Analytix

Advances in Analytical Chemistry

Issue 3 • 2005

Fluka
Riedel-de Haën®

Microbiology Base Ingredients

SIGMA-ALDRICH

Special issue on Microbiology: Find our state of the art products to to detect, isolate, differentiate, identify and cultivate microorganisms.

Picture: Jvo Siegrist, Product Manager Microbiology, Fluka / Sigma

Dear Colleague,

Sigma-Aldrich is known for its wide range of high-purity chemicals, biochemicals and reagents, but did you know that it is also a leading supplier of innovative products for microbiology?

Microorganisms comprise by far the largest mass of life forms on Earth. Their impact on human life is huge raging from beneficial to deadly. They form an integral part of the food chain and life, as we know it, could not function without them. Indeed, many Sigma-Aldrich products are derived from microorganisms, either as the source or to facilitate production. However, through our Sigma and Fluka brands we also offer a wide range of products to detect, isolate, differentiate, identify and cultivate microorganisms. We strive continually to expand our product line to bring you even more new and relevant products.

Some examples of our state of the art products for microbiologists are:

- **Peptones and Extracts, including new GMO and animal free products**
- **Media and Supplements for all types of microorganisms**
- **Reagents for differentiating and confirming species**
- **Discs and Strips used to verify quickly the presence or absence of specific microorganisms**

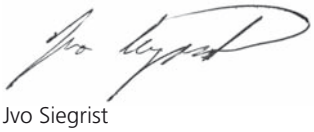
In this issue of Analytix we present information on the latest developments in our microbiology product line. We also have created a Microbiology CD and special literature, like the Microbiology Manual or Disks and Strips for Microbiology" brochure. If you can't wait for the mail, our award-winning website is a valuable source of products, techniques and technical information.
Please visit: **www.sigma-aldrich.com/microbiology**

If you're a practicing microbiologist, what can we help you with?

Apply the know-how of Sigma and Fluka scientists by contacting our Technical Service Team using the contact information on the back page. We enjoy being challenged by your questions!

I hope you enjoy reading this issue of Analytix, and can put the information to good use in your laboratory.

Cheers!



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Picture:
New Microbiology CD (IBG)

Microbiology Base Ingredients: Plant and animal derived, GMO free peptones, extracts and other ingredients for microbiological media.

By Jvo Siegrist, Product Manager Fluka / Sigma: isiegris@sial.com

Complex Ingredients

Although synthetic growth media is available, it lacks the complexity and richness of media and additives derived from natural sources.

Protein, Peptides and Amino Acids

Peptones and extracts are excellent natural sources of amino acids, peptides and proteins in growth media. They are most often obtained by enzymatic digestion or acid hydrolysis of natural products, such as animal tissues, milk, plants or microbial cultures. The number of available peptones and extract is enormous (see list), and can promote and sustain the growth of most organisms. However, because the resulting microbial culture takes up components from the growth media, we sought to develop peptones and extracts that were assured to be BSE- and GMO-free, two of today's major safety-related concerns. Using plants as the natural source not only eliminates the potential risk of BSE, but also offer better growth promotion for some microorganisms. **Pictures 1 - 3** show examples of agars or broth supplemented with Fluka Plant Peptone and Vegetable Extracts.

Carbohydrates

Carbohydrates present in extracts are an important energy source. Fluka brand natural carbohydrate sources provide mono, di, oligo and polysaccharides that build a rich nutritive substrate for mold or bacteria cultures.

Fatty Acids and Lipids

Fatty acids and lipids, like lecithin, are necessary nutrients. Fluka offers such compounds as egg powder and liquid sterile egg yolk supplements.

Vitamins and Trace Elements

Yeast extract, present in nearly every complex media, is the most common source for Vitamin B_{12}. It also contains a large number of amino acids, other vitamins and trace elements specially suited for this source

Bile Salts

Bile is often used as an inhibitory agent against most gram-positive bacteria. Cholates, biological detergent-like compounds with anti-microbial activity, are major constituents of bile.

Table 1: Biological Ingredients

Cat. No.	Brand	Peptones	Source
53283	Fluka	Brain Heart Infusion	animal
03077	Fluka	Liver Hydrolysate	animal
77180	Fluka	Peptone from animal proteins	animal
70951	Fluka	Peptone from gelatin, enzymatic digest	animal
70176	Fluka	Peptone from gelatine, pancreatic digest	animal
70175	Fluka	Peptone from meat, enzymatic digest	animal
82962	Fluka	Peptone from meat, enzymatic digest (for biotechnological purposes)	animal
70174	Fluka	Peptone from meat, peptic digest	animal
68971	Fluka	Peptone special (Neopeptone)	animal
82450	Fluka	Proteose-Peptone	animal
77199	Fluka	Peptone, mycological (Mycological Peptone)	animal / milk
70937	Fluka	Tryptose (Peptone from protein mixture, tryptic digest)	animal / milk
93490	Fluka	Peptone from fish	fish
22078	Fluka	Casein from bovine milk	milk
22080	Fluka	Casein from bovine milk	milk

Continued…

Cat. No.	Brand	Peptones	Source
22090	Fluka	Casein Hydrolysate	milk
61300	Fluka	Lactalbumin Hydrolysate	milk
61302	Fluka	Lactalbumin Hydrolysate	milk
70173	Fluka	Peptone from casein and other animal proteins	milk
70171	Fluka	Peptone from casein, acid digest	milk
82303	Fluka	Peptone from casein, enzymatic digest (for biotechnological purposes)	milk
70169	Fluka	Peptone from casein, pancreatic digest	milk
70177	Fluka	Peptone from lactalbumin, enzymatic digest, readily soluble	milk
82514	Fluka	Protein Hydrolysate Amicase (Amicase)	milk
82524	Fluka	Protein Hydrolysate N-Z-Amine® AS	milk
70172	Fluka	Tryptone (Peptone from casein, tryptic digest)	milk
95039	Fluka	Tryptone (Peptone from casein, tryptic digest, for biotechnological purposes)	milk
93733	Fluka	Tryptose (Peptone from protein mixture, tryptic digest)	milk
39396	Fluka	Casein Yeast Peptone	milk / microbial

Cat. No.	Brand	Plant Peptones	Replace
18332	Fluka	Peptone (vegetable)	Peptone from meat, enzymatic digest
51841	Fluka	Peptone (vegetable) acid hydrolysate	Casein acid hydrolysate
19942	Fluka	Peptone (vegetable), no 1	Peptone from meat, enzymatic digest
61854	Fluka	Peptone (vegetable), no 2	Peptone from gelatine
93491	Fluka	Peptone from broadbean	
83059	Fluka	Peptone from potatoes	
55273	Fluka	Peptone from soy AX	
70178	Fluka	Peptone from soybean meal, enzymatic digest	
07022	Fluka	Peptone from soybean, acid digest (Amisoy®)	
87972	Fluka	Peptone from soybean, enzymatic digest (for biotechnological purposes)	
93492	Fluka	Peptone from wheat	
92976	Fluka	Peptone special, vegetable (Neopeptone)	Peptone special (Neopeptone)
29185	Fluka	Proteose Peptone (vegetable)	Proteose Peptone
16922	Fluka	Tryptone (vegetable)	Tryptone
12331	Fluka	Tryptose (vegetable)	Tryptose
07436	Fluka	Vegetable hydrolysate no 2	Liver powder
67381	Fluka	Vegetable Infusion powder	Heart Infusion powder
95757	Fluka	Vegetable Special Infusion powder	Brain Heart Infusion powder

Cat. No.	Brand	Extracts	Source
70164	Fluka	Meat Extract	animal
73145	Fluka	Yeast Autolysate	microbial
09182	Fluka	Yeast Extract	microbial
70161	Fluka	Yeast Extract	microbial
92144	Fluka	Yeast Extract	microbial

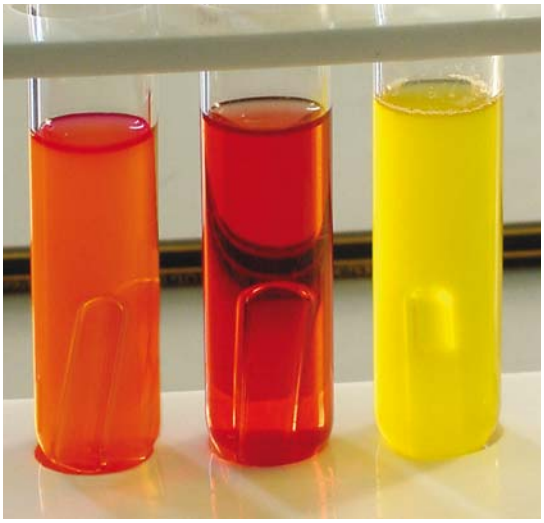
Continued...

Cat. No.	Brand	Plant Extracts	Replace
49760	Fluka	Gluten Hydrolysate from maize	
70167	Fluka	Malt Extract	
07915	Fluka	Potato Extract	
95261	Fluka	Rice extract	
05138	Fluka	Vegetable Extract	Meat extract
04316	Fluka	Vegetable Extract no 1	Meat extract
49869	Fluka	Vegetable Extract no 2	Liver Extract`

Cat. No.	Brand	Other Biological Ingredients	Source
48305	Fluka	Bile Salts	bile
55871	Fluka	Egg powder	egg
70168	Fluka	Ox-bile, dehydrated, purified	bile
70166	Fluka	Skim Milk Powder	milk

Picture 1: KF-Streptococcus Agar with Proteose Peptone (vegetable)

Picture 3: Triple Sugar Iron Agar with Peptone (vegetable) and Vegetable Extract



Picture 2: Phenol Red Broth Base with Proteose Peptone (vegetable) and Vegetable Extract

Saccharide Substrates For Microbiology: Specially suited for microbiology, these saccharides guarantee no unpleasant surprises in quality control or fermentation.

By Jvo Siegrist, Product Manager Fluka / Sigma: isiegris@sial.com

Fluka offers saccharides in a range specifically suited for microbiology applications. These saccharides are free of growth inhibiting substances like myxothiazol [1] and heavy metals [2]. Extensive testing ensures that these saccharides provide the intended microorganisms the best quality growth substrate for quality control, research and fermentation processes.

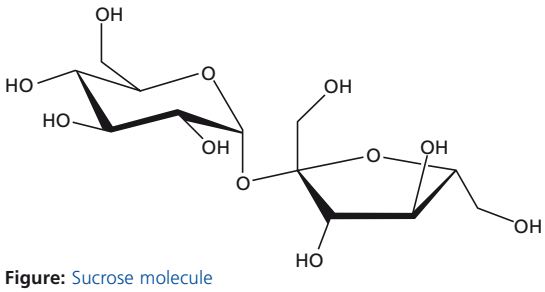


Figure: Sucrose molecule

Table 1: Saccharides for microbiology

Cat. No.	Brand	Saccharides (BioChemika for microbiology)
10850	Fluka	D-(-)-Arabinose
22150	Fluka	D-(+)-Cellobiose
22160	Fluka	D-(+)-Cellobiose octaacetate
44590	Fluka	Dulcitol
47740	Fluka	D-(-)-Fructose
48260	Fluka	D-(+)-Galactose
49140	Fluka	D-(+)-Glucose, anhydrous
49159	Fluka	D-(+)-Glucose, monohydrate
49210	Fluka	β-D-Glucose pentaacetate
57570	Fluka	myo-Inositol
63560	Fluka	D-Mannitol
63580	Fluka	D-(+)-Mannose
63582	Fluka	D-(+)-Mannose
63620	Fluka	D-(+)-Melezitose Monohydrate
63630	Fluka	D-(+)-Melibiose
83400	Fluka	D-(+)-Raffinose pentahydrate
83650	Fluka	L-(+)-Rhamnose, Monohydrate
84100	Fluka	Sucrose
90210	Fluka	D-(+)-Trehalose Dihydrate
95720	Fluka	L-(-)-Xylose

References:

[1] G. Thierbach, H. Reichenbach, Neutralizes growth inhibition by myxothiazol in *Saccharomyces cerevisiae, Mucor hiemalis* and *Candida albicans* et.al. Antimicrob. Agents Chemother. 19, 504 (1981)

[2] C.W. Forsberg, Effects of heavy metals and other trace elements on the fermentative activity of the rumen microflora and growth of functionally important rumen bacteria., Can J Microbiol., 24(3):298-306 (1978)

Agar for Microbiology: Agar and the solidifying agents in solid growth media should be well chosen, with certain criteria to consider.

By Jvo Siegrist, Product Manager Fluka / Sigma: isiegris@sial.com

Agar is available in a range of qualities dictated by the target application. For example, Fluka brand agar (Cat. No. 05038) is highly purified and ideal when high transparency and brightness is needed, as in nutritional studies (Vitamin Assay Media) and sensitivity testing procedures, or when high purity and good diffusion of substances is essential. For identification and differentiation we recommend using a purified or even highly purified agar. However, when isolating a single colony in most cases a standard quality will suffice. Typical solid media has an agar concentration of 1.0 - 1.5%, to accommodate the requirements of different applications and growth habits of the target microorganisms. For more details please contact our technical service **Flukatec@eurnotes.sial.com**.

Table 1: Agar qualities for microbiology

Cat. No.	Brand	Name
05038	Fluka	Agar, highly purified
05039	Fluka	Agar, purified
05040	Fluka	Agar, standard quality
05051	Fluka	Agar, fibers
A5054	Sigma	Select agar
A5306	Sigma	Bacteriological agar
A5431	Sigma	Noble Agar

www.sigma-aldrich.com/microbiology

Microbiology CD – 3rd Edition: New release of the Microbiology Media Data Bank CD, a valuable tool for all microbiologists

The 3rd Edition of the Microbiology Media Data Bank CD contains the most recent additions to the catalog, on top of a complete listing of growth media, base ingredients, supplements, reagents, discs, strips and tests for microbiology from Fluka and Sigma brands. The advanced search tool allows you to search for names, synonyms, keywords and the product numbers of Fluka, Sigma and other suppliers as well.

An excellent tool for all microbiologists. You will find a complete Microbiology Media Data Bank on this CD which gives detailed product information, including:

- **Product composition**
- **Directions for use**
- **Required additives**
- **Test strains**
- **Package sizes**
- **Background information about the application**
- **References and literature**

The detailed product information is printable as a working sheet. A link to our website gives you the prices in your local currency. But you must hurry; the stock of this valuable CD is limited. Please reserve your CD now by returning the enclosed reply card (Literature Code IBG).

www.sigma-aldrich.com/microbiology_cd

Use of Certified Reference Materials: Reference materials and especially certified reference materials are indispensable tools in ensuring analytical quality. They are used in calibration, method validation, routine quality control and establishing traceability.

Thomas Linsinger, EC-JRC, Institute for Reference Materials and Measurements (IRMM), Geel, Belgium: Thomas.Linsinger@cec.eu.int
With introduction by Rainer Walz, PhD, Product Manager, Fluka/Riedel-de Haën: rwalz@sial.com

Analytical chemists in industrial QC and international and regional governmental regulatory agencies are important players in the enforcement of quality and safety regulations of both domestic and imported products. The quality and reliability of their efforts, however, is in turn dependent on the quality and reliability of the reference standards used in their analytical methods. Sigma-Aldrich, through its Fluka brand, offers a wide selection of Certified Reference Materials (CRM) sanctioned by the Institute for Reference Materials and Measurements (IRMM) to ensure that our customers have available the most accurate, precise, stable, traceable and reliable single component and matrix reference standards. In this article, an official from the IRMM discusses some basic aspects of CRMs and how to use them to full advantage.

The use of highly accurate reference materials is an important aspect of quality assurance in analytical chemistry laboratories. Consequently, ISO 17025 [1] dedicates the whole paragraph 5.6.3 to reference materials. The Institute for Reference Materials and Measurements (IRMM) of the Joint Research Centre of the European Commission (EC-JRC) is responsible for storage, production, management and distribution of certified reference materials (CRM) for the European Commission. Although ISO guidelines exist for the use of CRM [2], the IRMM realizes that many questions and misunderstandings still remain.

Reference Materials, Certified Reference Materials and Standard Reference Materials

All reference materials must have the following characteristics specified and confirmed:

- **Homogeneity**
- **Stability**
- **Assigned values (concentration, purity, etc.)**

Certified Reference Materials (CRM) are a subgroup of reference materials with a higher degree of characterization, assigned and traceable values and written certification than the latter. Calibration standards are also reference materials. Arguably they should even be certified reference materials, since a standard without guaranteed purity and concentration is of very limited use. Recently, the IRMM launched a new brand of CRMs, European Reference Materials (ERM®) to address the need for CRMs of even higher quality. Other brands of CRMs available from IRMM include BCR® and IRMM branded materials.

Applications of RMs and CRMs

Every analytical chemistry application requires a reference material of some form. The term reference material gives only some basic requirements and therefore describes a wide range of materials. For several intended uses the higher degree of characterization achieved for CRMs is required.

Method Calibration

Calibration standards relate instrument response to the analyte concentration. The uncertainty of the stated analyte concentration or purity should be as low as possible, because this uncertainty is incorporated fully in the final analytical result. If, for example the concentration of the calibration standard is given as 10 ± 0.5 mg/L, the final uncertainty of the analytical result cannot be lower than 5% (0.5/10 mg/L). Using CRMs of pure powders or pure solutions as calibration standards is preferred. Typically, matrix reference materials are not suitable for calibration; uncertainties on the certified values are usually higher than for pure solutions due to the more difficult value assignment process.

Validation and Performance Assessment

A typical method validation study evaluates the repeatability, intermediate precision (within-laboratory reproducibility), robustness and trueness* of the method. Repeatability and intermediate precision could be assessed using normal laboratory samples (if they are homogeneous and stable over the period of the study). However, valuable personnel and instrument time can be saved by using CRMs also for this purpose as the assessment of trueness can be done using the data from these experiments.
In the assessment of trueness, results of measurements on a CRM are compared to the uncertainty of the certified value. Total uncertainty of the measurement (u_t) is found from the uncertainty of measurement (u_m) and the certified value of the reference material (u_{CRM}):

$$u_t = \sqrt{u_m^2 + u_{CRM}^2}$$

When the uncertainty of the certified value (u_{CRM}) is very small, the total uncertainty is essentially the uncertainty contributed by the experiment. The standard deviation of the measurements on the CRM divided by the square root of the number of measurements can be used as rough estimation for um. These measurements should be spread over several days to achieve conditions of intermediary precision.

Example: ERM-BB445 (PCBs in pork fat):
PCB 52: certified value = 12.9 ± 0.9 µg/kg.
Footnote 2 states that a coverage factor of 2 was applied. u_{CRM} is therefore 0.9 / 2 = 0.45 µg/kg.

The validation study gave an average of 14.3 ± 1.8 (single standard deviation of 6 measurements spread over 3 days). u_m is therefore estimated at 1.8/√6 = 0.73 µg/kg.

$$u_t = \sqrt{u_m^2 + u_{CRM}^2} = \sqrt{0.73^2 + 0.45^2} = 0.86 \text{ µg/kg}$$

The expanded uncertainty is 2 u_t = 1.7 µg/kg. This is larger than the difference between the certified and the found value (14.3 – 12.9 = 1.4 µg/kg). Therefore, the method does not have a significant bias and u_t is used as uncertainty contribution of trueness in the total uncertainty calculation.

Routine Quality Control

Using CRMs to produce quality control charts offers significant advantages over ordinary, laboratory prepared standards:

- **CRMs have been tested for homogeneity. Switching from one bottle to the other is possible without having to re-establish the control chart.**
- **CRMs have been stabilized so that even if opened can be assumed to be more stable than normal laboratory samples.**
- **CRMs are consistent and accurate allowing every result on the control chart to be checked against a true value.**
- **Labor costs in preparing, validating and rechecking home-made reference materials quickly exceed the additional cost of a CRM.**

References:

[1] ISO 17025 "General requirements for the competence of testing and calibration laboratories", ISO, Geneva, 2000

[2] ISO Guide 33 "Uses of Certified Reference Materials", ISO, Geneva, 2000

Establishment of Traceability

Most analytical techniques involve sample pre-treatment: dilution, extraction, etc. Each step breaks the traceability chain. Matrix CRMs are the tool of choice for proving that no significant errors in the sample preparation steps occurred, thereby maintaining traceability.

Reliable Sources of BCR® and ERM® and IRMM® Reference Materials

For quality-minded analytical laboratories, CRMs are indispensable tools to ensure the quality of the analytical results, and aid in compliance to ISO standards and guidelines. Fluka is among the few authorised distributors of CRMs produced by the European Commission, and in particular by the IRMM. These materials fulfill the highest requirements regarding uncertainty, homogeneity, stability and traceability.

Training course

„Selection and Use of Reference Materials"

Reference materials are considered key tools for achieving traceability of measurements, proving accuracy of methods and demonstrating proficiency of laboratories. The aim of this course is the practical demonstration of selection and use of reference materials:

- Selection of appropriate materials
- Evaluation of analytical results on reference materials
- Establishing traceability
- Uncertainty estimation
- Demonstrating trueness
- Proof of laboratory proficiency
- Proper material handling
- Making full use of existing information

Who should attend
Laboratory managers and practitioners in analytical laboratories who use reference materials for statistical quality control, method validation and calibration.

Course layout
Lectures as well as practical exercises for material selection and data evaluation.

For more information, please visit:
www.irmm.jrc.be/html/events/

* Trueness is defined as the "closeness of agreement between the average value obtained from a large series of test results and an accepted reference value" (ISO 5825:1994). Accuracy is defined as "closeness of agreement between a test result and the accepted reference value" (ISO 5725:1994), and is therefore a combined parameter comprising both precision and trueness. This means if a method is accurate, one gets the true result with a low variability. Inaccurate methods have poor precision, insufficient trueness or both.

EUROPEAN COMMISSION
DIRECTORATE-GENERAL
Joint Research Centre
irmm

European Reference Materials (ERM®): A new standard of certified reference materials.

By Rainer Walz, PhD, Product Manager, Fluka/Riedel-de Haën: rwalz@europe.sial.com

Since April 2000 Sigma-Aldrich has been an authorized distributor for the Institute for Reference Materials and Measurements (IRMM) at Geel, Belgium. As a result, analysts around the globe can obtain all 500+ IRMM Certified Reference Materials (CRM) from Sigma-Aldrich. Our customers profit from our fast and reliable delivery, competitive prices and expert technical service.

As part of our partnership with the IRMM, Sigma-Aldrich is pleased to offer the European Reference Materials (ERM®) line of chemical standards. ERM® is a new standard in certified reference materials that ensures reliability and comparability of results when they are used in chemical analyses. European Reference Materials (ERM®) are certified, undergo uncompromising peer evaluation and offer highest quality, traceability and reliability.

The key features and benefits of the European Reference Materials are:

- Full **transparency** of the certification principles and the evaluation report allows the user to see exactly how the material was tested and according to what specifications.
- Clearly defined and stated **traceability** of the certified values, meaning it is fully traceable to reference systems (i.e. reference materials and/or reference methods) ensures applicability of the materials to the intended analytical application.
- **Internationally recognized values** supported through the participation of the producing institutes in the key comparisons organized by the Bureau International des Poids et Mesures.

The full range of European Reference Materials (ERM®) spans many key analytical sectors, including:

- **Environmental** – polycyclic aromatic compounds, nitropolycyclic and oxygenated aromatic hydrocarbons, polychlorinated biphenyls (for purity), soils sludge, sediments, biological material, water, waste
- **Occupational hygiene** – filter media, charged tubes with Tenax or charcoal
- **Water and food microbiology** – milk powder, mycotoxins
- **Food and agriculture** – dairy products, alcohol, GMO standards, meat, cereals, vegetables, oils, fat, fish, mussels, animal feed, seeds
- **Clinical chemistry** – plasma, serum, body liquids, blood
- **Physical properties** – heat transmission, particle size, surface area, properties of films and surfaces, line-width measurements, color measurements, mechanical properties
- **Industrial raw materials and products** – ores, fuels, gas, oil, metals, semiconductors, plastics, glass, ceramics, fertilizers the method.
- **Isotopic standards**

Some of the latest innovations from ERM® and offered by Sigma-Aldrich include new CRM for food (aflatoxin) and isotopic (methylmercury) analysis **(Table 1)**.

Table 1: NEW! ERM® Standards Offered by Sigma-Aldrich

Cat. No	Brand	Certified Referemce Material	Pack Size
ERM-BD282	ERM®-IRMM	Aflatoxin M1 in Whole milk powder (zero level, < 0.02 µg/kg)	30 g
ERM-BD283	ERM®-IRMM	Aflatoxin M1 in Whole milk powder (low level, 0.111 +/- 0.018 µg/kg)	30 g
ERM-BD284	ERM®-IRMM	Aflatoxin M1 in Whole milk powder (high level, 0.44 +/- 0.06 µg/kg)	30 g
ERM-AE670	ERM®-IRMM	$CH_3{}^{202}HgCl$ in 2% ethanol/water	5 g

Looking for Analytical Standards?

Let Sigma-Aldrich Be Your Guide

Sigma-Aldrich Catalog of Analytical Standards

No matter what your analytical chemistry needs, the global resources and manufacturing expertise of Sigma-Aldrich are at your side, providing a full range of research tools to help you advance your work. Introducing: the new **Sigma-Aldrich Analytical Standards Catalog,** with over 7,000 standards from Fluka, Riedel-de Haën, Supelco, Isotec, Aldrich and Sigma – brought together for the first time in one comprehensive book.

From Chromatography to Spectroscopy and from Certified Standards to Special Packaging and Custom-made Standards, you'll find it here – all at competitive prices, every day. And all backed by service and technical support known the world over for excellence.

Let the Sigma-Aldrich Analytical Standards Catalog be your guide.

To reserve your free copy, visit us online at
sigma-aldrich.com/standardcatalog

For custom-made inquiries, please send an e-mail to
customstandards@sial.com.

SIGMA ALDRICH Fluka Riedel-de Haën SUPELCO ISOTEC

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SIGMA-ALDRICH

Quantitative Pesticide Mixes from Supelco: Sigma-Aldrich offers a large selection of Supelco brand pesticide mixes for use as chromatographic standards.

By Vicki Yearick, Product Manager, Supelco: vyearick@sial.com

Supelco brand quantitative pesticide mixes include organophosphorus, organochlorine and nitrogen containing pesticides and pesticide metabolites. They are appropriate for use in monitoring pesticide contamination in soil, food, drinking water and groundwater. All raw materials and solvents used in the preparation of these mixes are screened for purity. Mixtures are gravimetrically prepared and assayed by chromatography.

Each Supelco brand quantitative pesticide standard is supplied with a Certificate of Analysis. Data packets are also available free of charge upon request. Each data packet documents the rigorous analytical methods we use to verify raw material identity and purity, and provides certification of the purity and accuracy of the final concentration. An example is shown.

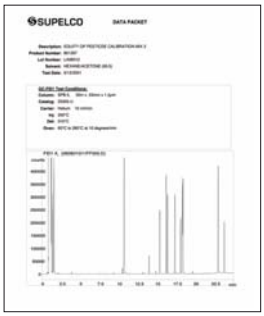
Supelco can also formulate, test and package custom pesticide mixtures for your specific application. Our custom standard chemists will gladly discuss stability and solubility concerns with you and make suggestions on how to maximize the quality and reliability of your standard.

Sigma-Aldrich custom pesticide standard solutions include:

- Raw materials and solvents screened for identity and purity
- Your choice of gravimetric, qualitative or quantitative testing
- Packaging choices from ampoules to bottles
- Manufacturing processes following ISO 9001:2000 guidelines
- Documentation and Material Safety Data Sheets
- Strict adherence to all shipping regulations
- Free technical support before and after the sale

To obtain a free quote, please send your request to **customstandards@sial.com**.

Figure 1: Data Packet



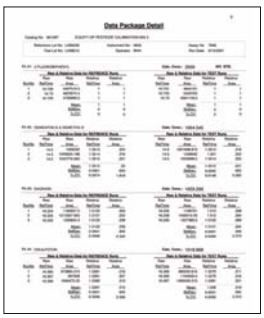


Figure 2: Data Packet (pages 1-3)

For a comprehensive **listing of Sigma-Aldrich analytical pesticide standards**, *request a copy of the 2004-2005 Sigma-Aldrich Analytical Standards catalog using the enclosed reply card or visit us on-line at* **sigma-aldrich.com/standardcatalog**.

Chlorinated Pesticdes

Cat. No.	Brand	Description	Composition (concentration)	Pack Size
47977	Supelco	Pesticide Std Mix A-1, 1 x 1 mL, Hexane:Toluene (99:1)	2,4,5,6-Tetrachloro-m-xylene, α-BHC, Endosulfan 1, γ-BHC, Heptachlor (0.5 µg/mL), 4,4′-DDD, 4,4′-DDT, Decachlorobiphenyl, (0.5 µg/mL); 4,4′-DDD; 4,4′-DDT; Decachlorobiphenyl; Dieldrin; Endrin (1 µg/mL); Methoxychlor (5 µg/mL)	1 mL
47978	Supelco	Pesticide Std Mix B-1, 1 x 1 mL, Hexane:Toluene (99.5:0.5)	2,4,5,6-Tetrachloro-m-xylene, Aldrin, α-Chlordane, β-BHC, δ-BHC, γ-Chlordane, Heptachlor epoxide isomer B (0.5 µg/mL); 4,4′-DDE, Decachlorobiphenyl, Endosulfan II (beta), Endosulfan sulfate, Endrin aldehyde, Endrin ketone (1 µg/mL)	1 mL
505935	Supelco	Pesticide Surrogate Spike Mix, 1 x 1 mL, Acetone, 200 µg/mL	2,4,5,6-Tetrachloro-m-xylene Decachlorobiphenyl (200 µg/mL)	1 mL
46960-U	Supelco	Appendix IX Organochlorine Pesticides Mix (2000 µg/mL)	Aldrin, α-BHC, β-BHC, γ-BHC, δ-BHC, 4,4′-DDD, 4,4′DDT, Dieldrin, Endosulfan I, Endosulfan sulfate, Endrin, Endrin aldehyde, Heptachlor, Heptachlor epoxide, Methoxychlor (2000 µg/mL)	1 mL
48282	Supelco	DDT-Endrin Mix, 1 x 1 mL, MeOH, 500 µg/mL, Each	4,4′-DDT, Endrin (500 µg/mL)	1 mL

Organophosphorous (OP) Pesticides

Cat. No.	Brand	Description	Composition (concentration)	Pack Size
861283	Supelco	OP Pesticide Mix 2, 1 x 1 mL	Alachlor, Atrazine, Bromacil, Butachlor, Metachlor (Dual), Prometone, Simazine (1000 µg/mL)	1 mL
507202	Supelco	EPA 8270 Organophosphorus Pesticide Mix, 1 x 1 mL, Hexane:Acetone, 2000 µg/mL	Dimethoate; Disulfoton, Famphur; Methyl Parathion; o,o,o,-Triethylphosphorothioate; Parathion; Phorate; Sulfotep, Thionazin (2000 µg/mL)	1 mL
861265	Supelco	OP Pesticide Calibration Mix 1, 1 x 1 mL, Hexane, 1000 µg/mL	Chlorpyrifos (Dursban), EPN (1000 µg/mL); Ethoprop (Prophos, Mocap) (100 µg/mL)	1 mL
861267	Supelco	OP Pesticide Calibration Mix 2, 1 x 1 mL, Hexane:Acetone (95:5,) 1000 µg/mL	Dementon S, Demonton O, Diazinon, Disulfoton, EPN, Fenthion, Malathion, Methyl azinphos (Guthion), Methyl parathion, Parathion (1000 µg/mL)	1 mL
861269	Supelco	OP Pesticide Calibration Mix 3, 1 x 1 mL, Hexane:Acetone (95:5), 1000 µg/mL	Chlorpyrifos (Dursban), Coumaphos, Dichlorovos, EPN, Fensulfothion, Mocap (Ethoprop), Naled, Phorate, Phosdrin (Mevinphos), Ronnel, Stirofos (Tetrachlorvinphos), Sulprofos (Bolstar), Tokuthion (1000 µg/mL)	1 mL
861162	Supelco	Pesticide 507 Mix, 1 x 1 mL, MTBE, Varied Concentrations	2,3-Dichloronitrobenzene, Bromacil (250 µg/mL); Alachlor, Metribuzin (50 µg/mL); Atrazine, Simazine (25 µg/mL); Butachlor, Metachlor (Dual) (100 µg/mL)	1 mL
861165	Supelco	Pesticide Mix, 1 x 1 mL, MTBE, Varied Concentrations	Dimethoate, Disulfoton, EPN, Ethion, Fonofos (Dyfonate), Malathion, Parathion, Sulfotep, Thionazin (200 µg/mL); TEPP (2000 µg/mL)	1 mL
861196	Supelco	EPA 8141 OP Pesticides Mix 1, 5x1mL, Hexane:Acetone (95:5), 200 µg/mL	Disulfoton, Fensulfothion, Malathion, Methyl azinphos (Guthion), Methyl Parathion, Parathion (200 µg/mL)	5 x 1 mL
861237	Supelco	OP Pesticide Mix, 1 x 1mL, Hexane, 100 µg/mL	Carbophenothion (Trithion), Ethion, Malathion, Parathion (100 µg/mL)	1 mL

New shipping carton for 4 x 2.5 L solvent bottles: Fully recyclable design is easier to use and reduces waste.

By Frederik Pillong, Product Manager Fluka/Riedel de Haën: fpillong@sial.com

There is a saying that first impressions last a lifetime. When we ship a product, often the first thing you see is its packaging. Our packaging engineers strive to make our shipping containers – bottles, bags and boxes – functional, safe, easy to open, space-conserving, environmentally friendly and aesthetically pleasing.

We've recently improved the design of the shipping carton that holds our popular 4 x 2.5 L solvent bottles. Obviously, organic solvents pose significant spill hazards and have stringent shipping restrictions. Carrying containers first must protect the bottles from breakage, but they have other important characteristics. Our existing design **(Figure 1)** already had very good environmental compatibility. It was recyclable, very stable and safe. However, it comprised six separate parts plus the covering carton that had to be broken down for recycling, and required air cushions for safety packaging. This resulted in more plastic and carton waste to dispose of.

The new shipping carton **(Figure 2)** has only three pieces: the outside covering box and two pulp-fiber forms custom-fit to the shape of the bottle. All components are recyclable. It is just as safe and stable as the old design, but it is easier to break down, recycle, has no plastic waste and less carton to dispose of. Also, in case of accidental spill, the pulp fiber acts as adsorbent.

Currently, the new shipping carton is used for all 4x2.5L solvents from Riedel-de Haën. Over the next few months we will be replacing all of our solvent shipping cartons with the new design.

Figure 1: Previous 4 x 2.5 L shipping carton

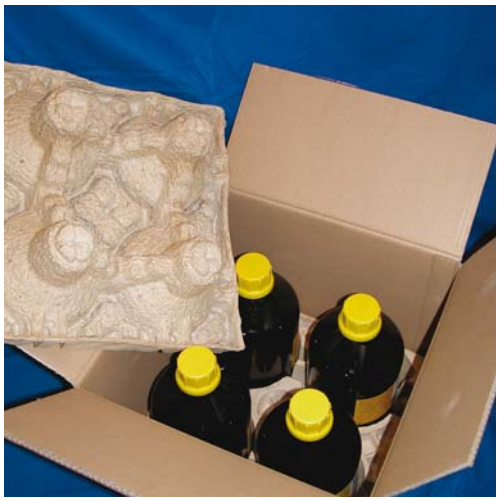


Figure 2: New 4 x 2.5 L shipping carton has fewer parts, easier to handle and recycle

Table 1: List of most popular Riedel-de Haën solvents

Cat. No.	Brand	Product	Description	Packaging Size
32222	Riedel-de Häen	Dichloromethane	puriss. p.a., ACS reagent, reag. ISO, ≥99.9% (GC)	1 L, 2.5 L, 6 x 1 L, 2.5 x 4 L
32299	Riedel-de Häen	Petroleum ether	puriss. p.a., ACS reagent, reag. ISO, bp 40-60 °C (min.95%)	1 L, 2.5 L, 6 x 1 L, 2.5 x 4 L
24201	Riedel-de Häen	Acetone	puriss., meets analytical specification of Ph. Eur., BP, NF, ≥99% (GC)	1 L, 2.5 L, 6 x 1 L, 2.5 x 4 L
34913	Riedel-de Häen	Hexane	SPECTRANAL™, ≥97.0% (GC)	1 L, 2.5 L, 6 x 1 L, 2.5 x 4 L
34851	Riedel-de Häen	Acetonitrile	for HPLC, CHROMASOLV™ gradient grade, ≥99.9% (GC)	1 L, 2.5 L, 6 x 1 L, 2.5 x 4 L
24216	Riedel-de Häen	Chloroform	puriss., meets analytical specification of DAB9, BP, 99-99.4% (GC)	1 L, 2.5 L, 6 x 1 L, 2.5 x 4 L
34966	Riedel-de Häen	Methanol	LC-MS CHROMASOLV™, ≥99.9%	1 L, 2.5 L, 6 x 1 L, 2.5 x 4 L

LC-MS CHROMASOLV® - The Highest Quality Solvents and Blends

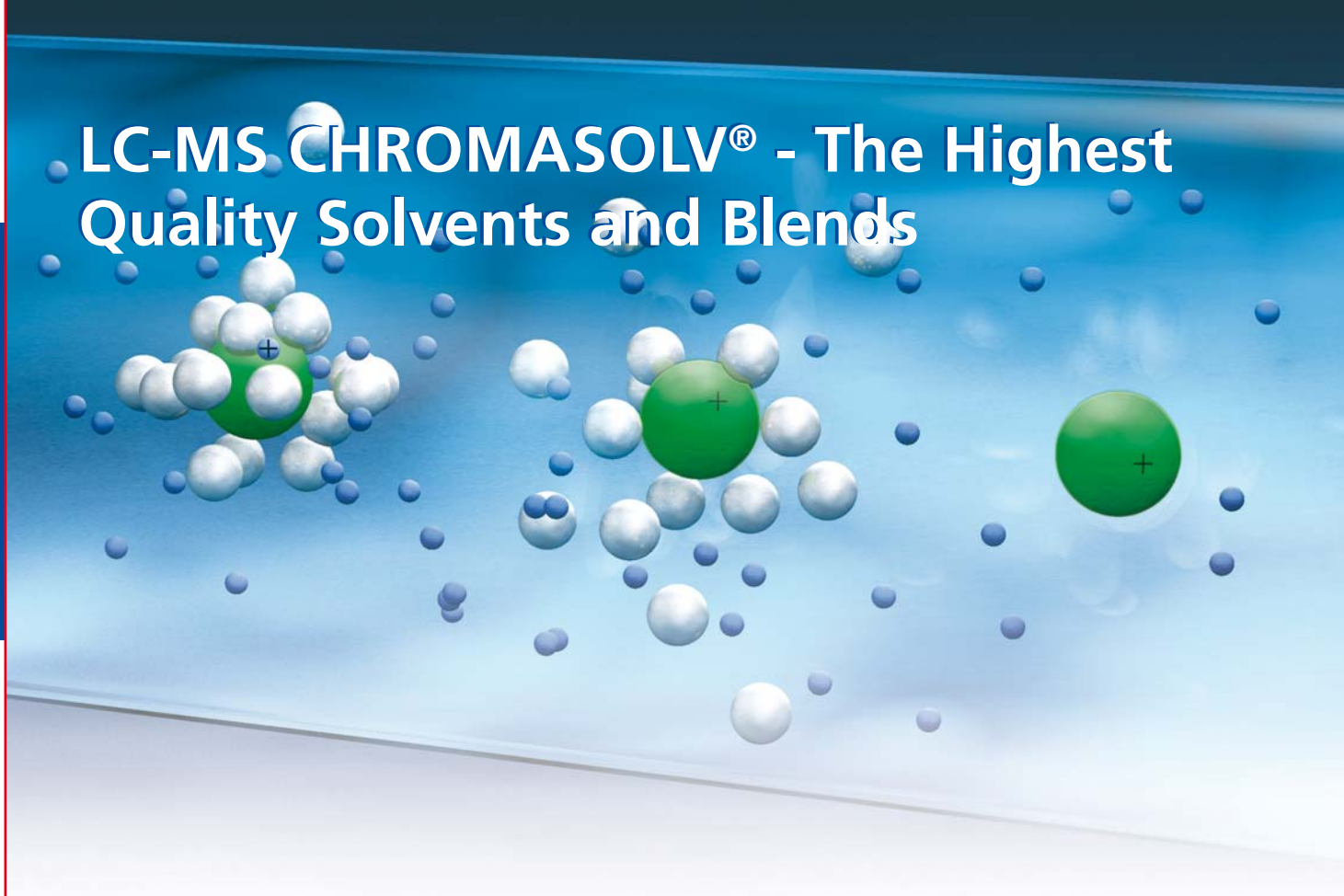


Table 1: Pure Solvents

Cat. No.	Brand	Solvent	Pack size
39253	Riedel-de Häen	Water	1 L
34967	Riedel-de Häen	Acetonitrile	1 L, 6 X 1 L, 4 X 2.5 L, 5 L
34966	Riedel-de Häen	Methanol	1 L, 6 X 1 L, 4 X 2.5 L, 2.5 L
34965	Riedel-de Häen	2-Propanol	1 L, 6 X 1 L, 4 X 2.5 L, 2.5 L
34972	Riedel-de Häen	Ethyl acetate	1 L-R, 2.5 L-R

Table 2: Solvent Blends

Cat. No.	Brand	Solvent Blend	Pack size
34978	Riedel-de Häen	Water with 0.1% TFA	2.5 L
34976	Riedel-de Häen	Acetonitrile with 0.1% TFA	2.5 L
34974	Riedel-de Häen	Methanol with 0.1% TFA	2.5 L
34673	Riedel-de Häen	Water with 0.1% formic acid	2.5 L
34668	Riedel-de Häen	Acetonitrile with 0.1% formic acid	2.5 L
34671	Riedel-de Häen	Methanol with 0.1% formic acid	2.5 L
34675	Riedel-de Häen	Water with 0.1% acetic acid	2.5 L
34678	Riedel-de Häen	Acetonitrile with 0.1% acetic acid	2.5 L
34672	Riedel-de Häen	Methanol with 0.1% acetic acid	2.5 L
34674	Riedel-de Häen	Water with 0.1% ammonium acetate	2.5 L
34669	Riedel-de Häen	Acetonitrile with 0.1% ammonium acetate	2.5 L
34670	Riedel-de Häen	Methanol with 0.1% ammonium acetate	2.5 L

Table 3: Rinsing Solution

Cat. No.	Brand	Composition	Pack size
34682	Riedel-de Häen	Water/2-Propanol 50/50	2.5 L

As an Analytical tool, LC-MS is often chosen for its sensitivity and specificity. However, impurities in the mobile phase can seriously diminish the ability to detect and identify compounds that exist at very low levels. LC-MS CHROMASOLV® solvents and blends undergo 34 distinct test to ensure they meet the stringent criteria required for sensitive LC-MS and LC-UV analysis.

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Application of MALDI-TOF for biomarker determination: A straightforward and reproducible tool for rapidly scanning serum proteome, detecting and distinguishing hundreds of low molecular weight proteins and peptides in seconds.

By Alicia Prieto, PhD, Chromatography Service, Centro de Investigaciones Biológicas,Consejo Superior de Investigaciones Cientificas Madrid, Spain: aliprieto@cib.csic.es

One of the most active MALDI-TOF application areas is in the analysis of disease-specific biomarker peptides and low abundance proteins in blood, urine, and other biological fluids. These molecules are used as disease-specific biomarkers. It is the aim of this type of research to use these biomarkers to aid in the diagnosis of disease and in the evaluation of its severity and progression.

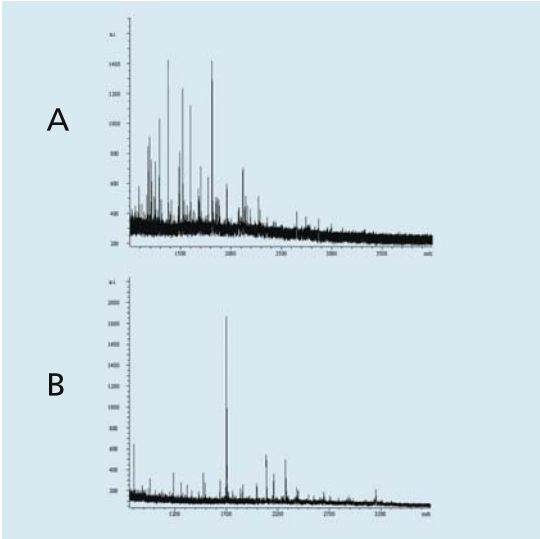
Of particular interest is the study of the serum proteome, a complex mixture comprising mainly highly abundant proteins, such as albumin and other carrier proteins, and proteins that originate from circulating blood cells. The population of proteins that enters the blood from the surrounding tissue constitutes a minor fraction, but it may contain most of the undiscovered biomarkers. MALDI-TOF has demonstrated it can be a straightforward and reproducible tool for rapidly scanning these samples, detecting and distinguishing hundreds of low molecular weight proteins and peptides in seconds.

The MALDI protocol first involves the capture and enrichment of peptides using magnetic beads or some other chromatographic method. In the second step a portion of the enriched sample is mixed with a matrix like α-cyano-4-hydroxycinnamic acid. Next, the mixture is spotted onto a target and allowed to dry at room temperature. The final step is the desorption of bulk portions of the solid sample by a short pulse of laser light. The matrix absorbs the laser energy, causing codesorption of the analyte and promoting analyte ionization. Liberated ions from the sample are swept by vacuum into the mass analyzer.

The resulting spectra can be recorded in the linear positive ion mode with external calibration in the range of analysis (1-15 kDa) using a mixture of peptide/protein standards. Up to 400 peptides can be detected and characterized in this mass range. This approach has been used in studies focused on the detection of biomarkers for asthma, acute lymphatic leukemia and brain tumors, among many others. In each case, specific profiles of peptides have been observed that can be used to predict if the sample is normal or diseased.

Two applications on protein identification by MALDI-TOF are shown below. The first one refers to identification of a bacterial protein (**A**), and the second one to porcine seminal protein from boar (PSP-II, **B**).

Sigma-Aldrich offers many MALDI products (matrices, validation and calibration sets), including those for analysis of peptides, proteins, oligonucleotides, synthetic polymers, organic molecules, carbohydrates, dendrimers.



Application: *MALDI-TOF analysis of tryptic digests of (**A**) unidentified bacterial protein and (**B**) PSP-II. The laser desorption/ionisation experiments were performed on a BIFLEX III time-of-flight instrument (Bruker-Franzen Analytik, Bremen, Germany) operated in the positive mode. A saturated solution of CCA in acetonitrile:water (1:2) with 0.1 % TFA was used as the matrix. Samples were analysed in the reflectron mode, and typically 50-100 laser shots were summed into a single mass spectrum. External calibration was performed, using peptide calibration standards. Equal volumes (0.5 microliters) of the sample solution and the matrix were spotted on the target and air-dried at room temperature.*

Table 1: List of most popular MALDI products

Cat. No.	Brand	Name
85429, 78867	Fluka	Sinapinic acid
85707, 39319	Fluka	2,5-Dihydroxybenzoic acid (DHB)
56197	Fluka	3-Hydroxpicolinic acid
70990, 55272	Fluka	α-Cyano-4-hydroxycinnamic acid
91928, 41711	Fluka	2',4',6'-Trihydroxyacetophenone monohydrate

HYDRANAL®-Molecular Sieve 0.3 nm: Drying agent for use in all Karl Fischer titration applications

By Michael Jeitziner, Product Manager, Fluka / Riedel-de Haën: mjeitziner@sial.com

"Which Molecular Sieve should I use with my Karl Fischer titrator? "

We often hear this question, and in response we now offer a Molecular Sieve chosen specifically for Karl Fischer applications: HYDRANAL®-Molecular Sieve 0.3 nm. Use it to fill the drying tubes on your reagent bottles, coulometric cell, volumetric titration vessel or Karl Fischer ovens and your system is ideally conditioned for reliable moisture determination. The table below shows the reproducibility of titre determinations of a sample of HYDRANAL®-Composite 5 over the course of one month using the same HYDRANAL®-Molecular Sieve 0.3 nm in the drying tubes.

Ideally designed and packaged for Karl Fischer applications

Molecular Sieve is the desiccant of choice for adsorbing moisture in Karl Fischer applications. HYDRANAL®-Molecular Sieve 0.3 nm (3Å) has an excellent water adsorption capacity of >15% w/w. And HYDRANAL®-Molecular Sieve 0.3 nm is supplied in glass bottles to keep it moisture-free over a long period of time. We offer HYDRANAL®-Molecular Sieve 0.3 nm in 250 g package sizes for coulometric cells and in 1 kg package sizes for volumetric titration vessels and Karl Fischer ovens.

Regeneration means savings

HYDRANAL®-Molecular Sieve 0.3 nm can be regenerated by heating it for at least 4 hours at 300°C. Higher temperatures cause a physical alteration of the structure. Drying at 180-250°C, in a vacuum oven under an inert gas stream is also possible.

Titre decrease of HYDRANAL®-Composite 5 using HYDRANAL®-Molecular Sieve 0.3 nm

Day	Reagent	Titre*	Std. dev.	Notes
1	HYDRANAL®-Composite 5	5.238	0.14	New bottle opened
2	HYDRANAL®-Composite 5	5.210	0.14	
7	HYDRANAL®-Composite 5	5.216	0.10	Very low temperature, titre therefore higher
22	HYDRANAL®-Composite 5	5.189	0.08	
24	HYDRANAL®-Composite 5	5.198	0.09	
32	HYDRANAL®-Composite 5	5.177	0.22	After 1 month the bottle was nearly empty. Titre determination was on the last few mL.

**The slight decrease in titre (5.238 – 5.177) was due to adjustment in the Molecular Sieve drying tube. The used reagent could be replaced with dried air.*

Special Offer *New* HYDRANAL®- *Molecular Sieve 0.3 nm*

Receive 35% off list price on the New HYDRANAL®- *Molecular Sieve 0.3 nm*
Please quote promo code 950 when placing your order.
Offer valid until 31st August 2005

Table 1: Ordering Information

Cat. No	Brand	Product	Used as.....	Pack Size
34241	Riedel-de Haën	HYDRANAL®- Molecular sieve 0.3 nm	Drying agent for Karl Fischer application	250 g, 1 kg

New Product Corner

Separate Source™ Aroclor Standards

Supelco now offers Separate Source™ (SS) Aroclor standards to meet US EPA requirements. These products have identical formulations but are prepared from independently sourced raw materials and quality controlled. Separate Source™ Aroclor standards provide the convenience of working with Supelco as a single vendor while enabling you to meet independent calibration and quality control requirements of the US EPA. Each standard is prepared in isooctane and offered at 1000 µg/mL.

Table 1: Ordering Information

Cat. No.	Brand	Standard (solution in isooctane, 1000 µg/mL)	Pack Size
48097	Supelco	Aroclor 1016	1 mL
4S8097	Supelco	NEW! SS AROCLOR 1016	1 mL
48098	Supelco	Aroclor 1221	1 mL
4S8098	Supelco	NEW! SS AROCLOR 1221	1 mL
44805	Supelco	Aroclor 1232	1 mL
4S4805	Supelco	NEW! SS AROCLOR 1232	1 mL
44806	Supelco	Aroclor 1242	1 mL
4S4806	Supelco	NEW! SS AROCLOR 1242	1 mL
44807	Supelco	Aroclor 1248	1 mL
4S4807	Supelco	NEW! SS AROCLOR 1248	1 mL
44808	Supelco	Aroclor 1254	1 mL
4S4808	Supelco	NEW! SS AROCLOR 1254	1 mL
44809	Supelco	Aroclor 1260	1 mL
4S4809	Supelco	NEW! SS AROCLOR 1260	1 mL
44810	Supelco	Aroclor 1262	1 mL
4S4810	Supelco	NEW! SS AROCLOR 1262	1 mL
502146	Supelco	Aroclor 1268	1 mL
5S02146	Supelco	NEW! SS AROCLOR 1268	1 mL

Multi-Pak Drinking Water Odor Standards

Our new multi-pak odor standards eliminate excess packaging and offer a more cost effective means of purchasing your standards. Each standard is prepared as 100 µg/mL in methanol.

Cat. No.	Brand	Standard (solution in methanol, 100 µg/m)	Qty.
47522-U	Supelco	(+/-)Geosmin	1 mL
4M7522-U	Supelco	NEW! (+/-)Geosmin	5 X 2 mL
47523-U	Supelco	2-Methylisoborneol	1 mL
4M7523-U	Supelco	NEW! 2-Methylisoborneol	5 X 2 mL
47525-U	Supelco	(+/-)Geosmin and 2-Methylisoborneol	1 mL
4M7525-U	Supelco	NEW! (+/-)Geosmin and 2-Methylisoborneol	5 X 2 mL

NIST-Traceable Alcohol Standards

Diluted in high purity water, each standard is delivered in a set of 10 x 1mL ampoules.

Table: Oekanal® Alcohol (Ethanol) Standard Solutions, NIST Traceable

Cat. No.	Brand	Concentration	Package size
33952	Riedel-de Haën	0.25mg/mL	10 x 1 mL ampoules
33953	Riedel-de Haën	0.3mg/mL	10 x 1 mL ampoules
33957	Riedel-de Haën	0.5mg/mL	10 x 1 mL ampoules
33958	Riedel-de Haën	0.8mg/mL	10 x 1 mL ampoules
33959	Riedel-de Haën	0.9mg/mL	10 x 1 mL ampoules
33961	Riedel-de Haën	1mg/mL	10 x 1 mL ampoules
33962	Riedel-de Haën	2mg/mL	10 x 1 mL ampoules
33963	Riedel-de Haën	3mg/mL	10 x 1 mL ampoules
33964	Riedel-de Haën	4mg/mL	10 x 1 mL ampoules

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