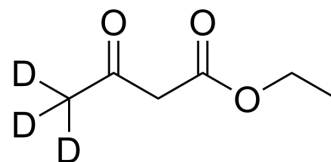


Ethyl acetoacetate-d₃

Cat. No.:	HY-Y1093S4
CAS No.:	1565868-21-4
Molecular Formula:	C ₆ H ₇ D ₃ O ₃
Molecular Weight:	133.16
Target:	Bacterial
Pathway:	Anti-infection
Storage:	4°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 200 mg/mL (1501.95 mM)
* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
	1 mM	7.5098 mL	37.5488 mL	75.0976 mL
	5 mM	1.5020 mL	7.5098 mL	15.0195 mL
	10 mM	0.7510 mL	3.7549 mL	7.5098 mL

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

BIOLOGICAL ACTIVITY

Description

Ethyl acetoacetate-d₃ is the deuterium labeled Ethyl acetoacetate. Ethyl acetoacetate (Ethyl acetylacetate) is an ester widely used as an intermediate in the synthesis of many varieties of compounds[1][2][3]. Ethyl acetoacetate is an inhibitor of bacterial biofilm[4].

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]. Rao M.Uppu, et al. Enantioselective catalytic asymmetric hydrogenation of ethyl acetoacetate in room temperature ionic liquids. Biochemical and Biophysical Research Communications. 1996 Dec; 229(3):764-769.

[2]. Leo F. Salter, et al. A dual-frequency Belousov Zhabotinskii oscillating reaction with ethyl acetoacetate as organic substrate. substrate. International Journal of Chemical Kinetics. 1982. 14(8), 815–821.

[3]. Iqbal S, et al. 2-Oxo-1,2,3,4-tetrahydropyrimidines Ethyl Esters as Potent β -Glucuronidase Inhibitors: One-pot Synthesis, In vitro and In silico Studies. Med Chem. 2018;14(8):818-830.

[4]. Horne SM, et al. Acetoacetate and ethyl acetoacetate as novel inhibitors of bacterial biofilm. Lett Appl Microbiol. 2018 Apr;66(4):329-339.

[5]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-223.

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

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