# SAFETY DATA SHEET

Version 6.2
Revision Date 04/29/2021
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : UR-144 5-Pentanoic acid-D5 metabolite (indole-D5)

Product Number : S-090
Brand : Cerilliant

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

Identified uses : Laboratory chemicals, Synthesis of substances

### 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)**

Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Specific target organ toxicity - single exposure (Category 1), H370

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



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Hazard statement(s)

| | |
|---|---|
| H225 | Highly flammable liquid and vapor. |
| H301 + H311 + H331 | Toxic if swallowed, in contact with skin or if inhaled. |
| H370 | Causes damage to organs. |

Precautionary statement(s)

| | |
|---|---|
| P210 | Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking. |
| P233 | Keep container tightly closed. |
| P240 | Ground/bond container and receiving equipment. |
| P241 | Use explosion-proof electrical/ ventilating/ lighting/ equipment. |
| P242 | Use only non-sparking tools. |
| P243 | Take precautionary measures against static discharge. |
| P260 | Do not breathe dust/ fume/ gas/ mist/ vapors/ spray. |
| P264 | Wash skin thoroughly after handling. |
| P270 | Do not eat, drink or smoke when using this product. |
| P271 | Use only outdoors or in a well-ventilated area. |
| P280 | Wear protective gloves/ eye protection/ face protection. |
| P301 + P310 + P330 | IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower. |
| P304 + P340 + P311 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor. |
| P307 + P311 | IF exposed: Call a POISON CENTER or doctor/ physician. |
| P362 | Take off contaminated clothing and wash before reuse. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed. |
| P403 + P235 | Store in a well-ventilated place. Keep cool. |
| 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

Molecular weight : 32.04 g/mol

| Component | | Classification | Concentration |
|---|---|---|---|
| **Methanol** | | | |
| CAS-No.<br>EC-No.<br>Index-No.<br>Registration number | 67-56-1<br>200-659-6<br>603-001-00-X<br>01-2119433307-44-XXXX | Flam. Liq. 2; Acute Tox. 3; STOT SE 1; H225, H301, H331, H311, H370<br>Concentration limits:<br>>= 10 %: STOT SE 1, H370; 3 - < 10 %: STOT SE 2, H371; | >= 90 - <= 100 % |

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



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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

**General advice**
Consult a physician. Show this material safety data sheet to the doctor in attendance.Move out of dangerous area.

**If inhaled**
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

**In case of eye contact**
Flush eyes with water as a precaution.

**If swallowed**
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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**
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture
Carbon oxides

### 5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information
Use water spray to cool unopened containers.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.
For personal protection see section 8.

### 6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.



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### 6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

### 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**
Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

**Advice on protection against fire and explosion**
Use explosion-proof equipment.**Advice on protection against fire and explosion**
Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.

**Hygiene measures**
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.
For precautions see section 2.2.

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

**Storage conditions**
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

**Storage stability**
Recommended storage temperature
-20 °C

Storage class (TRGS 510): 3: Flammable liquids

### 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 |
|---|---|---|---|---|
| Methanol | 67-56-1 | TWA | 200 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Danger of cutaneous absorption | | |
| | | STEL | 250 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Danger of cutaneous absorption | | |
| | | TWA | 200 ppm<br>260 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |



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| | | | | |
|---|---|---|---|---|
| | | ST | 250 ppm<br>325 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |
| | | TWA | 200 ppm<br>260 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | STEL | 250 ppm<br>325 mg/m3 | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | Skin notation | | |
| | | TWA | 200 ppm<br>260 mg/m3 | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000 |
| | | Skin notation | | |
| | | C | 1,000 ppm | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | PEL | 200 ppm<br>260 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | STEL | 250 ppm<br>325 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |

**Biological occupational exposure limits**

| Component | CAS-No. | Parameters | Value | Biological specimen | Basis |
|---|---|---|---|---|---|
| Methanol | 67-56-1 | Methanol | 15 mg/l | Urine | ACGIH - Biological Exposure Indices (BEI) |
| | Remarks | End of shift (As soon as possible after exposure ceases) | | | |

## 8.2 Exposure controls

**Appropriate engineering controls**
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

**Personal protective equipment**

**Eye/face protection**
Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

**Skin protection**
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.



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**Body Protection**
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory protection**
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**
Prevent further leakage or spillage if safe to do so. 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<br>Color: colorless |
| b) | Odor | pungent |
| c) | Odor Threshold | No data available |
| d) | pH | No data available |
| e) | Melting point/freezing point | Melting point/range: -98.0 °C (-144.4 °F) |
| f) | Initial boiling point and boiling range | 64.0 - 65.0 °C 147.2 - 149.0 °F at 1013 hPa |
| g) | Flash point | 9.7 °C (49.5 °F) - closed cup |
| h) | Evaporation rate | No data available |
| i) | Flammability (solid, gas) | No data available |
| j) | Upper/lower flammability or explosive limits | Upper explosion limit: 36 %(V)<br>Lower explosion limit: 6 %(V) |
| k) | Vapor pressure | 130.3 hPa at 20.0 °C (68.0 °F)<br>546.6 hPa at 50.0 °C(122.0 °F)<br>169.27 hPa at 25.0 °C(77.0 °F) |
| l) | Vapor density | 1.11 |
| m) | Relative density | No data available |
| n) | Water solubility | completely miscible |
| o) | Partition coefficient: n-octanol/water | log Pow: -0.77 |
| p) | Autoignition temperature | 455.0 °C (851.0 °F) at 1,013 hPa |
| q) | Decomposition temperature | No data available |



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| | | |
|---|---|---|
| r) | Viscosity | No data available |
| s) | Explosive properties | Not explosive |
| t) | Oxidizing properties | The substance or mixture is not classified as oxidizing. |

**9.2 Other safety information**

| | |
|---|---|
| Minimum ignition energy | 0.14 mJ |
| Conductivity | < 1 µS/cm |
| Relative vapor density | 1.11 |

## SECTION 10: Stability and reactivity

**10.1 Reactivity**
No data available

**10.2 Chemical stability**
Stable under recommended storage conditions.
Stable under recommended storage conditions.

**10.3 Possibility of hazardous reactions**

Vapors may form explosive mixture with air.

Vapors may form explosive mixture with air.

**10.4 Conditions to avoid**
Heat, flames and sparks.
Heat, flames and sparks.

**10.5 Incompatible materials**
Acid chlorides, Acid anhydrides, Oxidizing agents, Alkali metals, Reducing agents, Acids

**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**
No data available

Inhalation: No data available

Dermal: No data available

No data available



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**Skin corrosion/irritation**
No data available

**Serious eye damage/eye irritation**
No data available

**Respiratory or skin sensitization**
No data available

**Germ cell mutagenicity**
No data available

**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**
No data available

**Specific target organ toxicity - single exposure**
No data available**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
No data available

**11.2 Additional Information**
Not available

Methyl alcohol may be fatal or cause blindness if swallowed.
Effects due to ingestion may include:, Headache, Dizziness, Drowsiness, metabolic acidosis, Coma, Seizures.
Symptoms may be delayed., Damage of the:, Liver, Kidney

Stomach - Irregularities - Based on Human Evidence

**Components**

**Methanol**

**Acute toxicity**
Acute toxicity estimate Oral - 100.1 mg/kg
(Expert judgment)
Symptoms: Nausea, Vomiting
Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l
(Expert judgment)
Symptoms: Irritation symptoms in the respiratory tract.



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Acute toxicity estimate Dermal - 300.1 mg/kg
(Expert judgment)

**Skin corrosion/irritation**
Skin - Rabbit
Result: No skin irritation
Remarks:
(ECHA)
Drying-out effect resulting in rough and chapped skin.

**Serious eye damage/eye irritation**
Eyes - Rabbit
Result: No eye irritation
Remarks:
(ECHA)

**Respiratory or skin sensitization**
Sensitisation test: - Guinea pig
Result: negative
(OECD Test Guideline 406)

**Germ cell mutagenicity**
Based on available data the classification criteria are not met.
Ames test
Salmonella typhimurium
Result: negative
In vitro mammalian cell gene mutation test
Chinese hamster lung cells
Result: negative
OECD Test Guideline 474
Mouse - male and female - Bone marrow
Result: negative

**Carcinogenicity**
Did not show carcinogenic effects in animal experiments.

**Reproductive toxicity**
Based on available data the classification criteria are not met.

**Specific target organ toxicity - single exposure**
Causes damage to organs. - Eyes, Central nervous system
Remarks:
Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
Acute oral toxicity - Nausea, Vomiting
Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

**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



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### 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 Other adverse effects
No data available

**Components**

**Methanol**

| | |
|---|---|
| Toxicity to fish | flow-through test LC50 - Lepomis macrochirus (Bluegill) - 15,400.0 mg/l - 96 h<br>(US-EPA) |
| Toxicity to daphnia and other aquatic invertebrates | semi-static test EC50 - Daphnia magna (Water flea) - 18,260 mg/l - 96 h<br>(OECD Test Guideline 202) |
| Toxicity to algae | static test ErC50 - Pseudokirchneriella subcapitata (green algae) - ca. 22,000.0 mg/l - 96 h<br>(OECD Test Guideline 201) |
| Toxicity to bacteria | static test IC50 - activated sludge - > 1,000 mg/l - 3 h<br>(OECD Test Guideline 209) |

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

**Product**
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

**Contaminated packaging**
Dispose of as unused product.

## SECTION 14: Transport information

**DOT (US)**
UN number: 1230 Class: 3 Packing group: II
Proper shipping name: MethanolSOLUTION

Reportable Quantity (RQ):
Poison Inhalation Hazard: No

**IMDG**



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UN number: 1230 Class: 3 (6.1) Packing group: II EMS-No: F-E, S-D
Proper shipping name: METHANOLSOLUTION

**IATA**
UN number: 1230 Class: 3 (6.1) Packing group: II
Proper shipping name: MethanolSOLUTION

## SECTION 15: Regulatory information

**SARA 302 Components**
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |

**SARA 311/312 Hazards**
Fire Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |

**New Jersey Right To Know Components**

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |



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## SECTION 16: Other information

### Further information

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