Product Data Sheet

Muconic acid-d₄

Cat. No.: HY-113247S1 CAS No.: 1185239-59-1 Molecular Formula: $C_6H_2D_4O_4$

Molecular Weight: 146.13

Target: Isotope-Labeled Compounds

Pathway: Others

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

Analysis.

BIOLOGICAL ACTIVITY

Description	trans-trans-Muconic acid- d_4 -1 is a deuterium labeled trans-trans-Muconic acid (HY-113247). trans-trans-Muconic acid is a urinary metabolite of benzene and has been used as a biomarker of exposure to benzene in human.
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]. Bartczak A, ET AL. Evaluation of assays for the identification and quantitation of muconic acid, a benzene metabolite in human urine. J Toxicol Environ Health. 1994 Jul;42(3):245-58.

 $[2]. Russak \, EM, et \, al. \, Impact \, of \, Deuterium \, Substitution \, on \, the \, Pharmacokinetics \, of \, Pharmaceuticals. \, Ann \, Pharmacother. \, 2019 \, Feb; \\ 53(2): 211-246.$

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

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