CLEAR CHOICE
HIGH PURITY SOLVENTS FOR CHROMATOGRAPHY FROM MERCK

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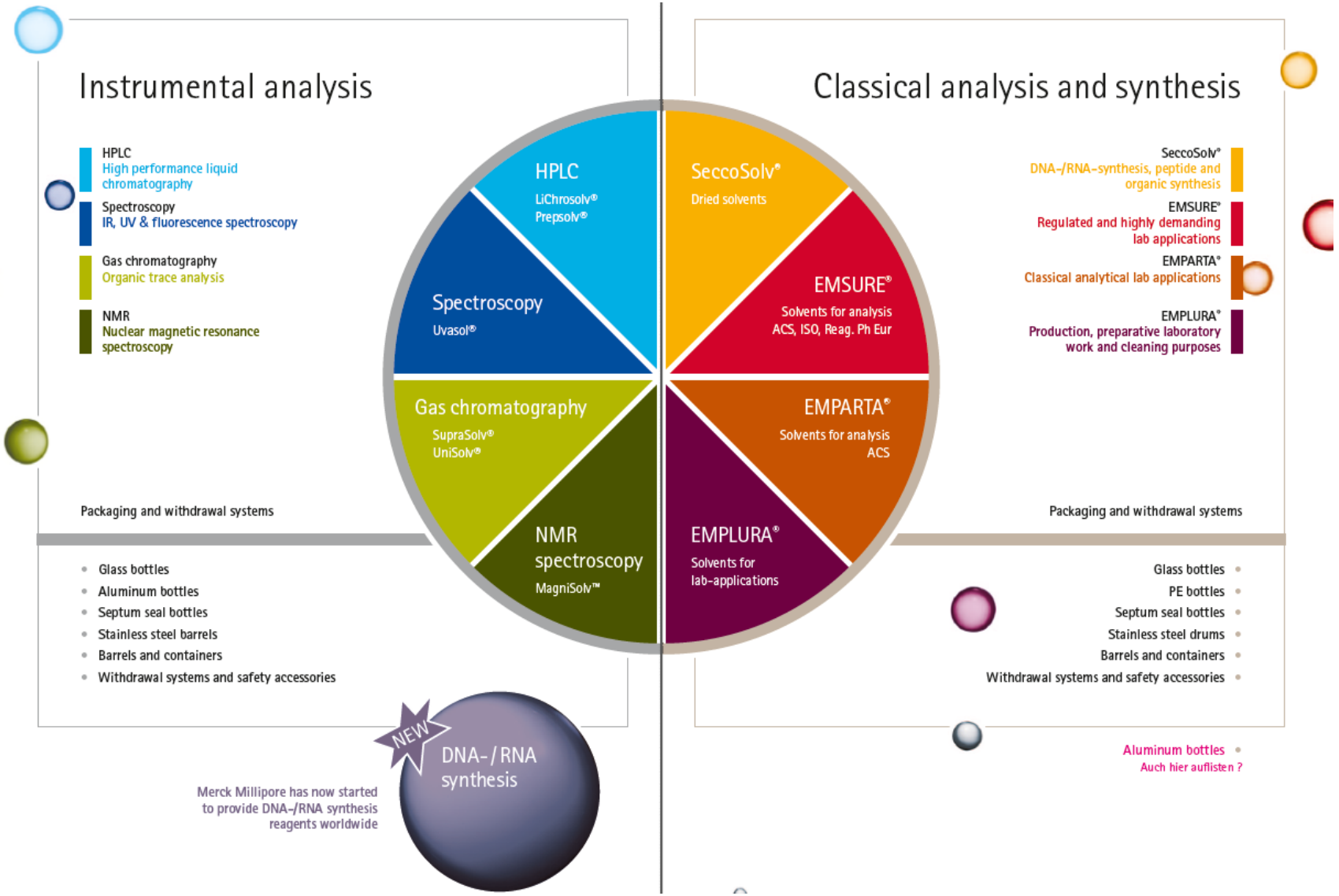
MERCK

Solvents for Instrumental Analysis



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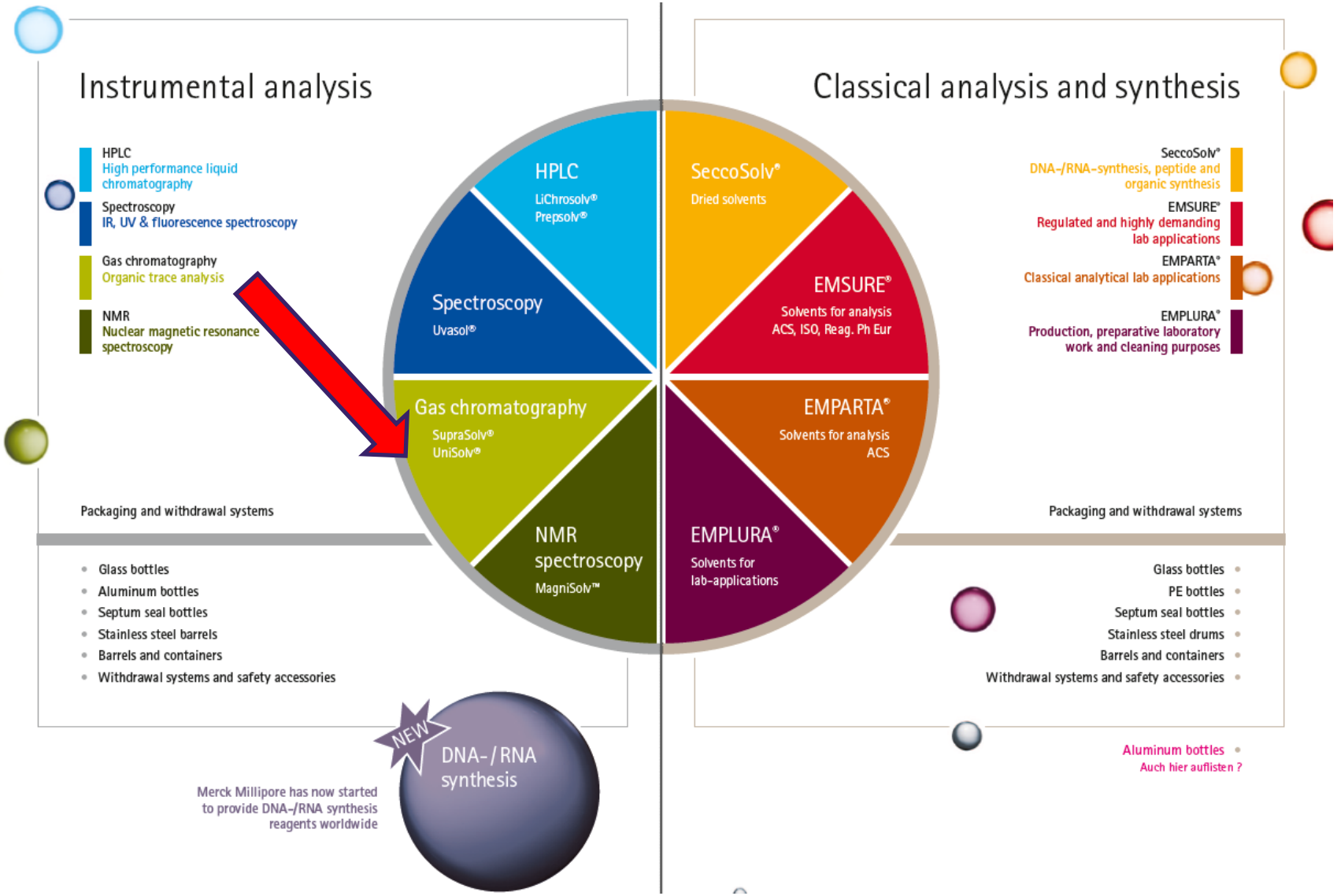
Solvents for gas chromatography – Suprasolv® and Unisolv®



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SOLVENTS FOR GASS CHROMATOGRAPHY SUPRASOLV® / UNISOLV®

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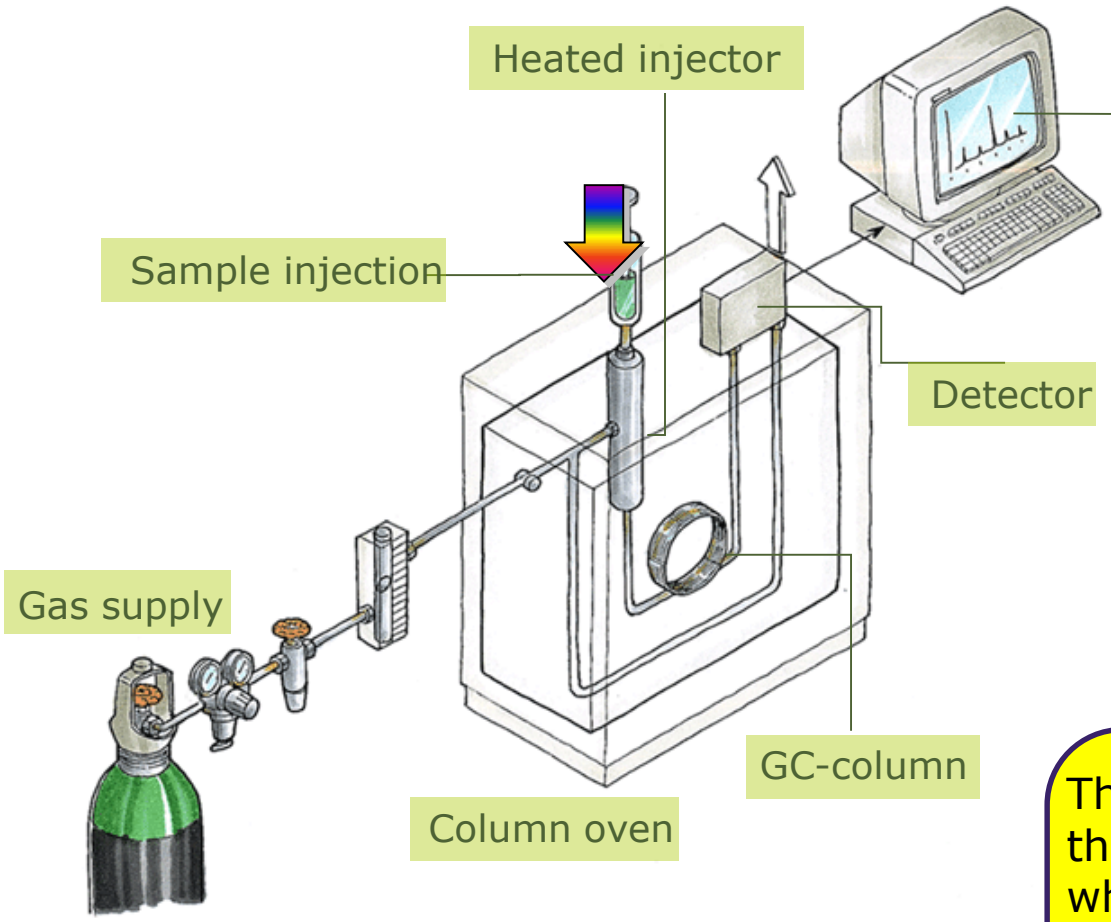
The principle of gas chromatography



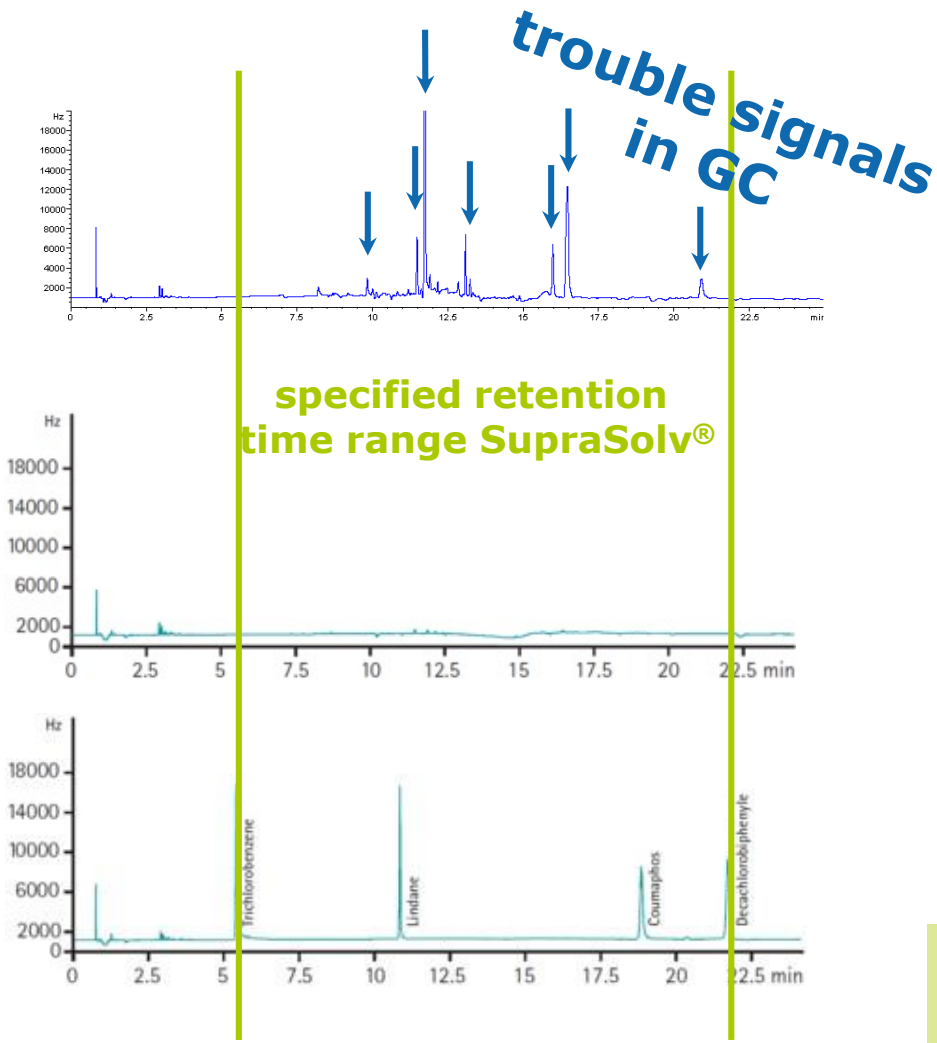
ECD = Electron Capture Detector

FID = Flame Ionization Detector

MS = Mass Spectrometric Detector

The sample solution injected into the instrument enters a gas stream which transports it through the column. The column separates the various components. The detector measures the quantity of the components that exit the column.

Why offering a special GC grade?



n-Hexane, purity (GC) 99.9%

Reagent grade
not specified for GC-application

n-Hexane SupraSolv® ECD and FID, Merck Millipore 1.04371

standard

Benefit:

Reliable and reproducible results due to constant minimal signal-noise-ratio (clear baseline)

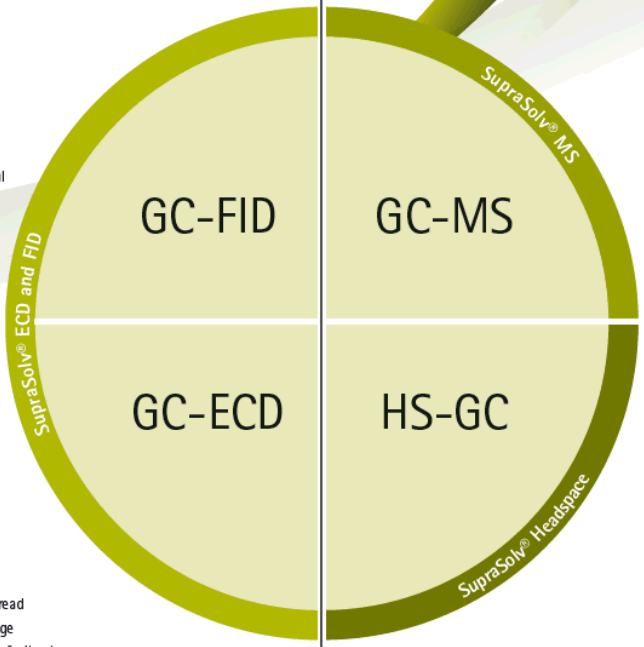
SupraSolv ® for Gas Chromatography
An Application Oriented program

SupraSolv

For all your needs in gas chromatography

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



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

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.

HS-GC
headspace gas chromatography

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

4 5

Solvents for GC - SupraSolv® & UniSolv®

UniSolv® for organic trace analysis
For ECD, FID and MS

„One for All"

SupraSolv®
For headspace GC

Application:
Analysis of residual solvents in drug substances and products acc. Ph Eur & USP

SupraSolv® ECD and FID
For gas chromatography ECD and FID

Applications
- Pesticide analysis
- Volatile halogenated hydrocarbons in water
- Polychlorinated biphenyls (PCB) in water
- Detection of Acrylamide in food

Applications
- BTX (Benzene, Toluene, Xylene) detection
- Hydrocarbon-oil-index in water
- Determination of emissions in car cockpit materials

SupraSolv® MS For GC-MS

Applications
- Analysis of Dioxins and Furans (PCDD/PCDF)
- Polycyclic aromatic hydrocarbons
- Pesticide analysis acc. QuEChERS
- Determination of phthalates in plastics

ECD
Electron Capture Detector

FID
Flame Ionization Detector

MS
Mass Spectrometric Detector

MERCK

Dedicated Specifications SupraSolv® & UniSolv®

1.04371.0000 n-Hexane for gas chromatography ECD and FID SupraSolv®

	Spec. Values	
Purity (GC)	≥ 98.0	%
Sum of hexane isomers + methylcyclopentane (GC)	≥ 99.8	%
Identity (IR)	conforms	
residue on evaporation	≤ 3.0	mg/l
Water	≤ 0.01	%
Colour	≤ 10	Hazen
GC/ECD (retention range 1,2,4-trichlorobenzene to decachlorobiphenyle individual signals (lindane standard))	≤ 3	pg/ml
GC/FID (retention range n-undecane - n-tetracontane individual signals (n- tetradecane standard))	≤ 3	ng/ml

suitable for residue analysis

1.00795.1000 n-Hexane for gas chromatography MS SupraSolv®

	Spec. Values	
Purity (GC)	≥ 98.0	%
Sum of hexane isomers + methylcyclopentane (GC)	≥ 99.8	%
Identity (IR)	conforms	
residue on evaporation	≤ 3.0	mg/l
Water	≤ 0.01	%
Colour	≤ 10	Hazen
GC/MSD (retention range n-undecane - n-tetracontane; scaning area 30 -600 amu individual signals (n- tetradecane standard))	≤ 3	ng/ml

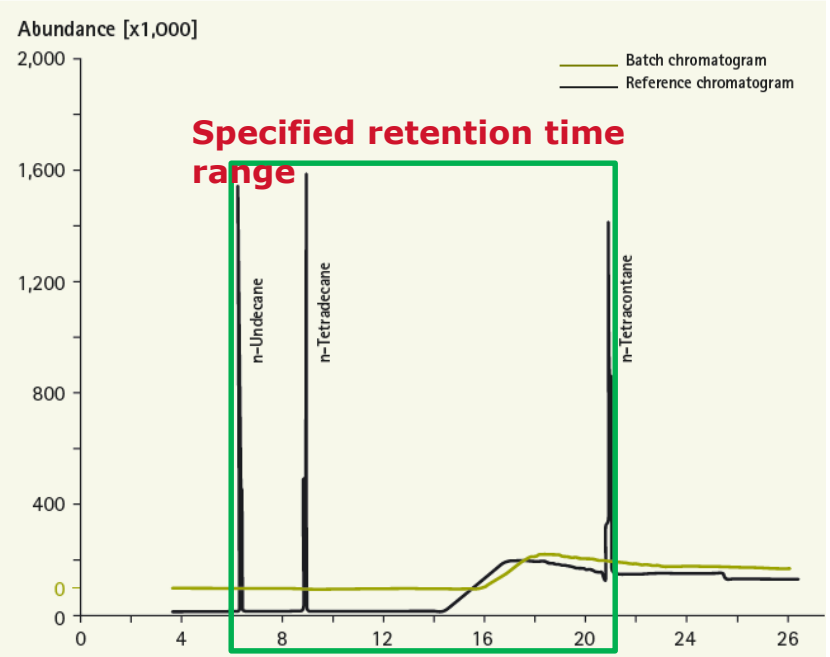
Suitable for residue analysis.

1.04369.0000 n-Hexane for organic trace analysis UniSolv®

	Spec. Values	
Purity (GC)	≥ 99.0	%
Sum of hexane isomers + methylcyclopentane (GC)	≥ 99.9	%
Identity (IR)	conforms	
residue on evaporation	≤ 3.0	mg/l
Water	≤ 0.005	%
Colour	≤ 10	Hazen
GC/ECD		
retention range 1,2,4-trichlorobenzene to decachlorobiphenyle		
individual signals (lindane standard)	≤ 2	pg/ml
retention range dichloromethane to 1,2,4-trichlorobenzene		
individual signals (tetrachloromethane)	≤ 1	ng/ml
GC/FID (retention range n-undecane - n-tetracontane		
individual signals (n- tetradecane standard))	≤ 2	ng/ml
GC/MSD (retention range n-undecane - n-tetracontane;		
scaning area 30 -600 amu		
individual signals (n- tetradecane standard))	≤ 2	ng/ml

Recommended for analysis of polychlorinated Dibenzodioxins and polychlorinated Dibenzofurans (PCDD/F).

SupraSolv® MS – marks the difference



Specification

1.00837.2500 Methanol for gas chromatography MS SupraSolv®

	Specification	
Purity (GC)	≥ 99.8	%
Identity (IR)	conforms	
Evaporation residue	≤ 3.0	mg/l
Water	≤ 0.1	%
Colour	≤ 10	Hazen
GC/MSD (retention range n-undecane to n-tetracontane, scaning area 30 - 600 amu, individual signals (n- tetradecane standard))	≤ 3	ng/ml

Suitable for residue analysis.

- Clear baseline – accurate, reliable & reproducible results (no risk of misinterpretation, no loss of valuable samples, no need for repeat analysis)
- Batch-to-batch consistency – time an cost saving
- Application tested quality – application security

Target groups

Contract Labs

Food analysis
Environmental analysis
Pharma analysis

Water & Environmental

Drinking water, (waste) water and soil analysis

Food & Beverage

Quality Control (e.g. pesticide analysis, dioxin detection, etc.)

Pharmaceutical Industry

Quality Control & R&D (e.g. analysis of residual solvents)

Chemical Industry

QC, R&D

Waste water control

Academia

R&D

Dioxin analysis by GC-MS

EPA method 3545A:
Determination of Dioxins and Furans in solid samples

→ Toluene, n-Hexane

VDI Guideline 3498/1:
Determination of Dioxins and Furans in indoor air

→ Acetone, Dichloromethane, n-Hexane, Toluene

Dioxin Analysis

DIN 38414-24: Determination of Dioxins and Furans in soil and sediments

→ Dichloromethane, n-Hexane, Toluene, Ethyl acetate, Cyclohexane

VDI Guideline 3499/1: Determination of Dioxins and Furans in filter dust, boiler ash and clinker

→ Dichloromethane, n-Hexane, Toluene,

Determination of pesticides in food & water according EPA method 508 by GC-ECD

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

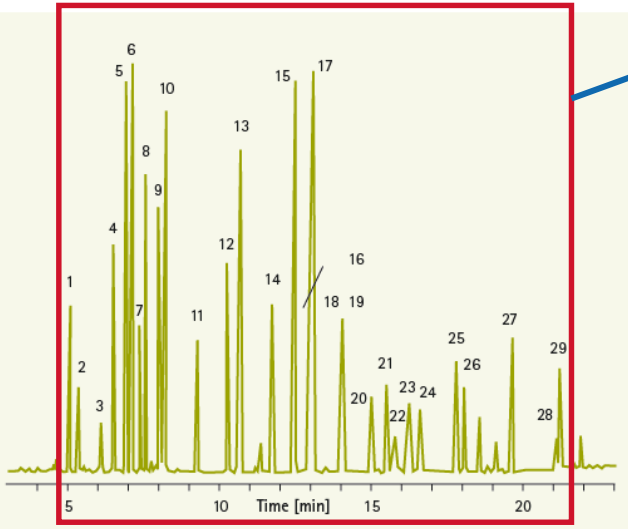


Fig. 3 *Chlorinated pesticides: EPA Method 508, GC-ECD.*

Retention time range of SupraSolv®

1. Etridiazole
2. Chloroneb
3. Propachlor
4. Trifluralin
5. α-BHC
6. Hexachlorobenzene
7. β-BHC
8. Ω-BHC
9. γ-BHC
10. Chlorothalonil
11. Heptachlor
12. Aldrin
13. DCPA
14. Heptachlor epoxide
15. γ-Chlordane
16. Endosulfan I
17. α-Chlordane
18. Dieldrin
19. 4,4'-DDE
20. Endrin
21. Endosulfan II
22. Chlorobenzilate
23. 4,4'-DDD
24. Endrin aldehyde
25. Endosulfan sulfate
26. 4,4'-DDT
27. Methoxichlor
28. cis-Permethrin
29. trans-Permethrin

- Solvents:
  - 1.00012 Acetone ECD and FID SupraSolv®
  - 1.06054 Dichloromethane ECD and FID SupraSolv®
  - 1.01995 tert-Butyl methyl ether ECD and FID SupraSolv®

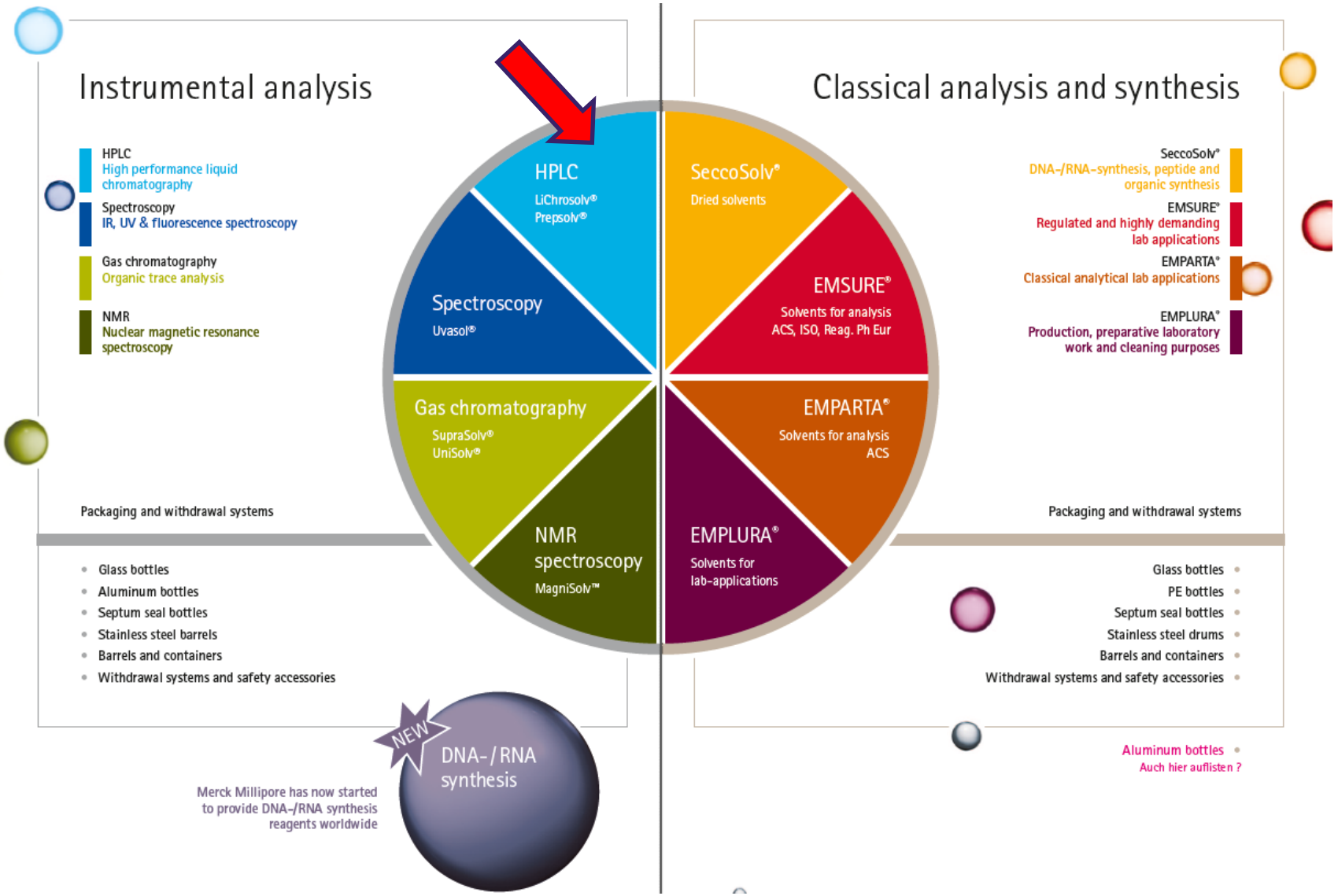
SupraSolv® & UniSolv® mark the difference

- **Lowest impurities/ clear baseline** – accurate, reliable & reproducible results (no risk of misinterpretation, no loss of valuable samples, no need for repeat analysis)
- **Widest retention time range** – most comprehensive range of applications
- **Batch-to-batch consistency** – time an cost saving (avoidance of analysis repetition)
- **Application tested quality** – application security
- **Flexibility** – Top-products are also offered in 10L stainless steel barrels as standard pack size
- **UniSolv®** is suitable **for all three main detection methods ECD, FID & MS** – one solvent quality for all applications

UNIQUE !

MERCK

Solvents for analytical liquid chromatography - LiChrosolv®



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HPLC – what can you do with it?

Qualitative analysis
Identification of compounds by their retention time (= time it takes to elute from the column after injection)

Quantitative analysis
Measurement of compound concentration via peak height and peak area

Preparative chromatography
Preparation of pure compound by collecting / concentrating the compound for further studies

Trace analysis
Of extremely low concentrations of harmful or toxic compounds with high resolution separations and very sensitive detectors

HPLC : High Performance (Pressure) Liquid Chromatography

Analytical technique to separate, identify & quantify chemical & biological compounds.

Separation is depending on:

- **Type of analysed substance**
- **Type of column**
- **Temperature**
- **ph value**
- **Flow rate of mobile phase**
- **Composition of mobile phase (solvent)**

02a

SOLVENTS FOR LIQUID CHROMATOGRAPHY LICHROSOLV® - AT A GLANCE

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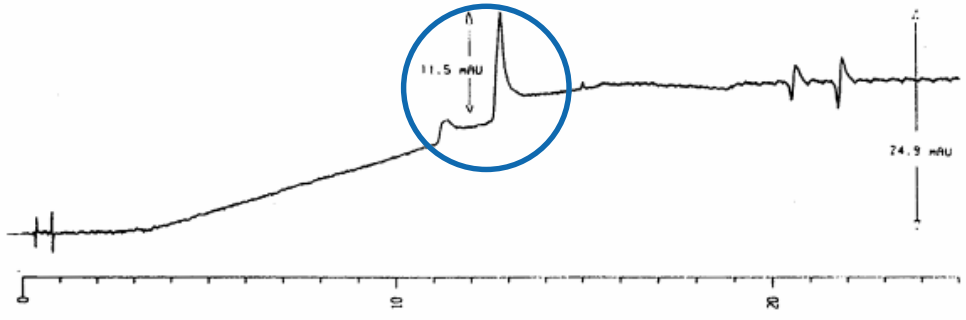
Why using a special HPLC grade?

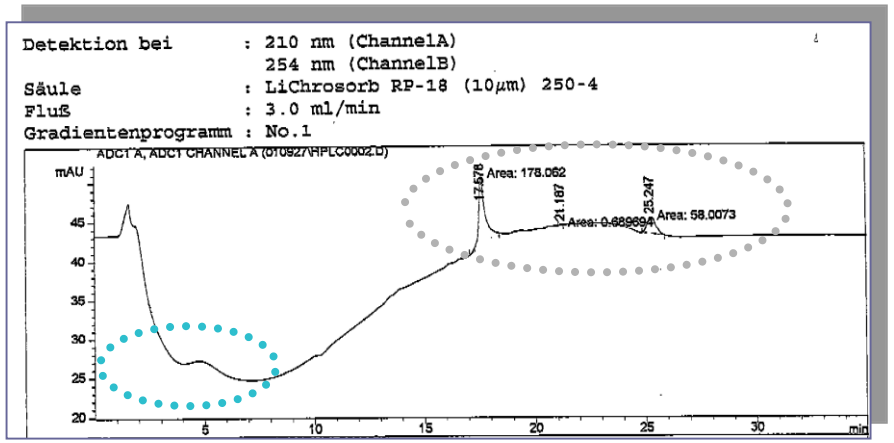
Solvent impurities can result in ghost peaks !



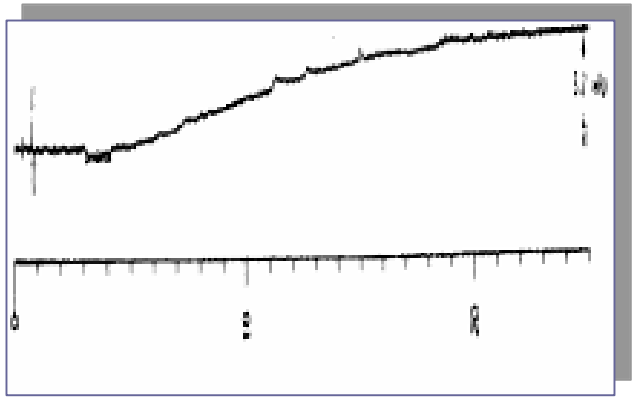
→HPLC peak resolution & quantitative results are effected by solvents with lower quality

Compounds producing artefacts: Additives, Peroxides, Phtalates

Risks „using non suitable Acetonitrile @ 210 nm“



Risk due to enrichment process of impurities



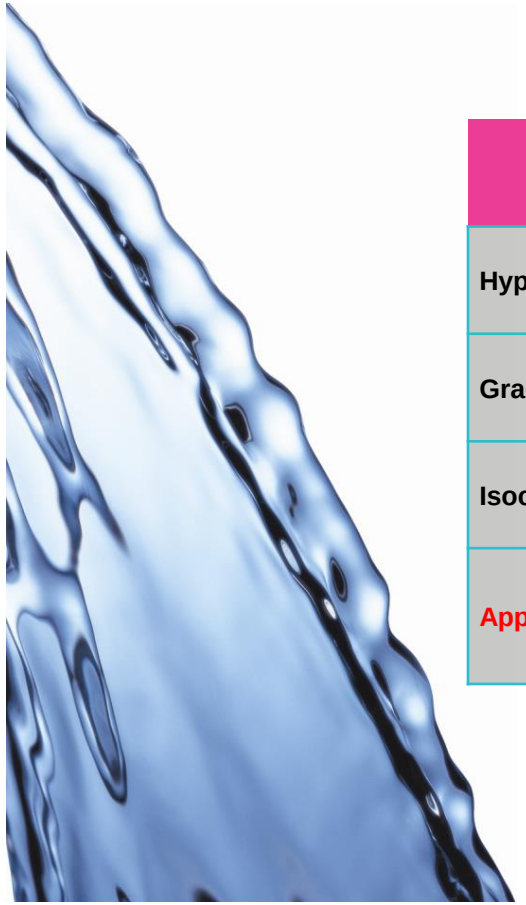
Baseline drift due to trace impurities

Solvent impurities

- No reliable HPLC result
- Loss in separation performance
- Reduced column lifetime

Solvents for liquid chromatography LiChrosolv®

Different applications require different purity

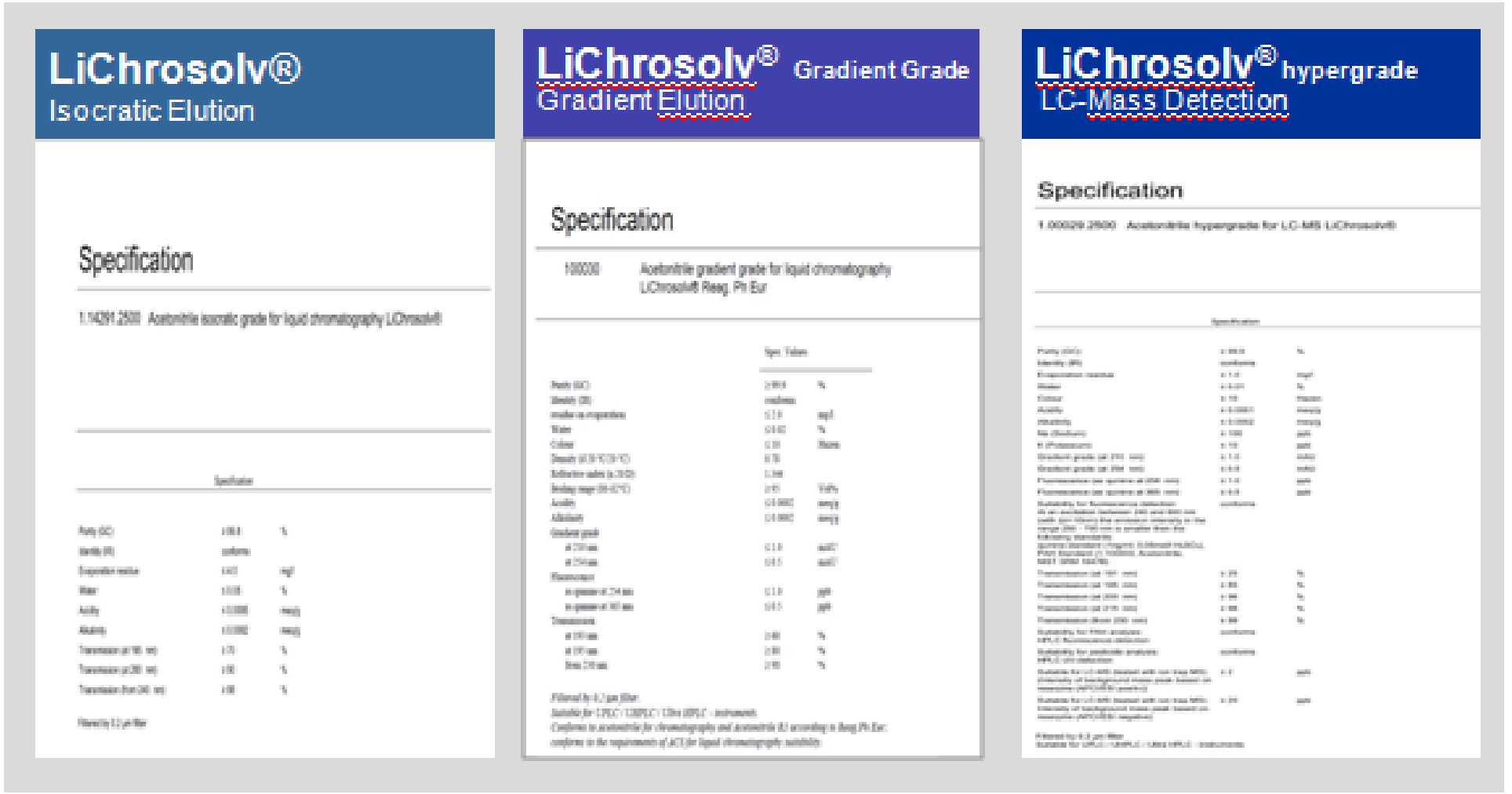


LiChrosolv®							
Hypergrade							
Gradient grade							
Isocratic grade							
Application	Isocratic HPLC	Far UV HPLC	Gradient Elution	Protein Profiling	Pesticide Analysis	PAHs	Proteomics LC-MS application

3 Grade-Program: Application Oriented

LiChrosolv® Isocratic Elution	**LiChrosolv®** **Gradient Grade** Gradient Elution	**LiChrosolv®** **hypergrade** LC-Mass Detection
▪ **Detection method: UV** ▪ For the analysis of simple matrix ▪ Applications: sample preparation & isocratic separation of similar polar, non polar compounds in QC ▪ Customer Segment: Food & Beverage, Environmental, Pharma , Chemical Industry	▪ **Detection method: UV, Fluorescence** ▪ Applications: sample preparation & analysis of complex, highly sensitive & demanding quality control, impurity profiling in QC, R&D for mixed samples of polar /non-polar compounds ▪ Customer Segment: Pharma, Chemistry, Cosmetics	▪ **Detection method: UV, Fluorescence, Mass** ▪ Applications: Protein Profiling Pesticide Analysis PAHs Proteomics LC-MS LC-MS routine analysis ▪ Customer Segment: Pharma, mainly R&D, Environmental QC

3 Grade – Application Oriented Program



Solvents for liquid chromatography LiChrosolv®

Different applications require different purity

LiChrosolv®							
Hypergrade							
Gradient grade							
Isocratic grade							
Application	Isocratic HPLC	Far UV HPLC	Gradient Elution	Protein Profiling	Pesticide Analysis	PAHs	Proteomics LC-MS application

Specification

1.00030.2500 Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

	Specification	
Purity (GC)	≥ 99.9	%
Identity (IR)	conforms	
Evaporation residue	≤ 2.0	mg/l
Water	≤ 0.02	%
Colour	≤ 10	Hazen
Density (d 20 °C/20 °C)	0.78	
Refractive index (n 20/D)	1.344	
Boiling range (80-82°C)	≥ 95	% (v/v)
Acidity	≤ 0.0002	meq/g
Alkalinity	≤ 0.0002	meq/g
Gradient grade (at 210 nm)	≤ 1.0	mAU
Gradient grade (at 254 nm)	≤ 0.5	mAU
Fluorescence (as quinine at 254 nm)	≤ 1.0	ppb
Fluorescence (as quinine at 365 nm)	≤ 0.5	ppb
Transmission (at 193 nm)	≥ 60	%
Transmission (at 195 nm)	≥ 80	%
Transmission (from 230 nm)	≥ 98	%

Filtered by 0.2 µm filter.
Suitable for UPLC / UHPLC /Ultra HPLC - instruments.
Conforms to Acetonitrile for chromatography and Acetonitrile R1 according to Reag.Ph Eur;
conforms to the requirements of ACS for liquid chromatography suitability.

What‘s different ?

Specification

1.00030.2500 Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

Reag. PhEur and ACS Specification

Specification		
Purity (GC)	*Conforms to Acetonitrile for chromatography and Acetonitrile R1 according to Reag.Ph Eur;*	
Identity (IR)	*conforms to the requirements of ACS for liquid chromatography suitability.*	
Evaporation		
Water		
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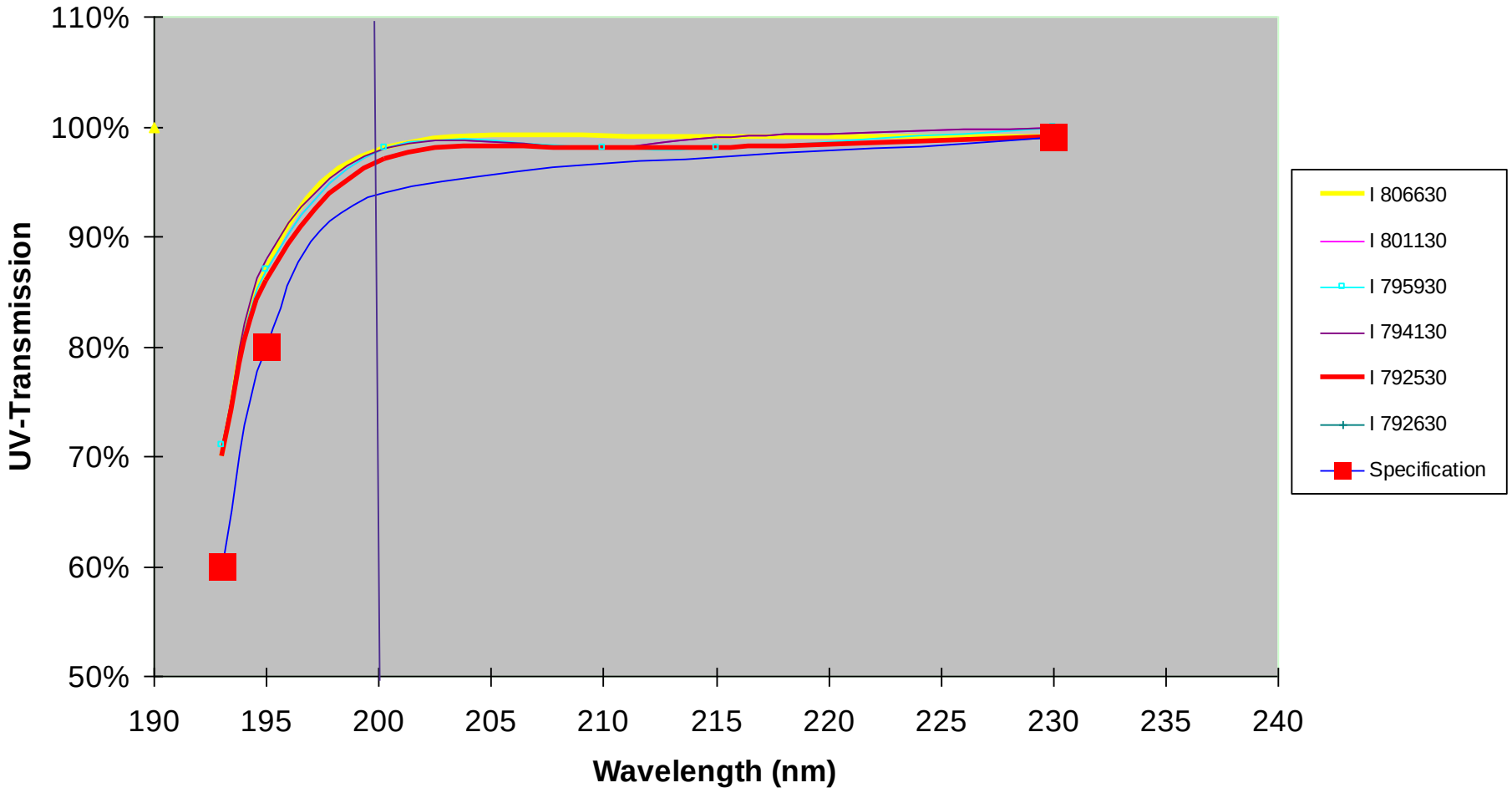
conforms to the requirements of ACS for liquid chromatography suitability.

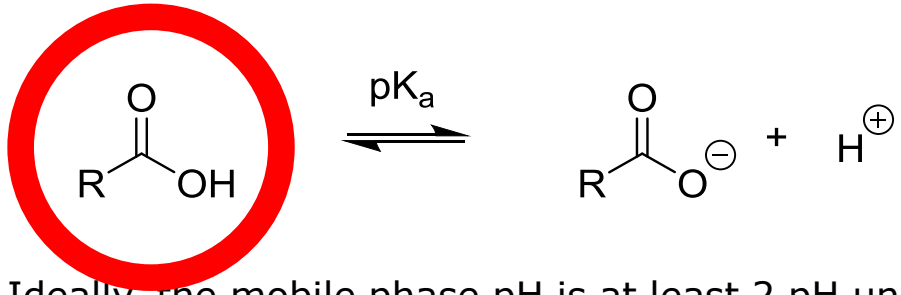
That‘s the difference

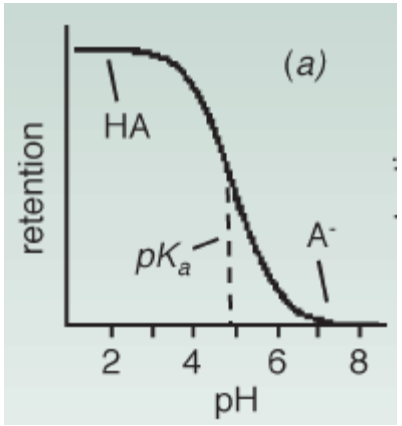
Quality Assurance (1) - **UV Transmission**



Why using buffers at all in HPLC and LC-MS…?

- Buffers are used in RP-HPLC separations to control the retention of ionizable compounds.
- This is to suppress ionization of analytes in order to maximize sample retention.





- Ideally, the mobile phase pH is at least 2 pH units below (acids) or above (bases) the sample *p*K*a*.
- For the most effective buffering, a buffer should be carefully chosen and used within ±1 pH unit of the buffer's *p*K*a*.
- For LC-UV assays, phosphate and acetate buffers are most popular.
- For LC-MS applications, the buffer must be volatile. Various combinations of formate, acetate, ammonia and bicarbonate are most popular for LC-MS work.

Lichropur® HPLC Reagents

Product No.	Name	Description	Package Size
5.43804	Formic acid	100%	100, 250 ml
5.43808	Acetic acid	100%	100, 250 ml
5.43827	Sulfuric acid	96%	100, 250 ml
5.43828	o-Phosphoric acid	85%	100, 250 ml
5.43830	Ammonia solution	25%	100, 250 ml
5.43832	Sodium chloride		100, 250 ml
5.43833	Sodium acetate trihydrate		100, 250 ml
5.43834	Ammonium acetate		100, 250 ml
5.43835	Ammonium hydrogen carbonate		100, 250 ml
5.43837	Ammonium dihydrogen phosphate		100, 250 ml
5.43838	Di-Sodium hydrogen phosphate anhydrous		100, 250 ml
5.43839	Di-Potassium hydrogen phosphate anhydrous		100, 250 ml
5.43840	Sodium dihydrogen phosphate anhydrous		100, 250 ml
5.43841	Potassium dihydrogen phosphate anhydrous		100, 250 ml

Lichropur® HPLC Reagents

HPLC Reagents

We offer LiChropur® reagents ideal for HPLC analysis.

These reagents are tested for inorganic impurities, including Al, Ca, Cu, Fe, K, Mg and Na.

- QC performed using a HPLC suitability gradient test at 220, 254 and 280 nm.
- Filled under clean room conditions
- Extensive impurity profile of the product on the Certificate of Analysis

→ High purity HPLC reagents for mobile phase improve performance and minimize interference!

Lichropur® HPLC Reagents
Product Specifications

- Assay (acidimetric): ≥ 98.0%
- Colour: ≤ 10 Hazen
- Evaporation Residue: ≤ 10 ppm
- Cation traces:
  - **Al: ≤ 0.050 ppm; Ca: ≤ 0.2 ppm; Cu: ≤ 0.020 ppm; Fe: ≤ 2.0 ppm; K: ≤ 0.10 ppm; Mg: ≤ 0.50 ppm; Na: ≤ 0.50 ppm**
  - HPLC-gradient suitability test (220, 254, 280 nm) chromophoric impurities based on 4’-hydroxyacetophenon
  - Chromophore purity: ≥ 99.999%

SOLVENTS FOR LIQUID CHROMATOGRAPHY LICHROSOLV® - FAST CHROMATOGRAPHY

b2b

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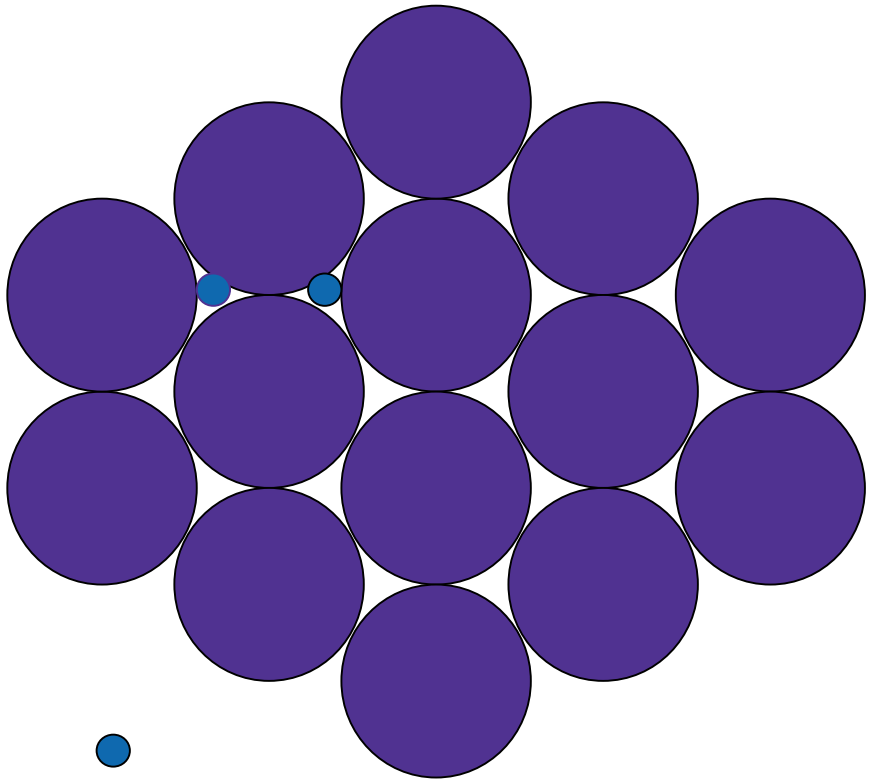
Fast chromatography – UHPLC

UHPLC column 1,7µm / 6 < 0,3µm **means high risk of blockage**



Faster
Short & thin columns
Higher separating capacity
Particle diameter > 2µm

Columns packed with 1.7µm particles tend to clogg easily, because the space in between the particles is only 0.3µm

1.00030.2500 Acetonitrile gradient grade for liquid chromatography LiChrosolv® Reag. Ph Eur

	Spec. Values	
Purity (GC)	≥ 99.9	%
Identity (IR)	conforms	
residue on evaporation	≤ 2.0	mg/l
Water	≤ 0.02	%
Colour	≤ 10	Hazen
Density (d 20 °C/20 °C)	0.78	
Refractive index (n 20/D)	1.344	
Boiling range (80-82°C)	≥ 95	Vol%
Acidity	≤ 0.0002	meq/g
Alkalinity	≤ 0.0002	meq/g
Gradient grade		
at 210 nm	≤ 1.0	mAU
at 254 nm	≤ 0.5	mAU
Fluorescence		
as quinine at 254 nm	≤ 1.0	ppb
as quinine at 365 nm	≤ 0.5	ppb
Transmission		
at 193 nm	≥ 60	%
at 195 nm	≥ 80	%
from 230 nm	≥ 98	%

Filtered by 0.2 µm filter
Suitable for UPLC / UHPLC / Ultra HPLC - instruments

SOLVENTS FOR LIQUID CHROMATOGRAPHY LICHROSOLV® LC – MASS DETECTION

D2C

MERCK

LC-MS Method

Is it necessary to have a better grade of solvent and better column purity for LC-MS?

YES!

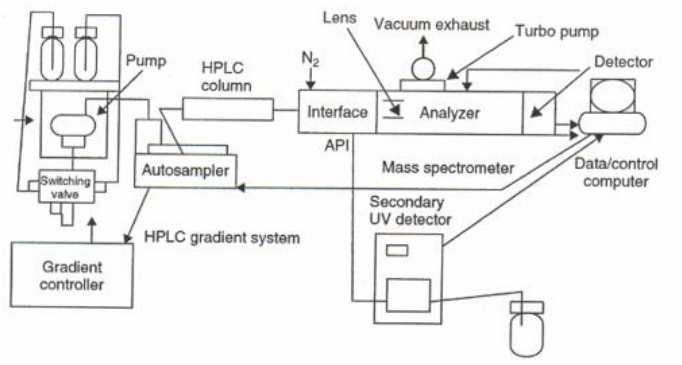
BECAUSE:

With standard solvents & columns, trace impurities cause unwanted background signals in LC-MS which reduce sensitivity and cause complex spectra with low reproducibility - compared to HPLC with standard UV detectors.

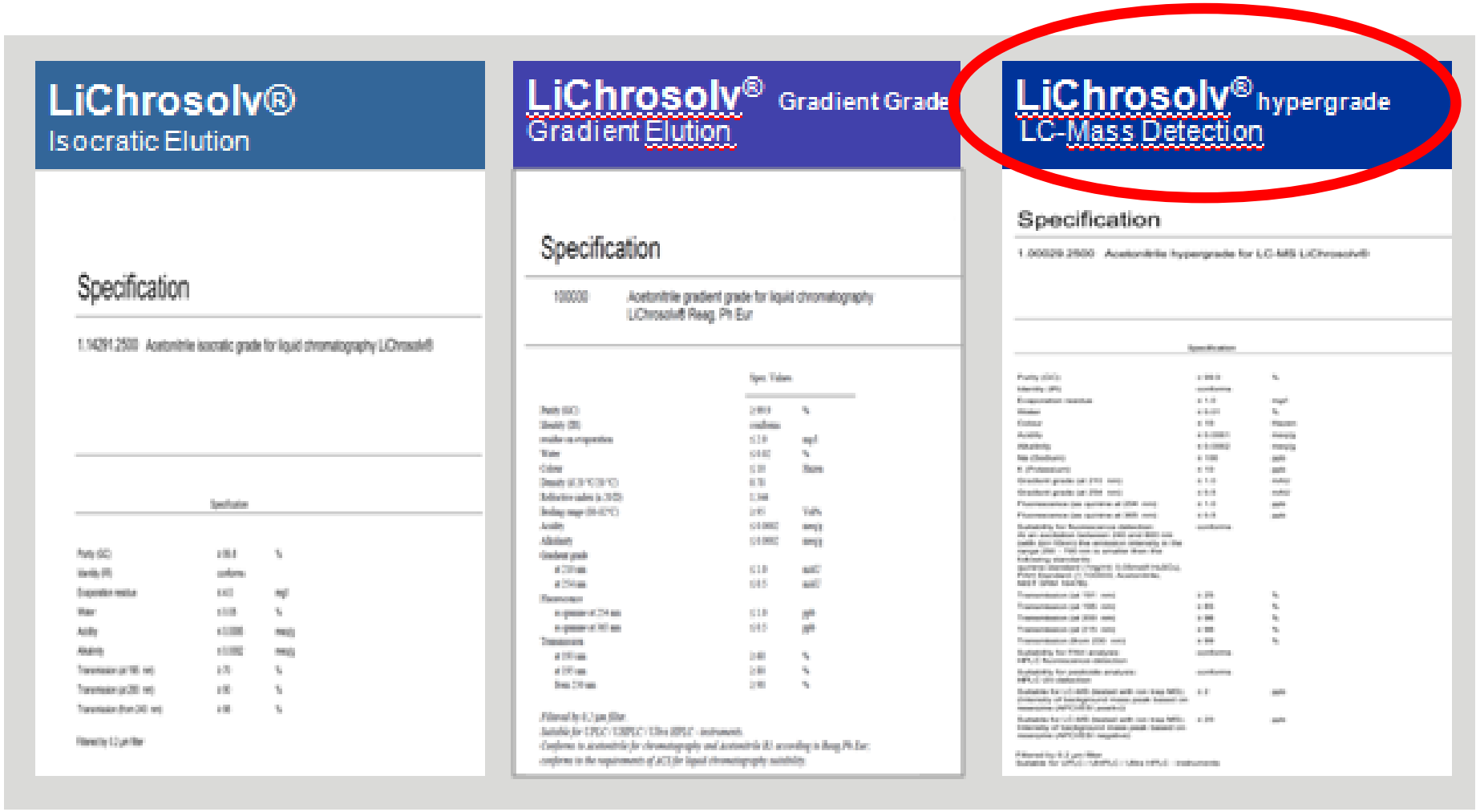
LC-MS requires improved procedures, compared to HPLC with UV detectors

Criteria LC-MS / Optimized Performance

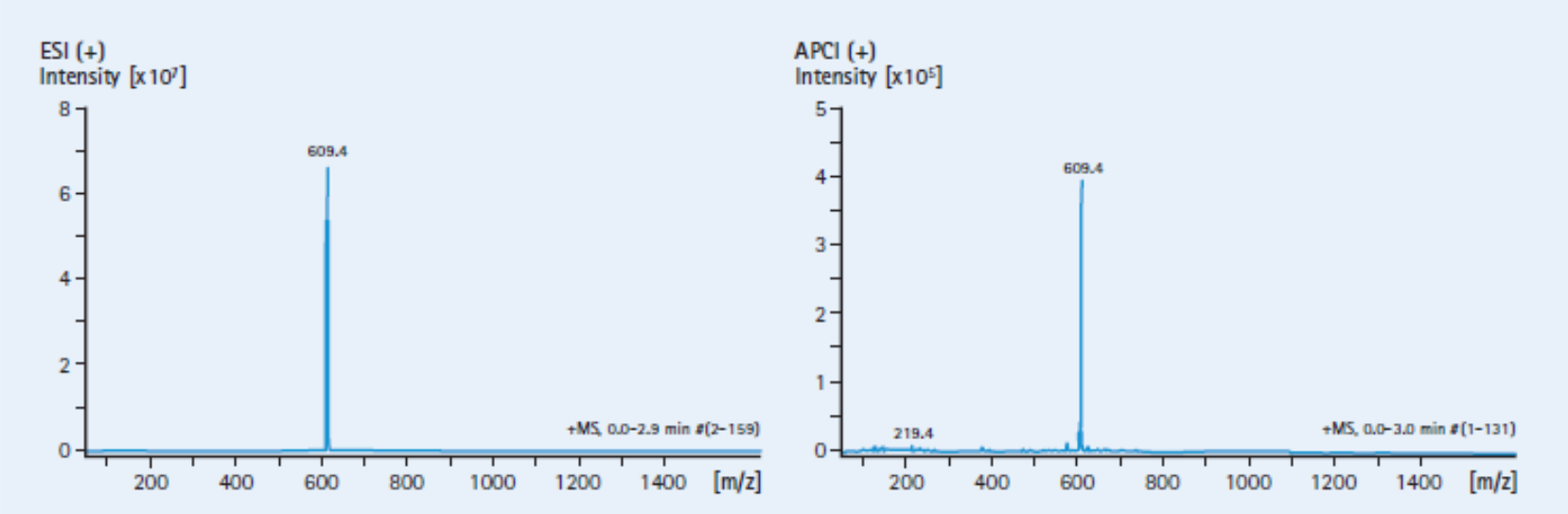
- High ionisation efficiency
- High reproducibility of the ionisation signal
- Low „background“ signals and low adduct formation
- Low „ion suppression“ due to solvents impurities
- Low contamination of the ionisation source



3 Grade – Application Oriented Program



Example: Acetonitrile LiChrosolv® hypergrade



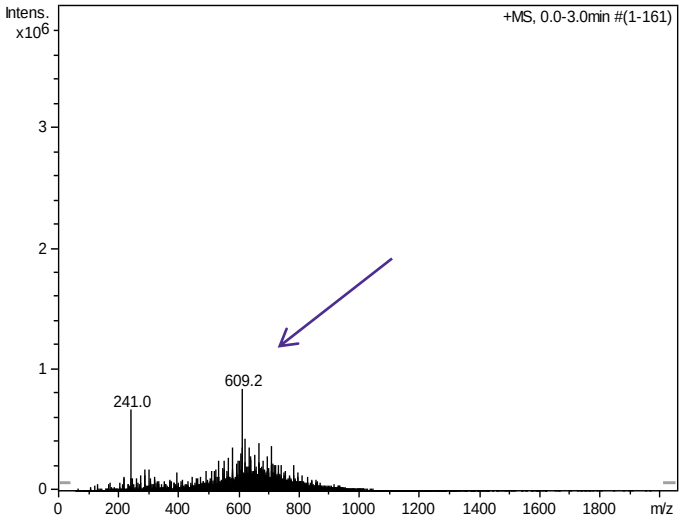
Mass spectrum of LiChrosolv® Acetonitrile hypergrade (100029). Mobile phase Acetonitrile special LC-MS grade. Intensity of single background mass peak based on resperine standard (m/z 609.4) in e.g. ESI (+) and APCI (+) mode.

ESI = Electron Spray Ionization

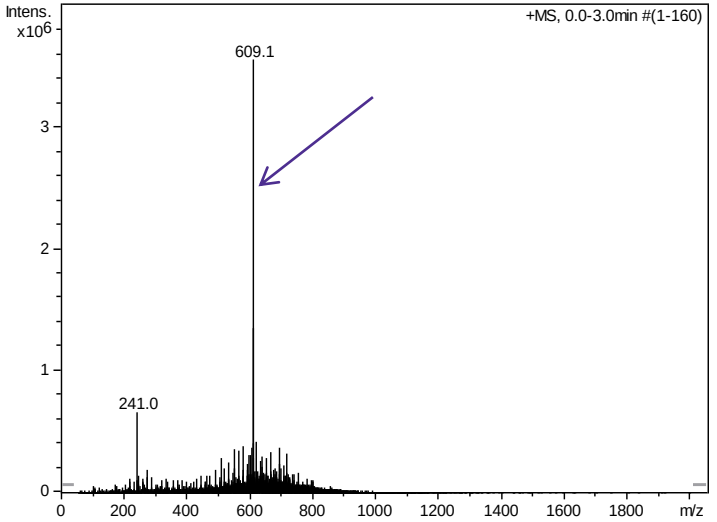
APCI = Atmospheric Pressure Chemical Ionization

Main problem: low ionization efficiency

Gradient Grade



Hypergrade LC-MS Grade



- The mass spectra of different acetonitrile grades show clearly the variation in the intensity of the reserpine signal ($[M+H]^+$ = 609) as well as the extent of the background signals.

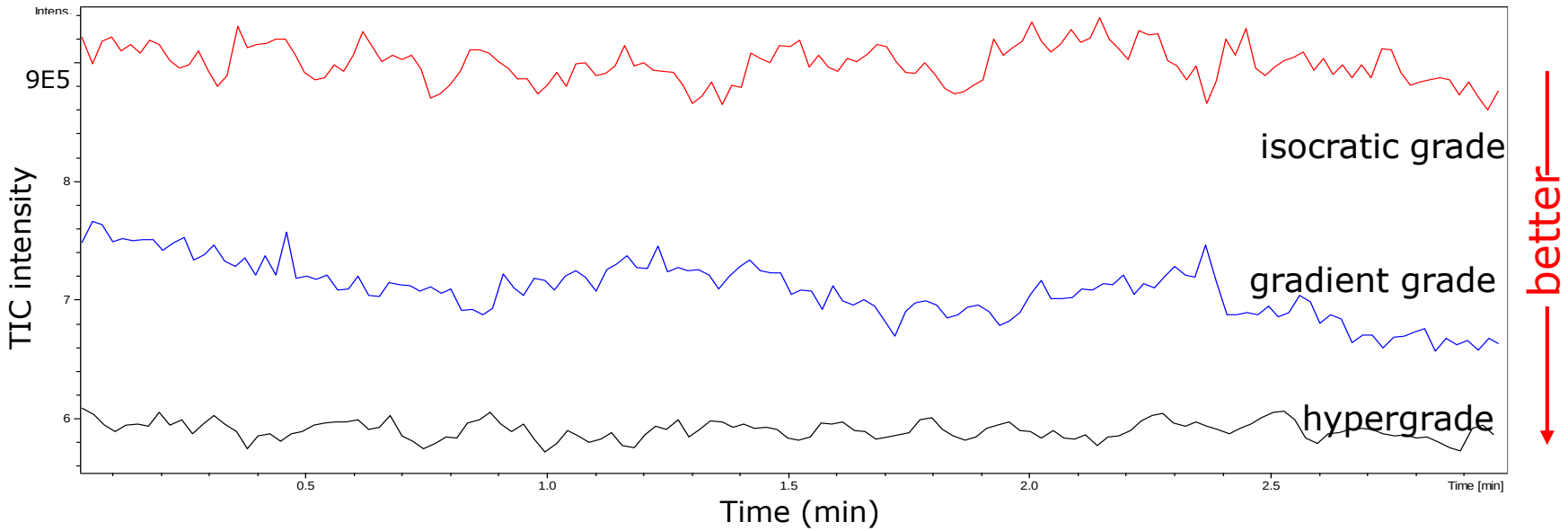
- The differences in the intensity of the reserpine signal are caused by ion suppression. This effect occurs due to interfering trace contaminants that can be present in acetonitrile.

TIC (Total Ion Current) in different eluent qualities

MS grade solvents prevent contamination

- Minimization of contaminant peaks & ion suppression
- Maximization of sensitivity (low background noise)

Combined TICs of the analysis of three different acetonitrile qualities:



Merck: Specification for ACN, Methanol, Water for LC-MS suitability

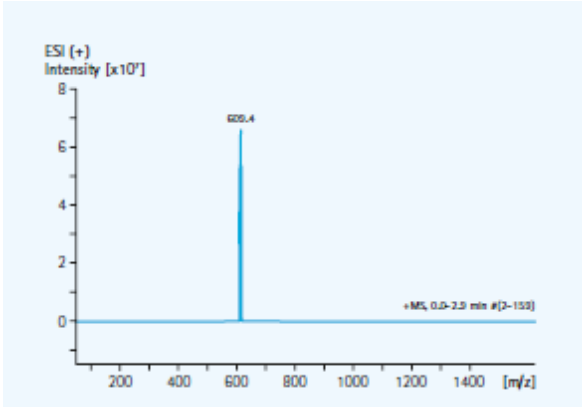
Acetonitrile hypergrade LC-MS suitability	Cat. No. 100029 Spec. values
Purity (GC)	≥ 99.9 %
Identity (IR)	conforms
Residue on evaporation	≤ 1.0 mg/l
Water	≤ 0.01 %
Color	≤ 10 Hazen
Acidity	≤ 0.0001 meq/g
Alkalinity	≤ 0.0002 meq/g
Al (Aluminum) *	≤ 10 ppb
Ca (Calcium) *	≤ 10 ppb
Fe (Iron) *	≤ 10 ppb
Mg (Magnesium) *	≤ 10 ppb
Na (Sodium) *	≤ 50 ppb
K (Potassium) *	≤ 5 ppb
Every other single metal (ICP-MS) *	≤ 5 ppb
Gradient grade	
at 210 nm	≤ 0.8 mAU
at 254 nm	≤ 0.3 mAU
Fluorescence	
as quinine at 254 nm	≤ 1 ppb
as quinine at 365 nm	≤ 0.5 ppb
Transmission	
at 191 nm	≥ 25 %
at 195 nm	≥ 85 %
at 200 nm	≥ 96 %
at 215 nm	≥ 98 %
from 230 nm	≥ 99 %
Suitability for PAH analysis (HPLC fluorescence-detection)	conforms
At an excitation between 240 and 600 nm (with t Δλ = 10 nm) the emission intensity in the range of 250 – 700 nm is smaller then the following standards: Chinin-Standard (1 ng/ml; 0.05 mol/l H_2SO_4), PAH Standard (1:100,000, Acetonitrile; NIST SRM 1647B)	
Suitability for pesticide analysis (HPLC UV-detection)	conforms
Suitability for LC-MS (tested with ion trap MS); Intensity of background mass peak based on reserpine:	
Mode: ESI 200 µl pos | APCI 200 µl pos	≤ 2 ppb
Mode: ESI 200 µl neg | APCI 200 µl neg	≤ 20 ppb

Filtered by 0.2 µm stainless steel filter | Suitable for PAH-analysis | Suitable for UPLC | UHPLC | Ultra Fast HPLC-instruments | Suitable for Q-TOF LC-MS | * = enhanced specifications

Methanol hypergrade LC-MS suitability	Cat. No. 106035 Spec. values
Purity (GC)	≥ 99.9 %
Identity (IR)	conforms
Residue on evaporation	≤ 1.0 mg/l
Water	≤ 0.01 %
Color	≤ 10 Hazen
Acidity	≤ 0.0002 meq/g
Alkalinity	≤ 0.0002 meq/g
Al (Aluminum) *	≤ 10 ppb
Ca (Calcium) *	≤ 10 ppb
Fe (Iron) *	≤ 10 ppb
Mg (Magnesium) *	≤ 10 ppb
Na (Sodium) *	≤ 100 ppb
K (Potassium) *	≤ 5 ppb
Every other single metal (ICP-MS) *	≤ 5 ppb
Gradient Grade	
at 220 nm	≤ 2.0 mAU
at 235 nm	≤ 1.0 mAU
Fluorescence	
as quinine at 254 nm	≤ 1 ppb
as quinine at 365 nm	≤ 0.5 ppb
Transmission	
at 210 nm	≥ 35 %
at 220 nm	≥ 60 %
at 230 nm	≥ 75 %
from 260 nm	≥ 98 %
Suitability for LC-MS (tested with ion trap MS); Intensity of single background mass peak based on reserpine:	
Mode: ESI 200 µl pos | APCI 200 µl pos	≤ 2 ppb
Mode: ESI 200 µl neg | APCI 200 µl neg	≤ 20 ppb

Filtered by 0.2 µm stainless steel filter | Suitable for PAH-analysis | Suitable for UPLC | UHPLC | Ultra Fast HPLC-instruments | * = enhanced specifications

Ion / Metal – information



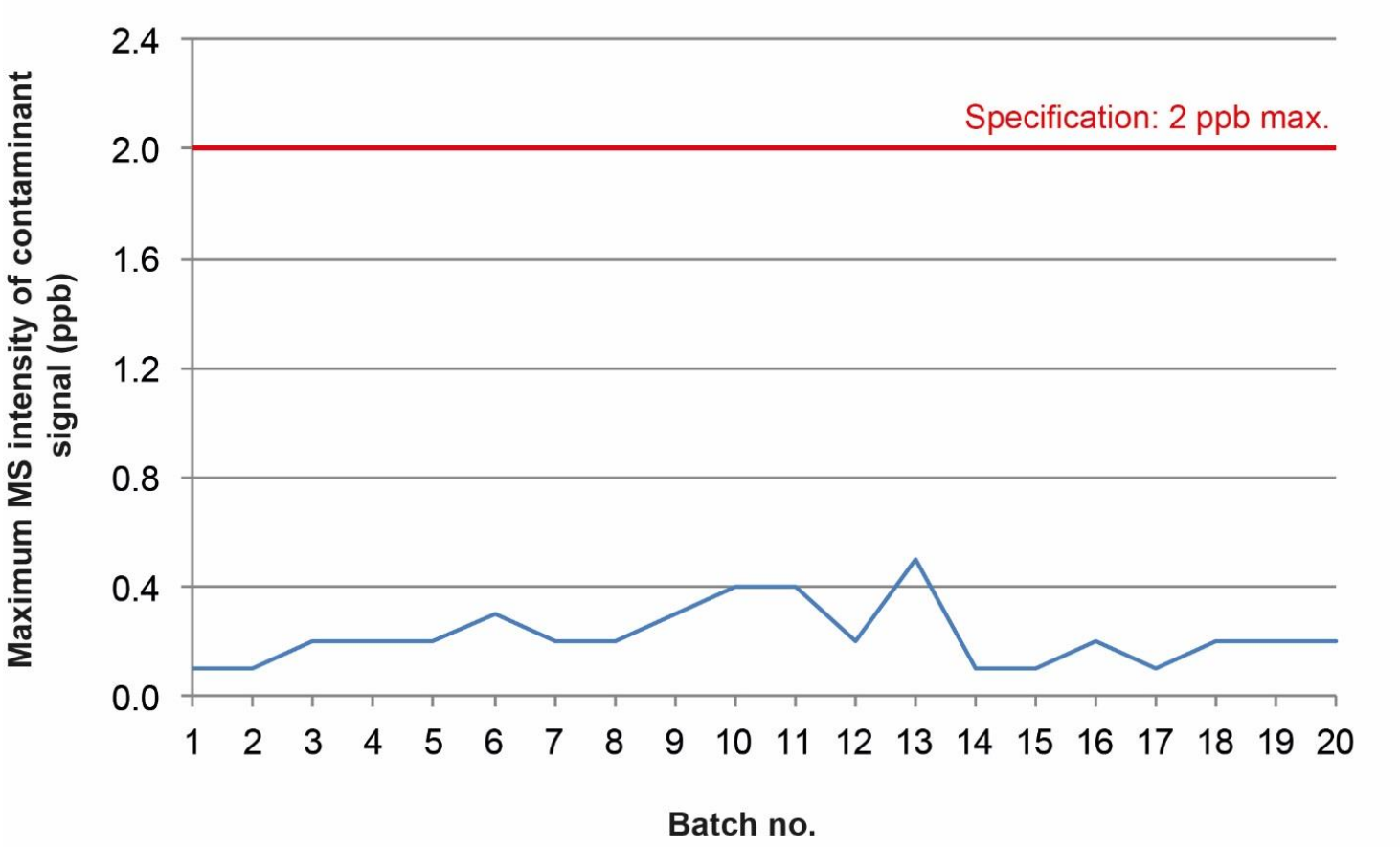
Suitability ESI/APCI (+) & ESI/APCI (-) mode

ESI = Electron Spray Ionization

APCI = Atmospheric Pressure Chemical Ionization

Sensitivity in MS

Batch-to-batch reproducibility of acetonitrile hypergrade for LC-MS LiChrosolv® in 20 consecutive batches



reproducibly low background noise
no or weak additional peaks/ signal suppression

Conditions	
System	Bruker Esquire 6000plus
Detection	Pos. ESI-MS, *m/z* range 50-2000
Flow rate	0.2 mL/min via syringe pump
Temp.	25 °C

LiChrosolv® hypergrade Portfolio – pure solvents

1.00029	Acetonitrile Lichrosolv® hypergrade for LC-MS
1.03649	Ethyl acetate Lichrosolv® hypergrade for LC-MS
1.03654	Heptane Lichrosolv® hypergrade for LC-MS
1.03701	Hexane Lichrosolv® hypergrade for LC-MS
1.06035	Methanol Lichrosolv® hypergrade for LC-MS
1.02781	2-Propanol LiChrosolv® hypergrade for LC-MS
1.15333	Water for chromatography LiChrosolv® (LC-MS grade)

LiChrosolv® hypergrade Portfolio- ready to use blends

1.59004	Acetonitrile with 0.1% (v/v) Acetic acid hypergrade for LC-MS LiChrosolv®
1.59002	Acetonitrile with 0.1% (v/v) Formic acid hypergrade for LC-MS LiChrosolv®
1.59014	Acetonitrile with 0.1% (v:v) Trifluoroacetic acid hypergrade for LC-MS LiChrosolv®
1.59007	Water with 0.1% (v/v) Acetic acid hypergrade for LC-MS LiChrosolv®
1.59013	Water with 0.1% (v/v) Formic acid hypergrade for LC-MS LiChrosolv®
4.80112	Water with 0.1% (v:v) trifluoroacetic acid hypergrade for LC-MS LiChrosolv®

Lichropur® LC-MS Reagents
Product Overview

Product No.	Name	Description	Package Size
5.33001	Acetic acid	100% for LC-MS Lichropur®	50 ml
5.33002	Formic acid	98-100% for LC-MS Lichropur®	50 ml
5.33003	Ammonia solution	25% for LC-MS Lichropur®	50 ml
5.33004	Ammonium acetate	for LC-MS Lichropur®	50 ml
5.33005	Ammonium hydrogen carbonate	for LC-MS Lichropur®	50 ml

Lichropur® LC-MS Reagents

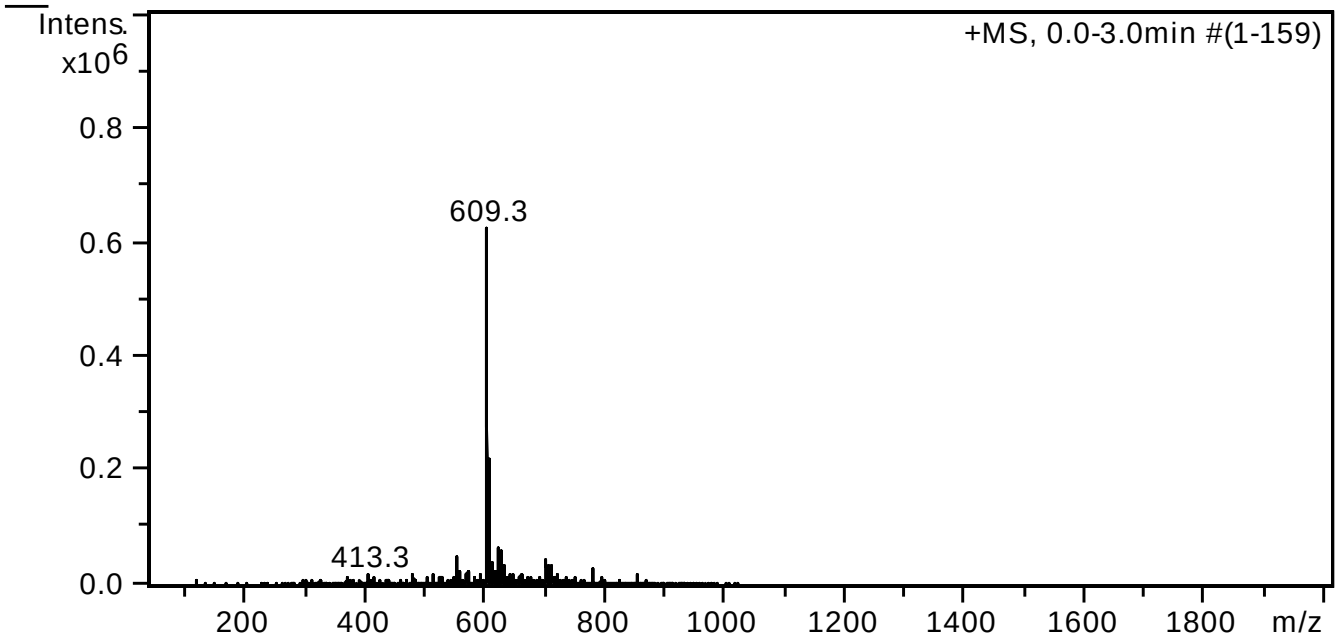
LC-MS Reagents

We offer LiChropur® products specific for LC-MS analysis.

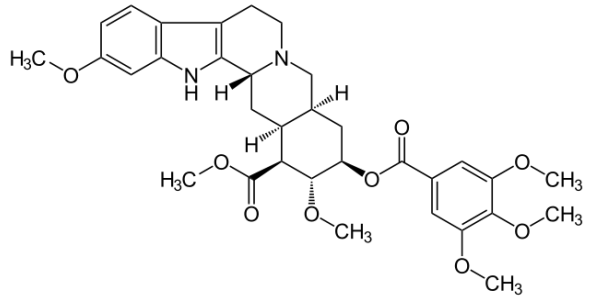
These reagents are tested for inorganic impurities, including Al, Ca, Cu, Fe, K, Mg and Na.

- QC performed using a standard reserpine test
- Filled under clean room conditions
- Extensive impurity profile of the product on the Certificate of Analysis
- Assay (acidimetric): ≥ 98.0%
- Colour: ≤ 10 Hazen
- Residue on ignition: ≤ 2 ppm
- Cation traces:
  - **Al: ≤ 5.0 ppb; Ca: ≤ 10.0 ppb; Cu: ≤ 1.0 ppb; Fe: ≤ 5.0 ppb; K: ≤ 5.0 ppb; Mg: ≤ 2.0 ppb; Na: ≤ 5.0 ppb; NH_4^+: ≤ 10 ppm**
- LC-MS suitability test

Lichropur® LC-MS Reagents
Reserpine test



Mass spectrum ESI positive
(flow injection analysis)



Reserpine

Measuring parameter	Specification value
ESI positive	< 2 ppb
ESI & APCI negative	< 20 ppb

No signal should be
greater than [M+H] = 609

LiChrosolv® hypergrade marks the difference

- High ionization efficiency
- Minimal baseline noise
- Low level of ionic background
- Reduced metal adduct formation

→ Superior resolution & sensitivity

Solvent storage

Solvent storage (water and organic) in

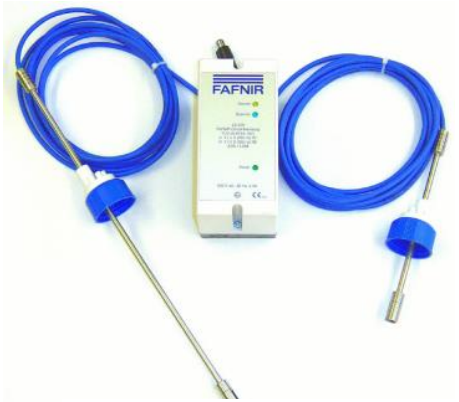
- surface treated amber glass
  (original Merck packaging) or
- borosilicate glass

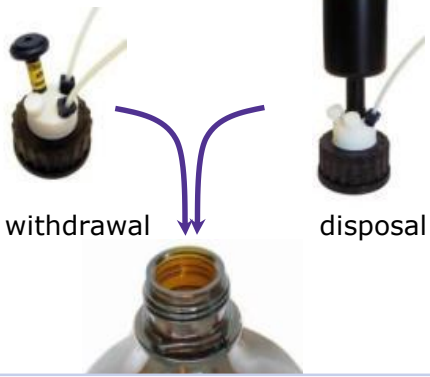
Standard clear glass bottles: Dissolution of silica and alkali, adduct formation $[M+X]^+$ possible

Bottle caps/adapters

- professional Merck equipment only,
  directly mounted to original bottle (see image)
- avoid decanting
- no homemade solvent tubing solutions

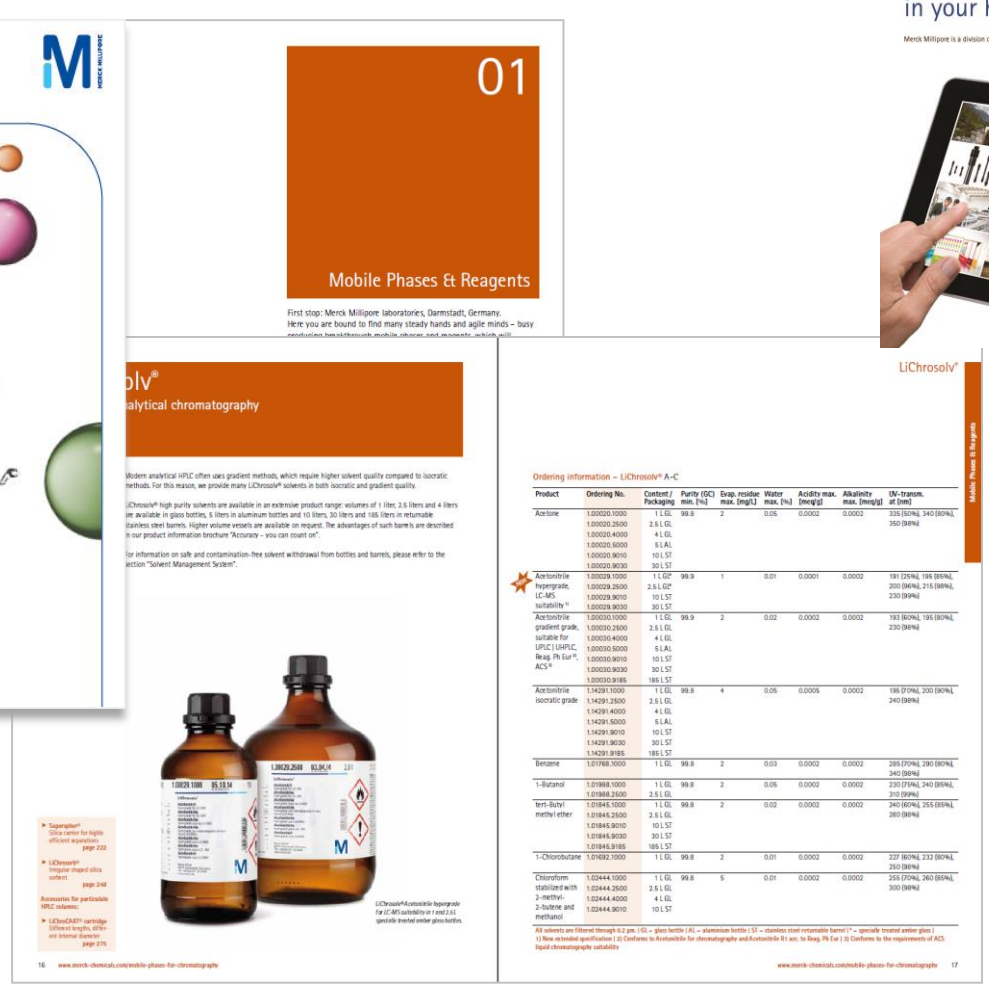
→ **solvent purity maintained, low background noise**

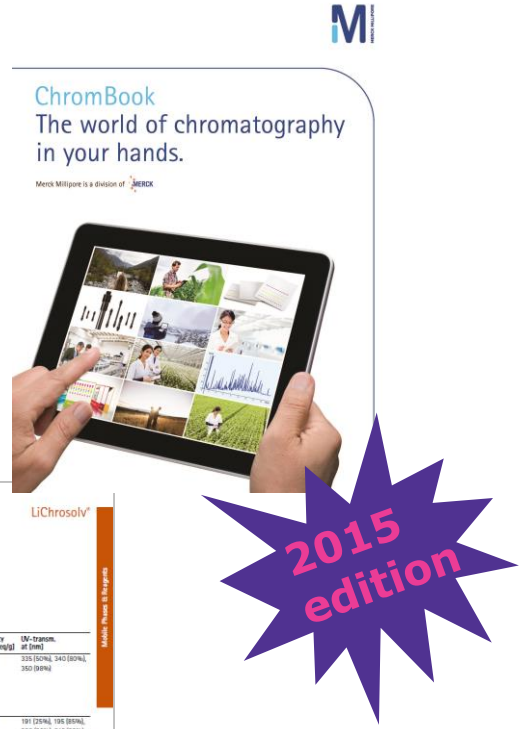




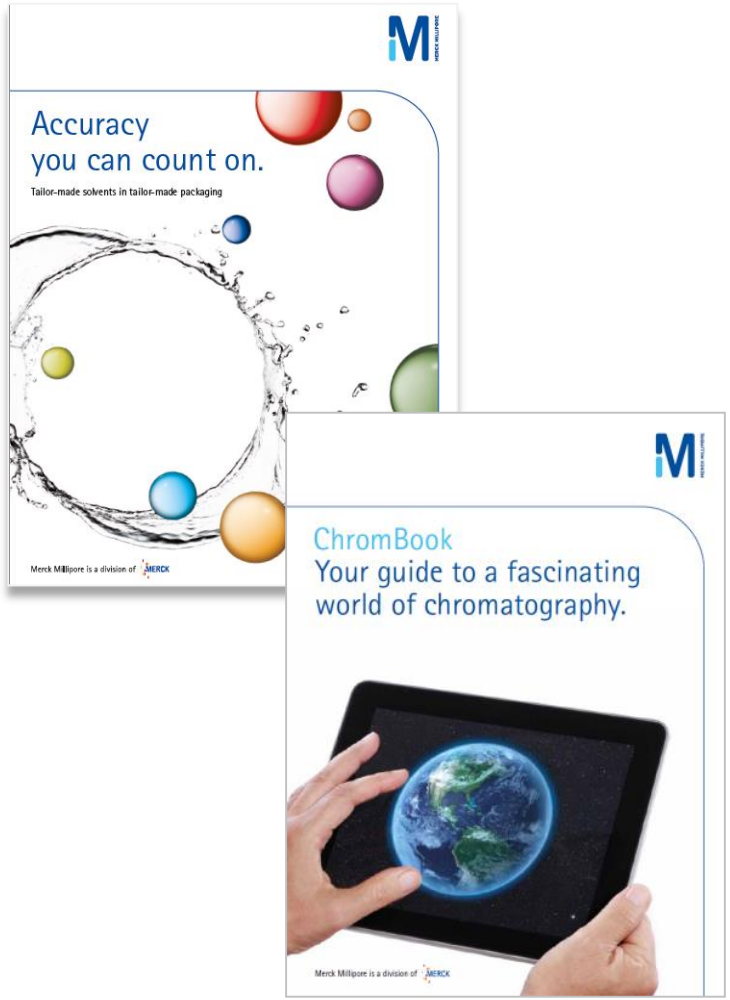
1.03830.0001 / 1.03831.0001
HPLC adapters for S40
(supply / disposal)

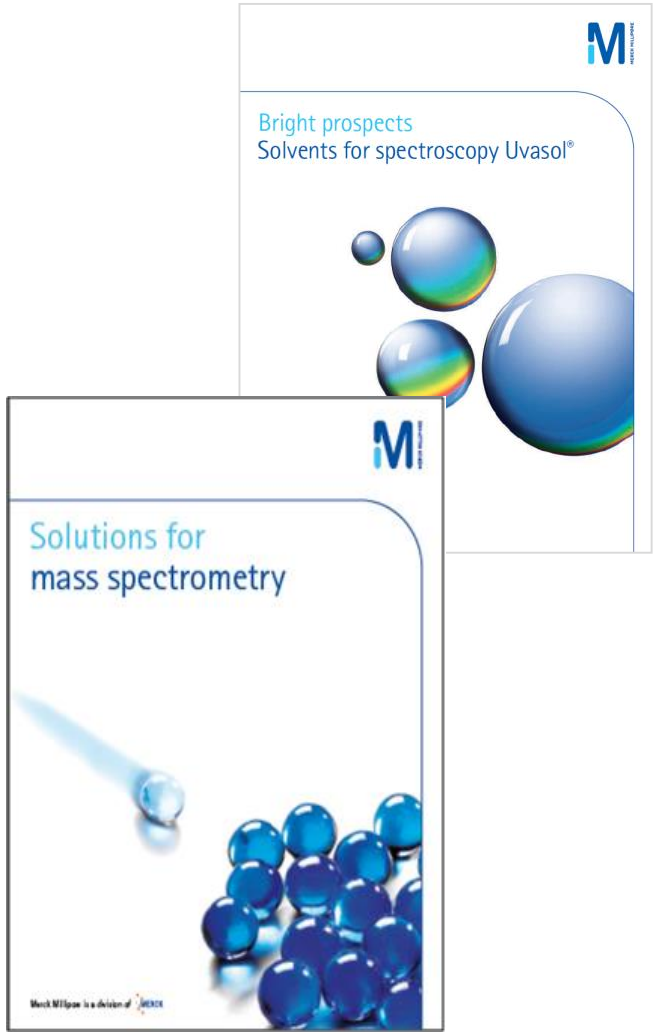
Supporting Literature





Information Variety





LiChrosolv® marks the difference

- Safety through reliable quality avoids misinterpretation of analytical results; saves cost- & time-intensive repetition of analysis
- Reduced baseline drift for better separation performance
- Interference free baseline for better reproducibility
- Enhanced sensitivity due to lower basic absorbance
- Convenience
  - No need for filtration, already done through 0.2 µm stainless steel filters (CoA)
  - No blank run necessary due to high batch-to-batch consistency (less solvent consumption, winning time & money)
  - "Audit resistant"