



Certificate of Analysis

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Product Name: VU 0155069 Catalog No.: 3575 Batch No.: 1

CAS Number: 1781834-89-6

IUPAC Name: N-[(1S)-2-[4-(5-Chloro-2,3-dihydro-2-oxo-1*H*-benzimidazol-1-yl)-1-piperidinyl]-1-methylethyl-2-

naphthalenecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{27}CIN_4O_2.HCl.1\frac{1}{2}H_2O$

Batch Molecular Weight: 526.45 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.3$ (Chloroform:Methanol [95:5])

HPLC: Shows 97.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = +81.2$ (Concentration = 1, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 59.32 5.93 10.64 Found 59.19 5.79 10.64



Product Information

Print Date: Feb 15th 2022

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Description:

VU 0155069 is a potent and selective phospholipase D1 (PLD1) inhibitor (IC_{50} values are 46 and 933 nM for PLD1 and PLD2 respectively). Inhibits migration of human and mouse breast cancer cell lines in transwell assays.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₆H₂₇CIN₄O₂.HCI.1½H₂O

Batch Molecular Weight: 526.45 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Lewis et al (2009) Design and synthesis of isoform-selective phospholipase D (PLD) inhibitors. Part I: Impact of alternative halogenated privileged structures for PLD1 specificity. Bioorg.Med.Chem.Lett. 19 1916. PMID: 19268584.

Scott *et al* (2009) Design of isoform-selective phospholipase D inhibitors that modulate cancer cell invasiveness. Nat.Chem.Biol. *5* 108. PMID: 19136975.

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