

# **Certificate of Analysis**

Print Date: Feb 2<sup>nd</sup> 2021

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Product Name: 8-MDP Catalog No.: 4588 Batch No.: 1

CAS Number: 29491-75-6

IUPAC Name: 2,2',2",2"'-[[4,8-Bis(hexahydro-1(2*H*)-azocinyl)pyrimido[5,4-*d*]pyrimidine-2,6-diyl]dinitrilo]tetrakisethanol

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{28}H_{48}N_8O_4.1/4H_2O$ 

Batch Molecular Weight: 565.23

Physical Appearance: Yellow solid

Solubility: DMSO to 20 mM Storage: Store at -20°C

**Batch Molecular Structure:** 

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.23$  (Acetone:Petrol [7:3])

**HPLC:** Shows 97.9% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 59.5 8.65 19.82 Found 59.53 8.66 19.97

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



# **Product Information**

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## **Description:**

Potent equilibrative nucleoside transporter 1 (ENT1) inhibitor ( $IC_{50} = 0.43$  nM). Inhibits hENT1 and hENT2 uptake of [H³] uridine in K562 cells and K15NTD cells respectively.

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

Batch Molecular Formula: C<sub>28</sub>H<sub>48</sub>N<sub>8</sub>O<sub>4</sub>. ½H<sub>2</sub>O

Batch Molecular Weight: 565.23 Physical Appearance: Yellow solid

**Minimum Purity:** ≥98%

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

Storage: Store at -20°C

# Solubility & Usage Info:

DMSO to 20 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.

#### References:

**Lin** *et al* (2011) Design, synthesis, and evaluation of 2-diethanolamino-4,8-diheptamethyleneimino-2-(N-aminoethyl-N-ethanolamino) -6-(N,N-diethanolamino)pyrimido[5,4-d]pyrimidine-fluorescein conjugate (8MDP-fluor), as a novel equilibrativ Bioconjug.Chem. **22** 1221. PMID: 21539390.

Lin et al (2007) Synthesis, flow cytometric evaluation, and identification of highly potent dipyrid. analogues as equilibrative nucleoside transporter 1 inhibitors. J.Med.Chem. **50** 3906. PMID: 17636949.

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