Inhibitors

Product Data Sheet

Cilastatin-15N,d₃

Cat. No.: HY-A0166S CAS No.: 2738376-83-3

Molecular Formula: $\mathsf{C}_{16}\mathsf{H}_{23}\mathsf{D}_{3}\mathsf{N}^{15}\mathsf{NO}_{5}\mathsf{S}$

Molecular Weight: 362.46

Target: Bacterial; Antibiotic Pathway: Anti-infection

Storage: Powder -20°C 3 years

> $4^{\circ}C$ 2 years

In solvent -80°C 6 months

> -20°C 1 month

SOLVENT & SOLUBILITY

In Vitro 1M NaOH: 100 mg/mL (275.89 mM; ultrasonic and adjust pH to 12 with NaOH)

DMSO: 100 mg/mL (275.89 mM; Need ultrasonic)

H2O: 12.5 mg/mL (34.49 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.7589 mL	13.7946 mL	27.5893 mL
	5 mM	0.5518 mL	2.7589 mL	5.5179 mL
	10 mM	0.2759 mL	1.3795 mL	2.7589 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description	Cilastatin- 15 N,d $_3$ is a 15 N-labeled and deuterium labeled Cilastatin. Cilastatin (MK0791) is a reversible, competitive renal dehydropeptidase I inhibitor with an IC50 of 0.1 μ M. Cilastatin inhibits the bacterial metallob-lactamase enzyme CphA with an IC50 of 178 μ M. Cilastatin is an antibacterial adjunct[1][2][3].
IC ₅₀ & Target	β-lactam
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 ^[5] . 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):211-223.
- [2]. Blanca Humanes, et al. Protective Effects of Cilastatin Against Vancomycin-Induced Nephrotoxicity. Biomed Res Int. 2015;2015:704382.
- [3]. P J Petersen, et al. In Vitro and in Vivo Activities of LJC10,627, a New Carbapenem With Stability to Dehydropeptidase I. Antimicrob Agents Chemother. 1991 Jan;35(1):203-7.
- [4]. The renal membrane dipeptidase (dehydropeptidase I) inhibitor, cilastatin, inhibits the bacterialmetallo-beta-lactamase enzyme CphA. Antimicrob Agents Chemother. 1995 Jul;39(7):1629-31.

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

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