

Product Name: VER 246608

Catalog No.: 6604

Batch No.: 1

CAS Number: 1684386-71-7

IUPAC Name: *N*-[4-(2-Chloro-5-methyl-4-pyrimidinyl)phenyl]-*N*-[[4-[[[(2,2-difluoroacetyl)amino]methyl]phenyl]methyl]-2,4-dihydroxybenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₂₃ClF₂N₄O₄·½H₂O

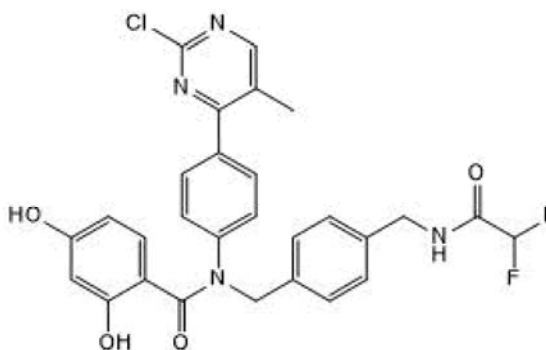
Batch Molecular Weight: 557.46

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.33	4.25	10.05
Found	60.01	4.22	9.94

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Description:

VER 246608 is a potent and ATP-competitive inhibitor of pyruvate dehydrogenase kinase (PDK; IC₅₀s = 35, 40, 84, and 91 nM for PDK-1, PDK-3, PDK-2, and PDK-4 respectively). It is selective for PDKs over a panel of 97 kinases and HSP90. VER 246608 increases pyruvate dehydrogenase complex activity, oxygen consumption and reduces glycolytic activity; it reduces the production of L-lactate in PC3 cells in D-glucose and L-glutamine depleted media. In PC3 cells, VER 246608 induces cell cycle arrest at the G₁ phase under glucose or serum-depleted conditions characteristic of the tumor microenvironment.

Physical and Chemical Properties:

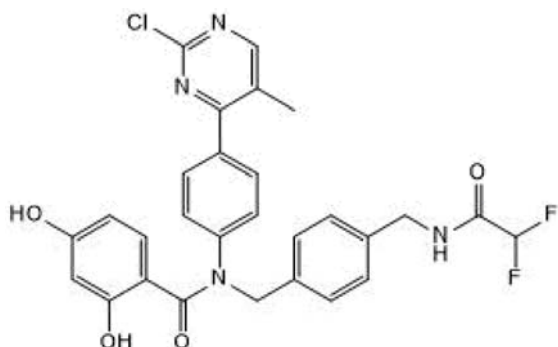
Batch Molecular Formula: C₂₈H₂₃ClF₂N₄O₄·¼H₂O

Batch Molecular Weight: 557.46

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Brough et al (2017) Application of off-rate screening in the identification of novel pan- isoform inhibitors of pyruvate dehydrogenase kinase. *J.Med.Chem.* **60** (6) 2271. PMID: 28199108.

Moore et al (2014) VER-246608, a novel pan-isoform ATP competitive inhibitor of pyruvate dehydrogenase kinase, disrupts Warburg metabolism and induces context-dependent cytostasis in cancer cells. *Oncotarget* **5** (24) 12862. PMID: 25404640.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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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