Product Data Sheet

Ethyl acetoacetate-13C4

Cat. No.: HY-Y1093S1 CAS No.: 84508-55-4 Molecular Formula: $C_2^{13}C_4H_{10}O_3$

Molecular Weight: 134.11

Target: Bacterial

Pathway: Anti-infection

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

 $H_3^{13}C^{13}G_3C^{13}C$

BIOLOGICAL ACTIVITY

Description	Ethyl acetoacetate- 13 C ₄ is the 13 C labeled Ethyl acetoacetate[1]. Ethyl acetoacetate (Ethyl acetylacetate) is an ester widely used as an intermediate in the synthesis of many varieties of compounds[2][3][4]. Ethyl acetoacetate is an inhibitor of bacterial biofilm[5].
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 Feb;53(2):211-216.

[2]. 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.

[3]. 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.

[4]. 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. 201814(8):818-830.

[5]. Horne SM, et al. Acetoacetate and ethyl acetoacetate as novel inhibitors of bacterial biofilm. Lett Appl Microbiol. 2018 Apr66(4):329-339.

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

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