



# Reagents and procedures for derivatization

## Derivatization reagents

- To improve volatility, increase thermal stability or to achieve a lower limit of detection in gas chromatography  
Prerequisite: quantitative, rapid and reproducible formation of only one derivative  
Halogen atoms inserted by derivatization, e.g., trifluoroacetates, allow the specific detection in an ECD with the advantage of high sensitivity.  
Specific derivatizations may influence elution orders and fragmentation patterns in a MS.
- We provide reagents for **acylation**, **alkylation (methylation)**, and **silylation**.

## Derivatization method development kits

| Designation  | Contents of the kit                         | REF    |
|--|---|--------|
| <b>Derivatization method development kit</b>   |   |        |
| Which type of derivatization is suited best for your sample (alkylation, acylation or silylation)? | 2 x 1 mL each of TMSH, MSTFA, MBTFA         | 701952 |
| <b>Acylation kit</b>   |   |        |
| Which is the proper reagent for acylation?   | 2 x 1 mL each of MBTFA, TFAA, MBHFBA        | 701950 |
| <b>Alkylation kit</b>  |   |        |
| Which is the proper reagent for methylation?   | 3 x 1 mL each of TMSH, DMF-DMA              | 701951 |
| <b>Silylation kit</b>  |   |        |
| Which is the proper reagent for silylation?  | 2 x 1 mL each of MSTFA, BSTFA, TSIM, MSHFBA | 701953 |

Reagents for GC

## Selection guide for derivatization of important functional groups in GC

| Function   | Method                            | Derivative   | Recommended reagents   |
|--|-----------------------------------|--|--|
| <b>Alcohols, Phenols</b><br>R'OH                   | silylation                        | R'O-TMS  | BSA, MSTFA, MSHFBA, TSIM, SILYL-2110, SILYL-21, SILYL-1139       |
|  | acylation                         | R'O-CO-R   | TFAA, HFBA, MBTFA, MBHFBA  |
|  | alkylation                        | R'O-R  | TMSH   |
|  | sterically hindered               | silylation   | R'O-TMS  |
| <b>Amines</b><br>primary, secondary hydrochlorides | silylation                        | R'-NR''-TMS  | BSA, MSTFA, MSHFBA, SILYL-991                                    |
|  | acylation                         | R'-NR''-CO-R   | TFAA, HFBA, MBTFA, MBHFBA  |
|  | silylation                        | R'-NR''-TMS  | MSTFA  |
| <b>Amides</b>                                      | silylation                        | not stable   |  |
|  | acylation                         | R'-CO-NH-CO-R  | TFAA, MBTFA, HFBA, MBHFBA  |
| <b>Amino acids</b>                                 | silylation                        | R'-CH(NH-TMS)-CO-O-TMS                                 | BSA, BSTFA, MSTFA, MSHFBA  |
|  | alkylation (a)<br>+ acylation (b) | R'-CH(NH-CO-R)-CO-O-R                                  | a) MeOH/TMCS, TMSH<br>b) TFAA, HFBA, MBTFA, MBHFBA               |
| <b>Carboxylic acids</b><br>(fatty acids)           | silylation                        | R'-CO-O-TMS<br>susceptible to hydrolysis               | BSA, MSTFA, MSHFBA, TMCS, TSIM, SILYL-2110, SILYL-21, Silyl 1139 |
|  | alkylation                        | R'-CO-O-R  | DMF-DMA, MeOH/TMCS (1 M), TMSH                                   |
|  | salts                             | silylation<br>R'-CO-O-TMS<br>susceptible to hydrolysis | TMCS   |
| <b>Carbohydrates</b>                               | silylation                        |  | MSTFA, TSIM, HMDS, SILYL-1139                                    |
|  | acylation                         |  | TFAA, MBTFA  |
| <b>Steroids</b>                                    | silylation                        |  | BSA, TSIM  |
|  | acylation                         |  | TFAA, MBTFA, HFBA, MBHFBA  |



## Acylation reagents

### Acyl halides

By-product of acylation with acyl halides: corresponding hydrohalic acids  
excess of reagent and acid have to be removed or trapped by a suitable base (e.g., pyridine)

#### Pentafluorobenzoyl chloride

**PFBC:**  $C_6F_5 - CO - Cl$

M 230.52 g/mol, Bp 158–159 °C (760 mm Hg),  
density  $d_{20^{\circ}/4^{\circ}} = 1.601$

### Anhydrides

By-products of acylation with anhydrides: corresponding acids  
excess reagent and the acid formed are to be removed

#### Trifluoroacetic acid anhydride

**TFAA:**  $CF_3 - CO - O - CO - CF_3$

M 210.04 g/mol, Bp 39.5–40.5 °C (760 mm Hg),  
density  $d_{20^{\circ}/4^{\circ}} = 1.490$

#### Heptafluorobutyric acid anhydride

**HFBA:**  $C_3F_7 - CO - O - CO - C_3F_7$

M 410.06 g/mol, Bp 106–107 °C (760 mm Hg),  
density  $d_{20^{\circ}/4^{\circ}} = 1.665$

### Bisacylamides

By-products: corresponding neutral acylamides: high volatility · easily removed; due to the neutral conditions and their favorable chromatographic characteristics, the removal of surplus bisacylamides and their by-products is often not necessary. Therefore, the sample preparation is much easier.

#### N-methyl-bis(trifluoroacetamide)

**MBTFA:**  $CF_3 - CO - N(CH_3) - CO - CF_3$

M 223.08 g/mol, Bp 123–124 °C (760 mm Hg),  
density  $d_{20^{\circ}/4^{\circ}} = 1.55$

#### N-methyl-bis(heptafluorobutyramide)

**MBHFBA:**  $C_3F_7 - CO - N(CH_3) - CO - C_3F_7$

M 423.1 g/mol, Bp 165–166 °C (760 mm Hg),  
density  $d_{20^{\circ}/4^{\circ}} = 1.673$

## Methods for acylation

### Acylation with fluorinated acid anhydrides:

The acylation with TFAA or HFBA, under formation of volatile, stable derivatives for FID or ECD detection, is applicable for alcohols, phenols, carboxylic acids, amines, amino acids and steroids.

#### Procedure:

Dissolve 0.1 to 1 mg sample in 0.1 mL solvent, add 0.1 mL of the anhydride and heat to 60–70 °C for 1–2 h. If the sample need not be concentrated prior to the analysis and if there is no danger of catalytically induced side reactions, pyridine is used as solvent. The reaction solution can be injected directly into the gas chromatograph. Otherwise, use a volatile solvent and evaporate solvent, excess reagent and free acid in a stream of nitrogen. Dissolve residue in 50 µL hexane, chloroform etc. and inject aliquot portions.

TFAA MN Appl. No. 213041 · HFBA MN Appl. No. 213042

### Acylation with fluorinated acid amides:

This method is recommended for alcohols, primary and secondary amines as well as for thiols under mild, neutral conditions. MBTFA also forms very volatile derivatives with carbohydrates [J. Sullivan and L. Schewe, J. Chromatogr. Sci. **15** (1977) 196–197].

#### Procedure:

Add 0.5 mL MBTFA or MBHFBA to about 2 mg sample. If there is no reaction at ambient temperature, heat the reaction mixture to 120 °C. Compounds difficult to dissolve, can be trifluoroacetylated in suitable solvent mixtures. It is recommended to use a ratio of solvent to MBTFA or MBHFBA of 4:1. The reaction mixture is chromatographed directly.

MBTFA MN Appl. No. 213051 · MBHFBA MN Appl. No. 213052

## Ordering information

| Substance | Packing unit |            |            |            |
|-----------|--------------|------------|------------|------------|
|           | 10 x 1 mL    | 20 x 1 mL  | 1 x 10 mL  | 5 x 10 mL  |
| HFBA*     |              | 701110.201 | 701110.110 | 701110.510 |
| MBTFA*    |              | 701410.201 | 701410.110 | 701410.510 |
| MBHFBA*   | 701420.101   | 701420.201 |            |            |
| PFBC*     | 701120.101   |            |            |            |
| TFAA*     |              |            | 701130.110 | 701130.510 |

\* These products contain harmful substances which must be specially labeled as hazardous. For detailed information please see MSDS. Due to their purpose, derivatization reagents are very reactive substances. For this reason, they should be stored cool and protected from moisture. For easy access with a syringe, our derivatization reagents are supplied in vials with crimp caps. Vials with pierced sealing disks have limited stability and should be used soon.





## Silylation reagents

The most common form of silylation in GC is the replacing of active hydrogen atoms with a trimethylsilyl group (TMS derivative). Less frequently, trialkylsilyl groups or dimethylsilyl groups with longer alkyl chains are also in use. The alkylsilyl group increases volatility and enhances thermal stability of the sample.

Silylation can be catalyzed either acidic by addition of TMCS or basic by addition of pyridine or TSIM (e.g., for sterically hindered functionalities like *tert.* alcohols).

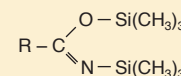
**Reactivity of silylation reagents** (acc. to M. Donike): TMS amides (e.g., BSA, MSTFA) > TMS amine = TSIM > Enol-O-TMS ether > S-TMS ether > O-TMS ether > TMS-O-TMS

**Stability of the TMS derivatives:** O-TMS ether > S-TMS ether > Enol-O-TMS ether > TMS amine > TMS amide

### BSA · BSTFA · SILYL-991

#### ◆ N,O-bis-trimethylsilyl-acetamide

**BSA:** R = CH<sub>3</sub>



M 203.4 g/mol, Bp 71–73 °C (35 mm Hg), density d<sub>20°/4°</sub> = 0.832

Strong silylation reagent, creating very stable TMS derivatives of a multitude of compounds, e.g., alcohols, amines, carboxylic acids, phenols, steroids, biogenic amines and alkaloids; not recommended for use with carbohydrates or very low molecular weight compounds; good solvent for polar compounds, but frequently used in combination with a solvent (pyridine, DMF etc.) or with other silylation reagents. Dissolved in DMF, BSA is the prime derivatization reagent for phenols.

#### ◆ N,O-bis-trimethylsilyl-trifluoroacetamide

**BSTFA:** R = CF<sub>3</sub>

M 257.4 g/mol, Bp 40 °C (12 mm Hg), density d<sub>20°/4°</sub> = 0.961

Powerful trimethylsilyl donor with approx. the same donor strength as the nonfluorinated analog BSA  
Advantage of BSTFA over BSA: greater volatility of its reaction products, particularly useful for GC analysis of low boiling TMS amino acids

BSTFA is nonpolar (less polar than MSTFA) and can be mixed with acetonitrile for improved solubility. For the silylation of fatty acid amides, hindered hydroxyl groups and other difficult to silylate compounds, e.g., secondary alcohols and amines, we recommend BSTFA + 1% trimethylchlorosilane (TMCS), available under the designation SILYL-991.

### Silylation with BSA, BSTFA or SILYL-991 (BSTFA + 1% TMCS)

#### Procedure:

Add 0.5 mL of the silylation reagent to 1–10 mg sample; if necessary, add some solvent (normally pyridine or DMF [dimethylformamide]). Heat to 60–80 °C for 20 min to increase the reaction rate. 1–2 drops of TMCS (trimethylchlorosilane) or TSIM will also speed up the reaction.

BSA MN Appl. No. 213091 · BSTFA MN Appl. No. 213092  
SILYL-991 MN Appl. No. 213093

### Silylation with BSA in combination with other silylation reagents

#### Procedure:

BSA alone silylates all sterically unhindered hydroxyl groups of the steroid skeleton; addition of TMCS will enable reaction of moderately hindered OH groups (reaction time 3–6 h at 60 °C). After addition of TSIM even strongly hindered hydroxyl groups will react (reaction time 6–24 h at 60 °C).

MN Appl. No. 213100

## Ordering information

| Substance                                  | Packing unit      |                   |                   |                   |                    |
|--|-------------------|-------------------|-------------------|-------------------|--------------------|
|  | 20 x 1 mL         | 1 x 10 mL         | 5 x 10 mL         | 1 x 50 mL         | 1 x 100 mL         |
| <b>BSA*</b>                                |                   | <b>701210.110</b> | <b>701210.510</b> | <b>701210.150</b> |                    |
| <b>BSTFA*</b>                              | <b>701220.201</b> | <b>701220.110</b> | <b>701220.510</b> |                   |                    |
| <b>SILYL-991*</b><br>(BSTFA – TMCS (99:1)) | <b>701490.201</b> |                   |                   | <b>701490.150</b> | <b>701490.1100</b> |

\* These products contain harmful substances which must be specially labeled as hazardous. For detailed information please see MSDS.



# Reagents and procedures for silylation

## MSTFA · MSHFBA · MBDSTFA

### ● N-methyl-N-trimethylsilyl-trifluoroacetamide

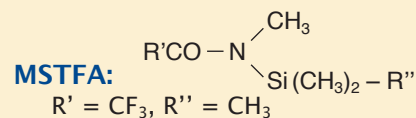
M 199.1 g/mol, Bp 70 °C (75 mm Hg), density  $d_{20}^{20}/4^{\circ} = 1.11$

The most volatile trimethylsilyl amide available

Very strong TMS donor which does not cause noticeable FID fouling even during long-time measuring series. The addition of protic solvents in submolar quantities, e.g., TFA for extremely polar compounds (hydrochlorides) or pyridine for carbohydrates), can improve the already good dissolving power of MSTFA.

Recommended applications: carboxylic acids, hydroxy and ketocarboxylic acids, amino acids, amines, alcohols, polyalcohols, sugars, mercaptans and similar compounds with active hydrogen atoms. Even amine hydrochlorides can be silylated directly.

Advantages: complete conversion with high reaction rates, even without a catalyst (1–2% TMCS or TSIM); the by-product of the reaction (N-methyltrifluoroacetamide) shows a high volatility and a short retention time



### ● N-methyl-N-trimethylsilyl-heptafluorobutyramide

**MSHFBA:** R' = C<sub>3</sub>F<sub>7</sub>, R'' = CH<sub>3</sub>

M 299.1 g/mol, Bp 148 °C (760 mm Hg)

Similar to MSTFA in reactivity and chromatography

Recommended applications: carboxylic acids, alcohols, phenols, primary and secondary amines and amino acids; either applied alone or in combination with a catalyst (TMCS, TSIM) or another silylation reagent with or without solvent; the by-product N-methylheptafluorobutyric amide has a lower retention time than the silylating reagent; especially useful for flame ionization detection due to the large ratio of fluorine to silicon of 7:1, since degradation of the surplus MSHFBA does not produce SiO<sub>2</sub> but volatile, non-corrosive silicon compounds

### ● N-methyl-N-tert-butyltrimethylsilyl-trifluoroacetamide

**MBDSTFA** (MTB-TFA):

M 241.3 g/mol, Bp 168–170 °C (760 mm Hg), density  $d_{20}^{20}/4^{\circ} = 1.121$  R' = CF<sub>3</sub>, R'' = C<sub>4</sub>H<sub>9</sub>

Silylation reagent that donates a *tert*-butyltrimethylsilyl group (TBDMS) for derivatizing active hydrogen atoms in hydroxyl, carboxyl and thiol groups as well as primary and secondary amines; fast reactions (typically 5–20 min) with high yields (> 96%); by-products are neutral volatiles

TBDMS ethers are 10<sup>4</sup> times more stable than the corresponding TMS ethers

Due to the large protecting group, chromatographic retention times are longer. This may have a beneficial impact on some separations. The high concentration of M<sup>+</sup>-57 ions is an interesting topic for GC/MS.

## Silylation with MSTFA, MSHFBA or MBDSTFA

### Procedure:

Dissolve 10–15 mg sample in 0.8 mL solvent, then add 0.2 mL of the silylation reagent. The reaction mixture can be heated to 60–70 °C for up to 1 h and can be analyzed directly. If TFA is used as a solvent, proceed as follows [M. Donike, J. Chromatogr. **85** (1973) 1–7]: dissolve 1–2 mg sample in 100 µL TFA. Dropwise add 0.9 mL of the silylating reagent. After cooling the sample can be chromatographed directly.

MSTFA MN Appl. No. 213111 · MSHFBA MN Appl. No. 213112 · MBDSTFA MN Appl. No. 213113

## Ordering information

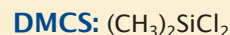
|                 |            | Packing unit |            |             |            |             |              |
|-----------------|------------|--------------|------------|-------------|------------|-------------|--------------|
| 10 x 1 mL       | 20 x 1 mL  | 1 x 10 mL    | 5 x 10 mL  | 1 x 100 mL  | 6 x 50 mL  | 6 x 100 mL  | 12 x 100 mL  |
| <b>MSHFBA*</b>  |            |              |            |             |            |             |              |
|                 | 701260.201 | 701260.110   | 701260.510 | 701260.1100 |            | 701260.6100 |              |
| <b>MSTFA*</b>   |            |              |            |             |            |             |              |
|                 | 701270.201 | 701270.110   | 701270.510 | 701270.1100 | 701270.650 | 701270.6100 | 701270.12100 |
| <b>MBDSTFA*</b> |            |              |            |             |            |             |              |
|                 | 701440.101 | 701440.201   |            |             |            |             |              |

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## DMCS · HMDS · TMCS · TSIM

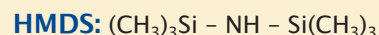
### Dimethyldichlorosilane



M 129.06 g/mol, Bp 70 °C (760 mm Hg), density  $d_{20}^{20}/4^\circ = 1.07$

Used to form dimethylsilyl (DMS) derivatives; DMS derivatives are much more susceptible to hydrolysis than TMS derivatives, it is therefore vital to have strictly anhydrous conditions during the conversion.

### Hexamethyldisilazane



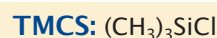
M 161.4 g/mol, Bp 126 °C (760 mm Hg), density  $d_{20}^{20}/4^\circ = 0.7742$

Weak TMS donor; used as a sole reagent, it is slow and not very effective.

With catalytic quantities, e.g., 1% of, or as a mixture with TMCS (2:1, v/v; SILYL-21 and SILYL-2110) it is perfectly suited for a quick and quantitative trimethylsilylation of organic compounds.

Aprotic solvents like acetonitrile, pyridine, dimethylformamide, carbon disulfide and dimethylacetamide recommend themselves for use with HMDS.

### Trimethylchlorosilane

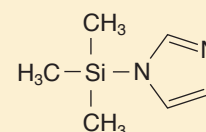


M 108.7 g/mol, Bp 57 °C (760 mm Hg), density  $d_{20}^{20}/4^\circ = 0.8580$

Often used as a catalyst with other trimethylsilyl reagents

As a sole reagent, it can be used to prepare TMS derivatives of organic acids.

### N-Trimethylsilyl-imidazole



M 140.3 g/mol, Bp 94–96 °C (760 mm Hg), density  $d_{20}^{20}/4^\circ = 0.961$

Strongest hydroxyl silylator; reagent of choice for carbohydrates and most steroids (even strongly hindered steroids)

It is remarkable that TSIM reacts quickly and smooth with hydroxyl (even *tert.* OH) and carboxyl groups, but not with amines. Hence it is especially suited for multiple derivatizations, when compounds with various functional groups are to be derivatized in different ways (e.g., -O-TMS, -N-HFB derivatives of catecholamines).

Recommended applications:

alcohols, phenols, organic acids, steroids, hormones, glycols, nucleotides, narcotics

## Silylation with TSIM or SILYL-1139 (TSIM - pyridine 11:39)

### Procedure:

Dissolve 10–15 mg sample in 0.8 mL solvent, then add 0.2 mL of the silylation reagent. The reaction mixture can be heated to 60–70 °C for up to 1 hour and can be analyzed directly.

Recommended solvent pyridine

**When using SILYL-1139, the presence of water does not interfere.**

TSIM MN Appl. No. 213121 · SILYL-1139 MN Appl. No. 213122

## Ordering information

| Substance | Packing unit  |            |            |               |
|-----------|---------------|------------|------------|---------------|
|           | 20 x 1 mL     | 1 x 10 mL  | 5 x 10 mL  | 6 x 50 mL     |
| DMCS*     |               |            |            | 701230.650 ** |
| HMDS*     |               |            | 701240.510 | 701240.650 ** |
| TMCS*     | 701280.201 ** |            |            | 701280.650 ** |
| TSIM      | 701310.201    | 701310.110 | 701310.510 |               |

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# Reagents and procedures for silylation

## Reagent mixtures for silylation

| Mixture    | Composition                     | 20 x 1 mL  | 1 x 10 mL  | 5 x 10 mL  | 1 x 50 mL  | 1 x 100 mL  |
|------------|---------------------------------|------------|------------|------------|------------|-------------|
| SILYL-271  | BSA – HMDS – TSIM (2:7:1)       | 701450.201 | 701450.110 | 701450.510 |            |             |
| SILYL-1139 | TSIM – pyridine (11:39)         | 701460.201 |            |            |            |             |
| SILYL-21   | HMDS – TMCS (2:1)               | 701470.201 |            |            |            |             |
| SILYL-2110 | HMDS – TMCS – pyridine (2:1:10) | 701480.201 |            |            |            |             |
| SILYL-991  | BSTFA – TMCS (99:1)             | 701490.201 |            |            | 701490.150 | 701490.1100 |

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## Silylation with SILYL-21 or SILYL-2110

### Procedure:

Carefully add SILYL-21 or SILYL-2110 to 1-10 mg of the sample. Precipitated ammonium chloride does not interfere. If the sample should not dissolve within 5 min, heat to 75-85 °C. If no mutarotation is to be expected, you may dissolve the sugar in warm pyridine first and then add the silylation reagent. In some cases it may be advantageous to use a different solvent instead of pyridine. For derivatization of 3-ketosteroids we recommend to use DMF (dimethylformamide).

SILYL-21 MN Appl. No. 213131 · SILYL-2110 MN Appl. No. 213132

- Recommended applications: sugars, glycols, sterically unhindered alcohols, carboxylic acids, acids in urine, hydroxy fatty acids, nucleotides, steroids, vitamin D, xanthone derivatives

## O-Trimethylsilylation with MSTFA followed by N-trifluoroacetylation with MBTFA

### Procedure:

Completely silylate 2 mg of the sample with 0.3 mL MSTFA, e.g., as described on page 286. After addition of 0.3 mL MBTFA the N-trimethylsilyl group is replaced by the N-trifluoroacetyl group. The mixture can be analyzed directly.

MN Appl. No. 213140





## Test mixtures for GC

- Test mixtures for GC capillary columns to control the performance of fused silica capillary columns and the GC system
- Test mixtures for chiral GC columns



## Ordering information

| Designation  | Composition  | Pack of | REF    |
|--|--|---------|--------|
| Polarity mixture POL <sub>5</sub> (qualitative) in <i>n</i> -pentane                       | 1-butanol, benzene, methyl butyrate, toluene, cyclopentanone, 1-octene, dibutyl ether  | 1 mL    | 722306 |
| Activity test mixture (FA-TMS test according to Donike) in MSTFA/ <i>n</i> -hexane (1 + 4) | 1 mg/mL each of TMS capric acid (C <sub>10</sub> ), TMS myristic acid (C <sub>14</sub> ), TMS stearic acid (C <sub>18</sub> ), TMS behenic acid (C <sub>22</sub> ), hexadecane (C <sub>16</sub> ), eicosane (C <sub>20</sub> ), tetra-cosane (C <sub>24</sub> ), octacosane (C <sub>28</sub> ) | 1 mL    | 722307 |
| Grob test mixture (modified) in <i>n</i> -hexane   | (in mg/mL) <i>n</i> -decane (~2.8), <i>n</i> -undecane (~2.9), <i>n</i> -octanol (~3.6), 2,6-dimethylphenol (~3.2), 2,6-dimethylaniline (~3.2), methyl decanoate (~4.2), dicyclohexylamine (~3.1), methyl undecanoate (~4.2), methyl dodecanoate (~4.1)  | 1 mL    | 722310 |
| MN OPTIMA <sup>®</sup> test mixture in pentane   | 0.1% each of undecane, dodecane, octanol, dimethylaniline, decylamine, methyl decanoate, methyl undecanoate, heneicosane, docosane, tricosane (chromatograms see page 240)   | 1 mL    | 722316 |
| MN OPTIMA <sup>®</sup> amine test mixture in ethanol                                       | 0.2% diisobutylamine, 1% diethanolamine, 0.2% 2,6-dimethylaniline, 0.2% <i>o</i> -propanol-pyridine, 0.2% dicyclohexylamine, 0.2% dibenzylamine  | 1 mL    | 722317 |
| FAME test mixture in hexane  | 0.1% each of FAMES C4, C6, C8, C10, C12, C14, C16, C18, C18:1 <i>cis</i> , C18:1 <i>trans</i> , C18:2, C18:3, C20, C22, C22:1, C24 (chromatogram see page 262)   | 1 mL    | 722320 |

## Test mixtures for chiral GC capillary columns

| Test mixture for   | Test compound (enantiomer mixture)                  | Pack of | REF    |
|--|---|---------|--------|
| LIPODEX <sup>®</sup> A, HYDRODEX β-PM, β-3P, β-6TBDM, β-TBDAC, γ-TBDAC | 1% phenylethanol in CH <sub>2</sub> Cl <sub>2</sub> | 1 mL    | 722321 |
| LIPODEX <sup>®</sup> B   | methylbutyrolactone                                 | 1 mL    | 722322 |
| LIPODEX <sup>®</sup> C, D  | phenylethylamine (TFA)                              | 1 mL    | 722323 |
| LIPODEX <sup>®</sup> E, G, HYDRODEX γ-DiMOM                            | phenylethanol (TFA)                                 | 1 mL    | 722319 |

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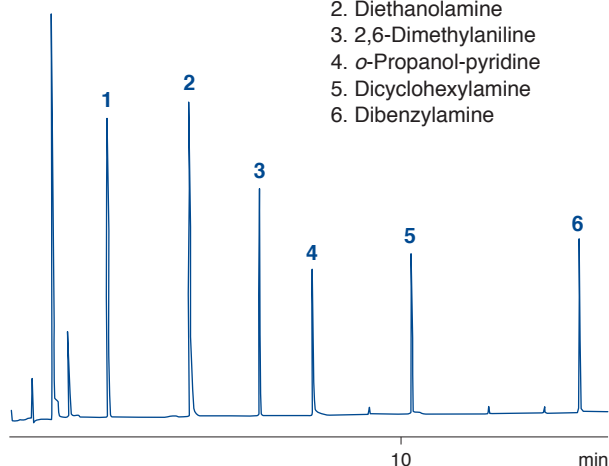


# Test mixtures for GC capillary columns

## OPTIMA® Amine test mixture (REF 722317)

Column: OPTIMA® 5 Amine, 1.0 µm film, 30 m x 0.32 mm ID  
 Injection: 1 µL, split 1:50  
 Carrier gas: 0.6 bar H<sub>2</sub>  
 Temperature: 100 °C → 290 °C, 10 °C/min  
 Detector: FID 280 °C

- Peaks:**
1. Diisobutylamine
  2. Diethanolamine
  3. 2,6-Dimethylaniline
  4. *o*-Propanol-pyridine
  5. Dicyclohexylamine
  6. Dibenzylamine

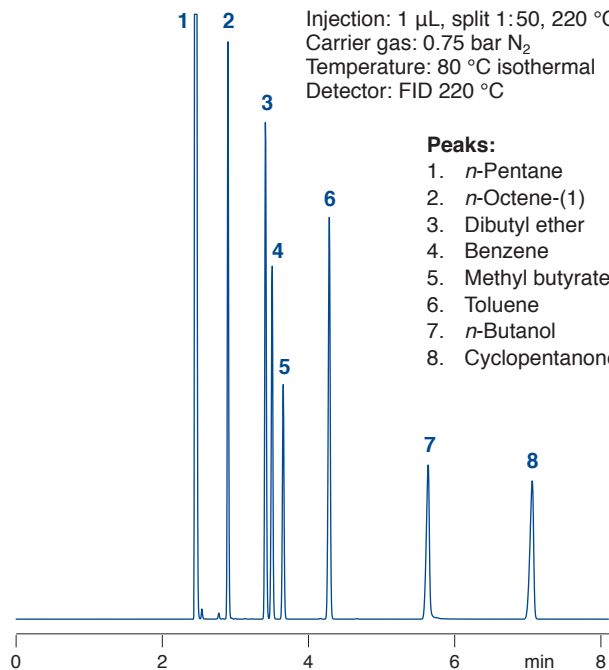


MN Appl. No. 250020

## Polarity mixture POL<sub>5</sub> (qualitative) (REF 722306)

Column: OPTIMA® Wax, 0.25 µm film, 25 m x 0.25 mm ID  
 Injection: 1 µL, split 1:50, 220 °C  
 Carrier gas: 0.75 bar N<sub>2</sub>  
 Temperature: 80 °C isothermal  
 Detector: FID 220 °C

- Peaks:**
1. *n*-Pentane
  2. *n*-Octene-(1)
  3. Dibutyl ether
  4. Benzene
  5. Methyl butyrate
  6. Toluene
  7. *n*-Butanol
  8. Cyclopentanone

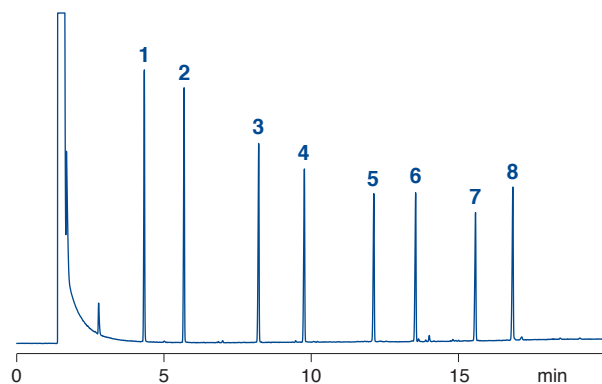


MN Appl. No. 211230

## Activity test mixture (REF 722307)

Column: OPTIMA® 5, 1.0 µm film, 25 m x 0.32 mm ID  
 Injection: 1 µL, split 1:40, 300 °C  
 Carrier gas: 0.6 bar H<sub>2</sub>  
 Temperature: 150 °C → 300 °C (8 min), 10 °C/min  
 Detector: FID 300 °C

- Peaks:**
1. TMS capric acid (C<sub>10</sub>)
  2. Hexadecane (C<sub>16</sub>)
  3. TMS myristic acid (C<sub>14</sub>)
  4. Eicosane (C<sub>20</sub>)
  5. TMS stearic acid (C<sub>18</sub>)
  6. Tetracosane (C<sub>24</sub>)
  7. TMS behenic acid (C<sub>22</sub>)
  8. Octacosane (C<sub>28</sub>)

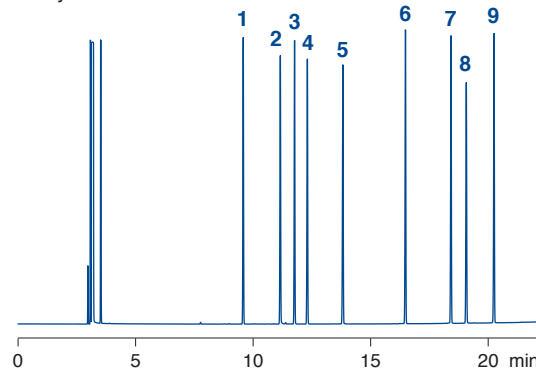


MN Appl. No. 211240

## Grob test mixture (modified) (REF 722310)

Column: OPTIMA® 5, 1.0 µm film, 50 m x 0.25 mm ID  
 Injection: 1 µL, split 1:40, 280 °C  
 Carrier gas: 1.5 bar H<sub>2</sub>  
 Temperature: 80 °C → 280 °C (10 min), 8 °C/min  
 Detector: FID 280 °C

- Peaks:**
1. *n*-Decane
  - 1-Octanol
  - n*-Undecane
  - 2,6-Dimethylphenol
  - 2,6-Dimethylaniline
  - Methyl decanoate
  - Methyl undecanoate
  - Dicyclohexylamine
  - Methyl dodecanoate



MN Appl. No. 211250



## Ordering information

| Designation  | Composition  | Pack of   | REF    |
|--|--|-----------|--------|
| Haloform test mixture in <i>n</i> -pentane (qualitative)                 | 9 halogenated hydrocarbons acc. to German drinking water specifications (in ng/mL): dichloromethane (795), chloroform (75), 1,1,1-trichloroethane (67), carbon tetrachloride (80), trichloroethylene (73), bromodichloromethane (100), dibromochloromethane (122), tetrachloroethylene (81), bromoform (145)   | 1 mL      | 722311 |
| Haloform test mixture in methanol for head-space analyses (qualitative)  | 9 halogenated hydrocarbons in increased concentration for calibration acc. to German Industrial Standard DIN 38407, part 5 (in µg/mL): dichloromethane (158.4), chloroform (14.9), 1,1,1-trichloroethane (13.4), carbon tetrachloride (15.9), trichloroethylene (14.6), bromodichloromethane (20), dibromochloromethane (24.5), tetrachloroethylene (16.2), bromoform (28.9) | 1 mL      | 722371 |
| Haloform test kit (qualitative)  | 1 mL each of 9 single undiluted halogenated hydrocarbons and 1 mL each of test mixtures REF 722311 and REF 722371  | 11 x 1 mL | 722312 |
| PAH test mixture acc. to EPA in toluene                                  | 20 µg/mL each of naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, anthracene, fluoranthene, pyrene, benz[a]anthracene, chrysene, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[a]pyrene, indeno[1,2,3-cd]pyrene, dibenz[a,h]anthracene, benzo[ghi]perylene   | 1 mL      | 722314 |
| PAH test mixture acc. to German drinking water specifications in toluene | 20 µg/mL each of fluoranthene, benzo[b]fluoranthene, benzo[k]fluoranthene, benzo[a]pyrene, indeno[1,2,3-cd]pyrene, benzo[ghi]perylene  | 1 mL      | 722331 |
| BTX test mixture in methanol   | 10 ng/µL each of benzene, ethylbenzene, toluene, <i>m</i> -, <i>o</i> -, <i>p</i> -xylene  | 1 mL      | 722372 |

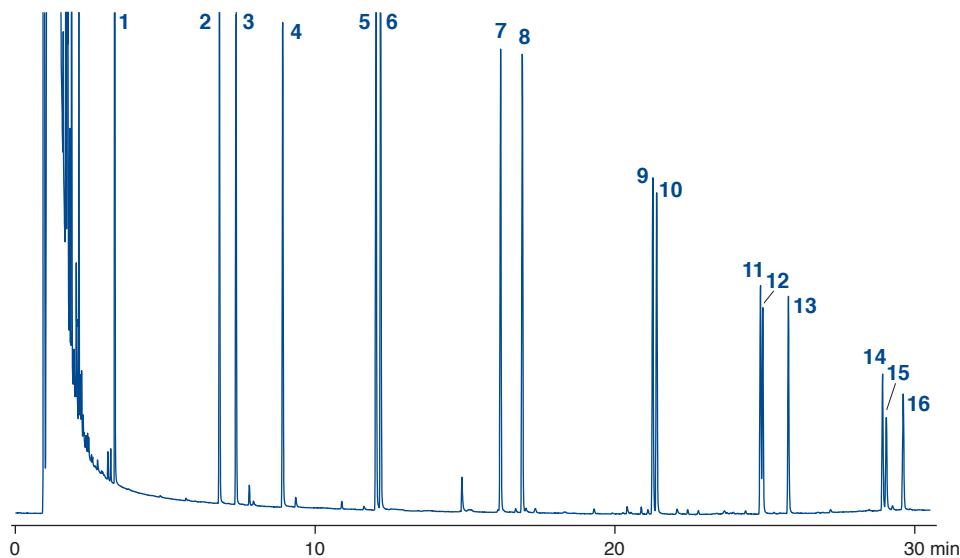
These products contain harmful substances which must be specially labeled as hazardous. For detailed information please see MSDS.

### PAH test mixture acc. to EPA for GC (REF 722314)

Column: OPTIMA® 5, 0.25 µm film, 30 m x 0.32 mm ID  
 Sample: PAH test mixture according to EPA (20 µg/mL each in toluene)  
 Injection: 1.0 µL, split 1:15  
 Carrier gas: H<sub>2</sub>, 70 kPa  
 Temperature: 100 °C, 7 °C/min → 300 °C  
 Detector: FID 300 °C

#### Peaks:

1. Naphthalene
2. Acenaphthylene
3. Acenaphthene
4. Fluorene
5. Phenanthrene
6. Anthracene
7. Fluoranthene
8. Pyrene
9. Benz[a]anthracene
10. Chrysene
11. Benzo[b]fluoranthene
12. Benzo[k]fluoranthene
13. Benzo[a]pyrene
14. Indeno[1,2,3-cd]pyrene
15. Dibenz[ah]anthracene
16. Benzo[ghi]perylene



MN Appl. No. 200510



# Test mixtures for environmental analyses

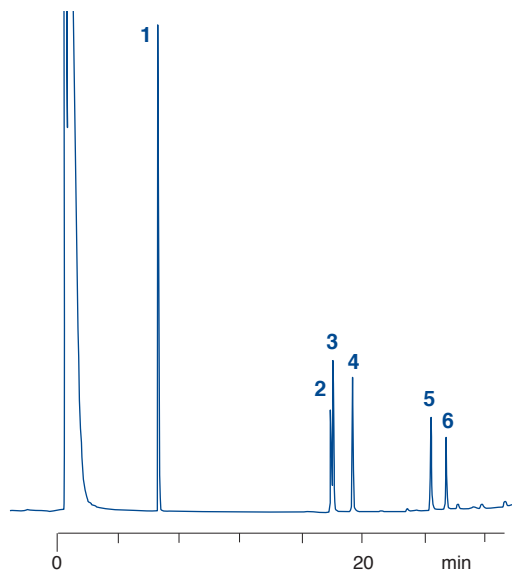
Reagents for GC

## PAH test mixture acc. to German drinking water specifications (REF 722331)

Column: OPTIMA® 5, 0.25 µm film, 25 m x 0.32 mm ID  
Injection: 2 µL, split 1:10  
Carrier gas: 0.6 bar H<sub>2</sub>  
Temperature: 80 °C ↑ 180 °C → 300 °C, 4 °C/min  
Detector: FID 300 °C

### Peaks:

1. Fluoranthene
2. Benzo[b]fluoranthene
3. Benzo[k]fluoranthene
4. Benzo[a]pyrene
5. Indeno[1,2,3-cd]pyrene
6. Benzo[ghi]perylene



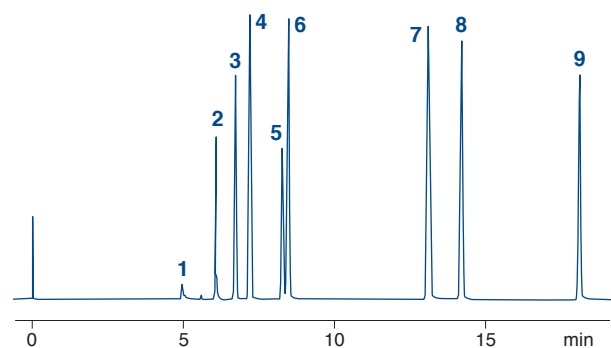
MN Appl. No. 200450

## Haloform test mixture (REF 722311)

Column: FS-SE-54, 0.35 µm film, 50 m x 0.25 mm ID  
Injection: 1 µL, split ~ 1:30  
Carrier gas: 1 bar N<sub>2</sub>  
Temperature: 45 °C (10 min) → 120 °C, 8 °C/min  
Detector: ECD 260 °C

### Peaks:

1. Dichloromethane
2. Trichloromethane
3. 1,1,1-Trichloroethane
4. Tetrachloromethane
5. Trichloroethene
6. Bromodichloromethane
7. Dibromochloromethane
8. Tetrachloroethene
9. Tribromomethane



MN Appl. No. 211190

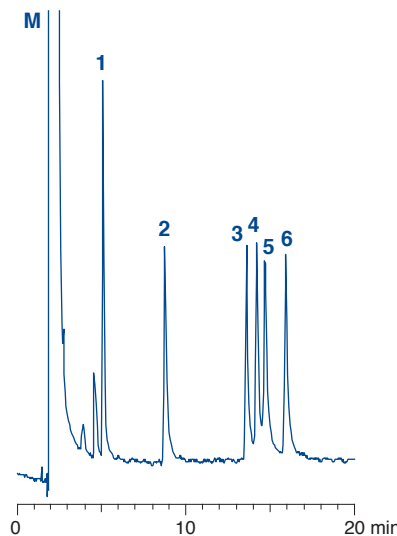
## BTX test mixture (REF 722372)

Column: HYDRODEX β-PM, 50 m x 0.25 mm ID  
Injection: 2 µL (10 ng/µL each in methanol), split 40 mL/min  
Carrier gas: 120 kPa H<sub>2</sub> (2.45 mL/min)  
Temperature: 60 °C → 100 °C, 2 °C/min  
Detector: FID 250 °C

### Peaks:

M = methanol

1. Benzene
2. Toluene
3. *p*-Xylene
4. *m*-Xylene
5. Ethylbenzene
6. *o*-Xylene



MN Appl. No. 211220