



Product Information

Captopril

Product Number **C4042**

Storage at Room Temperature

Product Description

Molecular Formula: $C_9H_{15}NO_3S$

Molecular Weight: 217.3

CAS Number: 62571-86-2

Optical Rotation: -131° (1.7 g/100 ml in 100% ethanol at 22 °C).¹

pK_a: pK₁: 3.7, pK₂: 9.8.¹

Captopril is a member of angiotensin-converting enzyme inhibitors and is very similar to enalapril. Captopril and enalapril differ only slightly in structure (enalapril lacks one sulfhydryl group). Both inhibit angiotensin-converting enzyme, but enalapril is more potent. The mechanisms of action are similar.²

Captopril inhibits porcine kidney angiotensin converting enzyme (Product No. A2580) with an IC₅₀ of $0.021 \pm 0.013 \mu M$. The substrate used is 1 mM Bz-Gly-His-Leu, pH 8.3, at 37 °C. The resulting His-Leu reaction products are measured fluorimetrically.³

Precautions and Disclaimer

For Laboratory Use Only. Not for drug, household or other uses.

Preparation Instructions

This product is freely soluble at >100 mg/ml in water, methanol, ethanol, isopropanol, chloroform, or methylene chloride. Solubility in sesame and corn oils was less than 1 mg/ml at 25 °C. Solubility in water at 25 °C is 160 mg/ml, and solubility vs. temperature is linear up to 40 °C, above which captopril showed extraordinarily high water solubility.⁴

Storage/Stability

This compound is very stable. No significant decomposition was detected in samples stored up to 50 °C for up to 6 months. Samples were examined for appearance, color, odor, LD₅₀, by quantitative TLC and HPLC, iodimetric titration, infrared, and optical rotation.^{1,5}

In solution, this product undergoes an oxygen-facilitated, first order, free radical oxidation at its thiol to yield captopril disulfide. Hydrolysis at the amide linkage occurs only under forcing conditions. Oxidation is delayed using lower pH, chelating agents, higher concentration, degassing, minimizing headspace, and incorporation of antioxidants. No degradation is seen in methanol (40 µg/ml) for up to 2 weeks at 5 °C. Transition metal ions (Cu and Fe in particular) catalyze its oxidation - as little as 1 ppm Cu has oxidized solutions.⁴

In McIlvaine's citrate-phosphate buffer, the stability at 50 °C was studied over a pH range of 2-5.6 and found to be most stable below pH 4.0.⁵

References

1. The Merck Index, 12th ed., Entry# 1817.
2. Vlasses, P. H., et al., Double-Blind Comparison of Captopril and Enalapril in Mild to Moderate Hypertension. *J. Am. College Cardiol.*, **7**, 651-660 (1986).
3. Hooper, N. M., and Turner, A. J., Isolation of Two Differentially Glycosylated Forms of Peptidyl-dipeptidase A (Angiotensin Converting Enzyme) from Pig Brain: A Re-evaluation of Their Role in Neuropeptide Metabolism. *Biochem. J.*, **241**(3), 625-633 (1987).
4. Kadin, H., *Anal. Profiles of Drug Substances*, **11**, 79-137 (1982).
5. *Intl. J. Pharm.*, **11**, 329-336 (1982).

MWM/RXR 5/06

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