

Product Name: ONO 6818

Catalog No.: 5651

Batch No.: 1

CAS Number: 208848-19-5

IUPAC Name: 5-Amino-*N*-[1-[[5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2-yl]carbonyl]-2-methylpropyl]-6-oxo-2-phenyl-1(6*H*)-pyrimidineacetamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₈N₆O₄·½H₂O

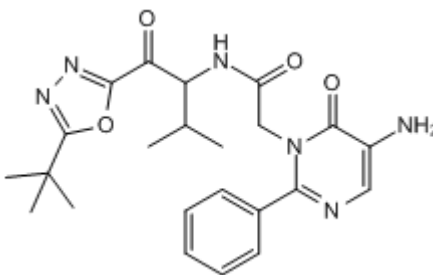
Batch Molecular Weight: 457.01

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.45	6.29	18.39
Found	60.69	6.25	18.03

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Description:

High affinity and selective human neutrophil elastase 1 (HNE1) inhibitor ($K_i = 12$ nM). Exhibits >100-fold less activity at other related proteases including trypsin, pancreatic elastase, collagenase and murine macrophage elastase. Inhibits HNE-induced lung hemorrhaging and suppresses leukocyte levels in an in vivo model of COPD. Orally active.

Physical and Chemical Properties:

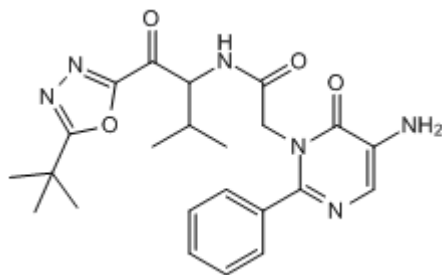
Batch Molecular Formula: $C_{23}H_{28}N_6O_4 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 457.01

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



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.

References:

Stevens et al (2011) AZD9668: pharmacological characterization of a novel oral inhibitor of neutrophil elastase. *J.Pharmacol.Exp.Ther.* **339** 313. PMID: 21791628.

Hirota et al (2004) Effects of the neutrophil elastase inhibitor (ONO-6818) on acetic acid induced colitis in Syrian hamsters. *J.Vet.Med.Sci.* **66** 1223. PMID: 15528853.

Aoshiba et al (2001) Serine proteases increase oxidative stress in lung cells. *Am.J.Physiol.Lung Cell Mol.Physiol.* **281** 556. PMID: 11504681.

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