FORENSICS

UCT

DERIVATIZING REAGENTS

SELECTRA-SIL®


Available in Sealed Glass Ampules!
itive - Nitrogen Packe
ELECTRA-SIL®
FA w/1%TM
BSTFA-1-1A

SELECTRA-SIL® Reagents are packaged by weight, but are liquid in form. UCT's derivatizing reagents are synthesized and purified by UCT to exacting standards of purity and consistency. The reagents are packaged under nitrogen, sealed with a PTFE stopper and crimp topped to maintain an inert atmosphere. If stability of the reagents are a concern, UCT offers reagents packaged in sealed glass ampules, packaged under an inert atmosphere.

Purpose of Derivatization:

Derivatization is performed for two significant reasons. The first of which is to reduce the polarity and enhance the volatility of high molecular weight polar drugs, making them more suitable for analysis via GC-MS (Figure 1).

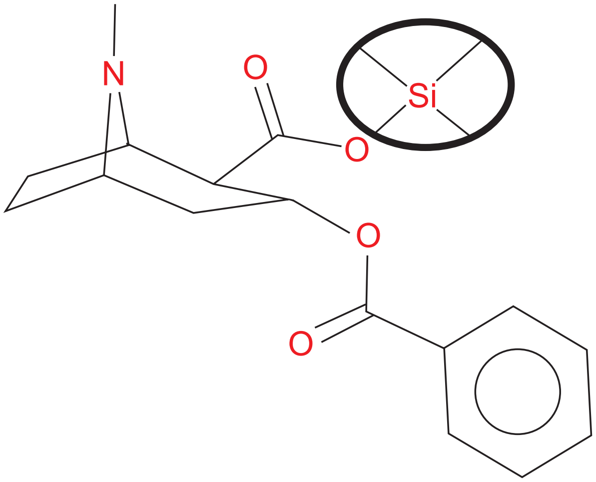

Figure 1. cccccderivative of benzoylecgonine. The underivatized compound has a carboxyl group and is too polar to pass through a GC column.

The second reason is to increase the molecular weight of very volatile drugs. This derivatization results in a more complex mass spectrum that improves the selectivity for that particular drug. When derivatizing drugs for GC/MS analysis, the spectrum of the resulting compounds should contain at least three ions that are unique to that analyte and not a result of the matrix.

Choosing a Derivatizing Agent

Silylation Reagents

Silylation is the most popular derivatization procedure for GC sample analysis. Of the silylation reagents, the most common is BSTFA (N,O-bis(trimethylsilyl)trifluoroacetamide). Silylation reagents are easy to use and readily form derivatives. In silylation, an active hydrogen found in molecules such as acids, alcohols, thiols, amines, amides, enolizable ketones and aldehydes is replaced by trimethylsilyl (TMS) or t-butyldimethylsilyl (t-BDMS). Compared to their parent compounds, silyl derivatives are more volatile, less polar, and more thermally stable. As a result, GC separation is improved and detection is enhanced. It is important to evaporate the analytes to complete dryness prior to derivatization. The higher boiling points of silylation reagents allow for greater room temperature stability, as long as the reagent is maintained in dry conditions.

Acylation Reagents

The next preferred derivatizing reagent is acylation reagents. These are typically available as acid anhydrides, acyl derivatives, or acyl halides. Common varieties of acylation reagents are TFAA (trifluoroacetic acid anhydride), PFAA (pentafluoropropionic acid anhydride) and HFAA (heptafluorobutyric acid anhydride). These reagents react with alcohols, phenols and amines to form fluoroacyl esters and amides. Acylation reagents offer similar advantages to silylation reagents. They create less polar, more volatile derivatives, however opposed to silylating reagents, acylating reagents target highly polar, multi-functional compounds, such as carbohydrates and amino acids. Acylating reagents also introduce electron capturing groups to the derivatized sample; enhancing analytical detection. Acyl halides and acyl derivatives are highly reactive. Typically they are used where steric hindrance may be an issue. Due to the corrosive nature of these reagents, any excess material or byproducts must be removed by evaporation prior to analysis. The derivatized analytes are then dissolved in another solvent and injected onto the GC-MS to prevent any column degradation.

Alkylation Reagents

Another group of derivatizing reagents are alkylation reagents, which replace active hydrogens with an alkyl group. These reagents are used to modify compounds having acidic hydrogens, such as carboxylic acids and phenols. Alkylation reagents can be used alone to form esters, ethers, and amides or they can be used in combination with acylation or silylation reagents. Esterification is the most popular method of alkylation. Alkyl esters are stable and form quickly and quantitatively. Alteration of the length of the substituted alkyl group can be used to alter the retention time of derivatives.

Derivatizing reagents are usually stored at room temperature or in a dessicator. Refrigeration should be avoided due to humid conditions shortening the life and effectiveness of the product. If refrigeration of reagents is desired, the reagent must come to room temperature in a dessicator prior to use. It is recommended to utilize reagents within six months of their ship date.

Common compounds found in a forensic/clinical setting along with the their targeted functional groups and derivatizatizing reagent of choice are listed below:

Drug	Derivatized Functional Group	Derivative
amphetamine	-NH2	4-carbethoxy-hexafluorobutyryl amide derivatized from 4-CB
methamphetamine	-NH2	4-carbethoxy-hexafluorobutyryl amide derivatized from 4-CB
phentermine	-NH2	4-carbethoxy-hexafluorobutyryl amide derivatized from 4-CB
cocaine	none	
benzoylecgonine	-CO2H	mono-TMS ester
morphine	-OH (two)	di-TMS ether
codeine	-OH	mono-TMS ether
6-monoacetylmorphine	-OH	mono-TMS ether
dihydrocodeine	-OH	mono-TMS ether
hydrocodone	enol –OH formed from =O	mono-TMS ether second peak corresponding to underivatized drug
oxycodone	-OH enol –OH formed from =O	mono and di-TMS ether
norcodeine	-OH -NH2	one peak: TMS ether and TMS amide
hydromorphone	OH enol –OH formed from =O	mono and di-TMS ether
oxymorphone	OH (two) enol –OH formed from =O	mono, di and tri-TMS ether
phencylidine (PCP)	none	
9-carboxy-11-nor-Δ9-tetrahydrocannabino	-OH -CO2H	One peak: mono-TMS ether and mono-TMS ester

Volatility of target compounds is an important consideration for gas chromatographic analysis. Polar functional groups such as amines, hydroxyls and carboxylic acids frequently hinder chromatographic resolution due to low volatility and/or hydrogen bonding effects with reactive sites on glassware, injector ports and analytical columns.

SILYLATION REAGENTS

Silyl derivatives are the most widely used chemical derivatization reagents. Silyl derivatization requires an "active" hydrogen as seen in acids, alcohols, thiols, amines, amide, enolizable ketones and aldehydes to be replaced by a trimethylsilyl group or tertiary butyl dimethylsilyl. Trimethylsilyl derivatives tend to be moisture sensitive, so a derivative with tertiary butyl dimethylsilyl may be preferred.

BSTFA N,O-bis(trimethylsilyl)trifluoroacetamide – CAS# 25561-30-2

Derivatizes most amines, alcohols, carboxylic acids and hydroxyls

Packaging	Units	Part Number
1 g sealed ampule	10 ampules / pack	SBSTFA-0-1-AMP
1 g vial	10 vials / pack	SBSTFA-0-1
10 g vial	1 vial	SBSTFA-0-10
25 g vial	1 vial	SBSTFA-0-25
100 g bottle	1 bottle	SBSTFA-0-100

BSTFA N,O-bis(trimethylsilyl)trifluoroacetamide with 1% TMCS trimethylchlorosilane

Derivatizes most amines, alcohols, carboxylic acids and hydroxyls, TMCS serves as a catalyst to improve reaction yield for sterically hindered hydroxyls, some amines and amides

Packaging	Units	Part Number
1 g sealed ampule	10 ampules / pack	SBSTFA-1-1-AMP
1 g vial	10 vials / pack	SBSTFA-1-1
10 g vial	1 vial	SBSTFA-1-10
25 g vial	1 vial	SBSTFA-1-25
100 g bottle	1 bottle	SBSTFA-1-100

BSTFA N,O-bis(trimethylsilyl)trifluoroacetamide with 10% TMCS trimethylchlorosilane

Derivatizes most amines, alcohols, carboxylic acids and hydroxyls, TMCS serves as a catalyst to improve reaction yield for sterically hindered hydroxyls, some amines and amides

Packaging	Units	Part Number
1 g sealed ampule	10 ampules / pack	SBSTFA-10-1-AMP
1 g vial	10 vials / pack	SBSTFA-10-1
10 g vial	1 vial	SBSTFA-10-10
25 g vial	1 vial	SBSTFA-10-25
100 g bottle	1 bottle	SBSTFA-10-100

MSTFA N-Methyl-N-trimethylsilyltrifluoroacetamide – CAS# 24589-78-4 Derivatizes most amines, alcohols, carboxylic acids and hydroxyls – most volatile of the trimethylsilyl derivatives, but with donor strength equal to BSTFA		
Packaging	**Units**	**Part Number**
1 g sealed ampule	10 ampules / pack	SMSTFA-0-1-AMP
1 g vial	10 vials / pack	SMSTFA-0-1
10 g vial	1 vial	SMSTFA-0-10
25 g vial	1 vial	SMSTFA-0-25
100 g bottle	1 bottle	SMSTFA-0-100

MSTFA N-Methyl-N-trimethylsilyltrifluoroacetamide with 1% Trimethylchlorosilane Derivatizes most amines, alcohols, carboxylic acids and hydroxyls – most volatile of the trimethylsilyl derivatives, but with donor strength equal to BSTFA. TMCS serves as a catalyst to improve reaction yield for sterically hindered hydroxyls, some amines and amides		
Packaging	**Units**	**Part Number**
1 g sealed ampule	10 ampules / pack	SMSTFA-1-1-AMP
1 g vial	10 vials / pack	SMSTFA-1-1
10 g vial	1 vial	SMSTFA-1-10
25 g vial	1 vial	SMSTFA-1-25
100 g bottle	1 bottle	SMSTFA-1-100

MTBSTFA N-Methyl-N-(tert-butyldimethylsilyl)trifluoroacetamide – CAS# 77377-52-7 Derivatizes hydroxyl, carboxyl, thiol and amines (primary and secondary).		
Packaging	**Units**	**Part Number**
1 g sealed ampule	10 ampules / pack	SMTBSTFA-0-1-AMP
1 g vial	10 vials / pack	SMTBSTFA-0-1
10 g vial	1 vial	SMTBSTFA-0-10
25 g vial	1 vial	SMTBSTFA-0-25
100 g bottle	1 bottle	SMTBSTFA-0-100

MTBSTFA N-Methyl-N-(tert-butyldimethylsilyl)trifluoroacetamide w/ 1% Tert-butyldimethylchlorosilane

Derivatizes hydroxyl, carboxyl, thiol and amines (primary and secondary). Addition of tert-butyldimethylchlorosilane increases the silylation ability to derivatize sterically hindered alcohols and amines. The TBDMCS derivatives are more stable than the related TMS analogs.

Packaging	Units	Part Number
1 g sealed ampule	10 ampules / pack	SMTBSTFA-1-1-AMP
1 g vial	10 vials / pack	SMTBSTFA-1-1
10 g vial	1 vial	SMTBSTFA-1-10
25 g vial	1 vial	SMTBSTFA-1-25
100 g bottle	1 bottle	SMTBSTFA-1-100

MTBSTFA N-Methyl-N-(tert-butyldimethylsilyl)trifluoroacetamide w/ 10% Tert-butyldimethylchlorosilane

Derivatizes hydroxyl, carboxyl, thiol and amines (primary and secondary). Addition of tert-butyldimethylchlorosilane increases the silylation ability to derivatize sterically hindered alcohols and amines. The TBDMCS derivatives are more stable than the related TMS analogs.

Packaging	Units	Part Number
1 g sealed ampule	10 ampules / pack	SMTBSTFA-10-1-AMP
1 g vial	10 vials / pack	SMTBSTFA-10-1
10 g vial	1 vial	SMTBSTFA-10-10
25 g vial	1 vial	SMTBSTFA-10-25
100 g bottle	1 bottle	SMTBSTFA-10-100

TMCS Trimethylchlorosilane – CAS# 75-77-4

Catalyst used to increase the reactivity of other silylation reagents.
Is also used to form trimethyl esters of organic acids.

Packaging	Units	Part Number
1 g sealed ampule	10 ampules / pack	STMCS-0-1-AMP
1 g vial	10 vials / pack	STMCS-0-1
10 g vial	1 vial	STMCS-0-10
25 g vial	1 vial	STMCS-0-25
100 g bottle	1 bottle	STMCS-0-100

ACYLATION REAGENTS

Acylation is the conversion of compounds with active hydrogens, such as thiols, hydroxyls, and amines, into thioesters, esters and amides respectively by forming a carboxylic acid derivative. The primary usage of acylation chemistry is to form compounds that chromatograph better than the parent molecule.

MBTFA N-Methyl-bis-trifluoroacetamide – CAS# 685-27-8

MBTFA reacts with primary and secondary amines, hydroxyl and thiol groups under mild, non-acidic conditions. It can also be used to selectively acelyate amines in the presence of hydroxyl and carboxyl groups that have been protected by silylation

Packaging	**Units**	**Part Number**
1 g vial	10 vials / pack	SMBTFA-0-1
10 g vial	1 vial	SMBTFA-0-10
25 g vial	1 vial	SMBTFA-0-25
100 g bottle	1 bottle	SMBTFA-0-100

TFAA Trifluoroacetic acid anhydride – CAS# 407-25-0

TFAA reacts readily with alcohols, phenols and amines producing stable volatile derivatives for TCD, FID, ECD and other detectors. Most reactive of all the perfluoroacid anhydrides and frequently used to identify methamphetamine

Packaging	**Units**	**Part Number**
1 g vial	10 vials / pack	STFAA-0-1
10 g vial	1 vial	STFAA-0-10
25 g vial	1 vial	STFAA-0-25
100 g bottle	1 bottle	STFAA-0-100

PFAA Pentafluoropropionic acid anhydride – CAS# 356-42-3

PFAA is commonly used in the determination of benzoylecgonine and opiates. Acidic by-products of this reaction must be removed before the derivative can be injected onto the GC

Packaging	**Units**	**Part Number**
1 g vial	10 vials / pack	SPFAA-0-1
10 g vial	1 vial	SPFAA-0-10
25 g vial	1 vial	SPFAA-0-25
100 g bottle	1 bottle	SPFAA-0-100

HFAA Heptafluorobutyric acid anhydride – CAS#336-59-4

HFAA is commonly used in the determination of benzoylecgonine and opiates.
Acidic by-products of this reaction must be removed before the derivative can be injected onto the GC

Packaging	Units	Part Number
1 g vial	10 vials / pack	SHFAA-0-1
10 g vial	1 vial	SHFAA-0-10
25 g vial	1 vial	SHFAA-0-25
100 g bottle	1 bottle	SHFAA-0-100

TFAI N-Trifluoroacetylimidazole – CAS#68739-25-3

TFAI offers considerable advantages over the anhydrides for the preparation of perfluoroacyl derivatives; the reactions are quantitative and produce relatively inert imidazole by-products.

Packaging	Units	Part Number
1 g vial	10 vials / pack	STFAI-0-1
10 g vial	1 vial	STFAI-0-10
25 g vial	1 vial	STFAI-0-25
100 g bottle	1 bottle	STFAI-0-100

PIA Propionic Anhydride – CAS#123-62-6

PIA is used in the derivatization of opiates if there is more morphine in the sample than 6-MAM.
This derivatization allows the 6-MAM peak to elute before morphine

Packaging	Units	Part Number
1 g sealed ampule	10 ampules / pack	SPIA-0-1-AMP
1 g vial	10 vials / pack	SPIA-0-1
10 g vial	1 vial	SPIA-0-10
25 g vial	1 vial	SPIA-0-25

Acetic Anhydride – CAS#108-24-7

Packaging	Units	Part Number
1 g sealed ampule	10 ampules / pack	SACETICANH-0-1-AMP

ALKYLATION REAGENTS

TMPAH 0.2M Trimethylanilium hydroxide in methanol

Packaging	Units	Part Number
1 g vial	10 vials / pack	STMPAH-0-1
10 g vial	1 vial	STMPAH-0-10
25 g vial	1 vial	STMPAH-0-25
100 g	2 x 50g vial	STMPAH-0-100
100 g bottle	1 bottle	SBSTFA-0-100

PFPOH Pentafluoropropanol – CAS# 771-61-9

Packaging	Units	Part Number
1 g vial	10 vials / pack	SPFPOH-0-1
10 g vial	1 vial	SPFPOH-0-10
25 g vial	1 vial	SPFPOH-0-25
100 g vial	1 vial	SPFPOH-0-100

4 CB 4-Carbethoxyhexafluorobutyryl Chloride – CAS# 18381-53-8

Packaging	Units	Part Number
1 g vial	10 vials / pack	S4CB-0-1
10 g vial	1 vial	S4CB-0-10
25 g vial	1 vial	S4CB-0-25

HFIP Hexafluoro-2-propanol – CAS# 920-66-1

Packaging	Units	Part Number
1 g vial	10 vials / pack	SHFIP-0-1
10 g vial	1 vial	SHFIP-0-10
25 g vial	1 vial	SHFIP-0-25
100 g vial	1 vial	SHFIP-0-100

DERIVATIZING REAGENT SOLVENTS

ACN Acetonitrile – CAS# 75-05-8

Packaging	Units	Part Number
50 g vial	1 vial	SACN-0-50

PYR Pyridine – CAS# 110-86-1

Packaging	Units	Part Number
25 g vial	1 vial	SPYR-0-25
50 g vial	1 vial	SPYR-0-50
100 g vial	1 vial	SPYR-0-100

PRICES AND TERMS

Our prices are subject to change without notice. The price in effect when we receive your order will apply. All prices are in US Dollars and are F.O.B. Terms of payment are net 30 days.

MINIMUM ORDERS

We welcome all orders, therefore, we do not have a minimum order requirement. When ordering, please include your purchase order number, complete "Ship To" and "Bill To" address, catalog number, quantity, and description of product(s). Also include your name and a phone number where you can be reached should we have any questions concerning your order.

SHIPMENTS

Normal processing is within 24 hours after receipt of an order. Unless special shipping requests have been made, our trained staff will send all orders by UPS Ground service. The appropriate shipping charges (freight & insurance costs) will be added to the invoice, unless otherwise instructed by the customer.

SPECIAL PRICING

We offer special pricing for volume purchases and standing orders. These discounts apply to bonded phase extraction column purchases only. Please call a sales representative for more information on special pricing qualifications.

RETURN POLICY

Our Quality Manager will handle all returns. Before returning merchandise, please call to obtain a return authorization number from the quality manager. We will need to know the reason for the return, date of purchase, purchase order number and invoice number in order to issue a return authorization number. Return merchandise must be received before a credit can be issued. Returns will not be accepted after 90 days. A restocking fee of 25% of the price paid, or a minimum of $25.00 (whichever is greater) will be charged on all returns.

WARRANTY

All products manufactured by UCT are guaranteed against defects in materials and workmanship for a period of 90 days after shipment. UCT will replace any items that prove to be defective during this time period. The exclusive remedy requires the end user to first advise UCT of the defective product by phone or in writing and must include order number, the lot number and the shipping date.

To initiate this action, photographs of the product, including packaging and labeling of the containers, must be submitted to the UCT Representative for approval. With approval a return authorization can be initiated, and must be received within 30 days. Once the materials arrive at UCT a further inspection of the materials must be completed and accepted by our Quality Manager prior to further action of credits or replacement. UCT's total liability is limited to the replacement cost of UCT products.

This warranty does not apply to damage resulting from misuse.

Contact Us

Phone: 215.781.9255
800.385.3153
Fax: 215.785.1226

UCT, Inc.
2731 Bartram Rd.
Bristol, PA 19007

Email: info@unitedchem.com
Web: www.unitedchem.com

MADE IN USA

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FORENSICS