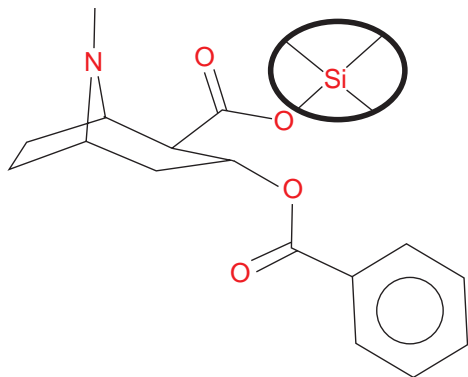


## Purpose of Derivatization:

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.** Trimethylsilyl derivative 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.

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## 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-butyl dimethylsilyl (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.

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.

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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

## 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

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**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.

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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 acylate amines in the presence of hydroxyl and carboxyl groups that have been protected by silylation

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

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### 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 sealed ampule	10 ampules / pack	STFAA-0-1-AMP
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 sealed ampule	10 ampules / pack	SPFAA-0-1-AMP
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 sealed ampule	10 ampules / pack	SHFAA-0-1-AMP
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

**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 sealed ampule	10 ampules / pack	STFAI-0-1-AMP
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 sealed ampule	10 ampules / pack	STMPAH-0-1-AMP
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

**PFPOH    Pentafluoropropanol – CAS# 771-61-9**

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

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**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

**PURIFIED  
BETA-GLUCURONIDASE FORMULA  
CLEAN, RAPID AND RELIABLE**

**Abalonase™**

Purified Beta-glucuronidase formula that has been designed to quickly hydrolyze conjugated drug metabolites in human samples within minutes.

Part Number	Vol. (mL)	Activity (units)
ASBETA-GLUC-10	10	≥50,000 units/mL
ASBETA-GLUC-25	25	≥50,000 units/mL
ASBETA-GLUC-50	50	≥50,000 units/mL
ASBETA-GLUC-100	100	≥50,000 units/mL

**Form:** Clear Aqueous Solution

**Sulfatase Activity:** None

**Storage:** +4°C to +8°C

**Effective pH:** 4.5

**Stability:** When properly stored, the enzyme will maintain activity for at least 1 Year. After 1 year, it is recommended that the activity level be reassessed.

**Abalonase™ +**

Designed for deconjugation of both glucuronidated and sulfated metabolites. The formula is enriched with 4 arylsulfatases making it ideal for the hydrolysis of steroid metabolites.

Part Number	Vol. (mL)	Activity (units)
ASFBETA-GLUC-10	10	≥50,000 units/mL
ASFBETA-GLUC-25	25	≥50,000 units/mL
ASFBETA-GLUC-50	50	≥50,000 units/mL
ASFBETA-GLUC-100	100	≥50,000 units/mL

**Form:** Clear Aqueous Solution

**Sulfatase Activity:** > 400 U/mL

**Storage:** +4°C to +8°C

**Effective pH:** 5.0

**Stability:** When properly stored, the enzyme will maintain activity for at least 1 year. After 1 year, it is recommended that the activity level be reassessed.

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Shown from left to right: Abalonase™ purified Beta-glucuronidase formula, Selectrazyme® and Red Abalone Beta-Glucuronidase enzyme from an alternate supplier

**Rapid Hydrolysis Buffer included in every order.**

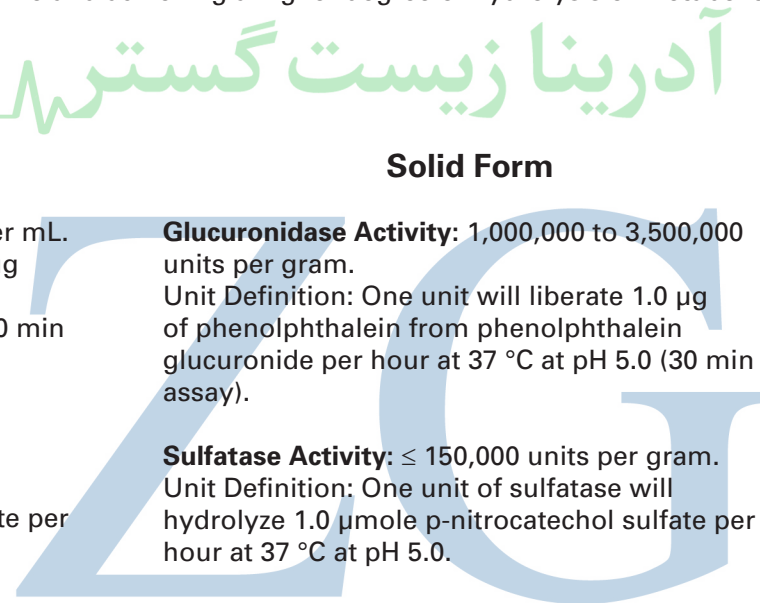
Every Abalonase™ and Abalonase™ + purified Beta-glucuronidase formula comes with a Rapid Hydrolysis Buffer to be used at your convenience. Through its usage, both purified Beta-glucuronidase formulas will achieve their maximum performance and it will significantly reduce sample preparation times and use of alternate reagents in addition to minimizing buffer preparation errors.





Abalone derived  $\beta$ -glucuronidase has been used for the enzymatic hydrolysis of glucuronides from urine, blood and serum prior to analysis by enzyme immunoassay, mass spectrometry, high performance liquid chromatography, and other means. Typically, between 1 to 10 units of glucuronidase is used per microliter of the sample matrix. The exact amount needed will depend on the specific conditions used and must be determined empirically.

Abalone derived  $\beta$ -glucuronidase is a crude solution of enzymes. Many  $\beta$ -glucuronidases derived from mollusks also contain sulfatase activity. For this reason, the sulfatase activity of the material is also determined. Abalone derived  $\beta$ -glucuronidase is more thermal tolerant as compared to enzymes derived from *E. coli*, *H. pomatia* and bovine liver. Therefore the hydrolysis reaction can be carried out at a higher temperature providing hydrolysis in less time and achieving a higher degree of hydrolysis of metabolites like morphine-3-glucuronide.



## Liquid Form

## Solid Form

**Glucuronidase Activity:**  $\geq 100,000$  units per mL.  
Unit Definition: One unit will liberate 1.0  $\mu$ g of phenolphthalein from phenolphthalein glucuronide per hour at 37 °C at pH 5.0 (30 min assay).

**Glucuronidase Activity:** 1,000,000 to 3,500,000 units per gram.  
Unit Definition: One unit will liberate 1.0  $\mu$ g of phenolphthalein from phenolphthalein glucuronide per hour at 37 °C at pH 5.0 (30 min assay).

**Sulfatase Activity:**  $\leq 8,000$  units per mL.  
Unit Definition: One unit of sulfatase will hydrolyze 1.0  $\mu$ mole p-nitrocatechol sulfate per hour at 37 °C at pH 5.0.

**Sulfatase Activity:**  $\leq 150,000$  units per gram.  
Unit Definition: One unit of sulfatase will hydrolyze 1.0  $\mu$ mole p-nitrocatechol sulfate per hour at 37 °C at pH 5.0.

**Storage / Stability**  
Store at +2 to +8 °C. When stored at +2 to +8 °C, the enzyme retains activity for at least 1 year. After this period we recommend retesting the activity.

**Storage / Stability**  
Store at -20 °C. When stored at -20 °C, the enzyme retains activity for at least 3 years. After this period we recommend retesting the activity.

Liquid		
Part Number	Vol. (mL)	Activity (units)
BETA-GLUC-10	10	$\geq 100,000$ units/mL
BETA-GLUC-25	25	$\geq 100,000$ units/mL
BETA-GLUC-50	50	$\geq 100,000$ units/mL

Lyophilized Powder	
Part Number	Activity (units)
BETA-GLUC-250KU	250,000
BETA-GLUC-500KU	500,000
BETA-GLUC-1MU	1,000,000
BETA-GLUC-2MU	2,000,000

# SELECT pH BUFFER POUCHES



To help simplify the process of sample preparation, UCT has developed a line of 'ready-to-use' phosphate and acetate buffer pouches. The UCT buffer pouches are a convenient way of accurately preparing the necessary reagents, at the proper pH and concentration, for solid phase extraction methods. These pre-measured pouches eliminate time and more importantly, any potential error in the buffer preparation, insuring the highest efficiency in the extraction method. As with all UCT products, these buffer pouches are prepared with the same high quality standards used in the manufacture of the entire line of SPE products.

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## SELECT pH BUFFER POUCHES 100mM ACETATE pH 4.5

**Instructions:** Add 300 mL of deionized water to a 500 mL volumetric flask. Mix in the contents of the buffer pouch and shake/stir well. Add 3.24 mL of glacial acetic acid to the volumetric flask and dilute to the mark with deionized water. Ensure pH is 4.5+/-0.5. **Yield:** 500 mL of solution

Contents	Units per Pack	Part Number
5.86 g Sodium Acetate Trihydrate	5	SPHACE4501-5
	10	SPHACE4501-10

## SELECT pH BUFFER POUCHES 100mM ACETATE pH 5.00

**Instructions:** Add 300 mL of deionized water to a 500 mL volumetric flask. Mix in the contents of the buffer pouch and shake/stir well. Add 1.04 mL of glacial acetic acid to the volumetric flask and dilute to the mark with deionized water. Ensure pH is 5.0+/-0.5. **Yield:** 500 mL of solution

Contents	Units per Pack	Part Number
4.29 g Sodium Acetate Trihydrate	5	SPHACE5001-5
	10	SPHACE5001-10

## SELECT pH BUFFER POUCHES 1M ACETATE pH 5.0

**Instructions:** Add 300 mL of deionized water to a 500 mL volumetric flask. Mix in the contents of the buffer pouch and shake/stir well. Add 10.4 mL of glacial acetic acid to the volumetric flask and dilute to the mark with deionized water. Ensure pH is 5.0+/-0.5. **Yield:** 500 mL of solution

Contents	Units per Pack	Part Number
42.9 g Sodium Acetate Trihydrate	5	SPHACE4501-5
	10	SPHACE4501-10

## SELECT pH BUFFER POUCHES 100mM PHOSPHATE pH 6.0

**Instructions:** Add 600 mL of deionized water to a 1000 mL volumetric flask. Add in the contents of the buffer pouch and mix/stir. Dilute to the mark with deionized water. Ensure the pH is 6.0+/-0.5. **Yield:** 1000 mL of solution

Contents	Units per Pack	Part Number
4.29 g Sodium Acetate Trihydrate	5	SPHPHO6001-5
	10	SPHPHO6001-10

## SELECT pH BUFFER POUCHES 100mM PHOSPHATE pH 7.0

**Instructions:** Add 600 mL of deionized water to a 1000 mL volumetric flask. Add in the contents of the buffer pouch and mix/stir. Dilute to the mark with deionized water. Ensure the pH is 7.0+/-0.5. **Yield:** 1000 mL of solution

Contents	Units per Pack	Part Number
7.82 g Disodium Hydrogen Phosphate and 6.22 g Sodium Dihydrogen Phosphate Hydrate	5	SPHPHO7001-5
	10	SPHPHO7001-10



GREEN EARTH

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