# Terephthalic acid-13C2

MedChemExpress

Cat. No.:	HY-W01009	8S1			
CAS No.:	121191-53-5				
Molecular Formula:	C <sub>6</sub> <sup>13</sup> C <sub>2</sub> H <sub>6</sub> O <sub>4</sub>				
Molecular Weight:	168.12				
Target:	Endogenous Metabolite				
Pathway:	Metabolic Enzyme/Protease				
Storage:	Powder	-20°C	3 years		
		4°C	2 years		
	In solvent	-80°C	6 months		
		-20°C	1 month		

### SOLVENT & SOLUBILITY

In Vitro	DMSO : 125 mg/mL (743.52 mM; Need ultrasonic)						
Preparing Stock Solutions		Solvent Mass Concentration	1 mg	5 mg	10 mg		
	1 mM	5.9481 mL	29.7407 mL	59.4813 mL			
		5 mM	1.1896 mL	5.9481 mL	11.8963 mL		
	10 mM	0.5948 mL	2.9741 mL	5.9481 mL			
	Please refer to the solubility information to select the appropriate solvent.						
In Vivo	1. Add each solvent Solubility: ≥ 2.08 r	one by one: 10% DMSO >> 90% cor ng/mL (12.37 mM); Clear solution	n oil				

BIOLOGICAL ACTIV					
Description	Terephthalic acid- <sup>13</sup> C <sub>2</sub> is the <sup>13</sup> C-labeled Terephthalic acid. Terephthalic acid is one isomer of the three phthalic, a precursor to the polyester PET, used to make clothing and plastic bottles.				
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 <sup>[1]</sup> . 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.

# Product Data Sheet

HO<sup>13</sup>C

OH

 $\mathbb{I}$ 

[2]. Heck HD, et al. The induction of bladder stones by terephthalic acid, dimethyl terephthalate, and melamine (2,4,6-triamino-s-triazine) and its relevance to risk assessment. Regul Toxicol Pharmacol. 1985 Sep;5(3):294-313.

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

 Tel: 609-228-6898
 Fax: 609-228-5909
 E-mail: tech@MedChemExpress.com

 Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA