

# Certificate of Analysis

[www.tocris.com](http://www.tocris.com)

**Product Name:** PD 404182

**Catalog No.:** 5124

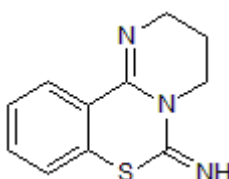
**Batch No.:** 1

CAS Number: 72596-74-8

IUPAC Name: 3,4-Dihydro-2*H*,6*H*-pyrimido[1,2-*c*][1,3]benzothiazin-6-imine

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>11</sub>H<sub>11</sub>N<sub>3</sub>S·½H<sub>2</sub>O  
**Batch Molecular Weight:** 226.3  
**Physical Appearance:** White solid  
**Solubility:** ethanol to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.3 (Ethyl acetate:Petroleum ether [5:4])  
**HPLC:** Shows 99.7% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

|             | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 58.38  | 5.34     | 18.57    |
| Found       | 58.68  | 5.04     | 18.68    |

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

**Product Name:** PD 404182

**Catalog No.:** 5124

**Batch No.:** 1

CAS Number: 72596-74-8

IUPAC Name: 3,4-Dihydro-2*H*,6*H*-pyrimido[1,2-*c*][1,3]benzothiazin-6-imine

**Description:**

High affinity inhibitor of KDO 8-P synthase ( $K_i = 26$  nM). Also inhibits dimethylarginine dimethylaminohydrolase 1 (DDAH1). Exhibits antiangiogenic and antiviral activity in vitro. Putative antibiotic against gram-negative bacteria.

**Physical and Chemical Properties:**

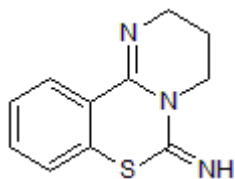
Batch Molecular Formula: C<sub>11</sub>H<sub>11</sub>N<sub>3</sub>S.½H<sub>2</sub>O

Batch Molecular Weight: 226.3

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Birck et al** (2000) Identification of a slow tight-binding inhibitor of 3-deoxy-*D*-manno-octulosonic acid 8-phosphate synthase. *J.Am.Chem.Soc.* **122** 9334.

**Ghebremariam et al** (2013) A novel and potent inhibitor of dimethylarginine dimethylaminohydrolase: a modulator of cardiovascular nitric oxide. *J.Pharmacol.Exp.Ther.* **348** 69. PMID: 24135074.

**Chamoun-Emanueli et al** (2014) Evaluation of PD 404,182 as an anti-HIV and anti-herpes simplex virus microbicide. *Antimicrob.Agents Chemother.* **58** 687. PMID: 24217696.

**Storage:** Store at -20°C

**Solubility & Usage Info:**

ethanol to 100 mM

**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.

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

**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel:+1 612 379 2956