

## **Safety Data Sheet**

## **1. PRODUCT AND COMPANY IDENTIFICATION**

1.1	Product identifier	
	Catalog Number	BP13498
	Chemical Name	Simurosertib
	CAS Number	1330782-76-7
1.2	Relevant identified uses of the substance or mixture and uses advised against	
	Identified uses	For Research Use Only, Not For Human or Veterinary Use.
1.3	Details of the supplier of the safety data sheet	
	Company	Purdue Bioscience Inc.
	Address	750 50th St, Brooklyn, NY 11220, USA
	Website	https://www.purduebio.com
1.4	Relevant identified uses of the substance or mixture and uses advised against	
	Emergency telephone number	1-877.618.7311

#### 2. HAZARDS IDENTIFICATION

2.1	Classification of the substance or mixture	
	Not a hazardous substance or mixture.	

2.2	GHS Label elements, including precautionary statements	
	Not a hazardous substance or mixture.	
2.3	Other hazards	
	None.	

### 3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1	Substances	
	Chemical Name	Simurosertib
	Solubility	DMSO: 75 mg/mL (219.66 mM), Need ultrasonic
	Synonyms	TAK-931
	CAS No.	1330782-76-7
	Chemical Formula	C17H19N5OS
	Molecular Weight	341.43

# 4. FIRST AID MEASURES

4.1	Description of first aid measures	
	In case of Inhalation	Immediately relocate self or casualty to fresh air. If breathing is difficult, give cardiopulmonary resuscitation (CPR). Avoid mouth-to-mouth resuscitation.
	In case of Skin	Rinse skin thoroughly with large amounts of water. Remove contaminated
	contact	clothing and shoes and call a physician.

	In case of Eye contact	Remove any contact lenses, locate eye-wash station, and flush eyes immediately with large amounts of water. Separate eyelids with fingers to ensure adequate flushing. Promptly call a physician.
	In case of Ingestion	Wash out mouth with water provided person is conscious. Never give anything by mouth to an unconscious person. Get medical attention. Do NOT induce vomiting unless directed to do so by medical personnel.
4.2	Most important symptoms and effects, both acute and delayed	
	No data available	
4.3	Indication of any immediate medical attention and special treatment needed	
	Treat symptomatically.	

## **5.FIRE FIGHTING MEASURES**

5.1	Suitable extinguishing media	
	Use water spray, dry chemical, foam, and carbon dioxide fire extinguisher.	
5.2	Special hazards arising from the substance or mixture	
	During combustion, may emit irritant fumes.	
5.3	Advice for firefighters	
	As in any fire, wear self-contained breathing apparatus and protective clothing.	

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#### **6. ACCIDENTAL RELEASE MEASURES**

6.1	Personal precautions, protective equipment and emergency procedures
	Use full personal protective equipment. Avoid breathing vapors, mist, dust or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Refer to protective measures listed in sections 8.

6.2	Environmental precautions	
	Try to prevent further leakage or spillage. Keep the product away from drains or water courses.	
6.3	Methods and materials for containment and cleaning up	
	Absorb solutions with finely-powdered liquid-binding material (diatomite, universal binders); Decontaminate surfaces and equipment by scrubbing with alcohol; Dispose of contaminated material according to Section 13.	

#### 7. HANDLING AND STORAGE

7.1	Precautions for safe handling	
	Avoid inhalation, contact with eyes and skin. Avoid dust and aerosol formation. Use only in areas with appropriate exhaust ventilation.	
7.2	Conditions for safe storage, including any incompatibilities	
	Keep container tightly sealed in cool, well-ventilated area. Keep away from direct sunlight and sources of ignition. Recommended storage temperature: Store at -20°C.	
7.3	Specific end use(s)	
	No data available.	
	No data available.	

## 8.EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1	Control parameters
	Components with workplace control parameters This product contains no substances with occupational exposure limit values.
8.2	Exposure controls
	Engineering controls Ensure adequate ventilation. Provide accessible safety shower and eye wash station. Personal protective equipment

Eye protection	Safety goggles with side-shields.
Hand protection	Protective gloves.
Protective gloves.	Impervious clothing.
Respiratory protection	Suitable respirator.
Environmental exposure controls	Keep the product away from drains, water courses or the soil. Clean spillages in a safe way as soon as possible.

#### 9.PHTSICAL AND CHEMICAL PROPERTIES

9.1	Information on basic physical and chemical properties	
	Physical states	Solid
	Odor	No data available
	Odor threshold	No data available
	рН	No data available
	Melting/freezing point	No data available
	Boiling point/range	No data available
	Flash point	No data available
	Evaporation rate	No data available
	Flammability (solid, gas)	No data available
	Upper/lower flammability or explosive limits	No data available
	Vapor pressure	No data available
	Vapor density	No data available

	Relative density	No data available
	Water solubility	Refer to protective measures listed in sections 3.1.
	Partition coefficient	No data available
	Auto-ignition temperature	No data available
	Decomposition temperature	No data available
	Viscosity	No data available
	Explosive properties	No data available
	Oxidizing properties	No data available
9.2	OOther safety information	No data available
10.STABILIT	10.STABILITY AND REACTIVITY	

## **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
	Under fire conditions, may decompose and emit toxic fumes. Other decomposition products - No Data Available.

## **11.TOXICOLOGICAL INFORMATION**

11.1	Information on toxicological effects
	The toxicological information has not been thoroughly studied and is based on our current knowledge. For more details, see section 2.
11.2	Carcinogenicity
	IARC Monographs? No ACGIH? No NTP? No OSHA Regulated? No

## **12.ECOLOGICAL INFORMATION**

12.1	Toxicity
	No Data Available
12.2	Persistence and degradability
	No Data Available
12.3	Mobility in soil
	No Data Available
12.4	Bioaccumlative potential
	No Data Available
12.5	Results of PBT and vPvB assessment

	PBT/vPvB assessment unavailable as chemical safety assessment not required or not conducted.
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#### **13.DISPOSAL CONSIDERATIONS**

13.1	Waste disposal methods
	Dispose substance in accordance with prevailing country, federal, state and local regulations.
13.2	Contaminated packaging
	Conduct recycling or disposal in accordance with prevailing country, federal, state and local regulations.

#### **14.TRANSPORT INFORMATION**

DOT (US)
This substance is considered to be non-hazardous for transport.
IMDG
This substance is considered to be non-hazardous for transport.
ΙΑΤΑ
This substance is considered to be non-hazardous for transport.

## **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

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.
SARA 311/312 hazards
No SARA Hazards.
Massachusetts Right to Know components
No components are subject to the Massachusetts Right to Know Act.
Pennsylvania Right to Know components
No components are subject to the Pennsylvania Right to Know Act.
New Jersey Right to Know components
No components are subject to the New Jersey Right to Know Act.
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.

#### **16. OTHER INFORMATION**

Copyright Purdue Bioscience Inc. The above information is believed to be correct based on our present knowledge but does not purport to be complete. The product is for research use only and for trained researchers. The burden of safe use of this material rests entirely with the user. Purdue Bioscience disclaims all liability for any damage resulting from use of this material.

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v2 Revision on 12/28/2022