



Certificate of Analysis

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Product Name: VTP 27999 trifluoroacetate Catalog No.: 5563 Batch No.: 1

CAS Number: 1013937-63-7

IUPAC Name: Methyl N-[2-[(R)-(3-Chlorophenyl)](3R)-1-[[(2S)-2-(methylamino)-3-[(3R)-tetrahydro-2H-pyran-3-yl]propyl]amino]

carbonyl]-3-piperidinyl]methoxy]ethyl]carbamate trifluoroacetate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{41}CIN_4O_5.CF_3CO_2H.\frac{1}{4}H_2O$

Batch Molecular Weight: 643.6

Physical Appearance: White solid

Solubility: water to 100 mM

DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

.CF₃CO₂H

2. ANALYTICAL DATA

HPLC: Shows 96.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 52.25 6.66 8.71 Found 52.08 6.96 8.8

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



Product Information

Print Date: Feb 18th 2020

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Description:

Highly potent and selective renin inhibitor ($IC_{50} = 0.47$ nM). Displays >1000-fold selectivity over related and unrelated off-targets. Blocks renin-stimulated ERK1/2 phosphorylation in vascular smooth muscle cells. Exhibits a different mode of action to aliskiren (Cat. No. 5491).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₆H₄₁CIN₄O₅.CF₃CO₂H.½H₂O

Batch Molecular Weight: 643.6 Physical Appearance: White solid

Minimum Purity: ≥97%

Batch Molecular Structure:

 $.CF_3CO_2H$

Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM 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).

Catalog No.: 5563

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:

Lu *et al* (2014) Renin inhibitor VTP-27999 differs from aliskiren: focus on their intracellular accumulation and the (pro)renin receptor. J.Hypertens. **32** 1255. PMID: 24637873.

Jia et al (2011) Discovery of VTP-27999, an alkyl amine renin inhibitor with potential for clinical utility. ACS Med.Chem.Lett. 2 747. PMID: 24900262.

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