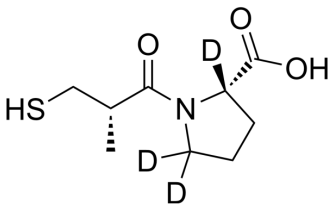
Captopril-d_3

Cat. No.:	HY-B0368S
CAS No.:	1356383-38-4
Molecular Formula:	$C_9H_{12}D_3NO_3S$
Molecular Weight:	220.3
Target:	Angiotensin-converting Enzyme (ACE); Isotope-Labeled Compounds
Pathway:	Metabolic Enzyme/Protease; Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Captopril-d_3 is deuterium labeled Captopril. Captopril (SQ 14225), antihypertensive agent, is a thiol-containing competitive, orally active angiotensin-converting enzyme (ACE) inhibitor (IC50=0.025 μM) and has been widely used for research of hypertension and congestive heart failure. Captopril is also a New Delhi metallo-β-lactamase-1 (NDM-1) inhibitor with an IC50 of 7.9 μM[1][2][3].
In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

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[3]. Esmaeili S, et al. Captopril/enalapril inhibit promiscuous esterase activity of carbonic anhydrase at micromolar concentrations: An in vitro study. Chem Biol Interact. 2017;265:24-35.

[4]. Li N, et al. Simplified captopril analogues as NDM-1 inhibitors. Bioorg Med Chem Lett. 2014;24(1):386-389.

[5]. 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.

[6]. 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.

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