

# **Certificate of Analysis**

Print Date: Sep 11th 2019

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Product Name: CM 10 Catalog No.: 6933 Batch No.: 1

CAS Number: 692269-09-3

IUPAC Name: 2-(2-Propen-1-yl)-6-[[(1-propyl-1*H*-benzimidazol-2-yl)amino]methyl]phenol

# 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{20}H_{23}N_3O$ Batch Molecular Weight:321.42Physical Appearance:White solid

Solubility: DMSO to 100 mM

ethanol to 20 mM with gentle warming

Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**HPLC:** Shows 97.8% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 73.7 7.27 12.89 Found 74.02 7.17 13.01



# **Product Information**

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#### **Description:**

Aldehyde dehydrogenase 1A (ALDH1A) inhibitor (IC $_{50}$  values are 0.64, 0.74 and 1.7  $\mu$ M for ALDH1A3, ALDH1A2 and ALDH1A1, respectively). Induces a necroptotic phenotype and preferentially depletes CD133+ ovarian cancer stem cells in vitro.

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

Batch Molecular Formula: C<sub>20</sub>H<sub>23</sub>N<sub>3</sub>O Batch Molecular Weight: 321.42 Physical Appearance: White solid

Minimum Purity: >98%

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

Storage: Store at -20°C

# Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 mM with gentle warming

#### 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:

**Chefetz** *et al* (2019) A pan-ALDH1A inhibitor induces necroptosis in ovarian cancer stem-like cells. Cell Rep. **26** 3061. PMID: 30865894. **Morgan & Hurley** (2015) Development of a high-throughput *in vitro* assay to identify selective inhibitors for human ALDH1A1. Chem.Biol.Interact. **234** 29. PMID: 25450233.