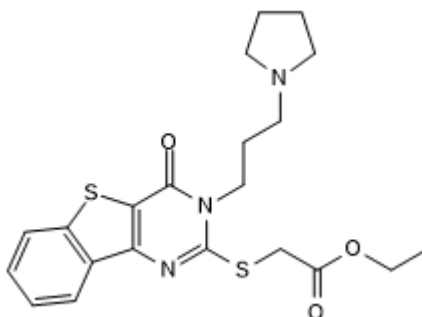


Certificate of Analysis

Product Name: A37 **Catalog No.:** 5802 **Batch No.:** 1
CAS Number: 896795-60-1
IUPAC Name: Ethyl 2-[[3,4-dihydro-4-oxo-3-[3-(1-pyrrolidinyl)propyl][1]benzothieno[3,2-d]pyrimidin-2-yl]thio]acetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₅N₃O₃S₂
Batch Molecular Weight: 431.57
Physical Appearance: Beige solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.45	5.84	9.74
Found	58.88	5.99	9.46

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

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Catalog No.: 5802

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CAS Number: 896795-60-1

IUPAC Name: Ethyl 2-[[3,4-dihydro-4-oxo-3-[3-(1-pyrrolidinyl)propyl][1]benzothieno[3,2-d]pyrimidin-2-yl]thio]acetate

Description:

ALDH1A1 inhibitor (IC_{50} = 4.6 μ M; K_i = 300 nM). Exhibits selectivity for ALDH1A1 over eight other ALDH isoforms. Disrupts spheroid formation and reduces cell viability of ovarian cancer cells in vitro.

Physical and Chemical Properties:

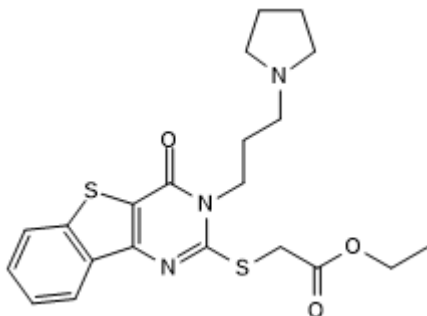
Batch Molecular Formula: $C_{21}H_{25}N_3O_3S_2$

Batch Molecular Weight: 431.57

Physical Appearance: Beige solid

Minimum Purity: >97%

Batch Molecular Structure:



References:

Condello et al (2015) β -Catenin-regulated ALDH1A1 is a target in ovarian cancer spheroids. *Oncogene* **34** 2297. PMID: 24954508 .

Morgan and Hurley (2015) Characterization of two distinct structural classes of selective aldehyde dehydrogenase 1A1 inhibitors. *J.Med.Chem* **58** 1964. PMID: 25634381 .

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
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.

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