



# CAMBRIDGE ISOTOPE LABORATORIES

## PRODUCT AND COMPANY IDENTIFICATION

Product Name: Metabolomics QC Kit

Catalog No: MSK-QC-KIT

Company: Cambridge Isotope Laboratories Inc.  
50 Frontage Road  
Andover, MA. 01810  
USA

Telephone: 1-800-322-1174 International information 1-978-749-8000  
Emergency: 1-800-424-9300 International Emergency 1-202-483-7616

## HAZARDS IDENTIFICATION

### Emergency Overview

### OSHA Hazards

Irritant

### GHS Classification(s)

Acute toxicity, oral, category 4

Skin irritation – Cat 2

Eye irritation – Cat 2

### GHS Label elements, including precautionary statements



Pictograms

Signal word

Warning

Hazard statement(s)

See individual Safety Data Sheets

## COMPOSITION

Each kit contains two vials:

Metabolomics QC Standard Mix 1

Metabolomics QC Standard Mix 2



# Metabolomics QC Standard Mix 1

## Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations  
Issue date: 5/20/2016 Revision date: 3/18/2024 Supersedes: 5/20/2016 Version: 2.0

### SECTION 1: Identification

#### 1.1. Identification

Product form : Mixture  
Product name : Metabolomics QC Standard Mix 1  
Product code : MSK-QC1

#### 1.2. Recommended use and restrictions on use

No additional information available

#### 1.3. Supplier

Cambridge Isotope Laboratories, Inc.  
50 Frontage Rd  
01810  
ANDOVER, MA, 01810  
USA  
T 1-800-322-1174  
[cilsales@isotope.com](mailto:cilsales@isotope.com) - [www.isotope.com](http://www.isotope.com)

#### 1.4. Emergency telephone number

Emergency number : 1-703-741-5970  
Chemtrec 1-800-424-9300 24 hours

### SECTION 2: Hazard(s) identification

#### 2.1. Classification of the substance or mixture

##### GHS US classification

Not classified

#### 2.2. GHS Label elements, including precautionary statements

##### GHS US labeling

No labeling applicable

#### 2.3. Other hazards which do not result in classification

No additional information available

#### 2.4. Unknown acute toxicity (GHS US)

Not applicable

### SECTION 3: Composition/Information on ingredients

#### 3.1. Substances

Not applicable

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### 3.2. Mixtures

Name	Product identifier	%	GHS US classification
L-LEUCINE (13C6, 99%)	CAS-No.: 201740-84-3	7.14	Not classified
L-ALANINE (13C3, 99%)	CAS-No.: 100108-77-8	7.14	Not classified
L-TYROSINE (RING-13C6, 99%)	CAS-No.: 201595-63-3	7.14	Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335
L-PHENYLALANINE (RING-13C6, 99%)	CAS-No.: 63-91-2 (Unlabeled)	7.14	Not classified

Full text of hazard classes and H-statements : see section 16

## SECTION 4: First-aid measures

### 4.1. Description of first aid measures

First-aid measures general	: Move out of dangerous area. Consult a physician and show this safety data sheet.
First-aid measures after inhalation	: If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
First-aid measures after skin contact	: Wash with soap and plenty of water. Consult a physician.
First-aid measures after eye contact	: Flush eye with water for 15 minutes. Get medical attention.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 4.2. Most important symptoms and effects (acute and delayed)

Potential Adverse human health effects and symptoms	: This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.
Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory tract irritation.
Symptoms/effects after skin contact	: May be harmful if absorbed through skin. May cause skin irritation.
Symptoms/effects after eye contact	: May cause eye irritation.
Symptoms/effects after ingestion	: May be harmful if swallowed.

### 4.3. Immediate medical attention and special treatment, if necessary

No additional information available

## SECTION 5: Fire-fighting measures

### 5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Use water spray, alcohol-resistant foam, dry chemical, or carbon dioxide.

### 5.2. Specific hazards arising from the chemical

Hazardous decomposition products in case of fire : Carbon oxides (CO, CO<sub>2</sub>). Nitrogen oxides. Phosgene.

### 5.3. Special protective equipment and precautions for fire-fighters

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

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### SECTION 6: Accidental release measures

#### 6.1. Personal precautions, protective equipment and emergency procedures

##### 6.1.1. For non-emergency personnel

Emergency procedures : Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust.

##### 6.1.2. For emergency responders

No additional information available

#### 6.2. Environmental precautions

Do not let product enter drains.

#### 6.3. Methods and material for containment and cleaning up

For containment : Take up mechanically (sweeping, shoveling) and collect in suitable container for disposal.

#### 6.4. Reference to other sections

For further information refer to section 13.

### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

#### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures : Keep container tightly closed in a cool, dry and well-ventilated place.  
Storage conditions : Store in freezer (-20°C). Protect from light.

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

##### Metabolomics QC Standard Mix 1

No additional information available

##### L-LEUCINE (13C6, 99%) (201740-84-3)

###### USA - ACGIH - Occupational Exposure Limits

ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
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##### L-ALANINE (13C3, 99%) (100108-77-8)

No additional information available

##### L-TYROSINE (RING-13C6, 99%) (201595-63-3)

###### USA - ACGIH - Occupational Exposure Limits

ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
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### L-PHENYLALANINE (RING-13C6, 99%) (63-91-2 (Unlabeled))

#### USA - ACGIH - Occupational Exposure Limits

ACGIH chemical category

No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.

### 8.2. Appropriate engineering controls

No additional information available

### 8.3. Individual protection measures/Personal protective equipment

#### Personal protective equipment:

Safety glasses. Gloves. Respiratory protection of the dependent type. Self-contained breathing apparatus. Protective clothing.

#### Hand protection:

Wear suitable protective clothing and gloves

#### Eye protection:

Wear safety glasses with side shields (or goggles) and a face shield.

#### Skin and body protection:

Choose body protection according to the amount and concentration of the dangerous substance at the work place.

#### Respiratory protection:

When appropriate, use NIOSH/CEN approved respirator.

#### Personal protective equipment symbol(s):



## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state	: Solid
Appearance	: Solid.
Color	: White to off-white
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Melting point	: No data available
Freezing point	: No data available
Boiling point	: No data available
Flash point	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: No data available
Relative vapor density at 20°C	: No data available
Relative density	: No data available
Solubility	: No data available
Partition coefficient n-octanol/water (Log Pow)	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available

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Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

No additional information available

### 10.2. Chemical stability

See storage and expiration date on CoA.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

No additional information available

### 10.5. Incompatible materials

No additional information available

### 10.6. Hazardous decomposition products

No additional information available

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity (oral)	: Not classified
Acute toxicity (dermal)	: Not classified
Acute toxicity (inhalation)	: Not classified

<b>L-LEUCINE (13C6, 99%) (201740-84-3)</b>	
LD50 oral rat	> 16000 mg/kg male and female

<b>L-ALANINE (13C3, 99%) (100108-77-8)</b>	
LD50 oral rat	> 5110 mg/kg male and female

Skin corrosion/irritation : Not classified

<b>L-ALANINE (13C3, 99%) (100108-77-8)</b>	
pH	5.5 – 7 at 89.1 g/l at 25 °C (77 °F)

<b>L-PHENYLALANINE (RING-13C6, 99%) (63-91-2 (Unlabeled))</b>	
pH	5 – 7 at 16.5 g/l at 25 °C (77 °F)

Serious eye damage/irritation : Not classified

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<b>L-ALANINE (13C3, 99%) (100108-77-8)</b>	
pH	5.5 – 7 at 89.1 g/l at 25 °C (77 °F)
<b>L-PHENYLALANINE (RING-13C6, 99%) (63-91-2 (Unlabeled))</b>	
pH	5 – 7 at 16.5 g/l at 25 °C (77 °F)
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
<b>L-TYROSINE (RING-13C6, 99%) (201595-63-3)</b>	
National Toxicology Program (NTP) Status	No component of this product present at levels greater than or equal to 0.1 % is identified as a known or anticipated carcinogen by NTP.
Reproductive toxicity	: Not classified
STOT-single exposure	: Not classified
<b>L-TYROSINE (RING-13C6, 99%) (201595-63-3)</b>	
STOT-single exposure	May cause respiratory irritation.
STOT-repeated exposure	: Not classified
<b>L-LEUCINE (13C6, 99%) (201740-84-3)</b>	
NOAEL (oral,rat,90 days)	3840 mg/kg bodyweight/day female
Aspiration hazard	: Not classified
Viscosity, kinematic	: No data available
Potential Adverse human health effects and symptoms	: This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.
Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory tract irritation.
Symptoms/effects after skin contact	: May be harmful if absorbed through skin. May cause skin irritation.
Symptoms/effects after eye contact	: May cause eye irritation.
Symptoms/effects after ingestion	: May be harmful if swallowed.

## SECTION 12: Ecological information

### 12.1. Toxicity

Ecology - general : The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.

<b>L-ALANINE (13C3, 99%) (100108-77-8)</b>	
EC50 - Crustacea [1]	> 100 mg/l static test - Daphnia magna (Water flea) - 48 h

### 12.2. Persistence and degradability

No additional information available

### 12.3. Bioaccumulative potential

<b>L-ALANINE (13C3, 99%) (100108-77-8)</b>	
Partition coefficient n-octanol/water (Log Pow)	-2.74 at 20 °C (68 °F)
<b>L-TYROSINE (RING-13C6, 99%) (201595-63-3)</b>	
Partition coefficient n-octanol/water (Log Pow)	-2.26 at 25 °C (77 °F)

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### 12.4. Mobility in soil

No additional information available

### 12.5. Other adverse effects

Other adverse effects : Disposal must be done according to official regulations. Avoid release to the environment.

## SECTION 13: Disposal considerations

### 13.1. Disposal methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and local environmental control regulations.  
Product/Packaging disposal recommendations : Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.  
Ecology - waste materials : Dispose of as unused product.

## SECTION 14: Transport information

In accordance with DOT / TDG / IMDG / IATA

### 14.1. UN number

Not regulated for transport

### 14.2. UN proper shipping name

Proper Shipping Name (DOT) : Not applicable  
Proper Shipping Name (TDG) : Not applicable  
Proper Shipping Name (IMDG) : Not applicable  
Proper Shipping Name (IATA) : Not applicable

### 14.3. Transport hazard class(es)

#### DOT

Transport hazard class(es) (DOT) : Not applicable

#### TDG

Transport hazard class(es) (TDG) : Not applicable

#### IMDG

Transport hazard class(es) (IMDG) : Not applicable

#### IATA

Transport hazard class(es) (IATA) : Not applicable

### 14.4. Packing group

Packing group (DOT) : Not applicable  
Packing group (TDG) : Not applicable  
Packing group (IMDG) : Not applicable  
Packing group (IATA) : Not applicable

### 14.5. Environmental hazards

Other information : No supplementary information available.



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### 14.6. Special precautions for user

Special transport precautions : Not dangerous goods.

#### DOT

No data available

#### TDG

No data available

#### IMDG

No data available

#### IATA

No data available

### 14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

Commercial status of components according to the United States Environmental Protection Agency's Toxic Substances Control Act (TSCA):

Name	CAS-No.	Listing	Commercial status	Flags
L-LEUCINE (13C6, 99%)	201740-84-3	Not present	-	
L-ALANINE (13C3, 99%)	100108-77-8	Not present	-	
L-TYROSINE (RING-13C6, 99%)	201595-63-3	Not present	-	
L-PHENYLALANINE (RING-13C6, 99%)	63-91-2 (Unlabeled)	Not present	-	

#### L-LEUCINE (13C6, 99%) (201740-84-3)

SARA Section 302 Threshold Planning Quantity (TPQ)	SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302
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#### L-TYROSINE (RING-13C6, 99%) (201595-63-3)

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard

#### L-PHENYLALANINE (RING-13C6, 99%) (63-91-2 (Unlabeled))

SARA Section 302 Threshold Planning Quantity (TPQ)	SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.
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### 15.2. International regulations

#### CANADA

#### L-LEUCINE (13C6, 99%) (201740-84-3)

Not listed on the Canadian DSL (Domestic Substances List)/NDSL (Non-Domestic Substances List)

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### L-ALANINE (13C3, 99%) (100108-77-8)

Not listed on the Canadian DSL (Domestic Substances List)/NDSL (Non-Domestic Substances List)

### L-TYROSINE (RING-13C6, 99%) (201595-63-3)

Not listed on the Canadian DSL (Domestic Substances List)/NDSL (Non-Domestic Substances List)

#### EU-Regulations

No additional information available

#### National regulations

No additional information available

### 15.3. US State regulations

No additional information available

## SECTION 16: Other information

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Revision date : 03/18/2024

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

#### Full text of H-phrases

H315	Causes skin irritation
H319	Causes serious eye irritation
H335	May cause respiratory irritation

Safety Data Sheet (SDS), USA

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.



# Metabolomics QC Standard Mix 2

## Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations  
Issue date: 5/20/2016 Revision date: 3/18/2024 Supersedes: 11/16/2022 Version: 3.0

### SECTION 1: Identification

#### 1.1. Identification

Product form : Mixture  
Product name : Metabolomics QC Standard Mix 2  
Product code : MSK-QC2

#### 1.2. Recommended use and restrictions on use

No additional information available

#### 1.3. Supplier

Cambridge Isotope Laboratories, Inc.  
50 Frontage Rd  
01810  
ANDOVER, MA, 01810  
USA  
T 1-800-322-1174  
[cilsales@isotope.com](mailto:cilsales@isotope.com) - [www.isotope.com](http://www.isotope.com)

#### 1.4. Emergency telephone number

Emergency number : 1-703-741-5970  
Chemtrec 1-800-424-9300 24 hours

### SECTION 2: Hazard(s) identification

#### 2.1. Classification of the substance or mixture

##### GHS US classification

Acute toxicity (oral) Category 4	H302	Harmful if swallowed
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2	H319	Causes serious eye irritation
Combustible Dust		May form combustible dust concentrations in air

Full text of H statements : see section 16

#### 2.2. GHS Label elements, including precautionary statements

##### GHS US labeling

Hazard pictograms (GHS US) :



Signal word (GHS US) : Warning

Hazard statements (GHS US) : May form combustible dust concentrations in air  
H302 - Harmful if swallowed  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation

Precautionary statements (GHS US) : P264 - Wash Both hands thoroughly after handling.  
P270 - Do not eat, drink or smoke when using this product.  
P280 - Wear eye protection, face protection, protective clothing, protective gloves.  
P301+P312 - If swallowed: Call a doctor, a POISON CENTER if you feel unwell.  
P302+P352 - If on skin: Wash with plenty of water.  
P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove

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contact lenses, if present and easy to do. Continue rinsing.  
P321 - Specific treatment (see Hazard pictograms (CLP) on this label).  
P330 - Rinse mouth.  
P332+P313 - If skin irritation occurs: Get medical advice/attention.  
P337+P313 - If eye irritation persists: Get medical advice/attention.  
P362+P364 - Take off contaminated clothing and wash it before reuse.  
P501 - Dispose of contents/container to Comply with applicable regulations.

### 2.3. Other hazards which do not result in classification

No additional information available

### 2.4. Unknown acute toxicity (GHS US)

Not applicable

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Not applicable

### 3.2. Mixtures

Name	Product identifier	%	GHS US classification
WATER UNLABELED	CAS-No.: 7732-18-5	99.996776	Not classified
CAFFEINE (TRIMETHYL-13C3, 99%)	CAS-No.: 78072-66-9	0.000401	Acute Tox. 4 (Oral), H302
SODIUM OCTANOATE (13C8, 99%)	CAS-No.: 1984-06-1 (Unlabeled)	0.000401	Skin Irrit. 2, H315 Eye Irrit. 2A, H319
SODIUM BENZOATE (RING-13C6, 99%)	CAS-No.: 532-32-1 (Unlabeled)	0.000401	Eye Irrit. 2A, H319
SODIUM SUCCINATE (13C4, 99%)	CAS-No.: 150-90-3	0.000401	Not classified
SODIUM CITRATE (1,5,6-CARBOXY-13C3, 99%)	CAS-No.: 18996-35-5	0.000398	Not classified
D-GLUCOSE (U-13C6, 99%)	CAS-No.: 50-99-7	0.000395	Not classified
D-SUCROSE (GLUCOSE-13C6, 98%)	CAS-No.: 57-50-1	0.000393	Not classified
SODIUM PROPIONATE (13C3, 99%)	CAS-No.: 152571-51-2	0.000393	Acute Tox. 4 (Dermal), H312
SODIUM STEARATE (U-13C18, 98%) 97% CHEMICAL PURITY	CAS-No.: 822-16-2	0.00004	Not classified

Full text of hazard classes and H-statements : see section 16

## SECTION 4: First-aid measures

### 4.1. Description of first aid measures

First-aid measures general : Call a poison center/doctor/physician if you feel unwell.  
First-aid measures after inhalation : Remove person to fresh air and keep comfortable for breathing.  
First-aid measures after skin contact : Wash skin with plenty of water. Take off contaminated clothing. If skin irritation occurs: Get medical advice/attention.  
First-aid measures after eye contact : Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice/attention.  
First-aid measures after ingestion : Rinse mouth. Call a poison center/doctor/physician if you feel unwell.

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### 4.2. Most important symptoms and effects (acute and delayed)

Potential Adverse human health effects and symptoms	: This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.
Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: Harmful if swallowed.

### 4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

## SECTION 5: Fire-fighting measures

### 5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Alcohol resistant foam. Dry chemical. Water spray. Dry powder. Foam.

### 5.2. Specific hazards arising from the chemical

Hazardous decomposition products in case of fire : Carbon oxides (CO, CO<sub>2</sub>).

### 5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions	: Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting	: Wear respiratory protection. Do not attempt to take action without suitable protective equipment. Self-contained breathing apparatus. Complete protective clothing.

## SECTION 6: Accidental release measures

### 6.1. Personal precautions, protective equipment and emergency procedures

#### 6.1.1. For non-emergency personnel

Protective equipment	: Wear recommended personal protective equipment. Avoid breathing dust, mist or spray. Avoid dust formation. Ensure there is adequate ventilation. Evacuate the danger area.
Emergency procedures	: Ventilate spillage area. Avoid contact with skin and eyes.

#### 6.1.2. For emergency responders

Protective equipment	: Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".
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### 6.2. Environmental precautions

Avoid release to the environment. Prevent entry to sewers and public waters.

### 6.3. Methods and material for containment and cleaning up

For containment	: Take up mechanically (sweeping, shoveling) and collect in suitable container for disposal.
Methods for cleaning up	: Mechanically recover the product. This material and its container must be disposed of in a safe way, and as per local legislation.
Other information	: Dispose of materials or solid residues at an authorized site.

### 6.4. Reference to other sections

For further information refer to section 13.

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### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

Precautions for safe handling	: Ensure good ventilation of the work station. Avoid dust formation. Provide good ventilation in process area to prevent formation of vapor. Avoid contact with skin and eyes. Wear personal protective equipment.
Hygiene measures	: Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

#### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures	: Store locked up. Store in a well-ventilated place. Keep container tightly closed.
Storage conditions	: Store in freezer (-20°C). Protect from light.

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

<b>Metabolomics QC Standard Mix 2</b>	
No additional information available	
<b>D-GLUCOSE (U-13C6, 99%) (50-99-7)</b>	
<b>USA - ACGIH - Occupational Exposure Limits</b>	
ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
<b>D-SUCROSE (GLUCOSE-13C6, 98%) (57-50-1)</b>	
<b>USA - ACGIH - Occupational Exposure Limits</b>	
ACGIH OEL TWA	10 mg/m <sup>3</sup> Dental erosion. Not classifiable as a human carcinogen.
ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
<b>USA - OSHA - Occupational Exposure Limits</b>	
OSHA PEL TWA [1]	5 mg/m <sup>3</sup>
<b>USA - NIOSH - Occupational Exposure Limits</b>	
NIOSH REL TWA	5 mg/m <sup>3</sup>
<b>CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)</b>	
No additional information available	
<b>SODIUM OCTANOATE (13C8, 99%) (1984-06-1 (Unlabeled))</b>	
<b>USA - ACGIH - Occupational Exposure Limits</b>	
ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
<b>SODIUM PROPIONATE (13C3, 99%) (152571-51-2)</b>	
<b>USA - ACGIH - Occupational Exposure Limits</b>	
ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.

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<b>SODIUM BENZOATE (RING-13C6, 99%) (532-32-1 (Unlabeled))</b>	
No additional information available	
<b>SODIUM CITRATE (1,5,6-CARBOXY-13C3, 99%) (18996-35-5)</b>	
No additional information available	
<b>SODIUM STEARATE (U-13C18, 98%) 97% CHEMICAL PURITY (822-16-2 )</b>	
<b>USA - ACGIH - Occupational Exposure Limits</b>	
ACGIH OEL TWA	10 mg/m <sup>3</sup> Basis: USA. ACGIH Threshold Limit Values (TLV)
Remark (ACGIH)	Upper Respiratory Tract irritation. Eye irritation. Skin irritation. Does not include stearates of toxic metals. Not classifiable as a human carcinogen.
<b>USA - OSHA - Occupational Exposure Limits</b>	
OSHA PEL C	10 mg/m <sup>3</sup> Basis: California permissible exposure limits for chemical contaminants (Title 8, Article 107)
<b>SODIUM SUCCINATE (13C4, 99%) (150-90-3)</b>	
No additional information available	
<b>WATER UNLABELED (7732-18-5)</b>	
<b>USA - ACGIH - Occupational Exposure Limits</b>	
ACGIH chemical category	No component of this product present at levels greater than or equal to 0.1% is identifiable as a carcinogen or potential carcinogen by ACGIH.
<b>8.2. Appropriate engineering controls</b>	
Appropriate engineering controls	: Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Ensure good ventilation of the work station.
Environmental exposure controls	: Avoid release to the environment.
<b>8.3. Individual protection measures/Personal protective equipment</b>	
<b>Personal protective equipment:</b> Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.	
<b>Materials for protective clothing:</b>	
Wear suitable protective clothing and gloves	
<b>Hand protection:</b>	
Wear suitable protective clothing and gloves	
<b>Eye protection:</b>	
Wear eye protection. Chemical goggles or face shield with safety glasses. Safety glasses	
<b>Skin and body protection:</b>	
Wear suitable protective clothing, gloves and eye/face protection	
<b>Respiratory protection:</b>	
In case of inadequate ventilation wear respiratory protection. Approved supplied air respirator	

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### Personal protective equipment symbol(s):



## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state	: Solid
Appearance	: Solid.
Color	: White to off-white
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Melting point	: No data available
Freezing point	: Not applicable
Boiling point	: No data available
Flash point	: Not applicable
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: Non flammable.
Vapor pressure	: No data available
Relative vapor density at 20°C	: No data available
Relative density	: Not applicable
Solubility	: No data available
Partition coefficient n-octanol/water (Log Pow)	: No data available
Auto-ignition temperature	: Not applicable
Decomposition temperature	: No data available
Viscosity, kinematic	: Not applicable
Viscosity, dynamic	: No data available
Explosion limits	: Not applicable
Explosive properties	: No data available
Oxidizing properties	: No data available

### 9.2. Other information

No additional information available

## SECTION 10: Stability and reactivity

### 10.1. Reactivity

The product is non-reactive under normal conditions of use, storage and transport.

### 10.2. Chemical stability

See storage and expiration date on CoA.

### 10.3. Possibility of hazardous reactions

No dangerous reactions known under normal conditions of use.

### 10.4. Conditions to avoid

None under recommended storage and handling conditions (see section 7).



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### 10.5. Incompatible materials

Strong oxidizing agents.

### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity (oral) : Harmful if swallowed.  
Acute toxicity (dermal) : Not classified  
Acute toxicity (inhalation) : Not classified

#### Metabolomics QC Standard Mix 2

ATE US (oral)	1600.694 mg/kg body weight
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#### D-GLUCOSE (U-13C6, 99%) (50-99-7)

LD50 oral rat	25800 mg/kg Remarks: Behavioral: Coma. Cyanosis. Diarrhea.
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ATE US (oral)	25800 mg/kg body weight
---------------	-------------------------

#### D-SUCROSE (GLUCOSE-13C6, 98%) (57-50-1)

LD50 oral rat	29700 mg/kg Somnolence (general depressed activity). Cynosis, diarrhea.
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ATE US (oral)	29700 mg/kg body weight
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#### CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)

LD50 oral rat	367.7 mg/kg - male and female (OECD Test Guideline 401)
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LD50 dermal	> 2000 mg/kg - male and female
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LC50 Inhalation - Rat	4.94 mg/l - male and female (Calculation method)
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ATE US (oral)	500 mg/kg body weight
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#### SODIUM PROPIONATE (13C3, 99%) (152571-51-2)

LD50 oral	6332 mg/kg mouse
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LD50 dermal rabbit	1640 mg/kg
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ATE US (dermal)	1640 mg/kg body weight
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#### SODIUM BENZOATE (RING-13C6, 99%) (532-32-1 (Unlabeled))

LD50 oral rat	2100 mg/kg
---------------	------------

ATE US (oral)	2100 mg/kg body weight
---------------	------------------------

Skin corrosion/irritation : Causes skin irritation.

#### D-SUCROSE (GLUCOSE-13C6, 98%) (57-50-1)

pH	5.5 – 7.5 at 342 g/l at 25 °C (77 °F)
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#### CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)

pH	5.5 – 6.5 at 10 g/l at 20 °C (68 °F)
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#### SODIUM BENZOATE (RING-13C6, 99%) (532-32-1 (Unlabeled))

pH	7 – 8.5 at 144.1 g/l at 25 °C (77 °F)
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<b>WATER UNLABELED (7732-18-5)</b>	
pH	6 – 8 at 25 °C (77 °F)
Serious eye damage/irritation	: Causes serious eye irritation.
<b>D-SUCROSE (GLUCOSE-13C6, 98%) (57-50-1)</b>	
pH	5.5 – 7.5 at 342 g/l at 25 °C (77 °F)
<b>CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)</b>	
pH	5.5 – 6.5 at 10 g/l at 20 °C (68 °F)
<b>SODIUM BENZOATE (RING-13C6, 99%) (532-32-1 (Unlabeled))</b>	
pH	7 – 8.5 at 144.1 g/l at 25 °C (77 °F)
<b>WATER UNLABELED (7732-18-5)</b>	
pH	6 – 8 at 25 °C (77 °F)
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
<b>CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)</b>	
IARC group	3 - Not classifiable
Reproductive toxicity	: Not classified
STOT-single exposure	: Not classified
STOT-repeated exposure	: Not classified
Aspiration hazard	: Not classified
Viscosity, kinematic	: Not applicable
Potential Adverse human health effects and symptoms	: This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.
Symptoms/effects after inhalation	: May be harmful if inhaled. May cause respiratory tract irritation. Vapours may cause drowsiness and dizziness.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious eye irritation.
Symptoms/effects after ingestion	: Harmful if swallowed.
<b>SECTION 12: Ecological information</b>	
<b>12.1. Toxicity</b>	
Ecology - general	: The product is not considered harmful to aquatic organisms or to cause long-term adverse effects in the environment.
<b>CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)</b>	
LC50 - Fish [1]	87 mg/l - <i>Leuciscus idus</i> (Golden orfe) - 96 h
EC50 - Crustacea [1]	182 mg/l static test - <i>Daphnia magna</i> (Water flea) - 48 h (DIN 38412)
ErC50 algae	Toxicity to algae static test - <i>Desmodesmus subspicatus</i> (green algae) - > 100 mg/l - 72 h (OECD Test Guideline 201)
<b>SODIUM OCTANOATE (13C8, 99%) (1984-06-1 (Unlabeled))</b>	
EC50 - Crustacea [1]	900 mg/l <i>Daphnia magna</i> (Water flea) - 24 h
<b>SODIUM PROPIONATE (13C3, 99%) (152571-51-2)</b>	
LC50 - Fish [1]	4740 mg/l <i>Pimephales promelas</i> (fathead minnow) - 96 h

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### SODIUM BENZOATE (RING-13C6, 99%) (532-32-1 (Unlabeled))

LC50 - Fish [1]	484 mg/l Pimephales promelas (fathead minnow) - 96 h
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### 12.2. Persistence and degradability

#### SODIUM OCTANOATE (13C8, 99%) (1984-06-1 (Unlabeled))

Persistence and degradability	Not available.
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#### SODIUM BENZOATE (RING-13C6, 99%) (532-32-1 (Unlabeled))

Biodegradation	90 % - Readily biodegradable. (OECD Test Guideline 301)
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### 12.3. Bioaccumulative potential

#### CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)

Partition coefficient n-octanol/water (Log Pow)	-0.091 at 23 °C (73 °F)
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#### SODIUM OCTANOATE (13C8, 99%) (1984-06-1 (Unlabeled))

Bioaccumulative potential	Not available.
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#### SODIUM BENZOATE (RING-13C6, 99%) (532-32-1 (Unlabeled))

Partition coefficient n-octanol/water (Log Pow)	-2.13
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### 12.4. Mobility in soil

#### SODIUM OCTANOATE (13C8, 99%) (1984-06-1 (Unlabeled))

Ecology - soil	Not available.
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### 12.5. Other adverse effects

Other adverse effects : Avoid release to the environment. Disposal must be done according to official regulations.

## SECTION 13: Disposal considerations

### 13.1. Disposal methods

Regional legislation (waste)	: Waste materials should be disposed of under conditions which meet Federal, State, and local environmental control regulations.
Product/Packaging disposal recommendations	: Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.
Ecology - waste materials	: Dispose of as unused product.

## SECTION 14: Transport information

In accordance with DOT / TDG / IMDG / IATA

### 14.1. UN number

Not regulated for transport

### 14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Not applicable
Proper Shipping Name (TDG)	: Not applicable
Proper Shipping Name (IMDG)	: Not applicable
Proper Shipping Name (IATA)	: Not applicable

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### 14.3. Transport hazard class(es)

#### DOT

Transport hazard class(es) (DOT) : Not applicable

#### TDG

Transport hazard class(es) (TDG) : Not applicable

#### IMDG

Transport hazard class(es) (IMDG) : Not applicable

#### IATA

Transport hazard class(es) (IATA) : Not applicable

### 14.4. Packing group

Packing group (DOT) : Not applicable

Packing group (TDG) : Not applicable

Packing group (IMDG) : Not applicable

Packing group (IATA) : Not applicable

### 14.5. Environmental hazards

Other information : No supplementary information available.

### 14.6. Special precautions for user

Special transport precautions : Not classified as dangerous in the meaning of transport regulations

#### DOT

No data available

#### TDG

No data available

#### IMDG

No data available

#### IATA

No data available

### 14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

#### Metabolomics QC Standard Mix 2

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
--	--

Commercial status of components according to the United States Environmental Protection Agency's Toxic Substances Control Act (TSCA):

Name	CAS-No.	Listing	Commercial status	Flags
D-GLUCOSE (U-13C6, 99%)	50-99-7	Not present	-	
D-SUCROSE (GLUCOSE-13C6, 98%)	57-50-1	Present	Active	

# Metabolomics QC Standard Mix 2

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Name	CAS-No.	Listing	Commercial status	Flags
CAFFEINE (TRIMETHYL-13C3, 99%)	78072-66-9	Not present	-	
SODIUM OCTANOATE (13C8, 99%)	1984-06-1 (Unlabeled)	Not present	-	
SODIUM PROPIONATE (13C3, 99%)	152571-51-2	Not present	-	
SODIUM BENZOATE (RING-13C6, 99%)	532-32-1 (Unlabeled)	Not present	-	
SODIUM CITRATE (1,5,6-CARBOXY-13C3, 99%)	18996-35-5	Present	Active	
SODIUM STEARATE (U-13C18, 98%) 97% CHEMICAL PURITY	822-16-2	Present	Active	
SODIUM SUCCINATE (13C4, 99%)	150-90-3	Present	Active	
WATER UNLABELED	7732-18-5	Not present	-	

### D-GLUCOSE (U-13C6, 99%) (50-99-7)

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
--	--

### D-SUCROSE (GLUCOSE-13C6, 98%) (57-50-1)

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
--	--

### CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Delayed (chronic) health hazard

### SODIUM OCTANOATE (13C8, 99%) (1984-06-1 (Unlabeled))

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard

### SODIUM PROPIONATE (13C3, 99%) (152571-51-2)

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard

### SODIUM BENZOATE (RING-13C6, 99%) (532-32-1 (Unlabeled))

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard

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### SODIUM CITRATE (1,5,6-CARBOXY-13C3, 99%) (18996-35-5)

SARA Section 302 Threshold Planning Quantity (TPQ)

Not subject to reporting requirements of the United States SARA Section 302.

### SODIUM STEARATE (U-13C18, 98%) 97% CHEMICAL PURITY (822-16-2)

SARA Section 302 Threshold Planning Quantity (TPQ)

Not subject to reporting requirements of the United States SARA Section 302.

### SODIUM SUCCINATE (13C4, 99%) (150-90-3)

SARA Section 302 Threshold Planning Quantity (TPQ)

Not subject to reporting requirements of the United States SARA Section 302.

### WATER UNLABELED (7732-18-5)

SARA Section 302 Threshold Planning Quantity (TPQ)

Not subject to reporting requirements of the United States SARA Section 302.

## 15.2. International regulations

### CANADA

#### D-GLUCOSE (U-13C6, 99%) (50-99-7)

Not listed on the Canadian DSL (Domestic Substances List)/NDSL (Non-Domestic Substances List)

#### D-SUCROSE (GLUCOSE-13C6, 98%) (57-50-1)

Listed on the Canadian DSL (Domestic Substances List)

#### CAFFEINE (TRIMETHYL-13C3, 99%) (78072-66-9)

Listed on the Canadian DSL (Domestic Substances List)

#### SODIUM PROPIONATE (13C3, 99%) (152571-51-2)

Not listed on the Canadian DSL (Domestic Substances List)/NDSL (Non-Domestic Substances List)

#### SODIUM CITRATE (1,5,6-CARBOXY-13C3, 99%) (18996-35-5)

Listed on the Canadian DSL (Domestic Substances List)

#### SODIUM STEARATE (U-13C18, 98%) 97% CHEMICAL PURITY (822-16-2)

Listed on the Canadian DSL (Domestic Substances List)

#### SODIUM SUCCINATE (13C4, 99%) (150-90-3)

Listed on the Canadian DSL (Domestic Substances List)

#### WATER UNLABELED (7732-18-5)

Listed on the Canadian DSL (Domestic Substances List)

### EU-Regulations

No additional information available

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### National regulations

#### D-SUCROSE (GLUCOSE-13C6, 98%) (57-50-1)

Listed on INSQ (Mexican National Inventory of Chemical Substances)

#### SODIUM CITRATE (1,5,6-CARBOXY-13C3, 99%) (18996-35-5)

Listed on INSQ (Mexican National Inventory of Chemical Substances)

#### SODIUM STEARATE (U-13C18, 98%) 97% CHEMICAL PURITY (822-16-2)

Listed on INSQ (Mexican National Inventory of Chemical Substances)

### 15.3. US State regulations

Component	State or local regulations
D-GLUCOSE (U-13C6, 99%)(50-99-7)	U.S. - Pennsylvania - RTK (Right to Know) List; U.S. - New Jersey - Right to Know Hazardous Substance List
D-SUCROSE (GLUCOSE-13C6, 98%)(57-50-1)	U.S. - Massachusetts - Right To Know List; U.S. - Pennsylvania - RTK (Right to Know) List
CAFFEINE (TRIMETHYL-13C3, 99%)(78072-66-9)	U.S. - Pennsylvania - RTK (Right to Know) List; U.S. - New Jersey - Right to Know Hazardous Substance List
WATER UNLABELED(7732-18-5)	U.S. - Pennsylvania - RTK (Right to Know) List; U.S. - New Jersey - Right to Know Hazardous Substance List

## SECTION 16: Other information

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Revision date : 03/18/2024

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Full text of H-phrases	
H302	Harmful if swallowed
H312	Harmful in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation

Safety Data Sheet (SDS), USA

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product.