



CAMBRIDGE ISOTOPE LABORATORIES

PRODUCT AND COMPANY IDENTIFICATION

Product Name: Metabolomics QReSS™ Kit (unlabeled)

Catalog No: MSK-QRESS-US-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 1-703-741-5970

HAZARDS IDENTIFICATION

Emergency Overview

OSHA Hazards

Irritant/Harmful

GHS Classification(s)

Skin irritation -Cat 2

Eye irritation -Cat 2A

Specific target organ toxicity - single exposure -Cat 3

GHS Label elements, including precautionary statements



Pictograms

Signal word Warning

Hazard statement(s)

See individual Safety Data Sheets

COMPOSITION

Each kit contains:

MSK-QRESS1-US-1	Metabolomics QReSS™ Standard Mix 1 Unlabeled
MSK-QRESS2-US-1	Metabolomics QReSS™ Standard Mix 2 Unlabeled



Metabolomics QReSS™ Standard Mix 1 (unlabeled)

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Issue date: 5/28/2020 Revision date: 3/19/2024 Supersedes: 7/7/2021 Version: 2.1

SECTION 1: Identification

1.1. Identification

Product form : Mixture
Product name : Metabolomics QReSS™ Standard Mix 1 (unlabeled)
Product code : MSK-QRESS1-US

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 - 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

Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2	H319	Causes serious eye irritation
Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation	H335	May cause respiratory irritation

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) : H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
Precautionary statements (GHS US) : P261 - Avoid breathing dust/fume/gas/mist/vapors/spray.
P264 - Wash hands, forearms and face thoroughly after handling.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear protective gloves/protective clothing/eye protection/face protection.
P302+P352 - If on skin: Wash with plenty of water.
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing.
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.
P312 - Call a poison center or doctor if you feel unwell.
P321 - Specific treatment (see supplemental first aid instruction on this label).
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.
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.
P405 - Store locked up.
P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation.

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
L-ALANINE UNLABELED	CAS-No.: 56-41-7	17.79	Not classified
CREATININE UNLABELED	CAS-No.: 60-27-5	17.79	Not classified
L-TRYPTOPHAN UNLABELED	CAS-No.: 73-22-3	17.79	Not classified
L-TYROSINE UNLABELED	CAS-No.: 60-18-4	17.79	Skin Irrit. 2, H315 Eye Irrit. 2, H319 STOT SE 3, H335
L-PHENYLALANINE UNLABELED	CAS-No.: 63-91-2	17.79	Not classified
THYMINE UNLABELED	CAS-No.: 65-71-4	3.56	Not classified
ETHANOLAMINE HCl UNLABELED	CAS-No.: 141-43-5	1.78	Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335
HYPOXANTHINE UNLABELED	CAS-No.: 68-94-0	1.78	Not classified
1,4-BUTANEDIAMINE:2HCl UNLABELED	CAS-No.: 333-93-7	1.78	Skin Irrit. 2, H315 Eye Irrit. 2, H319 STOT SE 3, H335
L-LEUCINE UNLABELED	CAS-No.: 61-90-5	0.89	Not classified
NICOTINAMIDE UNLABELED	CAS-No.: 98-92-0	0.89	Skin Irrit. 2, H315 Eye Irrit. 2, H319 STOT SE 3, H335
GUANOSINE UNLABELED	CAS-No.: 118-00-3	0.36	Not classified

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

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SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general	: If you feel unwell, seek medical advice (show the label where possible). Evacuate danger area.
First-aid measures after inhalation	: When symptoms occur: go into open air and ventilate suspected area. If not breathing give artificial respiration. Get medical advice/attention.
First-aid measures after skin contact	: Wash with plenty of soap and water. and soap. Get immediate medical advice/attention.
First-aid measures after eye contact	: Rinse cautiously with water for several minutes.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention.

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 irritation.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious 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 : Water spray. Dry chemical powder, alcohol-resistant foam, carbon dioxide (CO₂).

5.2. Specific hazards arising from the chemical

Hazardous decomposition products in case of fire : Carbon oxides (CO, CO₂).

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions	: Fight fire with normal precautions from a reasonable distance. Wear a self contained breathing apparatus. Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection. Wear recommended personal protective equipment.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Avoid breathing vapors, mist, gas. Avoid dust formation.

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".

6.2. Environmental precautions

Prevent entry to sewers and public waters. Do not allow to enter drains or water courses. Avoid release to the environment.

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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 : This material and its container must be disposed of in a safe way, and as per local legislation.

6.4. Reference to other sections

For further information refer to section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Provide adequate ventilation to minimize dust and/or vapor concentrations.
Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Handle in accordance with good industrial hygiene and safety practice.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : 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

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No additional information available

L-ALANINE UNLABELED (56-41-7)

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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CREATININE UNLABELED (60-27-5)

No additional information available

ETHANOLAMINE HCl UNLABELED (141-43-5)

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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HYPOXANTHINE UNLABELED (68-94-0)

No additional information available

L-LEUCINE UNLABELED (61-90-5)

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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NICOTINAMIDE UNLABELED (98-92-0)

No additional information available

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L-TRYPTOPHAN UNLABELED (73-22-3)	
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.
L-TYROSINE UNLABELED (60-18-4)	
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.
THYMINE UNLABELED (65-71-4)	
No additional information available	
L-PHENYLALANINE UNLABELED (63-91-2)	
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.
GUANOSINE UNLABELED (118-00-3)	
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.
1,4-BUTANEDIAMINE:2HCL UNLABELED (333-93-7)	
No additional information available	

8.2. Appropriate engineering controls

Appropriate engineering controls	: Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.
Environmental exposure controls	: Avoid release to the environment.

8.3. Individual protection measures/Personal protective equipment

Personal protective equipment:

Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.

Materials for protective clothing:
Wear suitable protective clothing and gloves
Hand protection:
Wear suitable protective clothing and gloves
Eye protection:
Wear eye protection. Chemical goggles or face shield with safety glasses
Skin and body protection:
Wear suitable protective clothing, gloves and eye/face protection
Respiratory protection:
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	: Powder.
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
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

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10.5. Incompatible materials

Strong oxidizing agents.

10.6. Hazardous decomposition products

Carbon oxides (CO, CO₂).

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

L-ALANINE UNLABELED (56-41-7)

LD50 oral rat	> 5110 mg/kg male and female
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HYPOXANTHINE UNLABELED (68-94-0)

LD50, intraperitoneal, mouse	750 mg/kg
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L-LEUCINE UNLABELED (61-90-5)

LD50 oral rat	> 16000 mg/kg male and female
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NICOTINAMIDE UNLABELED (98-92-0)

LD50 oral rat	3500 mg/kg
ATE US (oral)	3500 mg/kg body weight

L-TRYPTOPHAN UNLABELED (73-22-3)

LD50 oral rat	> 16000 mg/kg
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THYMINE UNLABELED (65-71-4)

LD50 oral	3500 mg/kg mouse
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Skin corrosion/irritation : Causes skin irritation.

L-ALANINE UNLABELED (56-41-7)

pH	5.5 – 7 at 89.1 g/l at 25 °C (77 °F)
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CREATININE UNLABELED (60-27-5)

pH	7.5 – 8.5 at 50 g/l at 20 °C (68 °F)
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L-PHENYLALANINE UNLABELED (63-91-2)

pH	5 – 7 at 16.5 g/l at 25 °C (77 °F)
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Serious eye damage/irritation : Causes serious eye irritation.

L-ALANINE UNLABELED (56-41-7)

pH	5.5 – 7 at 89.1 g/l at 25 °C (77 °F)
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CREATININE UNLABELED (60-27-5)

pH	7.5 – 8.5 at 50 g/l at 20 °C (68 °F)
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L-PHENYLALANINE UNLABELED (63-91-2)

pH	5 – 7 at 16.5 g/l at 25 °C (77 °F)
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Respiratory or skin sensitization : Not classified

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Germ cell mutagenicity : Not classified

Carcinogenicity : Not classified

L-TYROSINE UNLABELED (60-18-4)

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.
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Reproductive toxicity : Not classified

STOT-single exposure : May cause respiratory irritation.

ETHANOLAMINE HCl UNLABELED (141-43-5)

STOT-single exposure	May cause respiratory irritation.
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NICOTINAMIDE UNLABELED (98-92-0)

STOT-single exposure	May cause respiratory irritation.
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L-TYROSINE UNLABELED (60-18-4)

STOT-single exposure	May cause respiratory irritation.
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1,4-BUTANEDIAMINE:2HCl UNLABELED (333-93-7)

STOT-single exposure	May cause respiratory irritation.
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STOT-repeated exposure : Not classified

L-LEUCINE UNLABELED (61-90-5)

NOAEL (oral,rat,90 days)	3840 mg/kg bodyweight/day female
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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 irritation.

Symptoms/effects after skin contact : Causes skin irritation.

Symptoms/effects after eye contact : Causes serious 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.

L-ALANINE UNLABELED (56-41-7)

EC50 - Crustacea [1]	> 100 mg/l static test EC50 - Daphnia magna (Water flea) - 48 h (OECD Test Guideline 202)
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12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

L-ALANINE UNLABELED (56-41-7)

Partition coefficient n-octanol/water (Log Pow)	-2.74 at 20 °C (68 °F)
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L-TYROSINE UNLABELED (60-18-4)

Partition coefficient n-octanol/water (Log Pow)	-2.26 at 25 °C (77 °F)
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GUANOSINE UNLABELED (118-00-3)

Partition coefficient n-octanol/water (Log Pow)	1.918
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12.4. Mobility in soil

No additional information available

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

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

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14.5. Environmental hazards

Other information : No supplementary information available.

14.6. Special precautions for user

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

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SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
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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-ALANINE UNLABELED	56-41-7	Present	Active	
CREATININE UNLABELED	60-27-5	Present	Active	
ETHANOLAMINE HCl UNLABELED	141-43-5	Present	Active	
HYPOXANTHINE UNLABELED	68-94-0	Present	Active	
L-LEUCINE UNLABELED	61-90-5	Present	Active	
NICOTINAMIDE UNLABELED	98-92-0	Present	Active	
L-TRYPTOPHAN UNLABELED	73-22-3	Present	Active	
L-TYROSINE UNLABELED	60-18-4	Not present	-	
THYMINE UNLABELED	65-71-4	Present	Active	
L-PHENYLALANINE UNLABELED	63-91-2	Present	Active	
GUANOSINE UNLABELED	118-00-3	Present	Active	
1,4-BUTANEDIAMINE:2HCl UNLABELED	333-93-7	Present	Active	

L-ALANINE UNLABELED (56-41-7)

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
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CREATININE UNLABELED (60-27-5)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.

ETHANOLAMINE HCl UNLABELED (141-43-5)	
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
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard

HYPOXANTHINE UNLABELED (68-94-0)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.

L-LEUCINE UNLABELED (61-90-5)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.

NICOTINAMIDE UNLABELED (98-92-0)	
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

L-TRYPTOPHAN UNLABELED (73-22-3)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.

L-TYROSINE UNLABELED (60-18-4)	
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

THYMINE UNLABELED (65-71-4)	
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.

L-PHENYLALANINE UNLABELED (63-91-2)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.

GUANOSINE UNLABELED (118-00-3)	
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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1,4-BUTANEDIAMINE:2HCL UNLABELED (333-93-7)

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

15.2. International regulations

CANADA

L-ALANINE UNLABELED (56-41-7)

Listed on the Canadian DSL (Domestic Substances List)

CREATININE UNLABELED (60-27-5)

Listed on the Canadian DSL (Domestic Substances List)

ETHANOLAMINE HCI UNLABELED (141-43-5)

Listed on the Canadian DSL (Domestic Substances List)

HYPOXANTHINE UNLABELED (68-94-0)

Listed on the Canadian DSL (Domestic Substances List)

L-LEUCINE UNLABELED (61-90-5)

Listed on the Canadian DSL (Domestic Substances List)

NICOTINAMIDE UNLABELED (98-92-0)

Listed on the Canadian DSL (Domestic Substances List)

L-TRYPTOPHAN UNLABELED (73-22-3)

Listed on the Canadian DSL (Domestic Substances List)

L-TYROSINE UNLABELED (60-18-4)

Listed on the Canadian DSL (Domestic Substances List)

THYMINE UNLABELED (65-71-4)

Listed on the Canadian NDSL (Non-Domestic Substances List)

L-PHENYLALANINE UNLABELED (63-91-2)

Listed on the Canadian DSL (Domestic Substances List)

GUANOSINE UNLABELED (118-00-3)

Listed on the Canadian DSL (Domestic Substances List)

1,4-BUTANEDIAMINE:2HCL UNLABELED (333-93-7)

Listed on the Canadian NDSL (Non-Domestic Substances List)

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EU-Regulations

No additional information available

National regulations

L-ALANINE UNLABELED (56-41-7)
Listed on INSQ (Mexican National Inventory of Chemical Substances)

CREATININE UNLABELED (60-27-5)
Listed on INSQ (Mexican National Inventory of Chemical Substances)

ETHANOLAMINE HCl UNLABELED (141-43-5)
Listed on INSQ (Mexican National Inventory of Chemical Substances)

L-LEUCINE UNLABELED (61-90-5)
Listed on INSQ (Mexican National Inventory of Chemical Substances)

NICOTINAMIDE UNLABELED (98-92-0)
Listed on INSQ (Mexican National Inventory of Chemical Substances)

L-TRYPTOPHAN UNLABELED (73-22-3)
Listed on INSQ (Mexican National Inventory of Chemical Substances)

THYMINE UNLABELED (65-71-4)
Listed on INSQ (Mexican National Inventory of Chemical Substances)

15.3. US State regulations

Component	State or local regulations
ETHANOLAMINE HCl UNLABELED(141-43-5)	U.S. - Massachusetts - Right To Know List; U.S. - New Jersey - Right to Know Hazardous Substance List; U.S. - Pennsylvania - RTK (Right to Know) List
L-TYROSINE UNLABELED(60-18-4)	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

: 03/19/2024

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

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Full text of H-phrases	
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 QReSS™ Standard Mix 2 (unlabeled)

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Issue date: 5/28/2020 Revision date: 3/19/2024 Supersedes: 7/7/2021 Version: 2.1

SECTION 1: Identification

1.1. Identification

Product form : Mixture
Product name : Metabolomics QReSS™ Standard Mix 2 (unlabeled)
Product code : MSK-QRESS2-US

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 - 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

Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2	H319	Causes serious eye irritation
Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation	H335	May cause respiratory irritation

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) : H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
Precautionary statements (GHS US) : P261 - Avoid breathing dust/fume/gas/mist/vapors/spray.
P264 - Wash hands, forearms and face thoroughly after handling.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear protective gloves/protective clothing/eye protection/face protection.
P302+P352 - If on skin: Wash with plenty of water.
P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing.
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.
P312 - Call a poison center or doctor if you feel unwell.
P321 - Specific treatment (see supplemental first aid instruction on this label).
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.
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.
P405 - Store locked up.
P501 - Dispose of contents/container to hazardous or special waste collection point, in accordance with local, regional, national and/or international regulation.

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
FUMARIC ACID UNLABELED	CAS-No.: 110-17-8	24.1	Eye Irrit. 2A, H319
SODIUM PALMITATE UNLABELED	CAS-No.: 408-35-5	24.1	Eye Irrit. 2A, H319
SODIUM PYRUVATE UNLABELED	CAS-No.: 113-24-6	24.1	Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335
ALPHA-KETOGLUTARIC ACID, DISODIUM SALT DIHYDRATE UNLABELED	CAS-No.: 305-72-6	24.1	Not classified
CITRIC ACID UNLABELED	CAS-No.: 77-92-9	2.41	Eye Irrit. 2A, H319
INDOLE-3-ACETIC ACID UNLABELED	CAS-No.: 87-51-4	1.2	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 : If you feel unwell, seek medical advice (show the label where possible). Evacuate danger area.
First-aid measures after inhalation : When symptoms occur: go into open air and ventilate suspected area. If not breathing give artificial respiration. Get medical advice/attention.
First-aid measures after skin contact : Wash with plenty of soap and water. and soap. Get immediate medical advice/attention.
First-aid measures after eye contact : Rinse cautiously with water for several minutes.
First-aid measures after ingestion : Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get medical advice/attention.

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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 irritation.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious 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 : Water spray. Dry chemical powder, alcohol-resistant foam, carbon dioxide (CO₂).

5.2. Specific hazards arising from the chemical

Hazardous decomposition products in case of fire : Carbon oxides (CO, CO₂).

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions	: Fight fire with normal precautions from a reasonable distance. Wear a self contained breathing apparatus. Do not enter fire area without proper protective equipment, including respiratory protection.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection. Wear recommended personal protective equipment.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Emergency procedures : Avoid breathing vapors, mist, gas. Avoid dust formation.

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".

6.2. Environmental precautions

Prevent entry to sewers and public waters. Do not allow to enter drains or water courses. Avoid release to the environment.

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	: This material and its container must be disposed of in a safe way, and as per local legislation.

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 : Provide adequate ventilation to minimize dust and/or vapor concentrations.
Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Handle in accordance with good industrial hygiene and safety practice.

7.2. Conditions for safe storage, including any incompatibilities

Technical measures : 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

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No additional information available

CITRIC ACID UNLABELED (77-92-9)

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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FUMARIC ACID UNLABELED (110-17-8)

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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INDOLE-3-ACETIC ACID UNLABELED (87-51-4)

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.
-------------------------	--

SODIUM PALMITATE UNLABELED (408-35-5)

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.
-------------------------	--

SODIUM PYRUVATE UNLABELED (113-24-6)

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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ALPHA-KETOGLUTARIC ACID, DISODIUM SALT DIHYDRATE UNLABELED (305-72-6)

No additional information available

8.2. Appropriate engineering controls

Appropriate engineering controls : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.
Environmental exposure controls : Avoid release to the environment.

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8.3. Individual protection measures/Personal protective equipment

Personal protective equipment:

Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.

Materials for protective clothing:

Wear suitable protective clothing and gloves

Hand protection:

Wear suitable protective clothing and gloves

Eye protection:

Wear eye protection. Chemical goggles or face shield with safety glasses

Skin and body protection:

Wear suitable protective clothing, gloves and eye/face protection

Respiratory protection:

In case of inadequate ventilation wear respiratory protection. Approved supplied air 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	: Powder.
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
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

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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

Strong oxidizing agents.

10.6. Hazardous decomposition products

Carbon oxides (CO, CO₂).

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

CITRIC ACID UNLABELED (77-92-9)	
LD50 oral rat	5400 mg/kg (OECD Test Guideline 401)
LD50 dermal rat	> 2000 mg/kg (OECD Test Guideline 402)
ATE US (oral)	9300 mg/kg body weight
ATE US (dermal)	20000 mg/kg body weight

FUMARIC ACID UNLABELED (110-17-8)	
LD50 oral rat	9300 mg/kg female (OECD Test Guideline 401)
LD50 dermal rabbit	20000 mg/kg (OECD Test Guideline 402)
ATE US (oral)	9300 mg/kg body weight
ATE US (dermal)	20000 mg/kg body weight
LD50, intraperitoneal, mouse	100 mg/kg

Skin corrosion/irritation : Causes skin irritation.

CITRIC ACID UNLABELED (77-92-9)	
pH	1.8 at ca.50 g/l at °C (77 °F)

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FUMARIC ACID UNLABELED (110-17-8)	
pH	2.1 at 4.9 g/l at 20 °C (68 °F)
SODIUM PYRUVATE UNLABELED (113-24-6)	
pH	7
Serious eye damage/irritation	: Causes serious eye irritation.
CITRIC ACID UNLABELED (77-92-9)	
pH	1.8 at ca.50 g/l at °C (77 °F)
FUMARIC ACID UNLABELED (110-17-8)	
pH	2.1 at 4.9 g/l at 20 °C (68 °F)
SODIUM PYRUVATE UNLABELED (113-24-6)	
pH	7
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
STOT-single exposure	: May cause respiratory irritation.
SODIUM PYRUVATE UNLABELED (113-24-6)	
STOT-single exposure	May cause respiratory irritation.
STOT-repeated exposure	: Not classified
FUMARIC ACID UNLABELED (110-17-8)	
NOAEL (oral,rat,90 days)	600 mg/kg bodyweight/day male
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 irritation.
Symptoms/effects after skin contact	: Causes skin irritation.
Symptoms/effects after eye contact	: Causes serious 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.

CITRIC ACID UNLABELED (77-92-9)	
LC50 - Fish [1]	440 mg/l Mortality - Leuciscus idus melanotus - 48 h (OECD Test Guideline 203)
EC50 - Crustacea [1]	1535 mg/l Static test - Daphnia magna (Water flea) - 24 h
FUMARIC ACID UNLABELED (110-17-8)	
LC50 - Fish [1]	> 100 mg/l Danio rerio (Zebra fish) - 96 h (OECD Test Guideline 203)
EC50 - Crustacea [1]	212 mg/l Immobilization - Daphnia magna (Water flea) - 48 h (OECD Test Guideline 202)
EC50 - Other aquatic organisms [1]	> 300 mg/l Growth inhibition - activated sludge - 3 h (OECD Test Guideline 209)

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FUMARIC ACID UNLABELED (110-17-8)

ErC50 algae	> 100 mg/l Pseudokirchneriella subcapitata - 72 h (OECD Test Guideline 201)
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12.2. Persistence and degradability

FUMARIC ACID UNLABELED (110-17-8)

Persistence and degradability	Aerobic - exposure time: 28 d.
Biodegradation	67.5 % Readily biodegradable

12.3. Bioaccumulative potential

CITRIC ACID UNLABELED (77-92-9)

Partition coefficient n-octanol/water (Log Pow)	-1.639 at 20 °C (68 °F)
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FUMARIC ACID UNLABELED (110-17-8)

Partition coefficient n-octanol/water (Log Pow)	0.46 at 20 °C (68 °F)
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12.4. Mobility in soil

No additional information available

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

14.3. Transport hazard class(es)

DOT

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

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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

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 QReSS™ Standard Mix 2 (unlabeled)

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
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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
CITRIC ACID UNLABELED	77-92-9	Present	Active	
FUMARIC ACID UNLABELED	110-17-8	Present	Active	
INDOLE-3-ACETIC ACID UNLABELED	87-51-4	Present	Active	
SODIUM PALMITATE UNLABELED	408-35-5	Present	Active	
SODIUM PYRUVATE UNLABELED	113-24-6	Present	Active	
ALPHA-KETOGLUTARIC ACID, DISODIUM SALT DIHYDRATE UNLABELED	305-72-6	Not present	-	

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CITRIC ACID UNLABELED (77-92-9)	
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

FUMARIC ACID UNLABELED (110-17-8)	
Not subject to reporting requirements of the United States SARA Section 313	
CERCLA RQ	5000 lb
SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Delayed (chronic) health hazard

SODIUM PALMITATE UNLABELED (408-35-5)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302

SODIUM PYRUVATE UNLABELED (113-24-6)	
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

ALPHA-KETOGLUTARIC ACID, DISODIUM SALT DIHYDRATE UNLABELED (305-72-6)	
SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.

15.2. International regulations

CANADA

CITRIC ACID UNLABELED (77-92-9)	
Listed on the Canadian DSL (Domestic Substances List)	

FUMARIC ACID UNLABELED (110-17-8)	
Listed on the Canadian DSL (Domestic Substances List)	

INDOLE-3-ACETIC ACID UNLABELED (87-51-4)	
Listed on the Canadian NDSL (Non-Domestic Substances List)	

SODIUM PALMITATE UNLABELED (408-35-5)	
Listed on the Canadian DSL (Domestic Substances List)	

SODIUM PYRUVATE UNLABELED (113-24-6)	
Listed on the Canadian DSL (Domestic Substances List)	

ALPHA-KETOGLUTARIC ACID, DISODIUM SALT DIHYDRATE UNLABELED (305-72-6)	
Listed on the Canadian DSL (Domestic Substances List)	

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EU-Regulations

No additional information available

National regulations

CITRIC ACID UNLABELED (77-92-9)

Listed on INSQ (Mexican National Inventory of Chemical Substances)

FUMARIC ACID UNLABELED (110-17-8)

Listed on INSQ (Mexican National Inventory of Chemical Substances)

INDOLE-3-ACETIC ACID UNLABELED (87-51-4)

Listed on INSQ (Mexican National Inventory of Chemical Substances)

15.3. US State regulations

Component	State or local regulations
FUMARIC ACID UNLABELED(110-17-8)	U.S. - Massachusetts - Right To Know List; U.S. - New Jersey - Right to Know Hazardous Substance List; U.S. - Pennsylvania - RTK (Right to Know) List

SECTION 16: Other information

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

Revision date

: 03/19/2024

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.