

ENVIRONMENTAL TESTING

Organic certified reference materials

Zuzana Antalová
October 2017
Vilnius



Environmental

MERCK

Analytical Testing and Reference Standards go hand in hand



..... for **total confidence** in measurement

Results are only as accurate as the reference!

Why to buy Standards

Choosing a supplier for Reference Materials

**NO DOUBTS. NO DELAYS.
JUST PRECISION!**

Darmstadt, Germany
Certipur® inorganic and
elemental CRMs

Laramie, WY, USA
RT Pharma Secondary
standards, matrix
environmental CRMs,
proficiency testing
schemes

Round Rock TX, USA
Cerilliant® clinical,
toxicology and pharma
CRMs and RMs

Buchs, Switzerland
TraceCERT® organic and
inorganic CRMs, organic
RMs (pesticides), inorganic
custom standards

Trustful partner

- An accredited manufacturer of reference materials that you can **trust to**, we continually **develop new products** and solutions to make your analytical life and research **easier**

World renowned supply chain

- Global supply, with a majority of standards available to **ship same day**

Outstanding quality, service

- Supplying **over 22 000** different analytical standards and certified reference materials

Definition

What are Reference Materials?

Certified Reference Material	Reference Material
CRM	RM
<ul style="list-style-type: none">• Values(s) characterized by a metrologically valid procedure for the specified property(ies)• Certificate provides the<ul style="list-style-type: none">– Property Value– Associated Uncertainty– Metrological Traceability• Manufactured by an accredited Manufacturer and value(s) assigned by an accredited laboratory	<ul style="list-style-type: none">• Value is homogenous and stable with regard to the specified property(ies)• Fit for its intended use in measurement, calibration of an apparatus or assessment of analytical method

Type of standard

Acronyms

Quality attributes

References

- 1.) ISO Guide 30:2015 Reference materials – Selected terms and definitions
- 2.) ISO Guide 34:2009 General requirements for the competence of reference material producers
- 3.) JCGM 200:2012 International Vocabulary of Metrology

Certified Reference Materials Production to ISO (International Standardisation Organisation)

ISO/IEC 17025



Focuses on the
MEASUREMENT

Main objectives of the quality control lab:

- **Characterization of the CRM**
 - Certifying the measurement value and the uncertainty value according to Guide 35
 - Making the reference material traceable to a primary standard

ISO Guide 34 Changed to ISO17034 from November 2016



Accreditation as a producer of
certified reference materials

- **Production**
 - Raw material selection and purity
 - Production planning and control
- **Characterization** (*everything that is in ISO/IEC 17025*)
 - Measurement methods
 - Uncertainty evaluation
 - Traceability
- **Assessment of homogeneity and stability** (including packaging)

ISO Guide 31



Defines **content** of the Certificate of Analysis and product labelling

Certified Reference Materials (CRMs) Merck CRM Manufacture



Double accreditation as a Reference Material Producer

For CRM producers the combination of ISO/ IEC 17025 *and* ISO Guide 34 is the **highest achievable level of quality and confidence**

We also call it the **"gold standard"** for CRM producers

All MERCK standards manufacturing sites are at a minimum double accredited to ISO/IEC 17025 and ISO Guide 34, which is the highest achievable quality level for reference material producers

ISO Guide 34 & ISO 17025 Accreditation

Building on a solid foundation

ISO Guide 34: Accreditation as a producer of CRMs

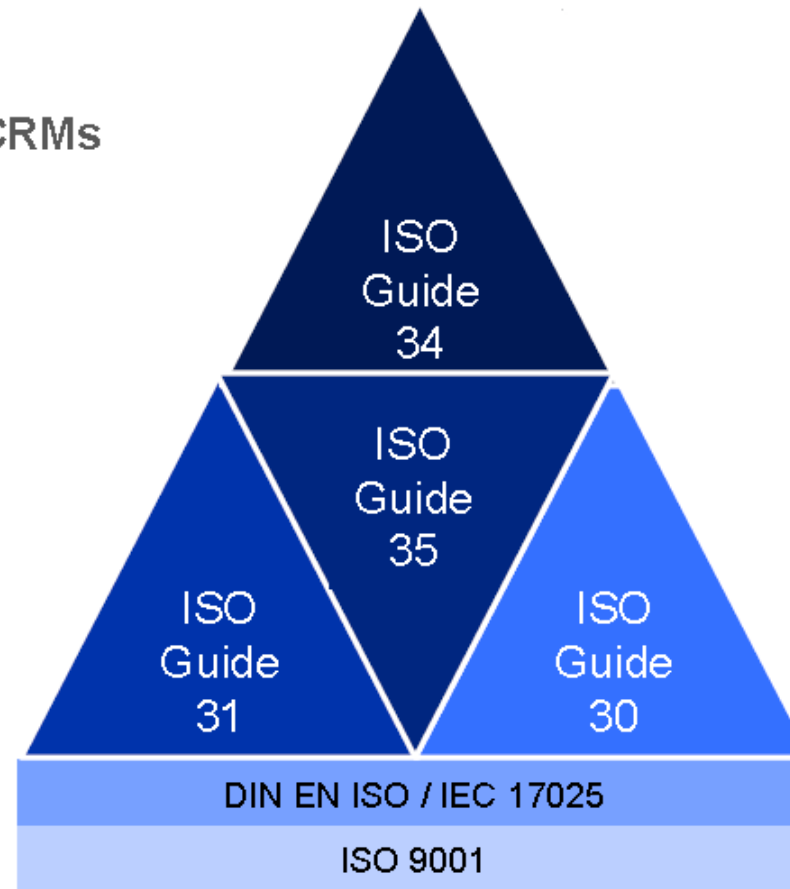
ISO Guide 35: Calculation of the uncertainty

ISO Guide 31: Certificate of Analysis

ISO Guide 30: CRM definition

ISO 17025: Accreditation of the analytical lab

ISO 9001: Documentation



ISO 17025 (General Requirements for the Competence of Testing and Calibration Laboratories) and ISO Guide 34 (General Requirements for the Competence of Reference Material Producers)

CRM Production

Merck Manufacturing Sites Having Double Accreditation

**Buchs,
CH**



Analytical standards and **TraceCERT®** CRMs

**Round
Rock,
TX**



Cerilliant® clinical, toxicology and pharma standards

**Laramie,
WY**



Secondary standards, matrix environmental CRMs, proficiency testing schemes

**Bellefonte,
PA**



Solutions, mixes and customer standards **Supelco®**

**Darmstadt,
DE**



Merck HQ, Certipure® inorganics

Why use Certified Reference Materials? Benefits

- **High Reliability**
- **Accurate Quantitative Values**
- **Comparable Results**

ISO/IEC 17025

General requirements for the competence of **testing and calibration laboratories**

- **Usage of CRMs is mandatory**

Supelco.
Quality Control Products

PRECISION
IS OUR
STRENGTH

Analytical Standards &
Certified Reference Materials

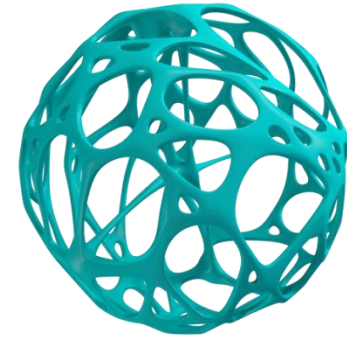
MERCK

© 2014 Merck KGaA, Darmstadt, Germany. The science business of Merck operates as MilliporeSigma Inc. in the U.S. and Canada.

The advertisement features a large satellite dish pointing towards the sky, with a bright yellow laser beam originating from the dish. The background is a vibrant green with a yellow and purple gradient at the top. The Supelco logo is in the top left, and the Merck logo is in the bottom right. The text 'PRECISION IS OUR STRENGTH' is prominently displayed in the center.

What are the different types of standards in our portfolio?

The Hierarchy of Standards



Metrology Reference Standard (NMI), and Pharmacopeial (Primary) Reference Standard

Certified Reference Material (CRM), ISO

A CRM is considered to provide the highest level of accuracy and traceability for a measurement outside of a National Metrology Institute (NMI) material

Analytical Standard

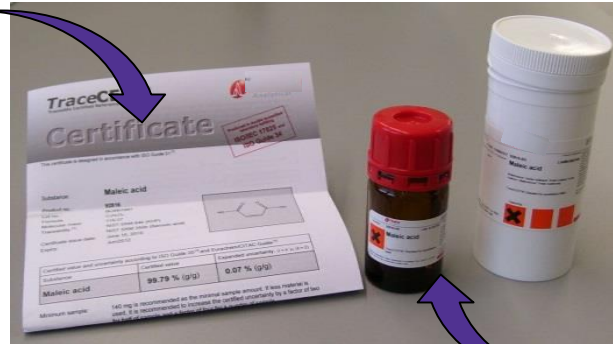
these are provided with a Certificate of Analysis, with high purity, this does not make them the same as a CRM, the certificate can be issued by anyone, no rules about who is authorized to issue certificates and who is not

Certified Reference Material (CRM) and Analytical Standard

What is the difference?

ISO/IEC 17025
(Guide for testing laboratories)

ISO Guide 31
(Guide for documentation, certificates)



ISO Guide 34
(Guide for the CRM Producer)

Parameters	Analytical Standard	CRM
Stability	✓	✓
Homogeneity		✓
Uncertainty		✓
Traceability		✓

Which type to choose from our portfolio?

Pure Chemical, Standard or CRM?

Research Grade Chemical

Used: *in a variety of applications, synthesis*

Is provided with a CoA

Purity varies

Is not suitable to be used as a standard

Analytical Standard

Used: *Where a standard is needed for calibration*

Qualitative identification (such as impurities) or quantitative

Method development

Performance controls

Impurity identification

Verification and checks of analytical systems

Also known as a:

- Standard, internal standard, calibrator, control

Certified Reference Material (CRM)

Used: *Where confidence in the measurement is critical*

As a calibration standard in 17025 regulated labs

Method validation

Where uncertainty of measurement is needed

Where traceability is needed (e.g. final product testing)

Instrument qualification (IQ/OQ)

Proficiency testing

Analytical Standards and Certified Reference Materials Formats available



Solid and liquid ('neats')

- To create your own calibration concentrations

Solutions

- Ready to use, for spiking biological samples or for use as calibrators

Mixes

- Convenient combinations of commonly screened compounds, such as multicomponent ICP CRMs

Proficiency Testing

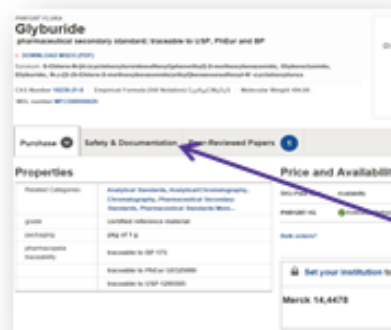
- More than 20 000 samples per year, from more than 2 500 labs in over the world

Analytical Standards and CRMs

Did you receive your Certificate of Analysis?

RM delivered with their CoAs:

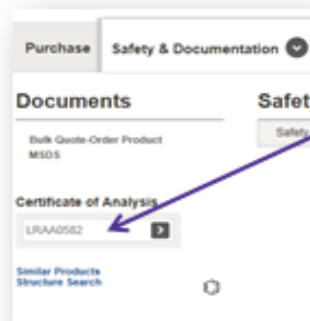
- TraceCERT® (organic)
- Pestanal®



RMs not delivered with CoA:

Cerilliant® Certified Reference Materials

- Electronic Certificate – product web page or CoA search tool



CoA

the real **value** behind

Analytical Standard Certificate of analysis

SIGMA-ALDRICH®

3050 Spruce Street, Saint Louis, MO 63103 USA
Email USA: techserv@sial.com Outside USA: eurtechserv@sial.com

Certificate of Analysis

Product Name: GLYPHOSATE
PESTANAL™, analytical standard

Product Number: 45521

Batch Number: BCBS2439V

Brand: Sigma-Aldrich

CAS Number: 1071-83-6

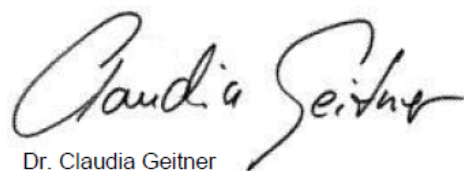
Formula: (HO)₂P(O)CH₂NHCH₂CO₂H

Formula Weight: 169.07

Expiration Date: AUG 2021

Quality Release Date: 08 SEP 2016

TEST	SPECIFICATION	RESULT
PURITY (HPLC AREA %)	≥ 98.0 %	98.7%
WATER	≤ 1.0 %	0.48%
PROTON NMR SPECTRUM	CONFORMS TO STRUCTURE	CONFORMS



Dr. Claudia Geitner
Manager Quality Control
Buchs, Switzerland

- High chromatographic purity
- Identity Confirmed (NMR)
- (sometimes) Tested for Impurities (Water, Solvents, inorganics)

45521 Glyphosate

Lot Number: BCBS2439V	Sample Name: T38562_001_LC
Dionex Ultimate 3000	
Pump: LPG-3400A	Injection Time: 07.09.16 19:43
Autosampler: WPS-3000	Processed By: Mikael Berthet
Detector: PDA-3000	Vial Number: BE4
Column: Supelco Ascentis Express C18, 2.7 um	Column S/N: -
Column Dim.: 100 x 4.6 mm	Sample Type: unknown
Mobile Phase:	Injection Volume: 2.0 µl
%A: Acetonitrile	Flow: 1.50 ml/min
%B: H ₂ O	Column Temp. (°C): 25.0
%C: TB pH 2.4	Run Time: 15.00 min
%D: HPS pH 2.4	
Gradient: see Figure 1	
Sample Prep.: 400 µl sample solution (1 mg/ml sample in Buffer pH 9) and 600 µl (5 mg/ml DNBC in acetonitrile)	

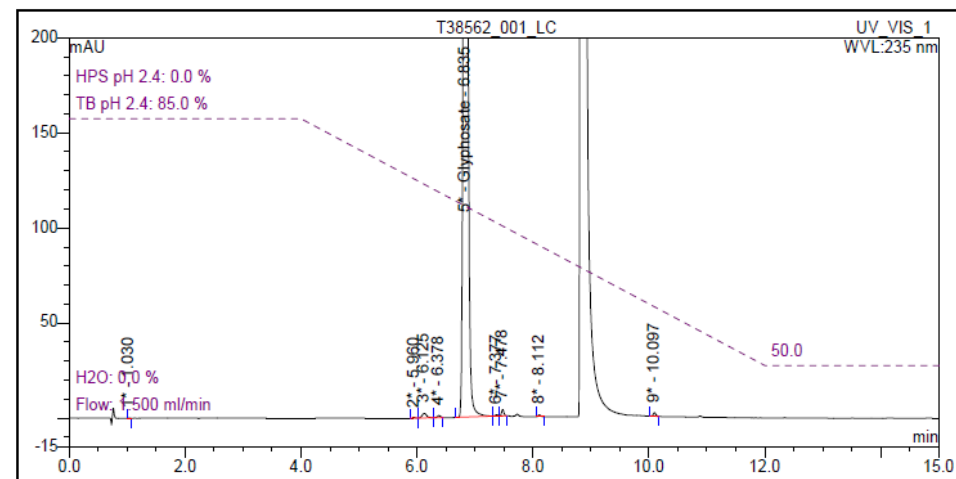


Figure 1: Zoomed Chromatogram

No.	Ret. Time min	Peak Name	Area mAU*min	Height mAU	Amount	Rel. Area %
1	1.030	n.a.	0.00695	0.21985	n.a.	0.01
2	5.960	n.a.	0.01555	0.23788	n.a.	0.03
3	6.125	n.a.	0.21857	2.38727	n.a.	0.43
4	6.378	n.a.	0.06830	1.05527	n.a.	0.14
5	6.835	Glyphosate	49.73302	638.84435	n.a.	98.73
6	7.377	n.a.	0.03779	0.67942	n.a.	0.08
7	7.478	n.a.	0.15080	3.30383	n.a.	0.30
8	8.112	n.a.	0.04084	0.92191	n.a.	0.08
9	10.097	n.a.	0.09856	1.87811	n.a.	0.20
Total:			50.37038	649.52789		100.00

Table 1: Integration

MERCK

Certified Reference Materials Certificate of Analysis

- Values **traceable** (NIST, SI)
- Proper calculated **uncertainty**
- **Homogeneity**
- **Stability** tested

All guaranteed if manufactured under **ISO 17025** and **ISO Guide 34**



TraceCERT® **SIGMA-ALDRICH®**
Traceable Certified Reference Materials

Certificate

This certificate is designed in accordance with ISO Guide 31[®].

Accredited in accordance with ISO/IEC 17025 and ISO Guide 34

Product name: **Pyrocatechol**

Product no.: **50550**

Lot no.: **BCBM6265V**

Formula: **C₆H₆O₂**

Molecular mass: **110.11 g/mol**

Traceability[®]: **NIST SRM 350b (Benzole assay)**

Certificate issue date: **February 29, 2016**

Expiry: **FEB 2018**

Certified value and uncertainty according to ISO Guide 35 [®] and Eurachem/CITAC Guide [®]		
Substance	Certified value as mass fraction (g/g)	Expanded uncertainty, $U = k \cdot u$ ($k = 2$) as mass fraction (g/g)
Pyrocatechol	99.8 %	0.2 %

Minimum sample: The sample is solid at room-temperature. 10 mg is recommended as the minimal sample amount. If less material is used, it is recommended to increase the certified uncertainty by a factor of two for half of sample and a factor of four for a quarter of sample.

Drying instruction: This material does not require drying before use.

Intended use: Use this certified reference material (CRM) as calibrant for chromatography or any other analytical technique.

Storage and handling: The CRM should be stored in the original bottle at room-temperature (20-25°C). After use the bottle should be tightly closed and protected from excessive moisture and light. Store under Argon.

CRM operations: *A. Rück*
Dr. A. Rück

Certification body: *Mano Bach*
Dr. K.D. Schmidt

Certificate page 1 of 4 Sigma-Aldrich Produkte GmbH, Industriestraße 25, 9471 Bucha/Schweizland, Tel. +41-81-756-2611, Fax +41-81-756-5856 **SIGMA-ALDRICH®**

ISO Guide 31

Traceability statement

Expiry date

Content

Expansion factor

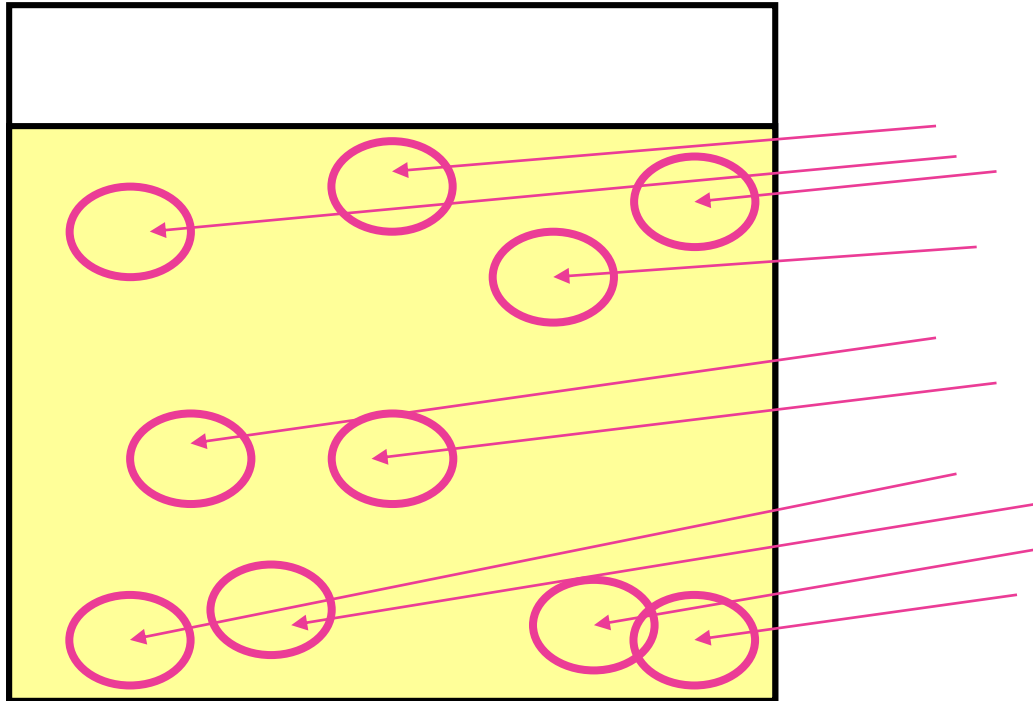
Expanded measurement uncertainty

Homogeneity

Stability

ISO/IEC 17025 + ISO Guide 34 accreditation

Certified Reference Materials
ISO Guide 34 Requirement: Homogeneity



- 10 samples measured
- Samples taken from randomly chosen spots
(top – middle – bottom)
- Contribute to overall uncertainty

Certified Reference Materials

ISO Guide 34 Requirement: : Stability Tests

- Long term stability tests at RT
- Stress tests: 3 months at 45°C



Certified Reference Materials

Standard and Expanded uncertainty

Certified value: is determined during batch release, stated in the respective CoA

Measurement uncertainty: during measurements, different influences need to be taken into account, which affect the measurement results and are represented as the "**Measurement uncertainty**"

The combined **standard uncertainty uc** is obtained from the standard uncertainties of the characterization(measurement), the homogeneity and the stability.

$$u_{CRM} = \sqrt{u^2_{\text{Characterisation}} + u^2_{\text{Homogeneity}} + u^2_{\text{Stability}}}$$

Ucharacterization is the uncertainty in accordance to DIN EN ISO/IEC 17025 which includes the contributions of the primary reference material and the measuring system (measurement uncertainty)

Uhomogeneity is the between-bottle variation in accordance to ISO Guide 34. The assessment of homogeneity is performed by analysis of a representative number of systematically chosen sample units,

Ustability is the uncertainty obtained from short-term and long-term stability in accordance to ISO Guide 34. The stability studies are the basis for the quantification of the minimum shelf life of this reference material for the unopened bottle.

Certified Reference Materials **Organics**

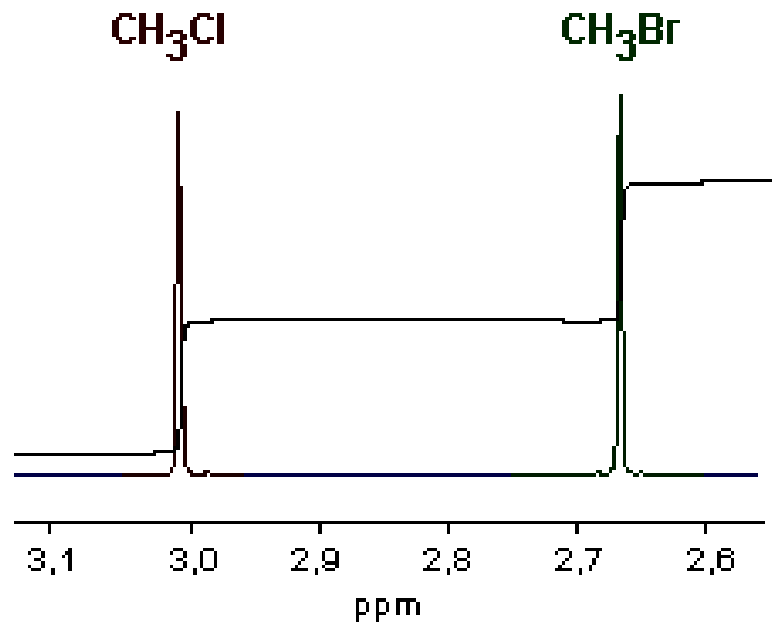
Traceability is a Challenge: ca. 50 Million Organic Compounds

-> Not always a Standard with known content is available

Quantitative $^1\text{H-NMR}$ (qNMR)

signal intensity is:

- proportional to the No. of protons
- independent of chemical structure
- no need of chemically identical reference material





Sigma-Aldrich Buchs:

ISO 17025 and ISO Guide 34
Double Accreditation
for CRM production using qNMR

600MHz Bruker NMR

^1H , ^{31}P and ^{19}F qNMR

Certified Reference Materials Prerequisites for qNMR

- Solubility
- No reaction between analyte and IS
- No Overlap for at least one signal
- No interfering impurities

Advantages of qNMR

- Traceability
- Low uncertainties for the measurement
- Non-Destructive
- Structure verification
- Information about impurities



Organic *TraceCERT*: CRMs for Chromatography

Product Groups

Amino Acids

Polyaromatic Hydrocarbons (PAHs)

Pesticides

Antibiotics

Phthalates

REACH SVHC



**More than 200 products available so far
-> Continuously growing
neats -> solutions**

www.sigma-aldrich.com/organiccrm

Reference Materials

... an overview of the
complete range for
chromatography

Complete Range for Chromatography



- Alcohol
- Pharmaceuticals & Illicit Drugs
- Steroids/Hormones
- Thyroid & Other Biomarkers
- Vitamins & Phytochemicals
- Internal Standards
- Environmental
- Explosives & Chemical Warfare
- View All

*Trace***CERT**[®]

- **Organic CRMs *TraceCERT***
 - CRMs for Chromatography (neats)
 - CRMs for Quantitative NMR (neats)
 - Supelco CRMs for Chromatography (solutions)

SIGMA-ALDRICH[®]

- Environmental Matrix

IRMM (Institute for Reference Materials and Measurements):

Merck is authorized distributor of their standards Certified Reference Materials (BCR, ERM, IRMM)

MERCK

Complete Range for Chromatography

PESTANAL®

TraceCERT®

SUPELCO®

Cerilliant®



Products are available as neat and single and multicomponent solution standards.

Extensive range of **organic pollutant** standards, available as Analytical Standards and CRMs

- Pesticides
- PAHs, PCBs, phenols, dioxins
- Volatiles and semi-volatiles
- Brominated Flame Retardants (PBDE)
- Phthalates, plasticizers
- Disinfectant by-products
- Chemical warfare degradation products
- Matrix standards
- Air monitoring/ -2,4-DNPH and DNPH derivatives
- Aldehydes
- Pharmaceuticals and their metabolites
- Proficiency Testing

TraceCERT®

CRMs for Chromatography (neats)

Organic TraceCERT® products are characterized by:

- Certified Content by quantitative NMR (qNMR)
- Manufactured under ISO/IEC 17025 and ISO Guide 34 double accreditation
- Superior level of accuracy, calculated uncertainties and lot-specific values
- Traceability to NIST
- Comprehensive documentation delivered with the product, CoA according to ISO Guide 31

Certified Standards for Chromatography

The organic TraceCERT products for chromatographic methods comprise many products for **environmental**, food and beverage as well as for clinical testing

- Organic CRMs Alphabetical - (183)
- Acids and Esters - (25)
- Alcohols - (2)
- Aldehydes and Aldehyde Derivatives - (3)
- Amines and Amides - (4)
- Amino Acids - (23)
- Antibiotics / Drugs - (17)
- Aromatics - (17)
- Dyes - (1)
- FA / FAME - (11)
- Flavors and Fragrances - (3)
- Hydrocarbons - (2)
- Natural Products - (32)
- Pesticides - (19)
- Phthalates/Parabens - (11)
- Polyaromatic Hydrocarbons (PAHs) - (17)
- SVHC - (11)
- Vitamins - (3)



Pesticides and Organic Pollutants Analytical Workflow

Sample collection



Sample preparation



Sample analysis



Quality assurance



- **Spiking standard**

- **Screening mixes**
 - **Internal standards**
 - **Calibration standards**
- (all as CRMs, RMs, analytical standards)**

- **Matrix material standards**
- **Proficiency testing**



- **SIL pesticides**
- **SIL organic pollutants**

- **Pesticides, neat & solutions**
- **Organic pollutants**

- **Proficiency testing**
- **Matrix material**

www.sigmaaldrich.com/pesticides

www.sigmaaldrich.com/popstandards

Organic Pollutants Portfolio

Organic Pollutant Standards

Analytical Standards and Certified Reference Materials



An extensive and broad selection of organic chemicals that are potentially harmful for people and for the environment are available as analytical standards and CRMs including PAHs, PCBs, phenols, air pollutants, explosives, chemical warfare degradation products, plasticizers, disinfectant by-products, flame retardants, phthalates, volatiles, semi-volatiles and many more. Products are available as neat and single and multicomponent certified solution standards.

➤ Air Pollutants, Aldehydes/DNPH

➤ Polycyclic Aromatic Hydrocarbons

➤ Plasticizers & Phthalates

➤ Disinfection By-Products

➤ PCBs & Dioxins

➤ Volatile & Semivolatile Standards

➤ Explosives & Chemical Warfare

➤ Perfluoro Compounds

➤ Additional Organic Pollutants

➤ Flame Retardants

➤ Phenols

➤ View All

➤ Organometallic Compounds

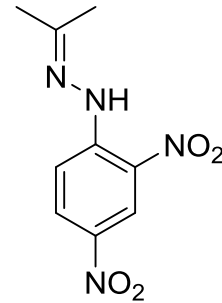
Organic pollutants

Air pollutants, aldehydes / DNPH

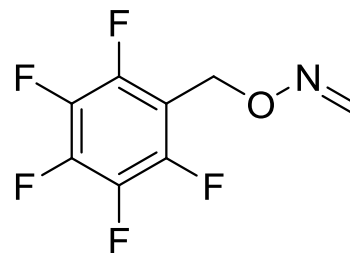
Product portfolio

- ~110 standards available, mainly 2 groups:
 - Aldehyde/ketone -dinitrophenylhydrazones (DNPHs)
 - Single solutions as CRMs
 - Neat as CRMs
 - Component mixes
 - Aldehyde O-pentafluorophenylmethyloximes
 - Neat
 - Hexamethylene diisocyanate amine adducts (HDI)
 - DNPH-cartridges

www.sigmaaldrich.com/analytical-chromatography/air-monitoring



Acetone-2,4-DNPH



Excellence in Air Monitoring

News On Air

2015 Volume 3

Formaldehyde Special

Formaldehyde was recently reclassified to carcinogenic category 1B and mutagen category 2A. Air formaldehyde can be frequently found in many indoor building materials such as varnishes, wallpaper and paints. It is important to monitor the quality of our indoor air. Long term exposure to formaldehyde can lead to serious health issues. It exacerbates respiratory tract diseases such as asthma. The volume of news on air concentrates on the measurement of formaldehyde in air.

Ethanol

The simplest way to diagnose and monitor indoor air quality inside buildings.

- Selective, sensitive and continuous measurement of formaldehyde
- Measurement of real exposure to pollutants and identification of pollution peaks
- Helps to define and validate good practices
- Simple controls to start/stop the campaign with a magnet
- Simple, user-friendly data management software
- Automated report generation with target values

Passive Sampling

radifier*

Radifier samplers are useful passive sampling devices that provide high sampling rates for formaldehyde in 90mL/min. It is comprised of a cylindrical diffuser body that is equipped with an adsorbent cartridge. The cartridge for aldehyde in the RAC165 consisting of a stainless steel net cartridge fixed with 2,4-dinitrophenylhydrazine (DNPH) coated fibers. Aldehydes react with 2,4-DNPH to give the corresponding 2,4-dinitrophenylhydrazones. The 2,4-dinitrophenylhydrazones are then extracted with acetonitrile and analysed by reverse phase HPLC and UV detection.

radifier components to be used:

- Blue diffusive body RAC120
- Support plate RAC121
- Vertical adapter RAC122 (optional, e.g. personal monitoring)
- Adsorbent Cartridge (DNPH) RAC165

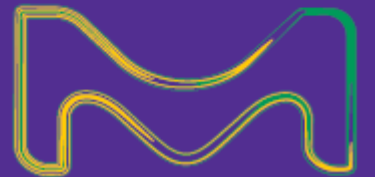
SIGMA ALDRICH Fluke SUPELCO

Organic pollutants

Disinfection by-products

Product portfolio

- ~ 38 standards, 36 CRMs, 2 analytical standards:
 - Halogenated acetic acids as solutions (18)
 - Neats (4)
 - EPA mixes, halogenated acetic acids/ trihalomethane (8)
 - **World Health Organization (WHO) sets guidelines for halomethanes – potential carcinogenic (20-200 µg/l)**

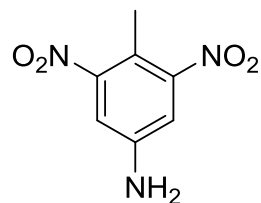


Organic pollutants

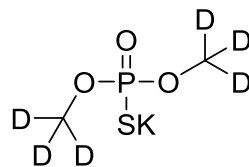
Explosives and chemical warfares

Product portfolio

- ~ 35 standards from Cerilliant, all CRMs
- all as solutions
- Nitrotoluene (explosives)
- phosphonic acids, thiophosphates (warfare)
- Product group might be linked to the local market, as there will be export/import restrictions



4-Amino-2,6-dinitrotoluene



O,O-Diethyl-hydrogen thiophosphate potassium salt solution

nitroglycerins/explosives standards

Cerilliant maintains a U.S. ATFE license for the manufacture of explosive materials. According to US Department of Transportation (DOT) regulations, these products are normally classified as Class 1 explosives, regardless of concentration, and legal shipment of these materials is highly regulated and restricted. Increasing homeland security measures are further restricting legal shipment of these materials increasing the cost and time required for delivery. To improve availability and reduce shipping costs for our customers, Cerilliant spent significant time and resources to obtain DOT exemptions for most of our solution based explosive standards allowing us to legally ship our products in categories other than Explosives. These exemptions apply only to Cerilliant products and cannot be relied upon by any other manufacturer.

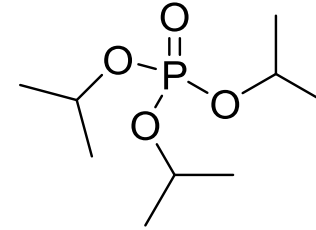
2-Amino-4,6-dinitrotoluene	100 mg	1 x 100 mg	ERA-017
4-Amino-2,6-dinitrotoluene	100 mg	1 x 100 mg	ERA-018
1,4-Butanediol	1.0 mg/mL in methanol	1 x 1 mL	B-020
Dinitroethylene glycol (EGDN)	100 µg/mL in acetonitrile	1 x 1 mL	D-004
Dinitroethylene glycol (EGDN)	1000 µg, mL in acetonitrile	1 x 1.2 mL	ERD-148S
1,2-Dinitroglycerin	1.0 mg/mL in acetonitrile	1 x 1 mL	D-010
1,2-Dinitroglycerin	100 µg/mL in acetonitrile	1 x 1 mL	D-002
1,3-Dinitroglycerin	1.0 mg/mL in acetonitrile	1 x 1 mL	D-011
1,3-Dinitroglycerin	100 µg/mL in acetonitrile	1 x 1 mL	D-003
2,4-Dinitrotoluene	1000 µg/mL in acetonitrile	1 x 1.2 mL	ERD-033S
2,4-Dinitrotoluene	10 mg/mL in acetonitrile	1 x 5 mL	ERD-152S
2,6-Dinitrotoluene	1000 µg/mL in acetonitrile	1 x 1.2 mL	ERD-034S
Ethyl centralite	500 µg/mL in acetonitrile	1 x 1.2 mL	ERE-032S
HMX	1000 µg/mL in acetonitrile	1 x 1.2 mL	ERH-004S
HMX	10 mg/mL in acetonitrile	1 x 5 mL	ERH-050S
1-Mononitroglycerin	1.0 mg/mL in acetonitrile	1 x 1 mL	M-077
1-Mononitroglycerin	100 µg/mL in acetonitrile	1 x 1 mL	M-001
2-Mononitroglycerin	1.0 mg/mL in acetonitrile	1 x 1 mL	M-078
2-Mononitroglycerin	100 µg/mL in acetonitrile	1 x 1 mL	M-002
Nitrobenzene	1000 µg/mL in acetonitrile	1 x 1.2 mL	ERN-004S
PETN	1000 µg/mL in acetonitrile	1 x 1 mL	P-037
PETN	10 mg/mL in acetonitrile	1 x 5 mL	ERP-109S
RDX	1000 µg/mL in acetonitrile	1 x 1.2 mL	ERR-001S
RDX	10 mg/mL in acetonitrile	1 x 5 mL	ERR-005S
Tetryl	1000 µg/mL in acetonitrile	1 x 1.2 mL	ERT-021S
Triclabendazole sulfone	25 mg	1 x 25 mg	NMIP1684
Triclabendazole sulfoxide	25 mg	1 x 25 mg	NMIP1685
1,3,5-Trinitrobenzene	1000 µg/mL in acetonitrile	1 x 1.2 mL	ERT-023S
Trinitroglycerin	1000 µg/mL in acetonitrile	1 x 1 mL	T-002
Trinitroglycerin	1 % w/w in propylene glycol	1 x 1 mL	T-021
Trinitroglycerin	1 % w/w in propylene glycol	5 x 0.2 mL	T-022
2,4,6-Trinitrotoluene (TNT)	1000 µg/mL in acetonitrile	1 x 1.2 mL	ERT-022S
2,4,6-Trinitrotoluene (TNT)	10 mg/mL in acetonitrile	1 x 5 mL	ERT-107S

Organic pollutants

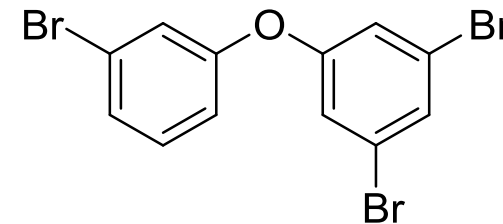
Flame retardants (FR)

Product portfolio

- ~ 33 standards, all analytical standard:
 - Mostly BDE solutions
 - 5 phosphates
 - Traditional:
 - Brominated diphenyl ethers (BDE)
 - Phosphate FRs



Triisopropyl phosphate



3,3',5-Tribromodiphenylether, BDE 36

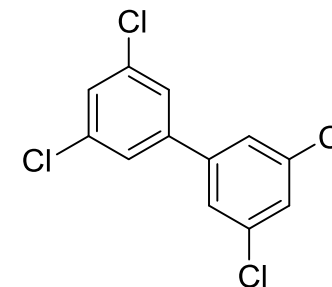
Organic pollutants

Polycyclic aromatic hydrocarbons (PAH)

Polychlorinated biphenyls (PCBs) & Dioxins

Product portfolio

- ~320 products in total:
 - 59 PCBs neat & solution, Pestanal/analytical standard, PCB as PT material, PCB mixes (CRMs)
 - Aroclor: a trademark from Monsanto for PCBs, sold under a 4 digit number from 1930-77; 69 products as CRMs (neats & solutions in oil)
 - 192 PAHs (anthracenes, pyrenes) as neat, solution and mixes; 20 isotope labeled ones to be used as internal standards
 - Wide product range



Aroclor 1248

Organic pollutants

Volatiles and semi-volatiles

Product portfolio

- ~ 1000 products
 - 280 EPA and other mixes (all CRMs)
 - ~200 solutions, single (all CRMs)
 - ~500 neats (analytical standard)



Environmental Testing

Organic Pollutants

Accredited to both ISO/IEC 17025 and ISO Guide 34, our manufacturing sites produce a multitude of **organic standards** as Certified Reference Materials (CRMs), Reference Materials (RMs), and analytical standards, for use as calibration standards, internal standards, surrogate standards, spiking solutions, and laboratory control samples (LCSs). You have the option of single-component solutions, multi-component mixtures, and highly characterized neat standards, plus separate source standards for many methods and analytes.

Water Framework Directive: An overview of analytical standards and certified reference materials for priority substances

The EU Water Framework Directive (2000/60/EC)[1] was established in the year 2000, committing member states to achieve “good” qualitative and quantitative status of all water bodies, including rivers, lakes, transitional waters, coastal waters and groundwater by the year 2015. Sigma Aldrich portfolio includes all 33 initial compounds, as well as the 15 newly proposed substances.

- Aldehydes
- Disinfection by-products
- Brominated Flame Retardants (PBDE)
- Organometallics
- PAHs, PCBs, Phenols, Perfluoro (PFC) compounds
- Plasticizers and phthalates
- Dioxins
- Pharmaceuticals
- Volatiles and semi-volatiles

www.sigmaaldrich.com/popstandards



Environmental Testing Organic Pollutants – VOCs

NEW ISO standard 17943:2016 for determination of VOCs in water by HS-SPME and GC-MS

- describes an improved and fully automated method for the determination of more than 60 VOCs in different water matrices. Method using headspace solid-phase micro-extraction (HS-SPME) followed by gas chromatography-mass spectrometry (GC-MS)

Certified Reference Materials have been developed specifically for ISO Standard 17943

These are split into:

- one mixture containing 57 VOCs TraceCERT®
- one mixture containing four odor compounds TraceCERT®
- two single compound solutions: Vinyl chloride (due to its high volatility) and 1,3,5-trichlorobenzene (due to compliance reasons - SVHC)

Order No.	Product Description
44926-U	ISO 17943 57 Component VOC Mix certified reference material, 200 µg/ml each component in methanol, ampule of 1 ml
44923-U	ISO 17943 Odor Compounds Mix certified reference material, 200 µg/ml each component in methanol, ampule of 1 ml
48625	Vinyl chloride solution 200 µg/ml in methanol, analytical standard, ampule of 1 ml
03824	1,3,5-Trichlorobenzene certified reference material, TraceCERT®, pack size of 100 mg

- www.sigmaaldrich.com/technical-documents/articles/analytical/sample-preparation/iso17943

GO GREEN
Make the world a greener place with high-quality products for environmental testing.

NEW ISO standard 17943 for determination of VOCs in water by HS-SPME and GC-MS

Contamination of water resources by Volatile Organic Compounds (VOCs) is a concern to human health as many of these compounds are toxic and are known or suspected to be carcinogenic. Consequently VOCs have to be monitored according to regulatory laws on water pollution such as European Council Directive 98/83/EC or the Safe Drinking Water Act (SDWA) in the US.

The new ISO Standard 17943 describes an improved and fully automated method for the determination of more than 60 VOCs in different water matrices, after extraction of the compounds from the headspace of the sample by SPME the analysis is conducted by GC-MS.

To support this, Certified Reference Materials have been developed specifically for ISO Standard 17943. These are split into one mixture containing 57 VOCs, one mixture containing four odor compounds and two single compound solutions: Vinyl chloride (due to its high volatility) and 1,3,5-trichlorobenzene (due to compliance reasons).

Order No.	Product Description
44926-U	ISO 17943 57 Component VOC Mix certified reference material, 200 µg/ml each component in methanol, ampule of 1 ml
44923-U	ISO 17943 Odor Compounds Mix certified reference material, 200 µg/ml each component in methanol, ampule of 1 ml
48625	Vinyl chloride solution 200 µg/ml in methanol, analytical standard, ampule of 1 ml
03824	1,3,5-Trichlorobenzene certified reference material, TraceCERT®, pack size of 100 mg

Materials

Order No.	Product Description
5066097	Headspace vial, screw top, rounded bottom (total vol) volume 20 ml, clear glass vial, thread 18, OD. x H 22.5 mm x 75.5 mm, packaging: 100 pc
5066099	Headspace vial, screw top, rounded bottom (total vol) volume 20 ml, amber glass vial, thread 18, OD. x H 22.5 mm x 75.5 mm, packaging: 100 pc
5066001	Magnetic Screw Cap for Headspace Vials, 18 mm thread PTFE/dichloro septum (white PTFE/transparent blue silicone septum thickness 1.5 mm), package of 100 pc
57234-U	SPME fiber assembly Carbowax/Polymethylsiloxane (CAR/PDMS) of 85 µm, needle size 24 ga, for use with manual holder, StabilFlex fiber, pack aging: 3 pc
57235-U	SPME fiber assembly Carbowax/Polymethylsiloxane (CAR/PDMS) of 85 µm, needle size 20 ga, StabilFlex, for use with autosampler, packaging: 3 pc
57238-U	SPME fiber assembly Divinylbenzene/Carbowax/Polymethylsiloxane (DVB/CAR/PDMS) needle size 24 ga, for use with manual holder, packaging: 3 pc
57239-U	SPME fiber assembly Divinylbenzene/Carbowax/Polymethylsiloxane (DVB/CAR/PDMS) needle size 23 ga, StabilFlex, for use with autosampler, packaging: 3 pc
57230-U	SPME Fiber Holder for use with manual sampling
57247-U	SPME Fiber Holder for use with CTC ComBPA, Gerstel MPS2 and Thermo TriPlus Autosamplers
24194	VOCLUB Capillary GC Column L x ID: 60 m x 0.25 mm, Ø 1.30 µm

For complete information, please visit:
www.sigmaaldrich.com/technical-documents/articles/analytical/sample-preparation/iso17943

Environmental Testing

Pesticides

- more than 1700 high purity pesticide and pesticide metabolite standards and CRMs for environmental analysis under the PESTANAL® and TraceCERT® brands

Products:

- Pesticides
- CRM Matrix Standards and Proficiency Testing (PT)
- Pesticide Metabolite Standards
- Isotope labeled internal standards
- Multi-component solutions

www.sigmaaldrich.com/pesticides

pesticides TRACECERT®

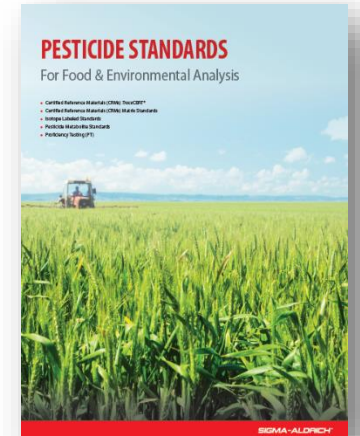
- the neat CRMs are certified by quantitative NMR (qNMR) and traceable to NIST SRM, 50 and 100 mg
- the CRM solutions are produced gravimetrically - Mass Balance Method (100% - impurities) using NIST traceable weights for balance calibration (various concentrations, solvents), 1 ml

pesticides Matrix CRMS sigma-Aldrich RTC

- “Real world” soil or sediment natural matrices or as natural matrices, in which selected analytes have been fortified to give analytical profiles that meet the needs of analysts
- CRMs for Solids, Non-Potable and Drinking Water (www.sigmaaldrich.com/ecrm)

pesticide Metabolite standards and isotope labeled standards pestanal®

- possible conversion of active compounds of some pesticides by the target insects or plants or degradation in the environment to their metabolites
- neat standards and solutions in various solvents, all are analytical standards – no CRMs



Environmental Testing Bioactive Compounds

Better Monitoring of Bioactive Compounds in Waste and Recycled Water

- micro pollutants, such as pharmaceutical and hormone active substances and their metabolites, constantly affect the chemical quality of water resources and cause detrimental effects on both health and the environment
- analytical standards and reference materials for convenient detection of APIs and their metabolites in wastewater
- certified by **qNMR**, and the measured value is traceable to NIST standard reference materials (**ISO / IEC 17025**)



www.sigmaaldrich.com/pharmametabolites

Analytical Standards and Certified Reference Material

Our Custom Capabilities

Organic Custom Standards

We can prepare chemical standards for you:

1. environmental

2. food & beverage
3. pesticide & metabolite
4. petroleum
5. chemical
6. Pharmaceutical

- Includes Safety Data Sheet (SDS)
- Certificate of Composition

Custom Services from Cerilliant®

- Custom Reference Standards
- Custom Organic Synthesis
- Analytical Services
- Custom Packaging
- Inventory Management and Distribution of Client Reference Materials

Specifications

Mixture Description (for label) :

Solvent(s) :

Volume or Weight / ampul:

1 mL 100 mg

5 mL 500 mg

10 mL Other (please specify)

Number of units :
(typically minimum order quantity is 4)

Concentration Units :

ng/mL vol / vol %

µg/mL wt. / wt. %

mg/mL wt. / vol.

Other (please specify)

Components	CAS No. (Optional)	Concentration

<http://www.sigmaaldrich.com/analytical-chromatography/analytical-standards/standards-quote.html>

Analytical Standards and Reference Materials

Further information sources

Further
information

Analytix

Journal for new topics in Standards and reagents

- Published 5 times per year.
- Subscribe at sigma-aldrich.com/analytix

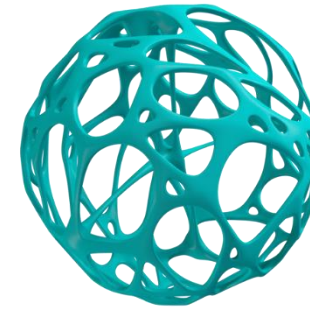
Standards Explorer

- Quickly find the standard you are looking for
- Various search parameters, including CAS #, agency method

News on Standards

- Quarterly newsletter highlighting new developments in Reference Materials
- Subscribe at sigmaaldrich.com/newsonstandards

Our Advantage



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Bundling Possibilities convenient & cost saving

One of the largest portfolio
Analytical reagents
Consumables, Sample Preparation,
Lab Water, Labware

Technical expertise

Five double accredited sites (ISO
17025 and ISO Guide 34)
High percentage of in-house
production



Let us know what else you need to better support your work

Thank you !

