Product Data Sheet

Cholic acid-d₅

 Cat. No.:
 HY-N0324S1

 CAS No.:
 53007-09-3

 Molecular Formula:
 C₂₄H₃₅D₅O₅

 Molecular Weight:
 413.6

Target: Endogenous Metabolite

Pathway: Metabolic Enzyme/Protease

Storage: 4°C, protect from light, stored under nitrogen

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

nitrogen)

SOLVENT & SOLUBILITY

In Vitro DMSO : ≥ 50 mg/mL (120.89 mM)

DMSO : ≥ 50 mg/mL (120.89 mM)

 $0.1\,M$ NaOH: 33.33 mg/mL (80.59 mM; ultrasonic and adjust pH to 9 with NaOH) $0.1\,M$ NaOH: 33.33 mg/mL (80.59 mM; ultrasonic and adjust pH to 9 with NaOH)

H₂O: 0.67 mg/mL (1.62 mM; Need ultrasonic) H₂O: 0.67 mg/mL (1.62 mM; Need ultrasonic) * "≥" means soluble, but saturation unknown.

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.4178 mL	12.0890 mL	24.1779 mL
	5 mM	0.4836 mL	2.4178 mL	4.8356 mL
	10 mM	0.2418 mL	1.2089 mL	2.4178 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 (6.04 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (6.04 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: \geq 2.5 mg/mL (6.04 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Cholic acid- d_5 is the deuterium labeled Cholic acid. Cholic acid is a major primary bile acid produced in the liver and usually conjugated with glycine or taurine. It facilitates fat absorption and cholesterol excretion.

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]. Li Y, et al. Mechanism of hepatic targeting via oral administration of DSPE-PEG-Cholic acid-modified nanoliposomes. Int J Nanomedicine. 2017 Feb 28;12:1673-1684.
- [3]. Pan X, et al. Cholic acid Feeding Leads to Increased CYP2D6 Expression in CYP2D6-Humanized Mice. Drug Metab Dispos. 2017 Apr;45(4):346-352.

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

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