Product Data Sheet

Ursodeoxycholic acid-2,2,4,4-d₄

Cat. No.: HY-113478S CAS No.: 347841-46-7 Molecular Formula: $C_{24}H_{36}D_4O_4$ Molecular Weight: 396.6

Target: Isotope-Labeled Compounds

Pathway: Others

Storage: -20°C, sealed storage, away from moisture

* In solvent: -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)

BIOLOGICAL ACTIVITY

Description

Ursodeoxycholic acid-2,2,4,4-d₄ is the deuterium labeled <u>Ursodeoxycholic acid</u> (HY-13771). Ursodeoxycholic acid is a secondary bile acid issued from the transformation of (cheno)deoxycholic acid by intestinal bacteria, acting as a key regulator of the intestinal barrier integrity and essential for lipid metabolism. Ursodeoxycholic acid acts as signaling molecule, exerting its effects by interacting with bile acid activated receptors, including G-protein coupled bile acid receptor 5 (TGR5, GPCR19) and the farnesoid X receptor (FXR). Ursodeoxycholic acid can be used for the research of a variety of hepatic and gastrointestinal diseases. Ursodeoxycholic acid also reduces ACE2 expression and is beneficial for reducing SARS-CoV-2 infection[1][2][3][4][5].

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 $^{[1]}$.

 $\label{eq:mce} \mbox{MCE has not independently confirmed the accuracy of these methods. They are for reference only.}$

REFERENCES

[1]. Kumar D, et al. Use of ursodeoxycholic acid in liver diseases. J Gastroenterol Hepatol. 2001 Jan;16(1):3-14.

[2]. Biao Nie, et al. Specific Bile Acids Inhibit Hepatic Fatty Acid Uptake in Mice. Hepatology. 2012 Oct;56(4):1300-10.

[3]. Brevini T, et al. FXR inhibition may protect from SARS-CoV-2 infection by reducing ACE2. Nature. 2022 Dec 5.

[4]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

[5]. Jackson H, et al. Influence of ursodeoxycholic acid on the mortality and malignancy associated with primary biliary cirrhosis: a population-based cohort study. Hepatology. 2007 Oct;46(4):1131-7.

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