

Naturally pure. SupraSolv[®] – high purity solvents for gas chromatography

EMD Millipore is a division of Merck KGaA, Darmstadt, Germany



SupraSolv[®]

Solvents for gas chromatography

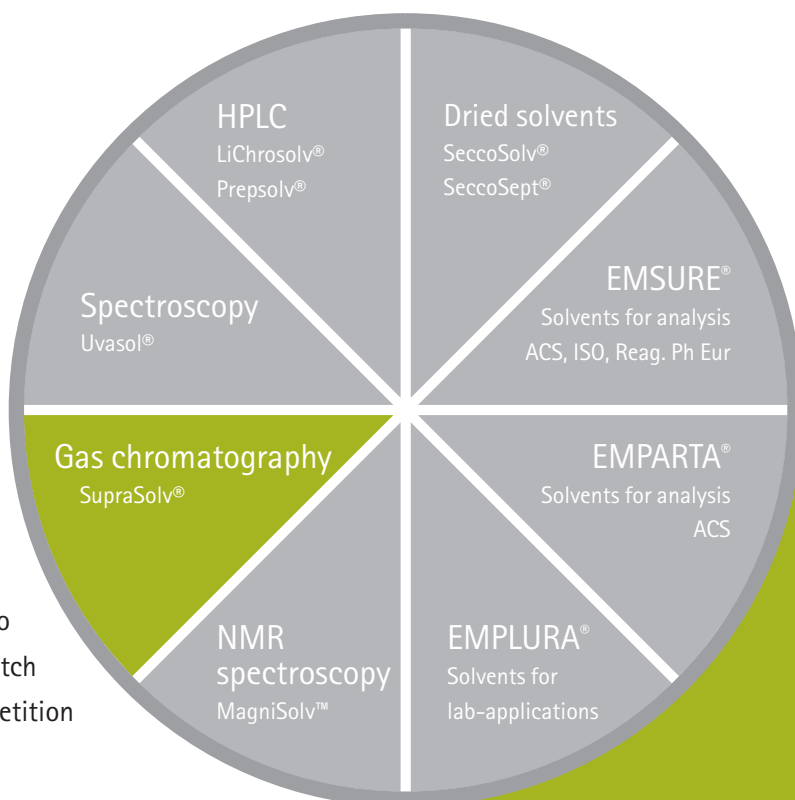
As the world's leading supplier of high-purity solvents, we offer a full range of products for every gas chromatography application in the laboratory – including highly sensitive pesticide and dioxin analyses. Our **SupraSolv[®]** solvents are developed specifically for sensitive detection processes in residue and environmental analysis. They cover all areas of application, and provide the highest level of reliability for your analytical results.

To ensure purity and suitability, we employ only the latest manufacturing processes. **SupraSolv[®]** solvents are recovered during special distillation cuts, and suitability testing involves a variety of detectors and highly concentrated solvents.

As a result, these high-purity products support you in countless ways during your daily work – with individual specifications that are tailored to their specific area of application.

SupraSolv[®] benefits

- The most comprehensive application area due to the largest retention time range
- Analytical reliability due to the highest possible purity and a minimal signal-to-noise ratio
- Time and cost savings due to the best possible batch consistency, thus avoiding analysis repetition





Quality for the widest range of applications

EMD Millipore solvents for gas chromatography offer the highest quality for the widest range of applications. The retention time window during which specified contaminants are lowest is broader than that of any competitor product.

Quality for the best batch consistency

Every batch that leaves our premises is tested to the same high standards of quality. This is your guarantee of consistently reliable analytical results.

Quality for reliable analyses

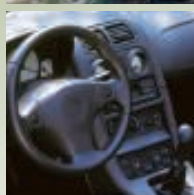
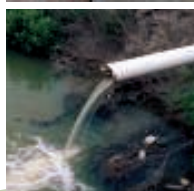
Our solvents for gas chromatography provide reliable, consistent analytical results without the need for costly purification and repeat analysis. As a result, they make your work easier, more efficient and more economical.

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FID flame ionization detector

- BTX (Benzene, Toluene, Xylene) – highly volatile aromatic hydrocarbons in sewage, ground-water, juices, canned fish etc.
- Hydrocarbon-oil index in water
- Determination of emissions in car cockpit material



GC-FID

GC-ECD

SupraSolv[®] ECD and FID

ECD electron capture detector

- Pesticide analysis in fruits and vegetables
- Acrylamide in e.g. potato chips, crisps and crisp bread
- Polychlorinated biphenyls (PCB) in water and sludge
- DDT (preserver and insecticide) in milk, fish, meat, fruits etc.
- Highly volatile halogenated hydrocarbons in water
- Nitrate in lettuce, radish etc.



GC-MS

SupraSolv[®] MS

HS-GC

SupraSolv[®] Headspace

MS mass spectrometry



- Dioxins and furans (PCDD/PCDF) in meat, fish and milk
- Polycyclic aromatic hydrocarbons (PAH) in vegetables, olive oil and broiled meat
- Pesticide analysis in fruits and vegetables according Anastassiades (QuEChERS)
- Determination of drugs (cocaine, cannabis, ecstasy, heroine, alcohol) in human hair
- Analysis of phthalates in child care products and toys

HS-GC headspace gas chromatography

- Analysis of residual solvents in drug substances, excipients, and drug products according to ICH, Ph Eur and USP



SupraSolv[®]

Solvents for gas chromatography

With gas chromatography, only solvents with the highest levels of purity are suitable for sample preparation tasks such as the extraction and concentration of the extracts before injection. SupraSolv[®] solvents are developed specially for this highly sophisticated application area.

Our comprehensive portfolio of GC solvents offers the right product for your specific application and detection method. SupraSolv[®] ECD and FID is specially developed and tested for ECD (Electron Capture Detector) and FID (Flame Ionization Detector). Typical applications include the determination of polychlorinated biphenyls (PCB) in water and soil or pesticides in fruits and vegetables.

SupraSolv[®] MS is dedicated for use in gas chromatography coupled with mass spectrometric detection. This method is of increasing importance and used e.g. for the analysis of dioxins and furans (PCDD/PCDF) in food and water samples or for the determination of PAH (polycyclic aromatic hydrocarbons) in food.

Both SupraSolv[®] qualities are carefully tested for the specific detectors and offer a clear baseline and minimal signal-to-noise ratio within a specified retention time range. Therefore SupraSolv[®] solvents help you achieve consistently accurate, reliable and reproducible results.

SupraSolv[®] Benefits:

- Minimal signal-to-noise ratio within a specified retention time range, leading to accurate, reliable and reproducible analytical results
- Tested for specific detectors, leading to high application security
- Widest retention time range for the most comprehensive range of applications

Specification at a glance

Specification at a glance		Specifications		
Tradenames	Analysis method	GC-ECD	GC-FID	GC-MS
		1,2,4-Trichlorobenzene to Decachlorobiphenyle (Lindane standard)	n-Undecane to n-Tetracontane (n-Tetradecane standard)	n-Undecane to n-Tetracontane; scan range 30-600 amu (n-Tetradecane standard)
SupraSolv [®] for gas chromatography ECD and FID	GC Detection methods: GC-ECD GC-FID	max. 3 pg/ml	max. 3 ng/ml	-
SupraSolv [®] for gas chromatography MS	GC Detection methods: GC-MS	-	-	max. 3 ng/ml



SupraSolv® – the reliable solution

SupraSolv® has minimal interference signals in the relevant retention time window (Fig. 1). This ensures reliable, reproducible and accurate analysis results. Thanks to outstanding batch consistency, SupraSolv® also saves you time and money by making repeat analyses a thing of the past.

SupraSolv® ECD specification

Outstanding analytical capabilities form the basis for providing you with comprehensive quality information – the specifications document our quality level and give you the reliability you need for your day-to-day laboratory decisions.

— Batch chromatogram
— Reference chromatogram

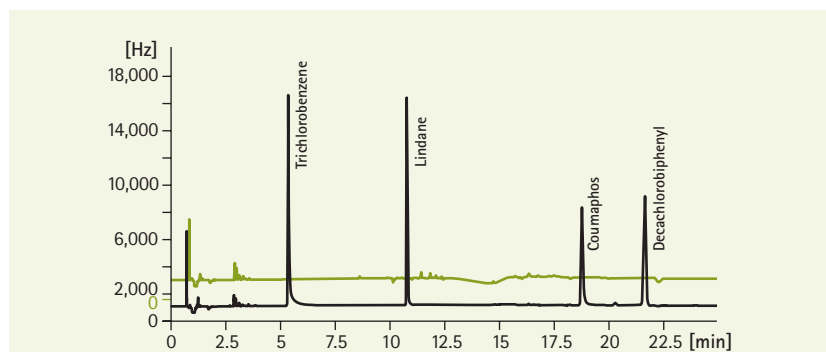


Fig. 1 GC-ECD, batch and reference chromatogram (Lindane = 3 pg/ml), n-Hexane SupraSolv® EDC and FID (104371)

Use of a non-specific solvent and competitor comparison

Both competitor chromatogram and the chromatogram of a non-GC-specific solvent (n-Hexane reagent grade) exhibit highly unstable baselines and many unidentifiable contaminant peaks. The competitor chromatogram also shows very low batch consistency. The bottom line: No clear analytical results, a risk of misinterpretation – and expensive, time-consuming repeat analyses.

— Batch 1 chromatogram
— Batch 2 chromatogram

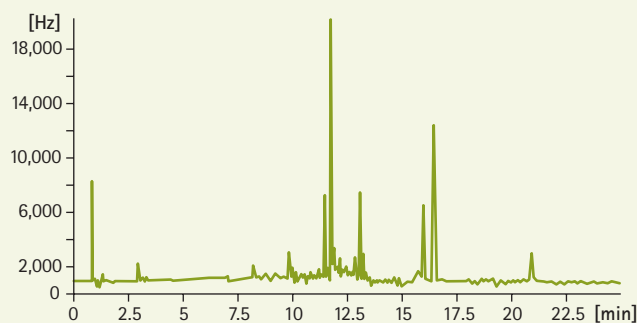


Fig. 2a GC-ECD, batch chromatogram of a non-GC-specific solvent, n-Hexane reagent grade

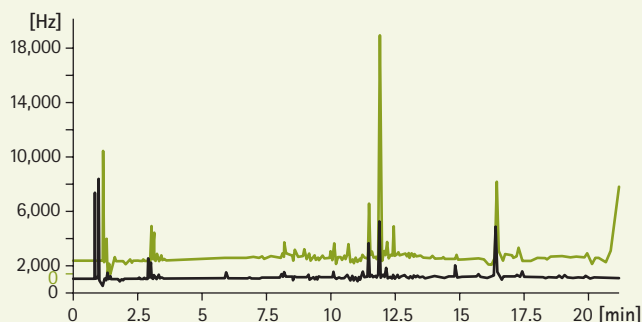


Fig. 2b GC-ECD, batch chromatogram, n-Hexane GC grade, competitor A

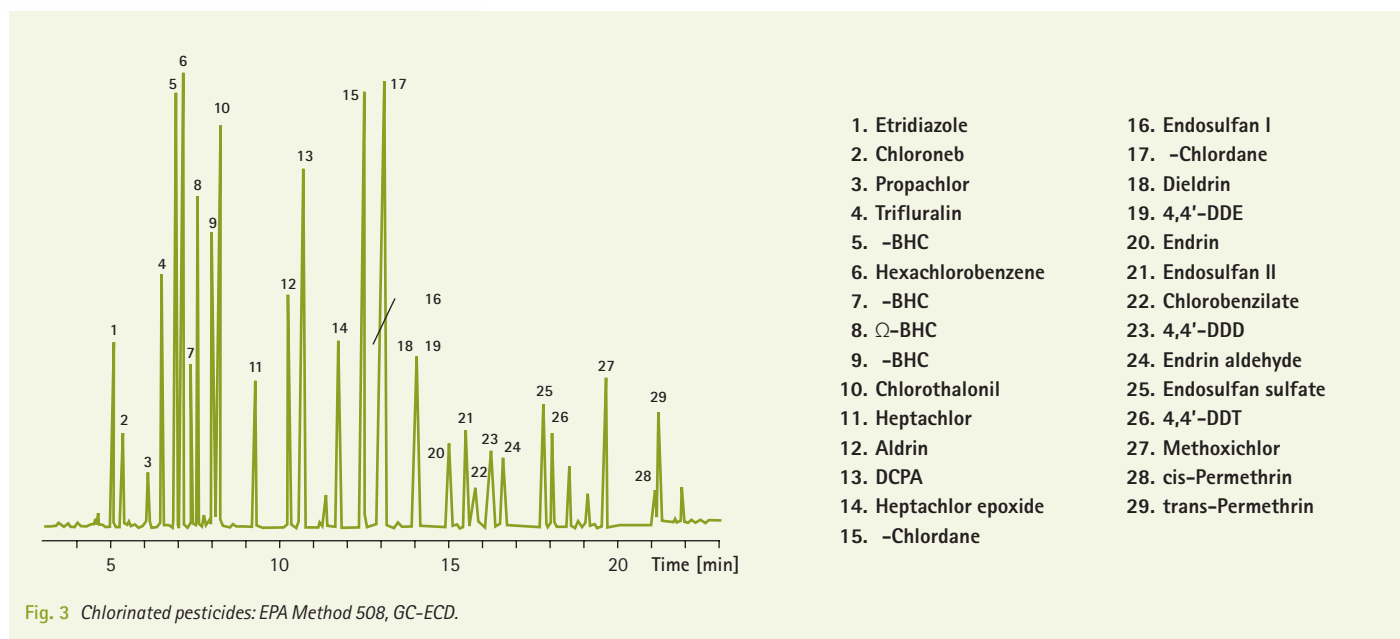
Important application: pesticide analysis

There are around 500 known pesticides in juices alone. Due to such substantial safety concerns, national and international regulations require that food and beverage manufacturers regularly test their products for pesticides.

Classical pesticide analysis according to EPA Method 508 is employed for the qualitative and quantitative determination of pesticides in food and environmental samples. This method uses gas chromatography coupled with ECD. For sample preparation the solvents n-Hexane, Ethyl acetate, Dichloromethane or Acetone are used. Due to their particular suitability for GC-ECD, as well as their high purity and minimal interference signals within the relevant retention time range, SupraSolv[®] solvents will help you to achieve consistently accurate, reliable and reproducible results in pesticide analysis. Furthermore the specified ECD retention time range of SupraSolv[®] ECD and FID covers all analytes of interest for this application, resulting in best application security.



EPA Method 508: Determination of chlorinated pesticides in water, standard chromatogram



The new, faster QuEChERS method for pesticide analysis according Anastassiades uses GC-MS instead. This method reduces manual effort, increases sample throughput, improves analytical safety, and extends the range of detectable pesticides. As **SupraSolv® MS** solvents are specially developed and tested for GC-MS, they are dedicated for this application.

Pesticide residue analysis in apple juice with GC-MS and Dichloromethane SupraSolv® MS

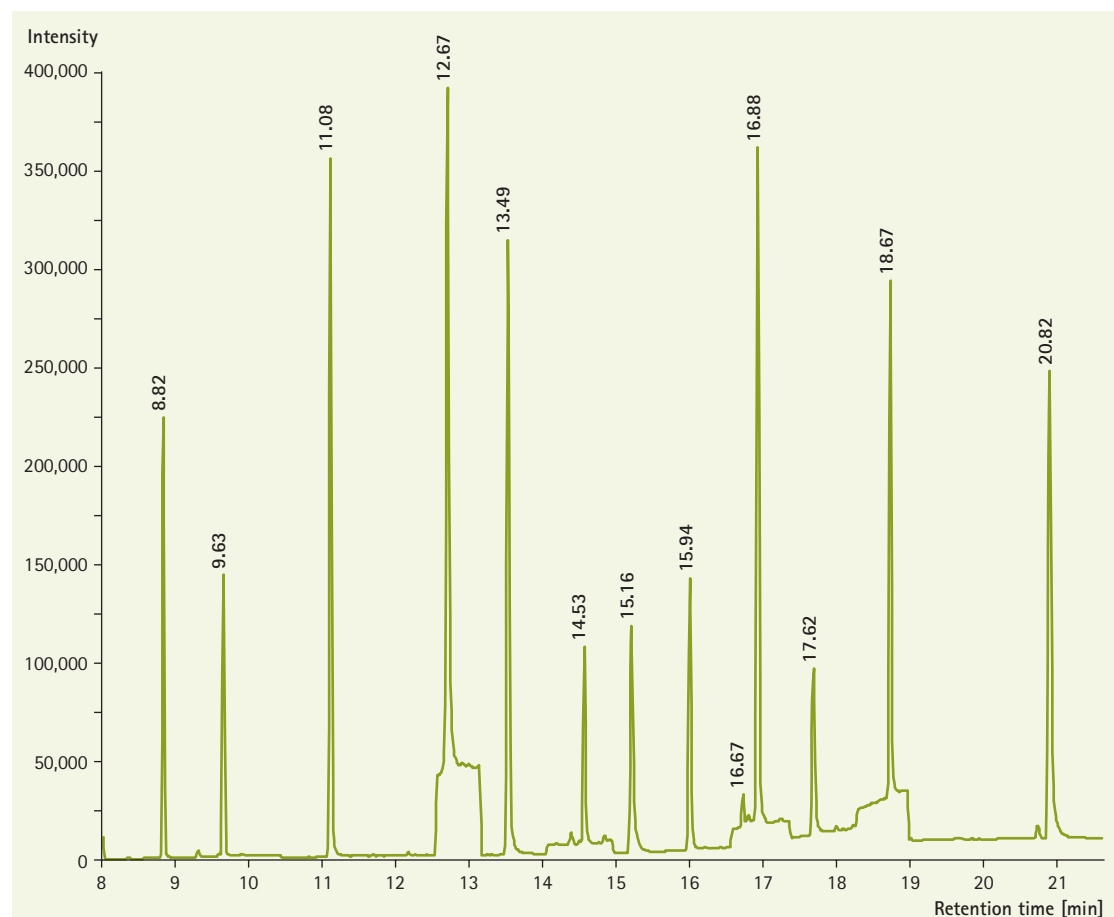


Fig. 4 Sample chromatogram (TIC) – apple juice spiked. Sample preparation via liquid-liquid-extraction with EXtrelut® NT20. Eluting solvent: Dichloromethane SupraSolv® MS (1.00668.1000)

Eluting solvent	Dichloromethane SupraSolv® MS [100668]	Sample			
Instrumentation	Agilent 7890A	RT [min]	Active substance	RT [min]	Active substance
Autosampler	Gerstel MPS	8.82	Trifluralin	15.94	Etoxazol
Capillary column	Phenomenex, ZB-MultiResidue; 30 m, 0.25 mm id, 0.25 µm ft	9.63	Profluralin	16.67	lambda-Cyhalothrin
Carrier gas	Helium; constant flow	11.08	Pirimiphos-methyl	16.88	lambda-Cyhalothrin
Injector	CIS 4 (cooled injection system, Gerstel)	12.67	Procymidon	17.62	Fenarimol
Injection volume	2 µl	13.49	p,p'-DDE	18.67	Halfenprox
Detector	MSD 5975C, inert XL MSD triple axis detector	14.53	Trifloxystrobin	20.82	Azoxystrobin
		15.16	Quinoxifen		

SupraSolv[®] headspace

Solvents for headspace gas chromatography

Headspace gas chromatography is a precise, well-accepted method for the analysis of residual solvents in drug substances and products. It is recommended as the preferred method of analysis for this application by the European Pharmacopoeia (Chapter 2.4.24) and the United States Pharmacopoeia (Chapter 467).

The ICH (International Conference on Harmonization of Technical Requirements for Registration of Pharmaceuticals for Human Use) Guideline Q3C »Impurities: Guideline for Residual Solvents« divides all residual solvents into three classes according to their harmfulness for human health, and defines permissible maximum concentrations in actives, excipients and drug products. Both the European and the United States Pharmacopoeia refer to this guideline. Accurate analysis with headspace gas chromatography demands the use of very pure solvents with extremely low concentrations of the defined residual solvents.

By specifying for **SupraSolv[®] headspace** the concentrations of all residual solvents of the three defined classes in the ICH guideline, EMD Millipore offers a precise purity window for this application – for unique, application-orientated quality. Since we also perform a headspace application test on each batch, every delivery gives you the reliability, accuracy and analytical safety you need.

Extract of specification

ICH = International Conference on Harmonisation of Technical Requirements for Registration of Pharmaceuticals for Human Use

Every residual solvent of **class 1** acc. ICH $\leq 1 \mu\text{g/g}$
Every residual solvent of **class 2** acc. ICH $\leq 10 \mu\text{g/g}$
Every residual solvent of **class 3** acc. ICH $\leq 50 \mu\text{g/g}$

Fig. 5 Chromatogram of DMSO Headspace SupraSolv[®] 101900 without addition compared to a chromatogram of DMSO Headspace SupraSolv[®] 101900 with 0.8 ppm benzene.

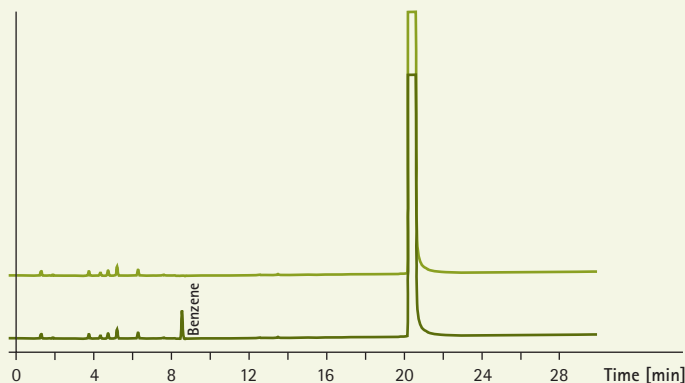
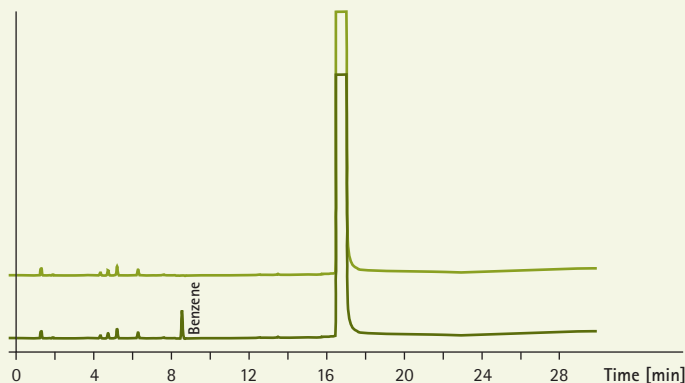


Fig. 6 Chromatogram of DMF Headspace SupraSolv[®] 100202 without addition compared to a chromatogram of DMF Headspace SupraSolv[®] 100202 with 0.8 ppm benzene.



SupraSolv® headspace solvents are specially designed for the analysis of residual solvents according to Ph Eur and USP. We have developed them in close cooperation with an experienced headspace laboratory, and manufacture them using special production processes. As a result, these high purity products ensure reliable, accurate analytical results.

Application: Quantification of residual solvents in an API

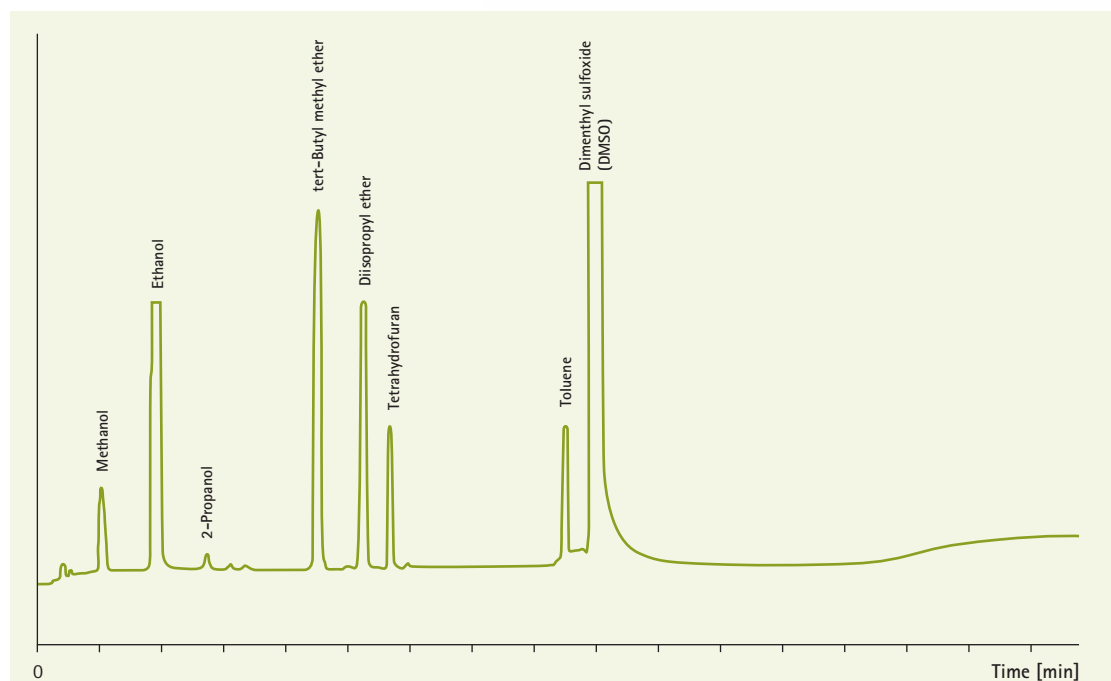


Fig. 7 Quantification of residual solvents in an API using Dimethyl sulfoxide (DMSO) SupraSolv® for headspace gas chromatography (101900).

Chromatographic conditions

Column fused silica capillary column, DB 1, length 30 m, ID 0.32 mm, film 5 µm

Pressure 0.6 bar / 8 psi (Helium)

Injection splitless, 150°C

Headspace conditions

thermostating temperature 80°C

transfer and needle temperature 130°C

thermostating time 30 min

pressurisation 1.0 min

injection time 0.04 min

withdrawal time 0.2 min

hHigh pressure 2 bar / 28 psi

Detection FID, 250°C

Temperature 50°C for 5 min, with 8°C/min up to 240°C, hold 240°C for 5 min

Method Quantification of residual solvents in an API

Chromatographic data

No.	Compound	Time [min]	Area
1	Methanol	2.0	12361
2	Ethanol	3.8	399048
3	2-Propanol	5.4	2368
4	tert-Butyl methyl ether	9.0	34637
5	Diisopropyl ether	10.5	43000
6	Tetrahydrofuran	11.4	14083
7	Toluene	11.5	11502

Ordering information

SupraSolv[®] solvents for gas chromatography ECD and FID

Product	Purity (GC) min. [%]	Evap. residue max. [mg/l]	Water max. [%]	Color max. [Hazen]	Content / Packaging	Ord. No.
A Acetone	99.8	3.0	0.05	10	1 GL	1.00012.1000
					2.5 GL	1.00012.2500
					4 GL	1.00012.4000
Acetonitrile	99.8	3.0	0.05	10	1 GL	1.00017.1000
					2.5 GL	1.00017.2500
					4 GL	1.00017.4000
B tert-Butyl methyl ether	99.8	3.0	0.02	10	1 GL	1.01995.1000
					2.5 GL	1.01995.2500
C Chloroform, stabilized	99.8	5.0	0.01	10	1 GL	1.02432.1000
					2.5 GL	1.02432.2500
Cyclohexane	99.8	3.0	0.01	10	1 GL	1.02817.1000
					2.5 GL	1.02817.2500
					4 GL	1.02817.4000
D Dichloromethane, stabilized	99.8	5.0	0.01	10	1 GL	1.06054.1000
					2.5 GL	1.06054.2500
					4 GL	1.06054.4000
Diethyl ether, stabilized	98.0	3.0	0.05	10	1 GL	1.00931.1000
					2.5 GL	1.00931.2500
					4 GL	1.00931.4000
N,N-Dimethylformamide	99.8	3.0	0.05	10	1 GL	1.10983.1000
					2.5 GL	1.10983.2500
E Ethyl acetate	99.8	3.0	0.02	10	1 GL	1.10972.1000
					2.5 GL	1.10972.2500
					4 GL	1.10972.4000
H n-Hexane	98.0*	3.0	0.01	10	1 GL	1.04371.1000
					2.5 GL	1.04371.2500
					4 GL	1.04371.4000
I Isohexane	99.8	3.0	0.01	10	2.5 GL	1.04340.2500
					1 GL	1.15440.1000
Isooctane	99.8	3.0	0.01	10	2.5 GL	1.15440.2500
					1 GL	1.15440.1000
M Methanol	99.8	3.0	0.1	10	1 GL	1.06011.1000
					2.5 GL	1.06011.2500
					4 GL	1.06011.4000
P Petroleum benzine (40 - 60°C)	-	3.0	0.01	10	1 GL	1.01772.1000
					2.5 GL	1.01772.2500
					4 GL	1.01772.4000
2-Propanol	99.8	3.0	0.1	10	1 GL	1.00998.1000
					2.5 GL	1.00998.2500
n-Pentane	99.8	3.0	0.02	10	1 GL	1.00882.1000
					2.5 GL	1.00882.2500
T Toluene	99.8	3.0	0.03	10	1 GL	1.08389.1000
					2.5 GL	1.08389.2500
					4 GL	1.08389.4000

GL = glass bottle | * = sum of hexane isomers + methyl cyclopentane (GC) ≥ 99.8 % | GC-ECD (retention range 1,2,4-Trichlorobenzene to Decachlorobiphenyle individual signals (Lindane standard)) ≤ 3 pg/ml | GC-FID (retention range n-Undecane to n-Tetracontane individual signals (n-Tetradecane standard)) ≤ 3 ng/ml

SupraSolv[®] solvents for gas chromatography MS

Product	Purity (GC) min. [%]	Evap. residue max. [mg/l]	Water max. [%]	Color max. [Hazen]	Content / Packaging	Ord. No.
A Acetone	99.8	3.0	0.05	10	1 l GL	1.00658.1000
					2.5 l GL	1.00658.2500
Acetonitrile	99.8	3.0	0.05	10	1 l GL	1.00665.1000
					2.5 l GL	1.00665.2500
C Cyclohexane	99.8	3.0	0.01	10	1 l GL	1.00667.1000
					2.5 l GL	1.00667.2500
D Dichloromethane, stabilized	99.8	5.0	0.01	10	1 l GL	1.00668.1000
					2.5 l GL	1.00668.2500
E Ethyl acetate	99.8	3.0	0.02	10	1 l GL	1.00789.1000
					2.5 l GL	1.00789.2500
H n-Hexane	98.0*	3.0	0.01	10	1 l GL	1.00795.1000
					2.5 l GL	1.00795.2500
M Methanol	99.8	3.0	0.1	10	1 l GL	1.00837.1000
					2.5 l GL	1.00837.2500
T Toluene	99.8	3.0	0.03	10	1 l GL	1.00849.1000
					2.5 l GL	1.00849.2500

GL = glass bottle | * = sum of hexane isomers + methyl cyclopentane (GC) ≥ 99.8 % | GC-MS (retention range n-undecane to n-tetracontane; scanning area 30-600 amu individual signals (n-tetradecane standard)) ≤ 3 ng/ml

SupraSolv[®] headspace For the analysis of residual solvents according to Ph Eur and USP

Product	Purity (GC) min. [%]	Evap. residue max. [mg/l]	Water max. [%]	Color max. [Hazen]	Content / Packaging	Ord. No.
D N,N-Dimethylacetamide	99.8	3.0	0.05	10	1 l GL	1.00399.1000
					2.5 l GL	1.00202.2500
N,N-Dimethylformamide	99.8	3.0	0.05	10	1 l GL	1.00202.1000
					2.5 l GL	1.00202.2500
Dimethyl sulfoxide	99.8	3.0	0.05	10	1 l GL	1.01900.1000
					2.5 l GL	1.01900.2500
W Water	-	5.0	-	-	1 l GL	1.00577.1000
					2.5 l GL	1.00577.2500

GL = glass bottle | Every residual solvent of class 1 acc. ICH ≤ 1 µg/g | Every residual solvent of class 2 acc. ICH ≤ 10 µg/g | Every residual solvent of class 3 acc. ICH ≤ 50 µg/g



Reference substances for gas chromatography

Most of the high-purity products in our »reference substances for GC« range are completely synthetic in origin, which means they are largely free from isomers that are difficult to separate by GC. Their assay is generally greater than 90 %, and is usually over 99.5 or 99.7 %. Every pack includes a gas chromatogram under the appropriate test conditions. These reference substances can be used when identifying unknown compounds in a gas chromatogram, as standards in quantitative GC analysis, or in the characterization of GC column properties. Reference substances belonging to the hydrocarbon group are packed in pierceable ampoules; fatty acid methyl esters and other reference substances come in screw-capped glass vials.

Ordering information

Hydrocarbons C 5 – C 7

	Designation	Empirical formula	Assay [%]	Content / Packaging	Ord. No.
B	Benzene	C ₆ H ₆	≥ 99.9	5 ml GA	1.09646.0005
H	n-Heptane	C ₇ H ₁₆	≥ 99.5	5 ml GA	1.09686.0005
	n-Hexane	C ₆ H ₁₄	≥ 99.7	5 ml GA	1.09687.0005
P	n-Pentane	C ₅ H ₁₂	≥ 99.7	5 ml GA	1.09719.0005
T	Toluene	C ₇ H ₈	≥ 99.7	5 ml GA	1.09768.0005

GA = glass ampoule

Hydrocarbons C 8

	Designation	Empirical formula	Assay [%]	Content / Packaging	Ord. No.
O	n-Octane	C ₈ H ₁₈	≥ 99.0	5 ml GA	1.09716.0005
X	o-Xylene	C ₈ H ₁₀	≥ 99.0	5 ml GA	1.09798.0005
	m-Xylene	C ₈ H ₁₀	≥ 99.3	5 ml GA	1.09797.0005
	p-Xylene	C ₈ H ₁₀	≥ 99.5	5 ml GA	1.09799.0005

GA = glass ampoule

Hydrocarbons C 9 – C 18

	Designation	Empirical formula	Assay [%]	Content / Packaging	Ord. No.
D	n-Decane	C ₁₀ H ₂₂	≥ 99.5	5 ml GA	1.09603.0005
	n-Dodecane	C ₁₂ H ₂₆	≥ 98.5	5 ml GA	1.09658.0005
H	n-Heptadecane	C ₁₇ H ₃₆	≥ 99.3	5 ml GA	1.09604.0005
	n-Hexadecane	C ₁₆ H ₃₄	≥ 99.5	5 ml GA	1.09605.0005
O	n-Octadecane	C ₁₈ H ₃₈	≥ 99.3	5 ml GA	1.09606.0005
P	n-Pentadecane	C ₁₅ H ₃₂	≥ 99.5	5 ml GA	1.09607.0005
T	n-Tetradecane	C ₁₄ H ₃₀	≥ 99.0	5 ml GA	1.09608.0005
	n-Tridecane	C ₁₃ H ₂₈	≥ 99.5	5 ml GA	1.09609.0005
U	n-Undecane	C ₁₁ H ₂₄	≥ 99.5	5 ml GA	1.09794.0005

GA = glass ampoule

Fatty acid methyl esters

Designation	Empirical formula	Assay [%]	Content / Packaging	Ord. No.
M Methyl decanoate	$C_{11}H_{22}O_2$	≥ 99.5	5 ml GV	1.09637.0005
Methyl laurate	$C_{13}H_{26}O_2$	≥ 99.0	5 ml GV	1.09693.0005
Methyl margarate	$C_{18}H_{36}O_2$	≥ 99.0	5 ml GV	1.09754.0005
Methyl myristate	$C_{15}H_{30}O_2$	≥ 99.5	5 ml GV	1.09736.0005
Methyl octanoate	$C_9H_{18}O_2$	≥ 99.5	5 ml GV	1.09633.0005
Methyl oleate	$C_{19}H_{36}O_2$	≥ 96.0	5 ml GV	1.09743.0005
Methyl stearate	$C_{19}H_{38}O_2$	≥ 99.0	5 g GV	1.09602.0005

GV = glass vial

Miscellaneous reference substance

Designation	Empirical formula	Assay [%]	Content / Packaging	Ord. No.
C D-Camphor	$C_{10}H_{16}O$	≥ 96.0	5 g GV	1.09656.0005
E Ethyl methyl ketone	C_4H_8O	≥ 99.5	5 ml GV	1.09709.0005

GV = glass vial



We provide information and advice to our customers to the best of our knowledge and ability, but without obligation or liability. Existing laws and regulations are to be observed in all cases by our customers. This also applies in respect to any rights of third parties. Our information and advice do not relieve our customers of their own responsibility for checking the suitability of our products for the envisaged purpose. SupraSolv® is a registered trademark of Merck KGaA, Darmstadt, Germany.



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