

# **Product** Data Sheet

## Glycoursodeoxycholic Acid-d<sub>4</sub>

Cat. No.: HY-N1424S CAS No.: 2044276-17-5 Molecular Formula:  $C_{26}H_{39}D_4NO_5$ Molecular Weight: 453.65

Target: **Endogenous Metabolite** Pathway: Metabolic Enzyme/Protease -20°C Storage: Powder 3 years

> In solvent -80°C 6 months

-20°C 1 month

### **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 50 mg/mL (110.22 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.2043 mL	11.0217 mL	22.0434 mL
	5 mM	0.4409 mL	2.2043 mL	4.4087 mL
	10 mM	0.2204 mL	1.1022 mL	2.2043 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: ≥ 1.25 mg/mL (2.76 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 1.25 mg/mL (2.76 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 1.25 mg/mL (2.76 mM); Clear solution

### BIOLOGICAL ACTIVITY

Description

Glycoursodeoxycholic acid-d4 (Ursodeoxycholylglycine-d4) is the deuterium labeled Glycoursodeoxycholic acid. Glycoursodeoxycholic acid, a acyl glycine and a bile acid-glycine conjugate, is a metabolite of ursodeoxycholic acid[1][2].

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.
- [2]. Vaz AR, et al. Bilirubin selectively inhibits cytochrome c oxidase activity and induces apoptosis in immature cortical neurons: assessment of the protective effects of glycoursodeoxycholic acid. J Neurochem. 2010 Jan;112(1):56-65.
- [3]. Vaz AR, et al. Glycoursodeoxycholic acid reduces matrix metalloproteinase-9 and caspase-9 activation in a cellular model of superoxide dismutase-1 neurodegeneration.
- [4]. Palmela I, et al. Hydrophilic bile acids protect human blood-brain barrier endothelial cells from disruption by unconjugated bilirubin: an in vitro study. Front Neurosci. 2015 Mar 13;9:80.

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