Screening Libraries

Product Data Sheet

Benzoic acid-13C₆

Cat. No.: HY-N0216S1 CAS No.: 125945-98-4 $\mathsf{C}^{13}\mathsf{C}_6\mathsf{H}_6\mathsf{O}_2$ Molecular Formula: Molecular Weight: 128.08

Target: Fungal; Bacterial; Endogenous Metabolite Pathway: Anti-infection; Metabolic Enzyme/Protease

4°C, stored under nitrogen, away from moisture

* In solvent: -80°C, 6 months; -20°C, 1 month (stored under nitrogen, away from

moisture)

SOLVENT & SOLUBILITY

In Vitro

Storage:

DMSO: 125 mg/mL (975.95 mM; Need ultrasonic) DMSO: 125 mg/mL (975.95 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	7.8076 mL	39.0381 mL	78.0762 mL
	5 mM	1.5615 mL	7.8076 mL	15.6152 mL
	10 mM	0.7808 mL	3.9038 mL	7.8076 mL

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

BIOLOGICAL ACTIVITY

Benzoic $acid-^{13}C_6$ is the ^{13}C -labeled Benzoic acid. Benzoic acid is an aromatic alcohol existing naturally in many plants and Description

is a common additive to food, drinks, cosmetics and other products. It acts as preservatives through inhibiting both bacteria

and fungi.

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.

2]. Nair B, et al. Final report on	the safety assessment of Benzy	l Alcohol, Benzoic Acid, and Sodiu	um Benzoate. Int J Toxicol. 2001;20 Su	ppl 3:23-50.		
Caution: Product has not been fully validated for medical applications. For research use only.						
	Tel: 609-228-6898 Address: 1 De	Fax: 609-228-5909 er Park Dr, Suite Q, Monmouth	E-mail: tech@MedChemExpress.on Junction, NJ 08852, USA	com		

Page 2 of 2 www.MedChemExpress.com