
- **DEUTERATED NMR SOLVENTS:** Offers a low cost alternative to ampoule packaging
- **ORGANICS:** Selective air/moisture sensitive organics



### Tamper-evident break ring at the lower end of the protective red cap.

Foolproof guarantee that the customer is the first to open the bottle. The lower ring breaks off with the first opening of the red cap.

### Triple sandwich septum with inner silicone layer and double outer PTFE resin coating.

Better chemical compatibility and re-closure of any puncture hole.

### Quadrant cap surface.

The quadrant cap promotes the durability of the septum because punctures can be spread over the large septum surface.



### Cushioning liner in outer protective cap.

Re-seals perfectly even after the septum has been punctured multiple times.

### Rim design at the inner surface of the septum holding quadrant cap will hold and stretch the septum.

Reduces the risk of bulging or deformation of the septum.

### Three-plus windings in the septum holding cap for extra security.

Large contact surface prevents infiltration of air and moisture through the screw neck.

### Special rim design inside the septum holding cap fits snugly over the glass rim of the bottle neck.

No risk of accidentally unscrewing the septum holding quadrant cap.

# Fisher Chemical Optima LC/MS Products Benefits

## OPTIMA LC/MS PRODUCTS

The joining of liquid chromatography (LC) with mass spectrometry (MS) has become an indispensable tool for various fields of research. The value of LC/MS derives from its ability to combine separation chemistry with selective mass ion detection. As instrumentation advances lead to ever-lower analyte detection limits, it is crucial for the chromatographer to consider the level of purity when selecting appropriate solvents for use in the LC/MS mobile phase. The Fisher Chemical product line offers superior high-purity solvents designed to meet the required purity level of advanced LC/MS systems.



## ULTRA-HIGH PURITY FOR MORE RELIABLE ANALYSIS AND COST SAVINGS

- Very low mass noise level contributed by Optima LC/MS Solvents for both positive and negative modes in total ion chromatography (TIC)
- Low levels of trace metals - including alkaline earth metals, which can interfere with MS ionization and MS interpretation
- Longer column life - due to minimal impurities in the mobile phase
- Low residue - clog-free operation of LC/MS system due to the absence of particles

## MANUFACTURED AND TESTED TO THE HIGHEST STANDARDS TO ENSURE TROUBLE-FREE ANALYSIS

- Tested specifically for LC/MS and LC/UV applications
- Stringent metal ion testing
- Assayed for free acid/alkali, nonvolatile matter, and other elements

## ACCURATE DATA AND REPRODUCIBLE PERFORMANCE

- Minimal metal mass adduct formation for better analyte identification
- Smooth, flat baselines from low solvent backgrounds using diode array detector and mass spectrometry detector (MSD)

- High ionization efficiency of mass spectrometry
- Solvent purity consistent from lot to lot
- Proprietary manufacturing process to ensure the highest quality of the product

## SPECIFICATIONS AND CHROMATOGRAPHIC DATA

Optima LC/MS Solvents have the lowest diode array detector (DAD) background with least drifting baseline; lowest mass spectrometry detector (MSD) noise level for both positive and negative modes in total ion chromatography (TIC); lowest metal ion content for many common elements; and lowest UV absorbances.

## CROSS-REFERENCES TO COMPETITOR PRODUCTS

Acetonitrile			
	1L	2.5L	4L
Fisher Chemical	A955-1	A955-212	A955-4
EMD	AX0156-6	NA	AX0156-1
Merck	1000291000	1000292500	NA
J.T. Baker	9829-2	NA	9829-3
Sigma-Aldrich	34967-1L	34967-2.5L	34967-4x4L
Biosolve	12041	NA	NA
Methanol			
	1L	2.5L	4L
Fisher Chemical	A456-1	A456-212	A456-4
EMD	MX0486-6	NA	MX0486-6
Merck	1060351000	1060352500	NA
J.T. Baker	9830-2	NA	9830-3
Sigma-Aldrich	34966-1L	34966-2.5L	34966-4x4L
Biosolve	136841	NA	NA
2-Propanol			
	1L	2.5L	4L
Fisher Chemical	A461-1	A461-212	A461-4
J.T. Baker	9627-2	NA	9627-3
Sigma-Aldrich	34965-1L	34965-2.5L	NA
Biosolve	162641	NA	162641
Water			
	1L	2.5L	4L
Fisher Chemical	W6-1	W6-212	W6-4
EMD	WX0001-6	NA	WX0001-1
J.T. Baker	9831-2	NA	9831-3
Sigma-Aldrich	39253-1L	NA	39253-4x4L
Biosolve	232141	NA	NA

For more information, including a white paper titled "Optimizing Mobile Phase Solvent Purity for LCMS," go to [www.FisherLCMS.com](http://www.FisherLCMS.com)

# Fisher Chemical Optima LC/MS Products List

## OPTIMA LC/MS ACETONITRILE A955

Assay (by GC), min	99.9%
Optical Abs, wavelength, nm	au max
280	0.005
254	0.005
230	0.01
225	0.015
220	0.015
215	0.025
210	0.03
205	0.04
200	0.05
195	0.15
190	1.00
LC/MS Gradient Suitability, nm	Single max peak (au)
254	0.0005
210	0.002
LC/MS at Positive Mode Max	50ppb Reserpine
LC/MS at Negative Mode Max	50ppb Aldicarb
Water (KF) %	0.01
Residue after Evaporation, ppm Max	0.8
Trace Ionic Impurities	ppb, Max
Aluminum (Al)	25
Barium (Ba)	5
Cadmium (Cd)	5
Calcium (Ca)	25
Chromium (Cr)	5
Cobalt (Co)	5
Copper (Cu)	5
Iron (Fe)	5
Lead (Pb)	5
Manganese (Mn)	5
Magnesium (Mg)	10
Nickel (Ni)	5
Potassium (K)	10
Silver (Ag)	5
Sodium (Na)	50
Tin (Sn)	5
Zinc (Zn)	10
Titratable Acid, mEQ/g	0.008
Titratable Base, mEQ/g	0.0006

## OPTIMA LC/MS 2-PROPANOL A461

Assay	99.9%
Color (APHA), Max	5
Optical Abs, wavelength, nm	au max
254	0.005
230	0.05
220	0.1
210	0.4
LCMS Suitability	Pass Test
Water (KF) %	0.05
Residue after Evaporation, ppm, Max	1
Titratable Acid or Base meq/g	0.0001
Trace Ionic Impurities	ppb, Max
Aluminum (Al)	10
Calcium (Ca)	10
Copper (Cu)	5
Iron (Fe)	5
Lead (Pb)	5
Magnesium (Mg)	5
Manganese (Mn)	5
Nickel (Ni)	5
Potassium (K)	10
Silver (Ag)	5
Sodium (Na)	50
Zinc (Zn)	10

## OPTIMA LC/MS METHANOL A456

Assay (by GC), min	99.9%
Optical Abs, wavelength, nm	au max
280	0.005
260	0.005
254	0.01
230	0.1
220	0.2
214	0.4
210	0.5
LC/MS Gradient Suitability, nm	Single max peak (au)
254	0.001
220	0.005
LC/MS at Positive Mode Max	50ppb Reserpine
LC/MS at Negative Mode Max	50ppb Aldicarb
Water (KF) %	0.02
Residue after Evaporation, ppm, Max	1
Trace Ionic Impurities	ppb, Max
Aluminum (Al)	10
Barium (Ba)	10
Cadmium (Cd)	10
Calcium (Ca)	20
Chromium (Cr)	10
Cobalt (Co)	10
Copper (Cu)	10
Iron (Fe)	10
Lead (Pb)	10
Magnesium (Mg)	10
Manganese (Mn)	10
Nickel (Ni)	10
Potassium (K)	10
Silver (Ag)	10
Sodium (Na)	50
Tin (Sn)	10
Zinc (Zn)	10
Titratable Acid, mEQ/g	0.0003
Titratable Base, mEQ/g	0.0002

## OPTIMA LC/MS WATER W6

Optical Abs, wavelength, nm	au max
280	0.005
260	0.005
254	0.005
240	0.01
230	0.01
220	0.01
210	0.01
LC/MS Gradient Suitability, nm	Single max peak (au)
254	0.0005
210	0.005
Protease	Not Detected
LC/MS at Positive Mode Max	50ppb Reserpine
LC/MS at Negative Mode Max	50ppb Aldicarb
Residue after Evaporation, ppm, Max	1
Trace Ionic Impurities	ppb, Max
Aluminum (Al)	10
Barium (Ba)	10
Cadmium (Cd)	10
Calcium (Ca)	20
Chromium (Cr)	10
Cobalt (Co)	10
Copper (Cu)	10
Iron (Fe)	10
Lead (Pb)	10
Magnesium (Mg)	10
Manganese (Mn)	10
Nickel (Ni)	10
Potassium (K)	10
Silver (Ag)	10
Sodium (Na)	20
Tin (Sn)	10
Zinc (Zn)	10
Total Halogens (as chloride)	Not Detected



## Quality Management

### PURITY OF OUR PRODUCTS

**Our priority is quality.** All products in this reference handbook have been subjected to meticulous purity analysis in our QC laboratories. The quality assays, purity levels and analytical values, and physico-chemical data, represent typical values. Values listed are valid at the time of going to press only.

### VALIDITY OF PRODUCT AND QUALITY SPECIFICATIONS


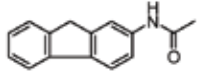
Specifications and typical values are subject to change during the reference handbook's period of validity. If you need the latest specifications or actual analytical profile of our products, we recommend checking our website, or requesting these at any time from your local customer service office.

### CERTIFICATES OF ANALYSIS AND SPECIFICATION SHEETS

If you wish to check the actual purity of a given batch, **request a Certificate of Analysis from our website.** You can also find on acros.com a feature to download a copy of the latest version of our specification sheets.

ACROS ORGANICS		Certificate of Analysis	
Product	17720 2-(5-Bromo-2-pyridylazo)-5-(diethylamino)phenol, 97%	General Product Data	
		Version	0
		CAS No.	14337-53-2
		Molecular weight	349.22
		Molecular formula	C <sub>15</sub> H <sub>17</sub> BrN <sub>4</sub> O
		Linear formula	#
Lot Specific Data	A0106679001		
Appearance	RED FINE CRYSTALLINE POWDER		
Infrared spectrometry	AUTHENTIC		
Melting point	158.4°C		
Assay Total base	101.17 %		

### Clear overview

2-Acetamidofluorene, 95%				
Acros Organics	Product code	Packaging	Pack size	Price
 R45 R22 S53 S45	102300050	Glass bottle	5 g	\$ 69.80
	102300250		25 g	\$ 218.80
	C <sub>16</sub> H <sub>13</sub> NO CAS: 53-96-3 MFCD00001116 F.W.: 223.27 mp: 192-196 °C			

### SPECIAL GRADES

Products which are documented with a quality description such as Pharmacopoeia, for Analysis, for HPLC, for NMR, for Biochemistry, were tested according to more specific and defined chemical criteria. We do NOT test for the referred to application itself, e.g. as a pharmaceutical raw material.

**The tests performed in our QC laboratories confirm that our products meet all the specific chemical quality criteria** you will find on our Certificates of Analysis, but do not imply that such products are always fit for a specific use. Fitness for any particular use remains the responsibility of the customer. Acros Organics and Maybridge branded products are marketed for research use only.

### EXPIRATION DATES

Acros Organics and Maybridge branded products are subject to regular inspection and, as long as we carry inventory, will be internally subject to re-testing at periodic intervals.

Most of our products maintain their original quality well beyond such re-testing period. We therefore do not assign expiration dates on our Certificates of Analysis. In case you need a 'best before' or 'use by' date, please contact your local customer service office.

Available from [www.acros.com](http://www.acros.com)





## Specifications

The majority of our Essentials are available in various qualities. The table below summarizes the different grades listed in this reference handbook.

### SPECIFICATIONS FOR CHEMICAL SYNTHESIS:

<b>Pure:</b>	Basic specification, suitable for chemical synthesis and general laboratory work.
<b>Extra pure:</b>	Extended specifications for exacting chemical synthesis.
<b>For analysis:</b>	Widest range of specifications for chemical synthesis and analysis, often designated "p.a."
<b>For analysis ACS:</b>	The specification complies with the recommendations of the American Chemical Society

### Detailed specifications

Acetonitrile, 99.9% conform Est. Ph.		for HPLC gradient grade		
Acros Organics	Product code	Packaging	Pack size	Price
 	<b>325730010</b>	Glass bottle	1 l	\$ 50.40
	<b>325730025</b>	Glass bottle	2.5 l	\$ 115.00
R11 R20/21/22 R36 S16 S36/37	<b>C<sub>2</sub>H<sub>3</sub>N</b>	CH <sub>3</sub> CN		
	CAS: 75-05-8	mp: -46 °C	d: 0.781	
	MFCDD0001878	bp: 81-82 °C (760 mm- Hg)	n <sub>D</sub> : 1.343-1.345	
	FW: 41.04	Fp: 2°C		
	Color: <math>\leq 10\text{ APHA}</math>			
	Assay: <math>\geq 99.9\%</math>			
	Water: <math>\leq 0.01\%</math>			
	Residue insoluble: <math>\leq 0.0001\%</math>			
	UV: <math>195\text{ nm } \leq 1</math>		200 nm <math>\leq 0.05</math>	
			210 nm <math>\leq 0.02</math>	
			230 nm <math>\leq 0.01</math>	
			250 nm <math>\leq 0.005</math>	

### SPECIFICATIONS FOR SPECIAL APPLICATIONS:

<b>Extra dry:</b>	Extra dry solvents with water content of 50 ppm or lower at the time of manufacture, filtered over 0.2 micron PTFE filter and filled er inert gas.
<b>Extra dry over molecular sieves:</b>	Extra dry solvents with water content of 50 ppm or lower at the time of manufacture, filled under inert gas and stored over molecular sieve for enduring shelflife.
<b>For peptide synthesis:</b>	Very pure and dry quality for usage in peptide synthesis.
<b>For biochemistry:</b>	Products are suitable for applications in biochemistry. Relevant parameters for this application are specified.
<b>For molecular biology:</b>	In addition to the parameters of the "Biochemistry" grade, specifications include the absence of DNase, RNase and Proteases.
<b>For spectroscopy:</b>	The solvents show a very low absorption in the UV or IR spectrum and a high purity.
<b>For residue analysis:</b>	Solvents used for the analysis of polyaromatic hydrocarbons, halogen containing pesticides and other residues.
<b>For NMR:</b>	Deuterium labeled compounds and solvents for NMR spectroscopy.
<b>For HPLC:</b>	Suitable for HPLC due to low absorption in UV, low residue of evaporation and other parameters.
<b>For HPLC gradient grade:</b>	A gradient analysis is part of the specification in addition to the parameters used for the "HPLC" grade.
<b>For electronic use:</b>	A special dust- and residue- free quality for applications in the electronic industry.
<b>For AAS:</b>	A special quality for use in atom-absorption spectroscopy

## Key to chemical listings

A new page layout was created to allow you to make searching and browsing through the Reference Handbook easier. The same type of product data is shown in the same position for every product.

Product description

1 Product name


2 Typical purity

3 Product description

4 Chemical grade

Brand name

Safety and storage information

Aluminium bromide, 98+% <sup>2</sup> anhydrous <sup>3</sup> extra pure <sup>4</sup>				
Acros Organics	Product code	Packaging	Pack size	Price
 R14 R22 R34 S8 S26 S36/37/39 S45 Hygroscopic	198410250	Glass bottle	25 g	\$ 34.00
	198411000	Glass bottle	100 g	\$ 76.60
AlBr <sub>3</sub>	AlBr <sub>3</sub>			
CAS: 7727-15-3	FW: 266.7		bp: 265 °C (760 mmHg)	
MFC000003421	mp: 97 °C			
Assay: 268.0 %	Fe: ≤ 50 ppm	Pb: ≤ 50 ppm		
Trace Analysis:	Cl: ≤ 2000 ppm	SO <sub>4</sub> : ≤ 200 ppm		

Aluminium sec-butoxide, see Aluminium tri-sec-butoxide on page 33

Ordering and packing information

Chemical and physical properties\*

Typical specifications

Synonym with reference to the listing in the alphabetic section

### FOR MORE INFORMATION ABOUT THE JOURNALS

Consult the dedicated pages "Table of abbreviations" and "Abbreviations for scientific journals used in the application guide" at the end of this reference handbook.

#### Application guide with transformation index and literature references

##### Aluminium bromide, anhydrous

##### APPLICATION GUIDE

##### Lewis acid catalysts

Synthesis of oxacyclic, cyclopentanone, conjugated cyclopentanone. JOC 1988, 911; TL 1983, 79; TL 1992, 7361

\* Carbonyl to methylolene. Accomplished by the diisobutylaluminum hydride. JOC 1992, 2143

\* Friedel-Crafts intramolecular Friedel-Crafts cyclization. CB 1960, 2693

\* Halogenation. JOC 1991, 5745

\* Isomerisation. Synthesis of adamantane, diamantane, and triformantane. CC 1978, 306

### \* CHEMICAL AND PHYSICAL PROPERTIES

The following physical and chemical information are given:

**Bp**: boiling point in °C at 760 mmHg unless a different pressure is specified

**Mp**: melting point in °C

**Fp**: flash point in °C

**d**: density in g/ml

$[\alpha]_D^{20}$ : specific optical rotation measured at 20°C with light having the frequency of the sodium D line

$n_D^{20}$ : refractive index measured at 20°C with light having the frequency of the sodium D line

### INDEXES

Products are indexed in this reference handbook by CAS, MFC, product number and molecular formula. These indexes can be found after the alphabetical listing at the end of this reference handbook.