

## SAFETY DATA SHEET

Version 6.3  
Revision Date 04/23/2019  
Print Date 10/30/2019**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : BIBN4096BS

Product Number : SML2426  
Brand : Sigma  
CAS-No. : 204697-65-4**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 STATESTelephone : +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**

Not a hazardous substance or mixture.

**2.2 GHS Label elements, including precautionary statements**

Not a hazardous substance or mixture.

**2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none****SECTION 3: Composition/information on ingredients****3.1 Substances**Synonyms : Olcegepant  
1-[3,5-Dibromo-N-[[4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-  
1-piperidinyl]carbonyl]-D-tyrosyl-L-lysyl]-4-(4-  
pyridinyl)piperazine

Formula : C38H47Br2N9O5

Sigma - SML2426

Page 1 of 7

Molecular weight : 869.65 g/mol  
CAS-No. : 204697-65-4

No components need to be disclosed according to the applicable regulations.

---

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### **If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration.

#### **In case of skin contact**

Wash off with soap and plenty of water.

#### **In case of eye contact**

Flush eyes with water as a precaution.

#### **If swallowed**

Never give anything by mouth to an unconscious person. Rinse mouth with water.

### 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 (NO<sub>x</sub>), Hydrogen bromide gas

### 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

Avoid dust formation. Avoid breathing vapours, mist or gas.  
For personal protection see section 8.

### 6.2 Environmental precautions

No special environmental precautions required.

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

Sweep up and shovel. Keep in suitable, closed containers for disposal.

## 6.4 Reference to other sections

For disposal see section 13.

---

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

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 -20 °C

Storage class (TRGS 510): 13: Non Combustible Solids

### 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

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

General industrial hygiene practice.

#### Personal protective equipment

##### Eye/face protection

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

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

##### Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**  
No special environmental precautions required.

---

**SECTION 9: Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

a) Appearance	Form: solid
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	( )Not applicable
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
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**

Strong oxidizing agents

### **10.6 Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>), Hydrogen bromide gas

Other decomposition products - No data available

In the event of fire: see section 5

---

## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

No data available

Inhalation: No data available

Dermal: No data available

No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

No data available

#### **Respiratory or skin sensitisation**

No data available

#### **Germ cell mutagenicity**

No data available

#### **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**

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

#### **Additional Information**

RTECS: Not available

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

---

## **SECTION 12: Ecological information**

### **12.1 Toxicity**

No data available

### **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

---

## **SECTION 13: Disposal considerations**

### **13.1 Waste treatment methods**

#### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company.

#### **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**

### **Massachusetts Right To Know Components**

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

**Pennsylvania Right To Know Components**

N-{(2S)-6-Amino-1-oxo-1-[4-(4-pyridinyl)-1-piperazinyl]-2-hexanyl}-3,5-dibromo-Na-[4-(2-oxo-1,4-dihydro-3(2H)-quinazolinyl)-1-piper	CAS-No. 204697-65-4	Revision Date
---	------------------------	---------------

N-{(2S)-6-Amino-1-oxo-1-[4-(4-pyridinyl)-1-piperazinyl]-2-hexanyl}-3,5-dibromo-Na-[4-(2-oxo-1,4-dihydro-3(2H)-quinazolinyl)-1-piper	CAS-No. 204697-65-4	Revision Date
---	------------------------	---------------

**New Jersey Right To Know Components**

N-{(2S)-6-Amino-1-oxo-1-[4-(4-pyridinyl)-1-piperazinyl]-2-hexanyl}-3,5-dibromo-Na-[4-(2-oxo-1,4-dihydro-3(2H)-quinazolinyl)-1-piper	CAS-No. 204697-65-4	Revision Date
---	------------------------	---------------

**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](http://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](mailto:mlsbranding@sial.com).

Version: 6.3

Revision Date: 04/23/2019

Print Date: 10/30/2019