# SAFETY DATA SHEET

Version 6.1
Revision Date 07/02/2019
Print Date 02/27/2020

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

### 1.1 Product identifiers

Product name : 6ß-Naltrexol-3-ß-D-glucuronide

Product Number : N-104
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 Street
ST. LOUIS MO 63103
UNITED STATES

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

### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

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

Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Eye irritation (Category 2A), H319

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 Warning

Hazard statement(s)
H302 + H312 + H332 Harmful if swallowed, in contact with skin or if inhaled.
H319 Causes serious eye irritation.



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

Precautionary statement(s)

| | |
|---|---|
| P261 | Avoid breathing dust/ fume/ gas/ mist/ vapours/ 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/ protective clothing/ eye protection/ face protection. |
| P301 + P312 + P330 | IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell. Rinse mouth. |
| P302 + P352 + P312 | IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor/ physician if you feel unwell. |
| P304 + P340 + P312 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor if you feel unwell. |
| P305 + P351 + P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P337 + P313 | If eye irritation persists: Get medical advice/ attention. |
| P363 | Wash contaminated clothing before reuse. |
| 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 |
|---|---|---|---|
| **Acetonitrile** | | | |
| CAS-No.<br>EC-No.<br>Index-No.<br>Registration number | 75-05-8<br>200-835-2<br>608-001-00-3<br>01-2119471307-38-XXXX | Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; H225, H302, H332, H312, H319 | >= 70 - < 90 % |
| **6ß-Naltrexol-3-ß-D-glucuronide** | | | |
| CAS-No. | 1391506-73-2 | Aquatic Acute 1; Aquatic Chronic 1; H400, H410<br>M-Factor - Aquatic Acute: 10 | < 0.1 % |

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**

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



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

**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. Consult a physician.

**In case of eye contact**
Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**
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, Nitrogen oxides (NOx)

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

**5.4 Further information**
No data available

## SECTION 6: Accidental release measures

**6.1 Personal precautions, protective equipment and emergency procedures**
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.
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**
Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

**6.4 Reference to other sections**
For disposal see section 13.



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
For precautions see section 2.2.

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

Keep container tightly closed in a dry and well-ventilated place.

Recommended storage temperature 2 - 8 °C
Storage class (TRGS 510): 12: Non Combustible 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

**Components with workplace control parameters**

| Component | CAS-No. | Value | Control parameters | Basis |
|---|---|---|---|---|
| Acetonitrile | 75-05-8 | TWA | 20 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Lower Respiratory Tract irritation<br>Not classifiable as a human carcinogen<br>Danger of cutaneous absorption | | |
| | | TWA | 20 ppm<br>34 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | Forms cyanide in the body. | | |
| | | TWA | 40 ppm<br>70 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | The value in mg/m3 is approximate. | | |
| | | PEL | 40 ppm<br>70 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | STEL | 60 ppm<br>105 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |

Hazardous components without workplace control parameters

### 8.2 Exposure controls

**Appropriate engineering controls**
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

**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.

**Body Protection**
Complete suit protecting against chemicals, 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 ABEK (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**
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 |
| b) | Odour | No data available |
| c) | Odour 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) | Vapour pressure | No data available |
| l) | Vapour density | No data available |
| m) | Relative density | No data available |
| n) | Water solubility | No data available |



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

| | | |
|---|---|---|
| o) | Partition coefficient: n-octanol/water | No data available |
| p) | Auto-ignition temperature | No data available |
| q) | Decomposition temperature | No data available |
| r) | Viscosity | No data available |
| s) | Explosive properties | No data available |
| t) | Oxidizing properties | No data available |

**9.2 Other safety information**
No data available

## SECTION 10: Stability and reactivity

**10.1 Reactivity**
No data available

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

**10.3 Possibility of hazardous reactions**
No data available

**10.4 Conditions to avoid**
No data available

**10.5 Incompatible materials**
No data available

**10.6 Hazardous decomposition products**
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)
In the event of fire: see section 5

## SECTION 11: Toxicological information

**11.1 Information on toxicological effects**

**Acute toxicity**
LD50 Oral - Mouse - male and female - 617 mg/kg (Acetonitrile)
(OECD Test Guideline 401)
LC50 Inhalation - Mouse - male and female - 4 h - 6.022 mg/l (Acetonitrile)
(OECD Test Guideline 403)
Inhalation: (Regulation (EC) No 1272/2008, Annex VI) (Acetonitrile)
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg (Acetonitrile)
(OECD Test Guideline 402)
Dermal: (Regulation (EC) No 1272/2008, Annex VI) (Acetonitrile)
No data available
No data available

**Skin corrosion/irritation**
No data available



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

Skin - Rabbit (Acetonitrile)
Result: No skin irritation - 4 h
(OECD Test Guideline 404)

**Serious eye damage/eye irritation**
No data available
Eyes - Rabbit (Acetonitrile)
Result: Eye irritation
(OECD Test Guideline 405)

**Respiratory or skin sensitisation**
No data available
Buehler Test - Guinea pig (Acetonitrile)
Result: negative
(OECD Test Guideline 406)

**Germ cell mutagenicity**
No data available
Ames test (Acetonitrile)
S. typhimurium
Result: negative
In vitro mammalian cell gene mutation test (Acetonitrile)
Chinese hamster ovary cells
Result: negative
Mutagenicity (mammal cell test): chromosome aberration. (Acetonitrile)
Chinese hamster ovary cells
Result: Positive results were obtained in some in vitro tests.
(National Toxicology Program)
sister chromatid exchange assay (Acetonitrile)
Chinese hamster ovary cells
Result: negative
Sister chromatid exchange
Saccharomyces cerevisiae
Result: positive
Cytogenetic analysis (ECHA)
In vitro mammalian cell gene mutation test (Acetonitrile)
Mouse lymphoma test
Result: negative
OECD Test Guideline 474 (Acetonitrile)
Mouse - male and female
Result: negative

**Carcinogenicity**
No evidence of carcinogenicity in animal studies. (Acetonitrile)

| | |
|---|---|
| IARC: | No component 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 component 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
No data available
Animal testing did not show any effects on fertility. (Acetonitrile)



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

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

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

**Aspiration hazard**
No data available

**Additional Information**
RTECS: Not available

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death (Acetonitrile)
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (Acetonitrile)

## SECTION 12: Ecological information

### 12.1 Toxicity
No data available

| | |
|---|---|
| Toxicity to fish | flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,640 mg/l - 96 h (Acetonitrile)<br>Remarks: (ECHA) |
| Toxicity to daphnia and other aquatic invertebrates | static test LC50 - Artemia salina (Brine shrimp) - 400 mg/l - 24 h (Acetonitrile)<br>Remarks: (ECHA) |
| Toxicity to algae | static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (Acetonitrile)<br>(ISO 10253) |
| | static test ErC50 - Phaeodactylum tricornutum - 9,696 mg/l - 72 h (Acetonitrile)<br>(ISO 10253) |
| Toxicity to bacteria | static test EC50 - activated sludge - > 1,000 mg/l - 30 min (Acetonitrile)<br>(OECD Test Guideline 209) |

### 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



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

### 12.6 Other adverse effects

No data available
Avoid release to the environment.

| | |
|---|---|
| Stability in water | DT50 - > 9,999 d pH 7 at 25 °C (Acetonitrile)<br>Remarks: (calculated)Hydrolyses slowly. |

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

**Product**
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)**
Not dangerous goods

**IMDG**
Not dangerous goods

**IATA**
Not dangerous goods

## 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 |
|---|---|---|
| Acetonitrile | 75-05-8 | 2007-07-01 |

**SARA 311/312 Hazards**
Acute Health Hazard

**Massachusetts Right To Know Components**

| | CAS-No. | Revision Date |
|---|---|---|
| Acetonitrile | 75-05-8 | 2007-07-01 |

**Pennsylvania Right To Know Components**

| | CAS-No. | Revision Date |
|---|---|---|
| Acetonitrile | 75-05-8 | 2007-07-01 |



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

| | |
|---|---|
| Water | 7732-18-5 |

**New Jersey Right To Know Components**

| | | |
|---|---|---|
| Acetonitrile | CAS-No.<br>75-05-8 | Revision Date<br>2007-07-01 |
| Water | 7732-18-5 | |

**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

## SECTION 16: Other information

**Further information**

Copyright 2018 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.1 Revision Date: 07/02/2019 Print Date: 02/27/2020



The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada