## **Product** Data Sheet

## Celecoxib-d<sub>4</sub>

**Cat. No.:** HY-118139S **CAS No.:** 544686-20-6

Molecular Formula:  $C_{17}H_{10}D_4F_3N_3O_2S$ 

Molecular Weight: 385.4

Target: COX; Isotope-Labeled Compounds
Pathway: Immunology/Inflammation; Others

Storage: Please store the product under the recommended conditions in the Certificate of

Analysis.

## **BIOLOGICAL ACTIVITY**

Description	Celecoxib- $d_4$ is the deuterium labeled Desmethyl Celecoxib. Desmethyl Celecoxib (compound 3b) is a selective cyclooxygenase-2 (COX-2) inhibitor (IC50=32 nM) with anti-inflammatory activities. Desmethyl Celecoxib is an analog of Celecoxib and with the optimal yield of 75%[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 <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]. Vinay Kumar Sthalam, et al. An Integrated Continuous Flow Micro-Total Ultrafast Process System ( $\mu$ -TUFPS) for the Synthesis of Celecoxib and Other Cyclooxygenase Inhibitors. RETURN TO ISSUEPREVARTICLENEXT

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

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