

# **Certificate of Analysis**

# www.tocris.com

### Product Name: Bengamide B

# Catalog No.: 5273 Batch No.: 2

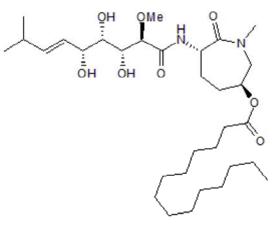
CAS Number: IUPAC Name:

(6*E*)-6,7,8,9-Tetradeoxy-N-[(3S,6S)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1*H*-azepin-3-yl]-8-methyl-2-O-methyl-D-gulo-Non-6-enonamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

104947-69-5

Batch Molecular Formula: Batch Molecular Weight: Physical Appearance: Solubility: Storage: Batch Molecular Structure: C<sub>32</sub>H<sub>58</sub>N<sub>2</sub>O<sub>8</sub> 598.81 Off White Iyophilised solid DMSO to 1 mg/ml Store at -20°C



### 2. ANALYTICAL DATA

HPLC: <sup>1</sup>H NMR: Mass Spectrum:

Shows >97% purity Consistent with structure Consistent with structure

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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CAS Number: 104947-69-5

**IUPAC Name:** 

(6*E*)-6,7,8,9-Tetradeoxy-N-[(3*S*,6*S*)-hexahydro-1-methyl-2-oxo-6-[(1-oxotetradecyl)oxy]-1*H*-azepin-3-yl]-8-methyl-2-O-methyl-D-gulo-Non-6-enonamide

#### **Description:**

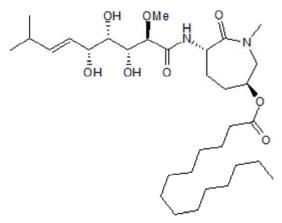
Potent inhibitor of NF- $\kappa$ B activation (IC<sub>50</sub> = 85 nM); decreases I $\kappa$ B $\alpha$  phosphorylation. Attenuates LPS-induced nitric oxide production and expression of TNF- $\alpha$ , IL-6 and MCP. Suppresses proliferation of HeLa and HCT116 cells. Anti-inflammatory and antitumor.

#### **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>32</sub>H<sub>58</sub>N<sub>2</sub>O<sub>8</sub> Batch Molecular Weight: 598.81 Physical Appearance: Off White lyophilised solid

#### Minimum Purity: >97%

#### **Batch Molecular Structure:**



#### Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Catalog No.: 5273

#### Solubility & Usage Info:

DMSO to 1 mg/ml

This product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

#### Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

#### **References:**

Johnson et al (2012) Myxobacteria versus sponge-derived alkaloids: the bengamide family identified as potent immune modulating agents by scrutiny of LC-MS/ELSD libraries. Bioorg.Med.Chem. 20 4348. PMID: 22705020.

Hu et al (2007) Regulation of c-Src nonreceptor tyrosine kinase activity by bengamide A through inhibition of methionine aminopeptidases. Chem.Biol. 14 764. PMID: 17656313.

Kinder et al (2001) Synthesis and antitumor activity of ester-modified analogues of bengamide B. J.Med.Chem. 44 3692. PMID: 11606134.

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