

# Recommended Reagents for GC Derivatization

Chemically Modify Your Sample to Improve the Chromatography

Recommended Reagents for GC Derivatization			
Compound	Type of Derivative	ECD*	Possible Reagent Choices
Alcohols	Acetate		Acetic Anhydride/Pyridine
	TMS		Sil-Prep™, BSTFA/TMCS
	<i>t</i> -Butyl Dimethyl Silyl Ether		<i>t</i> -Butyl-DMCS/Imidazole, MTBSTFA
Aldehydes	Dimethyl Acetal		DMF/DMA
Amines	TMS		Sil-Prep™
	Acetate		Pyridine-Plus
Amine (Primary and Secondary)	Acetate		Acetic Anhydride/Pyridine
	TMS		MSHFBA
Amino Acids	TMS		BSTFA
	HFB-Isobutyl Ester		HFB-IBA Kit
	Trifluoroacetate	X	Trifluoroacetic Anhydride
Bile Acids	Acetate		Pyridine-Plus
Carbohydrates	Acetate		Acetic Anhydride/Pyridine
	TMS		Power Sil-Prep™
Catecholamines	Trifluoroacetate	X	<i>N</i> -(Trifluoroacetyl)imidazole
<b>Drugs:</b>			
Alkaloids	Heptafluorobutyrate	X	Heptafluorobutyric Anhydride
	TMS		MSTFA, Sil-Prep™
Antibiotics	TMS		Sil-Prep™, Power Sil-Prep™
Anticonvulsants	TMS		MSTFA, BSA/TMCS
Barbiturates	<i>N</i> -Methyl		Barb-Prep™
	Dimethyl Ketal		DMF/DMA
Cannabinoids	Trifluoroacetate	X	<i>N</i> -(Trifluoroacetyl)imidazole
	TMS		BSTFA, MSTFA
Estrogens	Acetate		Pyridine-Plus
<b>Fatty Acids:</b>			
C9 and Longer	Methyl Ester		Methanolic HCl, Meth-Prep™ I
Short Chain (Up to C8)	TMS		MSTFA
	Methyl Ester		Methanolic HCl, Meth-Prep™ I
Glycerides (mono and di)	Acetate		Acetic Anhydride/Pyridine
Glycerides (mono, di, and tri)	Methyl Ester		Sodium Methoxide/Methanol, Meth-Prep™ II
Glycolipids, Sphingolipids	Methyl Ester		Sodium Methoxide/Methanol, Meth-Prep™ II
Hydroxyamines	TMS		BSTFA
Hydroxy Groups (Primary/Secondary)	Heptafluorobutyrate	X	Heptafluorobutylimidazole
	Trifluoroacetate	X	<i>N</i> -(Trifluoroacetyl)imidazole
17-Ketosteroids	TMS		DMF-Sil-Prep™
Phenols	Heptafluorobutyrate	X	Heptafluorobutyric Anhydride
	TMS		BSTFA
	Methyl Esters		DMF/DMA
Polyols	TMS		Sil-Prep™, Power Sil-Prep™
Steroids	TMS		Sil-Prep™
	Acetate		Pyridine-Plus
	Trifluoroacetate	X	Trifluoroacetic Anhydride

\*Derivatives suitable for use with Electron Capture Detector (ECD).

## tech tip

### When do you use derivatization?

When you need to:

1. Increase or decrease the volatility of the analytes to improve separation
2. Improve peak symmetry by reducing interaction of sample and column
3. Increase detector response (i.e., ECD)
4. Enhance thermal stability

## technical assistance

Contact Tech Support: Phone: 1.800.255.8324 (North America)

Email: [contact.alltech@grace.com](mailto:contact.alltech@grace.com)

Online: [www.discoverysciences.com](http://www.discoverysciences.com)

## Ready-To-Use Silylation Mixes

Silylation replaces an active hydrogen atom (-OH, -NH<sub>2</sub>, -NHR, -SH) with a silyl group. Generally, it reduces the polarity of the compound and decreases possibility of hydrogen bonding.



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### Sil-Prep™ (HMDS:TMCS:pyridine) Reagents

- General purpose reagent for making TMS derivatives

#### Sil-Prep™

Description	Qty.	Part No.
Sil-Prep™	10 x 1mL	<b>18013</b>

#### tech tip

Silylation Reagent Strength



HMDS  
TMCS  
Sil-Prep™  
MSTFA  
MSHFBA  
BSA  
BSTFA  
TMSIM  
BSTFA +1% TMCS  
POWER Sil-Prep™

### t-Butyldimethylchlorosilyl/Imidazole Reagents

- Derivatives of alcohols are more stable than TMS ethers to hydrolysis

#### t-Butyldimethylchlorosilyl/Imidazole

Description	Qty.	Part No.
t-BuDMCS/Imidazole	10 x 1mL	<b>18028</b>

### POWER Sil-Prep™ (TMSIM:BSA:TMCS) Reagents

- Powerful reagent for sterically hindered groups

#### POWER Sil-Prep™

Description	Qty.	Part No.
POWER Sil-Prep™	10 x 1mL	<b>18012</b>

### DMF Sil-Prep™ (HMDS:TMCS:DMF) Reagents

- Prevents enolization of keto groups

#### DMF Sil-Prep™

Description	Qty.	Part No.
DMF Sil-Prep™	10 x 1mL	<b>18015</b>

#### tech tip

What are the requirements for a good reagent?

It will:

1. Not cause any rearrangements or structural changes in the analyte
2. Produce a reaction that is 95–100% complete
3. Produce a stable derivative
4. Not contribute to loss of sample during the reaction
5. Produce a derivative that is inert to the column and connections
6. Not produce interfering byproducts

#### related product

Looking for a Safe and Easy Way to Open Ampoules?

Try the Ampule Cracker.  
See page 380.



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## Individual Silylation Reagents

### BSA [*N,O*-bis(trimethylsilyl)acetamide]

- Powerful silylating reagent and solvent for polar compounds

#### BSA

Description	Qty.	Part No.
BSA	10mL	<b>18056</b>
BSA	25mL	<b>18057</b>
BSA	10 x 1mL	<b>18034</b>

### BSTFA [*N,O*-bis(trimethylsilyl)trifluoroacetamide]

- More volatile reagent and byproducts compared to BSA
- Powerful silylating reagent; even more effective combined with TMCS as a catalyst

#### BSTFA

Description	Qty.	Part No.
BSTFA	10mL	<b>18085</b>
BSTFA	10 x 1mL	<b>18040</b>
BSTFA + 1% TMCS	10mL	<b>18087</b>
BSTFA + 1% TMCS	10 x 1mL	<b>18089</b>

### CMDMCS

- Longer retention times than TMCS derivatives
- Enhanced ECD response

#### CMDMCS

Description	Qty.	Part No.
CMDMCS	5mL	<b>18031</b>

### DMCS (Dimethylchlorosilane)

- DMS derivatives are more sensitive to hydrolysis than TMS derivatives

#### DMCS

Description	Qty.	Part No.
DMCS	3 x 10mL	<b>18071</b>

### HMDS (Hexamethyldisilazane)

- Slow and inefficient used alone
- Very effective in combination with TMCS

#### HMDS

Description	Qty.	Part No.
HMDS	25mL	<b>18069</b>
HMDS	10 x 1mL	<b>18003</b>

### MSHFBA [*N*-Methyl-*N*-trimethylsilylheptafluorobutyramide]

- Similar to MSTFA but does not produce harmful deposits in FID

#### MSHFBA

Description	Qty.	Part No.
MSHFBA	10mL	<b>214610</b>
MSHFBA	20 x 1mL	<b>2146201</b>

### MSTFA

#### (*N*-Methyl-*N*-trimethylsilyltrifluoroacetamide)

- Ideal reagent for drug analysis because excess reagent and byproducts elute during solvent delay
- May be used directly on HCl salts of compounds

#### MSTFA

Description	Qty.	Part No.
MSTFA	10mL	<b>18061</b>
MSTFA	1 x 1mL	<b>18038</b>

### MTBSTFA [*N*-(*tert*-butyldimethylsilyl)-*N*-methyltrifluoroacetamide]

- Derivatives more stable than common TMS derivatives
- Produces a distinct M-57 ion in GC/MS analysis
- Even more effective when combined with TBDMCS as a catalyst

#### MTBSTFA

Description	Qty.	Part No.
MTBSTFA	10 x 1mL	<b>18097</b>
MTBSTFA	10mL	<b>18102</b>
MTBSTFA + 1% TBDMCS	10 x 1mL	<b>18155</b>
MTBSTFA + 1% TBDMCS	10mL	<b>18148</b>

### TMCS (Trimethylchlorosilane)

- Similar to HMDS when used alone
- Very effective as a catalyst to other reagents

#### TMCS

Description	Qty.	Part No.
TMCS	3 x 10mL	<b>18091</b>
TMCS	10 x 1mL	<b>18084</b>

### TMSIM (*N*-Trimethylsilylimidazole)

- Preferentially silylates hydroxyl groups
- Best silylation reagent when water is present

#### TMSIM

Description	Qty.	Part No.
TMSIM	10 x 1mL	<b>18050</b>

### Glass Conditioning Reagent

#### Glass-Prep™ (5% DMDCS in toluene)

- Deactivate any glass surface

#### Glass-Prep™

Description	Qty.	Part No.
Glass-Prep™	100mL	<b>9700</b>
Glass-Prep™	400mL	<b>2233</b>
DMDCS, Neat	10 x 5mL	<b>18090</b>

## Alkylation (Esterification) Reagents

Alkylation replaces an acidic hydrogen (carboxylic acids, phenols) with an alkyl group. Alkyl esters are extremely stable and can be stored for long periods of time.

### Meth-Prep™ I

- On-column derivatization
- Aqueous solution does not give solvent peak

Meth-Prep™ I is a 0.2N aqueous solution of (m-trifluoromethylphenyl) trimethylammonium hydroxide. When the reagent is mixed with fatty acids and then injected into a GC injector at 240°C, the methyl esters are formed along with the by-product, m-trifluoromethylphenyl dimethylamine. The reaction is clean, fast, and quantitative. Meth-Prep™ I, being in aqueous solution, does not give a solvent peak. This may be advantageous in some cases.

#### Meth-Prep™ I

Description	Qty.	Part No.
Meth-Prep™ I	10 x 1mL	<b>18005</b>

### Instant Methanolic HCl Reagent Kit

- Acid catalyzed esterification of alcohols
- Reagent is generated before use and is stable for one week at room temperature

#### Instant Methanolic HCl Reagent Kit

Description	Qty.	Part No.
Instant Methanolic HCl Reagent Kit	ea	<b>18053</b>
Anhydrous Acetyl Chloride	5 x 2.8mL	<b>18095</b>
Anhydrous Methanol	10 x 5mL	<b>18157</b>



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**related product**  
Looking for syringes to use with reagents?  
See page 337–342.

## Transesterification Reagents

Transesterification is the process of converting one type of ester into another. Most commonly this is a very large ester (i.e., triglycerides, steryl esters, wax esters, phospholipids) converted into a methyl ester that is more easily analyzed.

### Meth-Prep™ II

- In one step forms fatty acid methyl esters from triglycerides at room temperature
- Requires no extraction before injecting into GC
- Faster than sodium methoxide reagents

Meth-Prep™ II is a 0.2N methanolic solution of m-trifluoromethylphenyl trimethylammonium hydroxide. This one-step reagent simplifies the transesterification of triglycerides to methyl esters. It is faster than sodium methoxide and the reaction occurs at room temperature. This quantitative reaction requires no extractions or additional treatment prior to gas chromatographic analysis.

#### Meth-Prep™ II

Description	Qty.	Part No.
Meth-Prep™ II	10 x 1mL	<b>18007</b>

### Sodium Methoxide/Methanol

- Converts a wide range of large esters to fatty acid methyl esters

#### Sodium Methoxide/Methanol

Description	Qty.	Part No.
Sodium Methoxide/Methanol	10 x 5mL	<b>18018</b>
Sodium Methoxide/Methanol	25mL	<b>218025</b>

### related product

Looking for amino acid derivatization kits?  
See page 63.

### technical assistance

Contact Tech Support: Phone: 1.800.255.8324 (North America)  
Email: [contact.alltech@grace.com](mailto:contact.alltech@grace.com)  
Online: [www.discoverysciences.com](http://www.discoverysciences.com)

## Acylation

Acylation reduces the polarity of amino, hydroxyl and thiol groups on multi-functional molecules such as carbohydrates and amino acids.

### Acetic Anhydride/Pyridine

- Used for acetylation of alcoholic and phenolic hydroxyl groups; and primary and secondary amino groups

#### Acetic Anhydride/Pyridine

Description	Qty.	Part No.
Acetic Anhydride/Pyridine Kit	ea	<b>18100</b>
Acetic Anhydride	10 x 1mL	<b>18103</b>

### Pyridine-Plus

- Much more powerful than acetic anhydride/pyridine
- Rapid reaction and fewer byproducts

#### Pyridine-Plus

Description	Qty.	Part No.
Pyridine-Plus Kit	ea	<b>18105</b>

### Fluorinated Imidazoles

- No acidic byproducts compared to anhydride reagents

#### Fluorinated Imidazoles

Description	Qty.	Part No.
TFAI ( <i>N</i> -Trifluoroacetylimidazole)	10 x 0.2g	<b>18046</b>
HFBI ( <i>N</i> -Heptafluorobutyrylimidazole)	10 x 0.2g	<b>18048</b>

### Perfluoroalkyl Anhydrides

- Produces derivatives suitable to electron capture detection

#### Perfluoroalkyl Anhydrides

Description	Qty.	Part No.
Trifluoroacetic Anhydride	5 x 1mL	<b>18083</b>
Pentafluoropropionic Anhydride	25g	<b>65192</b>
Pentafluoropropionic Anhydride	5 x 1mL	<b>18116</b>
Heptafluorobutyric Anhydride	25g	<b>63163</b>
Heptafluorobutyric Anhydride	5 x 1mL	<b>18118</b>



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#### related products

Looking for reaction vials to use with reagents? See page 375.

## Specialty Reagents

### Amino Acid Derivatization Kits

- Simple two-step procedure
- Three different reagents available: TFA, PFP, and HFB

#### Amino Acid Derivatization Kits

Description	Qty.	Part No.
TFA-IPA Derivatization Kit	ea	<b>18092</b>
PFP-IPA Derivatization Kit	ea	<b>18093</b>
HFB-IPA Derivatization Kit	ea	<b>18094</b>

### Barb-Prep™

- On-column methylation of barbiturates
- No byproduct formation

#### Barb-Prep™

Description	Qty.	Part No.
Barb-Prep™	10 x 1mL	<b>18009</b>

### DMF-DMA

- Novel reagent for derivatization of fatty acids, amino acids, amines, and barbiturates

#### DMF-DMA

Description	Qty.	Part No.
DMF-DMA	10 x 1mL	<b>18051</b>

## LC Reagents

### UV Enhancing

#### UV Enhancing

Description	Qty.	Part No.
<i>p</i> -Bromophenacyl Derivatization Kit	—	<b>18036</b>
<i>p</i> -Nitrobenzyloxyamine HCl (PNBA)	1g	<b>510113</b>

### Fluorescence Enhancing

#### Fluorescence Enhancing

Description	Qty.	Part No.
<i>o</i> -Phthalaldehyde (OPA)	5g	<b>35606</b>

## IPC™ Reagents

- Comparable to Waters® PIC® Reagents
- Preformulated at optimum concentration and pH
- Convenient—Simply dilute with HPLC grade solvents

### “A” Series

- Used for chromatography of acidic compounds

### “B” Series

- Used for chromatography of basic compounds

#### A Series and B Series

Description	Qty.	Part No.
IPC™ A, Tetrabutylammonium Phosphate	5 x 15mL	<b>185101</b>
IPC™ B5, Sodium Pentanesulfonate	5 x 25mL	<b>185110</b>
IPC™ B7, Sodium Heptanesulfonate	5 x 25mL	<b>185103</b>

### “Low UV”\* Series

- Suitable for use at wavelengths down to 200nm

#### Low UV Series

Description	Qty.	Part No.
Low UV IPC™ A, Tetrabutylammonium Sulfate	5 x 20mL	<b>185149</b>
Low UV IPC™ B5, Tetrabutylammonium Phosphate	5 x 20mL	<b>184198</b>
Low UV IPC™ B6, Tetrabutylammonium Phosphate	5 x 20mL	<b>184199</b>
Low UV IPC™ B7, Tetrabutylammonium Phosphate	5 x 20mL	<b>184282</b>
Low UV IPC™ B8, Tetrabutylammonium Phosphate	5 x 20mL	<b>184283</b>

\*For use at wavelengths below 240nm.

## Ion-Pair Salts

Grace offers high-purity ion-pairing salts for those wishing to formulate their own mobile phases.

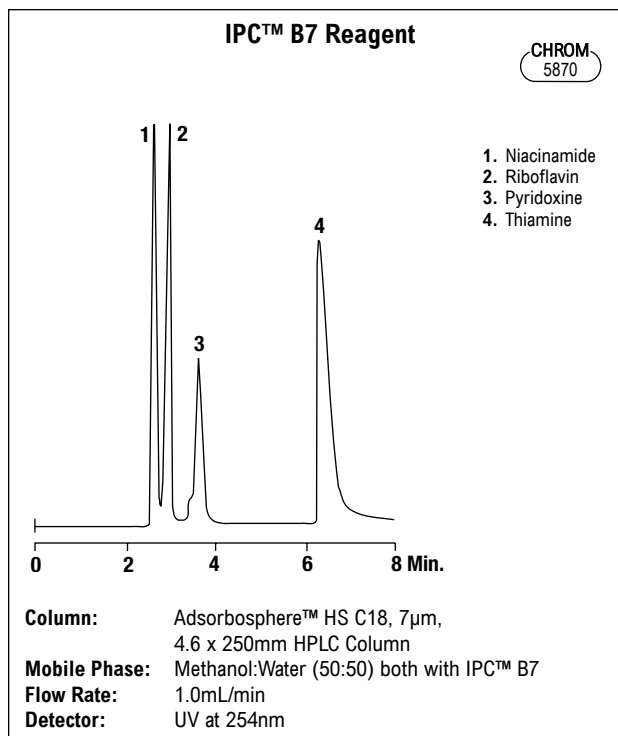
- High purity for HPLC applications

#### Ion-Pair Salts

Description	Qty.	Part No.
1-Pentanesulfonate	25g	<b>403125</b>
1-Hexanesulfonate	25g	<b>403126</b>
1-Heptanesulfonate	25g	<b>403127</b>
1-Octanesulfonate	25g	<b>403128</b>
Tetrabutylammonium Phosphate, 0.5M, pH 7.5)	10mL	<b>680502</b>

**Table 1—IPC™ Reagents**

Grace	Waters
IPC™ A	PIC® A
IPC™ B5	PIC® B5
IPC™ B6	PIC® B6
IPC™ B7	PIC® B7
IPC™ B8	PIC® B8
Low UV IPC™ A	Low UV PIC® A
Low UV IPC™ B5	Low UV PIC® B5
Low UV IPC™ B6	Low UV PIC® B6
Low UV IPC™ B7	Low UV PIC® B7
Low UV IPC™ B8	Low UV PIC® B8



### related products

Looking for mobile phase storage bottles?  
See page 125–127.

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