



Certificate of Analysis

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Product Name: Captopril Catalog No.: 4455 Batch No.: 3

CAS Number: 62571-86-2 EC Number: 263-607-1

IUPAC Name: 1-[(2S)-3-Mercapto-2-methyl-1-oxopropyl]-L-proline

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_9H_{15}NO_3S$ Batch Molecular Weight:217.29Physical Appearance:White solid

Solubility: water to 100 mM

DMSO to 100 mM ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.5% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = -126.9$ (Concentration = 1.7, Solvent = Ethanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 49.75 6.96 6.45 Found 49.89 6.99 6.43

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Product Information

Print Date: Apr 23rd 2020

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IUPAC Name: 1-[(2S)-3-Mercapto-2-methyl-1-oxopropyl]-L-proline

Description:

Angiotensin-converting enzyme (ACE) inhibitor (IC $_{50}$ = 0.022 μ M). Also displays reversible, competitive inhibition of leukotriene A $_4$ (LTA $_4$) hydrolase. Identified as targeting human host proteins that interact with SARS-CoV-2.

Physical and Chemical Properties:

Batch Molecular Formula: C₉H₁₅NO₃S Batch Molecular Weight: 217.29 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

water to 100 mM DMSO to 100 mM ethanol to 100 mM

In aqueous solutions, this compound undergoes an oxidative dimerisation to form captopril disulfide. This oxidation can be delayed by degassing solutions, minimizing headspace, using chelating agents or antioxidants and lowering the pH.

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:

Fujita and Yoshikawa (1999) LKPNM: a prodrug-type ACE-inhibitory peptide derived from fish protein. Immunopharmacology. **44** 123. PMID: 10604535.

Zhang et al (1996) Effects of early capt. treatment and its removal on plasma angiotensin converting enzyme (ACE) activity and arginine vasopressin in hypertensive rats (SHR) and normotensive rats (WKY). Clin.Exp.Hypertens. **18** 201. PMID: 8869001.

Orning et al (1991) Inhibition of leukotriene A₄ hydrolase/aminopeptidase by capt. J.Biol.Chem. **266** 16507. PMID: 1885582.

Gordon *et al* A SARS-CoV-2-human protein-protein interaction map reveals drug targets and potential drug-repurposing. BioRxiv - Paper not yet peer reviewed.

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