

# • SAFETY DATA SHEET

Version 6.8  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : PEMETREXED DISODIUM, UNITED STATES  
PHARMACOPEIA (USP) REFERENCE  
STANDARD

Product Number : 1500659  
Brand : US Pharmacopeia  
CAS-No. : 357166-29-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

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 number

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



## SECTION 2. HAZARDS IDENTIFICATION

### GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

#### Hazards for the product as supplied

- Skin irritation : Category 2
- Germ cell mutagenicity : Category 2
- Reproductive toxicity : Category 1A
- Specific target organ toxicity - repeated exposure : Category 1 (Blood, Immune system, Testes)
- Short-term (acute) aquatic hazard : Category 3

#### Other hazards

None known.

#### GHS label elements

Hazard pictograms : 

Signal word : Danger

Hazard statements : H315 Causes skin irritation.  
H341 Suspected of causing genetic defects.  
H360 May damage fertility or the unborn child.  
H372 Causes damage to organs (Blood, Immune system, Testes) through prolonged or repeated exposure.  
H402 Harmful to aquatic life.

Precautionary statements : **Prevention:**  
P201 Obtain special instructions before use.  
P202 Do not handle until all safety precautions have been read and understood.  
P260 Do not breathe dust.  
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.



**Response:**

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

P308 + P313 IF exposed or concerned: Get medical advice/ attention.

P332 + P313 If skin irritation occurs: Get medical advice/ attention.

P362 Take off contaminated clothing and wash before reuse.

**Storage:**

P405 Store locked up.

**Disposal:**

P501 Dispose of contents/ container to an approved waste disposal plant.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance

CAS-No. : 357166-29-1

**Components**

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
(2S)-2-([4-(2-(2-amino-4-oxo-1H,4H,7H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl)phenyl]formamido)pentanedioic acid heptahydrate disodium hydride	357166-29-1*	>= 90 - <= 100	-

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

**SECTION 4. FIRST AID MEASURES**

General advice : Show this 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.
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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

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## SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO <sub>2</sub> ) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.  Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	: Carbon oxides  Nitrogen oxides (NO <sub>x</sub> )  Sodium oxides
Specific extinguishing methods	: No data available
Further information	: Suppress (knock down) gases/vapours/mists with a water spray jet.



Prevent fire extinguishing water from contaminating surface water or the ground water system.

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

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:  
Avoid generation and inhalation of dusts in all circumstances.  
Avoid substance contact.  
Ensure adequate ventilation.  
Evacuate the danger area, observe emergency procedures, consult an expert.  
Advice for emergency responders:  
For personal protection see section 8.

Environmental precautions : Do not let product enter drains.

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. Dispose of properly. Clean up affected area.  
Avoid generation of dusts.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on safe handling : Work under hood. Do not inhale substance/mixture.

Further information on storage conditions : Tightly closed.  
Dry.  
Keep in a well-ventilated place.  
Keep locked up or in an area accessible only to qualified or authorised persons.

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

Recommended storage : Recommended storage temperature see product label.



temperature

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when dusts are generated.

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.

Recommended Filter type: : Filter type P3

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.

### Hand protection

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Full contact  
Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber  
Break through time : 480 min  
Glove thickness : 0.11 mm  
Protective index : Splash contact  
Manufacturer : KCL 741 Dermatril® L

Remarks : Handle with impervious gloves.  
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](http://www.kcl.de)).

- Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses
- Skin and body protection : protective clothing
- Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : solid
- Color : No data available
- Odor : No data available
- Odor Threshold : No data available  
pH : No data available
- Melting point : No data available
- Boiling point/boiling range : No data available
- Flash point : Not applicable
- Evaporation rate : No data available
- Flammability (solid, gas) : No data available
- Flammability (liquids) : No data available
- Burning rate : No data available
- Upper explosion limit /  
Upper flammability limit : No data available
- Lower explosion limit /  
Lower flammability limit : No data available
- Vapor pressure : No data available
- Relative vapour density : No data available



Relative density	: No data available
Density	: No data available
Water solubility	: No data available
Partition coefficient: n-octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 599.49 g/mol
Particle characteristics Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity	: The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Violent reactions possible with: Strong oxidizing agents
Conditions to avoid	: no information available
Incompatible materials	: Strong oxidizing agents
Hazardous decomposition products	: In the event of fire: see section 5



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## SECTION 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

Oral: No data available

Inhalation: No data available

Dermal: No data available

#### Skin corrosion/irritation

Remarks: Causes skin irritation.

(External MSDS)

#### Serious eye damage/eye irritation

No data available

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Suspected of causing genetic defects.

#### Carcinogenicity

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

May damage the unborn child. Positive evidence from human epidemiological studies.

May damage fertility.

#### Specific target organ toxicity - single exposure

No data available

#### Specific target organ toxicity - repeated exposure

Causes damage to organs through prolonged or repeated exposure.

- Blood, Immune system, Testes

#### Aspiration hazard

No data available

### 11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.



## SECTION 12. ECOLOGICAL INFORMATION

### Ecotoxicity

#### Components:

(2S)-2-{{[4-(2-{{2-amino-4-oxo-1H,4H,7H-pyrrolo[2,3-d]pyrimidin-5-yl}}ethyl)phenyl]formamido}pentanedioic acid heptahydrate disodium hydride:

- Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): > 1,099.6 mg/l  
Exposure time: 96 h  
Method: OECD Test Guideline 203  
Remarks: (External MSDS)
- Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 462 mg/l  
Exposure time: 48 h  
Method: OECD Test Guideline 202  
Remarks: (External MSDS)
- Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata): 63 mg/l  
Exposure time: 72 h  
Method: OECD Test Guideline 201  
Remarks: (External MSDS)
- NOEC (Pseudokirchneriella subcapitata): 11 mg/l  
Exposure time: 72 h  
Method: OECD Test Guideline 201  
Remarks: (External MSDS)
- Toxicity to fish (Chronic toxicity) : NOEC (Pimephales promelas (fathead minnow)): 13 mg/l  
Exposure time: 28 d  
Method: OECD Test Guideline 210  
Remarks: (External MSDS)
- Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : NOEC (Daphnia magna (Water flea)): 1.2 mg/l  
Exposure time: 21 d  
Method: OECD Test Guideline 211  
Remarks: (External MSDS)

### Persistence and degradability

#### Components:

(2S)-2-{{[4-(2-{{2-amino-4-oxo-1H,4H,7H-pyrrolo[2,3-d]pyrimidin-5-yl}}ethyl)phenyl]formamido}pentanedioic acid heptahydrate disodium hydride:

- Biodegradability : Result: Not readily biodegradable.  
Biodegradation: 20 %  
Exposure time: 29 d  
Method: OECD Test Guideline 301



**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**Other adverse effects**

No data available

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**SECTION 13. DISPOSAL CONSIDERATIONS****Disposal methods**

Waste from residues : 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.

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**SECTION 14. TRANSPORT INFORMATION****International Regulations****IATA-DGR**

Not regulated as a dangerous good

**IMDG-Code**

Not regulated as a dangerous good

**Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

**National Regulations****49 CFR Road**

Not regulated as a dangerous good

Poison Inhalation Hazard : No

**Special precautions for user**

Remarks : Not classified as dangerous in the meaning of transport regulations.

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

**SARA 313** : This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

## **US State Regulations**

### **Massachusetts Right To Know**

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

### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

## **The components 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.

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

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and

US Pharmacopeia - 1500659

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



Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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