



Metabolomics QReSS™ Standard Mix 2

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: 3/18/2024 Supersedes: 7/7/2021 Version: 2.1

SECTION 1: Identification

1.1. Identification

Product form : Mixture
Product name : Metabolomics QReSS™ Standard Mix 2
Product code : MSK-QRESS2

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 doctor, a POISON CENTER if you feel unwell.
P321 - Specific treatment (see Hazardous component(s) for labeling 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 (13C4, 99%)	CAS-No.: 201595-62-2	30.769	Eye Irrit. 2A, H319
SODIUM PYRUVATE (13C3, 99%)	CAS-No.: 142014-11-7	30.769	Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335
ALPHA-KETOGLUTARIC ACID, DISODIUM SALT (1,2,3,4-13C4, 99%)	CAS-No.: 305-72-6 (Unlabeled)	30.769	Not classified
CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%)	CAS-No.: 77-92-9 (Unlabeled)	3.077	Eye Irrit. 2A, H319
SODIUM PALMITATE (U-13C16, 98%+)	CAS-No.: 408-35-5 (unlabeled)	3.077	Eye Irrit. 2A, H319
INDOLE-3-ACETIC ACID (PHENYL-13C6, 99%)	CAS-No.: 87-51-4 (Unlabeled)	1.538	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 (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (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.
FUMARIC ACID (13C4, 99%) (201595-62-2)	
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.
INDOLE-3-ACETIC ACID (PHENYL-13C6, 99%) (87-51-4 (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.
SODIUM PALMITATE (U-13C16, 98%+) (408-35-5 (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.
SODIUM PYRUVATE (13C3, 99%) (142014-11-7)	
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.
ALPHA-KETOGLUTARIC ACID, DISODIUM SALT (1,2,3,4-13C4, 99%) (305-72-6 (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.

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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

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	: Mixture contains one or more component(s) which have the following odour:
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

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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

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 (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (Unlabeled))	
LD50 oral rat	5400 mg/kg
LD50 dermal rat	> 2000 mg/kg
ATE US (oral)	5400 mg/kg body weight
FUMARIC ACID (13C4, 99%) (201595-62-2)	
LD50 oral rat	9300 mg/kg female: (OECD Test Guideline 401)
LD50 oral	LD50 Intraperitoneal - Mouse - 100 mg/kg
LD50 dermal rabbit	20000 mg/kg female: (OECD Test Guideline 402)
ATE US (oral)	9300 mg/kg body weight
ATE US (dermal)	20000 mg/kg body weight

Skin corrosion/irritation : Causes skin irritation.

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CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (Unlabeled))	
pH	1.8 at ca.50 g/l at °C (77 °F)
FUMARIC ACID (13C4, 99%) (201595-62-2)	
pH	2.1 at 4.9 g/l at 20 °C (68 °F)
SODIUM PYRUVATE (13C3, 99%) (142014-11-7)	
pH	7

Serious eye damage/irritation : Causes serious eye irritation.

CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (Unlabeled))	
pH	1.8 at ca.50 g/l at °C (77 °F)
FUMARIC ACID (13C4, 99%) (201595-62-2)	
pH	2.1 at 4.9 g/l at 20 °C (68 °F)
SODIUM PYRUVATE (13C3, 99%) (142014-11-7)	
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 (13C3, 99%) (142014-11-7)	
STOT-single exposure	May cause respiratory irritation.
STOT-repeated exposure	: Not classified
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 (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (Unlabeled))	
LC50 - Fish [1]	440 mg/l <i>Leuciscus idus melanotus</i> - 48 h - mortality
EC50 - Crustacea [1]	1535 mg/l <i>Daphnia magna</i> (Water flea) - 24 h - static test
FUMARIC ACID (13C4, 99%) (201595-62-2)	
LC50 - Fish [1]	semi-static test > 100 mg/l - <i>Danio rerio</i> (zebra fish) - 96 h (OECD Test Guideline 203)
EC50 - Crustacea [1]	212 mg/l Immobilization: <i>Daphnia magna</i> (Water flea) - 48 h (OECD Test Guideline 202)
EC50 - Other aquatic organisms [1]	Respiration inhibition EC50 > 300 mg/l - activated sludge - 3 h (OECD Test Guideline 209)

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FUMARIC ACID (13C4, 99%) (201595-62-2)	
ErC50 algae	Growth inhibition EC50 > 100 mg/l - Pseudokirchneriella subcapitata - 72 h (OECD Test Guideline 201)

12.2. Persistence and degradability

CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (Unlabeled))	
Persistence and degradability	Not available.

FUMARIC ACID (13C4, 99%) (201595-62-2)	
Persistence and degradability	Biodegradability aerobic - Exposure time 28 d. Readily biodegradable.
Biodegradation	67.5 % (OECD Test Guideline 301B)

SODIUM PALMITATE (U-13C16, 98%+) (408-35-5 (unlabeled))	
Persistence and degradability	Not available.

12.3. Bioaccumulative potential

CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (Unlabeled))	
Partition coefficient n-octanol/water (Log Pow)	-1.639 at 20 °C (68 °F)
Bioaccumulative potential	Not available.

FUMARIC ACID (13C4, 99%) (201595-62-2)	
Partition coefficient n-octanol/water (Log Pow)	0.46 at 20 °C (68 °F)

SODIUM PALMITATE (U-13C16, 98%+) (408-35-5 (unlabeled))	
Bioaccumulative potential	Not available.

12.4. Mobility in soil

CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (Unlabeled))	
Ecology - soil	Not available.

SODIUM PALMITATE (U-13C16, 98%+) (408-35-5 (unlabeled))	
Ecology - soil	Not 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.

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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.

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

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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
CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%)	77-92-9 (Unlabeled)	Not present	-	
FUMARIC ACID (13C4, 99%)	201595-62-2	Not present	-	
INDOLE-3-ACETIC ACID (PHENYL-13C6, 99%)	87-51-4 (Unlabeled)	Not present	-	
SODIUM PALMITATE (U-13C16, 98%+)	408-35-5 (unlabeled)	Not present	-	
SODIUM PYRUVATE (13C3, 99%)	142014-11-7	Not present	-	
ALPHA-KETOGLUTARIC ACID, DISODIUM SALT (1,2,3,4-13C4, 99%)	305-72-6 (Unlabeled)	Not present	-	

CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%) (77-92-9 (Unlabeled))

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302.
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SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard
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FUMARIC ACID (13C4, 99%) (201595-62-2)

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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SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Delayed (chronic) health hazard
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SODIUM PALMITATE (U-13C16, 98%+) (408-35-5 (unlabeled))

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302
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SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard
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SODIUM PYRUVATE (13C3, 99%) (142014-11-7)

SARA Section 302 Threshold Planning Quantity (TPQ)	Not subject to reporting requirements of the United States SARA Section 302
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ALPHA-KETOGLUTARIC ACID, DISODIUM SALT (1,2,3,4-13C4, 99%) (305-72-6 (Unlabeled))

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

CANADA

FUMARIC ACID (13C4, 99%) (201595-62-2)

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

SODIUM PYRUVATE (13C3, 99%) (142014-11-7)

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

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State or local regulations	U.S. - New Jersey - Right to Know Hazardous Substance List U.S. - Pennsylvania - RTK (Right to Know) List
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Component	State or local regulations
CITRIC ACID (1,5,6-CARBOXYL-13C3, 99%)(77-92-9 (Unlabeled))	U.S. - Pennsylvania - RTK (Right to Know) List; U.S. - New Jersey - Right to Know Hazardous Substance List

SECTION 16: Other information

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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

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