

# MATERIAL SAFETY DATA SHEET

## (+)-Xestospongins A

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Cayman Chemical Company  
1180 E. Ellsworth Rd.  
Ann Arbor, MI 48108

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### 1. Product and Company Identification

**Product Code:** 10006794  
**Product Name:** (+)-Xestospongins A  
**Manufacturer Information**  
**Company Name:** Cayman Chemical Company  
**Emergency Contact:** Cayman Chemical Company (800)364-9897  
**Information:** Cayman Chemical Company (734)971-3335  
**Chemical Family:** PAFs & Polar Lipids  
**Synonyms:** [1R-(1R\*,4aR\*,11R\*,12aS\*,13R\*,16aR\*,23R\*,24aS\*)]-eicosahydro-5H, 17H-1,23:11,13-diethano-2H,14H-[1,11]dioxacycloeicosino[2,3-b:12,13-b']dipyridine; Araguspogin D; Xe A

### 2. Composition/Information on Ingredients

Hazardous Components (Chemical Name)	CAS #	Percentage	OSHA TWA	ACGIH TWA	Other Limits
1. (+)-Xestospongins A	88840-02-2	0.01 %	No data.	No data.	No data.
2. Acetone	67-64-1	99.99 %	8H TWA: 750 ppm (1800 mg/m <sup>3</sup> )	500 ppm	No data.

  

Hazardous Components (Chemical Name)	RTECS #	OSHA STEL	OSHA CEIL	ACGIH STEL	ACGIH CEIL
1. (+)-Xestospongins A	NA	No data.	No data.	No data.	No data.
2. Acetone	AL3150000	1000 ppm	No data.	750 ppm	No data.

### 3. Hazards Identification

**Emergency Overview:** No data available.  
**Route(s) of Entry:** Inhalation? Yes Skin? Yes Eyes? Yes Ingestion? Yes Other: Injection  
**Potential Health Effects (Acute and Chronic):** The hazards identified with this product are those associated with the solvent(s).  
Harmful by inhalation, ingestion, or skin absorption.  
Irritating to eyes, respiratory system and skin.  
Material is irritating to the mucous membranes and upper respiratory tract.  
The toxicological properties of this compound have not been fully evaluated.  
**LD 50/LC 50:** Please refer to Section 11.  
**Signs and Symptoms Of Exposure:** Inflammation of the eye; characterized by redness, watering, and itching.  
Skin inflammation; characterized by itching, scaling, reddening, or, occasionally, blistering.  
**Medical Conditions Generally Aggravated By Exposure:** Repeated exposure to a highly toxic material may produce general deterioration of health by an accumulation in one or many human organs.

### 4. First Aid Measures

**Emergency and First Aid Procedures:** If inhaled remove to fresh air. If not breathing, give artificial respiration or give oxygen by trained personnel. Get immediate medical attention.  
If swallowed, 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.  
In case of contact with eyes, hold eyelids apart and flush eyes with plenty of water. After initial flushings, remove any contact lenses and continue flushing for at least 20 minutes. Have eyes examined and tested by medical personnel.  
In case of skin contact, immediately wash skin with soap and plenty of water. Remove contaminated clothing. Get medical attention if symptoms occur. Wash clothing before reuse.

### 5. Fire Fighting Measures

<b>Flash Pt:</b>	-18.10 C Method Used: CC
<b>Explosive Limits:</b>	LEL: 2.6% at 25.0 C UEL: 12.8% at 25.0 C
<b>Autoignition Pt:</b>	464.90 C
<b>Fire Fighting Instructions:</b>	As in any fire, wear self-contained breathing apparatus pressure-demand (MSHA/NIOSH approved or equivalent), and full protective gear to prevent contact with skin and eyes.
<b>Flammable Properties and Hazards:</b>	Extremely explosive in presence of open flames, sparks and static discharge, of shocks, of heat, of oxidizing materials. Extremely flammable in presence of open flames, sparks and static discharge, of shocks, of heat, of oxidizing materials. Flammable liquid. Vapor may travel considerable distance to source of ignition and flash back.
<b>Hazardous Combustion Products:</b>	carbon dioxide carbon monoxide
<b>Extinguishing Media:</b>	Use alcohol-resistant foam, carbon dioxide, water, or dry chemical spray when fighting fires involving this material. Cool containing vessels with water jet in order to prevent pressure build-up, autoignition or explosion. Use of water spray when fire fighting may be inefficient.
<b>Unsuitable Extinguishing Media:</b>	No data available.

### 6. Accidental Release Measures

<b>Steps To Be Taken In Case Material Is Released Or Spilled:</b>	Wear a NIOSH/MSHA approved self-contained breathing apparatus and appropriate personal protection (rubber boots, safety goggles, and heavy rubber gloves). Absorb spill with inert material (e.g. dry sand or earth), then place in a chemical waste container. After removal, ventilate contaminated area and flush thoroughly with water.
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### 7. Handling and Storage

<b>Hazard Label Information:</b>	Avoid contact with skin and eyes. Do not reuse this container. Use with adequate ventilation. Wash thoroughly after handling.
<b>Precautions To Be Taken in Handling:</b>	Avoid breathing (dust, vapor, mist, gas). Avoid contact with eyes, skin, and clothing. Avoid prolonged or repeated exposure. Do not reuse this container. Use with adequate ventilation. Wash thoroughly after handling.
<b>Precautions To Be Taken in Storing:</b>	Store at correct temperature.
<b>Other Precautions:</b>	Keep away from heat, sparks, and flame.

### 8. Exposure Controls/Personal Protection

<b>Protective Equipment Summary - Hazard Label Information:</b>	Eye wash station in work area Lab coat Latex disposable gloves Safety glasses Safety shower in work area Vent Hood
<b>Respiratory Equipment (Specify Type):</b>	Government approved respirator as conditions warrant.
<b>Eye Protection:</b>	Safety glasses
<b>Protective Gloves:</b>	Latex disposable gloves
<b>Other Protective Clothing:</b>	Lab coat
<b>Engineering Controls (Ventilation etc.):</b>	Use process enclosures, local exhaust ventilation, or other engineering controls to control airborne levels below recommended exposure limits.
<b>Work/Hygienic/Maintenance Practices:</b>	Do not take internally. Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Wash thoroughly after handling.

## 9. Physical and Chemical Properties

<b>Physical States:</b>	[ ] Gas [ X ] Liquid [ ] Solid
<b>Melting Point:</b>	No data.
<b>Boiling Point:</b>	No data.
<b>Autoignition Pt:</b>	464.90 C
<b>Flash Pt:</b>	-18.10 C Method: CC
<b>Explosive Limits:</b>	LEL: 2.6% at 25.0 C UEL: 12.8% at 25.0 C
<b>Specific Gravity (Water = 1):</b>	No data.
<b>Vapor Pressure (vs. Air or mm Hg):</b>	No data.
<b>Vapor Density (vs. Air = 1):</b>	No data.
<b>Evaporation Rate (vs Butyl Acetate=1):</b>	No data.
<b>Solubility in Water:</b>	Soluble* at 25.0 C
<b>Other Solubility Notes:</b>	*Also sol. in EtOAc, MeOAc & DMSO
<b>Percent Volatile:</b>	N.A.
<b>Corrosion Rate:</b>	No data.
<b>Formula:</b>	C <sub>28</sub> H <sub>50</sub> N <sub>2</sub> O <sub>2</sub>
<b>Molecular Weight:</b>	446.70
<b>pH:</b>	No data.
<b>Appearance and Odor:</b>	A clear, colorless solution

## 10. Stability and Reactivity

<b>Stability:</b>	Unstable [ ] Stable [ X ]
<b>Conditions To Avoid - Instability:</b>	protect from flames protect from heat protect from ignition sources protect from impact or mechanical shock
<b>Incompatibility - Materials To Avoid:</b>	acids oxidizing agents
<b>Hazardous Decomposition Or Byproducts:</b>	carbon dioxide carbon monoxide
<b>Hazardous Polymerization:</b>	Will occur [ ] Will not occur [ X ]
<b>Conditions To Avoid - Hazardous Polymerization:</b>	No data available.

## 11. Toxicological Information

<b>Toxicological Information:</b>	The toxicological effects of this compound have not been thoroughly studied.  Acetone - Irritation Data: Skin (rabbit): 500 mg 24H mild effect Eyes (rabbit): 20 mg 24H moderate effect  Acetone - Toxicity Data: Oral LD50 (rabbit): 5340 mg/kg
<b>Chronic Toxicological Effects:</b>	Investigated as a mutagen and reproductive effector. Only select Registry of Toxic Effects of Chemical Substances (RTECS) data is presented here. See actual entry in RTECS for complete information. Acetone RTECS Number: AL3150000
<b>Carcinogenicity/Other Information:</b>	No data available.
<b>Carcinogenicity:</b>	NTP? No IARC Monographs? No OSHA Regulated? No

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**12. Ecological Information**

**Ecological Information:** Runoff from fire control or dilution water may cause pollution.

**13. Disposal Considerations**

**Waste Disposal Method:** Dispose in accordance with local, state and federal regulations.

**14. Transport Information**

**LAND TRANSPORT (US DOT)**

**DOT Proper Shipping Name:** Acetone  
**DOT Hazard Class:** 3  
**DOT Hazard Label:** FLAMMABLE LIQUID  
**UN/NA Number:** 1090  
**DOT Packing Group:** II

**Additional Transport Information:** Transport in accordance with local, state, and federal regulations.

**15. Regulatory Information**

**US EPA SARA Title III**

Hazardous Components (Chemical Name)	CAS #	Sec.302 (EHS)	Sec.304 RQ	Sec.313 (TRI)	Sec.110
1. (+)-Xestospongins A	88840-02-2	No	No	No	No
2. Acetone	67-64-1	No	Yes 5000 LB	No	Yes

**US EPA CAA, CWA, TSCA**

Hazardous Components (Chemical Name)	CAS #	EPA CAA	EPA CWA NPDES	EPA TSCA	CA PROP 65
1. (+)-Xestospongins A	88840-02-2	No	No	No	No
2. Acetone	67-64-1	No	No	No	No

**16. Other Information**

**Company Policy or Disclaimer**

For research use only, not for human or veterinary clinical use.

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