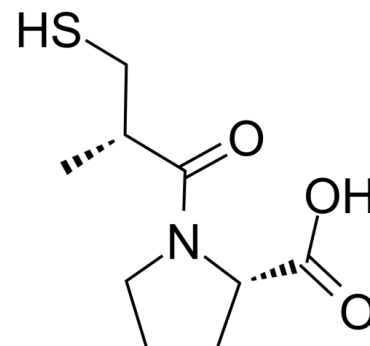


Data Sheet

Product Name:	Captopril
Cat. No.:	CS-2425
CAS No.:	62571-86-2
Molecular Formula:	C ₉ H ₁₅ NO ₃ S
Molecular Weight:	217.29
Target:	Angiotensin-converting Enzyme (ACE)
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 50 mg/mL (230.11 mM); H ₂ O : ≥ 50 mg/mL (230.11 mM)



BIOLOGICAL ACTIVITY:

Captopril (SQ-14534) is a potent, competitive inhibitor of angiotensin-converting enzyme (ACE). IC₅₀ & Target: ACE^[1]. **In Vitro:** Captopril (SQ-14534) has been shown to have similar morbidity and mortality benefits to those of diuretics and beta-blockers in hypertensive patients. Captopril (SQ-14534) has been shown to delay the progression of diabetic nephropathy, and enalapril and lisinopril prevent the development of nephropathy in normoalbuminuric patients with diabetes^[1]. An equimolar ratio of the cis and trans states of Captopril (SQ-14534) exists in solution and that the enzyme selects only the trans state of the inhibitor that presents architectural and stereoelectronic complementarity with its substrate binding groove^[2].

References:

[1]. Tzakos, A.G., et al., The molecular basis for the selection of captopril cis and trans conformations by angiotensin I converting enzyme. *Bioorg Med Chem Lett*, 2006. 16(19): p. 5084-7.

[2]. Song, J.C. and C.M. White, Clinical pharmacokinetics and selective pharmacodynamics of new angiotensin converting enzyme inhibitors: an update. *Clin Pharmacokinet*, 2002. 41(3): p. 207-24.

CAIndexNames:

L-Proline, 1-[(2S)-3-mercapto-2-methyl-1-oxopropyl]-

SMILES:

O=C(O)[C@H]1N(C([C@H](C)CS)=O)CCC1

Caution: Product has not been fully validated for medical applications. For research use only.

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