



Certificate of Analysis

www.tocris.com

Product Name: CVT 10216 Catalog No.: 5164 Batch No.: 1

CAS Number: 1005334-57-5

IUPAC Name: 3-[[[3-[4-[(Methylsulfonyl)amino]phenyl]-4-oxo-4*H*-1-benzopyran-7-yl]oxy]methyl]benzoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

 $\textbf{Batch Molecular Formula:} \qquad \qquad C_{24}H_{19}NO_7S$

Batch Molecular Weight: 465.48

Physical Appearance: Off White solid
Solubility: DMSO to 100 mM

1eq. NaOH to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 61.93 4.11 3.01 Found 61.88 4.03 3.07

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



Product Information

Print Date: Jan 10th 2020

www.tocris.com

Product Name: CVT 10216 Catalog No.: 5164 Batch No.: 1

CAS Number: 1005334-57-5

IUPAC Name: 3-[[[3-[4-[(Methylsulfonyl)amino]phenyl]-4-oxo-4*H*-1-benzopyran-7-yl]oxy]methyl]benzoic acid

Description:

Potent and selective, reversible inhibitor of aldehyde dehydrogenase 2 (ALDH2) (IC $_{50}$ values are 29 and 1300 nM for ALDH2 and ALDH1, respectively). Exhibits anxiolytic effects in rat models.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₄H₁₉NO₇S Batch Molecular Weight: 465.48 Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM 1eq. NaOH to 50 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:

Yao et al (2010) Inhibition of aldehyde dehydrogenase-2 suppresses cocaine seeking by generating THP, a cocaine use-dependent inhibitor of DA synthesis. Nat.Med. 16 1024. PMID: 20729865.

Overstreet et al (2009) A selective ALDH-2 inhibitor reduces anxiety in rats. Pharmacol.Biochem.Behav. 94 255. PMID: 19747934.

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