## **Product** Data Sheet

## Mono-Cyclohexyl Phthalate-3,4,5,6-d<sub>4</sub>

Cat. No.: HY-151911S

CAS No.: 1398066-18-6

Molecular Formula:  $C_{14}H_{12}D_4O_4$ Molecular Weight: 252.3

Target: Isotope-Labeled Compounds

Pathway: Others

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: 100 mg/mL (396.35 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	3.9635 mL	19.8177 mL	39.6354 mL
	5 mM	0.7927 mL	3.9635 mL	7.9271 mL
	10 mM	0.3964 mL	1.9818 mL	3.9635 mL

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

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (9.91 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE- $\beta$ -CD in saline) Solubility:  $\geq$  2.5 mg/mL (9.91 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.5 mg/mL (9.91 mM); Clear solution

## **BIOLOGICAL ACTIVITY**

Description

Mono-Cyclohexyl Phthalate-3,4,5,6-d<sub>4</sub> is the deuterium labeled Mono-Cyclohexyl Phthalate[1].

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.

<b>EFERENCES</b> J. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019 Feb;53(2):211-216.				
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