

Certificate of Analysis

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Product Name: VX 765

Catalog No.: 7143

Batch No.: 1

CAS Number: 273404-37-8

IUPAC Name: *N*-(4-Amino-3-chlorobenzoyl)-3-methyl-L-valyl-*N*-[(2*R*,3*S*)-2-ethoxytetrahydro-5-oxo-3-furanyl]-L-prolinamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₄ H ₃₃ ClN ₄ O ₆
Batch Molecular Weight:	509
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM ethanol to 100 mM
Storage:	Store at -20°C

2. ANALYTICAL DATA

HPLC:	Shows 98.7% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure

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

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Description:

High affinity and selective caspase-4 and caspase 1/ICE inhibitor (K_i of <0.6 and 0.8 nM, respectively). Prodrug of VRT-043198. Inhibits LPS-induced IL-1 β production ~ 60% in collagen-induced arthritis mouse model. Exhibits anticonvulsant effects in mouse model of acute seizures. Anti-inflammatory. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₄H₃₃ClN₄O₆

Batch Molecular Weight: 509

Physical Appearance: White solid

Minimum Purity: ≥98%

Storage: Store at -20°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.

References:

Wu *et al* (2019) Coptisine from *coptis chinensis* blocks NLRP3 inflammasome activation by inhibiting caspase-1. *Pharmacol.Res.* **147** 104348. PMID: 31336157.

Xu *et al* (2019) Caspase-1 inhibitor exerts brain-protective effects against sepsis-associated encephalopathy and cognitive impairments in a mouse model of sepsis. *Brain Behav.Immun.* **80** 859. PMID: 31145977.

Yang *et al* (2019) NLRP3 inflammasome activation promotes the development of allergic rhinitis via epithelium pyroptosis. *Biochem.Biophys.Res.Commun.* **522** 61. PMID: 31740004.

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