

SAFETY DATA SHEET

Version 8.13
Revision Date 08/05/2024
Print Date 08/06/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : CombiTitrant 5 Keto 1 ml \triangleq ca. 5 mg H₂O
Aquastar®

Product Number : 1.88006
Catalogue No. : 188006
Brand : Millipore

1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Reagent for analysis
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Skin irritation (Category 2), H315
Eye irritation (Category 2A), H319
Carcinogenicity (Category 2), H351
Reproductive toxicity (Category 1B), H360

Specific target organ toxicity - repeated exposure, Oral (Category 1), Thyroid, H372
Short-term (acute) aquatic hazard (Category 2), H401

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H315 Causes skin irritation.
H319 Causes serious eye irritation.
H351 Suspected of causing cancer.
H360 May damage fertility or the unborn child.
H372 Causes damage to organs (Thyroid) through prolonged or repeated exposure if swallowed.
H401 Toxic to aquatic life.

Precautionary Statements

P201 Obtain special instructions before use.
P202 Do not handle until all safety precautions have been read and understood.
P260 Do not breathe mist or vapors.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313 IF exposed or concerned: Get medical advice/ attention.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical advice/ attention.
P362 Take off contaminated clothing and wash before reuse.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Component	Classification	Concentration
diethylene glycol monoethyl ether		
CAS-No.	111-90-0	≥ 50 - < 70 %
EC-No.	203-919-7	

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Registration number	01-2119475105-42-XXXX		
Iodine			
CAS-No.	7553-56-2	Acute Tox. 4; Skin Irrit. 2;	≥ 10 - < 20 %
EC-No.	231-442-4	Eye Irrit. 2A; STOT SE 3;	
Index-No.	053-001-00-3	STOT RE 1; Aquatic Acute	
Registration number	01-2119485285-30-XXXX	1; H302, H332, H312, H315, H319, H335, H372, H400 M-Factor - Aquatic Acute: 1	
Imidazole			
CAS-No.	288-32-4	Acute Tox. 4; Skin Corr. 1C; Eye Dam. 1; Repr. 1B;	≥ 1 - < 5 %
EC-No.	206-019-2	H302, H314, H318, H360	
Index-No.	613-319-00-0		
Registration number	01-2119485825-24-XXXX		
2-Methylimidazole			
CAS-No.	693-98-1	Acute Tox. 4; Skin Corr. 1C; Eye Dam. 1; Carc. 2;	≥ 1 - < 5 %
EC-No.	211-765-7	Repr. 1B; H302, H314, H318, H351, H360	
Index-No.	613-330-00-0		

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Hydrogen iodide

Hydrogen cyanide (hydrocyanic acid)

Combustible.

Fire may cause evolution of:

Sulfur oxides, hydrogen iodide, nitrogen oxides

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

Storage class

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
diethylene glycol monoethyl ether	111-90-0	TWA	25 ppm	USA. Workplace Environmental Exposure Levels (WEEL)
Iodine	7553-56-2	C	0.1 ppm 1 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	0.001 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen Danger of cutaneous absorption		

		C	0.1 ppm 1 mg/m ³	USA. NIOSH Recommended Exposure Limits
		C	0.1 ppm 1 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Latex gloves

Minimum layer thickness: 0.6 mm

Break through time: 480 min

Material tested: Lapren® (KCL 706 / Aldrich Z677558, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 120 min

Material tested: KCL 741 Dermatril® L

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: filter ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

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required when vapours/aerosols are generated.

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Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Color: dark brown
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	No data available
g) Flash point	No data available
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	1.16 g/cm ³ at 20 °C (68 °F)
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	Not classified as explosive.
t) Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

10.2 Chemical stability

Reacts with air to form peroxides.

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Exothermic reaction with:

Strong oxidizing agents

Generates dangerous gases or fumes in contact with:

Aluminum

Possible formation of:

Hydrogen

Violent reactions possible with:

Metals

Acid chlorides

Acid anhydrides

Acids

10.4 Conditions to avoid

no information available

10.5 Incompatible materials

Aluminum, artificial and/or natural resins, Copper

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Acute toxicity estimate Oral - 2,537 mg/kg

(Calculation method)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute toxicity estimate Inhalation - 4 h - 12.85 mg/l - dust/mist(Calculation method)

Symptoms: Possible symptoms:, mucosal irritations

Acute toxicity estimate Dermal - > 5,000 mg/kg
(Calculation method)

Skin corrosion/irritation

Remarks: Mixture causes skin irritation.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

Evidence of a carcinogenic effect.

IARC: 2B - Group 2B: Possibly carcinogenic to humans (2-Methylimidazole)

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

May harm the unborn child.

May impair fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Mixture causes damage to organs through prolonged or repeated exposure.

- Thyroid

Aspiration hazard

No data available

11.2 Additional Information

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

Components

diethylene glycol monoethyl ether

Acute toxicity

LD50 Oral - Mouse - male - 6,031 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - > 5.24 mg/l - aerosol

(OECD Test Guideline 403)

Remarks: (ECHA)

LD50 Dermal - Rabbit - male - 9,143 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit
Result: Mild skin irritation - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: No eye irritation - 24 h
(OECD Test Guideline 405)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Remarks: (National Toxicology Program)
Method: OECD Test Guideline 474
Species: Mouse - male - Bone marrow
Result: negative
Method: OECD Test Guideline 486
Species: Rat - male - Liver cells
Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Aspiration hazard

No data available

Iodine

Acute toxicity

LD50 Oral - Rat - 315 mg/kg
(US-EPA)
Remarks: The GHS classification specified by the authority
LC50 Inhalation - Rat - male and female - 4 h - > 4.588 mg/l - dust/mist
(OECD Test Guideline 403)
Remarks: (Regulation (EC) No 1272/2008, Annex VI)
LD50 Dermal - Rabbit - male and female - 1,425 mg/kg
(US-EPA)
No data available

Skin corrosion/irritation

Skin - reconstructed human epidermis (RhE)
Result: Moderate skin irritation
(Regulation (EC) No. 440/2008, Annex, B.46)

Serious eye damage/eye irritation

Remarks: Causes serious eye irritation.

Respiratory or skin sensitization

In animal experiments: - Mouse
Result: negative
(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test):
Test system: Mouse lymphoma test
Result: negative
Method: Mutagenicity (micronucleus test)
Species: Mouse - male and female
Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory system

Specific target organ toxicity - repeated exposure

Oral - Causes damage to organs through prolonged or repeated exposure.
- Thyroid
Oral - Thyroid

Aspiration hazard

No data available

Imidazole**Acute toxicity**

LD50 Oral - Rat - 970 mg/kg
(OECD Test Guideline 401)
Inhalation: No data available
Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit
Result: Corrosive after 1 to 4 hours of exposure - 4 h
(OECD Test Guideline 404)
Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit
Result: Causes serious eye damage.

(OECD Test Guideline 405)
Remarks: Causes serious eye damage.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: negative

Test Type: unscheduled DNA synthesis assay

Test system: rat hepatocytes

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female - Bone marrow

Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

May damage the unborn child.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

Oral - Liver, Kidney

Aspiration hazard

No data available

2-Methylimidazole

Acute toxicity

LD50 Oral - Rat - male and female - 1,500 mg/kg

(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rat - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive after 1 to 4 hours of exposure - 4 h
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Corrosive

(OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male

Result: negative

Method: OECD Test Guideline 478

Species: Mouse - male and female

Result: negative

Carcinogenicity

Suspected of causing cancer.

Reproductive toxicity

May damage the unborn child.

Suspected of damaging fertility.

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

diethylene glycol monoethyl ether

Toxicity to fish	flow-through test LC50 - <i>Ictalurus punctatus</i> (channel catfish) - ca. 6,010 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test LC50 - <i>Daphnia magna</i> (Water flea) - 1,982 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> - 14,861 mg/l - 72 h (OECD Test Guideline 201)

Iodine

Toxicity to fish	static test LC50 - <i>Oncorhynchus mykiss</i> (rainbow trout) - 1.67 mg/l - 96 h Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 0.55 mg/l - 48 h Remarks: (ECHA)
	EC50 - <i>Daphnia magna</i> (Water flea) - 0.2 mg/l - 48 h
Toxicity to algae	Growth inhibition ErC50 - <i>Desmodesmus subspicatus</i> (green algae) - 0.13 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - activated sludge - 280 mg/l - 3 h (OECD Test Guideline 209)

Imidazole

Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 341.5 mg/l - 48 h (Regulation (EC) No. 440/2008, Annex, C.2)
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Toxicity to algae static test ErC50 - Desmodesmus subspicatus (green algae) - 133 mg/l - 72 h (DIN 38412)

Toxicity to bacteria static test EC50 - activated sludge - > 1,000 mg/l - 30 min (OECD Test Guideline 209)

2-Methylimidazole

Toxicity to fish static test LC50 - Leuciscus idus (Golden orfe) - 190 mg/l - 96 h (DIN 38412)

static test NOEC - Leuciscus idus (Golden orfe) - 100 mg/l - 96 h (DIN 38412)

Toxicity to daphnia and other aquatic invertebrates static test EC50 - Daphnia magna (Water flea) - 200 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae static test ErC50 - Desmodesmus subspicatus (green algae) - 256.3 mg/l - 72 h (DIN 38412)

Toxicity to bacteria static test EC50 - Pseudomonas putida - 459.9 mg/l - 7 h (DIN 38 412 Part 8)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

IATA

Not dangerous goods

Further information

Not classified as dangerous in the meaning of transport regulations.

SECTION 15: Regulatory information

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:

diethylene glycol monoethyl ether	111-90-0	>= 50 - < 70 %
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US State Regulations

Massachusetts Right To Know

Iodine	7553-56-2
Imidazole	288-32-4

Pennsylvania Right To Know

diethylene glycol monoethyl ether	111-90-0
Iodine	7553-56-2

Maine Chemicals of High Concern

Imidazole	288-32-4
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Vermont Chemicals of High Concern

Imidazole	288-32-4
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Washington Chemicals of High Concern

Imidazole	288-32-4
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California Prop. 65

WARNING: This product can expose you to chemicals including 2-Methylimidazole, which is/are known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.

The ingredients of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

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No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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